



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:20 AM UTC

PDB ID : 8GXS / pdb_00008gxs
EMDB ID : EMD-34360
Title : PIC-Mediator in complex with +1 nucleosome (T40N) in H-binding state
Authors : Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.
Deposited on : 2022-09-21
Resolution : 4.16 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

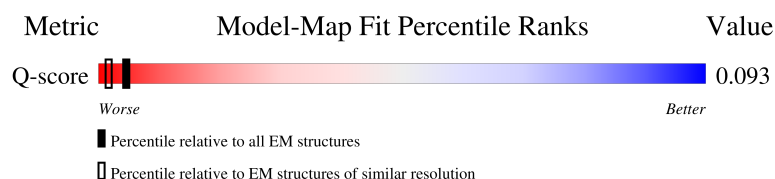
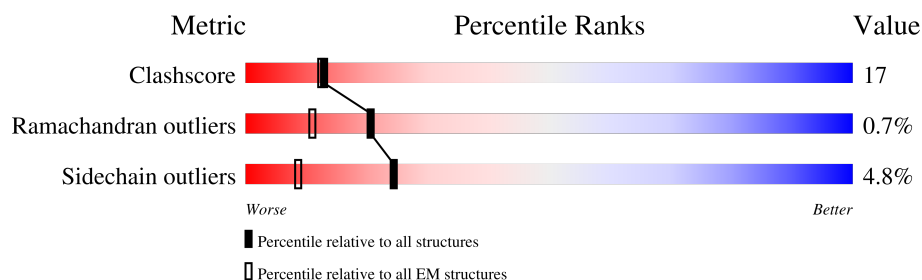
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.16 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.



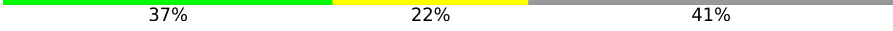
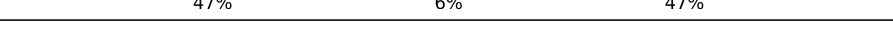
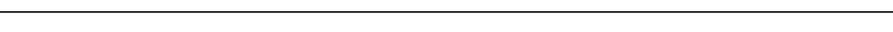
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5480 (3.66 - 4.66)

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

Mol	Chain	Length	Quality of chain
1	X	228	
2	Y	228	
3	NX	162	
4	NY	162	

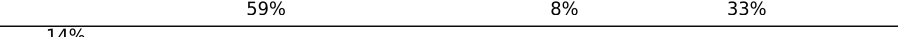
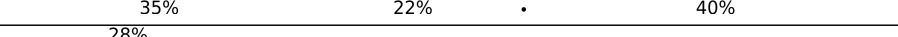
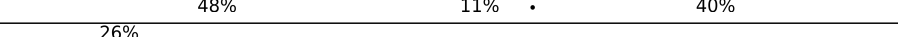
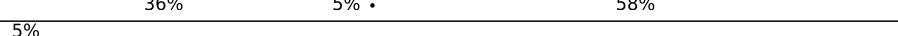
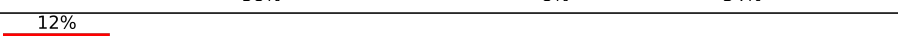
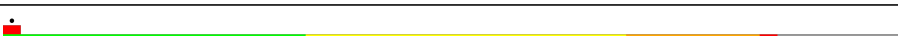
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Mol	Chain	Length	Quality of chain
5	BA	316	
6	DA	1872	
7	EA	439	
8	FA	517	
9	HA	760	
10	NA	136	
10	NE	136	
11	PA	1970	
12	DB	1199	
13	EB	291	
14	FB	249	
15	HB	548	
16	NB	103	
16	NF	103	
17	PB	1174	
18	HC	462	
19	DO	109	
20	DP	339	
21	DQ	376	
22	PC	275	
23	PE	210	
24	PF	127	
25	PH	150	
26	PI	125	
27	PJ	67	

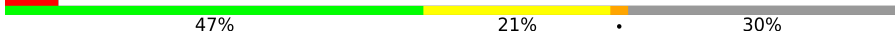
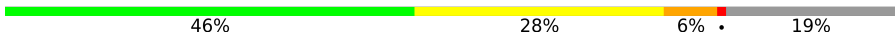
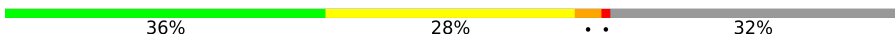
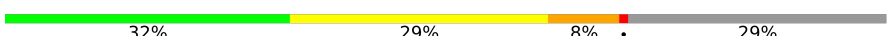
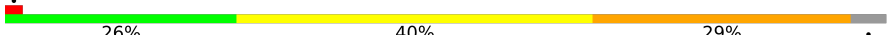
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Mol	Chain	Length	Quality of chain
28	PK	117	
29	PL	58	
30	HD	309	
31	HG	395	
32	HE	308	
33	HF	71	
34	HH	782	
35	DD	1085	
35	Dd	1085	
36	DE	800	
36	De	800	
37	DF	677	
37	Df	677	
38	DG	349	
39	DH	310	
40	DI	264	
40	Di	264	
41	DL	161	
41	Dl	161	
42	Dc	929	
43	DJ	218	
43	Dj	218	
44	Dk	211	
45	Dm	124	
46	HI	346	

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Mol	Chain	Length	Quality of chain
47	HJ	323	
48	PD	142	
49	PG	172	
50	g	233	
51	j	135	
52	n	1454	
53	s	244	
54	u	144	
55	a	1581	
56	d	270	
57	f	246	
58	i	146	
59	m	131	
60	q	651	
61	z	600	
62	b	200	
63	c	311	
64	e	178	
65	l	178	
66	o	788	
67	h	268	
68	k	117	
69	r	208	
70	t	212	
71	v	200	

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Mol	Chain	Length	Quality of chain
72	p	841	
73	w	1368	
74	x	989	
75	y	747	
76	NC	128	
76	NG	128	
77	ND	126	
77	NH	126	

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 185972 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 DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	67	Total	C	N	O	P	0	0
			1387	652	275	394	66		

- Molecule 2 is a DNA chain called DNA (228-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	67	Total	C	N	O	P	0	0
			1357	643	239	408	67		

- Molecule 3 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	NX	162	Total	C	N	O	P	0	0
			3078	1458	486	972	162		

- Molecule 4 is a DNA chain called DNA (162-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	NY	162	Total	C	N	O	P	0	0
			3561	1620	810	970	161		

- Molecule 5 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DA	558	Total	C	N	O	S	0	0
			4563	2913	791	832	27		

- Molecule 7 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	EA	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	FA	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 9 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	HA	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	NA	100	Total	C	N	O	0	0
			498	298	100	100		
10	NE	103	Total	C	N	O	0	0
			511	305	103	103		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	PA	1471	Total	C	N	O	S	0	0
			11628	7314	2064	2178	72		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 13 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	EB	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 14 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 15 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	HB	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	NB	80	Total	C	N	O	0	0
			391	231	80	80		
16	NF	86	Total	C	N	O	0	0
			421	249	86	86		

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	PB	1136	Total	C	N	O	S	0	0
			9076	5739	1597	1676	64		

- Molecule 18 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	HC	390	Total	C	N	O	S	0	0
			3158	2050	545	551	12		

- Molecule 19 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DO	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 20 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DP	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DQ	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	PE	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	PF	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 25 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	PI	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 28 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	PK	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 29 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	PL	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 30 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HD	306	Total	C	N	O	S	0	0
			2400	1498	424	465	13		

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	HG	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	HE	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	HF	66	Total	C	N	O	S	0	0
			523	337	83	100	3		

- Molecule 34 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	HH	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 6.

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

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DL	74	Total	C	N	O	S	0	0
			605	379	105	118	3		
41	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 3.

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

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

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

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 46 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	HI	299	Total	C	N	O	S	0	0
			2374	1532	405	426	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HI	41	ALA	LYS	engineered mutation	UNP P50613

- Molecule 47 is a protein called Cyclin-H.

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

- Molecule 48 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	PD	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 49 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	PG	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g	106	Total	C	N	O	S	0	0
			898	569	166	157	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	n	1015	Total	C	N	O	S	0	0
			7751	4941	1363	1405	42		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	93	Total	C	N	O	S	0	0
			723	463	121	135	4		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	117	Total	C	N	O	S	0	0
			886	552	146	184	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a	438	Total	C	N	O	S	0	0
			3430	2190	584	632	24		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	f	167	Total	C	N	O	S	0	0
			1365	882	235	243	5		

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	q	555	Total	C	N	O	S	0	0
			4373	2765	783	805	20		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	263	Total	C	N	O	S	0	0
			2131	1356	379	385	11		

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 67 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	r	192	Total	C	N	O	S	0	0
			1535	973	271	276	15		

- Molecule 70 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 72 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p	766	Total	C	N	O	S	0	0
			5983	3816	1026	1092	49		

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	w	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 74 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	x	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 75 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	y	210	Total	C	N	O	S	0	0
			1605	1030	264	302	9		

- Molecule 76 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	NC	103	Total	C	N	O		0	0
			506	300	103	103			
76	NG	107	Total	C	N	O		0	0
			524	310	107	107			

- Molecule 77 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ND	95	Total	C	N	O		0	0
			471	281	95	95			
77	NH	95	Total	C	N	O		0	0
			471	281	95	95			

- Molecule 78 is ZINC ION (CCD ID: ZN) (formula: Zn).

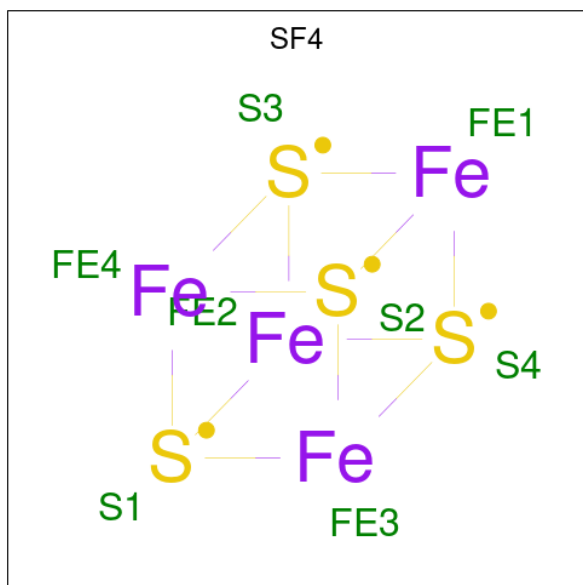
Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total	Zn	0
			1	1	
78	EA	1	Total	Zn	0
			1	1	
78	PA	2	Total	Zn	0
			2	2	
78	PB	1	Total	Zn	0
			1	1	
78	PC	1	Total	Zn	0
			1	1	
78	PI	2	Total	Zn	0
			2	2	
78	PJ	1	Total	Zn	0
			1	1	
78	PL	1	Total	Zn	0
			1	1	
78	HD	2	Total	Zn	0
			2	2	
78	HG	3	Total	Zn	0
			3	3	

Continued on next page...

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Mol	Chain	Residues	Atoms		AltConf
78	HE	2	Total	Zn	0
			2	2	
78	c	1	Total	Zn	0
			1	1	
78	p	1	Total	Zn	0
			1	1	

- Molecule 79 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
79	HA	1	Total	Fe	S	0
			8	4	4	

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

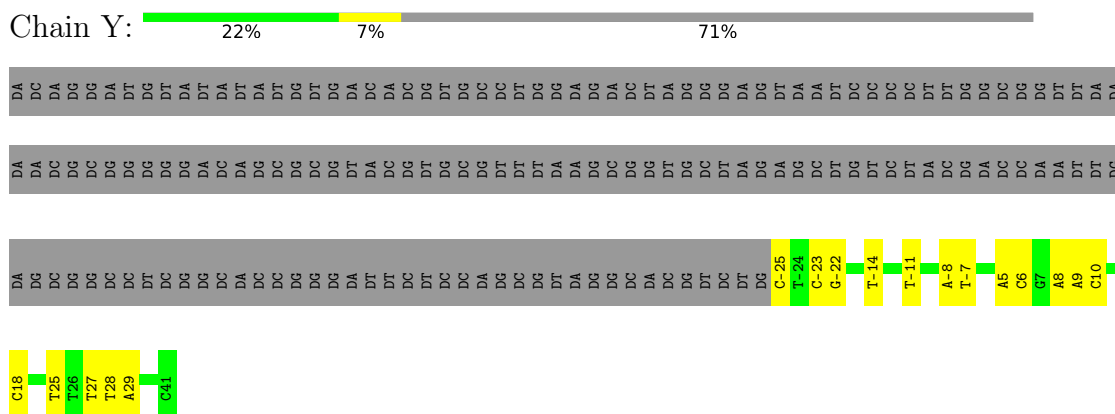
3 Residue-property plots [i](#)

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.

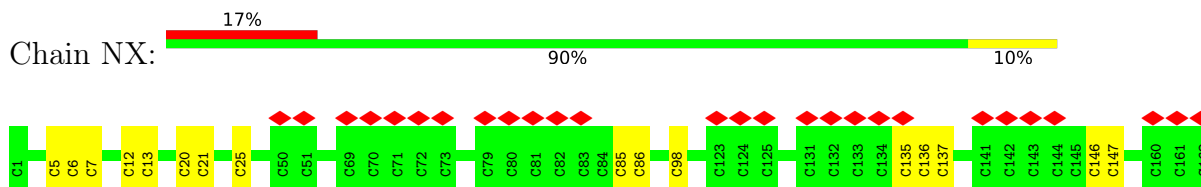
- Molecule 1: DNA (228-mer)



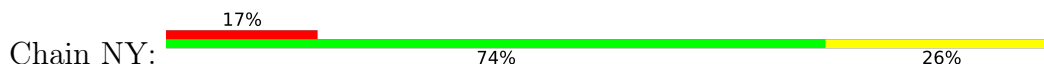
- Molecule 2: DNA (228-mer)



- Molecule 3: DNA (162-mer)



- Molecule 4: DNA (162-mer)

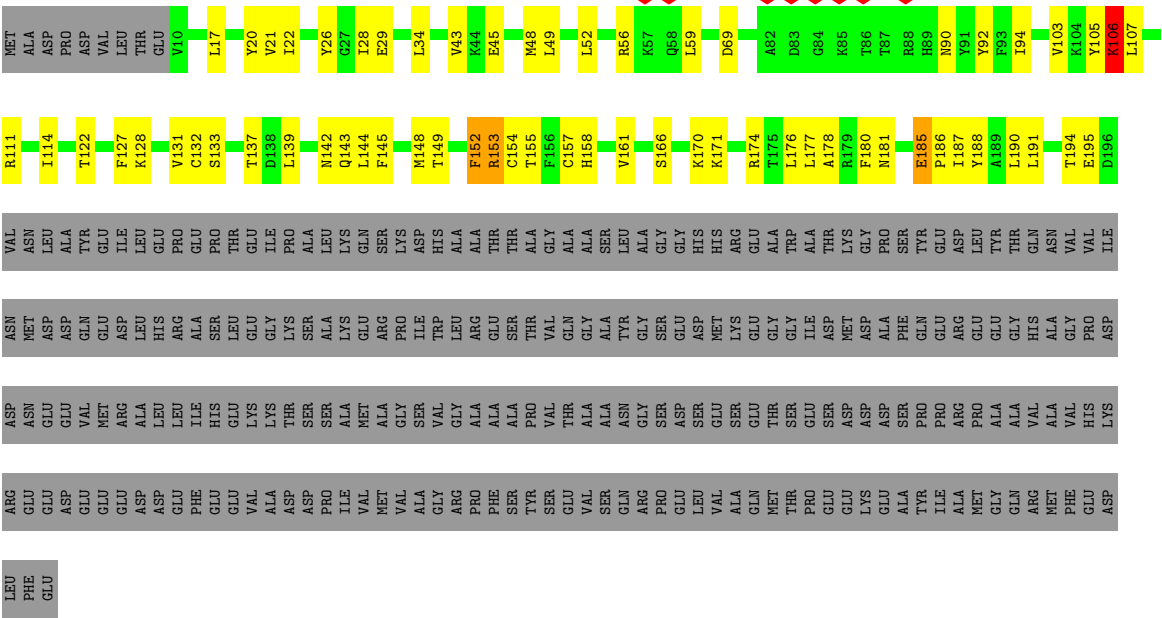




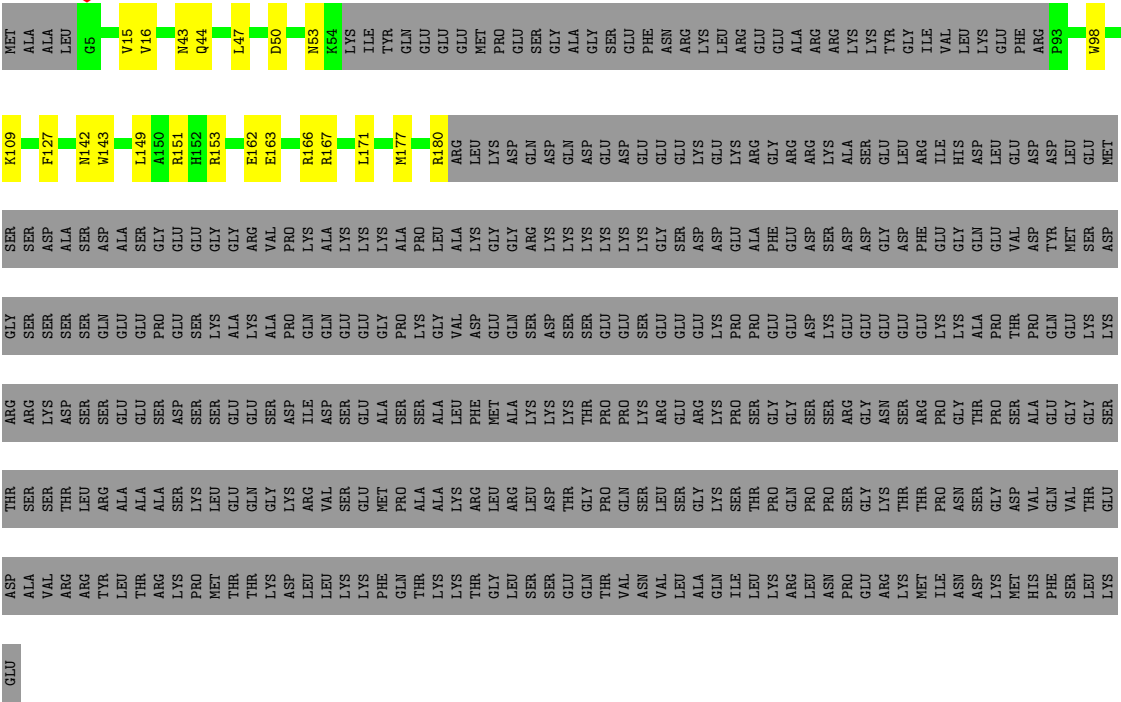


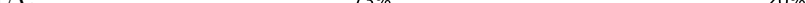
ILE
ALA
GLY
ASP
SER
ASP
SER
ASP
LEU
ASP
SER
ASP
GLU

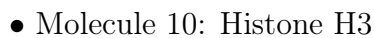
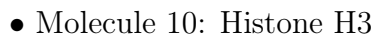
● Molecule 7: General transcription factor IIE subunit 1

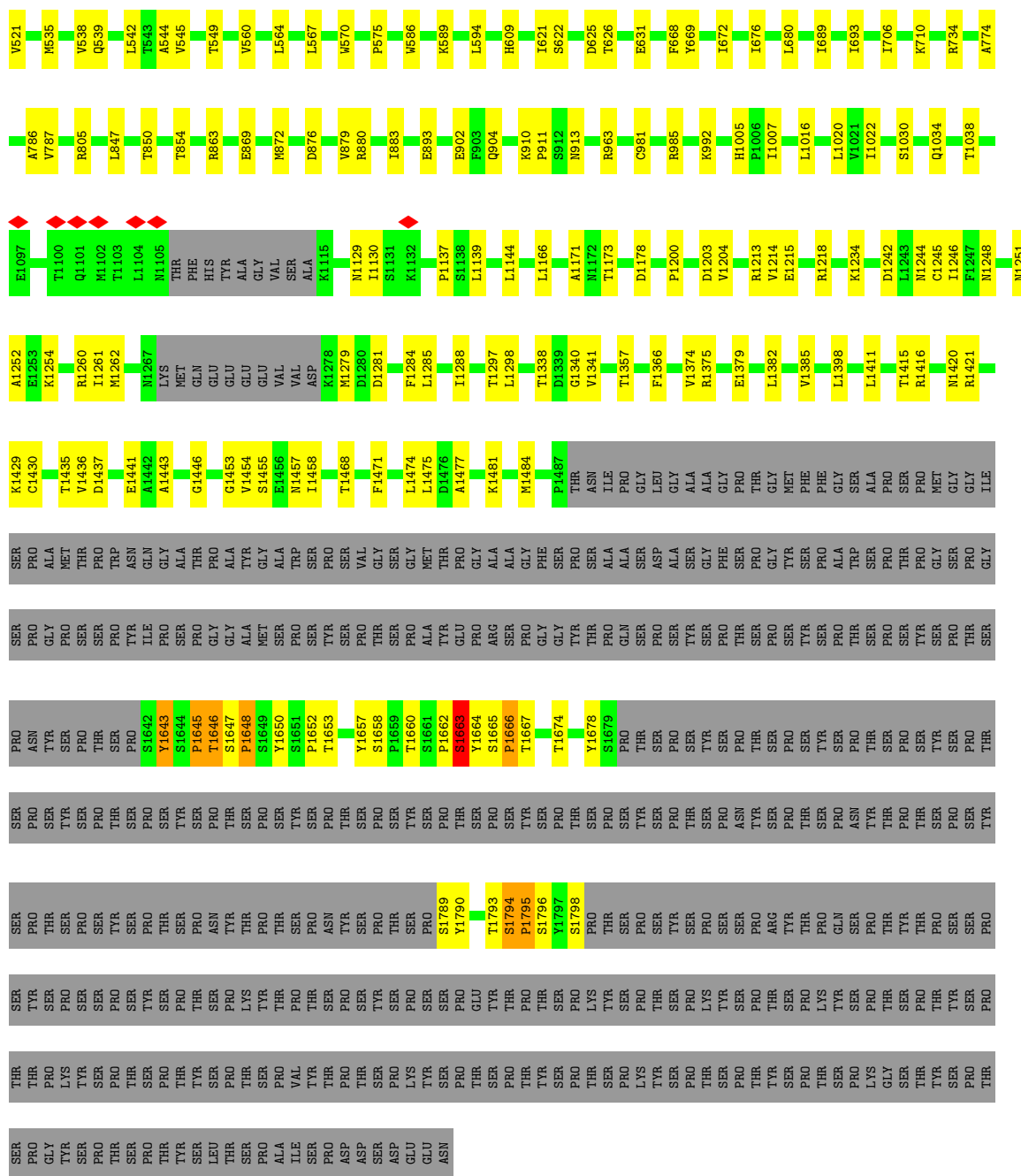


● Molecule 8: General transcription factor IIF subunit 1



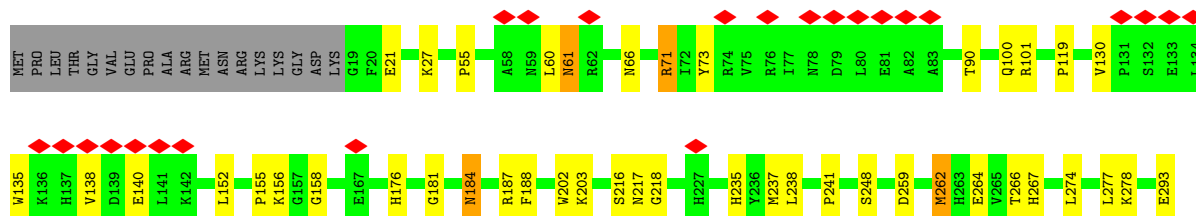
- Chain HA: 



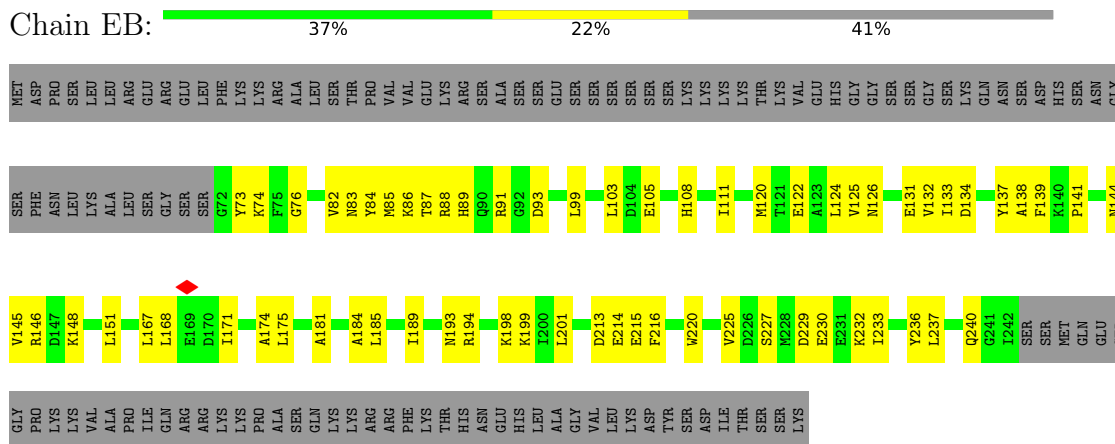


- Molecule 12: Transcription initiation factor TFIID subunit 2

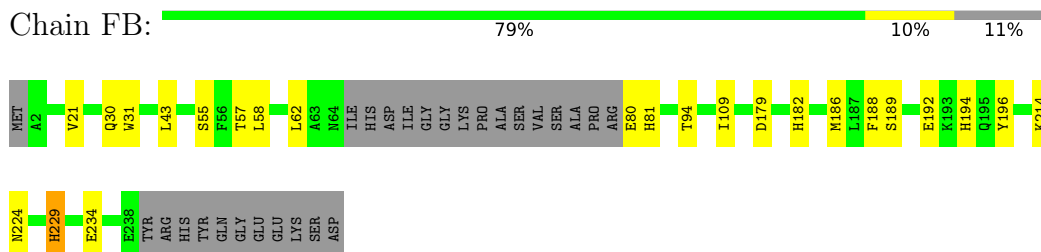
Chain DB:

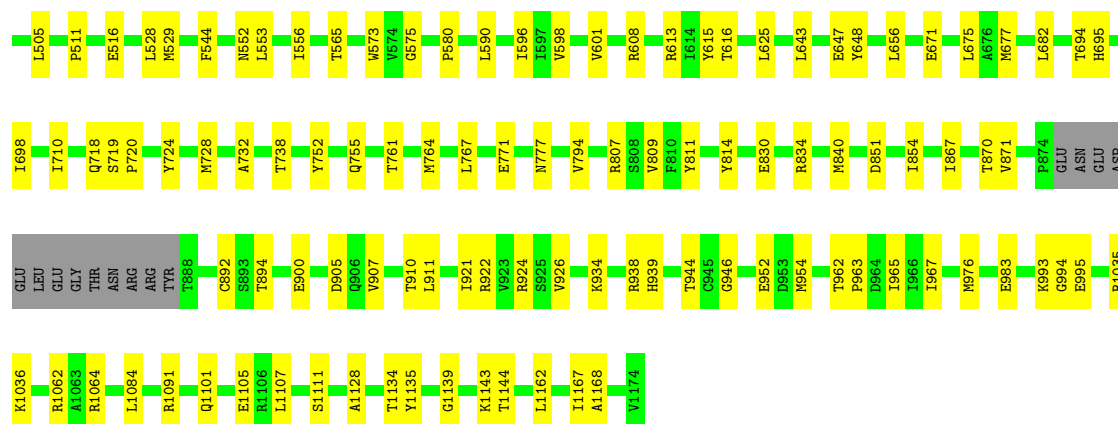


- Molecule 13: Transcription initiation factor IIE subunit beta

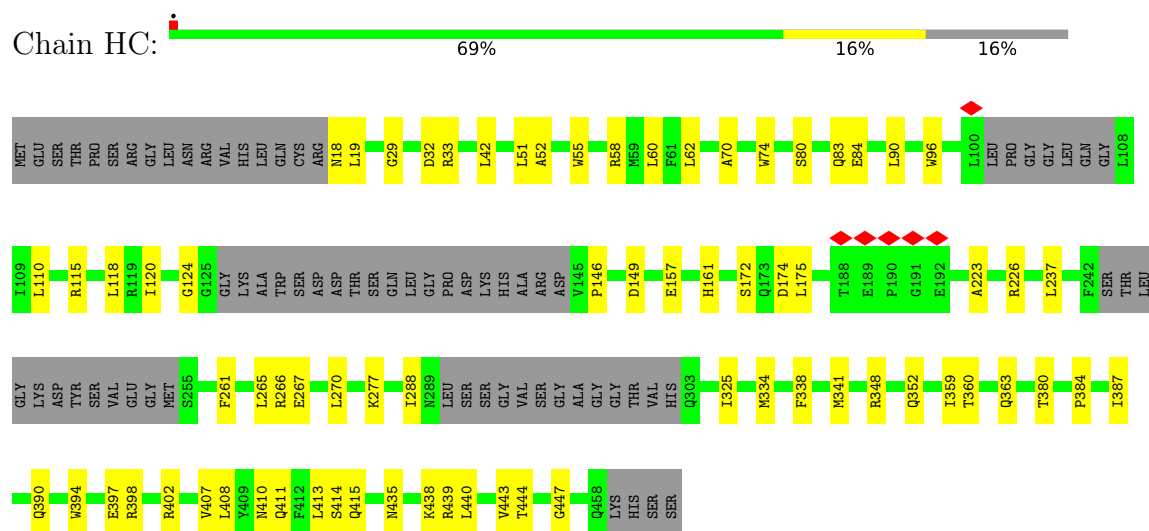


- Molecule 14: General transcription factor IIF subunit 2

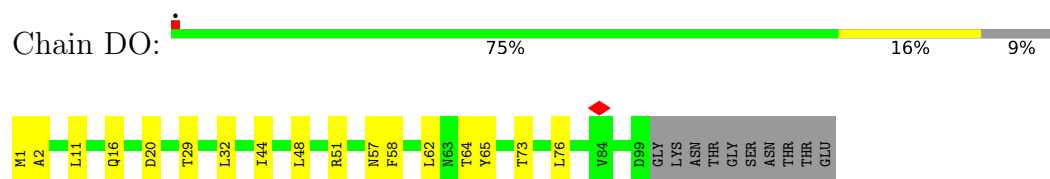




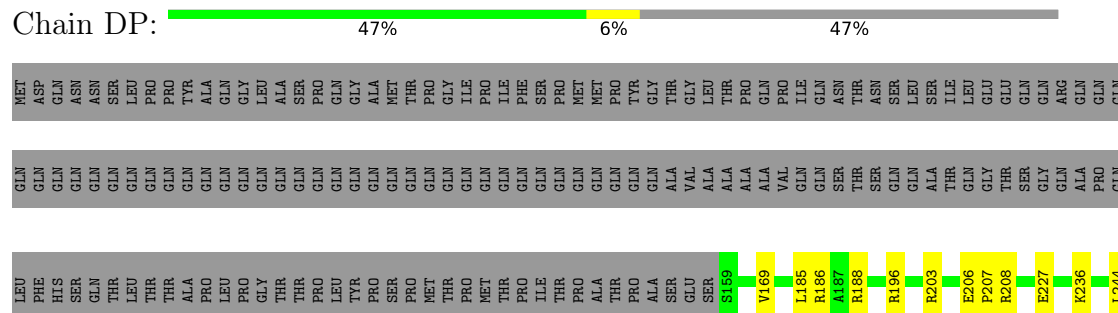
- Molecule 18: General transcription factor IIH subunit 4



- Molecule 19: Transcription initiation factor IIA subunit 2



- Molecule 20: TATA-box-binding protein

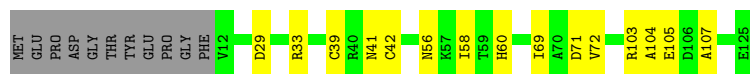


Chain PH:  91% 8% .



- Molecule 26: DNA-directed RNA polymerase II subunit RPB9

Chain PI:  79% 12% 9%



- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain PJ:  78% 18% .



- Molecule 28: RNA_pol_L_2 domain-containing protein

Chain PK:  89% 9% .



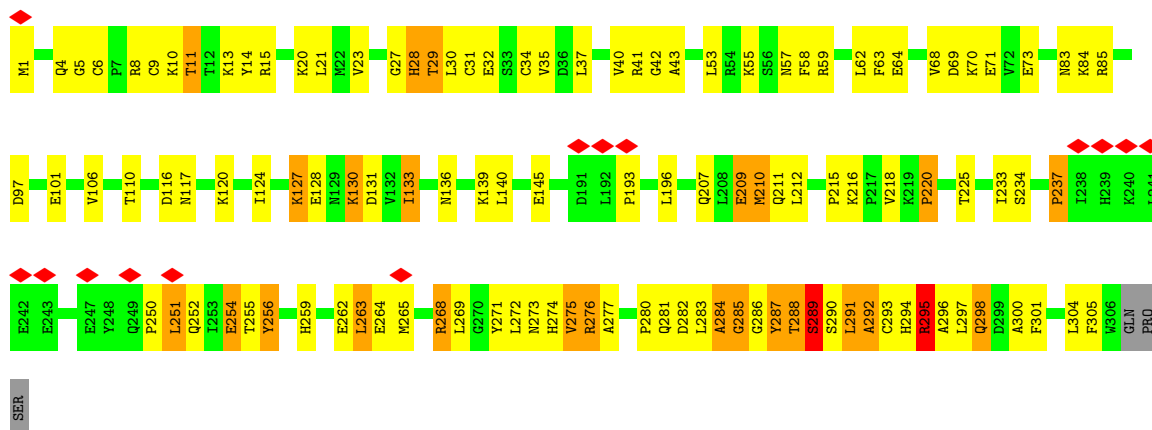
- Molecule 29: RPB12

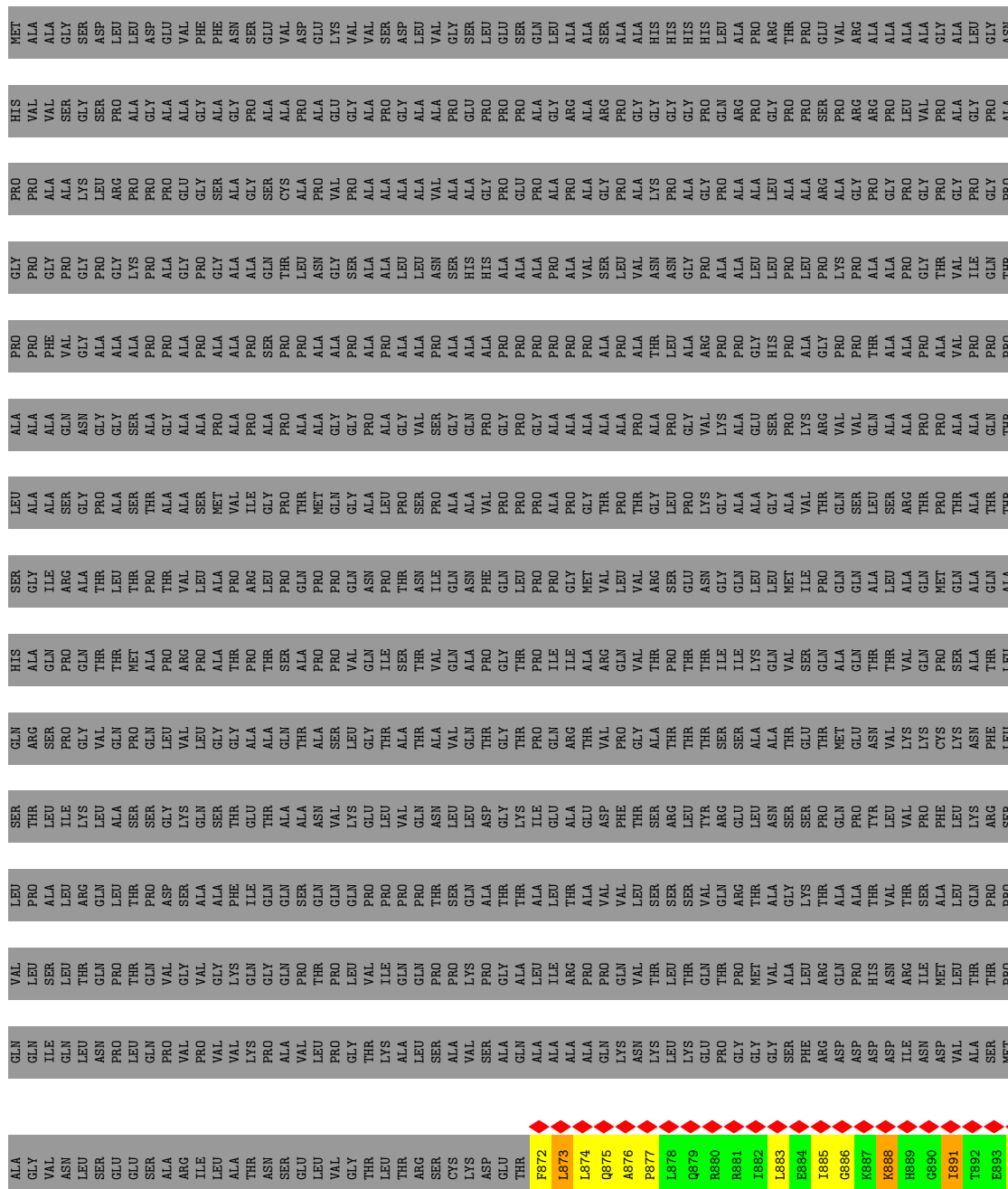
Chain PL:  60% 16% 24%

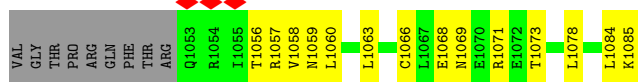


- Molecule 30: CDK-activating kinase assembly factor MAT1

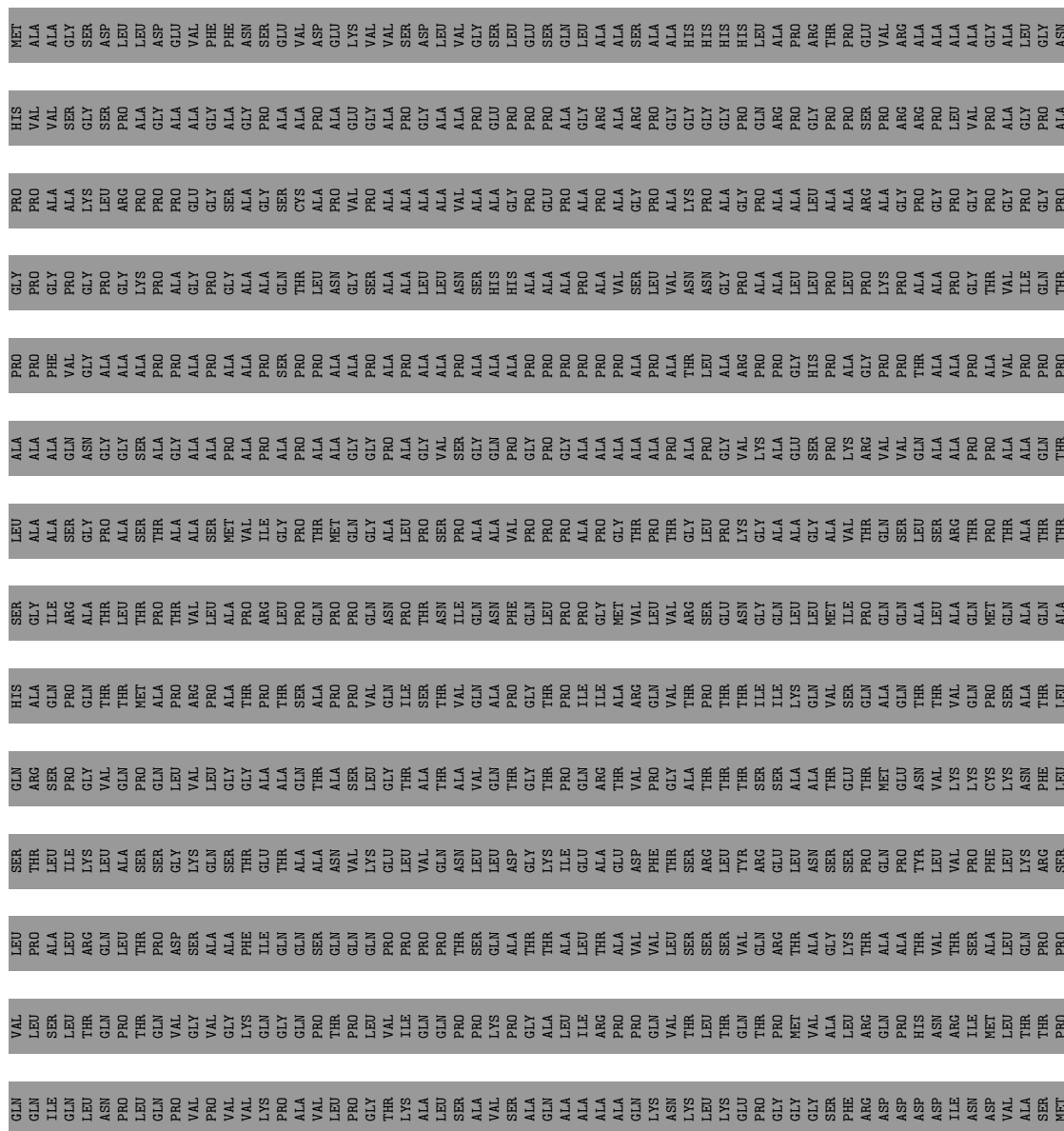
Chain HD:  5% 61% 30% 8% ..





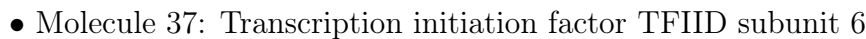


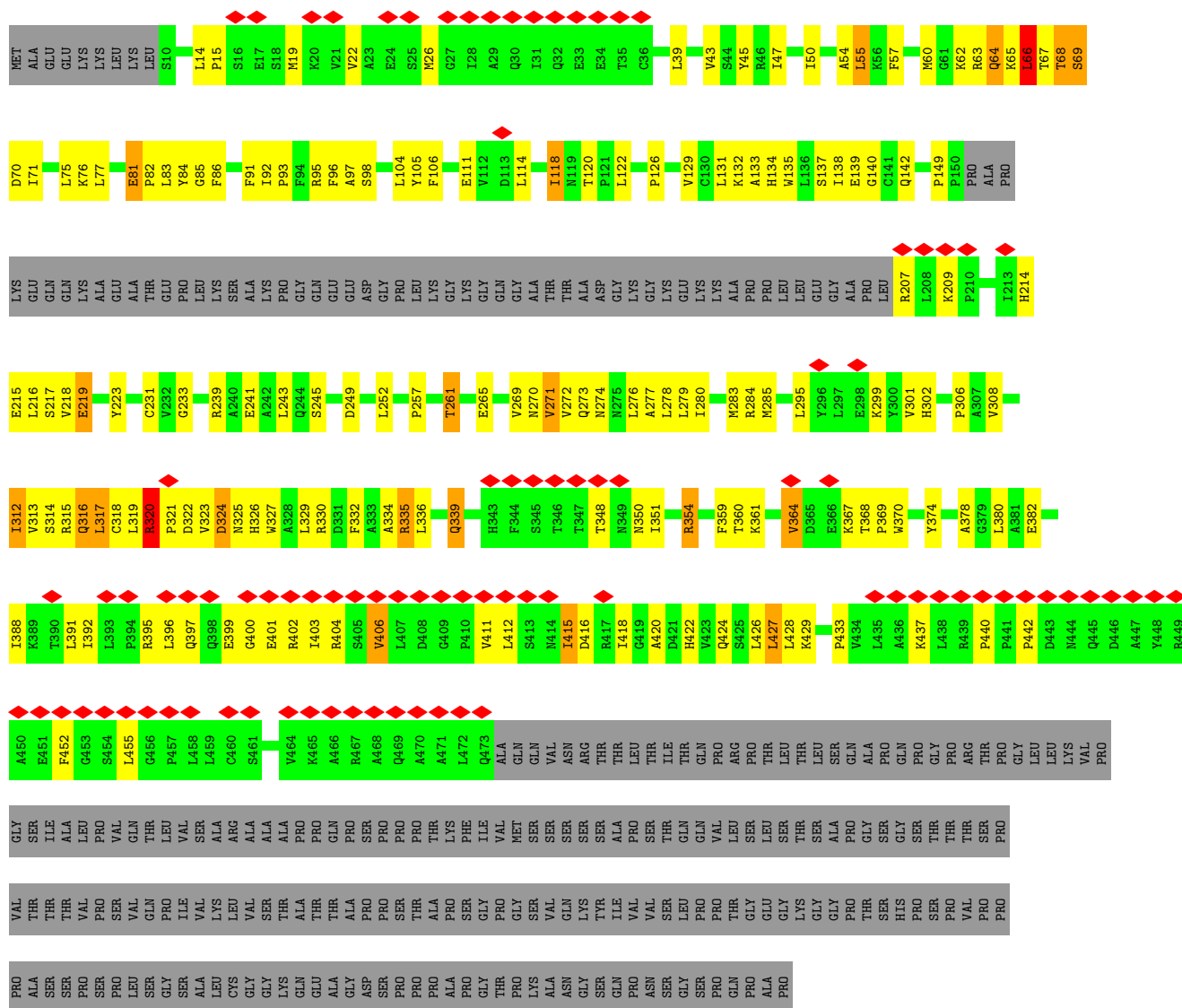
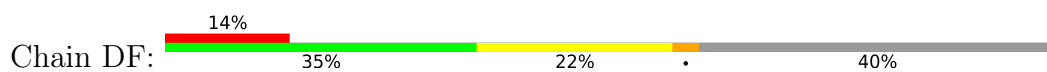
Chain Dd: 15%
13% . 85%



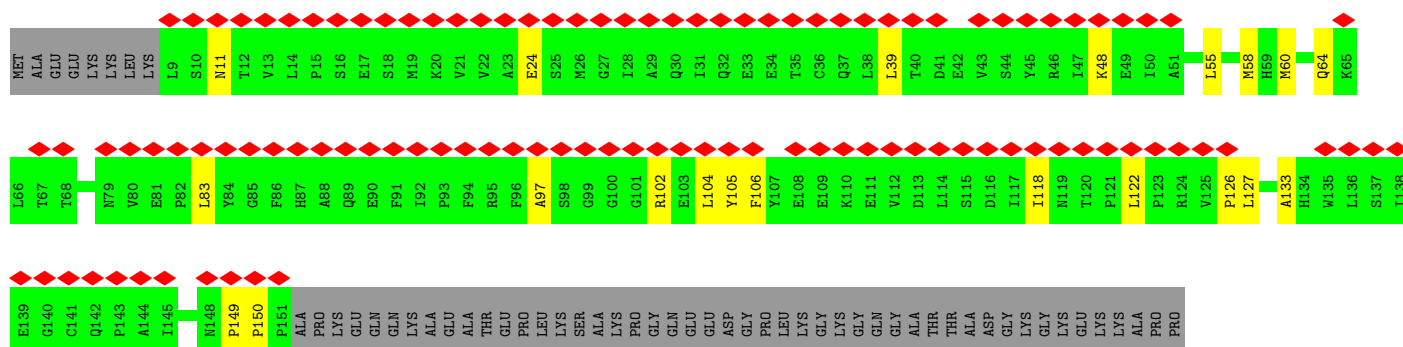


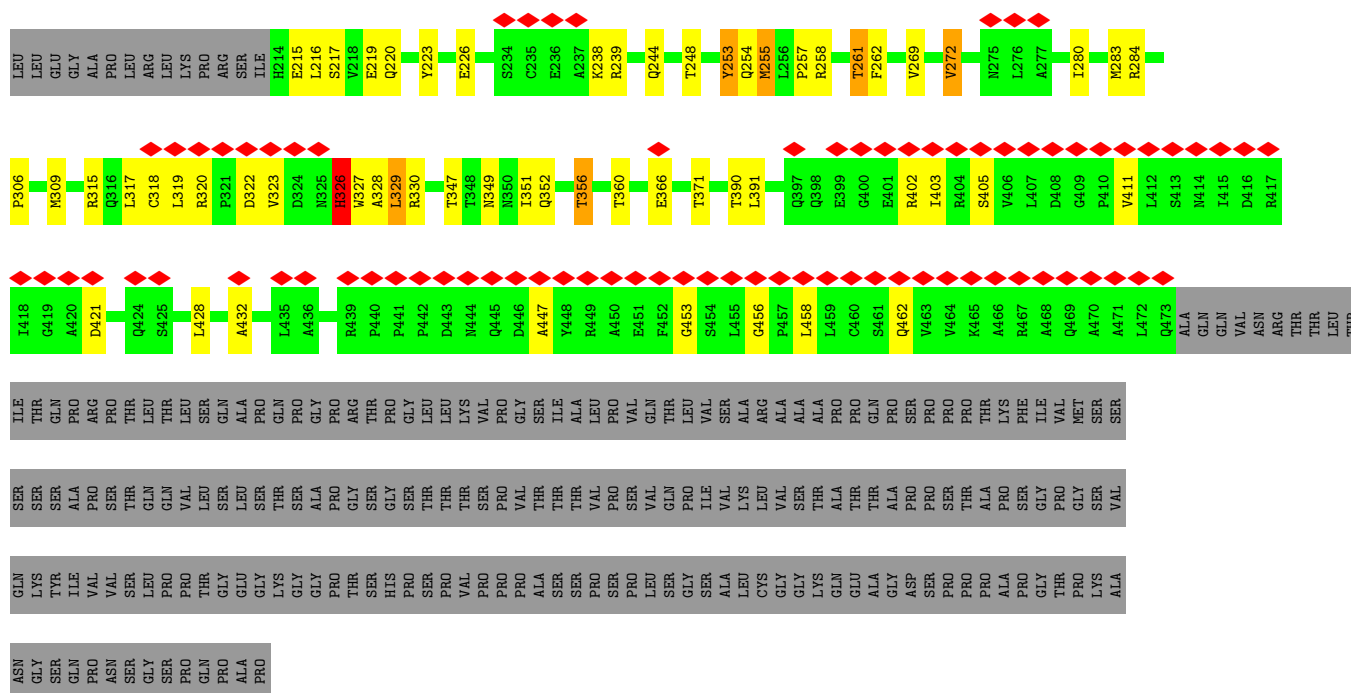
Chain De:



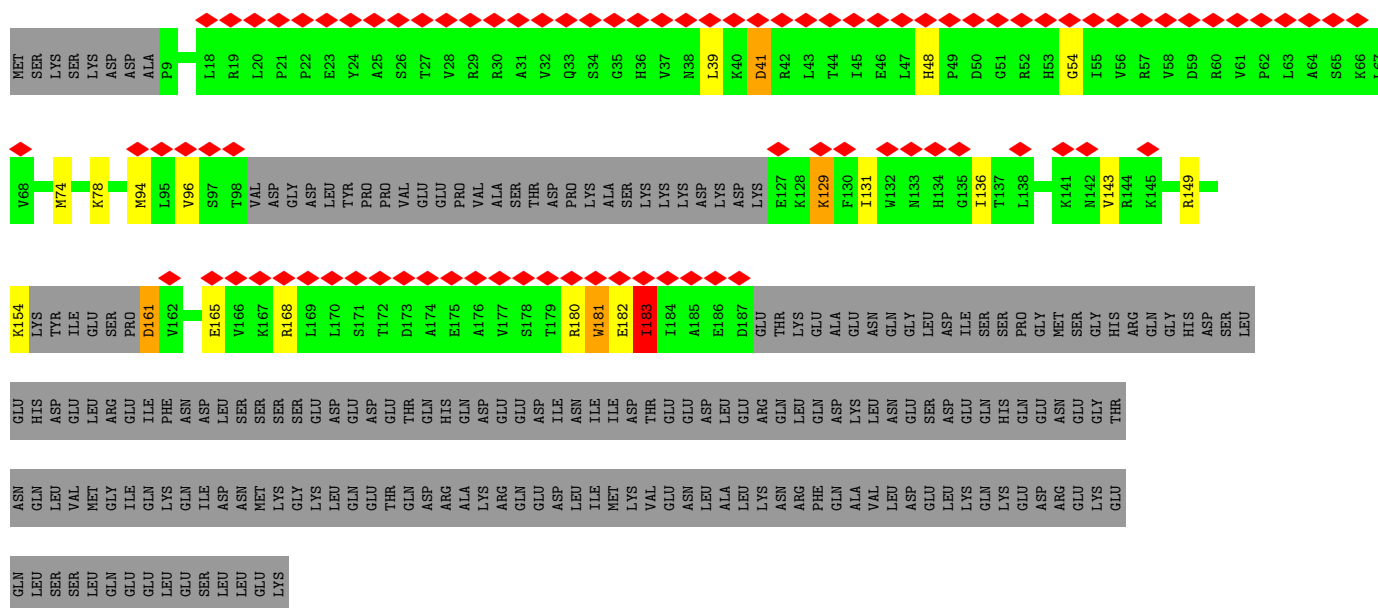
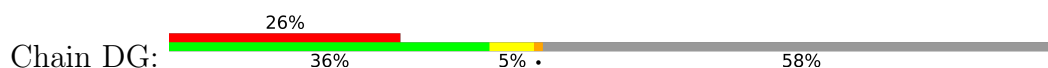


• Molecule 37: Transcription initiation factor TFIID subunit 6



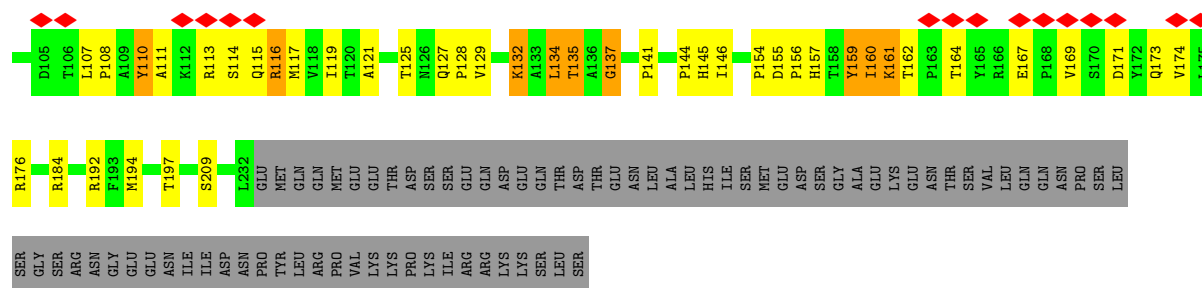


• Molecule 38: Transcription initiation factor TFIID subunit 7

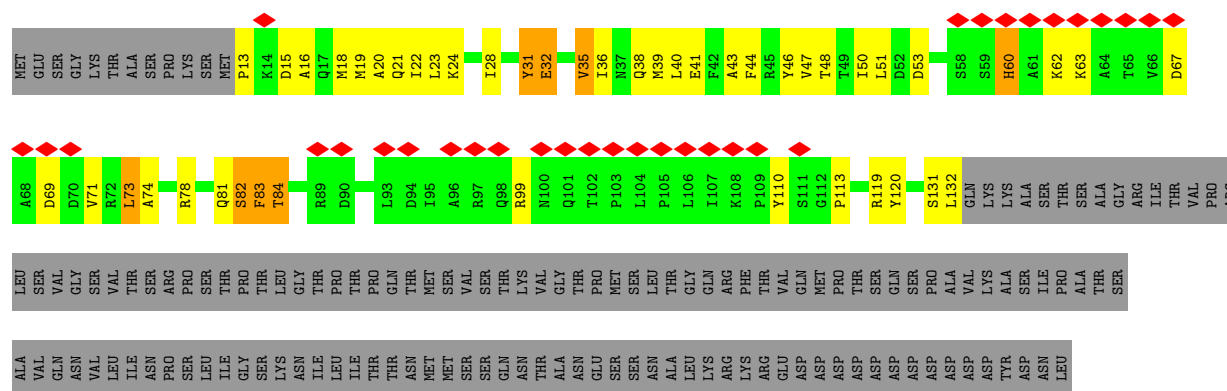
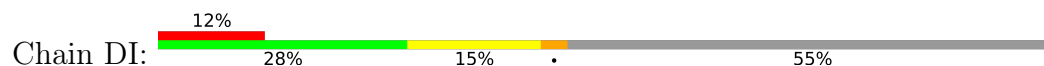


• Molecule 39: Transcription initiation factor TFIID subunit 8

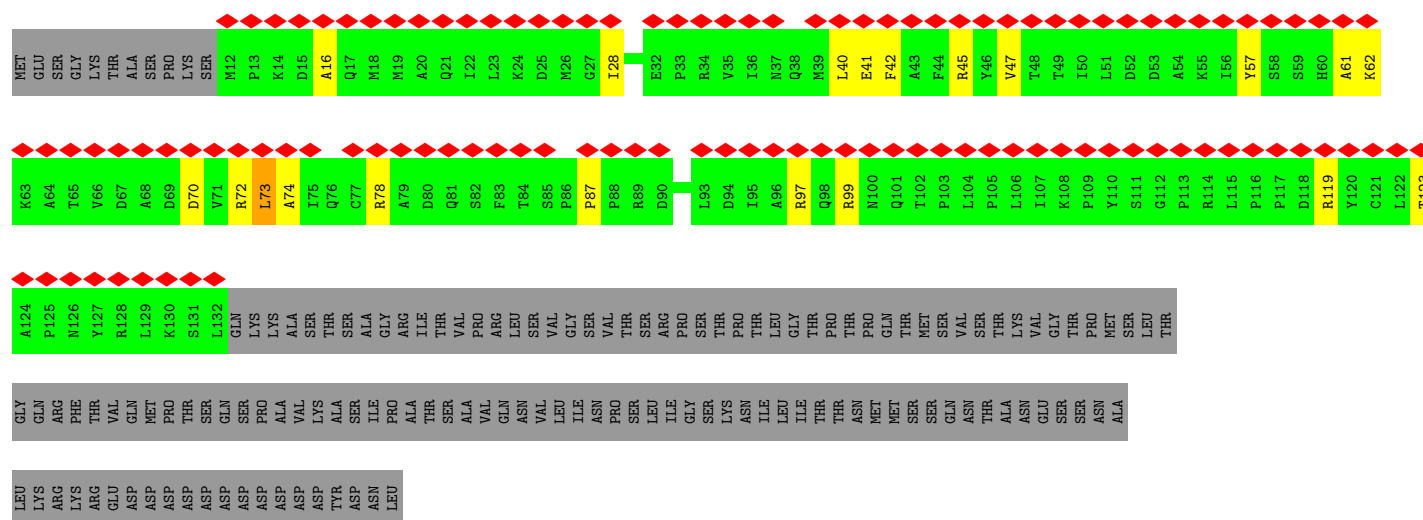
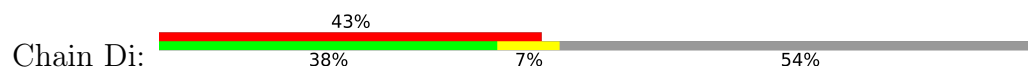




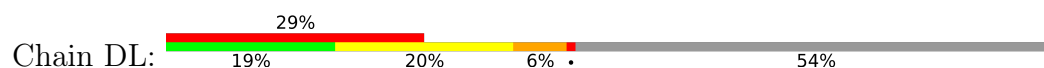
• Molecule 40: Transcription initiation factor TFIID subunit 9

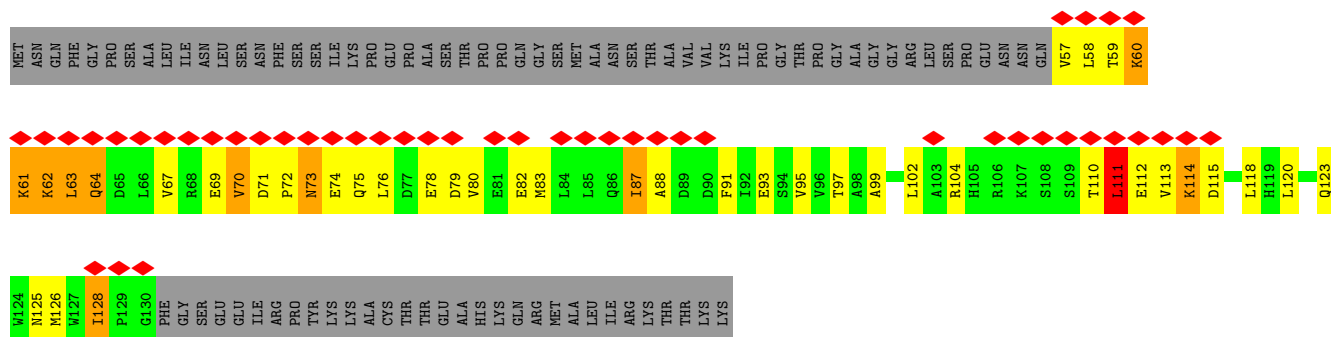


• Molecule 40: Transcription initiation factor TFIID subunit 9

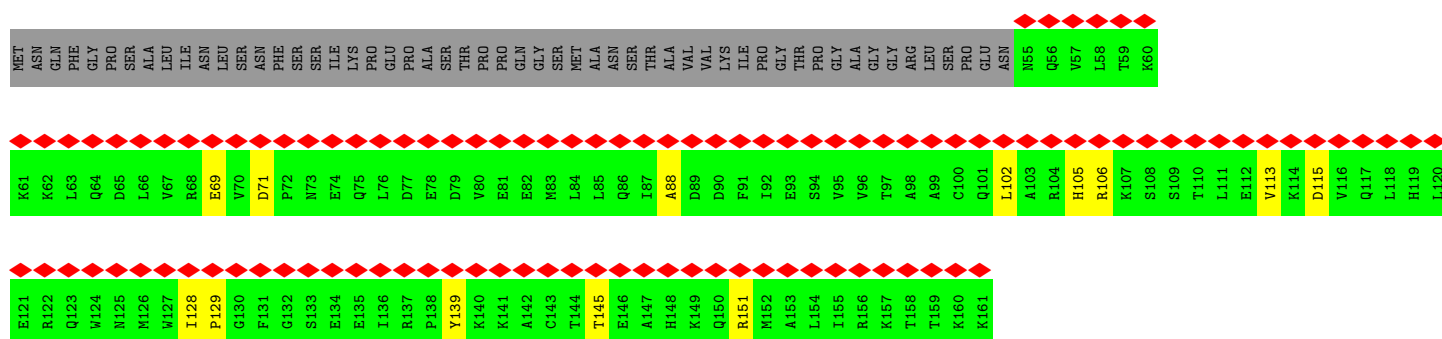


• Molecule 41: Transcription initiation factor TFIID subunit 12

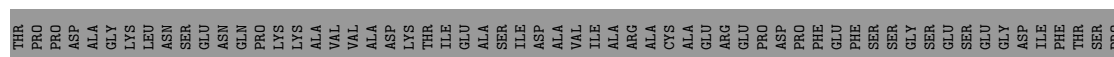
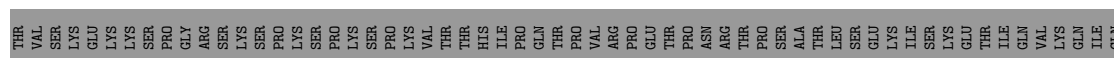
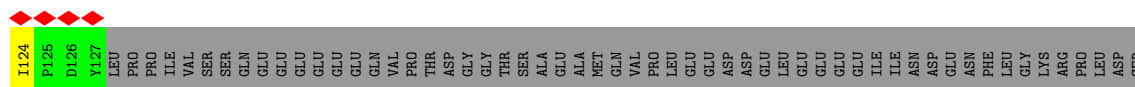
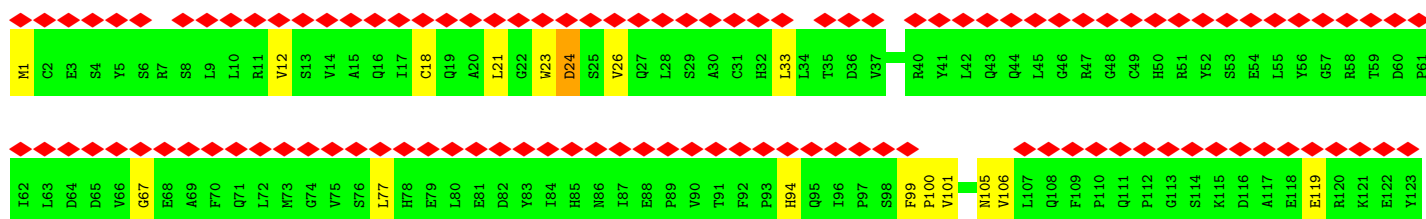




• Molecule 41: Transcription initiation factor TFIID subunit 12

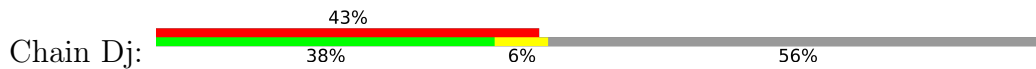


• Molecule 42: Transcription initiation factor TFIID subunit 3



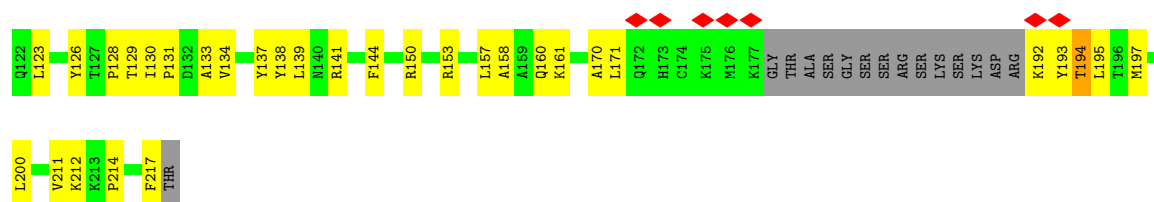
[illegible]

- Molecule 43: Transcription initiation factor TFIID subunit 10

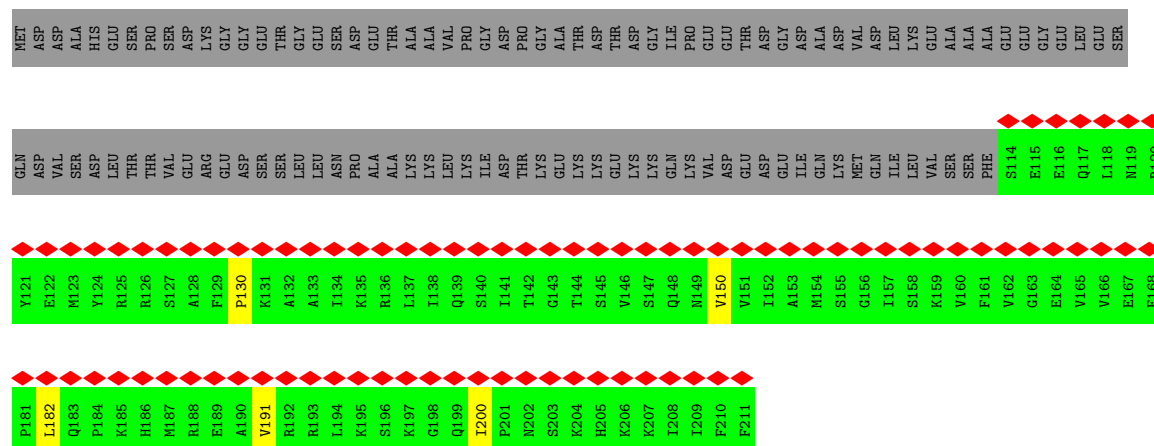
[illegible]

- Molecule 43: Transcription initiation factor TFIID subunit 10

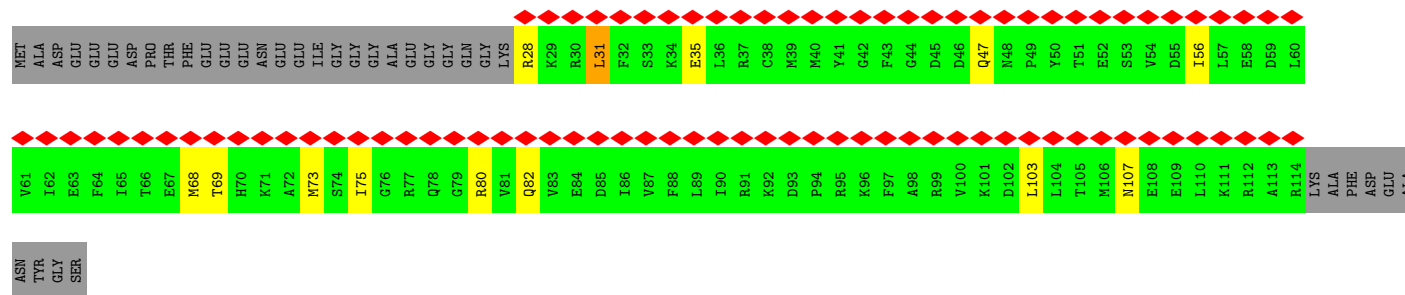
[illegible]



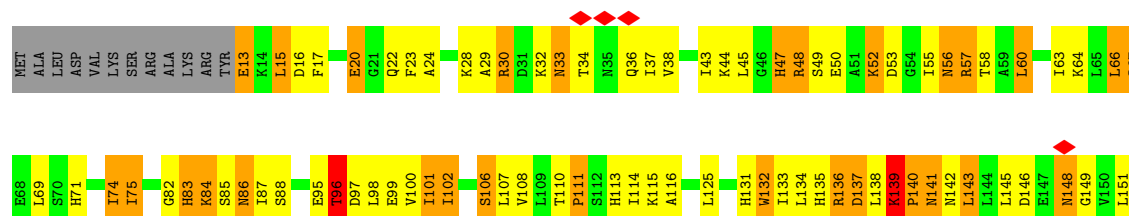
• Molecule 44: Transcription initiation factor TFIID subunit 11

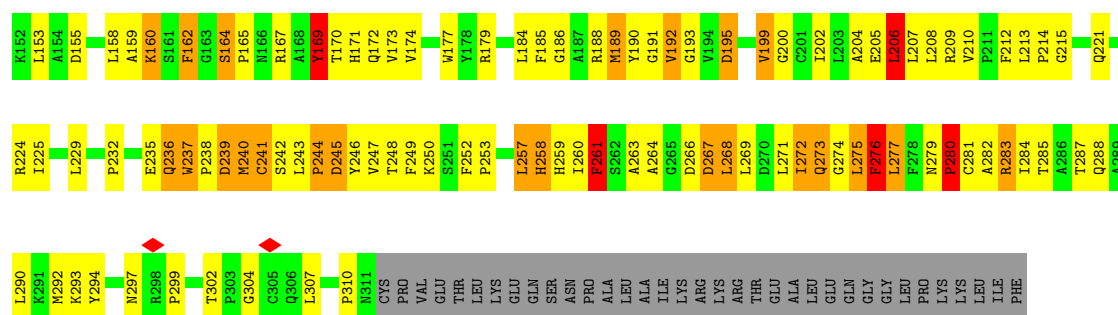


• Molecule 45: Transcription initiation factor TFIID subunit 13

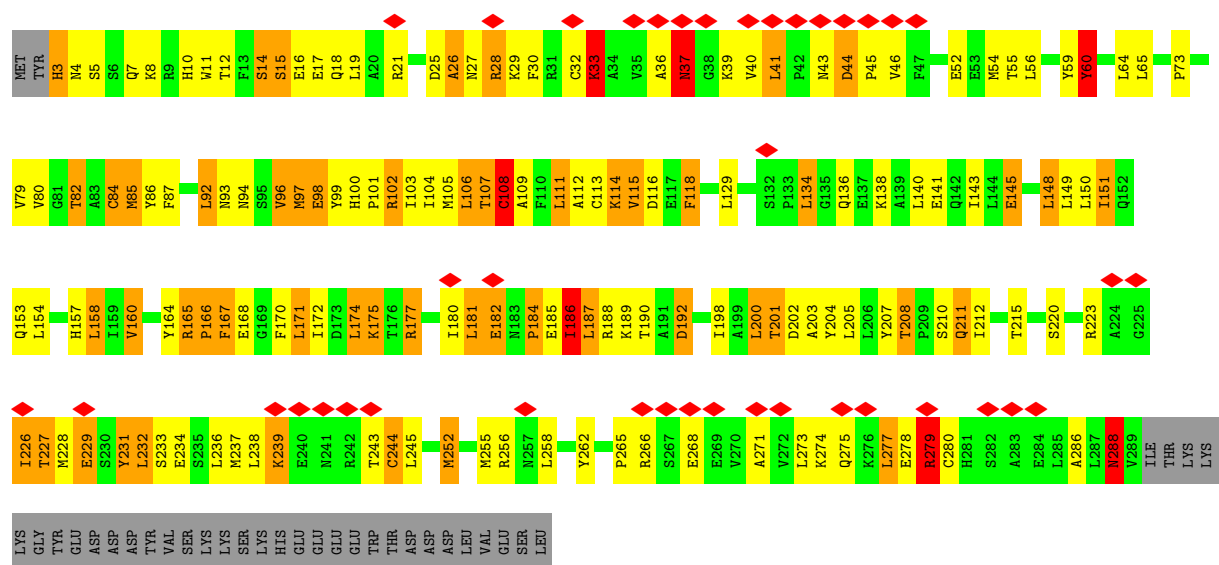
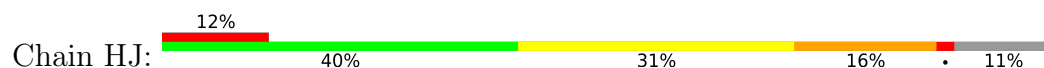


• Molecule 46: Cyclin-dependent kinase 7

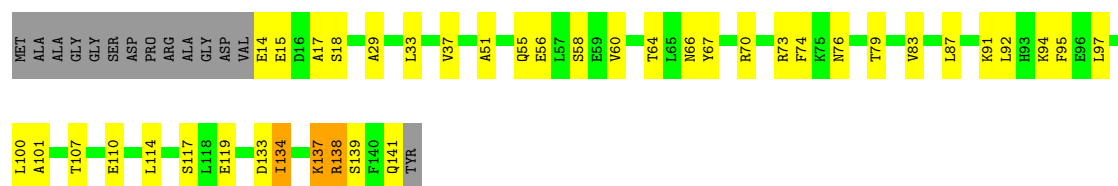




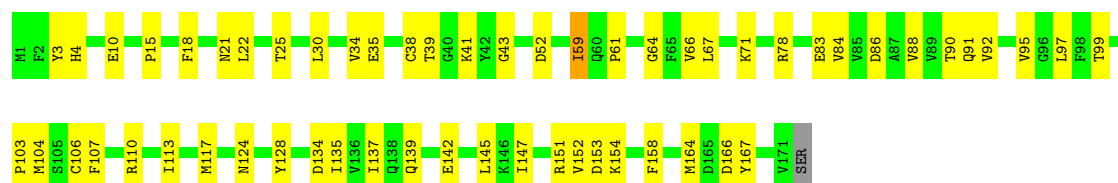
• Molecule 47: Cyclin-H



• Molecule 48: DNA-directed RNA polymerase II subunit RPB4

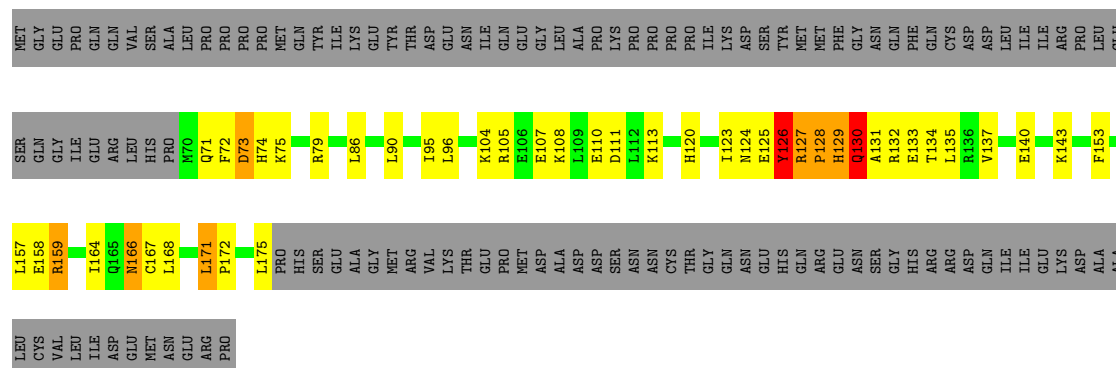


• Molecule 49: DNA-directed RNA polymerase II subunit RPB7



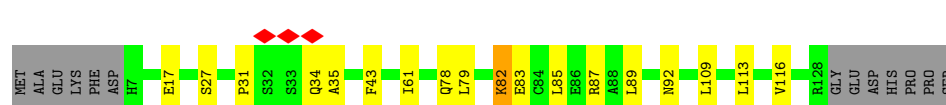
• Molecule 50: Mediator of RNA polymerase II transcription subunit 7

Chain g:  26% 15% 55%



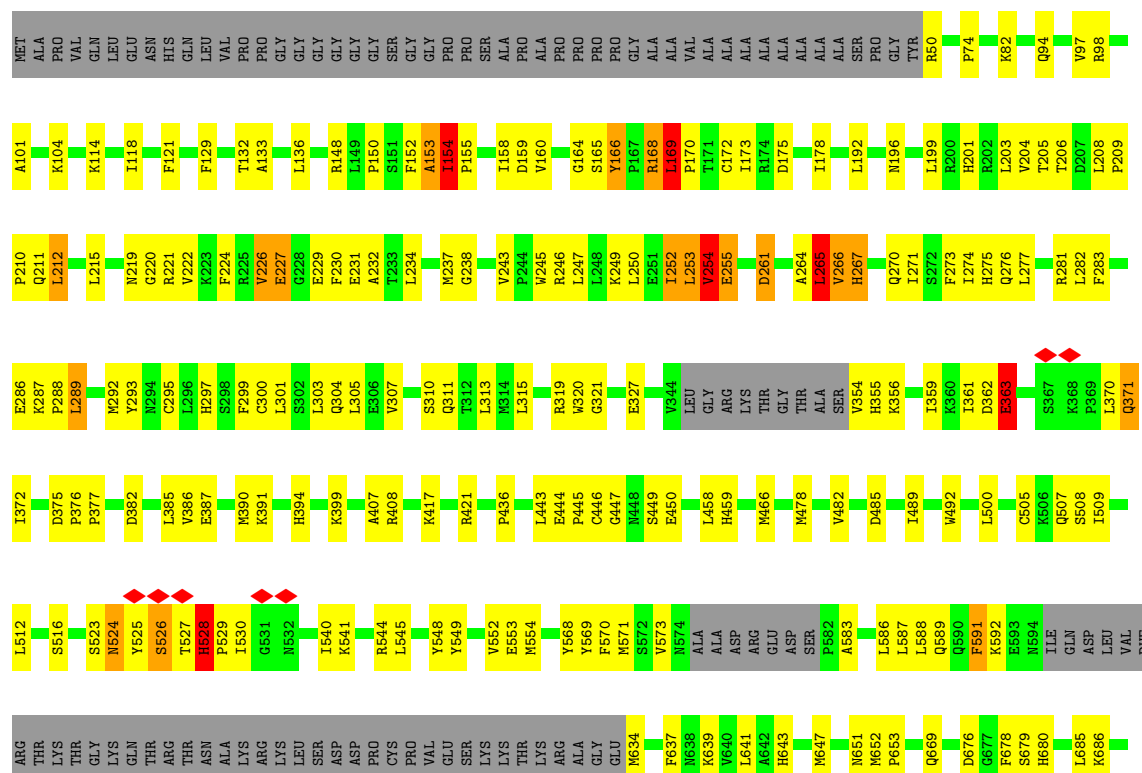
• Molecule 51: Mediator of RNA polymerase II transcription subunit 10

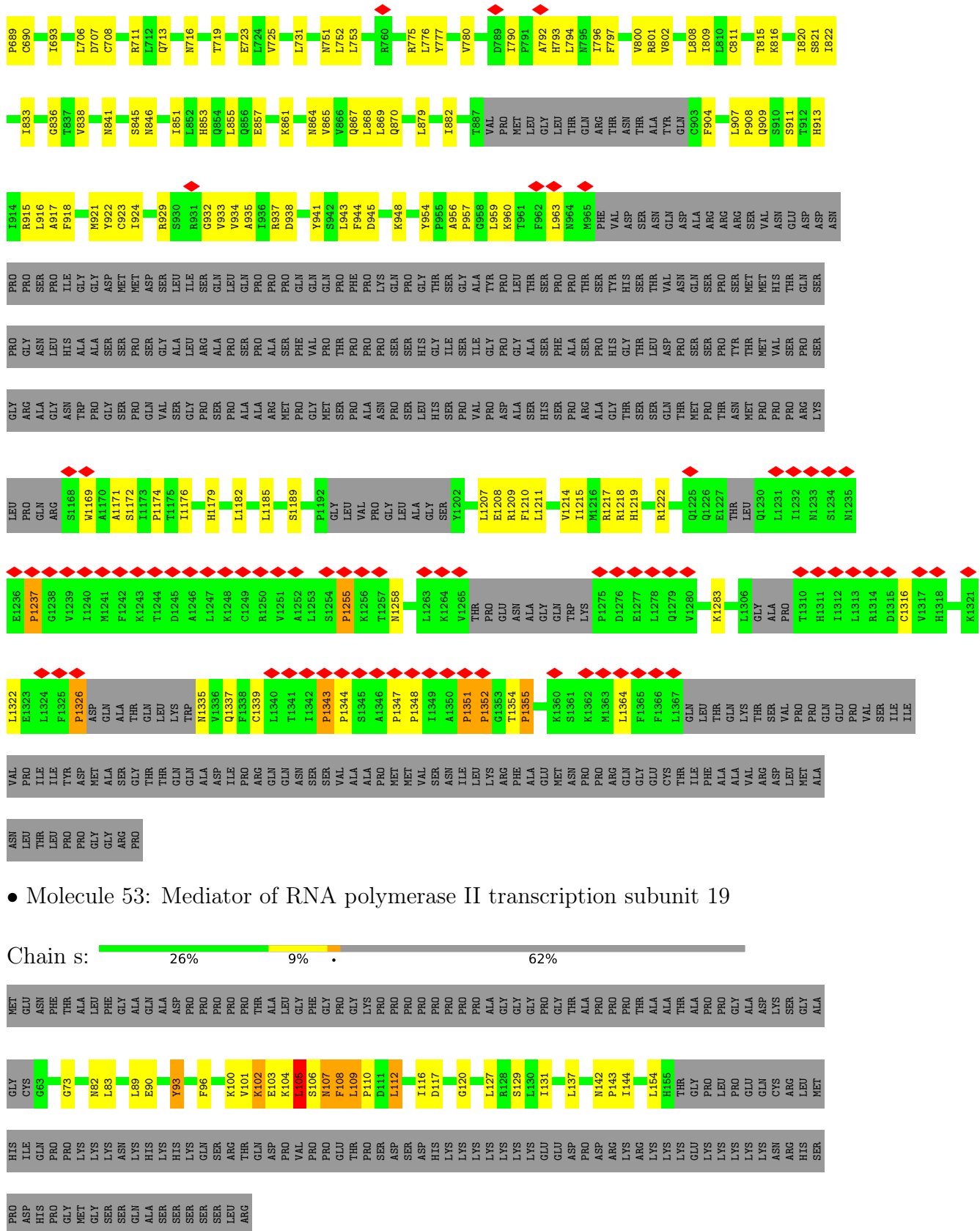
Chain j:  77% 13% 10%

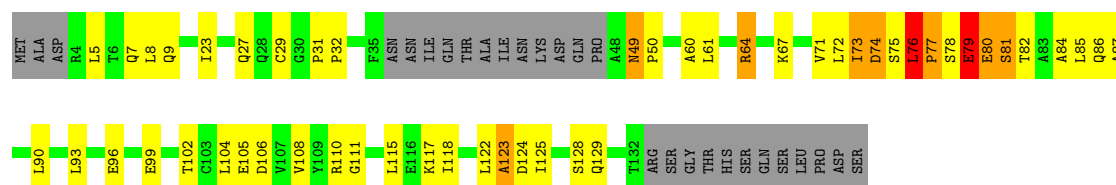


• Molecule 52: Mediator of RNA polymerase II transcription subunit 14

Chain n:  6% 47% 21% 30%



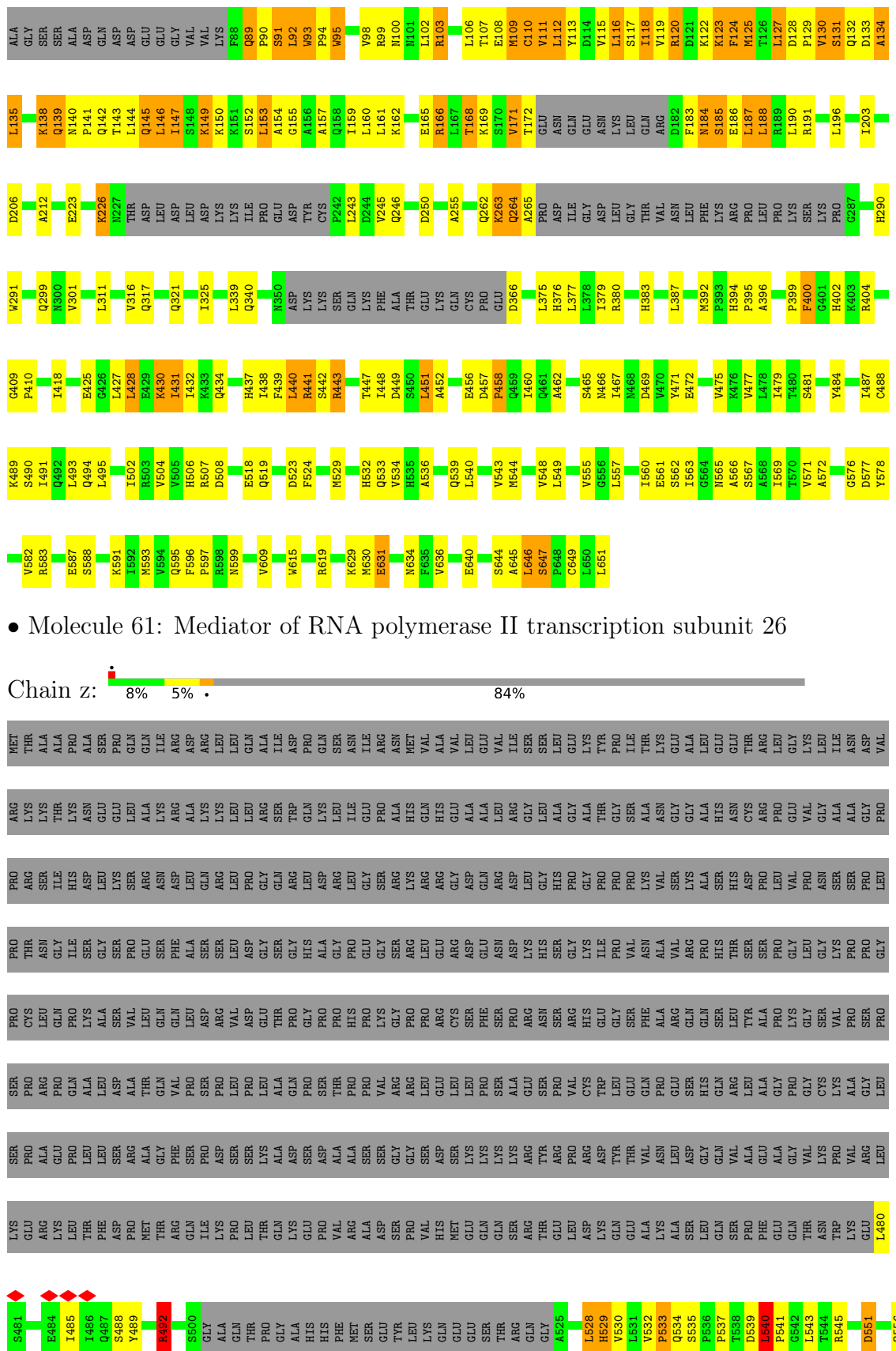


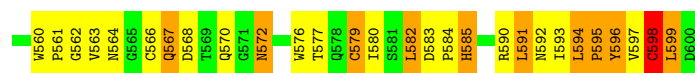


Chain a:

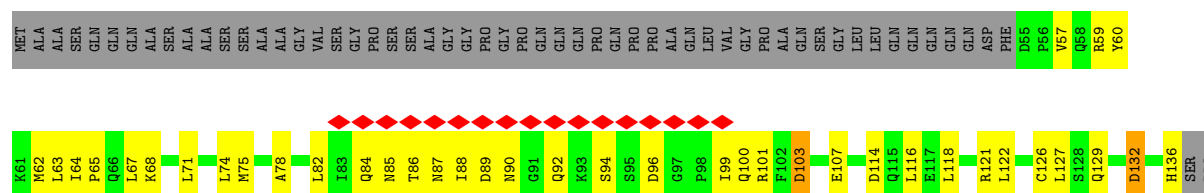
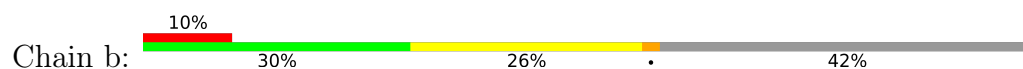




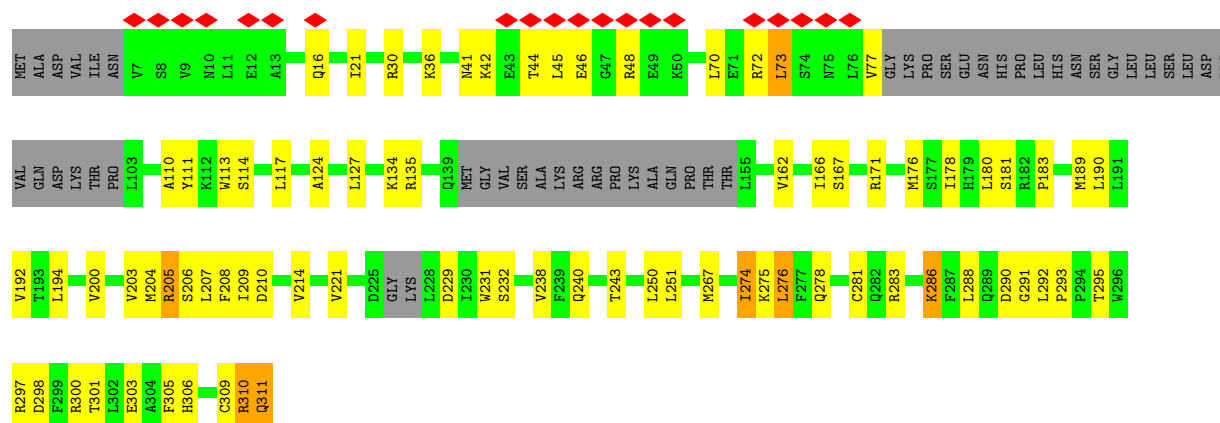




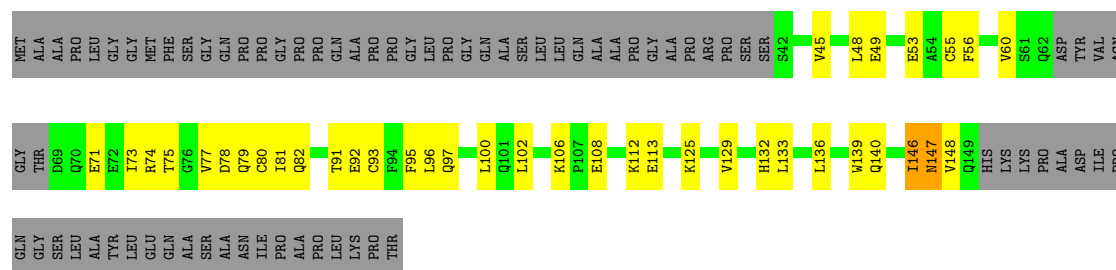
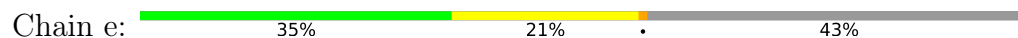
• Molecule 62: Mediator of RNA polymerase II transcription subunit 29



• Molecule 63: Mediator of RNA polymerase II transcription subunit 27

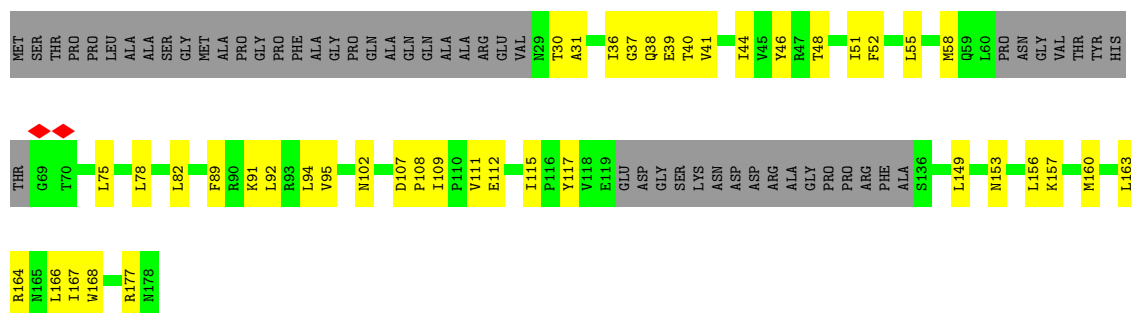


• Molecule 64: Mediator of RNA polymerase II transcription subunit 28



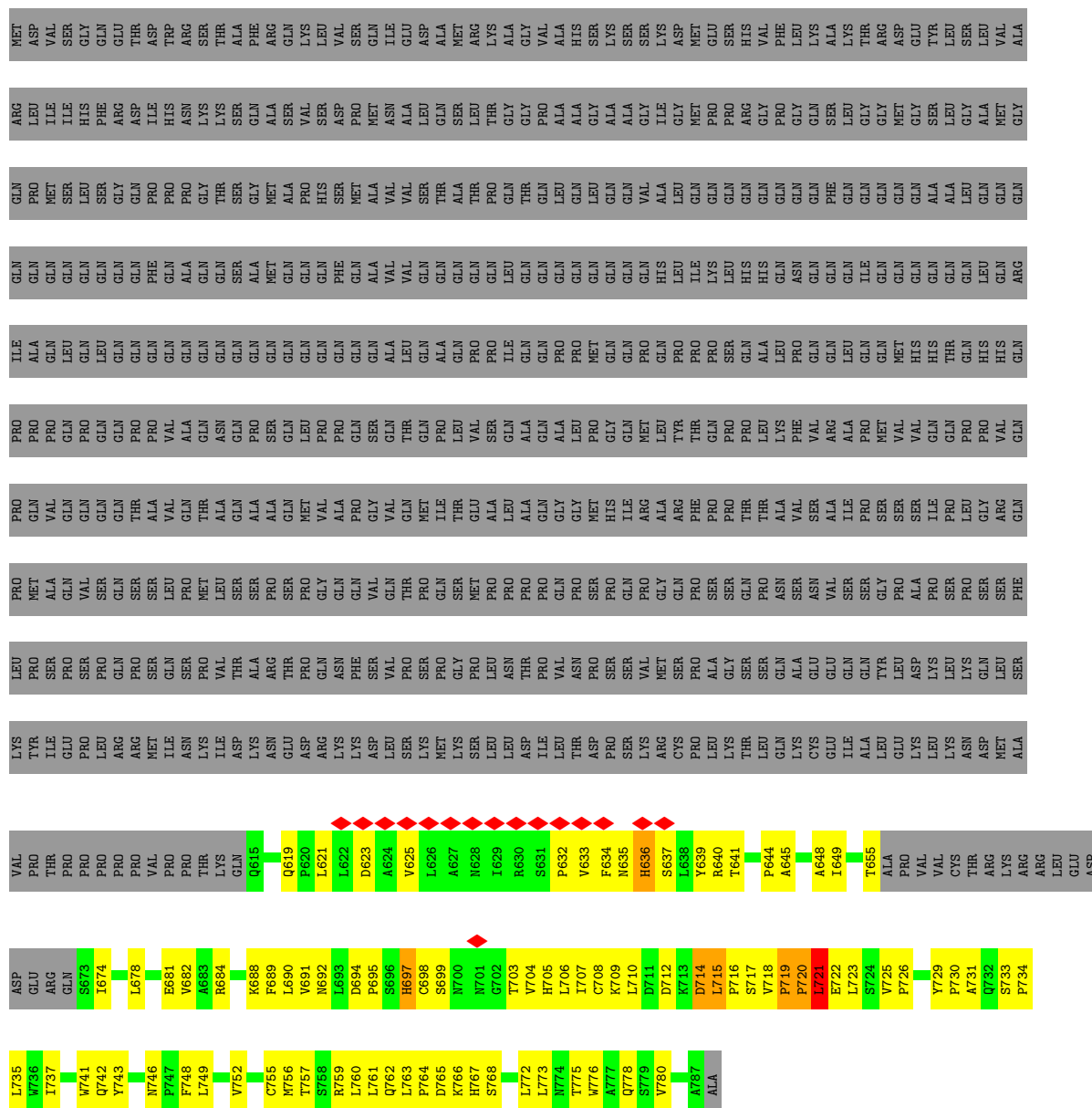
• Molecule 65: Mediator of RNA polymerase II transcription subunit 30



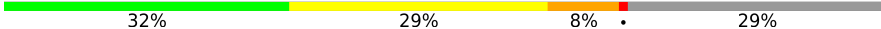


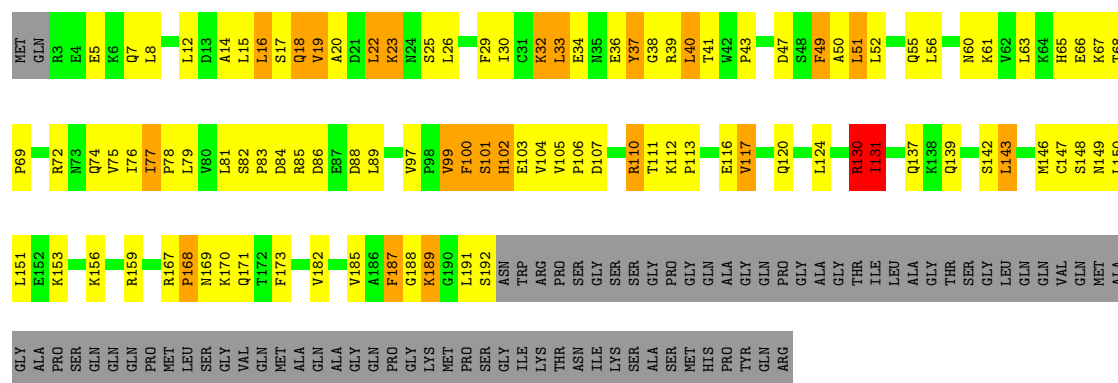
- Molecule 66: Mediator of RNA polymerase II transcription subunit 15

Chain o: 9% 10% 80%

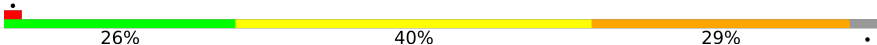


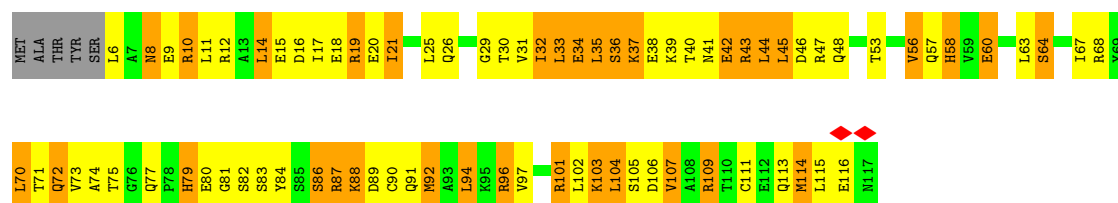
- Molecule 67: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

Chain h: 



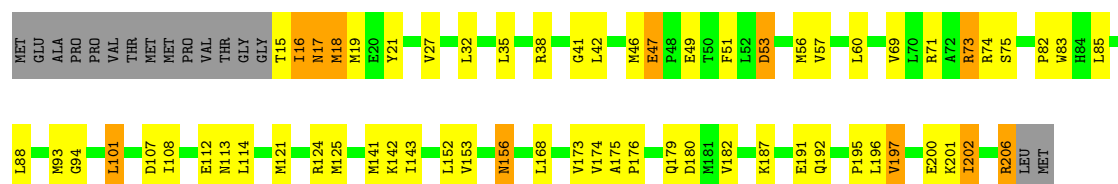
- Molecule 68: Mediator of RNA polymerase II transcription subunit 11

Chain k: 



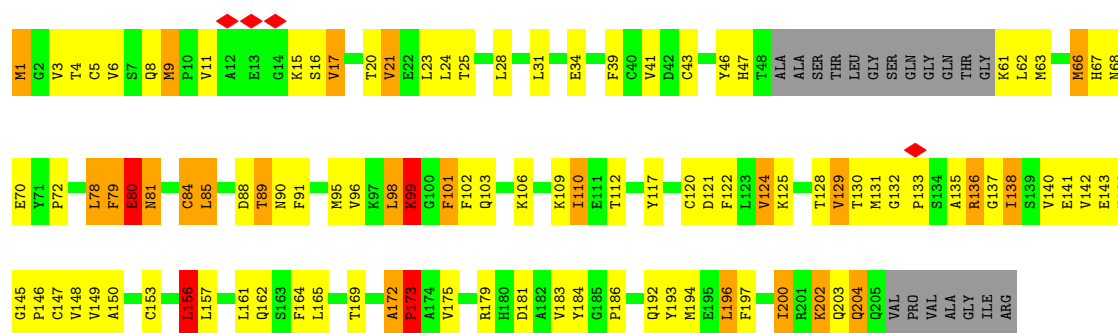
- Molecule 69: Mediator of RNA polymerase II transcription subunit 18

Chain r: 



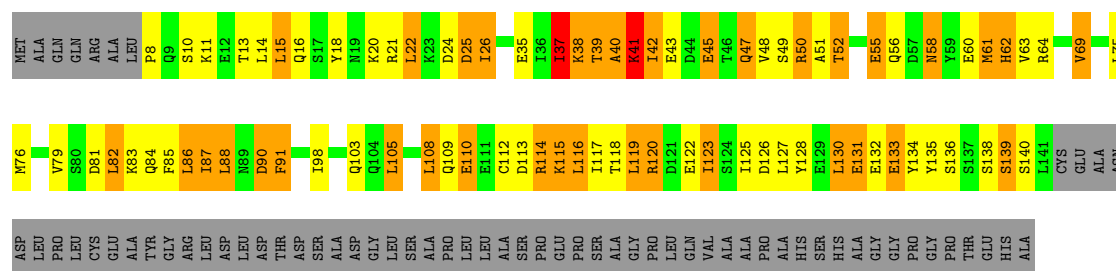
- Molecule 70: Mediator of RNA polymerase II transcription subunit 20

Chain t: 



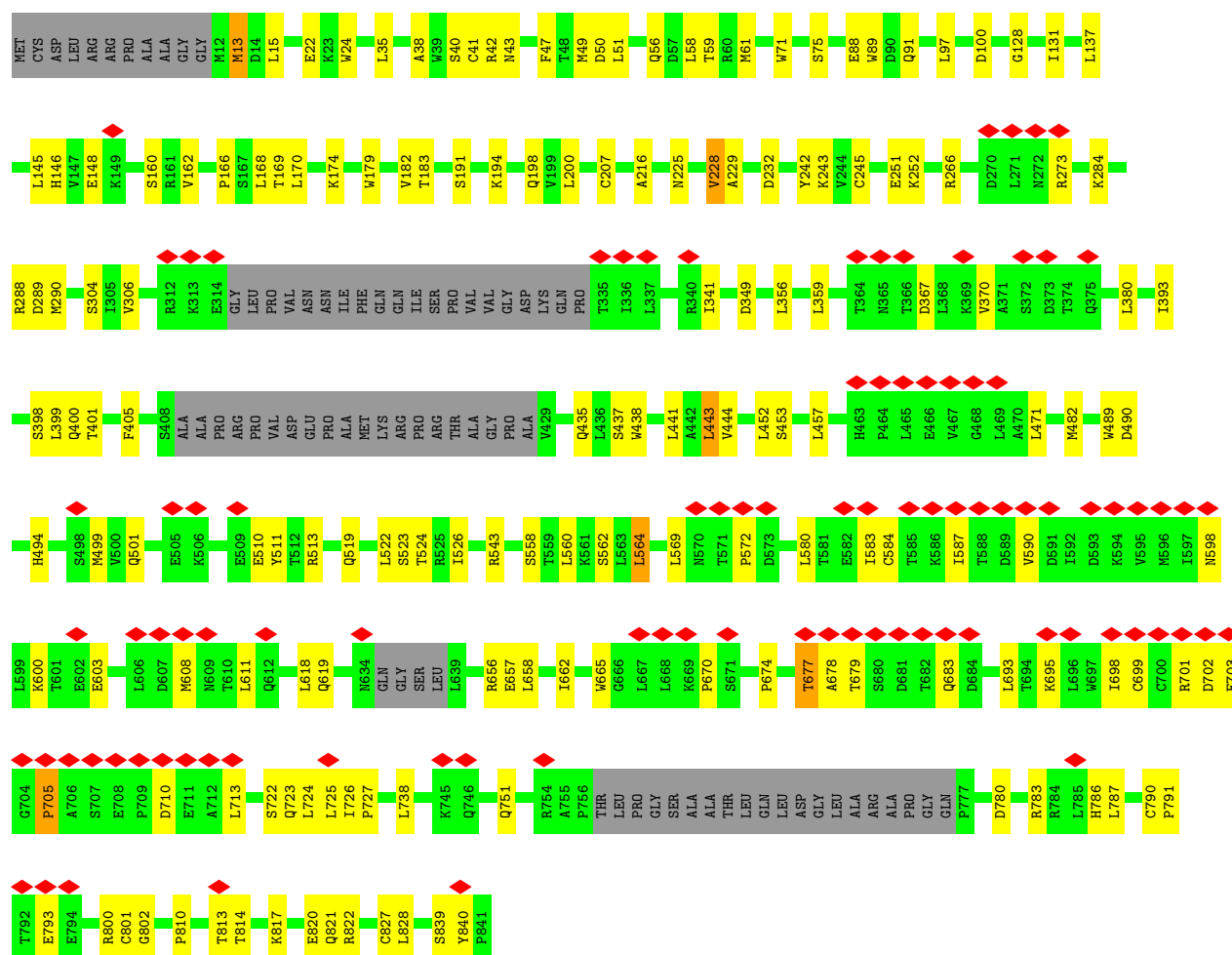
- Molecule 71: Mediator of RNA polymerase II transcription subunit 22

Chain v: 



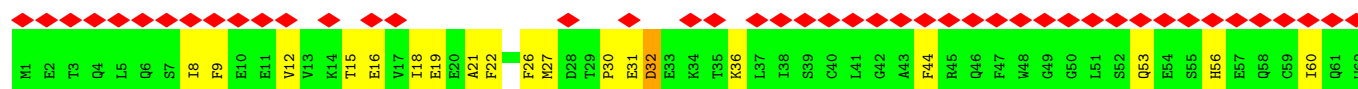
• Molecule 72: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p: 

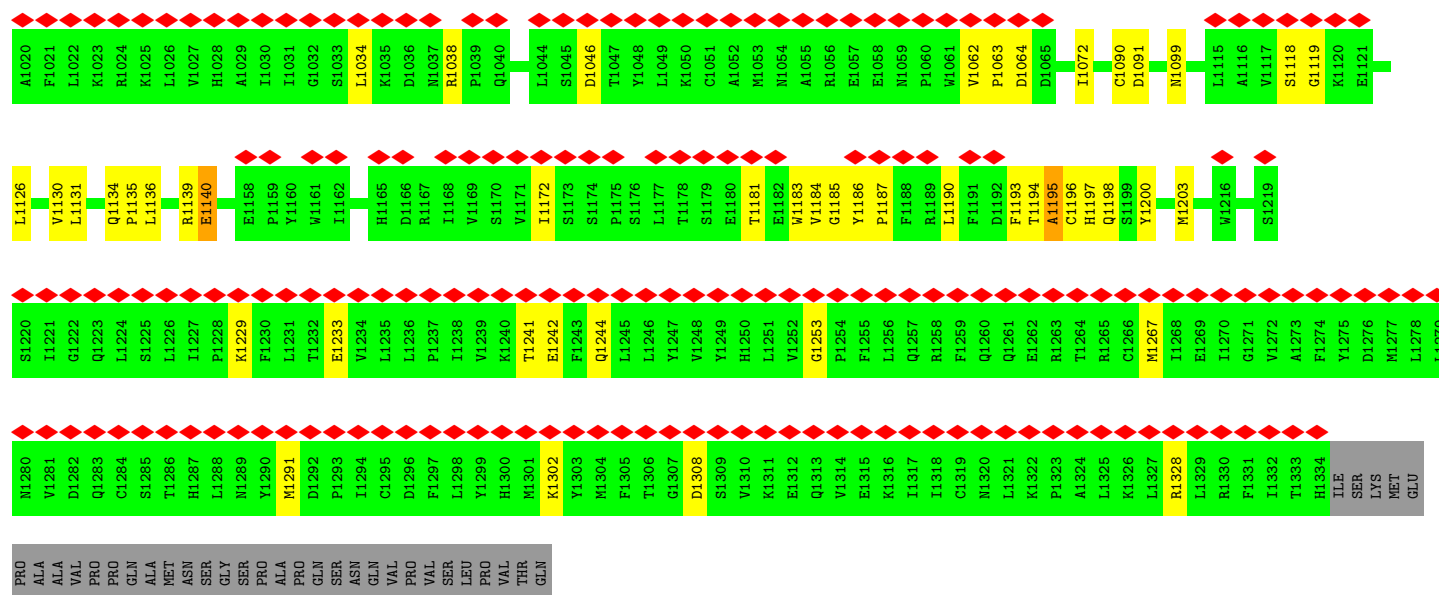


• Molecule 73: Mediator of RNA polymerase II transcription subunit 23

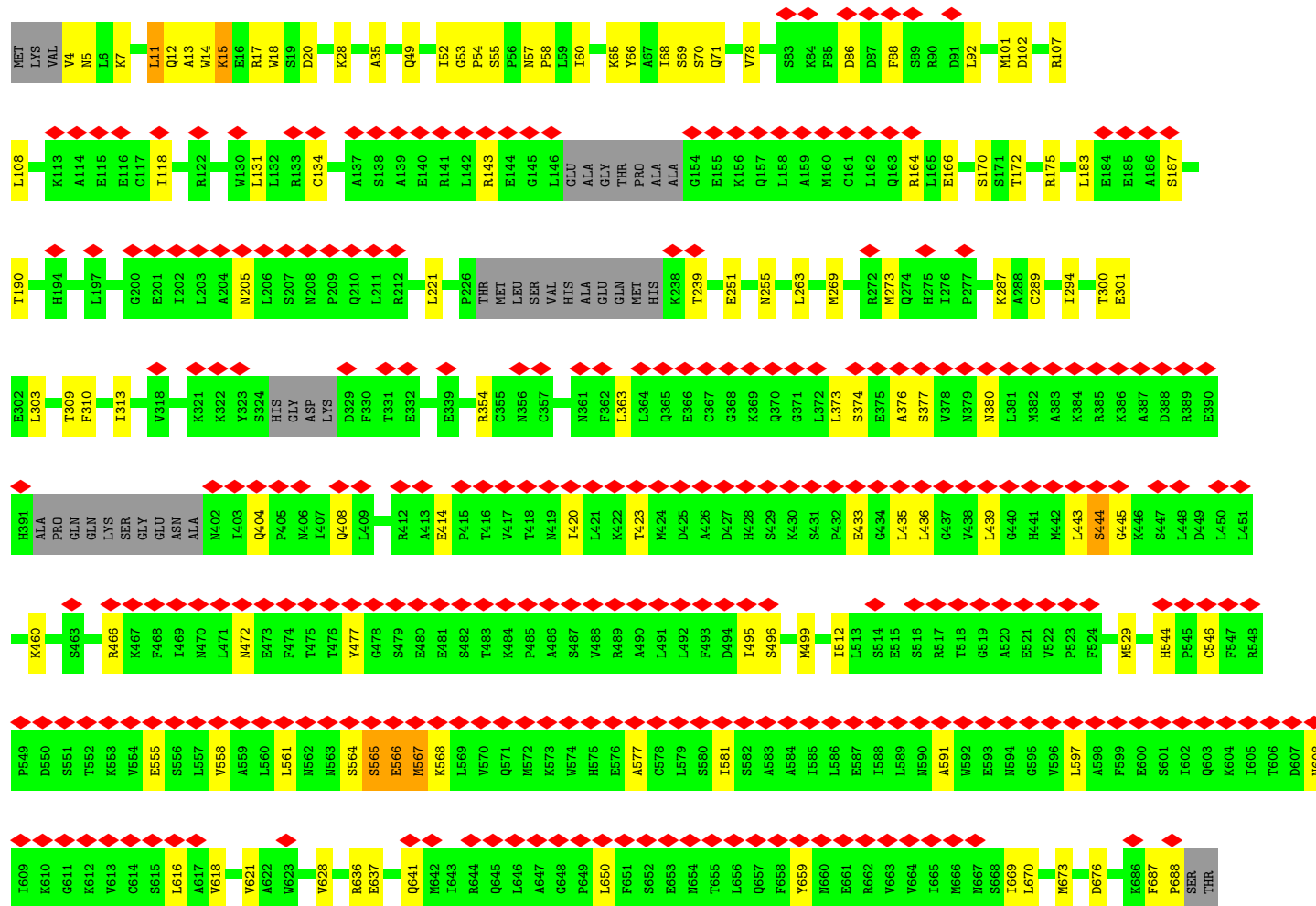
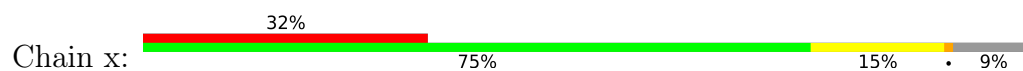
Chain w: 

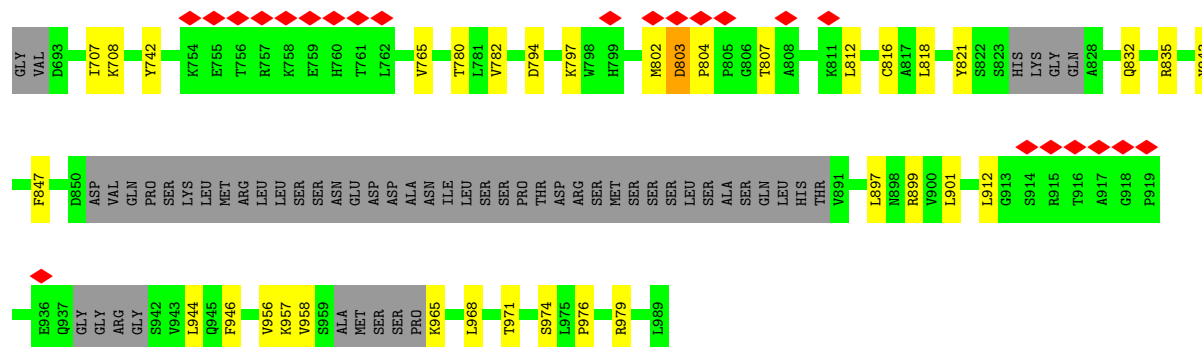


P950	Y951	L952	P953	I954	Y955	F956	G957	N958	V959	C960	L961	R962	F963	L964	P965	V966	F967	D968	I969	V970	I971	H972	R973	F974	L975	E976	L977	L978	P979	V980	K981	N982	S983	L984	E985	T986	L987	L988	D989	H990	L991	G992	G993	L994	Y995	K996	F997	H998	D999	Y1000	Y1001	E1002	M1003	H1004	L1005	L1006	L1007	D1008	R1009			
Q887	L888	L889	L890	L891	K892	F893	E894	N895	T896	S897	A898	G899	C900	Q901	D902	F903	V904	K905	E906	N907	S908	R909	Q910	N911	D912	W913	H914	W915	K916	T917	N918	L919	N920	Y921	H922	T923	L924	P925	L926	C927	Y928	P929	E930	K931	L932	F933	R934	E935	G936	L937	H938	D939	Y1000	Y1001	E1002	M1003	H1004	L1005	L1006	L1007	D1008	R1009
W767	K768	S769	M770	S771	M772	E773	M774	D775	T776	T777	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	L803	N804	Q805	T806	G807	Y808	R809	V810	L811	E812	R813	T814	G815	A816	R817	A818	L819	W820	A821	H822	V823	R824	T825	F826			
I707	Q708	G709	T710	W711	C712	K713	D714	T715	L716	Q717	T718	T719	W720	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	M746	W747	W748	P749	Q750	E751	S752	R753	F754	M755	L756	K757	K758	M759	V760	E761	E762	E763	Y764	R765	K766			
Q638	N639	Q640	L641	H642	L643	C644	V645	E646	L650	T653	E660	V661	Q662	P663	Q664	F665	T666	R667	F668	L669	S670	D671	P672	K673	T674	V675	L676	S677	A678	E679	S680	E681	E682	L683	M684	R685	A686	L687	L688	L689	T690	L691	A692	T695	H696	V697	T698	D699	F700	F701	T702	G703	S704	D705	S706							
L453	E456	F457	L458	Q459	Q460	S461	L462	R463	M464	K465	S466	L467	Q468	M469	M470	D471	Y472	K473	L474	L477	E486	G493	A494	L495	V496	E497	T498	G501	N502	G503	L504	M505	R506	L507	P508	L509	P510	G511	T512	N513	C514	M515	A516	S517	G518	S519	T520	P522	T532	V533	H534											
L343	F344	Q345	F346	A347	S348	H351	L356	R363	G364	L365	I366	R369	D370	H371	L372	Q378	S381	N387	A388	L389	A390	D391	F392	L402	Y408	L409	C410	V411	P412	D413	I414	M415	K416	P417	Q418	S419	T420	H421	M425	T426	C427	H431	L432	M433	T445	R452																
I187	R188	K189	L190	Y191	P192	E193	G194	K195	L196	P197	H198	V199	L200	L201	G202	N203	L204	V205	S206	D207	F208	V209	D210	T211	F212	R213	P214	T215	A216	R217	I218	N219	S220	R224	V231	S234	Q235	A236	I237	C238	N239	S240	W241	K242	L243	D244	P245	A246	T247	L248	R249	F250	P251	L252	K253	G254						
G127	G128	V129	D130	Y131	K132	G133	V134	R135	D136	L137	L138	K139	V140	I141	L142	E143	K144	I145	L146	T147	I148	P149	M150	T151	V152	S153	S154	A155	V156	C157	Q158	P159	L160	L161	A162	A163	R164	E165	V166	I167	E168	Y169	I170	L171	E172	Q173	L174	W175	A176	C177	L178	P179	Y180	F181	F182	A183	V184	T185	E186			
I63	V64	K65	F66	I67	H68	G69	H70	H71	R75		L79	Y80	D81	C82	L83	A84	M85	A86	V87	E88	T89	G90	L91	L92	P93	P94	R95	L96	V97	C98	E99	S100	L101	I102	M103	S104	D105	T106	L107	E108	W109	E110	R111	T112	Q113	L114	W115	A116	L117	T118	F119	K120	L121	V122	R123	K124	I125	I126				



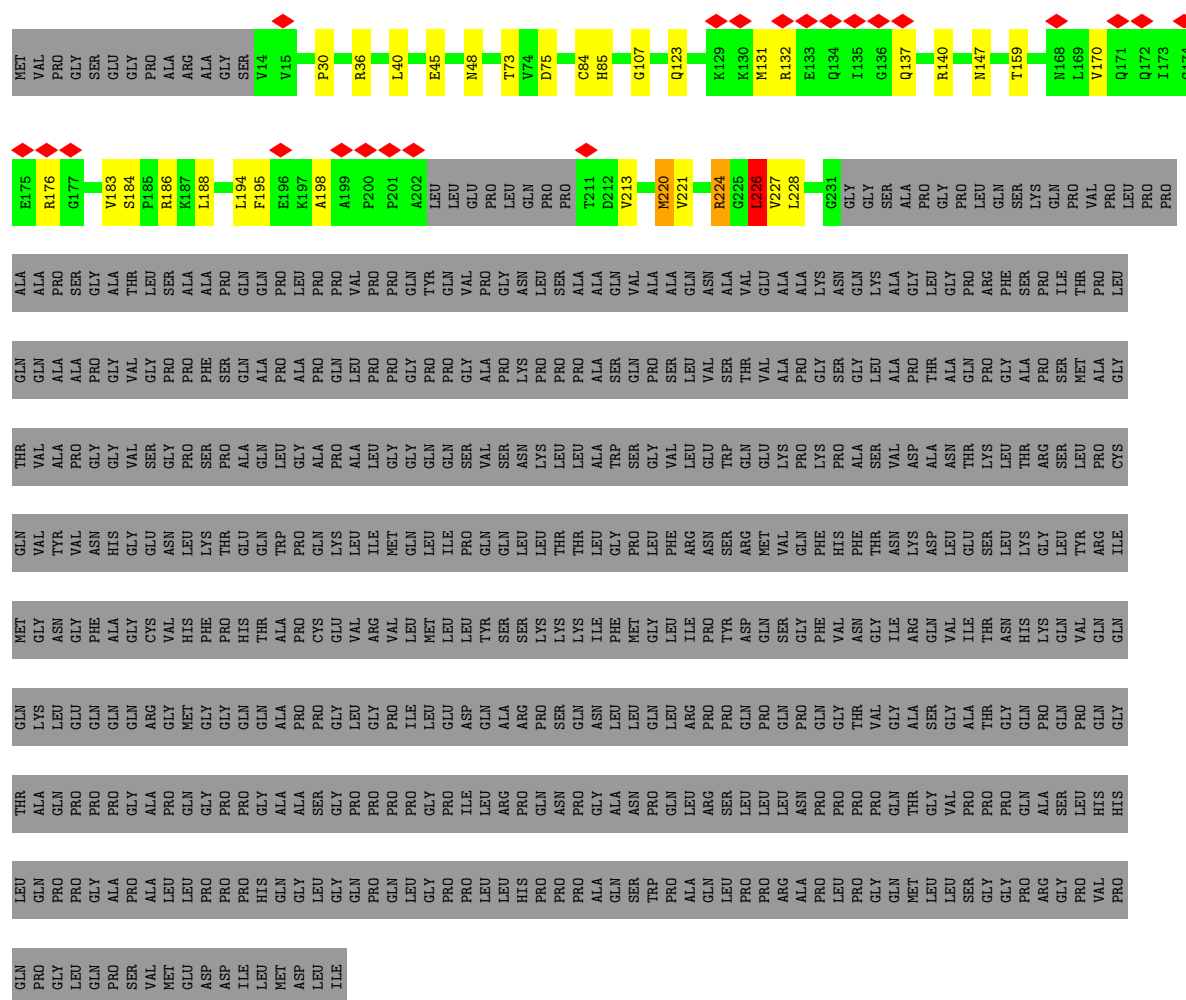
• Molecule 74: Mediator of RNA polymerase II transcription subunit 24





• Molecule 75: Mediator of RNA polymerase II transcription subunit 25

Chain y: 24% 72%

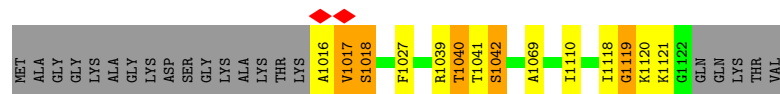


• Molecule 76: HISTONE H2A.Z

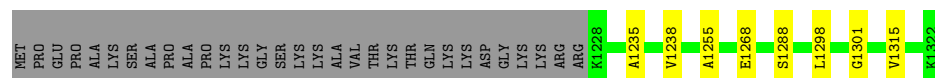
Chain NC: 70% 9% 20%



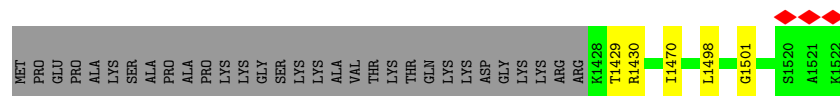
Chain NG:



Chain ND:



Chain NH:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-1.277	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.205	Depositor
Map size ($\text{\AA}$)	560.27997, 560.27997, 560.27997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3339999, 1.3339999, 1.3339999	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, ZN, MG

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	X	0.47	0/1561	0.64	2/2411 (0.1%)
2	Y	0.47	0/1516	0.63	1/2334 (0.0%)
3	NX	0.37	0/3401	0.65	1/5180 (0.0%)
4	NY	0.33	0/4046	0.55	0/6310
5	BA	0.14	0/1983	0.27	0/2679
6	DA	0.66	0/4679	0.90	6/6320 (0.1%)
7	EA	0.33	0/1560	0.58	1/2097 (0.0%)
8	FA	0.11	0/1167	0.27	0/1576
9	HA	0.16	0/5875	0.31	0/7955
10	NA	1.12	1/497 (0.2%)	1.44	2/693 (0.3%)
10	NE	1.27	0/510	1.54	6/710 (0.8%)
11	PA	0.24	0/11851	0.38	1/16014 (0.0%)
12	DB	0.49	1/7993 (0.0%)	0.71	8/10836 (0.1%)
13	EB	0.23	0/1427	0.44	0/1916
14	FB	0.20	0/1817	0.35	0/2445
15	HB	0.15	0/2210	0.31	0/2975
16	NB	1.23	0/390	1.46	5/539 (0.9%)
16	NF	1.40	5/420 (1.2%)	1.49	6/581 (1.0%)
17	PB	0.14	0/9257	0.29	0/12493
18	HC	0.21	0/3230	0.37	0/4376
19	DO	0.15	0/816	0.29	0/1105
20	DP	0.14	0/1448	0.28	0/1948
21	DQ	0.16	0/945	0.35	0/1274
22	PC	0.13	0/2102	0.29	0/2857
23	PE	0.16	0/1752	0.30	0/2366
24	PF	0.25	0/646	0.42	0/871
25	PH	0.12	0/1207	0.28	0/1628
26	PI	0.13	0/949	0.29	0/1284
27	PJ	0.14	0/516	0.25	0/696
28	PK	0.15	0/939	0.27	0/1271
29	PL	0.14	0/378	0.28	0/500
30	HD	0.70	0/2436	1.03	18/3286 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	HG	0.13	0/2793	0.28	0/3780
32	HE	0.25	0/2103	0.39	0/2846
33	HF	0.20	0/529	0.43	1/714 (0.1%)
34	HH	0.16	0/4994	0.31	1/6745 (0.0%)
35	DD	0.56	0/1343	0.83	2/1795 (0.1%)
35	Dd	0.23	0/1321	0.44	0/1772
36	DE	0.43	0/4469	0.64	1/6050 (0.0%)
36	De	0.30	0/4433	0.53	0/6004
37	DF	0.70	1/3167 (0.0%)	1.08	10/4303 (0.2%)
37	Df	0.48	0/3140	0.81	6/4268 (0.1%)
38	DG	0.71	0/1199	0.95	1/1612 (0.1%)
39	DH	0.46	0/1673	0.75	2/2285 (0.1%)
40	DI	0.58	0/981	0.90	5/1332 (0.4%)
40	Di	0.24	0/989	0.48	2/1343 (0.1%)
41	DL	0.65	0/613	1.03	1/829 (0.1%)
41	DI	0.54	0/888	0.80	0/1194
42	Dc	0.48	0/1035	0.67	0/1406
43	DJ	0.24	0/736	0.46	0/998
43	Dj	0.23	0/775	0.45	0/1049
44	Dk	0.30	0/799	0.53	1/1070 (0.1%)
45	Dm	0.31	0/733	0.55	0/977
46	HI	1.02	0/2433	1.64	45/3302 (1.4%)
47	HJ	1.10	3/2356 (0.1%)	1.72	54/3185 (1.7%)
48	PD	0.26	0/1064	0.43	1/1428 (0.1%)
49	PG	0.18	0/1382	0.28	0/1874
50	g	0.79	1/911 (0.1%)	1.40	8/1219 (0.7%)
51	j	0.38	0/849	0.61	0/1150
52	n	0.43	0/7901	0.73	17/10731 (0.2%)
53	s	0.93	0/741	1.26	6/1002 (0.6%)
54	u	0.75	1/895 (0.1%)	1.09	9/1215 (0.7%)
55	a	0.93	0/3507	1.34	11/4760 (0.2%)
56	d	0.92	0/1281	1.30	1/1718 (0.1%)
57	f	0.76	1/1402 (0.1%)	1.07	6/1905 (0.3%)
58	i	0.99	1/612 (0.2%)	1.35	1/815 (0.1%)
59	m	0.21	0/1010	0.39	0/1359
60	q	0.66	1/4456 (0.0%)	0.87	0/6019
61	z	0.95	0/781	1.41	6/1067 (0.6%)
62	b	0.75	0/911	1.13	1/1229 (0.1%)
63	c	0.58	0/2172	0.90	5/2935 (0.2%)
64	e	0.25	0/840	0.44	0/1128
65	l	0.20	0/1048	0.41	0/1405
66	o	0.53	0/1256	0.86	3/1724 (0.2%)
67	h	0.94	0/1485	1.33	4/2008 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	k	0.98	0/885	1.31	1/1190 (0.1%)
69	r	0.91	0/1565	1.26	3/2106 (0.1%)
70	t	1.05	2/1530 (0.1%)	1.49	11/2066 (0.5%)
71	v	0.98	0/1092	1.43	5/1468 (0.3%)
72	p	0.65	0/6116	0.76	3/8311 (0.0%)
73	w	0.52	0/11056	0.65	5/15023 (0.0%)
74	x	0.59	0/7191	0.78	11/9728 (0.1%)
75	y	0.63	0/1645	0.83	0/2240
76	NC	1.27	2/505 (0.4%)	1.53	9/700 (1.3%)
76	NG	1.08	1/523 (0.2%)	1.43	10/724 (1.4%)
77	ND	1.22	2/470 (0.4%)	1.46	5/654 (0.8%)
77	NH	1.09	0/470	1.44	4/654 (0.6%)
All	All	0.53	23/190578 (0.0%)	0.77	335/259940 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	q	452	ALA	C-N	9.12	1.47	1.33
57	f	110	ASP	C-N	-8.20	1.22	1.33
47	HJ	244	CYS	C-O	7.08	1.32	1.24
70	t	136	ARG	C-O	-6.88	1.15	1.23
70	t	89	THR	C-O	6.60	1.32	1.24
12	DB	61	ASN	C-O	-6.38	1.18	1.24
10	NA	518	THR	CA-CB	6.32	1.62	1.53
58	i	100	LEU	C-O	6.21	1.31	1.24
16	NF	250	ILE	CA-CB	6.19	1.62	1.54
37	DF	395	ARG	C-O	5.96	1.32	1.24
47	HJ	258	LEU	C-O	5.78	1.30	1.24
76	NG	1110	ILE	CA-C	5.66	1.58	1.53
16	NF	297	LEU	C-O	-5.54	1.17	1.24
76	NC	857	ILE	CA-CB	5.48	1.60	1.54
47	HJ	201	THR	N-CA	5.46	1.52	1.45
76	NC	913	ILE	CA-CB	-5.37	1.47	1.54
50	g	130	GLN	C-O	-5.32	1.18	1.24
16	NF	300	PHE	CA-C	5.25	1.59	1.52
16	NF	231	LYS	CA-C	5.24	1.59	1.52
77	ND	1255	ALA	CA-CB	-5.23	1.45	1.53
16	NF	243	VAL	CA-CB	-5.20	1.47	1.54
77	ND	1238	VAL	CA-CB	5.09	1.60	1.54
54	u	77	PRO	C-O	-5.08	1.17	1.23

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g	128	PRO	N-CA-C	-13.22	92.27	114.75
10	NA	464	LYS	N-CA-C	12.63	124.58	111.07
50	g	130	GLN	N-CA-C	-12.41	97.80	111.07
74	x	12	GLN	N-CA-C	-11.51	99.19	113.01
10	NE	635	VAL	N-CA-C	-10.85	102.26	111.91
30	HD	291	LEU	N-CA-C	-10.23	99.95	111.71
47	HJ	186	ILE	N-CA-C	-10.14	100.27	110.62
12	DB	491	HIS	N-CA-C	-9.69	100.72	111.28
10	NE	717	VAL	N-CA-C	-9.40	103.98	113.10
1	X	18	DG	C2'-C3'-O3'	-9.40	97.40	111.50
47	HJ	37	ASN	N-CA-C	-9.37	101.06	111.28
52	n	1351	PRO	N-CA-CB	9.34	112.14	103.08
52	n	1343	PRO	N-CA-CB	9.20	112.01	103.08
37	Df	149	PRO	O-C-N	9.10	125.50	121.31
52	n	288	PRO	N-CA-C	8.94	127.07	113.75
55	a	505	PRO	N-CA-C	-8.81	101.76	113.65
55	a	505	PRO	CA-C-N	8.78	132.49	120.46
55	a	505	PRO	C-N-CA	8.78	132.49	120.46
16	NB	28	GLY	N-CA-C	-8.77	103.79	114.66
50	g	126	TYR	N-CA-C	-8.62	102.89	112.72
40	DI	84	THR	CB-CA-C	8.53	122.44	109.13
52	n	591	PHE	CA-CB-CG	8.45	122.25	113.80
47	HJ	108	CYS	N-CA-C	-8.41	102.11	111.28
76	NC	839	ARG	N-CA-C	-8.38	103.17	112.72
70	t	80	GLU	CB-CA-C	-8.31	106.99	116.54
46	HI	275	LEU	N-CA-C	-8.15	102.39	111.28
63	c	274	ILE	N-CA-C	-8.06	105.63	113.53
47	HJ	184	PRO	CB-CA-C	-7.99	102.22	113.09
46	HI	280	PRO	N-CA-C	-7.97	102.90	113.65
57	f	64	VAL	CA-C-N	-7.94	116.04	122.16
57	f	64	VAL	C-N-CA	-7.94	116.04	122.16
46	HI	280	PRO	CB-CA-C	-7.93	99.83	112.21
52	n	1355	PRO	N-CA-CB	7.92	111.57	103.25
70	t	153	CYS	N-CA-C	-7.81	103.64	113.02
37	DF	320	ARG	CB-CG-CD	7.75	129.13	111.30
50	g	128	PRO	CA-N-CD	-7.75	101.15	112.00
52	n	1344	PRO	N-CA-CB	7.65	110.20	102.17
54	u	64	ARG	CB-CA-C	-7.63	98.91	110.88
39	DH	110	TYR	CB-CA-C	-7.56	99.00	110.88
46	HI	85	SER	N-CA-C	-7.50	103.08	111.71
46	HI	199	VAL	N-CA-C	-7.49	102.98	110.62
53	s	107	ASN	N-CA-C	-7.36	95.13	110.80
52	n	526	SER	N-CA-C	-7.35	104.31	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	HD	256	TYR	N-CA-C	-7.32	99.60	110.06
46	HI	142	ASN	N-CA-C	-7.31	104.83	113.38
52	n	1352	PRO	N-CA-CB	7.29	110.91	103.25
76	NG	1118	ILE	N-CA-C	-7.26	100.22	109.58
6	DA	640	LEU	N-CA-C	-7.23	103.56	113.18
11	PA	1795	PRO	N-CA-C	-7.21	99.73	111.77
6	DA	715	PRO	N-CA-C	-7.12	100.07	111.03
37	DF	271	VAL	N-CA-C	-7.07	106.11	112.90
50	g	71	GLN	N-CA-C	-7.07	103.58	111.71
55	a	437	LEU	N-CA-C	-7.07	101.49	111.24
52	n	591	PHE	CB-CA-C	7.05	120.94	111.70
55	a	412	ARG	CB-CA-C	7.02	122.40	110.74
46	HI	140	PRO	CB-CA-C	-7.02	101.34	113.20
12	DB	495	GLN	N-CA-C	-7.00	104.74	113.28
52	n	1326	PRO	N-CA-CB	6.99	110.69	103.00
10	NE	664	LYS	N-CA-C	6.99	118.68	111.14
52	n	1347	PRO	N-CA-CB	6.95	109.82	103.08
30	HD	284	ALA	N-CA-C	-6.89	103.78	111.71
70	t	137	GLY	CA-C-O	-6.88	114.81	122.24
54	u	74	ASP	N-CA-C	-6.87	103.40	112.34
46	HI	271	LEU	CA-C-N	-6.84	111.80	120.56
46	HI	271	LEU	C-N-CA	-6.84	111.80	120.56
6	DA	498	PRO	N-CA-CB	6.83	110.42	103.25
40	DI	84	THR	N-CA-C	-6.81	105.91	114.56
76	NG	1039	ARG	N-CA-C	-6.81	102.22	111.55
46	HI	136	ARG	CA-C-N	-6.79	113.93	123.03
46	HI	136	ARG	C-N-CA	-6.79	113.93	123.03
34	HH	64	GLN	N-CA-C	-6.79	100.24	111.37
50	g	129	HIS	N-CA-C	-6.76	104.67	113.12
52	n	1255	PRO	N-CA-CB	6.74	110.32	103.25
35	DD	923	GLN	N-CA-C	-6.74	105.03	113.18
77	ND	1298	LEU	N-CA-C	6.73	120.71	112.23
74	x	444	SER	CA-C-N	-6.70	114.95	120.98
74	x	444	SER	C-N-CA	-6.70	114.95	120.98
46	HI	287	THR	CB-CA-C	-6.68	99.70	110.79
16	NF	219	ARG	N-CA-C	6.68	125.02	110.80
61	z	595	PRO	CB-CA-C	-6.67	101.09	110.63
44	Dk	180	PRO	N-CA-C	6.67	118.83	110.70
52	n	1237	PRO	N-CA-CB	6.66	110.24	103.25
16	NB	46	ILE	N-CA-C	6.63	117.40	108.11
71	v	24	ASP	N-CA-C	-6.63	104.06	111.28
37	Df	326	HIS	N-CA-C	-6.60	104.33	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	o	719	PRO	N-CA-C	6.59	118.74	110.70
47	HJ	45	PRO	CB-CA-C	-6.58	101.76	112.62
47	HJ	29	LYS	CA-C-N	-6.54	111.52	120.28
47	HJ	29	LYS	C-N-CA	-6.54	111.52	120.28
37	Df	319	LEU	N-CA-C	-6.53	103.99	112.68
52	n	1348	PRO	N-CA-CB	6.52	110.21	103.23
47	HJ	14	SER	N-CA-C	6.52	119.71	111.69
55	a	231	LEU	N-CA-C	-6.51	104.18	111.28
57	f	110	ASP	O-C-N	-6.47	114.99	122.89
74	x	53	GLY	CA-C-O	-6.47	116.19	122.46
76	NC	827	PHE	CA-C-N	6.46	127.91	119.84
76	NC	827	PHE	C-N-CA	6.46	127.91	119.84
47	HJ	82	THR	N-CA-C	-6.44	104.26	111.28
30	HD	220	PRO	N-CA-CB	6.42	109.99	103.25
46	HI	53	ASP	N-CA-C	-6.41	106.18	112.97
74	x	804	PRO	CB-CA-C	6.39	118.72	110.92
37	DF	81	GLU	CA-C-N	6.39	126.14	119.05
37	DF	81	GLU	C-N-CA	6.39	126.14	119.05
47	HJ	232	LEU	N-CA-C	-6.39	104.31	111.28
50	g	125	GLU	N-CA-C	-6.39	105.34	113.01
52	n	1343	PRO	N-CA-C	-6.39	102.91	110.70
6	DA	1076	VAL	N-CA-C	6.34	117.13	110.72
53	s	108	PHE	N-CA-C	-6.32	99.10	109.40
47	HJ	118	PHE	N-CA-C	-6.31	105.58	113.28
70	t	156	LEU	CA-C-N	-6.30	111.84	120.28
70	t	156	LEU	C-N-CA	-6.30	111.84	120.28
47	HJ	103	ILE	CA-C-N	-6.29	111.84	120.46
47	HJ	103	ILE	C-N-CA	-6.29	111.84	120.46
52	n	74	PRO	N-CA-CB	6.29	110.19	103.52
55	a	509	ARG	CB-CA-C	-6.23	101.10	110.88
47	HJ	187	LEU	N-CA-C	-6.18	104.46	111.07
54	u	31	PRO	N-CA-C	-6.18	103.97	110.58
37	DF	325	ASN	N-CA-C	-6.18	104.62	111.36
74	x	35	ALA	CA-C-N	6.18	133.34	121.54
74	x	35	ALA	C-N-CA	6.18	133.34	121.54
16	NF	246	ILE	N-CA-C	6.17	116.76	107.75
30	HD	237	PRO	N-CA-CB	6.17	109.73	103.25
37	DF	316	GLN	CB-CA-C	6.17	120.30	110.19
63	c	306	HIS	N-CA-C	-6.16	100.47	110.20
40	DI	83	PHE	CA-C-N	-6.16	112.65	122.08
40	DI	83	PHE	C-N-CA	-6.16	112.65	122.08
46	HI	268	LEU	N-CA-C	-6.16	104.67	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	h	168	PRO	N-CA-CB	6.15	109.71	103.25
48	PD	138	ARG	N-CA-C	-6.15	105.49	112.87
30	HD	295	ARG	CA-C-N	-6.15	112.44	120.44
30	HD	295	ARG	C-N-CA	-6.15	112.44	120.44
54	u	80	GLU	N-CA-C	-6.15	104.41	112.41
54	u	77	PRO	N-CA-C	6.13	120.83	111.15
76	NC	879	LYS	N-CA-C	6.09	120.88	112.90
72	p	780	ASP	N-CA-C	-6.08	98.82	108.73
46	HI	287	THR	N-CA-C	-6.08	104.65	111.28
47	HJ	39	LYS	N-CA-C	-6.08	104.66	111.28
76	NG	1119	GLY	N-CA-C	6.06	127.53	113.18
6	DA	822	PRO	N-CA-C	-6.05	100.01	112.47
47	HJ	82	THR	CB-CA-C	-6.04	100.76	110.79
76	NC	883	PRO	N-CA-C	-6.04	105.13	113.53
46	HI	240	MET	N-CA-C	-6.03	104.71	111.28
16	NB	44	LYS	N-CA-C	6.02	120.65	113.12
46	HI	96	THR	CB-CA-C	-6.02	98.45	110.42
46	HI	261	PHE	N-CA-C	-6.01	98.94	108.73
37	DF	364	VAL	N-CA-C	6.01	116.75	110.62
67	h	49	PHE	CB-CA-C	-6.01	101.45	110.88
47	HJ	84	CYS	CB-CA-C	-6.00	100.82	110.79
30	HD	285	GLY	N-CA-C	-5.99	107.75	114.40
46	HI	50	GLU	N-CA-C	-5.98	105.84	113.01
47	HJ	30	PHE	CB-CA-C	-5.97	100.87	110.79
70	t	133	PRO	CB-CA-C	-5.97	101.72	111.56
76	NC	842	SER	CB-CA-C	-5.97	109.11	117.23
47	HJ	274	LYS	CB-CA-C	-5.94	101.55	110.88
73	w	30	PRO	N-CA-C	-5.94	101.86	111.19
37	Df	255	MET	N-CA-C	-5.92	104.91	114.09
47	HJ	80	VAL	CB-CA-C	-5.92	104.15	112.14
70	t	90	ASN	N-CA-C	-5.92	105.91	113.01
47	HJ	204	TYR	N-CA-C	-5.89	104.86	111.28
47	HJ	60	TYR	CB-CA-C	5.89	120.86	110.85
2	Y	-14	DT	C4'-C3'-O3'	5.87	118.80	110.00
12	DB	181	GLY	CA-C-O	-5.87	118.09	122.37
46	HI	173	VAL	N-CA-C	5.85	116.59	111.56
46	HI	290	LEU	N-CA-C	-5.85	104.91	111.28
47	HJ	288	ASN	N-CA-C	5.85	118.07	109.24
77	ND	1235	ALA	N-CA-C	5.84	118.39	111.33
61	z	529	HIS	CA-CB-CG	-5.81	107.99	113.80
55	a	278	HIS	CB-CA-C	5.80	118.69	109.52
47	HJ	278	GLU	CB-CA-C	-5.80	101.17	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	HJ	19	LEU	CA-C-N	-5.78	112.54	120.28
47	HJ	19	LEU	C-N-CA	-5.78	112.54	120.28
46	HI	204	ALA	N-CA-C	-5.77	104.89	111.07
46	HI	253	PRO	N-CA-C	-5.77	105.50	113.53
77	ND	1315	VAL	N-CA-C	-5.77	105.49	110.74
46	HI	238	PRO	CA-C-O	-5.76	114.88	121.56
71	v	90	ASP	CA-C-O	-5.76	114.95	121.00
10	NA	517	VAL	N-CA-C	-5.76	107.67	113.20
33	HF	3	ASN	CB-CA-C	-5.76	99.16	110.10
46	HI	206	LEU	CA-C-N	-5.75	112.63	120.44
46	HI	206	LEU	C-N-CA	-5.75	112.63	120.44
47	HJ	202	ASP	N-CA-C	-5.74	106.61	113.21
37	Df	150	PRO	N-CA-C	5.73	117.69	110.70
47	HJ	29	LYS	CB-CA-C	-5.72	101.89	110.88
52	n	525	TYR	CB-CA-C	5.70	118.27	110.06
47	HJ	33	LYS	CA-C-N	-5.70	112.65	120.28
47	HJ	33	LYS	C-N-CA	-5.70	112.65	120.28
46	HI	139	LYS	CB-CA-C	5.69	118.16	109.56
16	NF	251	TYR	N-CA-C	5.69	117.16	111.07
46	HI	280	PRO	CA-C-N	-5.68	112.67	120.28
46	HI	280	PRO	C-N-CA	-5.68	112.67	120.28
76	NG	1110	ILE	CA-C-N	-5.67	113.92	119.76
76	NG	1110	ILE	C-N-CA	-5.67	113.92	119.76
53	s	73	GLY	CA-C-N	5.66	128.18	120.54
53	s	73	GLY	C-N-CA	5.66	128.18	120.54
70	t	173	PRO	N-CA-CB	-5.65	97.32	103.25
10	NE	655	GLN	CA-C-N	-5.65	113.22	122.54
10	NE	655	GLN	C-N-CA	-5.65	113.22	122.54
47	HJ	116	ASP	CA-C-N	-5.64	114.50	122.34
47	HJ	116	ASP	C-N-CA	-5.64	114.50	122.34
73	w	1198	GLN	N-CA-C	-5.64	102.18	110.52
16	NB	29	ILE	N-CA-C	-5.63	98.54	107.15
30	HD	298	GLN	CA-C-N	-5.63	112.74	120.28
30	HD	298	GLN	C-N-CA	-5.63	112.74	120.28
7	EA	106	LYS	N-CA-C	-5.62	105.05	111.07
77	NH	1429	THR	N-CA-C	5.62	118.48	110.10
47	HJ	271	ALA	CA-C-N	-5.62	113.48	120.56
47	HJ	271	ALA	C-N-CA	-5.62	113.48	120.56
47	HJ	109	ALA	CA-C-N	-5.60	112.78	120.28
47	HJ	109	ALA	C-N-CA	-5.60	112.78	120.28
35	DD	962	GLU	N-CA-C	-5.59	105.33	111.82
41	DL	112	GLU	CB-CA-C	-5.58	110.12	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	HJ	187	LEU	CA-C-N	-5.58	113.01	120.54
47	HJ	187	LEU	C-N-CA	-5.58	113.01	120.54
30	HD	289	SER	CA-C-N	-5.58	113.19	120.44
30	HD	289	SER	C-N-CA	-5.58	113.19	120.44
76	NC	849	THR	N-CA-C	5.56	120.06	113.16
55	a	162	ASN	N-CA-C	-5.56	106.58	113.19
47	HJ	278	GLU	N-CA-C	-5.56	105.22	111.28
47	HJ	167	PHE	CA-C-N	-5.54	112.85	120.28
47	HJ	167	PHE	C-N-CA	-5.54	112.85	120.28
16	NF	228	GLY	N-CA-C	-5.54	107.79	114.66
16	NF	229	ILE	N-CA-C	-5.54	98.52	106.55
12	DB	583	GLU	CB-CA-C	-5.54	101.60	110.79
77	NH	1498	LEU	N-CA-C	5.53	120.15	112.90
6	DA	638	PRO	CB-CA-C	-5.53	106.37	111.40
54	u	79	GLU	CB-CG-CD	5.52	121.99	112.60
71	v	37	ILE	CB-CA-C	5.51	119.62	112.24
76	NG	1040	THR	N-CA-C	5.51	118.55	109.85
74	x	565	SER	N-CA-C	-5.49	101.92	110.10
16	NB	40	ARG	N-CA-C	-5.48	105.69	112.38
46	HI	276	PHE	CA-C-O	-5.48	114.61	120.42
63	c	311	GLN	CA-CB-CG	5.47	125.04	114.10
1	X	18	DG	N9-C1'-C2'	5.47	121.70	113.50
3	NX	25	DC	C2'-C3'-O3'	-5.47	103.30	111.50
37	Df	329	LEU	N-CA-C	-5.45	106.33	112.87
12	DB	264	GLU	N-CA-C	-5.45	106.31	113.17
46	HI	137	ASP	N-CA-C	5.45	117.48	108.49
76	NG	1027	PHE	CA-C-N	5.44	126.64	119.84
76	NG	1027	PHE	C-N-CA	5.44	126.64	119.84
76	NC	832	ILE	N-CA-C	-5.44	105.23	110.72
61	z	570	GLN	CB-CA-C	5.44	115.21	109.83
46	HI	138	LEU	N-CA-C	-5.43	101.81	109.96
58	i	135	TYR	CB-CA-C	5.43	120.58	109.55
61	z	492	ARG	CB-CA-C	-5.43	102.36	110.88
47	HJ	177	ARG	CB-CA-C	5.41	120.05	110.85
55	a	136	PRO	N-CA-C	-5.40	106.03	113.53
54	u	81	SER	CA-C-O	-5.40	115.58	121.14
77	NH	1430	ARG	N-CA-C	5.40	118.00	109.96
40	Di	72	ARG	CA-C-N	-5.39	111.60	121.52
40	Di	72	ARG	C-N-CA	-5.39	111.60	121.52
73	w	1195	ALA	N-CA-C	-5.38	105.53	111.71
36	DE	449	LYS	N-CA-C	-5.37	105.98	112.54
47	HJ	26	ALA	CA-C-N	-5.37	113.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	HJ	26	ALA	C-N-CA	-5.37	113.09	120.28
63	c	205	ARG	N-CA-C	-5.36	106.91	113.50
46	HI	283	ARG	CB-CA-C	5.35	117.87	109.84
53	s	105	LEU	N-CA-C	-5.34	99.42	110.80
47	HJ	33	LYS	N-CA-C	-5.34	105.46	111.28
70	t	202	LYS	CA-C-N	-5.33	113.07	120.38
70	t	202	LYS	C-N-CA	-5.33	113.07	120.38
47	HJ	86	TYR	N-CA-C	-5.33	105.47	111.28
69	r	15	THR	CA-C-N	-5.32	113.34	120.95
69	r	15	THR	C-N-CA	-5.32	113.34	120.95
37	DF	324	ASP	N-CA-C	-5.31	105.60	111.71
56	d	179	ASP	N-CA-C	-5.31	108.56	114.62
46	HI	148	ASN	N-CA-C	-5.30	105.50	111.28
63	c	221	VAL	N-CA-C	-5.30	106.70	112.80
53	s	102	LYS	N-CA-C	-5.30	106.99	112.93
66	o	720	PRO	N-CA-C	5.29	121.04	113.47
47	HJ	279	ARG	N-CA-C	-5.28	105.52	111.28
12	DB	491	HIS	CB-CA-C	5.27	119.54	110.79
37	DF	272	VAL	N-CA-C	-5.27	105.25	110.62
38	DG	183	ILE	N-CA-C	-5.27	102.72	109.30
71	v	25	ASP	CA-C-N	-5.27	113.24	120.46
71	v	25	ASP	C-N-CA	-5.27	113.24	120.46
68	k	72	GLN	N-CA-C	-5.26	105.71	111.82
46	HI	169	TYR	CB-CA-C	5.26	118.43	109.80
54	u	27	GLN	N-CA-C	-5.26	106.93	113.55
76	NC	895	GLU	N-CA-C	5.25	117.08	111.36
76	NG	1069	ALA	N-CA-C	-5.25	105.64	111.36
47	HJ	112	ALA	CA-C-N	-5.24	113.25	120.28
47	HJ	112	ALA	C-N-CA	-5.24	113.25	120.28
39	DH	134	LEU	CB-CA-C	-5.24	110.52	116.54
57	f	62	GLN	N-CA-C	-5.24	105.47	111.07
47	HJ	233	SER	CA-C-O	-5.22	115.02	120.55
46	HI	283	ARG	N-CA-C	-5.21	102.58	110.24
46	HI	173	VAL	CA-C-O	-5.19	115.75	120.73
50	g	73	ASP	CA-CB-CG	-5.18	107.42	112.60
57	f	109	PRO	O-C-N	5.18	129.31	123.10
30	HD	263	LEU	CA-C-N	-5.17	114.41	122.42
30	HD	263	LEU	C-N-CA	-5.17	114.41	122.42
40	DI	84	THR	O-C-N	5.16	127.57	122.10
47	HJ	79	VAL	CA-C-N	-5.16	113.39	120.46
47	HJ	79	VAL	C-N-CA	-5.16	113.39	120.46
74	x	445	GLY	N-CA-C	5.16	119.01	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	HJ	92	LEU	N-CA-C	-5.15	107.00	113.28
46	HI	271	LEU	N-CA-C	-5.15	105.67	111.28
62	b	88	ILE	N-CA-C	-5.14	104.96	110.36
12	DB	644	GLN	O-C-N	5.13	128.39	121.83
46	HI	100	VAL	CA-C-N	-5.12	114.10	120.56
46	HI	100	VAL	C-N-CA	-5.12	114.10	120.56
73	w	1140	GLU	CA-CB-CG	5.12	124.35	114.10
30	HD	292	ALA	CA-C-N	-5.12	112.91	120.28
30	HD	292	ALA	C-N-CA	-5.12	112.91	120.28
61	z	598	CYS	N-CA-C	-5.12	104.34	111.30
77	ND	1268	GLU	N-CA-C	-5.10	105.61	111.07
77	ND	1288	SER	N-CA-C	-5.10	106.32	112.54
46	HI	244	PRO	CB-CA-C	-5.10	104.96	113.06
10	NE	685	GLN	N-CA-C	-5.10	102.73	110.28
57	f	63	MET	N-CA-C	-5.09	103.96	110.53
72	p	380	LEU	CA-C-N	-5.09	118.61	122.33
72	p	380	LEU	C-N-CA	-5.09	118.61	122.33
54	u	80	GLU	CB-CG-CD	5.09	121.25	112.60
66	o	636	HIS	O-C-N	5.09	127.51	122.12
74	x	435	LEU	N-CA-C	-5.09	105.63	111.07
30	HD	298	GLN	CB-CA-C	-5.08	102.36	110.79
74	x	310	PHE	CB-CA-C	5.07	119.47	110.85
46	HI	195	ASP	CA-C-N	-5.07	113.85	120.44
46	HI	195	ASP	C-N-CA	-5.07	113.85	120.44
76	NG	1120	LYS	N-CA-C	-5.07	100.00	110.80
55	a	502	MET	N-CA-CB	5.07	119.05	110.49
70	t	181	ASP	N-CA-C	-5.06	106.94	113.02
30	HD	298	GLN	N-CA-C	-5.06	105.77	111.28
37	DF	219	GLU	N-CA-C	-5.06	105.84	111.36
46	HI	273	GLN	N-CA-C	-5.05	105.77	111.28
77	NH	1470	ILE	N-CA-C	5.05	115.27	110.53
61	z	596	TYR	CB-CA-C	-5.04	102.53	110.86
12	DB	541	ARG	CB-CA-C	-5.04	101.65	110.17
73	w	1253	GLY	N-CA-C	5.02	122.59	112.34
47	HJ	96	VAL	N-CA-C	-5.02	105.50	110.62
69	r	174	VAL	CA-C-O	-5.01	118.27	122.63
67	h	51	LEU	CA-C-N	-5.01	113.93	120.44
67	h	51	LEU	C-N-CA	-5.01	113.93	120.44
46	HI	204	ALA	CB-CA-C	-5.00	103.02	110.88
16	NF	243	VAL	N-CA-C	5.00	115.50	108.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1387	0	747	14	0
2	Y	1357	0	752	14	0
3	NX	3078	0	1783	11	0
4	NY	3561	0	1784	26	0
5	BA	1953	0	1987	20	0
6	DA	4563	0	4485	99	0
7	EA	1535	0	1539	140	0
8	FA	1138	0	1103	15	0
9	HA	5751	0	5794	105	0
10	NA	498	0	230	2	0
10	NE	511	0	238	5	0
11	PA	11628	0	11712	210	0
12	DB	7796	0	7751	148	0
13	EB	1403	0	1428	57	0
14	FB	1788	0	1819	32	0
15	HB	2167	0	2175	34	0
16	NB	391	0	185	0	0
16	NF	421	0	197	1	0
17	PB	9076	0	9116	130	0
18	HC	3158	0	3213	130	0
19	DO	806	0	818	31	0
20	DP	1422	0	1514	17	0
21	DQ	930	0	888	15	0
22	PC	2059	0	2007	22	0
23	PE	1721	0	1737	16	0
24	PF	636	0	665	11	0
25	PH	1186	0	1147	8	0
26	PI	928	0	859	11	0
27	PJ	507	0	523	14	0
28	PK	920	0	942	12	0
29	PL	373	0	378	8	0
30	HD	2400	0	2295	225	0
31	HG	2732	0	2698	42	0
32	HE	2066	0	2097	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	HF	523	0	530	52	0
34	HH	4890	0	4949	66	0
35	DD	1330	0	1351	138	0
35	Dd	1307	0	1318	13	0
36	DE	4364	0	4244	150	0
36	De	4327	0	4197	44	0
37	DF	3109	0	3045	310	0
37	Df	3081	0	3012	66	0
38	DG	1180	0	1235	18	0
39	DH	1633	0	1621	165	0
40	DI	959	0	969	135	0
40	Di	967	0	977	31	0
41	DL	605	0	606	76	0
41	Dl	876	0	893	25	0
42	Dc	1011	0	975	25	0
43	DJ	720	0	719	136	0
43	Dj	759	0	759	18	0
44	Dk	785	0	818	8	0
45	Dm	724	0	744	13	0
46	HI	2374	0	2389	172	0
47	HJ	2307	0	2314	148	0
48	PD	1050	0	1033	76	0
49	PG	1351	0	1358	139	0
50	g	898	0	936	77	0
51	j	840	0	718	37	0
52	n	7751	0	7530	593	0
53	s	723	0	727	57	0
54	u	886	0	871	138	0
55	a	3430	0	3461	423	0
56	d	1268	0	1305	279	0
57	f	1365	0	1337	153	0
58	i	605	0	628	210	0
59	m	983	0	968	91	0
60	q	4373	0	4433	546	0
61	z	765	0	728	79	0
62	b	899	0	908	114	0
63	c	2131	0	2140	133	0
64	e	832	0	824	101	0
65	l	1040	0	1065	85	0
66	o	1221	0	1212	120	0
67	h	1465	0	1460	213	0
68	k	879	0	886	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	r	1535	0	1545	54	0
70	t	1499	0	1482	105	0
71	v	1083	0	1059	196	0
72	p	5983	0	6071	134	0
73	w	10774	0	10838	146	0
74	x	7061	0	7223	226	0
75	y	1605	0	1576	24	0
76	NC	506	0	250	4	0
76	NG	524	0	260	7	0
77	ND	471	0	221	0	0
77	NH	471	0	221	0	0
78	BA	1	0	0	0	0
78	EA	1	0	0	0	0
78	HD	2	0	0	0	0
78	HE	2	0	0	0	0
78	HG	3	0	0	0	0
78	PA	2	0	0	0	0
78	PB	1	0	0	0	0
78	PC	1	0	0	0	0
78	PI	2	0	0	0	0
78	PJ	1	0	0	0	0
78	PL	1	0	0	0	0
78	c	1	0	0	0	0
78	p	1	0	0	0	0
79	HA	8	0	0	0	0
80	PA	1	0	0	0	0
All	All	185972	0	179545	6043	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (6043) 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)
56:d:49:ALA:HB2	58:i:76:MET:SD	1.21	1.70
12:DB:672:PHE:CD1	18:HC:414:SER:HB3	1.22	1.69
11:PA:1795:PRO:HD2	56:d:169:PRO:CB	1.24	1.63
7:EA:139:LEU:HD11	49:PG:151:ARG:CD	1.25	1.61
48:PD:79:THR:HG22	67:h:51:LEU:CD2	1.29	1.61
60:q:451:LEU:CD1	60:q:529:MET:HE1	1.30	1.61
62:b:174:ILE:CD1	65:l:75:LEU:HD21	1.23	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:HD:55:LYS:HG3	49:PG:166:ASP:CB	1.29	1.60
30:HD:55:LYS:CG	49:PG:166:ASP:HB2	1.25	1.60
52:n:941:TYR:CD2	52:n:1172:SER:HB3	1.39	1.57
52:n:647:MET:HE3	73:w:22:PHE:CB	1.34	1.55
7:EA:139:LEU:CD1	49:PG:151:ARG:HD2	1.10	1.54
52:n:359:ILE:CG1	52:n:372:ILE:HD11	1.37	1.53
7:EA:143:GLN:HG2	49:PG:158:PHE:CZ	1.44	1.52
54:u:115:LEU:HB2	56:d:121:LEU:CD1	1.07	1.52
48:PD:79:THR:CG2	67:h:51:LEU:HD22	1.04	1.51
56:d:76:PHE:HZ	58:i:65:PHE:CE2	1.29	1.51
12:DB:672:PHE:CE1	18:HC:413:LEU:HG	1.46	1.49
56:d:45:ILE:HG23	58:i:76:MET:CB	1.43	1.49
55:a:445:LEU:CG	74:x:55:SER:HB3	1.41	1.48
52:n:647:MET:CE	73:w:22:PHE:HB3	1.44	1.47
36:DE:694:LEU:HD13	36:DE:703:MET:CE	1.44	1.46
56:d:126:TYR:CE2	60:q:36:MET:HB3	1.50	1.46
66:o:639:TYR:CD2	72:p:786:HIS:HB3	1.48	1.46
54:u:90:LEU:HD22	60:q:9:ILE:CD1	1.45	1.46
12:DB:672:PHE:HD1	18:HC:414:SER:CB	1.24	1.46
52:n:960:LYS:HB2	52:n:1210:PHE:CE2	1.50	1.45
52:n:168:ARG:HG3	59:m:104:HIS:CE1	1.50	1.43
56:d:76:PHE:CZ	58:i:65:PHE:CE2	2.04	1.43
67:h:146:MET:CG	68:k:39:LYS:HZ2	1.31	1.42
52:n:941:TYR:CD2	52:n:1172:SER:CB	2.03	1.41
60:q:451:LEU:HD12	60:q:529:MET:CE	1.51	1.40
55:a:445:LEU:HD13	74:x:55:SER:N	1.26	1.40
54:u:90:LEU:CD2	60:q:9:ILE:HD11	1.50	1.40
56:d:45:ILE:CG2	58:i:76:MET:HB2	1.50	1.39
62:b:174:ILE:CG1	65:l:75:LEU:HD21	1.49	1.39
52:n:941:TYR:CE2	52:n:1172:SER:CB	2.05	1.38
19:DO:2:ALA:CA	35:DD:1000:ARG:HD3	1.53	1.38
52:n:686:LYS:HZ3	66:o:730:PRO:CG	1.32	1.38
71:v:16:GLN:NE2	71:v:20:LYS:HE2	1.07	1.38
52:n:359:ILE:HG12	52:n:372:ILE:CD1	1.54	1.36
54:u:115:LEU:CB	56:d:121:LEU:CD1	2.02	1.36
56:d:76:PHE:CE2	58:i:65:PHE:CD2	2.12	1.36
55:a:445:LEU:CD1	74:x:55:SER:H	1.37	1.35
56:d:49:ALA:CB	58:i:76:MET:SD	2.12	1.35
41:DL:111:LEU:HA	41:DL:114:LYS:NZ	1.39	1.35
52:n:957:PRO:CG	52:n:1210:PHE:CE1	2.09	1.35
66:o:639:TYR:CD2	72:p:786:HIS:CB	2.08	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:66:GLN:NE2	56:d:44:LEU:HD11	1.41	1.35
52:n:545:LEU:HD11	52:n:653:PRO:CG	1.56	1.34
56:d:76:PHE:CZ	58:i:65:PHE:CD2	2.14	1.34
55:a:364:TYR:HB3	55:a:430:LEU:CD1	1.57	1.34
7:EA:139:LEU:CD2	49:PG:151:ARG:HB3	1.55	1.34
55:a:70:LYS:HB2	58:i:70:HIS:ND1	1.39	1.34
56:d:45:ILE:O	58:i:76:MET:HG2	1.22	1.33
11:PA:1475:LEU:HD22	49:PG:66:VAL:CG2	1.58	1.33
55:a:70:LYS:NZ	58:i:74:LYS:HE2	1.36	1.33
62:b:181:CYS:SG	65:l:82:LEU:HD13	1.69	1.33
55:a:417:TYR:HD1	55:a:469:VAL:CG2	1.40	1.32
52:n:267:HIS:CD2	57:f:174:ARG:HD3	1.64	1.32
36:DE:694:LEU:CD1	36:DE:703:MET:HE1	1.59	1.32
60:q:89:GLN:CG	60:q:90:PRO:HD2	1.60	1.31
55:a:462:LEU:H	74:x:49:GLN:CG	1.43	1.31
30:HD:300:ALA:CB	47:HJ:166:PRO:HA	1.60	1.31
60:q:186:GLU:HG3	60:q:243:LEU:CD2	1.59	1.31
62:b:174:ILE:CD1	65:l:75:LEU:CD2	2.08	1.30
37:DF:104:LEU:HB3	43:DJ:217:PHE:CE2	1.66	1.30
67:h:146:MET:HB2	68:k:39:LYS:NZ	1.45	1.30
11:PA:1795:PRO:CD	56:d:169:PRO:HB3	1.61	1.30
55:a:445:LEU:HB3	74:x:55:SER:CB	1.61	1.30
52:n:267:HIS:HB3	52:n:270:GLN:OE1	1.30	1.29
60:q:451:LEU:CD1	60:q:529:MET:CE	2.08	1.29
30:HD:85:ARG:HH22	30:HD:139:LYS:C	1.40	1.29
52:n:250:LEU:HD21	52:n:275:HIS:CD2	1.67	1.29
52:n:960:LYS:CB	52:n:1210:PHE:CE2	2.15	1.29
52:n:921:MET:SD	52:n:1215:ILE:HD11	1.74	1.28
62:b:175:HIS:HB2	63:c:113:TRP:CH2	1.66	1.28
52:n:941:TYR:CE2	52:n:1172:SER:HB3	1.66	1.28
37:DF:218:VAL:HG12	39:DH:162:THR:OG1	1.31	1.28
39:DH:51:GLU:OE1	43:DJ:193:TYR:HB3	1.13	1.28
11:PA:1795:PRO:CD	56:d:169:PRO:CB	2.13	1.27
66:o:633:VAL:CG1	72:p:810:PRO:CB	2.13	1.27
12:DB:672:PHE:HE1	18:HC:413:LEU:CG	1.48	1.27
60:q:392:MET:SD	69:r:46:MET:HE1	1.72	1.27
55:a:417:TYR:CE1	55:a:450:PHE:CD1	2.23	1.27
60:q:441:ARG:NH1	65:l:168:TRP:CD2	2.01	1.27
36:DE:696:TRP:CH2	36:DE:703:MET:SD	2.28	1.27
55:a:445:LEU:HD13	74:x:55:SER:CA	1.64	1.26
67:h:147:CYS:SG	71:v:41:LYS:HG2	1.75	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:171:VAL:HG21	68:k:17:ILE:CG2	1.64	1.26
68:k:87:ARG:HA	71:v:105:LEU:CD1	1.65	1.26
55:a:462:LEU:N	74:x:49:GLN:HG2	1.50	1.26
60:q:186:GLU:CG	60:q:243:LEU:CD2	2.12	1.26
52:n:245:TRP:HB2	52:n:282:LEU:CD1	1.64	1.26
41:DL:71:ASP:OD2	41:DL:74:GLU:HG3	1.33	1.26
52:n:904:PHE:CE2	52:n:1208:GLU:HG3	1.68	1.26
60:q:479:ILE:HG22	60:q:532:HIS:CD2	1.71	1.26
7:EA:143:GLN:NE2	49:PG:158:PHE:HE1	1.31	1.25
30:HD:85:ARG:NH1	30:HD:140:LEU:HG	1.51	1.25
55:a:59:VAL:HG21	56:d:51:SER:CB	1.62	1.25
55:a:445:LEU:CD2	74:x:55:SER:HB3	1.65	1.25
11:PA:1475:LEU:CD2	49:PG:66:VAL:HG21	1.63	1.25
64:e:129:VAL:CG1	68:k:111:CYS:SG	2.23	1.25
52:n:273:PHE:CZ	57:f:185:ARG:HD2	1.70	1.25
60:q:458:PRO:HG3	60:q:533:GLN:NE2	1.49	1.25
37:DF:323:VAL:CG2	37:DF:326:HIS:HB2	1.65	1.25
37:DF:218:VAL:HG12	39:DH:162:THR:CB	1.66	1.24
55:a:445:LEU:CB	74:x:55:SER:HB3	1.66	1.24
60:q:458:PRO:CG	60:q:533:GLN:HE21	1.50	1.24
12:DB:672:PHE:CE1	18:HC:413:LEU:CG	2.20	1.24
60:q:647:SER:HB3	64:e:93:CYS:SG	1.78	1.23
60:q:191:ARG:HD3	71:v:87:ILE:O	1.35	1.23
67:h:146:MET:CB	68:k:39:LYS:HZ2	1.50	1.23
52:n:250:LEU:CD2	52:n:275:HIS:CD2	2.20	1.23
11:PA:1475:LEU:CD2	49:PG:66:VAL:CG2	2.17	1.23
30:HD:55:LYS:HE2	49:PG:166:ASP:OD2	1.32	1.22
37:DF:219:GLU:CB	39:DH:160:ILE:HG21	1.68	1.22
52:n:250:LEU:HD23	52:n:275:HIS:CG	1.73	1.22
52:n:545:LEU:HD11	52:n:653:PRO:CD	1.68	1.22
14:FB:186:MET:HE1	35:DD:995:GLU:OE2	1.40	1.22
7:EA:174:ARG:CB	30:HD:8:ARG:HH21	1.53	1.21
60:q:186:GLU:CG	60:q:243:LEU:HD22	1.71	1.21
14:FB:186:MET:HE1	35:DD:995:GLU:CD	1.65	1.21
67:h:182:VAL:HG21	69:r:202:ILE:CD1	1.68	1.21
52:n:957:PRO:HG2	52:n:1210:PHE:CE1	1.71	1.21
60:q:596:PHE:HZ	65:l:117:TYR:OH	1.24	1.21
71:v:16:GLN:NE2	71:v:20:LYS:CE	2.04	1.20
7:EA:181:ASN:CB	30:HD:10:LYS:HG2	1.69	1.20
48:PD:79:THR:HA	67:h:51:LEU:CD2	1.71	1.20
60:q:138:LYS:HB3	60:q:140:ASN:OD1	1.42	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DD:895:HIS:CG	35:DD:896:PRO:HD2	1.76	1.20
52:n:957:PRO:HB2	52:n:1210:PHE:CZ	1.74	1.20
55:a:417:TYR:HE1	55:a:450:PHE:CD1	1.58	1.20
55:a:417:TYR:CD1	55:a:469:VAL:HG21	1.77	1.19
60:q:441:ARG:NH1	65:l:168:TRP:CE3	2.09	1.19
12:DB:621:ALA:HB2	18:HC:438:LYS:NZ	1.55	1.19
37:DF:219:GLU:CB	39:DH:160:ILE:CG2	2.21	1.19
55:a:445:LEU:CB	74:x:55:SER:CB	2.19	1.19
30:HD:21:LEU:HD22	30:HD:69:ASP:OD2	1.43	1.19
40:Di:62:LYS:HD2	41:Dl:106:ARG:NH1	1.56	1.19
18:HC:352:GLN:NE2	33:HF:61:MET:SD	2.14	1.19
63:c:204:MET:CE	63:c:208:PHE:H	1.56	1.18
55:a:462:LEU:CG	74:x:49:GLN:HB3	1.70	1.18
64:e:129:VAL:HG21	68:k:114:MET:CE	1.73	1.18
36:DE:696:TRP:CZ3	36:DE:703:MET:SD	2.36	1.18
48:PD:76:ASN:CG	67:h:47:ASP:HB3	1.67	1.18
52:n:686:LYS:NZ	66:o:730:PRO:CG	2.05	1.18
68:k:20:GLU:OE1	71:v:76:MET:SD	2.02	1.18
39:DH:57:SER:HB2	43:DJ:197:MET:SD	1.83	1.17
52:n:169:LEU:HB3	52:n:170:PRO:CD	1.73	1.17
7:EA:181:ASN:HB3	30:HD:10:LYS:CG	1.75	1.17
11:PA:1475:LEU:HD22	49:PG:66:VAL:HG22	1.19	1.17
37:DF:71:ILE:HD12	40:DI:38:GLN:HE21	1.03	1.17
19:DO:2:ALA:HA	35:DD:1000:ARG:CD	1.72	1.17
52:n:957:PRO:HG2	52:n:1210:PHE:HE1	1.00	1.17
60:q:168:THR:OG1	68:k:21:ILE:HD12	1.44	1.17
63:c:204:MET:HE1	63:c:208:PHE:N	1.59	1.17
55:a:417:TYR:CD1	55:a:469:VAL:CG2	2.27	1.16
55:a:461:SER:CA	74:x:49:GLN:HE21	1.57	1.16
56:d:45:ILE:HG22	58:i:76:MET:HE2	1.25	1.16
67:h:146:MET:CB	68:k:39:LYS:NZ	2.08	1.16
48:PD:79:THR:CG2	67:h:51:LEU:CD2	2.01	1.16
67:h:150:LEU:HD21	68:k:45:LEU:HD11	1.21	1.16
30:HD:43:ALA:HB1	49:PG:164:MET:HG3	1.24	1.16
52:n:192:LEU:HD12	52:n:220:GLY:CA	1.75	1.16
7:EA:174:ARG:HB3	30:HD:8:ARG:NH2	1.61	1.16
62:b:174:ILE:HD11	65:l:75:LEU:HD21	1.22	1.16
57:f:145:TYR:CZ	67:h:43:PRO:HG3	1.79	1.16
52:n:169:LEU:HA	59:m:104:HIS:CG	1.81	1.15
52:n:904:PHE:CE2	52:n:1208:GLU:CG	2.29	1.15
68:k:87:ARG:CA	71:v:105:LEU:CD1	2.23	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:545:LEU:CD1	52:n:653:PRO:CD	2.25	1.15
56:d:31:LEU:HD23	58:i:103:THR:HG21	1.15	1.15
60:q:171:VAL:CG2	68:k:17:ILE:CG2	2.24	1.15
54:u:115:LEU:HB2	56:d:121:LEU:HD12	1.24	1.14
55:a:461:SER:HA	74:x:49:GLN:NE2	1.61	1.14
56:d:31:LEU:CD2	58:i:103:THR:HG21	1.76	1.14
67:h:147:CYS:SG	71:v:41:LYS:CG	2.34	1.14
52:n:904:PHE:HE2	52:n:1208:GLU:CG	1.59	1.14
55:a:375:PHE:CD2	74:x:17:ARG:NE	2.15	1.14
66:o:633:VAL:HG12	72:p:810:PRO:CB	1.73	1.14
67:h:182:VAL:HG21	69:r:202:ILE:HD12	1.20	1.14
55:a:364:TYR:HB3	55:a:430:LEU:HD12	1.26	1.14
52:n:270:GLN:NE2	57:f:174:ARG:HG3	1.61	1.14
52:n:545:LEU:HD11	52:n:653:PRO:HG3	1.24	1.13
7:EA:174:ARG:CG	30:HD:8:ARG:NH2	2.12	1.13
68:k:87:ARG:N	71:v:105:LEU:HD12	1.62	1.13
68:k:87:ARG:CA	71:v:105:LEU:HD11	1.77	1.13
60:q:89:GLN:HG2	60:q:90:PRO:CD	1.79	1.13
60:q:171:VAL:CG2	68:k:17:ILE:HG21	1.77	1.12
7:EA:139:LEU:HD21	49:PG:151:ARG:CB	1.77	1.12
30:HD:85:ARG:HH22	30:HD:140:LEU:N	1.46	1.12
52:n:957:PRO:CB	52:n:1210:PHE:CZ	2.32	1.12
54:u:128:SER:HB2	58:i:131:LEU:HD21	1.23	1.12
55:a:417:TYR:CE1	55:a:450:PHE:CE1	2.35	1.12
7:EA:174:ARG:HG2	30:HD:8:ARG:NH2	1.64	1.12
55:a:70:LYS:HB2	58:i:70:HIS:CE1	1.83	1.12
60:q:410:PRO:HG3	69:r:82:PRO:HB3	1.17	1.12
64:e:56:PHE:O	64:e:60:VAL:HG22	1.44	1.12
70:t:129:VAL:HG21	70:t:200:ILE:HD12	1.32	1.12
30:HD:284:ALA:CB	46:HI:243:LEU:HD13	1.79	1.12
52:n:686:LYS:NZ	66:o:730:PRO:HG3	1.60	1.12
30:HD:85:ARG:NH2	30:HD:139:LYS:C	2.07	1.12
52:n:265:LEU:HD12	52:n:303:LEU:HD21	1.28	1.12
71:v:16:GLN:HE21	71:v:20:LYS:CE	1.60	1.12
68:k:87:ARG:N	71:v:105:LEU:CD1	2.11	1.11
37:DF:83:LEU:HD11	37:DF:97:ALA:O	1.49	1.11
52:n:753:LEU:HD11	63:c:311:GLN:HA	1.31	1.11
52:n:957:PRO:HG3	52:n:1210:PHE:CE1	1.81	1.11
60:q:339:LEU:HD13	60:q:439:PHE:CE2	1.82	1.11
64:e:129:VAL:HG13	68:k:111:CYS:SG	1.90	1.11
64:e:146:ILE:HG22	64:e:147:ASN:H	0.96	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:323:VAL:HG22	37:DF:326:HIS:HB2	1.22	1.11
62:b:174:ILE:HG12	65:l:75:LEU:HD11	1.29	1.11
37:DF:428:LEU:HD13	37:DF:455:LEU:CB	1.81	1.11
52:n:209:PRO:HG3	52:n:293:TYR:HB2	1.30	1.11
58:i:85:GLN:HG3	58:i:86:ASP:N	1.53	1.11
11:PA:1795:PRO:HD3	56:d:169:PRO:HA	1.33	1.11
52:n:166:TYR:OH	59:m:70:PRO:HB2	1.50	1.11
52:n:254:VAL:CG2	52:n:303:LEU:HD22	1.81	1.11
52:n:686:LYS:HZ1	66:o:730:PRO:HD3	1.00	1.11
56:d:45:ILE:HG12	58:i:73:ILE:HA	1.26	1.11
66:o:633:VAL:CG1	72:p:810:PRO:HB2	1.72	1.11
12:DB:674:THR:HG21	18:HC:415:GLN:HG2	1.31	1.10
55:a:445:LEU:HD22	74:x:55:SER:CB	1.81	1.10
67:h:146:MET:HG2	68:k:39:LYS:HZ2	1.03	1.10
55:a:375:PHE:CD2	74:x:17:ARG:NH2	2.18	1.10
60:q:155:GLY:HA3	71:v:62:HIS:CE1	1.83	1.10
68:k:87:ARG:HA	71:v:105:LEU:HD11	1.12	1.10
52:n:686:LYS:HZ3	66:o:730:PRO:HG3	0.97	1.10
56:d:167:TRP:CH2	59:m:102:ILE:CG2	2.34	1.10
7:EA:174:ARG:HG2	30:HD:8:ARG:HH22	1.04	1.10
35:DD:872:PHE:CZ	41:DL:57:VAL:HG12	1.87	1.10
37:DF:219:GLU:HG2	39:DH:160:ILE:CG2	1.80	1.10
54:u:115:LEU:CB	56:d:121:LEU:HD13	1.68	1.10
55:a:445:LEU:CD1	74:x:55:SER:HB3	1.81	1.10
67:h:146:MET:CG	68:k:39:LYS:NZ	2.13	1.10
18:HC:397:GLU:HB3	33:HF:61:MET:HE3	1.27	1.09
48:PD:79:THR:HA	67:h:51:LEU:HD21	1.24	1.09
58:i:85:GLN:CG	58:i:86:ASP:H	1.60	1.09
63:c:204:MET:CE	63:c:208:PHE:N	2.14	1.09
55:a:462:LEU:HG	74:x:49:GLN:CB	1.81	1.09
7:EA:143:GLN:CG	49:PG:158:PHE:CZ	2.34	1.09
36:DE:433:LYS:HD3	40:DI:110:TYR:OH	1.50	1.09
60:q:152:SER:HB2	71:v:58:ASN:HA	1.19	1.09
52:n:545:LEU:HD12	52:n:653:PRO:HD3	1.34	1.09
55:a:461:SER:HA	74:x:49:GLN:HE21	1.13	1.09
30:HD:284:ALA:HB3	46:HI:243:LEU:CD1	1.81	1.09
54:u:67:LYS:HE3	61:z:528:LEU:CD2	1.82	1.09
55:a:449:ARG:NH2	74:x:54:PRO:HB2	1.67	1.09
7:EA:143:GLN:CD	49:PG:158:PHE:CE1	2.32	1.08
7:EA:174:ARG:CB	30:HD:8:ARG:NH2	2.15	1.08
54:u:90:LEU:HD11	60:q:7:VAL:HB	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:461:SER:C	74:x:49:GLN:HE21	1.59	1.08
56:d:38:GLU:CD	58:i:96:GLU:HG2	1.77	1.08
60:q:129:PRO:HB3	67:h:74:GLN:NE2	1.67	1.08
30:HD:43:ALA:CB	49:PG:164:MET:HG3	1.81	1.08
52:n:209:PRO:HG3	52:n:293:TYR:CB	1.83	1.08
55:a:462:LEU:HG	74:x:49:GLN:HB3	1.32	1.08
30:HD:43:ALA:O	49:PG:164:MET:SD	2.11	1.08
18:HC:397:GLU:OE1	33:HF:61:MET:SD	2.11	1.08
40:DI:16:ALA:HA	40:DI:40:LEU:HD11	1.34	1.08
55:a:445:LEU:HB3	74:x:55:SER:HB2	1.09	1.08
56:d:45:ILE:HG22	58:i:76:MET:CE	1.83	1.08
60:q:186:GLU:HG3	60:q:243:LEU:HD21	1.19	1.08
36:DE:433:LYS:CD	40:DI:110:TYR:OH	2.01	1.08
37:DF:15:PRO:HD3	40:DI:18:MET:HG2	1.34	1.08
52:n:960:LYS:HG3	52:n:1210:PHE:CD2	1.88	1.08
55:a:321:LEU:HD21	55:a:407:ILE:HG23	1.33	1.08
62:b:174:ILE:HD11	65:l:75:LEU:CD2	1.76	1.08
12:DB:646:ASP:HB3	18:HC:413:LEU:O	1.52	1.07
30:HD:83:ASN:OD1	30:HD:140:LEU:HD11	1.54	1.07
68:k:9:GLU:HG3	71:v:86:LEU:HG	1.28	1.07
68:k:86:SER:C	71:v:105:LEU:HD12	1.78	1.07
7:EA:143:GLN:NE2	49:PG:158:PHE:CE1	2.21	1.07
12:DB:672:PHE:CZ	18:HC:413:LEU:HD12	1.89	1.07
50:g:166:ASN:OD1	50:g:167:CYS:N	1.85	1.07
48:PD:79:THR:CB	67:h:51:LEU:HD22	1.83	1.07
52:n:168:ARG:CD	59:m:104:HIS:NE2	2.17	1.07
52:n:957:PRO:HB2	52:n:1210:PHE:HZ	0.93	1.07
67:h:150:LEU:HD21	68:k:45:LEU:CD1	1.84	1.07
52:n:168:ARG:CG	59:m:104:HIS:CE1	2.37	1.07
55:a:380:ALA:HB3	55:a:444:PRO:HD2	1.36	1.07
60:q:487:ILE:CG2	60:q:543:VAL:HG21	1.82	1.07
64:e:125:LYS:HE2	71:v:133:GLU:OE2	1.53	1.07
35:DD:895:HIS:ND1	35:DD:896:PRO:HD2	1.67	1.07
52:n:921:MET:SD	52:n:1215:ILE:CD1	2.42	1.07
55:a:321:LEU:CD2	55:a:407:ILE:HD12	1.83	1.07
68:k:29:GLY:O	68:k:33:LEU:HG	1.55	1.06
7:EA:139:LEU:HD21	49:PG:151:ARG:HB3	1.10	1.06
37:DF:82:PRO:HG3	37:DF:96:PHE:O	1.55	1.06
37:DF:219:GLU:CG	39:DH:160:ILE:CG2	2.32	1.06
52:n:245:TRP:CB	52:n:282:LEU:HD13	1.84	1.06
60:q:418:ILE:CD1	70:t:72:PRO:HG2	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:115:LEU:HD12	56:d:121:LEU:HB3	1.37	1.06
60:q:138:LYS:HD2	60:q:140:ASN:OD1	1.54	1.06
62:b:174:ILE:HG12	65:l:75:LEU:HD21	1.33	1.06
12:DB:674:THR:HG21	18:HC:415:GLN:CG	1.84	1.06
30:HD:295:ARG:NH1	47:HJ:165:ARG:HH21	1.52	1.06
42:Dc:67:GLY:HA3	43:Dj:116:LEU:CD1	1.85	1.06
55:a:445:LEU:HD13	74:x:55:SER:CB	1.85	1.06
60:q:155:GLY:HA3	71:v:62:HIS:HE1	0.94	1.06
30:HD:5:GLY:HA3	30:HD:10:LYS:HB2	1.37	1.06
60:q:458:PRO:HG3	60:q:533:GLN:HE21	0.90	1.06
62:b:179:LEU:CG	64:e:60:VAL:HB	1.85	1.06
18:HC:348:ARG:NE	33:HF:65:ALA:HB1	1.71	1.05
37:DF:316:GLN:HG2	37:DF:318:CYS:O	1.56	1.05
52:n:265:LEU:CD1	52:n:303:LEU:HD21	1.85	1.05
56:d:126:TYR:CE2	60:q:36:MET:CB	2.39	1.05
58:i:68:LEU:HD13	58:i:95:GLN:HG2	1.15	1.05
39:DH:51:GLU:OE1	43:DJ:193:TYR:CB	2.03	1.05
55:a:375:PHE:CD2	74:x:17:ARG:CZ	2.39	1.05
52:n:267:HIS:HD2	57:f:174:ARG:CD	1.67	1.05
52:n:545:LEU:CD1	52:n:653:PRO:HD3	1.83	1.05
66:o:633:VAL:CG1	72:p:810:PRO:HB3	1.80	1.05
52:n:570:PHE:CE2	73:w:18:ILE:HG21	1.92	1.05
52:n:957:PRO:CG	52:n:1210:PHE:CZ	2.39	1.05
56:d:167:TRP:HH2	59:m:102:ILE:HG21	1.15	1.05
66:o:633:VAL:HG11	72:p:810:PRO:HB2	1.09	1.05
37:DF:47:ILE:HD11	40:DI:43:ALA:HB2	1.39	1.04
56:d:167:TRP:HH2	59:m:102:ILE:CG2	1.68	1.04
11:PA:1475:LEU:HD23	49:PG:66:VAL:HG21	1.35	1.04
35:DD:997:ALA:O	35:DD:1001:GLN:HG3	1.55	1.04
60:q:102:LEU:HD11	67:h:29:PHE:CE2	1.92	1.04
60:q:155:GLY:CA	71:v:62:HIS:HE1	1.71	1.04
52:n:250:LEU:CD2	52:n:275:HIS:CG	2.37	1.04
60:q:134:ALA:H	67:h:72:ARG:NH1	1.54	1.04
60:q:149:LYS:CE	71:v:40:ALA:HA	1.87	1.04
60:q:487:ILE:HG21	60:q:543:VAL:HG21	1.07	1.04
50:g:167:CYS:SG	56:d:113:GLN:NE2	2.31	1.04
56:d:45:ILE:O	58:i:76:MET:CG	2.06	1.04
41:DL:111:LEU:O	41:DL:114:LYS:HG2	1.54	1.04
11:PA:1643:TYR:HB2	59:m:96:PHE:CG	1.93	1.03
40:Di:62:LYS:HD2	41:DI:106:ARG:HH12	1.05	1.03
56:d:31:LEU:HD21	58:i:103:THR:OG1	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:396:ALA:HB2	69:r:51:PHE:CE2	1.92	1.03
60:q:479:ILE:O	60:q:532:HIS:CE1	2.11	1.03
41:DL:111:LEU:CA	41:DL:114:LYS:HZ2	1.71	1.03
52:n:267:HIS:CB	52:n:270:GLN:OE1	2.05	1.03
54:u:90:LEU:CD1	60:q:9:ILE:HG13	1.88	1.03
56:d:45:ILE:HD11	58:i:73:ILE:N	1.73	1.03
30:HD:84:LYS:HA	30:HD:136:ASN:ND2	1.73	1.03
37:DF:219:GLU:CG	39:DH:160:ILE:HG21	1.86	1.03
40:DI:81:GLN:HE22	41:DL:123:GLN:NE2	1.55	1.03
52:n:861:LYS:HE3	63:c:30:ARG:HE	1.17	1.03
55:a:462:LEU:H	74:x:49:GLN:HG2	0.94	1.03
30:HD:300:ALA:HB2	47:HJ:166:PRO:HA	1.04	1.03
60:q:188:LEU:HA	71:v:87:ILE:CD1	1.89	1.03
62:b:174:ILE:HG12	65:l:75:LEU:CD1	1.89	1.03
62:b:179:LEU:CD1	64:e:60:VAL:HB	1.88	1.03
64:e:49:GLU:HG2	65:l:89:PHE:CE1	1.93	1.03
66:o:639:TYR:CE2	72:p:786:HIS:HB3	1.94	1.03
54:u:67:LYS:HE3	61:z:528:LEU:HD21	1.39	1.02
56:d:27:ARG:HD2	58:i:108:HIS:HA	1.40	1.02
60:q:339:LEU:HD13	60:q:439:PHE:CD2	1.94	1.02
60:q:647:SER:CB	64:e:93:CYS:SG	2.45	1.02
63:c:204:MET:HE3	63:c:208:PHE:H	1.21	1.02
37:DF:83:LEU:HD23	37:DF:86:PHE:CZ	1.93	1.02
52:n:169:LEU:HA	59:m:104:HIS:CD2	1.94	1.02
53:s:104:LYS:C	53:s:106:SER:H	1.59	1.02
55:a:70:LYS:NZ	58:i:74:LYS:CE	2.22	1.02
55:a:109:TYR:CZ	55:a:154:LEU:HD21	1.94	1.02
55:a:382:LEU:HD22	55:a:446:SER:HA	1.40	1.02
60:q:113:TYR:HB2	67:h:19:VAL:CG1	1.87	1.02
60:q:418:ILE:HD12	70:t:72:PRO:CG	1.88	1.02
52:n:270:GLN:NE2	57:f:174:ARG:CG	2.23	1.02
56:d:45:ILE:CG1	58:i:73:ILE:HA	1.89	1.02
60:q:171:VAL:HG22	68:k:17:ILE:HG21	1.40	1.02
68:k:104:LEU:HD21	71:v:123:ILE:HD11	1.39	1.02
60:q:186:GLU:HG2	60:q:243:LEU:CD2	1.90	1.02
11:PA:1798:SER:HA	60:q:25:ASP:OD2	1.59	1.02
37:DF:219:GLU:HB3	39:DH:160:ILE:CG2	1.89	1.02
52:n:261:ASP:HB2	60:q:250:ASP:OD1	1.60	1.02
52:n:686:LYS:HZ3	66:o:730:PRO:CB	1.71	1.02
60:q:171:VAL:HG21	68:k:17:ILE:HG23	1.37	1.02
63:c:204:MET:HE3	63:c:206:SER:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:DB:621:ALA:HB2	18:HC:438:LYS:CE	1.90	1.01
37:DF:104:LEU:CB	43:DJ:217:PHE:CE2	2.42	1.01
48:PD:79:THR:CA	67:h:51:LEU:CD2	2.37	1.01
62:b:179:LEU:HD12	64:e:60:VAL:CA	1.90	1.01
68:k:86:SER:C	71:v:105:LEU:CD1	2.34	1.01
37:DF:219:GLU:HB2	39:DH:160:ILE:HG21	1.41	1.01
54:u:90:LEU:HD13	60:q:9:ILE:CG1	1.88	1.01
57:f:16:VAL:HG12	57:f:103:GLY:O	1.60	1.01
36:DE:429:LEU:HB3	36:DE:430:PRO:HD2	1.41	1.01
52:n:273:PHE:HZ	57:f:185:ARG:CD	1.71	1.01
52:n:941:TYR:CD2	52:n:1172:SER:HB2	1.92	1.01
58:i:85:GLN:CG	58:i:86:ASP:OD1	2.09	1.01
11:PA:1475:LEU:HD21	49:PG:18:PHE:CZ	1.96	1.01
12:DB:645:ALA:HA	18:HC:413:LEU:HA	1.42	1.01
66:o:633:VAL:HG12	72:p:810:PRO:HB3	1.03	1.01
11:PA:1795:PRO:HD2	56:d:169:PRO:HB2	1.42	1.00
11:PA:1795:PRO:CD	56:d:169:PRO:CA	2.38	1.00
18:HC:397:GLU:CD	33:HF:61:MET:HG3	1.84	1.00
40:DI:23:LEU:HD11	40:DI:39:MET:HE1	1.40	1.00
52:n:169:LEU:CD2	59:m:101:GLN:HA	1.90	1.00
52:n:254:VAL:HG21	52:n:303:LEU:HD22	1.04	1.00
52:n:686:LYS:HZ1	66:o:730:PRO:CD	1.74	1.00
58:i:72:ILE:CD1	58:i:92:SER:HB2	1.91	1.00
59:m:116:GLN:NE2	61:z:579:CYS:SG	2.34	1.00
7:EA:143:GLN:CD	49:PG:158:PHE:HE1	1.69	1.00
48:PD:79:THR:HG22	67:h:51:LEU:CG	1.90	1.00
52:n:203:LEU:HD13	52:n:215:LEU:CD1	1.91	1.00
52:n:921:MET:CE	52:n:1215:ILE:HD11	1.90	1.00
55:a:462:LEU:N	74:x:49:GLN:NE2	2.10	1.00
58:i:85:GLN:HG3	58:i:86:ASP:OD1	1.56	1.00
47:HJ:181:LEU:HD13	47:HJ:181:LEU:H	1.26	1.00
52:n:359:ILE:CG1	52:n:372:ILE:CD1	2.26	1.00
54:u:128:SER:CB	58:i:131:LEU:CD2	2.39	1.00
55:a:462:LEU:H	74:x:49:GLN:CD	1.68	1.00
56:d:168:VAL:HB	56:d:169:PRO:HD2	1.43	1.00
52:n:170:PRO:HG3	59:m:100:GLN:HB3	1.44	1.00
52:n:941:TYR:CE2	52:n:1172:SER:HB2	1.96	1.00
59:m:56:LEU:HD21	59:m:80:GLN:NE2	1.76	1.00
60:q:191:ARG:CD	71:v:87:ILE:O	2.10	1.00
56:d:45:ILE:CD1	58:i:73:ILE:N	2.24	1.00
60:q:410:PRO:HG3	69:r:82:PRO:CB	1.89	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:e:129:VAL:HG21	68:k:114:MET:HE2	1.39	1.00
69:r:27:VAL:HG22	69:r:197:VAL:HG11	1.40	1.00
55:a:417:TYR:HD1	55:a:469:VAL:HG23	1.25	1.00
64:e:129:VAL:HG12	68:k:111:CYS:SG	2.00	1.00
14:FB:189:SER:HB3	35:DD:991:MET:HE1	1.41	0.99
60:q:481:SER:CB	60:q:636:VAL:HG21	1.91	0.99
55:a:445:LEU:HD22	74:x:55:SER:HB3	1.39	0.99
52:n:934:VAL:HG21	52:n:1182:LEU:HD22	1.42	0.99
60:q:89:GLN:CG	60:q:90:PRO:CD	2.38	0.99
55:a:462:LEU:N	74:x:49:GLN:HE21	1.60	0.99
62:b:174:ILE:HG12	65:l:75:LEU:CD2	1.92	0.99
67:h:146:MET:HG2	68:k:39:LYS:NZ	1.77	0.99
55:a:445:LEU:CG	74:x:55:SER:CB	2.36	0.99
68:k:89:ASP:HB3	71:v:109:GLN:OE1	1.61	0.99
7:EA:143:GLN:CG	49:PG:158:PHE:HZ	1.73	0.99
7:EA:188:TYR:HD2	30:HD:14:TYR:CD1	1.81	0.99
39:DH:57:SER:CB	43:DJ:197:MET:SD	2.49	0.99
52:n:686:LYS:NZ	66:o:730:PRO:CD	2.26	0.99
52:n:921:MET:CE	52:n:1215:ILE:CD1	2.40	0.99
52:n:359:ILE:CB	52:n:372:ILE:HD11	1.91	0.99
37:DF:43:VAL:HG23	40:DI:46:TYR:HB3	1.43	0.98
60:q:129:PRO:HA	67:h:74:GLN:HA	1.44	0.98
62:b:181:CYS:SG	65:l:82:LEU:CD1	2.51	0.98
35:DD:1078:LEU:HD21	41:DL:83:MET:HE3	1.44	0.98
64:e:129:VAL:HG21	68:k:114:MET:HE1	1.43	0.98
52:n:252:ILE:HD11	52:n:271:ILE:HG12	1.43	0.98
52:n:686:LYS:NZ	66:o:730:PRO:HD3	1.78	0.98
56:d:45:ILE:HD13	58:i:72:ILE:C	1.86	0.98
64:e:95:PHE:HB3	65:l:38:GLN:HG2	1.44	0.98
41:DL:71:ASP:OD2	41:DL:74:GLU:CG	2.10	0.98
52:n:270:GLN:HE22	57:f:174:ARG:CG	1.74	0.98
55:a:59:VAL:HG21	56:d:51:SER:HB3	1.42	0.98
30:HD:55:LYS:HG3	49:PG:166:ASP:CA	1.92	0.98
52:n:169:LEU:HB3	52:n:170:PRO:HD3	1.42	0.98
30:HD:55:LYS:CD	49:PG:166:ASP:HB2	1.92	0.98
56:d:41:SER:HB2	58:i:69:VAL:HG13	1.41	0.98
41:DL:71:ASP:CG	41:DL:74:GLU:HG3	1.89	0.98
42:Dc:77:LEU:CD1	43:Dj:116:LEU:HD23	1.94	0.98
30:HD:287:TYR:CD1	46:HI:189:MET:SD	2.56	0.98
39:DH:154:PRO:HD2	39:DH:159:TYR:OH	1.63	0.98
52:n:647:MET:CE	73:w:22:PHE:CB	2.18	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:462:LEU:CB	74:x:49:GLN:HB3	1.93	0.98
60:q:451:LEU:HD11	60:q:529:MET:CE	1.94	0.98
52:n:904:PHE:CZ	52:n:1208:GLU:HG3	1.98	0.97
6:DA:725:CYS:SG	6:DA:725:CYS:O	2.22	0.97
41:DL:111:LEU:CA	41:DL:114:LYS:NZ	2.26	0.97
50:g:127:ARG:HA	50:g:130:GLN:HB3	1.42	0.97
52:n:904:PHE:HE2	52:n:1208:GLU:CD	1.72	0.97
60:q:149:LYS:HE2	71:v:40:ALA:C	1.89	0.97
60:q:437:HIS:CE1	60:q:472:GLU:N	2.33	0.97
60:q:484:TYR:CD1	60:q:636:VAL:CG1	2.47	0.97
37:DF:83:LEU:HD23	37:DF:86:PHE:HZ	1.23	0.97
18:HC:397:GLU:CB	33:HF:61:MET:HE3	1.93	0.97
55:a:321:LEU:HD22	55:a:407:ILE:HD12	1.42	0.97
60:q:89:GLN:CB	60:q:90:PRO:HD2	1.94	0.97
52:n:957:PRO:CB	52:n:1210:PHE:HZ	1.72	0.97
60:q:17:LYS:HE2	60:q:30:TYR:CE2	2.00	0.97
66:o:639:TYR:CD2	72:p:786:HIS:CG	2.52	0.97
47:HJ:184:PRO:HB3	47:HJ:187:LEU:HD12	1.47	0.96
12:DB:762:ASP:OD1	12:DB:768:PRO:HG3	1.64	0.96
54:u:90:LEU:HD13	60:q:9:ILE:HG13	0.97	0.96
60:q:392:MET:SD	69:r:46:MET:CE	2.52	0.96
63:c:305:PHE:HB3	63:c:311:GLN:OE1	1.63	0.96
11:PA:1795:PRO:CD	56:d:169:PRO:HA	1.95	0.96
40:DI:28:ILE:HG22	40:DI:31:TYR:HD1	1.30	0.96
52:n:273:PHE:HZ	57:f:185:ARG:HD2	1.20	0.96
55:a:335:THR:O	55:a:391:THR:CG2	2.12	0.96
55:a:462:LEU:HB2	74:x:49:GLN:CB	1.95	0.96
47:HJ:239:LYS:HZ2	47:HJ:239:LYS:H	1.01	0.96
52:n:545:LEU:CD1	52:n:653:PRO:HG3	1.95	0.96
62:b:179:LEU:HG	64:e:60:VAL:HB	1.46	0.96
37:DF:323:VAL:HG23	37:DF:326:HIS:HB2	1.47	0.96
66:o:636:HIS:HA	72:p:786:HIS:O	1.66	0.96
40:DI:81:GLN:HE22	41:DL:123:GLN:CD	1.73	0.96
54:u:128:SER:CB	58:i:131:LEU:HD21	1.95	0.96
60:q:263:LYS:HE2	60:q:439:PHE:CE2	1.99	0.96
39:DH:50:PHE:CE1	43:DJ:195:LEU:HD13	2.01	0.96
52:n:270:GLN:HE22	57:f:174:ARG:CD	1.78	0.96
55:a:417:TYR:CE1	55:a:450:PHE:HD1	1.74	0.95
40:DI:132:LEU:HD21	43:DJ:121:MET:HE1	1.47	0.95
52:n:273:PHE:CZ	57:f:185:ARG:CD	2.47	0.95
55:a:375:PHE:HD2	74:x:17:ARG:NH2	1.58	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:71:ILE:HD12	40:DI:38:GLN:NE2	1.80	0.95
55:a:66:GLN:HE22	56:d:44:LEU:HD11	1.30	0.95
56:d:41:SER:CB	58:i:69:VAL:HG13	1.96	0.95
62:b:174:ILE:HD13	65:l:75:LEU:HD21	1.43	0.95
35:DD:872:PHE:CE1	41:DL:57:VAL:HG12	2.00	0.95
52:n:545:LEU:CD1	52:n:653:PRO:CG	2.45	0.95
55:a:70:LYS:HZ1	58:i:74:LYS:HE2	0.96	0.95
55:a:70:LYS:HZ3	58:i:74:LYS:HE2	1.29	0.95
55:a:383:PRO:HG3	74:x:92:LEU:HD22	1.48	0.95
60:q:93:TRP:CE3	60:q:93:TRP:HA	2.02	0.95
66:o:639:TYR:HE2	72:p:786:HIS:ND1	1.64	0.95
55:a:364:TYR:HB3	55:a:430:LEU:CG	1.96	0.95
63:c:281:CYS:SG	63:c:311:GLN:NE2	2.40	0.95
11:PA:1643:TYR:OH	59:m:93:CYS:HB2	1.67	0.95
52:n:192:LEU:CD1	52:n:220:GLY:CA	2.45	0.95
52:n:270:GLN:CB	57:f:181:LEU:HD11	1.96	0.95
55:a:59:VAL:HG11	56:d:51:SER:OG	1.67	0.95
67:h:146:MET:HE2	68:k:45:LEU:HD12	1.48	0.95
19:DO:2:ALA:O	35:DD:1000:ARG:HB3	1.65	0.95
56:d:31:LEU:HD21	58:i:103:THR:CB	1.96	0.95
56:d:76:PHE:CE2	58:i:65:PHE:HD2	1.72	0.95
56:d:123:THR:HG22	60:q:37:SER:HB3	1.49	0.95
60:q:578:TYR:CD1	60:q:646:LEU:CD1	2.49	0.95
64:e:146:ILE:HG22	64:e:147:ASN:N	1.78	0.95
48:PD:79:THR:HG23	67:h:51:LEU:HD22	1.44	0.94
54:u:90:LEU:HD11	60:q:7:VAL:CB	1.96	0.94
55:a:441:GLU:HB2	74:x:17:ARG:HH22	1.29	0.94
66:o:715:LEU:HD13	74:x:66:TYR:OH	1.66	0.94
67:h:146:MET:HB2	68:k:39:LYS:HZ3	1.13	0.94
12:DB:622:ASP:HB3	33:HF:36:GLN:HA	1.46	0.94
52:n:270:GLN:HE22	57:f:174:ARG:HG3	1.29	0.94
55:a:375:PHE:CD1	74:x:17:ARG:HG3	2.02	0.94
56:d:126:TYR:CD2	60:q:36:MET:HB3	2.01	0.94
35:DD:1078:LEU:CD2	41:DL:83:MET:CE	2.46	0.94
42:Dc:67:GLY:HA3	43:Dj:116:LEU:HD11	1.48	0.94
7:EA:174:ARG:HB3	30:HD:8:ARG:HH21	0.78	0.94
39:DH:37:LEU:HD11	43:DJ:138:TYR:CE2	2.03	0.94
18:HC:398:ARG:HH22	33:HF:58:GLY:HA2	1.30	0.94
37:DF:274:ASN:HB2	37:DF:317:LEU:HD23	1.48	0.94
46:HI:143:LEU:HD13	46:HI:143:LEU:O	1.68	0.94
60:q:418:ILE:CD1	70:t:72:PRO:CG	2.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:179:LEU:HD12	64:e:60:VAL:CB	1.97	0.94
56:d:45:ILE:HG13	58:i:73:ILE:HG12	1.48	0.94
7:EA:122:THR:HG23	30:HD:40:VAL:HG23	1.47	0.93
30:HD:284:ALA:HB3	46:HI:243:LEU:HD13	0.95	0.93
46:HI:86:ASN:ND2	46:HI:86:ASN:O	2.00	0.93
52:n:273:PHE:CE2	57:f:185:ARG:HD2	2.03	0.93
54:u:125:ILE:HG12	58:i:135:TYR:CE2	2.03	0.93
7:EA:139:LEU:CD2	49:PG:151:ARG:CB	2.39	0.93
56:d:34:LEU:HD22	58:i:99:LYS:HD3	1.47	0.93
7:EA:188:TYR:CD2	30:HD:14:TYR:CD1	2.57	0.93
35:DD:899:VAL:HG13	35:DD:900:SER:N	1.82	0.93
35:DD:1078:LEU:CD2	41:DL:83:MET:HE3	1.97	0.93
52:n:192:LEU:HB3	52:n:219:ASN:O	1.66	0.93
52:n:267:HIS:HD2	57:f:174:ARG:HD3	0.77	0.93
52:n:1218:ARG:HH22	52:n:1222:ARG:HB2	1.32	0.93
60:q:540:LEU:HD21	60:q:640:GLU:HG3	1.51	0.93
54:u:122:LEU:HD21	56:d:111:GLN:HG2	1.50	0.93
55:a:445:LEU:CD1	74:x:55:SER:CB	2.46	0.93
60:q:168:THR:OG1	68:k:21:ILE:HG21	1.68	0.93
62:b:136:HIS:CD2	63:c:111:TYR:CE1	2.57	0.93
62:b:179:LEU:HD12	64:e:60:VAL:HB	1.50	0.93
30:HD:85:ARG:HH12	30:HD:140:LEU:HG	1.34	0.93
55:a:417:TYR:HE1	55:a:450:PHE:HD1	1.07	0.93
68:k:87:ARG:HH11	68:k:87:ARG:HG3	1.33	0.93
46:HI:52:LYS:HA	46:HI:52:LYS:HE3	1.51	0.92
48:PD:134:ILE:HA	48:PD:137:LYS:HE2	1.51	0.92
60:q:149:LYS:CD	71:v:40:ALA:HA	1.99	0.92
39:DH:57:SER:OG	43:DJ:200:LEU:HD12	1.69	0.92
55:a:321:LEU:CD2	55:a:407:ILE:HG23	1.98	0.92
62:b:174:ILE:CG1	65:l:75:LEU:CD2	2.39	0.92
7:EA:17:LEU:HD22	7:EA:194:THR:HG21	1.50	0.92
37:DF:219:GLU:HG2	39:DH:160:ILE:HG22	1.50	0.92
56:d:45:ILE:HD11	58:i:73:ILE:HG13	1.51	0.92
54:u:115:LEU:HB2	56:d:121:LEU:HD11	1.48	0.92
66:o:735:LEU:HD21	73:w:113:GLN:CD	1.95	0.92
60:q:377:LEU:HD13	65:l:177:ARG:HA	1.52	0.92
52:n:932:GLY:HA2	52:n:1179:HIS:CE1	2.04	0.92
7:EA:122:THR:OG1	30:HD:40:VAL:HG21	1.70	0.92
36:DE:446:GLU:OE1	36:DE:788:ARG:NE	2.01	0.92
46:HI:239:ASP:HA	46:HI:242:SER:HB3	1.51	0.92
55:a:66:GLN:NE2	56:d:44:LEU:CD1	2.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:d:38:GLU:CG	58:i:96:GLU:HG2	1.99	0.92
62:b:136:HIS:CD2	63:c:111:TYR:CD1	2.58	0.92
17:PB:1143:LYS:HE3	49:PG:152:VAL:CG1	2.00	0.92
37:DF:105:TYR:O	43:DJ:217:PHE:CG	2.23	0.92
37:DF:323:VAL:CG2	37:DF:326:HIS:CB	2.48	0.92
56:d:45:ILE:HG23	58:i:76:MET:HB3	1.50	0.92
30:HD:55:LYS:HE2	49:PG:166:ASP:CG	1.95	0.91
52:n:359:ILE:HG12	52:n:372:ILE:HD11	0.92	0.91
58:i:72:ILE:HD13	58:i:92:SER:CB	2.00	0.91
60:q:479:ILE:CG2	60:q:532:HIS:CD2	2.52	0.91
30:HD:27:GLY:HA3	30:HD:70:LYS:HD3	1.51	0.91
52:n:224:PHE:CD2	52:n:292:MET:CE	2.53	0.91
55:a:462:LEU:HD21	74:x:11:LEU:HB3	1.51	0.91
51:j:82:LYS:HZ2	53:s:101:VAL:HG12	1.35	0.91
56:d:45:ILE:CD1	58:i:73:ILE:CA	2.48	0.91
67:h:182:VAL:CG2	69:r:202:ILE:HD12	2.01	0.91
52:n:261:ASP:HB2	60:q:250:ASP:CG	1.94	0.91
54:u:128:SER:HB2	58:i:131:LEU:CD2	1.99	0.91
55:a:375:PHE:HD2	74:x:17:ARG:HH21	0.93	0.91
12:DB:158:GLY:HA2	12:DB:188:PHE:HB3	1.53	0.91
52:n:192:LEU:HD12	52:n:220:GLY:HA2	1.52	0.91
60:q:392:MET:CE	69:r:46:MET:HE1	1.99	0.91
66:o:639:TYR:CE2	72:p:786:HIS:CG	2.58	0.91
55:a:449:ARG:HH22	74:x:54:PRO:HB2	1.32	0.91
60:q:157:ALA:HB2	68:k:31:VAL:HG23	1.52	0.91
18:HC:397:GLU:HB3	33:HF:61:MET:CE	2.00	0.91
36:DE:463:PHE:O	37:DF:133:ALA:HA	1.70	0.91
39:DH:60:THR:HG21	43:DJ:211:VAL:HG23	1.53	0.91
52:n:254:VAL:HG21	52:n:303:LEU:CD2	1.99	0.91
60:q:124:PHE:CE2	67:h:89:LEU:HD11	2.05	0.91
7:EA:139:LEU:HD12	49:PG:151:ARG:HD2	1.52	0.91
7:EA:143:GLN:HG2	49:PG:158:PHE:CE1	2.05	0.91
35:DD:966:LEU:HD11	35:DD:982:LEU:CD2	2.01	0.91
35:DD:1078:LEU:HD23	41:DL:83:MET:CE	2.01	0.91
52:n:359:ILE:HG23	52:n:372:ILE:CD1	2.01	0.91
37:DF:218:VAL:HG11	39:DH:162:THR:HG21	1.51	0.91
37:DF:323:VAL:HG23	37:DF:326:HIS:CB	2.01	0.91
54:u:90:LEU:HB2	60:q:9:ILE:HG12	1.53	0.91
62:b:186:THR:HG21	64:e:49:GLU:CD	1.96	0.91
70:t:98:LEU:HB3	70:t:102:PHE:HD1	1.36	0.90
55:a:70:LYS:HZ3	58:i:74:LYS:CE	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:i:72:ILE:CD1	58:i:92:SER:CB	2.49	0.90
67:h:142:SER:OG	68:k:39:LYS:HE3	1.72	0.90
52:n:203:LEU:HD13	52:n:215:LEU:HD12	1.53	0.90
37:DF:105:TYR:O	43:DJ:217:PHE:HB3	1.71	0.90
37:DF:218:VAL:CG1	39:DH:162:THR:CB	2.48	0.90
52:n:253:LEU:O	52:n:255:GLU:HG3	1.71	0.90
55:a:375:PHE:CE1	74:x:17:ARG:HG3	2.05	0.90
30:HD:21:LEU:CD2	30:HD:69:ASP:OD2	2.18	0.90
55:a:416:ALA:CB	55:a:472:SER:O	2.19	0.90
12:DB:672:PHE:CD1	18:HC:414:SER:CB	2.14	0.90
35:DD:966:LEU:HD11	35:DD:982:LEU:HD23	1.54	0.90
52:n:172:CYS:SG	60:q:21:GLU:HA	2.12	0.90
52:n:957:PRO:CG	52:n:1210:PHE:HE1	1.65	0.90
55:a:380:ALA:CB	74:x:58:PRO:HG3	2.01	0.90
60:q:89:GLN:CD	60:q:90:PRO:HD2	1.97	0.90
12:DB:672:PHE:HZ	18:HC:413:LEU:HD12	1.31	0.90
52:n:166:TYR:HE2	59:m:71:GLN:HA	1.36	0.90
55:a:445:LEU:CD1	74:x:55:SER:N	2.08	0.90
39:DH:57:SER:CA	43:DJ:197:MET:SD	2.59	0.90
50:g:129:HIS:HA	50:g:132:ARG:HG2	1.51	0.90
56:d:45:ILE:HG23	58:i:76:MET:HB2	0.93	0.90
56:d:103:ARG:HG2	56:d:103:ARG:HH11	1.34	0.90
37:DF:219:GLU:HG2	39:DH:160:ILE:HG21	1.45	0.90
52:n:960:LYS:NZ	52:n:1185:LEU:HD13	1.87	0.90
59:m:56:LEU:CD2	59:m:80:GLN:NE2	2.33	0.90
56:d:45:ILE:CG1	58:i:73:ILE:HG12	2.00	0.89
62:b:101:ARG:HH12	72:p:677:THR:CB	1.85	0.89
11:PA:1795:PRO:HD2	56:d:169:PRO:CA	1.99	0.89
40:DI:132:LEU:HG	43:DJ:121:MET:CE	2.02	0.89
47:HJ:165:ARG:HH11	47:HJ:165:ARG:HB2	1.35	0.89
60:q:89:GLN:HG2	60:q:90:PRO:HD3	1.55	0.89
55:a:364:TYR:CB	55:a:430:LEU:HG	2.03	0.89
62:b:62:MET:HE2	62:b:62:MET:HA	1.52	0.89
62:b:136:HIS:HD2	63:c:111:TYR:CD2	1.90	0.89
56:d:31:LEU:CD2	58:i:103:THR:CG2	2.51	0.89
51:j:35:ALA:HB3	53:s:154:LEU:HD23	1.54	0.89
41:DL:111:LEU:HA	41:DL:114:LYS:HZ2	0.78	0.89
50:g:124:ASN:O	50:g:128:PRO:HD3	1.72	0.89
52:n:224:PHE:HD2	52:n:292:MET:HE2	1.37	0.89
52:n:870:GLN:HG2	66:o:655:THR:HG22	1.53	0.89
56:d:126:TYR:CZ	60:q:36:MET:HB3	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:645:ALA:HB2	64:e:100:LEU:CD2	2.03	0.89
52:n:960:LYS:CG	52:n:1210:PHE:CD2	2.56	0.89
55:a:70:LYS:CB	58:i:70:HIS:ND1	2.34	0.89
60:q:437:HIS:HE1	60:q:472:GLU:C	1.81	0.89
60:q:484:TYR:CD1	60:q:636:VAL:HG12	2.06	0.89
35:DD:899:VAL:CG1	35:DD:900:SER:N	2.36	0.88
36:DE:432:LEU:HG	36:DE:436:ASP:OD2	1.73	0.88
56:d:45:ILE:CG2	58:i:76:MET:CB	2.27	0.88
40:DI:62:LYS:CD	41:DI:106:ARG:NH1	2.36	0.88
52:n:861:LYS:HE3	63:c:30:ARG:NE	1.87	0.88
56:d:156:SER:HA	56:d:161:VAL:HG12	1.55	0.88
60:q:410:PRO:CG	69:r:82:PRO:HB3	2.00	0.88
56:d:31:LEU:HD23	58:i:103:THR:CG2	2.00	0.88
39:DH:60:THR:HG21	43:DJ:211:VAL:CG2	2.02	0.88
7:EA:143:GLN:CG	49:PG:158:PHE:CE1	2.56	0.88
35:DD:899:VAL:CG1	35:DD:900:SER:H	1.86	0.88
47:HJ:175:LYS:HA	47:HJ:175:LYS:CE	2.04	0.88
56:d:45:ILE:HA	56:d:48:LEU:HD12	1.55	0.88
39:DH:171:ASP:HB3	39:DH:174:VAL:HG12	1.54	0.88
40:DI:132:LEU:HG	43:DJ:121:MET:SD	2.13	0.88
52:n:753:LEU:HD12	63:c:311:GLN:HG3	1.55	0.88
54:u:90:LEU:HD22	60:q:9:ILE:CG1	2.03	0.88
67:h:142:SER:O	68:k:39:LYS:NZ	2.05	0.88
52:n:651:ASN:HB3	73:w:21:ALA:HB1	1.56	0.88
55:a:417:TYR:CB	55:a:469:VAL:HG21	2.02	0.88
58:i:72:ILE:HD11	58:i:92:SER:HB2	1.54	0.88
12:DB:648:MET:HE3	18:HC:411:GLN:HG2	1.56	0.88
35:DD:1071:ARG:HB2	37:DF:91:PHE:CD2	2.08	0.88
60:q:102:LEU:CD1	67:h:29:PHE:CE2	2.57	0.88
17:PB:1134:THR:HG21	49:PG:153:ASP:OD1	1.74	0.88
37:DF:14:LEU:HD21	40:DI:19:MET:CE	2.04	0.88
59:m:124:GLN:CD	61:z:590:ARG:HB2	1.99	0.88
67:h:146:MET:HG3	68:k:39:LYS:HD2	1.52	0.88
68:k:37:LYS:H	68:k:37:LYS:HE3	1.35	0.88
11:PA:1795:PRO:HD2	56:d:169:PRO:HB3	0.88	0.87
35:DD:895:HIS:CG	35:DD:896:PRO:CD	2.56	0.87
37:DF:219:GLU:HB3	39:DH:160:ILE:HG23	1.55	0.87
46:HI:140:PRO:HA	46:HI:202:ILE:HD11	1.53	0.87
52:n:169:LEU:CA	59:m:104:HIS:CD2	2.57	0.87
12:DB:621:ALA:HB2	18:HC:438:LYS:HZ1	1.36	0.87
60:q:120:ARG:HG2	60:q:120:ARG:HH11	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EA:139:LEU:HD21	49:PG:151:ARG:CG	2.03	0.87
11:PA:1005:HIS:CD2	11:PA:1007:ILE:HG22	2.09	0.87
52:n:237:MET:HE1	60:q:45:GLN:CB	2.03	0.87
54:u:90:LEU:CD1	60:q:7:VAL:HB	2.01	0.87
60:q:418:ILE:HD12	70:t:72:PRO:HG3	1.56	0.87
60:q:451:LEU:HD11	60:q:529:MET:SD	2.13	0.87
60:q:149:LYS:CE	71:v:40:ALA:CA	2.52	0.87
62:b:179:LEU:HD12	64:e:60:VAL:HA	1.56	0.87
66:o:639:TYR:CE2	72:p:786:HIS:ND1	2.42	0.87
7:EA:139:LEU:CD1	49:PG:151:ARG:CD	2.06	0.87
47:HJ:175:LYS:HA	47:HJ:175:LYS:HE3	1.56	0.87
62:b:175:HIS:CB	63:c:113:TRP:CH2	2.57	0.87
66:o:639:TYR:HD2	72:p:786:HIS:CB	1.75	0.87
37:DF:43:VAL:CG2	40:DI:46:TYR:HB3	2.04	0.87
52:n:265:LEU:HD11	52:n:307:VAL:CG2	2.05	0.87
55:a:445:LEU:HD12	74:x:54:PRO:HG2	1.55	0.87
57:f:16:VAL:CG1	57:f:103:GLY:O	2.23	0.87
63:c:204:MET:HE1	63:c:208:PHE:C	1.99	0.87
63:c:288:LEU:HD11	70:t:122:PHE:CZ	2.08	0.87
18:HC:352:GLN:NE2	33:HF:61:MET:CE	2.38	0.87
55:a:417:TYR:CD1	55:a:469:VAL:HG23	2.03	0.87
17:PB:1143:LYS:HE3	49:PG:152:VAL:HG13	1.54	0.86
18:HC:120:ILE:O	32:HE:100:LYS:NZ	2.07	0.86
30:HD:55:LYS:CG	49:PG:166:ASP:CB	2.12	0.86
35:DD:960:GLU:HG3	35:DD:983:ARG:HH12	1.37	0.86
52:n:245:TRP:HB2	52:n:282:LEU:HD13	0.88	0.86
19:DO:2:ALA:HA	35:DD:1000:ARG:HD3	0.89	0.86
12:DB:646:ASP:CB	18:HC:413:LEU:O	2.23	0.86
30:HD:300:ALA:HB2	47:HJ:166:PRO:CA	1.99	0.86
39:DH:50:PHE:HB2	43:DJ:195:LEU:HB2	1.57	0.86
54:u:115:LEU:CD1	56:d:121:LEU:HB3	2.06	0.86
30:HD:300:ALA:CB	47:HJ:166:PRO:CA	2.52	0.86
52:n:192:LEU:HD12	52:n:220:GLY:HA3	1.57	0.86
55:a:59:VAL:HG21	56:d:51:SER:HB2	1.55	0.86
56:d:45:ILE:CD1	58:i:73:ILE:HA	2.04	0.86
62:b:78:ALA:HB3	66:o:621:LEU:HD21	1.58	0.86
54:u:77:PRO:HA	61:z:562:GLY:O	1.74	0.86
56:d:126:TYR:CZ	60:q:36:MET:CB	2.59	0.86
60:q:139:GLN:NE2	60:q:139:GLN:O	2.08	0.86
35:DD:922:GLN:HG3	35:DD:1056:THR:HG21	1.56	0.86
52:n:169:LEU:HB3	52:n:170:PRO:HD2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:707:ASP:HB2	66:o:684:ARG:HH21	1.40	0.86
57:f:94:PRO:HB2	60:q:130:VAL:HG22	1.55	0.86
58:i:96:GLU:HA	58:i:99:LYS:HG3	1.57	0.86
60:q:188:LEU:HA	71:v:87:ILE:HD11	1.57	0.86
60:q:484:TYR:CE1	60:q:636:VAL:HG12	2.09	0.86
30:HD:83:ASN:CG	30:HD:140:LEU:CD1	2.47	0.86
58:i:105:PRO:HD2	58:i:107:ILE:HG13	1.58	0.86
39:DH:50:PHE:CZ	43:DJ:170:ALA:C	2.54	0.86
52:n:168:ARG:HD3	59:m:104:HIS:NE2	1.87	0.86
52:n:224:PHE:CD2	52:n:292:MET:HE1	2.10	0.86
55:a:377:ASN:HD21	74:x:58:PRO:HG2	1.41	0.86
58:i:68:LEU:HD13	58:i:95:GLN:CG	2.05	0.86
58:i:85:GLN:HG3	58:i:86:ASP:H	0.73	0.86
11:PA:1475:LEU:HB2	49:PG:59:ILE:HG13	1.55	0.86
52:n:192:LEU:CD1	52:n:220:GLY:HA3	2.05	0.86
54:u:108:VAL:HG21	56:d:128:ALA:HB1	1.55	0.86
55:a:59:VAL:CG1	56:d:48:LEU:HA	2.05	0.86
55:a:509:ARG:HB2	55:a:509:ARG:NH1	1.89	0.86
47:HJ:186:ILE:HD13	47:HJ:186:ILE:H	1.39	0.85
54:u:75:SER:HB3	61:z:566:CYS:SG	2.16	0.85
55:a:228:PRO:HB2	55:a:502:MET:HB2	1.58	0.85
55:a:367:LEU:HD13	55:a:509:ARG:CZ	2.05	0.85
60:q:152:SER:HB2	71:v:58:ASN:CA	2.06	0.85
30:HD:55:LYS:C	30:HD:57:ASN:H	1.82	0.85
30:HD:295:ARG:HH11	47:HJ:165:ARG:NH2	1.73	0.85
39:DH:53:ALA:HA	43:DJ:195:LEU:O	1.75	0.85
52:n:166:TYR:HH	59:m:70:PRO:HB2	1.38	0.85
52:n:261:ASP:CG	60:q:250:ASP:OD2	2.17	0.85
63:c:204:MET:SD	63:c:208:PHE:O	2.35	0.85
48:PD:74:PHE:CZ	48:PD:137:LYS:HE3	2.10	0.85
52:n:1218:ARG:NH2	52:n:1222:ARG:HB2	1.90	0.85
57:f:145:TYR:CZ	67:h:43:PRO:CG	2.60	0.85
60:q:578:TYR:CD1	60:q:646:LEU:HD13	2.11	0.85
64:e:146:ILE:CG2	64:e:147:ASN:H	1.82	0.85
76:NG:1119:GLY:C	76:NG:1121:LYS:H	1.84	0.85
41:DL:71:ASP:HB3	41:DL:74:GLU:CD	2.02	0.85
7:EA:142:ASN:HD21	49:PG:107:PHE:HB2	1.41	0.85
12:DB:672:PHE:CZ	18:HC:413:LEU:HB2	2.10	0.85
55:a:377:ASN:HB3	55:a:442:VAL:O	1.75	0.85
55:a:462:LEU:HD12	74:x:60:ILE:CD1	2.06	0.85
63:c:204:MET:CE	63:c:208:PHE:O	2.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DI:28:ILE:HG22	40:DI:31:TYR:CD1	2.11	0.85
53:s:104:LYS:C	53:s:106:SER:N	2.30	0.85
55:a:417:TYR:CG	55:a:469:VAL:HG21	2.12	0.85
67:h:22:LEU:HA	67:h:56:LEU:HD13	1.58	0.85
68:k:45:LEU:O	68:k:45:LEU:HD22	1.76	0.85
40:DI:23:LEU:HD21	40:DI:39:MET:HE1	1.58	0.85
56:d:76:PHE:HE2	58:i:65:PHE:HD2	1.17	0.85
12:DB:672:PHE:CZ	18:HC:413:LEU:CD1	2.59	0.85
52:n:224:PHE:HD2	52:n:292:MET:CE	1.89	0.85
55:a:380:ALA:HB3	55:a:444:PRO:CD	2.06	0.85
55:a:462:LEU:HG	74:x:49:GLN:CD	2.01	0.85
60:q:487:ILE:HG21	60:q:543:VAL:CG2	2.02	0.85
13:EB:230:GLU:HA	13:EB:233:ILE:HD13	1.58	0.85
37:DF:83:LEU:CD1	37:DF:97:ALA:O	2.25	0.85
37:DF:218:VAL:CG1	39:DH:162:THR:OG1	2.21	0.85
52:n:907:LEU:HD11	62:b:118:LEU:HB2	1.58	0.85
57:f:145:TYR:CE1	67:h:43:PRO:CG	2.60	0.85
52:n:706:LEU:HD22	60:q:615:TRP:CZ3	2.12	0.84
54:u:108:VAL:CG2	56:d:128:ALA:HB1	2.07	0.84
56:d:38:GLU:HG2	58:i:96:GLU:HG2	1.59	0.84
55:a:335:THR:O	55:a:391:THR:HG21	1.76	0.84
54:u:115:LEU:CB	56:d:121:LEU:HD12	1.87	0.84
55:a:375:PHE:CG	74:x:17:ARG:CZ	2.59	0.84
56:d:42:ARG:HH22	58:i:93:LYS:HA	1.40	0.84
60:q:134:ALA:H	67:h:72:ARG:HH12	1.19	0.84
37:DF:104:LEU:CB	43:DJ:217:PHE:CZ	2.60	0.84
55:a:462:LEU:CA	74:x:49:GLN:HG2	2.07	0.84
72:p:702:ASP:HB2	72:p:705:PRO:HB3	1.58	0.84
11:PA:1795:PRO:CG	56:d:169:PRO:HB3	2.07	0.84
37:DF:219:GLU:CG	39:DH:160:ILE:HG22	2.05	0.84
37:DF:323:VAL:HG23	37:DF:326:HIS:CG	2.13	0.84
55:a:416:ALA:HB2	55:a:472:SER:O	1.77	0.84
17:PB:1143:LYS:CE	49:PG:152:VAL:HG13	2.07	0.84
47:HJ:60:TYR:HB3	47:HJ:105:MET:HE1	1.59	0.84
52:n:960:LYS:NZ	52:n:1185:LEU:CD1	2.41	0.84
62:b:175:HIS:CG	63:c:113:TRP:CZ2	2.66	0.84
14:FB:186:MET:CE	35:DD:995:GLU:CD	2.48	0.84
47:HJ:229:GLU:OE1	47:HJ:229:GLU:N	2.11	0.84
54:u:71:VAL:HG13	61:z:529:HIS:HB2	1.57	0.84
55:a:462:LEU:HB2	74:x:49:GLN:HB3	1.52	0.84
60:q:102:LEU:HD11	67:h:29:PHE:HE2	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:481:SER:HB3	60:q:636:VAL:HG21	1.57	0.84
37:DF:104:LEU:HB2	43:DJ:217:PHE:CZ	2.13	0.84
49:PG:41:LYS:O	49:PG:78:ARG:NH2	2.11	0.84
55:a:70:LYS:CB	58:i:70:HIS:CE1	2.59	0.84
56:d:167:TRP:CH2	59:m:102:ILE:HG21	2.03	0.84
48:PD:79:THR:CA	67:h:51:LEU:HD21	2.07	0.83
56:d:167:TRP:CH2	59:m:102:ILE:HG23	2.13	0.83
59:m:124:GLN:OE1	61:z:590:ARG:HB2	1.78	0.83
67:h:22:LEU:HD12	67:h:22:LEU:O	1.78	0.83
72:p:13:MET:HG3	72:p:405:PHE:HB2	1.59	0.83
7:EA:142:ASN:HB3	49:PG:158:PHE:CE2	2.13	0.83
39:DH:50:PHE:HZ	43:DJ:170:ALA:CB	1.90	0.83
52:n:169:LEU:H	59:m:104:HIS:CD2	1.94	0.83
52:n:960:LYS:HG3	52:n:1210:PHE:HD2	1.42	0.83
66:o:765:ASP:OD2	73:w:71:HIS:HB2	1.78	0.83
55:a:59:VAL:HG11	56:d:48:LEU:HA	1.59	0.83
62:b:174:ILE:HD13	65:l:75:LEU:CD2	2.03	0.83
7:EA:142:ASN:ND2	49:PG:107:PHE:CB	2.42	0.83
37:Df:447:ALA:HA	37:Df:456:GLY:HA3	1.61	0.83
50:g:164:ILE:HD13	58:i:140:MET:HG2	1.59	0.83
57:f:15:TRP:CH2	57:f:35:GLU:OE1	2.32	0.83
37:DF:104:LEU:HD13	43:DJ:217:PHE:HE2	1.43	0.83
67:h:142:SER:OG	68:k:39:LYS:CE	2.26	0.83
52:n:295:CYS:SG	57:f:188:PHE:CD2	2.72	0.83
60:q:186:GLU:OE2	60:q:291:TRP:CZ2	2.32	0.83
64:e:140:GLN:NE2	68:k:105:SER:HA	1.93	0.83
67:h:23:LYS:NZ	67:h:23:LYS:HB3	1.92	0.83
7:EA:139:LEU:CG	49:PG:151:ARG:HD2	2.07	0.83
7:EA:142:ASN:ND2	49:PG:107:PHE:HB2	1.93	0.83
18:HC:348:ARG:NE	33:HF:65:ALA:CB	2.42	0.83
37:DF:316:GLN:HB2	37:DF:327:TRP:CZ3	2.13	0.83
51:j:43:PHE:CB	53:s:144:ILE:CG2	2.56	0.83
56:d:38:GLU:OE2	58:i:96:GLU:HG2	1.79	0.83
55:a:462:LEU:H	74:x:49:GLN:NE2	1.70	0.83
63:c:305:PHE:CD1	63:c:311:GLN:HB3	2.13	0.83
66:o:714:ASP:O	74:x:28:LYS:NZ	2.10	0.83
30:HD:85:ARG:NH2	30:HD:140:LEU:N	2.25	0.83
36:DE:433:LYS:NZ	40:DI:110:TYR:CE1	2.46	0.83
37:DF:14:LEU:HD21	40:DI:19:MET:HE1	1.59	0.83
60:q:458:PRO:CB	60:q:533:GLN:HE21	1.91	0.83
41:DL:111:LEU:O	41:DL:114:LYS:CG	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:192:LEU:HD12	52:n:219:ASN:O	1.78	0.82
55:a:423:SER:OG	55:a:505:PRO:HD3	1.79	0.82
55:a:462:LEU:HG	74:x:49:GLN:CG	2.08	0.82
52:n:359:ILE:HA	52:n:372:ILE:HD12	1.60	0.82
54:u:115:LEU:HB2	56:d:121:LEU:HD13	0.83	0.82
55:a:380:ALA:CB	55:a:444:PRO:HD2	2.09	0.82
60:q:443:ARG:NE	60:q:443:ARG:HA	1.92	0.82
30:HD:145:GLU:OE1	67:h:67:LYS:HE2	1.80	0.82
41:DL:64:GLN:HA	41:DL:67:VAL:HG22	1.59	0.82
52:n:250:LEU:HD21	52:n:275:HIS:HD2	1.38	0.82
54:u:128:SER:CB	58:i:131:LEU:HD22	2.08	0.82
63:c:204:MET:HE1	63:c:208:PHE:CA	2.08	0.82
14:FB:186:MET:SD	35:DD:995:GLU:HG2	2.20	0.82
36:DE:747:LEU:HD22	36:DE:747:LEU:H	1.43	0.82
42:Dc:67:GLY:HA3	43:Dj:116:LEU:HD13	1.60	0.82
55:a:417:TYR:HB2	55:a:469:VAL:HG21	1.61	0.82
56:d:41:SER:CB	58:i:69:VAL:CG1	2.57	0.82
52:n:192:LEU:CD1	52:n:220:GLY:HA2	2.08	0.82
55:a:321:LEU:HD21	55:a:407:ILE:CG2	2.08	0.82
7:EA:139:LEU:HD23	49:PG:151:ARG:HB3	1.56	0.82
47:HJ:198:ILE:HD12	47:HJ:255:MET:HE2	1.62	0.82
52:n:680:HIS:HE2	60:q:557:LEU:HD11	1.44	0.82
57:f:32:TYR:CD1	57:f:35:GLU:OE2	2.33	0.82
57:f:32:TYR:HD1	57:f:35:GLU:OE2	1.63	0.82
46:HI:267:ASP:OD1	46:HI:267:ASP:N	2.08	0.82
52:n:686:LYS:CE	66:o:730:PRO:HG3	2.09	0.82
56:d:115:LYS:HE2	56:d:115:LYS:HA	1.60	0.82
65:l:166:LEU:HD12	68:k:103:LYS:HB3	1.60	0.82
11:PA:1643:TYR:O	59:m:96:PHE:HB2	1.80	0.82
30:HD:43:ALA:HB3	49:PG:164:MET:HE3	1.62	0.82
30:HD:83:ASN:ND2	30:HD:140:LEU:CD1	2.43	0.82
39:DH:50:PHE:CZ	43:DJ:170:ALA:HB3	2.15	0.82
42:Dc:77:LEU:HD13	43:Dj:116:LEU:HD23	1.61	0.82
60:q:441:ARG:NH1	65:l:168:TRP:CE2	2.48	0.82
63:c:305:PHE:CD1	63:c:311:GLN:CG	2.63	0.82
67:h:18:GLN:HA	67:h:18:GLN:NE2	1.92	0.82
31:HG:109:THR:HG1	31:HG:148:SER:HG	1.22	0.81
60:q:187:LEU:HD23	71:v:84:GLN:HG2	1.62	0.81
71:v:16:GLN:HE22	71:v:20:LYS:HE2	1.41	0.81
58:i:75:CYS:HB3	58:i:88:ASN:ND2	1.95	0.81
60:q:437:HIS:HE1	60:q:472:GLU:CA	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:359:ILE:CB	52:n:372:ILE:CD1	2.54	0.81
20:DP:206:GLU:OE1	20:DP:236:LYS:NZ	2.13	0.81
39:DH:57:SER:HA	43:DJ:197:MET:SD	2.20	0.81
54:u:128:SER:OG	58:i:131:LEU:HD22	1.80	0.81
60:q:149:LYS:HE2	71:v:40:ALA:O	1.79	0.81
62:b:174:ILE:HG12	65:l:75:LEU:CG	2.11	0.81
63:c:204:MET:CE	63:c:208:PHE:C	2.54	0.81
50:g:166:ASN:OD1	50:g:166:ASN:C	2.24	0.81
63:c:309:CYS:HB2	63:c:311:GLN:OE1	1.79	0.81
36:DE:526:ARG:NH1	36:DE:526:ARG:HA	1.96	0.81
55:a:364:TYR:CB	55:a:430:LEU:HD12	2.11	0.81
67:h:139:GLN:HE22	68:k:37:LYS:HB2	1.45	0.81
60:q:93:TRP:HA	60:q:93:TRP:HE3	1.41	0.81
70:t:144:TYR:HD2	70:t:147:CYS:HB2	1.46	0.81
18:HC:348:ARG:CZ	33:HF:65:ALA:HB3	2.10	0.81
30:HD:298:GLN:NE2	46:HI:132:TRP:CD1	2.49	0.81
36:DE:694:LEU:HD13	36:DE:703:MET:HE2	1.61	0.81
41:DL:71:ASP:HB3	41:DL:74:GLU:CG	2.11	0.81
56:d:110:LEU:O	56:d:110:LEU:HD22	1.79	0.81
59:m:124:GLN:OE1	61:z:590:ARG:CB	2.28	0.81
7:EA:142:ASN:HB3	49:PG:158:PHE:HE2	1.45	0.81
30:HD:55:LYS:CB	49:PG:166:ASP:HB2	2.11	0.81
39:DH:51:GLU:O	43:DJ:194:THR:HA	1.80	0.81
60:q:186:GLU:CG	60:q:243:LEU:HD21	1.91	0.81
60:q:462:ALA:O	71:v:131:GLU:HG2	1.80	0.81
5:BA:43:ASP:OD1	17:PB:1064:ARG:NH2	2.14	0.81
11:PA:1795:PRO:HD3	56:d:169:PRO:CA	2.05	0.81
30:HD:287:TYR:CE1	46:HI:189:MET:SD	2.73	0.81
39:DH:108:PRO:CG	43:DJ:116:LEU:CD2	2.59	0.81
40:DI:23:LEU:CD1	40:DI:39:MET:HE1	2.11	0.81
60:q:339:LEU:CD1	60:q:439:PHE:CD2	2.63	0.81
68:k:16:ASP:OD2	71:v:79:VAL:HG21	1.80	0.81
37:DF:276:LEU:HA	37:DF:330:ARG:NH2	1.96	0.80
40:DI:23:LEU:HD11	40:DI:39:MET:CE	2.11	0.80
54:u:8:LEU:HD11	54:u:73:ILE:HG13	1.60	0.80
60:q:339:LEU:CD1	60:q:439:PHE:CE2	2.63	0.80
60:q:596:PHE:CZ	65:l:117:TYR:OH	2.11	0.80
62:b:136:HIS:CD2	63:c:111:TYR:CZ	2.69	0.80
18:HC:348:ARG:NH2	33:HF:65:ALA:HB3	1.96	0.80
47:HJ:52:GLU:HB3	47:HJ:273:LEU:HD11	1.61	0.80
62:b:136:HIS:HD2	63:c:111:TYR:CE2	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:c:305:PHE:CG	63:c:311:GLN:HB3	2.16	0.80
6:DA:1065:GLU:OE1	6:DA:1065:GLU:HA	1.78	0.80
11:PA:911:PRO:O	11:PA:963:ARG:NH2	2.14	0.80
12:DB:672:PHE:CE1	18:HC:413:LEU:CD1	2.65	0.80
19:DO:2:ALA:CA	35:DD:1000:ARG:CD	2.44	0.80
46:HI:143:LEU:C	46:HI:143:LEU:HD22	2.07	0.80
55:a:461:SER:C	74:x:49:GLN:NE2	2.38	0.80
57:f:145:TYR:CE1	67:h:43:PRO:HG3	2.15	0.80
60:q:149:LYS:HE3	71:v:40:ALA:HA	1.64	0.80
60:q:263:LYS:CE	60:q:439:PHE:CE2	2.65	0.80
30:HD:55:LYS:CD	49:PG:166:ASP:CB	2.53	0.80
36:DE:513:LEU:HD13	36:DE:513:LEU:H	1.45	0.80
39:DH:50:PHE:HZ	43:DJ:170:ALA:C	1.88	0.80
50:g:127:ARG:HH21	54:u:5:LEU:HB3	1.46	0.80
60:q:129:PRO:HB3	67:h:74:GLN:CD	2.05	0.80
72:p:15:LEU:HD11	72:p:453:SER:HB2	1.63	0.80
52:n:274:ILE:HD13	52:n:299:PHE:CE1	2.16	0.80
60:q:437:HIS:HE1	60:q:472:GLU:N	1.77	0.80
66:o:735:LEU:CD2	73:w:113:GLN:CD	2.54	0.80
12:DB:672:PHE:CZ	18:HC:413:LEU:CG	2.63	0.80
34:HH:266:GLN:N	34:HH:266:GLN:HE21	1.79	0.80
56:d:45:ILE:C	58:i:76:MET:HG2	2.07	0.80
67:h:139:GLN:NE2	68:k:37:LYS:HB2	1.97	0.80
6:DA:491:MET:HE2	6:DA:491:MET:H	1.45	0.80
40:Di:61:ALA:HA	41:DI:106:ARG:HG2	1.64	0.80
52:n:169:LEU:N	59:m:104:HIS:CD2	2.50	0.80
55:a:66:GLN:OE1	56:d:44:LEU:HD21	1.82	0.80
64:e:95:PHE:HB3	65:l:38:GLN:CG	2.12	0.80
37:DF:43:VAL:HG23	40:DI:46:TYR:CB	2.12	0.80
52:n:956:ALA:CB	52:n:1217:ARG:NH2	2.45	0.80
68:k:87:ARG:HA	71:v:105:LEU:HD13	1.62	0.80
55:a:462:LEU:CB	74:x:49:GLN:CB	2.58	0.80
7:EA:143:GLN:HE21	49:PG:158:PHE:HE1	1.30	0.80
35:DD:886:GLY:HA3	35:DD:891:ILE:HG13	1.62	0.80
47:HJ:177:ARG:NH1	47:HJ:177:ARG:HB2	1.97	0.80
52:n:960:LYS:HB2	52:n:1210:PHE:HE2	0.98	0.80
54:u:122:LEU:HG	56:d:111:GLN:HE21	1.46	0.80
35:DD:917:ILE:HG22	35:DD:1066:CYS:SG	2.22	0.79
52:n:203:LEU:CD1	52:n:215:LEU:HD12	2.11	0.79
55:a:321:LEU:HD21	55:a:407:ILE:HD12	1.63	0.79
60:q:395:PRO:HA	69:r:53:ASP:OD2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:462:LEU:CD1	74:x:60:ILE:CD1	2.61	0.79
67:h:182:VAL:HG21	69:r:202:ILE:HD11	1.63	0.79
12:DB:621:ALA:CB	18:HC:438:LYS:HE2	2.11	0.79
47:HJ:165:ARG:HB2	47:HJ:165:ARG:NH1	1.96	0.79
53:s:106:SER:C	53:s:108:PHE:H	1.87	0.79
55:a:462:LEU:CB	74:x:49:GLN:HG2	2.12	0.79
60:q:102:LEU:CD1	67:h:29:PHE:HE2	1.93	0.79
60:q:644:SER:O	64:e:97:GLN:HG2	1.82	0.79
30:HD:83:ASN:CG	30:HD:140:LEU:HD11	2.07	0.79
35:DD:960:GLU:HG3	35:DD:983:ARG:NH1	1.95	0.79
36:DE:694:LEU:HD13	36:DE:703:MET:HE1	0.81	0.79
12:DB:674:THR:CG2	18:HC:415:GLN:HG3	2.11	0.79
52:n:545:LEU:HD11	52:n:653:PRO:N	1.97	0.79
52:n:753:LEU:HD12	63:c:311:GLN:CG	2.12	0.79
56:d:42:ARG:NH2	58:i:96:GLU:OE2	2.14	0.79
67:h:146:MET:CE	68:k:45:LEU:HD12	2.12	0.79
37:DF:324:ASP:HA	37:DF:327:TRP:HB3	1.64	0.79
52:n:172:CYS:SG	60:q:21:GLU:HB2	2.22	0.79
69:r:191:GLU:OE2	71:v:8:PRO:HA	1.82	0.79
18:HC:352:GLN:NE2	33:HF:61:MET:HE1	1.98	0.79
30:HD:295:ARG:NH1	47:HJ:165:ARG:NH2	2.26	0.79
37:DF:43:VAL:HA	40:DI:46:TYR:CD2	2.17	0.79
52:n:169:LEU:CB	52:n:170:PRO:CD	2.59	0.79
54:u:80:GLU:HB2	61:z:563:VAL:HG21	1.64	0.79
55:a:449:ARG:CZ	74:x:54:PRO:HB2	2.11	0.79
56:d:45:ILE:HG12	58:i:73:ILE:CA	2.10	0.79
56:d:46:GLU:HA	58:i:76:MET:HE3	1.65	0.79
11:PA:902:GLU:OE2	11:PA:985:ARG:NH2	2.16	0.79
35:DD:1058:VAL:HG21	41:DL:76:LEU:HD23	1.64	0.79
36:DE:433:LYS:HE2	40:DI:110:TYR:CZ	2.18	0.79
55:a:445:LEU:HD22	74:x:55:SER:OG	1.82	0.79
60:q:460:ILE:HD12	60:q:529:MET:CE	2.13	0.79
68:k:70:LEU:HD21	71:v:85:PHE:HD1	1.45	0.79
36:DE:605:HIS:NE2	37:DF:77:LEU:HD21	1.98	0.79
40:DI:132:LEU:HG	43:DJ:121:MET:HE2	1.62	0.79
45:Dm:31:LEU:H	45:Dm:31:LEU:HD23	1.47	0.79
47:HJ:28:ARG:CZ	47:HJ:28:ARG:HB2	2.11	0.79
52:n:204:VAL:O	56:d:108:GLN:NE2	2.16	0.79
60:q:644:SER:HA	60:q:647:SER:OG	1.83	0.79
6:DA:638:PRO:HB3	38:DG:39:LEU:HD23	1.63	0.79
37:DF:105:TYR:O	43:DJ:217:PHE:CB	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:188:LEU:HD22	71:v:87:ILE:HG13	1.65	0.79
11:PA:1475:LEU:CD2	49:PG:66:VAL:HG22	1.99	0.78
37:DF:218:VAL:HG12	39:DH:162:THR:HB	1.63	0.78
47:HJ:239:LYS:H	47:HJ:239:LYS:NZ	1.80	0.78
60:q:186:GLU:HG3	60:q:243:LEU:HD22	1.41	0.78
39:DH:56:ALA:CB	43:DJ:214:PRO:CG	2.61	0.78
55:a:380:ALA:HB2	74:x:58:PRO:HG3	1.65	0.78
37:DF:361:LYS:HA	37:DF:364:VAL:HG22	1.65	0.78
56:d:42:ARG:NH2	58:i:93:LYS:HA	1.97	0.78
56:d:167:TRP:HZ3	59:m:106:GLN:NE2	1.81	0.78
60:q:647:SER:HB2	64:e:97:GLN:NE2	1.97	0.78
12:DB:621:ALA:CB	18:HC:438:LYS:CE	2.61	0.78
39:DH:50:PHE:HZ	43:DJ:170:ALA:HB3	1.48	0.78
48:PD:94:LYS:NZ	49:PG:3:TYR:OH	2.17	0.78
50:g:175:LEU:HD21	58:i:132:LEU:HD12	1.64	0.78
52:n:199:LEU:HD22	52:n:222:VAL:CG1	2.13	0.78
67:h:182:VAL:CG2	69:r:202:ILE:CD1	2.56	0.78
18:HC:348:ARG:CZ	33:HF:65:ALA:CB	2.62	0.78
30:HD:83:ASN:OD1	30:HD:140:LEU:CD1	2.31	0.78
36:DE:433:LYS:HD3	40:DI:110:TYR:CZ	2.19	0.78
37:DF:273:GLN:NE2	37:DF:273:GLN:H	1.81	0.78
52:n:359:ILE:HG12	52:n:372:ILE:HD13	1.64	0.78
56:d:115:LYS:HE2	56:d:115:LYS:CA	2.13	0.78
62:b:174:ILE:HD11	65:l:75:LEU:HD23	1.65	0.78
12:DB:645:ALA:HB2	18:HC:411:GLN:HB3	1.64	0.78
50:g:168:LEU:O	50:g:172:PRO:HD2	1.83	0.78
11:PA:22:GLN:NE2	11:PA:1446:GLY:O	2.17	0.78
12:DB:674:THR:CG2	18:HC:415:GLN:CG	2.61	0.78
35:DD:1060:LEU:HD13	41:DL:79:ASP:HB3	1.65	0.78
37:DF:71:ILE:CD1	40:DI:38:GLN:HE21	1.91	0.78
52:n:270:GLN:HB3	57:f:181:LEU:HD11	1.64	0.78
52:n:706:LEU:O	66:o:684:ARG:NH2	2.16	0.78
56:d:45:ILE:HD11	58:i:73:ILE:CG1	2.14	0.78
67:h:150:LEU:CD2	68:k:45:LEU:HD11	2.09	0.78
13:EB:120:MET:HA	13:EB:124:LEU:HD12	1.66	0.78
14:FB:179:ASP:OD1	35:DD:1002:ARG:NH2	2.16	0.78
39:DH:110:TYR:CD1	43:DJ:161:LYS:HD3	2.18	0.78
57:f:78:LEU:HD11	67:h:81:LEU:HD23	1.65	0.78
7:EA:139:LEU:HD11	49:PG:151:ARG:CG	2.13	0.78
20:DP:188:ARG:NH2	21:DQ:321:SER:OG	2.16	0.78
47:HJ:28:ARG:HB2	47:HJ:28:ARG:NH1	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:382:LEU:HD22	55:a:446:SER:CA	2.13	0.78
70:t:98:LEU:HB3	70:t:102:PHE:CD1	2.18	0.78
55:a:375:PHE:CG	74:x:17:ARG:NE	2.51	0.78
37:DF:323:VAL:O	37:DF:327:TRP:N	2.17	0.77
48:PD:76:ASN:OD1	67:h:47:ASP:HB3	1.83	0.77
52:n:224:PHE:CD2	52:n:292:MET:HE2	2.18	0.77
60:q:484:TYR:CD1	60:q:636:VAL:HG11	2.19	0.77
55:a:462:LEU:CG	74:x:49:GLN:CB	2.47	0.77
56:d:45:ILE:CG2	58:i:76:MET:HE2	2.12	0.77
66:o:639:TYR:CD2	72:p:786:HIS:HB2	2.17	0.77
68:k:37:LYS:H	68:k:37:LYS:CE	1.96	0.77
19:DO:1:MET:HB3	35:DD:997:ALA:HB1	1.67	0.77
39:DH:50:PHE:CZ	43:DJ:170:ALA:CB	2.67	0.77
36:De:747:LEU:HD23	36:De:747:LEU:H	1.47	0.77
52:n:209:PRO:HD2	52:n:289:LEU:HD12	1.67	0.77
52:n:941:TYR:CG	52:n:1172:SER:HB3	2.14	0.77
55:a:509:ARG:HB2	55:a:509:ARG:CZ	2.15	0.77
60:q:168:THR:OG1	68:k:21:ILE:CD1	2.31	0.77
62:b:178:LEU:HD11	65:l:78:LEU:HD13	1.64	0.77
14:FB:182:HIS:CD2	35:DD:998:GLN:OE1	2.38	0.77
35:DD:1063:LEU:HD12	41:DL:80:VAL:HG13	1.65	0.77
37:DF:274:ASN:ND2	37:DF:316:GLN:HA	1.99	0.77
51:j:35:ALA:CB	53:s:154:LEU:HD23	2.13	0.77
36:DE:433:LYS:CE	40:DI:110:TYR:OH	2.31	0.77
39:DH:44:LEU:HD21	43:DJ:129:THR:HG21	1.67	0.77
39:DH:121:ALA:HB1	43:DJ:133:ALA:HB3	1.65	0.77
52:n:678:PHE:HB2	60:q:555:VAL:HG21	1.66	0.77
60:q:149:LYS:HG3	71:v:42:ILE:HG13	1.64	0.77
60:q:263:LYS:HE2	60:q:439:PHE:HE2	1.43	0.77
52:n:957:PRO:HD3	52:n:1214:VAL:HG21	1.64	0.77
63:c:290:ASP:O	70:t:120:CYS:CB	2.33	0.77
32:HE:56:LYS:NZ	32:HE:143:TYR:OH	2.17	0.77
35:DD:961:GLN:NE2	36:DE:434:ASP:OD2	2.18	0.77
39:DH:50:PHE:CD1	43:DJ:195:LEU:HD13	2.18	0.77
52:n:359:ILE:CG2	52:n:372:ILE:CD1	2.62	0.77
55:a:504:ILE:HA	55:a:507:THR:HG23	1.67	0.77
61:z:543:LEU:HD23	61:z:545:ARG:HD3	1.65	0.77
19:DO:2:ALA:C	35:DD:1000:ARG:HD3	2.10	0.77
35:DD:1063:LEU:CD1	41:DL:80:VAL:HG13	2.15	0.77
56:d:167:TRP:CZ3	59:m:106:GLN:NE2	2.53	0.77
60:q:168:THR:OG1	68:k:21:ILE:CG2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PA:1643:TYR:HB2	59:m:96:PHE:CD2	2.19	0.77
52:n:168:ARG:HG3	59:m:104:HIS:HE1	0.96	0.77
56:d:42:ARG:NH2	58:i:96:GLU:CD	2.42	0.77
60:q:113:TYR:HB2	67:h:19:VAL:HG11	1.65	0.77
62:b:178:LEU:HD23	65:l:82:LEU:HD11	1.64	0.77
68:k:33:LEU:HA	68:k:36:SER:OG	1.85	0.77
9:HA:722:ARG:NH2	31:HG:202:SER:OG	2.18	0.77
12:DB:672:PHE:CE1	18:HC:414:SER:HB3	2.13	0.77
39:DH:56:ALA:CB	43:DJ:214:PRO:HG3	2.15	0.77
39:DH:108:PRO:CG	43:DJ:116:LEU:HD23	2.14	0.77
66:o:717:SER:HA	74:x:70:SER:HB2	1.67	0.77
11:PA:1173:THR:OG1	26:PI:56:ASN:OD1	2.03	0.76
19:DO:1:MET:HE1	35:DD:993:GLN:HB3	1.65	0.76
30:HD:298:GLN:HE22	46:HI:132:TRP:CD1	2.03	0.76
54:u:61:LEU:HA	54:u:64:ARG:HD3	1.66	0.76
18:HC:397:GLU:CG	33:HF:61:MET:HE3	2.15	0.76
40:DI:16:ALA:CA	40:DI:40:LEU:HD11	2.13	0.76
52:n:921:MET:HE1	52:n:1215:ILE:HD11	1.66	0.76
18:HC:352:GLN:HE21	33:HF:61:MET:HE1	1.50	0.76
37:DF:218:VAL:HG12	39:DH:162:THR:HG1	1.49	0.76
46:HI:171:HIS:CE1	46:HI:188:ARG:HA	2.20	0.76
52:n:944:PHE:HE2	62:b:101:ARG:HH22	1.32	0.76
56:d:45:ILE:CD1	58:i:72:ILE:C	2.56	0.76
60:q:186:GLU:HG2	60:q:243:LEU:HD22	1.58	0.76
35:DD:961:GLN:O	35:DD:965:ILE:HG12	1.84	0.76
60:q:458:PRO:CB	60:q:533:GLN:NE2	2.49	0.76
67:h:85:ARG:HA	67:h:99:VAL:HG12	1.67	0.76
68:k:88:LYS:HD2	68:k:88:LYS:O	1.85	0.76
48:PD:79:THR:CB	67:h:51:LEU:CD2	2.53	0.76
60:q:138:LYS:CB	60:q:140:ASN:OD1	2.28	0.76
62:b:174:ILE:CG1	65:l:75:LEU:HD11	2.14	0.76
37:DF:316:GLN:CD	37:DF:320:ARG:HG3	2.11	0.76
52:n:168:ARG:CG	59:m:104:HIS:NE2	2.44	0.76
55:a:337:ALA:HB1	55:a:338:PRO:CD	2.16	0.76
55:a:375:PHE:HB3	74:x:17:ARG:NH2	2.00	0.76
55:a:417:TYR:HE1	55:a:450:PHE:CE1	1.88	0.76
61:z:540:LEU:HB3	61:z:541:PRO:HD3	1.68	0.76
62:b:136:HIS:CD2	63:c:111:TYR:CG	2.73	0.76
37:DF:82:PRO:HB2	37:DF:98:SER:HB3	1.67	0.76
39:DH:49:GLY:O	43:DJ:171:LEU:HD13	1.84	0.76
39:DH:56:ALA:HB1	43:DJ:214:PRO:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:83:VAL:HG22	48:PD:137:LYS:HD2	1.68	0.76
62:b:175:HIS:HB2	63:c:113:TRP:HH2	1.48	0.76
37:DF:43:VAL:HA	40:DI:46:TYR:HD2	1.50	0.76
40:DI:81:GLN:NE2	41:DL:123:GLN:NE2	2.34	0.76
55:a:412:ARG:HB3	55:a:472:SER:HB3	1.67	0.76
37:DF:418:ILE:H	37:DF:418:ILE:HD12	1.50	0.76
55:a:109:TYR:OH	55:a:154:LEU:HD21	1.83	0.76
52:n:222:VAL:HG22	52:n:234:LEU:O	1.86	0.76
60:q:102:LEU:HD11	67:h:29:PHE:CD2	2.19	0.76
7:EA:181:ASN:ND2	30:HD:10:LYS:N	2.33	0.75
37:DF:217:SER:OG	39:DH:162:THR:N	2.19	0.75
37:DF:323:VAL:HA	37:DF:326:HIS:HD2	1.51	0.75
52:n:921:MET:HE1	52:n:1215:ILE:CD1	2.15	0.75
7:EA:181:ASN:HB3	30:HD:10:LYS:HG2	0.83	0.75
25:PH:2:ALA:O	25:PH:84:ARG:NH2	2.20	0.75
37:DF:104:LEU:HB3	43:DJ:217:PHE:CZ	2.21	0.75
40:DI:132:LEU:CD2	43:DJ:121:MET:CE	2.64	0.75
52:n:647:MET:CE	73:w:22:PHE:HB2	2.15	0.75
68:k:104:LEU:CD2	71:v:123:ILE:HD11	2.16	0.75
69:r:108:ILE:HD13	70:t:91:PHE:HA	1.66	0.75
70:t:172:ALA:HB1	70:t:173:PRO:CD	2.16	0.75
60:q:188:LEU:HD13	71:v:87:ILE:HG13	1.68	0.75
68:k:16:ASP:OD2	71:v:79:VAL:CG2	2.34	0.75
62:b:101:ARG:NH1	72:p:677:THR:HA	2.01	0.75
35:DD:1071:ARG:HB2	37:DF:91:PHE:CG	2.20	0.75
37:DF:241:GLU:OE2	39:DH:135:THR:OG1	2.05	0.75
52:n:270:GLN:HE22	57:f:174:ARG:HD2	1.50	0.75
60:q:120:ARG:HG2	60:q:120:ARG:NH1	1.98	0.75
60:q:186:GLU:OE2	60:q:291:TRP:HZ2	1.70	0.75
9:HA:711:ASP:OD1	9:HA:715:GLN:NE2	2.20	0.75
30:HD:300:ALA:HA	47:HJ:166:PRO:HG3	1.66	0.75
34:HH:371:VAL:HG23	34:HH:407:ILE:HG22	1.68	0.75
35:DD:874:LEU:HD23	35:DD:874:LEU:H	1.51	0.75
35:DD:1078:LEU:HD21	41:DL:83:MET:CE	2.14	0.75
39:DH:108:PRO:HG3	43:DJ:116:LEU:HD23	1.68	0.75
46:HI:169:TYR:HB3	46:HI:190:TYR:CE2	2.22	0.75
47:HJ:181:LEU:HD13	47:HJ:181:LEU:N	2.01	0.75
67:h:153:LYS:HE3	68:k:46:ASP:OD2	1.85	0.75
6:DA:396:LEU:H	6:DA:396:LEU:HD13	1.50	0.75
30:HD:85:ARG:HH22	30:HD:140:LEU:CA	1.98	0.75
52:n:960:LYS:HB3	52:n:1210:PHE:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:h:8:LEU:HA	67:h:69:PRO:HG3	1.68	0.75
11:PA:1242:ASP:HA	11:PA:1262:MET:HE2	1.68	0.75
30:HD:128:GLU:HB3	30:HD:133:ILE:HB	1.69	0.75
40:DI:132:LEU:CG	43:DJ:121:MET:CE	2.65	0.75
50:g:128:PRO:HB3	56:d:149:ILE:HD13	1.69	0.75
55:a:413:HIS:CD2	55:a:471:ASP:HA	2.22	0.75
57:f:64:VAL:HG11	57:f:88:SER:C	2.11	0.75
62:b:136:HIS:CB	63:c:111:TYR:CZ	2.70	0.75
30:HD:84:LYS:CA	30:HD:136:ASN:ND2	2.49	0.74
37:DF:274:ASN:HB2	37:DF:317:LEU:H	1.51	0.74
47:HJ:288:ASN:C	47:HJ:288:ASN:HD22	1.94	0.74
55:a:224:TYR:CE2	55:a:253:MET:HB3	2.21	0.74
56:d:45:ILE:HD11	58:i:73:ILE:CA	2.14	0.74
66:o:707:ILE:HG23	66:o:720:PRO:HA	1.69	0.74
68:k:101:ARG:HB3	68:k:101:ARG:CZ	2.16	0.74
36:DE:433:LYS:HE2	40:DI:110:TYR:OH	1.87	0.74
36:DE:605:HIS:CE1	37:DF:77:LEU:HD11	2.22	0.74
39:DH:114:SER:O	39:DH:116:ARG:N	2.20	0.74
60:q:134:ALA:N	67:h:72:ARG:NH1	2.33	0.74
50:g:127:ARG:HD2	52:n:152:PHE:HB2	1.69	0.74
52:n:359:ILE:HG13	52:n:372:ILE:HD11	1.64	0.74
56:d:164:PRO:HD2	56:d:167:TRP:CB	2.17	0.74
67:h:102:HIS:CD2	67:h:102:HIS:H	2.03	0.74
60:q:135:LEU:HD12	60:q:135:LEU:O	1.86	0.74
62:b:136:HIS:HB2	63:c:111:TYR:OH	1.88	0.74
16:Nf:297:LEU:O	16:Nf:302:GLY:HA2	1.86	0.74
39:DH:107:LEU:HD21	43:DJ:158:ALA:HB2	1.70	0.74
40:DI:132:LEU:CD2	43:DJ:121:MET:HE1	2.17	0.74
47:HJ:102:ARG:HG2	47:HJ:102:ARG:HH11	1.53	0.74
52:n:753:LEU:HD11	63:c:311:GLN:CA	2.15	0.74
37:DF:404:ARG:NH2	37:DF:452:PHE:O	2.21	0.74
57:f:145:TYR:CD2	67:h:43:PRO:HD3	2.21	0.74
64:e:129:VAL:CG2	68:k:114:MET:HE2	2.17	0.74
12:DB:674:THR:HG21	18:HC:415:GLN:HG3	1.66	0.74
36:DE:359:LEU:O	36:DE:359:LEU:HD12	1.87	0.74
46:HI:47:HIS:HA	46:HI:52:LYS:HG2	1.70	0.74
48:PD:87:LEU:HD11	48:PD:100:LEU:HD11	1.70	0.74
52:n:169:LEU:H	59:m:104:HIS:CE1	2.05	0.74
52:n:957:PRO:CD	52:n:1214:VAL:HG21	2.17	0.74
55:a:337:ALA:HB1	55:a:338:PRO:HD2	1.70	0.74
17:PB:59:VAL:HG21	17:PB:91:ILE:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:134:ILE:HD12	48:PD:137:LYS:HD3	1.69	0.74
52:n:904:PHE:CE2	52:n:1208:GLU:CD	2.58	0.74
55:a:364:TYR:CB	55:a:430:LEU:CG	2.64	0.74
62:b:136:HIS:HD2	63:c:111:TYR:CG	2.05	0.74
12:DB:672:PHE:HE1	18:HC:413:LEU:HG	0.62	0.74
18:HC:398:ARG:NH2	33:HF:58:GLY:HA2	2.02	0.74
36:DE:433:LYS:HD3	40:DI:110:TYR:HH	1.50	0.74
37:DF:63:ARG:O	37:DF:65:LYS:N	2.19	0.74
56:d:167:TRP:O	59:m:106:GLN:OE1	2.06	0.74
58:i:68:LEU:CD1	58:i:95:GLN:HG2	2.09	0.74
11:PA:1005:HIS:HD2	11:PA:1007:ILE:HG22	1.50	0.74
18:HC:348:ARG:HD3	33:HF:66:PHE:O	1.87	0.74
55:a:364:TYR:HB3	55:a:430:LEU:HG	1.66	0.74
56:d:123:THR:CG2	60:q:37:SER:HB3	2.18	0.74
60:q:34:LEU:N	60:q:34:LEU:HD23	2.01	0.74
70:t:131:MET:HB2	70:t:136:ARG:HD2	1.67	0.74
30:HD:287:TYR:CG	30:HD:287:TYR:O	2.40	0.73
56:d:126:TYR:CD2	60:q:36:MET:SD	2.81	0.73
57:f:101:ILE:HD11	67:h:105:VAL:HG11	1.70	0.73
59:m:124:GLN:HB2	61:z:590:ARG:HD2	1.68	0.73
70:t:8:GLN:HE22	70:t:200:ILE:HG23	1.52	0.73
41:DL:61:LYS:O	41:DL:61:LYS:NZ	2.21	0.73
47:HJ:175:LYS:N	47:HJ:175:LYS:HZ2	1.85	0.73
55:a:412:ARG:HB3	55:a:472:SER:CB	2.18	0.73
60:q:481:SER:HB2	60:q:636:VAL:HG21	1.70	0.73
63:c:135:ARG:NH2	64:e:92:GLU:OE1	2.21	0.73
2:Y:29:DA:OP1	21:DQ:346:LYS:NZ	2.20	0.73
18:HC:398:ARG:HH22	33:HF:58:GLY:CA	2.01	0.73
41:DL:111:LEU:HA	41:DL:114:LYS:HZ1	1.52	0.73
56:d:126:TYR:CZ	60:q:36:MET:HB2	2.23	0.73
68:k:70:LEU:HD21	71:v:85:PHE:CD1	2.22	0.73
42:Dc:77:LEU:HD12	43:Dj:116:LEU:HD23	1.68	0.73
67:h:85:ARG:HA	67:h:99:VAL:CG1	2.18	0.73
11:PA:279:LYS:O	11:PA:283:ILE:HD12	1.88	0.73
52:n:937:ARG:NE	52:n:943:LEU:HD21	2.03	0.73
56:d:45:ILE:CG1	58:i:73:ILE:CG1	2.66	0.73
58:i:75:CYS:CB	58:i:88:ASN:ND2	2.50	0.73
37:DF:214:HIS:CE1	37:DF:216:LEU:HB2	2.23	0.73
37:DF:274:ASN:HB2	37:DF:317:LEU:CD2	2.16	0.73
53:s:104:LYS:HB2	53:s:106:SER:O	1.88	0.73
46:HI:95:GLU:H	46:HI:146:ASP:HA	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:g:171:LEU:HD21	56:d:110:LEU:HG	1.69	0.73
58:i:72:ILE:HD11	58:i:92:SER:CB	2.18	0.73
68:k:101:ARG:HB3	68:k:101:ARG:NH1	2.02	0.73
9:HA:231:VAL:HG13	9:HA:454:VAL:HG23	1.70	0.73
11:PA:869:GLU:OE1	11:PA:1455:SER:OG	2.07	0.73
36:DE:605:HIS:CE1	37:DF:77:LEU:HD21	2.23	0.73
37:DF:279:LEU:HB2	37:DF:330:ARG:NH2	2.04	0.73
49:PG:21:ASN:O	49:PG:25:THR:OG1	2.05	0.73
52:n:301:LEU:HD13	52:n:361:ILE:HD12	1.68	0.73
54:u:73:ILE:HA	54:u:76:LEU:HB3	1.71	0.73
56:d:45:ILE:C	58:i:76:MET:HE3	2.13	0.73
60:q:395:PRO:HA	69:r:53:ASP:CG	2.14	0.73
60:q:544:MET:SD	60:q:640:GLU:HG2	2.28	0.73
60:q:645:ALA:HB2	64:e:100:LEU:HD21	1.69	0.73
37:DF:68:THR:O	37:DF:68:THR:HG22	1.86	0.73
52:n:154:ILE:HB	52:n:155:PRO:HD3	1.69	0.73
52:n:169:LEU:HD22	59:m:101:GLN:HA	1.71	0.73
52:n:956:ALA:HB1	52:n:1217:ARG:HH22	1.52	0.73
55:a:417:TYR:CZ	55:a:450:PHE:CD1	2.77	0.73
55:a:462:LEU:CB	74:x:49:GLN:CG	2.65	0.73
57:f:95:LEU:C	60:q:130:VAL:HG11	2.14	0.73
60:q:184:ASN:CG	71:v:83:LYS:HD2	2.14	0.73
7:EA:178:ALA:HA	30:HD:8:ARG:O	1.89	0.73
36:DE:429:LEU:HB3	36:DE:430:PRO:CD	2.16	0.73
39:DH:156:PRO:O	39:DH:160:ILE:HB	1.88	0.73
52:n:545:LEU:CD1	52:n:653:PRO:N	2.50	0.73
57:f:95:LEU:O	60:q:130:VAL:CG1	2.37	0.73
60:q:109:MET:CA	60:q:109:MET:HE3	2.19	0.73
60:q:428:LEU:HD12	60:q:428:LEU:O	1.89	0.73
41:DL:71:ASP:CB	41:DL:74:GLU:HG3	2.19	0.72
51:j:82:LYS:NZ	53:s:101:VAL:HG12	2.04	0.72
52:n:652:MET:HE1	73:w:18:ILE:HG23	1.71	0.72
70:t:122:PHE:CZ	70:t:156:LEU:HD11	2.24	0.72
56:d:38:GLU:OE2	58:i:99:LYS:HD2	1.89	0.72
70:t:172:ALA:HB1	70:t:173:PRO:HD2	1.69	0.72
50:g:134:THR:HB	61:z:597:VAL:HG13	1.71	0.72
37:DF:241:GLU:CD	39:DH:135:THR:OG1	2.32	0.72
37:DF:428:LEU:CD1	37:DF:455:LEU:CB	2.64	0.72
37:DF:429:LYS:O	37:DF:433:PRO:HD2	1.89	0.72
47:HJ:167:PHE:O	47:HJ:167:PHE:HD1	1.72	0.72
52:n:237:MET:HE1	60:q:45:GLN:CA	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:482:VAL:HG22	52:n:489:ILE:HG12	1.70	0.72
11:PA:1481:LYS:HE3	49:PG:22:LEU:CD2	2.20	0.72
12:DB:672:PHE:CZ	18:HC:413:LEU:CB	2.72	0.72
30:HD:85:ARG:NH2	30:HD:139:LYS:O	2.23	0.72
48:PD:74:PHE:HE1	48:PD:137:LYS:HB2	1.54	0.72
52:n:266:VAL:HG22	57:f:177:VAL:CG1	2.19	0.72
56:d:42:ARG:NH2	58:i:93:LYS:HG2	2.04	0.72
56:d:46:GLU:CA	58:i:76:MET:HE3	2.20	0.72
60:q:479:ILE:O	60:q:532:HIS:ND1	2.22	0.72
30:HD:23:VAL:HG21	30:HD:73:GLU:HG3	1.71	0.72
32:HE:160:ARG:NH2	32:HE:234:ASP:OD1	2.23	0.72
33:HF:24:ASP:OD1	33:HF:25:GLU:N	2.22	0.72
36:DE:433:LYS:CE	40:DI:110:TYR:CE1	2.73	0.72
37:DF:279:LEU:HB2	37:DF:330:ARG:HH21	1.53	0.72
52:n:359:ILE:HA	52:n:372:ILE:CD1	2.19	0.72
54:u:90:LEU:CB	60:q:9:ILE:HG12	2.19	0.72
55:a:467:MET:HE2	55:a:504:ILE:HD11	1.70	0.72
58:i:72:ILE:HD13	58:i:92:SER:HB3	1.72	0.72
60:q:123:LYS:NZ	67:h:88:ASP:OD2	2.23	0.72
41:DL:60:LYS:O	41:DL:60:LYS:NZ	2.18	0.72
63:c:288:LEU:CD1	70:t:122:PHE:CZ	2.72	0.72
30:HD:145:GLU:CD	67:h:67:LYS:HE2	2.14	0.72
30:HD:300:ALA:HB1	47:HJ:166:PRO:HA	1.67	0.72
52:n:707:ASP:HB2	66:o:684:ARG:NH2	2.04	0.72
52:n:941:TYR:CE2	52:n:1172:SER:OG	2.43	0.72
54:u:90:LEU:HD22	60:q:9:ILE:HD11	0.75	0.72
55:a:417:TYR:CE1	55:a:450:PHE:HE1	2.00	0.72
60:q:168:THR:HG1	68:k:21:ILE:HG21	1.51	0.72
60:q:184:ASN:CG	71:v:83:LYS:CD	2.63	0.72
61:z:567:GLN:O	61:z:567:GLN:NE2	2.23	0.72
70:t:8:GLN:NE2	70:t:200:ILE:HG23	2.04	0.72
52:n:250:LEU:HG	52:n:275:HIS:HB2	1.71	0.72
56:d:38:GLU:CD	58:i:96:GLU:CG	2.61	0.72
62:b:136:HIS:HB2	63:c:111:TYR:CZ	2.25	0.72
63:c:305:PHE:HB3	63:c:311:GLN:CD	2.14	0.72
70:t:6:VAL:HG22	70:t:141:GLU:HB2	1.71	0.72
7:EA:17:LEU:HD22	7:EA:194:THR:CG2	2.19	0.72
7:EA:181:ASN:ND2	30:HD:9:CYS:HA	2.05	0.72
41:DI:102:LEU:HA	41:DI:105:HIS:HD2	1.55	0.72
52:n:168:ARG:HG3	59:m:104:HIS:NE2	1.99	0.72
52:n:234:LEU:HD21	52:n:282:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:d:45:ILE:HD13	58:i:73:ILE:N	2.00	0.72
60:q:102:LEU:CD1	67:h:29:PHE:CD2	2.72	0.72
11:PA:322:LEU:O	11:PA:327:ARG:NH2	2.23	0.71
47:HJ:207:TYR:HB3	47:HJ:211:GLN:HE22	1.55	0.71
48:PD:67:TYR:OH	49:PG:86:ASP:OD1	2.06	0.71
52:n:206:THR:HG22	52:n:289:LEU:HB2	1.71	0.71
52:n:261:ASP:OD1	60:q:250:ASP:OD2	2.06	0.71
52:n:960:LYS:CG	52:n:1210:PHE:CE2	2.72	0.71
60:q:418:ILE:HD13	70:t:72:PRO:HG2	1.72	0.71
71:v:119:LEU:C	71:v:119:LEU:HD12	2.15	0.71
20:DP:185:LEU:CD2	35:DD:1006:LEU:HD13	2.20	0.71
36:DE:433:LYS:CE	40:DI:110:TYR:CZ	2.73	0.71
37:DF:218:VAL:CG1	39:DH:162:THR:HG21	2.18	0.71
47:HJ:239:LYS:HZ2	47:HJ:239:LYS:N	1.85	0.71
50:g:73:ASP:CG	61:z:535:SER:HB2	2.14	0.71
50:g:128:PRO:CB	56:d:149:ILE:HD13	2.20	0.71
52:n:192:LEU:CB	52:n:219:ASN:O	2.38	0.71
56:d:110:LEU:HD22	56:d:110:LEU:C	2.14	0.71
58:i:110:SER:HB2	58:i:111:PRO:HD2	1.72	0.71
60:q:263:LYS:CE	60:q:439:PHE:HE2	2.02	0.71
60:q:595:GLN:HG2	60:q:619:ARG:HB2	1.70	0.71
68:k:87:ARG:HG3	68:k:87:ARG:NH1	2.01	0.71
74:x:566:GLU:C	74:x:568:LYS:H	1.98	0.71
47:HJ:236:LEU:O	47:HJ:238:LEU:N	2.22	0.71
55:a:109:TYR:CZ	55:a:154:LEU:CD2	2.72	0.71
56:d:31:LEU:CD2	58:i:103:THR:CB	2.67	0.71
68:k:86:SER:C	71:v:105:LEU:HD13	2.14	0.71
73:w:510:PRO:HD3	73:w:922:MET:HE1	1.71	0.71
12:DB:241:PRO:HG2	12:DB:496:MET:HE1	1.72	0.71
32:HE:67:SER:O	32:HE:139:LYS:NZ	2.24	0.71
52:n:172:CYS:SG	60:q:21:GLU:CA	2.78	0.71
55:a:56:GLN:NE2	56:d:51:SER:O	2.22	0.71
56:d:168:VAL:HB	56:d:169:PRO:CD	2.20	0.71
60:q:112:LEU:CD2	67:h:19:VAL:HG21	2.20	0.71
60:q:212:ALA:HB1	60:q:380:ARG:NH2	2.04	0.71
60:q:437:HIS:CE1	60:q:472:GLU:CA	2.71	0.71
60:q:481:SER:HB2	60:q:636:VAL:CG2	2.20	0.71
18:HC:408:LEU:HD21	33:HF:36:GLN:CD	2.16	0.71
30:HD:55:LYS:CE	49:PG:166:ASP:OD2	2.27	0.71
33:HF:36:GLN:HE21	33:HF:38:ILE:HG13	1.54	0.71
52:n:274:ILE:CD1	52:n:299:PHE:CE1	2.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:115:LEU:CA	56:d:121:LEU:HD12	2.21	0.71
60:q:263:LYS:HE2	60:q:439:PHE:CZ	2.25	0.71
67:h:22:LEU:HD12	67:h:22:LEU:C	2.13	0.71
32:HE:272:LEU:O	32:HE:272:LEU:HD23	1.90	0.71
56:d:154:ARG:NH2	59:m:66:TYR:O	2.23	0.71
61:z:529:HIS:HE1	61:z:580:ILE:HG21	1.56	0.71
55:a:383:PRO:HG3	74:x:92:LEU:CD2	2.19	0.71
55:a:462:LEU:CD1	74:x:60:ILE:HD11	2.21	0.71
56:d:42:ARG:HH22	58:i:93:LYS:CA	2.03	0.71
70:t:129:VAL:HG21	70:t:200:ILE:CD1	2.17	0.71
71:v:120:ARG:HG2	71:v:120:ARG:HH11	1.56	0.71
30:HD:289:SER:O	30:HD:292:ALA:HB3	1.90	0.71
60:q:152:SER:CB	71:v:58:ASN:HA	2.09	0.71
6:DA:357:GLU:HG3	6:DA:497:PRO:HB3	1.73	0.71
37:DF:22:VAL:HG13	40:DI:44:PHE:CE1	2.25	0.71
40:DI:73:LEU:HD13	41:DI:105:HIS:NE2	2.05	0.71
46:HI:263:ALA:HB3	57:f:48:GLU:HG3	1.72	0.70
52:n:104:LYS:HZ2	53:s:108:PHE:HA	1.54	0.70
52:n:237:MET:CE	60:q:45:GLN:HB2	2.21	0.70
55:a:465:VAL:HG21	55:a:511:ILE:HD13	1.73	0.70
58:i:122:ARG:C	58:i:122:ARG:HD3	2.15	0.70
6:DA:489:GLN:HB2	37:Df:315:ARG:HH11	1.56	0.70
52:n:270:GLN:CA	57:f:181:LEU:HD11	2.20	0.70
60:q:109:MET:HE3	60:q:109:MET:HA	1.74	0.70
37:DF:104:LEU:CD1	43:DJ:217:PHE:HE2	2.04	0.70
52:n:101:ALA:HB2	53:s:109:LEU:HD21	1.73	0.70
52:n:168:ARG:HD2	59:m:104:HIS:NE2	2.04	0.70
55:a:214:ARG:CZ	55:a:214:ARG:HB2	2.21	0.70
55:a:462:LEU:N	74:x:49:GLN:CD	2.43	0.70
56:d:103:ARG:HG2	56:d:103:ARG:NH1	2.05	0.70
60:q:116:LEU:HB3	67:h:16:LEU:CD2	2.22	0.70
60:q:134:ALA:N	67:h:72:ARG:HH12	1.87	0.70
13:EB:82:VAL:HG12	13:EB:86:LYS:NZ	2.06	0.70
52:n:229:GLU:C	52:n:253:LEU:HB2	2.15	0.70
52:n:686:LYS:HZ3	66:o:730:PRO:HB3	1.55	0.70
60:q:171:VAL:CG2	68:k:17:ILE:HG23	2.06	0.70
60:q:190:LEU:HD12	60:q:196:LEU:HD11	1.73	0.70
60:q:206:ASP:O	68:k:84:TYR:OH	2.08	0.70
60:q:437:HIS:CE1	60:q:472:GLU:C	2.69	0.70
60:q:630:MET:HE3	60:q:631:GLU:H	1.55	0.70
67:h:12:LEU:C	67:h:12:LEU:HD13	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:HD:287:TYR:CG	46:HI:189:MET:SD	2.84	0.70
52:n:295:CYS:SG	57:f:188:PHE:CE2	2.84	0.70
60:q:106:LEU:HD23	60:q:106:LEU:C	2.15	0.70
30:HD:254:GLU:CD	30:HD:254:GLU:H	1.99	0.70
30:HD:287:TYR:CD1	30:HD:287:TYR:O	2.45	0.70
41:DL:114:LYS:O	41:DL:118:LEU:HG	1.91	0.70
55:a:441:GLU:HG2	55:a:453:SER:OG	1.90	0.70
64:e:95:PHE:CE1	65:l:37:GLY:HA3	2.26	0.70
52:n:169:LEU:CA	59:m:104:HIS:CG	2.68	0.70
60:q:491:ILE:HD12	60:q:532:HIS:CA	2.21	0.70
66:o:633:VAL:HG11	72:p:810:PRO:CB	1.87	0.70
35:DD:950:LEU:C	35:DD:950:LEU:HD13	2.16	0.70
37:DF:81:GLU:OE2	37:DF:91:PHE:HD1	1.75	0.70
47:HJ:174:LEU:HD13	47:HJ:231:TYR:HE2	1.56	0.70
52:n:960:LYS:HZ1	52:n:1185:LEU:HD13	1.55	0.70
55:a:388:LEU:HD21	55:a:447:GLU:HG3	1.72	0.70
60:q:147:ILE:HG21	67:h:124:LEU:HD22	1.72	0.70
60:q:458:PRO:CG	60:q:533:GLN:NE2	2.24	0.70
71:v:119:LEU:HD12	71:v:119:LEU:O	1.91	0.70
1:X:-5:DT:H3	2:Y:5:DA:H61	1.38	0.70
30:HD:120:LYS:O	30:HD:124:ILE:HD12	1.91	0.70
55:a:160:LEU:CD1	55:a:214:ARG:HH21	2.03	0.70
60:q:149:LYS:HE2	71:v:40:ALA:CA	2.20	0.70
60:q:644:SER:HB3	64:e:96:LEU:HB3	1.74	0.70
39:DH:110:TYR:OH	43:DJ:160:GLN:HB3	1.92	0.70
46:HI:111:PRO:HG3	57:f:63:MET:HE3	1.74	0.70
60:q:187:LEU:CD2	71:v:84:GLN:HG2	2.22	0.70
5:BA:23:LEU:HD12	5:BA:32:MET:HE2	1.74	0.69
47:HJ:82:THR:HG23	47:HJ:160:VAL:HG11	1.73	0.69
55:a:445:LEU:CD1	74:x:55:SER:CA	2.59	0.69
71:v:120:ARG:HG2	71:v:120:ARG:NH1	2.05	0.69
75:y:170:VAL:HG22	75:y:198:ALA:HB2	1.74	0.69
9:HA:252:THR:HG22	9:HA:432:ILE:HG22	1.74	0.69
17:PB:254:GLN:OE1	17:PB:254:GLN:N	2.24	0.69
22:PC:193:ARG:NH2	22:PC:218:ALA:O	2.25	0.69
44:Dk:191:VAL:HG13	44:Dk:200:ILE:HD13	1.74	0.69
50:g:159:ARG:O	50:g:159:ARG:HD3	1.93	0.69
55:a:109:TYR:OH	55:a:154:LEU:CD2	2.40	0.69
55:a:223:LYS:HZ1	55:a:251:LEU:C	2.00	0.69
18:HC:397:GLU:CD	33:HF:61:MET:CG	2.62	0.69
50:g:79:ARG:HH21	54:u:74:ASP:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EA:20:TYR:CD2	7:EA:190:LEU:HD11	2.26	0.69
51:j:43:PHE:CB	53:s:144:ILE:HG23	2.22	0.69
52:n:97:VAL:HG22	53:s:109:LEU:HG	1.74	0.69
55:a:145:LYS:HA	55:a:145:LYS:HE3	1.74	0.69
55:a:259:ILE:HD12	55:a:259:ILE:H	1.56	0.69
60:q:113:TYR:HB2	67:h:19:VAL:HG12	1.75	0.69
60:q:212:ALA:HB1	60:q:380:ARG:HH22	1.56	0.69
11:PA:1248:ASN:ND2	11:PA:1254:LYS:O	2.26	0.69
12:DB:762:ASP:OD1	12:DB:768:PRO:CG	2.38	0.69
13:EB:84:TYR:OH	13:EB:105:GLU:OE1	2.05	0.69
34:HH:611:GLY:O	34:HH:642:ARG:NH2	2.26	0.69
47:HJ:64:LEU:HD13	47:HJ:105:MET:HB3	1.73	0.69
54:u:67:LYS:HE3	61:z:528:LEU:HD22	1.74	0.69
55:a:131:ASN:ND2	55:a:131:ASN:H	1.90	0.69
55:a:364:TYR:HB3	55:a:430:LEU:HD11	1.71	0.69
64:e:95:PHE:CB	65:l:38:GLN:HG2	2.22	0.69
9:HA:637:LEU:HD11	9:HA:648:GLU:HA	1.74	0.69
30:HD:55:LYS:HE2	49:PG:166:ASP:CB	2.22	0.69
60:q:481:SER:CB	60:q:636:VAL:CG2	2.71	0.69
65:l:167:ILE:HD11	71:v:123:ILE:HG22	1.75	0.69
30:HD:55:LYS:HG3	49:PG:166:ASP:N	2.06	0.69
40:DI:20:ALA:HB2	40:DI:36:ILE:HD13	1.73	0.69
6:DA:571:GLU:CD	6:DA:571:GLU:H	2.00	0.69
24:PF:100:ARG:NH2	24:PF:121:ASP:O	2.26	0.69
30:HD:85:ARG:NH1	30:HD:140:LEU:CG	2.45	0.69
30:HD:262:GLU:HA	30:HD:294:HIS:CE1	2.28	0.69
30:HD:287:TYR:HB3	46:HI:189:MET:HG2	1.73	0.69
34:HH:191:ASP:O	34:HH:195:ARG:NH1	2.25	0.69
35:DD:1078:LEU:CD2	41:DL:83:MET:HE1	2.23	0.69
56:d:164:PRO:HD2	56:d:167:TRP:HB2	1.74	0.69
57:f:115:ILE:HG23	60:q:112:LEU:HD11	1.74	0.69
66:o:639:TYR:HD2	72:p:786:HIS:CG	2.03	0.69
67:h:8:LEU:C	67:h:8:LEU:HD23	2.18	0.69
12:DB:618:ALA:HB1	18:HC:439:ARG:NH2	2.07	0.69
36:DE:605:HIS:ND1	37:DF:77:LEU:HD11	2.08	0.69
52:n:229:GLU:HB3	52:n:300:CYS:SG	2.33	0.69
52:n:591:PHE:HB3	73:w:26:PHE:HD1	1.58	0.69
56:d:42:ARG:NH2	58:i:93:LYS:CA	2.55	0.69
57:f:15:TRP:HH2	57:f:35:GLU:OE1	1.72	0.69
60:q:112:LEU:HD23	67:h:19:VAL:HG21	1.73	0.69
62:b:136:HIS:CB	63:c:111:TYR:OH	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p:13:MET:CG	72:p:405:PHE:HB2	2.22	0.69
9:HA:382:LEU:O	9:HA:385:THR:OG1	2.11	0.69
11:PA:373:LEU:O	11:PA:485:ASN:ND2	2.25	0.69
11:PA:1477:ALA:HB1	49:PG:22:LEU:HD11	1.75	0.69
41:DL:99:ALA:HB1	41:DL:115:ASP:HB3	1.75	0.69
55:a:336:TYR:CZ	55:a:391:THR:OG1	2.45	0.69
56:d:76:PHE:HZ	58:i:65:PHE:HE2	1.26	0.69
60:q:187:LEU:O	60:q:187:LEU:HD12	1.93	0.69
63:c:305:PHE:CD1	63:c:311:GLN:HG2	2.28	0.69
63:c:309:CYS:O	63:c:311:GLN:CG	2.41	0.69
39:DH:56:ALA:HB2	43:DJ:214:PRO:CG	2.24	0.68
57:f:95:LEU:C	60:q:130:VAL:CG1	2.67	0.68
60:q:168:THR:HG1	68:k:21:ILE:HD12	1.55	0.68
60:q:171:VAL:HG22	68:k:17:ILE:HD13	1.75	0.68
61:z:529:HIS:CE1	61:z:580:ILE:HG21	2.27	0.68
40:DI:28:ILE:CG2	40:DI:31:TYR:CD1	2.76	0.68
37:Df:447:ALA:CA	37:Df:456:GLY:HA3	2.23	0.68
52:n:237:MET:HE1	60:q:45:GLN:HA	1.76	0.68
56:d:45:ILE:HG23	58:i:76:MET:CG	2.22	0.68
19:DO:1:MET:CB	35:DD:997:ALA:CB	2.71	0.68
30:HD:295:ARG:HA	46:HI:132:TRP:NE1	2.08	0.68
52:n:169:LEU:N	59:m:104:HIS:NE2	2.33	0.68
52:n:245:TRP:CB	52:n:282:LEU:CD1	2.57	0.68
55:a:374:TYR:HA	55:a:440:PHE:O	1.93	0.68
56:d:64:GLN:HE21	56:d:68:LEU:HD12	1.58	0.68
60:q:299:GLN:OE1	68:k:87:ARG:NH2	2.25	0.68
63:c:291:GLY:HA3	70:t:120:CYS:HB3	1.74	0.68
65:l:156:LEU:HD22	71:v:134:TYR:HB2	1.75	0.68
39:DH:44:LEU:CD2	43:DJ:129:THR:HG21	2.23	0.68
46:HI:241:CYS:HA	46:HI:246:TYR:CD2	2.28	0.68
47:HJ:60:TYR:CB	47:HJ:105:MET:HE1	2.24	0.68
50:g:172:PRO:HA	50:g:175:LEU:HG	1.75	0.68
52:n:359:ILE:HG23	52:n:372:ILE:HD13	1.74	0.68
56:d:41:SER:HB2	58:i:69:VAL:CG1	2.19	0.68
60:q:149:LYS:HD2	71:v:40:ALA:O	1.93	0.68
67:h:14:ALA:HB1	67:h:63:LEU:HD11	1.76	0.68
6:DA:480:TRP:HB2	37:Df:306:PRO:HG3	1.74	0.68
17:PB:777:ASN:O	27:PJ:47:ARG:NH1	2.27	0.68
18:HC:29:GLY:O	18:HC:33:ARG:NE	2.24	0.68
36:DE:426:ARG:HH11	36:DE:640:ASN:HD22	1.41	0.68
39:DH:50:PHE:CG	43:DJ:195:LEU:HB2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:60:ALA:O	54:u:64:ARG:HG3	1.93	0.68
55:a:375:PHE:CE2	74:x:17:ARG:NE	2.45	0.68
64:e:49:GLU:CG	65:l:89:PHE:CE1	2.76	0.68
70:t:8:GLN:HA	70:t:138:ILE:O	1.94	0.68
71:v:10:SER:HB2	71:v:11:LYS:HE2	1.75	0.68
6:DA:410:TRP:HH2	37:DF:351:ILE:HA	1.59	0.68
37:DF:329:LEU:HD23	37:DF:329:LEU:O	1.93	0.68
52:n:305:LEU:HD11	52:n:361:ILE:HG12	1.75	0.68
60:q:184:ASN:OD1	71:v:83:LYS:HD2	1.93	0.68
15:HB:468:VAL:HG21	15:HB:525:ILE:HD11	1.74	0.68
18:HC:60:LEU:HD13	18:HC:118:LEU:HD23	1.76	0.68
40:DI:23:LEU:CD2	40:DI:39:MET:HE1	2.23	0.68
47:HJ:175:LYS:HZ2	47:HJ:175:LYS:CA	2.07	0.68
52:n:545:LEU:HD11	52:n:653:PRO:CA	2.24	0.68
54:u:125:ILE:CG1	58:i:135:TYR:CE2	2.77	0.68
55:a:219:LEU:HD13	55:a:258:THR:HB	1.75	0.68
55:a:382:LEU:CD2	55:a:446:SER:HA	2.23	0.68
66:o:735:LEU:HD21	73:w:113:GLN:OE1	1.94	0.68
67:h:147:CYS:SG	71:v:41:LYS:CD	2.81	0.68
7:EA:174:ARG:CG	30:HD:8:ARG:HH22	1.81	0.68
50:g:79:ARG:NH2	54:u:74:ASP:HA	2.09	0.68
52:n:937:ARG:HE	52:n:943:LEU:CD2	2.07	0.68
56:d:71:HIS:CE1	56:d:72:ARG:HD3	2.29	0.68
37:DF:83:LEU:HD12	37:DF:98:SER:HA	1.75	0.68
37:DF:329:LEU:HD23	37:DF:329:LEU:C	2.19	0.68
51:j:92:ASN:HD21	53:s:82:ASN:HA	1.58	0.68
52:n:250:LEU:HD23	52:n:275:HIS:CD2	2.00	0.68
55:a:466:VAL:HG21	74:x:54:PRO:HG3	1.75	0.68
58:i:136:LYS:HE2	58:i:136:LYS:O	1.94	0.68
60:q:15:CYS:SG	60:q:15:CYS:O	2.52	0.68
11:PA:1481:LYS:HE3	49:PG:22:LEU:HD22	1.74	0.67
36:DE:773:TYR:OH	37:DF:140:GLY:HA2	1.94	0.67
39:DH:50:PHE:HE2	43:DJ:170:ALA:O	1.77	0.67
46:HI:191:GLY:C	46:HI:193:GLY:H	2.02	0.67
49:PG:97:LEU:HD23	49:PG:113:ILE:HD11	1.75	0.67
52:n:192:LEU:HD12	52:n:219:ASN:C	2.19	0.67
52:n:685:LEU:HD22	66:o:729:TYR:HE2	1.60	0.67
55:a:62:LEU:HG	56:d:62:GLU:N	2.09	0.67
55:a:211:LEU:HD13	55:a:222:LEU:HD23	1.76	0.67
63:c:183:PRO:HD2	63:c:189:MET:HE2	1.76	0.67
68:k:87:ARG:CA	71:v:105:LEU:HD13	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:PC:109:GLU:OE1	22:PC:109:GLU:N	2.28	0.67
37:DF:317:LEU:H	37:DF:317:LEU:HD22	1.59	0.67
37:DF:361:LYS:HA	37:DF:364:VAL:CG2	2.25	0.67
41:DL:71:ASP:CB	41:DL:74:GLU:CD	2.66	0.67
52:n:937:ARG:HE	52:n:943:LEU:HD21	1.57	0.67
60:q:31:LEU:N	60:q:32:PRO:HD2	2.09	0.67
68:k:86:SER:O	71:v:105:LEU:HD13	1.95	0.67
9:HA:72:TYR:OH	9:HA:234:ASP:OD2	2.12	0.67
11:PA:1794:SER:HB2	11:PA:1795:PRO:HD3	1.77	0.67
31:HG:88:LEU:CD2	31:HG:131:LEU:HD21	2.25	0.67
51:j:17:GLU:CB	53:s:112:LEU:HD11	2.24	0.67
52:n:960:LYS:CB	52:n:1210:PHE:CD2	2.76	0.67
55:a:70:LYS:CA	58:i:70:HIS:CE1	2.77	0.67
55:a:364:TYR:HB2	55:a:430:LEU:HG	1.76	0.67
64:e:132:HIS:HD2	71:v:126:ASP:OD2	1.77	0.67
68:k:45:LEU:HD22	68:k:45:LEU:C	2.19	0.67
70:t:122:PHE:HZ	70:t:156:LEU:HD11	1.57	0.67
71:v:130:LEU:N	71:v:130:LEU:HD23	2.08	0.67
7:EA:122:THR:CG2	30:HD:40:VAL:HG23	2.20	0.67
11:PA:1475:LEU:HD21	49:PG:18:PHE:CE2	2.29	0.67
40:DI:132:LEU:CG	43:DJ:121:MET:SD	2.82	0.67
52:n:634:MET:HE2	60:q:519:GLN:NE2	2.10	0.67
52:n:815:THR:HG21	52:n:841:ASN:HB3	1.75	0.67
52:n:861:LYS:CE	63:c:30:ARG:HE	2.01	0.67
55:a:367:LEU:HD13	55:a:509:ARG:NH1	2.08	0.67
60:q:186:GLU:CB	60:q:243:LEU:HD22	2.25	0.67
60:q:644:SER:HB3	64:e:96:LEU:CB	2.25	0.67
63:c:292:LEU:HG	70:t:120:CYS:SG	2.35	0.67
68:k:70:LEU:HG	71:v:82:LEU:CD2	2.24	0.67
7:EA:139:LEU:HD21	49:PG:151:ARG:HG2	1.75	0.67
17:PB:814:TYR:OH	17:PB:900:GLU:OE1	2.13	0.67
35:DD:873:LEU:HD12	35:DD:873:LEU:N	2.10	0.67
40:DI:23:LEU:HD21	40:DI:39:MET:CE	2.23	0.67
55:a:412:ARG:C	55:a:472:SER:HB3	2.19	0.67
55:a:462:LEU:HB2	74:x:49:GLN:CG	2.25	0.67
56:d:41:SER:HB3	58:i:69:VAL:CG1	2.23	0.67
56:d:46:GLU:N	58:i:76:MET:HE3	2.09	0.67
63:c:305:PHE:CD1	63:c:311:GLN:CB	2.77	0.67
66:o:765:ASP:OD1	66:o:766:LYS:N	2.27	0.67
13:EB:89:HIS:CE1	13:EB:139:PHE:HB3	2.29	0.67
30:HD:207:GLN:HA	30:HD:210:MET:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DD:897:ASP:O	35:DD:898:VAL:HG23	1.95	0.67
46:HI:266:ASP:O	46:HI:269:LEU:HB3	1.93	0.67
60:q:28:GLU:HA	60:q:28:GLU:OE2	1.94	0.67
63:c:283:ARG:HB3	63:c:311:GLN:NE2	2.10	0.67
63:c:291:GLY:O	70:t:120:CYS:O	2.12	0.67
39:DH:41:VAL:O	39:DH:45:LEU:HG	1.94	0.67
55:a:461:SER:CA	74:x:49:GLN:NE2	2.32	0.67
59:m:67:LEU:HD13	59:m:73:LEU:HD11	1.77	0.67
60:q:116:LEU:HB3	67:h:16:LEU:HD23	1.77	0.67
60:q:149:LYS:CE	71:v:40:ALA:C	2.68	0.67
60:q:376:HIS:CB	68:k:92:MET:HE3	2.25	0.67
5:BA:26:ASP:OD1	11:PA:430:ARG:NH2	2.28	0.67
5:BA:128:ILE:HG23	5:BA:183:VAL:HG11	1.77	0.67
37:Df:239:ARG:HD3	37:Df:284:ARG:HH11	1.60	0.67
52:n:686:LYS:NZ	66:o:730:PRO:HB3	2.10	0.67
55:a:462:LEU:CD2	74:x:11:LEU:HB3	2.24	0.67
58:i:86:ASP:N	58:i:86:ASP:OD1	2.24	0.67
73:w:1291:MET:SD	73:w:1328:ARG:NH2	2.67	0.67
9:HA:60:GLN:OE1	9:HA:61:ARG:NH1	2.28	0.67
17:PB:1143:LYS:HE3	49:PG:152:VAL:HG11	1.75	0.67
31:HG:137:MET:SD	31:HG:139:CYS:N	2.68	0.67
37:DF:106:PHE:CE1	40:DI:13:PRO:HD3	2.30	0.67
39:DH:50:PHE:CB	43:DJ:195:LEU:HB2	2.23	0.67
36:De:645:GLY:H	36:De:675:LEU:HD11	1.59	0.67
46:HI:98:LEU:HB3	46:HI:143:LEU:HD21	1.77	0.67
52:n:166:TYR:OH	59:m:70:PRO:CB	2.36	0.67
60:q:89:GLN:CB	60:q:90:PRO:CD	2.68	0.67
65:l:164:ARG:NH2	71:v:131:GLU:OE2	2.26	0.67
33:HF:66:PHE:HB2	34:HH:674:THR:OG1	1.95	0.67
35:DD:899:VAL:HG12	35:DD:900:SER:H	1.58	0.67
36:DE:463:PHE:HB3	37:DF:134:HIS:CD2	2.30	0.67
40:DI:132:LEU:CD1	43:DJ:121:MET:SD	2.83	0.67
47:HJ:28:ARG:HG3	47:HJ:28:ARG:O	1.94	0.67
47:HJ:111:LEU:HD12	47:HJ:111:LEU:O	1.95	0.66
52:n:169:LEU:HD23	59:m:104:HIS:HB3	1.77	0.66
52:n:270:GLN:NE2	57:f:174:ARG:HD2	2.09	0.66
56:d:41:SER:HB3	58:i:69:VAL:HG11	1.76	0.66
60:q:212:ALA:CB	60:q:380:ARG:HH22	2.07	0.66
60:q:457:ASP:HB2	60:q:458:PRO:HD3	1.77	0.66
12:DB:490:SER:HA	12:DB:493:TRP:HB2	1.77	0.66
30:HD:106:VAL:O	30:HD:110:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:237:MET:CE	60:q:45:GLN:CB	2.73	0.66
52:n:270:GLN:HG2	57:f:177:VAL:HG12	1.77	0.66
60:q:35:SER:HB3	60:q:42:ARG:HH22	1.58	0.66
60:q:109:MET:HA	60:q:109:MET:CE	2.23	0.66
60:q:263:LYS:CE	60:q:439:PHE:CZ	2.77	0.66
60:q:428:LEU:HD12	60:q:428:LEU:C	2.18	0.66
71:v:131:GLU:O	71:v:135:TYR:HD2	1.79	0.66
74:x:912:LEU:HD22	74:x:958:VAL:HG21	1.77	0.66
46:HI:111:PRO:CG	57:f:63:MET:HE3	2.25	0.66
52:n:104:LYS:HZ1	53:s:109:LEU:N	1.92	0.66
60:q:129:PRO:CB	67:h:74:GLN:NE2	2.53	0.66
66:o:695:PRO:HA	66:o:699:SER:HB2	1.75	0.66
12:DB:621:ALA:HB2	18:HC:438:LYS:HZ3	1.56	0.66
35:DD:875:GLN:C	35:DD:877:PRO:HD3	2.20	0.66
37:DF:14:LEU:HD23	40:DI:22:ILE:CD1	2.25	0.66
37:DF:138:ILE:HG13	39:DH:159:TYR:HE2	1.59	0.66
37:DF:320:ARG:CG	37:DF:415:ILE:HD12	2.25	0.66
39:DH:57:SER:OG	43:DJ:200:LEU:CD1	2.43	0.66
58:i:68:LEU:O	58:i:72:ILE:HG13	1.96	0.66
12:DB:402:ILE:HD12	12:DB:455:LEU:HD12	1.78	0.66
13:EB:229:ASP:O	13:EB:233:ILE:HD12	1.95	0.66
40:DI:31:TYR:HD2	40:DI:35:VAL:HB	1.60	0.66
50:g:75:LYS:HG2	54:u:76:LEU:HD23	1.76	0.66
52:n:956:ALA:HB1	52:n:1217:ARG:NH2	2.08	0.66
54:u:85:LEU:HD11	61:z:551:ASP:HB2	1.76	0.66
54:u:115:LEU:CA	56:d:121:LEU:CD1	2.74	0.66
55:a:69:LEU:HG	56:d:70:ILE:HG21	1.77	0.66
60:q:95:TRP:HZ3	67:h:33:LEU:HD21	1.59	0.66
6:DA:970:ASN:OD1	6:DA:970:ASN:N	2.21	0.66
19:DO:51:ARG:NH2	21:DQ:20:ASP:OD2	2.28	0.66
30:HD:43:ALA:HB3	49:PG:164:MET:HG3	1.72	0.66
52:n:669:GLN:NE2	66:o:681:GLU:HG3	2.11	0.66
60:q:171:VAL:HG22	68:k:17:ILE:CG2	2.10	0.66
60:q:479:ILE:HG22	60:q:532:HIS:CG	2.30	0.66
62:b:65:PRO:HA	62:b:68:LYS:HE2	1.76	0.66
7:EA:142:ASN:ND2	49:PG:107:PHE:HB3	2.09	0.66
56:d:156:SER:CB	56:d:161:VAL:HG11	2.26	0.66
67:h:147:CYS:SG	71:v:41:LYS:HG3	2.34	0.66
71:v:61:MET:HE2	71:v:64:ARG:NH1	2.10	0.66
37:DF:126:PRO:HA	39:DH:125:THR:HB	1.78	0.66
39:DH:56:ALA:HB2	43:DJ:214:PRO:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:134:ILE:HA	48:PD:137:LYS:CE	2.25	0.66
60:q:578:TYR:CD1	60:q:646:LEU:HD12	2.29	0.66
73:w:318:GLU:HG2	73:w:320:LYS:H	1.59	0.66
7:EA:34:LEU:HD11	7:EA:94:ILE:HD12	1.76	0.66
11:PA:805:ARG:NH2	17:PB:671:GLU:O	2.28	0.66
35:DD:922:GLN:CG	35:DD:1056:THR:HG21	2.26	0.66
37:DF:43:VAL:CA	40:DI:46:TYR:HD2	2.08	0.66
55:a:67:LYS:HB3	55:a:83:SER:HB2	1.77	0.66
56:d:97:GLU:HA	56:d:97:GLU:OE2	1.95	0.66
63:c:290:ASP:O	70:t:120:CYS:HB3	1.95	0.66
63:c:309:CYS:O	63:c:311:GLN:HG3	1.96	0.66
70:t:165:LEU:HD23	70:t:169:THR:HA	1.78	0.66
25:PH:91:VAL:HG22	25:PH:144:LEU:CD2	2.26	0.66
37:DF:317:LEU:HD22	37:DF:317:LEU:N	2.11	0.66
47:HJ:200:LEU:O	47:HJ:200:LEU:HD22	1.96	0.66
48:PD:134:ILE:CA	48:PD:137:LYS:HE2	2.24	0.66
55:a:462:LEU:CG	74:x:49:GLN:CG	2.72	0.66
7:EA:111:ARG:HD3	30:HD:11:THR:OG1	1.96	0.65
12:DB:645:ALA:HB3	12:DB:648:MET:HG3	1.78	0.65
30:HD:27:GLY:CA	30:HD:70:LYS:HD3	2.26	0.65
34:HH:701:LEU:O	34:HH:704:SER:OG	2.14	0.65
48:PD:74:PHE:HZ	48:PD:137:LYS:HE3	1.60	0.65
52:n:265:LEU:HD12	52:n:303:LEU:CD2	2.15	0.65
52:n:921:MET:SD	52:n:1215:ILE:HD13	2.35	0.65
52:n:922:TYR:OH	52:n:1214:VAL:HG12	1.96	0.65
55:a:160:LEU:HD11	55:a:219:LEU:HD21	1.77	0.65
55:a:232:LEU:C	55:a:232:LEU:HD13	2.21	0.65
55:a:462:LEU:CD1	74:x:49:GLN:HB3	2.26	0.65
58:i:72:ILE:CD1	58:i:92:SER:HB3	2.24	0.65
60:q:644:SER:O	64:e:97:GLN:CG	2.44	0.65
11:PA:1660:THR:N	57:f:14:SER:O	2.27	0.65
39:DH:110:TYR:HB2	43:DJ:161:LYS:HD3	1.77	0.65
46:HI:33:ASN:N	46:HI:33:ASN:OD1	2.29	0.65
6:DA:784:GLN:H	6:DA:1073:GLN:HE22	1.45	0.65
60:q:149:LYS:HD2	71:v:40:ALA:HA	1.77	0.65
60:q:487:ILE:CD1	60:q:540:LEU:HD12	2.26	0.65
67:h:147:CYS:SG	71:v:41:LYS:HD2	2.36	0.65
7:EA:122:THR:OG1	30:HD:40:VAL:CG2	2.43	0.65
7:EA:188:TYR:CE2	30:HD:14:TYR:CG	2.85	0.65
19:DO:1:MET:HB3	35:DD:997:ALA:CB	2.25	0.65
32:HE:43:VAL:HG11	32:HE:224:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:359:LEU:HD13	36:DE:627:LEU:HD12	1.76	0.65
36:DE:462:CYS:HA	37:DF:134:HIS:O	1.97	0.65
62:b:101:ARG:NH1	72:p:677:THR:CB	2.57	0.65
64:e:133:LEU:HG	68:k:111:CYS:SG	2.37	0.65
67:h:146:MET:CG	68:k:39:LYS:CE	2.75	0.65
70:t:78:LEU:HD12	70:t:84:CYS:HB3	1.77	0.65
72:p:827:CYS:SG	72:p:828:LEU:N	2.69	0.65
9:HA:238:ASN:ND2	9:HA:662:GLN:OE1	2.29	0.65
11:PA:513:ALA:HB2	24:PF:90:LEU:HD21	1.78	0.65
12:DB:672:PHE:CD1	18:HC:414:SER:CA	2.79	0.65
26:PI:60:HIS:ND1	26:PI:60:HIS:O	2.30	0.65
37:DF:82:PRO:HG3	37:DF:96:PHE:C	2.21	0.65
60:q:168:THR:CB	68:k:21:ILE:HD12	2.27	0.65
60:q:184:ASN:OD1	71:v:83:LYS:CD	2.45	0.65
68:k:43:ARG:HB2	68:k:43:ARG:HH11	1.62	0.65
73:w:1183:TRP:CZ2	73:w:1185:GLY:HA3	2.32	0.65
6:DA:491:MET:H	6:DA:491:MET:CE	2.10	0.65
11:PA:122:ASN:O	11:PA:127:LYS:NZ	2.30	0.65
12:DB:672:PHE:CE1	18:HC:413:LEU:CB	2.78	0.65
30:HD:255:THR:HA	47:HJ:4:ASN:HB2	1.79	0.65
46:HI:241:CYS:HA	46:HI:246:TYR:CG	2.32	0.65
50:g:167:CYS:HG	56:d:113:GLN:NE2	1.93	0.65
52:n:680:HIS:NE2	60:q:557:LEU:HD11	2.09	0.65
60:q:166:ARG:CZ	60:q:166:ARG:HB3	2.27	0.65
60:q:631:GLU:HA	60:q:631:GLU:OE2	1.97	0.65
67:h:146:MET:HG3	68:k:39:LYS:CD	2.24	0.65
68:k:56:VAL:HG13	71:v:26:ILE:HD12	1.77	0.65
12:DB:674:THR:HB	18:HC:415:GLN:HE21	1.62	0.65
17:PB:677:MET:H	17:PB:682:LEU:HD22	1.62	0.65
37:DF:19:MET:SD	40:DI:47:VAL:HG11	2.37	0.65
39:DH:50:PHE:CE2	43:DJ:170:ALA:O	2.50	0.65
50:g:74:HIS:H	54:u:79:GLU:HB2	1.60	0.65
52:n:170:PRO:HB3	60:q:22:VAL:HG23	1.79	0.65
52:n:937:ARG:HH21	52:n:943:LEU:HD23	1.62	0.65
58:i:65:PHE:HE1	58:i:99:LYS:HA	1.62	0.65
59:m:121:GLU:O	59:m:124:GLN:HG2	1.96	0.65
60:q:484:TYR:OH	60:q:640:GLU:HB2	1.96	0.65
12:DB:645:ALA:CA	18:HC:413:LEU:HA	2.23	0.65
18:HC:172:SER:OG	18:HC:267:GLU:OE2	2.13	0.65
31:HG:377:ASP:O	31:HG:380:HIS:NE2	2.30	0.65
39:DH:54:GLU:OE1	43:DJ:197:MET:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DH:107:LEU:HD11	43:DJ:158:ALA:HA	1.78	0.65
46:HI:106:SER:HB2	57:f:59:HIS:CE1	2.31	0.65
55:a:380:ALA:HB1	74:x:58:PRO:HG3	1.76	0.65
60:q:162:LYS:O	60:q:166:ARG:HG2	1.96	0.65
64:e:45:VAL:HG13	65:l:92:LEU:HD11	1.79	0.65
70:t:112:THR:HG22	70:t:129:VAL:HG22	1.77	0.65
70:t:130:THR:HA	70:t:135:ALA:HA	1.77	0.65
18:HC:397:GLU:OE1	33:HF:61:MET:CG	2.44	0.65
37:DF:312:ILE:HG13	37:DF:334:ALA:CB	2.27	0.65
38:DG:129:LYS:O	38:DG:129:LYS:NZ	2.23	0.65
52:n:790:ILE:HG22	52:n:792:ALA:H	1.62	0.65
54:u:49:ASN:H	54:u:49:ASN:ND2	1.94	0.65
60:q:441:ARG:NH1	65:l:168:TRP:CZ3	2.59	0.65
18:HC:172:SER:OG	18:HC:174:ASP:OD1	2.15	0.65
36:DE:745:GLU:OE1	36:DE:745:GLU:HA	1.97	0.65
46:HI:191:GLY:O	46:HI:193:GLY:N	2.30	0.65
55:a:375:PHE:CD1	74:x:17:ARG:CG	2.79	0.65
68:k:44:LEU:HD22	68:k:47:ARG:HH22	1.62	0.65
71:v:50:ARG:HD2	71:v:51:ALA:H	1.61	0.65
6:DA:1168:TYR:HB2	38:DG:180:ARG:HB3	1.78	0.64
32:HE:168:GLU:N	32:HE:168:GLU:OE1	2.31	0.64
39:DH:108:PRO:HG3	43:DJ:116:LEU:CD2	2.25	0.64
52:n:250:LEU:HG	52:n:275:HIS:CB	2.26	0.64
53:s:107:ASN:H	53:s:110:PRO:HB3	1.62	0.64
60:q:168:THR:CA	68:k:21:ILE:HD12	2.26	0.64
63:c:305:PHE:HD1	63:c:311:GLN:NE2	1.95	0.64
66:o:719:PRO:HD2	74:x:71:GLN:HG3	1.79	0.64
68:k:77:GLN:HG3	69:r:192:GLN:HG2	1.79	0.64
72:p:490:ASP:N	72:p:490:ASP:OD1	2.30	0.64
37:DF:83:LEU:HD21	39:DH:67:SER:OG	1.97	0.64
41:DL:71:ASP:HB3	41:DL:74:GLU:HG3	1.76	0.64
55:a:109:TYR:CE2	55:a:154:LEU:CD2	2.80	0.64
56:d:38:GLU:OE2	58:i:96:GLU:CB	2.45	0.64
57:f:70:LEU:HD21	57:f:73:ALA:HB2	1.79	0.64
60:q:375:LEU:HD23	60:q:427:LEU:HD11	1.79	0.64
60:q:487:ILE:CG2	60:q:543:VAL:CG2	2.68	0.64
62:b:179:LEU:CD1	64:e:60:VAL:CB	2.62	0.64
70:t:31:LEU:HD11	70:t:164:PHE:HB3	1.79	0.64
30:HD:298:GLN:NE2	46:HI:132:TRP:NE1	2.45	0.64
36:DE:746:ASP:OD1	36:DE:746:ASP:N	2.30	0.64
39:DH:51:GLU:HB2	43:DJ:193:TYR:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Di:73:LEU:HD22	41:Dl:105:HIS:CE1	2.33	0.64
50:g:95:ILE:HG21	50:g:105:ARG:HB3	1.79	0.64
55:a:424:CYS:HA	55:a:505:PRO:HG3	1.79	0.64
67:h:146:MET:HG2	68:k:39:LYS:CE	2.26	0.64
12:DB:583:GLU:CD	12:DB:583:GLU:H	2.06	0.64
34:HH:330:ASN:OD1	34:HH:334:ARG:NH2	2.31	0.64
57:f:99:TYR:HB3	67:h:77:ILE:HG22	1.79	0.64
37:DF:332:PHE:HA	37:DF:335:ARG:HD3	1.78	0.64
47:HJ:268:GLU:H	47:HJ:268:GLU:CD	2.04	0.64
48:PD:74:PHE:CE1	48:PD:137:LYS:HE3	2.31	0.64
52:n:270:GLN:HA	57:f:181:LEU:HD11	1.78	0.64
52:n:904:PHE:CE2	52:n:1208:GLU:CB	2.81	0.64
57:f:181:LEU:O	57:f:185:ARG:HG3	1.96	0.64
60:q:129:PRO:HB3	67:h:74:GLN:HE21	1.61	0.64
62:b:116:LEU:HB3	63:c:21:ILE:HD13	1.79	0.64
63:c:166:ILE:HD13	63:c:190:LEU:HD21	1.80	0.64
74:x:780:THR:HG22	74:x:816:CYS:HB3	1.80	0.64
17:PB:116:ARG:HG2	17:PB:910:THR:HG21	1.79	0.64
17:PB:926:VAL:HG21	22:PC:62:GLU:HG3	1.78	0.64
37:DF:218:VAL:CG1	39:DH:162:THR:CG2	2.75	0.64
37:Df:320:ARG:HB3	37:Df:320:ARG:NH1	2.12	0.64
57:f:71:LEU:HD12	57:f:82:ARG:HE	1.61	0.64
60:q:212:ALA:O	60:q:383:HIS:HB3	1.98	0.64
61:z:576:TRP:HB3	61:z:596:TYR:HB3	1.79	0.64
66:o:639:TYR:CG	72:p:786:HIS:HB3	2.25	0.64
67:h:142:SER:C	68:k:39:LYS:HZ1	2.04	0.64
72:p:50:ASP:HA	72:p:59:THR:HG22	1.79	0.64
72:p:569:LEU:HG	72:p:569:LEU:O	1.97	0.64
17:PB:910:THR:HG22	17:PB:911:LEU:H	1.62	0.64
37:DF:314:SER:O	37:DF:327:TRP:HH2	1.81	0.64
48:PD:14:GLU:N	48:PD:14:GLU:OE1	2.31	0.64
51:j:82:LYS:CE	53:s:101:VAL:HG12	2.28	0.64
52:n:166:TYR:HB2	59:m:74:HIS:HB2	1.79	0.64
52:n:359:ILE:CA	52:n:372:ILE:CD1	2.75	0.64
56:d:42:ARG:CZ	58:i:96:GLU:OE2	2.46	0.64
60:q:150:LYS:HE3	68:k:37:LYS:HB3	1.80	0.64
60:q:647:SER:OG	64:e:93:CYS:SG	2.56	0.64
9:HA:571:THR:OG1	9:HA:576:GLU:OE1	2.08	0.64
48:PD:87:LEU:HB3	48:PD:97:LEU:HD22	1.78	0.64
60:q:467:ILE:HD11	63:c:203:VAL:HG11	1.78	0.64
60:q:491:ILE:HD12	60:q:532:HIS:HA	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:c:305:PHE:CD1	63:c:311:GLN:CD	2.76	0.64
12:DB:621:ALA:HB3	18:HC:438:LYS:HE2	1.80	0.64
12:DB:648:MET:CE	18:HC:411:GLN:HG2	2.26	0.64
18:HC:55:TRP:CZ2	18:HC:83:GLN:NE2	2.66	0.64
46:HI:37:ILE:HD12	46:HI:37:ILE:N	2.12	0.64
46:HI:215:GLY:HA3	46:HI:221:GLN:HB2	1.80	0.64
50:g:130:GLN:HB2	54:u:5:LEU:HD13	1.80	0.64
60:q:458:PRO:HB3	60:q:533:GLN:NE2	2.12	0.64
11:PA:140:ARG:NH1	11:PA:234:PHE:O	2.30	0.64
13:EB:145:VAL:HG13	13:EB:175:LEU:HB2	1.79	0.64
36:DE:359:LEU:HD11	36:DE:648:ASP:HB2	1.80	0.64
36:DE:451:VAL:O	36:DE:453:LEU:N	2.31	0.64
40:DI:28:ILE:CG2	40:DI:31:TYR:HD1	2.07	0.64
40:DI:132:LEU:HD21	43:DJ:121:MET:CE	2.22	0.64
52:n:265:LEU:CD1	52:n:303:LEU:CD2	2.70	0.64
59:m:124:GLN:OE1	61:z:590:ARG:HB3	1.98	0.64
63:c:293:PRO:HD3	70:t:144:TYR:OH	1.96	0.64
73:w:1184:VAL:O	73:w:1184:VAL:HG22	1.98	0.64
30:HD:295:ARG:HA	46:HI:132:TRP:HE1	1.62	0.63
46:HI:47:HIS:CG	46:HI:47:HIS:O	2.50	0.63
46:HI:214:PRO:HD2	46:HI:224:ARG:HG2	1.80	0.63
48:PD:29:ALA:HB3	49:PG:3:TYR:CE2	2.33	0.63
50:g:132:ARG:HG3	54:u:86:GLN:HG3	1.80	0.63
60:q:93:TRP:N	60:q:94:PRO:CD	2.62	0.63
71:v:42:ILE:H	71:v:42:ILE:HD12	1.61	0.63
34:HH:517:GLU:O	34:HH:521:GLU:OE1	2.16	0.63
46:HI:24:ALA:HA	46:HI:44:LYS:HB2	1.80	0.63
50:g:130:GLN:HB2	54:u:5:LEU:CD1	2.28	0.63
52:n:104:LYS:NZ	53:s:109:LEU:H	1.96	0.63
52:n:359:ILE:HG23	52:n:372:ILE:HD12	1.78	0.63
58:i:96:GLU:HA	58:i:99:LYS:CG	2.27	0.63
60:q:489:LYS:O	60:q:507:ARG:NH2	2.30	0.63
62:b:136:HIS:CD2	63:c:111:TYR:CE2	2.81	0.63
68:k:39:LYS:HG3	68:k:39:LYS:O	1.97	0.63
74:x:637:GLU:O	74:x:641:GLN:NE2	2.31	0.63
12:DB:361:ARG:HD2	12:DB:367:GLU:HB2	1.80	0.63
20:DP:297:LYS:NZ	20:DP:323:GLU:OE2	2.31	0.63
36:DE:433:LYS:HD3	40:DI:110:TYR:CE1	2.33	0.63
51:j:78:GLN:O	51:j:82:LYS:HE2	1.98	0.63
52:n:359:ILE:CA	52:n:372:ILE:HD11	2.28	0.63
55:a:417:TYR:CD1	55:a:450:PHE:HE1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:179:LEU:CD1	64:e:60:VAL:CA	2.72	0.63
15:HB:195:SER:O	15:HB:199:THR:OG1	2.06	0.63
30:HD:42:GLY:O	49:PG:164:MET:HE3	1.98	0.63
35:DD:872:PHE:CE1	41:DL:57:VAL:CG1	2.79	0.63
52:n:651:ASN:ND2	73:w:22:PHE:H	1.94	0.63
56:d:156:SER:HA	56:d:161:VAL:CG1	2.27	0.63
60:q:93:TRP:H	60:q:94:PRO:CD	2.11	0.63
60:q:93:TRP:H	60:q:94:PRO:HD2	1.63	0.63
60:q:149:LYS:CE	71:v:40:ALA:O	2.47	0.63
60:q:265:ALA:HB3	60:q:340:GLN:OE1	1.98	0.63
62:b:103:ASP:HB3	66:o:645:ALA:HB2	1.80	0.63
65:l:108:PRO:HD2	65:l:109:ILE:HD12	1.81	0.63
71:v:108:LEU:C	71:v:108:LEU:HD12	2.23	0.63
74:x:143:ARG:HH22	74:x:205:ASN:HB2	1.62	0.63
9:HA:2:LYS:HB3	9:HA:9:LEU:HD11	1.81	0.63
11:PA:589:LYS:NZ	11:PA:625:ASP:OD2	2.23	0.63
17:PB:529:MET:HE1	17:PB:698:ILE:HD12	1.79	0.63
30:HD:145:GLU:OE2	67:h:67:LYS:HE2	1.99	0.63
31:HG:379:LEU:HD22	31:HG:381:CYS:O	1.99	0.63
34:HH:128:SER:OG	34:HH:163:TYR:OH	2.17	0.63
39:DH:37:LEU:CD1	43:DJ:138:TYR:CE2	2.81	0.63
52:n:192:LEU:CD1	52:n:219:ASN:O	2.47	0.63
55:a:160:LEU:HD11	55:a:214:ARG:HH21	1.61	0.63
55:a:373:CYS:H	55:a:439:GLN:HA	1.63	0.63
55:a:463:VAL:HG11	55:a:488:ILE:HD12	1.80	0.63
72:p:232:ASP:OD1	72:p:232:ASP:N	2.31	0.63
20:DP:186:ARG:NH1	20:DP:244:LEU:O	2.31	0.63
30:HD:83:ASN:ND2	30:HD:140:LEU:HD12	2.14	0.63
36:DE:465:THR:N	37:DF:132:LYS:O	2.31	0.63
37:DF:43:VAL:CB	40:DI:46:TYR:HD2	2.11	0.63
37:DF:68:THR:HA	40:DI:32:GLU:CD	2.23	0.63
37:DF:106:PHE:CD1	40:DI:13:PRO:HD3	2.33	0.63
37:DF:392:ILE:O	37:DF:392:ILE:HG22	1.99	0.63
55:a:462:LEU:HD11	74:x:60:ILE:HD11	1.81	0.63
61:z:580:ILE:HB	61:z:593:ILE:HB	1.79	0.63
64:e:146:ILE:C	64:e:148:VAL:H	2.07	0.63
5:BA:171:GLU:O	17:PB:101:ARG:NH2	2.32	0.63
7:EA:188:TYR:CE2	30:HD:14:TYR:HB3	2.34	0.63
23:PE:9:ARG:O	23:PE:13:ILE:HD12	1.99	0.63
34:HH:266:GLN:HG2	34:HH:267:THR:HG23	1.81	0.63
35:DD:874:LEU:HD23	35:DD:874:LEU:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:241:GLU:CD	39:DH:135:THR:HG1	2.07	0.63
52:n:172:CYS:SG	60:q:21:GLU:CB	2.86	0.63
55:a:462:LEU:HB2	74:x:49:GLN:HG2	1.80	0.63
6:DA:481:GLU:CD	6:DA:481:GLU:H	2.04	0.63
7:EA:188:TYR:CE2	30:HD:14:TYR:CB	2.81	0.63
12:DB:156:LYS:O	12:DB:963:HIS:HB2	1.99	0.63
57:f:143:LYS:HG2	60:q:226:LYS:HG3	1.81	0.63
64:e:129:VAL:CG2	68:k:114:MET:CE	2.64	0.63
70:t:25:THR:HB	70:t:117:TYR:OH	1.97	0.63
9:HA:343:ARG:O	9:HA:346:VAL:HG12	1.99	0.63
22:PC:24:GLU:OE2	22:PC:228:ARG:NH1	2.31	0.63
35:DD:874:LEU:H	35:DD:874:LEU:CD2	2.10	0.63
37:DF:71:ILE:HD11	40:DI:35:VAL:HG22	1.81	0.63
52:n:209:PRO:HG3	52:n:293:TYR:CG	2.33	0.63
52:n:944:PHE:CE2	62:b:101:ARG:NH2	2.67	0.63
55:a:377:ASN:HD21	74:x:58:PRO:CG	2.12	0.63
56:d:34:LEU:CD2	58:i:99:LYS:HD3	2.26	0.63
57:f:145:TYR:CE1	67:h:43:PRO:HG2	2.32	0.63
70:t:8:GLN:HE21	70:t:200:ILE:HD13	1.63	0.63
34:HH:287:LEU:HD23	34:HH:287:LEU:O	1.98	0.62
39:DH:53:ALA:HB2	43:DJ:195:LEU:HB3	1.80	0.62
51:j:78:GLN:HB3	51:j:82:LYS:HE2	1.81	0.62
66:o:723:LEU:HD11	66:o:734:PRO:HB2	1.78	0.62
9:HA:335:ARG:NH1	30:HD:71:GLU:OE2	2.32	0.62
31:HG:242:SER:O	31:HG:245:SER:OG	2.17	0.62
50:g:120:HIS:CE1	52:n:148:ARG:HB3	2.33	0.62
52:n:196:ASN:OD1	52:n:219:ASN:HA	1.99	0.62
55:a:321:LEU:HA	55:a:410:LEU:HD12	1.81	0.62
55:a:445:LEU:CD2	74:x:55:SER:CB	2.43	0.62
57:f:145:TYR:CE2	67:h:43:PRO:HD3	2.34	0.62
58:i:72:ILE:HD13	58:i:92:SER:HB2	1.65	0.62
74:x:13:ALA:HA	74:x:18:TRP:CE3	2.34	0.62
30:HD:300:ALA:O	47:HJ:210:SER:HB3	1.99	0.62
35:DD:950:LEU:HD13	35:DD:950:LEU:O	1.99	0.62
39:DH:121:ALA:HB1	43:DJ:133:ALA:CB	2.27	0.62
55:a:220:MET:HB2	55:a:257:VAL:HG12	1.80	0.62
56:d:38:GLU:OE2	58:i:96:GLU:CG	2.46	0.62
56:d:100:VAL:HG13	58:i:128:LYS:NZ	2.14	0.62
2:Y:18:DC:OP2	14:FB:214:LYS:NZ	2.22	0.62
23:PE:29:THR:HG23	23:PE:32:GLU:H	1.65	0.62
52:n:169:LEU:HG	59:m:104:HIS:ND1	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:265:LEU:HD11	52:n:307:VAL:HG21	1.80	0.62
52:n:417:LYS:HG3	52:n:421:ARG:HE	1.64	0.62
55:a:109:TYR:CE2	55:a:154:LEU:HD21	2.34	0.62
55:a:441:GLU:HG3	55:a:442:VAL:N	2.08	0.62
56:d:27:ARG:HG2	58:i:107:ILE:HG22	1.79	0.62
17:PB:354:SER:HG	17:PB:357:CYS:HG	1.35	0.62
33:HF:49:LEU:HD12	33:HF:52:VAL:CG1	2.29	0.62
40:DI:32:GLU:HB2	40:DI:35:VAL:HG23	1.82	0.62
52:n:512:LEU:HD21	60:q:565:ASN:HD22	1.64	0.62
54:u:72:LEU:O	54:u:75:SER:HB2	1.99	0.62
54:u:115:LEU:CD1	56:d:121:LEU:HD13	2.30	0.62
70:t:98:LEU:HD13	70:t:102:PHE:HE1	1.64	0.62
11:PA:1475:LEU:CD2	49:PG:18:PHE:CZ	2.80	0.62
35:DD:891:ILE:H	35:DD:891:ILE:HD12	1.63	0.62
35:DD:966:LEU:HD11	35:DD:982:LEU:HD21	1.82	0.62
40:DI:15:ASP:O	40:DI:40:LEU:HD21	1.99	0.62
48:PD:119:GLU:N	48:PD:119:GLU:OE1	2.33	0.62
52:n:753:LEU:CD1	63:c:311:GLN:CG	2.77	0.62
52:n:957:PRO:HD3	52:n:1214:VAL:CG2	2.30	0.62
56:d:167:TRP:HE3	59:m:106:GLN:CD	2.08	0.62
57:f:46:ASN:ND2	57:f:63:MET:SD	2.72	0.62
66:o:735:LEU:CD2	73:w:113:GLN:OE1	2.46	0.62
70:t:96:VAL:O	70:t:99:LYS:HB2	2.00	0.62
72:p:13:MET:HE1	72:p:393:ILE:HD11	1.82	0.62
73:w:1181:THR:O	73:w:1184:VAL:HB	1.99	0.62
11:PA:1471:PHE:O	24:PF:64:ARG:NH1	2.33	0.62
12:DB:618:ALA:HB1	18:HC:439:ARG:HH22	1.62	0.62
17:PB:407:MET:HE1	17:PB:444:LEU:HG	1.80	0.62
68:k:109:ARG:HH11	68:k:109:ARG:HG3	1.65	0.62
72:p:47:PHE:HE2	72:p:49:MET:HE2	1.64	0.62
6:DA:349:TRP:HB3	37:Df:269:VAL:HG21	1.81	0.62
13:EB:189:ILE:HD11	13:EB:201:LEU:HD13	1.79	0.62
30:HD:43:ALA:CB	49:PG:164:MET:CG	2.69	0.62
47:HJ:229:GLU:H	47:HJ:229:GLU:CD	2.04	0.62
55:a:59:VAL:HG21	56:d:51:SER:OG	1.99	0.62
66:o:695:PRO:O	74:x:957:LYS:HE2	1.99	0.62
67:h:23:LYS:HB3	67:h:23:LYS:HZ3	1.64	0.62
7:EA:17:LEU:CD2	7:EA:194:THR:HG21	2.27	0.62
23:PE:168:ASN:OD1	23:PE:172:ARG:NH2	2.33	0.62
47:HJ:277:LEU:HD12	47:HJ:277:LEU:O	1.99	0.62
54:u:90:LEU:CD2	60:q:9:ILE:CD1	2.36	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:228:PRO:HB2	55:a:502:MET:CB	2.30	0.62
55:a:316:ALA:HB2	55:a:447:GLU:HG2	1.82	0.62
57:f:95:LEU:O	60:q:130:VAL:HG11	1.96	0.62
63:c:288:LEU:HD21	70:t:122:PHE:HZ	1.64	0.62
19:DO:1:MET:HB2	35:DD:997:ALA:HB2	1.81	0.62
22:PC:9:VAL:HG11	28:PK:105:PHE:CD1	2.35	0.62
40:DI:132:LEU:CG	43:DJ:121:MET:HE2	2.30	0.62
47:HJ:167:PHE:CD1	47:HJ:167:PHE:C	2.78	0.62
58:i:85:GLN:HG2	58:i:86:ASP:OD1	1.98	0.62
73:w:196:LEU:HD13	74:x:802:MET:HB2	1.80	0.62
5:BA:273:GLU:O	5:BA:277:ILE:HD12	1.99	0.61
7:EA:174:ARG:HG3	30:HD:37:LEU:HD11	1.82	0.61
7:EA:176:LEU:HD11	13:EB:215:GLU:HG3	1.82	0.61
19:DO:1:MET:HB2	35:DD:997:ALA:CB	2.30	0.61
30:HD:288:THR:C	30:HD:290:SER:N	2.57	0.61
31:HG:112:LYS:O	31:HG:147:ASN:ND2	2.32	0.61
34:HH:473:GLU:OE1	34:HH:473:GLU:N	2.33	0.61
40:DI:23:LEU:HD21	40:DI:39:MET:SD	2.40	0.61
55:a:66:GLN:HE21	56:d:44:LEU:HD11	1.53	0.61
58:i:109:LEU:CD2	58:i:117:GLN:HE22	2.13	0.61
69:r:121:MET:HE2	70:t:102:PHE:CZ	2.35	0.61
4:NY:-157:DG:H2'	4:NY:-156:DG:C8	2.34	0.61
11:PA:1375:ARG:NH1	11:PA:1379:GLU:OE1	2.31	0.61
15:HB:130:ASP:OD2	15:HB:463:HIS:NE2	2.33	0.61
37:DF:106:PHE:CD1	40:DI:13:PRO:HG3	2.35	0.61
46:HI:237:TRP:CG	46:HI:237:TRP:O	2.53	0.61
48:PD:29:ALA:HB3	49:PG:3:TYR:CZ	2.35	0.61
48:PD:79:THR:HG22	67:h:51:LEU:CD1	2.31	0.61
52:n:121:PHE:CD2	53:s:83:LEU:HD21	2.35	0.61
52:n:169:LEU:HD23	59:m:101:GLN:HA	1.80	0.61
52:n:172:CYS:SG	60:q:20:HIS:O	2.52	0.61
52:n:634:MET:N	52:n:634:MET:SD	2.73	0.61
52:n:922:TYR:CE2	52:n:1215:ILE:HD13	2.35	0.61
54:u:111:GLY:O	56:d:121:LEU:HD11	2.00	0.61
55:a:59:VAL:HG12	56:d:48:LEU:HD23	1.82	0.61
56:d:45:ILE:CD1	58:i:73:ILE:CG1	2.78	0.61
60:q:89:GLN:HB3	60:q:90:PRO:HD2	1.77	0.61
60:q:149:LYS:CD	71:v:40:ALA:O	2.48	0.61
68:k:42:GLU:HA	68:k:42:GLU:OE2	2.00	0.61
11:PA:1643:TYR:CZ	59:m:93:CYS:HB2	2.35	0.61
30:HD:274:HIS:H	30:HD:277:ALA:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:HE:16:ASP:OD1	32:HE:131:THR:OG1	2.16	0.61
35:DD:895:HIS:CE1	35:DD:896:PRO:HD2	2.35	0.61
39:DH:137:GLY:HA3	39:DH:155:ASP:OD2	2.00	0.61
46:HI:140:PRO:CA	46:HI:202:ILE:HD11	2.30	0.61
52:n:1189:SER:O	52:n:1209:ARG:NH1	2.33	0.61
56:d:46:GLU:HA	58:i:76:MET:CE	2.30	0.61
56:d:100:VAL:HG13	58:i:128:LYS:HZ3	1.63	0.61
60:q:109:MET:HE3	60:q:109:MET:O	2.00	0.61
60:q:265:ALA:CB	60:q:340:GLN:OE1	2.48	0.61
67:h:142:SER:OG	68:k:39:LYS:HE2	2.00	0.61
72:p:698:ILE:HA	72:p:701:ARG:HG2	1.82	0.61
11:PA:1648:PRO:O	59:m:92:GLN:NE2	2.34	0.61
18:HC:397:GLU:OE2	33:HF:61:MET:HG3	1.99	0.61
52:n:679:SER:H	60:q:557:LEU:HD22	1.64	0.61
56:d:109:GLN:HA	56:d:112:LYS:HZ1	1.66	0.61
60:q:138:LYS:CD	60:q:140:ASN:OD1	2.40	0.61
60:q:142:GLN:H	60:q:142:GLN:CD	2.08	0.61
74:x:251:GLU:HG3	74:x:263:LEU:HD13	1.82	0.61
34:HH:371:VAL:HG23	34:HH:407:ILE:CG2	2.30	0.61
36:DE:613:ALA:HB2	36:DE:620:LEU:HD11	1.81	0.61
39:DH:54:GLU:OE1	43:DJ:197:MET:CG	2.48	0.61
47:HJ:175:LYS:HA	47:HJ:175:LYS:NZ	2.16	0.61
52:n:270:GLN:CG	57:f:181:LEU:HD11	2.29	0.61
54:u:90:LEU:HD21	60:q:7:VAL:HG23	1.82	0.61
55:a:514:LYS:HE2	55:a:518:ILE:HD11	1.82	0.61
71:v:120:ARG:HH11	71:v:120:ARG:CG	2.13	0.61
18:HC:265:LEU:CD1	18:HC:270:LEU:HD12	2.31	0.61
36:DE:526:ARG:HA	36:DE:526:ARG:CZ	2.29	0.61
37:DF:83:LEU:CD2	37:DF:86:PHE:CZ	2.79	0.61
37:DF:323:VAL:HG22	37:DF:323:VAL:O	2.00	0.61
60:q:647:SER:CB	64:e:93:CYS:HG	2.12	0.61
7:EA:139:LEU:CG	49:PG:151:ARG:CD	2.72	0.61
31:HG:87:LEU:HD22	31:HG:232:LEU:HD12	1.82	0.61
42:Dc:18:CYS:O	42:Dc:23:TRP:HB2	2.01	0.61
35:Dd:884:GLU:HA	35:Dd:887:LYS:HE3	1.82	0.61
54:u:80:GLU:HB2	61:z:563:VAL:CG2	2.31	0.61
55:a:127:HIS:CE1	55:a:171:THR:HG22	2.35	0.61
58:i:65:PHE:CE1	58:i:99:LYS:HG2	2.36	0.61
72:p:656:ARG:HG3	72:p:693:LEU:HD22	1.82	0.61
9:HA:405:THR:O	9:HA:409:THR:OG1	2.16	0.61
15:HB:422:LEU:HD22	32:HE:225:GLN:HE22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:104:LEU:HB3	43:DJ:217:PHE:HE2	1.51	0.61
52:n:206:THR:CG2	52:n:289:LEU:HB2	2.29	0.61
52:n:266:VAL:HG22	57:f:177:VAL:HG11	1.82	0.61
52:n:932:GLY:HA2	52:n:1179:HIS:NE2	2.15	0.61
58:i:119:GLN:OE1	58:i:119:GLN:HA	2.01	0.61
60:q:451:LEU:HD12	60:q:529:MET:HE1	0.63	0.61
69:r:195:PRO:HG3	71:v:8:PRO:N	2.16	0.61
72:p:148:GLU:HB3	72:p:370:VAL:HG21	1.82	0.61
74:x:650:LEU:HB2	74:x:659:TYR:HE2	1.64	0.61
22:PC:78:ILE:HD11	22:PC:126:ARG:HB3	1.82	0.61
30:HD:55:LYS:CE	49:PG:166:ASP:CB	2.79	0.61
36:DE:290:HIS:HB3	37:DF:45:TYR:CZ	2.36	0.61
52:n:199:LEU:HD22	52:n:222:VAL:HG13	1.83	0.61
52:n:274:ILE:CG1	57:f:181:LEU:CD2	2.79	0.61
52:n:320:TRP:HA	60:q:316:VAL:HG11	1.81	0.61
52:n:960:LYS:HZ1	52:n:1185:LEU:CD1	2.09	0.61
60:q:34:LEU:HD23	60:q:34:LEU:H	1.64	0.61
60:q:212:ALA:HA	60:q:387:LEU:HD22	1.82	0.61
63:c:214:VAL:H	63:c:243:THR:HG22	1.65	0.61
63:c:305:PHE:HD1	63:c:311:GLN:CD	2.09	0.61
67:h:99:VAL:O	67:h:99:VAL:HG23	2.01	0.61
67:h:151:LEU:HD21	71:v:37:ILE:HB	1.83	0.61
68:k:109:ARG:HH11	68:k:109:ARG:CG	2.14	0.61
72:p:225:ASN:ND2	72:p:245:CYS:SG	2.74	0.61
73:w:425:MET:N	73:w:425:MET:SD	2.72	0.61
52:n:354:VAL:HG12	52:n:355:HIS:H	1.64	0.61
52:n:651:ASN:CB	73:w:21:ALA:HB1	2.30	0.61
52:n:957:PRO:HG3	52:n:1214:VAL:HG21	1.83	0.61
73:w:281:ASP:OD1	73:w:281:ASP:N	2.31	0.61
1:X:-27:DA:C2	20:DP:169:VAL:HG21	2.36	0.60
9:HA:513:ASP:OD1	9:HA:516:VAL:N	2.29	0.60
11:PA:1477:ALA:HB1	49:PG:22:LEU:CD1	2.31	0.60
30:HD:53:LEU:HB3	30:HD:57:ASN:HB2	1.83	0.60
35:DD:996:LEU:O	35:DD:1000:ARG:HG3	2.01	0.60
40:Di:57:TYR:CE2	40:Di:73:LEU:HD11	2.36	0.60
46:HI:276:PHE:O	46:HI:277:LEU:C	2.43	0.60
48:PD:29:ALA:HB1	49:PG:4:HIS:O	2.01	0.60
50:g:159:ARG:HD3	50:g:159:ARG:C	2.26	0.60
52:n:1316:CYS:HA	52:n:1339:CYS:H	1.65	0.60
55:a:455:GLN:HB2	74:x:11:LEU:CD2	2.30	0.60
62:b:59:ARG:HH21	62:b:63:LEU:HD11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:e:71:GLU:OE1	64:e:74:ARG:NH2	2.33	0.60
68:k:101:ARG:HG2	68:k:101:ARG:HH11	1.66	0.60
70:t:175:VAL:HG21	70:t:192:GLN:HG3	1.82	0.60
71:v:127:LEU:HD12	71:v:127:LEU:O	2.01	0.60
72:p:443:LEU:HD23	72:p:457:LEU:HD21	1.82	0.60
74:x:944:LEU:HD13	74:x:971:THR:HG22	1.83	0.60
7:EA:69:ASP:HA	13:EB:225:VAL:HG23	1.84	0.60
7:EA:181:ASN:HD21	30:HD:9:CYS:HA	1.65	0.60
17:PB:794:VAL:HG13	17:PB:965:ILE:HG23	1.82	0.60
30:HD:42:GLY:O	49:PG:164:MET:CE	2.48	0.60
42:Dc:99:PHE:HB2	42:Dc:100:PRO:HD3	1.83	0.60
61:z:529:HIS:HA	61:z:568:ASP:HA	1.83	0.60
66:o:749:LEU:HD11	74:x:69:SER:C	2.26	0.60
70:t:136:ARG:HG3	70:t:136:ARG:O	2.00	0.60
9:HA:609:ASP:OD1	9:HA:669:ARG:NH2	2.34	0.60
12:DB:203:LYS:HD3	12:DB:237:MET:HE3	1.83	0.60
17:PB:851:ASP:OD2	29:PL:17:TYR:OH	2.19	0.60
37:DF:276:LEU:HD22	37:DF:323:VAL:CG2	2.31	0.60
37:DF:314:SER:O	37:DF:327:TRP:CH2	2.54	0.60
40:DI:23:LEU:CG	40:DI:39:MET:HE1	2.31	0.60
37:Df:330:ARG:HH22	37:Df:371:THR:HB	1.66	0.60
56:d:47:MET:HA	56:d:47:MET:HE3	1.82	0.60
57:f:101:ILE:CD1	67:h:105:VAL:CG1	2.80	0.60
60:q:155:GLY:CA	71:v:62:HIS:CE1	2.63	0.60
67:h:61:LYS:HG2	67:h:65:HIS:CE1	2.37	0.60
7:EA:105:TYR:OH	13:EB:237:LEU:HG	2.00	0.60
11:PA:29:ASP:OD2	11:PA:33:ARG:NH2	2.34	0.60
42:Dc:67:GLY:CA	43:Dj:116:LEU:CD1	2.70	0.60
56:d:126:TYR:CD2	60:q:36:MET:CB	2.77	0.60
57:f:108:ALA:HB2	67:h:77:ILE:HG23	1.83	0.60
58:i:96:GLU:CA	58:i:99:LYS:HG3	2.29	0.60
62:b:175:HIS:HB2	63:c:113:TRP:CZ2	2.33	0.60
63:c:238:VAL:HG22	63:c:292:LEU:CD2	2.31	0.60
30:HD:83:ASN:HD21	30:HD:140:LEU:HD13	1.67	0.60
34:HH:189:LEU:O	34:HH:195:ARG:NH1	2.33	0.60
37:DF:15:PRO:HD3	40:DI:18:MET:CG	2.23	0.60
42:Dc:67:GLY:CA	43:Dj:116:LEU:HD11	2.25	0.60
52:n:254:VAL:CG1	52:n:304:GLN:HG2	2.32	0.60
52:n:274:ILE:HG13	57:f:181:LEU:CD2	2.32	0.60
59:m:56:LEU:HG	59:m:80:GLN:HE22	1.65	0.60
60:q:534:VAL:HG11	60:q:567:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p:97:LEU:HD11	72:p:179:TRP:HB3	1.83	0.60
18:HC:18:ASN:OD1	18:HC:19:LEU:N	2.35	0.60
34:HH:707:GLU:O	34:HH:711:GLN:OE1	2.20	0.60
36:DE:447:THR:HA	36:DE:450:ARG:HB3	1.84	0.60
47:HJ:164:TYR:O	47:HJ:167:PHE:N	2.33	0.60
51:j:78:GLN:C	51:j:82:LYS:HE2	2.26	0.60
57:f:63:MET:HE2	57:f:64:VAL:H	1.66	0.60
60:q:36:MET:HE2	60:q:40:LEU:HD23	1.84	0.60
60:q:113:TYR:CB	67:h:19:VAL:HG11	2.30	0.60
60:q:504:VAL:HG11	60:q:524:PHE:CE2	2.37	0.60
31:HG:357:VAL:HG13	31:HG:366:VAL:HG23	1.83	0.60
37:Df:219:GLU:OE1	37:Df:219:GLU:N	2.26	0.60
47:HJ:33:LYS:O	47:HJ:33:LYS:HD3	2.00	0.60
50:g:171:LEU:HG	58:i:132:LEU:HD22	1.83	0.60
52:n:203:LEU:HD21	52:n:224:PHE:HZ	1.67	0.60
52:n:937:ARG:NE	52:n:943:LEU:CD2	2.65	0.60
52:n:941:TYR:HD2	52:n:1172:SER:CB	2.02	0.60
55:a:224:TYR:CZ	55:a:253:MET:HB3	2.36	0.60
55:a:443:CYS:SG	74:x:57:ASN:HB3	2.41	0.60
55:a:467:MET:HB3	55:a:475:VAL:HG11	1.84	0.60
64:e:91:THR:OG1	65:l:41:VAL:HG21	2.01	0.60
68:k:88:LYS:HD2	68:k:88:LYS:C	2.27	0.60
73:w:765:ARG:HA	73:w:768:LYS:HE2	1.84	0.60
9:HA:461:LEU:HD23	9:HA:464:LEU:CD2	2.31	0.60
11:PA:1652:PRO:HG3	67:h:107:ASP:OD1	2.02	0.60
17:PB:57:ARG:NE	17:PB:227:ASN:O	2.34	0.60
34:HH:128:SER:HG	34:HH:163:TYR:HH	1.47	0.60
40:DI:32:GLU:CB	40:DI:35:VAL:HG23	2.31	0.60
49:PG:10:GLU:HG2	49:PG:67:LEU:HD12	1.84	0.60
52:n:155:PRO:HA	52:n:158:ILE:HD12	1.83	0.60
52:n:651:ASN:OD1	52:n:680:HIS:NE2	2.34	0.60
52:n:904:PHE:CZ	52:n:1208:GLU:CG	2.74	0.60
55:a:232:LEU:HD13	55:a:232:LEU:O	2.02	0.60
55:a:503:SER:HB3	55:a:505:PRO:HD2	1.84	0.60
58:i:95:GLN:O	58:i:99:LYS:HG3	2.01	0.60
60:q:168:THR:CA	68:k:21:ILE:CD1	2.80	0.60
60:q:487:ILE:HD11	60:q:540:LEU:CD1	2.32	0.60
67:h:156:LYS:HG2	67:h:159:ARG:HH21	1.66	0.60
1:X:-27:DA:OP1	20:DP:299:ARG:NH2	2.35	0.60
9:HA:372:LEU:HD11	9:HA:404:ALA:HB1	1.84	0.60
35:DD:1058:VAL:CG2	41:DL:76:LEU:HD23	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:449:LYS:HG2	39:DH:144:PRO:HB2	1.83	0.60
36:DE:463:PHE:O	37:DF:134:HIS:N	2.34	0.60
45:Dm:31:LEU:HD23	45:Dm:31:LEU:N	2.16	0.60
48:PD:79:THR:HG22	67:h:51:LEU:HD22	0.60	0.60
54:u:78:SER:HB3	61:z:563:VAL:HG23	1.84	0.60
55:a:380:ALA:HB3	55:a:444:PRO:CG	2.32	0.60
63:c:238:VAL:HG23	70:t:121:ASP:OD2	2.02	0.60
9:HA:462:SER:OG	9:HA:463:PRO:HD2	2.02	0.60
12:DB:400:ASP:HA	12:DB:403:VAL:HG22	1.83	0.60
12:DB:672:PHE:CE1	18:HC:413:LEU:C	2.80	0.60
34:HH:415:HIS:NE2	34:HH:417:THR:OG1	2.35	0.60
36:DE:474:THR:OG1	36:DE:546:VAL:O	2.19	0.60
37:DF:65:LYS:O	37:DF:66:LEU:HB2	2.01	0.60
37:DF:274:ASN:CB	37:DF:317:LEU:HD23	2.28	0.60
52:n:168:ARG:NH1	59:m:108:TYR:CZ	2.69	0.60
52:n:315:LEU:HD22	52:n:319:ARG:HD2	1.84	0.60
56:d:27:ARG:HD2	58:i:108:HIS:CA	2.25	0.60
71:v:48:VAL:CG2	71:v:52:THR:OG1	2.49	0.60
7:EA:139:LEU:CG	49:PG:151:ARG:CB	2.80	0.59
30:HD:287:TYR:CB	46:HI:189:MET:HG2	2.32	0.59
37:DF:14:LEU:HD11	40:DI:19:MET:HE1	1.84	0.59
37:Df:349:ASN:HB3	37:Df:351:ILE:HG13	1.84	0.59
50:g:75:LYS:HZ2	61:z:562:GLY:HA3	1.67	0.59
52:n:226:VAL:HG13	52:n:230:PHE:H	1.66	0.59
52:n:545:LEU:HD11	52:n:653:PRO:CB	2.30	0.59
60:q:19:VAL:O	60:q:19:VAL:HG22	2.01	0.59
60:q:168:THR:HA	68:k:21:ILE:HD12	1.83	0.59
68:k:101:ARG:HH11	68:k:101:ARG:CG	2.14	0.59
11:PA:261:ARG:O	11:PA:261:ARG:HD2	2.02	0.59
27:PJ:8:PHE:CD2	27:PJ:48:MET:HE1	2.36	0.59
33:HF:36:GLN:NE2	33:HF:38:ILE:HG13	2.16	0.59
52:n:104:LYS:NZ	53:s:109:LEU:N	2.50	0.59
54:u:122:LEU:CD2	56:d:111:GLN:HG2	2.29	0.59
60:q:130:VAL:O	60:q:130:VAL:HG12	2.01	0.59
66:o:741:TRP:HE1	74:x:107:ARG:HB2	1.66	0.59
69:r:191:GLU:OE2	71:v:8:PRO:CA	2.50	0.59
7:EA:154:CYS:HB2	7:EA:157:CYS:SG	2.42	0.59
9:HA:628:THR:O	9:HA:628:THR:HG22	2.02	0.59
9:HA:664:VAL:HG22	9:HA:677:MET:HG2	1.83	0.59
35:DD:960:GLU:O	35:DD:963:ARG:HB2	2.00	0.59
41:DL:111:LEU:O	41:DL:114:LYS:HE3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:70:ARG:NH2	49:PG:142:GLU:OE2	2.35	0.59
54:u:67:LYS:CE	61:z:528:LEU:CD1	2.80	0.59
56:d:44:LEU:HD22	56:d:48:LEU:HD11	1.84	0.59
62:b:136:HIS:CG	63:c:111:TYR:CZ	2.90	0.59
75:y:45:GLU:O	75:y:48:ASN:O	2.21	0.59
7:EA:139:LEU:HD12	49:PG:151:ARG:NH1	2.17	0.59
12:DB:431:LEU:O	12:DB:431:LEU:HD23	2.02	0.59
22:PC:9:VAL:HG11	28:PK:105:PHE:HD1	1.68	0.59
32:HE:195:VAL:HG12	32:HE:203:LEU:HD23	1.85	0.59
37:DF:43:VAL:HG23	40:DI:46:TYR:CD2	2.37	0.59
37:DF:316:GLN:NE2	37:DF:320:ARG:HG3	2.18	0.59
39:DH:192:ARG:NH1	39:DH:209:SER:O	2.34	0.59
40:DI:23:LEU:CD1	40:DI:31:TYR:CZ	2.85	0.59
52:n:192:LEU:HD12	52:n:220:GLY:N	2.16	0.59
55:a:509:ARG:CZ	55:a:509:ARG:CB	2.79	0.59
60:q:184:ASN:CG	71:v:83:LYS:HD3	2.28	0.59
68:k:70:LEU:HD13	68:k:74:ALA:HB2	1.84	0.59
33:HF:36:GLN:HG2	33:HF:37:ASP:N	2.17	0.59
47:HJ:239:LYS:NZ	47:HJ:239:LYS:HB2	2.17	0.59
52:n:265:LEU:O	52:n:265:LEU:HD22	2.02	0.59
52:n:821:SER:O	52:n:833:ILE:HA	2.02	0.59
52:n:870:GLN:HG2	66:o:655:THR:CG2	2.31	0.59
57:f:106:TYR:CE2	67:h:106:PRO:HG3	2.38	0.59
60:q:190:LEU:HD23	60:q:291:TRP:CE3	2.38	0.59
64:e:136:LEU:CD1	68:k:107:VAL:HG12	2.32	0.59
6:DA:511:LEU:H	6:DA:511:LEU:HD12	1.68	0.59
37:DF:85:GLY:O	43:DJ:212:LYS:HG2	2.02	0.59
39:DH:50:PHE:CE2	43:DJ:170:ALA:C	2.80	0.59
54:u:122:LEU:HD22	54:u:125:ILE:HB	1.84	0.59
60:q:543:VAL:HG11	63:c:135:ARG:HE	1.66	0.59
62:b:179:LEU:CD1	64:e:60:VAL:C	2.76	0.59
66:o:639:TYR:CE2	72:p:786:HIS:CB	2.61	0.59
74:x:11:LEU:HB2	74:x:14:TRP:HE3	1.66	0.59
30:HD:55:LYS:HG3	49:PG:166:ASP:HB2	0.66	0.59
30:HD:55:LYS:CE	49:PG:166:ASP:HB2	2.33	0.59
35:DD:960:GLU:CG	35:DD:983:ARG:HH12	2.10	0.59
37:DF:104:LEU:HD13	43:DJ:217:PHE:CE2	2.33	0.59
47:HJ:181:LEU:O	47:HJ:181:LEU:HD22	2.03	0.59
48:PD:18:SER:O	48:PD:117:SER:OG	2.09	0.59
55:a:367:LEU:HD22	55:a:509:ARG:HH11	1.67	0.59
72:p:22:GLU:HB3	72:p:751:GLN:HE21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:w:895:ASP:O	73:w:899:ARG:NH1	2.35	0.59
11:PA:1796:SER:HB2	60:q:24:LEU:HD22	1.85	0.59
13:EB:144:ASN:HB3	13:EB:174:ALA:HB1	1.84	0.59
31:HG:88:LEU:HD22	31:HG:131:LEU:HD21	1.84	0.59
36:DE:433:LYS:CD	40:DI:110:TYR:CZ	2.83	0.59
37:DF:122:LEU:HD12	37:DF:122:LEU:N	2.18	0.59
37:DF:317:LEU:H	37:DF:317:LEU:CD2	2.15	0.59
55:a:462:LEU:CG	74:x:49:GLN:CD	2.73	0.59
57:f:142:SER:OG	60:q:183:PHE:CD2	2.55	0.59
70:t:6:VAL:HA	70:t:140:VAL:O	2.03	0.59
74:x:414:GLU:OE2	74:x:460:LYS:NZ	2.34	0.59
5:BA:248:ARG:NH2	5:BA:287:GLN:OE1	2.36	0.59
6:DA:1068:ARG:HD2	6:DA:1068:ARG:C	2.27	0.59
15:HB:417:LYS:HA	15:HB:421:VAL:HG23	1.85	0.59
17:PB:274:ARG:NH2	17:PB:281:ASP:OD1	2.36	0.59
34:HH:625:GLN:OE1	34:HH:639:ARG:NH1	2.36	0.59
35:DD:1057:ARG:HA	41:DL:75:GLN:O	2.02	0.59
46:HI:207:LEU:HD22	57:f:52:MET:HE1	1.85	0.59
54:u:122:LEU:HB2	56:d:114:LEU:HD21	1.84	0.59
55:a:375:PHE:CG	74:x:17:ARG:NH2	2.69	0.59
56:d:42:ARG:NH2	58:i:96:GLU:OE1	2.35	0.59
66:o:636:HIS:HE2	66:o:640:ARG:HH21	1.50	0.59
14:FB:80:GLU:OE2	14:FB:81:HIS:N	2.35	0.59
24:PF:64:ARG:HH21	49:PG:61:PRO:CG	2.15	0.59
24:PF:72:GLN:HE22	49:PG:59:ILE:HD11	1.68	0.59
37:DF:82:PRO:HB2	37:DF:98:SER:CB	2.33	0.59
36:De:562:SER:OG	36:De:564:ASP:OD1	2.21	0.59
47:HJ:177:ARG:HB2	47:HJ:177:ARG:CZ	2.32	0.59
48:PD:76:ASN:ND2	67:h:47:ASP:HB3	2.15	0.59
52:n:237:MET:HE1	60:q:45:GLN:CG	2.32	0.59
54:u:67:LYS:HE3	61:z:528:LEU:CD1	2.32	0.59
60:q:591:LYS:NZ	60:q:593:MET:SD	2.76	0.59
60:q:597:PRO:HA	60:q:619:ARG:HA	1.84	0.59
7:EA:178:ALA:CA	30:HD:8:ARG:O	2.49	0.58
15:HB:471:LEU:HD12	15:HB:472:LEU:HD22	1.84	0.58
36:De:484:LEU:HD21	36:De:504:LEU:HD21	1.85	0.58
52:n:234:LEU:HD21	52:n:282:LEU:CD2	2.33	0.58
52:n:250:LEU:HG	52:n:275:HIS:HA	1.85	0.58
52:n:375:ASP:HB3	52:n:376:PRO:HD3	1.85	0.58
52:n:377:PRO:HG2	52:n:408:ARG:HH21	1.66	0.58
54:u:90:LEU:HD21	60:q:9:ILE:HD11	1.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:o:718:VAL:HG11	66:o:743:TYR:CE1	2.38	0.58
67:h:8:LEU:HD23	67:h:8:LEU:O	2.03	0.58
70:t:131:MET:O	70:t:131:MET:HE3	2.03	0.58
72:p:61:MET:HE2	72:p:75:SER:HB3	1.85	0.58
6:DA:401:ASN:H	6:DA:401:ASN:HD22	1.51	0.58
7:EA:144:LEU:HD22	7:EA:155:THR:H	1.68	0.58
14:FB:189:SER:HB3	35:DD:991:MET:CE	2.25	0.58
35:DD:898:VAL:O	35:DD:902:VAL:HG23	2.03	0.58
36:DE:432:LEU:HG	36:DE:436:ASP:CG	2.28	0.58
37:DF:14:LEU:HD23	40:DI:22:ILE:HD12	1.84	0.58
37:DF:83:LEU:HD12	37:DF:83:LEU:N	2.17	0.58
40:DI:23:LEU:HD12	40:DI:31:TYR:CZ	2.37	0.58
46:HI:239:ASP:CA	46:HI:242:SER:HB3	2.28	0.58
52:n:960:LYS:HZ3	52:n:1185:LEU:HD13	1.66	0.58
54:u:75:SER:CB	61:z:566:CYS:SG	2.91	0.58
55:a:131:ASN:H	55:a:131:ASN:HD22	1.50	0.58
60:q:102:LEU:HD22	67:h:26:LEU:HD22	1.84	0.58
60:q:124:PHE:CD2	67:h:89:LEU:HD11	2.38	0.58
67:h:97:VAL:HG23	67:h:104:VAL:HG21	1.85	0.58
67:h:150:LEU:HD21	68:k:45:LEU:HD13	1.81	0.58
70:t:8:GLN:HG3	70:t:196:LEU:HD21	1.84	0.58
71:v:48:VAL:HG22	71:v:52:THR:OG1	2.03	0.58
72:p:166:PRO:HG2	72:p:169:THR:HG22	1.84	0.58
54:u:115:LEU:HD12	56:d:121:LEU:CB	2.24	0.58
55:a:375:PHE:CB	74:x:17:ARG:CZ	2.81	0.58
60:q:157:ALA:HB1	68:k:32:ILE:HG13	1.85	0.58
73:w:53:GLN:O	73:w:56:HIS:HB2	2.04	0.58
12:DB:489:GLN:OE1	12:DB:489:GLN:N	2.34	0.58
30:HD:288:THR:O	30:HD:290:SER:N	2.36	0.58
32:HE:52:ASN:OD1	32:HE:53:ARG:N	2.37	0.58
37:DF:320:ARG:O	37:DF:322:ASP:N	2.36	0.58
41:DL:71:ASP:CB	41:DL:74:GLU:CG	2.79	0.58
47:HJ:114:LYS:HA	47:HJ:114:LYS:HE2	1.84	0.58
52:n:371:GLN:HG3	52:n:390:MET:HE1	1.84	0.58
54:u:90:LEU:HB2	60:q:9:ILE:CG1	2.31	0.58
55:a:160:LEU:CD1	55:a:214:ARG:NH2	2.67	0.58
59:m:56:LEU:CD2	59:m:80:GLN:HE22	2.12	0.58
60:q:162:LYS:O	60:q:166:ARG:CG	2.51	0.58
60:q:400:PHE:CE2	69:r:142:LYS:HB2	2.39	0.58
62:b:136:HIS:CG	63:c:111:TYR:CE1	2.91	0.58
66:o:691:VAL:HA	66:o:708:CYS:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:o:749:LEU:HD12	74:x:69:SER:HB2	1.84	0.58
25:PH:102:ASP:OD2	25:PH:110:THR:OG1	2.21	0.58
39:DH:114:SER:C	39:DH:116:ARG:H	2.11	0.58
47:HJ:201:THR:C	47:HJ:203:ALA:H	2.11	0.58
48:PD:74:PHE:HA	48:PD:141:GLN:HE22	1.68	0.58
50:g:128:PRO:HB3	56:d:149:ILE:HG21	1.86	0.58
51:j:82:LYS:HD2	53:s:101:VAL:HG11	1.85	0.58
52:n:528:HIS:HB3	52:n:530:ILE:HG22	1.84	0.58
52:n:544:ARG:HD3	52:n:716:ASN:O	2.04	0.58
56:d:167:TRP:CE3	59:m:106:GLN:CD	2.82	0.58
69:r:192:GLN:HE22	71:v:11:LYS:HG3	1.69	0.58
9:HA:262:ASN:O	9:HA:266:LEU:HD23	2.03	0.58
27:PJ:64:PRO:O	29:PL:23:HIS:NE2	2.36	0.58
34:HH:266:GLN:N	34:HH:266:GLN:NE2	2.49	0.58
37:DF:323:VAL:HA	37:DF:326:HIS:CD2	2.36	0.58
40:Di:57:TYR:CD2	40:Di:73:LEU:HD21	2.39	0.58
46:HI:132:TRP:HA	46:HI:132:TRP:CE3	2.38	0.58
52:n:250:LEU:HG	52:n:275:HIS:CA	2.33	0.58
54:u:117:LYS:HD3	58:i:140:MET:HA	1.85	0.58
57:f:145:TYR:OH	67:h:43:PRO:HG3	2.03	0.58
60:q:184:ASN:ND2	71:v:83:LYS:HD2	2.17	0.58
64:e:129:VAL:HG11	68:k:114:MET:HE2	1.84	0.58
17:PB:407:MET:HE1	17:PB:444:LEU:CD2	2.33	0.58
36:DE:432:LEU:HG	36:DE:436:ASP:CB	2.34	0.58
37:DF:118:ILE:HA	39:DH:39:VAL:HG13	1.86	0.58
37:DF:320:ARG:C	37:DF:322:ASP:H	2.12	0.58
46:HI:86:ASN:ND2	46:HI:86:ASN:C	2.58	0.58
52:n:169:LEU:HA	59:m:104:HIS:CB	2.31	0.58
52:n:234:LEU:HD22	52:n:245:TRP:HB3	1.86	0.58
60:q:188:LEU:HA	71:v:87:ILE:CG1	2.34	0.58
70:t:78:LEU:HD22	70:t:78:LEU:N	2.18	0.58
7:EA:122:THR:HG23	30:HD:40:VAL:CG2	2.29	0.58
11:PA:111:CYS:SG	11:PA:188:GLN:NE2	2.77	0.58
11:PA:357:LYS:NZ	17:PB:1107:LEU:O	2.33	0.58
11:PA:1662:PRO:HD3	57:f:16:VAL:O	2.04	0.58
13:EB:141:PRO:O	13:EB:146:ARG:NH1	2.36	0.58
37:DF:316:GLN:HB2	37:DF:327:TRP:CE3	2.39	0.58
56:d:45:ILE:CG2	58:i:76:MET:CG	2.81	0.58
71:v:16:GLN:HE21	71:v:20:LYS:HE2	0.76	0.58
12:DB:769:LYS:O	12:DB:769:LYS:HG3	2.03	0.58
30:HD:145:GLU:OE1	67:h:67:LYS:CE	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:HH:281:GLN:NE2	34:HH:482:PHE:O	2.37	0.58
35:DD:910:LEU:HD11	41:DL:88:ALA:HB2	1.85	0.58
36:DE:586:TYR:HB3	36:DE:605:HIS:HB3	1.84	0.58
37:DF:316:GLN:HE22	37:DF:320:ARG:HA	1.68	0.58
62:b:78:ALA:CB	66:o:621:LEU:HD21	2.31	0.58
70:t:9:MET:H	70:t:138:ILE:HG22	1.68	0.58
17:PB:867:ILE:HB	17:PB:894:THR:HG22	1.85	0.58
17:PB:1143:LYS:HE2	49:PG:152:VAL:HG13	1.84	0.58
30:HD:43:ALA:HB3	49:PG:164:MET:CE	2.33	0.58
41:DL:91:PHE:O	41:DL:95:VAL:HG23	2.03	0.58
46:HI:30:ARG:CZ	46:HI:30:ARG:HB3	2.34	0.58
46:HI:136:ARG:HB2	46:HI:159:ALA:HA	1.85	0.58
63:c:162:VAL:HG13	63:c:207:LEU:HD13	1.86	0.58
67:h:86:ASP:H	67:h:99:VAL:HG12	1.67	0.58
70:t:124:VAL:HG13	70:t:142:VAL:HG22	1.86	0.58
73:w:726:ASN:ND2	73:w:726:ASN:H	2.02	0.58
12:DB:672:PHE:HZ	18:HC:413:LEU:HB2	1.65	0.57
15:HB:422:LEU:HD22	32:HE:225:GLN:NE2	2.19	0.57
36:DE:450:ARG:HG3	36:DE:789:ASN:ND2	2.19	0.57
52:n:956:ALA:HB3	52:n:1217:ARG:NH2	2.18	0.57
55:a:66:GLN:HA	56:d:66:LEU:HD21	1.86	0.57
60:q:93:TRP:N	60:q:94:PRO:HD2	2.19	0.57
62:b:178:LEU:CD2	65:l:82:LEU:HD11	2.33	0.57
71:v:122:GLU:OE1	71:v:122:GLU:HA	2.05	0.57
6:DA:929:THR:HG22	6:DA:954:ALA:HA	1.86	0.57
11:PA:1650:TYR:CD1	60:q:111:VAL:HG21	2.40	0.57
12:DB:732:CYS:SG	39:DH:173:GLN:HB2	2.44	0.57
13:EB:167:LEU:HD23	13:EB:198:LYS:HD3	1.86	0.57
22:PC:7:PRO:O	28:PK:104:ARG:NH1	2.37	0.57
36:DE:694:LEU:CD1	36:DE:703:MET:CE	2.39	0.57
36:DE:742:LYS:HA	36:DE:745:GLU:HG2	1.85	0.57
48:PD:134:ILE:HD12	48:PD:137:LYS:CD	2.34	0.57
50:g:164:ILE:HD12	58:i:140:MET:HE3	1.86	0.57
52:n:685:LEU:CD2	66:o:729:TYR:HE2	2.17	0.57
52:n:944:PHE:HE2	72:p:677:THR:OG1	1.86	0.57
55:a:267:LYS:H	55:a:267:LYS:HD2	1.69	0.57
65:l:160:MET:HE1	71:v:134:TYR:CD2	2.39	0.57
67:h:85:ARG:HD2	67:h:99:VAL:HG11	1.85	0.57
8:FA:142:ASN:OD1	8:FA:143:TRP:N	2.37	0.57
18:HC:58:ARG:HD2	32:HE:229:TRP:CE3	2.39	0.57
46:HI:135:HIS:HD2	46:HI:137:ASP:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:HJ:114:LYS:HA	47:HJ:114:LYS:CE	2.33	0.57
54:u:80:GLU:HB3	61:z:539:ASP:CG	2.28	0.57
56:d:38:GLU:OE2	58:i:96:GLU:HB3	2.02	0.57
73:w:9:PHE:HE2	73:w:63:ILE:HG12	1.69	0.57
73:w:764:TYR:OH	73:w:799:GLU:OE2	2.22	0.57
74:x:404:GLN:NE2	74:x:408:GLN:OE1	2.37	0.57
7:EA:181:ASN:ND2	30:HD:10:LYS:H	2.01	0.57
30:HD:282:ASP:O	30:HD:285:GLY:N	2.36	0.57
42:Dc:21:LEU:C	42:Dc:21:LEU:HD12	2.29	0.57
47:HJ:87:PHE:CD1	47:HJ:87:PHE:C	2.82	0.57
49:PG:38:CYS:SG	49:PG:39:THR:N	2.78	0.57
57:f:101:ILE:CD1	67:h:105:VAL:HG11	2.33	0.57
60:q:38:GLN:HB2	60:q:42:ARG:HH21	1.70	0.57
60:q:113:TYR:HD2	67:h:19:VAL:HG12	1.67	0.57
60:q:645:ALA:HB2	64:e:100:LEU:HD22	1.85	0.57
66:o:756:MET:O	66:o:760:LEU:HG	2.05	0.57
67:h:151:LEU:CD2	71:v:37:ILE:HB	2.34	0.57
73:w:369:ARG:NH1	73:w:402:LEU:O	2.37	0.57
19:DO:62:LEU:HA	19:DO:76:LEU:HD23	1.86	0.57
30:HD:35:VAL:HG13	30:HD:58:PHE:CE2	2.39	0.57
30:HD:43:ALA:HB1	49:PG:164:MET:CG	2.17	0.57
32:HE:215:LEU:HD22	32:HE:230:VAL:HG21	1.86	0.57
37:DF:312:ILE:HG13	37:DF:334:ALA:HB3	1.86	0.57
39:DH:50:PHE:CZ	43:DJ:171:LEU:N	2.72	0.57
55:a:160:LEU:CD1	55:a:219:LEU:HD21	2.33	0.57
55:a:504:ILE:N	55:a:505:PRO:CD	2.67	0.57
62:b:101:ARG:HH12	72:p:677:THR:HB	1.68	0.57
6:DA:1063:LYS:C	6:DA:1063:LYS:HD3	2.28	0.57
30:HD:84:LYS:CB	30:HD:136:ASN:ND2	2.68	0.57
40:DI:53:ASP:HB2	40:DI:74:ALA:HB1	1.87	0.57
47:HJ:275:GLN:CD	47:HJ:275:GLN:C	2.73	0.57
52:n:166:TYR:HH	59:m:70:PRO:C	2.12	0.57
52:n:274:ILE:HD11	57:f:181:LEU:CD2	2.34	0.57
52:n:647:MET:HE1	73:w:22:PHE:HB2	1.87	0.57
52:n:651:ASN:HB3	73:w:21:ALA:CB	2.33	0.57
52:n:933:VAL:CG2	52:n:1176:ILE:HB	2.34	0.57
60:q:437:HIS:CE1	60:q:472:GLU:H	2.21	0.57
67:h:33:LEU:HD23	67:h:40:LEU:HD23	1.86	0.57
1:X:-5:DT:H3	2:Y:5:DA:N6	2.00	0.57
11:PA:223:GLU:OE2	13:EB:232:LYS:NZ	2.38	0.57
11:PA:668:PHE:CE1	11:PA:672:ILE:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PA:1245:CYS:O	11:PA:1246:ILE:HD13	2.03	0.57
12:DB:672:PHE:HZ	18:HC:413:LEU:CD1	2.06	0.57
13:EB:122:GLU:OE2	13:EB:126:ASN:OD1	2.22	0.57
17:PB:1144:THR:HG21	49:PG:41:LYS:HB2	1.85	0.57
18:HC:397:GLU:OE1	33:HF:61:MET:CE	2.53	0.57
40:DI:132:LEU:CD2	43:DJ:121:MET:HE2	2.35	0.57
52:n:237:MET:CE	60:q:45:GLN:CG	2.83	0.57
52:n:686:LYS:NZ	66:o:730:PRO:CB	2.48	0.57
52:n:904:PHE:CZ	52:n:1208:GLU:CB	2.88	0.57
71:v:108:LEU:HD12	71:v:108:LEU:O	2.04	0.57
74:x:11:LEU:C	74:x:13:ALA:N	2.59	0.57
75:y:183:VAL:HG13	75:y:221:VAL:HG22	1.86	0.57
4:NY:-84:DG:H2''	4:NY:-83:DG:C8	2.39	0.57
7:EA:114:ILE:HG23	7:EA:177:LEU:HD22	1.86	0.57
55:a:462:LEU:HB2	74:x:49:GLN:CA	2.35	0.57
60:q:110:CYS:SG	67:h:23:LYS:HD3	2.45	0.57
62:b:103:ASP:OD1	62:b:103:ASP:N	2.23	0.57
69:r:38:ARG:NH1	69:r:192:GLN:HG3	2.19	0.57
72:p:443:LEU:C	72:p:443:LEU:HD12	2.30	0.57
73:w:855:TRP:O	73:w:858:ASN:ND2	2.37	0.57
9:HA:240:ASP:OD1	9:HA:241:ASN:N	2.37	0.57
9:HA:345:ARG:CD	30:HD:1:MET:SD	2.93	0.57
30:HD:55:LYS:CD	49:PG:166:ASP:HB3	2.34	0.57
30:HD:84:LYS:HA	30:HD:136:ASN:CG	2.29	0.57
36:DE:345:MET:HE3	36:DE:346:PRO:HD2	1.87	0.57
40:DI:131:SER:CB	43:DJ:150:ARG:HH12	2.16	0.57
46:HI:52:LYS:HA	46:HI:52:LYS:CE	2.14	0.57
46:HI:146:ASP:OD1	46:HI:149:GLY:N	2.33	0.57
47:HJ:175:LYS:HA	47:HJ:175:LYS:HZ2	1.70	0.57
52:n:319:ARG:HG3	52:n:320:TRP:HD1	1.70	0.57
52:n:321:GLY:HA3	60:q:317:GLN:HE21	1.70	0.57
54:u:122:LEU:CG	56:d:111:GLN:HE21	2.17	0.57
55:a:416:ALA:HB1	55:a:472:SER:O	2.04	0.57
58:i:118:LEU:HD23	58:i:118:LEU:C	2.30	0.57
66:o:741:TRP:NE1	74:x:107:ARG:HB2	2.20	0.57
67:h:139:GLN:NE2	68:k:37:LYS:CB	2.68	0.57
68:k:63:LEU:HD23	71:v:22:LEU:HD13	1.87	0.57
6:DA:675:ASP:OD1	38:DG:78:LYS:NZ	2.37	0.57
9:HA:664:VAL:HG21	9:HA:679:PHE:CE1	2.40	0.57
37:DF:81:GLU:OE2	37:DF:91:PHE:CD1	2.57	0.57
37:DF:86:PHE:HA	43:DJ:212:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:315:ARG:CZ	37:DF:369:PRO:HB3	2.35	0.57
40:DI:16:ALA:HA	40:DI:40:LEU:CD1	2.23	0.57
52:n:944:PHE:CE2	72:p:677:THR:OG1	2.57	0.57
52:n:957:PRO:CG	52:n:1214:VAL:HG21	2.35	0.57
55:a:316:ALA:CB	55:a:447:GLU:HG2	2.34	0.57
55:a:382:LEU:CD2	55:a:446:SER:CA	2.82	0.57
60:q:168:THR:HA	68:k:21:ILE:CD1	2.34	0.57
71:v:47:GLN:OE1	71:v:47:GLN:HA	2.05	0.57
7:EA:185:GLU:HB2	30:HD:14:TYR:OH	2.04	0.56
13:EB:83:ASN:O	13:EB:87:THR:HG23	2.05	0.56
25:PH:33:GLU:OE2	25:PH:55:LYS:NZ	2.38	0.56
37:DF:22:VAL:HG13	40:DI:44:PHE:HE1	1.68	0.56
42:Dc:12:VAL:HG23	37:Df:118:ILE:HA	1.86	0.56
40:Di:73:LEU:HD13	41:DI:105:HIS:CE1	2.40	0.56
46:HI:15:LEU:H	46:HI:29:ALA:HB2	1.69	0.56
52:n:250:LEU:CG	52:n:275:HIS:HB2	2.34	0.56
52:n:820:ILE:HD11	52:n:833:ILE:HB	1.86	0.56
55:a:259:ILE:HD12	55:a:259:ILE:N	2.20	0.56
59:m:116:GLN:HG2	61:z:595:PRO:HD3	1.86	0.56
72:p:580:LEU:HD21	72:p:657:GLU:HB3	1.86	0.56
9:HA:345:ARG:HD3	30:HD:1:MET:SD	2.45	0.56
17:PB:223:SER:HG	17:PB:350:HIS:CE1	2.20	0.56
30:HD:283:LEU:HD23	30:HD:283:LEU:C	2.29	0.56
31:HG:261:SER:OG	31:HG:265:GLN:O	2.23	0.56
32:HE:241:LEU:HD23	32:HE:243:LEU:HD11	1.86	0.56
35:DD:966:LEU:CD1	35:DD:982:LEU:HD23	2.32	0.56
37:DF:276:LEU:HA	37:DF:330:ARG:HH22	1.70	0.56
39:DH:194:MET:HE1	37:Df:226:GLU:HG3	1.86	0.56
40:DI:81:GLN:NE2	41:DL:123:GLN:CD	2.56	0.56
46:HI:84:LYS:HZ2	46:HI:84:LYS:HA	1.70	0.56
46:HI:239:ASP:C	46:HI:239:ASP:OD1	2.48	0.56
72:p:251:GLU:HG2	72:p:252:LYS:HG2	1.86	0.56
9:HA:44:SER:OG	9:HA:46:THR:O	2.17	0.56
17:PB:91:ILE:HD13	17:PB:126:VAL:HG12	1.87	0.56
35:DD:873:LEU:CD1	35:DD:873:LEU:H	2.18	0.56
39:DH:137:GLY:O	39:DH:155:ASP:CG	2.47	0.56
41:DL:71:ASP:O	41:DL:73:ASN:N	2.37	0.56
41:DL:113:VAL:HG13	41:DL:113:VAL:O	2.06	0.56
37:Df:223:TYR:HD2	37:Df:255:MET:HE1	1.71	0.56
47:HJ:228:MET:HB3	47:HJ:231:TYR:HB2	1.88	0.56
48:PD:100:LEU:HD12	48:PD:101:ALA:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:154:ILE:HB	52:n:155:PRO:CD	2.35	0.56
52:n:706:LEU:HD22	60:q:615:TRP:CH2	2.40	0.56
52:n:960:LYS:HG3	52:n:1210:PHE:CE2	2.38	0.56
54:u:108:VAL:HG22	56:d:128:ALA:HB1	1.86	0.56
55:a:430:LEU:N	55:a:430:LEU:HD23	2.20	0.56
55:a:463:VAL:HG11	55:a:488:ILE:CD1	2.35	0.56
57:f:101:ILE:HD11	67:h:78:PRO:HG3	1.86	0.56
60:q:109:MET:HG3	67:h:22:LEU:HG	1.86	0.56
63:c:176:MET:HE1	63:c:267:MET:HB3	1.86	0.56
67:h:12:LEU:HD13	67:h:12:LEU:O	2.05	0.56
68:k:60:GLU:HG2	71:v:22:LEU:HD11	1.86	0.56
73:w:433:ASN:ND2	73:w:445:ILE:O	2.35	0.56
74:x:376:ALA:O	74:x:380:ASN:ND2	2.38	0.56
76:NC:840:THR:O	76:NC:841:THR:CB	2.53	0.56
8:FA:171:LEU:HD21	11:PA:1279:MET:HA	1.88	0.56
40:DI:31:TYR:CD2	40:DI:35:VAL:HB	2.41	0.56
54:u:128:SER:OG	58:i:131:LEU:CD2	2.49	0.56
55:a:364:TYR:CB	55:a:430:LEU:CD1	2.54	0.56
11:PA:1030:SER:OG	23:PE:162:ARG:NE	2.34	0.56
15:HB:432:THR:O	15:HB:435:SER:OG	2.10	0.56
17:PB:643:LEU:HD11	17:PB:656:LEU:HD11	1.87	0.56
17:PB:694:THR:HG22	17:PB:695:HIS:CE1	2.41	0.56
17:PB:910:THR:HG22	17:PB:911:LEU:N	2.18	0.56
35:DD:873:LEU:HD12	35:DD:873:LEU:H	1.69	0.56
36:DE:773:TYR:HA	37:DF:142:GLN:OE1	2.05	0.56
39:DH:50:PHE:CZ	43:DJ:195:LEU:HD13	2.40	0.56
35:Dd:917:ILE:HD11	35:Dd:1063:LEU:HD13	1.87	0.56
37:Df:320:ARG:CB	37:Df:320:ARG:HH11	2.18	0.56
52:n:507:GLN:HE22	52:n:637:PHE:HA	1.69	0.56
55:a:401:PRO:O	55:a:405:PRO:HD3	2.04	0.56
55:a:441:GLU:HB3	74:x:14:TRP:HE1	1.69	0.56
60:q:112:LEU:CD2	67:h:19:VAL:CG2	2.84	0.56
60:q:186:GLU:OE2	60:q:291:TRP:CE2	2.58	0.56
60:q:188:LEU:HA	71:v:87:ILE:HD12	1.81	0.56
60:q:188:LEU:HD22	71:v:87:ILE:CG1	2.35	0.56
62:b:179:LEU:HD11	64:e:60:VAL:C	2.30	0.56
64:e:140:GLN:HE22	68:k:105:SER:HA	1.65	0.56
65:l:156:LEU:CD2	71:v:134:TYR:HB2	2.34	0.56
74:x:581:ILE:HD11	74:x:616:LEU:HD22	1.87	0.56
75:y:195:PHE:O	75:y:224:ARG:NH1	2.38	0.56
76:NC:842:SER:C	76:NC:844:GLY:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:DB:61:ASN:O	12:DB:130:VAL:HG23	2.06	0.56
12:DB:560:TYR:CD2	12:DB:581:ILE:HD11	2.40	0.56
37:DF:71:ILE:CD1	40:DI:35:VAL:HG22	2.36	0.56
37:DF:217:SER:OG	39:DH:161:LYS:HA	2.05	0.56
39:DH:108:PRO:CG	43:DJ:116:LEU:HD21	2.34	0.56
40:DI:132:LEU:HD11	43:DJ:121:MET:SD	2.45	0.56
52:n:706:LEU:HB2	52:n:725:VAL:HG23	1.87	0.56
55:a:127:HIS:HE1	55:a:171:THR:CG2	2.19	0.56
56:d:45:ILE:HD13	58:i:72:ILE:O	2.05	0.56
56:d:47:MET:HE3	56:d:47:MET:CA	2.35	0.56
73:w:261:ASP:OD1	73:w:261:ASP:N	2.38	0.56
11:PA:1796:SER:CB	60:q:24:LEU:HD22	2.36	0.56
13:EB:108:HIS:O	13:EB:111:ILE:HG22	2.06	0.56
17:PB:346:GLU:N	17:PB:346:GLU:OE1	2.38	0.56
36:DE:433:LYS:CG	40:DI:110:TYR:OH	2.52	0.56
36:DE:464:TYR:HA	37:DF:133:ALA:HA	1.87	0.56
36:DE:645:GLY:H	36:DE:675:LEU:HD11	1.70	0.56
36:DE:697:ASP:HB2	36:DE:704:VAL:HG21	1.88	0.56
37:DF:360:THR:O	37:DF:364:VAL:HG22	2.06	0.56
47:HJ:167:PHE:HD1	47:HJ:167:PHE:C	2.12	0.56
49:PG:166:ASP:OD1	49:PG:167:TYR:N	2.38	0.56
52:n:250:LEU:CD2	52:n:275:HIS:CB	2.84	0.56
52:n:685:LEU:HD22	66:o:729:TYR:CE2	2.40	0.56
52:n:693:ILE:HD11	52:n:775:ARG:HG2	1.88	0.56
55:a:462:LEU:HG	74:x:49:GLN:OE1	2.05	0.56
61:z:551:ASP:OD1	61:z:551:ASP:N	2.37	0.56
61:z:577:THR:O	61:z:595:PRO:HB3	2.04	0.56
72:p:710:ASP:OD1	72:p:710:ASP:N	2.34	0.56
74:x:172:THR:HB	74:x:965:LYS:HE2	1.88	0.56
6:DA:353:LEU:HD21	37:Df:272:VAL:HG21	1.88	0.56
7:EA:22:ILE:HD11	7:EA:26:TYR:CD2	2.41	0.56
11:PA:1411:LEU:O	11:PA:1421:ARG:NH2	2.39	0.56
17:PB:755:GLN:HE22	27:PJ:48:MET:HE2	1.70	0.56
39:DH:50:PHE:CD1	39:DH:50:PHE:N	2.73	0.56
52:n:104:LYS:HZ1	53:s:109:LEU:H	1.50	0.56
52:n:199:LEU:HD13	52:n:222:VAL:HG13	1.88	0.56
56:d:42:ARG:NH2	58:i:93:LYS:CG	2.69	0.56
58:i:75:CYS:HB3	58:i:88:ASN:HD21	1.70	0.56
58:i:103:THR:O	58:i:107:ILE:HB	2.05	0.56
60:q:395:PRO:HG3	69:r:75:SER:HB3	1.87	0.56
60:q:578:TYR:CE1	60:q:646:LEU:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:t:66:MET:HG2	70:t:78:LEU:HD21	1.87	0.56
6:DA:396:LEU:HD13	6:DA:396:LEU:N	2.19	0.56
19:DO:29:THR:HG23	19:DO:32:LEU:H	1.69	0.56
36:DE:290:HIS:CD2	37:DF:45:TYR:CD2	2.94	0.56
39:DH:108:PRO:HG2	43:DJ:116:LEU:HD23	1.88	0.56
42:Dc:67:GLY:CA	43:Dj:116:LEU:HD13	2.33	0.56
46:HI:241:CYS:O	46:HI:241:CYS:SG	2.63	0.56
52:n:97:VAL:CG2	53:s:109:LEU:HG	2.35	0.56
52:n:643:HIS:CE1	60:q:560:ILE:HG13	2.41	0.56
54:u:67:LYS:CE	61:z:528:LEU:HD11	2.36	0.56
55:a:462:LEU:HD12	74:x:60:ILE:HD12	1.87	0.56
60:q:562:SER:HB2	60:q:587:GLU:HB2	1.87	0.56
63:c:305:PHE:CG	63:c:311:GLN:CB	2.86	0.56
67:h:81:LEU:HD12	67:h:101:SER:O	2.06	0.56
67:h:102:HIS:CD2	67:h:102:HIS:N	2.73	0.56
11:PA:621:ILE:HG23	11:PA:621:ILE:O	2.06	0.56
11:PA:1793:THR:H	67:h:102:HIS:HE1	1.54	0.56
11:PA:1798:SER:CA	60:q:25:ASP:OD2	2.47	0.56
15:HB:456:ASP:OD1	15:HB:457:ILE:HD12	2.06	0.56
17:PB:474:THR:OG1	17:PB:732:ALA:O	2.24	0.56
31:HG:345:CYS:O	31:HG:349:GLN:N	2.36	0.56
34:HH:361:CYS:SG	34:HH:405:VAL:HG13	2.46	0.56
34:HH:444:HIS:O	34:HH:472:ARG:NH1	2.39	0.56
37:DF:104:LEU:HB2	43:DJ:217:PHE:HZ	1.70	0.56
37:Df:352:GLN:O	37:Df:356:THR:OG1	2.24	0.56
52:n:118:ILE:HG12	53:s:83:LEU:HB3	1.87	0.56
53:s:106:SER:C	53:s:108:PHE:N	2.56	0.56
56:d:164:PRO:HD2	56:d:167:TRP:CG	2.40	0.56
57:f:82:ARG:HD2	57:f:84:GLN:HE21	1.71	0.56
60:q:437:HIS:HD2	60:q:437:HIS:O	1.89	0.56
62:b:136:HIS:CD2	63:c:111:TYR:CD2	2.82	0.56
63:c:283:ARG:HD3	63:c:309:CYS:HB3	1.87	0.56
71:v:37:ILE:C	71:v:39:THR:N	2.64	0.56
30:HD:85:ARG:NH2	30:HD:140:LEU:CA	2.69	0.55
37:DF:265:GLU:OE2	37:DF:265:GLU:HA	2.06	0.55
37:DF:367:LYS:HG2	37:DF:367:LYS:O	2.06	0.55
37:Df:280:ILE:O	37:Df:284:ARG:HG3	2.05	0.55
47:HJ:98:GLU:HA	47:HJ:98:GLU:OE2	2.05	0.55
48:PD:137:LYS:HG2	67:h:55:GLN:CD	2.32	0.55
52:n:941:TYR:HD2	52:n:1172:SER:HB2	1.62	0.55
55:a:94:LEU:HD23	55:a:94:LEU:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:c:204:MET:HE3	63:c:208:PHE:O	2.05	0.55
66:o:735:LEU:HD21	73:w:113:GLN:NE2	2.21	0.55
6:DA:475:LEU:HD13	6:DA:475:LEU:C	2.30	0.55
31:HG:59:ARG:NH2	31:HG:166:GLU:OE1	2.39	0.55
52:n:592:LYS:HB3	73:w:27:MET:HE3	1.87	0.55
54:u:122:LEU:O	54:u:125:ILE:N	2.39	0.55
57:f:118:ARG:HB3	60:q:108:GLU:OE2	2.06	0.55
66:o:748:PHE:O	66:o:752:VAL:HG13	2.06	0.55
68:k:86:SER:HB2	71:v:105:LEU:HD12	1.87	0.55
69:r:17:ASN:OD1	69:r:17:ASN:N	2.35	0.55
75:y:45:GLU:O	75:y:48:ASN:C	2.49	0.55
15:HB:486:LEU:O	15:HB:490:VAL:HG23	2.07	0.55
17:PB:764:MET:HE1	17:PB:938:ARG:NH1	2.21	0.55
17:PB:934:LYS:HG3	17:PB:944:THR:HG22	1.87	0.55
35:DD:891:ILE:HA	41:DL:104:ARG:HH21	1.70	0.55
36:DE:290:HIS:CG	37:DF:45:TYR:CD2	2.94	0.55
37:DF:368:THR:HG23	37:DF:369:PRO:HD2	1.87	0.55
60:q:477:VAL:HB	60:q:493:LEU:HB2	1.88	0.55
72:p:619:GLN:HA	72:p:674:PRO:HB3	1.88	0.55
6:DA:1157:ASN:O	6:DA:1159:SER:N	2.35	0.55
9:HA:606:GLU:O	9:HA:666:ARG:NH2	2.40	0.55
11:PA:1234:LYS:NZ	11:PA:1298:LEU:O	2.39	0.55
12:DB:544:LEU:HD23	12:DB:590:ILE:HD11	1.89	0.55
30:HD:20:LYS:HE3	30:HD:62:LEU:HD13	1.87	0.55
46:HI:143:LEU:HD23	46:HI:151:LEU:HD11	1.87	0.55
46:HI:191:GLY:C	46:HI:193:GLY:N	2.59	0.55
47:HJ:171:LEU:O	47:HJ:171:LEU:HD13	2.06	0.55
52:n:172:CYS:HB2	59:m:100:GLN:HE22	1.70	0.55
52:n:836:GLY:O	52:n:846:ASN:ND2	2.38	0.55
52:n:904:PHE:CE2	52:n:1208:GLU:HB2	2.41	0.55
55:a:199:PRO:HG2	55:a:244:GLU:O	2.06	0.55
56:d:154:ARG:NH2	59:m:66:TYR:C	2.65	0.55
60:q:188:LEU:HD22	71:v:87:ILE:HB	1.88	0.55
60:q:596:PHE:CZ	65:l:117:TYR:CZ	2.94	0.55
61:z:540:LEU:C	61:z:540:LEU:CD2	2.78	0.55
67:h:78:PRO:HG3	67:h:105:VAL:HG11	1.87	0.55
11:PA:1475:LEU:HD21	49:PG:18:PHE:HZ	1.63	0.55
12:DB:259:ASP:HB3	12:DB:262:MET:O	2.06	0.55
12:DB:762:ASP:CG	12:DB:766:LEU:O	2.49	0.55
32:HE:44:LEU:HD21	32:HE:162:LEU:HD13	1.89	0.55
39:DH:53:ALA:CA	43:DJ:195:LEU:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:137:LYS:HG2	67:h:55:GLN:NE2	2.21	0.55
52:n:956:ALA:CB	52:n:1217:ARG:HH21	2.17	0.55
55:a:449:ARG:NH1	74:x:54:PRO:CB	2.69	0.55
55:a:460:ASP:O	74:x:7:LYS:HB3	2.06	0.55
60:q:113:TYR:CB	67:h:19:VAL:CG1	2.75	0.55
64:e:139:TRP:HE1	71:v:122:GLU:HG3	1.71	0.55
66:o:639:TYR:HD2	72:p:786:HIS:HB2	1.59	0.55
68:k:43:ARG:HH11	68:k:43:ARG:CB	2.19	0.55
73:w:1034:LEU:HD22	73:w:1038:ARG:HD2	1.87	0.55
73:w:1185:GLY:O	73:w:1186:TYR:C	2.50	0.55
4:NY:-19:DG:H5"	10:NE:642:ARG:H	1.71	0.55
9:HA:309:VAL:O	9:HA:309:VAL:HG12	2.06	0.55
11:PA:1789:SER:O	57:f:76:PRO:HB3	2.06	0.55
14:FB:186:MET:SD	35:DD:995:GLU:CG	2.93	0.55
34:HH:87:GLU:OE2	34:HH:145:LYS:NZ	2.40	0.55
37:DF:406:VAL:HG11	37:DF:420:ALA:HB2	1.88	0.55
37:Df:253:TYR:O	37:Df:254:GLN:HB3	2.06	0.55
47:HJ:212:ILE:HG12	47:HJ:255:MET:HE1	1.89	0.55
48:PD:74:PHE:CZ	48:PD:137:LYS:CE	2.88	0.55
52:n:201:HIS:CE1	56:d:111:GLN:NE2	2.75	0.55
59:m:56:LEU:CG	59:m:80:GLN:HE22	2.20	0.55
66:o:722:GLU:HG3	66:o:737:ILE:HB	1.89	0.55
72:p:243:LYS:NZ	72:p:245:CYS:SG	2.79	0.55
9:HA:114:ASN:C	9:HA:114:ASN:HD22	2.15	0.55
11:PA:734:ARG:NE	26:PI:107:ALA:O	2.40	0.55
12:DB:248:SER:OG	12:DB:322:MET:SD	2.65	0.55
15:HB:524:HIS:ND1	31:HG:270:SER:OG	2.38	0.55
34:HH:83:HIS:ND1	34:HH:115:GLU:OE2	2.40	0.55
34:HH:664:SER:O	34:HH:667:THR:OG1	2.25	0.55
36:De:636:HIS:HD2	36:De:638:ASN:H	1.53	0.55
47:HJ:41:LEU:HG	47:HJ:41:LEU:O	2.07	0.55
48:PD:74:PHE:HZ	48:PD:137:LYS:CE	2.20	0.55
50:g:96:LEU:HD21	52:n:132:THR:HG21	1.87	0.55
52:n:545:LEU:CG	52:n:653:PRO:HG3	2.36	0.55
55:a:420:LEU:CD1	55:a:475:VAL:HG21	2.37	0.55
55:a:441:GLU:CB	74:x:17:ARG:HH22	2.11	0.55
60:q:418:ILE:CD1	70:t:72:PRO:HG3	2.26	0.55
64:e:45:VAL:HG13	65:l:92:LEU:CD1	2.35	0.55
68:k:16:ASP:CG	71:v:79:VAL:HG21	2.31	0.55
71:v:25:ASP:HB3	71:v:75:LEU:HD21	1.88	0.55
71:v:35:GLU:OE2	71:v:64:ARG:CZ	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:w:231:VAL:O	73:w:1099:ASN:ND2	2.39	0.55
8:FA:163:GLU:OE1	8:FA:163:GLU:N	2.40	0.55
17:PB:938:ARG:NH2	17:PB:983:GLU:OE2	2.38	0.55
35:DD:1078:LEU:HD23	41:DL:83:MET:HE1	1.85	0.55
37:DF:219:GLU:OE2	39:DH:157:HIS:HB3	2.06	0.55
46:HI:133:ILE:HG22	46:HI:133:ILE:O	2.07	0.55
66:o:757:THR:O	66:o:761:LEU:HG	2.06	0.55
72:p:695:LYS:HB3	72:p:713:LEU:HD11	1.88	0.55
6:DA:851:ASP:OD1	6:DA:851:ASP:N	2.38	0.55
19:DO:16:GLN:NE2	19:DO:20:ASP:OD2	2.40	0.55
30:HD:55:LYS:C	30:HD:57:ASN:N	2.52	0.55
36:DE:561:SER:HB2	36:DE:588:VAL:HB	1.88	0.55
37:DF:106:PHE:CD1	40:DI:13:PRO:CG	2.90	0.55
39:DH:137:GLY:O	39:DH:155:ASP:OD1	2.25	0.55
47:HJ:227:THR:HB	47:HJ:229:GLU:OE1	2.07	0.55
52:n:237:MET:HE1	60:q:45:GLN:HB2	1.77	0.55
55:a:66:GLN:CD	56:d:44:LEU:HD21	2.32	0.55
55:a:106:ASP:N	55:a:106:ASP:OD1	2.40	0.55
55:a:383:PRO:HD3	55:a:445:LEU:O	2.07	0.55
55:a:455:GLN:HB2	74:x:11:LEU:HG	1.89	0.55
57:f:82:ARG:HH11	57:f:94:PRO:HB3	1.72	0.55
60:q:147:ILE:CG2	67:h:124:LEU:HD22	2.36	0.55
60:q:409:GLY:HA3	70:t:88:ASP:OD1	2.07	0.55
62:b:101:ARG:NH1	72:p:677:THR:CA	2.69	0.55
63:c:288:LEU:HD21	70:t:122:PHE:CZ	2.42	0.55
73:w:1072:ILE:HD11	73:w:1126:LEU:HD22	1.89	0.55
11:PA:850:THR:O	11:PA:854:THR:HG23	2.06	0.55
30:HD:281:GLN:HA	30:HD:281:GLN:NE2	2.20	0.55
32:HE:242:ILE:C	32:HE:243:LEU:HD12	2.31	0.55
36:DE:697:ASP:HB3	36:DE:700:HIS:HB2	1.89	0.55
46:HI:135:HIS:C	46:HI:135:HIS:CD2	2.84	0.55
47:HJ:288:ASN:C	47:HJ:288:ASN:ND2	2.57	0.55
52:n:169:LEU:O	60:q:19:VAL:HG13	2.07	0.55
56:d:76:PHE:CZ	58:i:65:PHE:CZ	2.88	0.55
59:m:95:LYS:HE3	67:h:103:GLU:OE2	2.07	0.55
60:q:394:HIS:O	69:r:51:PHE:HB2	2.07	0.55
60:q:437:HIS:ND1	60:q:472:GLU:N	2.53	0.55
70:t:131:MET:C	70:t:131:MET:SD	2.89	0.55
11:PA:362:SER:HB2	17:PB:1084:LEU:HD12	1.89	0.54
30:HD:85:ARG:NH2	30:HD:140:LEU:HA	2.22	0.54
55:a:107:MET:O	55:a:107:MET:HE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:440:PHE:CE2	55:a:508:MET:HB3	2.41	0.54
58:i:85:GLN:HG3	58:i:86:ASP:CG	2.32	0.54
64:e:49:GLU:HG2	65:l:89:PHE:CD1	2.42	0.54
65:l:107:ASP:N	65:l:108:PRO:HD3	2.22	0.54
74:x:11:LEU:C	74:x:13:ALA:H	2.15	0.54
35:DD:963:ARG:HG2	35:DD:982:LEU:H	1.71	0.54
52:n:266:VAL:HG22	57:f:177:VAL:HG13	1.88	0.54
60:q:376:HIS:HB2	68:k:92:MET:HE3	1.89	0.54
60:q:437:HIS:C	60:q:437:HIS:CD2	2.86	0.54
60:q:451:LEU:HD12	60:q:460:ILE:HD12	1.89	0.54
61:z:480:LEU:HD23	61:z:480:LEU:O	2.08	0.54
66:o:715:LEU:CD1	74:x:66:TYR:OH	2.48	0.54
73:w:203:ASN:HD21	74:x:807:THR:HG21	1.73	0.54
75:y:226:LEU:HD11	75:y:228:LEU:HG	1.89	0.54
12:DB:571:LEU:HD21	12:DB:619:MET:HE1	1.89	0.54
36:DE:563:GLU:HG2	36:DE:587:PRO:HG3	1.90	0.54
37:DF:320:ARG:HB2	37:DF:415:ILE:CD1	2.37	0.54
41:DL:58:LEU:HA	41:DL:62:LYS:HD2	1.89	0.54
36:De:610:ARG:HD3	36:De:619:PRO:HG3	1.89	0.54
51:j:82:LYS:CD	53:s:96:PHE:CD1	2.89	0.54
52:n:82:LYS:HE2	53:s:154:LEU:HA	1.89	0.54
52:n:175:ASP:OD2	60:q:20:HIS:CE1	2.61	0.54
60:q:149:LYS:HE3	71:v:40:ALA:CA	2.30	0.54
60:q:166:ARG:CZ	60:q:166:ARG:CB	2.85	0.54
60:q:191:ARG:HD3	71:v:87:ILE:C	2.25	0.54
64:e:60:VAL:HG23	64:e:60:VAL:O	2.08	0.54
65:l:30:THR:OG1	65:l:102:ASN:ND2	2.40	0.54
66:o:767:HIS:CD2	66:o:772:LEU:HD21	2.42	0.54
70:t:4:THR:HG22	70:t:143:GLU:HB2	1.89	0.54
71:v:39:THR:C	71:v:41:LYS:H	2.15	0.54
73:w:32:ASP:OD1	73:w:32:ASP:N	2.39	0.54
5:BA:173:VAL:O	5:BA:175:ARG:NH1	2.40	0.54
9:HA:17:ILE:HD11	9:HA:22:PHE:CZ	2.42	0.54
17:PB:260:LEU:HB2	17:PB:263:ILE:HD12	1.89	0.54
35:DD:1068:GLU:OE2	36:DE:582:LYS:NZ	2.41	0.54
36:DE:278:ASP:OD2	36:DE:649:ARG:NH2	2.40	0.54
52:n:192:LEU:HD11	52:n:220:GLY:HA3	1.84	0.54
52:n:273:PHE:HZ	57:f:185:ARG:NE	2.03	0.54
52:n:301:LEU:HB3	52:n:361:ILE:HG13	1.89	0.54
55:a:462:LEU:N	74:x:49:GLN:CG	2.23	0.54
58:i:65:PHE:HE1	58:i:99:LYS:CA	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:i:65:PHE:CE1	58:i:99:LYS:HA	2.41	0.54
61:z:576:TRP:HB3	61:z:596:TYR:CB	2.38	0.54
73:w:625:SER:HB2	73:w:674:THR:HG22	1.89	0.54
9:HA:420:PRO:HA	9:HA:431:PRO:HB3	1.89	0.54
11:PA:193:ARG:NH1	11:PA:195:GLY:O	2.38	0.54
11:PA:1484:MET:N	11:PA:1484:MET:SD	2.80	0.54
26:PI:29:ASP:O	26:PI:33:ARG:N	2.40	0.54
37:DF:219:GLU:CD	39:DH:156:PRO:HB2	2.33	0.54
47:HJ:102:ARG:HG2	47:HJ:102:ARG:NH1	2.22	0.54
50:g:90:LEU:HD21	51:j:109:LEU:HD22	1.90	0.54
52:n:777:TYR:HA	52:n:780:VAL:HG22	1.89	0.54
55:a:226:VAL:HG12	55:a:226:VAL:O	2.08	0.54
55:a:336:TYR:CE1	55:a:391:THR:OG1	2.52	0.54
60:q:647:SER:HB2	64:e:97:GLN:HE21	1.73	0.54
12:DB:66:ASN:HD21	12:DB:119:PRO:HB3	1.73	0.54
14:FB:186:MET:CE	35:DD:995:GLU:OE2	2.34	0.54
18:HC:265:LEU:HD12	18:HC:270:LEU:HD12	1.90	0.54
30:HD:85:ARG:HH22	30:HD:140:LEU:HA	1.72	0.54
32:HE:195:VAL:CG1	32:HE:203:LEU:HD23	2.38	0.54
35:DD:891:ILE:HD12	35:DD:891:ILE:N	2.23	0.54
35:DD:961:GLN:HE22	36:DE:434:ASP:CG	2.16	0.54
35:DD:997:ALA:O	35:DD:1001:GLN:CG	2.43	0.54
55:a:417:TYR:HH	55:a:450:PHE:HB3	1.73	0.54
73:w:101:LEU:HD22	73:w:118:THR:HG23	1.90	0.54
73:w:339:ILE:O	73:w:343:LEU:HB2	2.08	0.54
1:X:-27:DA:H2	20:DP:169:VAL:HG21	1.71	0.54
11:PA:350:VAL:HG12	11:PA:1435:THR:HG21	1.90	0.54
11:PA:1475:LEU:HD23	49:PG:66:VAL:CG2	2.08	0.54
18:HC:42:LEU:HD13	32:HE:50:PHE:CE1	2.42	0.54
37:DF:83:LEU:CD1	37:DF:98:SER:HA	2.38	0.54
37:Df:390:THR:HG23	37:Df:391:LEU:HD22	1.90	0.54
46:HI:171:HIS:NE2	46:HI:188:ARG:HA	2.21	0.54
49:PG:92:VAL:HG23	49:PG:139:GLN:HG2	1.89	0.54
52:n:870:GLN:CG	66:o:655:THR:HG22	2.32	0.54
55:a:412:ARG:CB	55:a:472:SER:HB3	2.35	0.54
56:d:47:MET:HA	56:d:47:MET:CE	2.37	0.54
56:d:166:THR:HG23	56:d:166:THR:O	2.08	0.54
73:w:781:SER:O	73:w:783:GLN:NE2	2.41	0.54
74:x:976:PRO:HA	74:x:979:ARG:HE	1.73	0.54
6:DA:639:LEU:HD12	6:DA:639:LEU:O	2.07	0.54
9:HA:133:LYS:O	9:HA:137:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:EB:99:LEU:HD22	13:EB:120:MET:HE2	1.88	0.54
17:PB:1134:THR:CG2	49:PG:153:ASP:OD1	2.53	0.54
39:DH:50:PHE:HB2	43:DJ:195:LEU:CB	2.34	0.54
36:De:368:ASN:ND2	36:De:701:GLY:HA3	2.23	0.54
48:PD:110:GLU:O	48:PD:114:LEU:HD23	2.07	0.54
51:j:43:PHE:CB	53:s:144:ILE:HG21	2.36	0.54
55:a:160:LEU:CG	55:a:219:LEU:HD21	2.38	0.54
55:a:248:SER:HB3	55:a:251:LEU:HB2	1.90	0.54
55:a:367:LEU:HD22	55:a:509:ARG:NH1	2.23	0.54
62:b:160:TYR:O	62:b:164:ILE:HG12	2.07	0.54
62:b:186:THR:CG2	64:e:49:GLU:CD	2.77	0.54
66:o:746:ASN:HD21	74:x:65:LYS:HB3	1.72	0.54
76:NG:1119:GLY:C	76:NG:1121:LYS:N	2.57	0.54
15:HB:503:THR:OG1	15:HB:533:TYR:OH	2.01	0.54
17:PB:752:TYR:HE1	17:PB:809:VAL:HG23	1.72	0.54
18:HC:348:ARG:HE	33:HF:65:ALA:HB1	1.65	0.54
36:DE:665:PHE:HE1	36:DE:701:GLY:HA2	1.73	0.54
41:DL:111:LEU:HB2	41:DL:115:ASP:OD2	2.07	0.54
52:n:508:SER:OG	52:n:637:PHE:O	2.14	0.54
54:u:29:CYS:O	54:u:29:CYS:SG	2.66	0.54
55:a:59:VAL:CG1	56:d:48:LEU:HD23	2.37	0.54
60:q:166:ARG:CG	60:q:166:ARG:HH11	2.21	0.54
6:DA:1052:ARG:HD2	6:DA:1052:ARG:O	2.07	0.54
21:DQ:15:ARG:HA	21:DQ:18:ILE:HD12	1.89	0.54
36:DE:433:LYS:CD	40:DI:110:TYR:CE1	2.90	0.54
36:DE:433:LYS:NZ	40:DI:110:TYR:HE1	1.97	0.54
37:DF:418:ILE:HD12	37:DF:418:ILE:N	2.21	0.54
39:DH:159:TYR:N	39:DH:159:TYR:CD1	2.75	0.54
35:Dd:911:GLN:NE2	41:DI:69:GLU:OE2	2.41	0.54
46:HI:98:LEU:CB	46:HI:143:LEU:HD21	2.36	0.54
52:n:780:VAL:HG12	52:n:808:LEU:HD11	1.90	0.54
55:a:374:TYR:CE2	55:a:440:PHE:HB2	2.43	0.54
62:b:101:ARG:NH1	72:p:677:THR:HB	2.23	0.54
64:e:129:VAL:HG12	68:k:111:CYS:HG	1.73	0.54
67:h:110:ARG:C	67:h:110:ARG:HD3	2.33	0.54
5:BA:133:ASN:OD1	5:BA:134:ILE:N	2.40	0.53
7:EA:188:TYR:CD2	30:HD:14:TYR:CG	2.96	0.53
9:HA:80:ILE:HD11	9:HA:206:VAL:HB	1.90	0.53
11:PA:1660:THR:O	57:f:15:TRP:HA	2.09	0.53
17:PB:501:LEU:HD12	17:PB:505:LEU:HD12	1.90	0.53
20:DP:208:ARG:NH2	21:DQ:346:LYS:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:747:LEU:HD22	36:DE:747:LEU:N	2.20	0.53
36:De:251:LEU:O	36:De:256:HIS:HB2	2.07	0.53
52:n:208:LEU:HD12	52:n:208:LEU:O	2.08	0.53
52:n:904:PHE:HD1	52:n:916:LEU:HD11	1.74	0.53
55:a:109:TYR:HE1	55:a:150:PHE:HZ	1.56	0.53
55:a:127:HIS:CE1	55:a:171:THR:CG2	2.91	0.53
56:d:31:LEU:CD2	58:i:103:THR:OG1	2.44	0.53
56:d:163:ALA:CB	59:m:106:GLN:HA	2.38	0.53
58:i:110:SER:CB	58:i:111:PRO:HD2	2.38	0.53
9:HA:289:VAL:HG22	9:HA:324:ARG:NH1	2.23	0.53
9:HA:365:VAL:O	9:HA:365:VAL:HG22	2.08	0.53
11:PA:261:ARG:NH1	11:PA:277:THR:OG1	2.40	0.53
12:DB:345:CYS:HA	12:DB:348:GLN:HE21	1.73	0.53
34:HH:632:SER:OG	34:HH:676:ARG:NH2	2.41	0.53
36:DE:463:PHE:HB3	37:DF:134:HIS:NE2	2.22	0.53
37:DF:82:PRO:HG2	37:DF:83:LEU:HD12	1.91	0.53
39:DH:108:PRO:CD	43:DJ:116:LEU:HD21	2.39	0.53
40:DI:23:LEU:HD12	40:DI:31:TYR:OH	2.09	0.53
46:HI:22:GLN:CD	46:HI:22:GLN:H	2.17	0.53
55:a:336:TYR:CD1	55:a:391:THR:HG23	2.43	0.53
57:f:32:TYR:HD1	57:f:35:GLU:CD	2.16	0.53
60:q:484:TYR:CE2	60:q:540:LEU:HD11	2.44	0.53
60:q:487:ILE:HD11	60:q:540:LEU:HD12	1.89	0.53
63:c:167:SER:OG	63:c:171:ARG:NH1	2.41	0.53
63:c:238:VAL:HG22	63:c:292:LEU:HD23	1.89	0.53
72:p:13:MET:HB2	72:p:405:PHE:CD1	2.43	0.53
75:y:123:GLN:NE2	75:y:159:THR:O	2.42	0.53
5:BA:39:LEU:HD11	11:PA:425:ASP:HB2	1.91	0.53
7:EA:122:THR:HG1	30:HD:40:VAL:HG21	1.70	0.53
7:EA:148:MET:SD	7:EA:149:THR:N	2.81	0.53
12:DB:628:ILE:O	12:DB:644:GLN:NE2	2.42	0.53
12:DB:629:ARG:NH1	12:DB:658:ASP:OD2	2.37	0.53
17:PB:613:ARG:NH1	17:PB:615:TYR:OH	2.41	0.53
25:PH:49:PRO:O	25:PH:147:LYS:NZ	2.30	0.53
30:HD:288:THR:C	30:HD:290:SER:H	2.15	0.53
37:DF:320:ARG:C	37:DF:322:ASP:N	2.66	0.53
37:Df:318:CYS:SG	37:Df:326:HIS:HB3	2.49	0.53
46:HI:304:GLY:HA2	46:HI:307:LEU:HB2	1.90	0.53
48:PD:29:ALA:O	48:PD:94:LYS:NZ	2.39	0.53
50:g:128:PRO:CD	50:g:129:HIS:H	2.21	0.53
55:a:127:HIS:HE1	55:a:171:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:411:ILE:O	55:a:412:ARG:C	2.51	0.53
62:b:136:HIS:HD2	63:c:111:TYR:CZ	2.16	0.53
63:c:309:CYS:HB2	63:c:311:GLN:CD	2.33	0.53
64:e:136:LEU:HD22	68:k:104:LEU:HD22	1.89	0.53
71:v:90:ASP:O	71:v:91:PHE:HB2	2.08	0.53
73:w:161:LEU:HD22	73:w:164:ARG:HD2	1.91	0.53
73:w:627:LEU:HD22	73:w:645:VAL:HG23	1.89	0.53
5:BA:222:LEU:CD2	5:BA:277:ILE:HD13	2.38	0.53
9:HA:437:CYS:SG	9:HA:438:MET:N	2.81	0.53
11:PA:1453:GLY:O	11:PA:1457:ASN:ND2	2.35	0.53
18:HC:80:SER:O	18:HC:84:GLU:OE1	2.25	0.53
30:HD:85:ARG:HH12	30:HD:140:LEU:N	2.06	0.53
35:DD:958:LYS:HD3	35:DD:961:GLN:OE1	2.08	0.53
36:DE:517:ASP:HA	36:DE:520:SER:HB3	1.91	0.53
47:HJ:33:LYS:HD3	47:HJ:33:LYS:C	2.34	0.53
52:n:166:TYR:HH	59:m:70:PRO:CB	2.15	0.53
52:n:864:ASN:ND2	52:n:867:GLN:OE1	2.41	0.53
63:c:127:LEU:HB2	64:e:81:ILE:HD13	1.89	0.53
67:h:25:SER:OG	67:h:52:LEU:HB2	2.09	0.53
67:h:139:GLN:HE22	68:k:37:LYS:CB	2.16	0.53
68:k:109:ARG:CB	68:k:109:ARG:CZ	2.86	0.53
71:v:61:MET:HE2	71:v:64:ARG:HH12	1.74	0.53
73:w:1302:LYS:NZ	73:w:1308:ASP:OD1	2.41	0.53
12:DB:937:THR:HG23	12:DB:939:ASN:H	1.74	0.53
17:PB:552:ASN:OD1	17:PB:553:LEU:N	2.42	0.53
20:DP:206:GLU:HB3	20:DP:207:PRO:HD3	1.91	0.53
21:DQ:327:GLU:HG3	35:DD:1010:ALA:O	2.08	0.53
30:HD:275:VAL:HG13	30:HD:276:ARG:HE	1.73	0.53
35:DD:1069:ASN:O	37:DF:95:ARG:HD3	2.08	0.53
46:HI:239:ASP:C	46:HI:242:SER:H	2.17	0.53
47:HJ:17:GLU:OE2	47:HJ:17:GLU:HA	2.08	0.53
51:j:82:LYS:CD	53:s:101:VAL:HG11	2.39	0.53
52:n:261:ASP:CB	60:q:250:ASP:OD2	2.57	0.53
52:n:270:GLN:HG3	57:f:181:LEU:CD1	2.39	0.53
52:n:923:CYS:SG	52:n:924:ILE:N	2.82	0.53
54:u:90:LEU:CD2	60:q:9:ILE:CG1	2.78	0.53
57:f:15:TRP:CH2	57:f:35:GLU:HB2	2.44	0.53
58:i:105:PRO:CD	58:i:107:ILE:HG13	2.34	0.53
60:q:17:LYS:HE2	60:q:30:TYR:CD2	2.43	0.53
60:q:437:HIS:ND1	60:q:471:TYR:C	2.67	0.53
68:k:9:GLU:CG	71:v:86:LEU:HG	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:NY:-149:DG:H2"	4:NY:-148:DG:C8	2.44	0.53
34:HH:568:LEU:HD11	34:HH:606:PHE:HB3	1.91	0.53
36:DE:774:MET:HG3	37:DF:149:PRO:HG3	1.91	0.53
37:DF:359:PHE:HB3	37:DF:380:LEU:HG	1.91	0.53
39:DH:108:PRO:HG2	43:DJ:116:LEU:CD2	2.36	0.53
47:HJ:190:THR:HB	47:HJ:223:ARG:HH21	1.73	0.53
52:n:199:LEU:HD22	52:n:222:VAL:HG11	1.88	0.53
54:u:71:VAL:CG2	61:z:528:LEU:HD21	2.39	0.53
55:a:128:HIS:CG	55:a:128:HIS:O	2.60	0.53
55:a:321:LEU:C	55:a:321:LEU:HD13	2.34	0.53
55:a:375:PHE:CB	74:x:17:ARG:NH2	2.70	0.53
57:f:32:TYR:CD1	57:f:35:GLU:CD	2.87	0.53
58:i:75:CYS:CB	58:i:88:ASN:HD21	2.22	0.53
60:q:113:TYR:CD2	67:h:19:VAL:HG12	2.44	0.53
60:q:188:LEU:HD21	68:k:6:LEU:CD1	2.39	0.53
61:z:572:ASN:N	61:z:572:ASN:OD1	2.42	0.53
66:o:632:PRO:O	72:p:793:GLU:OE1	2.27	0.53
66:o:634:PHE:O	66:o:637:SER:OG	2.25	0.53
68:k:71:THR:HA	68:k:74:ALA:HB3	1.91	0.53
72:p:677:THR:HG23	72:p:725:LEU:HB2	1.90	0.53
73:w:958:ASN:N	73:w:958:ASN:OD1	2.40	0.53
75:y:137:GLN:OE1	75:y:140:ARG:NH1	2.37	0.53
43:DJ:130:ILE:HG13	43:DJ:160:GLN:HE21	1.73	0.53
6:DA:410:TRP:CD1	37:DF:306:PRO:HD3	2.44	0.53
9:HA:373:ARG:O	9:HA:405:THR:OG1	2.24	0.53
30:HD:124:ILE:HA	30:HD:127:LYS:HE2	1.91	0.53
30:HD:295:ARG:NE	47:HJ:165:ARG:HE	2.07	0.53
37:DF:76:LYS:HG3	37:DF:96:PHE:HB3	1.91	0.53
37:DF:403:ILE:O	37:DF:406:VAL:HG22	2.08	0.53
42:Dc:33:LEU:HD13	43:Dj:197:MET:HE1	1.91	0.53
37:Df:283:MET:HG3	37:Df:329:LEU:HD11	1.90	0.53
46:HI:171:HIS:HB3	46:HI:172:GLN:NE2	2.24	0.53
52:n:549:TYR:HB2	52:n:571:MET:HE2	1.90	0.53
55:a:373:CYS:O	55:a:440:PHE:N	2.40	0.53
66:o:690:LEU:O	66:o:692:ASN:ND2	2.42	0.53
66:o:776:TRP:O	66:o:780:VAL:HG23	2.08	0.53
73:w:16:GLU:OE2	73:w:19:GLU:N	2.40	0.53
12:DB:808:PRO:HA	12:DB:864:ASN:HB3	1.90	0.53
17:PB:410:ASN:O	17:PB:414:GLU:OE1	2.27	0.53
35:DD:1063:LEU:HD13	41:DL:80:VAL:HG13	1.91	0.53
46:HI:241:CYS:HB2	46:HI:246:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:272:ILE:O	46:HI:273:GLN:C	2.50	0.53
48:PD:134:ILE:HD12	48:PD:137:LYS:CE	2.39	0.53
52:n:941:TYR:HE2	52:n:1172:SER:CB	2.06	0.53
54:u:81:SER:HB3	54:u:86:GLN:HE21	1.74	0.53
73:w:109:TRP:HB2	73:w:160:LEU:HD21	1.90	0.53
74:x:566:GLU:C	74:x:568:LYS:N	2.63	0.53
7:EA:142:ASN:O	7:EA:145:PHE:HB3	2.08	0.53
7:EA:152:PHE:CE1	49:PG:95:VAL:HG11	2.44	0.53
11:PA:459:ASN:OD1	11:PA:460:ARG:N	2.42	0.53
11:PA:1790:TYR:CG	67:h:83:PRO:HD3	2.44	0.53
17:PB:939:HIS:NE2	17:PB:983:GLU:OE1	2.35	0.53
23:PE:111:THR:HG23	23:PE:114:ALA:H	1.74	0.53
31:HG:337:GLU:O	31:HG:340:ASN:ND2	2.38	0.53
37:DF:86:PHE:HA	43:DJ:212:LYS:HZ3	1.74	0.53
37:DF:274:ASN:H	37:DF:317:LEU:HB2	1.73	0.53
50:g:75:LYS:NZ	61:z:562:GLY:HA3	2.24	0.53
52:n:250:LEU:HD23	52:n:275:HIS:CB	2.36	0.53
52:n:458:LEU:HD12	60:q:325:ILE:HG12	1.90	0.53
55:a:348:LEU:HD13	55:a:425:VAL:HG12	1.89	0.53
57:f:181:LEU:HD23	57:f:184:LEU:HD21	1.91	0.53
67:h:147:CYS:SG	67:h:148:SER:N	2.81	0.53
75:y:132:ARG:HH21	75:y:140:ARG:HD3	1.71	0.53
75:y:188:LEU:H	75:y:220:MET:HE2	1.74	0.53
7:EA:127:PHE:HE2	7:EA:152:PHE:CE2	2.27	0.53
11:PA:233:CYS:SG	11:PA:244:ARG:NH1	2.81	0.53
19:DO:1:MET:CB	35:DD:997:ALA:HB2	2.38	0.53
22:PC:175:LYS:NZ	29:PL:57:ALA:O	2.42	0.53
51:j:79:LEU:HA	51:j:82:LYS:HG2	1.91	0.53
52:n:209:PRO:CG	52:n:293:TYR:CG	2.92	0.53
54:u:73:ILE:C	54:u:75:SER:N	2.61	0.53
55:a:440:PHE:CD1	55:a:454:PHE:HB3	2.43	0.53
60:q:109:MET:HE3	60:q:109:MET:C	2.32	0.53
60:q:113:TYR:CA	67:h:19:VAL:HG11	2.39	0.53
61:z:560:TRP:CD1	61:z:561:PRO:HD2	2.43	0.53
72:p:43:ASN:HD22	72:p:489:TRP:HB3	1.74	0.53
1:X:-6:DG:H1	2:Y:6:DC:N4	2.07	0.52
11:PA:521:VAL:HG13	11:PA:535:MET:HE1	1.90	0.52
11:PA:1674:THR:HB	46:HI:214:PRO:HG2	1.91	0.52
13:EB:82:VAL:HG12	13:EB:86:LYS:HZ2	1.72	0.52
18:HC:32:ASP:OD1	18:HC:33:ARG:N	2.42	0.52
18:HC:58:ARG:NH1	32:HE:229:TRP:CZ3	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:304:LYS:NZ	36:DE:335:GLU:O	2.42	0.52
36:DE:432:LEU:HD21	36:DE:436:ASP:HB3	1.91	0.52
36:DE:653:LEU:HB2	36:DE:663:ARG:HB2	1.91	0.52
40:DI:73:LEU:HG	40:DI:74:ALA:N	2.23	0.52
52:n:254:VAL:HG11	52:n:304:GLN:HG2	1.91	0.52
52:n:449:SER:OG	52:n:450:GLU:N	2.41	0.52
54:u:80:GLU:HB3	61:z:539:ASP:OD2	2.09	0.52
56:d:86:GLN:OE1	58:i:107:ILE:HA	2.09	0.52
60:q:263:LYS:HE3	60:q:439:PHE:CZ	2.42	0.52
60:q:479:ILE:CG2	60:q:532:HIS:CG	2.90	0.52
60:q:577:ASP:HB2	60:q:597:PRO:HG3	1.91	0.52
65:l:44:ILE:O	65:l:48:THR:HG23	2.09	0.52
73:w:522:PRO:HG3	73:w:565:GLU:HG2	1.90	0.52
73:w:681:GLU:OE2	73:w:685:ARG:NH1	2.41	0.52
75:y:73:THR:OG1	75:y:75:ASP:OD2	2.27	0.52
9:HA:488:VAL:HG23	9:HA:488:VAL:O	2.09	0.52
12:DB:529:VAL:HG11	12:DB:560:TYR:HB2	1.91	0.52
17:PB:128:ILE:HG21	17:PB:431:LEU:HD21	1.90	0.52
34:HH:463:LYS:O	34:HH:484:ILE:HG23	2.10	0.52
37:DF:218:VAL:CG1	39:DH:162:THR:HB	2.29	0.52
36:De:595:PRO:HD2	36:De:639:SER:HB3	1.91	0.52
36:De:646:SER:OG	36:De:647:ALA:N	2.41	0.52
47:HJ:229:GLU:N	47:HJ:229:GLU:CD	2.62	0.52
52:n:707:ASP:CB	66:o:684:ARG:NH2	2.72	0.52
55:a:375:PHE:HB3	74:x:17:ARG:CZ	2.39	0.52
57:f:78:LEU:HD11	67:h:81:LEU:CD2	2.39	0.52
64:e:132:HIS:HD2	71:v:126:ASP:CG	2.16	0.52
64:e:132:HIS:CD2	71:v:126:ASP:OD2	2.62	0.52
66:o:707:ILE:HG23	66:o:720:PRO:CA	2.37	0.52
68:k:101:ARG:NH1	68:k:101:ARG:CB	2.72	0.52
74:x:175:ARG:HH21	74:x:221:LEU:HD22	1.74	0.52
31:HG:54:ARG:NH2	31:HG:245:SER:O	2.43	0.52
36:DE:461:ILE:O	37:DF:135:TRP:HA	2.08	0.52
37:DF:273:GLN:H	37:DF:273:GLN:CD	2.17	0.52
37:DF:312:ILE:HG13	37:DF:334:ALA:HB1	1.91	0.52
46:HI:132:TRP:HA	46:HI:132:TRP:HE3	1.73	0.52
53:s:100:LYS:HE3	53:s:102:LYS:HB2	1.89	0.52
55:a:335:THR:O	55:a:391:THR:HG22	2.07	0.52
60:q:123:LYS:HG2	60:q:124:PHE:CE2	2.43	0.52
60:q:311:LEU:HD21	60:q:427:LEU:HG	1.91	0.52
63:c:204:MET:SD	63:c:208:PHE:C	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:x:472:ASN:ND2	74:x:496:SER:OG	2.42	0.52
12:DB:646:ASP:N	18:HC:413:LEU:O	2.42	0.52
17:PB:718:GLN:HG2	17:PB:720:PRO:HD2	1.90	0.52
30:HD:43:ALA:HB3	49:PG:164:MET:CG	2.38	0.52
37:DF:320:ARG:CD	37:DF:415:ILE:HD12	2.39	0.52
48:PD:76:ASN:ND2	67:h:47:ASP:C	2.68	0.52
52:n:921:MET:CE	52:n:1215:ILE:HD13	2.37	0.52
55:a:270:ILE:O	55:a:270:ILE:HG22	2.07	0.52
55:a:364:TYR:CD1	55:a:430:LEU:HB2	2.44	0.52
55:a:445:LEU:HD11	55:a:451:SER:HB3	1.90	0.52
56:d:42:ARG:HH22	58:i:93:LYS:HG2	1.71	0.52
60:q:223:GLU:HB2	60:q:246:GLN:HB3	1.90	0.52
64:e:125:LYS:NZ	65:l:153:ASN:OD1	2.43	0.52
66:o:759:ARG:O	66:o:762:GLN:HG3	2.08	0.52
4:NY:-64:DG:H2"	4:NY:-63:DG:C8	2.44	0.52
9:HA:709:THR:HG22	9:HA:710:VAL:N	2.25	0.52
12:DB:622:ASP:CB	33:HF:36:GLN:HA	2.29	0.52
13:EB:82:VAL:HG12	13:EB:86:LYS:HZ3	1.75	0.52
15:HB:127:LEU:HD12	15:HB:467:ALA:HA	1.91	0.52
17:PB:752:TYR:CE2	17:PB:807:ARG:HG2	2.43	0.52
17:PB:794:VAL:O	17:PB:946:GLY:N	2.42	0.52
31:HG:87:LEU:HD11	31:HG:229:LYS:HG2	1.91	0.52
34:HH:181:HIS:O	34:HH:184:VAL:HG12	2.10	0.52
46:HI:140:PRO:O	46:HI:143:LEU:HD12	2.09	0.52
49:PG:52:ASP:N	49:PG:71:LYS:O	2.42	0.52
52:n:160:VAL:HG22	52:n:166:TYR:HE1	1.75	0.52
52:n:261:ASP:CB	60:q:250:ASP:CG	2.76	0.52
52:n:362:ASP:O	52:n:363:GLU:C	2.52	0.52
52:n:1219:HIS:HD2	52:n:1222:ARG:HH11	1.58	0.52
54:u:90:LEU:CG	60:q:9:ILE:CG1	2.88	0.52
55:a:321:LEU:HD21	55:a:407:ILE:CD1	2.35	0.52
61:z:540:LEU:C	61:z:540:LEU:HD22	2.34	0.52
61:z:560:TRP:HD1	61:z:561:PRO:HD2	1.75	0.52
72:p:600:LYS:NZ	72:p:603:GLU:OE1	2.42	0.52
5:BA:222:LEU:HD21	5:BA:277:ILE:HD13	1.92	0.52
15:HB:136:VAL:HG11	15:HB:502:VAL:HG12	1.92	0.52
34:HH:340:LEU:HD23	34:HH:491:ALA:HB2	1.91	0.52
35:DD:918:SER:HB3	41:DL:74:GLU:CD	2.34	0.52
36:DE:433:LYS:HZ3	40:DI:110:TYR:HE1	1.41	0.52
37:DF:14:LEU:HD23	40:DI:22:ILE:HD11	1.91	0.52
37:DF:43:VAL:CG2	40:DI:43:ALA:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:276:LEU:HD22	37:DF:323:VAL:HG21	1.92	0.52
39:DH:50:PHE:HZ	43:DJ:170:ALA:CA	2.22	0.52
35:Dd:963:ARG:NH2	35:Dd:964:GLU:OE2	2.42	0.52
37:Df:320:ARG:NH1	37:Df:320:ARG:CB	2.73	0.52
60:q:99:ARG:CZ	60:q:103:ARG:HH22	2.23	0.52
62:b:96:ASP:OD2	72:p:670:PRO:HB2	2.10	0.52
64:e:45:VAL:CG1	65:l:92:LEU:HD11	2.39	0.52
66:o:775:THR:HA	66:o:778:GLN:HG2	1.91	0.52
68:k:77:GLN:HE21	69:r:192:GLN:HB2	1.75	0.52
8:FA:43:ASN:OD1	8:FA:44:GLN:N	2.43	0.52
13:EB:89:HIS:CE1	13:EB:139:PHE:CB	2.93	0.52
37:DF:241:GLU:OE1	39:DH:135:THR:OG1	2.27	0.52
39:DH:60:THR:CG2	43:DJ:211:VAL:HG23	2.35	0.52
36:De:607:ARG:NH1	40:Di:87:PRO:O	2.43	0.52
52:n:270:GLN:CG	57:f:181:LEU:CD1	2.87	0.52
52:n:879:LEU:HA	52:n:882:ILE:HG22	1.90	0.52
67:h:82:SER:C	67:h:84:ASP:H	2.18	0.52
70:t:8:GLN:NE2	70:t:200:ILE:HD13	2.24	0.52
74:x:439:LEU:HB3	74:x:495:ILE:HG21	1.92	0.52
43:DJ:128:PRO:HB2	43:DJ:160:GLN:HE22	1.75	0.52
43:DJ:137:TYR:OH	43:DJ:141:ARG:NH2	2.43	0.52
6:DA:483:ASN:HA	6:DA:493:ARG:HH11	1.73	0.52
11:PA:1139:LEU:HD13	11:PA:1341:VAL:HA	1.91	0.52
35:DD:883:LEU:HD23	35:DD:891:ILE:HG12	1.92	0.52
37:DF:14:LEU:CD2	40:DI:22:ILE:HD12	2.40	0.52
41:DL:60:LYS:HE3	41:DL:60:LYS:H	1.74	0.52
47:HJ:192:ASP:C	47:HJ:192:ASP:OD1	2.53	0.52
50:g:129:HIS:CG	54:u:82:THR:HG22	2.45	0.52
62:b:89:ASP:OD2	66:o:636:HIS:HD2	1.93	0.52
74:x:618:VAL:HG13	74:x:673:MET:HE1	1.92	0.52
74:x:628:VAL:HG13	74:x:636:ARG:HG2	1.91	0.52
1:X:-12:DG:H4'	14:FB:229:HIS:HA	1.91	0.52
4:NY:-132:DG:H5''	76:NG:1018:SER:HA	1.90	0.52
9:HA:28:LEU:HD22	9:HA:55:LEU:HD23	1.91	0.52
12:DB:983:ARG:HG3	12:DB:983:ARG:HH11	1.75	0.52
36:DE:463:PHE:O	37:DF:133:ALA:CA	2.51	0.52
36:DE:676:THR:HG22	36:DE:685:ALA:HB3	1.92	0.52
36:De:269:GLY:O	40:Di:97:ARG:NH2	2.43	0.52
52:n:327:GLU:HG3	52:n:356:LYS:HG2	1.91	0.52
52:n:651:ASN:HD22	73:w:22:PHE:H	1.58	0.52
52:n:845:SER:OG	52:n:846:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:223:LYS:NZ	55:a:251:LEU:C	2.68	0.52
56:d:103:ARG:NH1	56:d:103:ARG:CG	2.73	0.52
62:b:67:LEU:HD22	62:b:116:LEU:HD12	1.91	0.52
63:c:178:ILE:HG23	63:c:192:VAL:HG22	1.92	0.52
66:o:725:VAL:HA	66:o:734:PRO:HB3	1.92	0.52
70:t:131:MET:SD	70:t:132:GLY:N	2.83	0.52
71:v:86:LEU:HD12	71:v:86:LEU:O	2.10	0.52
4:NY:-63:DG:H2''	4:NY:-62:DG:C8	2.45	0.52
6:DA:487:ASP:OD1	6:DA:487:ASP:N	2.42	0.52
12:DB:66:ASN:OD1	12:DB:187:ARG:NH1	2.43	0.52
26:PI:69:ILE:HG22	26:PI:71:ASP:H	1.74	0.52
30:HD:83:ASN:CG	30:HD:140:LEU:HD12	2.34	0.52
35:Dd:943:GLN:NE2	36:De:509:GLN:O	2.41	0.52
36:De:423:PRO:HG2	36:De:426:ARG:HB2	1.91	0.52
46:HI:98:LEU:HD12	46:HI:98:LEU:O	2.10	0.52
46:HI:283:ARG:CZ	46:HI:283:ARG:HB2	2.40	0.52
47:HJ:252:MET:O	47:HJ:256:ARG:HG2	2.10	0.52
48:PD:79:THR:HA	67:h:51:LEU:HD23	1.84	0.52
60:q:523:ASP:HB3	60:q:563:ILE:HD12	1.92	0.52
68:k:43:ARG:CB	68:k:43:ARG:NH1	2.73	0.52
71:v:110:GLU:OE1	71:v:110:GLU:HA	2.09	0.52
72:p:398:SER:OG	72:p:400:GLN:NE2	2.43	0.52
74:x:565:SER:O	74:x:566:GLU:C	2.54	0.52
2:Y:25:DT:O3'	20:DP:196:ARG:NH1	2.43	0.51
18:HC:338:PHE:N	18:HC:341:MET:O	2.44	0.51
24:PF:64:ARG:HH21	49:PG:61:PRO:HG2	1.73	0.51
25:PH:91:VAL:HG22	25:PH:144:LEU:HD23	1.91	0.51
28:PK:63:VAL:HG23	28:PK:63:VAL:O	2.10	0.51
37:Df:447:ALA:O	37:Df:453:GLY:HA2	2.10	0.51
46:HI:43:ILE:HG23	46:HI:43:ILE:O	2.09	0.51
46:HI:111:PRO:HD3	57:f:63:MET:HG2	1.92	0.51
55:a:449:ARG:NH1	74:x:54:PRO:HB2	2.25	0.51
56:d:64:GLN:HE21	56:d:68:LEU:CD1	2.23	0.51
62:b:62:MET:HA	62:b:62:MET:CE	2.34	0.51
63:c:200:VAL:HG13	63:c:214:VAL:HG12	1.91	0.51
65:l:51:ILE:O	65:l:55:LEU:HG	2.09	0.51
68:k:29:GLY:O	68:k:33:LEU:CG	2.42	0.51
72:p:91:GLN:NE2	72:p:137:LEU:O	2.43	0.51
74:x:566:GLU:O	74:x:568:LYS:N	2.43	0.51
8:FA:109:LYS:O	8:FA:149:LEU:N	2.38	0.51
9:HA:115:LEU:HD13	9:HA:191:PRO:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HA:393:ASP:OD1	9:HA:394:PHE:N	2.42	0.51
15:HB:412:GLU:N	15:HB:412:GLU:OE1	2.44	0.51
17:PB:528:LEU:HD21	17:PB:767:LEU:HD21	1.93	0.51
18:HC:397:GLU:CD	33:HF:61:MET:HE3	2.36	0.51
31:HG:88:LEU:HD23	31:HG:131:LEU:HD21	1.91	0.51
35:DD:963:ARG:HD3	35:DD:983:ARG:CZ	2.41	0.51
46:HI:143:LEU:O	46:HI:143:LEU:CD1	2.52	0.51
47:HJ:100:HIS:CG	47:HJ:101:PRO:HD2	2.46	0.51
50:g:158:GLU:OE2	50:g:158:GLU:HA	2.10	0.51
52:n:861:LYS:HE3	63:c:30:ARG:CD	2.39	0.51
53:s:104:LYS:CB	53:s:106:SER:H	2.22	0.51
54:u:49:ASN:N	54:u:50:PRO:HD2	2.26	0.51
54:u:71:VAL:HG13	61:z:529:HIS:CB	2.35	0.51
54:u:71:VAL:HG22	61:z:528:LEU:HD23	1.92	0.51
60:q:166:ARG:CB	60:q:166:ARG:NH1	2.73	0.51
61:z:582:LEU:HD23	61:z:591:LEU:HB3	1.90	0.51
62:b:181:CYS:SG	65:l:82:LEU:HD22	2.50	0.51
72:p:304:SER:OG	72:p:349:ASP:O	2.28	0.51
11:PA:95:PHE:N	11:PA:311:GLN:OE1	2.43	0.51
12:DB:656:GLU:HG2	12:DB:661:ALA:HB3	1.93	0.51
17:PB:625:LEU:HD13	17:PB:675:LEU:HD21	1.91	0.51
36:DE:562:SER:OG	36:DE:564:ASP:OD1	2.27	0.51
37:DF:63:ARG:NH2	37:DF:70:ASP:OD1	2.41	0.51
46:HI:143:LEU:C	46:HI:143:LEU:CD2	2.80	0.51
47:HJ:73:PRO:HB2	47:HJ:118:PHE:HZ	1.75	0.51
48:PD:137:LYS:C	48:PD:139:SER:N	2.67	0.51
55:a:60:SER:O	55:a:63:GLU:HG2	2.11	0.51
55:a:493:PHE:CE2	55:a:514:LYS:HB2	2.45	0.51
60:q:186:GLU:OE2	60:q:291:TRP:NE1	2.43	0.51
60:q:479:ILE:HG22	60:q:532:HIS:NE2	2.19	0.51
71:v:130:LEU:N	71:v:130:LEU:CD2	2.73	0.51
73:w:86:ALA:HB1	73:w:92:LEU:HD13	1.92	0.51
73:w:767:TRP:HE1	73:w:804:ASN:HD21	1.58	0.51
6:DA:411:GLU:N	6:DA:411:GLU:OE2	2.41	0.51
6:DA:470:ILE:HG23	37:DF:214:HIS:HA	1.92	0.51
7:EA:49:LEU:HD22	7:EA:56:ARG:HD3	1.93	0.51
11:PA:1284:PHE:CE2	11:PA:1288:ILE:HD11	2.46	0.51
12:DB:152:LEU:HD23	12:DB:155:PRO:HB3	1.91	0.51
12:DB:618:ALA:CB	18:HC:439:ARG:HH22	2.24	0.51
12:DB:781:TYR:O	39:DH:176:ARG:NH2	2.44	0.51
17:PB:905:ASP:N	17:PB:922:ARG:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:PB:1134:THR:HG22	49:PG:154:LYS:H	1.73	0.51
30:HD:55:LYS:HD3	49:PG:166:ASP:HB3	1.93	0.51
36:DE:324:LYS:HG2	36:DE:327:ASN:HD22	1.74	0.51
51:j:61:ILE:O	52:n:50:ARG:N	2.43	0.51
52:n:643:HIS:CD2	60:q:560:ILE:HA	2.45	0.51
56:d:42:ARG:CZ	58:i:93:LYS:HG2	2.41	0.51
56:d:44:LEU:CD2	56:d:48:LEU:HD11	2.40	0.51
58:i:109:LEU:CD2	58:i:117:GLN:NE2	2.73	0.51
65:l:36:ILE:O	65:l:39:GLU:HG2	2.11	0.51
67:h:182:VAL:CG2	69:r:202:ILE:HD11	2.32	0.51
68:k:38:GLU:HG3	68:k:38:GLU:O	2.10	0.51
72:p:801:CYS:SG	72:p:802:GLY:N	2.83	0.51
6:DA:1065:GLU:O	6:DA:1069:ILE:HG12	2.10	0.51
7:EA:103:VAL:O	7:EA:107:LEU:HG	2.10	0.51
11:PA:904:GLN:NE2	11:PA:981:CYS:O	2.42	0.51
11:PA:1382:LEU:HD23	11:PA:1398:LEU:HD13	1.93	0.51
12:DB:90:THR:O	12:DB:968:ARG:NH2	2.43	0.51
32:HE:44:LEU:HD22	32:HE:227:LEU:HB3	1.90	0.51
34:HH:274:GLN:OE1	34:HH:459:GLN:NE2	2.44	0.51
34:HH:363:VAL:HG21	34:HH:378:PHE:HE2	1.75	0.51
36:DE:601:VAL:HG21	36:DE:642:VAL:HG11	1.91	0.51
37:DF:122:LEU:HD23	39:DH:36:THR:HG23	1.91	0.51
37:DF:243:LEU:HD21	37:DF:284:ARG:HB3	1.92	0.51
41:DL:111:LEU:O	41:DL:114:LYS:CE	2.59	0.51
42:Dc:21:LEU:HD12	42:Dc:21:LEU:O	2.11	0.51
35:Dd:916:LYS:NZ	35:Dd:1070:GLU:OE2	2.42	0.51
46:HI:232:PRO:HB2	46:HI:240:MET:SD	2.51	0.51
47:HJ:228:MET:O	47:HJ:229:GLU:C	2.53	0.51
52:n:203:LEU:HD13	52:n:215:LEU:HD11	1.88	0.51
52:n:321:GLY:HA3	60:q:317:GLN:NE2	2.25	0.51
57:f:101:ILE:HD13	67:h:105:VAL:HB	1.92	0.51
60:q:576:GLY:O	60:q:619:ARG:NH2	2.43	0.51
68:k:14:LEU:N	68:k:14:LEU:HD23	2.25	0.51
72:p:437:SER:OG	72:p:438:TRP:N	2.43	0.51
72:p:683:GLN:HE22	72:p:723:GLN:HB3	1.75	0.51
73:w:633:VAL:O	73:w:817:ARG:NH2	2.43	0.51
73:w:1118:SER:OG	73:w:1119:GLY:N	2.43	0.51
5:BA:107:MET:O	5:BA:112:ARG:NH2	2.43	0.51
6:DA:639:LEU:HD11	6:DA:774:ARG:HG2	1.93	0.51
9:HA:126:PHE:CE2	9:HA:128:LYS:HB2	2.46	0.51
12:DB:537:PHE:CE2	12:DB:539:ARG:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DG:181:TRP:CE3	38:DG:181:TRP:O	2.63	0.51
39:DH:32:ALA:O	39:DH:36:THR:OG1	2.29	0.51
48:PD:73:ARG:HD2	48:PD:138:ARG:HE	1.76	0.51
50:g:153:PHE:CZ	56:d:125:VAL:HG12	2.46	0.51
55:a:373:CYS:HB3	55:a:439:GLN:HG2	1.92	0.51
58:i:66:LEU:HD13	58:i:66:LEU:C	2.35	0.51
60:q:490:SER:OG	60:q:539:GLN:NE2	2.40	0.51
60:q:491:ILE:HD12	60:q:532:HIS:N	2.25	0.51
65:l:166:LEU:HD22	71:v:123:ILE:CD1	2.41	0.51
66:o:682:VAL:HG22	66:o:691:VAL:HG11	1.93	0.51
68:k:41:ASN:O	68:k:45:LEU:CB	2.59	0.51
68:k:109:ARG:CG	68:k:109:ARG:NH1	2.73	0.51
70:t:3:VAL:HG22	70:t:150:ALA:HB2	1.92	0.51
71:v:16:GLN:O	71:v:20:LYS:HG2	2.11	0.51
71:v:133:GLU:OE1	71:v:133:GLU:HA	2.10	0.51
72:p:822:ARG:NH1	75:y:107:GLY:O	2.38	0.51
74:x:86:ASP:O	74:x:88:PHE:N	2.43	0.51
11:PA:863:ARG:NH2	11:PA:1415:THR:OG1	2.44	0.51
15:HB:471:LEU:HD13	15:HB:475:PHE:HE2	1.75	0.51
35:DD:922:GLN:HG2	35:DD:1056:THR:OG1	2.11	0.51
36:DE:299:ASP:OD2	36:DE:607:ARG:NH2	2.38	0.51
36:DE:423:PRO:HG2	36:DE:426:ARG:HB2	1.92	0.51
41:DL:78:GLU:O	41:DL:82:GLU:HG3	2.11	0.51
36:De:747:LEU:O	36:De:747:LEU:HG	2.10	0.51
46:HI:15:LEU:HD23	46:HI:15:LEU:C	2.36	0.51
51:j:85:LEU:HD13	53:s:93:TYR:HA	1.93	0.51
52:n:446:CYS:SG	52:n:447:GLY:N	2.84	0.51
54:u:108:VAL:HG22	56:d:128:ALA:CB	2.41	0.51
55:a:465:VAL:HG21	55:a:511:ILE:CD1	2.41	0.51
56:d:90:HIS:C	56:d:90:HIS:CD2	2.89	0.51
57:f:29:VAL:HG11	57:f:79:PHE:HB3	1.92	0.51
57:f:36:ARG:HA	57:f:41:TYR:HE1	1.76	0.51
58:i:65:PHE:HE1	58:i:99:LYS:CB	2.23	0.51
60:q:441:ARG:CZ	65:l:168:TRP:CE3	2.90	0.51
11:PA:1643:TYR:CB	59:m:96:PHE:CD2	2.92	0.51
12:DB:202:TRP:HB2	12:DB:238:LEU:HB3	1.92	0.51
13:EB:193:ASN:OD1	13:EB:194:ARG:N	2.43	0.51
30:HD:27:GLY:HA3	30:HD:70:LYS:CD	2.34	0.51
34:HH:377:GLN:OE1	34:HH:381:TRP:NE1	2.40	0.51
36:DE:754:THR:OG1	36:DE:755:ALA:N	2.43	0.51
37:DF:323:VAL:HG23	37:DF:326:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DI:131:SER:OG	43:DJ:150:ARG:NH1	2.44	0.51
41:DL:111:LEU:HA	41:DL:114:LYS:CE	2.36	0.51
36:De:500:THR:HG22	36:De:502:LYS:H	1.76	0.51
52:n:907:LEU:HD21	62:b:118:LEU:HA	1.93	0.51
54:u:90:LEU:CD1	60:q:9:ILE:CG1	2.68	0.51
55:a:107:MET:HE2	55:a:107:MET:C	2.35	0.51
55:a:340:TYR:O	55:a:344:THR:HG23	2.11	0.51
57:f:169:SER:OG	57:f:170:SER:N	2.44	0.51
59:m:64:ALA:HA	59:m:67:LEU:HD12	1.92	0.51
68:k:75:THR:C	68:k:77:GLN:H	2.19	0.51
72:p:471:LEU:HD22	72:p:499:MET:HE3	1.93	0.51
72:p:790:CYS:SG	72:p:839:SER:OG	2.68	0.51
43:DJ:139:LEU:HB3	43:DJ:144:PHE:HB3	1.93	0.51
7:EA:170:LYS:O	7:EA:174:ARG:HD3	2.10	0.51
9:HA:3:LEU:O	9:HA:9:LEU:HD12	2.11	0.51
22:PC:51:GLN:NE2	29:PL:52:LEU:HD13	2.26	0.51
37:DF:299:LYS:HD3	37:Df:347:THR:HG22	1.91	0.51
40:DI:60:HIS:CE1	41:DL:102:LEU:HB3	2.46	0.51
46:HI:49:SER:HB2	46:HI:52:LYS:HD2	1.92	0.51
47:HJ:165:ARG:HB3	47:HJ:166:PRO:HD3	1.92	0.51
50:g:75:LYS:CD	54:u:78:SER:HA	2.40	0.51
50:g:157:LEU:HD23	50:g:157:LEU:C	2.36	0.51
52:n:226:VAL:HG22	52:n:229:GLU:H	1.75	0.51
52:n:935:ALA:HB1	52:n:1174:PRO:HB2	1.91	0.51
56:d:45:ILE:HD13	58:i:73:ILE:CA	2.38	0.51
60:q:113:TYR:HE2	67:h:20:ALA:HB2	1.76	0.51
60:q:645:ALA:O	65:l:111:VAL:CG2	2.59	0.51
62:b:84:GLN:OE1	62:b:94:SER:HB3	2.11	0.51
63:c:297:ARG:HA	63:c:303:GLU:O	2.11	0.51
67:h:143:LEU:HD21	68:k:34:GLU:O	2.11	0.51
70:t:78:LEU:HD22	70:t:78:LEU:H	1.74	0.51
70:t:144:TYR:CD2	70:t:147:CYS:HB2	2.36	0.51
73:w:378:GLN:HE22	73:w:532:THR:HA	1.75	0.51
7:EA:180:PHE:HA	13:EB:216:PHE:CZ	2.46	0.51
8:FA:162:GLU:OE1	8:FA:162:GLU:N	2.43	0.51
12:DB:274:LEU:HG	12:DB:278:LYS:HE2	1.92	0.51
12:DB:622:ASP:OD1	33:HF:36:GLN:HG3	2.11	0.51
17:PB:809:VAL:HG11	17:PB:811:TYR:CE2	2.46	0.51
35:DD:1071:ARG:HG3	37:DF:91:PHE:CE1	2.46	0.51
37:DF:335:ARG:HE	37:DF:382:GLU:HB2	1.74	0.51
39:DH:44:LEU:HD23	39:DH:47:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:22:GLN:CD	46:HI:22:GLN:N	2.69	0.51
47:HJ:212:ILE:HA	47:HJ:255:MET:HE1	1.93	0.51
52:n:915:ARG:NE	52:n:923:CYS:SG	2.84	0.51
53:s:102:LYS:O	53:s:103:GLU:C	2.53	0.51
54:u:5:LEU:HD11	61:z:596:TYR:CZ	2.45	0.51
54:u:71:VAL:CG2	61:z:528:LEU:CD2	2.89	0.51
54:u:80:GLU:HA	61:z:539:ASP:CG	2.36	0.51
55:a:94:LEU:O	55:a:94:LEU:HG	2.10	0.51
55:a:445:LEU:CA	74:x:55:SER:CB	2.86	0.51
60:q:188:LEU:CD1	71:v:87:ILE:HG13	2.40	0.51
62:b:186:THR:HG21	64:e:49:GLU:CG	2.41	0.51
64:e:77:VAL:HA	64:e:80:CYS:SG	2.51	0.51
69:r:206:ARG:HE	69:r:206:ARG:C	2.18	0.51
4:NY:-125:DG:H2"	4:NY:-124:DG:C8	2.46	0.50
6:DA:828:GLU:HA	6:DA:831:LYS:HB2	1.92	0.50
7:EA:137:THR:CG2	7:EA:139:LEU:HD13	2.41	0.50
35:DD:873:LEU:N	35:DD:873:LEU:CD1	2.73	0.50
36:DE:324:LYS:O	36:DE:327:ASN:ND2	2.44	0.50
36:DE:461:ILE:O	37:DF:135:TRP:HE3	1.94	0.50
36:DE:506:SER:HB2	36:DE:575:PHE:HD2	1.76	0.50
40:DI:82:SER:HB3	40:DI:83:PHE:HD1	1.76	0.50
45:Dm:28:ARG:HH21	45:Dm:31:LEU:HD21	1.75	0.50
52:n:261:ASP:HB2	60:q:250:ASP:OD2	2.12	0.50
52:n:274:ILE:HG13	57:f:181:LEU:HD22	1.93	0.50
54:u:67:LYS:HE2	61:z:528:LEU:CD1	2.41	0.50
58:i:66:LEU:N	58:i:67:PRO:HD2	2.25	0.50
60:q:561:GLU:OE2	60:q:588:SER:OG	2.28	0.50
6:DA:1163:ARG:HB3	38:DG:183:ILE:HG22	1.91	0.50
7:EA:139:LEU:HD12	49:PG:151:ARG:HH11	1.75	0.50
18:HC:408:LEU:HD21	33:HF:36:GLN:OE1	2.11	0.50
36:DE:463:PHE:N	37:DF:134:HIS:O	2.45	0.50
40:DI:83:PHE:HD1	40:DI:83:PHE:H	1.59	0.50
46:HI:83:HIS:HD2	46:HI:84:LYS:HG2	1.76	0.50
47:HJ:25:ASP:OD1	47:HJ:26:ALA:N	2.45	0.50
52:n:169:LEU:CB	52:n:170:PRO:HD3	2.26	0.50
52:n:960:LYS:CB	52:n:1210:PHE:CZ	2.86	0.50
66:o:718:VAL:HG13	66:o:742:GLN:OE1	2.10	0.50
68:k:96:ARG:CD	71:v:116:LEU:HD12	2.41	0.50
68:k:101:ARG:CZ	68:k:101:ARG:CB	2.87	0.50
73:w:418:GLN:HA	73:w:421:HIS:HD2	1.75	0.50
73:w:571:LEU:HB2	73:w:612:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HA:637:LEU:HD13	9:HA:651:PHE:CD2	2.47	0.50
11:PA:1674:THR:HB	46:HI:214:PRO:CG	2.42	0.50
18:HC:390:GLN:HE21	18:HC:394:TRP:NE1	2.09	0.50
19:DO:57:ASN:OD1	19:DO:58:PHE:N	2.44	0.50
31:HG:204:GLU:OE1	31:HG:209:THR:OG1	2.28	0.50
37:DF:279:LEU:HD22	37:DF:330:ARG:NH2	2.27	0.50
39:DH:54:GLU:OE1	43:DJ:197:MET:HB2	2.11	0.50
39:DH:110:TYR:CZ	39:DH:113:ARG:NH1	2.78	0.50
47:HJ:268:GLU:OE1	47:HJ:268:GLU:N	2.29	0.50
56:d:34:LEU:HD22	58:i:99:LYS:CD	2.31	0.50
9:HA:284:GLU:HA	9:HA:287:ARG:HG2	1.93	0.50
18:HC:410:ASN:HB2	33:HF:3:ASN:OD1	2.11	0.50
41:DI:102:LEU:HB2	41:DI:115:ASP:HB2	1.94	0.50
46:HI:151:LEU:C	46:HI:151:LEU:HD23	2.36	0.50
48:PD:79:THR:CA	67:h:51:LEU:HD22	2.19	0.50
50:g:164:ILE:CD1	58:i:140:MET:HG2	2.37	0.50
50:g:172:PRO:HA	50:g:175:LEU:CG	2.42	0.50
52:n:234:LEU:HD23	52:n:247:LEU:HA	1.92	0.50
52:n:267:HIS:CD2	57:f:174:ARG:CD	2.58	0.50
52:n:466:MET:HG3	60:q:321:GLN:HE21	1.75	0.50
55:a:377:ASN:CB	55:a:442:VAL:O	2.55	0.50
55:a:461:SER:CA	74:x:7:LYS:HD3	2.42	0.50
58:i:65:PHE:HZ	58:i:102:SER:HG	1.57	0.50
60:q:140:ASN:N	60:q:141:PRO:HD2	2.24	0.50
66:o:688:LYS:HG2	66:o:712:ASP:HB3	1.93	0.50
68:k:44:LEU:HD22	68:k:47:ARG:HH12	1.76	0.50
72:p:560:LEU:HD12	72:p:658:LEU:HD22	1.93	0.50
73:w:366:ILE:HG23	73:w:369:ARG:HD3	1.93	0.50
73:w:1193:PHE:C	73:w:1195:ALA:H	2.19	0.50
7:EA:152:PHE:O	7:EA:153:ARG:HB2	2.10	0.50
9:HA:377:GLU:N	9:HA:377:GLU:OE1	2.44	0.50
12:DB:818:THR:OG1	12:DB:819:LEU:N	2.44	0.50
15:HB:481:VAL:HG23	15:HB:483:THR:HG23	1.94	0.50
17:PB:834:ARG:HG2	17:PB:840:MET:HE2	1.93	0.50
17:PB:907:VAL:HG22	17:PB:921:ILE:HG12	1.94	0.50
22:PC:67:ARG:NH2	27:PJ:2:ILE:HG23	2.27	0.50
28:PK:105:PHE:CE2	28:PK:109:ILE:HD11	2.46	0.50
36:DE:449:LYS:O	39:DH:145:HIS:HB3	2.12	0.50
47:HJ:184:PRO:CB	47:HJ:187:LEU:HD12	2.33	0.50
50:g:127:ARG:HD3	50:g:130:GLN:HB3	1.93	0.50
52:n:203:LEU:HD21	52:n:224:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:104:LEU:O	54:u:108:VAL:HG23	2.10	0.50
55:a:417:TYR:HB2	55:a:469:VAL:HG11	1.92	0.50
60:q:113:TYR:HA	67:h:19:VAL:HG11	1.93	0.50
62:b:186:THR:HG21	64:e:49:GLU:OE1	2.11	0.50
68:k:109:ARG:CB	68:k:109:ARG:NH1	2.74	0.50
76:NC:841:THR:HA	76:NG:1040:THR:O	2.11	0.50
1:X:-6:DG:H1	2:Y:6:DC:H42	1.59	0.50
6:DA:396:LEU:N	6:DA:396:LEU:HD22	2.27	0.50
13:EB:88:ARG:NH2	13:EB:93:ASP:OD2	2.45	0.50
18:HC:402:ARG:NH1	33:HF:11:GLU:OE2	2.43	0.50
34:HH:369:VAL:HG11	34:HH:615:PHE:HA	1.93	0.50
36:DE:462:CYS:SG	37:DF:133:ALA:HB1	2.52	0.50
46:HI:261:PHE:CZ	46:HI:272:ILE:HD12	2.46	0.50
49:PG:90:THR:OG1	49:PG:91:GLN:OE1	2.11	0.50
49:PG:97:LEU:HD21	49:PG:128:TYR:CE1	2.46	0.50
52:n:201:HIS:ND1	56:d:111:GLN:NE2	2.59	0.50
54:u:74:ASP:O	61:z:532:VAL:HG21	2.11	0.50
56:d:115:LYS:CA	56:d:115:LYS:CE	2.86	0.50
57:f:15:TRP:HH2	57:f:35:GLU:HB2	1.77	0.50
62:b:96:ASP:CB	72:p:670:PRO:HG2	2.41	0.50
62:b:132:ASP:C	62:b:132:ASP:OD1	2.54	0.50
68:k:16:ASP:OD2	71:v:79:VAL:HG22	2.11	0.50
68:k:41:ASN:O	68:k:45:LEU:HB2	2.10	0.50
76:NG:1041:THR:O	76:NG:1042:SER:C	2.54	0.50
6:DA:481:GLU:HA	6:DA:484:ILE:HD12	1.93	0.50
9:HA:284:GLU:HG2	9:HA:385:THR:HG21	1.94	0.50
13:EB:124:LEU:HD13	13:EB:137:TYR:CD1	2.47	0.50
34:HH:363:VAL:HG21	34:HH:378:PHE:CE2	2.47	0.50
45:Dm:69:THR:HG23	45:Dm:80:ARG:HE	1.77	0.50
46:HI:192:VAL:O	46:HI:192:VAL:HG12	2.12	0.50
46:HI:229:LEU:HD11	46:HI:276:PHE:HB3	1.92	0.50
52:n:153:ALA:HB3	56:d:152:ALA:HB1	1.92	0.50
62:b:96:ASP:HB2	72:p:670:PRO:HG2	1.94	0.50
62:b:162:ALA:HA	62:b:165:LYS:HD3	1.94	0.50
62:b:179:LEU:HD12	64:e:60:VAL:C	2.37	0.50
62:b:186:THR:CG2	64:e:49:GLU:OE1	2.60	0.50
63:c:124:ALA:HA	64:e:81:ILE:HD11	1.94	0.50
63:c:200:VAL:HA	63:c:214:VAL:HA	1.93	0.50
73:w:1200:TYR:CD2	73:w:1200:TYR:O	2.64	0.50
1:X:25:DG:H1	2:Y:-25:DC:H42	1.60	0.50
4:NY:-147:DG:H2"	4:NY:-146:DG:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DA:931:PRO:O	6:DA:935:THR:OG1	2.25	0.50
7:EA:17:LEU:HD13	7:EA:194:THR:OG1	2.12	0.50
7:EA:20:TYR:HD2	7:EA:190:LEU:HD11	1.77	0.50
7:EA:174:ARG:NE	30:HD:37:LEU:HD11	2.27	0.50
11:PA:1016:LEU:O	11:PA:1020:LEU:HG	2.10	0.50
12:DB:540:LYS:HA	33:HF:32:LYS:O	2.11	0.50
17:PB:296:GLU:OE2	26:PI:103:ARG:NH2	2.44	0.50
30:HD:284:ALA:HB1	46:HI:243:LEU:HD22	1.94	0.50
42:Dc:1:MET:HG3	37:Df:126:PRO:HB3	1.94	0.50
37:Df:24:GLU:HG2	41:DI:145:THR:HG21	1.93	0.50
50:g:129:HIS:HB2	54:u:82:THR:HG22	1.93	0.50
51:j:78:GLN:O	51:j:82:LYS:HG2	2.12	0.50
58:i:118:LEU:HD23	58:i:118:LEU:O	2.11	0.50
68:k:77:GLN:CG	69:r:192:GLN:HG2	2.40	0.50
70:t:98:LEU:O	70:t:101:PHE:N	2.43	0.50
12:DB:983:ARG:HG3	12:DB:983:ARG:NH1	2.26	0.50
30:HD:295:ARG:O	30:HD:295:ARG:HD2	2.12	0.50
38:DG:94:MET:HE3	38:DG:96:VAL:HG22	1.94	0.50
39:DH:117:MET:HB2	43:DJ:129:THR:HG23	1.94	0.50
36:De:693:VAL:HB	36:De:707:LEU:HB2	1.94	0.50
54:u:115:LEU:CD1	56:d:121:LEU:CD1	2.88	0.50
57:f:123:VAL:HB	71:v:55:GLU:OE1	2.12	0.50
60:q:488:CYS:SG	60:q:536:ALA:HA	2.52	0.50
67:h:12:LEU:C	67:h:12:LEU:CD1	2.85	0.50
70:t:128:THR:O	70:t:128:THR:OG1	2.27	0.50
70:t:138:ILE:O	70:t:138:ILE:HG22	2.11	0.50
72:p:511:TYR:HB2	72:p:526:ILE:HD13	1.94	0.50
72:p:587:ILE:HD13	72:p:598:ASN:HD22	1.77	0.50
73:w:872:ARG:HB3	73:w:874:HIS:HD2	1.76	0.50
74:x:566:GLU:H	74:x:566:GLU:CD	2.20	0.50
7:EA:114:ILE:CG2	7:EA:177:LEU:HD22	2.42	0.49
11:PA:485:ASN:O	11:PA:488:VAL:HG22	2.10	0.49
12:DB:217:ASN:ND2	12:DB:320:ALA:O	2.35	0.49
47:HJ:46:VAL:HG22	47:HJ:279:ARG:HH12	1.76	0.49
55:a:467:MET:HB3	55:a:475:VAL:CG1	2.41	0.49
58:i:121:LEU:O	58:i:125:VAL:HG23	2.11	0.49
59:m:107:HIS:O	59:m:111:LYS:HB3	2.12	0.49
60:q:188:LEU:CA	71:v:87:ILE:CD1	2.78	0.49
60:q:644:SER:CA	60:q:647:SER:OG	2.58	0.49
73:w:1187:PRO:HA	73:w:1190:LEU:HB3	1.94	0.49
4:NY:-10:DG:H2"	4:NY:-9:DG:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DA:569:ASN:HB3	6:DA:572:TYR:HD2	1.76	0.49
7:EA:20:TYR:HB3	7:EA:190:LEU:HD13	1.94	0.49
7:EA:132:CYS:O	7:EA:133:SER:OG	2.18	0.49
7:EA:181:ASN:ND2	30:HD:9:CYS:CA	2.74	0.49
7:EA:191:LEU:O	7:EA:195:GLU:OE1	2.30	0.49
30:HD:5:GLY:HA3	30:HD:10:LYS:CB	2.25	0.49
31:HG:285:THR:O	31:HG:297:LYS:NZ	2.46	0.49
35:DD:950:LEU:HD13	35:DD:954:GLU:HG2	1.94	0.49
37:DF:368:THR:CG2	37:DF:369:PRO:HD2	2.42	0.49
39:DH:110:TYR:CD1	43:DJ:161:LYS:CD	2.92	0.49
36:De:586:TYR:HB3	36:De:605:HIS:HB3	1.94	0.49
36:De:650:THR:HG22	36:De:666:THR:HG22	1.93	0.49
37:Df:97:ALA:HB2	37:Df:106:PHE:HE1	1.77	0.49
52:n:776:LEU:O	52:n:780:VAL:HG13	2.12	0.49
55:a:443:CYS:HB3	74:x:58:PRO:HD2	1.93	0.49
56:d:31:LEU:CG	58:i:103:THR:HG21	2.39	0.49
60:q:95:TRP:N	60:q:95:TRP:CD1	2.79	0.49
60:q:523:ASP:CB	60:q:563:ILE:HD12	2.41	0.49
63:c:41:ASN:HB3	72:p:840:TYR:HA	1.92	0.49
64:e:108:GLU:O	64:e:112:LYS:HG3	2.12	0.49
67:h:85:ARG:HA	67:h:99:VAL:HG11	1.93	0.49
43:DJ:126:TYR:HE2	43:DJ:157:LEU:HD11	1.77	0.49
7:EA:43:VAL:HB	7:EA:48:MET:HE3	1.94	0.49
9:HA:118:HIS:HB3	9:HA:121:VAL:HG22	1.94	0.49
17:PB:404:PHE:HA	17:PB:407:MET:HE3	1.94	0.49
17:PB:738:THR:HG21	27:PJ:58:LYS:HG3	1.93	0.49
36:DE:693:VAL:HB	36:DE:707:LEU:HB2	1.95	0.49
37:DF:273:GLN:CD	37:DF:273:GLN:N	2.70	0.49
41:DL:111:LEU:CA	41:DL:114:LYS:CE	2.90	0.49
42:Dc:77:LEU:O	42:Dc:77:LEU:HD23	2.11	0.49
46:HI:37:ILE:HD12	46:HI:37:ILE:H	1.75	0.49
50:g:124:ASN:O	50:g:127:ARG:HB3	2.11	0.49
52:n:274:ILE:HD11	57:f:181:LEU:HD21	1.93	0.49
52:n:707:ASP:HA	66:o:684:ARG:NH2	2.27	0.49
55:a:62:LEU:HD21	56:d:62:GLU:HB2	1.94	0.49
55:a:274:ILE:HG22	55:a:274:ILE:O	2.11	0.49
55:a:441:GLU:HB2	74:x:17:ARG:NH2	2.10	0.49
56:d:115:LYS:CD	56:d:115:LYS:C	2.85	0.49
60:q:188:LEU:CD2	71:v:87:ILE:HG13	2.38	0.49
62:b:175:HIS:CB	63:c:113:TRP:CZ2	2.92	0.49
67:h:102:HIS:H	67:h:102:HIS:HD2	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:k:71:THR:HG21	71:v:15:LEU:HB2	1.94	0.49
69:r:112:GLU:C	69:r:114:LEU:H	2.20	0.49
70:t:6:VAL:HG22	70:t:141:GLU:CB	2.41	0.49
75:y:147:ASN:O	75:y:186:ARG:NH2	2.45	0.49
12:DB:674:THR:HG22	18:HC:415:GLN:HG3	1.92	0.49
18:HC:266:ARG:HE	18:HC:277:LYS:HZ2	1.58	0.49
37:DF:106:PHE:HA	43:DJ:217:PHE:HB3	1.94	0.49
46:HI:57:ARG:HH22	46:HI:158:LEU:HD23	1.78	0.49
49:PG:134:ASP:OD1	49:PG:135:ILE:N	2.45	0.49
54:u:78:SER:HB3	61:z:563:VAL:CG2	2.41	0.49
54:u:122:LEU:O	54:u:123:ALA:C	2.53	0.49
55:a:460:ASP:OD2	74:x:5:ASN:ND2	2.45	0.49
55:a:460:ASP:HB3	74:x:7:LYS:HB2	1.93	0.49
60:q:149:LYS:HD2	71:v:40:ALA:CA	2.41	0.49
60:q:451:LEU:CD1	60:q:529:MET:SD	2.84	0.49
73:w:726:ASN:ND2	73:w:726:ASN:N	2.60	0.49
74:x:555:GLU:HA	74:x:558:VAL:HG12	1.94	0.49
6:DA:504:PRO:HD3	37:DF:207:ARG:HB3	1.94	0.49
7:EA:152:PHE:CD1	49:PG:95:VAL:HG11	2.47	0.49
9:HA:243:CYS:SG	9:HA:443:ALA:HB3	2.53	0.49
13:EB:181:ALA:O	13:EB:185:LEU:HD23	2.13	0.49
17:PB:601:VAL:HG22	17:PB:616:THR:HG23	1.93	0.49
17:PB:962:THR:O	27:PJ:9:THR:HG23	2.12	0.49
31:HG:63:VAL:HG11	31:HG:88:LEU:HD11	1.95	0.49
39:DH:27:ASP:OD1	39:DH:27:ASP:N	2.45	0.49
39:DH:57:SER:HB2	43:DJ:197:MET:CG	2.42	0.49
52:n:592:LYS:HB3	73:w:27:MET:CE	2.42	0.49
60:q:155:GLY:C	71:v:62:HIS:HE1	2.20	0.49
63:c:240:GLN:O	63:c:243:THR:OG1	2.26	0.49
63:c:298:ASP:HB2	63:c:305:PHE:HE2	1.76	0.49
70:t:41:VAL:HG22	70:t:68:ASN:HA	1.93	0.49
7:EA:174:ARG:CG	30:HD:37:LEU:HD11	2.42	0.49
9:HA:81:GLU:O	9:HA:84:ILE:HG22	2.13	0.49
11:PA:1382:LEU:HD23	11:PA:1398:LEU:CD1	2.42	0.49
13:EB:131:GLU:N	13:EB:138:ALA:O	2.42	0.49
15:HB:471:LEU:HD13	15:HB:475:PHE:CE2	2.47	0.49
19:DO:65:TYR:OH	20:DP:203:ARG:NE	2.46	0.49
30:HD:4:GLN:OE1	30:HD:10:LYS:HD3	2.13	0.49
37:DF:22:VAL:CG1	40:DI:44:PHE:CE1	2.94	0.49
40:DI:32:GLU:HB2	40:DI:35:VAL:CG2	2.43	0.49
46:HI:179:ARG:HH21	46:HI:184:LEU:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:279:ASN:O	46:HI:282:ALA:N	2.45	0.49
49:PG:83:GLU:OE2	49:PG:147:ILE:HD12	2.13	0.49
52:n:870:GLN:CG	66:o:655:THR:CG2	2.90	0.49
52:n:937:ARG:NH2	52:n:943:LEU:HD23	2.27	0.49
55:a:160:LEU:HD12	55:a:214:ARG:NH2	2.26	0.49
55:a:420:LEU:HB3	55:a:504:ILE:HD12	1.94	0.49
55:a:443:CYS:SG	74:x:57:ASN:CB	3.00	0.49
57:f:16:VAL:HG13	57:f:104:VAL:HA	1.94	0.49
60:q:396:ALA:HB2	69:r:51:PHE:CZ	2.43	0.49
60:q:396:ALA:HB2	69:r:51:PHE:HE2	1.67	0.49
73:w:122:VAL:O	73:w:126:ILE:HB	2.13	0.49
6:DA:927:VAL:O	6:DA:933:ASN:ND2	2.45	0.49
11:PA:1658:SER:HB3	57:f:12:GLY:O	2.13	0.49
17:PB:388:TYR:CE2	17:PB:505:LEU:HD21	2.48	0.49
34:HH:578:PRO:HG3	34:HH:602:ILE:HD11	1.94	0.49
37:DF:312:ILE:HG22	37:DF:313:VAL:HG13	1.94	0.49
36:De:439:ASP:OD1	36:De:555:ARG:NH2	2.44	0.49
50:g:127:ARG:H	50:g:128:PRO:HD3	1.77	0.49
52:n:254:VAL:CG2	52:n:303:LEU:CD2	2.73	0.49
52:n:305:LEU:CD1	52:n:361:ILE:HG12	2.42	0.49
52:n:529:PRO:HB2	52:n:588:LEU:HD22	1.94	0.49
52:n:544:ARG:NE	52:n:716:ASN:HA	2.28	0.49
55:a:197:ALA:HB1	55:a:201:ASP:HB2	1.94	0.49
55:a:223:LYS:NZ	55:a:251:LEU:O	2.46	0.49
56:d:34:LEU:HD21	58:i:65:PHE:CD1	2.47	0.49
60:q:168:THR:N	68:k:21:ILE:CD1	2.76	0.49
67:h:110:ARG:C	67:h:110:ARG:CD	2.85	0.49
6:DA:824:ARG:HB3	6:DA:863:VAL:HG12	1.95	0.49
9:HA:134:CYS:O	9:HA:138:THR:HG22	2.12	0.49
15:HB:440:LEU:HD11	32:HE:218:PRO:CD	2.43	0.49
20:DP:185:LEU:HD21	35:DD:1006:LEU:HD13	1.93	0.49
34:HH:61:TYR:O	34:HH:62:ARG:C	2.56	0.49
35:DD:918:SER:HB3	41:DL:74:GLU:OE2	2.13	0.49
37:DF:320:ARG:HB2	37:DF:415:ILE:HD12	1.95	0.49
39:DH:50:PHE:CD1	43:DJ:195:LEU:HB2	2.48	0.49
47:HJ:207:TYR:HB3	47:HJ:211:GLN:NE2	2.27	0.49
48:PD:114:LEU:CD1	49:PG:84:VAL:HG21	2.43	0.49
49:PG:39:THR:O	49:PG:43:GLY:N	2.42	0.49
52:n:101:ALA:N	53:s:109:LEU:HD11	2.27	0.49
55:a:70:LYS:HA	58:i:70:HIS:CE1	2.46	0.49
55:a:246:ASN:N	55:a:246:ASN:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:417:TYR:HB2	55:a:469:VAL:CG2	2.36	0.49
57:f:142:SER:HB3	60:q:183:PHE:CE2	2.48	0.49
68:k:37:LYS:HE3	68:k:37:LYS:N	2.16	0.49
3:NX:20:DC:H1'	3:NX:21:DC:C2	2.48	0.49
11:PA:539:GLN:HA	11:PA:774:ALA:HB1	1.93	0.49
17:PB:952:GLU:OE2	22:PC:39:ILE:HG22	2.13	0.49
19:DO:73:THR:O	19:DO:73:THR:HG22	2.12	0.49
30:HD:55:LYS:CG	49:PG:166:ASP:H	2.25	0.49
31:HG:87:LEU:HD11	31:HG:229:LYS:CG	2.43	0.49
36:De:234:ALA:HB2	36:De:648:ASP:HB2	1.94	0.49
46:HI:140:PRO:HA	46:HI:202:ILE:CD1	2.33	0.49
46:HI:143:LEU:O	46:HI:143:LEU:HD22	2.13	0.49
51:j:82:LYS:CD	53:s:101:VAL:CG1	2.90	0.49
55:a:374:TYR:CD2	55:a:440:PHE:HB2	2.47	0.49
59:m:121:GLU:HG2	61:z:592:ASN:ND2	2.28	0.49
60:q:109:MET:HE1	60:q:112:LEU:HD22	1.95	0.49
68:k:70:LEU:HD11	71:v:85:PHE:CD1	2.47	0.49
71:v:49:SER:HB3	71:v:50:ARG:CZ	2.42	0.49
71:v:108:LEU:C	71:v:108:LEU:CD1	2.86	0.49
72:p:482:MET:HG2	72:p:522:LEU:HD13	1.93	0.49
73:w:1193:PHE:C	73:w:1195:ALA:N	2.70	0.49
11:PA:1178:ASP:OD2	11:PA:1260:ARG:NH2	2.45	0.49
12:DB:27:LYS:HE3	12:DB:490:SER:HB3	1.95	0.49
12:DB:598:ARG:HH11	12:DB:619:MET:HE3	1.77	0.49
12:DB:739:ASN:ND2	12:DB:782:ASN:OD1	2.44	0.49
18:HC:435:ASN:ND2	33:HF:38:ILE:O	2.45	0.49
34:HH:650:MET:SD	34:HH:656:ASN:ND2	2.82	0.49
36:DE:690:ASP:OD1	36:DE:690:ASP:N	2.43	0.49
37:DF:329:LEU:C	37:DF:329:LEU:CD2	2.86	0.49
60:q:428:LEU:C	60:q:428:LEU:CD1	2.85	0.49
67:h:8:LEU:C	67:h:8:LEU:CD2	2.86	0.49
67:h:36:GLU:O	67:h:38:GLY:N	2.45	0.49
68:k:109:ARG:CZ	68:k:109:ARG:HB3	2.41	0.49
11:PA:1251:ASN:OD1	11:PA:1252:ALA:N	2.46	0.48
12:DB:560:TYR:HD2	12:DB:581:ILE:HD11	1.78	0.48
18:HC:440:LEU:HD22	33:HF:36:GLN:OE1	2.13	0.48
34:HH:575:LEU:O	34:HH:576:ASN:OD1	2.31	0.48
39:DH:111:ALA:HB2	43:DJ:157:LEU:HD13	1.94	0.48
39:DH:116:ARG:HD3	43:DJ:126:TYR:CE1	2.48	0.48
35:Dd:1080:TYR:OH	36:De:606:ASP:OD2	2.26	0.48
36:De:720:SER:OG	36:De:721:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:HJ:177:ARG:HB2	47:HJ:177:ARG:HH11	1.76	0.48
47:HJ:226:ILE:HD13	47:HJ:226:ILE:N	2.28	0.48
49:PG:124:ASN:ND2	67:h:169:ASN:O	2.46	0.48
55:a:441:GLU:O	55:a:452:VAL:HA	2.13	0.48
63:c:46:GLU:H	63:c:46:GLU:CD	2.17	0.48
66:o:644:PRO:O	66:o:648:ALA:N	2.44	0.48
72:p:38:ALA:HA	72:p:435:GLN:HE21	1.78	0.48
72:p:783:ARG:NH1	72:p:820:GLU:OE2	2.45	0.48
73:w:980:VAL:O	73:w:983:SER:OG	2.30	0.48
11:PA:1203:ASP:OD2	11:PA:1244:ASN:ND2	2.44	0.48
14:FB:43:LEU:HD12	14:FB:55:SER:O	2.13	0.48
17:PB:830:GLU:OE2	17:PB:870:THR:OG1	2.21	0.48
21:DQ:18:ILE:HD11	21:DQ:46:TRP:CZ3	2.48	0.48
35:DD:924:LYS:HB2	39:DH:83:THR:HG22	1.94	0.48
36:DE:481:ASP:HB3	36:DE:787:ARG:HH22	1.77	0.48
37:DF:279:LEU:CB	37:DF:330:ARG:NH2	2.75	0.48
39:DH:54:GLU:OE1	43:DJ:197:MET:CB	2.62	0.48
37:Df:39:LEU:HD22	40:Di:47:VAL:HG13	1.94	0.48
47:HJ:59:TYR:HB2	47:HJ:265:PRO:HG2	1.94	0.48
54:u:108:VAL:CG2	56:d:128:ALA:CB	2.86	0.48
57:f:137:CYS:O	57:f:138:ARG:HD2	2.12	0.48
58:i:109:LEU:HD22	58:i:117:GLN:NE2	2.28	0.48
58:i:133:GLN:O	58:i:133:GLN:CD	2.56	0.48
60:q:19:VAL:CG2	60:q:22:VAL:HG22	2.43	0.48
60:q:106:LEU:HD23	60:q:106:LEU:O	2.12	0.48
60:q:117:SER:O	60:q:120:ARG:HB3	2.12	0.48
60:q:155:GLY:C	71:v:62:HIS:CE1	2.91	0.48
71:v:131:GLU:HG3	71:v:135:TYR:HE2	1.78	0.48
73:w:70:GLN:HG3	73:w:75:ARG:HG2	1.94	0.48
74:x:803:ASP:OD1	74:x:803:ASP:N	2.45	0.48
6:DA:571:GLU:OE1	6:DA:571:GLU:N	2.36	0.48
8:FA:153:ARG:NH1	8:FA:180:ARG:O	2.47	0.48
9:HA:45:GLY:O	9:HA:48:LYS:NZ	2.44	0.48
9:HA:310:LEU:HG	9:HA:409:THR:HG21	1.95	0.48
11:PA:1242:ASP:O	11:PA:1262:MET:N	2.46	0.48
19:DO:2:ALA:N	35:DD:1000:ARG:HD3	2.22	0.48
35:DD:1071:ARG:HB2	37:DF:91:PHE:CE2	2.45	0.48
41:DL:70:VAL:HG12	41:DL:74:GLU:OE1	2.13	0.48
46:HI:155:ASP:C	46:HI:155:ASP:OD1	2.55	0.48
47:HJ:185:GLU:O	47:HJ:188:ARG:HB3	2.14	0.48
50:g:124:ASN:HA	50:g:127:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:g:168:LEU:HD11	58:i:136:LYS:HA	1.94	0.48
51:j:82:LYS:HD2	53:s:101:VAL:CG1	2.43	0.48
54:u:71:VAL:HG22	61:z:528:LEU:CD2	2.43	0.48
55:a:412:ARG:C	55:a:472:SER:CB	2.84	0.48
55:a:441:GLU:CB	74:x:14:TRP:HE1	2.26	0.48
56:d:45:ILE:CG1	58:i:73:ILE:CA	2.69	0.48
56:d:64:GLN:NE2	56:d:68:LEU:HD12	2.27	0.48
56:d:133:LYS:HB2	56:d:133:LYS:HE3	1.44	0.48
60:q:191:ARG:HE	71:v:87:ILE:HG12	1.78	0.48
61:z:529:HIS:CD2	61:z:566:CYS:HB3	2.48	0.48
64:e:56:PHE:HE1	65:l:52:PHE:CE1	2.32	0.48
72:p:51:LEU:HB2	72:p:58:LEU:HB3	1.94	0.48
7:EA:181:ASN:ND2	30:HD:9:CYS:C	2.71	0.48
11:PA:1218:ARG:NH2	11:PA:1252:ALA:O	2.46	0.48
12:DB:646:ASP:CA	18:HC:413:LEU:O	2.60	0.48
18:HC:360:THR:HG22	18:HC:363:GLN:OE1	2.13	0.48
32:HE:13:ILE:HD13	32:HE:41:VAL:HG13	1.94	0.48
35:DD:1059:ASN:O	41:DL:80:VAL:CG2	2.61	0.48
36:DE:651:VAL:HB	36:DE:665:PHE:HB2	1.94	0.48
37:DF:68:THR:O	37:DF:69:SER:HB3	2.13	0.48
37:DF:223:TYR:HH	37:DF:245:SER:HG	1.61	0.48
50:g:159:ARG:C	50:g:159:ARG:CD	2.86	0.48
51:j:27:SER:HA	53:s:154:LEU:HD21	1.95	0.48
55:a:148:ASP:OD1	55:a:148:ASP:N	2.47	0.48
60:q:134:ALA:H	67:h:72:ARG:HH11	1.48	0.48
60:q:187:LEU:HD12	60:q:187:LEU:C	2.38	0.48
63:c:283:ARG:CB	63:c:311:GLN:HE21	2.27	0.48
70:t:128:THR:O	70:t:130:THR:N	2.46	0.48
73:w:671:ASP:OD1	73:w:671:ASP:N	2.44	0.48
73:w:777:ILE:HA	73:w:810:VAL:HG22	1.95	0.48
5:BA:53:ARG:NE	17:PB:892:CYS:SG	2.87	0.48
6:DA:1063:LYS:NZ	6:DA:1067:GLN:OE1	2.42	0.48
7:EA:45:GLU:HB2	7:EA:90:ASN:HB2	1.96	0.48
7:EA:105:TYR:OH	13:EB:237:LEU:N	2.47	0.48
9:HA:115:LEU:O	9:HA:115:LEU:HD12	2.13	0.48
11:PA:1173:THR:HG22	11:PA:1214:VAL:HG23	1.94	0.48
37:DF:257:PRO:O	37:DF:261:THR:OG1	2.26	0.48
37:DF:388:ILE:HG22	37:DF:392:ILE:HG13	1.95	0.48
38:DG:48:HIS:HD2	38:DG:54:GLY:HA2	1.78	0.48
40:DI:73:LEU:HD12	40:DI:73:LEU:O	2.14	0.48
40:Di:73:LEU:HB2	41:DI:105:HIS:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:116:ALA:HB2	46:HI:302:THR:H	1.78	0.48
51:j:82:LYS:CE	53:s:101:VAL:CG1	2.91	0.48
52:n:851:ILE:HD11	52:n:911:SER:HA	1.96	0.48
64:e:75:THR:O	64:e:79:GLN:HG2	2.14	0.48
70:t:11:VAL:HA	70:t:20:THR:HG21	1.95	0.48
72:p:88:GLU:OE2	72:p:288:ARG:NH1	2.47	0.48
72:p:441:LEU:HB3	72:p:494:HIS:CE1	2.49	0.48
75:y:140:ARG:NH2	75:y:176:ARG:O	2.47	0.48
4:NY:-65:DG:H2''	4:NY:-64:DG:C8	2.48	0.48
12:DB:135:TRP:HA	12:DB:138:VAL:HG12	1.95	0.48
22:PC:92:GLU:O	22:PC:93:PHE:CG	2.67	0.48
31:HG:348:CYS:O	32:HE:146:ARG:NH2	2.46	0.48
36:DE:526:ARG:HA	36:DE:526:ARG:HH11	1.73	0.48
42:Dc:26:VAL:HG23	43:Dj:195:LEU:HB3	1.96	0.48
42:Dc:119:GLU:HG3	36:De:790:LEU:HD11	1.96	0.48
36:De:651:VAL:HG13	36:De:665:PHE:HB2	1.95	0.48
44:Dk:173:CYS:SG	44:Dk:179:MET:O	2.72	0.48
47:HJ:40:VAL:HB	47:HJ:44:ASP:OD2	2.13	0.48
47:HJ:190:THR:OG1	47:HJ:220:SER:HB3	2.14	0.48
50:g:128:PRO:CD	50:g:129:HIS:N	2.72	0.48
54:u:125:ILE:HG12	58:i:135:TYR:CD2	2.49	0.48
55:a:157:LEU:HD23	55:a:217:GLY:HA2	1.96	0.48
55:a:321:LEU:HA	55:a:410:LEU:CD1	2.44	0.48
55:a:393:VAL:HG13	55:a:393:VAL:O	2.13	0.48
55:a:449:ARG:HH12	74:x:54:PRO:CB	2.27	0.48
60:q:171:VAL:CG1	68:k:17:ILE:HG21	2.43	0.48
61:z:528:LEU:HA	61:z:582:LEU:HD12	1.95	0.48
62:b:86:THR:O	62:b:90:ASN:N	2.44	0.48
62:b:178:LEU:HD13	65:l:55:LEU:CD2	2.43	0.48
63:c:204:MET:CE	63:c:206:SER:O	2.47	0.48
72:p:367:ASP:HA	72:p:370:VAL:HG22	1.96	0.48
72:p:817:LYS:HB2	75:y:30:PRO:HG3	1.96	0.48
73:w:726:ASN:N	73:w:726:ASN:HD22	2.11	0.48
1:X:-28:DA:H5'	20:DP:301:VAL:HG21	1.94	0.48
6:DA:953:VAL:O	38:DG:149:ARG:NH2	2.47	0.48
7:EA:131:VAL:HB	7:EA:157:CYS:HB2	1.94	0.48
9:HA:136:SER:O	9:HA:142:VAL:HG21	2.13	0.48
11:PA:363:ALA:O	17:PB:1084:LEU:HD11	2.13	0.48
18:HC:397:GLU:OE1	33:HF:61:MET:HE3	2.14	0.48
32:HE:192:ASP:OD1	32:HE:213:LEU:N	2.45	0.48
37:DF:316:GLN:NE2	37:DF:320:ARG:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Df:102:ARG:HD3	41:Dl:151:ARG:HG3	1.96	0.48
50:g:153:PHE:HZ	56:d:125:VAL:HG12	1.79	0.48
52:n:247:LEU:HB3	52:n:275:HIS:CD2	2.49	0.48
52:n:361:ILE:HA	52:n:370:LEU:HD21	1.95	0.48
52:n:808:LEU:HB2	52:n:822:ILE:HB	1.94	0.48
60:q:188:LEU:CD1	60:q:188:LEU:C	2.86	0.48
60:q:191:ARG:NE	71:v:87:ILE:O	2.46	0.48
61:z:582:LEU:HG	61:z:584:PRO:HD3	1.95	0.48
67:h:86:ASP:N	67:h:99:VAL:HG12	2.28	0.48
67:h:151:LEU:HD11	71:v:37:ILE:O	2.13	0.48
72:p:24:TRP:HD1	72:p:51:LEU:HD12	1.79	0.48
72:p:501:GLN:OE1	72:p:543:ARG:NH1	2.45	0.48
73:w:337:GLN:HE21	73:w:341:PHE:HE2	1.59	0.48
73:w:1195:ALA:C	73:w:1197:HIS:H	2.21	0.48
75:y:184:SER:HB3	75:y:220:MET:HE3	1.96	0.48
9:HA:722:ARG:NH1	31:HG:222:ILE:O	2.46	0.48
11:PA:1415:THR:HG22	11:PA:1416:ARG:N	2.29	0.48
15:HB:374:LEU:O	15:HB:374:LEU:HD12	2.13	0.48
35:DD:966:LEU:CD1	35:DD:982:LEU:CD2	2.85	0.48
48:PD:76:ASN:OD1	67:h:47:ASP:CB	2.59	0.48
52:n:196:ASN:HD21	52:n:219:ASN:C	2.22	0.48
52:n:371:GLN:HG3	52:n:390:MET:CE	2.44	0.48
55:a:160:LEU:HG	55:a:219:LEU:HD21	1.96	0.48
55:a:455:GLN:HB2	74:x:11:LEU:HD21	1.96	0.48
60:q:17:LYS:CE	60:q:30:TYR:CD2	2.97	0.48
69:r:21:TYR:HE1	69:r:175:ALA:HB3	1.78	0.48
74:x:621:VAL:HG11	74:x:670:LEU:HD22	1.96	0.48
6:DA:740:LEU:CD2	6:DA:1070:PHE:HZ	2.27	0.48
11:PA:1657:TYR:HB3	11:PA:1658:SER:H	1.52	0.48
17:PB:407:MET:HE1	17:PB:444:LEU:CG	2.43	0.48
18:HC:174:ASP:OD1	18:HC:175:LEU:N	2.45	0.48
20:DP:297:LYS:HG2	20:DP:298:PRO:HD3	1.96	0.48
30:HD:63:PHE:HB2	30:HD:69:ASP:OD1	2.13	0.48
37:DF:43:VAL:CA	40:DI:46:TYR:CD2	2.90	0.48
39:DH:54:GLU:CD	43:DJ:197:MET:HG2	2.39	0.48
35:Dd:922:GLN:NE2	41:Dl:71:ASP:OD2	2.47	0.48
36:De:556:ASN:HA	36:De:572:LEU:HB2	1.96	0.48
49:PG:30:LEU:O	49:PG:34:VAL:HG22	2.14	0.48
52:n:904:PHE:CZ	52:n:1208:GLU:HB2	2.49	0.48
55:a:364:TYR:CD1	55:a:430:LEU:HD12	2.49	0.48
55:a:441:GLU:CG	55:a:442:VAL:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:f:100:ILE:HG12	57:f:105:ILE:HG12	1.96	0.48
66:o:678:LEU:HD11	66:o:725:VAL:HG11	1.96	0.48
66:o:742:GLN:HG2	74:x:107:ARG:NH2	2.29	0.48
68:k:64:SER:HB2	68:k:68:ARG:CZ	2.43	0.48
68:k:101:ARG:NH1	68:k:101:ARG:CG	2.73	0.48
69:r:206:ARG:C	69:r:206:ARG:NE	2.72	0.48
70:t:5:CYS:O	70:t:141:GLU:HA	2.14	0.48
71:v:133:GLU:O	71:v:136:SER:N	2.46	0.48
6:DA:464:TRP:O	6:DA:464:TRP:HE3	1.97	0.48
6:DA:488:ALA:H	37:Df:315:ARG:HG2	1.79	0.48
14:FB:58:LEU:HD11	14:FB:62:LEU:HD23	1.96	0.48
14:FB:182:HIS:NE2	35:DD:998:GLN:OE1	2.47	0.48
17:PB:167:THR:HG23	17:PB:170:ASP:H	1.79	0.48
17:PB:598:VAL:CG2	17:PB:601:VAL:HG23	2.44	0.48
24:PF:68:THR:O	24:PF:72:GLN:HG3	2.14	0.48
35:DD:924:LYS:C	35:DD:926:PHE:H	2.22	0.48
37:DF:317:LEU:CD2	37:DF:317:LEU:N	2.76	0.48
37:DF:415:ILE:HG12	37:DF:415:ILE:O	2.14	0.48
39:DH:110:TYR:CE1	39:DH:113:ARG:CZ	2.97	0.48
39:DH:110:TYR:CG	43:DJ:161:LYS:HD3	2.48	0.48
46:HI:110:THR:HB	46:HI:113:HIS:ND1	2.29	0.48
48:PD:51:ALA:HA	57:f:172:PHE:CZ	2.49	0.48
52:n:101:ALA:HB2	53:s:109:LEU:CD2	2.44	0.48
52:n:678:PHE:HA	60:q:557:LEU:HB2	1.95	0.48
55:a:59:VAL:CG2	56:d:51:SER:HB3	2.30	0.48
55:a:420:LEU:HD22	55:a:504:ILE:HG13	1.96	0.48
60:q:92:LEU:HD11	60:q:99:ARG:HD2	1.95	0.48
65:l:177:ARG:CZ	71:v:113:ASP:OD2	2.61	0.48
70:t:80:GLU:HB2	70:t:81:ASN:H	1.45	0.48
73:w:787:PRO:HB3	73:w:822:HIS:CD2	2.49	0.48
74:x:107:ARG:O	74:x:108:LEU:C	2.56	0.48
10:NE:734:ARG:O	10:NE:735:ALA:HB2	2.13	0.48
11:PA:689:ILE:O	11:PA:693:ILE:HG12	2.14	0.47
11:PA:1454:VAL:HG12	11:PA:1458:ILE:HD12	1.95	0.47
12:DB:537:PHE:HE2	12:DB:539:ARG:HB2	1.79	0.47
12:DB:570:GLU:HA	12:DB:625:LEU:HA	1.95	0.47
22:PC:190:ASN:ND2	22:PC:195:THR:O	2.39	0.47
38:DG:181:TRP:CD2	38:DG:181:TRP:C	2.88	0.47
47:HJ:85:MET:HE2	47:HJ:160:VAL:HB	1.95	0.47
47:HJ:215:THR:HG23	47:HJ:252:MET:HG3	1.96	0.47
48:PD:55:GLN:NE2	48:PD:56:GLU:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:74:PHE:CE1	48:PD:137:LYS:HB2	2.42	0.47
50:g:110:GLU:O	50:g:113:LYS:HB3	2.14	0.47
54:u:115:LEU:HA	56:d:121:LEU:HD12	1.96	0.47
60:q:456:GLU:HG2	71:v:140:SER:HA	1.95	0.47
61:z:582:LEU:CD2	61:z:591:LEU:HB3	2.44	0.47
64:e:146:ILE:O	64:e:148:VAL:N	2.46	0.47
73:w:1195:ALA:C	73:w:1197:HIS:N	2.69	0.47
73:w:1241:THR:OG1	73:w:1242:GLU:N	2.44	0.47
74:x:544:HIS:HD2	74:x:546:CYS:H	1.62	0.47
6:DA:402:PHE:HE1	37:Df:391:LEU:HD11	1.79	0.47
9:HA:572:GLN:H	9:HA:572:GLN:HG2	1.40	0.47
12:DB:564:LEU:HB2	12:DB:581:ILE:HD13	1.97	0.47
12:DB:953:LEU:HD12	12:DB:979:PHE:HE2	1.79	0.47
17:PB:718:GLN:OE1	17:PB:976:MET:HE3	2.14	0.47
17:PB:752:TYR:CD2	17:PB:807:ARG:HB3	2.49	0.47
24:PF:72:GLN:HG2	49:PG:64:GLY:CA	2.44	0.47
36:DE:702:LEU:HD22	36:DE:702:LEU:N	2.30	0.47
37:DF:104:LEU:CD1	43:DJ:217:PHE:CE2	2.91	0.47
35:Dd:910:LEU:HD11	41:DI:88:ALA:HB2	1.96	0.47
36:De:724:GLU:OE1	36:De:789:ASN:ND2	2.46	0.47
52:n:796:ILE:O	52:n:816:LYS:NZ	2.34	0.47
55:a:108:PHE:O	55:a:108:PHE:CD1	2.66	0.47
56:d:72:ARG:HE	56:d:72:ARG:HB2	1.33	0.47
56:d:109:GLN:HA	56:d:112:LYS:HE3	1.95	0.47
57:f:145:TYR:HB2	67:h:41:THR:OG1	2.14	0.47
60:q:106:LEU:C	60:q:106:LEU:CD2	2.85	0.47
60:q:187:LEU:HD11	71:v:88:LEU:HD21	1.95	0.47
63:c:288:LEU:HD11	70:t:156:LEU:HD11	1.96	0.47
72:p:608:MET:HA	72:p:611:LEU:HB3	1.96	0.47
73:w:270:LEU:HD23	73:w:303:GLN:HG3	1.95	0.47
73:w:863:ASP:OD1	73:w:863:ASP:N	2.45	0.47
7:EA:139:LEU:HG	49:PG:151:ARG:CB	2.42	0.47
11:PA:33:ARG:NH1	17:PB:1139:GLY:O	2.47	0.47
11:PA:89:GLU:O	11:PA:287:ASN:ND2	2.46	0.47
12:DB:636:VAL:HG23	12:DB:638:ARG:HB3	1.96	0.47
12:DB:644:GLN:O	18:HC:413:LEU:HB3	2.14	0.47
15:HB:422:LEU:HD13	32:HE:225:GLN:NE2	2.29	0.47
17:PB:438:ARG:NH2	17:PB:442:ASP:OD2	2.47	0.47
24:PF:77:ALA:HA	49:PG:15:PRO:HB2	1.96	0.47
27:PJ:6:ARG:HD3	27:PJ:13:ILE:HD13	1.95	0.47
31:HG:382:CYS:HB3	31:HG:385:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:HE:20:ILE:H	32:HE:20:ILE:HD12	1.79	0.47
37:DF:43:VAL:HG23	40:DI:46:TYR:HD2	1.78	0.47
36:De:474:THR:OG1	36:De:546:VAL:O	2.28	0.47
47:HJ:82:THR:HG23	47:HJ:160:VAL:CG1	2.42	0.47
47:HJ:98:GLU:HG3	47:HJ:99:TYR:CZ	2.49	0.47
52:n:209:PRO:CG	52:n:293:TYR:CB	2.75	0.47
52:n:227:GLU:O	52:n:253:LEU:HD12	2.14	0.47
55:a:187:MET:HE1	55:a:401:PRO:HB2	1.96	0.47
58:i:65:PHE:CD1	58:i:99:LYS:HG2	2.49	0.47
59:m:116:GLN:CG	61:z:595:PRO:HD3	2.43	0.47
61:z:488:SER:HB2	61:z:492:ARG:NH2	2.29	0.47
63:c:134:LYS:HD3	65:l:46:TYR:HB2	1.97	0.47
68:k:60:GLU:HG3	71:v:26:ILE:HG13	1.95	0.47
73:w:1172:ILE:O	73:w:1244:GLN:NE2	2.41	0.47
74:x:529:MET:HE3	74:x:529:MET:HB3	1.77	0.47
11:PA:350:VAL:CG1	11:PA:1435:THR:HG21	2.44	0.47
11:PA:542:LEU:O	11:PA:545:VAL:HG12	2.14	0.47
17:PB:501:LEU:HD11	17:PB:511:PRO:HA	1.95	0.47
31:HG:87:LEU:HD13	31:HG:228:TYR:HD2	1.79	0.47
35:DD:886:GLY:CA	35:DD:891:ILE:HG13	2.39	0.47
37:DF:335:ARG:HD2	37:DF:378:ALA:HB1	1.96	0.47
44:Dk:191:VAL:HG13	44:Dk:200:ILE:CD1	2.42	0.47
48:PD:33:LEU:O	48:PD:37:VAL:HG23	2.13	0.47
52:n:277:LEU:CD1	57:f:185:ARG:HG2	2.45	0.47
55:a:441:GLU:HB3	74:x:14:TRP:NE1	2.29	0.47
56:d:45:ILE:HG22	58:i:76:MET:HE3	1.86	0.47
56:d:121:LEU:HD22	56:d:125:VAL:HG13	1.97	0.47
56:d:165:LEU:HA	59:m:110:ARG:NH1	2.29	0.47
60:q:645:ALA:O	65:l:111:VAL:HG21	2.14	0.47
62:b:107:GLU:HB3	66:o:649:ILE:HD11	1.96	0.47
63:c:176:MET:HG2	63:c:194:LEU:HG	1.96	0.47
70:t:130:THR:O	70:t:130:THR:OG1	2.25	0.47
72:p:100:ASP:OD1	72:p:100:ASP:N	2.48	0.47
7:EA:152:PHE:CZ	7:EA:161:VAL:HB	2.49	0.47
11:PA:1144:LEU:HD23	11:PA:1144:LEU:H	1.78	0.47
12:DB:184:ASN:N	12:DB:184:ASN:ND2	2.63	0.47
12:DB:431:LEU:HD23	12:DB:431:LEU:C	2.39	0.47
13:EB:148:LYS:HD2	13:EB:184:ALA:HB3	1.95	0.47
17:PB:1035:ARG:NH1	17:PB:1036:LYS:O	2.44	0.47
30:HD:55:LYS:CG	49:PG:166:ASP:N	2.74	0.47
31:HG:253:GLY:N	31:HG:310:LEU:HD21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:702:LEU:HD23	36:DE:704:VAL:HG23	1.95	0.47
37:DF:67:THR:O	37:DF:69:SER:N	2.47	0.47
46:HI:136:ARG:HG3	46:HI:136:ARG:NH1	2.28	0.47
50:g:129:HIS:O	50:g:133:GLU:N	2.41	0.47
54:u:122:LEU:HD13	54:u:122:LEU:C	2.39	0.47
60:q:157:ALA:HB2	68:k:31:VAL:CG2	2.36	0.47
60:q:484:TYR:O	60:q:488:CYS:HB2	2.14	0.47
68:k:94:LEU:HD21	71:v:108:LEU:HD11	1.97	0.47
74:x:289:CYS:HB3	74:x:309:THR:HG22	1.96	0.47
6:DA:483:ASN:HA	6:DA:493:ARG:NH1	2.29	0.47
6:DA:1195:VAL:HG22	6:DA:1198:ARG:HH12	1.80	0.47
7:EA:144:LEU:HD13	7:EA:154:CYS:HA	1.97	0.47
7:EA:145:PHE:HB2	7:EA:152:PHE:HA	1.97	0.47
33:HF:38:ILE:H	33:HF:38:ILE:HD12	1.80	0.47
35:DD:947:PHE:CD2	40:DI:113:PRO:HD3	2.50	0.47
36:DE:465:THR:HG22	37:DF:132:LYS:O	2.13	0.47
37:DF:68:THR:HA	40:DI:32:GLU:OE1	2.15	0.47
47:HJ:277:LEU:HA	47:HJ:280:CYS:SG	2.54	0.47
51:j:17:GLU:CB	53:s:112:LEU:CD1	2.93	0.47
52:n:387:GLU:HG3	52:n:391:LYS:HE3	1.97	0.47
52:n:711:ARG:HH12	52:n:723:GLU:CD	2.21	0.47
54:u:64:ARG:HB3	61:z:585:HIS:HE1	1.79	0.47
55:a:109:TYR:OH	55:a:150:PHE:CZ	2.65	0.47
55:a:259:ILE:HD12	55:a:259:ILE:O	2.14	0.47
59:m:56:LEU:CD2	59:m:80:GLN:HE21	2.23	0.47
59:m:107:HIS:O	59:m:111:LYS:CB	2.62	0.47
64:e:129:VAL:CB	68:k:114:MET:HE2	2.44	0.47
72:p:584:CYS:O	72:p:656:ARG:NH1	2.43	0.47
7:EA:139:LEU:CG	49:PG:151:ARG:HB3	2.35	0.47
9:HA:52:LEU:HD21	9:HA:232:VAL:HG11	1.96	0.47
9:HA:617:ALA:HB2	9:HA:676:LEU:HD21	1.97	0.47
11:PA:484:LEU:HD11	11:PA:501:MET:SD	2.54	0.47
14:FB:179:ASP:CG	35:DD:1002:ARG:NH2	2.73	0.47
15:HB:488:GLU:O	15:HB:491:VAL:HG22	2.13	0.47
18:HC:348:ARG:CD	33:HF:65:ALA:HB1	2.41	0.47
19:DO:2:ALA:HA	35:DD:1000:ARG:HH11	1.79	0.47
22:PC:72:PRO:HD3	27:PJ:13:ILE:HD11	1.97	0.47
23:PE:25:GLY:O	23:PE:65:ASN:ND2	2.47	0.47
31:HG:357:VAL:CG1	31:HG:366:VAL:HG23	2.45	0.47
36:DE:461:ILE:O	37:DF:135:TRP:CE3	2.67	0.47
36:DE:481:ASP:OD1	36:DE:481:ASP:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DH:50:PHE:CE2	43:DJ:171:LEU:HA	2.49	0.47
37:Df:254:GLN:O	37:Df:258:ARG:NH2	2.47	0.47
37:Df:330:ARG:NH1	37:Df:371:THR:O	2.47	0.47
46:HI:114:ILE:HG23	46:HI:206:LEU:HD12	1.97	0.47
46:HI:280:PRO:HA	46:HI:283:ARG:NH1	2.29	0.47
47:HJ:234:GLU:C	47:HJ:234:GLU:CD	2.83	0.47
48:PD:15:GLU:OE2	49:PG:78:ARG:NH1	2.47	0.47
50:g:127:ARG:CD	52:n:152:PHE:HB2	2.40	0.47
52:n:591:PHE:HB3	73:w:26:PHE:CD1	2.45	0.47
52:n:960:LYS:HB3	52:n:1210:PHE:CZ	2.50	0.47
52:n:963:LEU:HD21	52:n:1258:ASN:CB	2.45	0.47
57:f:24:LEU:HD22	57:f:24:LEU:HA	1.79	0.47
57:f:32:TYR:CE1	57:f:35:GLU:OE2	2.67	0.47
60:q:160:LEU:HD23	71:v:69:VAL:HG23	1.97	0.47
60:q:188:LEU:HD22	71:v:87:ILE:CB	2.45	0.47
60:q:190:LEU:O	60:q:190:LEU:HD13	2.15	0.47
60:q:548:VAL:HA	60:q:571:VAL:HG12	1.96	0.47
63:c:209:ILE:HB	63:c:250:LEU:HD13	1.96	0.47
64:e:136:LEU:HD11	68:k:107:VAL:HG12	1.96	0.47
68:k:35:LEU:HD12	68:k:35:LEU:O	2.14	0.47
70:t:204:GLN:NE2	70:t:204:GLN:HA	2.29	0.47
71:v:18:TYR:HA	71:v:21:ARG:HD2	1.95	0.47
72:p:510:GLU:OE1	72:p:513:ARG:NH2	2.45	0.47
73:w:234:SER:HB2	73:w:660:GLU:HG3	1.97	0.47
73:w:999:ASP:N	73:w:999:ASP:OD1	2.41	0.47
73:w:1229:LYS:O	73:w:1233:GLU:HB2	2.14	0.47
73:w:1267:MET:HE2	73:w:1267:MET:HB3	1.80	0.47
74:x:374:SER:O	74:x:377:SER:OG	2.30	0.47
74:x:687:PHE:HB2	74:x:688:PRO:HD3	1.97	0.47
75:y:36:ARG:HA	75:y:40:LEU:HB2	1.96	0.47
7:EA:137:THR:HG22	7:EA:139:LEU:H	1.80	0.47
10:NA:533:GLU:O	10:NA:534:ARG:O	2.33	0.47
18:HC:348:ARG:NH2	33:HF:65:ALA:CB	2.73	0.47
30:HD:31:CYS:SG	30:HD:34:CYS:HB2	2.55	0.47
39:DH:110:TYR:CZ	43:DJ:160:GLN:HB3	2.50	0.47
47:HJ:102:ARG:HH11	47:HJ:102:ARG:CG	2.25	0.47
51:j:78:GLN:O	51:j:82:LYS:CE	2.61	0.47
57:f:82:ARG:NH1	57:f:94:PRO:HB3	2.30	0.47
60:q:609:VAL:HG23	66:o:674:ILE:HD13	1.96	0.47
60:q:644:SER:HB3	64:e:96:LEU:HB2	1.96	0.47
64:e:45:VAL:CG1	65:l:92:LEU:CD1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:p:71:TRP:HZ3	72:p:738:LEU:HD21	1.80	0.47
11:PA:1200:PRO:HG2	11:PA:1204:VAL:HG22	1.96	0.47
11:PA:1790:TYR:CD2	67:h:83:PRO:HD3	2.50	0.47
12:DB:645:ALA:HA	18:HC:413:LEU:CA	2.28	0.47
30:HD:281:GLN:N	30:HD:281:GLN:CD	2.73	0.47
32:HE:44:LEU:HD21	32:HE:162:LEU:CD1	2.45	0.47
37:DF:316:GLN:CG	37:DF:318:CYS:O	2.46	0.47
38:DG:41:ASP:OD1	38:DG:41:ASP:N	2.47	0.47
39:DH:56:ALA:CB	43:DJ:214:PRO:HG2	2.36	0.47
40:DI:31:TYR:OH	40:DI:36:ILE:HD11	2.15	0.47
40:DI:119:ARG:NH1	40:DI:120:TYR:OH	2.48	0.47
37:Df:326:HIS:O	37:Df:330:ARG:HG2	2.15	0.47
43:Dj:149:PRO:O	43:Dj:153:ARG:NH1	2.46	0.47
46:HI:95:GLU:N	46:HI:145:LEU:O	2.47	0.47
47:HJ:3:HIS:ND1	47:HJ:3:HIS:N	2.59	0.47
49:PG:110:ARG:HA	49:PG:113:ILE:HD12	1.97	0.47
52:n:929:ARG:HB2	52:n:933:VAL:HG13	1.97	0.47
54:u:7:GLN:OE1	61:z:593:ILE:HA	2.15	0.47
55:a:421:ILE:HD11	55:a:450:PHE:CD1	2.50	0.47
60:q:494:GLN:HB2	63:c:251:LEU:HD11	1.95	0.47
68:k:80:GLU:N	68:k:80:GLU:OE1	2.48	0.47
71:v:82:LEU:HD23	71:v:82:LEU:HA	1.75	0.47
72:p:191:SER:HA	72:p:200:LEU:O	2.15	0.47
9:HA:563:ARG:NH2	31:HG:142:GLU:OE1	2.48	0.47
17:PB:207:VAL:HG11	17:PB:375:ALA:CB	2.45	0.47
31:HG:112:LYS:N	31:HG:142:GLU:O	2.41	0.47
32:HE:42:MET:SD	32:HE:108:ASN:ND2	2.86	0.47
36:DE:324:LYS:HA	36:DE:327:ASN:HB3	1.97	0.47
40:DI:83:PHE:N	40:DI:83:PHE:CD1	2.82	0.47
36:De:589:TRP:HB3	37:Df:60:MET:HE3	1.96	0.47
47:HJ:151:ILE:H	47:HJ:151:ILE:HG12	1.45	0.47
52:n:941:TYR:HE2	52:n:1172:SER:HB2	1.71	0.47
55:a:449:ARG:HH12	74:x:54:PRO:HB3	1.79	0.47
56:d:110:LEU:C	56:d:110:LEU:CD2	2.86	0.47
63:c:310:ARG:O	63:c:311:GLN:HB2	2.15	0.47
67:h:187:PHE:HE2	67:h:189:LYS:HD3	1.80	0.47
11:PA:491:PRO:HG3	11:PA:535:MET:HE2	1.96	0.46
11:PA:609:HIS:ND1	11:PA:626:THR:HG23	2.31	0.46
12:DB:674:THR:CB	18:HC:415:GLN:HE21	2.28	0.46
17:PB:1036:LYS:H	22:PC:186:TYR:HH	1.62	0.46
37:DF:82:PRO:HG2	37:DF:83:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DH:110:TYR:CE1	43:DJ:161:LYS:HA	2.50	0.46
41:DL:61:LYS:HA	41:DL:61:LYS:HD2	1.55	0.46
35:Dd:1061:ARG:NH1	40:Di:119:ARG:O	2.48	0.46
46:HI:101:ILE:HD13	46:HI:101:ILE:N	2.29	0.46
49:PG:104:MET:HE1	49:PG:106:CYS:HB2	1.96	0.46
52:n:153:ALA:O	52:n:154:ILE:C	2.58	0.46
52:n:904:PHE:HE2	52:n:1208:GLU:CB	2.20	0.46
55:a:445:LEU:HA	74:x:55:SER:OG	2.15	0.46
57:f:106:TYR:CZ	67:h:106:PRO:HG3	2.50	0.46
58:i:96:GLU:HA	58:i:99:LYS:CD	2.45	0.46
66:o:752:VAL:HA	66:o:755:CYS:SG	2.56	0.46
70:t:15:LYS:HB3	70:t:15:LYS:HE2	1.68	0.46
74:x:11:LEU:HB2	74:x:14:TRP:CE3	2.47	0.46
74:x:301:GLU:OE2	74:x:301:GLU:N	2.39	0.46
5:BA:128:ILE:HG23	5:BA:183:VAL:CG1	2.44	0.46
9:HA:28:LEU:O	9:HA:32:LEU:HD23	2.16	0.46
17:PB:128:ILE:CG2	17:PB:431:LEU:HD21	2.46	0.46
26:PI:69:ILE:O	26:PI:72:VAL:HG22	2.15	0.46
34:HH:605:ILE:HD12	34:HH:607:ILE:HD11	1.96	0.46
34:HH:656:ASN:OD1	34:HH:657:ALA:N	2.49	0.46
37:DF:92:ILE:HG13	37:DF:93:PRO:HD3	1.97	0.46
40:DI:38:GLN:HA	40:DI:41:GLU:HB2	1.97	0.46
46:HI:99:GLU:C	46:HI:99:GLU:CD	2.83	0.46
47:HJ:134:LEU:H	47:HJ:134:LEU:HG	1.42	0.46
50:g:107:GLU:O	50:g:111:ASP:N	2.47	0.46
52:n:270:GLN:NE2	57:f:174:ARG:CD	2.53	0.46
52:n:478:MET:HE3	52:n:492:TRP:HB3	1.97	0.46
52:n:801:ARG:NE	52:n:811:CYS:HB3	2.31	0.46
52:n:855:LEU:HD11	52:n:868:LEU:HD22	1.98	0.46
55:a:145:LYS:HA	55:a:145:LYS:CE	2.41	0.46
55:a:417:TYR:CD1	55:a:450:PHE:CE1	2.89	0.46
56:d:40:LEU:HB3	56:d:65:VAL:HG13	1.97	0.46
62:b:129:GLN:NE2	62:b:129:GLN:HA	2.31	0.46
62:b:174:ILE:HD13	65:l:58:MET:HE2	1.97	0.46
65:l:166:LEU:CD2	71:v:123:ILE:HD12	2.45	0.46
68:k:44:LEU:CD1	68:k:44:LEU:C	2.87	0.46
68:k:96:ARG:HD3	71:v:116:LEU:HD12	1.97	0.46
70:t:8:GLN:HG3	70:t:196:LEU:CD2	2.45	0.46
70:t:202:LYS:O	70:t:203:GLN:C	2.56	0.46
74:x:843:TYR:HD1	74:x:847:PHE:HE2	1.62	0.46
11:PA:225:PHE:HA	11:PA:228:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PA:1643:TYR:CZ	59:m:93:CYS:HA	2.50	0.46
12:DB:820:ASP:OD1	12:DB:820:ASP:N	2.37	0.46
17:PB:724:TYR:HB3	17:PB:728:MET:HE3	1.97	0.46
35:DD:950:LEU:HD23	36:DE:523:VAL:HG11	1.97	0.46
36:DE:321:LEU:HB3	36:DE:330:TRP:HB2	1.97	0.46
37:DF:106:PHE:CD1	40:DI:13:PRO:CD	2.98	0.46
40:DI:19:MET:HG2	40:DI:40:LEU:HG	1.97	0.46
52:n:199:LEU:CD2	52:n:222:VAL:HG13	2.45	0.46
55:a:450:PHE:CZ	55:a:467:MET:HB2	2.50	0.46
55:a:455:GLN:HB2	74:x:11:LEU:CG	2.45	0.46
56:d:45:ILE:HG22	58:i:76:MET:HB2	1.77	0.46
56:d:126:TYR:CD2	60:q:36:MET:CG	2.98	0.46
57:f:74:GLN:HB3	57:f:78:LEU:HB2	1.97	0.46
63:c:205:ARG:NH2	71:v:128:TYR:HD2	2.13	0.46
68:k:87:ARG:NH1	68:k:87:ARG:CG	2.73	0.46
72:p:207:CYS:HB3	72:p:242:TYR:HE2	1.79	0.46
6:DA:900:ASP:HB3	38:DG:154:LYS:HD2	1.98	0.46
6:DA:1165:LEU:HB2	6:DA:1191:ILE:HG12	1.97	0.46
17:PB:596:ILE:HG22	17:PB:596:ILE:O	2.15	0.46
17:PB:910:THR:HG23	29:PL:42:ARG:O	2.15	0.46
18:HC:261:PHE:O	18:HC:265:LEU:HD23	2.15	0.46
30:HD:250:PRO:HD2	30:HD:251:LEU:HD22	1.97	0.46
36:DE:773:TYR:CE1	37:DF:137:SER:HB2	2.50	0.46
37:DF:427:LEU:HD12	37:DF:427:LEU:HA	1.72	0.46
40:DI:131:SER:HB2	43:DJ:150:ARG:HH12	1.80	0.46
46:HI:37:ILE:N	46:HI:37:ILE:CD1	2.79	0.46
47:HJ:177:ARG:CZ	47:HJ:177:ARG:CB	2.93	0.46
54:u:90:LEU:HD11	60:q:7:VAL:CG2	2.45	0.46
56:d:45:ILE:O	58:i:76:MET:SD	2.73	0.46
56:d:163:ALA:HB2	59:m:106:GLN:HA	1.96	0.46
57:f:94:PRO:C	60:q:130:VAL:HG13	2.41	0.46
63:c:309:CYS:O	63:c:311:GLN:N	2.49	0.46
68:k:58:HIS:ND1	68:k:58:HIS:C	2.73	0.46
70:t:110:ILE:HD12	70:t:197:PHE:HB3	1.97	0.46
71:v:16:GLN:HE21	71:v:20:LYS:CD	2.23	0.46
74:x:565:SER:O	74:x:567:MET:N	2.48	0.46
3:NX:5:DC:H2''	3:NX:6:DC:O5'	2.16	0.46
7:EA:181:ASN:CG	30:HD:10:LYS:C	2.84	0.46
12:DB:329:LEU:HB3	12:DB:342:THR:HG23	1.96	0.46
13:EB:145:VAL:HG11	13:EB:171:ILE:HG23	1.98	0.46
14:FB:31:TRP:HD1	14:FB:62:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:HD:287:TYR:O	30:HD:288:THR:C	2.58	0.46
32:HE:165:LYS:NZ	32:HE:167:ALA:O	2.37	0.46
36:DE:702:LEU:HD23	36:DE:702:LEU:C	2.39	0.46
37:DF:276:LEU:HD13	37:DF:323:VAL:HG11	1.96	0.46
38:DG:161:ASP:OD1	38:DG:161:ASP:N	2.48	0.46
46:HI:241:CYS:HB2	46:HI:246:TYR:CD1	2.51	0.46
52:n:548:TYR:CE2	52:n:652:MET:HE2	2.51	0.46
55:a:56:GLN:CD	56:d:51:SER:O	2.58	0.46
55:a:431:LYS:HD3	55:a:431:LYS:HA	1.70	0.46
55:a:455:GLN:OE1	74:x:11:LEU:HD11	2.15	0.46
60:q:112:LEU:HD23	67:h:19:VAL:CG2	2.45	0.46
60:q:188:LEU:C	60:q:188:LEU:HD12	2.40	0.46
65:l:149:LEU:HD11	71:v:139:SER:HA	1.97	0.46
70:t:150:ALA:HB2	70:t:184:TYR:HB2	1.97	0.46
72:p:266:ARG:HH11	72:p:341:ILE:HD13	1.81	0.46
7:EA:22:ILE:HG12	7:EA:34:LEU:HD22	1.97	0.46
11:PA:510:GLU:CD	17:PB:1101:GLN:HE22	2.24	0.46
11:PA:1261:ILE:HG22	11:PA:1262:MET:N	2.31	0.46
17:PB:993:LYS:NZ	17:PB:995:GLU:OE1	2.44	0.46
19:DO:64:THR:HG22	19:DO:65:TYR:N	2.31	0.46
37:DF:411:VAL:HG13	37:DF:411:VAL:O	2.16	0.46
40:DI:131:SER:HA	43:DJ:150:ARG:HH22	1.81	0.46
36:De:633:THR:O	36:De:634:ARG:NH2	2.45	0.46
50:g:166:ASN:OD1	50:g:167:CYS:CA	2.63	0.46
52:n:938:ASP:HB2	52:n:1171:ALA:C	2.40	0.46
55:a:297:VAL:HG12	55:a:299:LEU:HG	1.97	0.46
57:f:63:MET:SD	57:f:64:VAL:N	2.88	0.46
60:q:110:CYS:SG	67:h:23:LYS:CD	3.03	0.46
60:q:506:HIS:CD2	60:q:508:ASP:H	2.34	0.46
60:q:644:SER:CB	64:e:96:LEU:HB3	2.44	0.46
62:b:71:LEU:O	62:b:75:MET:HG2	2.15	0.46
64:e:132:HIS:CD2	71:v:126:ASP:HB3	2.50	0.46
66:o:714:ASP:C	74:x:28:LYS:HZ2	2.15	0.46
66:o:720:PRO:O	66:o:721:LEU:C	2.58	0.46
68:k:37:LYS:CE	68:k:37:LYS:N	2.73	0.46
4:NY:-93:DG:H2"	4:NY:-92:DG:C8	2.50	0.46
9:HA:361:LEU:O	9:HA:365:VAL:HG12	2.16	0.46
11:PA:400:ASP:OD1	11:PA:401:ARG:N	2.49	0.46
11:PA:1357:THR:O	23:PE:142:HIS:NE2	2.46	0.46
11:PA:1643:TYR:CE1	59:m:93:CYS:HA	2.50	0.46
12:DB:71:ARG:HD3	12:DB:73:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:PK:105:PHE:CD2	28:PK:109:ILE:HD11	2.51	0.46
30:HD:28:HIS:HB3	30:HD:30:LEU:HG	1.96	0.46
30:HD:301:PHE:CE1	47:HJ:170:PHE:CZ	3.04	0.46
32:HE:13:ILE:HG21	32:HE:41:VAL:HG13	1.97	0.46
35:DD:874:LEU:HG	35:DD:877:PRO:HD2	1.97	0.46
36:DE:232:HIS:HD1	36:DE:313:SER:HG	1.56	0.46
36:DE:464:TYR:CD2	37:DF:133:ALA:HB2	2.51	0.46
37:DF:83:LEU:HD12	37:DF:83:LEU:H	1.81	0.46
37:DF:122:LEU:N	37:DF:122:LEU:CD1	2.78	0.46
37:DF:424:GLN:O	37:DF:428:LEU:HG	2.16	0.46
52:n:237:MET:HE1	60:q:45:GLN:HG2	1.96	0.46
52:n:802:VAL:HG22	52:n:809:ILE:HB	1.97	0.46
55:a:160:LEU:HG	55:a:219:LEU:HD11	1.98	0.46
55:a:432:GLU:OE1	55:a:432:GLU:HA	2.14	0.46
57:f:57:LEU:HD13	57:f:57:LEU:HA	1.78	0.46
60:q:466:ASN:ND2	63:c:205:ARG:HG3	2.30	0.46
61:z:597:VAL:O	61:z:598:CYS:C	2.59	0.46
71:v:26:ILE:HD13	71:v:26:ILE:HA	1.71	0.46
72:p:128:GLY:HA3	74:x:708:LYS:HB2	1.97	0.46
72:p:787:LEU:HB3	72:p:791:PRO:HB3	1.97	0.46
73:w:615:ILE:O	73:w:620:ARG:NH2	2.48	0.46
11:PA:1468:THR:HG21	17:PB:1101:GLN:HG3	1.97	0.46
12:DB:568:VAL:HG22	12:DB:628:ILE:HG23	1.98	0.46
13:EB:139:PHE:HZ	13:EB:144:ASN:OD1	1.99	0.46
17:PB:1143:LYS:CE	49:PG:152:VAL:CG1	2.75	0.46
18:HC:407:VAL:N	18:HC:443:VAL:O	2.47	0.46
18:HC:440:LEU:HD22	33:HF:36:GLN:CD	2.41	0.46
34:HH:173:ASN:N	34:HH:434:GLU:OE2	2.49	0.46
34:HH:185:ILE:HG22	34:HH:189:LEU:HD13	1.98	0.46
41:DL:111:LEU:N	41:DL:114:LYS:NZ	2.64	0.46
36:De:717:LEU:HD22	36:De:726:LEU:HD11	1.97	0.46
37:Df:257:PRO:O	37:Df:261:THR:OG1	2.32	0.46
50:g:175:LEU:HD22	58:i:129:ASN:OD1	2.15	0.46
52:n:170:PRO:HG2	52:n:173:ILE:HD11	1.97	0.46
54:u:87:ALA:HB1	60:q:7:VAL:HG21	1.97	0.46
60:q:166:ARG:HH11	60:q:166:ARG:HG3	1.80	0.46
65:l:149:LEU:CD1	71:v:139:SER:HA	2.45	0.46
66:o:710:LEU:HG	66:o:776:TRP:CH2	2.50	0.46
68:k:88:LYS:C	68:k:88:LYS:CD	2.89	0.46
69:r:125:MET:HE3	69:r:125:MET:HB3	1.82	0.46
73:w:1064:ASP:OD1	73:w:1064:ASP:N	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EA:17:LEU:O	7:EA:21:VAL:HG22	2.16	0.46
8:FA:163:GLU:O	8:FA:166:ARG:N	2.49	0.46
9:HA:107:LEU:HD12	9:HA:195:ALA:HB1	1.98	0.46
9:HA:137:LEU:O	9:HA:142:VAL:HG11	2.15	0.46
11:PA:458:PHE:HE2	11:PA:484:LEU:HD11	1.80	0.46
12:DB:559:LYS:HB2	12:DB:559:LYS:NZ	2.31	0.46
13:EB:220:TRP:CD1	13:EB:220:TRP:C	2.94	0.46
17:PB:553:LEU:HD23	17:PB:556:ILE:HD11	1.98	0.46
18:HC:444:THR:HG23	18:HC:447:GLY:H	1.81	0.46
26:PI:39:CYS:SG	26:PI:42:CYS:HB3	2.56	0.46
37:DF:83:LEU:CD1	37:DF:83:LEU:H	2.29	0.46
39:DH:110:TYR:CG	43:DJ:161:LYS:HB2	2.50	0.46
36:De:554:ASP:OD1	36:De:554:ASP:N	2.45	0.46
37:Df:83:LEU:HD22	40:Di:41:GLU:HG2	1.98	0.46
37:Df:327:TRP:O	37:Df:330:ARG:HB2	2.16	0.46
46:HI:258:HIS:C	46:HI:258:HIS:ND1	2.73	0.46
47:HJ:207:TYR:HD2	47:HJ:255:MET:HE3	1.81	0.46
51:j:113:LEU:HA	51:j:116:VAL:HG12	1.98	0.46
52:n:201:HIS:CE1	56:d:111:GLN:HE22	2.34	0.46
52:n:238:GLY:N	52:n:243:VAL:HG21	2.31	0.46
52:n:444:GLU:HB3	52:n:445:PRO:HD3	1.97	0.46
55:a:417:TYR:CZ	55:a:450:PHE:HD1	2.21	0.46
57:f:19:SER:O	57:f:22:PRO:HD2	2.16	0.46
58:i:109:LEU:HD21	58:i:117:GLN:HE22	1.79	0.46
59:m:93:CYS:O	59:m:97:ILE:HG22	2.16	0.46
60:q:102:LEU:CD1	67:h:29:PHE:HD2	2.26	0.46
60:q:449:ASP:OD2	65:l:157:LYS:HD3	2.16	0.46
74:x:847:PHE:HB2	74:x:899:ARG:HG2	1.97	0.46
6:DA:1063:LYS:HD3	6:DA:1063:LYS:O	2.16	0.46
9:HA:460:THR:HB	9:HA:661:ALA:HB1	1.98	0.46
11:PA:340:LYS:HE2	11:PA:1436:VAL:HG11	1.98	0.46
18:HC:52:ALA:HB1	18:HC:90:LEU:HD21	1.99	0.46
33:HF:49:LEU:HD12	33:HF:52:VAL:HG11	1.96	0.46
36:DE:646:SER:OG	36:DE:647:ALA:N	2.48	0.46
39:DH:119:ILE:O	43:DJ:131:PRO:HG3	2.15	0.46
39:DH:161:LYS:HB2	39:DH:161:LYS:HE3	1.32	0.46
37:Df:326:HIS:ND1	37:Df:326:HIS:N	2.63	0.46
46:HI:134:LEU:HG	46:HI:162:PHE:CD1	2.50	0.46
46:HI:141:ASN:C	46:HI:143:LEU:N	2.70	0.46
47:HJ:175:LYS:CE	47:HJ:175:LYS:CA	2.85	0.46
52:n:226:VAL:HG13	52:n:230:PHE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:252:ILE:HG21	52:n:303:LEU:HD13	1.97	0.46
52:n:509:ILE:HG21	52:n:540:ILE:HD13	1.97	0.46
52:n:959:LEU:HD12	52:n:963:LEU:HD23	1.98	0.46
53:s:104:LYS:O	53:s:106:SER:N	2.48	0.46
55:a:224:TYR:HE1	55:a:254:ASN:C	2.23	0.46
55:a:518:ILE:HG22	55:a:518:ILE:O	2.17	0.46
58:i:85:GLN:CG	58:i:86:ASP:N	2.32	0.46
60:q:103:ARG:HH11	60:q:103:ARG:HB2	1.81	0.46
63:c:288:LEU:CD2	70:t:122:PHE:CZ	2.99	0.46
66:o:733:SER:HB3	66:o:766:LYS:HA	1.98	0.46
67:h:26:LEU:HD23	67:h:26:LEU:HA	1.75	0.46
73:w:31:GLU:HB2	73:w:36:LYS:HD3	1.97	0.46
73:w:1183:TRP:CH2	73:w:1185:GLY:HA3	2.51	0.46
1:X:-6:DG:H2"	1:X:-5:DT:C6	2.51	0.45
9:HA:109:LEU:HD12	9:HA:207:TYR:CD2	2.52	0.45
12:DB:27:LYS:CE	12:DB:490:SER:HB3	2.45	0.45
13:EB:213:ASP:OD1	13:EB:214:GLU:N	2.49	0.45
30:HD:37:LEU:O	30:HD:40:VAL:HG12	2.16	0.45
37:DF:279:LEU:HB3	37:DF:330:ARG:HD2	1.97	0.45
37:Df:58:MET:HE3	37:Df:64:GLN:HA	1.98	0.45
37:Df:328:ALA:C	37:Df:330:ARG:N	2.72	0.45
40:Di:62:LYS:CG	41:Dl:106:ARG:NH1	2.79	0.45
43:Dj:176:MET:HE1	45:Dm:75:ILE:HD11	1.97	0.45
47:HJ:279:ARG:HH21	47:HJ:279:ARG:HG3	1.81	0.45
50:g:129:HIS:CB	54:u:82:THR:HG22	2.46	0.45
52:n:527:THR:O	52:n:528:HIS:HB2	2.15	0.45
54:u:102:THR:O	54:u:105:GLU:HG2	2.16	0.45
55:a:99:THR:HG22	55:a:112:VAL:HG13	1.96	0.45
59:m:21:GLU:O	59:m:25:VAL:HG23	2.16	0.45
60:q:113:TYR:CE2	67:h:20:ALA:HB2	2.51	0.45
60:q:113:TYR:CD1	60:q:113:TYR:C	2.93	0.45
60:q:418:ILE:HD13	70:t:72:PRO:CG	2.36	0.45
63:c:290:ASP:O	70:t:120:CYS:SG	2.74	0.45
64:e:74:ARG:HD2	64:e:78:ASP:OD2	2.17	0.45
70:t:46:TYR:HB2	70:t:63:MET:HB2	1.98	0.45
72:p:511:TYR:OH	72:p:519:GLN:O	2.31	0.45
73:w:623:LEU:HD12	73:w:623:LEU:HA	1.74	0.45
74:x:20:ASP:OD1	74:x:20:ASP:N	2.44	0.45
6:DA:404:MET:HE2	6:DA:404:MET:HA	1.99	0.45
7:EA:106:LYS:HD3	13:EB:220:TRP:CH2	2.51	0.45
11:PA:502:ASN:HB3	17:PB:1084:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:FB:194:HIS:ND1	14:FB:196:TYR:O	2.49	0.45
17:PB:809:VAL:HG11	17:PB:811:TYR:CZ	2.51	0.45
21:DQ:321:SER:OG	21:DQ:322:ASP:N	2.48	0.45
30:HD:21:LEU:HD21	30:HD:29:THR:HG23	1.98	0.45
34:HH:294:GLU:OE2	34:HH:334:ARG:NH1	2.49	0.45
35:DD:888:LYS:HB2	35:DD:888:LYS:NZ	2.32	0.45
36:DE:702:LEU:HD22	36:DE:702:LEU:H	1.81	0.45
36:DE:702:LEU:N	36:DE:702:LEU:CD2	2.78	0.45
49:PG:117:MET:HE3	49:PG:137:ILE:HD13	1.98	0.45
52:n:359:ILE:CG2	52:n:372:ILE:HD13	2.42	0.45
53:s:106:SER:HA	53:s:108:PHE:O	2.16	0.45
54:u:106:ASP:O	54:u:110:ARG:HG3	2.16	0.45
62:b:136:HIS:HB3	63:c:111:TYR:OH	2.14	0.45
4:NY:-74:DG:P	34:HH:63:LEU:H	2.39	0.45
6:DA:730:PHE:CD1	6:DA:730:PHE:N	2.83	0.45
9:HA:77:VAL:HA	9:HA:80:ILE:HG22	1.97	0.45
12:DB:539:ARG:O	12:DB:540:LYS:C	2.58	0.45
17:PB:694:THR:HG22	17:PB:695:HIS:ND1	2.31	0.45
19:DO:1:MET:CE	35:DD:993:GLN:HB3	2.42	0.45
37:DF:71:ILE:HD11	40:DI:35:VAL:CG2	2.45	0.45
37:Df:317:LEU:HD12	37:Df:329:LEU:HD23	1.98	0.45
47:HJ:15:SER:O	47:HJ:18:GLN:HG3	2.16	0.45
47:HJ:52:GLU:HB3	47:HJ:273:LEU:CD1	2.42	0.45
52:n:637:PHE:HD2	52:n:639:LYS:HG2	1.82	0.45
52:n:1335:ASN:C	52:n:1337:GLN:H	2.25	0.45
55:a:466:VAL:HB	74:x:54:PRO:CD	2.46	0.45
56:d:126:TYR:CE1	60:q:36:MET:HB2	2.51	0.45
56:d:167:TRP:CE3	59:m:106:GLN:NE2	2.84	0.45
60:q:188:LEU:HA	71:v:87:ILE:HG13	1.96	0.45
60:q:190:LEU:HD13	60:q:190:LEU:C	2.41	0.45
68:k:37:LYS:H	68:k:37:LYS:CD	2.27	0.45
72:p:569:LEU:HD23	72:p:569:LEU:H	1.81	0.45
72:p:583:ILE:HG23	72:p:587:ILE:HD12	1.98	0.45
74:x:289:CYS:SG	74:x:313:ILE:HG13	2.56	0.45
4:NY:-11:DG:H2''	4:NY:-10:DG:H5'	1.98	0.45
7:EA:181:ASN:CG	30:HD:10:LYS:N	2.74	0.45
11:PA:348:GLY:O	11:PA:352:GLY:N	2.46	0.45
11:PA:1034:GLN:HE22	11:PA:1038:THR:HG21	1.82	0.45
21:DQ:22:ILE:HG22	21:DQ:39:LEU:HD11	1.99	0.45
35:DD:949:GLN:HA	35:DD:952:GLN:HG2	1.97	0.45
36:DE:447:THR:HG23	36:DE:450:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:50:ILE:O	37:DF:54:ALA:N	2.47	0.45
44:Dk:150:VAL:HG22	45:Dm:82:GLN:HB3	1.98	0.45
46:HI:280:PRO:HA	46:HI:283:ARG:HH12	1.81	0.45
48:PD:83:VAL:O	48:PD:87:LEU:HD23	2.15	0.45
50:g:128:PRO:HD2	50:g:129:HIS:N	2.31	0.45
52:n:249:LYS:C	52:n:250:LEU:HD22	2.42	0.45
55:a:131:ASN:ND2	55:a:131:ASN:N	2.63	0.45
55:a:439:GLN:HB2	74:x:15:LYS:HG2	1.99	0.45
55:a:443:CYS:SG	74:x:57:ASN:HA	2.56	0.45
60:q:255:ALA:HB3	60:q:301:VAL:HG22	1.97	0.45
68:k:103:LYS:HD3	68:k:103:LYS:HA	1.69	0.45
69:r:16:ILE:H	69:r:16:ILE:HG12	1.55	0.45
70:t:89:THR:C	70:t:91:PHE:N	2.74	0.45
70:t:96:VAL:HA	70:t:99:LYS:HG2	1.98	0.45
73:w:44:PHE:HE2	73:w:92:LEU:HD11	1.81	0.45
73:w:315:SER:OG	73:w:319:GLU:OE1	2.31	0.45
6:DA:464:TRP:O	6:DA:464:TRP:CE3	2.70	0.45
7:EA:48:MET:HE1	7:EA:92:TYR:HB2	1.97	0.45
9:HA:345:ARG:HD2	30:HD:1:MET:SD	2.57	0.45
11:PA:24:GLY:O	17:PB:1168:ALA:HB3	2.16	0.45
17:PB:710:ILE:HA	17:PB:764:MET:HE2	1.99	0.45
30:HD:254:GLU:CD	30:HD:254:GLU:N	2.62	0.45
30:HD:284:ALA:C	30:HD:286:GLY:N	2.73	0.45
31:HG:199:ILE:CG2	31:HG:222:ILE:HD11	2.47	0.45
36:DE:470:TYR:CD1	39:DH:26:ALA:HA	2.51	0.45
37:DF:233:GLY:HA2	37:DF:239:ARG:HE	1.82	0.45
50:g:75:LYS:HD2	54:u:77:PRO:C	2.42	0.45
52:n:443:LEU:HD12	52:n:500:LEU:HD22	1.98	0.45
52:n:707:ASP:CG	66:o:684:ARG:HD3	2.42	0.45
55:a:74:LEU:HD22	55:a:74:LEU:HA	1.74	0.45
62:b:178:LEU:HD13	65:l:55:LEU:HD21	1.98	0.45
69:r:101:LEU:HD23	69:r:101:LEU:HA	1.79	0.45
72:p:618:LEU:HD13	72:p:662:ILE:HG12	1.99	0.45
73:w:370:ASP:OD1	73:w:370:ASP:N	2.49	0.45
74:x:832:GLN:NE2	74:x:835:ARG:HH21	2.15	0.45
6:DA:565:TRP:HA	6:DA:565:TRP:CE3	2.51	0.45
9:HA:329:PHE:O	9:HA:333:LEU:HD23	2.17	0.45
9:HA:600:ALA:HB1	9:HA:659:HIS:HD2	1.82	0.45
11:PA:495:ASP:C	11:PA:495:ASP:OD1	2.60	0.45
15:HB:472:LEU:HD12	15:HB:476:TRP:CD1	2.52	0.45
31:HG:121:SER:OG	31:HG:127:HIS:NE2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DD:947:PHE:HB3	40:DI:113:PRO:HD3	1.98	0.45
36:DE:447:THR:HG23	36:DE:450:ARG:HD2	1.98	0.45
35:Dd:860:VAL:HA	45:Dm:47:GLN:HG2	1.98	0.45
49:PG:153:ASP:OD1	49:PG:154:LYS:N	2.49	0.45
50:g:86:LEU:HD22	51:j:113:LEU:HD11	1.97	0.45
52:n:270:GLN:HG3	57:f:181:LEU:HD12	1.98	0.45
52:n:865:VAL:O	52:n:869:LEU:HG	2.17	0.45
54:u:96:GLU:O	54:u:99:GLU:HG3	2.17	0.45
55:a:462:LEU:HD11	74:x:60:ILE:CD1	2.39	0.45
55:a:509:ARG:HB2	55:a:509:ARG:HH11	1.77	0.45
58:i:100:LEU:C	58:i:100:LEU:HD13	2.41	0.45
58:i:108:HIS:C	58:i:109:LEU:HG	2.42	0.45
60:q:118:ILE:CG2	60:q:125:MET:HG2	2.46	0.45
60:q:440:LEU:CD2	60:q:502:ILE:HD11	2.47	0.45
66:o:703:THR:HB	66:o:726:PRO:HA	1.98	0.45
71:v:115:LYS:HD3	71:v:115:LYS:HA	1.46	0.45
73:w:512:THR:OG1	73:w:513:ASN:ND2	2.50	0.45
8:FA:127:PHE:CE2	14:FB:21:VAL:HG21	2.51	0.45
11:PA:1474:LEU:HA	49:PG:59:ILE:H	1.82	0.45
14:FB:179:ASP:CG	35:DD:1002:ARG:HH21	2.24	0.45
36:DE:290:HIS:CG	37:DF:45:TYR:CE2	3.05	0.45
37:DF:276:LEU:HD22	37:DF:323:VAL:HG22	1.98	0.45
39:DH:50:PHE:HB3	43:DJ:194:THR:C	2.42	0.45
40:Di:73:LEU:HD13	41:DI:105:HIS:HE2	1.78	0.45
46:HI:269:LEU:HD13	46:HI:269:LEU:C	2.42	0.45
54:u:122:LEU:HG	56:d:111:GLN:NE2	2.25	0.45
57:f:111:LEU:O	57:f:115:ILE:HG13	2.15	0.45
59:m:116:GLN:CG	61:z:594:LEU:HG	2.47	0.45
60:q:263:LYS:CE	60:q:439:PHE:HZ	2.29	0.45
70:t:173:PRO:CD	70:t:173:PRO:O	2.65	0.45
73:w:485:SER:OG	73:w:486:GLU:N	2.49	0.45
74:x:742:TYR:HA	74:x:782:VAL:HG11	1.99	0.45
2:Y:-11:DT:H5'	34:HH:412:MET:HE3	1.99	0.45
2:Y:9:DA:H2'	2:Y:10:DC:C6	2.51	0.45
3:NX:98:DC:H5'	10:NE:643:PRO:HA	1.99	0.45
6:DA:346:ALA:HB2	37:Df:262:PHE:HA	1.98	0.45
6:DA:396:LEU:H	6:DA:396:LEU:HD22	1.81	0.45
7:EA:187:ILE:HD12	7:EA:187:ILE:H	1.82	0.45
11:PA:360:ASP:OD1	17:PB:1062:ARG:NE	2.42	0.45
11:PA:910:LYS:N	11:PA:911:PRO:HD2	2.32	0.45
11:PA:1653:THR:O	59:m:39:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:HB:400:ILE:H	15:HB:400:ILE:HD12	1.82	0.45
22:PC:260:GLN:HB2	28:PK:91:ILE:HG21	1.97	0.45
30:HD:207:GLN:HB3	30:HD:211:GLN:HE21	1.82	0.45
32:HE:235:GLN:O	32:HE:235:GLN:NE2	2.47	0.45
40:DI:67:ASP:OD1	40:DI:67:ASP:C	2.60	0.45
35:Dd:941:ARG:NH2	40:Di:123:THR:O	2.48	0.45
47:HJ:181:LEU:N	47:HJ:181:LEU:CD1	2.72	0.45
48:PD:134:ILE:HD12	48:PD:137:LYS:NZ	2.32	0.45
52:n:201:HIS:HE1	54:u:122:LEU:HG	1.81	0.45
52:n:273:PHE:O	52:n:276:GLN:HG3	2.17	0.45
52:n:523:SER:OG	52:n:583:ALA:O	2.34	0.45
52:n:1185:LEU:HD12	52:n:1185:LEU:O	2.17	0.45
55:a:64:THR:HG22	55:a:86:ARG:HD2	1.98	0.45
55:a:200:LEU:C	55:a:200:LEU:HD13	2.42	0.45
55:a:259:ILE:O	55:a:259:ILE:CD1	2.64	0.45
57:f:111:LEU:HD22	60:q:127:LEU:HD11	1.97	0.45
60:q:479:ILE:C	60:q:532:HIS:CE1	2.92	0.45
70:t:78:LEU:CD1	70:t:84:CYS:HB3	2.46	0.45
73:w:673:LYS:HE2	73:w:678:ALA:HB2	1.99	0.45
74:x:676:ASP:OD1	74:x:676:ASP:N	2.49	0.45
43:DJ:123:LEU:O	43:DJ:153:ARG:NH1	2.50	0.45
7:EA:105:TYR:OH	13:EB:236:TYR:HB3	2.17	0.45
7:EA:188:TYR:HE2	30:HD:14:TYR:CG	2.33	0.45
11:PA:68:THR:HG23	11:PA:68:THR:O	2.16	0.45
11:PA:622:SER:OG	11:PA:626:THR:HG22	2.17	0.45
17:PB:851:ASP:CG	29:PL:15:MET:HE2	2.42	0.45
19:DO:2:ALA:N	35:DD:1000:ARG:CD	2.80	0.45
20:DP:227:GLU:OE1	20:DP:318:ARG:NH2	2.46	0.45
30:HD:6:CYS:O	30:HD:10:LYS:HE3	2.17	0.45
36:DE:250:GLU:O	36:DE:254:ASN:ND2	2.50	0.45
37:DF:426:LEU:C	37:DF:426:LEU:HD23	2.42	0.45
41:DL:63:LEU:O	41:DL:67:VAL:HG13	2.17	0.45
46:HI:258:HIS:CD2	57:f:36:ARG:HH12	2.35	0.45
52:n:281:ARG:CG	57:f:190:PRO:HA	2.46	0.45
52:n:436:PRO:HG3	52:n:458:LEU:HD21	1.99	0.45
52:n:753:LEU:HG	63:c:305:PHE:CE1	2.52	0.45
52:n:918:PHE:HB2	52:n:1211:LEU:HD12	1.99	0.45
55:a:69:LEU:HD13	55:a:69:LEU:HA	1.86	0.45
58:i:112:GLU:H	58:i:112:GLU:HG3	1.43	0.45
60:q:17:LYS:HB3	60:q:30:TYR:HE2	1.82	0.45
60:q:543:VAL:CG1	63:c:135:ARG:HE	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:156:PRO:HD2	62:b:159:GLN:HG2	1.99	0.45
69:r:57:VAL:HG22	69:r:71:ARG:HG2	1.98	0.45
70:t:46:TYR:HD2	70:t:63:MET:HB3	1.81	0.45
72:p:131:ILE:HD13	72:p:183:THR:HG22	1.99	0.45
73:w:339:ILE:HD11	73:w:378:GLN:HB3	1.99	0.45
9:HA:434:HIS:CB	9:HA:632:ILE:HD11	2.47	0.45
11:PA:1382:LEU:O	11:PA:1385:VAL:HG22	2.18	0.45
18:HC:325:ILE:H	18:HC:325:ILE:HD12	1.82	0.45
39:DH:132:LYS:HA	39:DH:132:LYS:HD2	1.69	0.45
55:a:145:LYS:HD2	55:a:145:LYS:N	2.32	0.45
56:d:167:TRP:O	56:d:167:TRP:HE3	2.00	0.45
57:f:64:VAL:HG11	57:f:88:SER:CA	2.47	0.45
60:q:32:PRO:HB2	60:q:34:LEU:HD21	1.99	0.45
60:q:116:LEU:HD22	60:q:116:LEU:HA	1.73	0.45
60:q:469:ASP:HB2	63:c:231:TRP:CD2	2.52	0.45
62:b:178:LEU:HD21	65:l:78:LEU:HB3	1.98	0.45
66:o:681:GLU:OE1	66:o:768:SER:OG	2.34	0.45
70:t:81:ASN:N	70:t:81:ASN:OD1	2.50	0.45
72:p:41:CYS:SG	72:p:42:ARG:N	2.90	0.45
74:x:956:VAL:HG11	74:x:968:LEU:HD21	1.98	0.45
11:PA:72:GLN:N	11:PA:72:GLN:OE1	2.50	0.44
11:PA:1665:SER:HB2	56:d:180:LEU:HD21	1.99	0.44
17:PB:738:THR:HG21	27:PJ:58:LYS:CG	2.48	0.44
35:DD:948:GLU:CD	35:DD:948:GLU:C	2.85	0.44
35:DD:1085:LYS:NZ	41:DL:83:MET:SD	2.85	0.44
36:DE:507:VAL:HG11	36:DE:513:LEU:HD12	1.97	0.44
36:DE:774:MET:O	37:DF:142:GLN:NE2	2.49	0.44
40:DI:16:ALA:CB	40:DI:40:LEU:HD11	2.46	0.44
35:Dd:1084:LEU:HB3	40:Di:99:ARG:HH21	1.81	0.44
47:HJ:268:GLU:CD	47:HJ:268:GLU:N	2.74	0.44
48:PD:91:LYS:C	48:PD:92:LEU:HD22	2.42	0.44
56:d:44:LEU:O	56:d:44:LEU:HD23	2.17	0.44
56:d:45:ILE:HG12	58:i:73:ILE:HG12	1.95	0.44
60:q:17:LYS:CE	60:q:30:TYR:CE2	2.88	0.44
60:q:190:LEU:CD2	60:q:291:TRP:CE3	3.00	0.44
60:q:549:LEU:HD11	60:q:572:ALA:HB2	1.99	0.44
63:c:41:ASN:HD22	63:c:41:ASN:C	2.24	0.44
64:e:113:GLU:OE2	65:l:31:ALA:HB3	2.16	0.44
1:X:20:DG:OP2	1:X:20:DG:H8	2.01	0.44
6:DA:857:MET:HE3	6:DA:858:ASP:H	1.81	0.44
6:DA:1061:ARG:HD3	6:DA:1061:ARG:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PA:273:GLN:HB3	11:PA:277:THR:HG21	2.00	0.44
12:DB:414:LEU:HB2	12:DB:523:VAL:HG13	1.99	0.44
14:FB:30:GLN:O	14:FB:62:LEU:HD11	2.16	0.44
18:HC:157:GLU:O	18:HC:161:HIS:ND1	2.51	0.44
18:HC:334:MET:HB3	34:HH:58:ALA:HB2	1.98	0.44
26:PI:58:ILE:HD12	26:PI:58:ILE:H	1.81	0.44
30:HD:271:TYR:CE2	30:HD:273:ASN:HB3	2.51	0.44
35:DD:891:ILE:C	35:DD:891:ILE:CD1	2.90	0.44
37:DF:418:ILE:H	37:DF:418:ILE:CD1	2.23	0.44
39:DH:44:LEU:HD21	43:DJ:129:THR:CG2	2.44	0.44
39:DH:110:TYR:CB	43:DJ:161:LYS:HD3	2.44	0.44
40:Di:57:TYR:CD2	40:Di:73:LEU:HD11	2.52	0.44
45:Dm:103:LEU:O	45:Dm:107:ASN:ND2	2.51	0.44
46:HI:141:ASN:C	46:HI:143:LEU:H	2.24	0.44
47:HJ:36:ALA:O	47:HJ:37:ASN:C	2.60	0.44
52:n:204:VAL:HB	54:u:129:GLN:OE1	2.17	0.44
52:n:1219:HIS:CD2	52:n:1222:ARG:HH11	2.35	0.44
54:u:61:LEU:HD22	54:u:64:ARG:HD3	2.00	0.44
56:d:131:LYS:HB2	56:d:131:LYS:HE2	1.35	0.44
57:f:60:LEU:H	57:f:60:LEU:HG	1.35	0.44
60:q:465:SER:OG	63:c:210:ASP:OD2	2.34	0.44
64:e:129:VAL:CG2	68:k:114:MET:HE1	2.32	0.44
66:o:706:LEU:HG	66:o:723:LEU:HB3	1.99	0.44
70:t:161:LEU:O	70:t:165:LEU:N	2.49	0.44
71:v:133:GLU:C	71:v:133:GLU:CD	2.85	0.44
72:p:40:SER:HB3	72:p:89:TRP:CD2	2.52	0.44
73:w:381:SER:O	73:w:534:HIS:ND1	2.48	0.44
73:w:726:ASN:H	73:w:726:ASN:HD22	1.64	0.44
73:w:1139:ARG:O	73:w:1140:GLU:HG3	2.17	0.44
74:x:294:ILE:HA	74:x:354:ARG:HD3	1.99	0.44
74:x:420:ILE:HA	74:x:423:THR:HG22	1.98	0.44
74:x:495:ILE:HG22	74:x:499:MET:HE2	1.99	0.44
1:X:-7:DC:H2"	1:X:-6:DG:C8	2.52	0.44
8:FA:151:ARG:HG2	8:FA:151:ARG:O	2.18	0.44
12:DB:540:LYS:HE2	33:HF:31:LYS:NZ	2.32	0.44
13:EB:133:ILE:O	13:EB:134:ASP:OD1	2.35	0.44
14:FB:220:ILE:HG13	14:FB:221:GLY:H	1.82	0.44
15:HB:457:ILE:HG22	15:HB:461:LEU:HD13	1.98	0.44
22:PC:245:VAL:HG11	28:PK:105:PHE:CZ	2.52	0.44
23:PE:159:LEU:HD12	23:PE:163:TYR:CD2	2.53	0.44
30:HD:97:ASP:O	30:HD:101:GLU:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:HE:16:ASP:HA	32:HE:62:SER:HB3	2.00	0.44
32:HE:201:GLY:O	32:HE:204:GLN:HG2	2.17	0.44
34:HH:99:PHE:CZ	34:HH:103:ILE:HD13	2.53	0.44
36:DE:521:ASP:C	36:DE:521:ASP:OD1	2.61	0.44
37:DF:350:ASN:OD1	37:DF:350:ASN:N	2.51	0.44
40:DI:19:MET:HB2	40:DI:40:LEU:HD21	1.99	0.44
36:De:542:HIS:CE1	36:De:568:ARG:HG3	2.52	0.44
46:HI:279:ASN:O	46:HI:280:PRO:C	2.60	0.44
46:HI:282:ALA:O	46:HI:283:ARG:C	2.59	0.44
48:PD:79:THR:HG22	67:h:51:LEU:CB	2.46	0.44
55:a:103:ILE:HG23	55:a:108:PHE:HB2	1.99	0.44
55:a:109:TYR:CE1	55:a:150:PHE:CZ	3.05	0.44
55:a:321:LEU:HD21	55:a:407:ILE:CG1	2.47	0.44
56:d:174:ARG:HD2	56:d:174:ARG:HA	1.70	0.44
60:q:437:HIS:O	60:q:437:HIS:CD2	2.70	0.44
65:l:167:ILE:HD12	71:v:127:LEU:CD2	2.47	0.44
68:k:79:HIS:CD2	69:r:41:GLY:HA2	2.53	0.44
68:k:86:SER:CB	71:v:105:LEU:HD12	2.47	0.44
69:r:192:GLN:OE1	71:v:11:LYS:HE3	2.17	0.44
2:Y:-8:DA:H2"	2:Y:-7:DT:H5"	1.99	0.44
7:EA:26:TYR:CD1	13:EB:220:TRP:CZ2	3.06	0.44
7:EA:181:ASN:OD1	30:HD:10:LYS:C	2.60	0.44
9:HA:475:PRO:HG3	9:HA:478:MET:HE2	1.99	0.44
31:HG:242:SER:N	31:HG:245:SER:OG	2.50	0.44
32:HE:123:ASP:OD1	32:HE:124:ILE:N	2.45	0.44
36:DE:458:LEU:O	37:DF:139:GLU:HA	2.16	0.44
39:DH:37:LEU:HD21	43:DJ:134:VAL:HG12	1.99	0.44
46:HI:247:VAL:O	46:HI:248:THR:C	2.58	0.44
48:PD:70:ARG:NH2	49:PG:88:VAL:HG22	2.32	0.44
51:j:82:LYS:NZ	53:s:96:PHE:CD1	2.85	0.44
57:f:29:VAL:HG21	57:f:79:PHE:CD1	2.53	0.44
60:q:153:LEU:HD22	68:k:34:GLU:HB3	1.99	0.44
60:q:185:SER:CB	68:k:10:ARG:HH22	2.31	0.44
60:q:402:HIS:HE1	60:q:404:ARG:HH21	1.64	0.44
60:q:491:ILE:HG23	60:q:506:HIS:HE1	1.81	0.44
63:c:229:ASP:OD1	63:c:232:SER:OG	2.34	0.44
65:l:167:ILE:HD12	71:v:127:LEU:HD23	1.98	0.44
66:o:698:CYS:HB2	66:o:705:HIS:CD2	2.52	0.44
74:x:255:ASN:OD1	74:x:255:ASN:N	2.47	0.44
76:NG:1016:ALA:O	76:NG:1017:VAL:CB	2.65	0.44
6:DA:1182:CYS:O	6:DA:1182:CYS:SG	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HA:462:SER:OG	9:HA:463:PRO:CD	2.66	0.44
11:PA:1341:VAL:O	11:PA:1341:VAL:HG23	2.17	0.44
11:PA:1481:LYS:CE	49:PG:22:LEU:CD2	2.93	0.44
30:HD:295:ARG:CD	30:HD:295:ARG:C	2.91	0.44
35:DD:947:PHE:HE1	36:DE:573:GLN:HE22	1.66	0.44
36:DE:784:HIS:HB3	36:DE:792:LEU:HB2	1.99	0.44
37:DF:47:ILE:HD11	40:DI:43:ALA:CB	2.28	0.44
41:DL:62:LYS:O	41:DL:62:LYS:NZ	2.21	0.44
46:HI:66:LEU:HD12	46:HI:66:LEU:HA	1.70	0.44
46:HI:139:LYS:NZ	46:HI:139:LYS:HB3	2.32	0.44
47:HJ:60:TYR:HD1	47:HJ:60:TYR:HA	1.73	0.44
47:HJ:145:GLU:H	47:HJ:145:GLU:HG2	1.50	0.44
52:n:98:ARG:HH22	53:s:120:GLY:N	2.16	0.44
52:n:231:GLU:HB2	52:n:253:LEU:HD21	1.98	0.44
52:n:273:PHE:CZ	57:f:185:ARG:CG	3.00	0.44
52:n:273:PHE:HD2	57:f:181:LEU:HD13	1.83	0.44
52:n:274:ILE:CD1	57:f:181:LEU:CD2	2.96	0.44
52:n:385:LEU:HD23	52:n:407:ALA:HA	1.99	0.44
55:a:109:TYR:CE2	55:a:154:LEU:HD23	2.52	0.44
55:a:168:LYS:HE3	55:a:168:LYS:HB3	1.49	0.44
55:a:357:LEU:HD22	55:a:357:LEU:HA	1.77	0.44
56:d:89:ILE:HG21	58:i:114:GLN:HG3	1.99	0.44
56:d:156:SER:HB3	56:d:161:VAL:HG11	1.99	0.44
67:h:38:GLY:C	67:h:40:LEU:H	2.26	0.44
67:h:130:ARG:O	67:h:131:ILE:C	2.61	0.44
68:k:113:GLN:HA	68:k:116:GLU:OE1	2.17	0.44
69:r:180:ASP:C	69:r:182:VAL:H	2.25	0.44
5:BA:245:VAL:HG23	5:BA:245:VAL:O	2.17	0.44
6:DA:690:LEU:HD22	6:DA:747:LEU:HD22	1.99	0.44
7:EA:105:TYR:N	7:EA:105:TYR:HD1	2.15	0.44
7:EA:105:TYR:CE2	13:EB:233:ILE:HA	2.52	0.44
7:EA:128:LYS:HZ1	7:EA:166:SER:N	2.16	0.44
7:EA:139:LEU:HG	49:PG:151:ARG:HB2	1.98	0.44
12:DB:539:ARG:C	12:DB:542:ASN:H	2.25	0.44
17:PB:379:ARG:O	17:PB:608:ARG:NH2	2.51	0.44
17:PB:761:THR:H	17:PB:764:MET:HE3	1.82	0.44
30:HD:291:LEU:HA	30:HD:291:LEU:HD12	1.74	0.44
31:HG:89:GLU:OE2	31:HG:132:LYS:NZ	2.42	0.44
35:DD:875:GLN:O	35:DD:877:PRO:HD3	2.18	0.44
37:DF:83:LEU:CD1	37:DF:83:LEU:N	2.79	0.44
37:DF:219:GLU:HB2	39:DH:160:ILE:CG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DF:323:VAL:O	37:DF:326:HIS:HB2	2.18	0.44
39:DH:194:MET:HE2	39:DH:194:MET:HB2	1.85	0.44
45:Dm:80:ARG:HD2	45:Dm:80:ARG:HA	1.85	0.44
46:HI:57:ARG:HE	46:HI:57:ARG:HB2	1.63	0.44
47:HJ:208:THR:O	47:HJ:212:ILE:HG13	2.18	0.44
48:PD:133:ASP:OD1	48:PD:134:ILE:N	2.50	0.44
50:g:127:ARG:HD3	50:g:130:GLN:CB	2.47	0.44
52:n:237:MET:HB2	52:n:246:ARG:HD2	2.00	0.44
54:u:115:LEU:CG	56:d:121:LEU:HD13	2.41	0.44
55:a:177:LEU:HB2	55:a:259:ILE:HG13	1.99	0.44
55:a:466:VAL:HG13	55:a:478:LYS:H	1.82	0.44
56:d:167:TRP:O	56:d:167:TRP:CE3	2.70	0.44
58:i:71:ASN:HA	58:i:74:LYS:HD2	1.99	0.44
60:q:487:ILE:HD11	60:q:540:LEU:HD13	1.98	0.44
63:c:283:ARG:CB	63:c:311:GLN:NE2	2.78	0.44
64:e:45:VAL:O	64:e:48:LEU:HG	2.18	0.44
68:k:17:ILE:HG12	71:v:76:MET:HE1	2.00	0.44
68:k:60:GLU:HG3	71:v:26:ILE:CG1	2.47	0.44
72:p:611:LEU:HD11	72:p:665:TRP:HB3	1.99	0.44
73:w:316:GLU:OE2	73:w:366:ILE:N	2.49	0.44
73:w:1135:PRO:O	73:w:1136:LEU:HB2	2.17	0.44
73:w:1195:ALA:O	73:w:1197:HIS:N	2.50	0.44
1:X:4:DC:H2''	1:X:5:DC:C6	2.53	0.44
4:NY:-18:DG:H2''	4:NY:-17:DG:H5'	1.99	0.44
6:DA:405:VAL:HA	37:DF:302:HIS:HB3	1.99	0.44
9:HA:285:TYR:O	9:HA:289:VAL:HG23	2.17	0.44
9:HA:613:HIS:O	9:HA:613:HIS:ND1	2.50	0.44
13:EB:132:VAL:HG22	13:EB:137:TYR:CD1	2.53	0.44
14:FB:94:THR:HG22	14:FB:109:ILE:HG22	2.00	0.44
37:DF:270:ASN:HD22	37:DF:270:ASN:HA	1.62	0.44
37:DF:320:ARG:CB	37:DF:415:ILE:HD12	2.48	0.44
39:DH:40:VAL:O	39:DH:44:LEU:HG	2.18	0.44
40:DI:20:ALA:HB2	40:DI:36:ILE:CD1	2.44	0.44
41:DL:111:LEU:C	41:DL:114:LYS:HE3	2.43	0.44
37:Df:105:TYR:O	43:Dj:217:PHE:N	2.51	0.44
40:Di:73:LEU:HD22	41:DI:105:HIS:ND1	2.32	0.44
46:HI:16:ASP:HB3	46:HI:28:LYS:HB3	1.98	0.44
48:PD:17:ALA:HB1	48:PD:95:PHE:CE2	2.52	0.44
50:g:168:LEU:HD23	50:g:168:LEU:C	2.43	0.44
51:j:78:GLN:O	51:j:82:LYS:CD	2.65	0.44
51:j:82:LYS:NZ	53:s:96:PHE:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:676:ASP:OD1	60:q:593:MET:HE2	2.18	0.44
52:n:948:LYS:HD2	52:n:948:LYS:HA	1.70	0.44
54:u:67:LYS:HE2	61:z:528:LEU:HD13	1.99	0.44
57:f:43:ARG:H	57:f:43:ARG:HD2	1.82	0.44
60:q:120:ARG:HH11	60:q:120:ARG:CG	2.14	0.44
60:q:127:LEU:HG	60:q:127:LEU:O	2.17	0.44
68:k:19:ARG:HG3	68:k:58:HIS:CD2	2.53	0.44
70:t:85:LEU:HD23	70:t:85:LEU:HA	1.77	0.44
72:p:145:LEU:HD22	72:p:359:LEU:HD21	2.00	0.44
4:NY:-123:DG:H2"	4:NY:-122:DG:C8	2.52	0.44
5:BA:25:GLU:OE1	5:BA:46:ILE:HD12	2.18	0.44
6:DA:491:MET:N	6:DA:491:MET:SD	2.91	0.44
7:EA:22:ILE:CD1	7:EA:26:TYR:CD2	3.01	0.44
11:PA:105:LYS:HD2	11:PA:141:LEU:HD22	1.99	0.44
11:PA:913:ASN:OD1	11:PA:963:ARG:NH1	2.48	0.44
36:DE:613:ALA:HB3	36:DE:616:HIS:HD2	1.83	0.44
37:DF:39:LEU:HD11	40:DI:51:LEU:HG	2.00	0.44
37:DF:370:TRP:CZ3	37:DF:420:ALA:HA	2.53	0.44
39:DH:59:GLU:HA	39:DH:62:THR:HG22	1.99	0.44
39:DH:121:ALA:CB	43:DJ:133:ALA:HB3	2.43	0.44
41:DL:64:GLN:N	41:DL:64:GLN:CD	2.75	0.44
46:HI:102:ILE:HD13	46:HI:102:ILE:HA	1.77	0.44
46:HI:243:LEU:HD12	46:HI:243:LEU:HA	1.84	0.44
50:g:127:ARG:HH22	54:u:9:GLN:CD	2.26	0.44
52:n:274:ILE:CD1	57:f:181:LEU:HD21	2.47	0.44
54:u:49:ASN:H	54:u:49:ASN:HD22	1.63	0.44
60:q:145:GLN:NE2	71:v:45:GLU:HB3	2.33	0.44
60:q:379:ILE:HD12	60:q:379:ILE:HA	1.87	0.44
60:q:577:ASP:N	60:q:577:ASP:OD1	2.51	0.44
65:l:91:LYS:O	65:l:94:LEU:HG	2.18	0.44
66:o:712:ASP:N	66:o:712:ASP:OD1	2.48	0.44
67:h:18:GLN:HB3	67:h:60:ASN:ND2	2.33	0.44
73:w:547:VAL:HG13	73:w:559:LEU:HD11	2.00	0.44
74:x:11:LEU:HA	74:x:14:TRP:HB3	2.00	0.44
11:PA:495:ASP:OD1	11:PA:497:ASP:OD1	2.36	0.44
13:EB:122:GLU:O	13:EB:125:VAL:HG22	2.18	0.44
23:PE:94:MET:HE1	23:PE:127:LEU:HD11	2.00	0.44
30:HD:193:PRO:HG2	30:HD:196:LEU:HD12	1.99	0.44
35:DD:899:VAL:HG13	35:DD:900:SER:H	1.55	0.44
37:DF:400:GLY:O	37:DF:404:ARG:HG2	2.18	0.44
36:De:747:LEU:H	36:De:747:LEU:CD2	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:48:ARG:HA	46:HI:48:ARG:HD3	1.77	0.44
48:PD:17:ALA:HB1	48:PD:95:PHE:HE2	1.83	0.44
50:g:126:TYR:C	50:g:130:GLN:H	2.26	0.44
52:n:232:ALA:HB1	52:n:247:LEU:HD11	2.00	0.44
52:n:485:ASP:N	52:n:485:ASP:OD1	2.51	0.44
52:n:509:ILE:HD11	52:n:516:SER:HB2	2.00	0.44
52:n:647:MET:HG2	52:n:651:ASN:ND2	2.32	0.44
52:n:904:PHE:CD1	52:n:916:LEU:HD11	2.53	0.44
52:n:938:ASP:HB2	52:n:1171:ALA:CB	2.47	0.44
52:n:1322:LEU:O	52:n:1326:PRO:N	2.51	0.44
54:u:115:LEU:HA	54:u:118:ILE:HG22	2.00	0.44
55:a:357:LEU:HD12	55:a:359:HIS:HB3	2.00	0.44
55:a:400:HIS:HE1	55:a:403:ARG:HG2	1.83	0.44
55:a:466:VAL:CG1	55:a:478:LYS:H	2.31	0.44
56:d:139:ARG:HD3	56:d:139:ARG:HA	1.76	0.44
60:q:171:VAL:HG21	68:k:17:ILE:HG22	1.83	0.44
60:q:437:HIS:HE1	60:q:472:GLU:O	1.99	0.44
61:z:485:ILE:H	61:z:485:ILE:HG13	1.68	0.44
62:b:71:LEU:HD23	62:b:71:LEU:HA	1.87	0.44
62:b:85:ASN:ND2	66:o:641:THR:HB	2.32	0.44
63:c:42:LYS:HB2	63:c:48:ARG:HB3	1.99	0.44
67:h:173:PHE:HB3	69:r:197:VAL:HG12	1.99	0.44
68:k:71:THR:HA	68:k:74:ALA:CB	2.48	0.44
70:t:39:PHE:O	70:t:39:PHE:CG	2.71	0.44
73:w:782:MET:HE3	73:w:782:MET:HB2	1.90	0.44
74:x:669:ILE:HG22	74:x:673:MET:HE2	1.99	0.44
75:y:213:VAL:O	75:y:213:VAL:CG1	2.66	0.44
75:y:220:MET:HE3	75:y:220:MET:HB3	1.76	0.44
6:DA:784:GLN:H	6:DA:1073:GLN:NE2	2.12	0.43
7:EA:180:PHE:HA	13:EB:216:PHE:CE1	2.52	0.43
11:PA:428:ASP:OD2	11:PA:430:ARG:NH1	2.51	0.43
23:PE:71:GLN:HB2	23:PE:99:ILE:HD12	2.00	0.43
30:HD:289:SER:O	30:HD:290:SER:C	2.56	0.43
36:DE:790:LEU:HD13	39:DH:146:ILE:HG12	2.00	0.43
37:DF:14:LEU:CD2	40:DI:19:MET:CE	2.88	0.43
37:DF:43:VAL:CG2	40:DI:46:TYR:HD2	2.30	0.43
37:DF:55:LEU:HD22	37:DF:55:LEU:HA	1.73	0.43
40:DI:35:VAL:HG12	40:DI:39:MET:HE2	1.99	0.43
36:De:718:ARG:HD3	36:De:718:ARG:HA	1.77	0.43
46:HI:267:ASP:HB2	46:HI:294:TYR:HB2	2.00	0.43
47:HJ:279:ARG:O	47:HJ:279:ARG:NE	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:g:123:ILE:HA	50:g:126:TYR:HB2	1.99	0.43
56:d:156:SER:CA	56:d:161:VAL:CG1	2.95	0.43
57:f:94:PRO:O	60:q:130:VAL:HG13	2.18	0.43
62:b:168:ILE:HG13	63:c:110:ALA:HB3	1.99	0.43
73:w:274:LEU:O	73:w:333:HIS:NE2	2.40	0.43
73:w:549:LYS:HA	73:w:549:LYS:HD3	1.84	0.43
74:x:313:ILE:HD13	74:x:313:ILE:HA	1.84	0.43
74:x:591:ALA:HB1	74:x:597:LEU:HD23	2.00	0.43
9:HA:332:PHE:CZ	9:HA:367:ILE:HG23	2.53	0.43
9:HA:354:PRO:HB2	9:HA:355:PRO:HD3	2.00	0.43
11:PA:1203:ASP:N	11:PA:1203:ASP:OD1	2.51	0.43
11:PA:1366:PHE:HB2	11:PA:1374:VAL:HG21	1.99	0.43
12:DB:859:ARG:HD2	12:DB:859:ARG:HA	1.80	0.43
18:HC:288:ILE:H	18:HC:288:ILE:HD12	1.83	0.43
28:PK:37:LYS:N	28:PK:69:HIS:O	2.49	0.43
34:HH:133:THR:HB	34:HH:160:THR:HG21	2.00	0.43
40:DI:21:GLN:HE22	40:DI:24:LYS:HE2	1.84	0.43
37:Df:317:LEU:HG	37:Df:330:ARG:HE	1.83	0.43
46:HI:247:VAL:O	46:HI:247:VAL:HG13	2.17	0.43
49:PG:145:LEU:HD23	49:PG:145:LEU:H	1.82	0.43
52:n:554:MET:HE3	52:n:554:MET:HB2	1.88	0.43
55:a:63:GLU:HG3	55:a:86:ARG:NH1	2.33	0.43
55:a:206:GLY:H	55:a:412:ARG:HH12	1.65	0.43
55:a:340:TYR:HB2	55:a:378:LYS:HB3	2.00	0.43
56:d:111:GLN:CD	56:d:111:GLN:C	2.86	0.43
58:i:75:CYS:HB3	58:i:88:ASN:HD22	1.81	0.43
60:q:264:GLN:H	60:q:264:GLN:HG3	1.57	0.43
64:e:146:ILE:C	64:e:148:VAL:N	2.71	0.43
71:v:39:THR:C	71:v:41:LYS:N	2.76	0.43
74:x:420:ILE:HA	74:x:420:ILE:HD13	1.92	0.43
4:NY:-96:DG:H2"	4:NY:-95:DG:C8	2.53	0.43
7:EA:178:ALA:HB2	30:HD:8:ARG:HA	2.00	0.43
23:PE:134:GLU:OE1	23:PE:181:ARG:NH2	2.50	0.43
30:HD:287:TYR:CZ	46:HI:189:MET:SD	3.11	0.43
31:HG:291:CYS:SG	31:HG:294:CYS:N	2.82	0.43
33:HF:36:GLN:CG	33:HF:37:ASP:N	2.80	0.43
34:HH:133:THR:HG23	34:HH:134:SER:N	2.32	0.43
37:DF:138:ILE:HG13	39:DH:159:TYR:CE2	2.46	0.43
37:DF:219:GLU:CD	37:DF:219:GLU:C	2.86	0.43
39:DH:116:ARG:HG2	43:DJ:126:TYR:OH	2.19	0.43
40:DI:23:LEU:HD13	40:DI:31:TYR:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DL:93:GLU:O	41:DL:97:THR:HG23	2.18	0.43
42:Dc:24:ASP:CB	43:Dj:192:LYS:HD2	2.48	0.43
52:n:169:LEU:N	59:m:104:HIS:CE1	2.82	0.43
52:n:793:HIS:CD2	52:n:794:LEU:HG	2.54	0.43
52:n:909:GLN:OE1	62:b:114:ASP:OD1	2.36	0.43
54:u:73:ILE:C	54:u:75:SER:H	2.25	0.43
54:u:77:PRO:HG2	61:z:596:TYR:OH	2.17	0.43
55:a:66:GLN:OE1	56:d:44:LEU:CD2	2.62	0.43
56:d:42:ARG:NH2	58:i:93:LYS:N	2.66	0.43
56:d:44:LEU:HD23	56:d:44:LEU:C	2.44	0.43
60:q:119:VAL:CG1	60:q:127:LEU:HD13	2.48	0.43
60:q:134:ALA:CB	67:h:72:ARG:HH11	2.32	0.43
64:e:95:PHE:CZ	65:l:37:GLY:HA3	2.54	0.43
65:l:166:LEU:HD22	71:v:123:ILE:HD12	2.01	0.43
70:t:125:LYS:HE2	70:t:125:LYS:HB2	1.52	0.43
74:x:765:VAL:HG13	74:x:812:LEU:HB2	1.99	0.43
6:DA:409:HIS:CE1	6:DA:411:GLU:HB2	2.53	0.43
7:EA:52:LEU:CD1	7:EA:59:LEU:HD13	2.49	0.43
11:PA:872:MET:O	11:PA:879:VAL:HA	2.18	0.43
17:PB:752:TYR:O	27:PJ:1:MET:N	2.51	0.43
19:DO:48:LEU:HG	21:DQ:366:ILE:HD11	2.00	0.43
34:HH:408:SER:HB3	34:HH:413:LEU:HD11	2.01	0.43
35:DD:1073:THR:HG21	41:DL:87:ILE:HD11	2.00	0.43
36:DE:369:LYS:HD3	36:DE:369:LYS:HA	1.74	0.43
36:DE:476:VAL:HB	36:DE:782:HIS:HB2	2.01	0.43
36:DE:650:THR:HG22	36:DE:666:THR:HG22	1.99	0.43
37:DF:433:PRO:O	37:DF:437:LYS:N	2.33	0.43
37:Df:11:ASN:OD1	37:Df:48:LYS:NZ	2.51	0.43
46:HI:15:LEU:HD23	46:HI:16:ASP:HB2	1.99	0.43
46:HI:164:SER:N	46:HI:165:PRO:HD2	2.34	0.43
47:HJ:98:GLU:OE2	47:HJ:98:GLU:CA	2.66	0.43
52:n:932:GLY:C	52:n:1179:HIS:NE2	2.76	0.43
55:a:373:CYS:O	55:a:439:GLN:HA	2.19	0.43
55:a:466:VAL:HG22	55:a:467:MET:N	2.34	0.43
55:a:467:MET:HE3	55:a:475:VAL:HG11	2.00	0.43
56:d:45:ILE:CD1	58:i:73:ILE:HG13	2.32	0.43
60:q:157:ALA:CB	68:k:31:VAL:HG23	2.36	0.43
63:c:283:ARG:HB3	63:c:311:GLN:HE21	1.82	0.43
73:w:326:THR:HA	73:w:329:LEU:HD13	1.99	0.43
6:DA:484:ILE:HD13	37:Df:309:MET:HG2	2.00	0.43
6:DA:496:GLU:OE2	6:DA:496:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PA:1663:SER:HB3	11:PA:1664:TYR:H	1.55	0.43
17:PB:544:PHE:CE1	17:PB:590:LEU:HD11	2.54	0.43
18:HC:380:THR:HG23	18:HC:380:THR:O	2.18	0.43
23:PE:106:VAL:HG12	23:PE:107:GLN:N	2.34	0.43
30:HD:116:ASP:OD1	30:HD:117:ASN:N	2.51	0.43
37:DF:105:TYR:O	43:DJ:217:PHE:CD1	2.70	0.43
37:DF:336:LEU:HD23	37:DF:336:LEU:HA	1.84	0.43
38:DG:165:GLU:HA	38:DG:168:ARG:HD2	2.00	0.43
46:HI:13:GLU:OE2	46:HI:15:LEU:HB2	2.19	0.43
46:HI:47:HIS:HA	46:HI:52:LYS:CG	2.44	0.43
50:g:130:GLN:O	50:g:134:THR:OG1	2.30	0.43
52:n:909:GLN:HB2	52:n:913:HIS:O	2.18	0.43
56:d:156:SER:CB	56:d:161:VAL:CG1	2.96	0.43
56:d:163:ALA:HA	59:m:105:TRP:CE2	2.53	0.43
60:q:569:ILE:HG22	60:q:582:VAL:HB	2.01	0.43
67:h:5:GLU:C	67:h:5:GLU:CD	2.86	0.43
67:h:146:MET:CB	68:k:39:LYS:HZ3	1.97	0.43
73:w:273:VAL:HG21	73:w:286:MET:HE1	1.99	0.43
73:w:770:MET:HB3	73:w:776:ILE:HD11	1.99	0.43
74:x:57:ASN:OD1	74:x:57:ASN:N	2.52	0.43
74:x:577:ALA:O	74:x:581:ILE:HG13	2.18	0.43
6:DA:474:ASP:N	6:DA:474:ASP:OD1	2.52	0.43
11:PA:786:ALA:O	11:PA:787:VAL:HG23	2.19	0.43
12:DB:622:ASP:HB3	33:HF:36:GLN:CA	2.33	0.43
12:DB:766:LEU:HA	12:DB:807:THR:HG21	2.00	0.43
17:PB:218:THR:O	17:PB:218:THR:HG23	2.18	0.43
26:PI:104:ALA:O	26:PI:105:GLU:HG2	2.18	0.43
31:HG:87:LEU:HD23	31:HG:87:LEU:O	2.18	0.43
31:HG:369:VAL:HG13	31:HG:370:ASP:N	2.32	0.43
34:HH:63:LEU:O	34:HH:64:GLN:C	2.61	0.43
35:DD:872:PHE:CZ	41:DL:57:VAL:CG1	2.79	0.43
35:DD:958:LYS:HD3	35:DD:958:LYS:HA	1.53	0.43
35:DD:963:ARG:HG2	35:DD:982:LEU:N	2.33	0.43
39:DH:49:GLY:O	43:DJ:171:LEU:CD1	2.60	0.43
40:DI:23:LEU:HD22	40:DI:28:ILE:HD12	2.01	0.43
36:De:332:ILE:HA	36:De:336:HIS:HD2	1.84	0.43
46:HI:135:HIS:HD2	46:HI:137:ASP:N	2.14	0.43
46:HI:169:TYR:CG	46:HI:190:TYR:CZ	3.06	0.43
46:HI:243:LEU:HD12	46:HI:244:PRO:HD3	2.00	0.43
46:HI:274:GLY:O	46:HI:275:LEU:C	2.61	0.43
47:HJ:64:LEU:HD22	47:HJ:105:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:808:LEU:O	52:n:821:SER:HA	2.18	0.43
55:a:420:LEU:HD22	55:a:504:ILE:CG1	2.49	0.43
58:i:109:LEU:HD22	58:i:117:GLN:HE22	1.84	0.43
60:q:475:VAL:HG22	60:q:495:LEU:HB2	2.01	0.43
62:b:175:HIS:CD2	63:c:113:TRP:CZ2	3.07	0.43
63:c:238:VAL:HG22	63:c:292:LEU:HD22	1.98	0.43
64:e:79:GLN:O	64:e:82:GLN:HG2	2.18	0.43
66:o:694:ASP:HB2	66:o:705:HIS:HB2	2.00	0.43
70:t:11:VAL:HG11	70:t:17:VAL:HA	2.00	0.43
70:t:196:LEU:HD22	70:t:196:LEU:HA	1.85	0.43
72:p:194:LYS:HG3	72:p:198:GLN:HB3	2.00	0.43
73:w:248:LEU:HD23	73:w:248:LEU:HA	1.83	0.43
4:NY:-160:DG:H2''	4:NY:-159:DG:O5'	2.18	0.43
4:NY:-73:DG:H2'	4:NY:-72:DG:C8	2.54	0.43
6:DA:396:LEU:H	6:DA:396:LEU:CD1	2.20	0.43
6:DA:847:LYS:HB3	6:DA:847:LYS:HE2	1.77	0.43
9:HA:576:GLU:OE2	15:HB:308:ASN:ND2	2.49	0.43
11:PA:1213:ARG:NH2	11:PA:1215:GLU:OE2	2.51	0.43
13:EB:88:ARG:O	13:EB:91:ARG:HB2	2.19	0.43
30:HD:283:LEU:O	30:HD:284:ALA:C	2.59	0.43
34:HH:193:VAL:HG11	34:HH:283:ARG:CD	2.49	0.43
37:DF:82:PRO:HD2	37:DF:96:PHE:HA	2.01	0.43
37:DF:336:LEU:O	37:DF:339:GLN:HG3	2.19	0.43
37:Df:55:LEU:HD13	40:Di:28:ILE:HG12	2.01	0.43
41:Dl:113:VAL:O	41:Dl:113:VAL:HG22	2.17	0.43
46:HI:162:PHE:CD1	46:HI:162:PHE:N	2.86	0.43
46:HI:297:ASN:HB3	46:HI:299:PRO:HD2	2.00	0.43
47:HJ:85:MET:HE3	47:HJ:85:MET:C	2.44	0.43
50:g:175:LEU:HD21	58:i:132:LEU:CD1	2.43	0.43
52:n:482:VAL:HG13	52:n:489:ILE:HD11	2.00	0.43
55:a:107:MET:O	55:a:107:MET:SD	2.77	0.43
55:a:378:LYS:O	55:a:379:ASP:HB2	2.18	0.43
55:a:417:TYR:OH	55:a:450:PHE:CD1	2.70	0.43
55:a:489:CYS:SG	55:a:514:LYS:HB3	2.58	0.43
56:d:119:GLN:HE21	56:d:119:GLN:HB2	1.48	0.43
60:q:95:TRP:CZ3	67:h:33:LEU:HD21	2.47	0.43
60:q:245:VAL:HG22	60:q:291:TRP:HB3	2.01	0.43
60:q:377:LEU:CD1	65:l:177:ARG:HA	2.36	0.43
67:h:146:MET:CG	68:k:39:LYS:CD	2.95	0.43
67:h:149:ASN:O	67:h:153:LYS:HG2	2.19	0.43
68:k:30:THR:HA	68:k:33:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:r:53:ASP:HB3	69:r:73:ARG:NE	2.33	0.43
74:x:433:GLU:C	74:x:433:GLU:CD	2.86	0.43
6:DA:645:LYS:HD2	6:DA:645:LYS:HA	1.76	0.43
6:DA:1052:ARG:O	6:DA:1052:ARG:CG	2.66	0.43
6:DA:1053:PHE:HB2	6:DA:1057:GLU:HB2	2.00	0.43
9:HA:49:THR:HG23	9:HA:50:VAL:N	2.34	0.43
30:HD:133:ILE:HD12	30:HD:133:ILE:HA	1.62	0.43
34:HH:184:VAL:HG13	34:HH:185:ILE:N	2.33	0.43
37:Df:405:SER:O	37:Df:405:SER:OG	2.34	0.43
44:Dk:179:MET:HB3	44:Dk:180:PRO:HD2	2.01	0.43
46:HI:24:ALA:CA	46:HI:44:LYS:HB2	2.47	0.43
46:HI:245:ASP:N	46:HI:245:ASP:OD1	2.51	0.43
47:HJ:138:LYS:HE3	47:HJ:138:LYS:HB3	1.85	0.43
48:PD:83:VAL:HG13	48:PD:137:LYS:HZ2	1.83	0.43
48:PD:107:THR:HG23	48:PD:110:GLU:H	1.83	0.43
51:j:89:LEU:HD23	51:j:89:LEU:HA	1.88	0.43
52:n:166:TYR:OH	59:m:70:PRO:C	2.62	0.43
52:n:273:PHE:CD2	57:f:181:LEU:HD13	2.54	0.43
55:a:467:MET:HB3	55:a:467:MET:HE3	1.97	0.43
55:a:468:ASP:OD1	55:a:468:ASP:O	2.36	0.43
57:f:127:GLN:HE22	71:v:62:HIS:HD2	1.66	0.43
58:i:133:GLN:O	58:i:136:LYS:HB3	2.18	0.43
63:c:309:CYS:O	63:c:310:ARG:C	2.61	0.43
63:c:309:CYS:CB	63:c:311:GLN:OE1	2.61	0.43
64:e:73:ILE:O	64:e:77:VAL:HG13	2.18	0.43
64:e:132:HIS:CE1	65:l:163:LEU:HD11	2.54	0.43
70:t:197:PHE:HA	70:t:200:ILE:HD11	2.00	0.43
71:v:131:GLU:CG	71:v:135:TYR:HE2	2.31	0.43
2:Y:27:DT:H72	2:Y:28:DT:C7	2.49	0.43
6:DA:406:THR:O	37:DF:354:ARG:NH2	2.51	0.43
6:DA:1068:ARG:HD2	6:DA:1068:ARG:O	2.18	0.43
9:HA:67:VAL:O	9:HA:67:VAL:HG23	2.19	0.43
9:HA:143:ARG:NH1	9:HA:159:GLU:OE1	2.48	0.43
9:HA:338:GLU:HG2	30:HD:68:VAL:HG11	2.00	0.43
12:DB:431:LEU:H	12:DB:431:LEU:CD2	2.32	0.43
12:DB:674:THR:HB	18:HC:415:GLN:NE2	2.30	0.43
12:DB:887:ARG:NH2	12:DB:917:ASP:OD2	2.49	0.43
15:HB:303:ILE:HG22	15:HB:307:PHE:CE2	2.54	0.43
17:PB:239:MET:HB2	17:PB:372:LEU:HD21	2.01	0.43
30:HD:300:ALA:HB1	47:HJ:166:PRO:CA	2.37	0.43
33:HF:24:ASP:OD1	33:HF:24:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:HH:409:THR:O	34:HH:413:LEU:HD13	2.19	0.43
35:DD:950:LEU:C	35:DD:950:LEU:CD1	2.86	0.43
37:DF:26:MET:HE2	40:DI:48:THR:HG22	2.01	0.43
37:DF:327:TRP:CD1	37:DF:327:TRP:C	2.97	0.43
42:Dc:124:ILE:HD11	37:Df:133:ALA:HB1	2.00	0.43
50:g:130:GLN:O	50:g:134:THR:N	2.44	0.43
52:n:201:HIS:CE1	54:u:122:LEU:HD12	2.54	0.43
52:n:210:PRO:HD2	52:n:211:GLN:HE21	1.83	0.43
52:n:954:TYR:OH	52:n:1169:TRP:HA	2.19	0.43
55:a:67:LYS:HD3	55:a:70:LYS:HE2	2.00	0.43
55:a:384:ASP:OD1	55:a:384:ASP:N	2.52	0.43
60:q:36:MET:SD	60:q:37:SER:N	2.92	0.43
60:q:646:LEU:HD21	65:l:115:ILE:CD1	2.49	0.43
64:e:146:ILE:CG2	64:e:147:ASN:N	2.52	0.43
66:o:625:VAL:HG23	66:o:634:PHE:HZ	1.84	0.43
68:k:109:ARG:NH1	68:k:109:ARG:HB2	2.34	0.43
70:t:21:VAL:HG22	70:t:138:ILE:HD11	2.01	0.43
72:p:569:LEU:HD12	72:p:572:PRO:HB3	2.01	0.43
72:p:817:LYS:O	72:p:821:GLN:HB2	2.18	0.43
74:x:11:LEU:HD22	74:x:15:LYS:HG3	2.01	0.43
74:x:187:SER:O	74:x:190:THR:OG1	2.35	0.43
75:y:226:LEU:HD12	75:y:227:VAL:N	2.34	0.43
3:NX:12:DC:H2''	3:NX:13:DC:O5'	2.18	0.43
4:NY:-82:DG:H2''	4:NY:-81:DG:C8	2.54	0.43
7:EA:105:TYR:CE2	13:EB:236:TYR:HB3	2.53	0.43
9:HA:168:VAL:O	9:HA:168:VAL:HG13	2.19	0.43
12:DB:653:LEU:HG	12:DB:684:ILE:HG13	2.00	0.43
13:EB:73:TYR:O	13:EB:74:LYS:HG2	2.18	0.43
13:EB:168:LEU:HD22	13:EB:199:LYS:HB2	2.01	0.43
18:HC:261:PHE:CZ	18:HC:265:LEU:HD21	2.54	0.43
25:PH:91:VAL:HG22	25:PH:144:LEU:HD22	1.98	0.43
30:HD:280:PRO:HB2	30:HD:281:GLN:OE1	2.19	0.43
34:HH:532:LEU:CD2	34:HH:716:VAL:HG13	2.49	0.43
37:DF:14:LEU:HD21	40:DI:19:MET:HE2	1.95	0.43
37:DF:402:ARG:O	37:DF:406:VAL:HG13	2.19	0.43
39:DH:57:SER:N	43:DJ:197:MET:SD	2.92	0.43
41:DL:69:GLU:O	41:DL:70:VAL:C	2.62	0.43
42:Dc:101:VAL:HG22	37:Df:127:LEU:HA	2.00	0.43
46:HI:102:ILE:O	46:HI:102:ILE:CG2	2.67	0.43
46:HI:185:PHE:HE2	46:HI:237:TRP:CH2	2.37	0.43
47:HJ:107:THR:O	47:HJ:108:CYS:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:HJ:182:GLU:O	47:HJ:182:GLU:OE2	2.37	0.43
55:a:321:LEU:CD2	55:a:407:ILE:CD1	2.75	0.43
56:d:109:GLN:HA	56:d:112:LYS:NZ	2.32	0.43
56:d:164:PRO:CD	56:d:167:TRP:HB2	2.45	0.43
57:f:145:TYR:CG	67:h:43:PRO:HD3	2.53	0.43
58:i:88:ASN:C	58:i:88:ASN:OD1	2.62	0.43
60:q:19:VAL:HG22	60:q:22:VAL:HG22	2.01	0.43
72:p:398:SER:O	72:p:400:GLN:N	2.51	0.43
73:w:236:ALA:HB2	73:w:663:PRO:HG3	2.00	0.43
73:w:470:ASN:OD1	73:w:470:ASN:N	2.52	0.43
7:EA:105:TYR:N	7:EA:105:TYR:CD1	2.87	0.42
7:EA:157:CYS:O	7:EA:158:HIS:HB2	2.19	0.42
11:PA:154:CYS:SG	11:PA:155:GLU:N	2.92	0.42
11:PA:511:THR:HG21	17:PB:1105:GLU:OE1	2.19	0.42
11:PA:1171:ALA:N	11:PA:1215:GLU:O	2.47	0.42
11:PA:1234:LYS:NZ	11:PA:1297:THR:O	2.52	0.42
12:DB:216:SER:OG	12:DB:217:ASN:N	2.52	0.42
12:DB:431:LEU:CD2	12:DB:431:LEU:N	2.82	0.42
17:PB:752:TYR:CE1	17:PB:809:VAL:HG23	2.52	0.42
17:PB:1128:ALA:HB1	17:PB:1135:TYR:HD1	1.84	0.42
17:PB:1162:LEU:HB3	17:PB:1167:ILE:HB	2.00	0.42
18:HC:70:ALA:HB1	18:HC:74:TRP:CZ2	2.54	0.42
30:HD:85:ARG:CZ	30:HD:140:LEU:HG	2.38	0.42
30:HD:295:ARG:NH2	30:HD:295:ARG:HG2	2.33	0.42
36:DE:731:MET:HE3	36:DE:731:MET:HB3	1.91	0.42
37:Df:432:ALA:HB1	37:Df:462:GLN:CB	2.49	0.42
46:HI:71:HIS:HB3	46:HI:74:ILE:HG13	2.00	0.42
47:HJ:85:MET:HE3	47:HJ:85:MET:HB3	1.34	0.42
50:g:140:GLU:OE2	61:z:556:GLN:HG2	2.19	0.42
50:g:140:GLU:HG2	54:u:93:LEU:HD21	2.01	0.42
52:n:1185:LEU:HD11	52:n:1207:LEU:HB2	2.01	0.42
55:a:503:SER:O	55:a:506:VAL:HB	2.19	0.42
56:d:63:ASN:HD22	56:d:63:ASN:HA	1.56	0.42
60:q:186:GLU:HB3	60:q:243:LEU:HD22	1.97	0.42
60:q:431:ILE:HD13	60:q:431:ILE:HA	1.75	0.42
66:o:719:PRO:N	66:o:720:PRO:HD2	2.34	0.42
71:v:116:LEU:HD23	71:v:116:LEU:HA	1.70	0.42
73:w:356:LEU:HD21	73:w:372:LEU:HD11	2.01	0.42
3:NX:85:DC:H2"	3:NX:86:DC:C6	2.54	0.42
15:HB:496:ASN:HB3	15:HB:536:LEU:HD11	2.01	0.42
17:PB:565:THR:HG21	17:PB:580:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:PB:719:SER:OG	17:PB:720:PRO:HD3	2.18	0.42
17:PB:854:ILE:O	17:PB:907:VAL:HG21	2.18	0.42
18:HC:58:ARG:HD2	32:HE:229:TRP:CZ3	2.54	0.42
32:HE:257:CYS:HB2	32:HE:258:HIS:CD2	2.54	0.42
35:DD:1084:LEU:HB3	40:DI:99:ARG:HH21	1.84	0.42
37:DF:67:THR:O	37:DF:68:THR:C	2.62	0.42
37:DF:82:PRO:CD	37:DF:96:PHE:HA	2.47	0.42
37:DF:85:GLY:C	43:DJ:212:LYS:HG2	2.43	0.42
37:DF:283:MET:HE1	37:DF:308:VAL:HG12	2.01	0.42
37:DF:312:ILE:HG22	37:DF:313:VAL:CG1	2.49	0.42
39:DH:116:ARG:HD3	43:DJ:126:TYR:HE1	1.82	0.42
40:DI:73:LEU:CB	41:DI:105:HIS:CE1	3.02	0.42
46:HI:37:ILE:H	46:HI:37:ILE:CD1	2.32	0.42
46:HI:160:LYS:HG2	46:HI:167:ARG:HH22	1.84	0.42
52:n:250:LEU:CG	52:n:275:HIS:CB	2.94	0.42
55:a:111:GLU:OE2	55:a:111:GLU:O	2.37	0.42
55:a:305:LEU:HD22	55:a:305:LEU:HA	1.83	0.42
55:a:383:PRO:CG	74:x:92:LEU:CD2	2.95	0.42
57:f:64:VAL:HG21	57:f:88:SER:HA	2.01	0.42
57:f:78:LEU:CD1	67:h:81:LEU:HD23	2.42	0.42
58:i:118:LEU:C	58:i:118:LEU:CD2	2.91	0.42
60:q:166:ARG:CG	60:q:166:ARG:NH1	2.79	0.42
63:c:114:SER:O	63:c:117:LEU:HG	2.19	0.42
68:k:70:LEU:HG	71:v:82:LEU:HD21	1.98	0.42
68:k:104:LEU:HD23	68:k:104:LEU:HA	1.75	0.42
70:t:91:PHE:O	70:t:95:MET:HG2	2.20	0.42
70:t:145:GLY:N	70:t:146:PRO:HD2	2.33	0.42
74:x:269:MET:O	74:x:273:MET:HG2	2.20	0.42
9:HA:345:ARG:NH2	30:HD:64:GLU:OE1	2.52	0.42
11:PA:560:VAL:HG21	11:PA:586:TRP:HB2	2.02	0.42
11:PA:883:ILE:O	11:PA:883:ILE:HG22	2.19	0.42
11:PA:1338:THR:OG1	11:PA:1340:GLY:O	2.36	0.42
13:EB:103:LEU:HD22	13:EB:108:HIS:CB	2.49	0.42
30:HD:32:GLU:OE1	30:HD:32:GLU:N	2.47	0.42
34:HH:532:LEU:HD23	34:HH:532:LEU:O	2.19	0.42
36:DE:485:ILE:HD12	37:DF:131:LEU:HD21	2.02	0.42
36:DE:564:ASP:OD1	36:DE:564:ASP:N	2.51	0.42
42:Dc:21:LEU:HD11	42:Dc:23:TRP:CD1	2.54	0.42
42:Dc:94:HIS:CD2	37:Df:122:LEU:HD22	2.55	0.42
46:HI:276:PHE:CD1	46:HI:276:PHE:N	2.87	0.42
47:HJ:3:HIS:C	47:HJ:5:SER:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:64:THR:HG22	49:PG:103:PRO:HD3	2.01	0.42
52:n:921:MET:HE2	52:n:1215:ILE:CD1	2.41	0.42
53:s:105:LEU:HB3	53:s:117:ASP:OD1	2.20	0.42
54:u:122:LEU:C	54:u:124:ASP:N	2.75	0.42
55:a:231:LEU:O	55:a:241:ILE:HB	2.19	0.42
55:a:437:LEU:HA	55:a:437:LEU:HD23	1.63	0.42
55:a:461:SER:N	74:x:7:LYS:HD3	2.35	0.42
56:d:115:LYS:HE2	56:d:115:LYS:O	2.19	0.42
57:f:127:GLN:NE2	71:v:62:HIS:HD2	2.17	0.42
60:q:152:SER:HB2	71:v:58:ASN:CB	2.50	0.42
62:b:187:GLY:O	64:e:53:GLU:OE2	2.37	0.42
67:h:23:LYS:NZ	67:h:23:LYS:CB	2.73	0.42
69:r:47:GLU:CD	69:r:47:GLU:H	2.26	0.42
70:t:197:PHE:O	70:t:200:ILE:HG12	2.20	0.42
71:v:41:LYS:HB3	71:v:41:LYS:HE2	1.79	0.42
71:v:114:ARG:HH12	71:v:115:LYS:HZ3	1.67	0.42
72:p:216:ALA:HA	72:p:229:ALA:O	2.19	0.42
73:w:389:LEU:HA	73:w:392:PHE:HD2	1.84	0.42
11:PA:106:VAL:O	11:PA:110:VAL:HG12	2.19	0.42
11:PA:1281:ASP:O	11:PA:1285:LEU:HD13	2.19	0.42
11:PA:1795:PRO:HG2	56:d:169:PRO:HB3	1.98	0.42
13:EB:145:VAL:HG21	13:EB:151:LEU:HB2	2.01	0.42
13:EB:148:LYS:CD	13:EB:184:ALA:HB3	2.49	0.42
15:HB:374:LEU:HD12	15:HB:374:LEU:C	2.45	0.42
19:DO:1:MET:C	35:DD:1000:ARG:HD2	2.44	0.42
21:DQ:18:ILE:HD11	21:DQ:46:TRP:CH2	2.54	0.42
29:PL:32:ASP:OD1	29:PL:32:ASP:N	2.50	0.42
36:DE:651:VAL:HG21	36:DE:686:THR:HG21	2.01	0.42
37:DF:104:LEU:CB	43:DJ:217:PHE:HE2	2.12	0.42
39:DH:127:GLN:N	39:DH:128:PRO:HD2	2.34	0.42
40:DI:32:GLU:HB3	40:DI:35:VAL:HG23	2.00	0.42
41:DL:120:LEU:O	41:DL:125:ASN:N	2.52	0.42
37:Df:223:TYR:CD2	37:Df:255:MET:HE1	2.52	0.42
40:Di:16:ALA:HB2	40:Di:40:LEU:HD11	2.00	0.42
46:HI:192:VAL:O	46:HI:192:VAL:CG1	2.66	0.42
52:n:266:VAL:CG2	57:f:177:VAL:HG13	2.49	0.42
52:n:273:PHE:CE2	57:f:185:ARG:CD	2.88	0.42
52:n:274:ILE:CG1	57:f:181:LEU:HD22	2.49	0.42
52:n:541:LYS:HG3	52:n:549:TYR:CZ	2.54	0.42
54:u:78:SER:C	54:u:80:GLU:H	2.26	0.42
55:a:204:LEU:HD23	55:a:204:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:i:94:PHE:O	58:i:94:PHE:HD1	2.01	0.42
58:i:135:TYR:HA	58:i:138:LEU:HB2	2.00	0.42
60:q:226:LYS:HD3	60:q:226:LYS:H	1.84	0.42
63:c:309:CYS:O	63:c:311:GLN:CB	2.67	0.42
72:p:35:LEU:HD22	72:p:49:MET:HA	2.00	0.42
72:p:523:SER:OG	72:p:524:THR:N	2.52	0.42
73:w:237:ILE:HG21	73:w:285:ASN:HB3	2.02	0.42
6:DA:925:ASP:OD1	6:DA:925:ASP:N	2.51	0.42
9:HA:661:ALA:HA	9:HA:664:VAL:HG12	2.02	0.42
11:PA:706:ILE:O	11:PA:710:LYS:HG2	2.19	0.42
17:PB:399:LEU:HB3	17:PB:453:TRP:CZ2	2.55	0.42
17:PB:446:TYR:CE1	17:PB:450:THR:HG21	2.55	0.42
17:PB:994:GLY:O	27:PJ:31:GLU:HB2	2.20	0.42
30:HD:23:VAL:HG12	30:HD:59:ARG:HB2	2.01	0.42
30:HD:85:ARG:NH2	30:HD:139:LYS:HB3	2.34	0.42
30:HD:130:LYS:HE2	30:HD:130:LYS:HB3	1.65	0.42
30:HD:301:PHE:CE1	47:HJ:170:PHE:CE1	3.08	0.42
36:DE:460:SER:HB3	37:DF:135:TRP:CZ3	2.55	0.42
36:DE:696:TRP:HH2	36:DE:703:MET:SD	2.25	0.42
39:DH:110:TYR:CE1	39:DH:113:ARG:NH1	2.87	0.42
40:Di:78:ARG:HD3	40:Di:78:ARG:HA	1.78	0.42
41:Dl:139:TYR:HD2	45:Dm:73:MET:HE3	1.84	0.42
46:HI:67:GLN:HE22	47:HJ:157:HIS:HA	1.83	0.42
47:HJ:97:MET:H	47:HJ:97:MET:HG2	1.66	0.42
50:g:127:ARG:NH2	54:u:5:LEU:HB3	2.26	0.42
51:j:82:LYS:HZ3	53:s:96:PHE:HD1	1.63	0.42
51:j:83:GLU:HB3	51:j:87:ARG:HH12	1.84	0.42
52:n:152:PHE:C	52:n:154:ILE:H	2.26	0.42
52:n:178:ILE:HD11	59:m:84:PHE:HB2	2.01	0.42
52:n:857:GLU:O	52:n:861:LYS:HG2	2.19	0.42
55:a:321:LEU:HD21	55:a:407:ILE:CB	2.50	0.42
55:a:407:ILE:HD13	55:a:407:ILE:N	2.35	0.42
56:d:96:LEU:HD12	56:d:96:LEU:HA	1.81	0.42
60:q:366:ASP:OD1	60:q:366:ASP:N	2.50	0.42
60:q:395:PRO:HA	69:r:53:ASP:OD1	2.19	0.42
61:z:489:TYR:HA	61:z:492:ARG:HD2	2.00	0.42
65:l:92:LEU:HA	65:l:95:VAL:HG22	1.99	0.42
69:r:57:VAL:HG13	69:r:69:VAL:HG13	2.00	0.42
69:r:196:LEU:HA	69:r:196:LEU:HD23	1.77	0.42
72:p:56:GLN:O	72:p:59:THR:OG1	2.35	0.42
73:w:1046:ASP:N	73:w:1046:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:x:68:ILE:HD11	74:x:78:VAL:HG11	2.01	0.42
74:x:101:MET:HE1	74:x:131:LEU:HD11	2.01	0.42
74:x:273:MET:HE1	74:x:818:LEU:HB2	2.01	0.42
75:y:40:LEU:HD12	75:y:40:LEU:N	2.35	0.42
3:NX:135:DC:H4'	3:NX:136:DC:OP1	2.20	0.42
6:DA:401:ASN:H	6:DA:401:ASN:ND2	2.16	0.42
11:PA:575:PRO:HG3	11:PA:594:LEU:HD11	2.01	0.42
11:PA:668:PHE:CZ	11:PA:672:ILE:HD11	2.54	0.42
12:DB:562:GLY:O	12:DB:581:ILE:HG12	2.19	0.42
12:DB:835:ARG:HE	12:DB:835:ARG:HB2	1.73	0.42
36:DE:645:GLY:N	36:DE:675:LEU:HD11	2.34	0.42
37:DF:14:LEU:CD2	40:DI:19:MET:HE1	2.40	0.42
38:DG:181:TRP:O	38:DG:181:TRP:CD2	2.72	0.42
36:De:238:GLN:H	36:De:238:GLN:HG2	1.64	0.42
40:Di:45:ARG:HG3	43:Dj:212:LYS:HB3	2.01	0.42
44:Dk:182:LEU:HD23	44:Dk:182:LEU:HA	1.85	0.42
47:HJ:3:HIS:C	47:HJ:5:SER:H	2.26	0.42
50:g:131:ALA:O	50:g:135:LEU:HG	2.20	0.42
52:n:199:LEU:CD1	52:n:222:VAL:HG13	2.49	0.42
52:n:945:ASP:OD1	52:n:945:ASP:N	2.53	0.42
55:a:259:ILE:H	55:a:259:ILE:CD1	2.22	0.42
56:d:64:GLN:NE2	56:d:68:LEU:CD1	2.82	0.42
56:d:115:LYS:O	56:d:115:LYS:HD3	2.20	0.42
58:i:89:ALA:O	58:i:93:LYS:HG3	2.19	0.42
70:t:194:MET:HE3	70:t:194:MET:HB3	1.91	0.42
73:w:758:LYS:HA	73:w:758:LYS:HD3	1.81	0.42
6:DA:342:ARG:O	6:DA:347:ARG:HB2	2.20	0.42
6:DA:727:THR:HG23	6:DA:727:THR:O	2.19	0.42
9:HA:109:LEU:HD11	9:HA:199:ILE:HD11	2.01	0.42
9:HA:323:ILE:O	9:HA:378:ARG:NH1	2.53	0.42
9:HA:557:ILE:HG22	9:HA:561:ILE:HD12	2.01	0.42
11:PA:1129:ASN:O	11:PA:1130:ILE:C	2.63	0.42
11:PA:1430:CYS:O	11:PA:1435:THR:OG1	2.38	0.42
15:HB:524:HIS:NE2	15:HB:528:MET:SD	2.93	0.42
17:PB:871:VAL:O	17:PB:871:VAL:HG13	2.18	0.42
30:HD:288:THR:O	30:HD:289:SER:C	2.62	0.42
36:DE:377:LEU:HD21	36:DE:422:PRO:HG2	2.00	0.42
37:DF:249:ASP:HB3	37:DF:252:LEU:HB2	2.02	0.42
37:DF:401:GLU:C	37:DF:401:GLU:CD	2.87	0.42
37:Df:447:ALA:CB	37:Df:456:GLY:HA3	2.49	0.42
46:HI:75:ILE:HD12	46:HI:75:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:141:ASN:O	46:HI:143:LEU:N	2.53	0.42
46:HI:208:LEU:HD23	46:HI:208:LEU:HA	1.77	0.42
46:HI:257:LEU:H	46:HI:257:LEU:HG	1.61	0.42
47:HJ:201:THR:C	47:HJ:203:ALA:N	2.78	0.42
52:n:133:ALA:HB2	54:u:23:ILE:HG22	2.02	0.42
52:n:166:TYR:CE2	59:m:71:GLN:HA	2.29	0.42
55:a:257:VAL:HG23	55:a:305:LEU:HD23	2.02	0.42
55:a:501:CYS:O	55:a:502:MET:HB2	2.19	0.42
57:f:111:LEU:HD22	60:q:127:LEU:CD1	2.49	0.42
58:i:65:PHE:HZ	58:i:102:SER:OG	2.03	0.42
60:q:188:LEU:HD13	71:v:87:ILE:CG1	2.46	0.42
60:q:451:LEU:HD22	60:q:451:LEU:HA	1.85	0.42
60:q:460:ILE:HD12	60:q:529:MET:HE2	1.99	0.42
60:q:523:ASP:HA	60:q:563:ILE:HD12	2.02	0.42
63:c:180:LEU:HD12	63:c:181:SER:H	1.84	0.42
64:e:129:VAL:CG1	68:k:114:MET:HE2	2.48	0.42
65:l:167:ILE:CD1	71:v:123:ILE:HG22	2.48	0.42
66:o:729:TYR:C	66:o:731:ALA:H	2.27	0.42
67:h:191:LEU:HD23	67:h:191:LEU:HA	1.89	0.42
69:r:19:MET:HE2	69:r:19:MET:HB3	1.80	0.42
69:r:74:ARG:HD3	69:r:83:TRP:CZ2	2.54	0.42
73:w:314:ARG:NH1	73:w:326:THR:OG1	2.48	0.42
73:w:952:LEU:HD23	73:w:952:LEU:HA	1.80	0.42
73:w:1090:CYS:SG	73:w:1091:ASP:N	2.88	0.42
74:x:269:MET:HE2	74:x:269:MET:HB2	1.76	0.42
5:BA:127:ARG:NH1	17:PB:435:ILE:O	2.51	0.42
6:DA:344:GLY:O	6:DA:347:ARG:HB3	2.19	0.42
6:DA:825:ILE:HD12	6:DA:830:ILE:HD11	2.01	0.42
8:FA:50:ASP:OD1	8:FA:53:ASN:ND2	2.52	0.42
12:DB:839:MET:HE1	12:DB:843:LEU:HD13	2.00	0.42
14:FB:58:LEU:CD1	14:FB:62:LEU:HD23	2.49	0.42
15:HB:456:ASP:OD1	15:HB:456:ASP:N	2.47	0.42
17:PB:905:ASP:OD1	17:PB:924:ARG:NH1	2.49	0.42
23:PE:13:ILE:HD12	23:PE:13:ILE:H	1.83	0.42
24:PF:72:GLN:HG2	49:PG:64:GLY:HA2	2.01	0.42
30:HD:254:GLU:CD	30:HD:254:GLU:O	2.62	0.42
32:HE:175:MET:HE3	32:HE:179:ASN:ND2	2.35	0.42
36:DE:464:TYR:CG	37:DF:133:ALA:HB2	2.55	0.42
39:DH:53:ALA:CB	43:DJ:195:LEU:HB3	2.49	0.42
36:De:667:GLY:O	36:De:692:ARG:NH2	2.52	0.42
52:n:94:GLN:HA	52:n:97:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:237:MET:CE	60:q:45:GLN:HG2	2.48	0.42
52:n:707:ASP:CA	66:o:684:ARG:NH2	2.83	0.42
54:u:78:SER:H	61:z:562:GLY:C	2.28	0.42
55:a:373:CYS:HB3	55:a:439:GLN:CG	2.49	0.42
57:f:57:LEU:HB3	57:f:58:GLU:H	1.50	0.42
57:f:63:MET:SD	57:f:65:GLY:N	2.93	0.42
59:m:103:LEU:HD23	59:m:103:LEU:HA	1.95	0.42
60:q:146:LEU:HD22	60:q:150:LYS:HG3	2.00	0.42
60:q:203:ILE:HG13	60:q:203:ILE:O	2.18	0.42
63:c:276:LEU:C	63:c:278:GLN:H	2.28	0.42
70:t:3:VAL:HG22	70:t:150:ALA:CB	2.50	0.42
72:p:174:LYS:HG3	75:y:84:CYS:HB3	2.01	0.42
72:p:182:VAL:HG21	72:p:228:VAL:HG21	2.02	0.42
73:w:60:ILE:HA	73:w:63:ILE:HD12	2.01	0.42
4:NY:-67:DG:H2"	4:NY:-66:DG:C8	2.55	0.42
6:DA:571:GLU:CD	6:DA:571:GLU:N	2.74	0.42
10:NA:534:ARG:O	10:NA:535:ALA:HB2	2.20	0.42
11:PA:672:ILE:HG23	11:PA:676:ILE:HD13	2.02	0.42
11:PA:893:GLU:OE1	23:PE:197:SER:OG	2.33	0.42
13:EB:240:GLN:HG3	30:HD:15:ARG:HH21	1.84	0.42
30:HD:209:GLU:H	30:HD:209:GLU:HG3	1.58	0.42
30:HD:294:HIS:O	30:HD:295:ARG:C	2.62	0.42
40:DI:78:ARG:O	40:DI:82:SER:HB2	2.20	0.42
41:DL:62:LYS:HD3	41:DL:62:LYS:C	2.44	0.42
37:Df:320:ARG:HH11	37:Df:320:ARG:HB2	1.83	0.42
46:HI:151:LEU:C	46:HI:151:LEU:CD2	2.93	0.42
46:HI:200:GLY:HA3	46:HI:276:PHE:HE1	1.84	0.42
48:PD:60:VAL:HG22	49:PG:103:PRO:HG3	2.02	0.42
52:n:114:LYS:HB3	53:s:89:LEU:HD11	2.02	0.42
52:n:908:PRO:HG3	62:b:121:ARG:NH2	2.34	0.42
54:u:7:GLN:HG3	61:z:594:LEU:HB2	2.02	0.42
55:a:383:PRO:CG	74:x:92:LEU:HD22	2.35	0.42
55:a:457:PRO:HB3	55:a:512:ARG:HD2	2.00	0.42
55:a:466:VAL:CG2	74:x:54:PRO:HG3	2.47	0.42
67:h:137:GLN:OE1	67:h:137:GLN:HA	2.20	0.42
70:t:122:PHE:CE2	70:t:156:LEU:HD11	2.55	0.42
72:p:273:ARG:HD2	72:p:273:ARG:HA	1.83	0.42
73:w:363:ARG:HD2	73:w:365:LEU:HD11	2.01	0.42
5:BA:195:PHE:CZ	5:BA:199:LEU:HD11	2.55	0.42
7:EA:26:TYR:HD1	13:EB:220:TRP:CZ2	2.37	0.42
8:FA:153:ARG:O	8:FA:177:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HA:111:SER:N	9:HA:211:TYR:OH	2.52	0.42
12:DB:464:ILE:HG12	12:DB:513:LYS:HE2	2.02	0.42
12:DB:594:SER:OG	12:DB:595:LYS:N	2.52	0.42
12:DB:957:MET:O	12:DB:968:ARG:NH1	2.53	0.42
18:HC:118:LEU:HD11	32:HE:50:PHE:CZ	2.55	0.42
19:DO:2:ALA:C	35:DD:1000:ARG:HB3	2.40	0.42
21:DQ:330:ASP:OD2	35:DD:1011:ALA:CB	2.68	0.42
28:PK:64:PRO:HG3	28:PK:72:ILE:HD12	2.02	0.42
30:HD:255:THR:OG1	30:HD:256:TYR:N	2.53	0.42
35:DD:1001:GLN:O	35:DD:1002:ARG:C	2.62	0.42
36:De:270:ASP:OD1	36:De:271:GLN:NE2	2.42	0.42
37:Df:428:LEU:HD13	37:Df:458:LEU:CB	2.50	0.42
44:Dk:179:MET:HB3	44:Dk:180:PRO:CD	2.50	0.42
46:HI:60:LEU:HD12	46:HI:60:LEU:HA	1.86	0.42
46:HI:235:GLU:O	46:HI:236:GLN:C	2.63	0.42
46:HI:266:ASP:HA	46:HI:269:LEU:CB	2.49	0.42
47:HJ:288:ASN:ND2	47:HJ:288:ASN:O	2.53	0.42
48:PD:70:ARG:HG2	71:v:20:LYS:HG3	2.01	0.42
49:PG:88:VAL:O	49:PG:99:THR:OG1	2.24	0.42
52:n:1283:LYS:HE2	52:n:1283:LYS:HB2	1.85	0.42
52:n:1354:THR:HA	52:n:1364:LEU:O	2.20	0.42
55:a:109:TYR:C	55:a:109:TYR:CD1	2.97	0.42
56:d:45:ILE:HG12	58:i:73:ILE:CB	2.49	0.42
56:d:49:ALA:HB3	58:i:76:MET:SD	2.41	0.42
63:c:16:GLN:HB3	63:c:73:LEU:HD21	2.02	0.42
66:o:619:GLN:NE2	66:o:623:ASP:OD1	2.38	0.42
66:o:772:LEU:HA	66:o:775:THR:HG22	2.02	0.42
67:h:151:LEU:CG	71:v:37:ILE:HB	2.50	0.42
68:k:8:ASN:OD1	68:k:8:ASN:N	2.52	0.42
68:k:75:THR:C	68:k:77:GLN:N	2.78	0.42
71:v:45:GLU:CD	71:v:45:GLU:C	2.88	0.42
74:x:436:LEU:HD23	74:x:436:LEU:HA	1.79	0.42
3:NX:136:DC:H2"	3:NX:137:DC:C5	2.55	0.41
6:DA:397:LEU:HD22	37:Df:360:THR:HG22	2.00	0.41
6:DA:511:LEU:HD12	6:DA:511:LEU:N	2.31	0.41
6:DA:620:LEU:HD11	6:DA:766:ARG:HD3	2.02	0.41
7:EA:17:LEU:HD22	7:EA:194:THR:CB	2.50	0.41
9:HA:56:ILE:HG21	9:HA:70:LEU:HD22	2.01	0.41
9:HA:618:VAL:HG11	9:HA:664:VAL:HA	2.03	0.41
11:PA:567:LEU:HB2	11:PA:570:TRP:HB2	2.01	0.41
12:DB:544:LEU:HD22	12:DB:625:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:FB:31:TRP:CD1	14:FB:62:LEU:HD21	2.55	0.41
18:HC:359:ILE:HG22	18:HC:360:THR:N	2.34	0.41
22:PC:36:ARG:HD3	28:PK:41:THR:OG1	2.20	0.41
26:PI:41:ASN:OD1	26:PI:41:ASN:C	2.63	0.41
30:HD:43:ALA:HB3	49:PG:164:MET:SD	2.60	0.41
30:HD:284:ALA:C	30:HD:286:GLY:H	2.28	0.41
34:HH:193:VAL:HG11	34:HH:283:ARG:HD3	2.01	0.41
35:DD:885:ILE:HA	35:DD:888:LYS:HE3	2.02	0.41
35:DD:949:GLN:O	35:DD:952:GLN:HB2	2.20	0.41
37:DF:43:VAL:HG23	40:DI:46:TYR:CG	2.55	0.41
37:DF:219:GLU:OE1	39:DH:156:PRO:HB2	2.20	0.41
37:DF:396:LEU:HA	37:DF:399:GLU:OE1	2.20	0.41
36:De:504:LEU:HD22	36:De:575:PHE:HZ	1.84	0.41
37:Df:104:LEU:HD22	43:Dj:216:TYR:HB2	2.02	0.41
44:Dk:130:PRO:HD3	45:Dm:35:GLU:HG2	2.02	0.41
52:n:376:PRO:HD2	52:n:377:PRO:HD3	2.01	0.41
52:n:382:ASP:O	52:n:386:VAL:HG22	2.20	0.41
52:n:553:GLU:OE2	52:n:569:TYR:OH	2.37	0.41
52:n:586:LEU:HD23	52:n:587:LEU:HD22	2.02	0.41
53:s:108:PHE:O	53:s:109:LEU:C	2.63	0.41
55:a:493:PHE:HE2	55:a:514:LYS:HB2	1.85	0.41
60:q:129:PRO:HB3	67:h:74:GLN:CG	2.49	0.41
61:z:597:VAL:HG11	61:z:599:LEU:HD12	2.02	0.41
62:b:87:ASN:HA	62:b:90:ASN:HB2	2.00	0.41
67:h:151:LEU:HG	71:v:37:ILE:HB	2.01	0.41
73:w:8:ILE:O	73:w:12:VAL:HG23	2.20	0.41
73:w:1131:LEU:HA	73:w:1131:LEU:HD13	1.88	0.41
74:x:821:TYR:HE2	74:x:946:PHE:HE2	1.67	0.41
4:NY:-143:DG:H2"	4:NY:-142:DG:C8	2.55	0.41
4:NY:-94:DG:H2"	4:NY:-93:DG:C8	2.54	0.41
7:EA:152:PHE:HZ	7:EA:161:VAL:HB	1.85	0.41
8:FA:15:VAL:HG12	8:FA:16:VAL:N	2.34	0.41
11:PA:219:GLU:OE1	13:EB:227:SER:HA	2.20	0.41
11:PA:544:ALA:CB	11:PA:680:LEU:HD13	2.50	0.41
11:PA:1793:THR:H	67:h:102:HIS:CE1	2.34	0.41
12:DB:371:LYS:HD3	12:DB:371:LYS:HA	1.87	0.41
12:DB:984:PRO:HG2	12:DB:987:LEU:HD22	2.02	0.41
13:EB:99:LEU:HD12	13:EB:124:LEU:HD11	2.01	0.41
18:HC:51:LEU:HD23	32:HE:237:GLN:CD	2.45	0.41
32:HE:217:VAL:HG23	32:HE:217:VAL:O	2.20	0.41
36:DE:452:ARG:O	36:DE:453:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DE:589:TRP:HH2	37:DF:57:PHE:CE1	2.37	0.41
38:DG:129:LYS:HA	38:DG:129:LYS:HD2	1.77	0.41
39:DH:61:LEU:HD11	43:DJ:200:LEU:HD21	2.02	0.41
39:DH:197:THR:HB	37:Df:238:LYS:HG2	2.02	0.41
41:DI:128:ILE:HA	41:DI:129:PRO:HD3	1.93	0.41
52:n:154:ILE:CB	52:n:155:PRO:HD3	2.43	0.41
52:n:212:LEU:HD22	52:n:226:VAL:HA	2.02	0.41
52:n:459:HIS:CE1	60:q:316:VAL:HG22	2.55	0.41
52:n:751:ASN:OD1	52:n:752:LEU:N	2.52	0.41
52:n:916:LEU:HD12	52:n:917:ALA:H	1.85	0.41
55:a:161:TYR:C	55:a:163:LEU:H	2.27	0.41
55:a:424:CYS:CA	55:a:505:PRO:HG3	2.48	0.41
56:d:42:ARG:HH21	58:i:93:LYS:N	2.18	0.41
57:f:114:VAL:O	57:f:118:ARG:HG2	2.20	0.41
62:b:64:ILE:HD13	62:b:64:ILE:HA	1.79	0.41
62:b:157:TYR:N	62:b:158:PRO:HD2	2.35	0.41
62:b:159:GLN:O	62:b:163:VAL:HG13	2.20	0.41
66:o:764:PRO:HA	73:w:15:THR:HG21	2.01	0.41
67:h:50:ALA:O	67:h:51:LEU:C	2.62	0.41
67:h:68:THR:HB	67:h:69:PRO:HD2	2.03	0.41
73:w:301:GLU:HG3	73:w:347:ALA:HB1	2.02	0.41
74:x:561:LEU:O	74:x:608:ASN:ND2	2.51	0.41
74:x:707:ILE:HD12	74:x:707:ILE:HA	1.88	0.41
74:x:794:ASP:HB3	74:x:797:LYS:HB2	2.02	0.41
3:NX:20:DC:H1'	3:NX:21:DC:N3	2.35	0.41
4:NY:-8:DG:H2''	4:NY:-7:DG:C8	2.55	0.41
8:FA:47:LEU:HD11	8:FA:98:TRP:HB3	2.01	0.41
9:HA:249:VAL:HG21	9:HA:403:PHE:HB2	2.00	0.41
11:PA:1007:ILE:HD12	11:PA:1007:ILE:HA	1.89	0.41
11:PA:1437:ASP:O	11:PA:1441:GLU:HG2	2.20	0.41
17:PB:718:GLN:CD	17:PB:976:MET:HE3	2.45	0.41
18:HC:96:TRP:HB3	18:HC:110:LEU:HD23	2.02	0.41
24:PF:75:MET:HE2	24:PF:75:MET:HB3	1.93	0.41
30:HD:259:HIS:ND1	30:HD:259:HIS:N	2.68	0.41
30:HD:281:GLN:NE2	30:HD:281:GLN:CA	2.79	0.41
30:HD:290:SER:O	30:HD:291:LEU:C	2.63	0.41
30:HD:295:ARG:CZ	47:HJ:165:ARG:HH21	2.25	0.41
32:HE:175:MET:HE3	32:HE:179:ASN:CG	2.45	0.41
34:HH:535:THR:HG23	34:HH:627:SER:HB2	2.02	0.41
40:DI:50:ILE:HG22	40:DI:71:VAL:HG13	2.03	0.41
46:HI:250:LYS:HB3	46:HI:252:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:PD:137:LYS:C	48:PD:139:SER:H	2.28	0.41
50:g:127:ARG:CA	50:g:130:GLN:H	2.33	0.41
51:j:82:LYS:HD3	53:s:96:PHE:CD1	2.55	0.41
52:n:220:GLY:C	52:n:221:ARG:HG3	2.46	0.41
52:n:907:LEU:HD11	62:b:118:LEU:CB	2.40	0.41
54:u:49:ASN:ND2	54:u:49:ASN:N	2.67	0.41
55:a:361:MET:HE3	55:a:376:LEU:HB2	2.02	0.41
55:a:500:ARG:HA	55:a:500:ARG:HD2	1.64	0.41
56:d:126:TYR:CD1	56:d:126:TYR:C	2.98	0.41
60:q:89:GLN:OE1	60:q:90:PRO:HD2	2.16	0.41
60:q:147:ILE:HD12	60:q:147:ILE:HA	1.80	0.41
69:r:18:MET:SD	69:r:176:PRO:HA	2.59	0.41
69:r:141:MET:HA	69:r:173:VAL:HG22	2.01	0.41
71:v:35:GLU:HB3	71:v:64:ARG:HD2	2.02	0.41
71:v:131:GLU:O	71:v:135:TYR:CD2	2.66	0.41
72:p:146:HIS:NE2	72:p:160:SER:OG	2.49	0.41
73:w:805:GLN:HE22	73:w:809:ARG:HE	1.68	0.41
73:w:916:ASP:OD1	73:w:916:ASP:N	2.53	0.41
4:NY:-12:DG:H2''	4:NY:-11:DG:O5'	2.20	0.41
9:HA:225:LEU:O	9:HA:227:ARG:NH1	2.54	0.41
11:PA:497:ASP:OD1	11:PA:497:ASP:C	2.63	0.41
11:PA:910:LYS:N	11:PA:911:PRO:CD	2.84	0.41
11:PA:1443:ALA:HB2	17:PB:1167:ILE:HG23	2.01	0.41
12:DB:176:HIS:HE1	12:DB:310:ASP:H	1.68	0.41
12:DB:835:ARG:CZ	39:DH:184:ARG:HH11	2.33	0.41
19:DO:11:LEU:HD23	19:DO:44:ILE:HD12	2.01	0.41
30:HD:13:LYS:N	30:HD:13:LYS:HD3	2.36	0.41
30:HD:85:ARG:HH12	30:HD:140:LEU:H	1.66	0.41
31:HG:333:GLU:O	31:HG:333:GLU:HG2	2.21	0.41
32:HE:255:CYS:HB2	32:HE:276:CYS:N	2.35	0.41
33:HF:21:LEU:O	33:HF:24:ASP:OD1	2.38	0.41
34:HH:559:ILE:HG22	34:HH:561:PHE:CE1	2.55	0.41
37:DF:279:LEU:HD22	37:DF:330:ARG:CZ	2.51	0.41
36:De:636:HIS:CD2	36:De:638:ASN:H	2.36	0.41
37:Df:219:GLU:H	37:Df:219:GLU:CD	2.21	0.41
47:HJ:54:MET:HE3	47:HJ:54:MET:HB3	1.89	0.41
51:j:82:LYS:HE3	53:s:101:VAL:HB	2.02	0.41
52:n:647:MET:HG2	52:n:651:ASN:HD21	1.85	0.41
52:n:909:GLN:NE2	62:b:114:ASP:OD1	2.53	0.41
52:n:922:TYR:HH	52:n:1214:VAL:HG12	1.85	0.41
53:s:105:LEU:HD23	53:s:105:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:q:102:LEU:HD13	67:h:29:PHE:CD2	2.54	0.41
66:o:763:LEU:HD11	66:o:775:THR:HG21	2.02	0.41
68:k:64:SER:HB2	68:k:68:ARG:NH2	2.35	0.41
70:t:79:PHE:C	70:t:80:GLU:HG3	2.44	0.41
71:v:35:GLU:OE2	71:v:64:ARG:NH2	2.53	0.41
72:p:252:LYS:HD3	72:p:252:LYS:HA	1.85	0.41
74:x:363:LEU:HA	74:x:363:LEU:HD23	1.81	0.41
74:x:466:ARG:NH2	74:x:512:ILE:O	2.53	0.41
74:x:687:PHE:CD1	74:x:687:PHE:N	2.88	0.41
10:NE:734:ARG:O	10:NE:735:ALA:CB	2.69	0.41
2:Y:-23:DC:H2''	2:Y:-22:DG:C8	2.55	0.41
4:NY:-18:DG:C2'	4:NY:-17:DG:H5'	2.51	0.41
11:PA:1645:PRO:HB2	11:PA:1646:THR:H	1.67	0.41
18:HC:223:ALA:HA	18:HC:226:ARG:HG2	2.02	0.41
36:DE:513:LEU:HD13	36:DE:513:LEU:N	2.25	0.41
36:DE:695:LEU:O	36:DE:704:VAL:HB	2.20	0.41
37:DF:85:GLY:C	43:DJ:212:LYS:CG	2.93	0.41
39:DH:155:ASP:OD1	39:DH:155:ASP:N	2.51	0.41
37:Df:244:GLN:O	37:Df:248:THR:OG1	2.34	0.41
52:n:104:LYS:HZ2	53:s:108:PHE:CA	2.28	0.41
52:n:573:VAL:HG21	52:n:583:ALA:HB1	2.02	0.41
52:n:689:PRO:O	52:n:690:CYS:HB2	2.21	0.41
52:n:753:LEU:HD12	63:c:311:GLN:HG2	1.99	0.41
55:a:87:GLN:HE21	55:a:87:GLN:HB2	1.64	0.41
55:a:359:HIS:HD2	55:a:361:MET:H	1.68	0.41
55:a:462:LEU:HB2	74:x:49:GLN:HA	2.02	0.41
57:f:96:ALA:HA	60:q:130:VAL:HG11	2.03	0.41
57:f:114:VAL:HG12	57:f:115:ILE:N	2.36	0.41
58:i:65:PHE:HD1	58:i:99:LYS:CD	2.33	0.41
59:m:116:GLN:HG2	61:z:595:PRO:CD	2.50	0.41
60:q:36:MET:O	60:q:39:ASN:N	2.54	0.41
60:q:596:PHE:HE2	65:l:112:GLU:CG	2.33	0.41
60:q:644:SER:HB2	64:e:97:GLN:N	2.35	0.41
67:h:151:LEU:HD11	71:v:37:ILE:C	2.45	0.41
68:k:106:ASP:HA	68:k:109:ARG:NE	2.36	0.41
70:t:1:MET:HG2	70:t:186:PRO:HD3	2.01	0.41
72:p:168:LEU:HD12	72:p:168:LEU:HA	1.92	0.41
72:p:564:LEU:H	72:p:564:LEU:HG	1.77	0.41
73:w:684:ASN:HD22	73:w:723:THR:HG21	1.85	0.41
2:Y:8:DA:H1'	2:Y:9:DA:C8	2.56	0.41
7:EA:28:ILE:HG13	7:EA:29:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:HA:56:ILE:HD12	9:HA:230:VAL:HG11	2.03	0.41
11:PA:1420:ASN:O	11:PA:1429:LYS:NZ	2.53	0.41
18:HC:58:ARG:CD	32:HE:229:TRP:CE3	3.03	0.41
20:DP:258:MET:N	20:DP:315:ALA:O	2.54	0.41
30:HD:295:ARG:O	30:HD:296:ALA:C	2.61	0.41
40:DI:35:VAL:CG1	40:DI:39:MET:HE2	2.50	0.41
40:DI:73:LEU:CB	41:DI:105:HIS:HE1	2.32	0.41
41:DI:129:PRO:HB2	45:Dm:56:ILE:HG23	2.01	0.41
46:HI:56:ASN:HD22	46:HI:56:ASN:HA	1.67	0.41
47:HJ:27:ASN:OD1	47:HJ:27:ASN:C	2.62	0.41
47:HJ:167:PHE:O	47:HJ:168:GLU:C	2.62	0.41
52:n:281:ARG:HG2	57:f:190:PRO:HA	2.02	0.41
52:n:287:LYS:HA	52:n:287:LYS:HD2	1.87	0.41
52:n:394:HIS:CD2	52:n:399:LYS:HD2	2.56	0.41
52:n:707:ASP:OD1	52:n:708:CYS:N	2.53	0.41
52:n:713:GLN:O	52:n:719:THR:HB	2.20	0.41
52:n:853:HIS:O	52:n:857:GLU:HG2	2.21	0.41
55:a:66:GLN:HE21	55:a:66:GLN:HB3	1.47	0.41
55:a:351:ASP:O	55:a:351:ASP:CG	2.63	0.41
63:c:70:LEU:HD12	63:c:70:LEU:HA	1.83	0.41
64:e:102:LEU:HD23	64:e:106:LYS:HE3	2.03	0.41
64:e:133:LEU:HD12	68:k:115:LEU:CD1	2.51	0.41
67:h:113:PRO:HB2	67:h:117:VAL:CG2	2.50	0.41
68:k:63:LEU:HD12	68:k:63:LEU:HA	1.89	0.41
6:DA:475:LEU:HD13	6:DA:475:LEU:O	2.21	0.41
6:DA:954:ALA:HA	38:DG:149:ARG:HH22	1.85	0.41
7:EA:17:LEU:HD22	7:EA:194:THR:OG1	2.20	0.41
7:EA:111:ARG:HD3	30:HD:11:THR:CB	2.50	0.41
7:EA:171:LYS:HZ1	30:HD:41:ARG:NE	2.18	0.41
9:HA:12:PHE:CE2	9:HA:14:TYR:HB2	2.56	0.41
9:HA:46:THR:HG22	9:HA:670:GLY:HA3	2.03	0.41
11:PA:549:THR:O	11:PA:549:THR:HG22	2.19	0.41
11:PA:869:GLU:OE2	17:PB:1091:ARG:NH1	2.46	0.41
11:PA:876:ASP:OD2	11:PA:880:ARG:NH2	2.53	0.41
11:PA:1166:LEU:HA	11:PA:1298:LEU:HD11	2.03	0.41
12:DB:644:GLN:O	18:HC:413:LEU:CB	2.69	0.41
12:DB:831:GLU:OE1	12:DB:835:ARG:NH2	2.52	0.41
13:EB:76:GLY:N	14:FB:192:GLU:OE2	2.53	0.41
13:EB:83:ASN:OD1	14:FB:188:PHE:CZ	2.74	0.41
13:EB:103:LEU:HD22	13:EB:108:HIS:HB3	2.02	0.41
14:FB:224:ASN:ND2	14:FB:234:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:PC:72:PRO:HG3	27:PJ:13:ILE:HD11	2.03	0.41
32:HE:42:MET:HE3	32:HE:108:ASN:HA	2.02	0.41
36:DE:236:LEU:HD21	36:DE:317:LEU:HB2	2.03	0.41
36:DE:704:VAL:HA	36:DE:759:ILE:HD11	2.01	0.41
36:DE:747:LEU:N	36:DE:747:LEU:HD13	2.35	0.41
37:DF:66:LEU:HB3	40:DI:32:GLU:OE2	2.21	0.41
37:DF:233:GLY:CA	37:DF:239:ARG:HE	2.33	0.41
38:DG:74:MET:HE1	38:DG:136:ILE:HD12	2.03	0.41
39:DH:114:SER:C	39:DH:116:ARG:N	2.76	0.41
37:Df:216:LEU:HD21	37:Df:254:GLN:O	2.21	0.41
46:HI:20:GLU:CD	46:HI:20:GLU:N	2.79	0.41
46:HI:139:LYS:O	46:HI:140:PRO:C	2.64	0.41
46:HI:279:ASN:C	46:HI:281:CYS:N	2.74	0.41
47:HJ:181:LEU:HD22	47:HJ:181:LEU:C	2.46	0.41
52:n:548:TYR:CE2	52:n:652:MET:CE	3.03	0.41
52:n:870:GLN:HG3	66:o:655:THR:HG21	2.03	0.41
52:n:944:PHE:O	52:n:945:ASP:C	2.64	0.41
55:a:62:LEU:HD22	56:d:48:LEU:HD21	2.03	0.41
55:a:63:GLU:O	55:a:67:LYS:HB2	2.21	0.41
57:f:34:SER:C	57:f:36:ARG:N	2.78	0.41
57:f:63:MET:CE	57:f:64:VAL:H	2.31	0.41
58:i:140:MET:SD	58:i:140:MET:N	2.93	0.41
61:z:583:ASP:HB2	61:z:590:ARG:HG2	2.02	0.41
68:k:106:ASP:HA	68:k:109:ARG:HE	1.85	0.41
70:t:204:GLN:CA	70:t:204:GLN:HE21	2.33	0.41
72:p:590:VAL:HG11	72:p:695:LYS:HE3	2.02	0.41
72:p:679:THR:OG1	72:p:722:SER:O	2.33	0.41
72:p:703:GLU:CD	72:p:703:GLU:N	2.79	0.41
11:PA:847:LEU:HD21	17:PB:720:PRO:HB3	2.02	0.41
12:DB:367:GLU:OE2	12:DB:371:LYS:NZ	2.39	0.41
13:EB:85:MET:HE2	13:EB:139:PHE:H	1.86	0.41
17:PB:516:GLU:OE1	17:PB:516:GLU:N	2.54	0.41
17:PB:573:TRP:NE1	17:PB:575:GLY:O	2.51	0.41
37:DF:75:LEU:HG	37:DF:84:TYR:OH	2.21	0.41
37:DF:231:CYS:HB3	37:DF:285:MET:HE2	2.02	0.41
37:DF:392:ILE:O	37:DF:392:ILE:CG2	2.69	0.41
41:DL:128:ILE:O	41:DL:128:ILE:HG22	2.19	0.41
37:Df:83:LEU:HD11	40:Di:42:PHE:HB2	2.03	0.41
45:Dm:68:MET:HE3	45:Dm:68:MET:HB3	1.95	0.41
47:HJ:25:ASP:OD1	47:HJ:25:ASP:C	2.63	0.41
52:n:205:THR:HA	56:d:108:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:237:MET:HE2	60:q:45:GLN:CG	2.51	0.41
52:n:861:LYS:HA	52:n:861:LYS:HD3	1.91	0.41
55:a:211:LEU:HD11	55:a:220:MET:SD	2.61	0.41
58:i:65:PHE:CE1	58:i:99:LYS:CG	3.03	0.41
60:q:20:HIS:HB3	60:q:31:LEU:HB2	2.02	0.41
60:q:430:LYS:HG2	60:q:471:TYR:OH	2.21	0.41
64:e:55:CYS:SG	65:l:52:PHE:HZ	2.43	0.41
68:k:77:GLN:NE2	69:r:192:GLN:HB2	2.36	0.41
72:p:50:ASP:OD1	72:p:50:ASP:N	2.42	0.41
72:p:306:VAL:HG23	72:p:399:LEU:HD13	2.02	0.41
72:p:558:SER:O	72:p:562:SER:N	2.53	0.41
72:p:678:ALA:HA	72:p:724:LEU:HD23	2.03	0.41
73:w:427:CYS:O	73:w:431:HIS:ND1	2.40	0.41
74:x:101:MET:HB3	74:x:101:MET:HE2	1.87	0.41
74:x:183:LEU:HD21	74:x:974:SER:HB3	2.03	0.41
6:DA:731:LEU:HD23	6:DA:731:LEU:HA	1.92	0.41
6:DA:797:LYS:HB3	6:DA:797:LYS:HE2	1.90	0.41
7:EA:21:VAL:HG23	7:EA:22:ILE:N	2.36	0.41
9:HA:195:ALA:O	9:HA:199:ILE:HG12	2.21	0.41
9:HA:383:LEU:HD21	9:HA:388:ILE:HD11	2.02	0.41
9:HA:604:VAL:O	9:HA:608:ILE:HG22	2.21	0.41
11:PA:478:PRO:HD2	28:PK:67:LEU:HD13	2.03	0.41
11:PA:1643:TYR:CZ	59:m:93:CYS:CB	3.04	0.41
11:PA:1666:PRO:HB2	11:PA:1667:THR:H	1.62	0.41
12:DB:218:GLY:HA2	12:DB:238:LEU:HD13	2.03	0.41
14:FB:186:MET:SD	35:DD:995:GLU:CD	3.04	0.41
17:PB:794:VAL:HG22	17:PB:967:ILE:HG22	2.02	0.41
17:PB:1107:LEU:O	17:PB:1111:SER:OG	2.30	0.41
18:HC:146:PRO:HA	18:HC:149:ASP:OD2	2.21	0.41
21:DQ:330:ASP:OD2	35:DD:1011:ALA:HB1	2.21	0.41
30:HD:264:GLU:HB2	30:HD:269:LEU:HB2	2.01	0.41
31:HG:186:ILE:HG12	31:HG:211:LEU:HD12	2.03	0.41
34:HH:364:LEU:HD23	34:HH:410:TYR:CD1	2.56	0.41
36:DE:239:LEU:HB3	36:DE:307:LEU:HD21	2.03	0.41
36:DE:359:LEU:HD12	36:DE:359:LEU:C	2.45	0.41
37:DF:215:GLU:H	37:DF:215:GLU:CD	2.29	0.41
37:DF:370:TRP:CH2	37:DF:402:ARG:HB3	2.56	0.41
37:DF:374:TYR:CE1	37:DF:422:HIS:HB3	2.56	0.41
40:DI:19:MET:CE	40:DI:40:LEU:HD23	2.51	0.41
36:De:774:MET:HE2	36:De:774:MET:HB2	1.91	0.41
46:HI:261:PHE:CZ	46:HI:272:ILE:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:HI:266:ASP:HA	46:HI:269:LEU:HB2	2.01	0.41
46:HI:293:LYS:HA	46:HI:293:LYS:HD3	1.92	0.41
47:HJ:186:ILE:HD13	47:HJ:186:ILE:N	2.21	0.41
47:HJ:239:LYS:N	47:HJ:239:LYS:HE3	2.36	0.41
48:PD:58:SER:OG	49:PG:35:GLU:OE2	2.35	0.41
48:PD:66:ASN:HD21	71:v:13:THR:HG21	1.86	0.41
52:n:129:PHE:O	52:n:132:THR:OG1	2.37	0.41
52:n:297:HIS:HA	52:n:300:CYS:SG	2.61	0.41
52:n:310:SER:O	52:n:313:LEU:HG	2.21	0.41
52:n:311:GLN:O	52:n:315:LEU:HG	2.20	0.41
52:n:907:LEU:HD21	62:b:118:LEU:CA	2.50	0.41
55:a:161:TYR:C	55:a:163:LEU:N	2.79	0.41
55:a:427:ARG:HE	55:a:427:ARG:HB3	1.50	0.41
56:d:42:ARG:HH22	58:i:93:LYS:CG	2.32	0.41
58:i:104:MET:HE3	58:i:104:MET:HB3	1.84	0.41
60:q:160:LEU:HD23	60:q:160:LEU:HA	1.81	0.41
60:q:495:LEU:HD22	60:q:504:VAL:HG22	2.03	0.41
61:z:543:LEU:HD12	61:z:543:LEU:HA	1.87	0.41
62:b:60:TYR:OH	63:c:70:LEU:O	2.36	0.41
65:l:160:MET:CE	71:v:134:TYR:CD2	3.04	0.41
66:o:697:HIS:HB2	66:o:698:CYS:H	1.78	0.41
67:h:32:LYS:NZ	67:h:40:LEU:HD11	2.36	0.41
68:k:33:LEU:CA	68:k:36:SER:OG	2.63	0.41
72:p:284:LYS:HB3	72:p:356:LEU:HD11	2.03	0.41
72:p:444:VAL:HG22	72:p:452:LEU:HD11	2.02	0.41
72:p:813:THR:OG1	72:p:814:THR:N	2.54	0.41
73:w:727:TRP:HB2	73:w:732:LEU:HD13	2.02	0.41
73:w:844:ASN:HA	73:w:847:ILE:HG22	2.02	0.41
73:w:1200:TYR:HD1	74:x:287:LYS:HD3	1.85	0.41
74:x:303:LEU:HD13	74:x:303:LEU:HA	1.87	0.41
74:x:687:PHE:H	74:x:687:PHE:HD1	1.67	0.41
76:NG:1017:VAL:O	76:NG:1018:SER:CB	2.69	0.41
3:NX:6:DC:H2''	3:NX:7:DC:H5'	2.02	0.41
11:PA:353:ASN:O	11:PA:357:LYS:HG3	2.21	0.41
11:PA:1022:ILE:N	11:PA:1034:GLN:OE1	2.45	0.41
17:PB:647:GLU:O	17:PB:648:TYR:CG	2.74	0.41
18:HC:58:ARG:HD2	32:HE:229:TRP:HE3	1.83	0.41
21:DQ:19:GLU:O	21:DQ:22:ILE:HG12	2.21	0.41
22:PC:62:GLU:OE1	22:PC:62:GLU:N	2.52	0.41
25:PH:136:GLU:O	25:PH:139:SER:OG	2.31	0.41
30:HD:287:TYR:CG	46:HI:189:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:HD:297:LEU:O	30:HD:298:GLN:C	2.61	0.41
34:HH:128:SER:O	34:HH:334:ARG:NH2	2.51	0.41
37:DF:118:ILE:HD12	37:DF:118:ILE:O	2.21	0.41
43:Dj:213:LYS:HA	43:Dj:214:PRO:HD3	1.97	0.41
46:HI:17:PHE:C	46:HI:17:PHE:CD1	2.96	0.41
46:HI:135:HIS:CD2	46:HI:137:ASP:H	2.35	0.41
46:HI:141:ASN:OD1	46:HI:141:ASN:N	2.53	0.41
46:HI:185:PHE:HE2	46:HI:237:TRP:HH2	1.68	0.41
47:HJ:15:SER:N	47:HJ:18:GLN:OE1	2.42	0.41
47:HJ:43:ASN:CG	47:HJ:43:ASN:O	2.63	0.41
48:PD:79:THR:HG22	67:h:51:LEU:HD13	2.02	0.41
50:g:104:LYS:O	50:g:108:LYS:N	2.47	0.41
52:n:136:LEU:HD23	52:n:136:LEU:HA	1.84	0.41
52:n:152:PHE:CE1	56:d:149:ILE:HG23	2.56	0.41
52:n:505:CYS:HB3	52:n:641:LEU:HD21	2.03	0.41
53:s:142:ASN:HB2	53:s:143:PRO:HD2	2.03	0.41
54:u:115:LEU:HD12	56:d:121:LEU:CD1	2.51	0.41
55:a:221:ASN:HB3	55:a:254:ASN:ND2	2.35	0.41
55:a:317:PHE:CD1	55:a:317:PHE:C	2.98	0.41
56:d:79:LEU:HD12	56:d:79:LEU:HA	1.76	0.41
57:f:50:VAL:HG11	57:f:56:THR:HB	2.03	0.41
60:q:188:LEU:CA	71:v:87:ILE:HD11	2.39	0.41
60:q:566:ALA:HB1	60:q:583:ARG:HD3	2.03	0.41
61:z:533:PRO:HB2	61:z:534:GLN:H	1.74	0.41
72:p:738:LEU:HD23	72:p:738:LEU:HA	1.91	0.41
73:w:711:TRP:CD1	73:w:711:TRP:H	2.39	0.41
6:DA:405:VAL:HG23	6:DA:410:TRP:HZ2	1.86	0.40
7:EA:185:GLU:HG3	7:EA:186:PRO:HD3	2.02	0.40
11:PA:375:ILE:HD13	11:PA:669:TYR:CD2	2.55	0.40
11:PA:457:ILE:HD11	11:PA:515:ILE:HG23	2.03	0.40
17:PB:428:ASP:OD1	17:PB:429:PHE:N	2.52	0.40
18:HC:415:GLN:HB3	18:HC:439:ARG:HD3	2.03	0.40
30:HD:84:LYS:CB	30:HD:136:ASN:HD21	2.32	0.40
30:HD:84:LYS:HB3	30:HD:136:ASN:ND2	2.36	0.40
30:HD:85:ARG:NH1	30:HD:140:LEU:N	2.68	0.40
31:HG:115:GLU:N	31:HG:115:GLU:OE1	2.54	0.40
34:HH:340:LEU:CD2	34:HH:491:ALA:HB2	2.51	0.40
37:DF:368:THR:O	37:DF:369:PRO:C	2.64	0.40
39:DH:40:VAL:HG11	43:DJ:130:ILE:HG12	2.03	0.40
39:DH:49:GLY:C	43:DJ:171:LEU:HD13	2.43	0.40
39:DH:111:ALA:CB	43:DJ:119:PHE:CZ	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DL:120:LEU:HD23	41:DL:126:MET:HG3	2.03	0.40
37:Df:402:ARG:HH22	37:Df:403:ILE:HD12	1.85	0.40
40:Di:73:LEU:HB2	41:Dl:105:HIS:CE1	2.56	0.40
46:HI:17:PHE:C	46:HI:17:PHE:HD1	2.30	0.40
46:HI:148:ASN:N	46:HI:148:ASN:OD1	2.54	0.40
47:HJ:158:LEU:HD12	47:HJ:158:LEU:HA	1.88	0.40
52:n:524:ASN:C	52:n:526:SER:H	2.29	0.40
52:n:678:PHE:CZ	60:q:583:ARG:HB2	2.56	0.40
52:n:794:LEU:HA	52:n:797:PHE:HB3	2.02	0.40
52:n:932:GLY:CA	52:n:1179:HIS:NE2	2.82	0.40
53:s:104:LYS:HB2	53:s:106:SER:H	1.87	0.40
55:a:70:LYS:N	58:i:70:HIS:HE1	2.20	0.40
55:a:402:GLY:O	55:a:405:PRO:HD2	2.20	0.40
55:a:462:LEU:HD12	74:x:49:GLN:HB3	1.99	0.40
55:a:498:VAL:CG2	55:a:507:THR:HG22	2.51	0.40
56:d:115:LYS:HE2	56:d:115:LYS:C	2.46	0.40
57:f:16:VAL:CG1	57:f:104:VAL:HA	2.50	0.40
57:f:77:ILE:HG13	57:f:78:LEU:N	2.37	0.40
60:q:35:SER:CB	60:q:42:ARG:HH22	2.30	0.40
67:h:116:GLU:O	67:h:120:GLN:HG2	2.20	0.40
72:p:800:ARG:HA	72:p:800:ARG:HD3	1.91	0.40
73:w:1183:TRP:HE1	73:w:1190:LEU:HD13	1.85	0.40
75:y:131:MET:HE2	75:y:131:MET:HB3	1.99	0.40
76:NC:842:SER:C	76:NC:844:GLY:N	2.79	0.40
11:PA:486:LEU:HB3	11:PA:538:VAL:HG21	2.03	0.40
12:DB:100:GLN:O	12:DB:101:ARG:NH1	2.46	0.40
14:FB:179:ASP:OD1	14:FB:179:ASP:N	2.54	0.40
15:HB:407:ILE:HD12	32:HE:22:TRP:CB	2.51	0.40
17:PB:954:MET:HE3	17:PB:963:PRO:O	2.22	0.40
18:HC:237:LEU:HD21	18:HC:261:PHE:HZ	1.86	0.40
30:HD:268:ARG:H	30:HD:268:ARG:HD3	1.87	0.40
37:DF:350:ASN:O	37:DF:354:ARG:NH1	2.54	0.40
46:HI:195:ASP:O	46:HI:199:VAL:HG23	2.22	0.40
47:HJ:111:LEU:O	47:HJ:115:VAL:HG12	2.21	0.40
48:PD:76:ASN:O	48:PD:79:THR:OG1	2.38	0.40
52:n:227:GLU:H	52:n:227:GLU:HG3	1.65	0.40
52:n:274:ILE:HG13	57:f:181:LEU:HD21	2.02	0.40
52:n:301:LEU:HD23	52:n:301:LEU:HA	1.89	0.40
52:n:731:LEU:HD12	52:n:800:VAL:HG11	2.03	0.40
52:n:793:HIS:HD2	52:n:794:LEU:HG	1.85	0.40
55:a:59:VAL:CG2	56:d:51:SER:HB2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:a:59:VAL:HA	55:a:62:LEU:HB2	2.03	0.40
55:a:336:TYR:CG	55:a:391:THR:HG23	2.57	0.40
60:q:139:GLN:C	60:q:139:GLN:CD	2.89	0.40
65:l:166:LEU:HD22	71:v:123:ILE:HD13	2.04	0.40
68:k:70:LEU:HD22	68:k:70:LEU:HA	1.44	0.40
73:w:213:ARG:HA	73:w:213:ARG:HD3	1.95	0.40
74:x:166:GLU:O	74:x:170:SER:CB	2.70	0.40
75:y:84:CYS:SG	75:y:85:HIS:N	2.94	0.40
3:NX:146:DC:H2''	3:NX:147:DC:C5	2.56	0.40
5:BA:282:ASP:OD1	5:BA:283:VAL:N	2.55	0.40
6:DA:410:TRP:HB3	37:DF:306:PRO:HD3	2.02	0.40
6:DA:470:ILE:H	6:DA:470:ILE:HD12	1.86	0.40
6:DA:1055:VAL:HG13	6:DA:1056:ALA:H	1.85	0.40
11:PA:1137:PRO:HB2	11:PA:1341:VAL:HG13	2.03	0.40
11:PA:1430:CYS:SG	11:PA:1435:THR:HG23	2.61	0.40
11:PA:1436:VAL:HG13	11:PA:1437:ASP:N	2.37	0.40
12:DB:267:HIS:HB3	12:DB:277:LEU:HD11	2.03	0.40
12:DB:294:ILE:HG13	12:DB:295:LEU:H	1.87	0.40
12:DB:463:ARG:HD2	12:DB:515:ILE:HG22	2.03	0.40
14:FB:57:THR:O	14:FB:57:THR:HG23	2.21	0.40
15:HB:422:LEU:HD21	32:HE:224:LEU:HB3	2.02	0.40
17:PB:771:GLU:O	27:PJ:55:LEU:HD21	2.21	0.40
18:HC:62:LEU:O	18:HC:115:ARG:NH2	2.54	0.40
18:HC:124:GLY:H	32:HE:100:LYS:NZ	2.20	0.40
18:HC:384:PRO:HB2	18:HC:387:ILE:HG12	2.03	0.40
19:DO:44:ILE:O	19:DO:48:LEU:HD13	2.21	0.40
29:PL:22:CYS:SG	29:PL:24:THR:OG1	2.69	0.40
30:HD:55:LYS:HG3	49:PG:166:ASP:H	1.78	0.40
30:HD:211:GLN:H	30:HD:211:GLN:HG3	1.72	0.40
34:HH:474:ASP:N	34:HH:474:ASP:OD1	2.54	0.40
37:DF:426:LEU:O	37:DF:429:LYS:HG2	2.21	0.40
39:DH:132:LYS:HE3	39:DH:134:LEU:H	1.86	0.40
36:De:282:LEU:HD23	36:De:282:LEU:HA	1.96	0.40
40:Di:70:ASP:HA	40:Di:73:LEU:HD23	2.03	0.40
46:HI:87:ILE:HD11	47:HJ:148:LEU:HD22	2.04	0.40
52:n:118:ILE:HG12	53:s:83:LEU:HD23	2.03	0.40
52:n:231:GLU:CB	52:n:253:LEU:HD21	2.51	0.40
52:n:552:VAL:HG22	52:n:568:TYR:HD1	1.86	0.40
52:n:634:MET:HE2	60:q:519:GLN:CD	2.45	0.40
52:n:907:LEU:HD23	52:n:907:LEU:HA	1.90	0.40
52:n:944:PHE:CD2	62:b:101:ARG:NH2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:n:957:PRO:HG2	52:n:1210:PHE:CZ	2.25	0.40
52:n:1210:PHE:HD1	52:n:1211:LEU:HD23	1.85	0.40
52:n:1215:ILE:HD12	52:n:1215:ILE:HA	1.94	0.40
55:a:160:LEU:HD12	55:a:214:ARG:HH21	1.80	0.40
55:a:388:LEU:CD2	55:a:447:GLU:HG3	2.46	0.40
56:d:107:ILE:HG12	58:i:132:LEU:HD21	2.03	0.40
57:f:78:LEU:HD21	67:h:81:LEU:HD23	2.04	0.40
60:q:102:LEU:HD13	67:h:29:PHE:HD2	1.85	0.40
60:q:188:LEU:CA	71:v:87:ILE:HD12	2.50	0.40
63:c:214:VAL:HG22	63:c:243:THR:HG23	2.03	0.40
68:k:96:ARG:CG	71:v:116:LEU:HD11	2.51	0.40
74:x:131:LEU:O	74:x:134:CYS:SG	2.79	0.40
74:x:373:LEU:HD23	74:x:373:LEU:HA	1.92	0.40
74:x:901:LEU:HD23	74:x:901:LEU:HA	1.91	0.40
9:HA:345:ARG:NH1	30:HD:1:MET:HG3	2.36	0.40
9:HA:354:PRO:HA	9:HA:416:ILE:HD12	2.02	0.40
11:PA:57:LEU:O	11:PA:261:ARG:NH2	2.54	0.40
11:PA:564:LEU:HD23	11:PA:567:LEU:HD12	2.04	0.40
12:DB:203:LYS:HZ3	12:DB:235:HIS:HB3	1.87	0.40
17:PB:598:VAL:HG22	17:PB:601:VAL:HG23	2.03	0.40
19:DO:32:LEU:HD13	21:DQ:32:ASP:OD2	2.21	0.40
23:PE:2:ASP:OD1	23:PE:4:GLU:N	2.54	0.40
23:PE:17:ILE:HD11	23:PE:135:LEU:HD21	2.03	0.40
34:HH:385:ASP:OD2	34:HH:387:SER:OG	2.29	0.40
37:DF:396:LEU:HA	37:DF:399:GLU:CD	2.46	0.40
42:Dc:105:ASN:OD1	42:Dc:105:ASN:N	2.55	0.40
36:De:256:HIS:O	36:De:257:GLU:HB2	2.21	0.40
47:HJ:106:LEU:HD22	47:HJ:106:LEU:HA	1.72	0.40
55:a:380:ALA:HB3	55:a:444:PRO:HG2	2.04	0.40
55:a:398:PHE:O	55:a:398:PHE:CG	2.74	0.40
56:d:109:GLN:HA	56:d:112:LYS:CE	2.52	0.40
56:d:145:SER:HB3	60:q:9:ILE:HD13	2.04	0.40
56:d:156:SER:HB2	56:d:161:VAL:HG11	2.01	0.40
58:i:110:SER:CB	58:i:111:PRO:CD	3.00	0.40
60:q:154:ALA:HB2	68:k:35:LEU:HD22	2.02	0.40
67:h:18:GLN:HB3	67:h:60:ASN:HD21	1.86	0.40
68:k:19:ARG:HA	68:k:19:ARG:HD3	1.51	0.40
70:t:156:LEU:O	70:t:157:LEU:C	2.64	0.40
72:p:290:MET:HE3	72:p:290:MET:HB2	1.86	0.40
3:NX:136:DC:H6	3:NX:136:DC:H2'	1.77	0.40
7:EA:143:GLN:HG2	49:PG:158:PHE:HZ	0.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:FA:167:ARG:NE	17:PB:307:GLU:OE2	2.46	0.40
9:HA:72:TYR:HE1	9:HA:83:VAL:HG21	1.86	0.40
9:HA:145:GLN:HG2	9:HA:150:THR:HG22	2.03	0.40
11:PA:141:LEU:HD23	11:PA:141:LEU:C	2.47	0.40
11:PA:631:GLU:OE2	11:PA:992:LYS:NZ	2.47	0.40
12:DB:55:PRO:HB3	12:DB:60:LEU:HD22	2.02	0.40
12:DB:560:TYR:CE2	12:DB:581:ILE:HD11	2.57	0.40
15:HB:303:ILE:HG22	15:HB:307:PHE:HE2	1.87	0.40
22:PC:183:ALA:HB3	22:PC:232:ASN:HB3	2.04	0.40
30:HD:83:ASN:H	30:HD:133:ILE:HD11	1.86	0.40
31:HG:318:LEU:HD12	32:HE:272:LEU:CD2	2.51	0.40
32:HE:254:ALA:CB	32:HE:260:ASN:O	2.70	0.40
34:HH:530:ARG:O	34:HH:534:TYR:CD2	2.75	0.40
35:DD:891:ILE:HA	41:DL:104:ARG:NH2	2.35	0.40
36:DE:694:LEU:HD12	36:DE:703:MET:HE1	1.82	0.40
37:DF:277:ALA:O	37:DF:278:LEU:C	2.64	0.40
37:Df:217:SER:H	37:Df:220:GLN:HE21	1.70	0.40
46:HI:96:THR:HB	46:HI:97:ASP:H	1.37	0.40
47:HJ:171:LEU:O	47:HJ:174:LEU:HB2	2.22	0.40
47:HJ:175:LYS:CA	47:HJ:175:LYS:NZ	2.77	0.40
47:HJ:205:LEU:HD23	47:HJ:205:LEU:HA	1.86	0.40
47:HJ:243:THR:O	47:HJ:244:CYS:C	2.65	0.40
49:PG:124:ASN:OD1	67:h:171:GLN:NE2	2.54	0.40
52:n:693:ILE:HD13	52:n:693:ILE:HA	1.97	0.40
52:n:838:VAL:HG23	52:n:838:VAL:O	2.21	0.40
55:a:109:TYR:HE1	55:a:150:PHE:CZ	2.36	0.40
55:a:160:LEU:HD23	55:a:160:LEU:O	2.22	0.40
55:a:211:LEU:HD12	55:a:212:THR:N	2.37	0.40
55:a:228:PRO:CB	55:a:502:MET:HB2	2.40	0.40
57:f:101:ILE:HD11	67:h:105:VAL:CG1	2.42	0.40
57:f:118:ARG:CB	60:q:108:GLU:OE2	2.70	0.40
57:f:142:SER:CB	60:q:183:PHE:CD2	3.04	0.40
59:m:124:GLN:NE2	61:z:590:ARG:HB2	2.35	0.40
60:q:599:ASN:OD1	60:q:599:ASN:C	2.64	0.40
63:c:276:LEU:HD22	63:c:276:LEU:HA	1.83	0.40
63:c:286:LYS:HD2	63:c:286:LYS:HA	1.80	0.40
64:e:71:GLU:O	64:e:75:THR:HG22	2.21	0.40
64:e:136:LEU:HD11	68:k:107:VAL:CG1	2.51	0.40
65:l:36:ILE:O	65:l:40:THR:HG23	2.22	0.40
66:o:689:PHE:CG	66:o:773:LEU:HD13	2.57	0.40
67:h:8:LEU:HG	67:h:69:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:h:33:LEU:HD23	67:h:33:LEU:HA	1.81	0.40
67:h:85:ARG:CA	67:h:99:VAL:HG12	2.45	0.40
70:t:99:LYS:HA	70:t:102:PHE:HB2	2.04	0.40
73:w:786:PRO:HA	73:w:787:PRO:HD3	1.81	0.40
73:w:850:LEU:HD23	73:w:889:LEU:HD13	2.03	0.40
73:w:1062:VAL:HA	73:w:1063:PRO:HD3	1.91	0.40
74:x:102:ASP:HB2	74:x:164:ARG:HE	1.86	0.40
74:x:301:GLU:N	74:x:301:GLU:CD	2.80	0.40
10:NE:733:GLU:O	10:NE:734:ARG:CB	2.70	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	
5	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
6	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	21	58
7	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	24	61
8	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
9	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
10	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	6	31
10	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	6	31
11	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	36	70
12	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
13	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
14	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	24	61
15	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
16	NB	78/103 (76%)	78 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	2	20
17	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
18	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
19	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
20	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
21	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
22	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
23	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
24	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
25	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
26	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
27	PJ	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
28	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
29	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
30	HD	304/309 (98%)	265 (87%)	29 (10%)	10 (3%)	3	21
31	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
32	HE	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
33	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
34	HH	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43	76
35	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	9	41
35	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
36	DE	540/800 (68%)	506 (94%)	32 (6%)	2 (0%)	30	65
36	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
37	DF	404/677 (60%)	377 (93%)	20 (5%)	7 (2%)	7	35
37	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	36	70
38	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
39	DH	207/310 (67%)	191 (92%)	12 (6%)	4 (2%)	6	32
40	DI	118/264 (45%)	113 (96%)	4 (3%)	1 (1%)	16	52
40	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
41	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	1	15
41	DI	105/161 (65%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
43	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
43	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
44	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
45	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
46	HI	297/346 (86%)	265 (89%)	20 (7%)	12 (4%)	2	19
47	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	11	44
48	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
49	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
50	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	12	46
51	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	7	35
52	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	6	32
53	s	91/244 (37%)	81 (89%)	8 (9%)	2 (2%)	5	29
54	u	113/144 (78%)	104 (92%)	5 (4%)	4 (4%)	3	21
55	a	430/1581 (27%)	387 (90%)	38 (9%)	5 (1%)	10	42
56	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	9	41
57	f	163/246 (66%)	150 (92%)	12 (7%)	1 (1%)	21	58
58	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	24
59	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
60	q	543/651 (83%)	486 (90%)	50 (9%)	7 (1%)	9	41
61	z	93/600 (16%)	83 (89%)	7 (8%)	3 (3%)	3	22
62	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	48
63	c	255/311 (82%)	239 (94%)	15 (6%)	1 (0%)	30	65
64	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	31
65	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
66	o	152/788 (19%)	135 (89%)	13 (9%)	4 (3%)	4	26
67	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	18
68	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	6	33
69	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	5	30
70	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	5	30
71	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	p	756/841 (90%)	707 (94%)	47 (6%)	2 (0%)	36	70
73	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	36	70
74	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	21	58
75	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	24	61
76	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	3	23
76	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	3	24
77	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	11	44
77	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	11	44
All	All	22102/36357 (61%)	20863 (94%)	1076 (5%)	163 (1%)	20	54

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	DA	498	PRO
6	DA	1158	SER
10	NA	534	ARG
11	PA	1666	PRO
14	FB	229	HIS
30	HD	215	PRO
30	HD	220	PRO
30	HD	237	PRO
34	HH	62	ARG
35	DD	876	ALA
36	DE	452	ARG
37	DF	68	THR
37	DF	69	SER
37	DF	442	PRO
39	DH	115	GLN
39	DH	141	PRO
41	DL	73	ASN
51	j	31	PRO
52	n	154	ILE
52	n	363	GLU
52	n	1351	PRO
52	n	1355	PRO
55	a	502	MET
56	d	187	LEU
60	q	131	SER
63	c	310	ARG

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Mol	Chain	Res	Type
67	h	100	PHE
67	h	130	ARG
67	h	167	ARG
67	h	168	PRO
70	t	173	PRO
71	v	91	PHE
72	p	705	PRO
74	x	15	LYS
74	x	567	MET
76	NC	841	THR
77	ND	1301	GLY
10	NE	636	LYS
76	NG	1017	VAL
77	NH	1501	GLY
11	PA	1645	PRO
11	PA	1663	SER
30	HD	233	ILE
30	HD	234	SER
35	DD	898	VAL
36	DE	704	VAL
39	DH	129	VAL
41	DL	111	LEU
41	DL	114	LYS
46	HI	96	THR
46	HI	111	PRO
46	HI	192	VAL
46	HI	236	GLN
46	HI	239	ASP
46	HI	310	PRO
52	n	169	LEU
52	n	254	VAL
52	n	1343	PRO
54	u	32	PRO
54	u	76	LEU
55	a	164	PRO
55	a	334	PRO
58	i	108	HIS
58	i	138	LEU
60	q	399	PRO
64	e	146	ILE
66	o	714	ASP
67	h	37	TYR

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Mol	Chain	Res	Type
67	h	131	ILE
70	t	99	LYS
71	v	40	ALA
71	v	41	LYS
71	v	42	ILE
71	v	139	SER
72	p	727	PRO
73	w	1196	CYS
74	x	444	SER
74	x	564	SER
76	NC	843	HIS
30	HD	289	SER
37	DF	321	PRO
46	HI	106	SER
46	HI	277	LEU
47	HJ	237	MET
52	n	150	PRO
52	n	153	ALA
52	n	165	SER
52	n	1237	PRO
53	s	105	LEU
53	s	129	SER
54	u	84	ALA
54	u	123	ALA
55	a	487	LEU
56	d	170	GLY
60	q	91	SER
60	q	458	PRO
66	o	709	LYS
69	r	156	ASN
71	v	38	LYS
73	w	1203	MET
74	x	566	GLU
76	NC	840	THR
37	DF	66	LEU
40	DI	62	LYS
46	HI	264	ALA
47	HJ	286	ALA
51	j	34	GLN
52	n	265	LEU
52	n	1255	PRO
55	a	208	VAL

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Mol	Chain	Res	Type
60	q	127	LEU
60	q	134	ALA
61	z	533	PRO
62	b	100	GLN
64	e	147	ASN
68	k	81	GLY
69	r	113	ASN
70	t	172	ALA
75	y	226	LEU
16	NF	220	LYS
16	NF	301	GLY
76	NG	1042	SER
7	EA	153	ARG
10	NA	438	PRO
30	HD	218	VAL
30	HD	225	THR
30	HD	265	MET
37	DF	64	GLN
37	DF	440	PRO
39	DH	137	GLY
47	HJ	16	GLU
50	g	127	ARG
52	n	264	ALA
52	n	286	GLU
52	n	524	ASN
52	n	1352	PRO
57	f	57	LEU
61	z	540	LEU
66	o	721	LEU
68	k	79	HIS
70	t	129	VAL
73	w	32	ASP
76	NG	1018	SER
6	DA	506	ASP
41	DL	72	PRO
37	Df	411	VAL
46	HI	82	GLY
46	HI	212	PHE
52	n	164	GLY
60	q	89	GLN
67	h	188	GLY
73	w	1194	THR

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Mol	Chain	Res	Type
10	NE	734	ARG
16	NF	219	ARG
61	z	537	PRO
69	r	94	GLY
69	r	153	VAL
52	n	528	HIS
11	PA	1648	PRO
46	HI	186	GLY
66	o	716	PRO
67	h	99	VAL
30	HD	216	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BA	215/268 (80%)	215 (100%)	0	100	100
6	DA	495/1665 (30%)	461 (93%)	34 (7%)	14	37
7	EA	169/373 (45%)	166 (98%)	3 (2%)	51	66
8	FA	121/448 (27%)	121 (100%)	0	100	100
9	HA	624/664 (94%)	623 (100%)	1 (0%)	87	85
11	PA	1302/1749 (74%)	1296 (100%)	6 (0%)	81	81
12	DB	876/1083 (81%)	861 (98%)	15 (2%)	53	67
13	EB	154/261 (59%)	154 (100%)	0	100	100
14	FB	196/218 (90%)	196 (100%)	0	100	100
15	HB	241/484 (50%)	241 (100%)	0	100	100
17	PB	994/1027 (97%)	994 (100%)	0	100	100
18	HC	342/399 (86%)	342 (100%)	0	100	100
19	DO	90/98 (92%)	90 (100%)	0	100	100
20	DP	154/293 (53%)	154 (100%)	0	100	100
21	DQ	105/324 (32%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	PC	234/252 (93%)	234 (100%)	0	100	100
23	PE	191/192 (100%)	190 (100%)	1 (0%)	81	81
24	PF	69/111 (62%)	68 (99%)	1 (1%)	59	70
25	PH	129/131 (98%)	129 (100%)	0	100	100
26	PI	103/112 (92%)	103 (100%)	0	100	100
27	PJ	53/56 (95%)	53 (100%)	0	100	100
28	PK	104/106 (98%)	104 (100%)	0	100	100
29	PL	41/55 (74%)	41 (100%)	0	100	100
30	HD	251/283 (89%)	227 (90%)	24 (10%)	8	26
31	HG	311/352 (88%)	311 (100%)	0	100	100
32	HE	234/272 (86%)	230 (98%)	4 (2%)	53	67
33	HF	59/64 (92%)	59 (100%)	0	100	100
34	HH	536/688 (78%)	533 (99%)	3 (1%)	78	80
35	DD	144/815 (18%)	131 (91%)	13 (9%)	9	29
35	Dd	146/815 (18%)	146 (100%)	0	100	100
36	DE	478/657 (73%)	465 (97%)	13 (3%)	39	60
36	De	475/657 (72%)	473 (100%)	2 (0%)	84	82
37	DF	324/574 (56%)	292 (90%)	32 (10%)	7	25
37	Df	322/574 (56%)	312 (97%)	10 (3%)	35	56
38	DG	133/322 (41%)	125 (94%)	8 (6%)	17	41
39	DH	181/270 (67%)	171 (94%)	10 (6%)	19	43
40	DI	106/235 (45%)	97 (92%)	9 (8%)	10	30
40	Di	107/235 (46%)	106 (99%)	1 (1%)	70	75
41	DL	69/141 (49%)	58 (84%)	11 (16%)	2	13
41	Dl	98/141 (70%)	98 (100%)	0	100	100
42	Dc	113/833 (14%)	111 (98%)	2 (2%)	51	66
43	DJ	79/154 (51%)	77 (98%)	2 (2%)	42	62
43	Dj	83/154 (54%)	83 (100%)	0	100	100
44	Dk	87/182 (48%)	87 (100%)	0	100	100
45	Dm	80/106 (76%)	79 (99%)	1 (1%)	61	71
46	HI	258/298 (87%)	183 (71%)	75 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	HJ	252/296 (85%)	173 (69%)	79 (31%)	0	2
48	PD	118/126 (94%)	116 (98%)	2 (2%)	53	67
49	PG	152/153 (99%)	151 (99%)	1 (1%)	76	78
50	g	102/216 (47%)	94 (92%)	8 (8%)	11	33
51	j	66/124 (53%)	65 (98%)	1 (2%)	57	70
52	n	807/1271 (64%)	785 (97%)	22 (3%)	39	60
53	s	83/208 (40%)	74 (89%)	9 (11%)	6	22
54	u	95/119 (80%)	91 (96%)	4 (4%)	26	49
55	a	393/1391 (28%)	316 (80%)	77 (20%)	1	9
56	d	139/230 (60%)	93 (67%)	46 (33%)	0	2
57	f	149/223 (67%)	131 (88%)	18 (12%)	5	19
58	i	71/133 (53%)	61 (86%)	10 (14%)	3	16
59	m	102/115 (89%)	101 (99%)	1 (1%)	68	75
60	q	491/577 (85%)	405 (82%)	86 (18%)	2	11
61	z	89/512 (17%)	74 (83%)	15 (17%)	2	12
62	b	102/163 (63%)	91 (89%)	11 (11%)	6	22
63	c	238/280 (85%)	225 (94%)	13 (6%)	19	43
64	e	94/152 (62%)	94 (100%)	0	100	100
65	l	116/155 (75%)	116 (100%)	0	100	100
66	o	141/697 (20%)	136 (96%)	5 (4%)	32	54
67	h	161/225 (72%)	125 (78%)	36 (22%)	1	6
68	k	94/98 (96%)	43 (46%)	51 (54%)	0	0
69	r	169/183 (92%)	140 (83%)	29 (17%)	2	12
70	t	166/178 (93%)	124 (75%)	42 (25%)	0	4
71	v	122/173 (70%)	76 (62%)	46 (38%)	0	1
72	p	681/736 (92%)	670 (98%)	11 (2%)	55	68
73	w	1203/1232 (98%)	1198 (100%)	5 (0%)	84	82
74	x	789/864 (91%)	779 (99%)	10 (1%)	61	71
75	y	175/601 (29%)	171 (98%)	4 (2%)	44	64
All	All	19036/30622 (62%)	18113 (95%)	923 (5%)	24	46

All (923) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	DA	353	LEU
6	DA	357	GLU
6	DA	396	LEU
6	DA	397	LEU
6	DA	401	ASN
6	DA	403	LEU
6	DA	404	MET
6	DA	405	VAL
6	DA	470	ILE
6	DA	474	ASP
6	DA	482	ASP
6	DA	484	ILE
6	DA	485	ILE
6	DA	491	MET
6	DA	496	GLU
6	DA	500	LEU
6	DA	502	LEU
6	DA	511	LEU
6	DA	574	TYR
6	DA	639	LEU
6	DA	661	GLU
6	DA	667	THR
6	DA	711	ASP
6	DA	727	THR
6	DA	730	PHE
6	DA	828	GLU
6	DA	925	ASP
6	DA	943	LYS
6	DA	970	ASN
6	DA	1052	ARG
6	DA	1058	HIS
6	DA	1062	TYR
6	DA	1165	LEU
6	DA	1203	GLU
7	EA	106	LYS
7	EA	152	PHE
7	EA	185	GLU
9	HA	572	GLN
11	PA	1643	TYR
11	PA	1646	THR
11	PA	1647	SER
11	PA	1663	SER
11	PA	1678	TYR

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Mol	Chain	Res	Type
11	PA	1794	SER
12	DB	21	GLU
12	DB	71	ARG
12	DB	140	GLU
12	DB	184	ASN
12	DB	262	MET
12	DB	266	THR
12	DB	293	GLU
12	DB	431	LEU
12	DB	559	LYS
12	DB	603	LYS
12	DB	640	VAL
12	DB	746	SER
12	DB	771	VAL
12	DB	818	THR
12	DB	987	LEU
23	PE	79	GLU
24	PF	71	LEU
30	HD	11	THR
30	HD	28	HIS
30	HD	29	THR
30	HD	127	LYS
30	HD	130	LYS
30	HD	131	ASP
30	HD	133	ILE
30	HD	209	GLU
30	HD	210	MET
30	HD	212	LEU
30	HD	251	LEU
30	HD	252	GLN
30	HD	254	GLU
30	HD	263	LEU
30	HD	268	ARG
30	HD	272	LEU
30	HD	275	VAL
30	HD	276	ARG
30	HD	287	TYR
30	HD	288	THR
30	HD	293	CYS
30	HD	295	ARG
30	HD	304	LEU
30	HD	305	PHE

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Mol	Chain	Res	Type
32	HE	62	SER
32	HE	222	SER
32	HE	257	CYS
32	HE	258	HIS
34	HH	62	ARG
34	HH	63	LEU
34	HH	266	GLN
35	DD	873	LEU
35	DD	888	LYS
35	DD	891	ILE
35	DD	894	LEU
35	DD	897	ASP
35	DD	898	VAL
35	DD	924	LYS
35	DD	953	ILE
35	DD	955	LYS
35	DD	958	LYS
35	DD	963	ARG
35	DD	1006	LEU
35	DD	1009	LEU
36	DE	432	LEU
36	DE	433	LYS
36	DE	450	ARG
36	DE	451	VAL
36	DE	507	VAL
36	DE	513	LEU
36	DE	515	LEU
36	DE	519	GLU
36	DE	521	ASP
36	DE	702	LEU
36	DE	745	GLU
36	DE	746	ASP
36	DE	747	LEU
37	DF	55	LEU
37	DF	60	MET
37	DF	62	LYS
37	DF	64	GLN
37	DF	66	LEU
37	DF	111	GLU
37	DF	114	LEU
37	DF	118	ILE
37	DF	120	THR

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Mol	Chain	Res	Type
37	DF	129	VAL
37	DF	209	LYS
37	DF	261	THR
37	DF	269	VAL
37	DF	271	VAL
37	DF	280	ILE
37	DF	295	LEU
37	DF	301	VAL
37	DF	312	ILE
37	DF	317	LEU
37	DF	319	LEU
37	DF	320	ARG
37	DF	335	ARG
37	DF	339	GLN
37	DF	348	THR
37	DF	354	ARG
37	DF	391	LEU
37	DF	397	GLN
37	DF	406	VAL
37	DF	412	LEU
37	DF	415	ILE
37	DF	416	ASP
37	DF	427	LEU
38	DG	41	ASP
38	DG	129	LYS
38	DG	131	ILE
38	DG	143	VAL
38	DG	161	ASP
38	DG	181	TRP
38	DG	182	GLU
38	DG	183	ILE
39	DH	50	PHE
39	DH	116	ARG
39	DH	132	LYS
39	DH	135	THR
39	DH	159	TYR
39	DH	160	ILE
39	DH	161	LYS
39	DH	164	THR
39	DH	167	GLU
39	DH	169	VAL
40	DI	31	TYR

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Mol	Chain	Res	Type
40	DI	32	GLU
40	DI	35	VAL
40	DI	60	HIS
40	DI	63	LYS
40	DI	69	ASP
40	DI	73	LEU
40	DI	82	SER
40	DI	84	THR
41	DL	59	THR
41	DL	60	LYS
41	DL	61	LYS
41	DL	62	LYS
41	DL	63	LEU
41	DL	64	GLN
41	DL	70	VAL
41	DL	87	ILE
41	DL	110	THR
41	DL	111	LEU
41	DL	128	ILE
42	Dc	24	ASP
42	Dc	106	VAL
36	De	546	VAL
36	De	579	VAL
37	Df	215	GLU
37	Df	253	TYR
37	Df	261	THR
37	Df	272	VAL
37	Df	322	ASP
37	Df	323	VAL
37	Df	326	HIS
37	Df	356	THR
37	Df	366	GLU
37	Df	421	ASP
40	Di	73	LEU
45	Dm	31	LEU
46	HI	13	GLU
46	HI	15	LEU
46	HI	20	GLU
46	HI	23	PHE
46	HI	30	ARG
46	HI	32	LYS
46	HI	33	ASN

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Mol	Chain	Res	Type
46	HI	34	THR
46	HI	36	GLN
46	HI	38	VAL
46	HI	45	LEU
46	HI	47	HIS
46	HI	48	ARG
46	HI	52	LYS
46	HI	55	ILE
46	HI	56	ASN
46	HI	57	ARG
46	HI	58	THR
46	HI	60	LEU
46	HI	63	ILE
46	HI	64	LYS
46	HI	66	LEU
46	HI	67	GLN
46	HI	69	LEU
46	HI	74	ILE
46	HI	75	ILE
46	HI	83	HIS
46	HI	84	LYS
46	HI	86	ASN
46	HI	88	SER
46	HI	96	THR
46	HI	101	ILE
46	HI	102	ILE
46	HI	107	LEU
46	HI	108	VAL
46	HI	115	LYS
46	HI	125	LEU
46	HI	131	HIS
46	HI	132	TRP
46	HI	139	LYS
46	HI	141	ASN
46	HI	143	LEU
46	HI	153	LEU
46	HI	160	LYS
46	HI	162	PHE
46	HI	164	SER
46	HI	169	TYR
46	HI	170	THR
46	HI	174	VAL

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Mol	Chain	Res	Type
46	HI	177	TRP
46	HI	189	MET
46	HI	205	GLU
46	HI	206	LEU
46	HI	209	ARG
46	HI	210	VAL
46	HI	213	LEU
46	HI	225	ILE
46	HI	237	TRP
46	HI	241	CYS
46	HI	245	ASP
46	HI	249	PHE
46	HI	257	LEU
46	HI	258	HIS
46	HI	259	HIS
46	HI	260	ILE
46	HI	261	PHE
46	HI	267	ASP
46	HI	268	LEU
46	HI	272	ILE
46	HI	276	PHE
46	HI	280	PRO
46	HI	284	ILE
46	HI	285	THR
46	HI	288	GLN
46	HI	292	MET
47	HJ	3	HIS
47	HJ	7	GLN
47	HJ	8	LYS
47	HJ	10	HIS
47	HJ	11	TRP
47	HJ	12	THR
47	HJ	14	SER
47	HJ	15	SER
47	HJ	21	ARG
47	HJ	28	ARG
47	HJ	32	CYS
47	HJ	33	LYS
47	HJ	37	ASN
47	HJ	41	LEU
47	HJ	44	ASP
47	HJ	55	THR

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Mol	Chain	Res	Type
47	HJ	56	LEU
47	HJ	60	TYR
47	HJ	65	LEU
47	HJ	84	CYS
47	HJ	85	MET
47	HJ	92	LEU
47	HJ	93	ASN
47	HJ	94	ASN
47	HJ	96	VAL
47	HJ	97	MET
47	HJ	98	GLU
47	HJ	102	ARG
47	HJ	104	ILE
47	HJ	106	LEU
47	HJ	107	THR
47	HJ	108	CYS
47	HJ	111	LEU
47	HJ	113	CYS
47	HJ	114	LYS
47	HJ	115	VAL
47	HJ	129	LEU
47	HJ	134	LEU
47	HJ	136	GLN
47	HJ	140	LEU
47	HJ	141	GLU
47	HJ	143	ILE
47	HJ	145	GLU
47	HJ	148	LEU
47	HJ	149	LEU
47	HJ	150	LEU
47	HJ	151	ILE
47	HJ	153	GLN
47	HJ	154	LEU
47	HJ	158	LEU
47	HJ	160	VAL
47	HJ	165	ARG
47	HJ	166	PRO
47	HJ	171	LEU
47	HJ	172	ILE
47	HJ	174	LEU
47	HJ	175	LYS
47	HJ	180	ILE

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Mol	Chain	Res	Type
47	HJ	181	LEU
47	HJ	182	GLU
47	HJ	186	ILE
47	HJ	189	LYS
47	HJ	192	ASP
47	HJ	200	LEU
47	HJ	208	THR
47	HJ	211	GLN
47	HJ	226	ILE
47	HJ	227	THR
47	HJ	229	GLU
47	HJ	231	TYR
47	HJ	232	LEU
47	HJ	239	LYS
47	HJ	245	LEU
47	HJ	252	MET
47	HJ	262	TYR
47	HJ	266	ARG
47	HJ	277	LEU
47	HJ	279	ARG
47	HJ	288	ASN
48	PD	134	ILE
48	PD	137	LYS
49	PG	59	ILE
50	g	72	PHE
50	g	126	TYR
50	g	130	GLN
50	g	137	VAL
50	g	143	LYS
50	g	159	ARG
50	g	166	ASN
50	g	171	LEU
51	j	82	LYS
52	n	154	ILE
52	n	159	ASP
52	n	166	TYR
52	n	168	ARG
52	n	169	LEU
52	n	212	LEU
52	n	226	VAL
52	n	227	GLU
52	n	252	ILE

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Mol	Chain	Res	Type
52	n	253	LEU
52	n	254	VAL
52	n	255	GLU
52	n	261	ASP
52	n	265	LEU
52	n	266	VAL
52	n	267	HIS
52	n	283	PHE
52	n	289	LEU
52	n	363	GLU
52	n	371	GLN
52	n	528	HIS
52	n	589	GLN
53	s	90	GLU
53	s	93	TYR
53	s	105	LEU
53	s	109	LEU
53	s	112	LEU
53	s	116	ILE
53	s	127	LEU
53	s	131	ILE
53	s	137	LEU
54	u	49	ASN
54	u	73	ILE
54	u	76	LEU
54	u	79	GLU
55	a	58	LEU
55	a	62	LEU
55	a	64	THR
55	a	66	GLN
55	a	70	LYS
55	a	71	VAL
55	a	72	THR
55	a	74	LEU
55	a	77	MET
55	a	78	THR
55	a	80	ARG
55	a	82	GLU
55	a	83	SER
55	a	86	ARG
55	a	87	GLN
55	a	93	HIS

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Mol	Chain	Res	Type
55	a	106	ASP
55	a	107	MET
55	a	108	PHE
55	a	109	TYR
55	a	111	GLU
55	a	128	HIS
55	a	131	ASN
55	a	133	VAL
55	a	135	CYS
55	a	145	LYS
55	a	148	ASP
55	a	160	LEU
55	a	162	ASN
55	a	167	ASN
55	a	168	LYS
55	a	173	MET
55	a	201	ASP
55	a	214	ARG
55	a	226	VAL
55	a	232	LEU
55	a	246	ASN
55	a	253	MET
55	a	254	ASN
55	a	258	THR
55	a	259	ILE
55	a	267	LYS
55	a	278	HIS
55	a	297	VAL
55	a	305	LEU
55	a	309	GLN
55	a	324	CYS
55	a	325	THR
55	a	327	ILE
55	a	329	LEU
55	a	332	THR
55	a	333	GLN
55	a	335	THR
55	a	339	LEU
55	a	348	LEU
55	a	357	LEU
55	a	367	LEU
55	a	373	CYS

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Mol	Chain	Res	Type
55	a	376	LEU
55	a	384	ASP
55	a	388	LEU
55	a	391	THR
55	a	400	HIS
55	a	414	GLN
55	a	421	ILE
55	a	427	ARG
55	a	430	LEU
55	a	432	GLU
55	a	433	ASP
55	a	437	LEU
55	a	438	LEU
55	a	441	GLU
55	a	443	CYS
55	a	501	CYS
55	a	502	MET
55	a	504	ILE
55	a	509	ARG
56	d	28	GLU
56	d	30	LEU
56	d	51	SER
56	d	62	GLU
56	d	63	ASN
56	d	64	GLN
56	d	66	LEU
56	d	67	GLU
56	d	69	LEU
56	d	70	ILE
56	d	71	HIS
56	d	72	ARG
56	d	73	ASP
56	d	78	GLU
56	d	79	LEU
56	d	80	MET
56	d	81	LYS
56	d	82	LEU
56	d	85	ASN
56	d	92	GLU
56	d	93	MET
56	d	98	LYS
56	d	101	GLU

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Mol	Chain	Res	Type
56	d	106	ASP
56	d	107	ILE
56	d	108	GLN
56	d	110	LEU
56	d	114	LEU
56	d	115	LYS
56	d	116	GLU
56	d	119	GLN
56	d	121	LEU
56	d	126	TYR
56	d	127	GLN
56	d	129	LYS
56	d	130	GLU
56	d	131	LYS
56	d	132	LEU
56	d	133	LYS
56	d	135	ILE
56	d	173	ARG
56	d	181	GLU
56	d	184	SER
56	d	186	LEU
56	d	187	LEU
56	d	189	GLN
57	f	16	VAL
57	f	19	SER
57	f	20	TRP
57	f	24	LEU
57	f	30	LEU
57	f	41	TYR
57	f	49	VAL
57	f	50	VAL
57	f	56	THR
57	f	57	LEU
57	f	60	LEU
57	f	63	MET
57	f	64	VAL
57	f	66	ILE
57	f	114	VAL
57	f	117	SER
57	f	120	LEU
57	f	192	PHE
58	i	86	ASP

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Mol	Chain	Res	Type
58	i	87	LEU
58	i	88	ASN
58	i	90	LEU
58	i	95	GLN
58	i	100	LEU
58	i	112	GLU
58	i	122	ARG
58	i	136	LYS
58	i	140	MET
59	m	59	LYS
60	q	1	MET
60	q	2	SER
60	q	7	VAL
60	q	16	GLU
60	q	19	VAL
60	q	22	VAL
60	q	28	GLU
60	q	29	THR
60	q	31	LEU
60	q	34	LEU
60	q	36	MET
60	q	91	SER
60	q	92	LEU
60	q	93	TRP
60	q	95	TRP
60	q	98	VAL
60	q	100	ASN
60	q	103	ARG
60	q	107	THR
60	q	109	MET
60	q	110	CYS
60	q	111	VAL
60	q	112	LEU
60	q	115	VAL
60	q	116	LEU
60	q	118	ILE
60	q	120	ARG
60	q	122	LYS
60	q	123	LYS
60	q	124	PHE
60	q	125	MET
60	q	128	ASP

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Mol	Chain	Res	Type
60	q	130	VAL
60	q	131	SER
60	q	132	GLN
60	q	133	ASP
60	q	135	LEU
60	q	138	LYS
60	q	139	GLN
60	q	143	THR
60	q	144	LEU
60	q	145	GLN
60	q	146	LEU
60	q	147	ILE
60	q	149	LYS
60	q	153	LEU
60	q	159	ILE
60	q	161	LEU
60	q	165	GLU
60	q	166	ARG
60	q	168	THR
60	q	169	LYS
60	q	171	VAL
60	q	172	THR
60	q	184	ASN
60	q	185	SER
60	q	187	LEU
60	q	188	LEU
60	q	226	LYS
60	q	262	GLN
60	q	263	LYS
60	q	264	GLN
60	q	290	HIS
60	q	400	PHE
60	q	425	GLU
60	q	428	LEU
60	q	430	LYS
60	q	431	ILE
60	q	432	ILE
60	q	434	GLN
60	q	438	ILE
60	q	440	LEU
60	q	441	ARG
60	q	442	SER

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Mol	Chain	Res	Type
60	q	443	ARG
60	q	447	THR
60	q	448	ILE
60	q	451	LEU
60	q	518	GLU
60	q	629	LYS
60	q	631	GLU
60	q	634	ASN
60	q	646	LEU
60	q	647	SER
60	q	649	CYS
60	q	651	LEU
61	z	492	ARG
61	z	528	LEU
61	z	530	VAL
61	z	540	LEU
61	z	551	ASP
61	z	564	ASN
61	z	567	GLN
61	z	572	ASN
61	z	579	CYS
61	z	582	LEU
61	z	585	HIS
61	z	591	LEU
61	z	594	LEU
61	z	598	CYS
61	z	599	LEU
62	b	57	VAL
62	b	74	LEU
62	b	82	LEU
62	b	92	GLN
62	b	99	ILE
62	b	103	ASP
62	b	122	LEU
62	b	126	CYS
62	b	127	LEU
62	b	132	ASP
62	b	168	ILE
63	c	36	LYS
63	c	44	THR
63	c	45	LEU
63	c	72	ARG

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Mol	Chain	Res	Type
63	c	73	LEU
63	c	77	VAL
63	c	274	ILE
63	c	275	LYS
63	c	276	LEU
63	c	286	LYS
63	c	295	THR
63	c	300	ARG
63	c	301	THR
66	o	635	ASN
66	o	697	HIS
66	o	704	VAL
66	o	715	LEU
66	o	721	LEU
67	h	7	GLN
67	h	15	LEU
67	h	16	LEU
67	h	17	SER
67	h	18	GLN
67	h	19	VAL
67	h	22	LEU
67	h	23	LYS
67	h	30	ILE
67	h	32	LYS
67	h	33	LEU
67	h	34	GLU
67	h	37	TYR
67	h	39	ARG
67	h	40	LEU
67	h	49	PHE
67	h	66	GLU
67	h	75	VAL
67	h	76	ILE
67	h	77	ILE
67	h	79	LEU
67	h	100	PHE
67	h	101	SER
67	h	102	HIS
67	h	110	ARG
67	h	111	THR
67	h	112	LYS
67	h	117	VAL

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Mol	Chain	Res	Type
67	h	130	ARG
67	h	131	ILE
67	h	143	LEU
67	h	170	LYS
67	h	185	VAL
67	h	187	PHE
67	h	189	LYS
67	h	192	SER
68	k	8	ASN
68	k	10	ARG
68	k	11	LEU
68	k	12	ARG
68	k	14	LEU
68	k	15	GLU
68	k	18	GLU
68	k	19	ARG
68	k	21	ILE
68	k	25	LEU
68	k	26	GLN
68	k	32	ILE
68	k	33	LEU
68	k	34	GLU
68	k	35	LEU
68	k	36	SER
68	k	37	LYS
68	k	40	THR
68	k	42	GLU
68	k	43	ARG
68	k	44	LEU
68	k	45	LEU
68	k	48	GLN
68	k	53	THR
68	k	56	VAL
68	k	57	GLN
68	k	58	HIS
68	k	60	GLU
68	k	64	SER
68	k	67	ILE
68	k	70	LEU
68	k	72	GLN
68	k	73	VAL
68	k	82	SER

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Mol	Chain	Res	Type
68	k	83	SER
68	k	86	SER
68	k	87	ARG
68	k	88	LYS
68	k	90	CYS
68	k	91	GLN
68	k	92	MET
68	k	94	LEU
68	k	96	ARG
68	k	97	VAL
68	k	101	ARG
68	k	102	LEU
68	k	103	LYS
68	k	104	LEU
68	k	107	VAL
68	k	109	ARG
68	k	114	MET
69	r	16	ILE
69	r	17	ASN
69	r	18	MET
69	r	32	LEU
69	r	35	LEU
69	r	42	LEU
69	r	47	GLU
69	r	49	GLU
69	r	53	ASP
69	r	56	MET
69	r	60	LEU
69	r	73	ARG
69	r	85	LEU
69	r	88	LEU
69	r	93	MET
69	r	101	LEU
69	r	107	ASP
69	r	124	ARG
69	r	143	ILE
69	r	152	LEU
69	r	156	ASN
69	r	168	LEU
69	r	179	GLN
69	r	187	LYS
69	r	197	VAL

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Mol	Chain	Res	Type
69	r	200	GLU
69	r	201	LYS
69	r	202	ILE
69	r	206	ARG
70	t	1	MET
70	t	9	MET
70	t	16	SER
70	t	17	VAL
70	t	21	VAL
70	t	23	LEU
70	t	24	LEU
70	t	28	LEU
70	t	34	GLU
70	t	43	CYS
70	t	47	HIS
70	t	61	LYS
70	t	62	LEU
70	t	66	MET
70	t	67	HIS
70	t	70	GLU
70	t	78	LEU
70	t	79	PHE
70	t	80	GLU
70	t	81	ASN
70	t	84	CYS
70	t	85	LEU
70	t	98	LEU
70	t	99	LYS
70	t	101	PHE
70	t	103	GLN
70	t	106	LYS
70	t	109	LYS
70	t	110	ILE
70	t	124	VAL
70	t	138	ILE
70	t	148	VAL
70	t	149	VAL
70	t	156	LEU
70	t	162	GLN
70	t	173	PRO
70	t	179	ARG
70	t	183	VAL

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Mol	Chain	Res	Type
70	t	193	TYR
70	t	196	LEU
70	t	200	ILE
70	t	204	GLN
71	v	14	LEU
71	v	15	LEU
71	v	22	LEU
71	v	26	ILE
71	v	37	ILE
71	v	38	LYS
71	v	39	THR
71	v	41	LYS
71	v	43	GLU
71	v	45	GLU
71	v	47	GLN
71	v	50	ARG
71	v	52	THR
71	v	55	GLU
71	v	56	GLN
71	v	58	ASN
71	v	60	GLU
71	v	61	MET
71	v	62	HIS
71	v	63	VAL
71	v	69	VAL
71	v	81	ASP
71	v	82	LEU
71	v	86	LEU
71	v	87	ILE
71	v	88	LEU
71	v	98	ILE
71	v	103	GLN
71	v	105	LEU
71	v	108	LEU
71	v	110	GLU
71	v	112	CYS
71	v	114	ARG
71	v	115	LYS
71	v	116	LEU
71	v	117	ILE
71	v	118	THR
71	v	119	LEU

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Mol	Chain	Res	Type
71	v	120	ARG
71	v	123	ILE
71	v	125	ILE
71	v	130	LEU
71	v	131	GLU
71	v	132	GLU
71	v	133	GLU
71	v	138	SER
72	p	13	MET
72	p	162	VAL
72	p	170	LEU
72	p	228	VAL
72	p	289	ASP
72	p	401	THR
72	p	443	LEU
72	p	564	LEU
72	p	677	THR
72	p	699	CYS
72	p	726	ILE
73	w	205	VAL
73	w	723	THR
73	w	726	ASN
73	w	1130	VAL
73	w	1134	GLN
74	x	4	VAL
74	x	11	LEU
74	x	52	ILE
74	x	118	ILE
74	x	239	THR
74	x	300	THR
74	x	443	LEU
74	x	477	TYR
74	x	803	ASP
74	x	897	LEU
75	y	194	LEU
75	y	220	MET
75	y	224	ARG
75	y	226	LEU
43	DJ	192	LYS
43	DJ	194	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (361) such sidechains are listed below:

Mol	Chain	Res	Type
5	BA	116	ASN
5	BA	139	ASN
6	DA	401	ASN
6	DA	407	GLN
6	DA	409	HIS
6	DA	630	GLN
6	DA	702	ASN
6	DA	755	HIS
6	DA	802	HIS
6	DA	860	ASN
6	DA	896	GLN
6	DA	1073	GLN
7	EA	142	ASN
7	EA	181	ASN
9	HA	201	HIS
9	HA	645	GLN
11	PA	700	GLN
11	PA	731	ASN
11	PA	905	ASN
11	PA	1078	GLN
11	PA	1310	HIS
12	DB	30	HIS
12	DB	36	ASN
12	DB	123	ASN
12	DB	137	HIS
12	DB	160	HIS
12	DB	176	HIS
12	DB	183	GLN
12	DB	235	HIS
12	DB	272	GLN
12	DB	348	GLN
12	DB	432	HIS
12	DB	439	HIS
12	DB	450	GLN
12	DB	509	ASN
12	DB	577	HIS
12	DB	644	GLN
12	DB	652	GLN
12	DB	663	GLN
12	DB	750	GLN
12	DB	813	ASN
12	DB	864	ASN
12	DB	908	GLN

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Mol	Chain	Res	Type
12	DB	912	ASN
12	DB	963	HIS
13	EB	126	ASN
13	EB	188	GLN
13	EB	217	GLN
14	FB	64	ASN
14	FB	152	ASN
14	FB	229	HIS
15	HB	420	GLN
15	HB	537	HIS
17	PB	90	GLN
17	PB	145	GLN
17	PB	420	GLN
17	PB	582	GLN
17	PB	631	GLN
17	PB	913	GLN
17	PB	1101	GLN
18	HC	211	GLN
18	HC	218	GLN
18	HC	390	GLN
18	HC	415	GLN
19	DO	35	GLN
19	DO	77	ASN
20	DP	229	GLN
20	DP	278	GLN
21	DQ	343	HIS
22	PC	66	HIS
22	PC	260	GLN
22	PC	265	HIS
23	PE	92	GLN
26	PI	91	HIS
26	PI	98	GLN
28	PK	55	GLN
30	HD	45	ASN
30	HD	129	ASN
30	HD	136	ASN
30	HD	249	GLN
30	HD	298	GLN
31	HG	227	HIS
31	HG	293	GLN
31	HG	317	HIS
32	HE	9	ASN

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Mol	Chain	Res	Type
33	HF	36	GLN
33	HF	51	ASN
34	HH	498	ASN
34	HH	598	HIS
35	DD	875	GLN
35	DD	912	ASN
35	DD	936	GLN
35	DD	1075	HIS
36	DE	254	ASN
36	DE	268	HIS
36	DE	290	HIS
36	DE	326	ASN
36	DE	327	ASN
36	DE	351	GLN
36	DE	509	GLN
36	DE	573	GLN
36	DE	616	HIS
36	DE	636	HIS
36	DE	640	ASN
36	DE	733	ASN
37	DF	37	GLN
37	DF	119	ASN
37	DF	214	HIS
37	DF	270	ASN
37	DF	273	GLN
37	DF	275	ASN
37	DF	316	GLN
37	DF	326	HIS
38	DG	10	HIS
38	DG	48	HIS
38	DG	142	ASN
39	DH	145	HIS
40	DI	21	GLN
40	DI	38	GLN
40	DI	81	GLN
40	DI	98	GLN
41	DL	73	ASN
41	DL	86	GLN
41	DL	117	GLN
41	DL	123	GLN
42	Dc	19	GLN
42	Dc	27	GLN

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Mol	Chain	Res	Type
42	Dc	50	HIS
35	Dd	912	ASN
36	De	223	HIS
36	De	256	HIS
36	De	320	HIS
36	De	368	ASN
36	De	420	ASN
36	De	424	GLN
36	De	660	ASN
36	De	733	ASN
37	Df	30	GLN
37	Df	37	GLN
37	Df	119	ASN
37	Df	134	HIS
37	Df	325	ASN
40	Di	38	GLN
44	Dk	186	HIS
44	Dk	205	HIS
41	Dl	73	ASN
41	Dl	105	HIS
41	Dl	119	HIS
45	Dm	107	ASN
46	HI	56	ASN
46	HI	67	GLN
46	HI	83	HIS
46	HI	135	HIS
46	HI	166	ASN
47	HJ	7	GLN
47	HJ	10	HIS
47	HJ	37	ASN
47	HJ	100	HIS
47	HJ	211	GLN
47	HJ	275	GLN
47	HJ	288	ASN
48	PD	38	HIS
48	PD	66	ASN
49	PG	28	GLN
49	PG	124	ASN
50	g	120	HIS
50	g	130	GLN
51	j	92	ASN
52	n	201	HIS

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Mol	Chain	Res	Type
52	n	211	GLN
52	n	267	HIS
52	n	330	HIS
52	n	410	HIS
52	n	411	GLN
52	n	459	HIS
52	n	494	GLN
52	n	507	GLN
52	n	532	ASN
52	n	668	HIS
52	n	669	GLN
52	n	672	GLN
52	n	698	GLN
52	n	716	ASN
52	n	825	ASN
52	n	841	ASN
52	n	848	HIS
52	n	880	ASN
52	n	883	ASN
52	n	909	GLN
52	n	1225	GLN
53	s	82	ASN
54	u	27	GLN
54	u	49	ASN
54	u	56	GLN
54	u	86	GLN
54	u	97	ASN
55	a	57	HIS
55	a	87	GLN
55	a	131	ASN
55	a	146	ASN
55	a	221	ASN
55	a	243	HIS
55	a	254	ASN
55	a	333	GLN
55	a	359	HIS
55	a	370	GLN
55	a	377	ASN
55	a	399	GLN
55	a	413	HIS
55	a	459	ASN
56	d	63	ASN

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Mol	Chain	Res	Type
56	d	64	GLN
56	d	71	HIS
56	d	85	ASN
56	d	90	HIS
56	d	94	GLN
56	d	111	GLN
56	d	113	GLN
56	d	119	GLN
56	d	127	GLN
56	d	189	GLN
56	d	191	ASN
57	f	84	GLN
57	f	107	GLN
57	f	127	GLN
58	i	70	HIS
58	i	85	GLN
58	i	108	HIS
58	i	113	GLN
58	i	117	GLN
59	m	35	ASN
59	m	80	GLN
59	m	106	GLN
59	m	116	GLN
60	q	139	GLN
60	q	142	GLN
60	q	262	GLN
60	q	310	GLN
60	q	321	GLN
60	q	334	GLN
60	q	347	HIS
60	q	402	HIS
60	q	411	GLN
60	q	434	GLN
60	q	437	HIS
60	q	461	GLN
60	q	463	HIS
60	q	492	GLN
60	q	496	ASN
60	q	506	HIS
60	q	533	GLN
60	q	539	GLN
60	q	547	GLN

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Mol	Chain	Res	Type
60	q	565	ASN
60	q	595	GLN
60	q	611	GLN
60	q	626	GLN
61	z	483	ASN
61	z	527	GLN
61	z	549	GLN
61	z	567	GLN
61	z	585	HIS
61	z	592	ASN
62	b	66	GLN
62	b	87	ASN
62	b	129	GLN
62	b	136	HIS
63	c	10	ASN
63	c	41	ASN
63	c	64	ASN
63	c	160	GLN
63	c	237	GLN
63	c	245	HIS
64	e	97	GLN
64	e	132	HIS
65	l	102	ASN
66	o	692	ASN
66	o	701	ASN
66	o	746	ASN
66	o	753	HIS
67	h	18	GLN
67	h	60	ASN
67	h	102	HIS
67	h	123	GLN
67	h	169	ASN
67	h	171	GLN
68	k	66	GLN
68	k	77	GLN
68	k	79	HIS
68	k	91	GLN
69	r	156	ASN
70	t	8	GLN
70	t	103	GLN
70	t	178	ASN
70	t	180	HIS

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Mol	Chain	Res	Type
70	t	204	GLN
71	v	16	GLN
71	v	32	ASN
71	v	62	HIS
71	v	103	GLN
72	p	63	HIS
72	p	225	ASN
72	p	272	ASN
72	p	400	GLN
72	p	435	GLN
72	p	570	ASN
72	p	598	ASN
72	p	619	GLN
72	p	683	GLN
72	p	723	GLN
72	p	751	GLN
72	p	781	HIS
73	w	158	GLN
73	w	203	ASN
73	w	239	ASN
73	w	295	GLN
73	w	357	HIS
73	w	358	GLN
73	w	378	GLN
73	w	385	GLN
73	w	421	HIS
73	w	433	ASN
73	w	438	ASN
73	w	513	ASN
73	w	596	HIS
73	w	616	GLN
73	w	618	HIS
73	w	638	GLN
73	w	726	ASN
73	w	822	HIS
73	w	841	GLN
73	w	851	ASN
73	w	874	HIS
73	w	923	ASN
73	w	972	HIS
73	w	1037	ASN
73	w	1040	GLN

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Mol	Chain	Res	Type
73	w	1059	ASN
73	w	1124	ASN
73	w	1320	ASN
74	x	8	GLN
74	x	49	GLN
74	x	179	HIS
74	x	214	GLN
74	x	217	GLN
74	x	356	ASN
74	x	361	ASN
74	x	380	ASN
74	x	402	ASN
74	x	404	GLN
74	x	472	ASN
74	x	502	HIS
74	x	544	HIS
74	x	737	HIS
74	x	799	HIS
75	y	72	ASN
75	y	85	HIS
75	y	134	GLN
75	y	179	HIS
43	DJ	160	GLN
43	DJ	173	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 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	$\# Z > 2$
79	SF4	HA	1000	9	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
79	SF4	HA	1000	9	-	-	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.

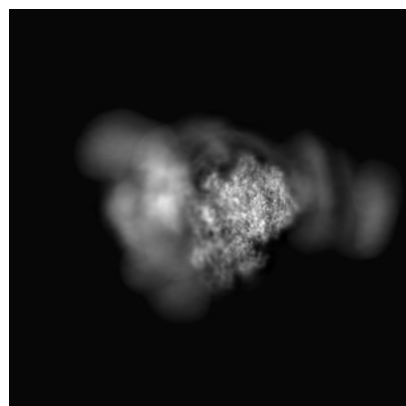
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34360. These allow visual inspection of the internal detail of the map and identification of artifacts.

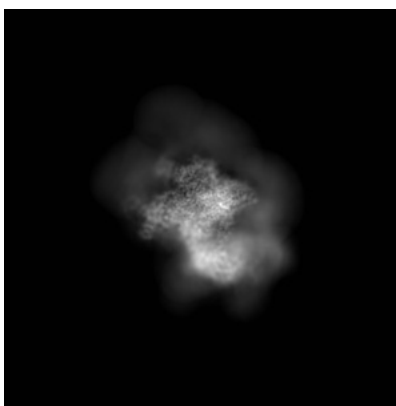
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

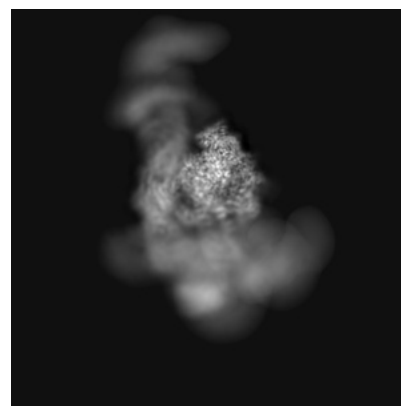
6.1.1 Primary map



X

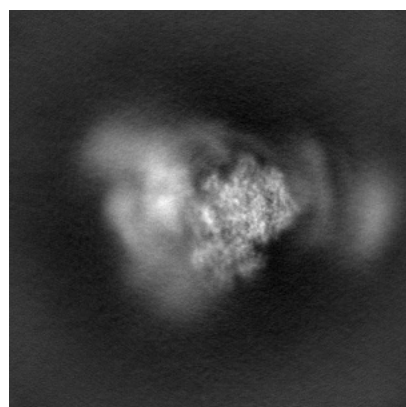


Y

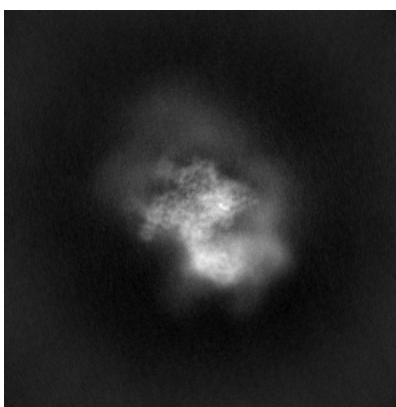


Z

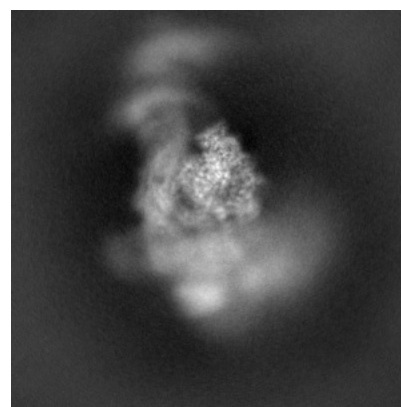
6.1.2 Raw map



X



Y

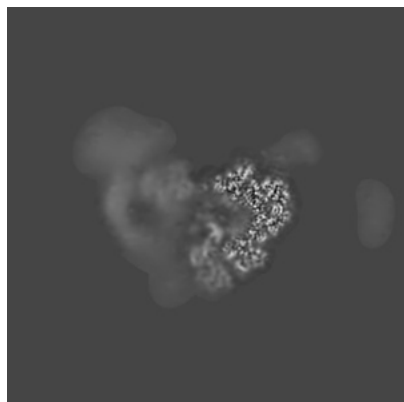


Z

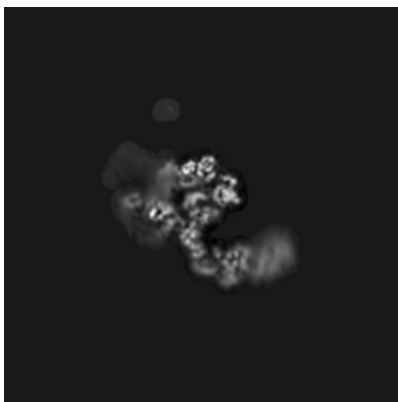
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

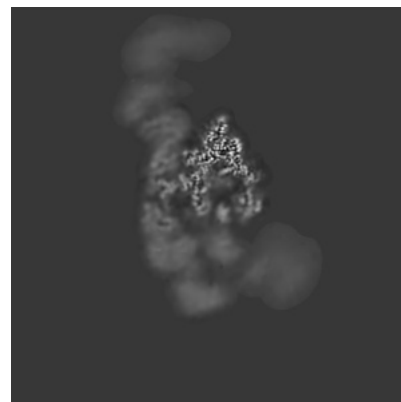
6.2.1 Primary map



X Index: 210

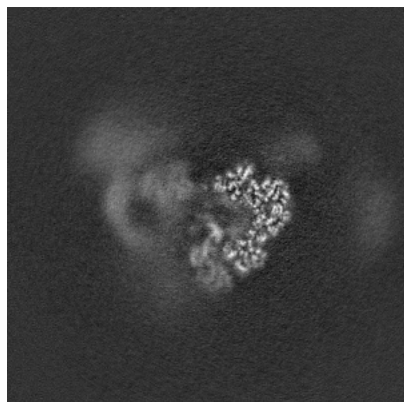


Y Index: 210

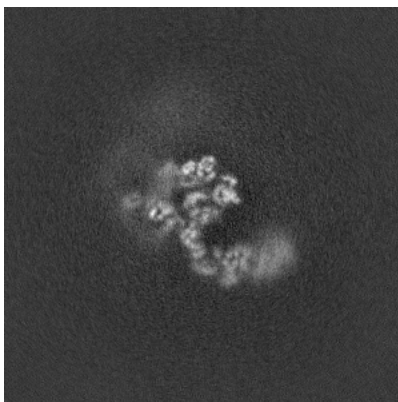


Z Index: 210

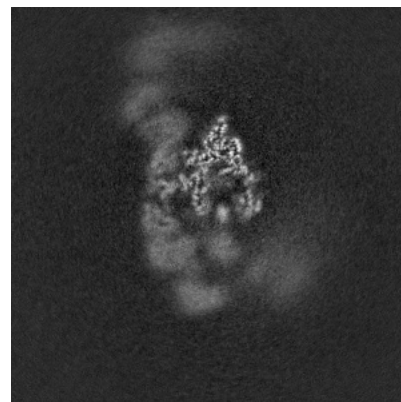
6.2.2 Raw map



X Index: 210



Y Index: 210

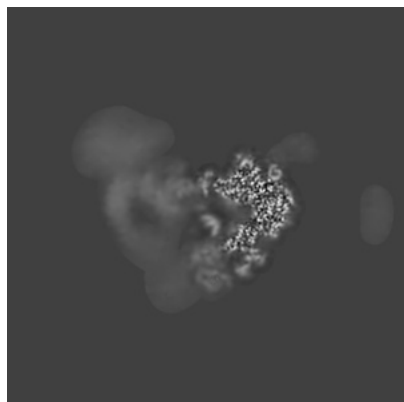


Z Index: 210

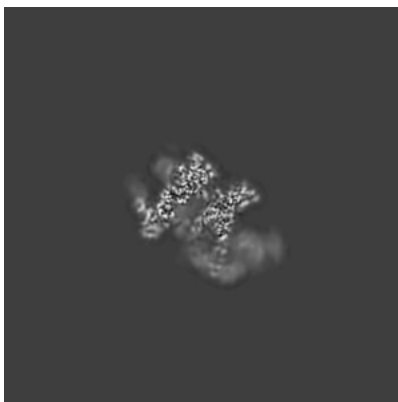
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

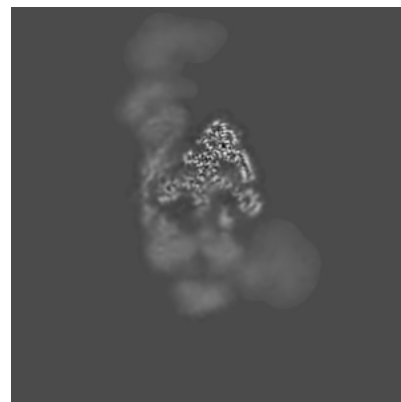
6.3.1 Primary map



X Index: 215

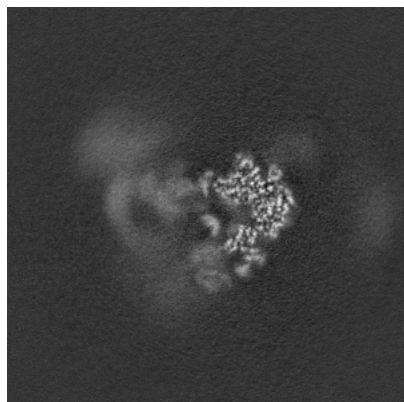


Y Index: 246

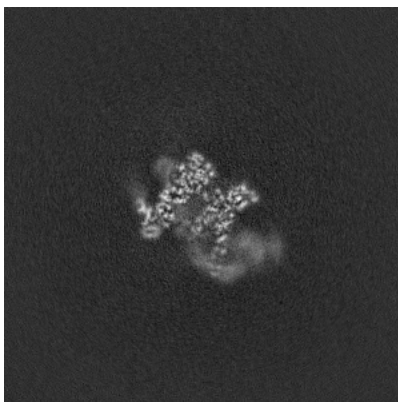


Z Index: 217

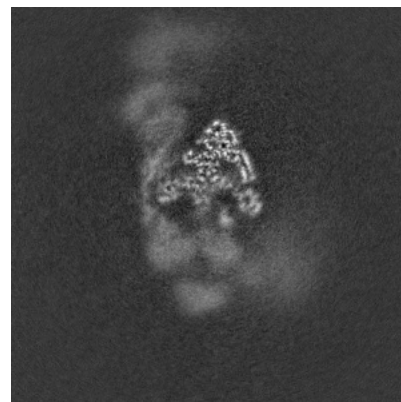
6.3.2 Raw map



X Index: 215



Y Index: 245

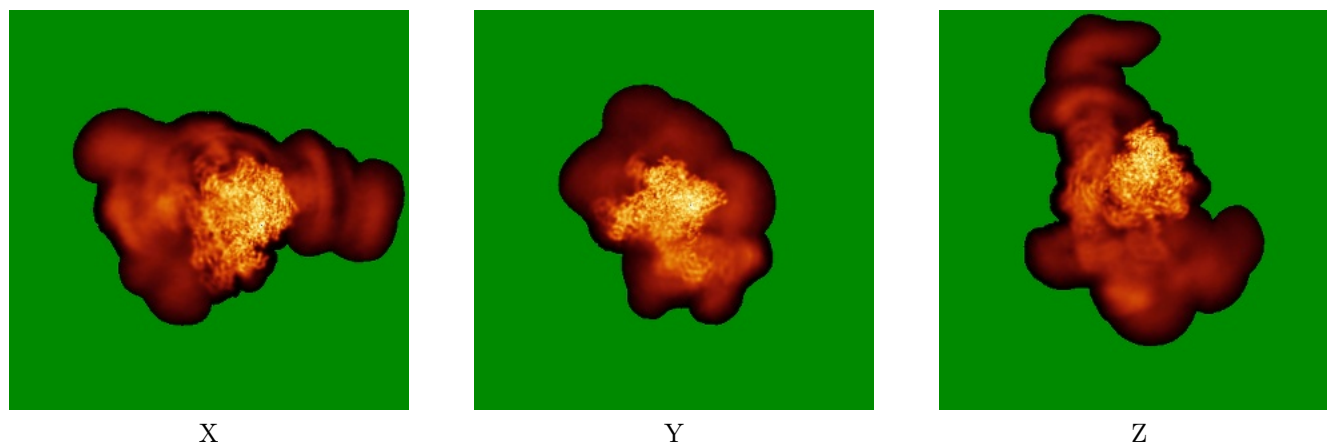


Z Index: 217

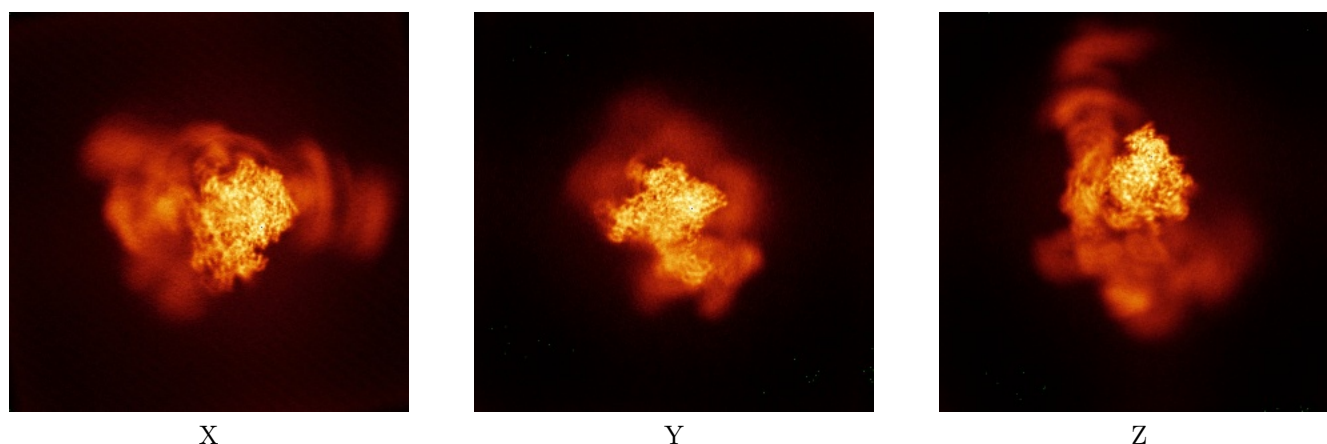
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

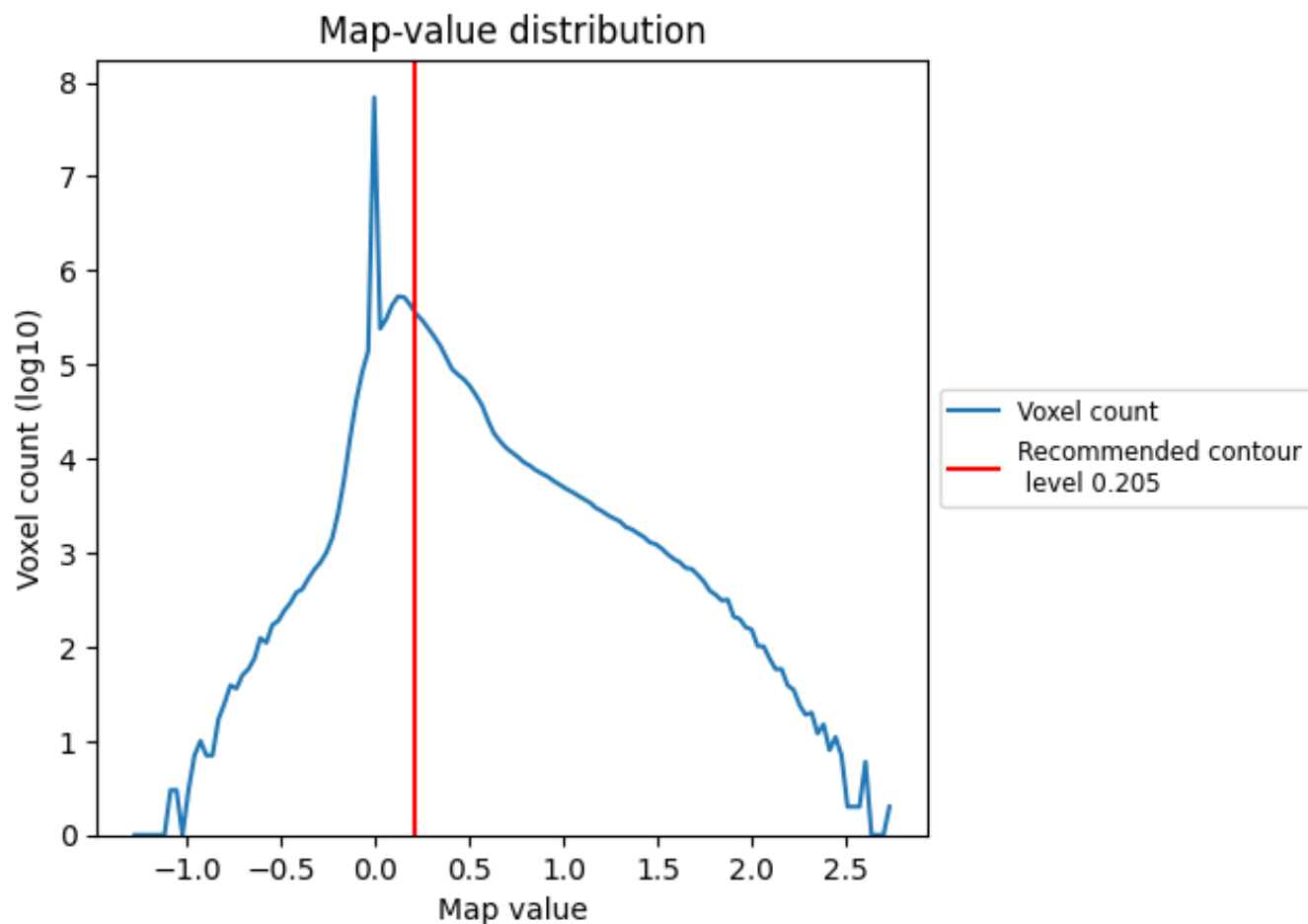
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

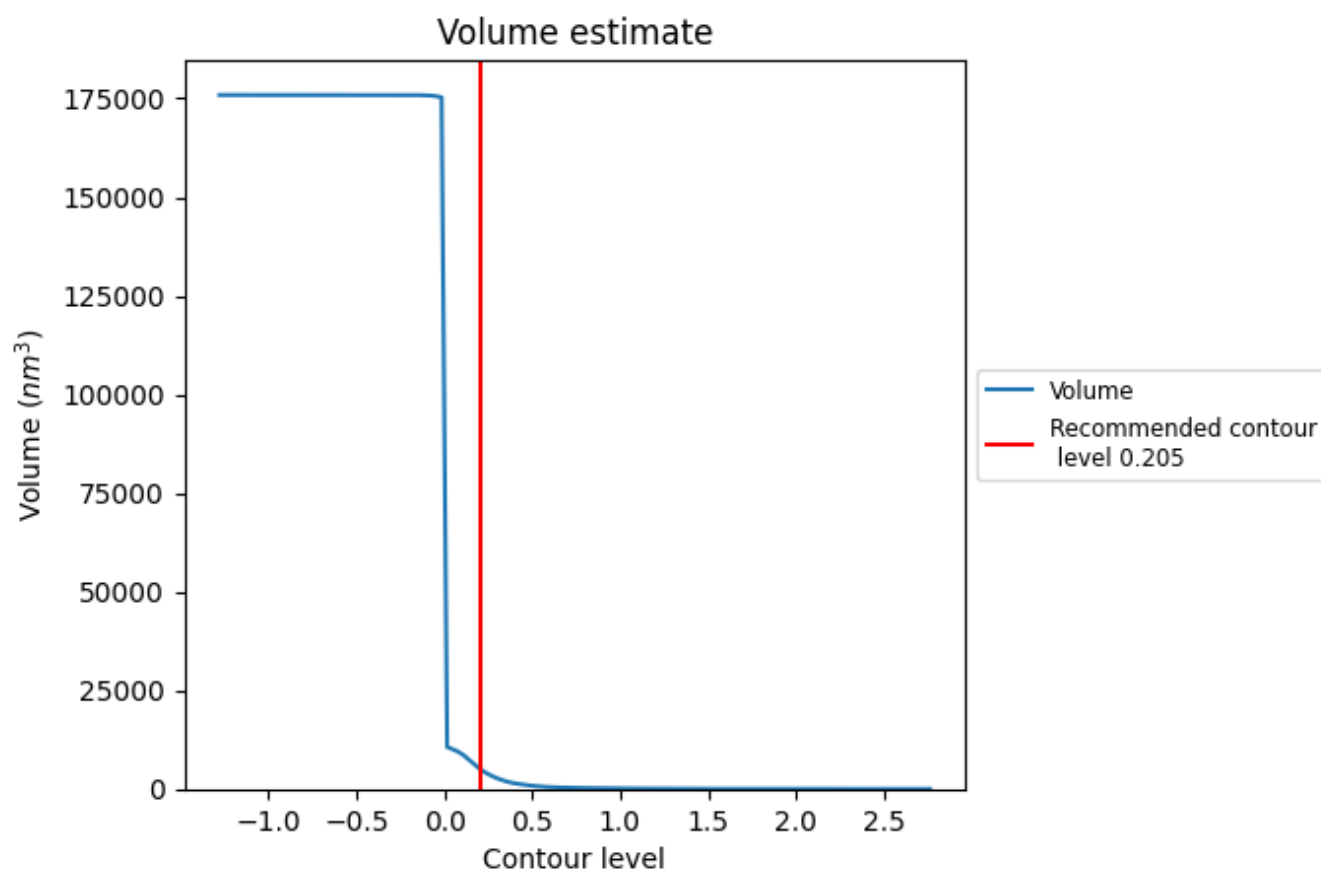
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

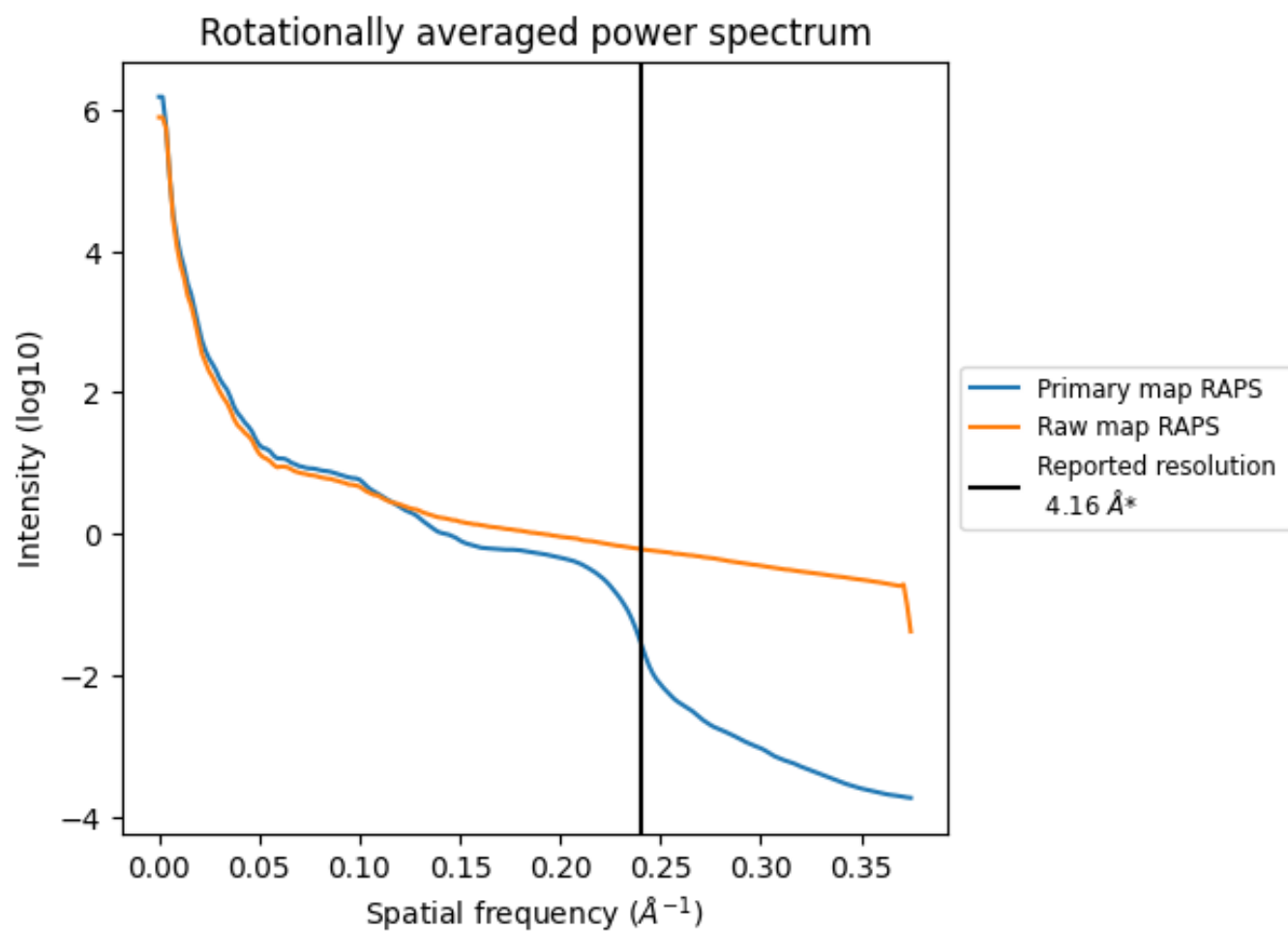
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4986 nm^3 ; this corresponds to an approximate mass of 4504 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

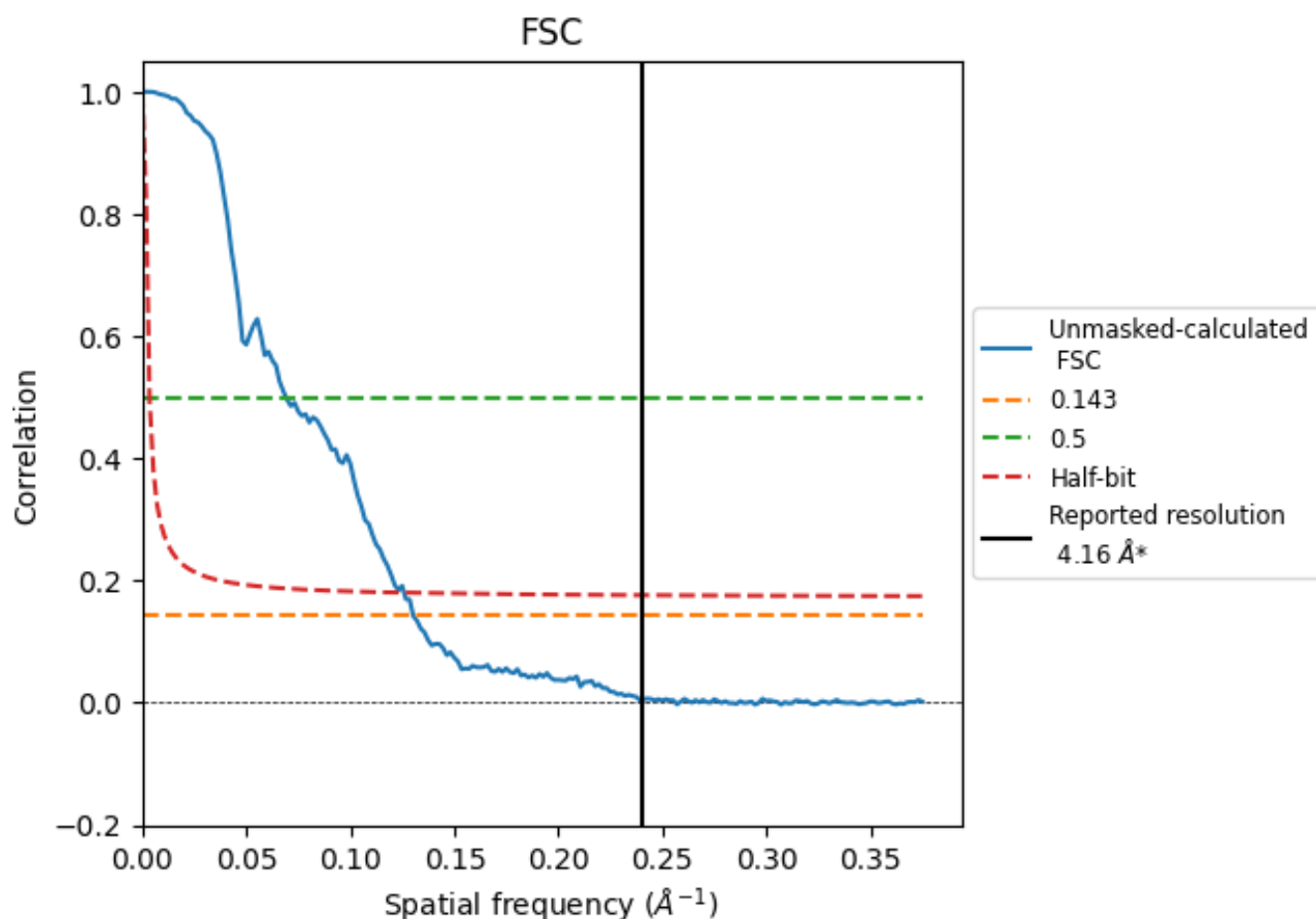


*Reported resolution corresponds to spatial frequency of $0.240 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.240 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.68	14.47	7.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.68 differs from the reported value 4.16 by more than 10 %

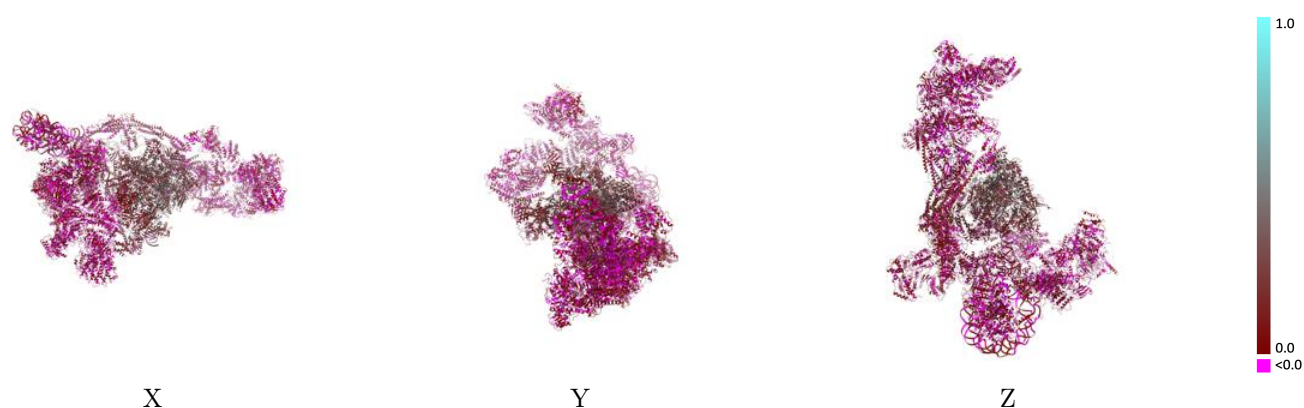
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34360 and PDB model 8GXS. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

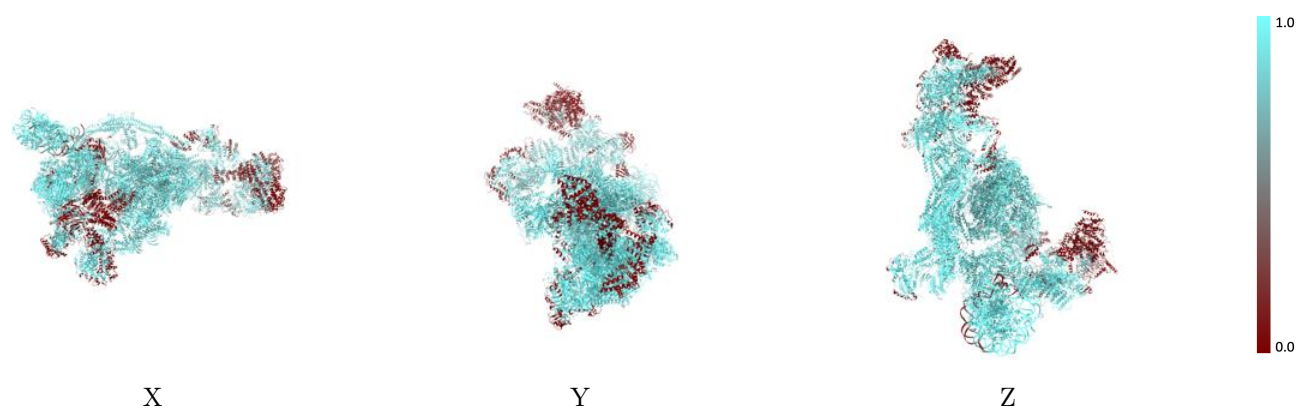
This section was not generated.

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



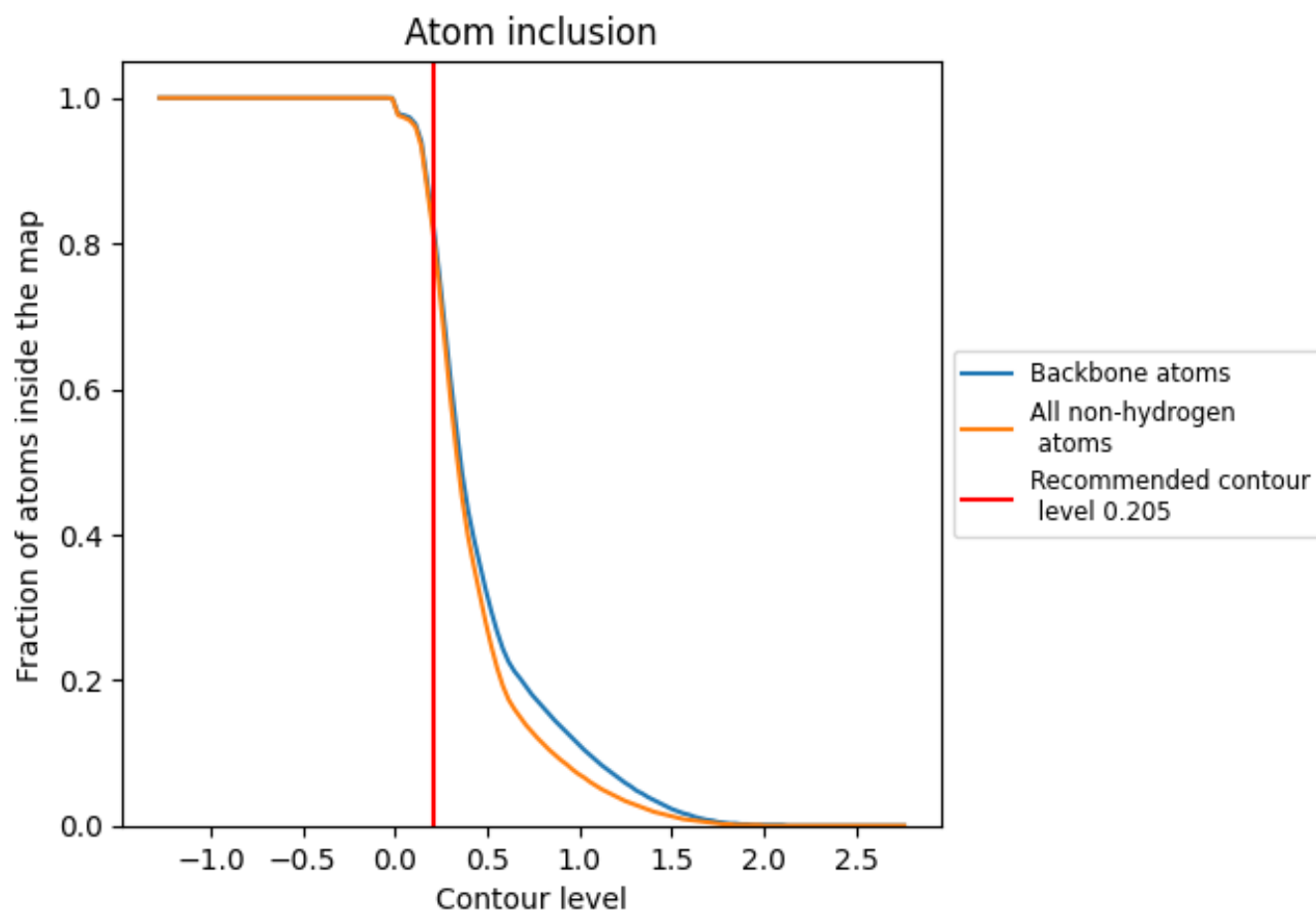
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.205).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.0930
BA	 0.9700	 0.2280
DA	 0.7100	 0.0220
DB	 0.9430	 0.0400
DD	 0.6540	 0.0380
DE	 0.8400	 0.0360
DF	 0.7870	 0.0420
DG	 0.3760	 0.0250
DH	 0.9100	 0.0420
DI	 0.7220	 0.0330
DJ	 0.8810	 0.0270
DL	 0.3730	 0.0400
DO	 0.9520	 0.1340
DP	 0.9860	 0.1680
DQ	 0.9410	 0.1180
Dc	 0.0650	 0.0310
Dd	 0.0020	 0.0010
De	 0.1900	 0.0150
Df	 0.5500	 0.0330
Di	 0.0590	 0.0290
Dj	 0.0170	 0.0500
Dk	 0.0000	 -0.0150
DI	 0.0000	 -0.0070
Dm	 0.0000	 -0.0110
EA	 0.9340	 0.1170
EB	 0.9760	 0.1150
FA	 0.9710	 0.1500
FB	 0.9780	 0.1680
HA	 0.9890	 0.0880
HB	 0.9870	 0.0480
HC	 0.9830	 0.0680
HD	 0.9190	 0.1020
HE	 0.9820	 0.0530
HF	 1.0000	 0.0510
HG	 0.9890	 0.0560



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Chain	Atom inclusion	Q-score
HH	 0.9900	 0.0720
HI	 0.9670	 0.0600
HJ	 0.8510	 0.0620
NA	 0.9420	 0.0310
NB	 1.0000	 0.0490
NC	 1.0000	 0.0050
ND	 1.0000	 0.0090
NE	 0.9770	 0.0330
NF	 0.9720	 0.0480
NG	 0.9850	 0.0410
NH	 0.9640	 0.0380
NX	 0.8070	 0.0300
NY	 0.7950	 0.0250
PA	 0.9580	 0.2510
PB	 0.9670	 0.3080
PC	 0.9740	 0.3060
PD	 0.9710	 0.1790
PE	 0.9610	 0.2250
PF	 0.9290	 0.2910
PG	 0.9770	 0.1770
PH	 0.9740	 0.2790
PI	 0.9770	 0.2320
PJ	 0.9720	 0.3180
PK	 0.9570	 0.3000
PL	 0.9640	 0.3100
X	 0.9990	 0.1960
Y	 0.9970	 0.2010
a	 0.6860	 0.0430
b	 0.8340	 0.0330
c	 0.9130	 0.0440
d	 0.8600	 0.0710
e	 0.9870	 0.0840
f	 0.9930	 0.1270
g	 1.0000	 0.0910
h	 0.9850	 0.1250
i	 0.6570	 0.0630
j	 0.9780	 0.0830
k	 0.9760	 0.1280
l	 0.9910	 0.0600
m	 1.0000	 0.0720
n	 0.9280	 0.0510
o	 0.8830	 0.0320

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Chain	Atom inclusion	Q-score
p	 0.8590	 0.0390
q	 0.9980	 0.0750
r	 0.9910	 0.0850
s	 0.9920	 0.0460
t	 0.9650	 0.0660
u	 1.0000	 0.0740
v	 0.9850	 0.1190
w	 0.3200	 0.0150
x	 0.6380	 0.0290
y	 0.8770	 0.0350
z	 0.9320	 0.0350