



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:41 PM JST

PDB ID : 8GXQ / pdb_00008gxq
EMDB ID : EMD-34359
Title : PIC-Mediator in complex with +1 nucleosome (T40N) in MH-binding state
Authors : Chen, X.; Wang, X.; Liu, W.; Ren, Y.; Qu, X.; Li, J.; Yin, X.; Xu, Y.
Deposited on : 2022-09-21
Resolution : 5.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

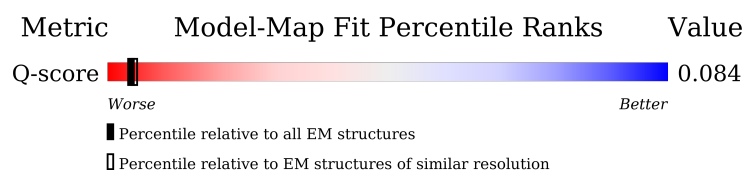
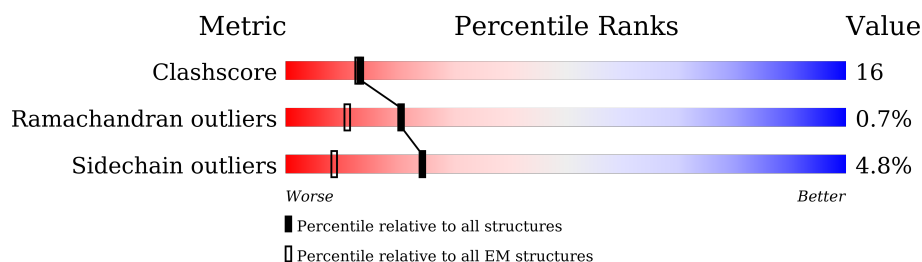
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.04 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.



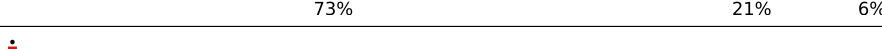
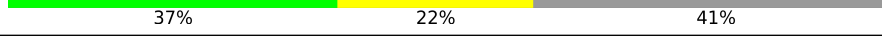
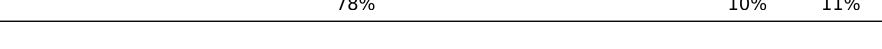
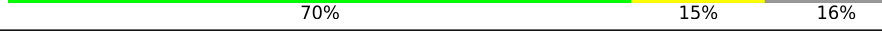
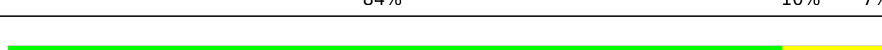
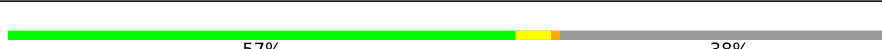
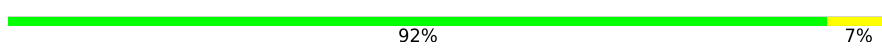
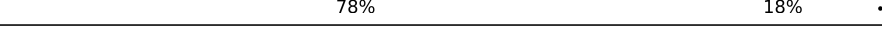
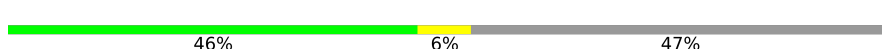
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	840 (4.54 - 5.51)

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	BA	316	
4	DA	1872	

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Mol	Chain	Length	Quality of chain
5	EA	439	
6	FA	517	
7	HA	760	
8	NA	136	
8	NE	136	
9	PA	1970	
10	DB	1199	
11	EB	291	
12	FB	249	
13	HB	548	
14	NB	103	
14	NF	103	
15	PB	1174	
16	HC	462	
17	PC	275	
18	PE	210	
19	PF	127	
20	PH	150	
21	PI	125	
22	PJ	67	
23	PK	117	
24	PL	58	
25	DP	339	
26	DQ	376	
27	DO	109	

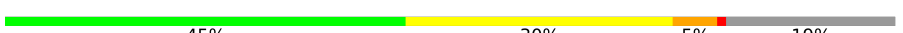
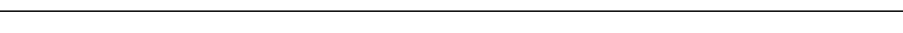
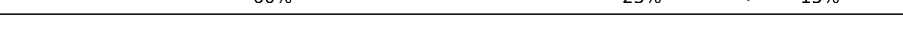
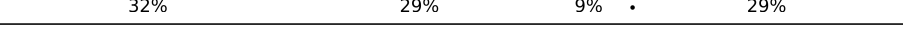
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Mol	Chain	Length	Quality of chain
28	Dc	929	
29	DD	1085	
29	Dd	1085	
30	DE	800	
30	De	800	
31	DF	677	
31	Df	677	
32	DI	264	
32	Di	264	
33	DJ	218	
33	Dj	218	
34	Dk	211	
35	DL	161	
35	DI	161	
36	Dm	124	
37	DG	349	
38	DH	310	
39	HD	309	
40	HE	308	
41	HG	395	
42	HH	782	
43	HF	71	
44	HI	346	
45	HJ	323	
46	PD	142	

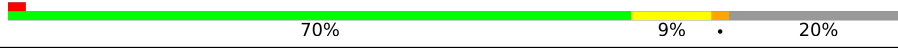
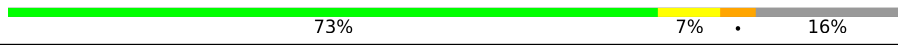
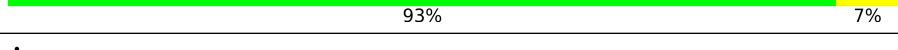
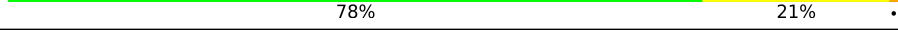
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Mol	Chain	Length	Quality of chain
47	PG	172	
48	g	233	
49	j	135	
50	n	1454	
51	s	244	
52	u	144	
53	a	1581	
54	d	270	
55	f	246	
56	i	146	
57	m	131	
58	q	651	
59	z	600	
60	b	200	
61	c	311	
62	e	178	
63	l	178	
64	o	788	
65	h	268	
66	k	117	
67	r	208	
68	t	212	
69	v	200	
70	p	841	
71	w	1368	

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Mol	Chain	Length	Quality of chain
72	x	989	
73	y	747	
74	NC	128	
74	NG	128	
75	ND	126	
75	NH	126	
76	NX	162	
77	NY	162	

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 protein called Transcription initiation factor IIB.

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

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 1.

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

- Molecule 5 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 6 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

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

- Molecule 8 is a protein called Histone H3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

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

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 11 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 12 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 13 is a protein called General transcription factor IIH subunit 1.

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

- Molecule 14 is a protein called Histone H4.

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

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

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

- Molecule 16 is a protein called General transcription factor IIH subunit 4.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

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

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

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 22 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 23 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 24 is a protein called RPB12.

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

- Molecule 25 is a protein called TATA-box-binding protein.

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

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 27 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 28 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 29 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 30 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 6.

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

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 10.

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

- Molecule 34 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 12.

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

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 39 is a protein called CDK-activating kinase assembly factor MAT1.

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

- Molecule 40 is a protein called General transcription factor IIH subunit 3.

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

- Molecule 41 is a protein called General transcription factor IIH subunit 2.

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

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

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

- Molecule 43 is a protein called General transcription factor IIH subunit 5.

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

- Molecule 44 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	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 45 is a protein called Cyclin-H.

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

- Molecule 46 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 47 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 10.

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

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 14.

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

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 19.

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

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 21.

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

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 1.

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

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 6.

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

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 58 is a protein called Mediator of RNA polymerase II transcription subunit 17.

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

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 27.

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

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 65 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 67 is a protein called Mediator of RNA polymerase II transcription subunit 18.

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

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

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

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

- Molecule 71 is a protein called Mediator of RNA polymerase II transcription subunit 23.

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

- Molecule 72 is a protein called Mediator of RNA polymerase II transcription subunit 24.

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

- Molecule 73 is a protein called Mediator of RNA polymerase II transcription subunit 25.

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

- Molecule 74 is a protein called HISTONE H2A.Z.

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

- Molecule 75 is a protein called Histone H2B.

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

- Molecule 76 is a DNA chain called DNA (162-mer).

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

- Molecule 77 is a DNA chain called DNA (162-mer).

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

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

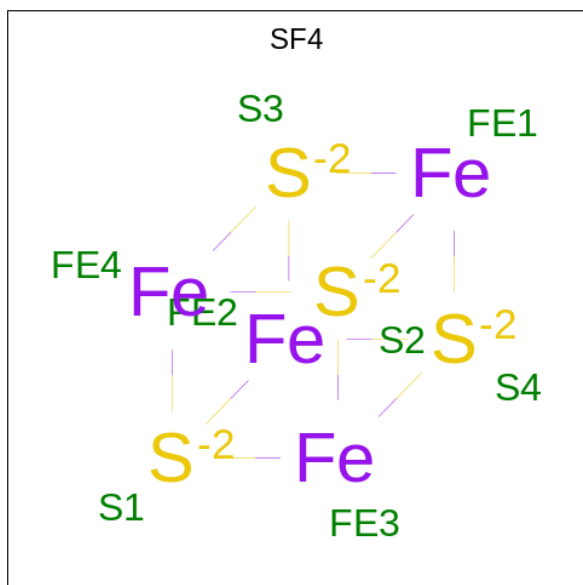
Mol	Chain	Residues	Atoms		AltConf
78	BA	1	Total	Zn	0
			1	1	
78	EA	1	Total	Zn	0
			1	1	
78	PA	2	Total	Zn	0
			2	2	
78	PB	1	Total	Zn	0
			1	1	
78	PC	1	Total	Zn	0
			1	1	
78	PI	2	Total	Zn	0
			2	2	
78	PJ	1	Total	Zn	0
			1	1	
78	PL	1	Total	Zn	0
			1	1	
78	HD	2	Total	Zn	0
			2	2	
78	HE	2	Total	Zn	0
			2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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
78	HG	3	Total	Zn	0
			3	3	
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	

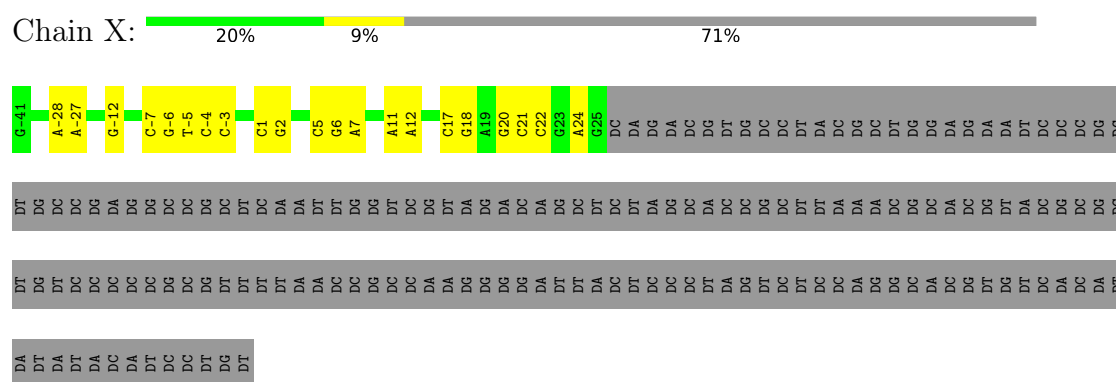
- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

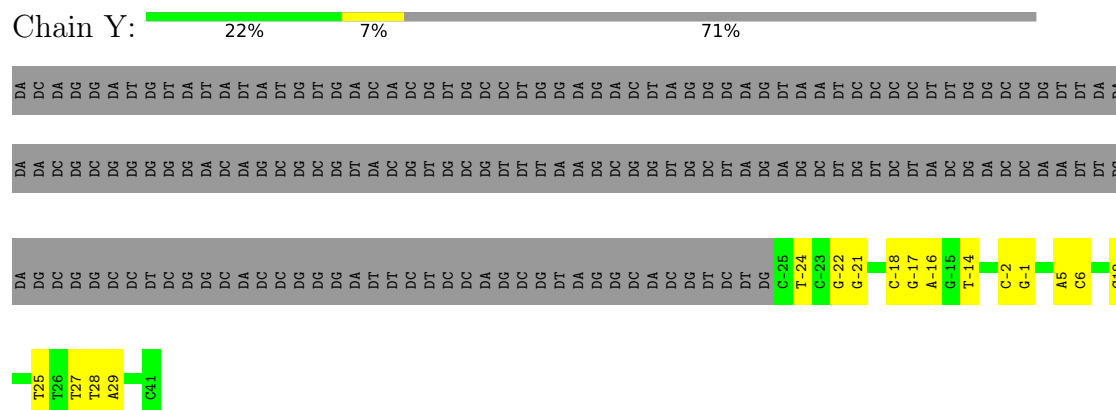
3 Residue-property plots

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.

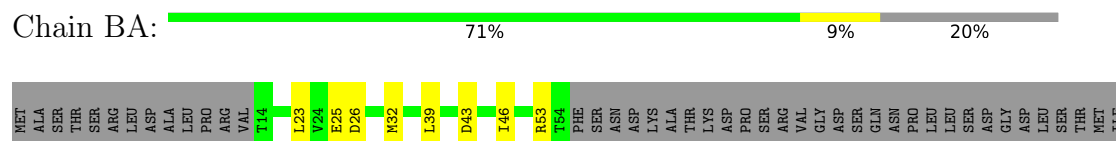
• Molecule 1: DNA (228-mer)



• Molecule 2: DNA (228-mer)

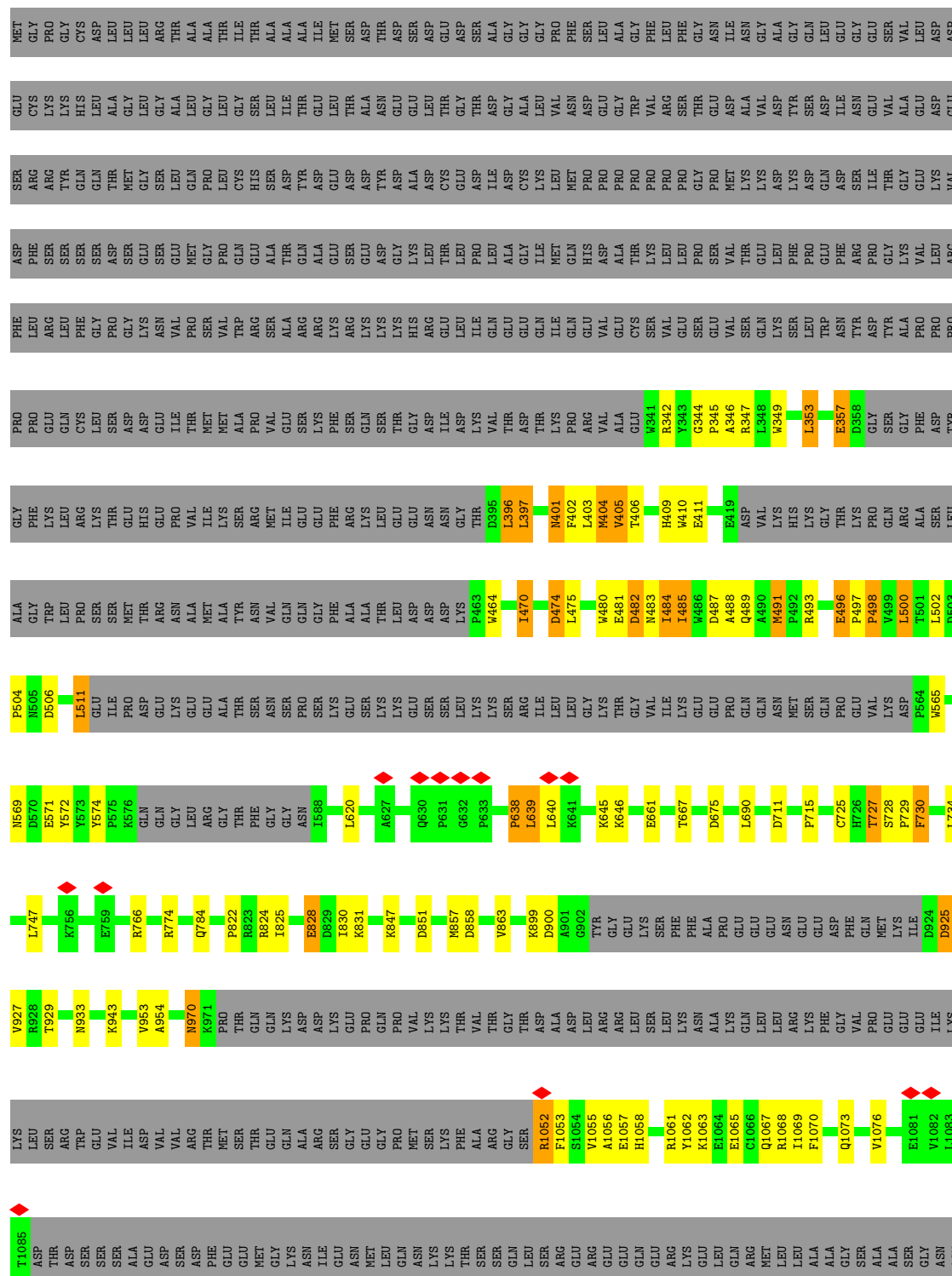


• Molecule 3: Transcription initiation factor IIB





● Molecule 4: Transcription initiation factor TFIID subunit 1





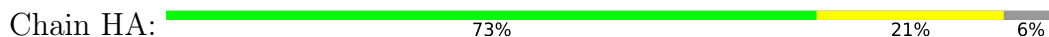
ASP GLU GLU GLU ASP ASP GLU PHE GLU GLU VAL ALA ASP ASP ASP PRO PRO PHE SER SER GLU VAL SER GLN GLN GLN MET GLN THR THR GLU GLU LYS GLU ALA ALA TYR TLE TLE ALA MET GLY GLN ARG MET PHE GLU ASP ASP LEU LEU PHE GLU

- Molecule 6: General transcription factor IIF subunit 1



GLU	ASP	THR	ARG	GLY	SER	K109	MET
	ALA	SER	ARG	SER	SER	ALA	ALA
	VAL	SER	LYS	SER	ASP	F127	ALA
	ARG	THR	ASP	SER	ALA		LEU
	ARG	LEU	SER	SER	SER	N142	G5
	TVR	ARG	SER	GLN	ASP	W143	
	LEU	ALA	GLU	GLU	ALA		V15
	THR	ALA	GLU	GLU	SER	L149	V16
	ARG	ALA	ASP	PRO	GLY	A150	
	LYS	SER	ASP	GLU	GLU	R151	N43
	PRO	LEU	SER	SER	GLU	H152	Q44
	MET	LEU	SER	LYS	GLY	R153	
	THR	GLU	GLU	ALA	GLY		L47
	THR	GLN	GLU	LYS	ARG	E163	
	LYS	GLY	SER	ALA	VAL	E162	D50
	ASP	ARG	PRO	PRO	PRO		
	LEU	ARG	ILE	GLN	LYS	R166	N53
	LEU	VAL	ASP	GLN	ALA	R167	K54
	LYS	SER	SER	GLU	LYS		LYS
	LYS	GLU	GLU	GLU	LYS	L171	ILE
	GLN	MET	ALA	GLY	LYS		TVR
	THR	PRO	SER	PRO	ALA	M177	GLN
	ALA	THR	SER	LYS	PRO		GLU
	LYS	ALA	ALA	GLY	LEU	R180	GLU
	LYS	LYS	LEU	VAL	ALA	ARG	GLU
	THR	ARG	PHE	ASP	LYS	LEU	GLU
	GLY	LEU	MET	GLU	GLY	LYS	MET
	LEU	ARG	ALA	GLN	GLY	ASP	GLU
	SER	LEU	LYS	SER	ARG	GLN	GLU
	SER	ASP	LYS	ASP	LYS	ASP	SER
	GLU	THR	LYS	SER	LYS	GLN	GLY
	GLN	GLY	THR	SER	LYS	ASP	ALA
	THR	PRO	PRO	GLU	LYS	GLU	GLY
	VAL	GLN	PRO	GLU	LYS	ASP	SER
	ASN	SER	LYS	SER	LYS	GLU	PHE
	VAL	LEU	ARG	GLU	GLY	GLU	ASN
	LEU	SER	GLU	GLU	SER	GLU	ASN
	ALA	GLY	ARG	GLU	ASP	LYS	ARG
	GLN	LYS	LYS	LYS	ASP	GLY	LYS
	ILE	SER	PRO	PRO	GLU	LYS	LEU
	LEU	THR	SER	PRO	GLU	LYS	ARG
	LYS	PRO	GLY	GLU	ALA	ARG	GLU
	ARG	GLN	GLY	GLU	PHE	GLY	GLU
	LEU	GLN	GLY	GLU	GLU	ARG	GLU
	LEU	PRO	SER	ASP	ASP	ARG	ALA
	ASN	SER	SER	LYS	SER	LYS	ARG
	PRO	GLY	GLY	GLU	ASP	ALA	LYS
	ARG	LYS	ASN	GLU	GLY	SER	LYS
	LYS	THR	ASN	GLU	ASP	GLU	TYR
	MET	THR	ARG	GLU	PHE	LEU	GLY
	ILE	PRO	PRO	LYS	GLU	ILE	VAL
	ASN	ASN	GLY	LYS	GLN	HIS	LEU
	ASN	SER	THR	ALA	GLU	ASP	LYS
	LYS	GLY	PRO	PRO	GLU	LEU	GLU
	MET	ASP	ALA	THR	VAL	GLU	PHE
	PHE	VAL	ALA	PRO	ASP	ASP	ARG
	SER	GLN	GLU	GLN	TYR	ASP	
	SER	VAL	GLY	GLU	MET	LEU	P93
	LEU	THR	SER	LYS	GLU	GLU	K98
	LYS	GLU	GLY	LYS	ASP	MET	

- Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPD



L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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SER
LEU
GLU
GLN
GLY
GLU
SER
GLU
GLU
THR
LYS
THR
LYS
LYS
ILE
GLU
GLN
ILE
ALA
GLN
LEU

● Molecule 8: Histone H3

Chain NA:  68% 26%

MET
ALA
ARG
THR
GLY
LYS
GLN
THR
ALA
ARG
LYS
SER
THR
LYS
GLY
GLY
LYS
ALA
PRO
ARG
LYS
GLN
LEU
THR
LYS
ALA
ALA
ARG
LYS
SER
SER
ALA
PRO
THR
THR
GLY
GLY
VAL
K436
K437
P438
K464
V517
T518
E533
R594
A535

● Molecule 8: Histone H3

Chain NE:  69% 6% 24%

MET
ALA
THR
GLY
LYS
PRO
ARG
LYS
SER
THR
LYS
GLY
GLY
LYS
ALA
PRO
ARG
LYS
GLN
LEU
THR
LYS
ALA
ALA
ARG
LYS
SER
SER
ALA
PRO
THR
THR
G833
G834
V835
K636
P643
Q655
K664
Q685
V717
R734
A735

● Molecule 9: DNA-directed RNA polymerase subunit

Chain PA:  63% 11% 25%

MET
HIS
GLY
GLY
ASP
GLY
LEU
PRO
PRO
SER
GLY
ASP
S11
Q22
F23
G24
D29
R33
L57
T68
Q72
E89
F95
K105
V106
V110
C111
M122
K127
R140
L141
C154
E155
GLY
GLY
GLU
GLU
MET
ASP
ASN
LYS
PHE
GLY
VAL
GLU
GLN
PRO
GLU

GLY
ASP
GLU
ASP
THR
LYS
GLU
GLY
HIS
G182
Q188
R193
S194
G195
V202
LYS
HIS
VAL
ASN
GLU
ASP
SER
GLN
GLU
K212
E219
E223
T224
F225
L228
C233
F234
R244
R261
Q273
T277
H278
K279
T283
N287
Q311
L322

R327
R340
G348
R349
V350
R351
G352
N353
K357
D360
F361
A363
L373
D400
R401
D425
D428
L429
R430
I457
F458
N459
R460
P478
L484
N485
L486
S487
V488
P491
D495
F496
D497
M501
N502
L509
E510
T511
R512
A513
S514
I515
V521

M535
V538
Q539
L542
T543
A544
V546
T549
V560
L564
L567
W570
P575
V586
K589
L594
H609
I621
S622
D625
T626
F668
I672
I676
L680
T689
I693
I706
K710
R734
A774
A786
V787

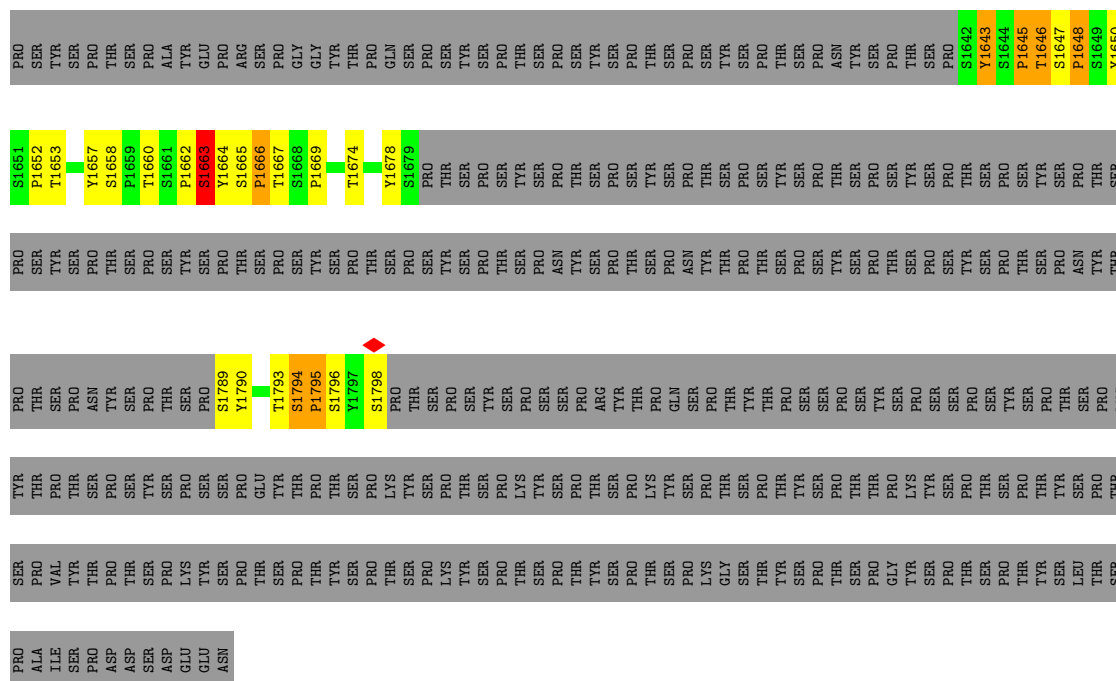
R805
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T850
T854
R863
E869
M872
Y875
D876
V879
R880
I883
E893
E902
F903
Q904
K910
P911
S912
N913
R963
C981
R985
H1005
P1006
I1007
L1016
L1020
V1021
I1022
S1030
Q1034
T1038
M1105
THR
PHE
HIS
TYR

ALA
GLY
VAL
SER
ASP
K1115
N1129
I1130
P1137
S1138
L1139
L1144
L1166
A1171
N1172
G1340
GLY
D1338
V1341
T1357
F1366
V1374
R1375
R1213
V1214
E1215
R1218
K1234
D1242
I1243
N1244
C1245
I1246
F1247
N1248
M1251
A1252
E1253
K1254
R1260
I1261
M1262
T1435
V1436
D1437
E1441
A1442
A1443
G1446
G1453

GLU
GLU
VAL
SER
ASP
K1278
M1279
D1280
D1281
F1284
L1285
I1288
T1297
L1298
T1338
D1339
G1340
GLY
T1357
F1366
V1374
R1375
R1213
V1214
E1215
R1218
K1234
D1242
I1243
N1244
C1245
I1246
F1247
N1248
M1251
A1252
E1253
K1254
R1260
I1261
M1262
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V1436
D1437
E1441
A1442
A1443
G1446
G1453

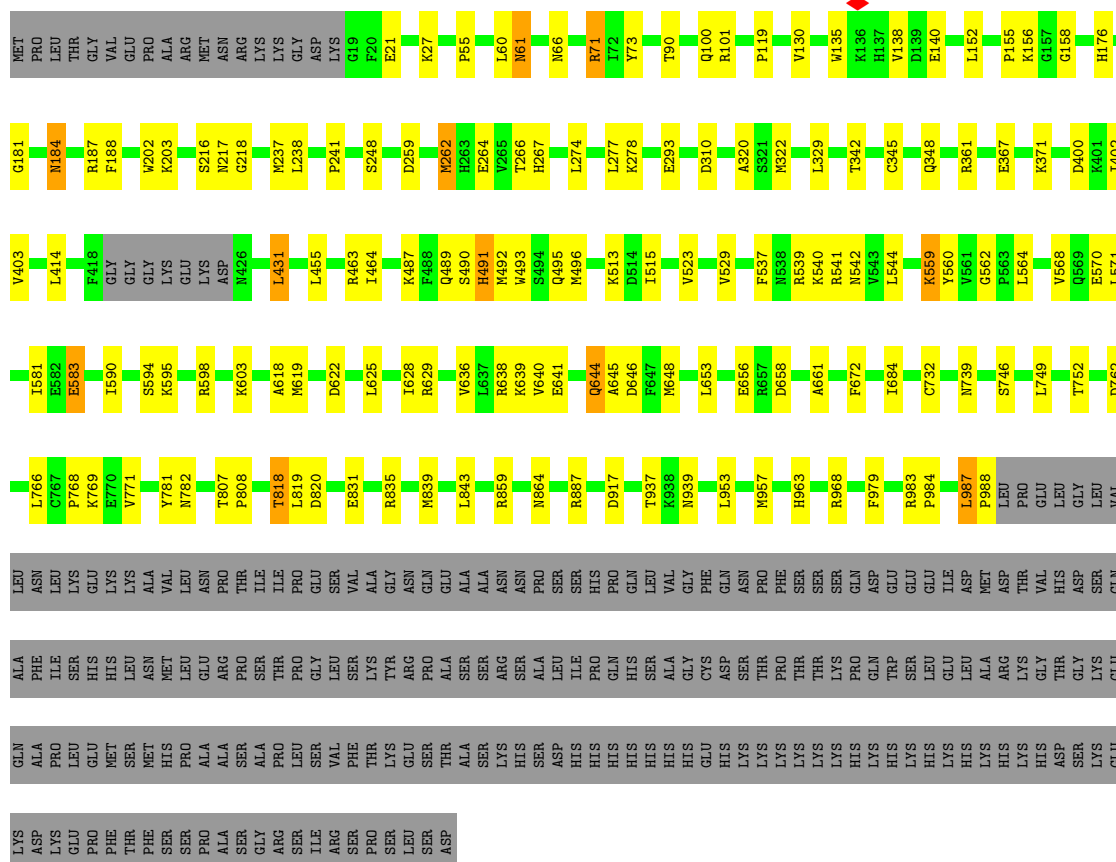
V1454
S1455
E1456
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I1458
T1468
F1471
L1475
K1481
M1484
F1487
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ASN
ILE
PRO
GLY
LEU
GLY
ALA
ALA
GLY
PHE
GLY
SER
PRO
THR
GLY
TYR
SER
PRO
PHE
GLY
TRP
SER
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THR
PRO
GLY
MET
SER
THR
TRP
ASN
ILE
PRO
SER
ALA
GLY
TYR
ALA
MET
SER

TRP
SER
PRO
SER
VAL
GLY
SER
GLY
MET
THR
PRO
GLY
ALA
ALA
GLY
PHE
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TYR
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TRP
SER
ALA
PRO
THR
PRO
GLY
MET
SER
THR
TRP
ASN
ILE
PRO
SER
ALA
GLY
TYR
ALA
MET
SER



● Molecule 10: Transcription initiation factor TFIID subunit 2

Chain DB:



[illegible]

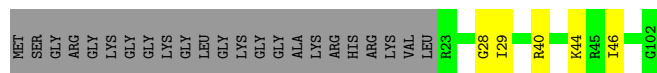
Chain FB:

Amino Acid	Percentage
MET	1%
A2	1%
V21	1%
Q30	1%
W31	1%
L43	1%
S55	1%
F56	1%
T57	1%
L58	1%
L62	1%
A63	1%
N64	1%
ILE	1%
HIS	1%
ASP	1%
ILE	1%
GLY	1%
GLY	1%
LYS	1%
PRO	1%
ALA	1%
SER	1%
VAL	1%
SER	1%
ALA	1%
PRO	1%
ARG	1%
E80	1%
H81	1%
T94	1%
I109	1%
N123	1%
D179	1%
H182	1%
M186	1%
L187	1%
F188	1%
S189	1%
E192	1%
K193	1%
H194	1%
Q195	1%
Y196	1%
K214	1%
T270	1%

[illegible]

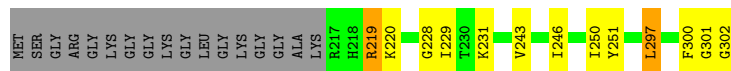
- Molecule 14: Histone H4

Chain NB:  73% 5% 22%



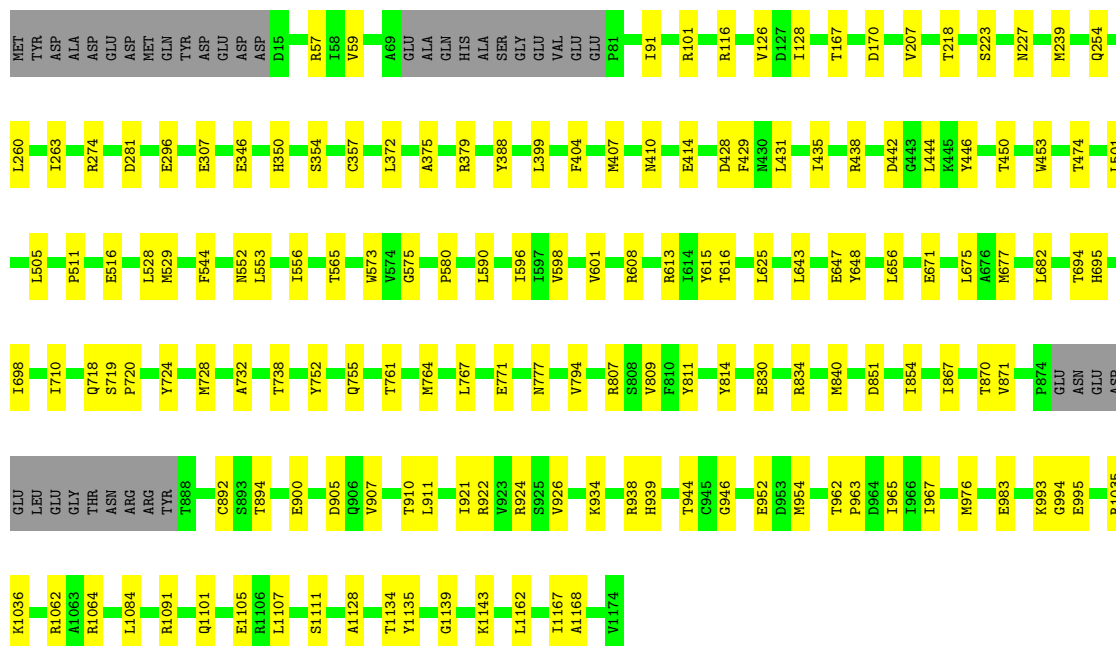
- Molecule 14: Histone H4

Chain NF:  71% 11% 17%



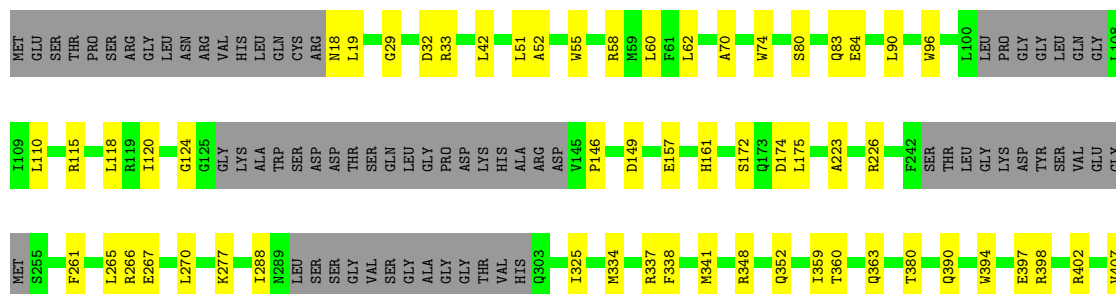
- Molecule 15: DNA-directed RNA polymerase subunit beta

Chain PB:  84% 13% .



- Molecule 16: General transcription factor IIH subunit 4

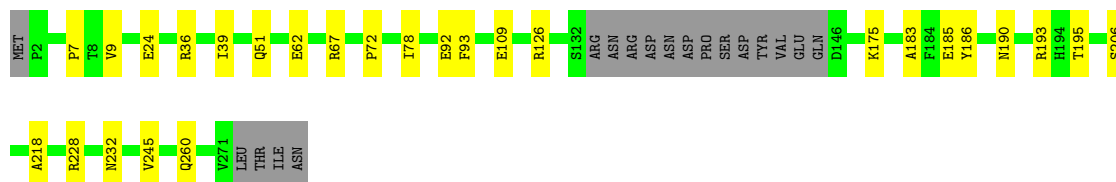
Chain HC:  70% 15% 16%





- Molecule 17: DNA-directed RNA polymerase II subunit RPB3

Chain PC: 84% 10% 7%



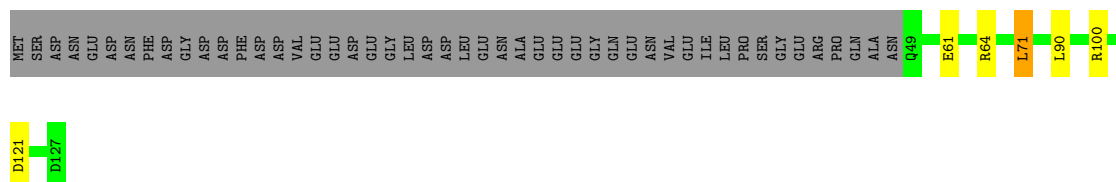
- Molecule 18: DNA-directed RNA polymerase II subunit E

Chain PE: 87% 13%



- Molecule 19: DNA-directed RNA polymerase II subunit F

Chain PF: 57% 38%



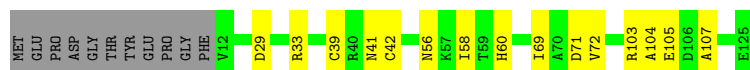
- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain PH: 92% 7%



- Molecule 21: DNA-directed RNA polymerase II subunit RPB9

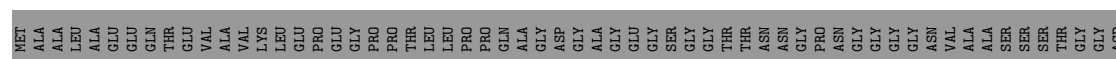
Chain PI: 79% 12% 9%

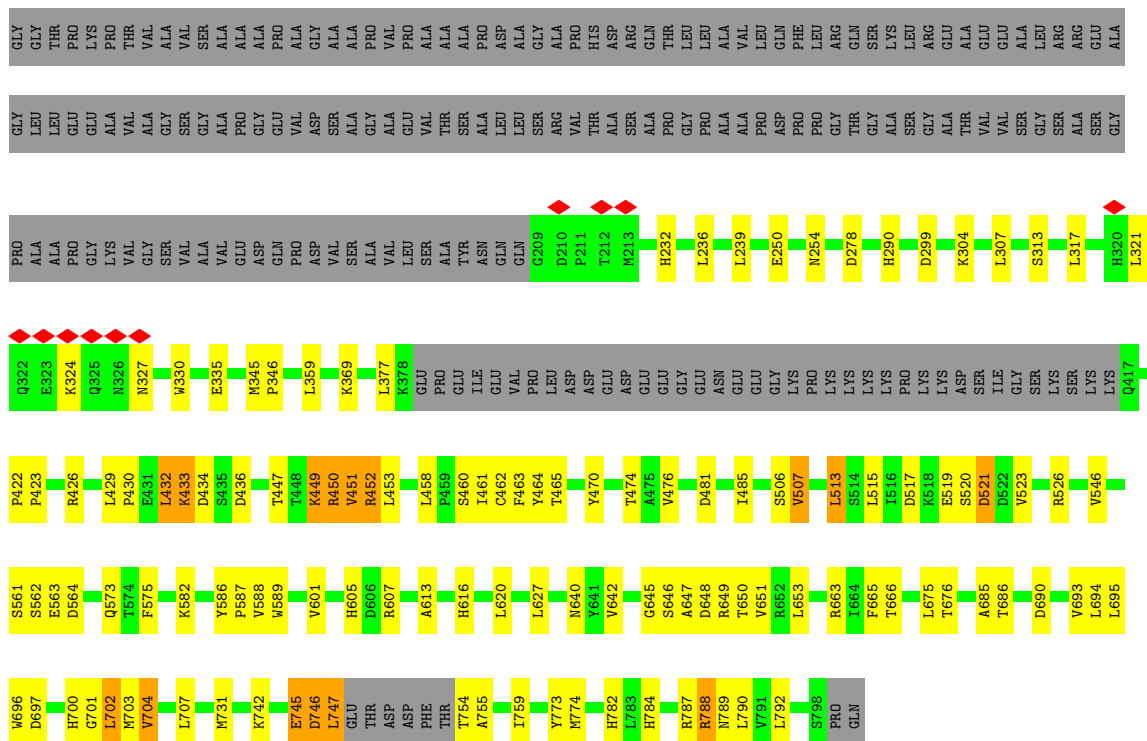


- Molecule 22: DNA-directed RNA polymerases I, II, and III subunit RPABC5

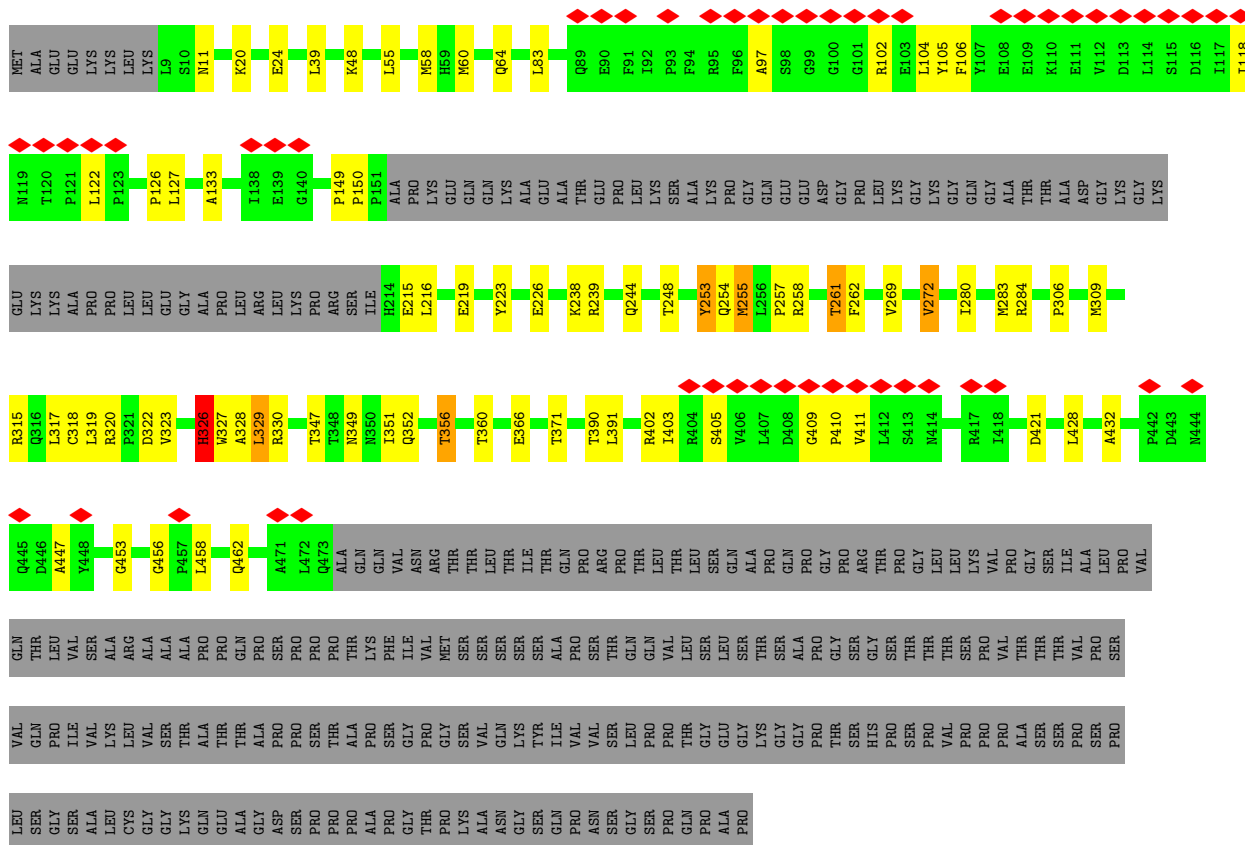
Chain PJ: 78% 18%

Chain Dd:

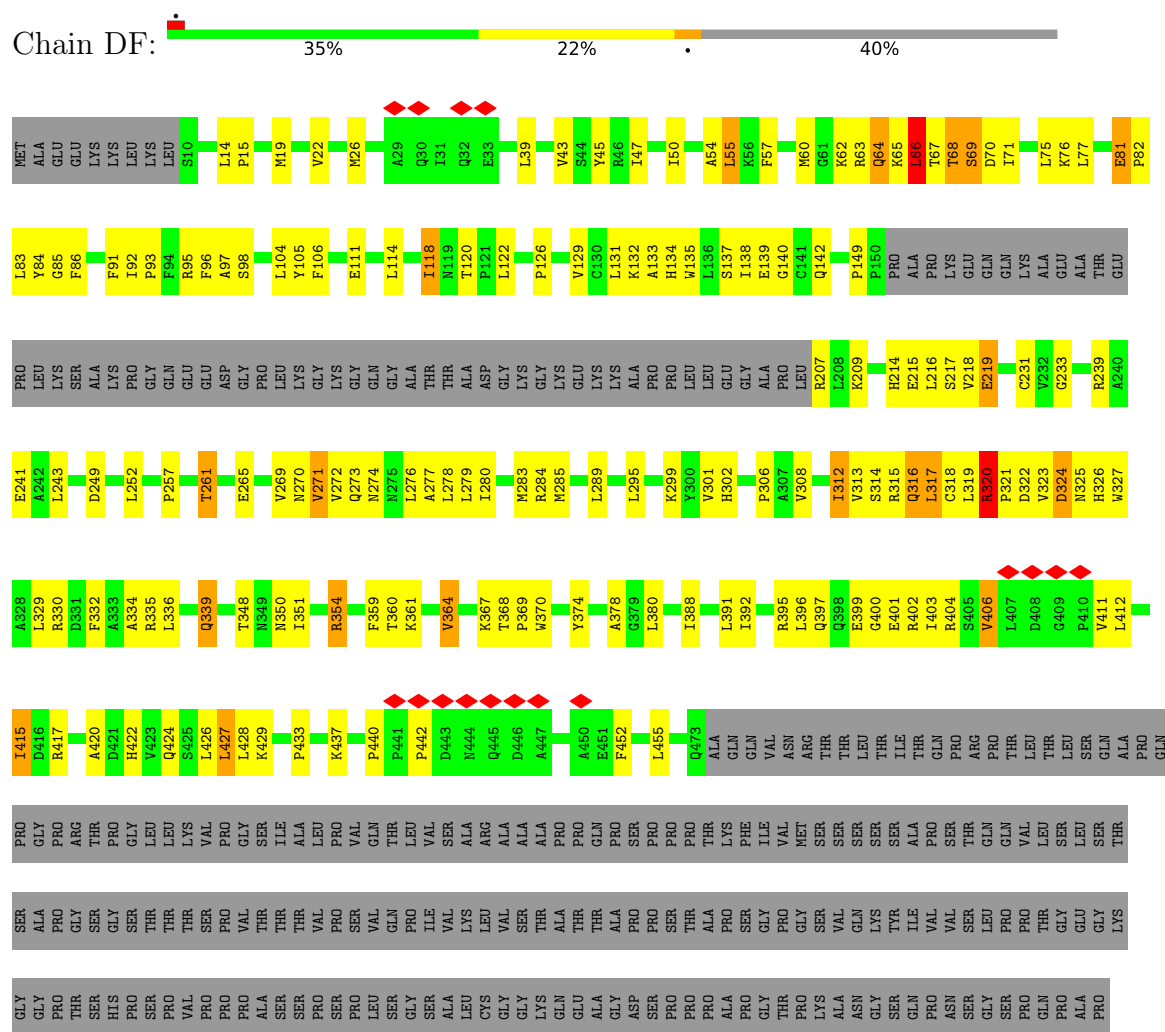




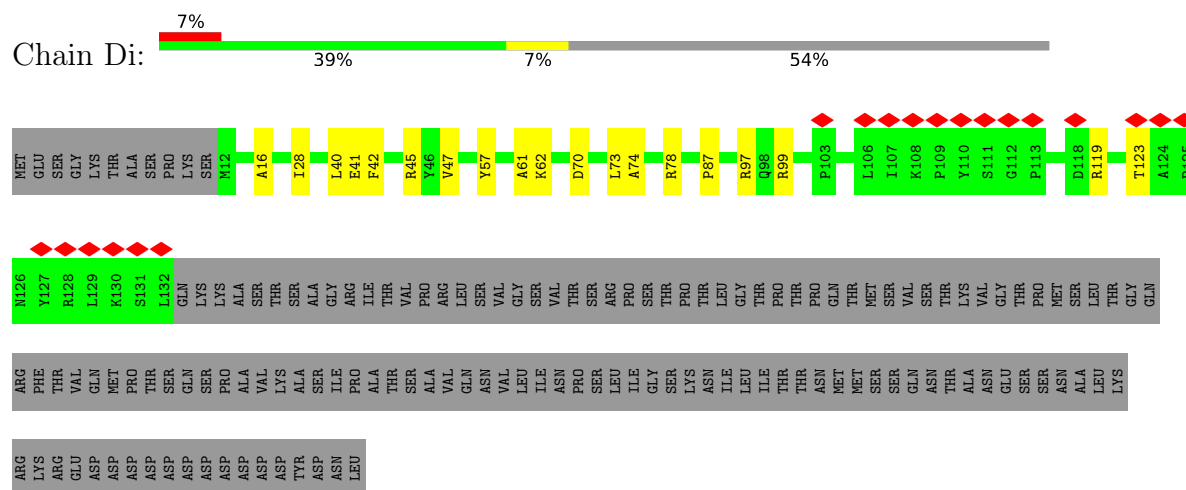
- Molecule 31: Transcription initiation factor TFIID subunit 6



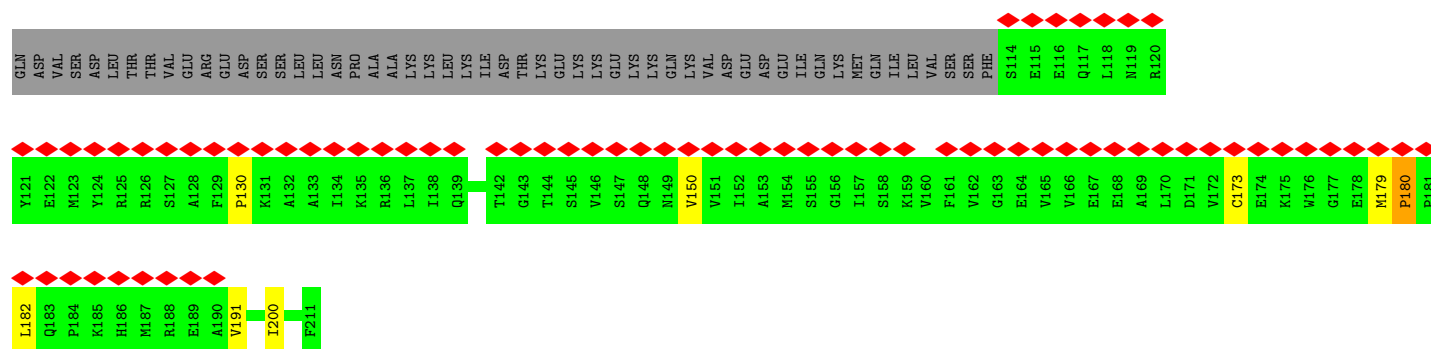
• Molecule 31: Transcription initiation factor TFIID subunit 6



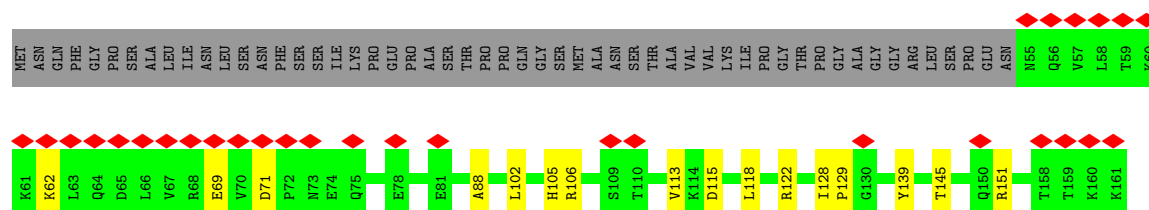
• Molecule 32: Transcription initiation factor TFIID subunit 9



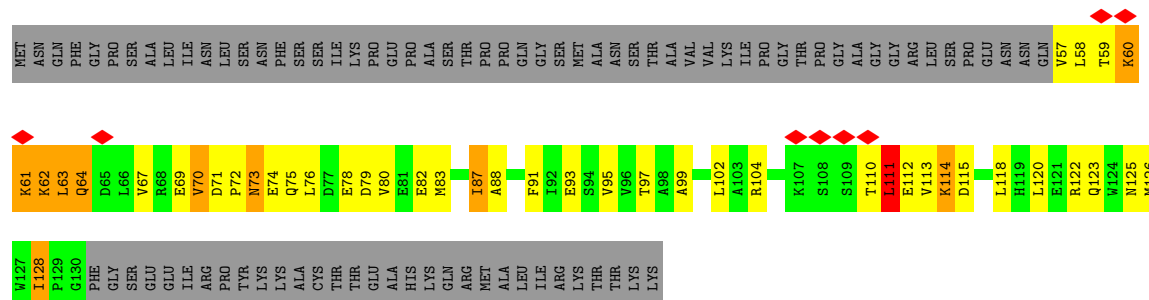
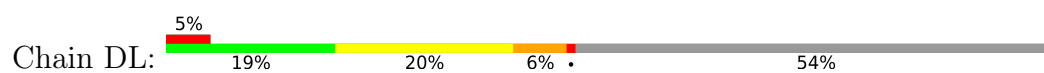
• Molecule 32: Transcription initiation factor TFIID subunit 9



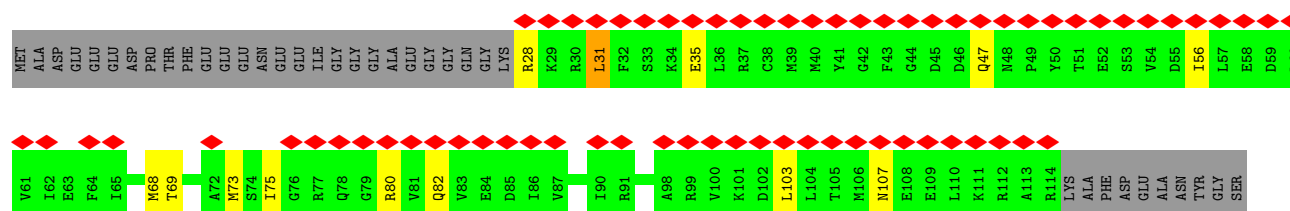
• Molecule 35: Transcription initiation factor TFIID subunit 12



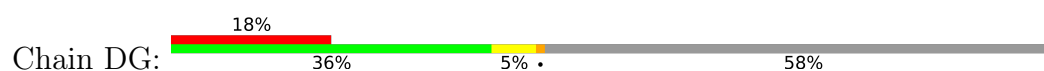
• Molecule 35: Transcription initiation factor TFIID subunit 12

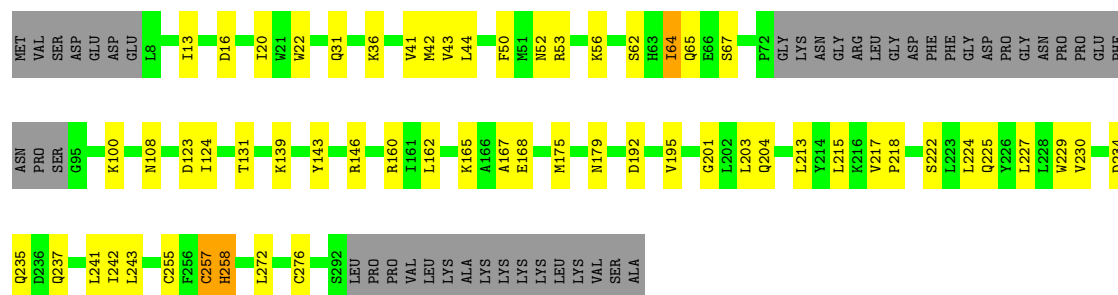


• Molecule 36: Transcription initiation factor TFIID subunit 13



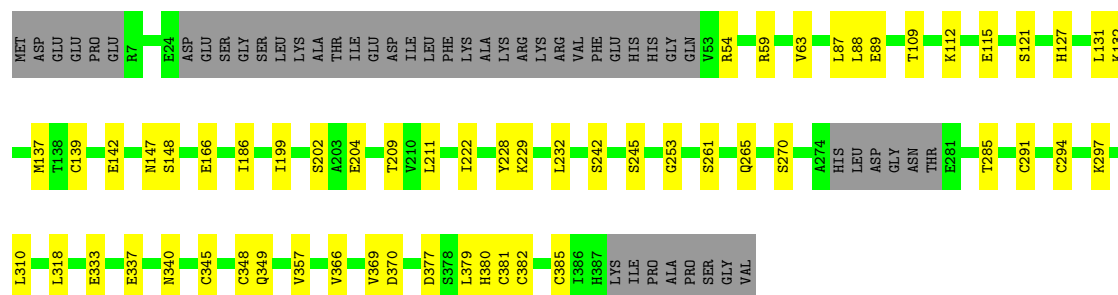
• Molecule 37: Transcription initiation factor TFIID subunit 7





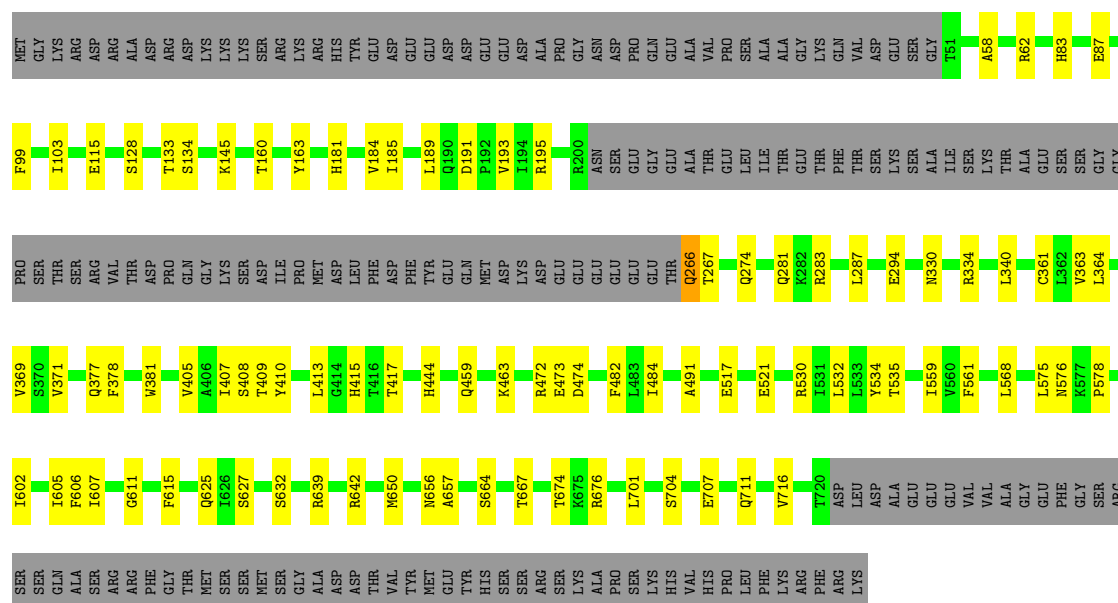
- Molecule 41: General transcription factor IIH subunit 2

Chain HG: 73% 14% 12%



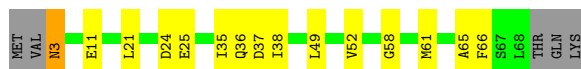
- Molecule 42: General transcription and DNA repair factor IIH helicase subunit XPB

Chain HH: 66% 11% 23%

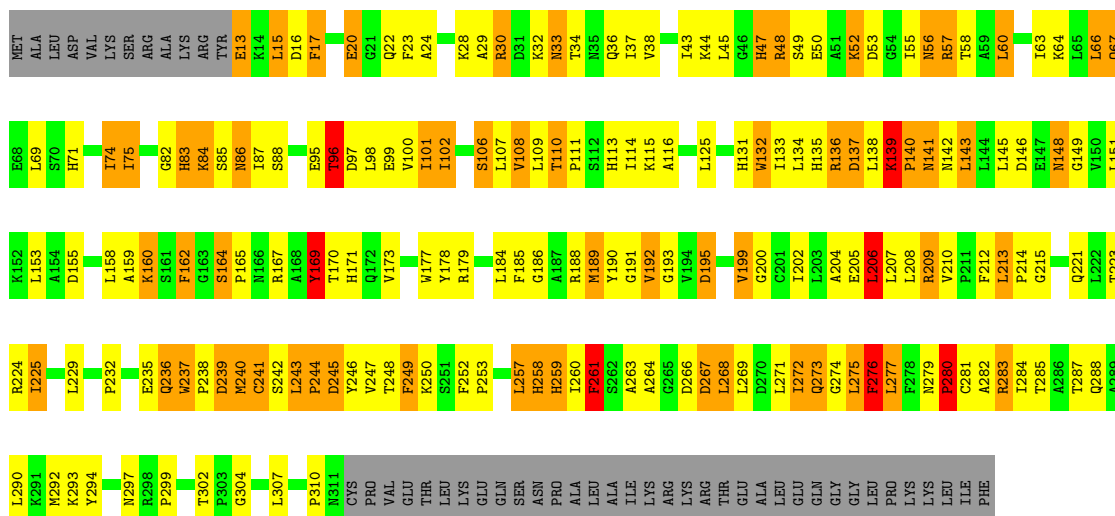


- Molecule 43: General transcription factor IIH subunit 5

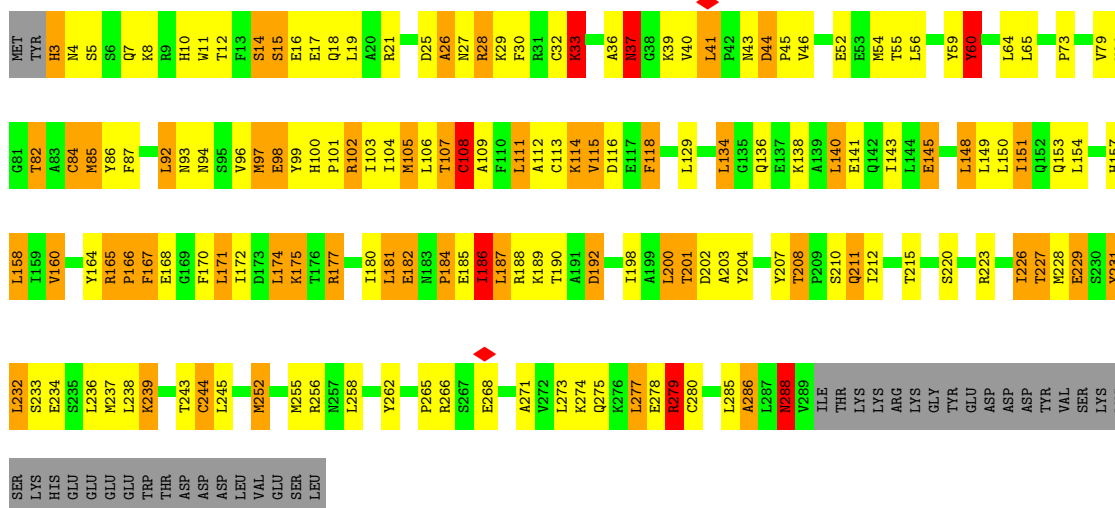
Chain HF: 72% 20% 7%



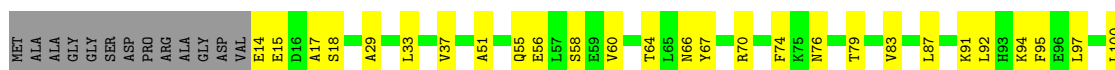
• Molecule 44: Cyclin-dependent kinase 7



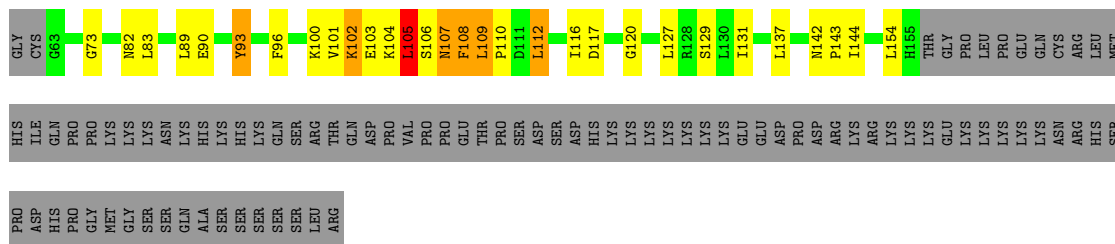
• Molecule 45: Cyclin-H



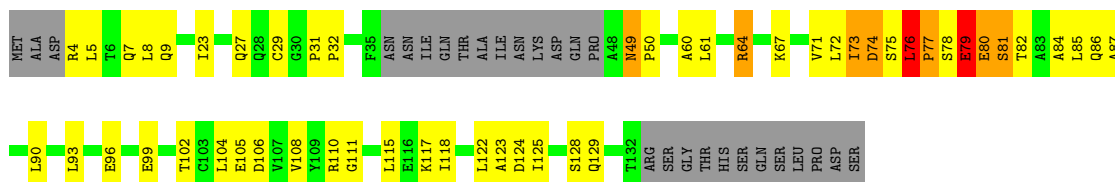
• Molecule 46: DNA-directed RNA polymerase II subunit RPB4



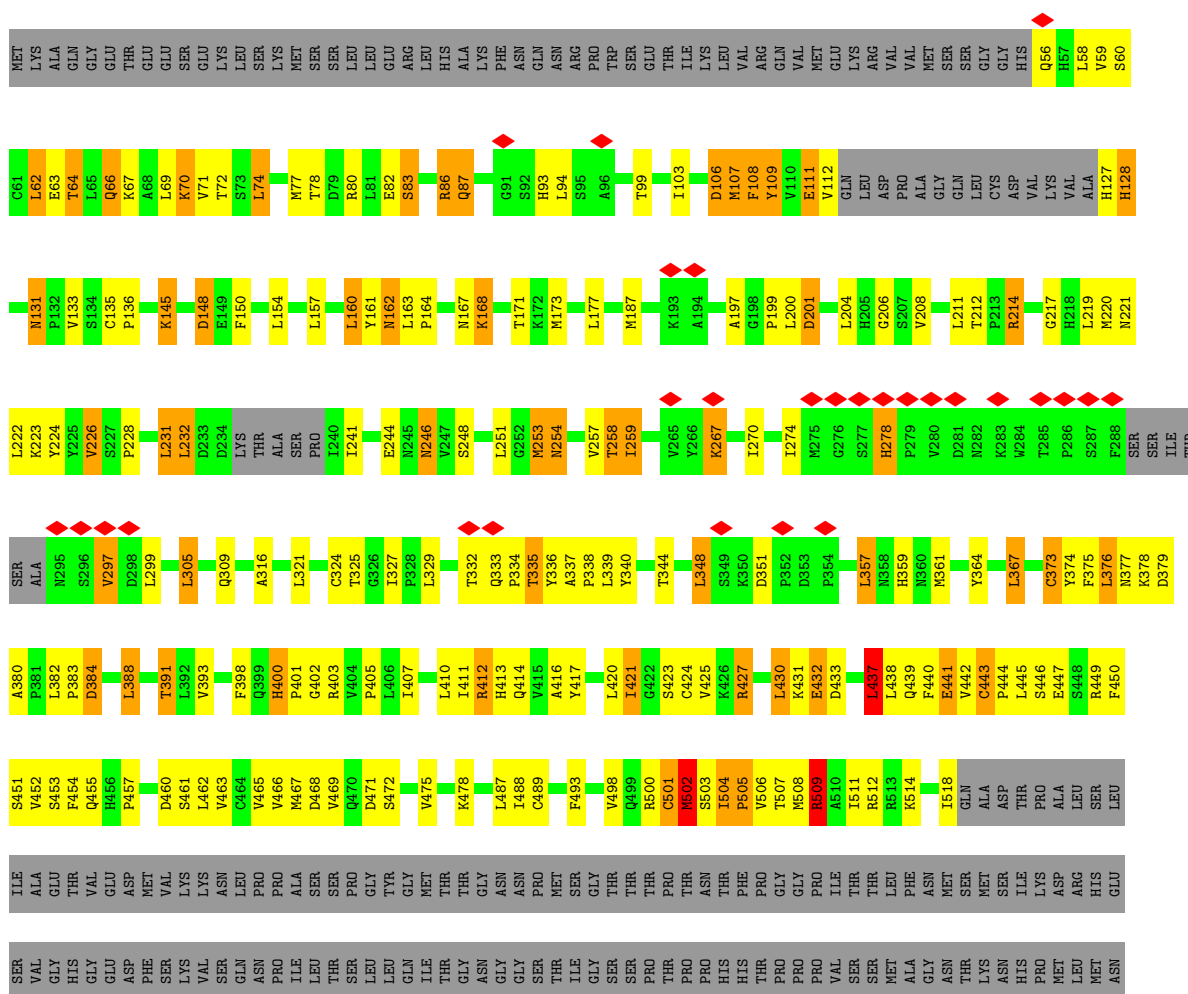




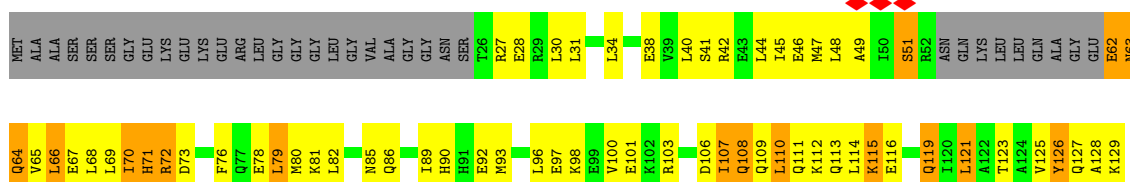
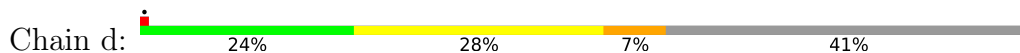
- Molecule 52: Mediator of RNA polymerase II transcription subunit 21

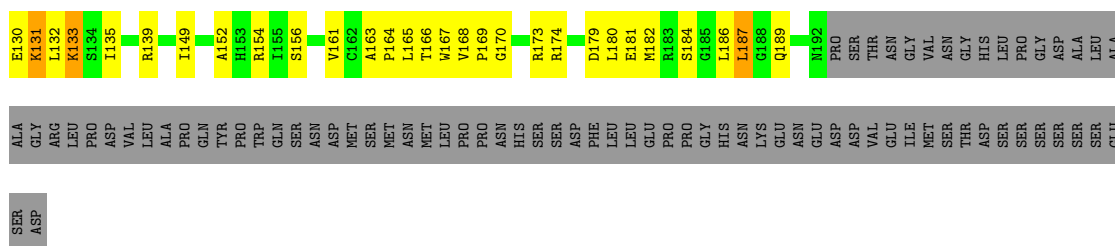


- Molecule 53: Mediator of RNA polymerase II transcription subunit 1

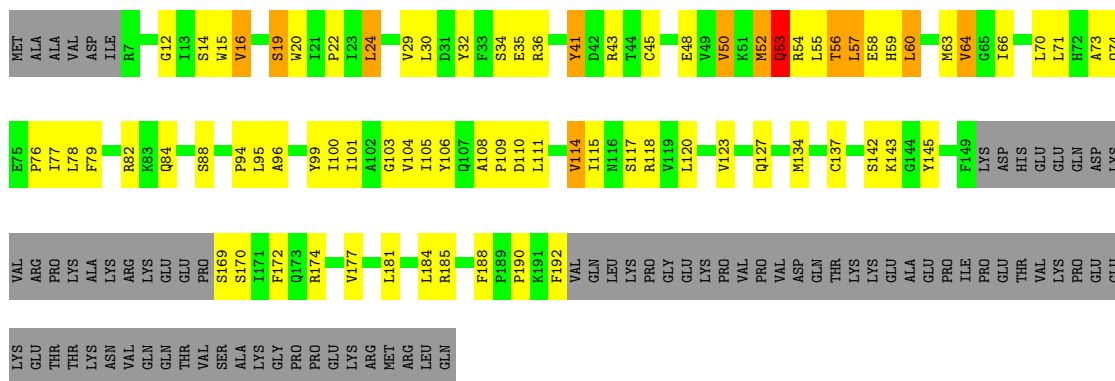
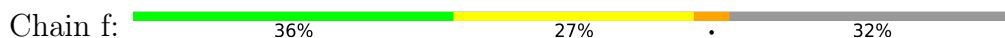


- Molecule 54: Mediator of RNA polymerase II transcription subunit 4

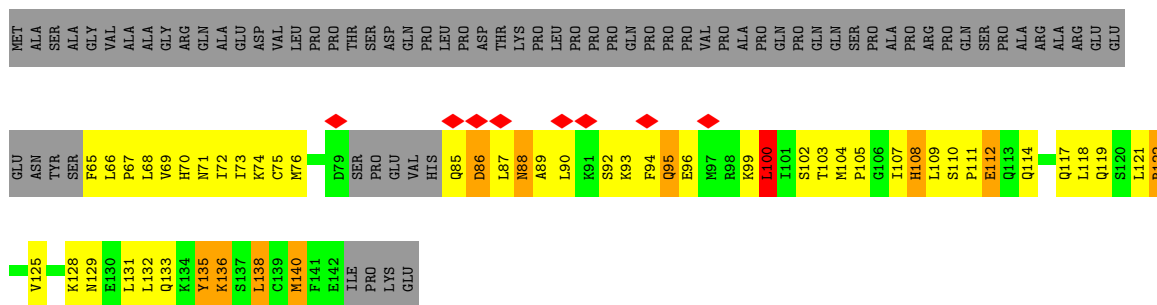




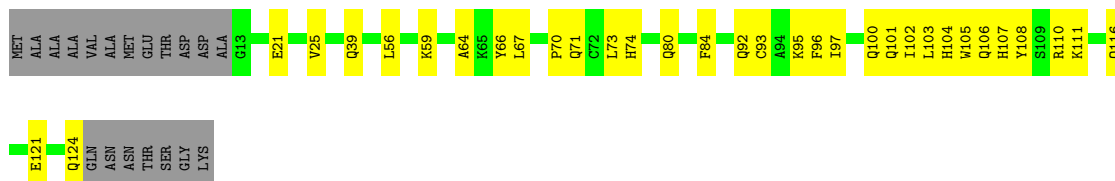
- Molecule 55: Mediator of RNA polymerase II transcription subunit 6



- Molecule 56: Mediator of RNA polymerase II transcription subunit 9

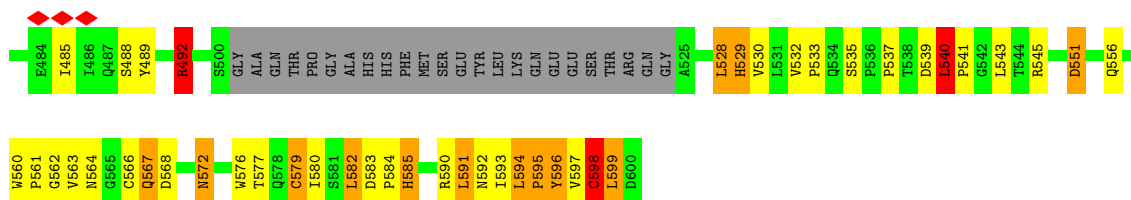


- Molecule 57: Mediator of RNA polymerase II transcription subunit 31



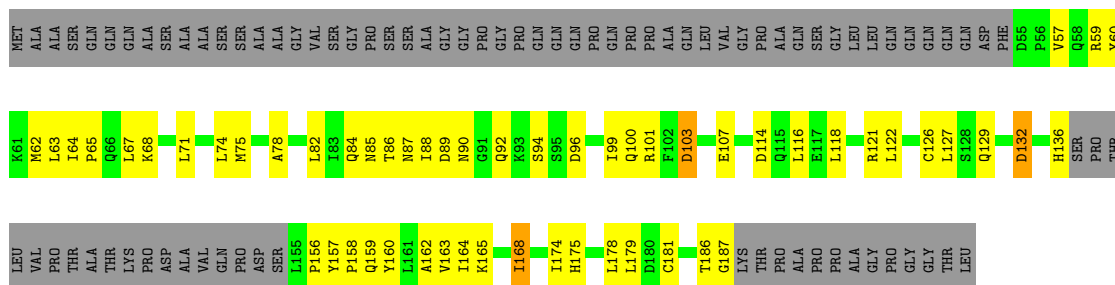
- Molecule 58: Mediator of RNA polymerase II transcription subunit 17





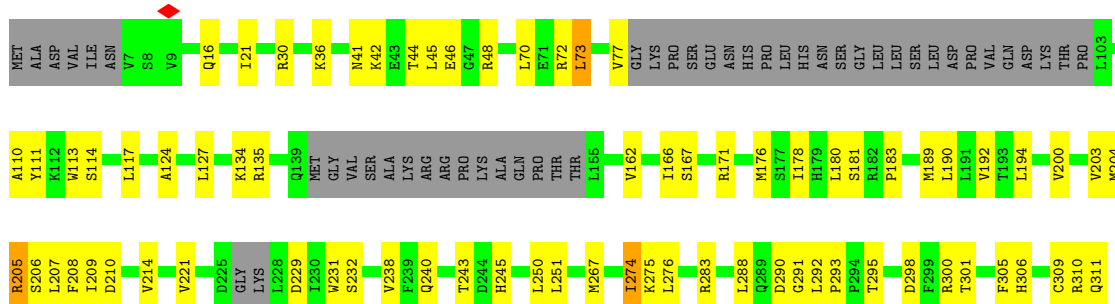
• Molecule 60: Mediator of RNA polymerase II transcription subunit 29

Chain b: 30% 26% 42%



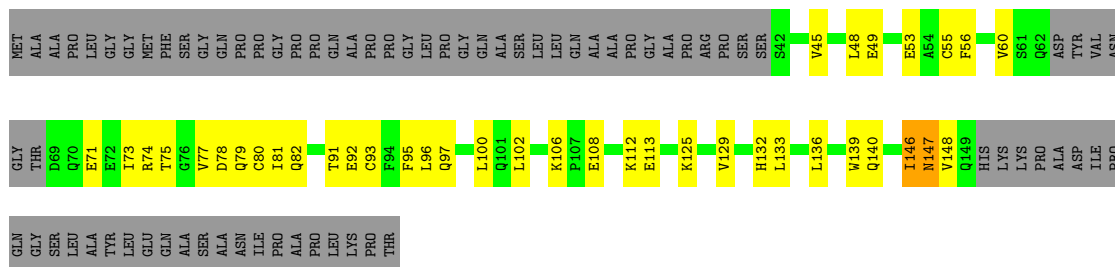
• Molecule 61: Mediator of RNA polymerase II transcription subunit 27

Chain c: 60% 23% 15%



• Molecule 62: Mediator of RNA polymerase II transcription subunit 28

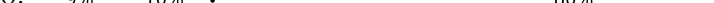
Chain e: 35% 21% 43%

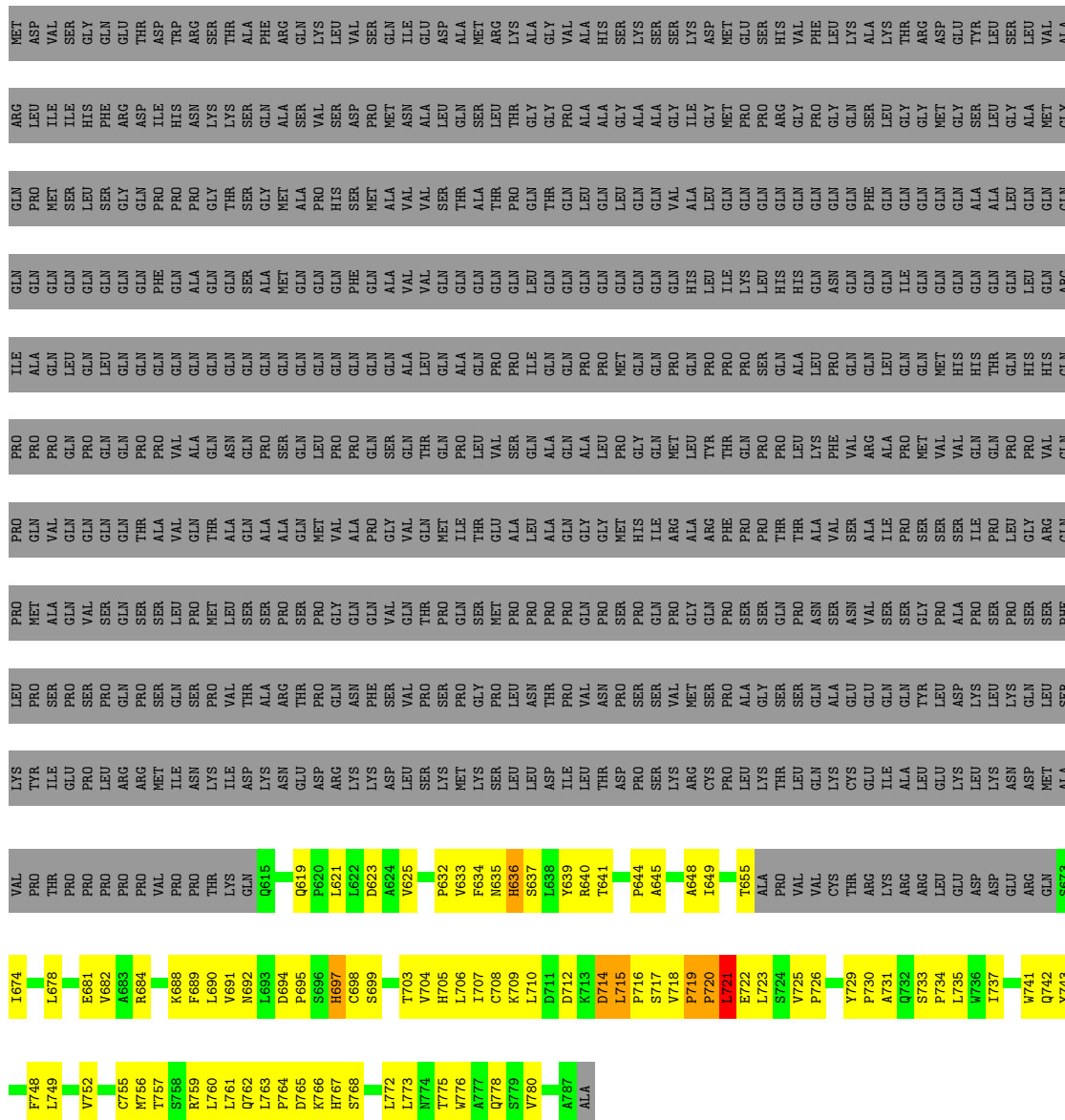


• Molecule 63: Mediator of RNA polymerase II transcription subunit 30

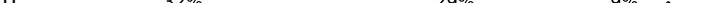
Chain l: 47% 24% 29%

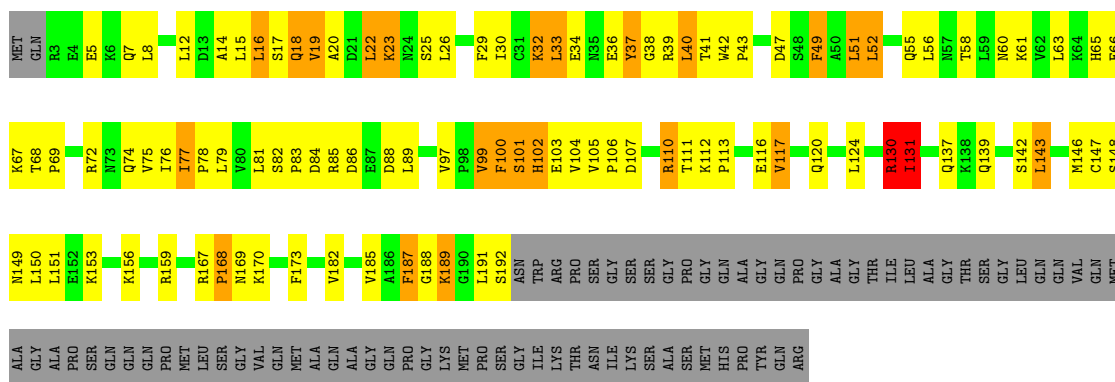
- Molecule 64: Mediator of RNA polymerase II transcription subunit 15

Chain o:  9% 10% 80%

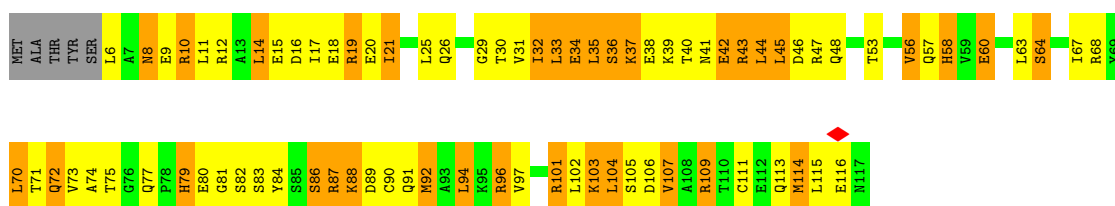
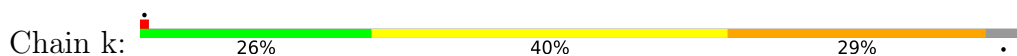


- Molecule 65: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

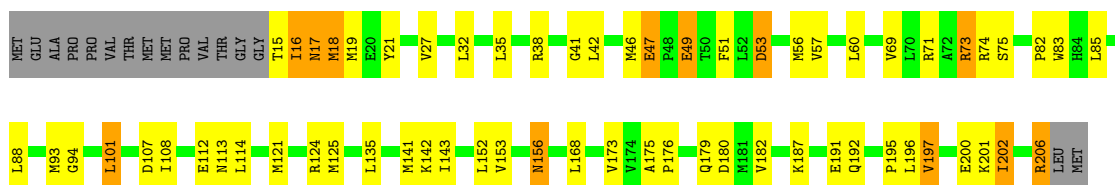
Chain h:  32% 29% 9% 29%



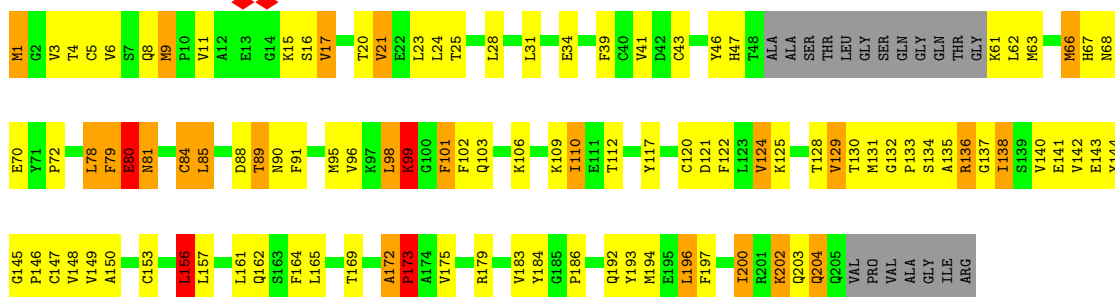
• Molecule 66: Mediator of RNA polymerase II transcription subunit 11



• Molecule 67: Mediator of RNA polymerase II transcription subunit 18

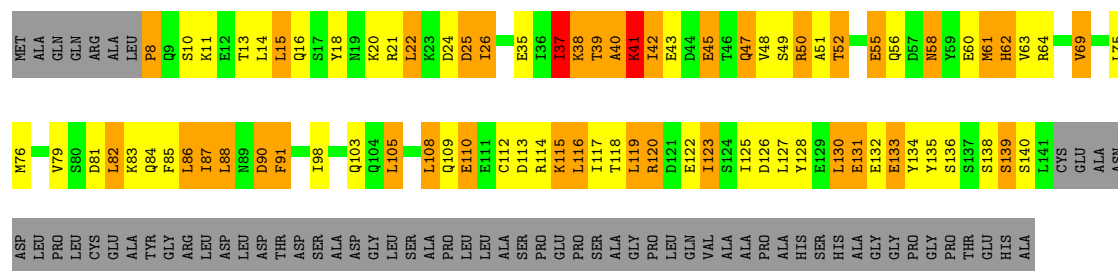


• Molecule 68: Mediator of RNA polymerase II transcription subunit 20



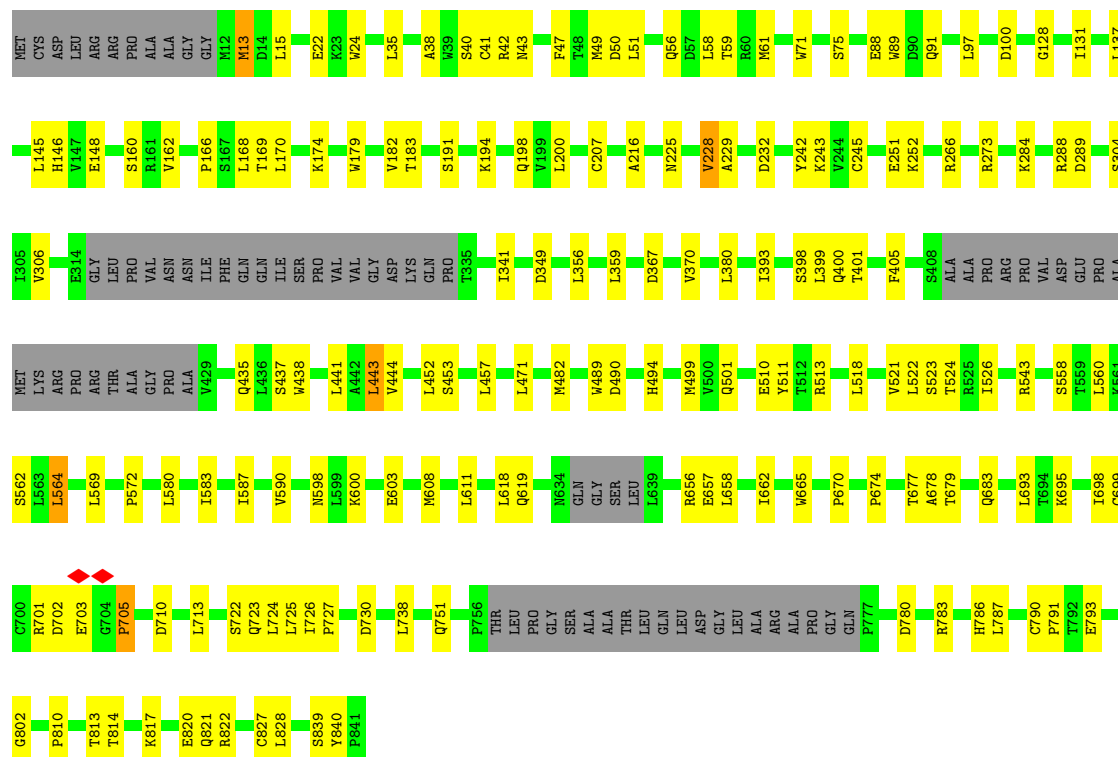
• Molecule 69: Mediator of RNA polymerase II transcription subunit 22





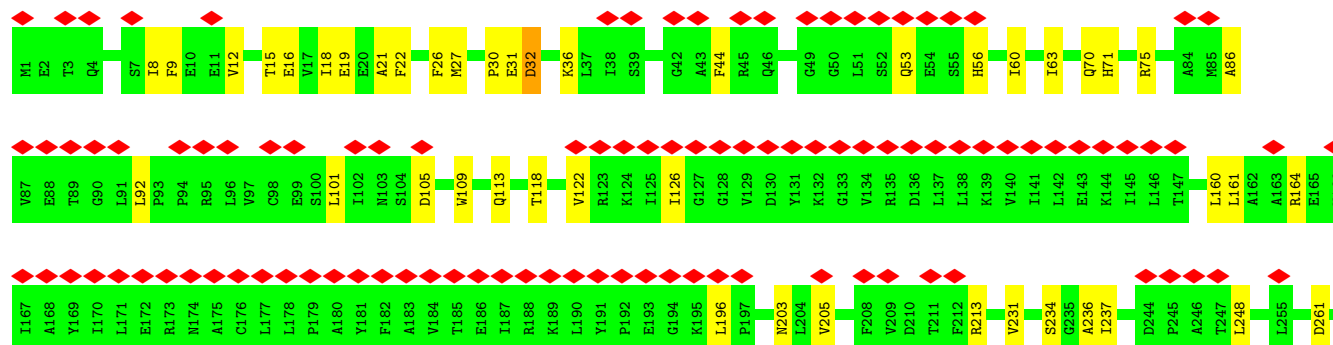
- Molecule 70: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

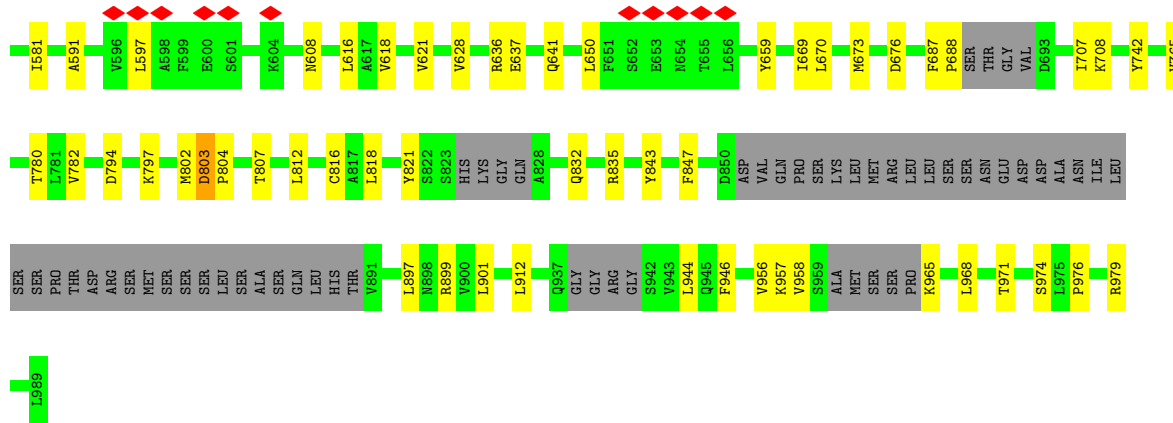
Chain p:



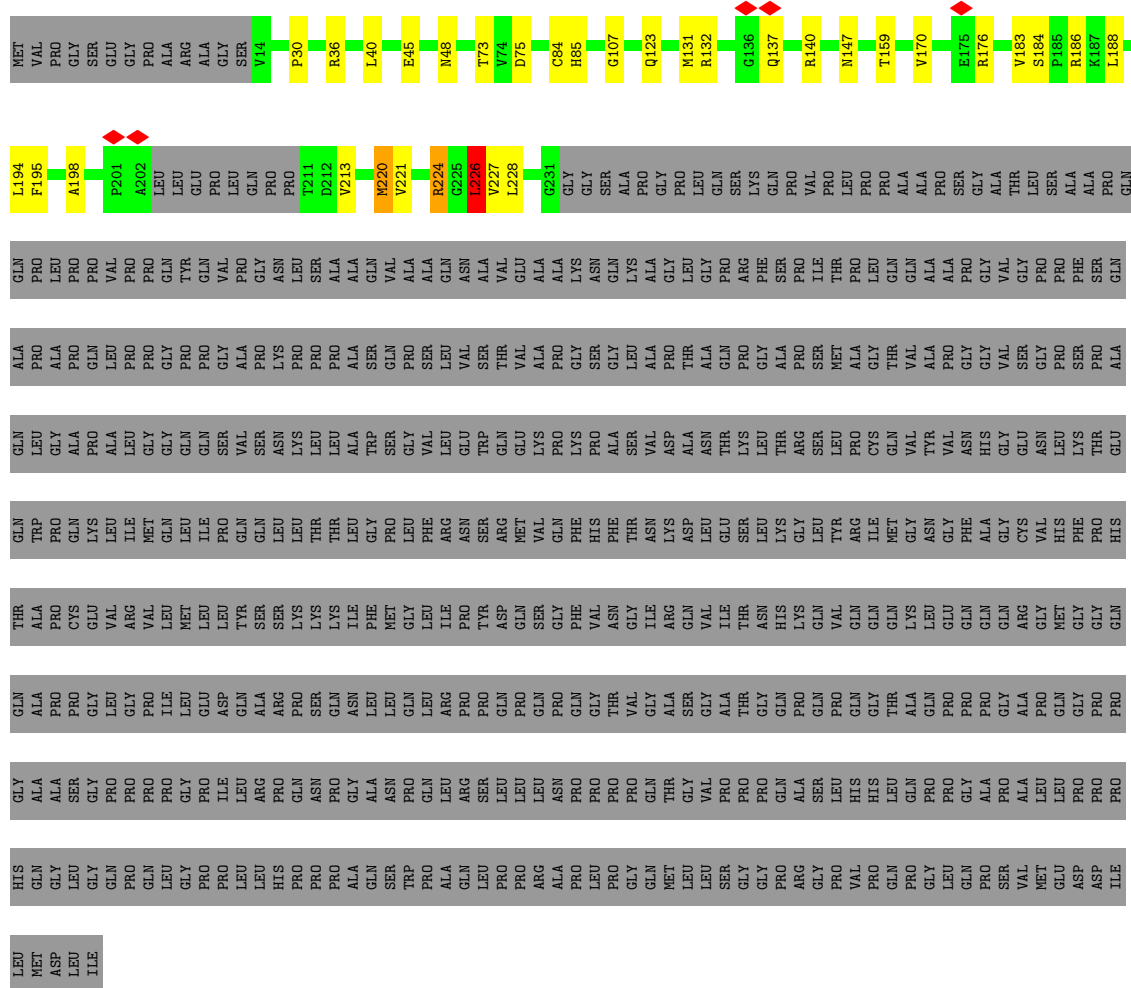
- Molecule 71: Mediator of RNA polymerase II transcription subunit 23

Chain w:





• Molecule 73: Mediator of RNA polymerase II transcription subunit 25

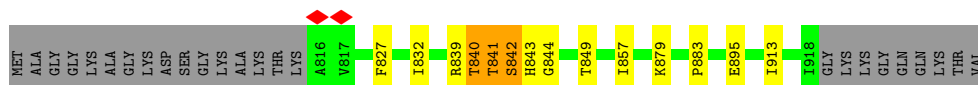


• Molecule 74: HISTONE H2A.Z

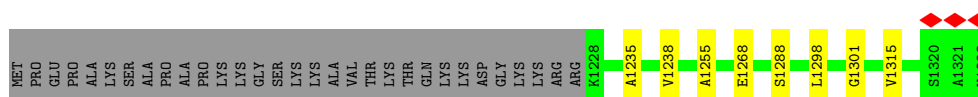




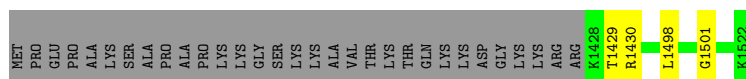
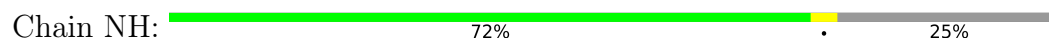
• Molecule 74: HISTONE H2A.Z



• Molecule 75: Histone H2B



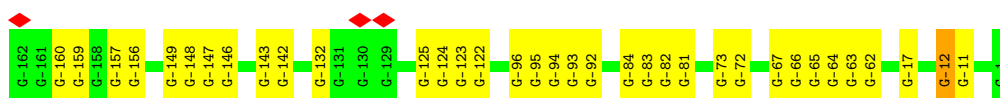
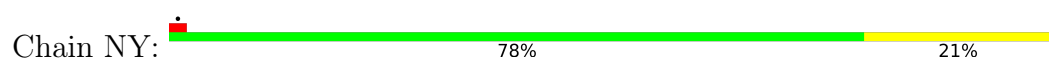
• Molecule 75: Histone H2B



• Molecule 76: DNA (162-mer)



• Molecule 77: DNA (162-mer)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26458	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	2.678	Depositor
Minimum map value	-1.034	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.156	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: MG, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	X	0.42	0/1561	0.60	1/2411 (0.0%)
2	Y	0.48	0/1516	0.63	1/2334 (0.0%)
3	BA	0.13	0/1983	0.27	0/2679
4	DA	0.66	0/4679	0.90	6/6320 (0.1%)
5	EA	0.32	0/1560	0.58	1/2097 (0.0%)
6	FA	0.11	0/1167	0.27	0/1576
7	HA	0.14	0/5875	0.30	0/7955
8	NA	1.12	1/497 (0.2%)	1.43	2/693 (0.3%)
8	NE	1.27	0/510	1.55	6/710 (0.8%)
9	PA	0.24	0/11851	0.38	1/16014 (0.0%)
10	DB	0.49	1/7993 (0.0%)	0.71	8/10836 (0.1%)
11	EB	0.23	0/1427	0.44	0/1916
12	FB	0.19	0/1817	0.35	0/2445
13	HB	0.15	0/2210	0.31	0/2975
14	NB	1.23	0/390	1.46	5/539 (0.9%)
14	NF	1.39	5/420 (1.2%)	1.49	5/581 (0.9%)
15	PB	0.13	0/9257	0.28	0/12493
16	HC	0.21	0/3230	0.37	0/4376
17	PC	0.13	0/2102	0.29	0/2857
18	PE	0.12	0/1752	0.28	0/2366
19	PF	0.24	0/646	0.40	0/871
20	PH	0.11	0/1207	0.28	0/1628
21	PI	0.12	0/949	0.29	0/1284
22	PJ	0.14	0/516	0.25	0/696
23	PK	0.15	0/939	0.26	0/1271
24	PL	0.13	0/378	0.27	0/500
25	DP	0.14	0/1448	0.28	0/1948
26	DQ	0.16	0/945	0.35	0/1274
27	DO	0.15	0/816	0.29	0/1105
28	Dc	0.48	0/1035	0.67	0/1406
29	DD	0.56	0/1343	0.85	2/1795 (0.1%)
29	Dd	0.22	0/1321	0.44	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	DE	0.43	0/4469	0.64	2/6050 (0.0%)
30	De	0.29	0/4433	0.53	0/6004
31	DF	0.70	1/3167 (0.0%)	1.07	10/4303 (0.2%)
31	Df	0.48	0/3140	0.81	6/4268 (0.1%)
32	DI	0.62	0/981	0.84	0/1332
32	Di	0.24	0/989	0.44	0/1343
33	DJ	0.24	0/736	0.46	0/998
33	Dj	0.23	0/775	0.45	0/1049
34	Dk	0.30	0/799	0.54	1/1070 (0.1%)
35	DL	0.65	0/613	1.03	1/829 (0.1%)
35	Dl	0.54	0/888	0.80	0/1194
36	Dm	0.32	0/733	0.55	0/977
37	DG	0.71	0/1199	0.95	1/1612 (0.1%)
38	DH	0.46	0/1673	0.75	2/2285 (0.1%)
39	HD	0.68	0/2436	1.05	23/3286 (0.7%)
40	HE	0.30	0/2103	0.42	0/2846
41	HG	0.13	0/2793	0.27	0/3780
42	HH	0.13	0/4994	0.29	0/6745
43	HF	0.19	0/529	0.43	1/714 (0.1%)
44	HI	1.02	0/2433	1.64	46/3302 (1.4%)
45	HJ	1.10	3/2356 (0.1%)	1.72	55/3185 (1.7%)
46	PD	0.28	0/1064	0.39	0/1428
47	PG	0.20	0/1382	0.33	0/1874
48	g	0.78	0/911	1.40	8/1219 (0.7%)
49	j	0.38	0/849	0.61	0/1150
50	n	0.43	0/7901	0.73	17/10731 (0.2%)
51	s	0.93	0/741	1.25	6/1002 (0.6%)
52	u	0.75	1/895 (0.1%)	1.10	9/1215 (0.7%)
53	a	0.93	0/3507	1.34	11/4760 (0.2%)
54	d	0.92	0/1281	1.30	1/1718 (0.1%)
55	f	0.75	1/1402 (0.1%)	1.00	2/1905 (0.1%)
56	i	0.99	1/612 (0.2%)	1.35	1/815 (0.1%)
57	m	0.21	0/1010	0.39	0/1359
58	q	0.66	1/4456 (0.0%)	0.87	0/6019
59	z	0.95	0/781	1.40	5/1067 (0.5%)
60	b	0.75	0/911	1.13	1/1229 (0.1%)
61	c	0.58	0/2172	0.88	4/2935 (0.1%)
62	e	0.25	0/840	0.44	0/1128
63	l	0.19	0/1048	0.40	0/1405
64	o	0.52	0/1256	0.86	3/1724 (0.2%)
65	h	0.93	0/1485	1.32	3/2008 (0.1%)
66	k	0.98	0/885	1.32	1/1190 (0.1%)
67	r	0.91	0/1565	1.27	2/2106 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	t	1.04	2/1530 (0.1%)	1.49	10/2066 (0.5%)
69	v	0.97	0/1092	1.43	6/1468 (0.4%)
70	p	0.65	0/6116	0.76	3/8311 (0.0%)
71	w	0.52	0/11056	0.65	4/15023 (0.0%)
72	x	0.59	0/7191	0.78	11/9728 (0.1%)
73	y	0.63	0/1645	0.83	0/2240
74	NC	1.27	2/505 (0.4%)	1.53	9/700 (1.3%)
74	NG	1.09	1/523 (0.2%)	1.44	10/724 (1.4%)
75	ND	1.22	2/470 (0.4%)	1.46	5/654 (0.8%)
75	NH	1.10	0/470	1.44	3/654 (0.5%)
76	NX	0.38	0/3401	0.67	2/5180 (0.0%)
77	NY	0.34	0/4046	0.57	1/6310 (0.0%)
All	All	0.53	22/190578 (0.0%)	0.77	324/259940 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
39	HD	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	q	452	ALA	C-N	9.13	1.47	1.33
55	f	110	ASP	C-N	-8.18	1.22	1.33
45	HJ	244	CYS	C-O	6.98	1.32	1.24
68	t	136	ARG	C-O	-6.86	1.15	1.23
68	t	89	THR	C-O	6.61	1.32	1.24
10	DB	61	ASN	C-O	-6.32	1.18	1.24
8	NA	518	THR	CA-CB	6.32	1.62	1.53
14	NF	250	ILE	CA-CB	6.25	1.62	1.54
56	i	100	LEU	C-O	6.15	1.31	1.24
31	DF	395	ARG	C-O	5.94	1.32	1.24
45	HJ	258	LEU	C-O	5.85	1.30	1.24
74	NG	1110	ILE	CA-C	5.66	1.58	1.53
14	NF	297	LEU	C-O	-5.54	1.17	1.24
74	NC	857	ILE	CA-CB	5.53	1.60	1.54
45	HJ	201	THR	N-CA	5.49	1.52	1.45
74	NC	913	ILE	CA-CB	-5.48	1.47	1.54
14	NF	243	VAL	CA-CB	-5.26	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	u	77	PRO	C-O	-5.22	1.17	1.23
14	NF	231	LYS	CA-C	5.18	1.59	1.52
75	ND	1255	ALA	CA-CB	-5.16	1.45	1.53
14	NF	300	PHE	CA-C	5.13	1.59	1.52
75	ND	1238	VAL	CA-CB	5.10	1.60	1.54

All (324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g	128	PRO	N-CA-C	-13.40	91.97	114.75
8	NA	464	LYS	N-CA-C	12.62	124.58	111.07
48	g	130	GLN	N-CA-C	-11.90	98.33	111.07
72	x	12	GLN	N-CA-C	-11.47	99.24	113.01
8	NE	635	VAL	N-CA-C	-10.90	102.21	111.91
39	HD	291	LEU	N-CA-C	-10.19	99.99	111.71
45	HJ	186	ILE	N-CA-C	-10.14	100.28	110.62
10	DB	491	HIS	N-CA-C	-9.70	100.70	111.28
8	NE	717	VAL	N-CA-C	-9.44	103.94	113.10
45	HJ	37	ASN	N-CA-C	-9.39	101.04	111.28
50	n	1351	PRO	N-CA-CB	9.33	112.13	103.08
48	g	126	TYR	N-CA-C	-9.21	102.22	112.72
50	n	1343	PRO	N-CA-CB	9.21	112.01	103.08
31	Df	149	PRO	O-C-N	9.11	125.50	121.31
50	n	288	PRO	N-CA-C	8.91	127.02	113.75
53	a	505	PRO	N-CA-C	-8.82	101.74	113.65
53	a	505	PRO	CA-C-N	8.74	132.44	120.46
53	a	505	PRO	C-N-CA	8.74	132.44	120.46
14	NB	28	GLY	N-CA-C	-8.69	103.88	114.66
45	HJ	108	CYS	N-CA-C	-8.39	102.13	111.28
50	n	591	PHE	CA-CB-CG	8.36	122.16	113.80
74	NC	839	ARG	N-CA-C	-8.33	103.22	112.72
68	t	80	GLU	CB-CA-C	-8.31	106.98	116.54
39	HD	55	LYS	CA-C-O	-8.22	112.36	122.64
31	DF	320	ARG	CB-CG-CD	8.14	130.03	111.30
44	HI	275	LEU	N-CA-C	-8.12	102.43	111.28
61	c	274	ILE	N-CA-C	-8.09	105.61	113.53
45	HJ	184	PRO	CB-CA-C	-7.98	102.23	113.09
44	HI	280	PRO	N-CA-C	-7.93	102.94	113.65
44	HI	280	PRO	CB-CA-C	-7.93	99.84	112.21
68	t	153	CYS	N-CA-C	-7.91	103.53	113.02
50	n	1355	PRO	N-CA-CB	7.87	111.51	103.25
48	g	128	PRO	CA-N-CD	-7.66	101.28	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	u	64	ARG	CB-CA-C	-7.65	98.87	110.88
50	n	1344	PRO	N-CA-CB	7.64	110.19	102.17
38	DH	110	TYR	CB-CA-C	-7.57	98.99	110.88
44	HI	199	VAL	N-CA-C	-7.56	102.91	110.62
44	HI	85	SER	N-CA-C	-7.52	103.06	111.71
50	n	526	SER	N-CA-C	-7.36	104.30	113.28
39	HD	256	TYR	N-CA-C	-7.35	99.56	110.06
51	s	107	ASN	N-CA-C	-7.33	95.18	110.80
44	HI	142	ASN	N-CA-C	-7.30	104.83	113.38
50	n	1352	PRO	N-CA-CB	7.28	110.89	103.25
4	DA	640	LEU	N-CA-C	-7.26	103.53	113.18
9	PA	1795	PRO	N-CA-C	-7.23	99.70	111.77
74	NG	1118	ILE	N-CA-C	-7.20	100.29	109.58
50	n	591	PHE	CB-CA-C	7.12	121.03	111.70
4	DA	715	PRO	N-CA-C	-7.07	100.14	111.03
53	a	437	LEU	N-CA-C	-7.05	101.51	111.24
50	n	1347	PRO	N-CA-CB	7.03	109.90	103.08
8	NE	664	LYS	N-CA-C	7.02	118.73	111.14
50	n	1326	PRO	N-CA-CB	7.02	110.72	103.00
39	HD	55	LYS	CB-CA-C	-7.02	100.70	112.00
48	g	71	GLN	N-CA-C	-7.01	103.64	111.71
53	a	412	ARG	CB-CA-C	7.01	122.37	110.74
31	DF	271	VAL	N-CA-C	-7.00	106.18	112.90
10	DB	495	GLN	N-CA-C	-7.00	104.74	113.28
44	HI	140	PRO	CB-CA-C	-7.00	101.38	113.20
52	u	74	ASP	N-CA-C	-6.92	103.35	112.34
48	g	129	HIS	N-CA-C	-6.91	104.49	113.12
4	DA	498	PRO	N-CA-CB	6.89	110.48	103.25
68	t	137	GLY	CA-C-O	-6.87	114.82	122.24
39	HD	284	ALA	N-CA-C	-6.86	103.82	111.71
44	HI	136	ARG	CA-C-N	-6.84	113.87	123.03
44	HI	136	ARG	C-N-CA	-6.84	113.87	123.03
44	HI	271	LEU	CA-C-N	-6.83	111.81	120.56
44	HI	271	LEU	C-N-CA	-6.83	111.81	120.56
74	NG	1039	ARG	N-CA-C	-6.82	102.21	111.55
72	x	444	SER	CA-C-N	-6.81	114.85	120.98
72	x	444	SER	C-N-CA	-6.81	114.85	120.98
75	ND	1298	LEU	N-CA-C	6.75	120.73	112.23
50	n	1255	PRO	N-CA-CB	6.74	110.33	103.25
29	DD	923	GLN	N-CA-C	-6.74	105.03	113.18
50	n	1237	PRO	N-CA-CB	6.70	110.29	103.25
34	Dk	180	PRO	N-CA-C	6.69	118.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	NB	46	ILE	N-CA-C	6.69	117.47	108.11
69	v	24	ASP	N-CA-C	-6.68	104.00	111.28
14	NF	219	ARG	N-CA-C	6.67	125.00	110.80
44	HI	287	THR	CB-CA-C	-6.66	99.74	110.79
61	c	306	HIS	N-CA-C	-6.64	100.44	110.28
59	z	595	PRO	CB-CA-C	-6.64	101.14	110.63
64	o	719	PRO	N-CA-C	6.62	118.78	110.70
45	HJ	45	PRO	CB-CA-C	-6.60	101.73	112.62
53	a	231	LEU	N-CA-C	-6.58	104.11	111.28
31	Df	326	HIS	N-CA-C	-6.57	104.37	112.38
45	HJ	29	LYS	CA-C-N	-6.54	111.52	120.28
45	HJ	29	LYS	C-N-CA	-6.54	111.52	120.28
50	n	1348	PRO	N-CA-CB	6.54	110.22	103.23
45	HJ	14	SER	N-CA-C	6.54	119.73	111.69
31	Df	319	LEU	N-CA-C	-6.50	104.03	112.68
55	f	110	ASP	O-C-N	-6.49	114.98	122.89
39	HD	220	PRO	N-CA-CB	6.46	110.03	103.25
72	x	53	GLY	CA-C-O	-6.44	116.21	122.46
72	x	804	PRO	CB-CA-C	6.43	118.76	110.92
74	NC	827	PHE	CA-C-N	6.42	127.86	119.84
74	NC	827	PHE	C-N-CA	6.42	127.86	119.84
44	HI	53	ASP	N-CA-C	-6.42	106.17	112.97
45	HJ	82	THR	N-CA-C	-6.40	104.30	111.28
68	t	156	LEU	CA-C-N	-6.39	111.72	120.28
68	t	156	LEU	C-N-CA	-6.39	111.72	120.28
45	HJ	232	LEU	N-CA-C	-6.37	104.34	111.28
31	DF	81	GLU	CA-C-N	6.35	126.10	119.05
31	DF	81	GLU	C-N-CA	6.35	126.10	119.05
45	HJ	118	PHE	N-CA-C	-6.35	105.53	113.28
51	s	108	PHE	N-CA-C	-6.34	99.07	109.40
50	n	1343	PRO	N-CA-C	-6.33	102.98	110.70
52	u	31	PRO	N-CA-C	-6.28	103.86	110.58
53	a	509	ARG	CB-CA-C	-6.28	101.02	110.88
45	HJ	103	ILE	CA-C-N	-6.27	111.87	120.46
45	HJ	103	ILE	C-N-CA	-6.27	111.87	120.46
50	n	74	PRO	N-CA-CB	6.26	110.15	103.52
4	DA	1076	VAL	N-CA-C	6.25	117.03	110.72
31	DF	325	ASN	N-CA-C	-6.25	104.55	111.36
39	HD	237	PRO	N-CA-CB	6.21	109.77	103.25
72	x	35	ALA	CA-C-N	6.18	133.35	121.54
72	x	35	ALA	C-N-CA	6.18	133.35	121.54
65	h	49	PHE	CB-CA-C	-6.17	101.46	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DF	316	GLN	CB-CA-C	6.16	120.29	110.19
52	u	80	GLU	N-CA-C	-6.14	104.43	112.41
70	p	780	ASP	N-CA-C	-6.13	98.73	108.73
52	u	77	PRO	N-CA-C	6.13	120.83	111.15
44	HI	268	LEU	N-CA-C	-6.12	104.72	111.82
39	HD	295	ARG	CA-C-N	-6.12	112.49	120.44
39	HD	295	ARG	C-N-CA	-6.12	112.49	120.44
14	NF	246	ILE	N-CA-C	6.11	116.68	107.75
45	HJ	187	LEU	N-CA-C	-6.09	104.55	111.07
45	HJ	39	LYS	N-CA-C	-6.09	104.64	111.28
74	NC	883	PRO	N-CA-C	-6.08	105.08	113.53
74	NG	1119	GLY	N-CA-C	6.05	127.53	113.18
65	h	168	PRO	N-CA-CB	6.05	109.61	103.25
74	NC	879	LYS	N-CA-C	6.04	120.81	112.90
44	HI	287	THR	N-CA-C	-6.03	104.71	111.28
4	DA	822	PRO	N-CA-C	-6.03	100.05	112.47
14	NB	44	LYS	N-CA-C	6.03	120.65	113.12
45	HJ	84	CYS	CB-CA-C	-6.02	100.79	110.79
68	t	133	PRO	CB-CA-C	-6.01	101.64	111.56
45	HJ	82	THR	CB-CA-C	-6.01	100.82	110.79
44	HI	240	MET	N-CA-C	-6.00	104.73	111.28
31	DF	364	VAL	N-CA-C	5.99	116.73	110.62
44	HI	96	THR	CB-CA-C	-5.99	98.51	110.42
44	HI	50	GLU	N-CA-C	-5.97	105.84	113.01
44	HI	261	PHE	N-CA-C	-5.97	98.99	108.73
45	HJ	30	PHE	CB-CA-C	-5.97	100.88	110.79
68	t	90	ASN	N-CA-C	-5.94	105.88	113.01
48	g	125	GLU	N-CA-C	-5.93	105.89	113.01
45	HJ	274	LYS	CB-CA-C	-5.93	101.57	110.88
74	NC	842	SER	CB-CA-C	-5.92	109.17	117.23
39	HD	285	GLY	N-CA-C	-5.92	107.83	114.40
71	w	30	PRO	N-CA-C	-5.92	101.90	111.19
29	DD	963	ARG	CB-CA-C	-5.91	100.98	110.79
45	HJ	60	TYR	CB-CA-C	5.89	120.86	110.85
75	ND	1235	ALA	N-CA-C	5.88	118.45	111.33
31	Df	255	MET	N-CA-C	-5.88	104.97	114.09
45	HJ	204	TYR	N-CA-C	-5.87	104.88	111.28
69	v	90	ASP	CA-C-O	-5.86	114.85	121.00
10	DB	181	GLY	CA-C-O	-5.86	118.09	122.37
45	HJ	80	VAL	CB-CA-C	-5.86	104.23	112.14
39	HD	217	PRO	N-CA-CB	5.85	109.77	103.33
53	a	278	HIS	CB-CA-C	5.84	118.75	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	ND	1315	VAL	N-CA-C	-5.83	105.43	110.74
45	HJ	288	ASN	N-CA-C	5.83	118.04	109.24
8	NA	517	VAL	N-CA-C	-5.81	107.62	113.20
59	z	529	HIS	CA-CB-CG	-5.81	107.99	113.80
44	HI	290	LEU	N-CA-C	-5.80	104.96	111.28
45	HJ	19	LEU	CA-C-N	-5.80	112.51	120.28
45	HJ	19	LEU	C-N-CA	-5.80	112.51	120.28
45	HJ	278	GLU	CB-CA-C	-5.79	101.18	110.79
2	Y	-14	DT	C4'-C3'-O3'	5.79	118.68	110.00
44	HI	204	ALA	N-CA-C	-5.77	104.89	111.07
44	HI	139	LYS	CB-CA-C	5.76	118.26	109.56
43	HF	3	ASN	CB-CA-C	-5.75	99.17	110.10
44	HI	238	PRO	CA-C-O	-5.75	114.89	121.56
44	HI	280	PRO	CA-C-N	-5.75	112.57	120.28
44	HI	280	PRO	C-N-CA	-5.75	112.57	120.28
44	HI	253	PRO	N-CA-C	-5.74	105.55	113.53
45	HJ	202	ASP	N-CA-C	-5.73	106.62	113.21
74	NG	1110	ILE	CA-C-N	-5.73	113.86	119.76
74	NG	1110	ILE	C-N-CA	-5.73	113.86	119.76
44	HI	206	LEU	CA-C-N	-5.70	112.69	120.44
44	HI	206	LEU	C-N-CA	-5.70	112.69	120.44
31	Df	150	PRO	N-CA-C	5.70	117.65	110.70
4	DA	638	PRO	CB-CA-C	-5.68	106.23	111.40
71	w	1198	GLN	N-CA-C	-5.68	102.11	110.52
50	n	525	TYR	CB-CA-C	5.67	118.22	110.06
51	s	73	GLY	CA-C-N	5.67	128.19	120.54
51	s	73	GLY	C-N-CA	5.67	128.19	120.54
45	HJ	29	LYS	CB-CA-C	-5.67	101.98	110.88
68	t	173	PRO	N-CA-CB	-5.67	97.30	103.25
45	HJ	33	LYS	CA-C-N	-5.66	112.69	120.28
45	HJ	33	LYS	C-N-CA	-5.66	112.69	120.28
14	NF	251	TYR	N-CA-C	5.66	117.13	111.07
14	NB	29	ILE	N-CA-C	-5.64	98.53	107.15
39	HD	298	GLN	CA-C-N	-5.63	112.74	120.28
39	HD	298	GLN	C-N-CA	-5.63	112.74	120.28
8	NE	655	GLN	CA-C-N	-5.63	113.26	122.54
8	NE	655	GLN	C-N-CA	-5.63	113.26	122.54
45	HJ	278	GLU	N-CA-C	-5.61	105.16	111.28
5	EA	106	LYS	N-CA-C	-5.61	105.07	111.07
35	DL	112	GLU	CB-CA-C	-5.59	110.12	116.54
14	NF	228	GLY	N-CA-C	-5.58	107.74	114.66
45	HJ	271	ALA	CA-C-N	-5.57	113.54	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	HJ	271	ALA	C-N-CA	-5.57	113.54	120.56
45	HJ	109	ALA	CA-C-N	-5.57	112.81	120.28
45	HJ	109	ALA	C-N-CA	-5.57	112.81	120.28
45	HJ	187	LEU	CA-C-N	-5.57	113.02	120.54
45	HJ	187	LEU	C-N-CA	-5.57	113.02	120.54
72	x	565	SER	N-CA-C	-5.57	101.80	110.10
45	HJ	116	ASP	CA-C-N	-5.57	114.60	122.34
45	HJ	116	ASP	C-N-CA	-5.57	114.60	122.34
52	u	79	GLU	CB-CG-CD	5.56	122.06	112.60
10	DB	583	GLU	CB-CA-C	-5.55	101.57	110.79
45	HJ	167	PHE	CA-C-N	-5.55	112.84	120.28
45	HJ	167	PHE	C-N-CA	-5.55	112.84	120.28
39	HD	289	SER	CA-C-N	-5.54	113.23	120.44
39	HD	289	SER	C-N-CA	-5.54	113.23	120.44
75	NH	1429	THR	N-CA-C	5.54	118.35	110.10
74	NC	849	THR	N-CA-C	5.53	120.02	113.16
75	NH	1498	LEU	N-CA-C	5.53	120.14	112.90
53	a	162	ASN	N-CA-C	-5.52	106.62	113.19
14	NF	229	ILE	N-CA-C	-5.52	98.54	106.55
74	NG	1040	THR	N-CA-C	5.51	118.56	109.85
77	NY	-12	DG	C2'-C3'-O3'	5.51	119.77	111.50
31	Df	329	LEU	N-CA-C	-5.49	106.28	112.87
14	NB	40	ARG	N-CA-C	-5.49	105.68	112.38
69	v	37	ILE	CB-CA-C	5.48	119.58	112.24
44	HI	276	PHE	CA-C-O	-5.47	114.62	120.42
76	NX	2	DC	C2'-C3'-O3'	-5.46	103.31	111.50
74	NC	832	ILE	N-CA-C	-5.45	105.22	110.72
10	DB	264	GLU	N-CA-C	-5.44	106.32	113.17
61	c	205	ARG	N-CA-C	-5.43	106.82	113.50
74	NG	1027	PHE	CA-C-N	5.43	126.62	119.84
74	NG	1027	PHE	C-N-CA	5.43	126.62	119.84
45	HJ	177	ARG	CB-CA-C	5.42	120.07	110.85
75	NH	1430	ARG	N-CA-C	5.42	118.04	109.96
76	NX	25	DC	C2'-C3'-O3'	-5.42	103.37	111.50
56	i	135	TYR	CB-CA-C	5.42	120.55	109.55
44	HI	138	LEU	N-CA-C	-5.41	101.84	109.96
59	z	492	ARG	CB-CA-C	-5.41	102.38	110.88
30	DE	449	LYS	N-CA-C	-5.39	105.96	112.54
53	a	136	PRO	N-CA-C	-5.39	106.04	113.53
44	HI	137	ASP	N-CA-C	5.39	117.38	108.49
31	DF	324	ASP	N-CA-C	-5.39	105.52	111.71
45	HJ	86	TYR	N-CA-C	-5.38	105.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	w	1195	ALA	N-CA-C	-5.38	105.52	111.71
68	t	202	LYS	CA-C-N	-5.37	113.03	120.38
68	t	202	LYS	C-N-CA	-5.37	113.03	120.38
51	s	105	LEU	N-CA-C	-5.36	99.38	110.80
54	d	179	ASP	N-CA-C	-5.36	108.52	114.62
45	HJ	279	ARG	N-CA-C	-5.35	105.45	111.28
39	HD	55	LYS	CA-C-N	-5.33	111.36	121.54
39	HD	55	LYS	C-N-CA	-5.33	111.36	121.54
45	HJ	26	ALA	CA-C-N	-5.33	113.14	120.28
45	HJ	26	ALA	C-N-CA	-5.33	113.14	120.28
67	r	15	THR	CA-C-N	-5.32	113.34	120.95
67	r	15	THR	C-N-CA	-5.32	113.34	120.95
30	DE	788	ARG	N-CA-C	-5.31	106.67	112.72
37	DG	183	ILE	N-CA-C	-5.31	102.66	109.30
52	u	81	SER	CA-C-O	-5.30	115.68	121.14
44	HI	283	ARG	CB-CA-C	5.30	117.79	109.84
45	HJ	33	LYS	N-CA-C	-5.30	105.50	111.28
45	HJ	233	SER	CA-C-O	-5.30	114.94	120.55
44	HI	169	TYR	CB-CA-C	5.29	118.48	109.80
45	HJ	112	ALA	CA-C-N	-5.29	113.19	120.28
45	HJ	112	ALA	C-N-CA	-5.29	113.19	120.28
61	c	221	VAL	N-CA-C	-5.29	106.72	112.80
51	s	102	LYS	N-CA-C	-5.29	107.01	112.93
10	DB	491	HIS	CB-CA-C	5.28	119.55	110.79
52	u	27	GLN	N-CA-C	-5.27	106.91	113.55
66	k	72	GLN	N-CA-C	-5.27	105.71	111.82
64	o	720	PRO	N-CA-C	5.26	120.99	113.47
69	v	25	ASP	CA-C-N	-5.26	113.26	120.46
69	v	25	ASP	C-N-CA	-5.26	113.26	120.46
44	HI	148	ASN	N-CA-C	-5.25	105.56	111.28
31	DF	272	VAL	N-CA-C	-5.24	105.27	110.62
38	DH	134	LEU	CB-CA-C	-5.24	110.52	116.54
74	NC	895	GLU	N-CA-C	5.24	117.07	111.36
44	HI	283	ARG	N-CA-C	-5.22	102.57	110.24
48	g	73	ASP	CA-CB-CG	-5.22	107.38	112.60
10	DB	644	GLN	O-C-N	5.21	128.50	121.83
74	NG	1069	ALA	N-CA-C	-5.21	105.68	111.36
45	HJ	79	VAL	CA-C-N	-5.20	113.34	120.46
45	HJ	79	VAL	C-N-CA	-5.20	113.34	120.46
60	b	88	ILE	N-CA-C	-5.20	104.90	110.36
72	x	435	LEU	N-CA-C	-5.19	105.52	111.07
1	X	20	DG	C4'-C3'-O3'	5.18	117.77	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	HI	271	LEU	N-CA-C	-5.17	105.64	111.28
39	HD	263	LEU	CA-C-N	-5.17	114.40	122.42
39	HD	263	LEU	C-N-CA	-5.17	114.40	122.42
64	o	636	HIS	O-C-N	5.17	127.60	122.12
39	HD	292	ALA	CA-C-N	-5.16	112.86	120.28
39	HD	292	ALA	C-N-CA	-5.16	112.86	120.28
72	x	445	GLY	N-CA-C	5.14	118.98	110.97
70	p	380	LEU	CA-C-N	-5.13	118.59	122.33
70	p	380	LEU	C-N-CA	-5.13	118.59	122.33
53	a	502	MET	N-CA-CB	5.11	119.13	110.49
55	f	109	PRO	O-C-N	5.11	129.24	123.10
59	z	598	CYS	N-CA-C	-5.11	104.34	111.30
75	ND	1288	SER	N-CA-C	-5.11	106.31	112.54
75	ND	1268	GLU	N-CA-C	-5.11	105.60	111.07
72	x	310	PHE	CB-CA-C	5.10	119.52	110.85
39	HD	298	GLN	CB-CA-C	-5.09	102.34	110.79
39	HD	298	GLN	N-CA-C	-5.08	105.74	111.28
71	w	1140	GLU	CA-CB-CG	5.08	124.26	114.10
74	NG	1120	LYS	N-CA-C	-5.08	99.99	110.80
31	DF	219	GLU	N-CA-C	-5.07	105.83	111.36
52	u	80	GLU	CB-CG-CD	5.07	121.22	112.60
44	HI	244	PRO	CB-CA-C	-5.07	105.00	113.06
44	HI	100	VAL	CA-C-N	-5.07	114.18	120.56
44	HI	100	VAL	C-N-CA	-5.07	114.18	120.56
44	HI	195	ASP	CA-C-N	-5.06	113.87	120.44
44	HI	195	ASP	C-N-CA	-5.06	113.87	120.44
44	HI	273	GLN	N-CA-C	-5.05	105.77	111.28
8	NE	685	GLN	N-CA-C	-5.05	102.80	110.28
45	HJ	92	LEU	N-CA-C	-5.05	107.12	113.28
44	HI	204	ALA	CB-CA-C	-5.05	102.95	110.88
69	v	8	PRO	N-CA-CB	5.04	108.55	103.00
10	DB	541	ARG	CB-CA-C	-5.04	101.65	110.17
44	HI	243	LEU	N-CA-CB	-5.04	103.34	110.04
65	h	58	THR	N-CA-C	-5.03	105.80	111.28
45	HJ	105	MET	CA-C-N	-5.02	113.55	120.28
45	HJ	105	MET	C-N-CA	-5.02	113.55	120.28
44	HI	17	PHE	CB-CA-C	-5.02	104.91	112.09
59	z	596	TYR	CB-CA-C	-5.02	102.57	110.86
44	HI	249	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	HD	126	GLN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1387	0	747	24	0
2	Y	1357	0	752	17	0
3	BA	1953	0	1987	20	0
4	DA	4563	0	4485	102	0
5	EA	1535	0	1539	133	0
6	FA	1138	0	1103	15	0
7	HA	5751	0	5794	104	0
8	NA	498	0	230	2	0
8	NE	511	0	238	3	0
9	PA	11628	0	11712	204	0
10	DB	7796	0	7751	116	0
11	EB	1403	0	1428	56	0
12	FB	1788	0	1819	33	0
13	HB	2167	0	2175	35	0
14	NB	391	0	185	0	0
14	NF	421	0	197	1	0
15	PB	9076	0	9116	123	0
16	HC	3158	0	3213	96	0
17	PC	2059	0	2007	23	0
18	PE	1721	0	1737	16	0
19	PF	636	0	665	7	0
20	PH	1186	0	1147	7	0
21	PI	928	0	859	11	0
22	PJ	507	0	523	14	0
23	PK	920	0	942	13	0
24	PL	373	0	378	8	0
25	DP	1422	0	1514	18	0
26	DQ	930	0	888	15	0
27	DO	806	0	818	31	0
28	Dc	1011	0	975	25	0
29	DD	1330	0	1351	127	0
29	Dd	1307	0	1318	14	0
30	DE	4364	0	4244	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	De	4327	0	4197	43	0
31	DF	3109	0	3045	310	0
31	Df	3081	0	3012	68	0
32	DI	959	0	969	133	0
32	Di	967	0	977	30	0
33	DJ	720	0	719	135	0
33	Dj	759	0	759	17	0
34	Dk	785	0	818	8	0
35	DL	605	0	606	77	0
35	Dl	876	0	893	27	0
36	Dm	724	0	744	13	0
37	DG	1180	0	1235	18	0
38	DH	1633	0	1621	165	0
39	HD	2400	0	2295	197	0
40	HE	2066	0	2097	52	0
41	HG	2732	0	2698	43	0
42	HH	4890	0	4949	63	0
43	HF	523	0	530	50	0
44	HI	2374	0	2389	205	0
45	HJ	2307	0	2314	149	0
46	PD	1050	0	1033	52	0
47	PG	1351	0	1358	98	0
48	g	898	0	936	79	0
49	j	840	0	718	37	0
50	n	7751	0	7530	586	0
51	s	723	0	727	53	0
52	u	886	0	871	143	0
53	a	3430	0	3461	420	0
54	d	1268	0	1305	277	0
55	f	1365	0	1337	172	0
56	i	605	0	628	210	0
57	m	983	0	968	90	0
58	q	4373	0	4433	550	0
59	z	765	0	728	78	0
60	b	899	0	908	116	0
61	c	2131	0	2140	100	0
62	e	832	0	824	101	0
63	l	1040	0	1065	86	0
64	o	1221	0	1212	123	0
65	h	1465	0	1460	198	0
66	k	879	0	886	192	0
67	r	1535	0	1545	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	t	1499	0	1482	105	0
69	v	1083	0	1059	197	0
70	p	5983	0	6071	134	0
71	w	10774	0	10838	146	0
72	x	7061	0	7223	229	0
73	y	1605	0	1576	24	0
74	NC	506	0	250	4	0
74	NG	524	0	260	7	0
75	ND	471	0	221	0	0
75	NH	471	0	221	0	0
76	NX	3078	0	1783	7	0
77	NY	3561	0	1784	20	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	5909	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (5909) 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)
54:d:49:ALA:HB2	56:i:76:MET:SD	1.22	1.71
60:b:174:ILE:CD1	63:l:75:LEU:HD21	1.22	1.61
9:PA:1795:PRO:HD2	54:d:169:PRO:CB	1.24	1.61
58:q:451:LEU:CD1	58:q:529:MET:HE1	1.30	1.61
5:EA:139:LEU:HD11	47:PG:151:ARG:CD	1.31	1.59
50:n:941:TYR:CD2	50:n:1172:SER:HB3	1.39	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:647:MET:HE3	71:w:22:PHE:CB	1.34	1.55
5:EA:139:LEU:CD1	47:PG:151:ARG:HD2	1.28	1.54
50:n:359:ILE:CG1	50:n:372:ILE:HD11	1.37	1.54
52:u:115:LEU:HB2	54:d:121:LEU:CD1	1.08	1.51
54:d:76:PHE:HZ	56:i:65:PHE:CE2	1.29	1.51
54:d:45:ILE:HG23	56:i:76:MET:CB	1.43	1.49
53:a:445:LEU:CG	72:x:55:SER:HB3	1.41	1.48
30:DE:694:LEU:HD13	30:DE:703:MET:CE	1.44	1.47
50:n:647:MET:CE	71:w:22:PHE:HB3	1.44	1.47
54:d:126:TYR:CE2	58:q:36:MET:HB3	1.50	1.47
52:u:90:LEU:HD22	58:q:9:ILE:CD1	1.45	1.46
64:o:639:TYR:CD2	70:p:786:HIS:HB3	1.48	1.46
50:n:960:LYS:HB2	50:n:1210:PHE:CE2	1.50	1.45
50:n:168:ARG:HG3	57:m:104:HIS:CE1	1.50	1.42
50:n:941:TYR:CD2	50:n:1172:SER:CB	2.03	1.41
54:d:76:PHE:CZ	56:i:65:PHE:CE2	2.04	1.41
65:h:146:MET:CG	66:k:39:LYS:HZ2	1.30	1.41
53:a:445:LEU:HD13	72:x:55:SER:N	1.26	1.41
58:q:451:LEU:HD12	58:q:529:MET:CE	1.51	1.41
52:u:90:LEU:CD2	58:q:9:ILE:HD11	1.50	1.40
54:d:45:ILE:CG2	56:i:76:MET:HB2	1.50	1.39
60:b:174:ILE:CG1	63:l:75:LEU:HD21	1.49	1.39
50:n:941:TYR:CE2	50:n:1172:SER:CB	2.05	1.39
27:DO:2:ALA:CA	29:DD:1000:ARG:HD3	1.53	1.38
69:v:16:GLN:NE2	69:v:20:LYS:HE2	1.07	1.38
50:n:359:ILE:HG12	50:n:372:ILE:CD1	1.54	1.37
54:d:76:PHE:CE2	56:i:65:PHE:CD2	2.12	1.35
50:n:957:PRO:CG	50:n:1210:PHE:CE1	2.09	1.35
53:a:445:LEU:CD1	72:x:55:SER:H	1.38	1.35
64:o:639:TYR:CD2	70:p:786:HIS:CB	2.08	1.35
52:u:115:LEU:CB	54:d:121:LEU:CD1	2.02	1.35
53:a:66:GLN:NE2	54:d:44:LEU:HD11	1.41	1.35
54:d:49:ALA:CB	56:i:76:MET:SD	2.12	1.35
5:EA:139:LEU:CD2	47:PG:151:ARG:HB3	1.55	1.34
53:a:364:TYR:HB3	53:a:430:LEU:CD1	1.58	1.34
54:d:76:PHE:CZ	56:i:65:PHE:CD2	2.14	1.34
50:n:545:LEU:HD11	50:n:653:PRO:CG	1.56	1.34
35:DL:111:LEU:HA	35:DL:114:LYS:NZ	1.39	1.34
53:a:70:LYS:NZ	56:i:74:LYS:HE2	1.36	1.34
53:a:70:LYS:HB2	56:i:70:HIS:ND1	1.39	1.33
60:b:181:CYS:SG	63:l:82:LEU:HD13	1.69	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:417:TYR:HD1	53:a:469:VAL:CG2	1.40	1.33
50:n:267:HIS:CD2	55:f:174:ARG:HD3	1.64	1.32
54:d:45:ILE:O	56:i:76:MET:HG2	1.22	1.32
30:DE:694:LEU:CD1	30:DE:703:MET:HE1	1.59	1.32
58:q:89:GLN:CG	58:q:90:PRO:HD2	1.60	1.31
58:q:186:GLU:HG3	58:q:243:LEU:CD2	1.59	1.31
39:HD:300:ALA:CB	45:HJ:166:PRO:HA	1.60	1.31
53:a:462:LEU:H	72:x:49:GLN:CG	1.43	1.31
31:DF:104:LEU:HB3	33:DJ:217:PHE:CE2	1.66	1.30
5:EA:143:GLN:HG2	47:PG:158:PHE:CZ	1.65	1.30
50:n:267:HIS:HB3	50:n:270:GLN:OE1	1.30	1.30
60:b:174:ILE:CD1	63:l:75:LEU:CD2	2.08	1.30
65:h:146:MET:HB2	66:k:39:LYS:NZ	1.45	1.30
53:a:445:LEU:HB3	72:x:55:SER:CB	1.61	1.30
58:q:451:LEU:CD1	58:q:529:MET:CE	2.08	1.30
9:PA:1795:PRO:CD	54:d:169:PRO:HB3	1.61	1.29
31:DF:218:VAL:HG12	38:DH:162:THR:OG1	1.31	1.29
39:HD:85:ARG:HH22	39:HD:139:LYS:C	1.40	1.29
10:DB:672:PHE:CE1	16:HC:414:SER:HB3	1.68	1.29
50:n:250:LEU:HD21	50:n:275:HIS:CD2	1.67	1.29
50:n:960:LYS:CB	50:n:1210:PHE:CE2	2.15	1.29
58:q:392:MET:SD	67:r:46:MET:HE1	1.72	1.28
5:EA:174:ARG:HB3	39:HD:8:ARG:NH2	1.47	1.28
50:n:921:MET:SD	50:n:1215:ILE:HD11	1.74	1.28
50:n:941:TYR:CE2	50:n:1172:SER:HB3	1.66	1.28
60:b:175:HIS:HB2	61:c:113:TRP:CH2	1.66	1.28
9:PA:1795:PRO:CD	54:d:169:PRO:CB	2.13	1.27
50:n:686:LYS:HZ3	64:o:730:PRO:CG	1.46	1.27
64:o:633:VAL:CG1	70:p:810:PRO:CB	2.13	1.27
35:DL:71:ASP:OD2	35:DL:74:GLU:HG3	1.33	1.27
53:a:417:TYR:CE1	53:a:450:PHE:CD1	2.23	1.27
30:DE:696:TRP:CH2	30:DE:703:MET:SD	2.28	1.27
38:DH:51:GLU:OE1	33:DJ:193:TYR:HB3	1.12	1.27
65:h:147:CYS:SG	69:v:41:LYS:HG2	1.75	1.27
50:n:904:PHE:CE2	50:n:1208:GLU:HG3	1.68	1.26
53:a:445:LEU:HD13	72:x:55:SER:CA	1.64	1.26
53:a:462:LEU:N	72:x:49:GLN:HG2	1.50	1.26
58:q:441:ARG:NH1	63:l:168:TRP:CD2	2.01	1.26
66:k:87:ARG:HA	69:v:105:LEU:CD1	1.65	1.26
53:a:59:VAL:HG21	54:d:51:SER:CB	1.62	1.26
58:q:171:VAL:HG21	66:k:17:ILE:CG2	1.64	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:HD:85:ARG:NH1	39:HD:140:LEU:HG	1.51	1.26
50:n:273:PHE:CZ	55:f:185:ARG:HD2	1.70	1.26
58:q:186:GLU:CG	58:q:243:LEU:CD2	2.13	1.26
58:q:479:ILE:HG22	58:q:532:HIS:CD2	1.71	1.26
53:a:445:LEU:CD2	72:x:55:SER:HB3	1.65	1.25
50:n:245:TRP:HB2	50:n:282:LEU:CD1	1.64	1.25
62:e:129:VAL:CG1	66:k:111:CYS:SG	2.23	1.25
65:h:146:MET:CB	66:k:39:LYS:HZ2	1.48	1.25
10:DB:672:PHE:CD1	16:HC:414:SER:HB3	1.72	1.24
58:q:458:PRO:HG3	58:q:533:GLN:NE2	1.49	1.24
31:DF:218:VAL:HG12	38:DH:162:THR:CB	1.66	1.24
53:a:445:LEU:CB	72:x:55:SER:HB3	1.65	1.24
58:q:458:PRO:CG	58:q:533:GLN:HE21	1.50	1.24
31:DF:323:VAL:CG2	31:DF:326:HIS:HB2	1.65	1.24
58:q:191:ARG:HD3	69:v:87:ILE:O	1.35	1.24
58:q:647:SER:HB3	62:e:93:CYS:SG	1.78	1.24
31:DF:219:GLU:CB	38:DH:160:ILE:HG21	1.68	1.23
50:n:250:LEU:CD2	50:n:275:HIS:CD2	2.21	1.23
50:n:545:LEU:HD11	50:n:653:PRO:CD	1.68	1.22
12:FB:186:MET:HE1	29:DD:995:GLU:OE2	1.40	1.22
12:FB:186:MET:HE1	29:DD:995:GLU:CD	1.65	1.21
50:n:250:LEU:HD23	50:n:275:HIS:CG	1.74	1.21
65:h:182:VAL:HG21	67:r:202:ILE:CD1	1.68	1.21
46:PD:76:ASN:CG	65:h:47:ASP:HB3	1.63	1.21
58:q:186:GLU:CG	58:q:243:LEU:HD22	1.70	1.21
58:q:596:PHE:HZ	63:l:117:TYR:OH	1.24	1.21
50:n:957:PRO:HG2	50:n:1210:PHE:CE1	1.71	1.21
50:n:957:PRO:HB2	50:n:1210:PHE:CZ	1.74	1.20
69:v:16:GLN:NE2	69:v:20:LYS:CE	2.04	1.20
44:HI:209:ARG:HG3	55:f:53:GLN:NE2	1.53	1.20
58:q:441:ARG:NH1	63:l:168:TRP:CE3	2.09	1.20
29:DD:895:HIS:CG	29:DD:896:PRO:HD2	1.76	1.20
58:q:138:LYS:HB3	58:q:140:ASN:OD1	1.42	1.20
32:Di:62:LYS:HD2	35:Dl:106:ARG:NH1	1.56	1.19
16:HC:352:GLN:NE2	43:HF:61:MET:SD	2.14	1.19
44:HI:209:ARG:CG	55:f:53:GLN:HE22	1.53	1.19
53:a:417:TYR:HE1	53:a:450:PHE:CD1	1.58	1.19
53:a:417:TYR:CD1	53:a:469:VAL:HG21	1.77	1.19
39:HD:21:LEU:HD22	39:HD:69:ASP:OD2	1.43	1.19
31:DF:219:GLU:CB	38:DH:160:ILE:CG2	2.20	1.19
53:a:462:LEU:CG	72:x:49:GLN:HB3	1.70	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:c:204:MET:CE	61:c:208:PHE:H	1.56	1.18
62:e:129:VAL:HG21	66:k:114:MET:CE	1.72	1.18
53:a:445:LEU:CB	72:x:55:SER:CB	2.19	1.18
38:DH:57:SER:HB2	33:DJ:197:MET:SD	1.83	1.18
44:HI:209:ARG:CG	55:f:53:GLN:NE2	2.06	1.18
50:n:686:LYS:NZ	64:o:730:PRO:CG	2.05	1.18
66:k:20:GLU:OE1	69:v:76:MET:SD	2.02	1.18
54:d:45:ILE:HG22	56:i:76:MET:HE2	1.25	1.18
30:DE:696:TRP:CZ3	30:DE:703:MET:SD	2.36	1.17
50:n:169:LEU:HB3	50:n:170:PRO:CD	1.72	1.17
64:o:633:VAL:CG1	70:p:810:PRO:HB2	1.72	1.17
50:n:957:PRO:HG2	50:n:1210:PHE:HE1	1.00	1.17
61:c:204:MET:HE1	61:c:208:PHE:N	1.59	1.17
27:DO:2:ALA:HA	29:DD:1000:ARG:CD	1.72	1.17
31:DF:71:ILE:HD12	32:DI:38:GLN:HE21	1.03	1.17
53:a:461:SER:CA	72:x:49:GLN:HE21	1.58	1.17
50:n:192:LEU:HD12	50:n:220:GLY:CA	1.75	1.16
58:q:168:THR:OG1	66:k:21:ILE:HD12	1.43	1.16
55:f:145:TYR:CZ	65:h:43:PRO:HG3	1.79	1.16
50:n:169:LEU:HA	57:m:104:HIS:CG	1.81	1.16
53:a:417:TYR:CD1	53:a:469:VAL:CG2	2.27	1.16
60:b:174:ILE:HD11	63:l:75:LEU:HD21	1.22	1.16
65:h:150:LEU:HD21	66:k:45:LEU:HD11	1.20	1.16
50:n:904:PHE:CE2	50:n:1208:GLU:CG	2.29	1.15
50:n:545:LEU:CD1	50:n:653:PRO:CD	2.25	1.15
5:EA:139:LEU:HD21	47:PG:151:ARG:CB	1.75	1.15
65:h:182:VAL:HG21	67:r:202:ILE:HD12	1.21	1.15
66:k:87:ARG:CA	69:v:105:LEU:CD1	2.23	1.15
44:HI:209:ARG:HB2	55:f:53:GLN:CD	1.69	1.15
50:n:904:PHE:HE2	50:n:1208:GLU:CG	1.59	1.15
54:d:31:LEU:HD23	56:i:103:THR:HG21	1.15	1.15
53:a:461:SER:HA	72:x:49:GLN:NE2	1.61	1.14
54:d:31:LEU:CD2	56:i:103:THR:HG21	1.76	1.14
58:q:171:VAL:CG2	66:k:17:ILE:CG2	2.24	1.14
65:h:146:MET:HG2	66:k:39:LYS:HZ2	1.05	1.14
53:a:375:PHE:CD2	72:x:17:ARG:NE	2.15	1.14
62:e:56:PHE:O	62:e:60:VAL:HG22	1.44	1.14
65:h:147:CYS:SG	69:v:41:LYS:CG	2.34	1.14
5:EA:181:ASN:HB3	39:HD:10:LYS:HG2	1.21	1.13
50:n:270:GLN:NE2	55:f:174:ARG:HG3	1.61	1.13
64:o:633:VAL:HG12	70:p:810:PRO:CB	1.73	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:k:87:ARG:N	69:v:105:LEU:HD12	1.62	1.13
50:n:265:LEU:HD12	50:n:303:LEU:HD21	1.28	1.13
52:u:115:LEU:HB2	54:d:121:LEU:HD12	1.24	1.13
58:q:171:VAL:CG2	66:k:17:ILE:HG21	1.77	1.13
50:n:545:LEU:HD11	50:n:653:PRO:HG3	1.24	1.13
58:q:410:PRO:HG3	67:r:82:PRO:HB3	1.18	1.13
39:HD:85:ARG:HH22	39:HD:140:LEU:N	1.46	1.12
50:n:686:LYS:NZ	64:o:730:PRO:HG3	1.60	1.12
50:n:957:PRO:CB	50:n:1210:PHE:CZ	2.32	1.12
53:a:364:TYR:HB3	53:a:430:LEU:HD12	1.26	1.12
53:a:417:TYR:CE1	53:a:450:PHE:CE1	2.35	1.12
58:q:89:GLN:HG2	58:q:90:PRO:CD	1.79	1.12
60:b:174:ILE:HG12	63:l:75:LEU:HD11	1.29	1.12
66:k:87:ARG:CA	69:v:105:LEU:HD11	1.77	1.12
69:v:16:GLN:HE21	69:v:20:LYS:CE	1.60	1.12
53:a:70:LYS:HB2	56:i:70:HIS:CE1	1.84	1.12
62:e:129:VAL:HG13	66:k:111:CYS:SG	1.90	1.12
62:e:146:ILE:HG22	62:e:147:ASN:H	0.96	1.12
66:k:87:ARG:N	69:v:105:LEU:CD1	2.11	1.12
31:DF:323:VAL:HG22	31:DF:326:HIS:HB2	1.22	1.12
39:HD:284:ALA:CB	44:HI:243:LEU:HD13	1.78	1.12
39:HD:85:ARG:NH2	39:HD:139:LYS:C	2.07	1.11
50:n:209:PRO:HG3	50:n:293:TYR:HB2	1.30	1.11
50:n:686:LYS:HZ1	64:o:730:PRO:CD	1.61	1.11
52:u:128:SER:HB2	56:i:131:LEU:HD21	1.23	1.11
54:d:45:ILE:HG12	56:i:73:ILE:HA	1.26	1.11
68:t:129:VAL:HG21	68:t:200:ILE:HD12	1.32	1.11
31:DF:428:LEU:HD13	31:DF:455:LEU:CB	1.80	1.11
58:q:339:LEU:HD13	58:q:439:PHE:CE2	1.82	1.11
31:DF:83:LEU:HD11	31:DF:97:ALA:O	1.49	1.11
50:n:957:PRO:HG3	50:n:1210:PHE:CE1	1.80	1.11
56:i:85:GLN:HG3	56:i:86:ASP:N	1.53	1.11
58:q:152:SER:HB2	69:v:58:ASN:HA	1.19	1.11
50:n:166:TYR:OH	57:m:70:PRO:HB2	1.49	1.11
52:u:115:LEU:CB	54:d:121:LEU:HD13	1.68	1.11
53:a:445:LEU:HD22	72:x:55:SER:CB	1.81	1.11
66:k:87:ARG:HA	69:v:105:LEU:HD11	1.12	1.11
9:PA:1795:PRO:HD3	54:d:169:PRO:HA	1.33	1.10
50:n:254:VAL:CG2	50:n:303:LEU:HD22	1.81	1.10
58:q:155:GLY:HA3	69:v:62:HIS:CE1	1.83	1.10
65:h:146:MET:CG	66:k:39:LYS:NZ	2.13	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:HC:397:GLU:HB3	43:HF:61:MET:HE3	1.27	1.10
53:a:375:PHE:CD2	72:x:17:ARG:NH2	2.18	1.10
54:d:167:TRP:CH2	57:m:102:ILE:CG2	2.34	1.10
31:DF:219:GLU:HG2	38:DH:160:ILE:CG2	1.80	1.10
44:HI:209:ARG:CB	55:f:53:GLN:NE2	2.14	1.10
30:DE:433:LYS:HD3	32:DI:110:TYR:OH	1.50	1.09
56:i:85:GLN:CG	56:i:86:ASP:H	1.60	1.09
29:DD:872:PHE:CZ	35:DL:57:VAL:HG12	1.87	1.09
50:n:545:LEU:HD12	50:n:653:PRO:HD3	1.34	1.09
53:a:445:LEU:CD1	72:x:55:SER:HB3	1.81	1.09
53:a:462:LEU:HG	72:x:49:GLN:CB	1.81	1.09
5:EA:181:ASN:ND2	39:HD:9:CYS:HA	1.68	1.09
50:n:686:LYS:HZ1	64:o:730:PRO:HD3	0.95	1.09
52:u:67:LYS:HE3	59:z:528:LEU:CD2	1.82	1.09
53:a:449:ARG:NH2	72:x:54:PRO:HB2	1.67	1.09
61:c:204:MET:CE	61:c:208:PHE:N	2.14	1.09
39:HD:284:ALA:HB3	44:HI:243:LEU:CD1	1.82	1.09
52:u:90:LEU:HD11	58:q:7:VAL:HB	1.10	1.09
31:DF:15:PRO:HD3	32:DI:18:MET:HG2	1.34	1.08
39:HD:43:ALA:O	47:PG:164:MET:SD	2.11	1.08
53:a:462:LEU:HG	72:x:49:GLN:HB3	1.32	1.08
50:n:209:PRO:HG3	50:n:293:TYR:CB	1.83	1.08
54:d:38:GLU:CD	56:i:96:GLU:HG2	1.77	1.08
58:q:129:PRO:HB3	65:h:74:GLN:NE2	1.67	1.08
60:b:174:ILE:HD11	63:l:75:LEU:CD2	1.76	1.08
16:HC:397:GLU:OE1	43:HF:61:MET:SD	2.11	1.08
48:g:166:ASN:OD1	48:g:167:CYS:N	1.85	1.08
54:d:45:ILE:HG22	56:i:76:MET:CE	1.83	1.08
50:n:960:LYS:HG3	50:n:1210:PHE:CD2	1.88	1.08
53:a:321:LEU:HD21	53:a:407:ILE:HG23	1.33	1.08
53:a:461:SER:C	72:x:49:GLN:HE21	1.59	1.08
66:k:86:SER:C	69:v:105:LEU:HD12	1.78	1.08
39:HD:43:ALA:HB1	47:PG:164:MET:HG3	1.33	1.08
39:HD:83:ASN:OD1	39:HD:140:LEU:HD11	1.54	1.08
53:a:445:LEU:HB3	72:x:55:SER:HB2	1.09	1.08
65:h:146:MET:CB	66:k:39:LYS:NZ	2.08	1.08
50:n:168:ARG:CD	57:m:104:HIS:NE2	2.17	1.07
32:DI:16:ALA:HA	32:DI:40:LEU:HD11	1.35	1.07
50:n:957:PRO:HB2	50:n:1210:PHE:HZ	0.93	1.07
53:a:461:SER:HA	72:x:49:GLN:HE21	1.13	1.07
58:q:418:ILE:CD1	68:t:72:PRO:HG2	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:487:ILE:CG2	58:q:543:VAL:HG21	1.82	1.07
53:a:321:LEU:CD2	53:a:407:ILE:HD12	1.83	1.07
66:k:9:GLU:HG3	69:v:86:LEU:HG	1.28	1.07
30:DE:433:LYS:CD	32:DI:110:TYR:OH	2.01	1.07
65:h:150:LEU:HD21	66:k:45:LEU:CD1	1.84	1.07
31:DF:82:PRO:HG3	31:DF:96:PHE:O	1.55	1.07
50:n:168:ARG:CG	57:m:104:HIS:CE1	2.37	1.07
53:a:380:ALA:HB3	53:a:444:PRO:HD2	1.37	1.07
56:i:68:LEU:HD13	56:i:95:GLN:HG2	1.15	1.07
58:q:186:GLU:HG3	58:q:243:LEU:HD21	1.19	1.07
60:b:174:ILE:HG12	63:l:75:LEU:HD21	1.34	1.07
52:u:115:LEU:HD12	54:d:121:LEU:HB3	1.37	1.06
66:k:29:GLY:O	66:k:33:LEU:HG	1.55	1.06
39:HD:295:ARG:NH1	45:HJ:165:ARG:HH21	1.52	1.06
58:q:138:LYS:HD2	58:q:140:ASN:OD1	1.54	1.06
62:e:125:LYS:HE2	69:v:133:GLU:OE2	1.53	1.06
29:DD:895:HIS:ND1	29:DD:896:PRO:HD2	1.67	1.06
53:a:445:LEU:HD13	72:x:55:SER:CB	1.85	1.06
31:DF:219:GLU:CG	38:DH:160:ILE:CG2	2.32	1.06
50:n:245:TRP:CB	50:n:282:LEU:HD13	1.84	1.06
50:n:921:MET:SD	50:n:1215:ILE:CD1	2.42	1.06
54:d:126:TYR:CE2	58:q:36:MET:CB	2.39	1.06
16:HC:348:ARG:NE	43:HF:65:ALA:HB1	1.71	1.05
39:HD:5:GLY:HA3	39:HD:10:LYS:HB2	1.37	1.05
50:n:265:LEU:CD1	50:n:303:LEU:HD21	1.85	1.05
50:n:267:HIS:HD2	55:f:174:ARG:CD	1.67	1.05
50:n:545:LEU:CD1	50:n:653:PRO:HD3	1.83	1.05
50:n:686:LYS:HZ3	64:o:730:PRO:HG3	1.10	1.05
28:Dc:67:GLY:HA3	33:Dj:116:LEU:CD1	1.85	1.05
58:q:155:GLY:HA3	69:v:62:HIS:HE1	0.93	1.05
58:q:458:PRO:HG3	58:q:533:GLN:HE21	0.90	1.05
31:DF:316:GLN:HG2	31:DF:318:CYS:O	1.56	1.05
50:n:570:PHE:CE2	71:w:18:ILE:HG21	1.92	1.05
54:d:167:TRP:HH2	57:m:102:ILE:CG2	1.68	1.05
64:o:633:VAL:CG1	70:p:810:PRO:HB3	1.80	1.05
29:DD:997:ALA:O	29:DD:1001:GLN:HG3	1.55	1.05
54:d:167:TRP:HH2	57:m:102:ILE:HG21	1.15	1.05
38:DH:51:GLU:OE1	33:DJ:193:TYR:CB	2.03	1.05
50:n:957:PRO:CG	50:n:1210:PHE:CZ	2.39	1.05
60:b:179:LEU:CG	62:e:60:VAL:HB	1.85	1.05
35:DL:111:LEU:O	35:DL:114:LYS:HG2	1.54	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:134:ALA:H	65:h:72:ARG:NH1	1.53	1.04
5:EA:174:ARG:HB3	39:HD:8:ARG:HH21	0.89	1.04
58:q:102:LEU:HD11	65:h:29:PHE:CE2	1.92	1.04
58:q:155:GLY:CA	69:v:62:HIS:HE1	1.71	1.04
31:DF:47:ILE:HD11	32:DI:43:ALA:HB2	1.39	1.04
50:n:861:LYS:HE3	61:c:30:ARG:HE	1.17	1.04
53:a:375:PHE:CD2	72:x:17:ARG:CZ	2.39	1.04
53:a:445:LEU:CG	72:x:55:SER:CB	2.36	1.04
58:q:89:GLN:HG2	58:q:90:PRO:HD2	1.38	1.04
31:DF:219:GLU:CG	38:DH:160:ILE:HG21	1.86	1.04
32:DI:81:GLN:HE22	35:DL:123:GLN:NE2	1.55	1.04
44:HI:209:ARG:HG3	55:f:53:GLN:HE22	0.97	1.04
48:g:167:CYS:SG	54:d:113:GLN:NE2	2.31	1.04
50:n:250:LEU:CD2	50:n:275:HIS:CG	2.37	1.04
50:n:267:HIS:CB	50:n:270:GLN:OE1	2.05	1.04
54:d:45:ILE:O	56:i:76:MET:CG	2.06	1.04
58:q:149:LYS:CE	69:v:40:ALA:HA	1.87	1.04
58:q:487:ILE:HG21	58:q:543:VAL:HG21	1.07	1.04
39:HD:84:LYS:HA	39:HD:136:ASN:ND2	1.73	1.04
53:a:445:LEU:CD1	72:x:55:SER:N	2.08	1.04
64:o:633:VAL:HG11	70:p:810:PRO:HB2	1.09	1.04
54:d:31:LEU:HD21	56:i:103:THR:OG1	1.58	1.03
54:d:45:ILE:HD11	56:i:73:ILE:N	1.73	1.03
9:PA:1643:TYR:HB2	57:m:96:PHE:CG	1.93	1.03
10:DB:645:ALA:HA	16:HC:413:LEU:HA	1.08	1.03
32:DI:62:LYS:HD2	35:DI:106:ARG:HH12	1.05	1.03
58:q:418:ILE:HD12	68:t:72:PRO:CG	1.87	1.03
58:q:479:ILE:O	58:q:532:HIS:CE1	2.11	1.03
62:e:49:GLU:HG2	63:l:89:PHE:CE1	1.93	1.03
39:HD:300:ALA:HB2	45:HJ:166:PRO:HA	1.04	1.03
52:u:90:LEU:CD1	58:q:9:ILE:HG13	1.89	1.03
53:a:382:LEU:HD22	53:a:446:SER:HA	1.40	1.03
58:q:171:VAL:HG21	66:k:17:ILE:HG23	1.37	1.03
60:b:174:ILE:HG12	63:l:75:LEU:CD1	1.89	1.03
61:c:204:MET:HE3	61:c:208:PHE:H	1.21	1.03
58:q:188:LEU:HA	69:v:87:ILE:CD1	1.89	1.03
58:q:339:LEU:HD13	58:q:439:PHE:CD2	1.93	1.03
58:q:647:SER:CB	62:e:93:CYS:SG	2.45	1.03
60:b:179:LEU:CD1	62:e:60:VAL:HB	1.88	1.03
64:o:639:TYR:CE2	70:p:786:HIS:HB3	1.94	1.03
66:k:104:LEU:HD21	69:v:123:ILE:HD11	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:462:LEU:H	72:x:49:GLN:HG2	0.94	1.02
50:n:169:LEU:HA	57:m:104:HIS:CD2	1.94	1.02
50:n:686:LYS:HZ3	64:o:730:PRO:CB	1.71	1.02
53:a:109:TYR:CZ	53:a:154:LEU:HD21	1.94	1.02
54:d:27:ARG:HD2	56:i:108:HIS:HA	1.40	1.02
58:q:396:ALA:HB2	67:r:51:PHE:CE2	1.94	1.02
10:DB:644:GLN:O	16:HC:413:LEU:CB	2.08	1.02
50:n:270:GLN:NE2	55:f:174:ARG:CG	2.23	1.02
50:n:941:TYR:CD2	50:n:1172:SER:HB2	1.92	1.02
52:u:67:LYS:HE3	59:z:528:LEU:HD21	1.39	1.02
31:DF:219:GLU:HB3	38:DH:160:ILE:CG2	1.89	1.02
53:a:70:LYS:NZ	56:i:74:LYS:CE	2.22	1.02
9:PA:1475:LEU:HD22	47:PG:66:VAL:HG22	1.41	1.02
9:PA:1798:SER:HA	58:q:25:ASP:OD2	1.59	1.02
31:DF:83:LEU:HD23	31:DF:86:PHE:CZ	1.93	1.02
54:d:45:ILE:CG1	56:i:73:ILE:HA	1.89	1.02
58:q:113:TYR:HB2	65:h:19:VAL:CG1	1.87	1.02
50:n:261:ASP:HB2	58:q:250:ASP:OD1	1.60	1.01
58:q:171:VAL:HG22	66:k:17:ILE:HG21	1.40	1.01
61:c:204:MET:HE3	61:c:206:SER:O	1.60	1.01
5:EA:174:ARG:CB	39:HD:8:ARG:NH2	2.23	1.01
60:b:179:LEU:HD12	62:e:60:VAL:CA	1.90	1.01
66:k:86:SER:C	69:v:105:LEU:CD1	2.33	1.01
50:n:169:LEU:CD2	57:m:101:GLN:HA	1.90	1.01
50:n:273:PHE:HZ	55:f:185:ARG:CD	1.71	1.01
52:u:90:LEU:HD13	58:q:9:ILE:CG1	1.88	1.01
55:f:16:VAL:HG12	55:f:103:GLY:O	1.60	1.01
58:q:186:GLU:HG2	58:q:243:LEU:CD2	1.90	1.01
64:o:633:VAL:HG12	70:p:810:PRO:HB3	1.03	1.01
9:PA:1795:PRO:HD2	54:d:169:PRO:HB2	1.42	1.01
9:PA:1795:PRO:CD	54:d:169:PRO:CA	2.38	1.01
31:DF:219:GLU:HB2	38:DH:160:ILE:HG21	1.41	1.01
35:DL:111:LEU:CA	35:DL:114:LYS:HZ2	1.73	1.01
56:i:72:ILE:CD1	56:i:92:SER:HB2	1.91	1.01
5:EA:142:ASN:HB3	47:PG:158:PHE:CE2	1.96	1.01
56:i:85:GLN:HG3	56:i:86:ASP:OD1	1.56	1.01
56:i:85:GLN:CG	56:i:86:ASP:OD1	2.09	1.01
62:e:129:VAL:HG21	66:k:114:MET:HE2	1.39	1.01
16:HC:397:GLU:CD	43:HF:61:MET:HG3	1.84	1.00
31:DF:104:LEU:CB	33:DJ:217:PHE:CE2	2.42	1.00
39:HD:43:ALA:HB3	47:PG:164:MET:HE3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:254:VAL:HG21	50:n:303:LEU:HD22	1.04	1.00
53:a:462:LEU:N	72:x:49:GLN:NE2	2.10	1.00
62:e:129:VAL:HG12	66:k:111:CYS:SG	2.00	1.00
67:r:27:VAL:HG22	67:r:197:VAL:HG11	1.40	1.00
5:EA:178:ALA:HA	39:HD:8:ARG:O	1.61	1.00
50:n:921:MET:CE	50:n:1215:ILE:HD11	1.90	1.00
57:m:56:LEU:HD21	57:m:80:GLN:NE2	1.75	1.00
57:m:116:GLN:NE2	59:z:579:CYS:SG	2.34	1.00
10:DB:672:PHE:CD1	16:HC:414:SER:CB	2.43	1.00
32:DI:23:LEU:HD11	32:DI:39:MET:HE1	1.40	1.00
52:u:128:SER:CB	56:i:131:LEU:CD2	2.39	1.00
54:d:45:ILE:CD1	56:i:73:ILE:N	2.24	1.00
50:n:170:PRO:HG3	57:m:100:GLN:HB3	1.44	1.00
50:n:203:LEU:HD13	50:n:215:LEU:CD1	1.91	1.00
50:n:934:VAL:HG21	50:n:1182:LEU:HD22	1.42	1.00
54:d:168:VAL:HB	54:d:169:PRO:HD2	1.43	1.00
53:a:445:LEU:HD22	72:x:55:SER:HB3	1.39	1.00
58:q:191:ARG:CD	69:v:87:ILE:O	2.10	1.00
45:HJ:181:LEU:HD13	45:HJ:181:LEU:H	1.26	1.00
53:a:462:LEU:H	72:x:49:GLN:CD	1.68	1.00
66:k:89:ASP:HB3	69:v:109:GLN:OE1	1.61	1.00
58:q:481:SER:CB	58:q:636:VAL:HG21	1.91	0.99
30:DE:429:LEU:HB3	30:DE:430:PRO:HD2	1.41	0.99
50:n:941:TYR:CE2	50:n:1172:SER:HB2	1.96	0.99
53:a:417:TYR:HD1	53:a:469:VAL:HG23	1.25	0.99
58:q:410:PRO:HG3	67:r:82:PRO:CB	1.90	0.99
38:DH:57:SER:CB	33:DJ:197:MET:SD	2.49	0.99
58:q:89:GLN:CG	58:q:90:PRO:CD	2.38	0.99
53:a:462:LEU:N	72:x:49:GLN:HE21	1.59	0.99
58:q:129:PRO:HA	65:h:74:GLN:HA	1.44	0.99
50:n:169:LEU:HB3	50:n:170:PRO:HD3	1.42	0.99
50:n:921:MET:CE	50:n:1215:ILE:CD1	2.40	0.99
60:b:174:ILE:HG12	63:l:75:LEU:CD2	1.92	0.99
10:DB:644:GLN:O	16:HC:413:LEU:HB2	1.62	0.99
54:d:45:ILE:HD13	56:i:72:ILE:C	1.86	0.99
62:e:129:VAL:HG21	66:k:114:MET:HE1	1.43	0.99
12:FB:189:SER:HB3	29:DD:991:MET:HE1	1.41	0.99
65:h:146:MET:HG2	66:k:39:LYS:NZ	1.77	0.99
53:a:59:VAL:HG21	54:d:51:SER:HB3	1.42	0.99
29:DD:1078:LEU:HD21	35:DL:83:MET:HE3	1.44	0.98
50:n:359:ILE:CG1	50:n:372:ILE:CD1	2.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:83:LEU:HD23	31:DF:86:PHE:HZ	1.23	0.98
35:DL:71:ASP:OD2	35:DL:74:GLU:CG	2.10	0.98
50:n:359:ILE:CB	50:n:372:ILE:HD11	1.91	0.98
50:n:686:LYS:NZ	64:o:730:PRO:HD3	1.78	0.98
50:n:252:ILE:HD11	50:n:271:ILE:HG12	1.43	0.98
50:n:647:MET:CE	71:w:22:PHE:CB	2.17	0.98
31:DF:43:VAL:HG23	32:DI:46:TYR:HB3	1.43	0.98
53:a:321:LEU:HD22	53:a:407:ILE:HD12	1.42	0.98
62:e:95:PHE:HB3	63:l:38:GLN:HG2	1.44	0.98
60:b:181:CYS:SG	63:l:82:LEU:CD1	2.51	0.98
38:DH:154:PRO:HD2	38:DH:159:TYR:OH	1.63	0.98
35:DL:71:ASP:CG	35:DL:74:GLU:HG3	1.89	0.98
39:HD:287:TYR:CD1	44:HI:189:MET:SD	2.56	0.98
28:Dc:77:LEU:CD1	33:Dj:116:LEU:HD23	1.94	0.98
50:n:270:GLN:HE22	55:f:174:ARG:CG	1.74	0.98
50:n:273:PHE:HZ	55:f:185:ARG:HD2	1.20	0.98
53:a:375:PHE:HD2	72:x:17:ARG:NH2	1.58	0.98
58:q:451:LEU:HD11	58:q:529:MET:CE	1.94	0.98
5:EA:143:GLN:HG2	47:PG:158:PHE:CE1	1.99	0.97
48:g:127:ARG:HA	48:g:130:GLN:HB3	1.42	0.97
50:n:904:PHE:CZ	50:n:1208:GLU:HG3	1.99	0.97
53:a:462:LEU:CB	72:x:49:GLN:HB3	1.93	0.97
58:q:484:TYR:CD1	58:q:636:VAL:CG1	2.47	0.97
54:d:41:SER:HB2	56:i:69:VAL:HG13	1.41	0.97
10:DB:762:ASP:OD1	10:DB:768:PRO:HG3	1.64	0.97
58:q:149:LYS:HE2	69:v:40:ALA:C	1.89	0.97
58:q:392:MET:SD	67:r:46:MET:CE	2.52	0.97
16:HC:397:GLU:CB	43:HF:61:MET:HE3	1.93	0.97
50:n:904:PHE:HE2	50:n:1208:GLU:CD	1.72	0.97
4:DA:725:CYS:O	4:DA:725:CYS:SG	2.22	0.97
35:DL:111:LEU:CA	35:DL:114:LYS:NZ	2.26	0.97
64:o:639:TYR:CD2	70:p:786:HIS:CG	2.52	0.97
45:HJ:239:LYS:HZ2	45:HJ:239:LYS:H	1.01	0.97
58:q:17:LYS:HE2	58:q:30:TYR:CE2	2.00	0.97
58:q:437:HIS:CE1	58:q:472:GLU:N	2.33	0.97
65:h:146:MET:HB2	66:k:39:LYS:HZ3	1.15	0.97
32:DI:28:ILE:HG22	32:DI:31:TYR:HD1	1.30	0.97
45:HJ:184:PRO:HB3	45:HJ:187:LEU:HD12	1.47	0.97
53:a:335:THR:O	53:a:391:THR:CG2	2.12	0.97
53:a:462:LEU:HB2	72:x:49:GLN:CB	1.95	0.96
58:q:89:GLN:CB	58:q:90:PRO:HD2	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:PA:1795:PRO:CD	54:d:169:PRO:HA	1.95	0.96
52:u:90:LEU:HD13	58:q:9:ILE:HG13	0.98	0.96
31:DF:323:VAL:HG23	31:DF:326:HIS:HB2	1.47	0.96
60:b:179:LEU:HG	62:e:60:VAL:HB	1.46	0.96
50:n:545:LEU:CD1	50:n:653:PRO:HG3	1.95	0.96
52:u:128:SER:CB	56:i:131:LEU:HD21	1.95	0.96
50:n:957:PRO:CB	50:n:1210:PHE:HZ	1.72	0.96
58:q:263:LYS:HE2	58:q:439:PHE:CE2	1.99	0.96
50:n:270:GLN:HE22	55:f:174:ARG:CD	1.78	0.96
38:DH:50:PHE:CE1	33:DJ:195:LEU:HD13	2.01	0.96
32:DI:81:GLN:HE22	35:DL:123:GLN:CD	1.73	0.96
64:o:636:HIS:HA	70:p:786:HIS:O	1.66	0.96
53:a:417:TYR:CE1	53:a:450:PHE:HD1	1.74	0.96
54:d:41:SER:CB	56:i:69:VAL:HG13	1.96	0.95
5:EA:171:LYS:NZ	39:HD:41:ARG:HG3	1.82	0.95
50:n:273:PHE:CZ	55:f:185:ARG:CD	2.47	0.95
53:a:441:GLU:HB2	72:x:17:ARG:HH22	1.29	0.95
29:DD:872:PHE:CE1	35:DL:57:VAL:HG12	2.00	0.95
44:HI:209:ARG:HB2	55:f:53:GLN:NE2	1.77	0.95
58:q:578:TYR:CD1	58:q:646:LEU:CD1	2.49	0.95
53:a:66:GLN:HE22	54:d:44:LEU:HD11	1.30	0.95
53:a:445:LEU:CD2	72:x:55:SER:CB	2.43	0.95
53:a:383:PRO:HG3	72:x:92:LEU:HD22	1.48	0.95
64:o:639:TYR:HE2	70:p:786:HIS:ND1	1.64	0.95
32:DI:132:LEU:HD21	33:DJ:121:MET:HE1	1.47	0.95
9:PA:1643:TYR:OH	57:m:93:CYS:HB2	1.67	0.95
27:DO:2:ALA:O	29:DD:1000:ARG:HB3	1.65	0.95
53:a:70:LYS:HZ3	56:i:74:LYS:HE2	1.29	0.95
53:a:364:TYR:HB3	53:a:430:LEU:CG	1.96	0.95
31:DF:71:ILE:HD12	32:DI:38:GLN:NE2	1.80	0.95
50:n:192:LEU:CD1	50:n:220:GLY:CA	2.45	0.95
50:n:545:LEU:CD1	50:n:653:PRO:CG	2.45	0.95
58:q:93:TRP:CE3	58:q:93:TRP:HA	2.02	0.95
60:b:174:ILE:HD13	63:l:75:LEU:HD21	1.43	0.95
65:h:146:MET:HE2	66:k:45:LEU:HD12	1.47	0.95
50:n:270:GLN:CB	55:f:181:LEU:HD11	1.96	0.94
53:a:59:VAL:HG11	54:d:51:SER:OG	1.67	0.94
53:a:70:LYS:HZ1	56:i:74:LYS:HE2	0.95	0.94
54:d:123:THR:HG22	58:q:37:SER:HB3	1.49	0.94
54:d:126:TYR:CD2	58:q:36:MET:HB3	2.01	0.94
64:o:715:LEU:HD13	72:x:66:TYR:OH	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:375:PHE:CD1	72:x:17:ARG:HG3	2.02	0.94
54:d:31:LEU:HD21	56:i:103:THR:CB	1.96	0.94
58:q:418:ILE:CD1	68:t:72:PRO:CG	2.45	0.94
54:d:34:LEU:HD22	56:i:99:LYS:HD3	1.47	0.94
29:DD:1078:LEU:CD2	35:DL:83:MET:CE	2.46	0.94
38:DH:37:LEU:HD11	33:DJ:138:TYR:CE2	2.03	0.94
44:HI:143:LEU:HD13	44:HI:143:LEU:O	1.68	0.94
52:u:90:LEU:HD11	58:q:7:VAL:CB	1.96	0.94
54:d:45:ILE:HG13	56:i:73:ILE:HG12	1.48	0.94
31:DF:274:ASN:HB2	31:DF:317:LEU:HD23	1.48	0.94
9:PA:1475:LEU:HD22	47:PG:66:VAL:CG2	1.97	0.94
16:HC:398:ARG:HH22	43:HF:58:GLY:HA2	1.30	0.94
62:e:146:ILE:HG22	62:e:147:ASN:N	1.78	0.94
39:HD:284:ALA:HB3	44:HI:243:LEU:HD13	0.94	0.94
50:n:270:GLN:HE22	55:f:174:ARG:HG3	1.29	0.94
10:DB:645:ALA:CA	16:HC:413:LEU:HA	1.98	0.94
52:u:125:ILE:HG12	56:i:135:TYR:CE2	2.03	0.94
54:d:76:PHE:CE2	56:i:65:PHE:HD2	1.72	0.94
60:b:179:LEU:HD12	62:e:60:VAL:CB	1.97	0.93
44:HI:86:ASN:ND2	44:HI:86:ASN:O	2.00	0.93
50:n:273:PHE:CE2	55:f:185:ARG:HD2	2.03	0.93
39:HD:85:ARG:HH12	39:HD:140:LEU:HG	1.34	0.93
28:Dc:67:GLY:HA3	33:Dj:116:LEU:HD11	1.48	0.93
50:n:192:LEU:HB3	50:n:219:ASN:O	1.66	0.93
50:n:267:HIS:HD2	55:f:174:ARG:HD3	0.77	0.93
58:q:540:LEU:HD21	58:q:640:GLU:HG3	1.51	0.93
60:b:174:ILE:CG1	63:l:75:LEU:CD2	2.39	0.93
5:EA:143:GLN:HG2	47:PG:158:PHE:HZ	1.15	0.93
29:DD:1078:LEU:CD2	35:DL:83:MET:HE3	1.97	0.93
66:k:87:ARG:HH11	66:k:87:ARG:HG3	1.33	0.93
38:DH:57:SER:OG	33:DJ:200:LEU:HD12	1.69	0.93
58:q:149:LYS:CD	69:v:40:ALA:HA	1.99	0.93
58:q:168:THR:OG1	66:k:21:ILE:HG21	1.68	0.93
10:DB:645:ALA:HA	16:HC:413:LEU:CA	1.97	0.92
52:u:115:LEU:HB2	54:d:121:LEU:HD11	1.48	0.92
53:a:321:LEU:CD2	53:a:407:ILE:HG23	1.98	0.92
54:d:45:ILE:HD11	56:i:73:ILE:HG13	1.51	0.92
60:b:136:HIS:CD2	61:c:111:TYR:CE1	2.57	0.92
44:HI:52:LYS:HA	44:HI:52:LYS:HE3	1.51	0.92
64:o:735:LEU:HD21	71:w:113:GLN:CD	1.95	0.92
44:HI:239:ASP:HA	44:HI:242:SER:HB3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:45:ILE:HG23	56:i:76:MET:HB3	1.50	0.92
57:m:56:LEU:CD2	57:m:80:GLN:NE2	2.33	0.92
60:b:179:LEU:HD12	62:e:60:VAL:HB	1.50	0.92
5:EA:17:LEU:HD22	5:EA:194:THR:HG21	1.50	0.92
31:DF:323:VAL:CG2	31:DF:326:HIS:CB	2.48	0.92
49:j:82:LYS:HZ2	51:s:101:VAL:HG12	1.35	0.92
29:DD:899:VAL:HG13	29:DD:900:SER:N	1.82	0.92
53:a:66:GLN:NE2	54:d:44:LEU:CD1	2.32	0.92
53:a:375:PHE:HD2	72:x:17:ARG:HH21	0.93	0.92
58:q:479:ILE:CG2	58:q:532:HIS:CD2	2.52	0.92
58:q:377:LEU:HD13	63:l:177:ARG:HA	1.52	0.92
31:DF:218:VAL:HG11	38:DH:162:THR:HG21	1.51	0.92
31:DF:219:GLU:HG2	38:DH:160:ILE:HG22	1.51	0.92
48:g:129:HIS:HA	48:g:132:ARG:HG2	1.51	0.92
50:n:932:GLY:HA2	50:n:1179:HIS:CE1	2.04	0.92
60:b:136:HIS:CD2	61:c:111:TYR:CD1	2.58	0.92
53:a:462:LEU:HD21	72:x:11:LEU:HB3	1.51	0.91
56:i:72:ILE:HD13	56:i:92:SER:CB	2.00	0.91
54:d:45:ILE:CD1	56:i:73:ILE:CA	2.48	0.91
50:n:957:PRO:CG	50:n:1210:PHE:HE1	1.64	0.91
51:s:104:LYS:C	51:s:106:SER:H	1.70	0.91
52:u:128:SER:HB2	56:i:131:LEU:CD2	1.99	0.91
53:a:449:ARG:HH22	72:x:54:PRO:HB2	1.31	0.91
54:d:38:GLU:CG	56:i:96:GLU:HG2	1.99	0.91
65:h:182:VAL:CG2	67:r:202:ILE:HD12	2.01	0.91
10:DB:158:GLY:HA2	10:DB:188:PHE:HB3	1.53	0.91
30:DE:463:PHE:O	31:DF:133:ALA:HA	1.70	0.91
31:DF:105:TYR:O	33:DJ:217:PHE:CG	2.23	0.91
50:n:224:PHE:CD2	50:n:292:MET:CE	2.53	0.91
50:n:359:ILE:HG12	50:n:372:ILE:HD11	0.91	0.91
58:q:124:PHE:CE2	65:h:89:LEU:HD11	2.05	0.91
5:EA:139:LEU:HD21	47:PG:151:ARG:HB3	0.92	0.91
35:DL:111:LEU:HA	35:DL:114:LYS:HZ2	0.81	0.91
39:HD:27:GLY:HA3	39:HD:70:LYS:HD3	1.51	0.91
29:DD:1078:LEU:HD23	35:DL:83:MET:CE	2.01	0.91
38:DH:60:THR:HG21	33:DJ:211:VAL:HG23	1.53	0.91
50:n:261:ASP:HB2	58:q:250:ASP:CG	1.95	0.91
58:q:392:MET:CE	67:r:46:MET:HE1	1.99	0.91
60:b:186:THR:HG21	62:e:49:GLU:CD	1.96	0.91
16:HC:397:GLU:HB3	43:HF:61:MET:CE	2.00	0.91
31:DF:323:VAL:HG23	31:DF:326:HIS:CB	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:192:LEU:HD12	50:n:220:GLY:HA2	1.52	0.91
50:n:359:ILE:HG23	50:n:372:ILE:CD1	2.01	0.91
68:t:98:LEU:HB3	68:t:102:PHE:HD1	1.36	0.91
31:DF:218:VAL:CG1	38:DH:162:THR:CB	2.48	0.90
50:n:166:TYR:HH	57:m:70:PRO:HB2	1.35	0.90
52:u:90:LEU:HB2	58:q:9:ILE:HG12	1.53	0.90
54:d:103:ARG:HG2	54:d:103:ARG:HH11	1.34	0.90
64:o:639:TYR:CE2	70:p:786:HIS:CG	2.58	0.90
50:n:254:VAL:HG21	50:n:303:LEU:CD2	1.99	0.90
53:a:70:LYS:HZ3	56:i:74:LYS:CE	1.81	0.90
56:i:72:ILE:CD1	56:i:92:SER:CB	2.49	0.90
58:q:157:ALA:HB2	66:k:31:VAL:HG23	1.52	0.90
65:h:142:SER:OG	66:k:39:LYS:HE3	1.72	0.90
53:a:375:PHE:CE1	72:x:17:ARG:HG3	2.05	0.90
53:a:416:ALA:CB	53:a:472:SER:O	2.19	0.90
39:HD:21:LEU:CD2	39:HD:69:ASP:OD2	2.18	0.90
50:n:166:TYR:HE2	57:m:71:GLN:HA	1.36	0.90
50:n:203:LEU:HD13	50:n:215:LEU:HD12	1.53	0.90
53:a:380:ALA:CB	72:x:58:PRO:HG3	2.01	0.90
53:a:445:LEU:CD1	72:x:55:SER:CB	2.46	0.90
5:EA:143:GLN:NE2	47:PG:158:PHE:HE1	1.69	0.90
31:DF:105:TYR:O	33:DJ:217:PHE:HB3	1.71	0.90
44:HI:209:ARG:CB	55:f:53:GLN:CD	2.44	0.90
54:d:45:ILE:CG1	56:i:73:ILE:HG12	2.00	0.90
58:q:89:GLN:CD	58:q:90:PRO:HD2	1.97	0.90
50:n:253:LEU:O	50:n:255:GLU:HG3	1.70	0.90
50:n:172:CYS:SG	58:q:21:GLU:HA	2.12	0.90
38:DH:57:SER:CA	33:DJ:197:MET:SD	2.59	0.90
50:n:686:LYS:NZ	64:o:730:PRO:CD	2.26	0.90
50:n:960:LYS:NZ	50:n:1185:LEU:HD13	1.87	0.90
54:d:45:ILE:HG23	56:i:76:MET:HB2	0.93	0.89
9:PA:1795:PRO:HD2	54:d:169:PRO:CA	1.99	0.89
50:n:870:GLN:HG2	64:o:655:THR:HG22	1.53	0.89
60:b:62:MET:HE2	60:b:62:MET:HA	1.52	0.89
60:b:101:ARG:HH12	70:p:677:THR:CB	1.85	0.89
1:X:1:DC:H42	2:Y:-1:DG:H1	1.19	0.89
58:q:89:GLN:HG2	58:q:90:PRO:HD3	1.55	0.89
44:HI:209:ARG:HG3	55:f:53:GLN:CD	1.97	0.89
50:n:224:PHE:HD2	50:n:292:MET:HE2	1.37	0.89
9:PA:1475:LEU:CD2	47:PG:66:VAL:CG2	2.49	0.89
53:a:364:TYR:CB	53:a:430:LEU:HG	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:31:LEU:CD2	56:i:103:THR:CG2	2.51	0.89
39:HD:55:LYS:HB2	47:PG:166:ASP:HB2	1.54	0.89
54:d:45:ILE:CG2	56:i:76:MET:CB	2.27	0.89
58:q:645:ALA:HB2	62:e:100:LEU:CD2	2.03	0.89
32:Di:62:LYS:CD	35:Dl:106:ARG:NH1	2.36	0.89
29:DD:899:VAL:CG1	29:DD:900:SER:N	2.36	0.89
54:d:126:TYR:CZ	58:q:36:MET:HB3	2.08	0.89
58:q:418:ILE:HD12	68:t:72:PRO:HG3	1.55	0.89
65:h:146:MET:HG3	66:k:39:LYS:HD2	1.52	0.89
38:DH:60:THR:HG21	33:DJ:211:VAL:CG2	2.02	0.89
54:d:156:SER:HA	54:d:161:VAL:HG12	1.55	0.89
60:b:136:HIS:HD2	61:c:111:TYR:CD2	1.90	0.89
49:j:35:ALA:HB3	51:s:154:LEU:HD23	1.54	0.88
58:q:484:TYR:CD1	58:q:636:VAL:HG12	2.06	0.88
29:DD:899:VAL:CG1	29:DD:900:SER:H	1.86	0.88
30:DE:432:LEU:HG	30:DE:436:ASP:OD2	1.73	0.88
32:DI:132:LEU:HG	33:DJ:121:MET:CE	2.02	0.88
45:HJ:165:ARG:HH11	45:HJ:165:ARG:HB2	1.35	0.88
50:n:960:LYS:CG	50:n:1210:PHE:CD2	2.56	0.88
54:d:45:ILE:HA	54:d:48:LEU:HD12	1.54	0.88
45:HJ:175:LYS:HA	45:HJ:175:LYS:CE	2.03	0.88
50:n:861:LYS:HE3	61:c:30:ARG:NE	1.87	0.88
66:k:37:LYS:H	66:k:37:LYS:HE3	1.35	0.88
39:HD:43:ALA:CB	47:PG:164:MET:HG3	2.02	0.88
53:a:70:LYS:CB	56:i:70:HIS:ND1	2.34	0.88
58:q:437:HIS:HE1	58:q:472:GLU:C	1.81	0.88
5:EA:174:ARG:HG3	39:HD:37:LEU:HD11	1.53	0.88
10:DB:672:PHE:HE1	16:HC:414:SER:HB3	1.35	0.88
32:DI:132:LEU:HG	33:DJ:121:MET:SD	2.13	0.88
53:a:417:TYR:CB	53:a:469:VAL:HG21	2.02	0.88
29:DD:1071:ARG:HB2	31:DF:91:PHE:CD2	2.08	0.88
48:g:124:ASN:O	48:g:128:PRO:HD3	1.74	0.88
50:n:651:ASN:HB3	71:w:21:ALA:HB1	1.55	0.88
58:q:102:LEU:CD1	65:h:29:PHE:CE2	2.57	0.88
58:q:410:PRO:CG	67:r:82:PRO:HB3	2.01	0.88
31:DF:14:LEU:HD21	32:DI:19:MET:CE	2.04	0.88
44:HI:140:PRO:HA	44:HI:202:ILE:HD11	1.53	0.88
29:DD:895:HIS:CG	29:DD:896:PRO:CD	2.56	0.88
50:n:169:LEU:CA	57:m:104:HIS:CD2	2.57	0.88
58:q:120:ARG:HG2	58:q:120:ARG:HH11	1.38	0.88
58:q:451:LEU:HD11	58:q:529:MET:SD	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:h:142:SER:O	66:k:39:LYS:NZ	2.05	0.88
10:DB:672:PHE:HD1	16:HC:414:SER:CB	1.83	0.88
60:b:179:LEU:HD12	62:e:60:VAL:HA	1.56	0.88
31:DF:219:GLU:HG2	38:DH:160:ILE:HG21	1.45	0.87
52:u:90:LEU:HD22	58:q:9:ILE:CG1	2.03	0.87
54:d:31:LEU:HD23	56:i:103:THR:CG2	2.00	0.87
56:i:72:ILE:HD11	56:i:92:SER:HB2	1.54	0.87
9:PA:1005:HIS:CD2	9:PA:1007:ILE:HG22	2.09	0.87
53:a:445:LEU:HD12	72:x:54:PRO:HG2	1.55	0.87
57:m:124:GLN:CD	59:z:590:ARG:HB2	1.99	0.87
9:PA:1795:PRO:HD2	54:d:169:PRO:HB3	0.88	0.87
50:n:237:MET:HE1	58:q:45:GLN:CB	2.03	0.87
45:HJ:175:LYS:HA	45:HJ:175:LYS:HE3	1.56	0.87
38:DH:171:ASP:HB3	38:DH:174:VAL:HG12	1.54	0.87
55:f:16:VAL:CG1	55:f:103:GLY:O	2.22	0.87
61:c:288:LEU:HD11	68:t:122:PHE:CZ	2.08	0.87
52:u:90:LEU:CD1	58:q:7:VAL:HB	2.01	0.87
61:c:204:MET:HE1	61:c:208:PHE:C	1.99	0.87
16:HC:352:GLN:NE2	43:HF:61:MET:CE	2.38	0.87
31:DF:43:VAL:CG2	32:DI:46:TYR:HB3	2.04	0.87
31:DF:219:GLU:HB3	38:DH:160:ILE:HG23	1.55	0.87
64:o:639:TYR:CE2	70:p:786:HIS:ND1	2.42	0.87
50:n:265:LEU:HD11	50:n:307:VAL:CG2	2.05	0.87
53:a:59:VAL:HG21	54:d:51:SER:HB2	1.55	0.87
58:q:149:LYS:CE	69:v:40:ALA:CA	2.52	0.87
27:DO:2:ALA:HA	29:DD:1000:ARG:HD3	0.89	0.86
55:f:94:PRO:HB2	58:q:130:VAL:HG22	1.55	0.86
50:n:168:ARG:HD3	57:m:104:HIS:NE2	1.87	0.86
52:u:115:LEU:CB	54:d:121:LEU:HD12	1.87	0.86
16:HC:120:ILE:O	40:HE:100:LYS:NZ	2.07	0.86
50:n:169:LEU:HB3	50:n:170:PRO:HD2	1.57	0.86
58:q:139:GLN:NE2	58:q:139:GLN:O	2.08	0.86
54:d:45:ILE:CD1	56:i:73:ILE:HA	2.04	0.86
60:b:175:HIS:CB	61:c:113:TRP:CH2	2.57	0.86
50:n:192:LEU:CD1	50:n:220:GLY:HA3	2.05	0.86
60:b:78:ALA:HB3	64:o:621:LEU:HD21	1.58	0.86
64:o:639:TYR:HD2	70:p:786:HIS:CB	1.75	0.86
50:n:245:TRP:HB2	50:n:282:LEU:HD13	0.88	0.86
52:u:77:PRO:HA	59:z:562:GLY:O	1.74	0.86
52:u:115:LEU:CD1	54:d:121:LEU:HB3	2.05	0.86
39:HD:83:ASN:CG	39:HD:140:LEU:CD1	2.47	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:HD:295:ARG:HH11	45:HJ:165:ARG:NH2	1.72	0.86
38:DH:50:PHE:CZ	33:DJ:170:ALA:C	2.54	0.86
38:DH:50:PHE:HB2	33:DJ:195:LEU:HB2	1.58	0.86
39:HD:300:ALA:CB	45:HJ:166:PRO:CA	2.53	0.86
50:n:707:ASP:HB2	64:o:684:ARG:HH21	1.40	0.86
52:u:75:SER:HB3	59:z:566:CYS:SG	2.16	0.86
53:a:417:TYR:CD1	53:a:469:VAL:HG23	2.03	0.86
54:d:76:PHE:HE2	56:i:65:PHE:HD2	1.17	0.86
54:d:126:TYR:CZ	58:q:36:MET:CB	2.59	0.86
56:i:85:GLN:HG3	56:i:86:ASP:H	0.73	0.86
58:q:188:LEU:HA	69:v:87:ILE:HD11	1.58	0.86
58:q:484:TYR:CE1	58:q:636:VAL:HG12	2.10	0.86
50:n:192:LEU:HD12	50:n:220:GLY:HA3	1.57	0.86
50:n:261:ASP:CG	58:q:250:ASP:OD2	2.17	0.86
53:a:509:ARG:HB2	53:a:509:ARG:NH1	1.89	0.86
56:i:68:LEU:HD13	56:i:95:GLN:CG	2.05	0.86
56:i:96:GLU:HA	56:i:99:LYS:HG3	1.57	0.86
56:i:105:PRO:HD2	56:i:107:ILE:HG13	1.58	0.86
5:EA:188:TYR:HD2	39:HD:14:TYR:CD1	1.94	0.85
38:DH:53:ALA:HA	33:DJ:195:LEU:O	1.76	0.85
50:n:224:PHE:CD2	50:n:292:MET:HE1	2.10	0.85
53:a:377:ASN:HD21	72:x:58:PRO:HG2	1.41	0.85
50:n:224:PHE:HD2	50:n:292:MET:CE	1.89	0.85
50:n:1218:ARG:HH22	50:n:1222:ARG:HB2	1.38	0.85
9:PA:1475:LEU:CD2	47:PG:66:VAL:HG21	2.05	0.85
53:a:228:PRO:HB2	53:a:502:MET:HB2	1.58	0.85
55:f:145:TYR:CZ	65:h:43:PRO:CG	2.60	0.85
61:c:204:MET:SD	61:c:208:PHE:O	2.35	0.85
9:PA:1475:LEU:HB2	47:PG:59:ILE:HG23	1.58	0.85
29:DD:922:GLN:HG3	29:DD:1056:THR:HG21	1.56	0.85
52:u:108:VAL:HG21	54:d:128:ALA:HB1	1.55	0.85
53:a:59:VAL:CG1	54:d:48:LEU:HA	2.06	0.85
53:a:367:LEU:HD13	53:a:509:ARG:CZ	2.05	0.85
53:a:462:LEU:HD12	72:x:60:ILE:CD1	2.06	0.85
66:k:45:LEU:O	66:k:45:LEU:HD22	1.76	0.85
31:DF:83:LEU:CD1	31:DF:97:ALA:O	2.25	0.85
35:DL:71:ASP:HB3	35:DL:74:GLU:CD	2.01	0.85
52:u:122:LEU:HG	54:d:111:GLN:HE21	1.40	0.85
58:q:578:TYR:CD1	58:q:646:LEU:HD13	2.11	0.85
65:h:22:LEU:HA	65:h:56:LEU:HD13	1.59	0.85
45:HJ:186:ILE:HD13	45:HJ:186:ILE:H	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:907:LEU:HD11	60:b:118:LEU:HB2	1.59	0.85
53:a:380:ALA:HB3	53:a:444:PRO:CD	2.06	0.85
32:DI:28:ILE:HG22	32:DI:31:TYR:CD1	2.11	0.85
53:a:417:TYR:CG	53:a:469:VAL:HG21	2.12	0.85
58:q:487:ILE:HG21	58:q:543:VAL:CG2	2.02	0.85
62:e:146:ILE:CG2	62:e:147:ASN:H	1.82	0.85
53:a:377:ASN:HB3	53:a:442:VAL:O	1.75	0.85
5:EA:139:LEU:HD11	47:PG:151:ARG:CG	2.07	0.85
31:DF:219:GLU:CG	38:DH:160:ILE:HG22	2.05	0.85
50:n:706:LEU:HD22	58:q:615:TRP:CZ3	2.12	0.85
52:u:108:VAL:CG2	54:d:128:ALA:HB1	2.07	0.85
53:a:335:THR:O	53:a:391:THR:HG21	1.76	0.85
54:d:38:GLU:HG2	56:i:96:GLU:HG2	1.59	0.85
55:f:145:TYR:CE1	65:h:43:PRO:CG	2.60	0.85
61:c:204:MET:CE	61:c:208:PHE:O	2.23	0.85
53:a:462:LEU:HG	72:x:49:GLN:CD	2.01	0.84
31:DF:218:VAL:CG1	38:DH:162:THR:OG1	2.21	0.84
60:b:174:ILE:HD13	63:l:75:LEU:CD2	2.03	0.84
11:EB:230:GLU:HA	11:EB:233:ILE:HD13	1.58	0.84
53:a:416:ALA:HB2	53:a:472:SER:O	1.77	0.84
58:q:102:LEU:HD11	65:h:29:PHE:HE2	1.36	0.84
9:PA:1795:PRO:CG	54:d:169:PRO:HB3	2.07	0.84
32:DI:23:LEU:HD21	32:DI:39:MET:HE1	1.58	0.84
52:u:71:VAL:HG13	59:z:529:HIS:HB2	1.57	0.84
54:d:42:ARG:HH22	56:i:93:LYS:HA	1.39	0.84
5:EA:122:THR:OG1	39:HD:40:VAL:HG21	1.77	0.84
50:n:960:LYS:HG3	50:n:1210:PHE:HD2	1.42	0.84
70:p:702:ASP:HB2	70:p:705:PRO:HB3	1.58	0.84
53:a:70:LYS:CB	56:i:70:HIS:CE1	2.59	0.84
53:a:462:LEU:HB2	72:x:49:GLN:HB3	1.52	0.84
31:DF:323:VAL:HG23	31:DF:326:HIS:CG	2.13	0.84
57:m:124:GLN:OE1	59:z:590:ARG:HB2	1.78	0.84
60:b:175:HIS:CG	61:c:113:TRP:CZ2	2.66	0.84
65:h:23:LYS:NZ	65:h:23:LYS:HB3	1.92	0.84
5:EA:174:ARG:HG2	39:HD:8:ARG:HH22	1.43	0.84
31:DF:104:LEU:CB	33:DJ:217:PHE:CZ	2.60	0.84
45:HJ:60:TYR:HB3	45:HJ:105:MET:HE1	1.59	0.84
45:HJ:229:GLU:OE1	45:HJ:229:GLU:N	2.11	0.84
48:g:164:ILE:HD13	56:i:140:MET:HG2	1.59	0.84
53:a:375:PHE:CG	72:x:17:ARG:CZ	2.59	0.84
53:a:462:LEU:CA	72:x:49:GLN:HG2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:h:22:LEU:HD12	65:h:22:LEU:O	1.78	0.84
50:n:960:LYS:NZ	50:n:1185:LEU:CD1	2.41	0.84
53:a:59:VAL:HG11	54:d:48:LEU:HA	1.59	0.84
47:PG:41:LYS:O	47:PG:78:ARG:NH2	2.11	0.83
70:p:13:MET:HG3	70:p:405:PHE:HB2	1.59	0.83
12:FB:186:MET:CE	29:DD:995:GLU:CD	2.48	0.83
31:DF:104:LEU:HB2	33:DJ:217:PHE:CZ	2.14	0.83
46:PD:76:ASN:OD1	65:h:47:ASP:HB3	1.78	0.83
50:n:169:LEU:H	57:m:104:HIS:CD2	1.94	0.83
54:d:167:TRP:CH2	57:m:102:ILE:HG21	2.03	0.83
62:e:140:GLN:NE2	66:k:105:SER:HA	1.93	0.83
64:o:765:ASP:OD2	71:w:71:HIS:HB2	1.78	0.83
31:DF:316:GLN:HB2	31:DF:327:TRP:CZ3	2.13	0.83
54:d:167:TRP:CH2	57:m:102:ILE:HG23	2.13	0.83
58:q:134:ALA:H	65:h:72:ARG:HH12	1.19	0.83
58:q:481:SER:HB3	58:q:636:VAL:HG21	1.57	0.83
64:o:714:ASP:O	72:x:28:LYS:NZ	2.10	0.83
74:NG:1119:GLY:C	74:NG:1121:LYS:H	1.84	0.83
16:HC:348:ARG:NE	43:HF:65:ALA:CB	2.42	0.83
31:Df:447:ALA:HA	31:Df:456:GLY:HA3	1.61	0.83
31:DF:104:LEU:HD13	33:DJ:217:PHE:HE2	1.43	0.83
31:DF:316:GLN:CD	31:DF:320:ARG:HG3	2.04	0.83
53:a:462:LEU:H	72:x:49:GLN:NE2	1.70	0.83
50:n:250:LEU:HD21	50:n:275:HIS:HD2	1.38	0.83
58:q:186:GLU:OE2	58:q:291:TRP:CZ2	2.32	0.83
31:DF:14:LEU:HD21	32:DI:19:MET:HE1	1.59	0.83
38:DH:50:PHE:HZ	33:DJ:170:ALA:CB	1.91	0.83
50:n:295:CYS:SG	55:f:188:PHE:CD2	2.72	0.83
65:h:142:SER:OG	66:k:39:LYS:CE	2.26	0.83
35:DL:64:GLN:HA	35:DL:67:VAL:HG22	1.60	0.83
55:f:15:TRP:CH2	55:f:35:GLU:OE1	2.32	0.83
30:DE:433:LYS:NZ	32:DI:110:TYR:CE1	2.46	0.83
35:DL:111:LEU:O	35:DL:114:LYS:CG	2.27	0.83
49:j:43:PHE:CB	51:s:144:ILE:CG2	2.56	0.83
54:d:38:GLU:OE2	56:i:96:GLU:HG2	1.79	0.83
30:DE:747:LEU:HD22	30:DE:747:LEU:H	1.44	0.83
50:n:192:LEU:HD12	50:n:219:ASN:O	1.78	0.83
58:q:458:PRO:CB	58:q:533:GLN:HE21	1.91	0.83
61:c:204:MET:HE1	61:c:208:PHE:CA	2.08	0.83
69:v:16:GLN:HE22	69:v:20:LYS:HE2	1.41	0.83
28:Dc:67:GLY:HA3	33:Dj:116:LEU:HD13	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:h:18:GLN:HA	65:h:18:GLN:NE2	1.92	0.82
54:d:41:SER:CB	56:i:69:VAL:CG1	2.57	0.82
53:a:423:SER:OG	53:a:505:PRO:HD3	1.79	0.82
53:a:462:LEU:HG	72:x:49:GLN:CG	2.08	0.82
12:FB:186:MET:SD	29:DD:995:GLU:HG2	2.20	0.82
39:HD:85:ARG:NH2	39:HD:140:LEU:N	2.25	0.82
52:u:115:LEU:HB2	54:d:121:LEU:HD13	0.83	0.82
53:a:417:TYR:HB2	53:a:469:VAL:HG21	1.61	0.82
45:HJ:198:ILE:HD12	45:HJ:255:MET:HE2	1.62	0.82
50:n:686:LYS:CE	64:o:730:PRO:HG3	2.09	0.82
53:a:380:ALA:CB	53:a:444:PRO:HD2	2.09	0.82
58:q:443:ARG:NE	58:q:443:ARG:HA	1.92	0.82
5:EA:142:ASN:HB3	47:PG:158:PHE:HE2	1.45	0.82
58:q:339:LEU:CD1	58:q:439:PHE:CD2	2.62	0.82
9:PA:1643:TYR:O	57:m:96:PHE:HB2	1.80	0.82
39:HD:55:LYS:HG3	47:PG:166:ASP:H	1.43	0.82
39:HD:83:ASN:ND2	39:HD:140:LEU:CD1	2.43	0.82
44:HI:214:PRO:HD2	44:HI:224:ARG:HG2	1.60	0.82
50:n:680:HIS:HE2	58:q:557:LEU:HD11	1.43	0.82
53:a:321:LEU:HD21	53:a:407:ILE:CG2	2.08	0.82
54:d:115:LYS:HE2	54:d:115:LYS:HA	1.60	0.82
55:f:32:TYR:CD1	55:f:35:GLU:OE2	2.33	0.82
50:n:192:LEU:CD1	50:n:220:GLY:HA2	2.09	0.82
50:n:359:ILE:HA	50:n:372:ILE:HD12	1.60	0.82
58:q:441:ARG:NH1	63:l:168:TRP:CE2	2.48	0.82
56:i:75:CYS:HB3	56:i:88:ASN:ND2	1.95	0.81
58:q:187:LEU:HD23	69:v:84:GLN:HG2	1.62	0.81
55:f:32:TYR:HD1	55:f:35:GLU:OE2	1.62	0.81
58:q:339:LEU:CD1	58:q:439:PHE:CE2	2.62	0.81
38:DH:50:PHE:CZ	33:DJ:170:ALA:HB3	2.15	0.81
44:HI:267:ASP:OD1	44:HI:267:ASP:N	2.08	0.81
52:u:8:LEU:HD11	52:u:73:ILE:HG13	1.60	0.81
52:u:128:SER:CB	56:i:131:LEU:HD22	2.08	0.81
54:d:110:LEU:O	54:d:110:LEU:HD22	1.79	0.81
58:q:437:HIS:HE1	58:q:472:GLU:CA	1.92	0.81
60:b:174:ILE:HG12	63:l:75:LEU:CG	2.10	0.81
65:h:139:GLN:HE22	66:k:37:LYS:HB2	1.45	0.81
25:DP:206:GLU:OE1	25:DP:236:LYS:NZ	2.13	0.81
30:DE:526:ARG:NH1	30:DE:526:ARG:HA	1.96	0.81
61:c:204:MET:CE	61:c:208:PHE:C	2.54	0.81
63:l:166:LEU:HD12	66:k:103:LYS:HB3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:HB:503:THR:HG1	13:HB:533:TYR:HH	1.24	0.81
28:Dc:77:LEU:HD13	33:Dj:116:LEU:HD23	1.62	0.81
52:u:128:SER:OG	56:i:131:LEU:HD22	1.80	0.81
4:DA:1065:GLU:OE1	4:DA:1065:GLU:HA	1.78	0.81
38:DH:51:GLU:O	33:DJ:194:THR:HA	1.80	0.81
39:HD:55:LYS:HA	47:PG:164:MET:O	1.81	0.81
39:HD:287:TYR:CE1	44:HI:189:MET:SD	2.73	0.81
39:HD:298:GLN:NE2	44:HI:132:TRP:CD1	2.49	0.81
50:n:1218:ARG:NH2	50:n:1222:ARG:HB2	1.94	0.81
53:a:364:TYR:CB	53:a:430:LEU:HD12	2.11	0.81
57:m:124:GLN:OE1	59:z:590:ARG:CB	2.28	0.81
58:q:149:LYS:HE2	69:v:40:ALA:O	1.79	0.81
68:t:144:TYR:HD2	68:t:147:CYS:HB2	1.46	0.81
5:EA:143:GLN:CG	47:PG:158:PHE:CE1	2.64	0.81
39:HD:300:ALA:HB2	45:HJ:166:PRO:CA	1.99	0.81
58:q:93:TRP:HA	58:q:93:TRP:HE3	1.41	0.81
5:EA:139:LEU:CD2	47:PG:151:ARG:CB	2.44	0.81
30:DE:513:LEU:HD13	30:DE:513:LEU:H	1.46	0.81
50:n:359:ILE:CB	50:n:372:ILE:CD1	2.54	0.81
50:n:960:LYS:HB2	50:n:1210:PHE:HE2	0.98	0.81
60:b:136:HIS:CD2	61:c:111:TYR:CZ	2.69	0.81
38:DH:57:SER:HA	33:DJ:197:MET:SD	2.20	0.81
58:q:129:PRO:HB3	65:h:74:GLN:CD	2.05	0.81
58:q:186:GLU:CG	58:q:243:LEU:HD21	1.91	0.81
66:k:16:ASP:OD2	69:v:79:VAL:HG21	1.80	0.81
3:BA:43:ASP:OD1	15:PB:1064:ARG:NH2	2.14	0.80
9:PA:911:PRO:O	9:PA:963:ARG:NH2	2.14	0.80
16:HC:348:ARG:NH2	43:HF:65:ALA:HB3	1.96	0.80
30:DE:694:LEU:HD13	30:DE:703:MET:HE2	1.61	0.80
38:DH:108:PRO:CG	33:DJ:116:LEU:CD2	2.59	0.80
32:DI:23:LEU:HD11	32:DI:39:MET:CE	2.11	0.80
32:DI:23:LEU:CD1	32:DI:39:MET:HE1	2.11	0.80
55:f:145:TYR:CE1	65:h:43:PRO:HG3	2.15	0.80
58:q:462:ALA:O	69:v:131:GLU:HG2	1.79	0.80
16:HC:348:ARG:CZ	43:HF:65:ALA:HB3	2.10	0.80
31:DF:276:LEU:HA	31:DF:330:ARG:NH2	1.96	0.80
53:a:462:LEU:CB	72:x:49:GLN:CB	2.57	0.80
70:p:15:LEU:HD11	70:p:453:SER:HB2	1.63	0.80
45:HJ:52:GLU:HB3	45:HJ:273:LEU:HD11	1.61	0.80
53:a:417:TYR:HE1	53:a:450:PHE:HD1	1.07	0.80
65:h:139:GLN:NE2	66:k:37:LYS:HB2	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DL:71:ASP:HB3	35:DL:74:GLU:CG	2.10	0.80
44:HI:143:LEU:C	44:HI:143:LEU:HD22	2.07	0.80
51:s:106:SER:C	51:s:108:PHE:H	1.87	0.80
58:q:263:LYS:CE	58:q:439:PHE:CE2	2.65	0.80
60:b:136:HIS:HD2	61:c:111:TYR:CE2	1.98	0.80
9:PA:1795:PRO:HD3	54:d:169:PRO:CA	2.06	0.80
42:HH:266:GLN:N	42:HH:266:GLN:HE21	1.79	0.80
44:HI:261:PHE:HB2	55:f:52:MET:HE2	1.64	0.80
50:n:169:LEU:N	57:m:104:HIS:CD2	2.50	0.80
50:n:274:ILE:HD13	50:n:299:PHE:CE1	2.16	0.80
58:q:149:LYS:HE3	69:v:40:ALA:HA	1.64	0.80
64:o:735:LEU:CD2	71:w:113:GLN:CD	2.54	0.80
50:n:956:ALA:CB	50:n:1217:ARG:NH2	2.45	0.80
53:a:66:GLN:OE1	54:d:44:LEU:HD21	1.82	0.80
62:e:95:PHE:HB3	63:l:38:GLN:CG	2.12	0.80
5:EA:174:ARG:CB	39:HD:8:ARG:HH21	1.83	0.80
31:DF:43:VAL:HG23	32:DI:46:TYR:CB	2.12	0.80
53:a:461:SER:C	72:x:49:GLN:NE2	2.38	0.80
27:DO:2:ALA:CA	29:DD:1000:ARG:CD	2.44	0.80
32:DI:61:ALA:HA	35:DL:106:ARG:HG2	1.64	0.80
31:DF:332:PHE:HA	31:DF:335:ARG:HD3	1.64	0.80
45:HJ:177:ARG:NH1	45:HJ:177:ARG:HB2	1.97	0.80
50:n:686:LYS:HZ3	64:o:730:PRO:HB3	1.45	0.80
54:d:45:ILE:C	56:i:76:MET:HG2	2.07	0.80
58:q:644:SER:O	62:e:97:GLN:HG2	1.82	0.80
65:h:146:MET:CE	66:k:45:LEU:HD12	2.11	0.80
4:DA:491:MET:HE2	4:DA:491:MET:H	1.45	0.80
50:n:169:LEU:CB	50:n:170:PRO:CD	2.59	0.80
58:q:102:LEU:CD1	65:h:29:PHE:HE2	1.93	0.80
39:HD:83:ASN:CG	39:HD:140:LEU:HD11	2.07	0.79
58:q:152:SER:HB2	69:v:58:ASN:CA	2.06	0.79
29:DD:1058:VAL:HG21	35:DL:76:LEU:HD23	1.64	0.79
30:DE:694:LEU:HD13	30:DE:703:MET:HE1	0.81	0.79
45:HJ:165:ARG:HB2	45:HJ:165:ARG:NH1	1.96	0.79
48:g:127:ARG:HD2	50:n:152:PHE:HB2	1.64	0.79
53:a:321:LEU:HD21	53:a:407:ILE:HD12	1.63	0.79
54:d:45:ILE:HG12	56:i:73:ILE:CA	2.10	0.79
32:DI:132:LEU:HG	33:DJ:121:MET:HE2	1.62	0.79
53:a:462:LEU:CD1	72:x:60:ILE:CD1	2.61	0.79
29:DD:917:ILE:HG22	29:DD:1066:CYS:SG	2.22	0.79
31:DF:324:ASP:HA	31:DF:327:TRP:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:HG:109:THR:HG1	41:HG:148:SER:HG	1.26	0.79
50:n:203:LEU:CD1	50:n:215:LEU:HD12	2.11	0.79
67:r:191:GLU:OE2	69:v:8:PRO:HA	1.82	0.79
29:DD:886:GLY:HA3	29:DD:891:ILE:HG13	1.63	0.79
53:a:449:ARG:CZ	72:x:54:PRO:HB2	2.11	0.79
58:q:437:HIS:HE1	58:q:472:GLU:N	1.77	0.79
58:q:647:SER:HB2	62:e:97:GLN:NE2	1.96	0.79
30:DE:433:LYS:HE2	32:DI:110:TYR:CZ	2.18	0.79
31:DF:105:TYR:O	33:DJ:217:PHE:CB	2.31	0.79
50:n:172:CYS:SG	58:q:21:GLU:HB2	2.22	0.79
52:u:80:GLU:HB2	59:z:563:VAL:HG21	1.64	0.79
53:a:445:LEU:HD22	72:x:55:SER:OG	1.82	0.79
53:a:462:LEU:CB	72:x:49:GLN:HG2	2.12	0.79
58:q:596:PHE:CZ	63:l:117:TYR:OH	2.11	0.79
16:HC:352:GLN:NE2	43:HF:61:MET:HE1	1.97	0.79
30:DE:605:HIS:NE2	31:DF:77:LEU:HD21	1.98	0.79
31:DF:43:VAL:HA	32:DI:46:TYR:CD2	2.17	0.79
39:HD:295:ARG:NH1	45:HJ:165:ARG:NH2	2.26	0.79
58:q:460:ILE:HD12	58:q:529:MET:CE	2.13	0.79
66:k:87:ARG:HA	69:v:105:LEU:HD13	1.62	0.79
31:DF:218:VAL:HG12	38:DH:162:THR:HB	1.63	0.79
38:DH:50:PHE:HZ	33:DJ:170:ALA:C	1.88	0.79
45:HJ:28:ARG:CZ	45:HJ:28:ARG:HB2	2.11	0.79
54:d:46:GLU:HA	56:i:76:MET:HE3	1.65	0.79
58:q:188:LEU:HD22	69:v:87:ILE:HG13	1.65	0.79
58:q:395:PRO:HA	67:r:53:ASP:OD2	1.83	0.79
65:h:182:VAL:HG21	67:r:202:ILE:HD11	1.63	0.79
9:PA:902:GLU:OE2	9:PA:985:ARG:NH2	2.16	0.79
50:n:204:VAL:O	54:d:108:GLN:NE2	2.16	0.79
50:n:545:LEU:HD11	50:n:653:PRO:N	1.97	0.79
66:k:70:LEU:HD21	69:v:85:PHE:HD1	1.45	0.79
45:HJ:239:LYS:H	45:HJ:239:LYS:NZ	1.80	0.79
48:g:127:ARG:HH21	52:u:5:LEU:HB3	1.47	0.79
53:a:380:ALA:HB2	72:x:58:PRO:HG3	1.65	0.79
54:d:42:ARG:NH2	56:i:93:LYS:HA	1.97	0.79
54:d:42:ARG:NH2	56:i:96:GLU:OE2	2.14	0.79
58:q:644:SER:HA	58:q:647:SER:OG	1.83	0.79
5:EA:143:GLN:CD	47:PG:158:PHE:CE1	2.61	0.78
48:g:175:LEU:HD21	56:i:132:LEU:HD12	1.64	0.78
54:d:115:LYS:HE2	54:d:115:LYS:CA	2.13	0.78
31:DF:273:GLN:NE2	31:DF:273:GLN:H	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:706:LEU:O	64:o:684:ARG:NH2	2.16	0.78
60:b:174:ILE:HD11	63:l:75:LEU:HD23	1.65	0.78
65:h:150:LEU:CD2	66:k:45:LEU:HD11	2.09	0.78
4:DA:638:PRO:HB3	37:DG:39:LEU:HD23	1.63	0.78
48:g:166:ASN:OD1	48:g:166:ASN:C	2.23	0.78
54:d:167:TRP:HZ3	57:m:106:GLN:NE2	1.81	0.78
32:Di:73:LEU:HD22	35:Dl:105:HIS:CE1	2.18	0.78
30:DE:433:LYS:HD3	32:DI:110:TYR:CZ	2.19	0.78
38:DH:56:ALA:CB	33:DJ:214:PRO:CG	2.61	0.78
12:FB:179:ASP:OD1	29:DD:1002:ARG:NH2	2.16	0.78
38:DH:110:TYR:CD1	33:DJ:161:LYS:HD3	2.18	0.78
46:PD:94:LYS:NZ	47:PG:3:TYR:OH	2.17	0.78
54:d:45:ILE:HD11	56:i:73:ILE:CG1	2.14	0.78
30:De:747:LEU:HD23	30:De:747:LEU:H	1.47	0.78
36:Dm:31:LEU:H	36:Dm:31:LEU:HD23	1.47	0.78
16:HC:348:ARG:CZ	43:HF:65:ALA:CB	2.62	0.78
39:HD:83:ASN:OD1	39:HD:140:LEU:CD1	2.31	0.78
55:f:78:LEU:HD11	65:h:81:LEU:HD23	1.65	0.78
5:EA:181:ASN:HD21	39:HD:9:CYS:HA	1.45	0.78
25:DP:188:ARG:NH2	26:DQ:321:SER:OG	2.16	0.78
50:n:199:LEU:HD22	50:n:222:VAL:CG1	2.13	0.78
58:q:484:TYR:CD1	58:q:636:VAL:HG11	2.19	0.78
45:HJ:28:ARG:HB2	45:HJ:28:ARG:NH1	1.99	0.78
48:g:168:LEU:O	48:g:172:PRO:HD2	1.83	0.78
9:PA:22:GLN:NE2	9:PA:1446:GLY:O	2.17	0.78
11:EB:120:MET:HA	11:EB:124:LEU:HD12	1.66	0.78
31:DF:323:VAL:O	31:DF:327:TRP:N	2.17	0.78
31:DF:361:LYS:HA	31:DF:364:VAL:HG22	1.65	0.78
58:q:168:THR:OG1	66:k:21:ILE:CD1	2.30	0.78
60:b:178:LEU:HD11	63:l:78:LEU:HD13	1.64	0.78
13:HB:503:THR:OG1	13:HB:533:TYR:OH	2.01	0.77
31:DF:218:VAL:HG12	38:DH:162:THR:HG1	1.48	0.77
38:DH:50:PHE:HZ	33:DJ:170:ALA:HB3	1.48	0.77
38:DH:121:ALA:HB1	33:DJ:133:ALA:HB3	1.65	0.77
50:n:678:PHE:HB2	58:q:555:VAL:HG21	1.66	0.77
58:q:263:LYS:HE2	58:q:439:PHE:HE2	1.43	0.77
59:z:543:LEU:HD23	59:z:545:ARG:HD3	1.65	0.77
64:o:639:TYR:CD2	70:p:786:HIS:HB2	2.17	0.77
10:DB:618:ALA:O	16:HC:439:ARG:NH2	2.17	0.77
31:DF:71:ILE:CD1	32:DI:38:GLN:HE21	1.91	0.77
53:a:382:LEU:HD22	53:a:446:SER:CA	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:149:LYS:HG3	69:v:42:ILE:HG13	1.64	0.77
68:t:98:LEU:HB3	68:t:102:PHE:CD1	2.18	0.77
29:DD:1060:LEU:HD13	35:DL:79:ASP:HB3	1.65	0.77
50:n:209:PRO:HD2	50:n:289:LEU:HD12	1.67	0.77
50:n:270:GLN:HB3	55:f:181:LEU:HD11	1.64	0.77
9:PA:1643:TYR:HB2	57:m:96:PHE:CD2	2.19	0.77
12:FB:182:HIS:CD2	29:DD:998:GLN:OE1	2.38	0.77
38:DH:50:PHE:CD1	33:DJ:195:LEU:HD13	2.18	0.77
50:n:957:PRO:HD3	50:n:1214:VAL:HG21	1.64	0.77
58:q:168:THR:OG1	66:k:21:ILE:CG2	2.32	0.77
58:q:168:THR:HG1	66:k:21:ILE:HG21	1.48	0.77
58:q:186:GLU:HG3	58:q:243:LEU:HD22	1.41	0.77
66:k:37:LYS:H	66:k:37:LYS:CE	1.96	0.77
40:HE:56:LYS:NZ	40:HE:143:TYR:OH	2.16	0.77
50:n:224:PHE:CD2	50:n:292:MET:HE2	2.17	0.77
50:n:941:TYR:CG	50:n:1172:SER:HB3	2.14	0.77
61:c:290:ASP:O	68:t:120:CYS:CB	2.33	0.77
65:h:182:VAL:CG2	67:r:202:ILE:CD1	2.56	0.77
27:DO:1:MET:HB3	29:DD:997:ALA:HB1	1.67	0.77
31:DF:274:ASN:ND2	31:DF:316:GLN:HA	1.99	0.77
53:a:375:PHE:CG	72:x:17:ARG:NE	2.51	0.77
27:DO:2:ALA:C	29:DD:1000:ARG:HD3	2.10	0.77
50:n:168:ARG:CG	57:m:104:HIS:NE2	2.44	0.77
54:d:45:ILE:CG2	56:i:76:MET:HE2	2.12	0.77
18:PE:79:GLU:OE2	18:PE:86:THR:OG1	2.01	0.77
27:DO:1:MET:HE1	29:DD:993:GLN:HB3	1.65	0.77
49:j:35:ALA:CB	51:s:154:LEU:HD23	2.13	0.77
54:d:42:ARG:NH2	56:i:96:GLU:CD	2.42	0.77
58:q:186:GLU:HG2	58:q:243:LEU:HD22	1.58	0.77
66:k:33:LEU:HA	66:k:36:SER:OG	1.85	0.77
29:DD:961:GLN:NE2	30:DE:434:ASP:OD2	2.18	0.77
29:DD:1063:LEU:HD12	35:DL:80:VAL:HG13	1.65	0.77
29:DD:1063:LEU:CD1	35:DL:80:VAL:HG13	2.15	0.77
30:DE:433:LYS:CE	32:DI:110:TYR:OH	2.31	0.77
50:n:359:ILE:CG2	50:n:372:ILE:CD1	2.62	0.77
60:b:175:HIS:HB2	61:c:113:TRP:HH2	1.48	0.77
38:DH:44:LEU:HD21	33:DJ:129:THR:HG21	1.67	0.77
52:u:61:LEU:HA	52:u:64:ARG:HD3	1.66	0.77
53:a:417:TYR:HE1	53:a:450:PHE:CE1	1.88	0.77
53:a:504:ILE:HA	53:a:507:THR:HG23	1.67	0.77
54:d:167:TRP:CZ3	57:m:106:GLN:NE2	2.53	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:113:TYR:HB2	65:h:19:VAL:HG11	1.65	0.77
60:b:178:LEU:HD23	63:l:82:LEU:HD11	1.64	0.77
9:PA:1173:THR:OG1	21:PI:56:ASN:OD1	2.03	0.76
16:HC:397:GLU:CG	43:HF:61:MET:HE3	2.15	0.76
54:d:45:ILE:CD1	56:i:72:ILE:C	2.56	0.76
64:o:717:SER:HA	72:x:70:SER:HB2	1.67	0.76
5:EA:174:ARG:CG	39:HD:8:ARG:NH2	2.48	0.76
16:HC:352:GLN:HE21	43:HF:61:MET:HE1	1.49	0.76
38:DH:56:ALA:CB	33:DJ:214:PRO:HG3	2.15	0.76
39:HD:298:GLN:HE22	44:HI:132:TRP:CD1	2.04	0.76
53:a:509:ARG:HB2	53:a:509:ARG:CZ	2.15	0.76
65:h:85:ARG:HA	65:h:99:VAL:HG12	1.67	0.76
7:HA:722:ARG:NH2	41:HG:202:SER:OG	2.18	0.76
5:EA:174:ARG:CG	39:HD:8:ARG:HH22	1.97	0.76
38:DH:108:PRO:CG	33:DJ:116:LEU:HD23	2.14	0.76
50:n:921:MET:HE1	50:n:1215:ILE:HD11	1.65	0.76
58:q:458:PRO:CB	58:q:533:GLN:NE2	2.49	0.76
38:DH:50:PHE:CZ	33:DJ:170:ALA:CB	2.67	0.76
39:HD:145:GLU:OE1	65:h:67:LYS:HE2	1.86	0.76
44:HI:171:HIS:CE1	44:HI:188:ARG:HA	2.20	0.76
53:a:375:PHE:HB3	72:x:17:ARG:NH2	2.00	0.76
29:DD:961:GLN:O	29:DD:965:ILE:HG12	1.84	0.76
32:DI:16:ALA:CA	32:DI:40:LEU:HD11	2.13	0.76
50:n:168:ARG:HG3	57:m:104:HIS:HE1	0.96	0.76
58:q:138:LYS:CB	58:q:140:ASN:OD1	2.28	0.76
50:n:944:PHE:HE2	60:b:101:ARG:HH22	1.32	0.76
53:a:337:ALA:HB1	53:a:338:PRO:CD	2.16	0.76
66:k:88:LYS:HD2	66:k:88:LYS:O	1.86	0.76
38:DH:56:ALA:HB1	33:DJ:214:PRO:HG3	1.68	0.76
50:n:222:VAL:HG22	50:n:234:LEU:O	1.86	0.76
53:a:109:TYR:OH	53:a:154:LEU:HD21	1.83	0.76
60:b:136:HIS:CD2	61:c:111:TYR:CG	2.73	0.76
60:b:174:ILE:CG1	63:l:75:LEU:HD11	2.14	0.76
31:DF:43:VAL:HA	32:DI:46:TYR:HD2	1.51	0.76
50:n:647:MET:CE	71:w:22:PHE:HB2	2.15	0.76
59:z:540:LEU:HB3	59:z:541:PRO:HD3	1.68	0.76
67:r:108:ILE:HD13	68:t:91:PHE:HA	1.66	0.76
31:DF:82:PRO:HB2	31:DF:98:SER:HB3	1.67	0.75
31:DF:217:SER:OG	38:DH:162:THR:N	2.19	0.75
31:DF:323:VAL:HA	31:DF:326:HIS:HD2	1.51	0.75
38:DH:49:GLY:O	33:DJ:171:LEU:HD13	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DI:132:LEU:CD2	33:DJ:121:MET:CE	2.64	0.75
4:DA:396:LEU:H	4:DA:396:LEU:HD13	1.50	0.75
58:q:102:LEU:HD11	65:h:29:PHE:CD2	2.19	0.75
5:EA:181:ASN:ND2	39:HD:9:CYS:CA	2.49	0.75
29:DD:874:LEU:HD23	29:DD:874:LEU:H	1.51	0.75
50:n:921:MET:HE1	50:n:1215:ILE:CD1	2.15	0.75
58:q:120:ARG:HG2	58:q:120:ARG:NH1	1.98	0.75
65:h:153:LYS:HE3	66:k:46:ASP:OD2	1.85	0.75
66:k:16:ASP:OD2	69:v:79:VAL:CG2	2.34	0.75
20:PH:2:ALA:O	20:PH:84:ARG:NH2	2.20	0.75
58:q:134:ALA:N	65:h:72:ARG:NH1	2.33	0.75
7:HA:711:ASP:OD1	7:HA:715:GLN:NE2	2.19	0.75
31:DF:104:LEU:HB3	33:DJ:217:PHE:HE2	1.51	0.75
39:HD:85:ARG:HH22	39:HD:140:LEU:CA	1.98	0.75
53:a:224:TYR:CE2	53:a:253:MET:HB3	2.21	0.75
66:k:104:LEU:CD2	69:v:123:ILE:HD11	2.16	0.75
29:DD:1071:ARG:HB2	31:DF:91:PHE:CG	2.20	0.75
30:DE:433:LYS:HE2	32:DI:110:TYR:OH	1.86	0.75
31:DF:274:ASN:HB2	31:DF:317:LEU:H	1.51	0.75
35:DL:111:LEU:HA	35:DL:114:LYS:HZ1	1.50	0.75
50:n:270:GLN:HE22	55:f:174:ARG:HD2	1.50	0.75
53:a:412:ARG:HB3	53:a:472:SER:HB3	1.67	0.75
58:q:186:GLU:OE2	58:q:291:TRP:HZ2	1.70	0.75
60:b:101:ARG:NH1	70:p:677:THR:HA	2.01	0.75
64:o:748:PHE:CD2	72:x:66:TYR:HE1	2.05	0.75
9:PA:1242:ASP:HA	9:PA:1262:MET:HE2	1.68	0.75
31:DF:241:GLU:OE2	38:DH:135:THR:OG1	2.05	0.75
42:HH:371:VAL:HG23	42:HH:407:ILE:HG22	1.68	0.75
58:q:188:LEU:HD13	69:v:87:ILE:HG13	1.68	0.75
68:t:172:ALA:HB1	68:t:173:PRO:CD	2.16	0.75
44:HI:169:TYR:HB3	44:HI:190:TYR:CE2	2.22	0.75
50:n:960:LYS:HB3	50:n:1210:PHE:CE2	2.21	0.75
60:b:136:HIS:CB	61:c:111:TYR:CZ	2.70	0.75
38:DH:108:PRO:HG3	33:DJ:116:LEU:HD23	1.68	0.75
45:HJ:181:LEU:HD13	45:HJ:181:LEU:N	2.01	0.75
14:NF:297:LEU:O	14:NF:302:GLY:HA2	1.86	0.75
30:DE:359:LEU:O	30:DE:359:LEU:HD12	1.87	0.74
30:DE:605:HIS:CE1	31:DF:77:LEU:HD11	2.22	0.74
39:HD:300:ALA:HA	45:HJ:166:PRO:HG3	1.66	0.74
53:a:413:HIS:CD2	53:a:471:ASP:HA	2.22	0.74
54:d:164:PRO:HD2	54:d:167:TRP:CB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:k:101:ARG:HB3	66:k:101:ARG:CZ	2.16	0.74
32:DI:132:LEU:CG	33:DJ:121:MET:CE	2.65	0.74
44:HI:207:LEU:O	55:f:53:GLN:CG	2.35	0.74
44:HI:207:LEU:O	55:f:53:GLN:HG2	1.87	0.74
45:HJ:288:ASN:C	45:HJ:288:ASN:HD22	1.94	0.74
54:d:45:ILE:HD11	56:i:73:ILE:CA	2.14	0.74
38:DH:107:LEU:HD21	33:DJ:158:ALA:HB2	1.70	0.74
32:DI:132:LEU:CD2	33:DJ:121:MET:HE1	2.17	0.74
55:f:145:TYR:CD2	65:h:43:PRO:HD3	2.21	0.74
58:q:135:LEU:HD12	58:q:135:LEU:O	1.86	0.74
64:o:707:ILE:HG23	64:o:720:PRO:HA	1.69	0.74
5:EA:143:GLN:CG	47:PG:158:PHE:CZ	2.60	0.74
31:DF:63:ARG:O	31:DF:65:LYS:N	2.19	0.74
39:HD:84:LYS:CA	39:HD:136:ASN:ND2	2.49	0.74
60:b:136:HIS:HB2	61:c:111:TYR:OH	1.88	0.74
15:PB:59:VAL:HG21	15:PB:91:ILE:HD11	1.70	0.74
38:DH:114:SER:O	38:DH:116:ARG:N	2.20	0.74
50:n:957:PRO:CD	50:n:1214:VAL:HG21	2.17	0.74
31:DF:404:ARG:NH2	31:DF:452:PHE:O	2.20	0.74
45:HJ:102:ARG:HG2	45:HJ:102:ARG:HH11	1.53	0.74
53:a:337:ALA:HB1	53:a:338:PRO:HD2	1.70	0.74
62:e:129:VAL:CG2	66:k:114:MET:HE2	2.17	0.74
65:h:8:LEU:HA	65:h:69:PRO:HG3	1.68	0.74
68:t:131:MET:HB2	68:t:136:ARG:HD2	1.67	0.74
16:HC:348:ARG:HD3	43:HF:66:PHE:O	1.87	0.74
50:n:169:LEU:H	57:m:104:HIS:CE1	2.05	0.74
50:n:359:ILE:HG13	50:n:372:ILE:HD11	1.64	0.74
57:m:124:GLN:HB2	59:z:590:ARG:HD2	1.68	0.74
65:h:102:HIS:CD2	65:h:102:HIS:H	2.03	0.74
9:PA:1475:LEU:HD23	47:PG:66:VAL:HG21	1.69	0.74
23:PK:77:THR:OG1	23:PK:81:TYR:O	2.05	0.74
46:PD:87:LEU:HD11	46:PD:100:LEU:HD11	1.70	0.74
1:X:21:DC:H42	2:Y:-21:DG:H1	1.36	0.74
5:EA:171:LYS:HZ2	39:HD:41:ARG:HG3	1.50	0.74
29:DD:1078:LEU:HD21	35:DL:83:MET:CE	2.14	0.74
44:HI:47:HIS:HA	44:HI:52:LYS:HG2	1.70	0.74
54:d:123:THR:CG2	58:q:37:SER:HB3	2.18	0.74
55:f:101:ILE:HD11	65:h:105:VAL:HG11	1.70	0.74
50:n:904:PHE:CE2	50:n:1208:GLU:CD	2.59	0.74
54:d:167:TRP:O	57:m:106:GLN:OE1	2.06	0.74
58:q:34:LEU:N	58:q:34:LEU:HD23	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:t:8:GLN:HE22	68:t:200:ILE:HG23	1.52	0.74
9:PA:279:LYS:O	9:PA:283:ILE:HD12	1.87	0.73
28:Dc:77:LEU:HD12	33:Dj:116:LEU:HD23	1.68	0.73
45:HJ:175:LYS:N	45:HJ:175:LYS:HZ2	1.85	0.73
53:a:364:TYR:HB3	53:a:430:LEU:HG	1.66	0.73
54:d:126:TYR:CD2	58:q:36:MET:SD	2.82	0.73
5:EA:188:TYR:CD2	39:HD:14:TYR:CD1	2.76	0.73
9:PA:1005:HIS:HD2	9:PA:1007:ILE:HG22	1.50	0.73
53:a:364:TYR:CB	53:a:430:LEU:CG	2.64	0.73
53:a:412:ARG:HB3	53:a:472:SER:CB	2.18	0.73
39:HD:287:TYR:CG	39:HD:287:TYR:O	2.40	0.73
48:g:171:LEU:HD21	54:d:110:LEU:HG	1.68	0.73
53:a:462:LEU:CB	72:x:49:GLN:CG	2.65	0.73
54:d:45:ILE:CG1	56:i:73:ILE:CG1	2.66	0.73
61:c:135:ARG:NH2	62:e:92:GLU:OE1	2.21	0.73
16:HC:398:ARG:NH2	43:HF:58:GLY:HA2	2.02	0.73
35:DL:61:LYS:O	35:DL:61:LYS:NZ	2.21	0.73
44:HI:95:GLU:H	44:HI:146:ASP:HA	1.54	0.73
2:Y:29:DA:OP1	26:DQ:346:LYS:NZ	2.20	0.73
16:HC:398:ARG:HH22	43:HF:58:GLY:CA	2.01	0.73
31:DF:68:THR:O	31:DF:68:THR:HG22	1.86	0.73
31:DF:279:LEU:HB2	31:DF:330:ARG:NH2	2.04	0.73
53:a:417:TYR:CZ	53:a:450:PHE:CD1	2.77	0.73
56:i:75:CYS:CB	56:i:88:ASN:ND2	2.50	0.73
58:q:481:SER:HB2	58:q:636:VAL:HG21	1.70	0.73
65:h:85:ARG:HA	65:h:99:VAL:CG1	2.18	0.73
66:k:101:ARG:HB3	66:k:101:ARG:NH1	2.02	0.73
9:PA:1475:LEU:CD2	47:PG:66:VAL:HG22	2.15	0.73
31:DF:274:ASN:HB2	31:DF:317:LEU:CD2	2.16	0.73
50:n:937:ARG:NE	50:n:943:LEU:HD21	2.03	0.73
56:i:68:LEU:CD1	56:i:95:GLN:HG2	2.09	0.73
58:q:184:ASN:CG	69:v:83:LYS:HD2	2.14	0.73
60:b:136:HIS:HD2	61:c:111:TYR:CG	2.05	0.73
7:HA:231:VAL:HG13	7:HA:454:VAL:HG23	1.70	0.73
30:DE:429:LEU:HB3	30:DE:430:PRO:CD	2.16	0.73
38:DH:156:PRO:O	38:DH:160:ILE:HB	1.88	0.73
54:d:45:ILE:C	56:i:76:MET:HE3	2.13	0.73
66:k:70:LEU:HD21	69:v:85:PHE:CD1	2.22	0.73
50:n:359:ILE:HG12	50:n:372:ILE:HD13	1.64	0.73
54:d:126:TYR:CZ	58:q:36:MET:HB2	2.23	0.73
68:t:172:ALA:HB1	68:t:173:PRO:HD2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:428:LEU:CD1	31:DF:455:LEU:CB	2.64	0.73
48:g:128:PRO:HB3	54:d:149:ILE:HD13	1.71	0.73
49:j:82:LYS:NZ	51:s:101:VAL:HG12	2.03	0.73
50:n:301:LEU:HD13	50:n:361:ILE:HD12	1.68	0.73
50:n:956:ALA:HB1	50:n:1217:ARG:HH22	1.52	0.73
58:q:428:LEU:HD12	58:q:428:LEU:O	1.89	0.73
9:PA:869:GLU:OE1	9:PA:1455:SER:OG	2.07	0.73
31:DF:214:HIS:CE1	31:DF:216:LEU:HB2	2.23	0.73
50:n:169:LEU:HD22	57:m:101:GLN:HA	1.71	0.73
50:n:545:LEU:CD1	50:n:653:PRO:N	2.50	0.73
52:u:73:ILE:HA	52:u:76:LEU:HB3	1.71	0.73
54:d:38:GLU:OE2	56:i:99:LYS:HD2	1.89	0.73
58:q:109:MET:CA	58:q:109:MET:HE3	2.19	0.73
68:t:122:PHE:CZ	68:t:156:LEU:HD11	2.24	0.73
5:EA:122:THR:OG1	39:HD:40:VAL:CG2	2.37	0.72
30:DE:433:LYS:HD3	32:DI:110:TYR:HH	1.50	0.72
35:DL:71:ASP:CB	35:DL:74:GLU:HG3	2.19	0.72
55:f:95:LEU:C	58:q:130:VAL:HG11	2.14	0.72
58:q:645:ALA:HB2	62:e:100:LEU:HD21	1.69	0.72
39:HD:55:LYS:C	39:HD:57:ASN:H	1.97	0.72
50:n:168:ARG:HG3	57:m:104:HIS:NE2	1.99	0.72
50:n:237:MET:HE1	58:q:45:GLN:CA	2.19	0.72
50:n:482:VAL:HG22	50:n:489:ILE:HG12	1.70	0.72
53:a:467:MET:HE2	53:a:504:ILE:HD11	1.70	0.72
58:q:544:MET:SD	58:q:640:GLU:HG2	2.29	0.72
5:EA:143:GLN:CD	47:PG:158:PHE:HE1	1.95	0.72
30:DE:605:HIS:CE1	31:DF:77:LEU:HD21	2.23	0.72
31:DF:241:GLU:CD	38:DH:135:THR:OG1	2.32	0.72
45:HJ:167:PHE:O	45:HJ:167:PHE:HD1	1.72	0.72
50:n:154:ILE:HB	50:n:155:PRO:HD3	1.69	0.72
50:n:206:THR:HG22	50:n:289:LEU:HB2	1.71	0.72
51:s:104:LYS:C	51:s:106:SER:N	2.41	0.72
55:f:95:LEU:O	58:q:130:VAL:CG1	2.37	0.72
5:EA:178:ALA:CA	39:HD:8:ARG:O	2.36	0.72
47:PG:21:ASN:O	47:PG:25:THR:OG1	2.05	0.72
50:n:652:MET:HE1	71:w:18:ILE:HG23	1.71	0.72
56:i:72:ILE:HD13	56:i:92:SER:HB3	1.72	0.72
68:t:6:VAL:HG22	68:t:141:GLU:HB2	1.71	0.72
30:DE:433:LYS:CE	32:DI:110:TYR:CE1	2.73	0.72
40:HE:160:ARG:NH2	40:HE:234:ASP:OD1	2.23	0.72
44:HI:207:LEU:HD22	55:f:52:MET:HE1	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:134:THR:HB	59:z:597:VAL:HG13	1.71	0.72
54:d:110:LEU:HD22	54:d:110:LEU:C	2.14	0.72
5:EA:139:LEU:HD12	47:PG:151:ARG:HD2	1.61	0.72
5:EA:143:GLN:NE2	47:PG:158:PHE:CE1	2.56	0.72
10:DB:672:PHE:HD1	16:HC:414:SER:HB2	1.53	0.72
50:n:960:LYS:CG	50:n:1210:PHE:CE2	2.72	0.72
52:u:90:LEU:CB	58:q:9:ILE:HG12	2.20	0.72
54:d:42:ARG:NH2	56:i:93:LYS:HG2	2.04	0.72
54:d:46:GLU:CA	56:i:76:MET:HE3	2.20	0.72
58:q:479:ILE:O	58:q:532:HIS:ND1	2.22	0.72
58:q:123:LYS:NZ	65:h:88:ASP:OD2	2.23	0.72
58:q:437:HIS:CE1	58:q:472:GLU:CA	2.71	0.72
59:z:567:GLN:O	59:z:567:GLN:NE2	2.23	0.72
35:DI:102:LEU:HA	35:DI:105:HIS:HD2	1.55	0.72
39:HD:85:ARG:NH2	39:HD:139:LYS:O	2.23	0.72
58:q:395:PRO:HA	67:r:53:ASP:CG	2.15	0.72
61:c:288:LEU:CD1	68:t:122:PHE:CZ	2.72	0.72
68:t:8:GLN:NE2	68:t:200:ILE:HG23	2.04	0.72
31:DF:279:LEU:HB2	31:DF:330:ARG:HH21	1.53	0.72
31:DF:429:LYS:O	31:DF:433:PRO:HD2	1.89	0.72
39:HD:23:VAL:HG21	39:HD:73:GLU:HG3	1.71	0.72
43:HF:24:ASP:OD1	43:HF:25:GLU:N	2.22	0.72
50:n:266:VAL:HG22	55:f:177:VAL:CG1	2.19	0.72
50:n:941:TYR:CE2	50:n:1172:SER:OG	2.43	0.72
53:a:56:GLN:NE2	54:d:51:SER:O	2.22	0.72
54:d:31:LEU:CD2	56:i:103:THR:CB	2.67	0.72
66:k:86:SER:C	69:v:105:LEU:HD13	2.14	0.72
30:DE:433:LYS:CE	32:DI:110:TYR:CZ	2.73	0.72
35:DL:60:LYS:O	35:DL:60:LYS:NZ	2.18	0.72
46:PD:67:TYR:OH	47:PG:86:ASP:OD1	2.06	0.72
50:n:250:LEU:HG	50:n:275:HIS:HB2	1.71	0.72
50:n:707:ASP:HB2	64:o:684:ARG:NH2	2.04	0.72
55:f:15:TRP:HH2	55:f:35:GLU:OE1	1.72	0.72
56:i:110:SER:HB2	56:i:111:PRO:HD2	1.72	0.72
58:q:184:ASN:CG	69:v:83:LYS:CD	2.63	0.72
60:b:136:HIS:HB2	61:c:111:TYR:CZ	2.25	0.72
71:w:510:PRO:HD3	71:w:922:MET:HE1	1.71	0.72
9:PA:322:LEU:O	9:PA:327:ARG:NH2	2.23	0.71
45:HJ:207:TYR:HB3	45:HJ:211:GLN:HE22	1.55	0.71
50:n:359:ILE:HA	50:n:372:ILE:CD1	2.19	0.71
52:u:90:LEU:HD22	58:q:9:ILE:HD11	0.75	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:38:GLU:CD	56:i:96:GLU:CG	2.61	0.71
58:q:102:LEU:CD1	65:h:29:PHE:CD2	2.72	0.71
58:q:418:ILE:HD13	68:t:72:PRO:HG2	1.72	0.71
65:h:22:LEU:HD12	65:h:22:LEU:C	2.13	0.71
48:g:73:ASP:CG	59:z:535:SER:HB2	2.14	0.71
72:x:566:GLU:C	72:x:568:LYS:H	1.98	0.71
25:DP:185:LEU:CD2	29:DD:1006:LEU:HD13	2.20	0.71
45:HJ:236:LEU:O	45:HJ:238:LEU:N	2.22	0.71
50:n:172:CYS:SG	58:q:21:GLU:CA	2.78	0.71
50:n:192:LEU:CB	50:n:219:ASN:O	2.39	0.71
50:n:234:LEU:HD21	50:n:282:LEU:HD22	1.72	0.71
50:n:261:ASP:OD1	58:q:250:ASP:OD2	2.06	0.71
56:i:122:ARG:C	56:i:122:ARG:HD3	2.14	0.71
69:v:119:LEU:C	69:v:119:LEU:HD12	2.15	0.71
5:EA:17:LEU:HD22	5:EA:194:THR:CG2	2.19	0.71
10:DB:241:PRO:HG2	10:DB:496:MET:HE1	1.72	0.71
31:DF:22:VAL:HG13	32:DI:44:PHE:CE1	2.25	0.71
52:u:115:LEU:CA	54:d:121:LEU:HD12	2.21	0.71
58:q:152:SER:CB	69:v:58:ASN:HA	2.09	0.71
58:q:212:ALA:HB1	58:q:380:ARG:NH2	2.04	0.71
39:HD:300:ALA:HB1	45:HJ:166:PRO:HA	1.67	0.71
40:HE:67:SER:O	40:HE:139:LYS:NZ	2.24	0.71
40:HE:272:LEU:O	40:HE:272:LEU:HD23	1.90	0.71
54:d:45:ILE:HD13	56:i:73:ILE:N	2.00	0.71
54:d:168:VAL:HB	54:d:169:PRO:CD	2.20	0.71
69:v:120:ARG:HG2	69:v:120:ARG:HH11	1.56	0.71
4:DA:357:GLU:HG3	4:DA:497:PRO:HB3	1.73	0.71
31:DF:218:VAL:CG1	38:DH:162:THR:HG21	2.18	0.71
50:n:274:ILE:CD1	50:n:299:PHE:CE1	2.74	0.71
58:q:263:LYS:CE	58:q:439:PHE:HE2	2.02	0.71
58:q:481:SER:HB2	58:q:636:VAL:CG2	2.21	0.71
64:o:633:VAL:HG11	70:p:810:PRO:CB	1.87	0.71
66:k:87:ARG:HG3	66:k:87:ARG:NH1	2.01	0.71
43:HF:36:GLN:HE21	43:HF:38:ILE:HG13	1.54	0.71
58:q:595:GLN:HG2	58:q:619:ARG:HB2	1.71	0.71
68:t:129:VAL:HG21	68:t:200:ILE:CD1	2.17	0.71
39:HD:289:SER:O	39:HD:292:ALA:HB3	1.90	0.71
53:a:109:TYR:CZ	53:a:154:LEU:CD2	2.72	0.71
53:a:465:VAL:HG21	53:a:511:ILE:HD13	1.72	0.71
54:d:42:ARG:HH22	56:i:93:LYS:CA	2.03	0.71
54:d:154:ARG:NH2	57:m:66:TYR:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:134:ALA:N	65:h:72:ARG:HH12	1.87	0.71
16:HC:408:LEU:HD21	43:HF:36:GLN:CD	2.16	0.71
31:DF:104:LEU:HB3	33:DJ:217:PHE:CZ	2.20	0.71
58:q:112:LEU:CD2	65:h:19:VAL:HG21	2.20	0.71
59:z:529:HIS:HE1	59:z:580:ILE:HG21	1.56	0.71
53:a:441:GLU:HG2	53:a:453:SER:OG	1.90	0.70
58:q:263:LYS:HE2	58:q:439:PHE:CZ	2.25	0.70
58:q:394:HIS:CD2	67:r:49:GLU:HG3	2.25	0.70
53:a:383:PRO:HG3	72:x:92:LEU:CD2	2.19	0.70
58:q:437:HIS:CE1	58:q:472:GLU:C	2.69	0.70
58:q:630:MET:HE3	58:q:631:GLU:H	1.55	0.70
11:EB:82:VAL:HG12	11:EB:86:LYS:NZ	2.06	0.70
50:n:101:ALA:HB2	51:s:109:LEU:HD21	1.74	0.70
50:n:237:MET:CE	58:q:45:GLN:HB2	2.21	0.70
50:n:270:GLN:CA	55:f:181:LEU:HD11	2.20	0.70
58:q:106:LEU:HD23	58:q:106:LEU:C	2.15	0.70
58:q:458:PRO:CG	58:q:533:GLN:NE2	2.25	0.70
31:DF:104:LEU:CD1	33:DJ:217:PHE:HE2	2.04	0.70
39:HD:254:GLU:CD	39:HD:254:GLU:H	1.99	0.70
53:a:160:LEU:CD1	53:a:214:ARG:HH21	2.03	0.70
53:a:417:TYR:CE1	53:a:450:PHE:HE1	2.00	0.70
53:a:462:LEU:CD1	72:x:60:ILE:HD11	2.21	0.70
58:q:116:LEU:HB3	65:h:16:LEU:CD2	2.22	0.70
5:EA:139:LEU:CD1	47:PG:151:ARG:CD	2.17	0.70
31:DF:81:GLU:OE2	31:DF:91:PHE:HD1	1.75	0.70
35:DL:114:LYS:O	35:DL:118:LEU:HG	1.91	0.70
46:PD:74:PHE:HE1	46:PD:137:LYS:HB2	1.53	0.70
50:n:168:ARG:HD2	57:m:104:HIS:NE2	2.04	0.70
54:d:103:ARG:HG2	54:d:103:ARG:NH1	2.05	0.70
5:EA:171:LYS:HZ1	39:HD:41:ARG:HG3	1.54	0.70
29:DD:950:LEU:C	29:DD:950:LEU:HD13	2.16	0.70
39:HD:120:LYS:O	39:HD:124:ILE:HD12	1.91	0.70
50:n:104:LYS:HZ2	51:s:108:PHE:HA	1.55	0.70
53:a:214:ARG:CZ	53:a:214:ARG:HB2	2.21	0.70
58:q:109:MET:HE3	58:q:109:MET:HA	1.74	0.70
58:q:491:ILE:HD12	58:q:532:HIS:CA	2.21	0.70
62:e:95:PHE:CE1	63:l:37:GLY:HA3	2.26	0.70
65:h:12:LEU:C	65:h:12:LEU:HD13	2.17	0.70
13:HB:195:SER:O	13:HB:199:THR:OG1	2.06	0.70
39:HD:287:TYR:CD1	39:HD:287:TYR:O	2.45	0.70
39:HD:287:TYR:CG	44:HI:189:MET:SD	2.84	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:147:ILE:HG21	65:h:124:LEU:HD22	1.72	0.70
58:q:190:LEU:HD12	58:q:196:LEU:HD11	1.74	0.70
4:DA:489:GLN:HB2	31:Df:315:ARG:HH11	1.56	0.70
34:Dk:191:VAL:HG13	34:Dk:200:ILE:HD13	1.74	0.70
32:DI:81:GLN:NE2	35:DL:123:GLN:NE2	2.34	0.70
45:HJ:174:LEU:HD13	45:HJ:231:TYR:HE2	1.56	0.70
50:n:295:CYS:SG	55:f:188:PHE:CE2	2.84	0.70
50:n:960:LYS:HZ1	50:n:1185:LEU:HD13	1.55	0.70
53:a:223:LYS:HZ1	53:a:251:LEU:C	1.99	0.70
53:a:259:ILE:HD12	53:a:259:ILE:H	1.56	0.70
58:q:206:ASP:O	66:k:84:TYR:OH	2.08	0.70
58:q:644:SER:HB3	62:e:96:LEU:HB3	1.74	0.70
45:HJ:82:THR:HG23	45:HJ:160:VAL:HG11	1.73	0.70
53:a:375:PHE:CE2	72:x:17:ARG:NE	2.45	0.70
69:v:120:ARG:HG2	69:v:120:ARG:NH1	2.05	0.70
38:DH:110:TYR:OH	33:DJ:160:GLN:HB3	1.92	0.70
53:a:388:LEU:HD21	53:a:447:GLU:HG3	1.72	0.70
54:d:76:PHE:HZ	56:i:65:PHE:HE2	1.27	0.70
58:q:187:LEU:CD2	69:v:84:GLN:HG2	2.22	0.70
73:y:170:VAL:HG22	73:y:198:ALA:HB2	1.74	0.70
3:BA:23:LEU:HD12	3:BA:32:MET:HE2	1.74	0.69
50:n:229:GLU:C	50:n:253:LEU:HB2	2.15	0.69
53:a:445:LEU:CD1	72:x:55:SER:CA	2.59	0.69
58:q:149:LYS:HE2	69:v:40:ALA:CA	2.19	0.69
1:X:-5:DT:H3	2:Y:5:DA:H61	1.38	0.69
10:DB:646:ASP:N	16:HC:413:LEU:O	2.25	0.69
17:PC:193:ARG:NH2	17:PC:218:ALA:O	2.26	0.69
48:g:159:ARG:O	48:g:159:ARG:HD3	1.92	0.69
49:j:43:PHE:CB	51:s:144:ILE:HG23	2.22	0.69
58:q:212:ALA:HB1	58:q:380:ARG:HH22	1.56	0.69
64:o:639:TYR:HD2	70:p:786:HIS:CG	2.03	0.69
69:v:119:LEU:HD12	69:v:119:LEU:O	1.91	0.69
15:PB:254:GLN:OE1	15:PB:254:GLN:N	2.24	0.69
39:HD:85:ARG:NH1	39:HD:140:LEU:CG	2.45	0.69
48:g:79:ARG:HH21	52:u:74:ASP:HA	1.56	0.69
50:n:97:VAL:HG22	51:s:109:LEU:HG	1.73	0.69
53:a:145:LYS:HA	53:a:145:LYS:HE3	1.74	0.69
7:HA:252:THR:HG22	7:HA:432:ILE:HG22	1.74	0.69
9:PA:1248:ASN:ND2	9:PA:1254:LYS:O	2.26	0.69
31:DF:316:GLN:HE22	31:DF:320:ARG:HA	1.57	0.69
42:HH:611:GLY:O	42:HH:642:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:462:LEU:N	72:x:49:GLN:CD	2.43	0.69
58:q:113:TYR:HB2	65:h:19:VAL:HG12	1.75	0.69
32:DI:20:ALA:HB2	32:DI:36:ILE:HD13	1.72	0.69
53:a:109:TYR:OH	53:a:154:LEU:CD2	2.40	0.69
39:HD:287:TYR:HB3	44:HI:189:MET:HG2	1.73	0.69
48:g:128:PRO:CB	54:d:149:ILE:HD13	2.23	0.69
52:u:67:LYS:HE3	59:z:528:LEU:HD22	1.74	0.69
53:a:336:TYR:CZ	53:a:391:THR:OG1	2.45	0.69
53:a:445:LEU:CB	72:x:55:SER:HB2	1.98	0.69
55:f:115:ILE:HG23	58:q:112:LEU:HD11	1.74	0.69
63:l:167:ILE:HD11	69:v:123:ILE:HG22	1.75	0.69
7:HA:637:LEU:HD11	7:HA:648:GLU:HA	1.74	0.69
45:HJ:64:LEU:HD13	45:HJ:105:MET:HB3	1.73	0.69
50:n:169:LEU:CA	57:m:104:HIS:CG	2.68	0.69
53:a:131:ASN:ND2	53:a:131:ASN:H	1.90	0.69
54:d:42:ARG:NH2	56:i:93:LYS:CA	2.55	0.69
58:q:171:VAL:CG2	66:k:17:ILE:HG23	2.06	0.69
58:q:481:SER:CB	58:q:636:VAL:CG2	2.71	0.69
5:EA:20:TYR:CD2	5:EA:190:LEU:HD11	2.26	0.69
7:HA:382:LEU:O	7:HA:385:THR:OG1	2.11	0.69
9:PA:373:LEU:O	9:PA:485:ASN:ND2	2.25	0.69
16:HC:397:GLU:CD	43:HF:61:MET:CG	2.62	0.69
30:DE:605:HIS:ND1	31:DF:77:LEU:HD11	2.08	0.69
42:HH:191:ASP:O	42:HH:195:ARG:NH1	2.25	0.69
50:n:591:PHE:HB3	71:w:26:PHE:HD1	1.58	0.69
58:q:112:LEU:HD23	65:h:19:VAL:HG21	1.73	0.69
58:q:187:LEU:O	58:q:187:LEU:HD12	1.93	0.69
70:p:13:MET:CG	70:p:405:PHE:HB2	2.22	0.69
19:PF:100:ARG:NH2	19:PF:121:ASP:O	2.26	0.69
39:HD:262:GLU:HA	39:HD:294:HIS:CE1	2.28	0.69
44:HI:106:SER:HB2	55:f:59:HIS:CE1	2.27	0.69
65:h:8:LEU:C	65:h:8:LEU:HD23	2.18	0.69
35:DL:99:ALA:HB1	35:DL:115:ASP:HB3	1.75	0.69
50:n:229:GLU:HB3	50:n:300:CYS:SG	2.33	0.69
31:Df:447:ALA:CA	31:Df:456:GLY:HA3	2.23	0.68
32:Di:73:LEU:HD22	35:DI:105:HIS:ND1	2.08	0.68
53:a:461:SER:CA	72:x:49:GLN:NE2	2.32	0.68
58:q:149:LYS:HD2	69:v:40:ALA:O	1.93	0.68
60:b:136:HIS:CB	61:c:111:TYR:OH	2.41	0.68
4:DA:480:TRP:HB2	31:Df:306:PRO:HG3	1.74	0.68
4:DA:571:GLU:CD	4:DA:571:GLU:H	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DH:44:LEU:CD2	33:DJ:129:THR:HG21	2.23	0.68
32:DI:28:ILE:CG2	32:DI:31:TYR:CD1	2.76	0.68
50:n:169:LEU:N	57:m:104:HIS:NE2	2.33	0.68
53:a:364:TYR:HB3	53:a:430:LEU:HD11	1.71	0.68
10:DB:762:ASP:OD1	10:DB:768:PRO:CG	2.38	0.68
27:DO:1:MET:CB	29:DD:997:ALA:CB	2.71	0.68
38:DH:56:ALA:HB2	33:DJ:214:PRO:CG	2.24	0.68
39:HD:295:ARG:HA	44:HI:132:TRP:NE1	2.08	0.68
44:HI:241:CYS:HA	44:HI:246:TYR:CD2	2.28	0.68
50:n:245:TRP:CB	50:n:282:LEU:CD1	2.57	0.68
54:d:41:SER:HB2	56:i:69:VAL:CG1	2.19	0.68
59:z:529:HIS:CE1	59:z:580:ILE:HG21	2.27	0.68
16:HC:29:GLY:O	16:HC:33:ARG:NE	2.24	0.68
48:g:172:PRO:HA	48:g:175:LEU:HG	1.75	0.68
50:n:237:MET:HE1	58:q:45:GLN:HA	1.75	0.68
52:u:122:LEU:HD22	52:u:125:ILE:HB	1.75	0.68
54:d:45:ILE:HG23	56:i:76:MET:CG	2.22	0.68
54:d:164:PRO:HD2	54:d:167:TRP:HB2	1.74	0.68
58:q:171:VAL:HG22	66:k:17:ILE:HD13	1.75	0.68
68:t:122:PHE:HZ	68:t:156:LEU:HD11	1.57	0.68
15:PB:777:ASN:O	22:PJ:47:ARG:NH1	2.27	0.68
29:DD:1078:LEU:CD2	35:DL:83:MET:HE1	2.23	0.68
30:DE:426:ARG:HH11	30:DE:640:ASN:HD22	1.41	0.68
38:DH:50:PHE:CG	33:DJ:195:LEU:HB2	2.29	0.68
45:HJ:60:TYR:CB	45:HJ:105:MET:HE1	2.24	0.68
55:f:95:LEU:C	58:q:130:VAL:CG1	2.67	0.68
68:t:8:GLN:HA	68:t:138:ILE:O	1.94	0.68
50:n:305:LEU:HD11	50:n:361:ILE:HG12	1.75	0.68
58:q:299:GLN:OE1	66:k:87:ARG:NH2	2.25	0.68
63:l:156:LEU:HD22	69:v:134:TYR:HB2	1.75	0.68
65:h:14:ALA:HB1	65:h:63:LEU:HD11	1.76	0.68
50:n:545:LEU:HD11	50:n:653:PRO:CA	2.24	0.68
53:a:374:TYR:HA	53:a:440:PHE:O	1.93	0.68
54:d:64:GLN:HE21	54:d:68:LEU:HD12	1.58	0.68
62:e:49:GLU:CG	63:l:89:PHE:CE1	2.76	0.68
13:HB:468:VAL:HG21	13:HB:525:ILE:HD11	1.74	0.68
16:HC:60:LEU:HD13	16:HC:118:LEU:HD23	1.76	0.68
45:HJ:175:LYS:HZ2	45:HJ:175:LYS:CA	2.07	0.68
48:g:79:ARG:NH2	52:u:74:ASP:HA	2.09	0.68
52:u:60:ALA:O	52:u:64:ARG:HG3	1.93	0.68
65:h:147:CYS:SG	69:v:41:LYS:CD	2.81	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:83:LEU:HD12	31:DF:98:SER:HA	1.75	0.68
32:DI:23:LEU:CD2	32:DI:39:MET:HE1	2.23	0.68
50:n:815:THR:HG21	50:n:841:ASN:HB3	1.75	0.68
54:d:71:HIS:CE1	54:d:72:ARG:HD3	2.29	0.68
58:q:184:ASN:OD1	69:v:83:LYS:HD2	1.93	0.68
62:e:95:PHE:CB	63:l:38:GLN:HG2	2.22	0.68
38:DH:50:PHE:HE2	33:DJ:170:ALA:O	1.77	0.68
50:n:960:LYS:CB	50:n:1210:PHE:CD2	2.76	0.68
52:u:125:ILE:CG1	56:i:135:TYR:CE2	2.77	0.68
53:a:219:LEU:HD13	53:a:258:THR:HB	1.75	0.68
53:a:382:LEU:CD2	53:a:446:SER:HA	2.22	0.68
58:q:15:CYS:SG	58:q:15:CYS:O	2.52	0.68
61:c:183:PRO:HD2	61:c:189:MET:HE2	1.76	0.68
61:c:291:GLY:HA3	68:t:120:CYS:HB3	1.74	0.68
64:o:735:LEU:HD21	71:w:113:GLN:OE1	1.94	0.68
69:v:10:SER:HB2	69:v:11:LYS:HE2	1.75	0.68
4:DA:410:TRP:HH2	31:DF:351:ILE:HA	1.59	0.67
31:DF:329:LEU:HD23	31:DF:329:LEU:C	2.19	0.67
31:DF:329:LEU:HD23	31:DF:329:LEU:O	1.94	0.67
31:DF:361:LYS:HA	31:DF:364:VAL:CG2	2.24	0.67
50:n:192:LEU:HD12	50:n:219:ASN:C	2.20	0.67
50:n:359:ILE:HG23	50:n:372:ILE:HD13	1.74	0.67
50:n:937:ARG:HE	50:n:943:LEU:CD2	2.07	0.67
11:EB:84:TYR:OH	11:EB:105:GLU:OE1	2.04	0.67
30:DE:773:TYR:OH	31:DF:140:GLY:HA2	1.94	0.67
35:DL:71:ASP:CB	35:DL:74:GLU:CD	2.66	0.67
41:HG:88:LEU:CD2	41:HG:131:LEU:HD21	2.25	0.67
44:HI:191:GLY:C	44:HI:193:GLY:H	2.02	0.67
49:j:17:GLU:CB	51:s:112:LEU:HD11	2.24	0.67
49:j:92:ASN:HD21	51:s:82:ASN:HA	1.58	0.67
50:n:861:LYS:CE	61:c:30:ARG:HE	2.01	0.67
54:d:41:SER:HB3	56:i:69:VAL:CG1	2.24	0.67
7:HA:72:TYR:OH	7:HA:234:ASP:OD2	2.12	0.67
9:PA:1794:SER:HB2	9:PA:1795:PRO:HD3	1.76	0.67
17:PC:109:GLU:OE1	17:PC:109:GLU:N	2.28	0.67
29:DD:963:ARG:HG2	29:DD:981:GLN:N	2.09	0.67
31:DF:317:LEU:H	31:DF:317:LEU:HD22	1.59	0.67
39:HD:55:LYS:O	39:HD:57:ASN:N	2.28	0.67
50:n:685:LEU:HD22	64:o:729:TYR:HE2	1.60	0.67
53:a:62:LEU:HG	54:d:62:GLU:N	2.09	0.67
53:a:367:LEU:HD13	53:a:509:ARG:NH1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:412:ARG:C	53:a:472:SER:HB3	2.19	0.67
53:a:462:LEU:HB2	72:x:49:GLN:CG	2.25	0.67
56:i:72:ILE:HD11	56:i:92:SER:CB	2.18	0.67
56:i:136:LYS:HE2	56:i:136:LYS:O	1.94	0.67
61:c:291:GLY:O	68:t:120:CYS:O	2.12	0.67
66:k:86:SER:O	69:v:105:LEU:HD13	1.95	0.67
71:w:1291:MET:SD	71:w:1328:ARG:NH2	2.67	0.67
29:DD:873:LEU:HD12	29:DD:873:LEU:N	2.10	0.67
38:DH:41:VAL:O	38:DH:45:LEU:HG	1.94	0.67
40:HE:65:GLN:HE22	40:HE:123:ASP:HB3	1.58	0.67
50:n:634:MET:HE2	58:q:519:GLN:NE2	2.10	0.67
50:n:937:ARG:HE	50:n:943:LEU:HD21	1.58	0.67
53:a:211:LEU:HD13	53:a:222:LEU:HD23	1.75	0.67
53:a:364:TYR:HB2	53:a:430:LEU:HG	1.76	0.67
64:o:765:ASP:OD1	64:o:766:LYS:N	2.27	0.67
66:k:45:LEU:HD22	66:k:45:LEU:C	2.19	0.67
66:k:70:LEU:HG	69:v:82:LEU:CD2	2.24	0.67
32:DI:132:LEU:CG	33:DJ:121:MET:SD	2.83	0.67
44:HI:86:ASN:HD22	44:HI:86:ASN:C	1.97	0.67
50:n:250:LEU:HD23	50:n:275:HIS:CD2	2.00	0.67
53:a:70:LYS:CA	56:i:70:HIS:CE1	2.77	0.67
58:q:28:GLU:HA	58:q:28:GLU:OE2	1.94	0.67
58:q:31:LEU:N	58:q:32:PRO:HD2	2.09	0.67
58:q:186:GLU:CB	58:q:243:LEU:HD22	2.25	0.67
58:q:644:SER:HB3	62:e:96:LEU:CB	2.25	0.67
62:e:132:HIS:HD2	69:v:126:ASP:OD2	1.77	0.67
11:EB:89:HIS:CE1	11:EB:139:PHE:HB3	2.29	0.67
29:DD:897:ASP:O	29:DD:898:VAL:HG23	1.95	0.67
32:DI:23:LEU:HD21	32:DI:39:MET:CE	2.24	0.67
44:HI:266:ASP:O	44:HI:269:LEU:HB3	1.93	0.67
47:PG:97:LEU:HD23	47:PG:113:ILE:HD11	1.75	0.67
53:a:466:VAL:HG21	72:x:54:PRO:HG3	1.75	0.67
54:d:46:GLU:N	56:i:76:MET:HE3	2.09	0.67
57:m:67:LEU:HD13	57:m:73:LEU:HD11	1.77	0.67
58:q:149:LYS:CE	69:v:40:ALA:C	2.68	0.67
58:q:376:HIS:CB	66:k:92:MET:HE3	2.25	0.67
61:c:292:LEU:HG	68:t:120:CYS:SG	2.35	0.67
4:DA:970:ASN:OD1	4:DA:970:ASN:N	2.21	0.67
5:EA:174:ARG:CB	39:HD:8:ARG:HH22	2.08	0.67
15:PB:814:TYR:OH	15:PB:900:GLU:OE1	2.13	0.67
45:HJ:28:ARG:HG3	45:HJ:28:ARG:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:PD:140:PHE:HB2	65:h:51:LEU:HD23	1.77	0.67
54:d:41:SER:HB3	56:i:69:VAL:HG11	1.76	0.67
15:PB:1134:THR:HG21	47:PG:153:ASP:OD1	1.94	0.67
31:Df:239:ARG:HD3	31:Df:284:ARG:HH11	1.60	0.67
44:HI:98:LEU:HB3	44:HI:143:LEU:HD21	1.76	0.67
52:u:85:LEU:HD11	59:z:551:ASP:HB2	1.76	0.67
7:HA:60:GLN:OE1	7:HA:61:ARG:NH1	2.28	0.67
31:DF:106:PHE:CE1	32:DI:13:PRO:HD3	2.30	0.67
31:DF:320:ARG:CG	31:DF:415:ILE:HD12	2.25	0.67
50:n:169:LEU:HD23	57:m:104:HIS:HB3	1.77	0.67
58:q:35:SER:HB3	58:q:42:ARG:HH22	1.58	0.67
58:q:428:LEU:HD12	58:q:428:LEU:C	2.18	0.67
69:v:130:LEU:N	69:v:130:LEU:HD23	2.08	0.67
3:BA:26:ASP:OD1	9:PA:430:ARG:NH2	2.28	0.67
3:BA:128:ILE:HG23	3:BA:183:VAL:HG11	1.77	0.67
42:HH:674:THR:OG1	43:HF:66:PHE:HB2	1.95	0.67
50:n:166:TYR:OH	57:m:70:PRO:CB	2.36	0.67
53:a:462:LEU:CD2	72:x:11:LEU:HB3	2.25	0.67
58:q:116:LEU:HB3	65:h:16:LEU:HD23	1.77	0.67
10:DB:490:SER:HA	10:DB:493:TRP:HB2	1.77	0.66
30:De:645:GLY:H	30:De:675:LEU:HD11	1.59	0.66
48:g:75:LYS:HG2	52:u:76:LEU:HD23	1.76	0.66
72:x:912:LEU:HD22	72:x:958:VAL:HG21	1.77	0.66
29:DD:875:GLN:C	29:DD:877:PRO:HD3	2.21	0.66
30:DE:463:PHE:HB3	31:DF:134:HIS:CD2	2.30	0.66
32:DI:132:LEU:CD1	33:DJ:121:MET:SD	2.83	0.66
41:HG:137:MET:SD	41:HG:139:CYS:N	2.68	0.66
45:HJ:111:LEU:HD12	45:HJ:111:LEU:O	1.96	0.66
50:n:270:GLN:HG2	55:f:177:VAL:HG12	1.77	0.66
58:q:457:ASP:HB2	58:q:458:PRO:HD3	1.77	0.66
69:v:131:GLU:O	69:v:135:TYR:HD2	1.79	0.66
5:EA:181:ASN:HD22	39:HD:9:CYS:HA	1.56	0.66
50:n:237:MET:CE	58:q:45:GLN:CB	2.73	0.66
50:n:270:GLN:NE2	55:f:174:ARG:HD2	2.09	0.66
58:q:171:VAL:HG22	66:k:17:ILE:CG2	2.10	0.66
32:DI:31:TYR:HD2	32:DI:35:VAL:HB	1.60	0.66
39:HD:106:VAL:O	39:HD:110:THR:HG23	1.95	0.66
46:PD:83:VAL:HG22	46:PD:137:LYS:HD3	1.77	0.66
52:u:115:LEU:CA	54:d:121:LEU:CD1	2.74	0.66
58:q:95:TRP:HZ3	65:h:33:LEU:HD21	1.59	0.66
58:q:263:LYS:CE	58:q:439:PHE:CZ	2.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:l:164:ARG:NH2	69:v:131:GLU:OE2	2.26	0.66
9:PA:1660:THR:N	55:f:14:SER:O	2.27	0.66
31:DF:138:ILE:HG13	38:DH:159:TYR:HE2	1.59	0.66
38:DH:50:PHE:CB	33:DJ:195:LEU:HB2	2.23	0.66
38:DH:57:SER:OG	33:DJ:200:LEU:CD1	2.43	0.66
46:PD:137:LYS:HE2	65:h:55:GLN:HE22	1.59	0.66
56:i:68:LEU:O	56:i:72:ILE:HG13	1.96	0.66
58:q:109:MET:HA	58:q:109:MET:CE	2.23	0.66
10:DB:402:ILE:HD12	10:DB:455:LEU:HD12	1.78	0.66
11:EB:229:ASP:O	11:EB:233:ILE:HD12	1.95	0.66
50:n:956:ALA:HB1	50:n:1217:ARG:NH2	2.08	0.66
53:a:69:LEU:HG	54:d:70:ILE:HG21	1.77	0.66
54:d:97:GLU:HA	54:d:97:GLU:OE2	1.95	0.66
54:d:156:SER:CB	54:d:161:VAL:HG11	2.26	0.66
56:i:72:ILE:CD1	56:i:92:SER:HB3	2.24	0.66
58:q:89:GLN:CB	58:q:90:PRO:CD	2.68	0.66
58:q:212:ALA:CB	58:q:380:ARG:HH22	2.07	0.66
26:DQ:20:ASP:OD2	27:DO:51:ARG:NH2	2.28	0.66
50:n:265:LEU:HD12	50:n:303:LEU:CD2	2.15	0.66
50:n:669:GLN:NE2	64:o:681:GLU:HG3	2.11	0.66
56:i:86:ASP:N	56:i:86:ASP:OD1	2.24	0.66
58:q:479:ILE:HG22	58:q:532:HIS:CG	2.30	0.66
64:o:695:PRO:HA	64:o:699:SER:HB2	1.75	0.66
29:DD:899:VAL:HG12	29:DD:900:SER:H	1.58	0.66
31:DF:14:LEU:HD23	32:DI:22:ILE:CD1	2.25	0.66
31:DF:126:PRO:HA	38:DH:125:THR:HB	1.78	0.66
38:DH:56:ALA:HB2	33:DJ:214:PRO:HG2	1.76	0.66
38:DH:110:TYR:HB2	33:DJ:161:LYS:HD3	1.77	0.66
45:HJ:200:LEU:O	45:HJ:200:LEU:HD22	1.96	0.66
58:q:129:PRO:CB	65:h:74:GLN:NE2	2.54	0.66
5:EA:34:LEU:HD11	5:EA:94:ILE:HD12	1.77	0.66
29:DD:922:GLN:CG	29:DD:1056:THR:HG21	2.26	0.66
42:HH:701:LEU:O	42:HH:704:SER:OG	2.14	0.66
50:n:686:LYS:NZ	64:o:730:PRO:HB3	2.10	0.66
53:a:67:LYS:HB3	53:a:83:SER:HB2	1.77	0.66
58:q:644:SER:O	62:e:97:GLN:CG	2.44	0.66
60:b:65:PRO:HA	60:b:68:LYS:HE2	1.76	0.66
71:w:318:GLU:HG2	71:w:320:LYS:H	1.59	0.66
30:DE:359:LEU:HD13	30:DE:627:LEU:HD12	1.76	0.66
31:DF:43:VAL:CA	32:DI:46:TYR:HD2	2.08	0.66
31:DF:317:LEU:HD22	31:DF:317:LEU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:160:LEU:HD11	53:a:219:LEU:HD21	1.77	0.66
58:q:578:TYR:CD1	58:q:646:LEU:HD12	2.29	0.66
9:PA:805:ARG:NH2	15:PB:671:GLU:O	2.28	0.65
32:Di:70:ASP:O	32:Di:73:LEU:HG	1.96	0.65
38:DH:108:PRO:HG3	33:DJ:116:LEU:CD2	2.25	0.65
44:HI:33:ASN:N	44:HI:33:ASN:OD1	2.29	0.65
65:h:147:CYS:SG	69:v:41:LYS:HD2	2.36	0.65
39:HD:27:GLY:CA	39:HD:70:LYS:HD3	2.26	0.65
53:a:232:LEU:C	53:a:232:LEU:HD13	2.22	0.65
53:a:462:LEU:CD1	72:x:49:GLN:HB3	2.26	0.65
58:q:149:LYS:HD2	69:v:40:ALA:HA	1.77	0.65
58:q:487:ILE:CG2	58:q:543:VAL:CG2	2.68	0.65
65:h:147:CYS:SG	69:v:41:LYS:HG3	2.35	0.65
69:v:61:MET:HE2	69:v:64:ARG:NH1	2.10	0.65
20:PH:91:VAL:HG22	20:PH:144:LEU:CD2	2.26	0.65
21:PI:60:HIS:ND1	21:PI:60:HIS:O	2.30	0.65
58:q:168:THR:CB	66:k:21:ILE:HD12	2.27	0.65
58:q:487:ILE:CD1	58:q:540:LEU:HD12	2.26	0.65
65:h:146:MET:CG	66:k:39:LYS:CE	2.75	0.65
4:DA:784:GLN:H	4:DA:1073:GLN:HE22	1.44	0.65
31:DF:82:PRO:HG3	31:DF:96:PHE:C	2.21	0.65
55:f:95:LEU:O	58:q:130:VAL:HG11	1.96	0.65
58:q:162:LYS:O	58:q:166:ARG:HG2	1.96	0.65
60:b:101:ARG:NH1	70:p:677:THR:CB	2.57	0.65
62:e:133:LEU:HG	66:k:111:CYS:SG	2.37	0.65
66:k:43:ARG:HB2	66:k:43:ARG:HH11	1.62	0.65
68:t:78:LEU:HD12	68:t:84:CYS:HB3	1.76	0.65
68:t:165:LEU:HD23	68:t:169:THR:HA	1.78	0.65
9:PA:122:ASN:O	9:PA:127:LYS:NZ	2.30	0.65
10:DB:645:ALA:HB3	10:DB:648:MET:HG3	1.78	0.65
13:HB:432:THR:O	13:HB:435:SER:OG	2.10	0.65
38:DH:50:PHE:CE2	33:DJ:170:ALA:O	2.50	0.65
39:HD:43:ALA:HB3	47:PG:164:MET:CE	2.22	0.65
50:n:790:ILE:HG22	50:n:792:ALA:H	1.62	0.65
50:n:922:TYR:OH	50:n:1214:VAL:HG12	1.96	0.65
53:a:462:LEU:CG	72:x:49:GLN:CG	2.73	0.65
58:q:631:GLU:HA	58:q:631:GLU:OE2	1.97	0.65
7:HA:238:ASN:ND2	7:HA:662:GLN:OE1	2.29	0.65
15:PB:677:MET:H	15:PB:682:LEU:HD22	1.62	0.65
37:DG:129:LYS:O	37:DG:129:LYS:NZ	2.23	0.65
53:a:380:ALA:HB1	72:x:58:PRO:HG3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:484:TYR:OH	58:q:640:GLU:HB2	1.96	0.65
65:h:146:MET:HG3	66:k:39:LYS:CD	2.24	0.65
70:p:827:CYS:SG	70:p:828:LEU:N	2.69	0.65
71:w:1183:TRP:CZ2	71:w:1185:GLY:HA3	2.32	0.65
4:DA:491:MET:H	4:DA:491:MET:CE	2.10	0.65
4:DA:1168:TYR:HB2	37:DG:180:ARG:HB3	1.78	0.65
9:PA:513:ALA:HB2	19:PF:90:LEU:HD21	1.78	0.65
27:DO:1:MET:HB3	29:DD:997:ALA:CB	2.25	0.65
30:DE:462:CYS:HA	31:DF:134:HIS:O	1.97	0.65
39:HD:255:THR:HA	45:HJ:4:ASN:HB2	1.79	0.65
40:HE:43:VAL:HG11	40:HE:224:LEU:HD21	1.78	0.65
44:HI:241:CYS:HA	44:HI:246:TYR:CG	2.32	0.65
48:g:74:HIS:H	52:u:79:GLU:HB2	1.60	0.65
16:HC:397:GLU:OE1	43:HF:61:MET:CG	2.44	0.65
31:DF:19:MET:SD	32:DI:47:VAL:HG11	2.37	0.65
50:n:680:HIS:NE2	58:q:557:LEU:HD11	2.09	0.65
50:n:937:ARG:HH21	50:n:943:LEU:HD23	1.62	0.65
53:a:109:TYR:CE2	53:a:154:LEU:CD2	2.80	0.65
58:q:166:ARG:CZ	58:q:166:ARG:HB3	2.27	0.65
58:q:184:ASN:OD1	69:v:83:LYS:CD	2.45	0.65
58:q:441:ARG:NH1	63:l:168:TRP:CZ3	2.59	0.65
60:b:179:LEU:CD1	62:e:60:VAL:CB	2.62	0.65
31:DF:312:ILE:HG13	31:DF:334:ALA:CB	2.27	0.65
38:DH:107:LEU:HD11	33:DJ:158:ALA:HA	1.78	0.65
56:i:65:PHE:HE1	56:i:99:LYS:HA	1.62	0.65
57:m:121:GLU:O	57:m:124:GLN:HG2	1.96	0.65
62:e:45:VAL:HG13	63:l:92:LEU:HD11	1.79	0.65
68:t:130:THR:HA	68:t:135:ALA:HA	1.77	0.65
7:HA:571:THR:OG1	7:HA:576:GLU:OE1	2.08	0.65
16:HC:172:SER:OG	16:HC:174:ASP:OD1	2.15	0.65
16:HC:172:SER:OG	16:HC:267:GLU:OE2	2.13	0.65
41:HG:377:ASP:O	41:HG:380:HIS:NE2	2.30	0.65
50:n:921:MET:SD	50:n:1215:ILE:HD13	2.35	0.65
58:q:129:PRO:HB3	65:h:74:GLN:HE21	1.61	0.65
61:c:290:ASP:O	68:t:120:CYS:HB3	1.95	0.65
66:k:56:VAL:HG13	69:v:26:ILE:HD12	1.77	0.65
68:t:31:LEU:HD11	68:t:164:PHE:HB3	1.79	0.65
69:v:50:ARG:HD2	69:v:51:ALA:H	1.61	0.65
10:DB:583:GLU:CD	10:DB:583:GLU:H	2.06	0.64
38:DH:54:GLU:OE1	33:DJ:197:MET:HG2	1.98	0.64
44:HI:191:GLY:O	44:HI:193:GLY:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:38:GLU:OE2	56:i:96:GLU:CB	2.45	0.64
55:f:70:LEU:HD21	55:f:73:ALA:HB2	1.79	0.64
64:o:719:PRO:HD2	72:x:71:GLN:HG3	1.79	0.64
66:k:44:LEU:HD22	66:k:47:ARG:HH22	1.62	0.64
68:t:112:THR:HG22	68:t:129:VAL:HG22	1.77	0.64
32:DI:28:ILE:CG2	32:DI:31:TYR:HD1	2.07	0.64
35:DL:71:ASP:HB3	35:DL:74:GLU:HG3	1.76	0.64
40:HE:168:GLU:N	40:HE:168:GLU:OE1	2.31	0.64
50:n:170:PRO:HB3	58:q:22:VAL:HG23	1.79	0.64
50:n:270:GLN:HA	55:f:181:LEU:HD11	1.78	0.64
58:q:168:THR:CA	66:k:21:ILE:HD12	2.26	0.64
58:q:375:LEU:HD23	58:q:427:LEU:HD11	1.79	0.64
58:q:467:ILE:HD11	61:c:203:VAL:HG11	1.78	0.64
65:h:146:MET:HG2	66:k:39:LYS:CE	2.26	0.64
66:k:77:GLN:HG3	67:r:192:GLN:HG2	1.80	0.64
15:PB:926:VAL:HG21	17:PC:62:GLU:HG3	1.78	0.64
29:DD:960:GLU:HA	29:DD:963:ARG:HG3	1.78	0.64
30:DE:745:GLU:OE1	30:DE:745:GLU:HA	1.98	0.64
48:g:95:ILE:HG21	48:g:105:ARG:HB3	1.79	0.64
70:p:50:ASP:HA	70:p:59:THR:HG22	1.79	0.64
31:DF:83:LEU:HD21	38:DH:67:SER:OG	1.97	0.64
42:HH:330:ASN:OD1	42:HH:334:ARG:NH2	2.31	0.64
50:n:104:LYS:HZ1	51:s:109:LEU:N	1.94	0.64
50:n:166:TYR:HB2	57:m:74:HIS:HB2	1.79	0.64
50:n:250:LEU:HG	50:n:275:HIS:CB	2.26	0.64
53:a:424:CYS:HA	53:a:505:PRO:HG3	1.79	0.64
55:f:71:LEU:HD12	55:f:82:ARG:HE	1.61	0.64
55:f:181:LEU:O	55:f:185:ARG:HG3	1.96	0.64
58:q:491:ILE:HD12	58:q:532:HIS:HA	1.77	0.64
59:z:576:TRP:HB3	59:z:596:TYR:HB3	1.79	0.64
60:b:116:LEU:HB3	61:c:21:ILE:HD13	1.79	0.64
60:b:179:LEU:CD1	62:e:60:VAL:CA	2.72	0.64
70:p:490:ASP:N	70:p:490:ASP:OD1	2.30	0.64
15:PB:910:THR:HG22	15:PB:911:LEU:H	1.62	0.64
32:DI:132:LEU:HD21	33:DJ:121:MET:CE	2.22	0.64
39:HD:298:GLN:NE2	44:HI:132:TRP:NE1	2.46	0.64
45:HJ:268:GLU:H	45:HJ:268:GLU:CD	2.05	0.64
46:PD:14:GLU:N	46:PD:14:GLU:OE1	2.31	0.64
50:n:508:SER:OG	50:n:637:PHE:O	2.14	0.64
51:s:107:ASN:H	51:s:110:PRO:HB3	1.63	0.64
54:d:42:ARG:CZ	56:i:96:GLU:OE2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:126:TYR:CD2	58:q:36:MET:CB	2.77	0.64
58:q:458:PRO:HB3	58:q:533:GLN:NE2	2.12	0.64
31:DF:314:SER:O	31:DF:327:TRP:HH2	1.81	0.64
38:DH:51:GLU:HB2	33:DJ:193:TYR:O	1.97	0.64
55:f:99:TYR:HB3	65:h:77:ILE:HG22	1.79	0.64
56:i:65:PHE:HZ	56:i:102:SER:HG	1.41	0.64
58:q:647:SER:OG	62:e:93:CYS:SG	2.56	0.64
61:c:166:ILE:HD13	61:c:190:LEU:HD21	1.80	0.64
72:x:780:THR:HG22	72:x:816:CYS:HB3	1.80	0.64
39:HD:295:ARG:HA	44:HI:132:TRP:HE1	1.62	0.64
46:PD:87:LEU:HB3	46:PD:97:LEU:HD22	1.78	0.64
49:j:82:LYS:CE	51:s:101:VAL:HG12	2.28	0.64
50:n:904:PHE:CE2	50:n:1208:GLU:CB	2.80	0.64
53:a:375:PHE:CD1	72:x:17:ARG:CG	2.80	0.64
58:q:212:ALA:O	58:q:383:HIS:HB3	1.98	0.64
58:q:265:ALA:HB3	58:q:340:GLN:OE1	1.97	0.64
64:o:639:TYR:CG	70:p:786:HIS:HB3	2.25	0.64
70:p:569:LEU:HG	70:p:569:LEU:O	1.97	0.64
11:EB:145:VAL:HG13	11:EB:175:LEU:HB2	1.79	0.64
30:DE:359:LEU:HD11	30:DE:648:ASP:HB2	1.80	0.64
31:DF:218:VAL:CG1	38:DH:162:THR:CG2	2.75	0.64
50:n:359:ILE:CA	50:n:372:ILE:CD1	2.75	0.64
52:u:49:ASN:H	52:u:49:ASN:ND2	1.94	0.64
58:q:150:LYS:HE3	66:k:37:LYS:HB3	1.80	0.64
61:c:293:PRO:HD3	68:t:144:TYR:OH	1.96	0.64
66:k:39:LYS:HG3	66:k:39:LYS:O	1.97	0.64
9:PA:589:LYS:NZ	9:PA:625:ASP:OD2	2.23	0.64
10:DB:644:GLN:O	16:HC:413:LEU:HB3	1.97	0.64
30:DE:451:VAL:O	30:DE:453:LEU:N	2.31	0.64
9:PA:140:ARG:NH1	9:PA:234:PHE:O	2.30	0.64
15:PB:116:ARG:HG2	15:PB:910:THR:HG21	1.80	0.64
16:HC:55:TRP:CZ2	16:HC:83:GLN:NE2	2.66	0.64
31:Df:320:ARG:HB3	31:Df:320:ARG:NH1	2.12	0.64
46:PD:18:SER:O	46:PD:117:SER:OG	2.09	0.64
50:n:265:LEU:CD1	50:n:303:LEU:CD2	2.70	0.64
56:i:96:GLU:HA	56:i:99:LYS:CG	2.27	0.64
44:HI:209:ARG:CG	55:f:53:GLN:CD	2.58	0.63
44:HI:215:GLY:HA3	44:HI:221:GLN:HB2	1.80	0.63
53:a:160:LEU:HD11	53:a:214:ARG:HH21	1.61	0.63
57:m:124:GLN:OE1	59:z:590:ARG:HB3	1.98	0.63
58:q:489:LYS:O	58:q:507:ARG:NH2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:x:637:GLU:O	72:x:641:GLN:NE2	2.31	0.63
5:EA:171:LYS:NZ	39:HD:41:ARG:CG	2.61	0.63
30:DE:433:LYS:HD3	32:DI:110:TYR:CE1	2.33	0.63
31:DF:68:THR:HA	32:DI:32:GLU:CD	2.23	0.63
44:HI:24:ALA:HA	44:HI:44:LYS:HB2	1.80	0.63
44:HI:37:ILE:HD12	44:HI:37:ILE:N	2.12	0.63
50:n:359:ILE:CA	50:n:372:ILE:HD11	2.28	0.63
53:a:417:TYR:CD1	53:a:450:PHE:HE1	2.15	0.63
69:v:42:ILE:H	69:v:42:ILE:HD12	1.61	0.63
72:x:143:ARG:HH22	72:x:205:ASN:HB2	1.62	0.63
5:EA:139:LEU:HD21	47:PG:151:ARG:CG	2.29	0.63
15:PB:529:MET:HE1	15:PB:698:ILE:HD12	1.79	0.63
25:DP:186:ARG:NH1	25:DP:244:LEU:O	2.31	0.63
25:DP:297:LYS:NZ	25:DP:323:GLU:OE2	2.30	0.63
49:j:78:GLN:O	49:j:82:LYS:HE2	1.98	0.63
50:n:359:ILE:HG23	50:n:372:ILE:HD12	1.78	0.63
50:n:651:ASN:ND2	71:w:22:PHE:H	1.94	0.63
58:q:93:TRP:H	58:q:94:PRO:CD	2.11	0.63
71:w:1184:VAL:O	71:w:1184:VAL:HG22	1.98	0.63
42:HH:517:GLU:O	42:HH:521:GLU:OE1	2.16	0.63
44:HI:47:HIS:CG	44:HI:47:HIS:O	2.50	0.63
46:PD:29:ALA:HB3	47:PG:3:TYR:CE2	2.33	0.63
50:n:104:LYS:NZ	51:s:109:LEU:H	1.96	0.63
53:a:462:LEU:HB2	72:x:49:GLN:HG2	1.80	0.63
54:d:156:SER:HA	54:d:161:VAL:CG1	2.27	0.63
58:q:93:TRP:N	58:q:94:PRO:CD	2.62	0.63
63:l:108:PRO:HD2	63:l:109:ILE:HD12	1.81	0.63
4:DA:481:GLU:CD	4:DA:481:GLU:H	2.04	0.63
10:DB:361:ARG:HD2	10:DB:367:GLU:HB2	1.80	0.63
30:DE:788:ARG:HD3	38:DH:145:HIS:HA	1.81	0.63
41:HG:379:LEU:HD22	41:HG:381:CYS:O	1.99	0.63
48:g:132:ARG:HG3	52:u:86:GLN:HG3	1.80	0.63
58:q:149:LYS:CE	69:v:40:ALA:O	2.47	0.63
69:v:108:LEU:C	69:v:108:LEU:HD12	2.23	0.63
7:HA:2:LYS:HB3	7:HA:9:LEU:HD11	1.81	0.63
31:DF:43:VAL:CB	32:DI:46:TYR:HD2	2.11	0.63
31:DF:106:PHE:CD1	32:DI:13:PRO:HD3	2.34	0.63
38:DH:37:LEU:CD1	33:DJ:138:TYR:CE2	2.81	0.63
38:DH:121:ALA:HB1	33:DJ:133:ALA:CB	2.27	0.63
39:HD:83:ASN:ND2	39:HD:140:LEU:HD12	2.14	0.63
42:HH:128:SER:OG	42:HH:163:TYR:OH	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:373:CYS:H	53:a:439:GLN:HA	1.63	0.63
60:b:103:ASP:HB3	64:o:645:ALA:HB2	1.80	0.63
64:o:723:LEU:HD11	64:o:734:PRO:HB2	1.79	0.63
68:t:8:GLN:HE21	68:t:200:ILE:HD13	1.63	0.63
68:t:25:THR:HB	68:t:117:TYR:OH	1.97	0.63
9:PA:1475:LEU:HD21	47:PG:18:PHE:CZ	2.34	0.63
29:DD:874:LEU:H	29:DD:874:LEU:CD2	2.10	0.63
48:g:120:HIS:CE1	50:n:148:ARG:HB3	2.33	0.63
53:a:220:MET:HB2	53:a:257:VAL:HG12	1.80	0.63
55:f:145:TYR:CE1	65:h:43:PRO:HG2	2.32	0.63
70:p:232:ASP:OD1	70:p:232:ASP:N	2.31	0.63
18:PE:9:ARG:O	18:PE:13:ILE:HD12	1.99	0.63
42:HH:287:LEU:HD23	42:HH:287:LEU:O	1.98	0.63
50:n:209:PRO:HG3	50:n:293:TYR:CG	2.33	0.63
53:a:463:VAL:HG11	53:a:488:ILE:HD12	1.80	0.63
54:d:34:LEU:CD2	56:i:99:LYS:HD3	2.26	0.63
62:e:146:ILE:C	62:e:148:VAL:H	2.07	0.63
29:DD:950:LEU:HD13	29:DD:950:LEU:O	1.99	0.63
42:HH:266:GLN:HG2	42:HH:267:THR:HG23	1.80	0.63
50:n:192:LEU:CD1	50:n:219:ASN:O	2.47	0.63
50:n:196:ASN:OD1	50:n:219:ASN:HA	1.99	0.63
53:a:377:ASN:HD21	72:x:58:PRO:CG	2.12	0.63
54:d:100:VAL:HG13	56:i:128:LYS:NZ	2.14	0.63
58:q:93:TRP:H	58:q:94:PRO:HD2	1.63	0.63
59:z:580:ILE:HB	59:z:593:ILE:HB	1.79	0.63
2:Y:18:DC:OP2	12:FB:214:LYS:NZ	2.22	0.62
7:HA:343:ARG:O	7:HA:346:VAL:HG12	1.99	0.62
29:DD:872:PHE:CE1	35:DL:57:VAL:CG1	2.79	0.62
49:j:78:GLN:HB3	49:j:82:LYS:HE2	1.81	0.62
50:n:172:CYS:SG	58:q:21:GLU:CB	2.86	0.62
50:n:944:PHE:CE2	60:b:101:ARG:NH2	2.67	0.62
52:u:90:LEU:CD2	58:q:9:ILE:CD1	2.36	0.62
72:x:13:ALA:HA	72:x:18:TRP:CE3	2.34	0.62
4:DA:349:TRP:HB3	31:Df:269:VAL:HG21	1.81	0.62
5:EA:152:PHE:CE1	47:PG:95:VAL:HG11	2.33	0.62
32:DI:32:GLU:HB2	32:DI:35:VAL:HG23	1.82	0.62
53:a:462:LEU:HD11	72:x:60:ILE:HD11	1.81	0.62
60:b:136:HIS:CD2	61:c:111:TYR:CE2	2.81	0.62
29:DD:891:ILE:H	29:DD:891:ILE:HD12	1.63	0.62
31:DF:241:GLU:CD	38:DH:135:THR:HG1	2.08	0.62
31:DF:392:ILE:O	31:DF:392:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:417:LYS:HG3	50:n:421:ARG:HE	1.64	0.62
53:a:109:TYR:CE2	53:a:154:LEU:HD21	2.34	0.62
55:f:143:LYS:HG2	58:q:226:LYS:HG3	1.81	0.62
55:f:145:TYR:CE2	65:h:43:PRO:HD3	2.34	0.62
5:EA:142:ASN:ND2	47:PG:107:PHE:HB2	2.14	0.62
10:DB:156:LYS:O	10:DB:963:HIS:HB2	1.99	0.62
15:PB:407:MET:HE1	15:PB:444:LEU:HG	1.80	0.62
18:PE:29:THR:HG23	18:PE:32:GLU:H	1.65	0.62
39:HD:300:ALA:O	45:HJ:210:SER:HB3	1.99	0.62
41:HG:242:SER:O	41:HG:245:SER:OG	2.17	0.62
43:HF:49:LEU:HD12	43:HF:52:VAL:CG1	2.29	0.62
52:u:72:LEU:O	52:u:75:SER:HB2	1.99	0.62
53:a:321:LEU:HA	53:a:410:LEU:HD12	1.81	0.62
54:d:100:VAL:HG13	56:i:128:LYS:HZ3	1.62	0.62
70:p:13:MET:HE1	70:p:393:ILE:HD11	1.82	0.62
7:HA:335:ARG:NH1	39:HD:71:GLU:OE2	2.32	0.62
11:EB:189:ILE:HD11	11:EB:201:LEU:HD13	1.79	0.62
15:PB:354:SER:HG	15:PB:357:CYS:HG	1.34	0.62
17:PC:24:GLU:OE2	17:PC:228:ARG:NH1	2.32	0.62
30:DE:465:THR:N	31:DF:132:LYS:O	2.31	0.62
46:PD:119:GLU:N	46:PD:119:GLU:OE1	2.33	0.62
46:PD:137:LYS:HA	65:h:51:LEU:HD21	1.79	0.62
52:u:115:LEU:CD1	54:d:121:LEU:HD13	2.30	0.62
64:o:695:PRO:O	72:x:957:LYS:HE2	1.99	0.62
66:k:109:ARG:HH11	66:k:109:ARG:HG3	1.65	0.62
31:DF:71:ILE:HD11	32:DI:35:VAL:HG22	1.81	0.62
38:DH:53:ALA:HB2	33:DJ:195:LEU:HB3	1.80	0.62
32:DI:15:ASP:O	32:DI:40:LEU:HD21	1.99	0.62
50:n:265:LEU:HD11	50:n:307:VAL:HG21	1.80	0.62
50:n:941:TYR:HD2	50:n:1172:SER:CB	2.02	0.62
50:n:957:PRO:HD3	50:n:1214:VAL:CG2	2.30	0.62
53:a:228:PRO:HB2	53:a:502:MET:CB	2.29	0.62
54:d:38:GLU:OE2	56:i:96:GLU:CG	2.46	0.62
54:d:167:TRP:HE3	57:m:106:GLN:CD	2.07	0.62
70:p:47:PHE:HE2	70:p:49:MET:HE2	1.64	0.62
9:PA:1471:PHE:O	19:PF:64:ARG:NH1	2.33	0.62
27:DO:1:MET:HB2	29:DD:997:ALA:CB	2.29	0.62
27:DO:1:MET:HB2	29:DD:997:ALA:HB2	1.80	0.62
29:DD:874:LEU:HD23	29:DD:874:LEU:N	2.12	0.62
58:q:89:GLN:HB3	58:q:90:PRO:HD2	1.78	0.62
61:c:288:LEU:HD21	68:t:122:PHE:HZ	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:t:96:VAL:O	68:t:99:LYS:HB2	2.00	0.62
5:EA:17:LEU:CD2	5:EA:194:THR:HG21	2.27	0.62
18:PE:168:ASN:OD1	18:PE:172:ARG:NH2	2.33	0.62
29:DD:895:HIS:CE1	29:DD:896:PRO:HD2	2.35	0.62
50:n:634:MET:N	50:n:634:MET:SD	2.73	0.62
53:a:59:VAL:HG21	54:d:51:SER:OG	1.99	0.62
56:i:109:LEU:CD2	56:i:117:GLN:HE22	2.13	0.62
64:o:735:LEU:CD2	71:w:113:GLN:OE1	2.46	0.62
68:t:98:LEU:HD13	68:t:102:PHE:HE1	1.64	0.62
32:DI:23:LEU:HD21	32:DI:39:MET:SD	2.40	0.62
44:HI:209:ARG:HG3	55:f:53:GLN:OE1	1.98	0.62
45:HJ:167:PHE:CD1	45:HJ:167:PHE:C	2.78	0.62
50:n:169:LEU:HG	57:m:104:HIS:ND1	2.13	0.62
53:a:316:ALA:HB2	53:a:447:GLU:HG2	1.82	0.62
54:d:27:ARG:HG2	56:i:107:ILE:HG22	1.79	0.62
71:w:1181:THR:O	71:w:1184:VAL:HB	2.00	0.62
3:BA:171:GLU:O	15:PB:101:ARG:NH2	2.32	0.62
15:PB:1143:LYS:HE3	47:PG:152:VAL:HG13	1.81	0.62
32:DI:132:LEU:CG	33:DJ:121:MET:HE2	2.30	0.62
45:HJ:229:GLU:H	45:HJ:229:GLU:CD	2.05	0.62
45:HJ:277:LEU:HD12	45:HJ:277:LEU:O	1.99	0.62
48:g:130:GLN:HB2	52:u:5:LEU:CD1	2.30	0.62
52:u:111:GLY:O	54:d:121:LEU:HD11	2.00	0.62
53:a:441:GLU:HG3	53:a:442:VAL:N	2.08	0.62
58:q:265:ALA:CB	58:q:340:GLN:OE1	2.48	0.62
77:NY:-157:DG:H2'	77:NY:-156:DG:C8	2.34	0.62
5:EA:176:LEU:HD11	11:EB:215:GLU:HG3	1.82	0.61
17:PC:9:VAL:HG11	23:PK:105:PHE:CD1	2.34	0.61
50:n:121:PHE:CD2	51:s:83:LEU:HD21	2.35	0.61
50:n:512:LEU:HD21	58:q:565:ASN:HD22	1.64	0.61
50:n:1189:SER:O	50:n:1209:ARG:NH1	2.33	0.61
58:q:149:LYS:CD	69:v:40:ALA:O	2.48	0.61
67:r:121:MET:HE2	68:t:102:PHE:CZ	2.34	0.61
9:PA:1643:TYR:CZ	57:m:93:CYS:HB2	2.35	0.61
31:DF:323:VAL:HG22	31:DF:323:VAL:O	2.00	0.61
39:HD:274:HIS:H	39:HD:277:ALA:HA	1.65	0.61
41:HG:112:LYS:O	41:HG:147:ASN:ND2	2.33	0.61
42:HH:473:GLU:OE1	42:HH:473:GLU:N	2.33	0.61
44:HI:140:PRO:CA	44:HI:202:ILE:HD11	2.30	0.61
44:HI:237:TRP:CG	44:HI:237:TRP:O	2.53	0.61
50:n:922:TYR:CE2	50:n:1215:ILE:HD13	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:45:ILE:CD1	56:i:73:ILE:CG1	2.78	0.61
69:v:120:ARG:HH11	69:v:120:ARG:CG	2.13	0.61
71:w:196:LEU:HD13	72:x:802:MET:HB2	1.80	0.61
3:BA:273:GLU:O	3:BA:277:ILE:HD12	1.99	0.61
16:HC:397:GLU:OE2	43:HF:61:MET:HG3	1.99	0.61
30:DE:290:HIS:HB3	31:DF:45:TYR:CZ	2.36	0.61
40:HE:16:ASP:OD1	40:HE:131:THR:OG1	2.16	0.61
46:PD:29:ALA:HB3	47:PG:3:TYR:CZ	2.35	0.61
50:n:169:LEU:HD23	57:m:101:GLN:HA	1.80	0.61
53:a:59:VAL:HG12	54:d:48:LEU:HD23	1.83	0.61
53:a:66:GLN:HE21	54:d:44:LEU:HD11	1.53	0.61
53:a:127:HIS:CE1	53:a:171:THR:HG22	2.35	0.61
58:q:647:SER:CB	62:e:93:CYS:HG	2.12	0.61
65:h:142:SER:OG	66:k:39:LYS:HE2	2.00	0.61
7:HA:44:SER:OG	7:HA:46:THR:O	2.16	0.61
9:PA:1375:ARG:NH1	9:PA:1379:GLU:OE1	2.31	0.61
30:DE:526:ARG:HA	30:DE:526:ARG:CZ	2.29	0.61
39:HD:288:THR:C	39:HD:290:SER:N	2.57	0.61
44:HI:263:ALA:HB3	55:f:48:GLU:HB3	1.83	0.61
50:n:270:GLN:CG	55:f:181:LEU:HD11	2.29	0.61
50:n:354:VAL:HG12	50:n:355:HIS:H	1.64	0.61
50:n:960:LYS:HZ1	50:n:1185:LEU:CD1	2.09	0.61
53:a:514:LYS:HE2	53:a:518:ILE:HD11	1.82	0.61
56:i:85:GLN:HG2	56:i:86:ASP:OD1	1.98	0.61
58:q:109:MET:HE3	58:q:109:MET:O	2.00	0.61
58:q:138:LYS:CD	58:q:140:ASN:OD1	2.40	0.61
58:q:212:ALA:HA	58:q:387:LEU:HD22	1.82	0.61
62:e:129:VAL:CG2	66:k:114:MET:CE	2.64	0.61
5:EA:181:ASN:CB	39:HD:10:LYS:HG2	2.14	0.61
7:HA:405:THR:O	7:HA:409:THR:OG1	2.16	0.61
30:DE:613:ALA:HB2	30:DE:620:LEU:HD11	1.81	0.61
31:DF:106:PHE:CD1	32:DI:13:PRO:HG3	2.35	0.61
38:DH:54:GLU:OE1	33:DJ:197:MET:CG	2.48	0.61
38:DH:137:GLY:HA3	38:DH:155:ASP:OD2	2.00	0.61
39:HD:55:LYS:C	39:HD:57:ASN:N	2.58	0.61
45:HJ:175:LYS:HA	45:HJ:175:LYS:NZ	2.15	0.61
50:n:274:ILE:CG1	55:f:181:LEU:CD2	2.79	0.61
52:u:80:GLU:HB2	59:z:563:VAL:CG2	2.31	0.61
54:d:46:GLU:HA	56:i:76:MET:CE	2.30	0.61
58:q:142:GLN:H	58:q:142:GLN:CD	2.08	0.61
66:k:42:GLU:HA	66:k:42:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:p:148:GLU:HB3	70:p:370:VAL:HG21	1.82	0.61
70:p:698:ILE:HA	70:p:701:ARG:HG2	1.82	0.61
9:PA:1648:PRO:O	57:m:92:GLN:NE2	2.34	0.61
13:HB:422:LEU:HD22	40:HE:225:GLN:HE22	1.66	0.61
41:HG:87:LEU:HD22	41:HG:232:LEU:HD12	1.82	0.61
42:HH:371:VAL:HG23	42:HH:407:ILE:CG2	2.30	0.61
53:a:455:GLN:HB2	72:x:11:LEU:CD2	2.30	0.61
61:c:214:VAL:H	61:c:243:THR:HG22	1.65	0.61
64:o:748:PHE:CD2	72:x:66:TYR:CE1	2.88	0.61
9:PA:1674:THR:HB	44:HI:214:PRO:CG	2.30	0.61
16:HC:265:LEU:CD1	16:HC:270:LEU:HD12	2.31	0.61
42:HH:128:SER:HG	42:HH:163:TYR:HH	1.46	0.61
50:n:172:CYS:SG	58:q:20:HIS:O	2.52	0.61
50:n:679:SER:H	58:q:557:LEU:HD22	1.63	0.61
52:u:90:LEU:HD21	58:q:7:VAL:HG23	1.82	0.61
58:q:34:LEU:HD23	58:q:34:LEU:H	1.64	0.61
70:p:656:ARG:HG3	70:p:693:LEU:HD22	1.82	0.61
17:PC:78:ILE:HD11	17:PC:126:ARG:HB3	1.82	0.61
28:Dc:18:CYS:O	28:Dc:23:TRP:HB2	2.01	0.61
50:n:206:THR:CG2	50:n:289:LEU:HB2	2.29	0.61
50:n:320:TRP:HA	58:q:316:VAL:HG11	1.81	0.61
62:e:140:GLN:HE22	66:k:105:SER:HA	1.65	0.61
68:t:175:VAL:HG21	68:t:192:GLN:HG3	1.82	0.61
70:p:225:ASN:ND2	70:p:245:CYS:SG	2.74	0.61
70:p:443:LEU:HD23	70:p:457:LEU:HD21	1.82	0.61
5:EA:132:CYS:O	5:EA:133:SER:OG	2.18	0.61
31:DF:276:LEU:HD22	31:DF:323:VAL:CG2	2.31	0.61
48:g:159:ARG:HD3	48:g:159:ARG:C	2.26	0.61
58:q:451:LEU:HD12	58:q:529:MET:HE1	0.63	0.61
65:h:151:LEU:HD21	69:v:37:ILE:HB	1.83	0.61
67:r:195:PRO:HG3	69:v:8:PRO:N	2.16	0.61
72:x:650:LEU:HB2	72:x:659:TYR:HE2	1.64	0.61
7:HA:513:ASP:OD1	7:HA:516:VAL:N	2.29	0.61
29:Dd:884:GLU:HA	29:Dd:887:LYS:HE3	1.82	0.61
46:PD:29:ALA:HB1	47:PG:4:HIS:O	2.01	0.61
50:n:651:ASN:CB	71:w:21:ALA:HB1	2.30	0.61
56:i:96:GLU:CA	56:i:99:LYS:HG3	2.29	0.61
56:i:119:GLN:OE1	56:i:119:GLN:HA	2.01	0.61
62:e:71:GLU:OE1	62:e:74:ARG:NH2	2.33	0.61
65:h:99:VAL:O	65:h:99:VAL:HG23	2.01	0.61
66:k:109:ARG:HH11	66:k:109:ARG:CG	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:x:251:GLU:HG3	72:x:263:LEU:HD13	1.82	0.61
5:EA:69:ASP:HA	11:EB:225:VAL:HG23	1.83	0.60
15:PB:794:VAL:HG13	15:PB:965:ILE:HG23	1.82	0.60
15:PB:851:ASP:OD2	24:PL:17:TYR:OH	2.19	0.60
28:Dc:99:PHE:HB2	28:Dc:100:PRO:HD3	1.83	0.60
29:DD:996:LEU:O	29:DD:1000:ARG:HG3	2.01	0.60
50:n:199:LEU:HD22	50:n:222:VAL:HG13	1.83	0.60
53:a:443:CYS:SG	72:x:57:ASN:HB3	2.41	0.60
55:f:101:ILE:CD1	65:h:105:VAL:CG1	2.79	0.60
56:i:65:PHE:CE1	56:i:99:LYS:HG2	2.36	0.60
64:o:749:LEU:HD11	72:x:69:SER:C	2.26	0.60
65:h:23:LYS:HB3	65:h:23:LYS:HZ3	1.65	0.60
66:k:101:ARG:HG2	66:k:101:ARG:HH11	1.66	0.60
72:x:944:LEU:HD13	72:x:971:THR:HG22	1.83	0.60
1:X:-27:DA:C2	25:DP:169:VAL:HG21	2.36	0.60
28:Dc:67:GLY:CA	33:Dj:116:LEU:CD1	2.70	0.60
31:DF:314:SER:O	31:DF:327:TRP:CH2	2.54	0.60
32:DI:23:LEU:CG	32:DI:39:MET:HE1	2.31	0.60
50:n:932:GLY:HA2	50:n:1179:HIS:NE2	2.15	0.60
58:q:36:MET:HE2	58:q:40:LEU:HD23	1.83	0.60
59:z:529:HIS:HA	59:z:568:ASP:HA	1.83	0.60
69:v:127:LEU:HD12	69:v:127:LEU:O	2.02	0.60
50:n:266:VAL:HG22	55:f:177:VAL:HG11	1.82	0.60
50:n:957:PRO:HG3	50:n:1214:VAL:HG21	1.83	0.60
60:b:59:ARG:HH21	60:b:63:LEU:HD11	1.66	0.60
65:h:61:LYS:HG2	65:h:65:HIS:CE1	2.37	0.60
71:w:281:ASP:OD1	71:w:281:ASP:N	2.31	0.60
15:PB:1143:LYS:HE3	47:PG:152:VAL:CG1	2.30	0.60
39:HD:83:ASN:HD21	39:HD:140:LEU:HD13	1.67	0.60
41:HG:357:VAL:HG13	41:HG:366:VAL:HG23	1.83	0.60
44:HI:276:PHE:O	44:HI:277:LEU:C	2.43	0.60
50:n:168:ARG:NH1	57:m:108:TYR:CZ	2.69	0.60
68:t:136:ARG:HG3	68:t:136:ARG:O	2.00	0.60
5:EA:105:TYR:OH	11:EB:237:LEU:HG	2.00	0.60
5:EA:188:TYR:CD2	39:HD:14:TYR:CG	2.89	0.60
7:HA:609:ASP:OD1	7:HA:669:ARG:NH2	2.34	0.60
9:PA:29:ASP:OD2	9:PA:33:ARG:NH2	2.34	0.60
16:HC:18:ASN:OD1	16:HC:19:LEU:N	2.35	0.60
30:DE:449:LYS:HG2	38:DH:144:PRO:HB2	1.83	0.60
50:n:1316:CYS:HA	50:n:1339:CYS:H	1.65	0.60
55:f:108:ALA:HB2	65:h:77:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:113:TYR:CB	65:h:19:VAL:HG11	2.30	0.60
65:h:156:LYS:HG2	65:h:159:ARG:HH21	1.66	0.60
71:w:425:MET:N	71:w:425:MET:SD	2.72	0.60
9:PA:1652:PRO:HG3	65:h:107:ASP:OD1	2.02	0.60
32:Di:73:LEU:CD2	35:Dl:105:HIS:CE1	2.84	0.60
42:HH:189:LEU:O	42:HH:195:ARG:NH1	2.34	0.60
49:j:78:GLN:C	49:j:82:LYS:HE2	2.26	0.60
50:n:254:VAL:CG1	50:n:304:GLN:HG2	2.32	0.60
50:n:545:LEU:HD11	50:n:653:PRO:CB	2.30	0.60
54:d:47:MET:HA	54:d:47:MET:HE3	1.83	0.60
60:b:175:HIS:HB2	61:c:113:TRP:CZ2	2.34	0.60
70:p:97:LEU:HD11	70:p:179:TRP:HB3	1.83	0.60
31:Df:330:ARG:HH22	31:Df:371:THR:HB	1.66	0.60
42:HH:707:GLU:O	42:HH:711:GLN:OE1	2.19	0.60
47:PG:124:ASN:ND2	65:h:169:ASN:O	2.35	0.60
50:n:203:LEU:HD21	50:n:224:PHE:HZ	1.67	0.60
50:n:274:ILE:HG13	55:f:181:LEU:CD2	2.32	0.60
53:a:380:ALA:HB3	53:a:444:PRO:CG	2.32	0.60
53:a:467:MET:HB3	53:a:475:VAL:HG11	1.84	0.60
57:m:56:LEU:HG	57:m:80:GLN:HE22	1.65	0.60
58:q:19:VAL:O	58:q:19:VAL:HG22	2.01	0.60
58:q:130:VAL:O	58:q:130:VAL:HG12	2.01	0.60
58:q:504:VAL:HG11	58:q:524:PHE:CE2	2.37	0.60
58:q:534:VAL:HG11	58:q:567:SER:HB3	1.84	0.60
62:e:91:THR:OG1	63:l:41:VAL:HG21	2.00	0.60
64:o:741:TRP:HE1	72:x:107:ARG:HB2	1.66	0.60
7:HA:461:LEU:HD23	7:HA:464:LEU:CD2	2.31	0.60
10:DB:203:LYS:HD3	10:DB:237:MET:HE3	1.83	0.60
10:DB:400:ASP:HA	10:DB:403:VAL:HG22	1.83	0.60
15:PB:57:ARG:NE	15:PB:227:ASN:O	2.34	0.60
28:Dc:67:GLY:CA	33:Dj:116:LEU:HD11	2.25	0.60
31:DF:274:ASN:CB	31:DF:317:LEU:HD23	2.28	0.60
35:DL:111:LEU:O	35:DL:114:LYS:HE3	2.01	0.60
42:HH:415:HIS:NE2	42:HH:417:THR:OG1	2.35	0.60
45:HJ:33:LYS:O	45:HJ:33:LYS:HD3	2.00	0.60
45:HJ:164:TYR:O	45:HJ:167:PHE:N	2.33	0.60
47:PG:10:GLU:HG2	47:PG:67:LEU:HD12	1.84	0.60
50:n:226:VAL:HG13	50:n:230:PHE:H	1.66	0.60
50:n:937:ARG:NE	50:n:943:LEU:CD2	2.65	0.60
52:u:78:SER:HB3	59:z:563:VAL:HG23	1.84	0.60
53:a:224:TYR:CZ	53:a:253:MET:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:i:95:GLN:O	56:i:99:LYS:HG3	2.01	0.60
61:c:238:VAL:HG22	61:c:292:LEU:CD2	2.31	0.60
66:k:88:LYS:HD2	66:k:88:LYS:C	2.27	0.60
69:v:48:VAL:CG2	69:v:52:THR:OG1	2.49	0.60
71:w:765:ARG:HA	71:w:768:LYS:HE2	1.84	0.60
1:X:-27:DA:OP1	25:DP:299:ARG:NH2	2.35	0.60
31:DF:83:LEU:CD2	31:DF:86:PHE:CZ	2.79	0.60
53:a:503:SER:HB3	53:a:505:PRO:HD2	1.84	0.60
60:b:136:HIS:CG	61:c:111:TYR:CZ	2.90	0.60
7:HA:372:LEU:HD11	7:HA:404:ALA:HB1	1.84	0.60
7:HA:664:VAL:HG22	7:HA:677:MET:HG2	1.83	0.60
30:DE:447:THR:HA	30:DE:450:ARG:HB3	1.84	0.60
32:DI:32:GLU:CB	32:DI:35:VAL:HG23	2.31	0.60
50:n:904:PHE:CZ	50:n:1208:GLU:CG	2.74	0.60
52:u:90:LEU:HD21	58:q:9:ILE:HD11	1.70	0.60
58:q:487:ILE:HD11	58:q:540:LEU:CD1	2.32	0.60
61:c:238:VAL:HG23	68:t:121:ASP:OD2	2.02	0.60
66:k:101:ARG:HH11	66:k:101:ARG:CG	2.14	0.60
5:EA:154:CYS:HB2	5:EA:157:CYS:SG	2.42	0.59
22:PJ:8:PHE:CD2	22:PJ:48:MET:HE1	2.36	0.59
31:DF:43:VAL:HG23	32:DI:46:TYR:CD2	2.37	0.59
48:g:171:LEU:HG	56:i:132:LEU:HD22	1.83	0.59
50:n:104:LYS:NZ	51:s:109:LEU:N	2.50	0.59
54:d:27:ARG:HD2	56:i:108:HIS:CA	2.25	0.59
58:q:168:THR:HA	66:k:21:ILE:HD12	1.83	0.59
58:q:543:VAL:HG11	61:c:135:ARG:HE	1.66	0.59
29:DD:1058:VAL:CG2	35:DL:76:LEU:HD23	2.32	0.59
36:Dm:31:LEU:HD23	36:Dm:31:LEU:N	2.16	0.59
38:DH:192:ARG:NH1	38:DH:209:SER:O	2.34	0.59
39:HD:287:TYR:CB	44:HI:189:MET:HG2	2.32	0.59
43:HF:36:GLN:NE2	43:HF:38:ILE:HG13	2.16	0.59
50:n:315:LEU:HD22	50:n:319:ARG:HD2	1.84	0.59
50:n:651:ASN:OD1	50:n:680:HIS:NE2	2.34	0.59
53:a:232:LEU:HD13	53:a:232:LEU:O	2.02	0.59
53:a:367:LEU:HD22	53:a:509:ARG:HH11	1.67	0.59
58:q:168:THR:CA	66:k:21:ILE:CD1	2.80	0.59
5:EA:139:LEU:CG	47:PG:151:ARG:CB	2.79	0.59
9:PA:261:ARG:O	9:PA:261:ARG:HD2	2.02	0.59
31:Df:349:ASN:HB3	31:Df:351:ILE:HG13	1.84	0.59
30:DE:463:PHE:O	31:DF:134:HIS:N	2.34	0.59
43:HF:36:GLN:HG2	43:HF:37:ASP:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:HJ:239:LYS:HZ2	45:HJ:239:LYS:N	1.85	0.59
53:a:509:ARG:CZ	53:a:509:ARG:CB	2.79	0.59
54:d:44:LEU:HD22	54:d:48:LEU:HD11	1.84	0.59
62:e:136:LEU:CD1	66:k:107:VAL:HG12	2.32	0.59
66:k:70:LEU:HD13	66:k:74:ALA:HB2	1.84	0.59
73:y:45:GLU:O	73:y:48:ASN:O	2.21	0.59
7:HA:462:SER:OG	7:HA:463:PRO:HD2	2.02	0.59
7:HA:628:THR:O	7:HA:628:THR:HG22	2.02	0.59
29:DD:1057:ARG:HA	35:DL:75:GLN:O	2.02	0.59
31:DF:14:LEU:HD11	32:DI:19:MET:HE1	1.84	0.59
31:DF:85:GLY:O	33:DJ:212:LYS:HG2	2.02	0.59
46:PD:70:ARG:NH2	47:PG:142:GLU:OE2	2.35	0.59
50:n:155:PRO:HA	50:n:158:ILE:HD12	1.83	0.59
50:n:192:LEU:HD12	50:n:220:GLY:N	2.16	0.59
52:u:67:LYS:HE3	59:z:528:LEU:CD1	2.32	0.59
52:u:67:LYS:CE	59:z:528:LEU:CD1	2.80	0.59
55:f:106:TYR:CE2	65:h:106:PRO:HG3	2.38	0.59
67:r:191:GLU:OE2	69:v:8:PRO:CA	2.50	0.59
17:PC:9:VAL:HG11	23:PK:105:PHE:HD1	1.68	0.59
30:DE:474:THR:OG1	30:DE:546:VAL:O	2.19	0.59
30:DE:694:LEU:CD1	30:DE:703:MET:CE	2.39	0.59
32:DI:23:LEU:HD12	32:DI:31:TYR:CZ	2.37	0.59
45:HJ:239:LYS:NZ	45:HJ:239:LYS:HB2	2.17	0.59
50:n:265:LEU:O	50:n:265:LEU:HD22	2.02	0.59
50:n:821:SER:O	50:n:833:ILE:HA	2.02	0.59
58:q:155:GLY:CA	69:v:62:HIS:CE1	2.63	0.59
58:q:597:PRO:HA	58:q:619:ARG:HA	1.84	0.59
60:b:179:LEU:CD1	62:e:60:VAL:C	2.75	0.59
65:h:150:LEU:HD21	66:k:45:LEU:HD13	1.81	0.59
4:DA:1157:ASN:O	4:DA:1159:SER:N	2.36	0.59
31:DF:65:LYS:O	31:DF:66:LEU:HB2	2.02	0.59
31:DF:122:LEU:HD12	31:DF:122:LEU:N	2.18	0.59
32:DI:23:LEU:CD1	32:DI:31:TYR:CZ	2.85	0.59
53:a:375:PHE:CG	72:x:17:ARG:NH2	2.69	0.59
54:d:42:ARG:NH2	56:i:96:GLU:OE1	2.35	0.59
68:t:8:GLN:HG3	68:t:196:LEU:HD21	1.84	0.59
70:p:22:GLU:HB3	70:p:751:GLN:HE21	1.68	0.59
12:FB:80:GLU:OE2	12:FB:81:HIS:N	2.35	0.59
13:HB:471:LEU:HD12	13:HB:472:LEU:HD22	1.84	0.59
31:DF:104:LEU:HD13	33:DJ:217:PHE:CE2	2.33	0.59
40:HE:195:VAL:HG12	40:HE:203:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:HG:88:LEU:HD22	41:HG:131:LEU:HD21	1.83	0.59
48:g:130:GLN:HB2	52:u:5:LEU:HD13	1.85	0.59
50:n:237:MET:HE1	58:q:45:GLN:CG	2.32	0.59
50:n:870:GLN:HG2	64:o:655:THR:CG2	2.31	0.59
58:q:184:ASN:CG	69:v:83:LYS:HD3	2.28	0.59
10:DB:431:LEU:O	10:DB:431:LEU:HD23	2.02	0.59
15:PB:274:ARG:NH2	15:PB:281:ASP:OD1	2.36	0.59
30:De:562:SER:OG	30:De:564:ASP:OD1	2.21	0.59
31:Df:219:GLU:OE1	31:Df:219:GLU:N	2.26	0.59
45:HJ:177:ARG:HB2	45:HJ:177:ARG:CZ	2.32	0.59
50:n:960:LYS:HZ3	50:n:1185:LEU:HD13	1.67	0.59
53:a:462:LEU:CG	72:x:49:GLN:CD	2.73	0.59
58:q:190:LEU:HD23	58:q:291:TRP:CE3	2.38	0.59
68:t:6:VAL:HA	68:t:140:VAL:O	2.03	0.59
3:BA:248:ARG:NH2	3:BA:287:GLN:OE1	2.36	0.59
5:EA:144:LEU:HD22	5:EA:155:THR:H	1.68	0.59
11:EB:144:ASN:HB3	11:EB:174:ALA:HB1	1.84	0.59
30:DE:432:LEU:HG	30:DE:436:ASP:CG	2.28	0.59
30:DE:433:LYS:CD	32:DI:110:TYR:CZ	2.83	0.59
30:DE:746:ASP:OD1	30:DE:746:ASP:N	2.30	0.59
31:DF:316:GLN:NE2	31:DF:320:ARG:HA	2.17	0.59
38:DH:50:PHE:CE2	33:DJ:170:ALA:C	2.80	0.59
45:HJ:181:LEU:O	45:HJ:181:LEU:HD22	2.03	0.59
50:n:375:ASP:HB3	50:n:376:PRO:HD3	1.85	0.59
50:n:686:LYS:NZ	64:o:730:PRO:CB	2.48	0.59
55:f:142:SER:OG	58:q:183:PHE:CD2	2.55	0.59
65:h:8:LEU:HD23	65:h:8:LEU:O	2.03	0.59
1:X:18:DG:H1	2:Y:-18:DC:H42	1.48	0.59
4:DA:401:ASN:H	4:DA:401:ASN:HD22	1.50	0.59
4:DA:511:LEU:H	4:DA:511:LEU:HD12	1.68	0.59
4:DA:1068:ARG:HD2	4:DA:1068:ARG:C	2.27	0.59
9:PA:1796:SER:HB2	58:q:24:LEU:HD22	1.85	0.59
10:DB:622:ASP:HB3	43:HF:36:GLN:HG3	1.84	0.59
31:DF:317:LEU:H	31:DF:317:LEU:CD2	2.15	0.59
44:HI:239:ASP:CA	44:HI:242:SER:HB3	2.28	0.59
64:o:749:LEU:HD12	72:x:69:SER:HB2	1.83	0.59
68:t:131:MET:O	68:t:131:MET:HE3	2.03	0.59
72:x:11:LEU:HB2	72:x:14:TRP:HE3	1.66	0.59
72:x:414:GLU:OE2	72:x:460:LYS:NZ	2.34	0.59
13:HB:417:LYS:HA	13:HB:421:VAL:HG23	1.85	0.58
39:HD:145:GLU:CD	65:h:67:LYS:HE2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:HH:625:GLN:OE1	42:HH:639:ARG:NH1	2.36	0.58
44:HI:207:LEU:O	55:f:53:GLN:HG3	2.03	0.58
45:HJ:114:LYS:HA	45:HJ:114:LYS:HE2	1.84	0.58
46:PD:76:ASN:ND2	65:h:47:ASP:HB3	2.17	0.58
52:u:75:SER:CB	59:z:566:CYS:SG	2.91	0.58
53:a:375:PHE:CB	72:x:17:ARG:CZ	2.81	0.58
64:o:718:VAL:HG11	64:o:743:TYR:CE1	2.38	0.58
65:h:97:VAL:HG23	65:h:104:VAL:HG21	1.85	0.58
69:v:48:VAL:HG22	69:v:52:THR:OG1	2.02	0.58
10:DB:489:GLN:OE1	10:DB:489:GLN:N	2.34	0.58
31:DF:82:PRO:HB2	31:DF:98:SER:CB	2.33	0.58
38:DH:114:SER:C	38:DH:116:ARG:H	2.11	0.58
39:HD:288:THR:O	39:HD:290:SER:N	2.36	0.58
52:u:115:LEU:HD12	54:d:121:LEU:CB	2.24	0.58
71:w:895:ASP:O	71:w:899:ARG:NH1	2.35	0.58
32:Di:73:LEU:HD12	32:Di:74:ALA:N	2.18	0.58
40:HE:52:ASN:OD1	40:HE:53:ARG:N	2.37	0.58
44:HI:86:ASN:ND2	44:HI:86:ASN:C	2.58	0.58
52:u:117:LYS:HD3	56:i:140:MET:HA	1.85	0.58
54:d:167:TRP:CE3	57:m:106:GLN:CD	2.81	0.58
55:f:137:CYS:HB3	65:h:42:TRP:HB2	1.85	0.58
58:q:124:PHE:CD2	65:h:89:LEU:HD11	2.38	0.58
58:q:162:LYS:O	58:q:166:ARG:CG	2.50	0.58
71:w:53:GLN:O	71:w:56:HIS:HB2	2.03	0.58
7:HA:262:ASN:O	7:HA:266:LEU:HD23	2.03	0.58
20:PH:102:ASP:OD2	20:PH:110:THR:OG1	2.21	0.58
30:De:484:LEU:HD21	30:De:504:LEU:HD21	1.85	0.58
29:DD:898:VAL:O	29:DD:902:VAL:HG23	2.04	0.58
31:DF:118:ILE:HA	38:DH:39:VAL:HG13	1.86	0.58
45:HJ:201:THR:C	45:HJ:203:ALA:H	2.11	0.58
50:n:234:LEU:HD21	50:n:282:LEU:CD2	2.33	0.58
50:n:377:PRO:HG2	50:n:408:ARG:HH21	1.66	0.58
50:n:528:HIS:HB3	50:n:530:ILE:HG22	1.84	0.58
53:a:131:ASN:H	53:a:131:ASN:HD22	1.50	0.58
58:q:157:ALA:HB1	66:k:32:ILE:HG13	1.85	0.58
58:q:184:ASN:ND2	69:v:83:LYS:HD2	2.17	0.58
58:q:400:PHE:CE2	67:r:142:LYS:HB2	2.39	0.58
58:q:591:LYS:NZ	58:q:593:MET:SD	2.75	0.58
65:h:86:ASP:H	65:h:99:VAL:HG12	1.67	0.58
9:PA:1674:THR:HB	44:HI:214:PRO:HG2	1.85	0.58
22:PJ:64:PRO:O	24:PL:23:HIS:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:250:LEU:HG	50:n:275:HIS:HA	1.86	0.58
50:n:250:LEU:HG	50:n:275:HIS:CA	2.33	0.58
53:a:160:LEU:CD1	53:a:214:ARG:NH2	2.67	0.58
54:d:45:ILE:CG2	56:i:76:MET:CG	2.81	0.58
55:f:145:TYR:OH	65:h:43:PRO:HG3	2.03	0.58
57:m:56:LEU:CD2	57:m:80:GLN:HE22	2.12	0.58
64:o:636:HIS:HE2	64:o:640:ARG:HH21	1.50	0.58
64:o:639:TYR:CE2	70:p:786:HIS:CB	2.61	0.58
67:r:192:GLN:HE22	69:v:11:LYS:HG3	1.69	0.58
70:p:61:MET:HE2	70:p:75:SER:HB3	1.85	0.58
70:p:166:PRO:HG2	70:p:169:THR:HG22	1.84	0.58
30:DE:432:LEU:HG	30:DE:436:ASP:CB	2.34	0.58
31:DF:14:LEU:HD23	32:DI:22:ILE:HD12	1.84	0.58
31:DF:83:LEU:HD12	31:DF:83:LEU:N	2.17	0.58
48:g:75:LYS:HZ2	59:z:562:GLY:HA3	1.68	0.58
50:n:371:GLN:HG3	50:n:390:MET:HE1	1.84	0.58
50:n:956:ALA:HB3	50:n:1217:ARG:NH2	2.18	0.58
58:q:102:LEU:HD22	65:h:26:LEU:HD22	1.84	0.58
60:b:103:ASP:OD1	60:b:103:ASP:N	2.23	0.58
68:t:78:LEU:HD22	68:t:78:LEU:N	2.18	0.58
9:PA:357:LYS:NZ	15:PB:1107:LEU:O	2.33	0.58
12:FB:189:SER:HB3	29:DD:991:MET:CE	2.25	0.58
13:HB:130:ASP:OD2	13:HB:463:HIS:NE2	2.33	0.58
29:DD:910:LEU:HD11	35:DL:88:ALA:HB2	1.85	0.58
30:DE:586:TYR:HB3	30:DE:605:HIS:HB3	1.84	0.58
35:DL:62:LYS:O	35:DL:62:LYS:NZ	2.21	0.58
44:HI:132:TRP:HA	44:HI:132:TRP:CE3	2.38	0.58
46:PD:76:ASN:ND2	65:h:47:ASP:C	2.62	0.58
50:n:544:ARG:HD3	50:n:716:ASN:O	2.03	0.58
4:DA:929:THR:HG22	4:DA:954:ALA:HA	1.86	0.58
10:DB:732:CYS:SG	38:DH:173:GLN:HB2	2.44	0.58
15:PB:407:MET:HE1	15:PB:444:LEU:CD2	2.33	0.58
31:DF:323:VAL:HA	31:DF:326:HIS:CD2	2.36	0.58
42:HH:266:GLN:N	42:HH:266:GLN:NE2	2.49	0.58
52:u:90:LEU:HB2	58:q:9:ILE:CG1	2.31	0.58
54:d:38:GLU:OE2	56:i:96:GLU:HB3	2.02	0.58
58:q:113:TYR:HD2	65:h:19:VAL:HG12	1.67	0.58
58:q:188:LEU:HA	69:v:87:ILE:CG1	2.34	0.58
64:o:691:VAL:HA	64:o:708:CYS:HA	1.84	0.58
9:PA:1481:LYS:HE3	47:PG:22:LEU:CD2	2.34	0.58
11:EB:141:PRO:O	11:EB:146:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:316:GLN:HB2	31:DF:327:TRP:CE3	2.39	0.58
42:HH:281:GLN:NE2	42:HH:482:PHE:O	2.37	0.58
49:j:82:LYS:HD2	51:s:101:VAL:HG11	1.86	0.58
50:n:234:LEU:HD22	50:n:245:TRP:HB3	1.86	0.58
58:q:93:TRP:N	58:q:94:PRO:HD2	2.19	0.58
60:b:78:ALA:CB	64:o:621:LEU:HD21	2.31	0.58
60:b:136:HIS:CG	61:c:111:TYR:CE1	2.91	0.58
60:b:178:LEU:CD2	63:l:82:LEU:HD11	2.33	0.58
69:v:16:GLN:HE21	69:v:20:LYS:HE2	0.76	0.58
9:PA:111:CYS:SG	9:PA:188:GLN:NE2	2.77	0.58
15:PB:867:ILE:HB	15:PB:894:THR:HG22	1.85	0.58
32:Di:73:LEU:CD2	35:Di:105:HIS:ND1	2.67	0.58
38:DH:108:PRO:CG	33:DJ:116:LEU:HD21	2.34	0.58
53:a:160:LEU:CD1	53:a:219:LEU:HD21	2.33	0.58
55:f:101:ILE:CD1	65:h:105:VAL:HG11	2.33	0.58
62:e:129:VAL:HG12	66:k:111:CYS:HG	1.68	0.58
72:x:404:GLN:NE2	72:x:408:GLN:OE1	2.37	0.58
9:PA:1662:PRO:HD3	55:f:16:VAL:O	2.04	0.57
11:EB:167:LEU:HD23	11:EB:198:LYS:HD3	1.86	0.57
13:HB:422:LEU:HD22	40:HE:225:GLN:NE2	2.18	0.57
35:DL:71:ASP:CB	35:DL:74:GLU:CG	2.79	0.57
44:HI:111:PRO:HD2	55:f:63:MET:HG3	1.86	0.57
44:HI:135:HIS:HD2	44:HI:137:ASP:H	1.51	0.57
50:n:685:LEU:CD2	64:o:729:TYR:HE2	2.17	0.57
58:q:645:ALA:HB2	62:e:100:LEU:HD22	1.85	0.57
61:c:162:VAL:HG13	61:c:207:LEU:HD13	1.86	0.57
62:e:129:VAL:HG11	66:k:114:MET:HE2	1.85	0.57
17:PC:7:PRO:O	23:PK:104:ARG:NH1	2.37	0.57
30:DE:450:ARG:HG3	30:DE:789:ASN:ND2	2.19	0.57
44:HI:30:ARG:CZ	44:HI:30:ARG:HB3	2.34	0.57
44:HI:136:ARG:HB2	44:HI:159:ALA:HA	1.85	0.57
50:n:169:LEU:HA	57:m:104:HIS:CB	2.31	0.57
50:n:944:PHE:HE2	70:p:677:THR:OG1	1.86	0.57
53:a:66:GLN:HA	54:d:66:LEU:HD21	1.86	0.57
54:d:109:GLN:HA	54:d:112:LYS:HZ1	1.69	0.57
64:o:748:PHE:HD2	72:x:66:TYR:HE1	1.53	0.57
68:t:124:VAL:HG13	68:t:142:VAL:HG22	1.86	0.57
69:v:108:LEU:HD12	69:v:108:LEU:O	2.04	0.57
71:w:726:ASN:ND2	71:w:726:ASN:H	2.02	0.57
6:FA:142:ASN:OD1	6:FA:143:TRP:N	2.38	0.57
9:PA:1650:TYR:CD1	58:q:111:VAL:HG21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:DB:769:LYS:O	10:DB:769:LYS:HG3	2.03	0.57
38:DH:50:PHE:CZ	33:DJ:171:LEU:N	2.72	0.57
35:DL:91:PHE:O	35:DL:95:VAL:HG23	2.03	0.57
50:n:274:ILE:HD11	55:f:181:LEU:CD2	2.34	0.57
65:h:33:LEU:HD23	65:h:40:LEU:HD23	1.86	0.57
65:h:85:ARG:HD2	65:h:99:VAL:HG11	1.85	0.57
68:t:9:MET:H	68:t:138:ILE:HG22	1.68	0.57
4:DA:1063:LYS:C	4:DA:1063:LYS:HD3	2.28	0.57
9:PA:668:PHE:CE1	9:PA:672:ILE:HD11	2.40	0.57
9:PA:1475:LEU:HD23	47:PG:66:VAL:CG2	2.31	0.57
16:HC:58:ARG:HD2	40:HE:229:TRP:CE3	2.39	0.57
47:PG:38:CYS:SG	47:PG:39:THR:N	2.78	0.57
53:a:267:LYS:H	53:a:267:LYS:HD2	1.70	0.57
53:a:504:ILE:N	53:a:505:PRO:CD	2.67	0.57
58:q:38:GLN:HB2	58:q:42:ARG:HH21	1.70	0.57
69:v:122:GLU:OE1	69:v:122:GLU:HA	2.05	0.57
71:w:764:TYR:OH	71:w:799:GLU:OE2	2.22	0.57
77:NY:-84:DG:H2''	77:NY:-83:DG:C8	2.39	0.57
27:DO:62:LEU:HA	27:DO:76:LEU:HD23	1.87	0.57
39:HD:35:VAL:HG13	39:HD:58:PHE:CE2	2.39	0.57
39:HD:282:ASP:O	39:HD:285:GLY:N	2.36	0.57
40:HE:215:LEU:HD22	40:HE:230:VAL:HG21	1.86	0.57
45:HJ:87:PHE:CD1	45:HJ:87:PHE:C	2.83	0.57
45:HJ:229:GLU:N	45:HJ:229:GLU:CD	2.62	0.57
48:g:164:ILE:HD12	56:i:140:MET:HE3	1.86	0.57
50:n:647:MET:HE1	71:w:22:PHE:HB2	1.87	0.57
64:o:756:MET:O	64:o:760:LEU:HG	2.05	0.57
65:h:151:LEU:CD2	69:v:37:ILE:HB	2.34	0.57
70:p:443:LEU:C	70:p:443:LEU:HD12	2.30	0.57
73:y:183:VAL:HG13	73:y:221:VAL:HG22	1.86	0.57
7:HA:240:ASP:OD1	7:HA:241:ASN:N	2.37	0.57
30:DE:433:LYS:CG	32:DI:110:TYR:OH	2.52	0.57
39:HD:84:LYS:CB	39:HD:136:ASN:ND2	2.68	0.57
39:HD:283:LEU:HD23	39:HD:283:LEU:C	2.29	0.57
45:HJ:275:GLN:CD	45:HJ:275:GLN:C	2.73	0.57
48:g:129:HIS:HB2	52:u:82:THR:HG22	1.86	0.57
50:n:651:ASN:HB3	71:w:21:ALA:CB	2.33	0.57
53:a:382:LEU:CD2	53:a:446:SER:CA	2.82	0.57
63:l:160:MET:HE1	69:v:134:TYR:CD2	2.40	0.57
71:w:9:PHE:HE2	71:w:63:ILE:HG12	1.69	0.57
5:EA:114:ILE:HG23	5:EA:177:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:HC:397:GLU:OE1	43:HF:61:MET:CE	2.53	0.57
31:DF:22:VAL:HG13	32:DI:44:PHE:HE1	1.68	0.57
45:HJ:114:LYS:HA	45:HJ:114:LYS:CE	2.33	0.57
50:n:321:GLY:HA3	58:q:317:GLN:HE21	1.70	0.57
50:n:904:PHE:CZ	50:n:1208:GLU:CB	2.88	0.57
50:n:933:VAL:CG2	50:n:1176:ILE:HB	2.34	0.57
58:q:110:CYS:SG	65:h:23:LYS:HD3	2.45	0.57
65:h:139:GLN:NE2	66:k:37:LYS:CB	2.68	0.57
71:w:855:TRP:O	71:w:858:ASN:ND2	2.37	0.57
7:HA:345:ARG:CD	39:HD:1:MET:SD	2.93	0.57
9:PA:223:GLU:OE2	11:EB:232:LYS:NZ	2.38	0.57
11:EB:122:GLU:OE2	11:EB:126:ASN:OD1	2.22	0.57
28:Dc:21:LEU:C	28:Dc:21:LEU:HD12	2.29	0.57
31:DF:312:ILE:HG13	31:DF:334:ALA:HB3	1.86	0.57
32:DI:53:ASP:HB2	32:DI:74:ALA:HB1	1.87	0.57
32:DI:132:LEU:CD2	33:DJ:121:MET:HE2	2.34	0.57
44:HI:261:PHE:CB	55:f:52:MET:HE2	2.34	0.57
50:n:237:MET:CE	58:q:45:GLN:CG	2.83	0.57
52:u:80:GLU:HB3	59:z:539:ASP:CG	2.29	0.57
53:a:462:LEU:HB2	72:x:49:GLN:CA	2.35	0.57
57:m:116:GLN:HG2	59:z:595:PRO:HD3	1.86	0.57
66:k:63:LEU:HD23	69:v:22:LEU:HD13	1.87	0.57
9:PA:1245:CYS:O	9:PA:1246:ILE:HD13	2.03	0.57
20:PH:33:GLU:OE2	20:PH:55:LYS:NZ	2.38	0.57
32:DI:16:ALA:HA	32:DI:40:LEU:CD1	2.23	0.57
32:DI:131:SER:CB	33:DJ:150:ARG:HH12	2.16	0.57
44:HI:52:LYS:HA	44:HI:52:LYS:CE	2.14	0.57
50:n:319:ARG:HG3	50:n:320:TRP:HD1	1.70	0.57
50:n:944:PHE:CE2	70:p:677:THR:OG1	2.57	0.57
50:n:957:PRO:CG	50:n:1214:VAL:HG21	2.35	0.57
52:u:108:VAL:HG22	54:d:128:ALA:HB1	1.86	0.57
53:a:416:ALA:HB1	53:a:472:SER:O	2.04	0.57
11:EB:83:ASN:O	11:EB:87:THR:HG23	2.05	0.57
28:Dc:12:VAL:HG23	31:Df:118:ILE:HA	1.86	0.57
38:DH:137:GLY:O	38:DH:155:ASP:CG	2.47	0.57
44:HI:15:LEU:H	44:HI:29:ALA:HB2	1.69	0.57
44:HI:239:ASP:C	44:HI:239:ASP:OD1	2.48	0.57
45:HJ:175:LYS:HA	45:HJ:175:LYS:HZ2	1.70	0.57
50:n:820:ILE:HD11	50:n:833:ILE:HB	1.86	0.57
53:a:316:ALA:CB	53:a:447:GLU:HG2	2.34	0.57
56:i:118:LEU:HD23	56:i:118:LEU:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:b:101:ARG:HH12	70:p:677:THR:HB	1.68	0.57
60:b:179:LEU:HD11	62:e:60:VAL:C	2.29	0.57
64:o:741:TRP:NE1	72:x:107:ARG:HB2	2.20	0.57
70:p:580:LEU:HD21	70:p:657:GLU:HB3	1.86	0.57
72:x:11:LEU:C	72:x:13:ALA:N	2.59	0.57
7:HA:664:VAL:HG21	7:HA:679:PHE:CE1	2.40	0.56
29:DD:873:LEU:CD1	29:DD:873:LEU:H	2.18	0.56
30:DE:345:MET:HE3	30:DE:346:PRO:HD2	1.87	0.56
39:HD:84:LYS:HA	39:HD:136:ASN:CG	2.29	0.56
41:HG:261:SER:OG	41:HG:265:GLN:O	2.23	0.56
44:HI:146:ASP:OD1	44:HI:149:GLY:N	2.33	0.56
50:n:941:TYR:HD2	50:n:1172:SER:HB2	1.62	0.56
53:a:259:ILE:HD12	53:a:259:ILE:N	2.20	0.56
53:a:441:GLU:HB3	72:x:14:TRP:HE1	1.69	0.56
58:q:109:MET:HG3	65:h:22:LEU:HG	1.86	0.56
58:q:437:HIS:CE1	58:q:472:GLU:H	2.21	0.56
1:X:-5:DT:H3	2:Y:5:DA:N6	2.00	0.56
30:DE:742:LYS:HA	30:DE:745:GLU:HG2	1.85	0.56
31:DF:86:PHE:HA	33:DJ:212:LYS:NZ	2.20	0.56
35:DL:71:ASP:O	35:DL:73:ASN:N	2.37	0.56
40:HE:241:LEU:HD23	40:HE:243:LEU:HD11	1.86	0.56
50:n:154:ILE:HB	50:n:155:PRO:CD	2.36	0.56
67:r:38:ARG:NH1	67:r:192:GLN:HG3	2.19	0.56
72:x:376:ALA:O	72:x:380:ASN:ND2	2.38	0.56
4:DA:475:LEU:HD13	4:DA:475:LEU:C	2.30	0.56
4:DA:675:ASP:OD1	37:DG:78:LYS:NZ	2.37	0.56
4:DA:851:ASP:OD1	4:DA:851:ASP:N	2.38	0.56
31:Df:223:TYR:HD2	31:Df:255:MET:HE1	1.71	0.56
31:Df:320:ARG:CB	31:Df:320:ARG:HH11	2.18	0.56
31:DF:276:LEU:HA	31:DF:330:ARG:HH22	1.70	0.56
31:DF:315:ARG:CZ	31:DF:369:PRO:HB3	2.35	0.56
31:DF:320:ARG:O	31:DF:322:ASP:N	2.38	0.56
35:DL:113:VAL:HG13	35:DL:113:VAL:O	2.06	0.56
44:HI:84:LYS:HZ2	44:HI:84:LYS:HA	1.70	0.56
50:n:250:LEU:CG	50:n:275:HIS:HB2	2.34	0.56
52:u:122:LEU:C	52:u:124:ASP:N	2.59	0.56
53:a:127:HIS:HE1	53:a:171:THR:CG2	2.19	0.56
58:q:186:GLU:OE2	58:q:291:TRP:CE2	2.58	0.56
58:q:188:LEU:HD22	69:v:87:ILE:CG1	2.35	0.56
58:q:437:HIS:ND1	58:q:472:GLU:N	2.53	0.56
65:h:12:LEU:HD13	65:h:12:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:k:60:GLU:HG2	69:v:22:LEU:HD11	1.86	0.56
69:v:47:GLN:OE1	69:v:47:GLN:HA	2.05	0.56
4:DA:396:LEU:HD13	4:DA:396:LEU:N	2.19	0.56
6:FA:109:LYS:O	6:FA:149:LEU:N	2.38	0.56
6:FA:171:LEU:HD21	9:PA:1279:MET:HA	1.88	0.56
7:HA:345:ARG:HD3	39:HD:1:MET:SD	2.45	0.56
15:PB:91:ILE:HD13	15:PB:126:VAL:HG12	1.88	0.56
15:PB:910:THR:HG22	15:PB:911:LEU:N	2.18	0.56
31:Df:226:GLU:HG3	38:DH:194:MET:HE1	1.86	0.56
29:DD:873:LEU:HD12	29:DD:873:LEU:H	1.69	0.56
31:DF:217:SER:OG	38:DH:161:LYS:HA	2.05	0.56
45:HJ:228:MET:HB3	45:HJ:231:TYR:HB2	1.88	0.56
46:PD:100:LEU:HD12	46:PD:101:ALA:N	2.20	0.56
47:PG:166:ASP:OD1	47:PG:167:TYR:N	2.38	0.56
50:n:201:HIS:HE1	52:u:122:LEU:HG	1.70	0.56
50:n:693:ILE:HD11	50:n:775:ARG:HG2	1.87	0.56
53:a:401:PRO:O	53:a:405:PRO:HD3	2.04	0.56
53:a:463:VAL:HG11	53:a:488:ILE:CD1	2.35	0.56
58:q:188:LEU:HA	69:v:87:ILE:HD12	1.81	0.56
59:z:577:THR:O	59:z:595:PRO:HB3	2.04	0.56
67:r:17:ASN:OD1	67:r:17:ASN:N	2.35	0.56
73:y:195:PHE:O	73:y:224:ARG:NH1	2.37	0.56
74:NC:840:THR:O	74:NC:841:THR:CB	2.53	0.56
9:PA:1798:SER:CA	58:q:25:ASP:OD2	2.46	0.56
29:Dd:917:ILE:HD11	29:Dd:1063:LEU:HD13	1.87	0.56
30:DE:773:TYR:HA	31:DF:142:GLN:OE1	2.05	0.56
31:DF:360:THR:O	31:DF:364:VAL:HG22	2.06	0.56
38:DH:50:PHE:CD1	38:DH:50:PHE:N	2.73	0.56
32:DI:31:TYR:CD2	32:DI:35:VAL:HB	2.41	0.56
46:PD:74:PHE:HA	46:PD:141:GLN:HE22	1.71	0.56
50:n:250:LEU:CD2	50:n:275:HIS:CB	2.84	0.56
50:n:706:LEU:HD22	58:q:615:TRP:CH2	2.40	0.56
50:n:706:LEU:HB2	50:n:725:VAL:HG23	1.87	0.56
53:a:430:LEU:N	53:a:430:LEU:HD23	2.21	0.56
55:f:101:ILE:HD11	65:h:78:PRO:HG3	1.86	0.56
56:i:103:THR:O	56:i:107:ILE:HB	2.05	0.56
58:q:409:GLY:HA3	68:t:88:ASP:OD1	2.05	0.56
58:q:578:TYR:CE1	58:q:646:LEU:HD13	2.41	0.56
72:x:172:THR:HB	72:x:965:LYS:HE2	1.88	0.56
72:x:581:ILE:HD11	72:x:616:LEU:HD22	1.87	0.56
9:PA:1030:SER:OG	18:PE:162:ARG:NE	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:DB:672:PHE:CE1	16:HC:414:SER:CB	2.63	0.56
15:PB:694:THR:HG22	15:PB:695:HIS:CE1	2.41	0.56
27:DO:29:THR:HG23	27:DO:32:LEU:H	1.69	0.56
31:DF:81:GLU:OE2	31:DF:91:PHE:CD1	2.57	0.56
50:n:685:LEU:HD22	64:o:729:TYR:CE2	2.40	0.56
58:q:112:LEU:CD2	65:h:19:VAL:CG2	2.84	0.56
63:l:156:LEU:CD2	69:v:134:TYR:HB2	2.34	0.56
9:PA:1481:LYS:HE3	47:PG:22:LEU:HD22	1.88	0.56
9:PA:1793:THR:H	65:h:102:HIS:HE1	1.54	0.56
30:DE:697:ASP:HB2	30:DE:704:VAL:HG21	1.88	0.56
38:DH:50:PHE:CZ	33:DJ:195:LEU:HD13	2.40	0.56
32:DI:81:GLN:NE2	35:DL:123:GLN:CD	2.56	0.56
32:DI:132:LEU:HD11	33:DJ:121:MET:SD	2.45	0.56
45:HJ:167:PHE:HD1	45:HJ:167:PHE:C	2.12	0.56
50:n:960:LYS:HG3	50:n:1210:PHE:CE2	2.38	0.56
54:d:164:PRO:HD2	54:d:167:TRP:CG	2.40	0.56
66:k:87:ARG:CA	69:v:105:LEU:HD13	2.22	0.56
5:EA:22:ILE:HD11	5:EA:26:TYR:CD2	2.41	0.56
10:DB:560:TYR:CD2	10:DB:581:ILE:HD11	2.39	0.56
11:EB:108:HIS:O	11:EB:111:ILE:HG22	2.06	0.56
15:PB:643:LEU:HD11	15:PB:656:LEU:HD11	1.87	0.56
29:DD:891:ILE:HA	35:DL:104:ARG:HH21	1.70	0.56
31:DF:104:LEU:HB2	33:DJ:217:PHE:HZ	1.70	0.56
38:DH:108:PRO:HG2	33:DJ:116:LEU:HD23	1.88	0.56
41:HG:345:CYS:O	41:HG:349:GLN:N	2.36	0.56
42:HH:444:HIS:O	42:HH:472:ARG:NH1	2.39	0.56
50:n:507:GLN:HE22	50:n:637:PHE:HA	1.69	0.56
52:u:128:SER:OG	56:i:131:LEU:CD2	2.49	0.56
55:f:82:ARG:HD2	55:f:84:GLN:HE21	1.71	0.56
61:c:176:MET:HE1	61:c:267:MET:HB3	1.86	0.56
65:h:81:LEU:HD12	65:h:101:SER:O	2.06	0.56
70:p:251:GLU:HG2	70:p:252:LYS:HG2	1.87	0.56
9:PA:1411:LEU:O	9:PA:1421:ARG:NH2	2.39	0.56
9:PA:1796:SER:CB	58:q:24:LEU:HD22	2.36	0.56
10:DB:61:ASN:O	10:DB:130:VAL:HG23	2.06	0.56
10:DB:259:ASP:HB3	10:DB:262:MET:O	2.06	0.56
13:HB:456:ASP:OD1	13:HB:457:ILE:HD12	2.06	0.56
15:PB:223:SER:HG	15:PB:350:HIS:CE1	2.21	0.56
15:PB:346:GLU:N	15:PB:346:GLU:OE1	2.38	0.56
15:PB:474:THR:OG1	15:PB:732:ALA:O	2.24	0.56
31:DF:71:ILE:CD1	32:DI:35:VAL:HG22	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:265:GLU:OE2	31:DF:265:GLU:HA	2.06	0.56
50:n:199:LEU:HD13	50:n:222:VAL:HG13	1.87	0.56
53:a:441:GLU:CB	72:x:17:ARG:HH22	2.11	0.56
54:d:45:ILE:HD13	56:i:72:ILE:O	2.05	0.56
54:d:47:MET:HE3	54:d:47:MET:CA	2.35	0.56
58:q:168:THR:HA	66:k:21:ILE:CD1	2.35	0.56
59:z:551:ASP:OD1	59:z:551:ASP:N	2.37	0.56
64:o:735:LEU:HD21	71:w:113:GLN:NE2	2.21	0.56
74:NC:842:SER:C	74:NC:844:GLY:H	2.14	0.56
15:PB:755:GLN:HE22	22:PJ:48:MET:HE2	1.70	0.56
31:DF:368:THR:HG23	31:DF:369:PRO:HD2	1.87	0.56
44:HI:111:PRO:CD	55:f:63:MET:HG3	2.35	0.56
53:a:462:LEU:HG	72:x:49:GLN:OE1	2.05	0.56
59:z:540:LEU:C	59:z:540:LEU:CD2	2.78	0.56
60:b:136:HIS:CD2	61:c:111:TYR:CD2	2.82	0.56
61:c:204:MET:HE3	61:c:208:PHE:O	2.04	0.56
68:t:66:MET:HG2	68:t:78:LEU:HD21	1.87	0.56
71:w:433:ASN:ND2	71:w:445:ILE:O	2.35	0.56
4:DA:353:LEU:HD21	31:Df:272:VAL:HG21	1.88	0.55
53:a:462:LEU:N	72:x:49:GLN:CG	2.23	0.55
58:q:437:HIS:HD2	58:q:437:HIS:O	1.89	0.55
58:q:477:VAL:HB	58:q:493:LEU:HB2	1.88	0.55
66:k:43:ARG:HH11	66:k:43:ARG:CB	2.19	0.55
73:y:45:GLU:O	73:y:48:ASN:C	2.49	0.55
9:PA:621:ILE:HG23	9:PA:621:ILE:O	2.07	0.55
31:Df:352:GLN:O	31:Df:356:THR:OG1	2.25	0.55
30:DE:290:HIS:CG	31:DF:45:TYR:CD2	2.94	0.55
31:DF:320:ARG:HB2	31:DF:415:ILE:CD1	2.35	0.55
31:DF:367:LYS:HG2	31:DF:367:LYS:O	2.06	0.55
41:HG:59:ARG:NH2	41:HG:166:GLU:OE1	2.39	0.55
42:HH:361:CYS:SG	42:HH:405:VAL:HG13	2.46	0.55
44:HI:143:LEU:HD23	44:HI:151:LEU:HD11	1.87	0.55
45:HJ:98:GLU:HA	45:HJ:98:GLU:OE2	2.05	0.55
48:g:96:LEU:HD21	50:n:132:THR:HG21	1.87	0.55
50:n:172:CYS:HB2	57:m:100:GLN:HE22	1.70	0.55
50:n:237:MET:HE1	58:q:45:GLN:HB2	1.77	0.55
50:n:592:LYS:HB3	71:w:27:MET:HE3	1.88	0.55
50:n:956:ALA:CB	50:n:1217:ARG:HH21	2.17	0.55
52:u:67:LYS:CE	59:z:528:LEU:HD11	2.36	0.55
55:f:118:ARG:HB3	58:q:108:GLU:OE2	2.06	0.55
56:i:75:CYS:HB3	56:i:88:ASN:HD21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:562:SER:HB2	58:q:587:GLU:HB2	1.87	0.55
61:c:204:MET:CE	61:c:206:SER:O	2.47	0.55
65:h:102:HIS:CD2	65:h:102:HIS:N	2.73	0.55
7:HA:606:GLU:O	7:HA:666:ARG:NH2	2.40	0.55
15:PB:764:MET:HE1	15:PB:938:ARG:NH1	2.21	0.55
30:DE:290:HIS:CD2	31:DF:45:TYR:CD2	2.94	0.55
30:DE:464:TYR:HA	31:DF:133:ALA:HA	1.88	0.55
39:HD:85:ARG:NH2	39:HD:140:LEU:CA	2.69	0.55
44:HI:241:CYS:O	44:HI:241:CYS:SG	2.64	0.55
50:n:118:ILE:HG12	51:s:83:LEU:HB3	1.87	0.55
50:n:904:PHE:CE2	50:n:1208:GLU:HB2	2.41	0.55
58:q:418:ILE:CD1	68:t:72:PRO:HG3	2.26	0.55
62:e:139:TRP:HE1	69:v:122:GLU:HG3	1.71	0.55
69:v:25:ASP:HB3	69:v:75:LEU:HD21	1.88	0.55
70:p:243:LYS:NZ	70:p:245:CYS:SG	2.79	0.55
10:DB:762:ASP:CG	10:DB:766:LEU:O	2.49	0.55
30:De:636:HIS:HD2	30:De:638:ASN:H	1.53	0.55
30:DE:645:GLY:H	30:DE:675:LEU:HD11	1.70	0.55
31:DF:406:VAL:HG11	31:DF:420:ALA:HB2	1.88	0.55
39:HD:20:LYS:HE3	39:HD:62:LEU:HD13	1.87	0.55
42:HH:87:GLU:OE2	42:HH:145:LYS:NZ	2.39	0.55
48:g:128:PRO:HB3	54:d:149:ILE:HG21	1.89	0.55
50:n:643:HIS:CE1	58:q:560:ILE:HG13	2.41	0.55
52:u:122:LEU:O	52:u:123:ALA:C	2.50	0.55
53:a:336:TYR:CE1	53:a:391:THR:OG1	2.52	0.55
53:a:460:ASP:O	72:x:7:LYS:HB3	2.06	0.55
54:d:154:ARG:NH2	57:m:66:TYR:C	2.65	0.55
58:q:596:PHE:CZ	63:l:117:TYR:CZ	2.95	0.55
61:c:283:ARG:HD3	61:c:309:CYS:HB3	1.87	0.55
62:e:45:VAL:HG13	63:l:92:LEU:CD1	2.35	0.55
69:v:37:ILE:C	69:v:39:THR:N	2.64	0.55
70:p:695:LYS:HB3	70:p:713:LEU:HD11	1.88	0.55
9:PA:1234:LYS:NZ	9:PA:1298:LEU:O	2.39	0.55
12:FB:186:MET:SD	29:DD:995:GLU:CG	2.93	0.55
13:HB:486:LEU:O	13:HB:490:VAL:HG23	2.07	0.55
15:PB:934:LYS:HG3	15:PB:944:THR:HG22	1.87	0.55
42:HH:83:HIS:ND1	42:HH:115:GLU:OE2	2.39	0.55
44:HI:191:GLY:C	44:HI:193:GLY:N	2.59	0.55
50:n:201:HIS:CE1	54:d:111:GLN:NE2	2.75	0.55
53:a:94:LEU:HD23	53:a:94:LEU:H	1.69	0.55
53:a:199:PRO:HG2	53:a:244:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:m:56:LEU:CG	57:m:80:GLN:HE22	2.20	0.55
65:h:78:PRO:HG3	65:h:105:VAL:HG11	1.88	0.55
69:v:35:GLU:OE2	69:v:64:ARG:CZ	2.54	0.55
70:p:710:ASP:OD1	70:p:710:ASP:N	2.34	0.55
71:w:231:VAL:O	71:w:1099:ASN:ND2	2.39	0.55
9:PA:734:ARG:NE	21:PI:107:ALA:O	2.40	0.55
10:DB:248:SER:OG	10:DB:322:MET:SD	2.65	0.55
10:DB:539:ARG:HB3	43:HF:35:ILE:O	2.07	0.55
10:DB:544:LEU:HD23	10:DB:590:ILE:HD11	1.89	0.55
30:DE:561:SER:HB2	30:DE:588:VAL:HB	1.88	0.55
40:HE:44:LEU:HD21	40:HE:162:LEU:HD13	1.89	0.55
45:HJ:212:ILE:HG12	45:HJ:255:MET:HE1	1.89	0.55
50:n:545:LEU:CG	50:n:653:PRO:HG3	2.36	0.55
53:a:449:ARG:NH1	72:x:54:PRO:CB	2.69	0.55
55:f:82:ARG:HH11	55:f:94:PRO:HB3	1.72	0.55
60:b:101:ARG:NH1	70:p:677:THR:CA	2.69	0.55
66:k:86:SER:HB2	69:v:105:LEU:HD12	1.87	0.55
70:p:619:GLN:HA	70:p:674:PRO:HB3	1.88	0.55
7:HA:114:ASN:C	7:HA:114:ASN:HD22	2.15	0.55
27:DO:16:GLN:NE2	27:DO:20:ASP:OD2	2.40	0.55
38:DH:137:GLY:O	38:DH:155:ASP:OD1	2.25	0.55
40:HE:242:ILE:C	40:HE:243:LEU:HD12	2.31	0.55
44:HI:133:ILE:HG22	44:HI:133:ILE:O	2.07	0.55
45:HJ:171:LEU:O	45:HJ:171:LEU:HD13	2.06	0.55
48:g:128:PRO:CD	48:g:129:HIS:H	2.19	0.55
51:s:106:SER:C	51:s:108:PHE:N	2.56	0.55
53:a:66:GLN:CD	54:d:44:LEU:HD21	2.31	0.55
64:o:722:GLU:HG3	64:o:737:ILE:HB	1.89	0.55
68:t:131:MET:C	68:t:131:MET:SD	2.89	0.55
71:w:1185:GLY:O	71:w:1186:TYR:C	2.50	0.55
7:HA:309:VAL:O	7:HA:309:VAL:HG12	2.07	0.55
28:Dc:67:GLY:CA	33:Dj:116:LEU:HD13	2.33	0.55
31:Df:280:ILE:O	31:Df:284:ARG:HG3	2.05	0.55
30:DE:697:ASP:HB3	30:DE:700:HIS:HB2	1.89	0.55
31:DF:106:PHE:CD1	32:DI:13:PRO:CG	2.90	0.55
42:HH:664:SER:O	42:HH:667:THR:OG1	2.25	0.55
45:HJ:41:LEU:HG	45:HJ:41:LEU:O	2.07	0.55
46:PD:70:ARG:HG2	69:v:20:LYS:HG3	1.89	0.55
50:n:169:LEU:O	58:q:19:VAL:HG13	2.07	0.55
53:a:383:PRO:HD3	53:a:445:LEU:O	2.07	0.55
57:m:95:LYS:HE3	65:h:103:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:188:LEU:HD22	69:v:87:ILE:HB	1.88	0.55
62:e:49:GLU:HG2	63:l:89:PHE:CD1	2.42	0.55
64:o:639:TYR:HD2	70:p:786:HIS:HB2	1.59	0.55
71:w:32:ASP:OD1	71:w:32:ASP:N	2.39	0.55
71:w:369:ARG:NH1	71:w:402:LEU:O	2.37	0.55
6:FA:163:GLU:OE1	6:FA:163:GLU:N	2.40	0.55
9:PA:1789:SER:O	55:f:76:PRO:HB3	2.07	0.55
13:HB:524:HIS:ND1	41:HG:270:SER:OG	2.38	0.55
31:DF:219:GLU:OE2	38:DH:157:HIS:HB3	2.06	0.55
53:a:106:ASP:N	53:a:106:ASP:OD1	2.40	0.55
53:a:420:LEU:CD1	53:a:475:VAL:HG21	2.37	0.55
61:c:288:LEU:HD21	68:t:122:PHE:CZ	2.42	0.55
71:w:1034:LEU:HD22	71:w:1038:ARG:HD2	1.87	0.55
72:x:11:LEU:C	72:x:13:ALA:H	2.14	0.55
12:FB:186:MET:CE	29:DD:995:GLU:OE2	2.34	0.55
30:De:610:ARG:HD3	30:De:619:PRO:HG3	1.89	0.55
45:HJ:227:THR:HB	45:HJ:229:GLU:OE1	2.07	0.55
50:n:82:LYS:HE2	51:s:154:LEU:HA	1.89	0.55
50:n:836:GLY:O	50:n:846:ASN:ND2	2.38	0.55
53:a:455:GLN:HB2	72:x:11:LEU:HG	1.89	0.55
58:q:149:LYS:HE3	69:v:40:ALA:CA	2.30	0.55
63:l:107:ASP:N	63:l:108:PRO:HD3	2.22	0.55
64:o:715:LEU:CD1	72:x:66:TYR:OH	2.47	0.55
64:o:757:THR:O	64:o:761:LEU:HG	2.06	0.55
64:o:767:HIS:CD2	64:o:772:LEU:HD21	2.42	0.55
1:X:11:DA:H2"	1:X:12:DA:C8	2.42	0.54
7:HA:17:ILE:HD11	7:HA:22:PHE:CZ	2.42	0.54
50:n:266:VAL:HG22	55:f:177:VAL:HG13	1.88	0.54
50:n:273:PHE:HZ	55:f:185:ARG:NE	2.03	0.54
53:a:462:LEU:HD12	72:x:60:ILE:HD12	1.87	0.54
58:q:376:HIS:HB2	66:k:92:MET:HE3	1.89	0.54
71:w:1072:ILE:HD11	71:w:1126:LEU:HD22	1.89	0.54
3:BA:173:VAL:O	3:BA:175:ARG:NH1	2.40	0.54
7:HA:420:PRO:HA	7:HA:431:PRO:HB3	1.89	0.54
9:PA:362:SER:HB2	15:PB:1084:LEU:HD12	1.89	0.54
31:DF:316:GLN:NE2	31:DF:320:ARG:HG3	2.23	0.54
39:HD:85:ARG:NH2	39:HD:140:LEU:HA	2.22	0.54
58:q:166:ARG:CZ	58:q:166:ARG:CB	2.85	0.54
58:q:191:ARG:HD3	69:v:87:ILE:C	2.25	0.54
58:q:451:LEU:HD12	58:q:460:ILE:HD12	1.89	0.54
66:k:16:ASP:CG	69:v:79:VAL:HG21	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:6:DG:H2''	1:X:7:DA:C8	2.42	0.54
10:DB:629:ARG:NH1	10:DB:658:ASP:OD2	2.37	0.54
15:PB:938:ARG:NH2	15:PB:983:GLU:OE2	2.38	0.54
31:Df:253:TYR:O	31:Df:254:GLN:HB3	2.06	0.54
30:DE:278:ASP:OD2	30:DE:649:ARG:NH2	2.40	0.54
31:DF:83:LEU:CD1	31:DF:98:SER:HA	2.37	0.54
38:DH:53:ALA:CA	33:DJ:195:LEU:O	2.54	0.54
35:DL:58:LEU:HA	35:DL:62:LYS:HD2	1.89	0.54
39:HD:281:GLN:HA	39:HD:281:GLN:NE2	2.20	0.54
44:HI:135:HIS:C	44:HI:135:HIS:CD2	2.84	0.54
44:HI:209:ARG:HB2	55:f:53:GLN:CG	2.35	0.54
50:n:254:VAL:CG2	50:n:303:LEU:CD2	2.72	0.54
50:n:301:LEU:HB3	50:n:361:ILE:HG13	1.89	0.54
53:a:440:PHE:CE2	53:a:508:MET:HB3	2.41	0.54
54:d:47:MET:HA	54:d:47:MET:CE	2.37	0.54
58:q:147:ILE:CG2	65:h:124:LEU:HD22	2.37	0.54
59:z:480:LEU:HD23	59:z:480:LEU:O	2.08	0.54
1:X:-27:DA:H2	25:DP:169:VAL:HG21	1.71	0.54
15:PB:260:LEU:HB2	15:PB:263:ILE:HD12	1.89	0.54
21:PI:29:ASP:O	21:PI:33:ARG:N	2.40	0.54
30:De:368:ASN:ND2	30:De:701:GLY:HA3	2.23	0.54
29:DD:1068:GLU:OE2	30:DE:582:LYS:NZ	2.41	0.54
38:DH:108:PRO:HG2	33:DJ:116:LEU:CD2	2.36	0.54
39:HD:85:ARG:HH22	39:HD:140:LEU:HA	1.72	0.54
45:HJ:102:ARG:HG2	45:HJ:102:ARG:NH1	2.22	0.54
49:j:43:PHE:CB	51:s:144:ILE:HG21	2.36	0.54
49:j:82:LYS:CD	51:s:96:PHE:CD1	2.89	0.54
50:n:166:TYR:HH	57:m:70:PRO:CB	2.16	0.54
58:q:647:SER:HB2	62:e:97:GLN:HE21	1.73	0.54
62:e:60:VAL:HG23	62:e:60:VAL:O	2.08	0.54
63:l:30:THR:OG1	63:l:102:ASN:ND2	2.40	0.54
69:v:39:THR:C	69:v:41:LYS:H	2.15	0.54
71:w:101:LEU:HD22	71:w:118:THR:HG23	1.90	0.54
71:w:203:ASN:HD21	72:x:807:THR:HG21	1.73	0.54
71:w:339:ILE:O	71:w:343:LEU:HB2	2.08	0.54
9:PA:850:THR:O	9:PA:854:THR:HG23	2.07	0.54
9:PA:1484:MET:N	9:PA:1484:MET:SD	2.80	0.54
11:EB:99:LEU:HD22	11:EB:120:MET:HE2	1.88	0.54
30:De:251:LEU:O	30:De:256:HIS:HB2	2.07	0.54
29:DD:997:ALA:O	29:DD:1001:GLN:CG	2.43	0.54
30:DE:563:GLU:HG2	30:DE:587:PRO:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:HJ:288:ASN:C	45:HJ:288:ASN:ND2	2.57	0.54
53:a:107:MET:O	53:a:107:MET:HE2	2.07	0.54
53:a:226:VAL:HG12	53:a:226:VAL:O	2.08	0.54
56:i:85:GLN:HG3	56:i:86:ASP:CG	2.32	0.54
4:DA:1052:ARG:HD2	4:DA:1052:ARG:O	2.07	0.54
7:HA:133:LYS:O	7:HA:137:LEU:HD23	2.08	0.54
30:DE:665:PHE:HE1	30:DE:701:GLY:HA2	1.73	0.54
35:DL:111:LEU:HB2	35:DL:115:ASP:OD2	2.07	0.54
46:PD:110:GLU:O	46:PD:114:LEU:HD23	2.07	0.54
48:g:90:LEU:HD21	49:j:109:LEU:HD22	1.90	0.54
50:n:97:VAL:CG2	51:s:109:LEU:HG	2.35	0.54
50:n:175:ASP:OD2	58:q:20:HIS:CE1	2.61	0.54
50:n:192:LEU:HD11	50:n:220:GLY:HA3	1.84	0.54
53:a:59:VAL:CG1	54:d:48:LEU:HD23	2.37	0.54
56:i:110:SER:CB	56:i:111:PRO:HD2	2.37	0.54
59:z:576:TRP:HB3	59:z:596:TYR:CB	2.38	0.54
9:PA:193:ARG:NH1	9:PA:195:GLY:O	2.38	0.54
9:PA:350:VAL:HG12	9:PA:1435:THR:HG21	1.89	0.54
29:Dd:911:GLN:NE2	35:DI:69:GLU:OE2	2.40	0.54
31:Df:390:THR:HG23	31:Df:391:LEU:HD22	1.90	0.54
31:DF:219:GLU:CD	38:DH:156:PRO:HB2	2.33	0.54
44:HI:171:HIS:NE2	44:HI:188:ARG:HA	2.21	0.54
56:i:65:PHE:HE1	56:i:99:LYS:CA	2.20	0.54
56:i:65:PHE:CE1	56:i:99:LYS:HA	2.42	0.54
58:q:395:PRO:HG3	67:r:75:SER:HB3	1.89	0.54
68:t:4:THR:HG22	68:t:143:GLU:HB2	1.88	0.54
71:w:781:SER:O	71:w:783:GLN:NE2	2.41	0.54
73:y:226:LEU:HD11	73:y:228:LEU:HG	1.90	0.54
10:DB:66:ASN:HD21	10:DB:119:PRO:HB3	1.73	0.54
10:DB:571:LEU:HD21	10:DB:619:MET:HE1	1.89	0.54
15:PB:752:TYR:HE1	15:PB:809:VAL:HG23	1.72	0.54
29:DD:891:ILE:HD12	29:DD:891:ILE:N	2.23	0.54
29:DD:961:GLN:HE22	30:DE:434:ASP:CG	2.16	0.54
40:HE:195:VAL:CG1	40:HE:203:LEU:HD23	2.38	0.54
47:PG:92:VAL:HG23	47:PG:139:GLN:HG2	1.89	0.54
50:n:777:TYR:HA	50:n:780:VAL:HG22	1.89	0.54
52:u:29:CYS:O	52:u:29:CYS:SG	2.66	0.54
53:a:248:SER:HB3	53:a:251:LEU:HB2	1.90	0.54
53:a:367:LEU:HD22	53:a:509:ARG:NH1	2.23	0.54
71:w:625:SER:HB2	71:w:674:THR:HG22	1.89	0.54
74:NG:1018:SER:HA	77:NY:-132:DG:H5"	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DA:639:LEU:HD12	4:DA:639:LEU:O	2.07	0.54
9:PA:261:ARG:NH1	9:PA:277:THR:OG1	2.40	0.54
9:PA:1453:GLY:O	9:PA:1457:ASN:ND2	2.35	0.54
16:HC:265:LEU:HD12	16:HC:270:LEU:HD12	1.90	0.54
29:DD:1069:ASN:O	31:DF:95:ARG:HD3	2.08	0.54
46:PD:29:ALA:O	46:PD:94:LYS:NZ	2.39	0.54
50:n:104:LYS:HZ1	51:s:109:LEU:H	1.53	0.54
53:a:127:HIS:CE1	53:a:171:THR:CG2	2.91	0.54
53:a:160:LEU:CG	53:a:219:LEU:HD21	2.38	0.54
53:a:336:TYR:CD1	53:a:391:THR:HG23	2.43	0.54
53:a:374:TYR:CE2	53:a:440:PHE:HB2	2.43	0.54
53:a:411:ILE:O	53:a:412:ARG:C	2.51	0.54
53:a:417:TYR:HH	53:a:450:PHE:HB3	1.73	0.54
54:d:42:ARG:NH2	56:i:93:LYS:CG	2.69	0.54
54:d:163:ALA:CB	57:m:106:GLN:HA	2.38	0.54
56:i:72:ILE:HD13	56:i:92:SER:HB2	1.65	0.54
58:q:113:TYR:CB	65:h:19:VAL:CG1	2.75	0.54
60:b:160:TYR:O	60:b:164:ILE:HG12	2.07	0.54
72:x:976:PRO:HA	72:x:979:ARG:HE	1.73	0.54
16:HC:42:LEU:HD13	40:HE:50:PHE:CE1	2.42	0.54
30:DE:433:LYS:NZ	32:DI:110:TYR:HE1	1.97	0.54
50:n:780:VAL:HG12	50:n:808:LEU:HD11	1.90	0.54
54:d:166:THR:HG23	54:d:166:THR:O	2.08	0.54
58:q:166:ARG:CG	58:q:166:ARG:HH11	2.22	0.54
61:c:167:SER:OG	61:c:171:ARG:NH1	2.41	0.54
65:h:110:ARG:C	65:h:110:ARG:HD3	2.33	0.54
66:k:109:ARG:CB	66:k:109:ARG:CZ	2.86	0.54
71:w:627:LEU:HD22	71:w:645:VAL:HG23	1.89	0.54
71:w:1302:LYS:NZ	71:w:1308:ASP:OD1	2.41	0.54
3:BA:133:ASN:OD1	3:BA:134:ILE:N	2.40	0.53
5:EA:171:LYS:HZ1	39:HD:41:ARG:CG	2.19	0.53
7:HA:80:ILE:HD11	7:HA:206:VAL:HB	1.90	0.53
9:PA:1660:THR:O	55:f:15:TRP:HA	2.08	0.53
10:DB:628:ILE:O	10:DB:644:GLN:NE2	2.42	0.53
15:PB:501:LEU:HD12	15:PB:505:LEU:HD12	1.90	0.53
26:DQ:15:ARG:HA	26:DQ:18:ILE:HD12	1.89	0.53
30:DE:433:LYS:CD	32:DI:110:TYR:CE1	2.90	0.53
44:HI:98:LEU:CB	44:HI:143:LEU:HD21	2.36	0.53
50:n:904:PHE:HD1	50:n:916:LEU:HD11	1.74	0.53
53:a:109:TYR:HE1	53:a:150:PHE:HZ	1.56	0.53
54:d:31:LEU:CD2	56:i:103:THR:OG1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:f:32:TYR:HD1	55:f:35:GLU:CD	2.16	0.53
69:v:90:ASP:O	69:v:91:PHE:HB2	2.08	0.53
3:BA:39:LEU:HD11	9:PA:425:ASP:HB2	1.91	0.53
5:EA:148:MET:SD	5:EA:149:THR:N	2.81	0.53
7:HA:289:VAL:HG22	7:HA:324:ARG:NH1	2.23	0.53
11:EB:82:VAL:HG12	11:EB:86:LYS:HZ3	1.74	0.53
15:PB:613:ARG:NH1	15:PB:615:TYR:OH	2.41	0.53
25:DP:208:ARG:NH2	26:DQ:346:LYS:O	2.41	0.53
30:DE:517:ASP:HA	30:DE:520:SER:HB3	1.91	0.53
38:DH:108:PRO:CD	33:DJ:116:LEU:HD21	2.38	0.53
32:DI:23:LEU:HD12	32:DI:31:TYR:OH	2.09	0.53
42:HH:632:SER:OG	42:HH:676:ARG:NH2	2.41	0.53
44:HI:22:GLN:CD	44:HI:22:GLN:H	2.16	0.53
48:g:129:HIS:CG	52:u:82:THR:HG22	2.43	0.53
52:u:90:LEU:CD2	58:q:9:ILE:CG1	2.78	0.53
54:d:76:PHE:CZ	56:i:65:PHE:CZ	2.88	0.53
60:b:186:THR:CG2	62:e:49:GLU:CD	2.77	0.53
64:o:634:PHE:O	64:o:637:SER:OG	2.25	0.53
73:y:137:GLN:OE1	73:y:140:ARG:NH1	2.38	0.53
3:BA:222:LEU:CD2	3:BA:277:ILE:HD13	2.39	0.53
7:HA:365:VAL:O	7:HA:365:VAL:HG22	2.08	0.53
16:HC:80:SER:O	16:HC:84:GLU:OE1	2.25	0.53
31:Df:318:CYS:SG	31:Df:326:HIS:HB3	2.49	0.53
31:DF:218:VAL:CG1	38:DH:162:THR:HB	2.29	0.53
50:n:870:GLN:CG	64:o:655:THR:HG22	2.32	0.53
53:a:412:ARG:CB	53:a:472:SER:HB3	2.35	0.53
55:f:32:TYR:CD1	55:f:35:GLU:CD	2.86	0.53
58:q:263:LYS:HE3	58:q:439:PHE:CZ	2.42	0.53
58:q:394:HIS:O	67:r:51:PHE:HB2	2.08	0.53
58:q:484:TYR:CE2	58:q:540:LEU:HD11	2.44	0.53
58:q:487:ILE:HD11	58:q:540:LEU:HD12	1.89	0.53
71:w:109:TRP:HB2	71:w:160:LEU:HD21	1.90	0.53
1:X:5:DC:H2"	1:X:6:DG:C8	2.44	0.53
5:EA:122:THR:HG23	39:HD:40:VAL:HG23	1.90	0.53
5:EA:127:PHE:HE2	5:EA:152:PHE:CE2	2.27	0.53
10:DB:345:CYS:HA	10:DB:348:GLN:HE21	1.73	0.53
28:Dc:33:LEU:HD13	33:Dj:197:MET:HE1	1.91	0.53
30:DE:433:LYS:HZ3	32:DI:110:TYR:HE1	1.41	0.53
30:DE:463:PHE:HB3	31:DF:134:HIS:NE2	2.22	0.53
31:DF:82:PRO:HG2	31:DF:83:LEU:HD12	1.91	0.53
31:DF:359:PHE:HB3	31:DF:380:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:HD:85:ARG:HH12	39:HD:140:LEU:N	2.06	0.53
41:HG:337:GLU:O	41:HG:340:ASN:ND2	2.38	0.53
45:HJ:33:LYS:HD3	45:HJ:33:LYS:C	2.34	0.53
53:a:128:HIS:CG	53:a:128:HIS:O	2.60	0.53
56:i:105:PRO:CD	56:i:107:ILE:HG13	2.34	0.53
58:q:113:TYR:CD2	65:h:19:VAL:HG12	2.44	0.53
60:b:101:ARG:NH1	70:p:677:THR:HB	2.24	0.53
60:b:136:HIS:HD2	61:c:111:TYR:CZ	2.16	0.53
62:e:136:LEU:HD22	66:k:104:LEU:HD22	1.89	0.53
64:o:748:PHE:O	64:o:752:VAL:HG13	2.09	0.53
64:o:776:TRP:O	64:o:780:VAL:HG23	2.08	0.53
65:h:139:GLN:HE22	66:k:37:LYS:CB	2.16	0.53
73:y:123:GLN:NE2	73:y:159:THR:O	2.42	0.53
4:DA:410:TRP:CD1	31:DF:306:PRO:HD3	2.43	0.53
7:HA:437:CYS:SG	7:HA:438:MET:N	2.81	0.53
10:DB:644:GLN:O	16:HC:413:LEU:CA	2.56	0.53
15:PB:410:ASN:O	15:PB:414:GLU:OE1	2.27	0.53
16:HC:348:ARG:HE	43:HF:65:ALA:HB1	1.65	0.53
25:DP:206:GLU:HB3	25:DP:207:PRO:HD3	1.91	0.53
29:DD:958:LYS:HD3	29:DD:961:GLN:OE1	2.08	0.53
38:DH:159:TYR:N	38:DH:159:TYR:CD1	2.75	0.53
39:HD:295:ARG:NE	45:HJ:165:ARG:HE	2.07	0.53
44:HI:239:ASP:C	44:HI:242:SER:H	2.17	0.53
44:HI:304:GLY:HA2	44:HI:307:LEU:HB2	1.90	0.53
48:g:75:LYS:NZ	59:z:562:GLY:HA3	2.24	0.53
48:g:124:ASN:HA	48:g:127:ARG:HB3	1.91	0.53
50:n:208:LEU:HD12	50:n:208:LEU:O	2.08	0.53
50:n:270:GLN:HG3	55:f:181:LEU:CD1	2.39	0.53
50:n:549:TYR:HB2	50:n:571:MET:HE2	1.90	0.53
58:q:168:THR:HG1	66:k:21:ILE:HD12	1.67	0.53
58:q:437:HIS:ND1	58:q:471:TYR:C	2.67	0.53
61:c:127:LEU:HB2	62:e:81:ILE:HD13	1.89	0.53
61:c:238:VAL:HG22	61:c:292:LEU:HD23	1.89	0.53
70:p:13:MET:HB2	70:p:405:PHE:CD1	2.44	0.53
71:w:161:LEU:HD22	71:w:164:ARG:HD2	1.91	0.53
26:DQ:327:GLU:HG3	29:DD:1010:ALA:O	2.08	0.53
31:DF:320:ARG:C	31:DF:322:ASP:H	2.17	0.53
39:HD:275:VAL:HG13	39:HD:276:ARG:HE	1.73	0.53
45:HJ:190:THR:HB	45:HJ:223:ARG:HH21	1.73	0.53
50:n:199:LEU:HD22	50:n:222:VAL:HG11	1.88	0.53
50:n:864:ASN:ND2	50:n:867:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:348:LEU:HD13	53:a:425:VAL:HG12	1.89	0.53
53:a:373:CYS:O	53:a:440:PHE:N	2.40	0.53
55:f:15:TRP:CH2	55:f:35:GLU:HB2	2.44	0.53
56:i:75:CYS:CB	56:i:88:ASN:HD21	2.22	0.53
58:q:188:LEU:HD21	66:k:6:LEU:CD1	2.39	0.53
66:k:71:THR:HA	66:k:74:ALA:HB3	1.90	0.53
77:NY:-149:DG:H2"	77:NY:-148:DG:C8	2.44	0.53
7:HA:373:ARG:O	7:HA:405:THR:OG1	2.24	0.53
29:DD:1063:LEU:HD13	35:DL:80:VAL:HG13	1.91	0.53
30:DE:747:LEU:HD22	30:DE:747:LEU:N	2.20	0.53
38:DH:50:PHE:HB2	33:DJ:195:LEU:CB	2.34	0.53
33:DJ:130:ILE:HG13	33:DJ:160:GLN:HE21	1.74	0.53
39:HD:288:THR:C	39:HD:290:SER:H	2.15	0.53
45:HJ:17:GLU:OE2	45:HJ:17:GLU:HA	2.08	0.53
49:j:82:LYS:CD	51:s:101:VAL:HG11	2.39	0.53
50:n:458:LEU:HD12	58:q:325:ILE:HG12	1.90	0.53
53:a:321:LEU:C	53:a:321:LEU:HD13	2.34	0.53
58:q:17:LYS:HE2	58:q:30:TYR:CD2	2.43	0.53
58:q:113:TYR:CA	65:h:19:VAL:HG11	2.39	0.53
66:k:9:GLU:CG	69:v:86:LEU:HG	2.20	0.53
70:p:677:THR:HG23	70:p:725:LEU:HB2	1.90	0.53
77:NY:-64:DG:H2"	77:NY:-63:DG:C8	2.44	0.53
9:PA:233:CYS:SG	9:PA:244:ARG:NH1	2.81	0.53
10:DB:937:THR:HG23	10:DB:939:ASN:H	1.74	0.53
15:PB:552:ASN:OD1	15:PB:553:LEU:N	2.42	0.53
17:PC:175:LYS:NZ	24:PL:57:ALA:O	2.42	0.53
18:PE:111:THR:HG23	18:PE:114:ALA:H	1.74	0.53
31:Df:283:MET:HG3	31:Df:329:LEU:HD11	1.90	0.53
31:DF:403:ILE:O	31:DF:406:VAL:HG22	2.08	0.53
42:HH:568:LEU:HD11	42:HH:606:PHE:HB3	1.91	0.53
44:HI:241:CYS:HB2	44:HI:246:TYR:CE1	2.43	0.53
47:PG:88:VAL:O	47:PG:99:THR:OG1	2.24	0.53
50:n:261:ASP:CB	58:q:250:ASP:OD2	2.57	0.53
50:n:449:SER:OG	50:n:450:GLU:N	2.41	0.53
50:n:923:CYS:SG	50:n:924:ILE:N	2.82	0.53
51:s:100:LYS:HE3	51:s:102:LYS:HB2	1.89	0.53
52:u:81:SER:HB3	52:u:86:GLN:HE21	1.74	0.53
58:q:123:LYS:HG2	58:q:124:PHE:CE2	2.43	0.53
58:q:577:ASP:HB2	58:q:597:PRO:HG3	1.90	0.53
69:v:61:MET:HE2	69:v:64:ARG:HH12	1.74	0.53
9:PA:459:ASN:OD1	9:PA:460:ARG:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:PA:1475:LEU:HD21	47:PG:18:PHE:CE2	2.44	0.53
9:PA:1475:LEU:N	47:PG:59:ILE:HG12	2.23	0.53
30:De:595:PRO:HD2	30:De:639:SER:HB3	1.91	0.53
32:Di:57:TYR:OH	35:Dl:122:ARG:NH1	2.41	0.53
30:DE:774:MET:HG3	31:DF:149:PRO:HG3	1.91	0.53
50:n:941:TYR:HE2	50:n:1172:SER:CB	2.06	0.53
53:a:375:PHE:CB	72:x:17:ARG:NH2	2.70	0.53
55:f:181:LEU:HD23	55:f:184:LEU:HD21	1.91	0.53
59:z:572:ASN:N	59:z:572:ASN:OD1	2.42	0.53
64:o:632:PRO:O	70:p:793:GLU:OE1	2.27	0.53
64:o:690:LEU:O	64:o:692:ASN:ND2	2.42	0.53
65:h:142:SER:C	66:k:39:LYS:HZ1	2.05	0.53
70:p:43:ASN:HD22	70:p:489:TRP:HB3	1.74	0.53
73:y:132:ARG:HH21	73:y:140:ARG:HD3	1.71	0.53
9:PA:1790:TYR:CG	65:h:83:PRO:HD3	2.44	0.53
44:HI:132:TRP:HA	44:HI:132:TRP:HE3	1.73	0.53
44:HI:272:ILE:O	44:HI:273:GLN:C	2.50	0.53
46:PD:76:ASN:OD1	65:h:47:ASP:CB	2.54	0.53
50:n:209:PRO:CG	50:n:293:TYR:CG	2.92	0.53
55:f:78:LEU:HD11	65:h:81:LEU:CD2	2.39	0.53
58:q:109:MET:HE3	58:q:109:MET:C	2.32	0.53
62:e:132:HIS:HD2	69:v:126:ASP:CG	2.16	0.53
73:y:73:THR:OG1	73:y:75:ASP:OD2	2.27	0.53
1:X:-6:DG:H1	2:Y:6:DC:N4	2.07	0.52
5:EA:142:ASN:O	5:EA:145:PHE:HB3	2.08	0.52
9:PA:521:VAL:HG13	9:PA:535:MET:HE1	1.90	0.52
10:DB:808:PRO:HA	10:DB:864:ASN:HB3	1.90	0.52
31:DF:14:LEU:HD23	32:DI:22:ILE:HD11	1.91	0.52
31:DF:76:LYS:HG3	31:DF:96:PHE:HB3	1.91	0.52
52:u:71:VAL:CG2	59:z:528:LEU:HD21	2.39	0.52
52:u:73:ILE:C	52:u:75:SER:N	2.61	0.52
61:c:204:MET:SD	61:c:208:PHE:C	2.92	0.52
64:o:759:ARG:O	64:o:762:GLN:HG3	2.08	0.52
71:w:16:GLU:OE2	71:w:19:GLU:N	2.40	0.52
71:w:522:PRO:HG3	71:w:565:GLU:HG2	1.90	0.52
71:w:681:GLU:OE2	71:w:685:ARG:NH1	2.41	0.52
72:x:175:ARG:HH21	72:x:221:LEU:HD22	1.74	0.52
7:HA:488:VAL:HG23	7:HA:488:VAL:O	2.09	0.52
15:PB:128:ILE:HG21	15:PB:431:LEU:HD21	1.91	0.52
15:PB:718:GLN:HG2	15:PB:720:PRO:HD2	1.90	0.52
27:DO:1:MET:CB	29:DD:997:ALA:HB2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Dd:963:ARG:NH2	29:Dd:964:GLU:OE2	2.42	0.52
30:DE:461:ILE:O	31:DF:135:TRP:HA	2.08	0.52
30:DE:653:LEU:HB2	30:DE:663:ARG:HB2	1.91	0.52
31:DF:406:VAL:HB	31:DF:417:ARG:HG2	1.91	0.52
42:HH:463:LYS:O	42:HH:484:ILE:HG23	2.10	0.52
49:j:79:LEU:HA	49:j:82:LYS:HG2	1.91	0.52
50:n:707:ASP:CB	64:o:684:ARG:NH2	2.72	0.52
50:n:879:LEU:HA	50:n:882:ILE:HG22	1.90	0.52
53:a:270:ILE:O	53:a:270:ILE:HG22	2.08	0.52
53:a:364:TYR:CD1	53:a:430:LEU:HB2	2.44	0.52
58:q:479:ILE:CG2	58:q:532:HIS:CG	2.90	0.52
71:w:958:ASN:N	71:w:958:ASN:OD1	2.40	0.52
5:EA:174:ARG:CG	39:HD:37:LEU:HD11	2.32	0.52
15:PB:752:TYR:CE2	15:PB:807:ARG:HG2	2.43	0.52
16:HC:32:ASP:OD1	16:HC:33:ARG:N	2.42	0.52
31:DF:274:ASN:H	31:DF:317:LEU:HB2	1.73	0.52
41:HG:54:ARG:NH2	41:HG:245:SER:O	2.43	0.52
41:HG:87:LEU:HD11	41:HG:229:LYS:HG2	1.91	0.52
50:n:254:VAL:HG11	50:n:304:GLN:HG2	1.91	0.52
50:n:921:MET:CE	50:n:1215:ILE:HD13	2.37	0.52
50:n:1219:HIS:HD2	50:n:1222:ARG:HH11	1.58	0.52
53:a:440:PHE:CD1	53:a:454:PHE:HB3	2.43	0.52
54:d:31:LEU:CG	56:i:103:THR:HG21	2.39	0.52
54:d:86:GLN:OE1	56:i:107:ILE:HA	2.09	0.52
59:z:560:TRP:CD1	59:z:561:PRO:HD2	2.43	0.52
62:e:125:LYS:NZ	63:l:153:ASN:OD1	2.43	0.52
63:l:44:ILE:O	63:l:48:THR:HG23	2.09	0.52
65:h:147:CYS:SG	65:h:148:SER:N	2.81	0.52
70:p:600:LYS:NZ	70:p:603:GLU:OE1	2.42	0.52
73:y:188:LEU:H	73:y:220:MET:HE2	1.74	0.52
7:HA:28:LEU:HD22	7:HA:55:LEU:HD23	1.91	0.52
16:HC:58:ARG:NH1	40:HE:229:TRP:CZ3	2.77	0.52
30:DE:304:LYS:NZ	30:DE:335:GLU:O	2.42	0.52
30:DE:432:LEU:HD21	30:DE:436:ASP:HB3	1.91	0.52
31:DF:273:GLN:H	31:DF:273:GLN:CD	2.17	0.52
31:DF:276:LEU:HD22	31:DF:323:VAL:HG21	1.92	0.52
52:u:122:LEU:HD23	54:d:111:GLN:HG2	1.91	0.52
53:a:335:THR:O	53:a:391:THR:HG22	2.07	0.52
60:b:96:ASP:OD2	70:p:670:PRO:HB2	2.10	0.52
66:k:77:GLN:HE21	67:r:192:GLN:HB2	1.75	0.52
10:DB:529:VAL:HG11	10:DB:560:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Df:320:ARG:NH1	31:Df:320:ARG:CB	2.73	0.52
31:DF:86:PHE:HA	33:DJ:212:LYS:HZ3	1.75	0.52
31:DF:335:ARG:HD2	31:DF:378:ALA:HB1	1.91	0.52
38:DH:50:PHE:HZ	33:DJ:170:ALA:CA	2.22	0.52
44:HI:140:PRO:O	44:HI:143:LEU:HD12	2.09	0.52
50:n:250:LEU:HD23	50:n:275:HIS:CB	2.36	0.52
50:n:362:ASP:O	50:n:363:GLU:C	2.52	0.52
53:a:375:PHE:HB3	72:x:17:ARG:CZ	2.38	0.52
59:z:540:LEU:C	59:z:540:LEU:HD22	2.34	0.52
64:o:707:ILE:HG23	64:o:720:PRO:CA	2.37	0.52
64:o:775:THR:HA	64:o:778:GLN:HG2	1.91	0.52
66:k:101:ARG:NH1	66:k:101:ARG:CB	2.72	0.52
72:x:472:ASN:ND2	72:x:496:SER:OG	2.42	0.52
4:DA:483:ASN:HA	4:DA:493:ARG:HH11	1.74	0.52
5:EA:142:ASN:ND2	47:PG:107:PHE:CB	2.73	0.52
7:HA:709:THR:HG22	7:HA:710:VAL:N	2.25	0.52
13:HB:136:VAL:HG11	13:HB:502:VAL:HG12	1.92	0.52
15:PB:794:VAL:O	15:PB:946:GLY:N	2.42	0.52
15:PB:939:HIS:NE2	15:PB:983:GLU:OE1	2.35	0.52
21:PI:69:ILE:HG22	21:PI:71:ASP:H	1.74	0.52
33:DJ:128:PRO:HB2	33:DJ:160:GLN:HE22	1.74	0.52
44:HI:143:LEU:O	44:HI:143:LEU:CD1	2.52	0.52
47:PG:52:ASP:N	47:PG:71:LYS:O	2.43	0.52
53:a:223:LYS:NZ	53:a:251:LEU:C	2.68	0.52
53:a:445:LEU:HD11	53:a:451:SER:HB3	1.90	0.52
58:q:99:ARG:CZ	58:q:103:ARG:HH22	2.23	0.52
58:q:223:GLU:HB2	58:q:246:GLN:HB3	1.90	0.52
59:z:560:TRP:HD1	59:z:561:PRO:HD2	1.75	0.52
60:b:89:ASP:OD2	64:o:636:HIS:HD2	1.93	0.52
68:t:8:GLN:NE2	68:t:200:ILE:HD13	2.24	0.52
4:DA:487:ASP:OD1	4:DA:487:ASP:N	2.42	0.52
6:FA:43:ASN:OD1	6:FA:44:GLN:N	2.43	0.52
9:PA:360:ASP:OD1	15:PB:1062:ARG:NE	2.42	0.52
11:EB:89:HIS:CE1	11:EB:139:PHE:CB	2.93	0.52
15:PB:1143:LYS:CE	47:PG:152:VAL:HG13	2.40	0.52
16:HC:266:ARG:HE	16:HC:277:LYS:HZ2	1.56	0.52
30:De:607:ARG:NH1	32:Di:87:PRO:O	2.43	0.52
30:DE:463:PHE:O	31:DF:133:ALA:CA	2.51	0.52
31:DF:312:ILE:HG13	31:DF:334:ALA:HB1	1.91	0.52
39:HD:83:ASN:CG	39:HD:140:LEU:HD12	2.34	0.52
42:HH:181:HIS:O	42:HH:184:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:HH:340:LEU:HD23	42:HH:491:ALA:HB2	1.91	0.52
50:n:651:ASN:HD22	71:w:22:PHE:H	1.58	0.52
52:u:80:GLU:HB3	59:z:539:ASP:OD2	2.09	0.52
58:q:311:LEU:HD21	58:q:427:LEU:HG	1.91	0.52
61:c:178:ILE:HG23	61:c:192:VAL:HG22	1.92	0.52
62:e:45:VAL:CG1	63:l:92:LEU:HD11	2.39	0.52
62:e:132:HIS:CD2	69:v:126:ASP:OD2	2.62	0.52
63:l:51:ILE:O	63:l:55:LEU:HG	2.09	0.52
64:o:725:VAL:HA	64:o:734:PRO:HB3	1.92	0.52
72:x:566:GLU:C	72:x:568:LYS:N	2.63	0.52
72:x:618:VAL:HG13	72:x:673:MET:HE1	1.92	0.52
1:X:-12:DG:H4'	12:FB:229:HIS:HA	1.91	0.52
4:DA:411:GLU:N	4:DA:411:GLU:OE2	2.41	0.52
30:De:646:SER:OG	30:De:647:ALA:N	2.41	0.52
29:DD:883:LEU:HD23	29:DD:891:ILE:HG12	1.92	0.52
44:HI:98:LEU:HD12	44:HI:98:LEU:O	2.10	0.52
50:n:160:VAL:HG22	50:n:166:TYR:HE1	1.75	0.52
50:n:861:LYS:HE3	61:c:30:ARG:CD	2.39	0.52
52:u:71:VAL:HG22	59:z:528:LEU:HD23	1.92	0.52
54:d:103:ARG:NH1	54:d:103:ARG:CG	2.73	0.52
58:q:186:GLU:OE2	58:q:291:TRP:NE1	2.43	0.52
59:z:582:LEU:HD23	59:z:591:LEU:HB3	1.91	0.52
65:h:82:SER:C	65:h:84:ASP:H	2.18	0.52
2:Y:25:DT:O3'	25:DP:196:ARG:NH1	2.43	0.52
3:BA:222:LEU:HD21	3:BA:277:ILE:HD13	1.92	0.52
5:EA:188:TYR:CE2	39:HD:14:TYR:CB	2.93	0.52
9:PA:1139:LEU:HD13	9:PA:1341:VAL:HA	1.91	0.52
10:DB:66:ASN:OD1	10:DB:187:ARG:NH1	2.43	0.52
13:HB:127:LEU:HD12	13:HB:467:ALA:HA	1.91	0.52
20:PH:91:VAL:HG22	20:PH:144:LEU:HD23	1.92	0.52
30:DE:562:SER:OG	30:DE:564:ASP:OD1	2.28	0.52
30:DE:676:THR:HG22	30:DE:685:ALA:HB3	1.92	0.52
30:DE:690:ASP:OD1	30:DE:690:ASP:N	2.43	0.52
31:DF:14:LEU:CD2	32:DI:22:ILE:HD12	2.40	0.52
31:DF:43:VAL:CG2	32:DI:43:ALA:HA	2.40	0.52
44:HI:17:PHE:CE2	50:n:68:VAL:CB	2.93	0.52
50:n:267:HIS:CD2	55:f:174:ARG:CD	2.58	0.52
52:u:90:LEU:CG	58:q:9:ILE:CG1	2.88	0.52
66:k:43:ARG:CB	66:k:43:ARG:NH1	2.73	0.52
72:x:439:LEU:HB3	72:x:495:ILE:HG21	1.92	0.52
77:NY:-63:DG:H2''	77:NY:-62:DG:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:PA:875:TYR:OH	19:PF:61:GLU:OE2	2.26	0.52
15:PB:625:LEU:HD13	15:PB:675:LEU:HD21	1.91	0.52
30:De:269:GLY:O	32:Di:97:ARG:NH2	2.43	0.52
29:DD:918:SER:HB3	35:DL:74:GLU:CD	2.34	0.52
29:DD:1071:ARG:HB2	31:DF:91:PHE:CE2	2.45	0.52
30:DE:324:LYS:HG2	30:DE:327:ASN:HD22	1.74	0.52
31:DF:15:PRO:HD3	32:DI:18:MET:CG	2.23	0.52
33:DJ:137:TYR:OH	33:DJ:141:ARG:NH2	2.43	0.52
44:HI:43:ILE:HG23	44:HI:43:ILE:O	2.09	0.52
45:HJ:192:ASP:C	45:HJ:192:ASP:OD1	2.53	0.52
48:g:158:GLU:OE2	48:g:158:GLU:HA	2.10	0.52
50:n:261:ASP:CB	58:q:250:ASP:CG	2.76	0.52
50:n:270:GLN:CG	55:f:181:LEU:CD1	2.87	0.52
50:n:321:GLY:HA3	58:q:317:GLN:NE2	2.24	0.52
53:a:321:LEU:HD21	53:a:407:ILE:CD1	2.35	0.52
54:d:64:GLN:HE21	54:d:68:LEU:CD1	2.23	0.52
58:q:441:ARG:CZ	63:l:168:TRP:CE3	2.90	0.52
68:t:131:MET:SD	68:t:132:GLY:N	2.83	0.52
69:v:86:LEU:HD12	69:v:86:LEU:O	2.10	0.52
69:v:110:GLU:OE1	69:v:110:GLU:HA	2.09	0.52
72:x:565:SER:O	72:x:566:GLU:C	2.53	0.52
72:x:628:VAL:HG13	72:x:636:ARG:HG2	1.91	0.52
74:NG:1041:THR:O	74:NG:1042:SER:C	2.54	0.52
9:PA:1284:PHE:CE2	9:PA:1288:ILE:HD11	2.46	0.51
10:DB:152:LEU:HD23	10:DB:155:PRO:HB3	1.91	0.51
13:HB:412:GLU:N	13:HB:412:GLU:OE1	2.44	0.51
31:Df:447:ALA:O	31:Df:453:GLY:HA2	2.09	0.51
38:DH:60:THR:CG2	33:DJ:211:VAL:HG23	2.34	0.51
44:HI:283:ARG:CZ	44:HI:283:ARG:HB2	2.41	0.51
45:HJ:252:MET:O	45:HJ:256:ARG:HG2	2.10	0.51
53:a:493:PHE:CE2	53:a:514:LYS:HB2	2.45	0.51
56:i:65:PHE:HE1	56:i:99:LYS:CB	2.23	0.51
58:q:523:ASP:HB3	58:q:563:ILE:HD12	1.92	0.51
71:w:86:ALA:HB1	71:w:92:LEU:HD13	1.92	0.51
72:x:566:GLU:O	72:x:568:LYS:N	2.44	0.51
4:DA:470:ILE:HG23	31:DF:214:HIS:HA	1.92	0.51
4:DA:639:LEU:HD11	4:DA:774:ARG:HG2	1.92	0.51
4:DA:1065:GLU:O	4:DA:1069:ILE:HG12	2.10	0.51
7:HA:115:LEU:HD13	7:HA:191:PRO:HB2	1.92	0.51
10:DB:983:ARG:HG3	10:DB:983:ARG:HH11	1.76	0.51
15:PB:528:LEU:HD21	15:PB:767:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:HC:397:GLU:CD	43:HF:61:MET:HE3	2.36	0.51
31:DF:241:GLU:OE1	38:DH:135:THR:OG1	2.27	0.51
50:n:845:SER:OG	50:n:846:ASN:N	2.43	0.51
53:a:60:SER:O	53:a:63:GLU:HG2	2.11	0.51
56:i:109:LEU:CD2	56:i:117:GLN:NE2	2.73	0.51
58:q:490:SER:OG	58:q:539:GLN:NE2	2.40	0.51
60:b:62:MET:HA	60:b:62:MET:CE	2.34	0.51
60:b:67:LEU:HD22	60:b:116:LEU:HD12	1.91	0.51
66:k:14:LEU:N	66:k:14:LEU:HD23	2.25	0.51
69:v:130:LEU:N	69:v:130:LEU:CD2	2.73	0.51
77:NY:-12:DG:H2'	77:NY:-11:DG:C8	2.45	0.51
5:EA:103:VAL:O	5:EA:107:LEU:HG	2.10	0.51
5:EA:143:GLN:HE21	47:PG:158:PHE:HE1	1.53	0.51
7:HA:393:ASP:OD1	7:HA:394:PHE:N	2.42	0.51
9:PA:1382:LEU:HD23	9:PA:1398:LEU:HD13	1.93	0.51
10:DB:202:TRP:HB2	10:DB:238:LEU:HB3	1.92	0.51
10:DB:537:PHE:CE2	10:DB:539:ARG:HB2	2.45	0.51
10:DB:656:GLU:HG2	10:DB:661:ALA:HB3	1.93	0.51
11:EB:82:VAL:HG12	11:EB:86:LYS:HZ2	1.73	0.51
16:HC:338:PHE:N	16:HC:341:MET:O	2.44	0.51
23:PK:63:VAL:HG23	23:PK:63:VAL:O	2.10	0.51
29:Dd:916:LYS:NZ	29:Dd:1070:GLU:OE2	2.42	0.51
41:HG:88:LEU:HD23	41:HG:131:LEU:HD21	1.91	0.51
44:HI:213:LEU:HD22	44:HI:225:ILE:HG12	1.92	0.51
45:HJ:100:HIS:CG	45:HJ:101:PRO:HD2	2.46	0.51
46:PD:70:ARG:HE	69:v:20:LYS:HE3	1.75	0.51
52:u:71:VAL:HG13	59:z:529:HIS:CB	2.35	0.51
55:f:101:ILE:HD13	65:h:105:VAL:HB	1.92	0.51
60:b:181:CYS:SG	63:l:82:LEU:HD22	2.50	0.51
61:c:200:VAL:HG13	61:c:214:VAL:HG12	1.91	0.51
66:k:109:ARG:CG	66:k:109:ARG:NH1	2.73	0.51
69:v:133:GLU:OE1	69:v:133:GLU:HA	2.10	0.51
70:p:91:GLN:NE2	70:p:137:LEU:O	2.43	0.51
70:p:398:SER:OG	70:p:400:GLN:NE2	2.43	0.51
70:p:683:GLN:HE22	70:p:723:GLN:HB3	1.75	0.51
71:w:767:TRP:HE1	71:w:804:ASN:HD21	1.58	0.51
72:x:86:ASP:O	72:x:88:PHE:N	2.43	0.51
9:PA:95:PHE:N	9:PA:311:GLN:OE1	2.43	0.51
10:DB:90:THR:O	10:DB:968:ARG:NH2	2.43	0.51
30:De:423:PRO:HG2	30:De:426:ARG:HB2	1.91	0.51
30:De:747:LEU:H	30:De:747:LEU:CD2	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DJ:139:LEU:HB3	33:DJ:144:PHE:HB3	1.93	0.51
35:DL:60:LYS:HE3	35:DL:60:LYS:H	1.74	0.51
35:DL:111:LEU:HA	35:DL:114:LYS:CE	2.36	0.51
45:HJ:73:PRO:HB2	45:HJ:118:PHE:HZ	1.75	0.51
50:n:327:GLU:HG3	50:n:356:LYS:HG2	1.91	0.51
52:u:49:ASN:N	52:u:50:PRO:HD2	2.26	0.51
52:u:108:VAL:HG22	54:d:128:ALA:CB	2.40	0.51
53:a:449:ARG:NH1	72:x:54:PRO:HB2	2.25	0.51
54:d:42:ARG:HH22	56:i:93:LYS:HG2	1.71	0.51
54:d:42:ARG:CZ	56:i:93:LYS:HG2	2.41	0.51
58:q:166:ARG:CB	58:q:166:ARG:NH1	2.73	0.51
70:p:304:SER:OG	70:p:349:ASP:O	2.28	0.51
70:p:437:SER:OG	70:p:438:TRP:N	2.43	0.51
70:p:801:CYS:SG	70:p:802:GLY:N	2.83	0.51
71:w:1118:SER:OG	71:w:1119:GLY:N	2.44	0.51
5:EA:49:LEU:HD22	5:EA:56:ARG:HD3	1.93	0.51
5:EA:111:ARG:HD3	39:HD:11:THR:OG1	2.10	0.51
10:DB:781:TYR:O	38:DH:176:ARG:NH2	2.44	0.51
29:Dd:943:GLN:NE2	30:De:509:GLN:O	2.41	0.51
31:DF:122:LEU:HD23	38:DH:36:THR:HG23	1.92	0.51
31:DF:243:LEU:HD21	31:DF:284:ARG:HB3	1.92	0.51
37:DG:181:TRP:CE3	37:DG:181:TRP:O	2.63	0.51
35:DL:78:GLU:O	35:DL:82:GLU:HG3	2.11	0.51
39:HD:27:GLY:HA3	39:HD:70:LYS:CD	2.35	0.51
44:HI:179:ARG:HH21	44:HI:184:LEU:HA	1.74	0.51
58:q:576:GLY:O	58:q:619:ARG:NH2	2.43	0.51
66:k:29:GLY:O	66:k:33:LEU:CG	2.42	0.51
66:k:38:GLU:HG3	66:k:38:GLU:O	2.10	0.51
70:p:471:LEU:HD22	70:p:499:MET:HE3	1.93	0.51
7:HA:126:PHE:CE2	7:HA:128:LYS:HB2	2.46	0.51
11:EB:193:ASN:OD1	11:EB:194:ARG:N	2.43	0.51
36:Dm:28:ARG:HH21	36:Dm:31:LEU:HD21	1.75	0.51
35:DL:111:LEU:O	35:DL:114:LYS:CE	2.59	0.51
44:HI:111:PRO:HA	44:HI:114:ILE:HB	1.93	0.51
44:HI:232:PRO:HB2	44:HI:240:MET:SD	2.51	0.51
46:PD:70:ARG:NE	69:v:20:LYS:HE3	2.26	0.51
48:g:153:PHE:CZ	54:d:125:VAL:HG12	2.46	0.51
50:n:446:CYS:SG	50:n:447:GLY:N	2.84	0.51
58:q:479:ILE:HG22	58:q:532:HIS:NE2	2.19	0.51
58:q:491:ILE:HD12	58:q:532:HIS:N	2.25	0.51
58:q:645:ALA:O	63:l:111:VAL:CG2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:l:36:ILE:O	63:l:39:GLU:HG2	2.11	0.51
64:o:682:VAL:HG22	64:o:691:VAL:HG11	1.93	0.51
69:v:16:GLN:O	69:v:20:LYS:HG2	2.11	0.51
3:BA:107:MET:O	3:BA:112:ARG:NH2	2.43	0.51
9:PA:863:ARG:NH2	9:PA:1415:THR:OG1	2.44	0.51
30:De:500:THR:HG22	30:De:502:LYS:H	1.76	0.51
30:De:747:LEU:O	30:De:747:LEU:HG	2.10	0.51
29:DD:1071:ARG:HG3	31:DF:91:PHE:CE1	2.46	0.51
32:DI:131:SER:OG	33:DJ:150:ARG:NH1	2.44	0.51
40:HE:44:LEU:HD22	40:HE:227:LEU:HB3	1.90	0.51
42:HH:274:GLN:OE1	42:HH:459:GLN:NE2	2.44	0.51
42:HH:363:VAL:HG21	42:HH:378:PHE:HE2	1.75	0.51
45:HJ:228:MET:O	45:HJ:229:GLU:C	2.54	0.51
48:g:75:LYS:CD	52:u:78:SER:HA	2.40	0.51
48:g:124:ASN:O	48:g:127:ARG:HB3	2.11	0.51
49:j:85:LEU:HD13	51:s:93:TYR:HA	1.92	0.51
54:d:44:LEU:CD2	54:d:48:LEU:HD11	2.40	0.51
56:i:66:LEU:HD13	56:i:66:LEU:C	2.35	0.51
56:i:66:LEU:N	56:i:67:PRO:HD2	2.25	0.51
58:q:140:ASN:N	58:q:141:PRO:HD2	2.24	0.51
58:q:188:LEU:CD1	69:v:87:ILE:HG13	2.40	0.51
63:l:166:LEU:HD22	69:v:123:ILE:CD1	2.41	0.51
66:k:75:THR:C	66:k:77:GLN:H	2.19	0.51
68:t:3:VAL:HG22	68:t:150:ALA:HB2	1.93	0.51
9:PA:904:GLN:NE2	9:PA:981:CYS:O	2.42	0.51
10:DB:217:ASN:ND2	10:DB:320:ALA:O	2.35	0.51
13:HB:471:LEU:HD13	13:HB:475:PHE:HE2	1.75	0.51
15:PB:905:ASP:N	15:PB:922:ARG:O	2.42	0.51
32:Di:73:LEU:CB	35:DI:105:HIS:CE1	2.94	0.51
29:DD:873:LEU:N	29:DD:873:LEU:CD1	2.73	0.51
42:HH:377:GLN:OE1	42:HH:381:TRP:NE1	2.40	0.51
44:HI:15:LEU:HD23	44:HI:15:LEU:C	2.36	0.51
48:g:157:LEU:HD23	48:g:157:LEU:C	2.36	0.51
49:j:61:ILE:O	50:n:50:ARG:N	2.43	0.51
52:u:71:VAL:CG2	59:z:528:LEU:CD2	2.89	0.51
53:a:340:TYR:O	53:a:344:THR:HG23	2.11	0.51
53:a:465:VAL:HG21	53:a:511:ILE:CD1	2.41	0.51
55:f:36:ARG:HA	55:f:41:TYR:HE1	1.76	0.51
66:k:41:ASN:O	66:k:45:LEU:CB	2.59	0.51
68:t:78:LEU:HD22	68:t:78:LEU:H	1.74	0.51
5:EA:137:THR:CG2	5:EA:139:LEU:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FA:162:GLU:OE1	6:FA:162:GLU:N	2.43	0.51
7:HA:3:LEU:O	7:HA:9:LEU:HD12	2.11	0.51
15:PB:809:VAL:HG11	15:PB:811:TYR:CE2	2.46	0.51
17:PC:51:GLN:NE2	24:PL:52:LEU:HD13	2.26	0.51
28:Dc:21:LEU:HD12	28:Dc:21:LEU:O	2.11	0.51
29:DD:922:GLN:HG2	29:DD:1056:THR:OG1	2.11	0.51
30:DE:324:LYS:O	30:DE:327:ASN:ND2	2.44	0.51
30:DE:423:PRO:HG2	30:DE:426:ARG:HB2	1.92	0.51
38:DH:44:LEU:HD23	38:DH:47:GLU:OE2	2.10	0.51
44:HI:22:GLN:CD	44:HI:22:GLN:N	2.69	0.51
50:n:643:HIS:CD2	58:q:560:ILE:HA	2.45	0.51
50:n:907:LEU:HD21	60:b:118:LEU:HA	1.93	0.51
51:s:102:LYS:O	51:s:103:GLU:C	2.53	0.51
52:u:67:LYS:HE2	59:z:528:LEU:CD1	2.41	0.51
52:u:122:LEU:CD2	54:d:111:GLN:HG2	2.39	0.51
53:a:107:MET:HE2	53:a:107:MET:C	2.35	0.51
54:d:45:ILE:HD13	56:i:73:ILE:CA	2.38	0.51
55:f:29:VAL:HG11	55:f:79:PHE:HB3	1.92	0.51
55:f:169:SER:OG	55:f:170:SER:N	2.44	0.51
58:q:561:GLU:OE2	58:q:588:SER:OG	2.28	0.51
62:e:77:VAL:HA	62:e:80:CYS:SG	2.51	0.51
71:w:633:VAL:O	71:w:817:ARG:NH2	2.43	0.51
74:NG:1119:GLY:C	74:NG:1121:LYS:N	2.57	0.51
4:DA:828:GLU:HA	4:DA:831:LYS:HB2	1.92	0.51
5:EA:170:LYS:O	5:EA:174:ARG:HD3	2.10	0.51
5:EA:180:PHE:HA	11:EB:216:PHE:CZ	2.46	0.51
16:HC:408:LEU:HD21	43:HF:36:GLN:OE1	2.11	0.51
38:DH:32:ALA:O	38:DH:36:THR:OG1	2.29	0.51
39:HD:129:ASN:O	39:HD:130:LYS:C	2.54	0.51
48:g:129:HIS:CB	52:u:82:THR:HG22	2.41	0.51
48:g:129:HIS:O	48:g:133:GLU:N	2.38	0.51
50:n:203:LEU:HD13	50:n:215:LEU:HD11	1.88	0.51
50:n:915:ARG:NE	50:n:923:CYS:SG	2.85	0.51
50:n:960:LYS:CB	50:n:1210:PHE:CZ	2.86	0.51
52:u:80:GLU:HA	59:z:539:ASP:CG	2.36	0.51
54:d:90:HIS:C	54:d:90:HIS:CD2	2.89	0.51
58:q:113:TYR:HE2	65:h:20:ALA:HB2	1.76	0.51
65:h:143:LEU:HD21	66:k:34:GLU:O	2.11	0.51
4:DA:1163:ARG:HB3	37:DG:183:ILE:HG22	1.91	0.50
30:DE:601:VAL:HG21	30:DE:642:VAL:HG11	1.92	0.50
30:DE:754:THR:OG1	30:DE:755:ALA:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:279:LEU:HD22	31:DF:330:ARG:NH2	2.26	0.50
31:DF:323:VAL:HG23	31:DF:326:HIS:CD2	2.45	0.50
32:DI:60:HIS:CE1	35:DL:102:LEU:HB3	2.46	0.50
44:HI:49:SER:HB2	44:HI:52:LYS:HD2	1.92	0.50
45:HJ:165:ARG:HB3	45:HJ:166:PRO:HD3	1.92	0.50
45:HJ:212:ILE:HA	45:HJ:255:MET:HE1	1.93	0.50
50:n:935:ALA:HB1	50:n:1174:PRO:HB2	1.91	0.50
52:u:5:LEU:HD11	59:z:596:TYR:CZ	2.45	0.50
53:a:373:CYS:HB3	53:a:439:GLN:HG2	1.92	0.50
53:a:441:GLU:HB2	72:x:17:ARG:NH2	2.10	0.50
57:m:64:ALA:HA	57:m:67:LEU:HD12	1.92	0.50
60:b:84:GLN:OE1	60:b:94:SER:HB3	2.11	0.50
60:b:186:THR:HG21	62:e:49:GLU:CG	2.41	0.50
64:o:718:VAL:HG13	64:o:742:GLN:OE1	2.10	0.50
70:p:790:CYS:SG	70:p:839:SER:OG	2.68	0.50
71:w:571:LEU:HB2	71:w:612:MET:HE1	1.93	0.50
77:NY:-147:DG:H2''	77:NY:-146:DG:C8	2.46	0.50
77:NY:-125:DG:H2''	77:NY:-124:DG:C8	2.47	0.50
4:DA:481:GLU:HA	4:DA:484:ILE:HD12	1.93	0.50
30:DE:463:PHE:N	31:DF:134:HIS:O	2.45	0.50
30:DE:506:SER:HB2	30:DE:575:PHE:HD2	1.76	0.50
41:HG:204:GLU:OE1	41:HG:209:THR:OG1	2.28	0.50
42:HH:369:VAL:HG11	42:HH:615:PHE:HA	1.93	0.50
52:u:104:LEU:O	52:u:108:VAL:HG23	2.10	0.50
53:a:94:LEU:O	53:a:94:LEU:HG	2.10	0.50
54:d:34:LEU:HD22	56:i:99:LYS:CD	2.31	0.50
58:q:113:TYR:HA	65:h:19:VAL:HG11	1.93	0.50
60:b:96:ASP:CB	70:p:670:PRO:HG2	2.41	0.50
66:k:96:ARG:CD	69:v:116:LEU:HD12	2.42	0.50
66:k:109:ARG:CB	66:k:109:ARG:NH1	2.74	0.50
67:r:206:ARG:HE	67:r:206:ARG:C	2.18	0.50
5:EA:152:PHE:O	5:EA:153:ARG:HB2	2.10	0.50
7:HA:284:GLU:HA	7:HA:287:ARG:HG2	1.93	0.50
7:HA:637:LEU:HD13	7:HA:651:PHE:CD2	2.47	0.50
23:PK:105:PHE:CE2	23:PK:109:ILE:HD11	2.45	0.50
27:DO:57:ASN:OD1	27:DO:58:PHE:N	2.44	0.50
44:HI:151:LEU:C	44:HI:151:LEU:HD23	2.36	0.50
44:HI:261:PHE:CZ	44:HI:272:ILE:HD12	2.46	0.50
45:HJ:25:ASP:OD1	45:HJ:26:ALA:N	2.45	0.50
48:g:164:ILE:CD1	56:i:140:MET:HG2	2.37	0.50
50:n:466:MET:HG3	58:q:321:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:417:TYR:HB2	53:a:469:VAL:HG11	1.93	0.50
58:q:437:HIS:C	58:q:437:HIS:CD2	2.86	0.50
65:h:182:VAL:CG2	67:r:202:ILE:HD11	2.32	0.50
71:w:418:GLN:HA	71:w:421:HIS:HD2	1.75	0.50
71:w:872:ARG:HB3	71:w:874:HIS:HD2	1.76	0.50
4:DA:396:LEU:N	4:DA:396:LEU:HD22	2.27	0.50
7:HA:377:GLU:N	7:HA:377:GLU:OE1	2.44	0.50
9:PA:1643:TYR:CB	57:m:96:PHE:CD2	2.92	0.50
10:DB:818:THR:OG1	10:DB:819:LEU:N	2.44	0.50
15:PB:834:ARG:HG2	15:PB:840:MET:HE2	1.93	0.50
16:HC:390:GLN:HE21	16:HC:394:TRP:NE1	2.09	0.50
30:DE:299:ASP:OD2	30:DE:607:ARG:NH2	2.38	0.50
30:DE:461:ILE:O	31:DF:135:TRP:HE3	1.94	0.50
38:DH:54:GLU:OE1	33:DJ:197:MET:HB2	2.12	0.50
50:n:226:VAL:HG22	50:n:229:GLU:H	1.75	0.50
50:n:234:LEU:HD23	50:n:247:LEU:HA	1.92	0.50
60:b:132:ASP:C	60:b:132:ASP:OD1	2.54	0.50
64:o:688:LYS:HG2	64:o:712:ASP:HB3	1.93	0.50
66:k:44:LEU:HD22	66:k:47:ARG:HH12	1.76	0.50
68:t:98:LEU:O	68:t:101:PHE:N	2.43	0.50
71:w:366:ILE:HG23	71:w:369:ARG:HD3	1.93	0.50
71:w:378:GLN:HE22	71:w:532:THR:HA	1.75	0.50
1:X:-6:DG:H1	2:Y:6:DC:H42	1.59	0.50
10:DB:274:LEU:HG	10:DB:278:LYS:HE2	1.92	0.50
13:HB:481:VAL:HG23	13:HB:483:THR:HG23	1.94	0.50
15:PB:907:VAL:HG22	15:PB:921:ILE:HG12	1.94	0.50
16:HC:410:ASN:HB2	43:HF:3:ASN:OD1	2.11	0.50
17:PC:67:ARG:NH2	22:PJ:2:ILE:HG23	2.27	0.50
31:Df:347:THR:HG22	31:DF:299:LYS:HD3	1.91	0.50
36:Dm:69:THR:HG23	36:Dm:80:ARG:HE	1.77	0.50
31:DF:320:ARG:HB2	31:DF:415:ILE:HD12	1.94	0.50
39:HD:125:TYR:O	39:HD:129:ASN:HB2	2.11	0.50
44:HI:83:HIS:HD2	44:HI:84:LYS:HG2	1.77	0.50
44:HI:229:LEU:HD11	44:HI:276:PHE:HB3	1.92	0.50
45:HJ:184:PRO:CB	45:HJ:187:LEU:HD12	2.33	0.50
48:g:172:PRO:HA	48:g:175:LEU:CG	2.42	0.50
50:n:153:ALA:HB3	54:d:152:ALA:HB1	1.93	0.50
50:n:203:LEU:HD21	50:n:224:PHE:CZ	2.46	0.50
54:d:115:LYS:CA	54:d:115:LYS:CE	2.86	0.50
56:i:121:LEU:O	56:i:125:VAL:HG23	2.11	0.50
60:b:186:THR:HG21	62:e:49:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:h:102:HIS:H	65:h:102:HIS:HD2	1.58	0.50
68:t:144:TYR:CD2	68:t:147:CYS:HB2	2.36	0.50
70:p:822:ARG:NH1	73:y:107:GLY:O	2.38	0.50
11:EB:88:ARG:NH2	11:EB:93:ASP:OD2	2.45	0.50
31:Df:24:GLU:HG2	35:DI:145:THR:HG21	1.93	0.50
50:n:201:HIS:ND1	54:d:111:GLN:NE2	2.60	0.50
50:n:261:ASP:HB2	58:q:250:ASP:OD2	2.12	0.50
50:n:274:ILE:HG13	55:f:181:LEU:HD22	1.93	0.50
53:a:461:SER:CA	72:x:7:LYS:HD3	2.42	0.50
60:b:162:ALA:HA	60:b:165:LYS:HD3	1.94	0.50
60:b:179:LEU:HD12	62:e:60:VAL:C	2.37	0.50
60:b:186:THR:CG2	62:e:49:GLU:OE1	2.60	0.50
61:c:124:ALA:HA	62:e:81:ILE:HD11	1.94	0.50
70:p:560:LEU:HD12	70:p:658:LEU:HD22	1.93	0.50
70:p:587:ILE:HD13	70:p:598:ASN:HD22	1.77	0.50
7:HA:284:GLU:HG2	7:HA:385:THR:HG21	1.93	0.50
9:PA:1016:LEU:O	9:PA:1020:LEU:HG	2.10	0.50
11:EB:124:LEU:HD13	11:EB:137:TYR:CD1	2.47	0.50
35:DI:102:LEU:HB2	35:DI:115:ASP:HB2	1.94	0.50
31:DF:22:VAL:CG1	32:DI:44:PHE:CE1	2.94	0.50
39:HD:284:ALA:HB1	44:HI:243:LEU:HD22	1.94	0.50
42:HH:363:VAL:HG21	42:HH:378:PHE:CE2	2.47	0.50
45:HJ:46:VAL:HG22	45:HJ:279:ARG:HH12	1.76	0.50
47:PG:97:LEU:HD21	47:PG:128:TYR:CE1	2.46	0.50
53:a:445:LEU:CA	72:x:55:SER:CB	2.86	0.50
55:f:123:VAL:HB	69:v:55:GLU:OE1	2.12	0.50
55:f:137:CYS:CB	65:h:42:TRP:HB2	2.41	0.50
58:q:451:LEU:CD1	58:q:529:MET:SD	2.84	0.50
71:w:1193:PHE:C	71:w:1195:ALA:H	2.19	0.50
71:w:1200:TYR:CD2	71:w:1200:TYR:O	2.64	0.50
5:EA:20:TYR:HB3	5:EA:190:LEU:HD13	1.94	0.50
30:DE:449:LYS:O	38:DH:145:HIS:HB3	2.11	0.50
38:DH:117:MET:HB2	33:DJ:129:THR:HG23	1.94	0.50
39:HD:295:ARG:O	39:HD:295:ARG:HD2	2.12	0.50
44:HI:192:VAL:O	44:HI:192:VAL:HG12	2.12	0.50
44:HI:261:PHE:HB2	55:f:52:MET:CE	2.40	0.50
48:g:127:ARG:CD	50:n:152:PHE:HB2	2.39	0.50
52:u:115:LEU:CD1	54:d:121:LEU:CD1	2.88	0.50
56:i:118:LEU:HD23	56:i:118:LEU:O	2.11	0.50
58:q:95:TRP:N	58:q:95:TRP:CD1	2.79	0.50
58:q:488:CYS:SG	58:q:536:ALA:HA	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:k:41:ASN:O	66:k:45:LEU:HB2	2.10	0.50
5:EA:17:LEU:HD13	5:EA:194:THR:OG1	2.12	0.50
9:PA:485:ASN:O	9:PA:488:VAL:HG22	2.10	0.50
16:HC:402:ARG:NH1	43:HF:11:GLU:OE2	2.43	0.50
30:DE:462:CYS:SG	31:DF:133:ALA:HB1	2.52	0.50
31:DF:106:PHE:HA	33:DJ:217:PHE:HB3	1.94	0.50
37:DG:94:MET:HE3	37:DG:96:VAL:HG22	1.94	0.50
50:n:707:ASP:HA	64:o:684:ARG:NH2	2.27	0.50
53:a:127:HIS:HE1	53:a:171:THR:HG22	1.73	0.50
55:f:15:TRP:HH2	55:f:35:GLU:HB2	1.77	0.50
58:q:149:LYS:HD2	69:v:40:ALA:CA	2.41	0.50
61:c:200:VAL:HA	61:c:214:VAL:HA	1.93	0.50
66:k:77:GLN:CG	67:r:192:GLN:HG2	2.40	0.50
68:t:138:ILE:O	68:t:138:ILE:HG22	2.11	0.50
71:w:261:ASP:OD1	71:w:261:ASP:N	2.38	0.50
71:w:1187:PRO:HA	71:w:1190:LEU:HB3	1.94	0.50
5:EA:114:ILE:CG2	5:EA:177:LEU:HD22	2.42	0.49
10:DB:983:ARG:HG3	10:DB:983:ARG:NH1	2.26	0.49
15:PB:296:GLU:OE2	21:PI:103:ARG:NH2	2.45	0.49
15:PB:738:THR:HG21	22:PJ:58:LYS:HG3	1.93	0.49
30:De:586:TYR:HB3	30:De:605:HIS:HB3	1.94	0.49
30:De:650:THR:HG22	30:De:666:THR:HG22	1.93	0.49
38:DH:110:TYR:CZ	38:DH:113:ARG:NH1	2.79	0.49
41:HG:285:THR:O	41:HG:297:LYS:NZ	2.45	0.49
49:j:78:GLN:O	49:j:82:LYS:HG2	2.12	0.49
52:u:74:ASP:O	59:z:532:VAL:HG21	2.11	0.49
53:a:467:MET:HB3	53:a:475:VAL:CG1	2.41	0.49
5:EA:143:GLN:CG	47:PG:158:PHE:HE1	2.17	0.49
10:DB:559:LYS:HZ3	10:DB:559:LYS:HB2	1.78	0.49
15:PB:830:GLU:OE2	15:PB:870:THR:OG1	2.21	0.49
31:Df:97:ALA:HB2	31:Df:106:PHE:HE1	1.78	0.49
45:HJ:268:GLU:OE1	45:HJ:268:GLU:N	2.29	0.49
50:n:274:ILE:HD11	55:f:181:LEU:HD21	1.93	0.49
50:n:529:PRO:HB2	50:n:588:LEU:HD22	1.94	0.49
50:n:776:LEU:O	50:n:780:VAL:HG13	2.13	0.49
53:a:62:LEU:HD21	54:d:62:GLU:HB2	1.93	0.49
53:a:160:LEU:HD12	53:a:214:ARG:NH2	2.26	0.49
53:a:197:ALA:HB1	53:a:201:ASP:HB2	1.94	0.49
53:a:377:ASN:CB	53:a:442:VAL:O	2.55	0.49
53:a:443:CYS:SG	72:x:57:ASN:CB	3.00	0.49
57:m:107:HIS:O	57:m:111:LYS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:b:175:HIS:CB	61:c:113:TRP:CZ2	2.92	0.49
61:c:41:ASN:HB3	70:p:840:TYR:HA	1.93	0.49
62:e:108:GLU:O	62:e:112:LYS:HG3	2.12	0.49
66:k:16:ASP:OD2	69:v:79:VAL:HG22	2.11	0.49
71:w:726:ASN:ND2	71:w:726:ASN:N	2.60	0.49
72:x:566:GLU:H	72:x:566:GLU:CD	2.20	0.49
5:EA:43:VAL:HB	5:EA:48:MET:HE3	1.94	0.49
7:HA:118:HIS:HB3	7:HA:121:VAL:HG22	1.94	0.49
11:EB:131:GLU:N	11:EB:138:ALA:O	2.42	0.49
28:Dc:1:MET:HG3	31:Df:126:PRO:HB3	1.94	0.49
38:DH:27:ASP:OD1	38:DH:27:ASP:N	2.45	0.49
50:n:169:LEU:CB	50:n:170:PRO:HD3	2.26	0.49
54:d:115:LYS:CD	54:d:115:LYS:C	2.86	0.49
58:q:188:LEU:CD2	69:v:87:ILE:HG13	2.38	0.49
70:p:511:TYR:HB2	70:p:526:ILE:HD13	1.94	0.49
73:y:147:ASN:O	73:y:186:ARG:NH2	2.45	0.49
74:NG:1040:THR:O	74:NC:841:THR:HA	2.11	0.49
4:DA:927:VAL:O	4:DA:933:ASN:ND2	2.45	0.49
5:EA:185:GLU:HB2	39:HD:14:TYR:OH	2.13	0.49
9:PA:1382:LEU:HD23	9:PA:1398:LEU:CD1	2.42	0.49
28:Dc:77:LEU:O	28:Dc:77:LEU:HD23	2.11	0.49
30:DE:693:VAL:HB	30:DE:707:LEU:HB2	1.94	0.49
35:DL:111:LEU:CA	35:DL:114:LYS:CE	2.90	0.49
44:HI:279:ASN:O	44:HI:282:ALA:N	2.45	0.49
50:n:870:GLN:CG	64:o:655:THR:CG2	2.90	0.49
53:a:460:ASP:HB3	72:x:7:LYS:HB2	1.93	0.49
58:q:523:ASP:CB	58:q:563:ILE:HD12	2.41	0.49
58:q:644:SER:CA	58:q:647:SER:OG	2.58	0.49
60:b:96:ASP:HB2	70:p:670:PRO:HG2	1.94	0.49
65:h:12:LEU:C	65:h:12:LEU:CD1	2.85	0.49
65:h:110:ARG:C	65:h:110:ARG:CD	2.85	0.49
67:r:112:GLU:C	67:r:114:LEU:H	2.20	0.49
68:t:128:THR:O	68:t:128:THR:OG1	2.27	0.49
70:p:482:MET:HG2	70:p:522:LEU:HD13	1.93	0.49
1:X:24:DA:H61	2:Y:-24:DT:H3	1.58	0.49
5:EA:191:LEU:O	5:EA:195:GLU:OE1	2.30	0.49
7:HA:243:CYS:SG	7:HA:443:ALA:HB3	2.53	0.49
11:EB:181:ALA:O	11:EB:185:LEU:HD23	2.13	0.49
15:PB:404:PHE:HA	15:PB:407:MET:HE3	1.94	0.49
15:PB:962:THR:O	22:PJ:9:THR:HG23	2.12	0.49
30:De:693:VAL:HB	30:De:707:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DD:950:LEU:HD13	29:DD:954:GLU:HG2	1.94	0.49
31:DF:368:THR:CG2	31:DF:369:PRO:HD2	2.42	0.49
38:DH:57:SER:HB2	33:DJ:197:MET:CG	2.42	0.49
38:DH:110:TYR:CD1	33:DJ:161:LYS:CD	2.92	0.49
32:DI:32:GLU:HB2	32:DI:35:VAL:CG2	2.43	0.49
41:HG:63:VAL:HG11	41:HG:88:LEU:HD11	1.95	0.49
44:HI:57:ARG:HH22	44:HI:158:LEU:HD23	1.78	0.49
47:PG:39:THR:O	47:PG:43:GLY:N	2.42	0.49
49:j:82:LYS:CD	51:s:101:VAL:CG1	2.90	0.49
52:u:78:SER:HB3	59:z:563:VAL:CG2	2.41	0.49
54:d:34:LEU:HD21	56:i:65:PHE:CD1	2.47	0.49
66:k:71:THR:HG21	69:v:15:LEU:HB2	1.94	0.49
4:DA:569:ASN:HB3	4:DA:572:TYR:HD2	1.76	0.49
10:DB:598:ARG:HH11	10:DB:619:MET:HE3	1.77	0.49
13:HB:471:LEU:HD13	13:HB:475:PHE:CE2	2.47	0.49
25:DP:203:ARG:NE	27:DO:65:TYR:OH	2.46	0.49
31:DF:320:ARG:CD	31:DF:415:ILE:HD12	2.42	0.49
38:DH:50:PHE:CD1	33:DJ:195:LEU:HB2	2.47	0.49
33:DJ:126:TYR:HE2	33:DJ:157:LEU:HD11	1.77	0.49
39:HD:4:GLN:OE1	39:HD:10:LYS:HD3	2.13	0.49
39:HD:5:GLY:HA3	39:HD:10:LYS:CB	2.25	0.49
47:PG:134:ASP:OD1	47:PG:135:ILE:N	2.45	0.49
50:n:592:LYS:HB3	71:w:27:MET:CE	2.42	0.49
50:n:937:ARG:NH2	50:n:943:LEU:HD23	2.27	0.49
53:a:274:ILE:HG22	53:a:274:ILE:O	2.11	0.49
53:a:374:TYR:CD2	53:a:440:PHE:HB2	2.47	0.49
53:a:443:CYS:HB3	72:x:58:PRO:HD2	1.93	0.49
67:r:49:GLU:OE1	67:r:135:LEU:HD22	2.12	0.49
72:x:555:GLU:HA	72:x:558:VAL:HG12	1.94	0.49
4:DA:824:ARG:HB3	4:DA:863:VAL:HG12	1.95	0.49
7:HA:81:GLU:O	7:HA:84:ILE:HG22	2.13	0.49
15:PB:388:TYR:CE2	15:PB:505:LEU:HD21	2.48	0.49
32:Di:57:TYR:CE1	35:DI:102:LEU:HD21	2.47	0.49
29:DD:918:SER:HB3	35:DL:74:GLU:OE2	2.13	0.49
31:DF:273:GLN:CD	31:DF:273:GLN:N	2.70	0.49
42:HH:578:PRO:HG3	42:HH:602:ILE:HD11	1.94	0.49
47:PG:83:GLU:OE2	47:PG:147:ILE:HD12	2.13	0.49
47:PG:90:THR:OG1	47:PG:91:GLN:OE1	2.11	0.49
52:u:128:SER:HB3	56:i:131:LEU:CD2	2.41	0.49
53:a:70:LYS:HA	56:i:70:HIS:CE1	2.46	0.49
53:a:223:LYS:NZ	53:a:251:LEU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:460:ASP:OD2	72:x:5:ASN:ND2	2.45	0.49
58:q:428:LEU:C	58:q:428:LEU:CD1	2.85	0.49
65:h:85:ARG:HA	65:h:99:VAL:HG11	1.94	0.49
66:k:109:ARG:CZ	66:k:109:ARG:HB3	2.41	0.49
68:t:41:VAL:HG22	68:t:68:ASN:HA	1.93	0.49
71:w:122:VAL:O	71:w:126:ILE:HB	2.13	0.49
72:x:803:ASP:N	72:x:803:ASP:OD1	2.45	0.49
9:PA:539:GLN:HA	9:PA:774:ALA:HB1	1.94	0.49
9:PA:1178:ASP:OD2	9:PA:1260:ARG:NH2	2.45	0.49
9:PA:1658:SER:HB3	55:f:12:GLY:O	2.13	0.49
15:PB:601:VAL:HG22	15:PB:616:THR:HG23	1.93	0.49
31:DF:257:PRO:O	31:DF:261:THR:OG1	2.26	0.49
31:DF:312:ILE:HG22	31:DF:313:VAL:HG13	1.94	0.49
44:HI:37:ILE:HD12	44:HI:37:ILE:H	1.75	0.49
44:HI:110:THR:O	44:HI:114:ILE:HG13	2.13	0.49
46:PD:114:LEU:CD1	47:PG:84:VAL:HG21	2.43	0.49
50:n:101:ALA:N	51:s:109:LEU:HD11	2.27	0.49
50:n:305:LEU:CD1	50:n:361:ILE:HG12	2.43	0.49
55:f:142:SER:HB3	58:q:183:PHE:CE2	2.48	0.49
57:m:121:GLU:HG2	59:z:592:ASN:ND2	2.28	0.49
58:q:117:SER:O	58:q:120:ARG:HB3	2.11	0.49
58:q:191:ARG:HE	69:v:87:ILE:HG12	1.78	0.49
59:z:529:HIS:CD2	59:z:566:CYS:HB3	2.48	0.49
65:h:36:GLU:O	65:h:38:GLY:N	2.45	0.49
66:k:70:LEU:HD11	69:v:85:PHE:CD1	2.47	0.49
70:p:783:ARG:NH1	70:p:820:GLU:OE2	2.45	0.49
76:NX:20:DC:H1'	76:NX:21:DC:C2	2.48	0.49
4:DA:504:PRO:HD3	31:DF:207:ARG:HB3	1.94	0.49
4:DA:1063:LYS:NZ	4:DA:1067:GLN:OE1	2.42	0.49
7:HA:134:CYS:O	7:HA:138:THR:HG22	2.12	0.49
7:HA:310:LEU:HG	7:HA:409:THR:HG21	1.95	0.49
9:PA:1251:ASN:OD1	9:PA:1252:ALA:N	2.46	0.49
10:DB:560:TYR:HD2	10:DB:581:ILE:HD11	1.78	0.49
13:HB:440:LEU:HD11	40:HE:218:PRO:CD	2.43	0.49
15:PB:952:GLU:OE2	17:PC:39:ILE:HG22	2.13	0.49
52:u:90:LEU:CD1	58:q:9:ILE:CG1	2.68	0.49
55:f:16:VAL:HG13	55:f:104:VAL:HA	1.94	0.49
58:q:106:LEU:HD23	58:q:106:LEU:O	2.11	0.49
58:q:109:MET:HE1	58:q:112:LEU:HD22	1.95	0.49
58:q:168:THR:N	66:k:21:ILE:CD1	2.76	0.49
61:c:240:GLN:O	61:c:243:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:o:644:PRO:O	64:o:648:ALA:N	2.44	0.49
68:t:125:LYS:HE2	68:t:125:LYS:HB2	1.52	0.49
70:p:40:SER:OG	70:p:42:ARG:O	2.24	0.49
71:w:980:VAL:O	71:w:983:SER:OG	2.31	0.49
16:HC:435:ASN:ND2	43:HF:38:ILE:O	2.45	0.49
25:DP:185:LEU:HD21	29:DD:1006:LEU:HD13	1.93	0.49
31:DF:329:LEU:C	31:DF:329:LEU:CD2	2.86	0.49
41:HG:87:LEU:HD11	41:HG:229:LYS:CG	2.43	0.49
44:HI:140:PRO:HA	44:HI:202:ILE:CD1	2.33	0.49
45:HJ:207:TYR:HB3	45:HJ:211:GLN:NE2	2.27	0.49
48:g:168:LEU:HD11	56:i:136:LYS:HA	1.94	0.49
53:a:59:VAL:CG2	54:d:51:SER:HB3	2.30	0.49
53:a:420:LEU:HB3	53:a:504:ILE:HD12	1.94	0.49
53:a:441:GLU:CB	72:x:14:TRP:HE1	2.26	0.49
69:v:131:GLU:HG3	69:v:135:TYR:HE2	1.77	0.49
70:p:38:ALA:HA	70:p:435:GLN:HE21	1.78	0.49
9:PA:1657:TYR:HB3	9:PA:1658:SER:H	1.53	0.48
10:DB:27:LYS:HE3	10:DB:490:SER:HB3	1.95	0.48
26:DQ:18:ILE:HD11	26:DQ:46:TRP:CZ3	2.48	0.48
27:DO:73:THR:O	27:DO:73:THR:HG22	2.12	0.48
30:De:439:ASP:OD1	30:De:555:ARG:NH2	2.44	0.48
29:DD:924:LYS:HB2	38:DH:83:THR:HG22	1.94	0.48
31:DF:279:LEU:CB	31:DF:330:ARG:NH2	2.75	0.48
42:HH:650:MET:SD	42:HH:656:ASN:ND2	2.82	0.48
44:HI:143:LEU:O	44:HI:143:LEU:HD22	2.13	0.48
48:g:128:PRO:CD	48:g:129:HIS:N	2.71	0.48
50:n:544:ARG:NE	50:n:716:ASN:HA	2.28	0.48
53:a:246:ASN:N	53:a:246:ASN:OD1	2.44	0.48
53:a:412:ARG:C	53:a:472:SER:CB	2.84	0.48
58:q:134:ALA:H	65:h:72:ARG:HH11	1.48	0.48
69:v:49:SER:HB3	69:v:50:ARG:CZ	2.42	0.48
71:w:1193:PHE:C	71:w:1195:ALA:N	2.70	0.48
5:EA:139:LEU:HG	47:PG:151:ARG:HB2	1.95	0.48
12:FB:43:LEU:HD12	12:FB:55:SER:O	2.13	0.48
16:HC:440:LEU:HD22	43:HF:36:GLN:OE1	2.14	0.48
37:DG:48:HIS:HD2	37:DG:54:GLY:HA2	1.78	0.48
37:DG:181:TRP:CD2	37:DG:181:TRP:C	2.88	0.48
38:DH:116:ARG:HD3	33:DJ:126:TYR:CE1	2.49	0.48
40:HE:13:ILE:HD13	40:HE:41:VAL:HG13	1.94	0.48
42:HH:575:LEU:O	42:HH:576:ASN:OD1	2.32	0.48
45:HJ:177:ARG:HB2	45:HJ:177:ARG:HH11	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:j:27:SER:HA	51:s:154:LEU:HD21	1.95	0.48
50:n:808:LEU:HB2	50:n:822:ILE:HB	1.94	0.48
53:a:441:GLU:O	53:a:452:VAL:HA	2.14	0.48
58:q:396:ALA:HB2	67:r:51:PHE:HE2	1.69	0.48
6:FA:153:ARG:NH1	6:FA:180:ARG:O	2.47	0.48
16:HC:360:THR:HG22	16:HC:363:GLN:OE1	2.13	0.48
31:DF:388:ILE:HG22	31:DF:392:ILE:HG13	1.95	0.48
44:HI:110:THR:HB	44:HI:113:HIS:ND1	2.28	0.48
44:HI:116:ALA:HB2	44:HI:302:THR:H	1.78	0.48
44:HI:155:ASP:C	44:HI:155:ASP:OD1	2.55	0.48
45:HJ:59:TYR:HB2	45:HJ:265:PRO:HG2	1.94	0.48
45:HJ:185:GLU:O	45:HJ:188:ARG:HB3	2.14	0.48
45:HJ:226:ILE:HD13	45:HJ:226:ILE:N	2.28	0.48
50:n:247:LEU:HB3	50:n:275:HIS:CD2	2.48	0.48
52:u:71:VAL:HG22	59:z:528:LEU:CD2	2.43	0.48
53:a:393:VAL:HG13	53:a:393:VAL:O	2.13	0.48
53:a:441:GLU:CG	53:a:442:VAL:N	2.75	0.48
56:i:109:LEU:HD22	56:i:117:GLN:NE2	2.27	0.48
56:i:133:GLN:O	56:i:133:GLN:CD	2.56	0.48
58:q:19:VAL:CG2	58:q:22:VAL:HG22	2.43	0.48
58:q:187:LEU:HD12	58:q:187:LEU:C	2.38	0.48
59:z:528:LEU:HA	59:z:582:LEU:HD12	1.95	0.48
65:h:8:LEU:C	65:h:8:LEU:CD2	2.85	0.48
65:h:86:ASP:N	65:h:99:VAL:HG12	2.28	0.48
68:t:11:VAL:HA	68:t:20:THR:HG21	1.95	0.48
69:v:108:LEU:C	69:v:108:LEU:CD1	2.86	0.48
71:w:1195:ALA:C	71:w:1197:HIS:N	2.69	0.48
9:PA:1242:ASP:O	9:PA:1262:MET:N	2.46	0.48
27:DO:2:ALA:N	29:DD:1000:ARG:HD3	2.22	0.48
28:Dc:26:VAL:HG23	33:Dj:195:LEU:HB3	1.96	0.48
28:Dc:119:GLU:HG3	30:De:790:LEU:HD11	1.96	0.48
30:De:651:VAL:HG13	30:De:665:PHE:HB2	1.95	0.48
30:De:720:SER:OG	30:De:721:ARG:N	2.47	0.48
30:DE:481:ASP:HB3	30:DE:787:ARG:HH22	1.77	0.48
40:HE:192:ASP:OD1	40:HE:213:LEU:N	2.45	0.48
58:q:171:VAL:CG1	66:k:17:ILE:HG21	2.43	0.48
58:q:191:ARG:NE	69:v:87:ILE:O	2.46	0.48
60:b:178:LEU:HD13	63:l:55:LEU:CD2	2.43	0.48
61:c:46:GLU:H	61:c:46:GLU:CD	2.17	0.48
62:e:56:PHE:HE1	63:l:52:PHE:CE1	2.32	0.48
66:k:101:ARG:NH1	66:k:101:ARG:CG	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:w:726:ASN:N	71:w:726:ASN:HD22	2.11	0.48
71:w:1172:ILE:O	71:w:1244:GLN:NE2	2.41	0.48
71:w:1195:ALA:C	71:w:1197:HIS:H	2.20	0.48
77:NY:-65:DG:H2"	77:NY:-64:DG:C8	2.48	0.48
5:EA:45:GLU:HB2	5:EA:90:ASN:HB2	1.95	0.48
5:EA:131:VAL:HB	5:EA:157:CYS:HB2	1.94	0.48
7:HA:45:GLY:O	7:HA:48:LYS:NZ	2.44	0.48
9:PA:1218:ARG:NH2	9:PA:1252:ALA:O	2.46	0.48
30:De:234:ALA:HB2	30:De:648:ASP:HB2	1.94	0.48
31:Df:39:LEU:HD22	32:Di:47:VAL:HG13	1.94	0.48
29:DD:1059:ASN:O	35:DL:80:VAL:CG2	2.61	0.48
30:DE:526:ARG:HA	30:DE:526:ARG:HH11	1.73	0.48
31:DF:317:LEU:CD2	31:DF:317:LEU:N	2.76	0.48
38:DH:54:GLU:OE1	33:DJ:197:MET:CB	2.62	0.48
39:HD:63:PHE:HB2	39:HD:69:ASP:OD1	2.13	0.48
45:HJ:190:THR:OG1	45:HJ:220:SER:HB3	2.14	0.48
49:j:82:LYS:CE	51:s:101:VAL:CG1	2.91	0.48
50:n:371:GLN:HG3	50:n:390:MET:CE	2.44	0.48
50:n:851:ILE:HD11	50:n:911:SER:HA	1.96	0.48
50:n:904:PHE:CZ	50:n:1208:GLU:HB2	2.48	0.48
52:u:108:VAL:CG2	54:d:128:ALA:CB	2.86	0.48
53:a:148:ASP:OD1	53:a:148:ASP:N	2.47	0.48
53:a:417:TYR:HB2	53:a:469:VAL:CG2	2.36	0.48
53:a:449:ARG:HH12	72:x:54:PRO:CB	2.27	0.48
62:e:75:THR:O	62:e:79:GLN:HG2	2.14	0.48
66:k:70:LEU:HD22	66:k:70:LEU:HA	1.45	0.48
70:p:367:ASP:HA	70:p:370:VAL:HG22	1.96	0.48
70:p:441:LEU:HB3	70:p:494:HIS:CE1	2.49	0.48
71:w:777:ILE:HA	71:w:810:VAL:HG22	1.95	0.48
3:BA:53:ARG:NE	15:PB:892:CYS:SG	2.87	0.48
7:HA:115:LEU:O	7:HA:115:LEU:HD12	2.13	0.48
9:PA:363:ALA:O	15:PB:1084:LEU:HD11	2.13	0.48
9:PA:1173:THR:HG22	9:PA:1214:VAL:HG23	1.94	0.48
9:PA:1203:ASP:OD2	9:PA:1244:ASN:ND2	2.44	0.48
10:DB:739:ASN:ND2	10:DB:782:ASN:OD1	2.44	0.48
13:HB:374:LEU:O	13:HB:374:LEU:HD12	2.13	0.48
13:HB:456:ASP:OD1	13:HB:456:ASP:N	2.47	0.48
17:PC:92:GLU:O	17:PC:93:PHE:CG	2.67	0.48
32:Di:73:LEU:HB3	35:DI:105:HIS:HE1	1.77	0.48
34:Dk:173:CYS:SG	34:Dk:179:MET:O	2.72	0.48
38:DH:161:LYS:HB2	38:DH:161:LYS:HE3	1.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DI:73:LEU:HD12	32:DI:73:LEU:O	2.14	0.48
48:g:159:ARG:C	48:g:159:ARG:CD	2.86	0.48
53:a:321:LEU:HA	53:a:410:LEU:CD1	2.44	0.48
53:a:455:GLN:HB2	72:x:11:LEU:HD21	1.96	0.48
54:d:64:GLN:NE2	54:d:68:LEU:HD12	2.27	0.48
60:b:86:THR:O	60:b:90:ASN:N	2.44	0.48
66:k:64:SER:HB2	66:k:68:ARG:CZ	2.43	0.48
70:p:88:GLU:OE2	70:p:288:ARG:NH1	2.47	0.48
70:p:817:LYS:HB2	73:y:30:PRO:HG3	1.96	0.48
7:HA:136:SER:O	7:HA:142:VAL:HG21	2.13	0.48
16:HC:397:GLU:OE1	43:HF:61:MET:HE3	2.14	0.48
25:DP:227:GLU:OE1	25:DP:318:ARG:NH2	2.46	0.48
31:Df:102:ARG:HD3	35:DL:151:ARG:HG3	1.96	0.48
29:DD:950:LEU:C	29:DD:950:LEU:CD1	2.86	0.48
38:DH:111:ALA:HB2	33:DJ:157:LEU:HD13	1.94	0.48
35:DL:70:VAL:HG12	35:DL:74:GLU:OE1	2.13	0.48
45:HJ:40:VAL:HB	45:HJ:44:ASP:OD2	2.14	0.48
47:PG:30:LEU:O	47:PG:34:VAL:HG22	2.14	0.48
50:n:196:ASN:HD21	50:n:219:ASN:C	2.22	0.48
50:n:678:PHE:HA	58:q:557:LEU:HB2	1.95	0.48
53:a:108:PHE:O	53:a:108:PHE:CD1	2.66	0.48
53:a:157:LEU:HD23	53:a:217:GLY:HA2	1.96	0.48
53:a:431:LYS:HD3	53:a:431:LYS:HA	1.70	0.48
57:m:56:LEU:CD2	57:m:80:GLN:HE21	2.23	0.48
67:r:206:ARG:C	67:r:206:ARG:NE	2.72	0.48
68:t:128:THR:O	68:t:130:THR:N	2.46	0.48
71:w:70:GLN:HG3	71:w:75:ARG:HG2	1.95	0.48
71:w:671:ASP:OD1	71:w:671:ASP:N	2.44	0.48
71:w:999:ASP:N	71:w:999:ASP:OD1	2.41	0.48
72:x:107:ARG:O	72:x:108:LEU:C	2.56	0.48
73:y:184:SER:HB3	73:y:220:MET:HE3	1.96	0.48
1:X:-28:DA:H5'	25:DP:301:VAL:HG21	1.94	0.48
5:EA:105:TYR:OH	11:EB:237:LEU:N	2.47	0.48
9:PA:1454:VAL:HG12	9:PA:1458:ILE:HD12	1.95	0.48
10:DB:636:VAL:HG23	10:DB:638:ARG:HB3	1.96	0.48
16:HC:174:ASP:OD1	16:HC:175:LEU:N	2.45	0.48
29:Dd:1080:TYR:OH	30:De:606:ASP:OD2	2.26	0.48
30:De:556:ASN:HA	30:De:572:LEU:HB2	1.96	0.48
31:DF:68:THR:O	31:DF:69:SER:HB3	2.13	0.48
40:HE:146:ARG:NH2	41:HG:348:CYS:O	2.46	0.48
46:PD:134:ILE:HA	46:PD:137:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:153:PHE:HZ	54:d:125:VAL:HG12	1.79	0.48
49:j:82:LYS:HD2	51:s:101:VAL:CG1	2.43	0.48
52:u:125:ILE:HG12	56:i:135:TYR:CD2	2.49	0.48
58:q:187:LEU:HD11	69:v:88:LEU:HD21	1.95	0.48
58:q:188:LEU:CD1	58:q:188:LEU:C	2.86	0.48
58:q:188:LEU:CA	69:v:87:ILE:CD1	2.78	0.48
58:q:456:GLU:HG2	69:v:140:SER:HA	1.95	0.48
59:z:582:LEU:HG	59:z:584:PRO:HD3	1.95	0.48
69:v:133:GLU:O	69:v:136:SER:N	2.46	0.48
70:p:24:TRP:HD1	70:p:51:LEU:HD12	1.79	0.48
70:p:51:LEU:HB2	70:p:58:LEU:HB3	1.94	0.48
71:w:337:GLN:HE21	71:w:341:PHE:HE2	1.59	0.48
4:DA:464:TRP:O	4:DA:464:TRP:HE3	1.97	0.48
4:DA:488:ALA:H	31:Df:315:ARG:HG2	1.79	0.48
5:EA:142:ASN:HD21	47:PG:107:PHE:HB2	1.78	0.48
5:EA:145:PHE:HB2	5:EA:152:PHE:HA	1.96	0.48
9:PA:1415:THR:HG22	9:PA:1416:ARG:N	2.29	0.48
10:DB:820:ASP:OD1	10:DB:820:ASP:N	2.37	0.48
15:PB:167:THR:HG23	15:PB:170:ASP:H	1.79	0.48
15:PB:718:GLN:OE1	15:PB:976:MET:HE3	2.14	0.48
29:Dd:910:LEU:HD11	35:Dl:88:ALA:HB2	1.96	0.48
30:DE:651:VAL:HB	30:DE:665:PHE:HB2	1.94	0.48
44:HI:263:ALA:O	55:f:52:MET:HE3	2.14	0.48
45:HJ:140:LEU:HD22	45:HJ:140:LEU:HA	1.73	0.48
48:g:131:ALA:O	48:g:135:LEU:HG	2.14	0.48
52:u:122:LEU:C	52:u:122:LEU:HD13	2.38	0.48
53:a:364:TYR:CD1	53:a:430:LEU:HD12	2.49	0.48
56:i:65:PHE:CD1	56:i:99:LYS:HG2	2.49	0.48
58:q:155:GLY:C	69:v:62:HIS:CE1	2.91	0.48
66:k:37:LYS:HE3	66:k:37:LYS:N	2.16	0.48
67:r:21:TYR:HE1	67:r:175:ALA:HB3	1.78	0.48
71:w:863:ASP:OD1	71:w:863:ASP:N	2.45	0.48
73:y:140:ARG:NH2	73:y:176:ARG:O	2.47	0.48
1:X:-4:DC:H2"	1:X:-3:DC:C6	2.49	0.48
4:DA:402:PHE:HE1	31:Df:391:LEU:HD11	1.79	0.48
4:DA:740:LEU:CD2	4:DA:1070:PHE:HZ	2.27	0.48
7:HA:722:ARG:NH1	41:HG:222:ILE:O	2.46	0.48
12:FB:58:LEU:HD11	12:FB:62:LEU:HD23	1.96	0.48
15:PB:598:VAL:CG2	15:PB:601:VAL:HG23	2.44	0.48
25:DP:297:LYS:HG2	25:DP:298:PRO:HD3	1.96	0.48
38:DH:110:TYR:CG	33:DJ:161:LYS:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:HI:110:THR:HG22	55:f:63:MET:HA	1.96	0.48
45:HJ:85:MET:HE2	45:HJ:160:VAL:HB	1.95	0.48
50:n:270:GLN:NE2	55:f:174:ARG:CD	2.53	0.48
50:n:361:ILE:HA	50:n:370:LEU:HD21	1.95	0.48
50:n:591:PHE:HB3	71:w:26:PHE:CD1	2.45	0.48
50:n:796:ILE:O	50:n:816:LYS:NZ	2.34	0.48
52:u:122:LEU:HG	54:d:111:GLN:NE2	2.19	0.48
53:a:160:LEU:HG	53:a:219:LEU:HD21	1.96	0.48
58:q:396:ALA:HB2	67:r:51:PHE:CZ	2.43	0.48
58:q:645:ALA:O	63:l:111:VAL:HG21	2.14	0.48
59:z:488:SER:HB2	59:z:492:ARG:NH2	2.29	0.48
59:z:582:LEU:CD2	59:z:591:LEU:HB3	2.44	0.48
61:c:176:MET:HG2	61:c:194:LEU:HG	1.96	0.48
63:l:177:ARG:CZ	69:v:113:ASP:OD2	2.61	0.48
64:o:742:GLN:HG2	72:x:107:ARG:NH2	2.29	0.48
68:t:5:CYS:O	68:t:141:GLU:HA	2.14	0.48
71:w:105:ASP:OD1	71:w:105:ASP:N	2.46	0.48
71:w:787:PRO:HB3	71:w:822:HIS:CD2	2.49	0.48
72:x:289:CYS:HB3	72:x:309:THR:HG22	1.96	0.48
4:DA:953:VAL:O	37:DG:149:ARG:NH2	2.47	0.47
5:EA:171:LYS:HZ1	39:HD:41:ARG:NE	2.12	0.47
9:PA:542:LEU:O	9:PA:545:VAL:HG12	2.14	0.47
10:DB:135:TRP:HA	10:DB:138:VAL:HG12	1.95	0.47
10:DB:953:LEU:HD12	10:DB:979:PHE:HE2	1.79	0.47
12:FB:182:HIS:NE2	29:DD:998:GLN:OE1	2.47	0.47
29:Dd:922:GLN:NE2	35:Dl:71:ASP:OD2	2.47	0.47
30:DE:702:LEU:HD22	30:DE:702:LEU:N	2.29	0.47
31:DF:415:ILE:HG12	31:DF:415:ILE:O	2.14	0.47
38:DH:54:GLU:CD	33:DJ:197:MET:HG2	2.39	0.47
38:DH:110:TYR:CE1	38:DH:113:ARG:CZ	2.97	0.47
46:PD:55:GLN:NE2	46:PD:56:GLU:O	2.46	0.47
48:g:110:GLU:O	48:g:113:LYS:HB3	2.14	0.47
53:a:420:LEU:HD22	53:a:504:ILE:HG13	1.96	0.47
54:d:45:ILE:CG1	56:i:73:ILE:CA	2.69	0.47
54:d:72:ARG:HE	54:d:72:ARG:HB2	1.33	0.47
55:f:145:TYR:HB2	65:h:41:THR:OG1	2.14	0.47
58:q:17:LYS:CE	58:q:30:TYR:CD2	2.97	0.47
72:x:621:VAL:HG11	72:x:670:LEU:HD22	1.96	0.47
9:PA:689:ILE:O	9:PA:693:ILE:HG12	2.14	0.47
10:DB:564:LEU:HB2	10:DB:581:ILE:HD13	1.96	0.47
16:HC:348:ARG:NH2	43:HF:65:ALA:CB	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DD:886:GLY:CA	29:DD:891:ILE:HG13	2.39	0.47
31:DF:43:VAL:CA	32:DI:46:TYR:CD2	2.90	0.47
31:DF:104:LEU:CD1	33:DJ:217:PHE:CE2	2.91	0.47
41:HG:382:CYS:HB3	41:HG:385:CYS:HB3	1.96	0.47
45:HJ:215:THR:HG23	45:HJ:252:MET:HG3	1.96	0.47
50:n:101:ALA:HB2	51:s:109:LEU:CD2	2.44	0.47
54:d:121:LEU:HD22	54:d:125:VAL:HG13	1.96	0.47
61:c:288:LEU:HD11	68:t:156:LEU:HD11	1.96	0.47
64:o:678:LEU:HD11	64:o:725:VAL:HG11	1.96	0.47
65:h:151:LEU:HD11	69:v:37:ILE:O	2.13	0.47
70:p:510:GLU:OE1	70:p:513:ARG:NH2	2.45	0.47
9:PA:33:ARG:NH1	15:PB:1139:GLY:O	2.47	0.47
9:PA:1144:LEU:HD23	9:PA:1144:LEU:H	1.78	0.47
10:DB:537:PHE:HE2	10:DB:539:ARG:HB2	1.79	0.47
15:PB:407:MET:HE1	15:PB:444:LEU:CG	2.43	0.47
15:PB:1035:ARG:NH1	15:PB:1036:LYS:O	2.44	0.47
17:PC:190:ASN:ND2	17:PC:195:THR:O	2.39	0.47
22:PJ:6:ARG:HD3	22:PJ:13:ILE:HD13	1.95	0.47
31:Df:254:GLN:O	31:Df:258:ARG:NH2	2.47	0.47
30:DE:465:THR:HG22	31:DF:132:LYS:O	2.13	0.47
35:DL:61:LYS:HA	35:DL:61:LYS:HD2	1.55	0.47
45:HJ:82:THR:HG23	45:HJ:160:VAL:CG1	2.42	0.47
46:PD:33:LEU:O	46:PD:37:VAL:HG23	2.13	0.47
54:d:45:ILE:HG22	56:i:76:MET:HB2	1.77	0.47
58:q:92:LEU:HD11	58:q:99:ARG:HD2	1.95	0.47
58:q:106:LEU:C	58:q:106:LEU:CD2	2.85	0.47
61:c:134:LYS:HD3	63:l:46:TYR:HB2	1.97	0.47
66:k:60:GLU:HG3	69:v:26:ILE:HG13	1.95	0.47
70:p:100:ASP:OD1	70:p:100:ASP:N	2.47	0.47
70:p:608:MET:HA	70:p:611:LEU:HB3	1.96	0.47
71:w:1241:THR:OG1	71:w:1242:GLU:N	2.44	0.47
8:NE:734:ARG:O	8:NE:735:ALA:HB2	2.13	0.47
9:PA:89:GLU:O	9:PA:287:ASN:ND2	2.46	0.47
9:PA:350:VAL:CG1	9:PA:1435:THR:HG21	2.43	0.47
11:EB:148:LYS:HD2	11:EB:184:ALA:HB3	1.95	0.47
13:HB:488:GLU:O	13:HB:491:VAL:HG22	2.13	0.47
15:PB:438:ARG:NH2	15:PB:442:ASP:OD2	2.47	0.47
31:Df:330:ARG:NH1	31:Df:371:THR:O	2.47	0.47
33:Dj:149:PRO:O	33:Dj:153:ARG:NH1	2.46	0.47
45:HJ:98:GLU:HG3	45:HJ:99:TYR:CZ	2.50	0.47
46:PD:15:GLU:OE2	47:PG:78:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:227:GLU:O	50:n:253:LEU:HD12	2.14	0.47
50:n:711:ARG:HH12	50:n:723:GLU:CD	2.21	0.47
53:a:187:MET:HE1	53:a:401:PRO:HB2	1.96	0.47
53:a:449:ARG:CZ	72:x:54:PRO:CB	2.90	0.47
55:f:100:ILE:HG12	55:f:105:ILE:HG12	1.96	0.47
57:m:116:GLN:CG	59:z:595:PRO:HD3	2.43	0.47
62:e:136:LEU:HD11	66:k:107:VAL:HG12	1.96	0.47
62:e:146:ILE:O	62:e:148:VAL:N	2.46	0.47
72:x:544:HIS:HD2	72:x:546:CYS:H	1.62	0.47
5:EA:144:LEU:HD13	5:EA:154:CYS:HA	1.97	0.47
5:EA:181:ASN:ND2	39:HD:10:LYS:N	2.63	0.47
10:DB:431:LEU:HD23	10:DB:431:LEU:C	2.39	0.47
13:HB:422:LEU:HD13	40:HE:225:GLN:NE2	2.29	0.47
15:PB:752:TYR:CD2	15:PB:807:ARG:HB3	2.49	0.47
16:HC:348:ARG:CD	43:HF:65:ALA:HB1	2.41	0.47
18:PE:25:GLY:O	18:PE:65:ASN:ND2	2.47	0.47
30:De:724:GLU:OE1	30:De:789:ASN:ND2	2.46	0.47
29:DD:961:GLN:O	29:DD:965:ILE:N	2.48	0.47
30:DE:702:LEU:HD23	30:DE:704:VAL:HG23	1.95	0.47
40:HE:20:ILE:H	40:HE:20:ILE:HD12	1.79	0.47
41:HG:87:LEU:HD13	41:HG:228:TYR:HD2	1.80	0.47
43:HF:38:ILE:H	43:HF:38:ILE:HD12	1.80	0.47
44:HI:178:TYR:CE2	44:HI:202:ILE:HG13	2.49	0.47
45:HJ:277:LEU:HA	45:HJ:280:CYS:SG	2.54	0.47
46:PD:51:ALA:HA	55:f:172:PHE:CZ	2.49	0.47
48:g:126:TYR:HD1	48:g:126:TYR:HA	1.57	0.47
53:a:441:GLU:HB3	72:x:14:TRP:NE1	2.29	0.47
58:q:157:ALA:HB2	66:k:31:VAL:CG2	2.36	0.47
60:b:107:GLU:HB3	64:o:649:ILE:HD11	1.96	0.47
66:k:35:LEU:HD12	66:k:35:LEU:O	2.14	0.47
66:k:94:LEU:HD21	69:v:108:LEU:HD11	1.96	0.47
71:w:234:SER:HB2	71:w:660:GLU:HG3	1.96	0.47
73:y:36:ARG:HA	73:y:40:LEU:HB2	1.96	0.47
4:DA:1195:VAL:HG22	4:DA:1198:ARG:HH12	1.80	0.47
7:HA:617:ALA:HB2	7:HA:676:LEU:HD21	1.97	0.47
9:PA:484:LEU:HD11	9:PA:501:MET:SD	2.54	0.47
10:DB:184:ASN:N	10:DB:184:ASN:ND2	2.63	0.47
10:DB:570:GLU:HA	10:DB:625:LEU:HA	1.95	0.47
15:PB:501:LEU:HD11	15:PB:511:PRO:HA	1.95	0.47
29:DD:924:LYS:C	29:DD:926:PHE:H	2.22	0.47
41:HG:253:GLY:N	41:HG:310:LEU:HD21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:HI:136:ARG:HG3	44:HI:136:ARG:NH1	2.28	0.47
49:j:17:GLU:CB	51:s:112:LEU:CD1	2.93	0.47
50:n:277:LEU:CD1	55:f:185:ARG:HG2	2.45	0.47
50:n:960:LYS:HB3	50:n:1210:PHE:CZ	2.50	0.47
50:n:963:LEU:HD21	50:n:1258:ASN:CB	2.45	0.47
54:d:109:GLN:HA	54:d:112:LYS:HE3	1.95	0.47
57:m:107:HIS:O	57:m:111:LYS:CB	2.62	0.47
58:q:160:LEU:HD23	69:v:69:VAL:HG23	1.97	0.47
58:q:484:TYR:O	58:q:488:CYS:HB2	2.14	0.47
69:v:26:ILE:HD13	69:v:26:ILE:HA	1.70	0.47
71:w:270:LEU:HD23	71:w:303:GLN:HG3	1.96	0.47
72:x:20:ASP:OD1	72:x:20:ASP:N	2.44	0.47
4:DA:483:ASN:HA	4:DA:493:ARG:NH1	2.29	0.47
5:EA:137:THR:HG22	5:EA:139:LEU:H	1.80	0.47
9:PA:1200:PRO:HG2	9:PA:1204:VAL:HG22	1.96	0.47
17:PC:72:PRO:HD3	22:PJ:13:ILE:HD11	1.97	0.47
30:De:474:THR:OG1	30:De:546:VAL:O	2.28	0.47
30:De:703:MET:HE2	30:De:703:MET:HB3	1.84	0.47
31:DF:68:THR:HA	32:DI:32:GLU:OE1	2.15	0.47
31:DF:276:LEU:HD13	31:DF:323:VAL:HG11	1.95	0.47
31:DF:427:LEU:HD12	31:DF:427:LEU:HA	1.72	0.47
38:DH:110:TYR:CZ	33:DJ:160:GLN:HB3	2.50	0.47
32:DI:31:TYR:OH	32:DI:36:ILE:HD11	2.15	0.47
41:HG:357:VAL:CG1	41:HG:366:VAL:HG23	2.45	0.47
44:HI:95:GLU:N	44:HI:145:LEU:O	2.47	0.47
44:HI:101:ILE:HD13	44:HI:101:ILE:N	2.29	0.47
44:HI:209:ARG:CA	55:f:53:GLN:NE2	2.76	0.47
44:HI:214:PRO:CD	44:HI:224:ARG:HG2	2.38	0.47
44:HI:280:PRO:HA	44:HI:283:ARG:NH1	2.29	0.47
45:HJ:3:HIS:ND1	45:HJ:3:HIS:N	2.59	0.47
45:HJ:134:LEU:H	45:HJ:134:LEU:HG	1.42	0.47
50:n:387:GLU:HG3	50:n:391:LYS:HE3	1.97	0.47
53:a:449:ARG:HH12	72:x:54:PRO:HB3	1.79	0.47
54:d:133:LYS:HB2	54:d:133:LYS:HE3	1.44	0.47
55:f:32:TYR:CE1	55:f:35:GLU:OE2	2.67	0.47
58:q:190:LEU:O	58:q:190:LEU:HD13	2.15	0.47
61:c:209:ILE:HB	61:c:250:LEU:HD13	1.96	0.47
61:c:310:ARG:O	61:c:311:GLN:C	2.57	0.47
68:t:204:GLN:NE2	68:t:204:GLN:HA	2.29	0.47
71:w:1229:LYS:O	71:w:1233:GLU:HB2	2.14	0.47
72:x:301:GLU:OE2	72:x:301:GLU:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:x:687:PHE:HB2	72:x:688:PRO:HD3	1.97	0.47
7:HA:52:LEU:HD21	7:HA:232:VAL:HG11	1.96	0.47
8:NA:533:GLU:O	8:NA:534:ARG:O	2.33	0.47
10:DB:329:LEU:HB3	10:DB:342:THR:HG23	1.96	0.47
15:PB:207:VAL:HG11	15:PB:375:ALA:CB	2.45	0.47
30:DE:481:ASP:OD1	30:DE:481:ASP:N	2.41	0.47
31:DF:43:VAL:HG23	32:DI:46:TYR:HD2	1.78	0.47
31:DF:67:THR:O	31:DF:69:SER:N	2.47	0.47
32:DI:119:ARG:NH1	32:DI:120:TYR:OH	2.48	0.47
40:HE:42:MET:SD	40:HE:108:ASN:ND2	2.86	0.47
40:HE:44:LEU:HD21	40:HE:162:LEU:CD1	2.45	0.47
40:HE:165:LYS:NZ	40:HE:167:ALA:O	2.38	0.47
44:HI:114:ILE:HG23	44:HI:206:LEU:HD12	1.97	0.47
47:PG:104:MET:HE1	47:PG:106:CYS:HB2	1.96	0.47
47:PG:110:ARG:HA	47:PG:113:ILE:HD12	1.97	0.47
48:g:127:ARG:HD3	48:g:130:GLN:HB3	1.97	0.47
52:u:7:GLN:OE1	59:z:593:ILE:HA	2.15	0.47
53:a:145:LYS:HA	53:a:145:LYS:CE	2.41	0.47
53:a:421:ILE:HD11	53:a:450:PHE:CD1	2.50	0.47
55:f:106:TYR:CZ	65:h:106:PRO:HG3	2.50	0.47
62:e:129:VAL:CB	66:k:114:MET:HE2	2.44	0.47
66:k:80:GLU:N	66:k:80:GLU:OE1	2.48	0.47
68:t:6:VAL:HG22	68:t:141:GLU:CB	2.41	0.47
69:v:16:GLN:HE21	69:v:20:LYS:CD	2.23	0.47
69:v:18:TYR:HA	69:v:21:ARG:HD2	1.95	0.47
4:DA:571:GLU:OE1	4:DA:571:GLU:N	2.37	0.47
5:EA:139:LEU:HG	47:PG:151:ARG:CB	2.45	0.47
9:PA:1790:TYR:CD2	65:h:83:PRO:HD3	2.50	0.47
29:Dd:1061:ARG:NH1	32:Di:119:ARG:O	2.48	0.47
30:De:589:TRP:HB3	31:Df:60:MET:HE3	1.96	0.47
31:Df:326:HIS:O	31:Df:330:ARG:HG2	2.15	0.47
32:Di:73:LEU:HB3	35:Dl:105:HIS:CE1	2.50	0.47
34:Dk:191:VAL:HG13	34:Dk:200:ILE:CD1	2.42	0.47
31:DF:82:PRO:HG2	31:DF:83:LEU:CD1	2.45	0.47
38:DH:50:PHE:CE2	33:DJ:171:LEU:HA	2.50	0.47
39:HD:281:GLN:N	39:HD:281:GLN:CD	2.73	0.47
44:HI:207:LEU:HD13	55:f:52:MET:HE1	1.96	0.47
50:n:209:PRO:CG	50:n:293:TYR:CB	2.75	0.47
52:u:64:ARG:HB3	59:z:585:HIS:HE1	1.79	0.47
53:a:259:ILE:HD12	53:a:259:ILE:O	2.14	0.47
53:a:417:TYR:CD1	53:a:450:PHE:CE1	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:165:LEU:HA	57:m:110:ARG:NH1	2.30	0.47
55:f:57:LEU:HD13	55:f:57:LEU:HA	1.78	0.47
55:f:82:ARG:NH1	55:f:94:PRO:HB3	2.30	0.47
58:q:188:LEU:HD22	69:v:87:ILE:CB	2.45	0.47
58:q:548:VAL:HA	58:q:571:VAL:HG12	1.96	0.47
68:t:80:GLU:HB2	68:t:81:ASN:H	1.44	0.47
70:p:71:TRP:HZ3	70:p:738:LEU:HD21	1.80	0.47
72:x:374:SER:O	72:x:377:SER:OG	2.29	0.47
5:EA:171:LYS:HZ2	39:HD:41:ARG:CG	2.24	0.47
7:HA:563:ARG:NH2	41:HG:142:GLU:OE1	2.48	0.47
9:PA:225:PHE:HA	9:PA:228:ILE:HD12	1.96	0.47
12:FB:179:ASP:CG	29:DD:1002:ARG:NH2	2.73	0.47
15:PB:1036:LYS:H	17:PC:186:TYR:HH	1.62	0.47
27:DO:2:ALA:HA	29:DD:1000:ARG:HH11	1.79	0.47
29:DD:947:PHE:CD2	32:DI:113:PRO:HD3	2.50	0.47
37:DG:41:ASP:OD1	37:DG:41:ASP:N	2.47	0.47
39:HD:31:CYS:SG	39:HD:34:CYS:HB2	2.55	0.47
45:HJ:151:ILE:H	45:HJ:151:ILE:HG12	1.45	0.47
45:HJ:234:GLU:C	45:HJ:234:GLU:CD	2.83	0.47
49:j:78:GLN:O	49:j:82:LYS:CE	2.61	0.47
54:d:126:TYR:CD2	58:q:36:MET:CG	2.98	0.47
56:i:85:GLN:CG	56:i:86:ASP:N	2.32	0.47
58:q:609:VAL:HG23	64:o:674:ILE:HD13	1.96	0.47
62:e:45:VAL:CG1	63:l:92:LEU:CD1	2.92	0.47
68:t:8:GLN:HG3	68:t:196:LEU:CD2	2.45	0.47
70:p:191:SER:HA	70:p:200:LEU:O	2.15	0.47
72:x:843:TYR:HD1	72:x:847:PHE:HE2	1.62	0.47
5:EA:188:TYR:CE2	39:HD:14:TYR:CG	3.03	0.46
9:PA:609:HIS:ND1	9:PA:626:THR:HG23	2.31	0.46
9:PA:1643:TYR:CZ	57:m:93:CYS:HA	2.49	0.46
10:DB:644:GLN:O	16:HC:413:LEU:HA	2.15	0.46
21:PI:69:ILE:O	21:PI:72:VAL:HG22	2.15	0.46
30:DE:461:ILE:O	31:DF:135:TRP:CE3	2.68	0.46
31:DF:412:LEU:HG	31:DF:412:LEU:O	2.15	0.46
48:g:107:GLU:O	48:g:111:ASP:N	2.47	0.46
50:n:929:ARG:HB2	50:n:933:VAL:HG13	1.97	0.46
53:a:450:PHE:CZ	53:a:467:MET:HB2	2.50	0.46
54:d:45:ILE:O	56:i:76:MET:SD	2.73	0.46
56:i:96:GLU:HA	56:i:99:LYS:CD	2.45	0.46
58:q:494:GLN:HB2	61:c:251:LEU:HD11	1.95	0.46
60:b:174:ILE:HD13	63:l:58:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:c:245:HIS:HD2	61:c:295:THR:O	1.97	0.46
63:l:166:LEU:CD2	69:v:123:ILE:HD12	2.45	0.46
65:h:187:PHE:HE2	65:h:189:LYS:HD3	1.80	0.46
66:k:44:LEU:CD1	66:k:44:LEU:C	2.88	0.46
77:NY:-93:DG:H2"	77:NY:-92:DG:C8	2.50	0.46
3:BA:128:ILE:HG23	3:BA:183:VAL:CG1	2.44	0.46
5:EA:106:LYS:HD3	11:EB:220:TRP:CH2	2.50	0.46
7:HA:28:LEU:O	7:HA:32:LEU:HD23	2.16	0.46
16:HC:261:PHE:O	16:HC:265:LEU:HD23	2.14	0.46
31:DF:316:GLN:CG	31:DF:318:CYS:O	2.46	0.46
38:DH:110:TYR:CE1	33:DJ:161:LYS:HA	2.49	0.46
32:DI:19:MET:HG2	32:DI:40:LEU:HG	1.98	0.46
32:DI:131:SER:HB2	33:DJ:150:ARG:HH12	1.80	0.46
42:HH:605:ILE:HD12	42:HH:607:ILE:HD11	1.96	0.46
44:HI:99:GLU:C	44:HI:99:GLU:CD	2.82	0.46
45:HJ:102:ARG:HH11	45:HJ:102:ARG:CG	2.25	0.46
48:g:166:ASN:OD1	48:g:167:CYS:CA	2.63	0.46
50:n:153:ALA:O	50:n:154:ILE:C	2.59	0.46
50:n:938:ASP:HB2	50:n:1171:ALA:C	2.40	0.46
50:n:941:TYR:HE2	50:n:1172:SER:HB2	1.71	0.46
58:q:644:SER:HB3	62:e:96:LEU:HB2	1.96	0.46
68:t:130:THR:O	68:t:130:THR:OG1	2.25	0.46
69:v:82:LEU:HD23	69:v:82:LEU:HA	1.75	0.46
70:p:501:GLN:OE1	70:p:543:ARG:NH1	2.45	0.46
71:w:1267:MET:HB3	71:w:1267:MET:HE2	1.80	0.46
4:DA:1165:LEU:HB2	4:DA:1191:ILE:HG12	1.97	0.46
15:PB:128:ILE:CG2	15:PB:431:LEU:HD21	2.46	0.46
15:PB:596:ILE:HG22	15:PB:596:ILE:O	2.15	0.46
15:PB:724:TYR:HB3	15:PB:728:MET:HE3	1.97	0.46
16:HC:407:VAL:N	16:HC:443:VAL:O	2.47	0.46
32:Di:57:TYR:CD2	32:Di:73:LEU:CD1	2.98	0.46
30:DE:321:LEU:HB3	30:DE:330:TRP:HB2	1.97	0.46
37:DG:161:ASP:OD1	37:DG:161:ASP:N	2.48	0.46
39:HD:287:TYR:O	39:HD:288:THR:C	2.58	0.46
44:HI:207:LEU:HD22	55:f:52:MET:CE	2.43	0.46
50:n:199:LEU:CD2	50:n:222:VAL:HG13	2.45	0.46
50:n:478:MET:HE3	50:n:492:TRP:HB3	1.97	0.46
50:n:855:LEU:HD11	50:n:868:LEU:HD22	1.98	0.46
53:a:455:GLN:OE1	72:x:11:LEU:HD11	2.15	0.46
58:q:102:LEU:CD1	65:h:29:PHE:HD2	2.26	0.46
60:b:136:HIS:HB3	61:c:111:TYR:OH	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:o:752:VAL:HA	64:o:755:CYS:SG	2.56	0.46
70:p:266:ARG:HH11	70:p:341:ILE:HD13	1.80	0.46
72:x:11:LEU:HB2	72:x:14:TRP:CE3	2.47	0.46
12:FB:31:TRP:HD1	12:FB:62:LEU:HD21	1.81	0.46
30:DE:702:LEU:HD23	30:DE:702:LEU:C	2.39	0.46
31:DF:219:GLU:HB2	38:DH:160:ILE:CG2	2.17	0.46
39:HD:250:PRO:HD2	39:HD:251:LEU:HD22	1.97	0.46
41:HG:112:LYS:N	41:HG:142:GLU:O	2.41	0.46
42:HH:656:ASN:OD1	42:HH:657:ALA:N	2.49	0.46
45:HJ:177:ARG:CZ	45:HJ:177:ARG:CB	2.93	0.46
50:n:170:PRO:HG2	50:n:173:ILE:HD11	1.97	0.46
50:n:548:TYR:CE2	50:n:652:MET:HE2	2.51	0.46
50:n:801:ARG:NE	50:n:811:CYS:HB3	2.31	0.46
52:u:90:LEU:HD11	58:q:7:VAL:CG2	2.45	0.46
53:a:432:GLU:OE1	53:a:432:GLU:HA	2.14	0.46
53:a:445:LEU:HA	72:x:55:SER:OG	2.15	0.46
54:d:40:LEU:HB3	54:d:65:VAL:HG13	1.97	0.46
54:d:45:ILE:HG22	56:i:76:MET:HE3	1.86	0.46
54:d:163:ALA:HB2	57:m:106:GLN:HA	1.96	0.46
58:q:188:LEU:C	58:q:188:LEU:HD12	2.40	0.46
58:q:466:ASN:ND2	61:c:205:ARG:HG3	2.30	0.46
60:b:71:LEU:O	60:b:75:MET:HG2	2.15	0.46
60:b:129:GLN:NE2	60:b:129:GLN:HA	2.31	0.46
61:c:205:ARG:NH2	69:v:128:TYR:HD2	2.14	0.46
68:t:110:ILE:HD12	68:t:197:PHE:HB3	1.97	0.46
68:t:150:ALA:HB2	68:t:184:TYR:HB2	1.97	0.46
9:PA:491:PRO:HG3	9:PA:535:MET:HE2	1.96	0.46
9:PA:1468:THR:HG21	15:PB:1101:GLN:HG3	1.97	0.46
11:EB:145:VAL:HG11	11:EB:171:ILE:HG23	1.98	0.46
15:PB:910:THR:HG23	24:PL:42:ARG:O	2.15	0.46
31:Df:326:HIS:ND1	31:Df:326:HIS:N	2.63	0.46
29:DD:950:LEU:HD23	30:DE:523:VAL:HG11	1.97	0.46
30:DE:232:HIS:HD1	30:DE:313:SER:HG	1.56	0.46
30:DE:324:LYS:HA	30:DE:327:ASN:HB3	1.97	0.46
31:DF:92:ILE:HG13	31:DF:93:PRO:HD3	1.98	0.46
31:DF:122:LEU:N	31:DF:122:LEU:CD1	2.78	0.46
31:DF:320:ARG:C	31:DF:322:ASP:N	2.73	0.46
44:HI:37:ILE:N	44:HI:37:ILE:CD1	2.79	0.46
44:HI:241:CYS:HB2	44:HI:246:TYR:CD1	2.51	0.46
53:a:56:GLN:CD	54:d:51:SER:O	2.58	0.46
55:f:94:PRO:C	58:q:130:VAL:HG13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:i:109:LEU:HD21	56:i:117:GLN:HE22	1.79	0.46
58:q:644:SER:CB	62:e:96:LEU:HB3	2.44	0.46
62:e:132:HIS:CD2	69:v:126:ASP:HB3	2.50	0.46
63:l:149:LEU:HD11	69:v:139:SER:HA	1.97	0.46
64:o:720:PRO:O	64:o:721:LEU:C	2.58	0.46
66:k:96:ARG:HD3	69:v:116:LEU:HD12	1.97	0.46
70:p:207:CYS:HB3	70:p:242:TYR:HE2	1.79	0.46
70:p:787:LEU:HB3	70:p:791:PRO:HB3	1.97	0.46
72:x:529:MET:HE3	72:x:529:MET:HB3	1.77	0.46
7:HA:137:LEU:O	7:HA:142:VAL:HG11	2.15	0.46
7:HA:361:LEU:O	7:HA:365:VAL:HG12	2.16	0.46
27:DO:64:THR:HG22	27:DO:65:TYR:N	2.31	0.46
31:Df:328:ALA:C	31:Df:330:ARG:N	2.72	0.46
30:DE:773:TYR:CE1	31:DF:137:SER:HB2	2.50	0.46
31:DF:106:PHE:CD1	32:DI:13:PRO:CD	2.99	0.46
31:DF:411:VAL:HG13	31:DF:411:VAL:O	2.16	0.46
37:DG:129:LYS:HA	37:DG:129:LYS:HD2	1.77	0.46
38:DH:56:ALA:CB	33:DJ:214:PRO:HG2	2.36	0.46
32:DI:38:GLN:HA	32:DI:41:GLU:HB2	1.98	0.46
32:DI:131:SER:HA	33:DJ:150:ARG:HH22	1.81	0.46
44:HI:106:SER:HB3	44:HI:109:LEU:HD22	1.96	0.46
45:HJ:175:LYS:CE	45:HJ:175:LYS:CA	2.86	0.46
55:f:45:CYS:O	55:f:48:GLU:HB2	2.15	0.46
56:i:112:GLU:H	56:i:112:GLU:HG3	1.43	0.46
58:q:113:TYR:CE2	65:h:20:ALA:HB2	2.51	0.46
58:q:506:HIS:CD2	58:q:508:ASP:H	2.34	0.46
68:t:202:LYS:O	68:t:203:GLN:C	2.56	0.46
71:w:615:ILE:O	71:w:620:ARG:NH2	2.48	0.46
72:x:565:SER:O	72:x:567:MET:N	2.48	0.46
72:x:847:PHE:HB2	72:x:899:ARG:HG2	1.97	0.46
4:DA:900:ASP:HB3	37:DG:154:LYS:HD2	1.97	0.46
5:EA:22:ILE:HG12	5:EA:34:LEU:HD22	1.97	0.46
5:EA:181:ASN:ND2	39:HD:9:CYS:C	2.74	0.46
9:PA:400:ASP:OD1	9:PA:401:ARG:N	2.49	0.46
10:DB:27:LYS:CE	10:DB:490:SER:HB3	2.45	0.46
10:DB:71:ARG:HD3	10:DB:73:TYR:CE1	2.51	0.46
10:DB:568:VAL:HG22	10:DB:628:ILE:HG23	1.98	0.46
23:PK:105:PHE:CD2	23:PK:109:ILE:HD11	2.51	0.46
31:Df:327:TRP:O	31:Df:330:ARG:HB2	2.16	0.46
29:DD:949:GLN:HA	29:DD:952:GLN:HG2	1.97	0.46
30:DE:464:TYR:CD2	31:DF:133:ALA:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:47:ILE:HD11	32:DI:43:ALA:CB	2.28	0.46
31:DF:424:GLN:O	31:DF:428:LEU:HG	2.16	0.46
38:DH:119:ILE:O	33:DJ:131:PRO:HG3	2.15	0.46
39:HD:28:HIS:HB3	39:HD:30:LEU:HG	1.96	0.46
42:HH:185:ILE:HG22	42:HH:189:LEU:HD13	1.97	0.46
44:HI:258:HIS:C	44:HI:258:HIS:ND1	2.73	0.46
50:n:237:MET:HE1	58:q:45:GLN:HG2	1.96	0.46
50:n:238:GLY:N	50:n:243:VAL:HG21	2.31	0.46
54:d:110:LEU:C	54:d:110:LEU:CD2	2.86	0.46
55:f:74:GLN:HB3	55:f:78:LEU:HB2	1.97	0.46
58:q:103:ARG:HH11	58:q:103:ARG:HB2	1.81	0.46
64:o:715:LEU:HD12	64:o:748:PHE:CZ	2.50	0.46
66:k:58:HIS:ND1	66:k:58:HIS:C	2.73	0.46
66:k:103:LYS:HD3	66:k:103:LYS:HA	1.70	0.46
70:p:128:GLY:HA3	72:x:708:LYS:HB2	1.97	0.46
1:X:-6:DG:H2"	1:X:-5:DT:C6	2.51	0.46
9:PA:1261:ILE:HG22	9:PA:1262:MET:N	2.31	0.46
15:PB:553:LEU:HD23	15:PB:556:ILE:HD11	1.98	0.46
15:PB:993:LYS:NZ	15:PB:995:GLU:OE1	2.44	0.46
16:HC:440:LEU:HD22	43:HF:36:GLN:CD	2.41	0.46
23:PK:37:LYS:N	23:PK:69:HIS:O	2.49	0.46
30:DE:646:SER:OG	30:DE:647:ALA:N	2.48	0.46
30:DE:702:LEU:HD22	30:DE:702:LEU:H	1.81	0.46
31:DF:83:LEU:HD12	31:DF:83:LEU:H	1.81	0.46
39:HD:301:PHE:CE1	45:HJ:170:PHE:CZ	3.04	0.46
40:HE:13:ILE:HG21	40:HE:41:VAL:HG13	1.97	0.46
44:HI:134:LEU:HG	44:HI:162:PHE:CD1	2.50	0.46
50:n:252:ILE:HG21	50:n:303:LEU:HD13	1.97	0.46
50:n:802:VAL:HG22	50:n:809:ILE:HB	1.97	0.46
50:n:904:PHE:HE2	50:n:1208:GLU:CB	2.20	0.46
53:a:297:VAL:HG12	53:a:299:LEU:HG	1.97	0.46
55:f:19:SER:O	55:f:22:PRO:HD2	2.16	0.46
58:q:112:LEU:HD23	65:h:19:VAL:CG2	2.45	0.46
58:q:166:ARG:HH11	58:q:166:ARG:HG3	1.80	0.46
58:q:449:ASP:OD2	63:l:157:LYS:HD3	2.16	0.46
59:z:597:VAL:O	59:z:598:CYS:C	2.59	0.46
61:c:288:LEU:CD2	68:t:122:PHE:CZ	2.99	0.46
63:l:149:LEU:CD1	69:v:139:SER:HA	2.45	0.46
68:t:15:LYS:HB3	68:t:15:LYS:HE2	1.68	0.46
71:w:31:GLU:HB2	71:w:36:LYS:HD3	1.97	0.46
5:EA:17:LEU:O	5:EA:21:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:PA:458:PHE:HE2	9:PA:484:LEU:HD11	1.80	0.46
9:PA:1357:THR:O	18:PE:142:HIS:NE2	2.46	0.46
10:DB:559:LYS:HB2	10:DB:559:LYS:NZ	2.31	0.46
27:DO:1:MET:CE	29:DD:993:GLN:HB3	2.42	0.46
30:De:717:LEU:HD22	30:De:726:LEU:HD11	1.97	0.46
31:Df:83:LEU:HD22	32:Di:41:GLU:HG2	1.98	0.46
32:Di:62:LYS:CG	35:Dl:106:ARG:NH1	2.79	0.46
29:DD:874:LEU:HG	29:DD:877:PRO:HD2	1.97	0.46
31:DF:50:ILE:O	31:DF:54:ALA:N	2.47	0.46
38:DH:110:TYR:CG	33:DJ:161:LYS:HB2	2.50	0.46
39:HD:21:LEU:HD21	39:HD:29:THR:HG23	1.98	0.46
39:HD:42:GLY:O	47:PG:164:MET:CE	2.64	0.46
45:HJ:15:SER:O	45:HJ:18:GLN:HG3	2.15	0.46
45:HJ:207:TYR:HD2	45:HJ:255:MET:HE3	1.81	0.46
48:g:127:ARG:HA	48:g:130:GLN:CB	2.30	0.46
50:n:166:TYR:HH	57:m:70:PRO:C	2.23	0.46
50:n:201:HIS:CE1	54:d:111:GLN:HE22	2.34	0.46
50:n:509:ILE:HG21	50:n:540:ILE:HD13	1.97	0.46
53:a:160:LEU:HG	53:a:219:LEU:HD11	1.98	0.46
53:a:462:LEU:HD11	72:x:60:ILE:CD1	2.40	0.46
58:q:443:ARG:NE	58:q:443:ARG:CA	2.73	0.46
61:c:290:ASP:O	68:t:120:CYS:SG	2.74	0.46
65:h:52:LEU:O	65:h:56:LEU:HD12	2.16	0.46
68:t:46:TYR:HB2	68:t:63:MET:HB2	1.98	0.46
7:HA:107:LEU:HD12	7:HA:195:ALA:HB1	1.98	0.46
7:HA:109:LEU:HD12	7:HA:207:TYR:CD2	2.51	0.46
7:HA:460:THR:HB	7:HA:661:ALA:HB1	1.98	0.46
9:PA:340:LYS:HE2	9:PA:1436:VAL:HG11	1.98	0.46
9:PA:1643:TYR:CE1	57:m:93:CYS:HA	2.50	0.46
10:DB:539:ARG:O	10:DB:540:LYS:C	2.58	0.46
11:EB:139:PHE:HZ	11:EB:144:ASN:OD1	1.99	0.46
11:EB:220:TRP:CD1	11:EB:220:TRP:C	2.94	0.46
16:HC:444:THR:HG23	16:HC:447:GLY:H	1.81	0.46
26:DQ:321:SER:OG	26:DQ:322:ASP:N	2.48	0.46
33:Dj:176:MET:HE1	36:Dm:75:ILE:HD11	1.97	0.46
31:DF:83:LEU:CD1	31:DF:83:LEU:H	2.29	0.46
38:DH:49:GLY:O	33:DJ:171:LEU:CD1	2.60	0.46
35:DL:111:LEU:N	35:DL:114:LYS:NZ	2.64	0.46
39:HD:145:GLU:OE2	65:h:67:LYS:HE2	2.16	0.46
39:HD:254:GLU:CD	39:HD:254:GLU:N	2.62	0.46
43:HF:49:LEU:HD12	43:HF:52:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:j:113:LEU:HA	49:j:116:VAL:HG12	1.98	0.46
50:n:226:VAL:HG13	50:n:230:PHE:N	2.31	0.46
50:n:959:LEU:HD12	50:n:963:LEU:HD23	1.98	0.46
52:u:87:ALA:HB1	58:q:7:VAL:HG21	1.97	0.46
53:a:69:LEU:HD13	53:a:69:LEU:HA	1.86	0.46
53:a:224:TYR:HE1	53:a:254:ASN:C	2.23	0.46
57:m:93:CYS:O	57:m:97:ILE:HG22	2.16	0.46
58:q:255:ALA:HB3	58:q:301:VAL:HG22	1.97	0.46
58:q:418:ILE:HD13	68:t:72:PRO:CG	2.36	0.46
60:b:178:LEU:HD13	63:l:55:LEU:HD21	1.98	0.46
64:o:710:LEU:HG	64:o:776:TRP:CH2	2.51	0.46
2:Y:-17:DG:H2"	2:Y:-16:DA:C8	2.51	0.45
4:DA:565:TRP:HA	4:DA:565:TRP:CE3	2.51	0.45
15:PB:809:VAL:HG11	15:PB:811:TYR:CZ	2.51	0.45
16:HC:52:ALA:HB1	16:HC:90:LEU:HD21	1.99	0.45
21:PI:39:CYS:SG	21:PI:42:CYS:HB3	2.56	0.45
29:Dd:941:ARG:NH2	32:Di:123:THR:O	2.48	0.45
34:Dk:150:VAL:HG22	36:Dm:82:GLN:HB3	1.98	0.45
29:DD:888:LYS:HB2	29:DD:888:LYS:NZ	2.32	0.45
45:HJ:279:ARG:HH21	45:HJ:279:ARG:HG3	1.81	0.45
51:s:106:SER:HA	51:s:108:PHE:O	2.16	0.45
53:a:455:GLN:HB2	72:x:11:LEU:CG	2.45	0.45
53:a:466:VAL:HB	72:x:54:PRO:CD	2.46	0.45
53:a:518:ILE:HG22	53:a:518:ILE:O	2.17	0.45
54:d:167:TRP:CE3	57:m:106:GLN:NE2	2.84	0.45
57:m:21:GLU:O	57:m:25:VAL:HG23	2.17	0.45
58:q:110:CYS:SG	65:h:23:LYS:CD	3.03	0.45
64:o:733:SER:HB3	64:o:766:LYS:HA	1.98	0.45
66:k:37:LYS:H	66:k:37:LYS:CD	2.27	0.45
67:r:16:ILE:H	67:r:16:ILE:HG12	1.55	0.45
71:w:1183:TRP:CH2	71:w:1185:GLY:HA3	2.52	0.45
4:DA:1063:LYS:HD3	4:DA:1063:LYS:O	2.16	0.45
6:FA:163:GLU:O	6:FA:166:ARG:N	2.49	0.45
7:HA:77:VAL:HA	7:HA:80:ILE:HG22	1.97	0.45
9:PA:502:ASN:HB3	15:PB:1084:LEU:HD13	1.98	0.45
12:FB:194:HIS:ND1	12:FB:196:TYR:O	2.49	0.45
38:DH:110:TYR:CB	33:DJ:161:LYS:HD3	2.44	0.45
42:HH:294:GLU:OE2	42:HH:334:ARG:NH1	2.49	0.45
44:HI:141:ASN:C	44:HI:143:LEU:N	2.70	0.45
46:PD:79:THR:HG22	65:h:51:LEU:CG	2.46	0.45
50:n:444:GLU:HB3	50:n:445:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:1335:ASN:C	50:n:1337:GLN:H	2.25	0.45
52:u:122:LEU:CD2	52:u:125:ILE:HB	2.46	0.45
54:d:126:TYR:CE1	58:q:36:MET:HB2	2.51	0.45
62:e:74:ARG:HD2	62:e:78:ASP:OD2	2.17	0.45
70:p:569:LEU:HD23	70:p:569:LEU:H	1.81	0.45
73:y:220:MET:HE3	73:y:220:MET:HB3	1.76	0.45
7:HA:600:ALA:HB1	7:HA:659:HIS:HD2	1.82	0.45
9:PA:1034:GLN:HE22	9:PA:1038:THR:HG21	1.82	0.45
17:PC:260:GLN:HB2	23:PK:91:ILE:HG21	1.97	0.45
26:DQ:22:ILE:HG22	26:DQ:39:LEU:HD11	1.99	0.45
31:Df:257:PRO:O	31:Df:261:THR:OG1	2.32	0.45
31:DF:279:LEU:HB3	31:DF:330:ARG:HD2	1.97	0.45
45:HJ:52:GLU:HB3	45:HJ:273:LEU:CD1	2.42	0.45
48:g:75:LYS:HD2	52:u:77:PRO:C	2.42	0.45
48:g:86:LEU:HD22	49:j:113:LEU:HD11	1.97	0.45
48:g:175:LEU:HD22	56:i:129:ASN:OD1	2.15	0.45
50:n:201:HIS:CE1	52:u:122:LEU:HG	2.50	0.45
50:n:249:LYS:C	50:n:250:LEU:HD22	2.41	0.45
50:n:359:ILE:CG2	50:n:372:ILE:HD13	2.42	0.45
50:n:637:PHE:HD2	50:n:639:LYS:HG2	1.82	0.45
52:u:102:THR:O	52:u:105:GLU:HG2	2.17	0.45
52:u:106:ASP:O	52:u:110:ARG:HG3	2.16	0.45
53:a:99:THR:HG22	53:a:112:VAL:HG13	1.96	0.45
53:a:439:GLN:HB2	72:x:15:LYS:HG2	1.99	0.45
57:m:116:GLN:CG	59:z:594:LEU:HG	2.47	0.45
58:q:113:TYR:CD1	58:q:113:TYR:C	2.93	0.45
58:q:188:LEU:HA	69:v:87:ILE:HG13	1.96	0.45
58:q:190:LEU:HD13	58:q:190:LEU:C	2.41	0.45
69:v:115:LYS:HD3	69:v:115:LYS:HA	1.45	0.45
4:DA:404:MET:HE2	4:DA:404:MET:HA	1.99	0.45
4:DA:464:TRP:O	4:DA:464:TRP:CE3	2.70	0.45
11:EB:213:ASP:OD1	11:EB:214:GLU:N	2.50	0.45
30:DE:447:THR:HG23	30:DE:450:ARG:CZ	2.46	0.45
31:DF:63:ARG:NH2	31:DF:70:ASP:OD1	2.41	0.45
31:DF:71:ILE:HD11	32:DI:35:VAL:CG2	2.45	0.45
39:HD:37:LEU:O	39:HD:40:VAL:HG12	2.16	0.45
39:HD:284:ALA:C	39:HD:286:GLY:N	2.73	0.45
44:HI:178:TYR:HE2	44:HI:202:ILE:HG13	1.81	0.45
46:PD:137:LYS:HE2	65:h:55:GLN:NE2	2.29	0.45
47:PG:117:MET:HE3	47:PG:137:ILE:HD13	1.98	0.45
48:g:128:PRO:HD2	48:g:129:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:n:443:LEU:HD12	50:n:500:LEU:HD22	1.98	0.45
53:a:443:CYS:SG	72:x:57:ASN:HA	2.56	0.45
56:i:100:LEU:C	56:i:100:LEU:HD13	2.41	0.45
65:h:26:LEU:HD23	65:h:26:LEU:HA	1.75	0.45
68:t:96:VAL:HA	68:t:99:LYS:HG2	1.99	0.45
70:p:618:LEU:HD13	70:p:662:ILE:HG12	1.99	0.45
71:w:370:ASP:OD1	71:w:370:ASP:N	2.49	0.45
72:x:289:CYS:SG	72:x:313:ILE:HG13	2.56	0.45
5:EA:48:MET:HE1	5:EA:92:TYR:HB2	1.97	0.45
12:FB:179:ASP:CG	29:DD:1002:ARG:HH21	2.24	0.45
15:PB:694:THR:HG22	15:PB:695:HIS:ND1	2.31	0.45
30:De:633:THR:O	30:De:634:ARG:NH2	2.45	0.45
31:Df:317:LEU:HD12	31:Df:329:LEU:HD23	1.98	0.45
30:DE:702:LEU:N	30:DE:702:LEU:CD2	2.78	0.45
31:DF:233:GLY:HA2	31:DF:239:ARG:HE	1.82	0.45
31:DF:276:LEU:HD22	31:DF:323:VAL:HG22	1.98	0.45
41:HG:199:ILE:CG2	41:HG:222:ILE:HD11	2.47	0.45
50:n:527:THR:O	50:n:528:HIS:HB2	2.15	0.45
50:n:1185:LEU:HD12	50:n:1185:LEU:O	2.16	0.45
53:a:509:ARG:HB2	53:a:509:ARG:HH11	1.77	0.45
55:f:111:LEU:O	55:f:115:ILE:HG13	2.15	0.45
56:i:108:HIS:C	56:i:109:LEU:HG	2.42	0.45
58:q:118:ILE:CG2	58:q:125:MET:HG2	2.46	0.45
64:o:714:ASP:C	72:x:28:LYS:HZ2	2.15	0.45
67:r:125:MET:HE3	67:r:125:MET:HB3	1.82	0.45
71:w:512:THR:OG1	71:w:513:ASN:ND2	2.50	0.45
4:DA:346:ALA:HB2	31:Df:262:PHE:HA	1.98	0.45
5:EA:105:TYR:OH	11:EB:236:TYR:HB3	2.17	0.45
7:HA:329:PHE:O	7:HA:333:LEU:HD23	2.17	0.45
9:PA:348:GLY:O	9:PA:352:GLY:N	2.46	0.45
9:PA:495:ASP:C	9:PA:495:ASP:OD1	2.60	0.45
9:PA:510:GLU:CD	15:PB:1101:GLN:HE22	2.25	0.45
13:HB:472:LEU:HD12	13:HB:476:TRP:CD1	2.52	0.45
15:PB:710:ILE:HA	15:PB:764:MET:HE2	1.99	0.45
29:Dd:860:VAL:HA	36:Dm:47:GLN:HG2	1.98	0.45
31:Df:58:MET:HE3	31:Df:64:GLN:HA	1.98	0.45
30:DE:290:HIS:CG	31:DF:45:TYR:CE2	3.05	0.45
30:DE:774:MET:O	31:DF:142:GLN:NE2	2.49	0.45
38:DH:50:PHE:HB3	33:DJ:194:THR:C	2.42	0.45
40:HE:235:GLN:O	40:HE:235:GLN:NE2	2.47	0.45
44:HI:280:PRO:HA	44:HI:283:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:PD:83:VAL:O	46:PD:87:LEU:HD23	2.15	0.45
47:PG:153:ASP:OD1	47:PG:154:LYS:N	2.50	0.45
50:n:707:ASP:CG	64:o:684:ARG:HD3	2.42	0.45
50:n:865:VAL:O	50:n:869:LEU:HG	2.17	0.45
50:n:948:LYS:HD2	50:n:948:LYS:HA	1.70	0.45
52:u:96:GLU:O	52:u:99:GLU:HG3	2.17	0.45
53:a:131:ASN:ND2	53:a:131:ASN:N	2.63	0.45
53:a:417:TYR:CZ	53:a:450:PHE:HD1	2.21	0.45
54:d:45:ILE:HG12	56:i:73:ILE:HG12	1.95	0.45
58:q:479:ILE:C	58:q:532:HIS:CE1	2.92	0.45
68:t:89:THR:C	68:t:91:PHE:N	2.74	0.45
70:p:583:ILE:HG23	70:p:587:ILE:HD12	1.98	0.45
72:x:832:GLN:NE2	72:x:835:ARG:HH21	2.15	0.45
5:EA:188:TYR:CD2	39:HD:14:TYR:HB3	2.52	0.45
30:DE:507:VAL:HG11	30:DE:513:LEU:HD12	1.97	0.45
39:HD:6:CYS:O	39:HD:10:LYS:HE3	2.17	0.45
45:HJ:145:GLU:H	45:HJ:145:GLU:HG2	1.50	0.45
50:n:270:GLN:HG3	55:f:181:LEU:HD12	1.98	0.45
50:n:273:PHE:O	50:n:276:GLN:HG3	2.17	0.45
50:n:436:PRO:HG3	50:n:458:LEU:HD21	1.99	0.45
58:q:116:LEU:HD22	58:q:116:LEU:HA	1.73	0.45
66:k:37:LYS:CE	66:k:37:LYS:N	2.73	0.45
68:t:46:TYR:HD2	68:t:63:MET:HB3	1.81	0.45
68:t:173:PRO:CD	68:t:173:PRO:O	2.65	0.45
71:w:44:PHE:HE2	71:w:92:LEU:HD11	1.81	0.45
71:w:315:SER:OG	71:w:319:GLU:OE1	2.31	0.45
72:x:956:VAL:HG11	72:x:968:LEU:HD21	1.98	0.45
4:DA:857:MET:HE3	4:DA:858:ASP:H	1.81	0.45
5:EA:187:ILE:HD12	5:EA:187:ILE:H	1.82	0.45
7:HA:345:ARG:HD2	39:HD:1:MET:SD	2.57	0.45
9:PA:24:GLY:O	15:PB:1168:ALA:HB3	2.17	0.45
9:PA:622:SER:OG	9:PA:626:THR:HG22	2.17	0.45
27:DO:2:ALA:N	29:DD:1000:ARG:CD	2.80	0.45
32:DI:67:ASP:OD1	32:DI:67:ASP:C	2.60	0.45
39:HD:145:GLU:OE1	65:h:67:LYS:CE	2.61	0.45
44:HI:141:ASN:C	44:HI:143:LEU:H	2.24	0.45
44:HI:269:LEU:HD13	44:HI:269:LEU:C	2.42	0.45
48:g:126:TYR:CE2	52:u:77:PRO:O	2.70	0.45
50:n:281:ARG:CG	55:f:190:PRO:HA	2.46	0.45
58:q:440:LEU:CD2	58:q:502:ILE:HD11	2.47	0.45
58:q:549:LEU:HD11	58:q:572:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:o:681:GLU:OE1	64:o:768:SER:OG	2.35	0.45
64:o:706:LEU:HG	64:o:723:LEU:HB3	1.99	0.45
71:w:549:LYS:HD3	71:w:549:LYS:HA	1.83	0.45
71:w:673:LYS:HE2	71:w:678:ALA:HB2	1.99	0.45
2:Y:-2:DC:H2"	2:Y:-1:DG:C8	2.51	0.45
4:DA:396:LEU:H	4:DA:396:LEU:HD22	1.81	0.45
7:HA:434:HIS:CB	7:HA:632:ILE:HD11	2.47	0.45
15:PB:851:ASP:CG	24:PL:15:MET:HE2	2.42	0.45
29:Dd:1084:LEU:HB3	32:Di:99:ARG:HH21	1.81	0.45
30:DE:250:GLU:O	30:DE:254:ASN:ND2	2.50	0.45
30:DE:447:THR:HG23	30:DE:450:ARG:HD2	1.98	0.45
38:DH:121:ALA:CB	33:DJ:133:ALA:HB3	2.43	0.45
33:DJ:123:LEU:O	33:DJ:153:ARG:NH1	2.50	0.45
39:HD:55:LYS:O	39:HD:56:SER:OG	2.33	0.45
39:HD:291:LEU:HD12	39:HD:291:LEU:HA	1.74	0.45
46:PD:70:ARG:CD	69:v:20:LYS:HE3	2.47	0.45
50:n:918:PHE:HB2	50:n:1211:LEU:HD12	1.99	0.45
53:a:145:LYS:HD2	53:a:145:LYS:N	2.32	0.45
53:a:168:LYS:HE3	53:a:168:LYS:HB3	1.48	0.45
53:a:200:LEU:C	53:a:200:LEU:HD13	2.42	0.45
53:a:259:ILE:O	53:a:259:ILE:CD1	2.64	0.45
54:d:167:TRP:O	54:d:167:TRP:HE3	2.00	0.45
58:q:17:LYS:HB3	58:q:30:TYR:HE2	1.82	0.45
58:q:491:ILE:HG23	58:q:506:HIS:HE1	1.81	0.45
60:b:178:LEU:HD21	63:l:78:LEU:HB3	1.98	0.45
61:c:41:ASN:HD22	61:c:41:ASN:C	2.24	0.45
68:t:78:LEU:CD1	68:t:84:CYS:HB3	2.46	0.45
71:w:381:SER:O	71:w:534:HIS:ND1	2.48	0.45
72:x:676:ASP:OD1	72:x:676:ASP:N	2.50	0.45
9:PA:910:LYS:N	9:PA:911:PRO:HD2	2.32	0.45
9:PA:1669:PRO:CB	44:HI:259:HIS:NE2	2.79	0.45
16:HC:325:ILE:H	16:HC:325:ILE:HD12	1.82	0.45
36:Dm:80:ARG:HD2	36:Dm:80:ARG:HA	1.86	0.45
30:DE:458:LEU:O	31:DF:139:GLU:HA	2.16	0.45
45:HJ:181:LEU:N	45:HJ:181:LEU:CD1	2.72	0.45
46:PD:91:LYS:C	46:PD:92:LEU:HD22	2.42	0.45
50:n:523:SER:OG	50:n:583:ALA:O	2.34	0.45
52:u:115:LEU:CG	54:d:121:LEU:HD13	2.41	0.45
66:k:79:HIS:CD2	67:r:41:GLY:HA2	2.52	0.45
72:x:294:ILE:HA	72:x:354:ARG:HD3	1.99	0.45
72:x:420:ILE:HA	72:x:423:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FA:127:PHE:CE2	12:FB:21:VAL:HG21	2.51	0.44
9:PA:68:THR:HG23	9:PA:68:THR:O	2.16	0.44
9:PA:1382:LEU:O	9:PA:1385:VAL:HG22	2.18	0.44
13:HB:400:ILE:H	13:HB:400:ILE:HD12	1.82	0.44
13:HB:457:ILE:HG22	13:HB:461:LEU:HD13	1.98	0.44
29:DD:872:PHE:CZ	35:DL:57:VAL:CG1	2.79	0.44
30:DE:470:TYR:CD1	38:DH:26:ALA:HA	2.51	0.44
31:DF:320:ARG:CB	31:DF:415:ILE:HD12	2.48	0.44
35:DL:63:LEU:O	35:DL:67:VAL:HG13	2.17	0.44
41:HG:121:SER:OG	41:HG:127:HIS:NE2	2.39	0.44
46:PD:70:ARG:NH2	47:PG:88:VAL:HG22	2.32	0.44
50:n:1219:HIS:CD2	50:n:1222:ARG:HH11	2.35	0.44
53:a:74:LEU:HD22	53:a:74:LEU:HA	1.74	0.44
53:a:103:ILE:HG23	53:a:108:PHE:HB2	1.99	0.44
54:d:89:ILE:HG21	56:i:114:GLN:HG3	1.99	0.44
54:d:156:SER:HB3	54:d:161:VAL:HG11	1.99	0.44
55:f:60:LEU:H	55:f:60:LEU:HG	1.35	0.44
55:f:111:LEU:HD22	58:q:127:LEU:HD11	1.97	0.44
58:q:32:PRO:HB2	58:q:34:LEU:HD21	1.99	0.44
58:q:543:VAL:CG1	61:c:135:ARG:HE	2.29	0.44
60:b:156:PRO:HD2	60:b:159:GLN:HG2	1.99	0.44
62:e:113:GLU:OE2	63:l:31:ALA:HB3	2.16	0.44
64:o:698:CYS:HB2	64:o:705:HIS:CD2	2.52	0.44
68:t:81:ASN:N	68:t:81:ASN:OD1	2.51	0.44
68:t:161:LEU:O	68:t:165:LEU:N	2.50	0.44
70:p:41:CYS:SG	70:p:42:ARG:N	2.90	0.44
71:w:274:LEU:O	71:w:333:HIS:NE2	2.40	0.44
71:w:339:ILE:HD11	71:w:378:GLN:HB3	1.99	0.44
71:w:1139:ARG:O	71:w:1140:GLU:HG3	2.17	0.44
72:x:742:TYR:HA	72:x:782:VAL:HG11	1.99	0.44
8:NE:643:PRO:HA	76:NX:98:DC:H5'	1.99	0.44
74:NG:1016:ALA:O	74:NG:1017:VAL:CB	2.65	0.44
4:DA:396:LEU:H	4:DA:396:LEU:CD1	2.20	0.44
5:EA:174:ARG:HH21	39:HD:40:VAL:HG11	1.83	0.44
9:PA:72:GLN:N	9:PA:72:GLN:OE1	2.50	0.44
9:PA:1665:SER:HB2	54:d:180:LEU:HD21	1.99	0.44
12:FB:30:GLN:O	12:FB:62:LEU:HD11	2.16	0.44
15:PB:738:THR:HG21	22:PJ:58:LYS:CG	2.48	0.44
16:HC:157:GLU:O	16:HC:161:HIS:ND1	2.51	0.44
17:PC:245:VAL:HG11	23:PK:105:PHE:CZ	2.52	0.44
21:PI:58:ILE:HD12	21:PI:58:ILE:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DD:948:GLU:CD	29:DD:948:GLU:C	2.85	0.44
36:Dm:103:LEU:O	36:Dm:107:ASN:ND2	2.51	0.44
41:HG:242:SER:N	41:HG:245:SER:OG	2.50	0.44
42:HH:99:PHE:CZ	42:HH:103:ILE:HD13	2.53	0.44
45:HJ:36:ALA:O	45:HJ:37:ASN:C	2.60	0.44
45:HJ:268:GLU:CD	45:HJ:268:GLU:N	2.74	0.44
48:g:127:ARG:H	48:g:128:PRO:HD3	1.81	0.44
49:j:82:LYS:NZ	51:s:96:PHE:CD1	2.85	0.44
52:u:61:LEU:HD22	52:u:64:ARG:HD3	1.99	0.44
53:a:64:THR:HG22	53:a:86:ARG:HD2	1.98	0.44
58:q:263:LYS:HD2	58:q:263:LYS:HA	1.34	0.44
58:q:425:GLU:HG2	58:q:429:GLU:HB3	1.97	0.44
65:h:25:SER:OG	65:h:52:LEU:HB2	2.17	0.44
66:k:86:SER:CB	69:v:105:LEU:HD12	2.47	0.44
70:p:131:ILE:HD13	70:p:183:THR:HG22	1.99	0.44
71:w:623:LEU:HD12	71:w:623:LEU:HA	1.74	0.44
71:w:1135:PRO:O	71:w:1136:LEU:HB2	2.17	0.44
4:DA:784:GLN:H	4:DA:1073:GLN:NE2	2.12	0.44
5:EA:139:LEU:HD12	47:PG:151:ARG:NH1	2.32	0.44
6:FA:151:ARG:HG2	6:FA:151:ARG:O	2.18	0.44
7:HA:475:PRO:HG3	7:HA:478:MET:HE2	1.99	0.44
11:EB:133:ILE:O	11:EB:134:ASP:OD1	2.35	0.44
25:DP:179:ASP:OD1	25:DP:182:THR:N	2.41	0.44
30:De:542:HIS:CE1	30:De:568:ARG:HG3	2.52	0.44
30:DE:521:ASP:C	30:DE:521:ASP:OD1	2.61	0.44
30:DE:784:HIS:HB3	30:DE:792:LEU:HB2	1.99	0.44
31:DF:350:ASN:OD1	31:DF:350:ASN:N	2.51	0.44
38:DH:194:MET:HE2	38:DH:194:MET:HB2	1.85	0.44
32:DI:16:ALA:CB	32:DI:40:LEU:HD11	2.47	0.44
32:DI:19:MET:HB2	32:DI:40:LEU:HD21	1.99	0.44
35:DL:64:GLN:CD	35:DL:64:GLN:N	2.75	0.44
39:HD:43:ALA:CB	47:PG:164:MET:CG	2.86	0.44
39:HD:97:ASP:O	39:HD:101:GLU:OE1	2.36	0.44
39:HD:271:TYR:CE2	39:HD:273:ASN:HB3	2.51	0.44
40:HE:201:GLY:O	40:HE:204:GLN:HG2	2.17	0.44
50:n:204:VAL:HB	52:u:129:GLN:OE1	2.17	0.44
50:n:231:GLU:HB2	50:n:253:LEU:HD21	1.98	0.44
52:u:67:LYS:HE2	59:z:528:LEU:HD13	1.99	0.44
53:a:109:TYR:CE1	53:a:150:PHE:CZ	3.05	0.44
54:d:139:ARG:HD3	54:d:139:ARG:HA	1.75	0.44
58:q:377:LEU:CD1	63:l:177:ARG:HA	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:437:HIS:O	58:q:437:HIS:CD2	2.71	0.44
64:o:703:THR:HB	64:o:726:PRO:HA	1.99	0.44
65:h:38:GLY:C	65:h:40:LEU:H	2.25	0.44
72:x:255:ASN:OD1	72:x:255:ASN:N	2.47	0.44
1:X:-7:DC:H2"	1:X:-6:DG:C8	2.52	0.44
5:EA:20:TYR:HD2	5:EA:190:LEU:HD11	1.77	0.44
5:EA:26:TYR:CD1	11:EB:220:TRP:CZ2	3.06	0.44
9:PA:273:GLN:HB3	9:PA:277:THR:HG21	2.00	0.44
9:PA:913:ASN:OD1	9:PA:963:ARG:NH1	2.48	0.44
9:PA:1341:VAL:O	9:PA:1341:VAL:HG23	2.17	0.44
9:PA:1653:THR:O	57:m:39:GLN:HG2	2.16	0.44
9:PA:1663:SER:HB3	9:PA:1664:TYR:H	1.55	0.44
10:DB:414:LEU:HB2	10:DB:523:VAL:HG13	1.99	0.44
10:DB:859:ARG:HD2	10:DB:859:ARG:HA	1.81	0.44
18:PE:159:LEU:HD12	18:PE:163:TYR:CD2	2.53	0.44
29:DD:947:PHE:HB3	32:DI:113:PRO:HD3	1.98	0.44
31:DF:83:LEU:CD1	31:DF:83:LEU:N	2.79	0.44
31:DF:426:LEU:C	31:DF:426:LEU:HD23	2.42	0.44
39:HD:295:ARG:CD	39:HD:295:ARG:C	2.91	0.44
44:HI:16:ASP:HB3	44:HI:28:LYS:HB3	1.98	0.44
44:HI:140:PRO:HD3	44:HI:178:TYR:CE1	2.52	0.44
44:HI:279:ASN:O	44:HI:280:PRO:C	2.60	0.44
50:n:273:PHE:CZ	55:f:185:ARG:CG	3.00	0.44
53:a:109:TYR:CE2	53:a:154:LEU:HD23	2.52	0.44
53:a:177:LEU:HB2	53:a:259:ILE:HG13	1.99	0.44
53:a:357:LEU:HD22	53:a:357:LEU:HA	1.77	0.44
53:a:466:VAL:HG13	53:a:478:LYS:H	1.82	0.44
54:d:44:LEU:O	54:d:44:LEU:HD23	2.17	0.44
54:d:109:GLN:HA	54:d:112:LYS:NZ	2.32	0.44
54:d:167:TRP:O	54:d:167:TRP:CE3	2.70	0.44
58:q:109:MET:CA	58:q:109:MET:CE	2.86	0.44
58:q:127:LEU:HG	58:q:127:LEU:O	2.17	0.44
58:q:185:SER:CB	66:k:10:ARG:HH22	2.31	0.44
58:q:465:SER:OG	61:c:210:ASP:OD2	2.34	0.44
58:q:469:ASP:HB2	61:c:231:TRP:CD2	2.52	0.44
63:l:167:ILE:HD12	69:v:127:LEU:CD2	2.47	0.44
66:k:88:LYS:C	66:k:88:LYS:CD	2.89	0.44
67:r:180:ASP:C	67:r:182:VAL:H	2.25	0.44
69:v:133:GLU:C	69:v:133:GLU:CD	2.85	0.44
70:p:40:SER:HB3	70:p:89:TRP:CD2	2.52	0.44
71:w:726:ASN:H	71:w:726:ASN:HD22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:x:495:ILE:HG22	72:x:499:MET:HE2	1.99	0.44
4:DA:690:LEU:HD22	4:DA:747:LEU:HD22	1.99	0.44
5:EA:105:TYR:CE2	11:EB:233:ILE:HA	2.52	0.44
7:HA:613:HIS:O	7:HA:613:HIS:ND1	2.50	0.44
10:DB:539:ARG:C	10:DB:542:ASN:H	2.25	0.44
12:FB:94:THR:HG22	12:FB:109:ILE:HG22	2.00	0.44
12:FB:220:ILE:HG13	12:FB:221:GLY:H	1.82	0.44
16:HC:334:MET:HB3	42:HH:58:ALA:HB2	1.98	0.44
27:DO:2:ALA:C	29:DD:1000:ARG:HB3	2.40	0.44
29:DD:947:PHE:HE1	30:DE:573:GLN:HE22	1.66	0.44
31:DF:323:VAL:O	31:DF:326:HIS:HB2	2.18	0.44
38:DH:59:GLU:HA	38:DH:62:THR:HG22	1.99	0.44
32:DI:23:LEU:HD13	32:DI:31:TYR:CZ	2.52	0.44
44:HI:48:ARG:HA	44:HI:48:ARG:HD3	1.77	0.44
44:HI:66:LEU:HD12	44:HI:66:LEU:HA	1.70	0.44
44:HI:209:ARG:CG	55:f:53:GLN:OE1	2.62	0.44
44:HI:247:VAL:O	44:HI:248:THR:C	2.58	0.44
45:HJ:208:THR:O	45:HJ:212:ILE:HG13	2.18	0.44
46:PD:79:THR:HG22	65:h:51:LEU:HG	1.99	0.44
49:j:78:GLN:O	49:j:82:LYS:CD	2.64	0.44
50:n:237:MET:HB2	50:n:246:ARG:HD2	2.00	0.44
50:n:274:ILE:CD1	55:f:181:LEU:CD2	2.96	0.44
50:n:781:LEU:HD23	50:n:781:LEU:HA	1.88	0.44
53:a:400:HIS:HE1	53:a:403:ARG:HG2	1.83	0.44
56:i:71:ASN:HA	56:i:74:LYS:HD2	1.99	0.44
58:q:263:LYS:CE	58:q:439:PHE:HZ	2.29	0.44
58:q:402:HIS:HE1	58:q:404:ARG:HH21	1.64	0.44
58:q:487:ILE:HD11	58:q:540:LEU:HD13	1.98	0.44
71:w:1195:ALA:O	71:w:1197:HIS:N	2.50	0.44
3:BA:245:VAL:HG23	3:BA:245:VAL:O	2.17	0.44
4:DA:1182:CYS:O	4:DA:1182:CYS:SG	2.75	0.44
7:HA:462:SER:OG	7:HA:463:PRO:CD	2.66	0.44
11:EB:132:VAL:HG22	11:EB:137:TYR:CD1	2.53	0.44
15:PB:761:THR:H	15:PB:764:MET:HE3	1.82	0.44
31:Df:105:TYR:O	33:Dj:217:PHE:N	2.51	0.44
31:DF:39:LEU:HD11	32:DI:51:LEU:HG	2.00	0.44
31:DF:55:LEU:HD22	31:DF:55:LEU:HA	1.73	0.44
38:DH:40:VAL:O	38:DH:44:LEU:HG	2.18	0.44
44:HI:139:LYS:NZ	44:HI:139:LYS:HB3	2.32	0.44
44:HI:282:ALA:O	44:HI:283:ARG:C	2.59	0.44
50:n:273:PHE:HD2	55:f:181:LEU:HD13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:321:LEU:HD21	53:a:407:ILE:CG1	2.48	0.44
54:d:119:GLN:HE21	54:d:119:GLN:HB2	1.48	0.44
54:d:174:ARG:HD2	54:d:174:ARG:HA	1.70	0.44
55:f:29:VAL:HG21	55:f:79:PHE:CD1	2.53	0.44
58:q:17:LYS:CE	58:q:30:TYR:CE2	2.88	0.44
58:q:145:GLN:NE2	69:v:45:GLU:HB3	2.33	0.44
58:q:153:LEU:HD22	66:k:34:GLU:HB3	1.99	0.44
58:q:190:LEU:CD2	58:q:291:TRP:CE3	3.00	0.44
62:e:45:VAL:O	62:e:48:LEU:HG	2.18	0.44
63:l:167:ILE:HD12	69:v:127:LEU:HD23	1.98	0.44
66:k:101:ARG:CZ	66:k:101:ARG:CB	2.87	0.44
66:k:113:GLN:HA	66:k:116:GLU:OE1	2.17	0.44
67:r:57:VAL:HG22	67:r:71:ARG:HG2	1.99	0.44
68:t:39:PHE:O	68:t:39:PHE:CG	2.71	0.44
68:t:85:LEU:HD23	68:t:85:LEU:HA	1.77	0.44
70:p:145:LEU:HD22	70:p:359:LEU:HD21	2.00	0.44
71:w:316:GLU:OE2	71:w:366:ILE:N	2.49	0.44
71:w:485:SER:OG	71:w:486:GLU:N	2.49	0.44
72:x:420:ILE:HA	72:x:420:ILE:HD13	1.92	0.44
1:X:18:DG:H1	2:Y:-18:DC:N4	2.15	0.44
5:EA:22:ILE:CD1	5:EA:26:TYR:CD2	3.01	0.44
5:EA:128:LYS:HZ1	5:EA:166:SER:N	2.16	0.44
5:EA:180:PHE:HA	11:EB:216:PHE:CE1	2.52	0.44
10:DB:672:PHE:HE1	16:HC:413:LEU:HG	1.83	0.44
15:PB:379:ARG:O	15:PB:608:ARG:NH2	2.51	0.44
29:DD:875:GLN:O	29:DD:877:PRO:HD3	2.18	0.44
29:DD:891:ILE:C	29:DD:891:ILE:CD1	2.90	0.44
31:DF:320:ARG:H	31:DF:320:ARG:NE	2.16	0.44
32:DI:20:ALA:HB2	32:DI:36:ILE:CD1	2.44	0.44
39:HD:42:GLY:O	47:PG:164:MET:HE3	2.17	0.44
39:HD:289:SER:O	39:HD:290:SER:C	2.56	0.44
40:HE:123:ASP:OD1	40:HE:124:ILE:N	2.45	0.44
41:HG:291:CYS:SG	41:HG:294:CYS:N	2.82	0.44
46:PD:76:ASN:CB	65:h:47:ASP:HB3	2.44	0.44
48:g:168:LEU:HD23	48:g:168:LEU:C	2.43	0.44
50:n:98:ARG:HH22	51:s:120:GLY:N	2.16	0.44
50:n:274:ILE:CD1	55:f:181:LEU:HD21	2.47	0.44
52:u:122:LEU:O	52:u:124:ASP:N	2.50	0.44
53:a:66:GLN:OE1	54:d:44:LEU:CD2	2.62	0.44
55:f:43:ARG:H	55:f:43:ARG:HD2	1.82	0.44
61:c:229:ASP:OD1	61:c:232:SER:OG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:c:298:ASP:HB2	61:c:305:PHE:HE2	1.82	0.44
65:h:130:ARG:O	65:h:131:ILE:C	2.61	0.44
67:r:192:GLN:OE1	69:v:11:LYS:HE3	2.18	0.44
4:DA:730:PHE:CD1	4:DA:730:PHE:N	2.83	0.44
7:HA:285:TYR:O	7:HA:289:VAL:HG23	2.17	0.44
9:PA:495:ASP:OD1	9:PA:497:ASP:OD1	2.36	0.44
11:EB:122:GLU:O	11:EB:125:VAL:HG22	2.18	0.44
18:PE:94:MET:HE1	18:PE:127:LEU:HD11	2.00	0.44
18:PE:134:GLU:OE1	18:PE:181:ARG:NH2	2.50	0.44
29:DD:958:LYS:HD3	29:DD:958:LYS:HA	1.53	0.44
31:DF:370:TRP:CZ3	31:DF:420:ALA:HA	2.53	0.44
38:DH:37:LEU:HD21	33:DJ:134:VAL:HG12	1.99	0.44
35:DL:111:LEU:C	35:DL:114:LYS:HE3	2.43	0.44
39:HD:193:PRO:HG2	39:HD:196:LEU:HD12	1.99	0.44
41:HG:89:GLU:OE2	41:HG:132:LYS:NZ	2.42	0.44
50:n:676:ASP:OD1	58:q:593:MET:HE2	2.18	0.44
52:u:115:LEU:HA	52:u:118:ILE:HG22	2.00	0.44
53:a:305:LEU:HD22	53:a:305:LEU:HA	1.83	0.44
54:d:63:ASN:HD22	54:d:63:ASN:HA	1.56	0.44
56:i:75:CYS:HB3	56:i:88:ASN:HD22	1.81	0.44
60:b:85:ASN:ND2	64:o:641:THR:HB	2.32	0.44
60:b:168:ILE:HG13	61:c:110:ALA:HB3	1.99	0.44
65:h:18:GLN:HB3	65:h:60:ASN:ND2	2.33	0.44
66:k:19:ARG:HG3	66:k:58:HIS:CD2	2.53	0.44
66:k:71:THR:HA	66:k:74:ALA:CB	2.48	0.44
72:x:591:ALA:HB1	72:x:597:LEU:HD23	2.00	0.44
3:BA:25:GLU:OE1	3:BA:46:ILE:HD12	2.18	0.44
4:DA:491:MET:N	4:DA:491:MET:SD	2.91	0.44
5:EA:105:TYR:N	5:EA:105:TYR:HD1	2.15	0.44
7:HA:332:PHE:CZ	7:HA:367:ILE:HG23	2.53	0.44
9:PA:1203:ASP:N	9:PA:1203:ASP:OD1	2.51	0.44
9:PA:1366:PHE:HB2	9:PA:1374:VAL:HG21	1.99	0.44
30:DE:650:THR:HG22	30:DE:666:THR:HG22	1.99	0.44
31:DF:43:VAL:CG2	32:DI:46:TYR:HD2	2.30	0.44
31:DF:400:GLY:O	31:DF:404:ARG:HG2	2.18	0.44
42:HH:133:THR:HG23	42:HH:134:SER:N	2.32	0.44
45:HJ:279:ARG:O	45:HJ:279:ARG:NE	2.44	0.44
46:PD:17:ALA:HB1	46:PD:95:PHE:HE2	1.83	0.44
48:g:130:GLN:O	48:g:134:THR:OG1	2.30	0.44
49:j:82:LYS:NZ	51:s:96:PHE:HD1	2.16	0.44
50:n:385:LEU:HD23	50:n:407:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:357:LEU:HD12	53:a:359:HIS:HB3	2.00	0.44
54:d:111:GLN:CD	54:d:111:GLN:C	2.86	0.44
58:q:157:ALA:CB	66:k:31:VAL:HG23	2.36	0.44
62:e:56:PHE:O	62:e:60:VAL:CG2	2.38	0.44
65:h:173:PHE:HB3	67:r:197:VAL:HG12	1.99	0.44
67:r:19:MET:HE2	67:r:19:MET:HB3	1.80	0.44
4:DA:405:VAL:HA	31:DF:302:HIS:HB3	1.99	0.43
5:EA:52:LEU:CD1	5:EA:59:LEU:HD13	2.48	0.43
9:PA:105:LYS:HD2	9:PA:141:LEU:HD22	2.00	0.43
16:HC:288:ILE:H	16:HC:288:ILE:HD12	1.83	0.43
16:HC:337:ARG:O	42:HH:62:ARG:NH1	2.48	0.43
18:PE:71:GLN:HB2	18:PE:99:ILE:HD12	2.00	0.43
29:Dd:871:THR:O	35:DI:62:LYS:NZ	2.42	0.43
31:Df:405:SER:O	31:Df:405:SER:OG	2.34	0.43
29:DD:1085:LYS:NZ	35:DL:83:MET:SD	2.85	0.43
30:DE:369:LYS:HD3	30:DE:369:LYS:HA	1.74	0.43
30:DE:613:ALA:HB3	30:DE:616:HIS:HD2	1.83	0.43
31:DF:219:GLU:CD	31:DF:219:GLU:C	2.86	0.43
38:DH:44:LEU:HD21	33:DJ:129:THR:CG2	2.44	0.43
38:DH:155:ASP:OD1	38:DH:155:ASP:N	2.51	0.43
35:DL:93:GLU:O	35:DL:97:THR:HG23	2.18	0.43
45:HJ:60:TYR:HD1	45:HJ:60:TYR:HA	1.73	0.43
46:PD:17:ALA:HB1	46:PD:95:PHE:CE2	2.52	0.43
46:PD:66:ASN:ND2	69:v:13:THR:CG2	2.81	0.43
50:n:485:ASP:N	50:n:485:ASP:OD1	2.51	0.43
50:n:509:ILE:HD11	50:n:516:SER:HB2	2.00	0.43
50:n:904:PHE:CD1	50:n:916:LEU:HD11	2.53	0.43
50:n:1322:LEU:O	50:n:1326:PRO:N	2.51	0.43
53:a:63:GLU:HG3	53:a:86:ARG:NH1	2.33	0.43
53:a:417:TYR:OH	53:a:450:PHE:CD1	2.70	0.43
54:d:156:SER:CB	54:d:161:VAL:CG1	2.96	0.43
58:q:119:VAL:CG1	58:q:127:LEU:HD13	2.48	0.43
58:q:577:ASP:N	58:q:577:ASP:OD1	2.51	0.43
61:c:42:LYS:HB2	61:c:48:ARG:HB3	1.99	0.43
63:l:91:LYS:O	63:l:94:LEU:HG	2.18	0.43
65:h:16:LEU:HD22	65:h:16:LEU:HA	1.91	0.43
65:h:146:MET:CG	66:k:39:LYS:CD	2.95	0.43
66:k:17:ILE:HG12	69:v:76:MET:HE1	2.00	0.43
66:k:60:GLU:HG3	69:v:26:ILE:CG1	2.47	0.43
71:w:547:VAL:HG13	71:w:559:LEU:HD11	2.00	0.43
72:x:313:ILE:HD13	72:x:313:ILE:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:y:213:VAL:O	73:y:213:VAL:CG1	2.66	0.43
7:HA:354:PRO:HB2	7:HA:355:PRO:HD3	2.00	0.43
9:PA:428:ASP:OD2	9:PA:430:ARG:NH1	2.51	0.43
26:DQ:366:ILE:HD11	27:DO:48:LEU:HG	2.00	0.43
40:HE:64:ILE:HG12	40:HE:65:GLN:N	2.33	0.43
44:HI:15:LEU:HD23	44:HI:16:ASP:HB2	1.99	0.43
44:HI:164:SER:N	44:HI:165:PRO:HD2	2.34	0.43
44:HI:267:ASP:HB2	44:HI:294:TYR:HB2	2.00	0.43
47:PG:59:ILE:HA	47:PG:65:PHE:O	2.18	0.43
50:n:136:LEU:HD23	50:n:136:LEU:HA	1.84	0.43
50:n:201:HIS:CE1	52:u:122:LEU:CD1	3.02	0.43
53:a:340:TYR:HB2	53:a:378:LYS:HB3	1.99	0.43
53:a:373:CYS:HB3	53:a:439:GLN:CG	2.49	0.43
53:a:466:VAL:HG22	53:a:467:MET:N	2.34	0.43
54:d:44:LEU:HD23	54:d:44:LEU:C	2.43	0.43
54:d:96:LEU:HD12	54:d:96:LEU:HA	1.81	0.43
55:f:53:GLN:HB3	55:f:54:ARG:H	1.57	0.43
58:q:120:ARG:HH11	58:q:120:ARG:CG	2.14	0.43
62:e:129:VAL:CG2	66:k:114:MET:HE1	2.32	0.43
65:h:5:GLU:C	65:h:5:GLU:CD	2.86	0.43
67:r:101:LEU:HD23	67:r:101:LEU:HA	1.79	0.43
69:v:39:THR:C	69:v:41:LYS:N	2.76	0.43
70:p:611:LEU:HD11	70:p:665:TRP:HB3	1.99	0.43
71:w:326:THR:HA	71:w:329:LEU:HD13	1.99	0.43
71:w:770:MET:HB3	71:w:776:ILE:HD11	1.99	0.43
72:x:11:LEU:HA	72:x:14:TRP:HB3	2.00	0.43
72:x:765:VAL:HG13	72:x:812:LEU:HB2	1.99	0.43
77:NY:-123:DG:H2"	77:NY:-122:DG:C8	2.52	0.43
29:DD:1073:THR:HG21	35:DL:87:ILE:HD11	2.00	0.43
37:DG:165:GLU:HA	37:DG:168:ARG:HD2	2.00	0.43
44:HI:135:HIS:HD2	44:HI:137:ASP:N	2.14	0.43
44:HI:243:LEU:HD12	44:HI:244:PRO:HD3	2.00	0.43
45:HJ:64:LEU:HD22	45:HJ:105:MET:HG2	2.00	0.43
45:HJ:85:MET:HB3	45:HJ:85:MET:HE3	1.34	0.43
47:PG:145:LEU:HD23	47:PG:145:LEU:H	1.82	0.43
48:g:127:ARG:CA	48:g:130:GLN:H	2.31	0.43
50:n:647:MET:HG2	50:n:651:ASN:ND2	2.32	0.43
50:n:793:HIS:CD2	50:n:794:LEU:HG	2.54	0.43
50:n:932:GLY:C	50:n:1179:HIS:NE2	2.76	0.43
53:a:206:GLY:H	53:a:412:ARG:HH12	1.66	0.43
53:a:466:VAL:CG1	53:a:478:LYS:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:f:94:PRO:O	58:q:130:VAL:HG13	2.18	0.43
58:q:569:ILE:HG22	58:q:582:VAL:HB	2.01	0.43
64:o:712:ASP:N	64:o:712:ASP:OD1	2.48	0.43
70:p:817:LYS:O	70:p:821:GLN:HB2	2.18	0.43
72:x:669:ILE:HG22	72:x:673:MET:HE2	1.99	0.43
4:DA:406:THR:O	31:DF:354:ARG:NH2	2.51	0.43
4:DA:496:GLU:HA	4:DA:496:GLU:OE2	2.19	0.43
30:De:718:ARG:HD3	30:De:718:ARG:HA	1.77	0.43
31:Df:317:LEU:HG	31:Df:330:ARG:HE	1.83	0.43
31:DF:14:LEU:HD21	32:DI:19:MET:HE2	1.95	0.43
41:HG:87:LEU:HD23	41:HG:87:LEU:O	2.18	0.43
42:HH:408:SER:HB3	42:HH:413:LEU:HD11	2.01	0.43
44:HI:17:PHE:HE2	50:n:68:VAL:CB	2.31	0.43
44:HI:57:ARG:HE	44:HI:57:ARG:HB2	1.63	0.43
44:HI:102:ILE:HD13	44:HI:102:ILE:HA	1.77	0.43
44:HI:274:GLY:O	44:HI:275:LEU:C	2.61	0.43
50:n:232:ALA:HB1	50:n:247:LEU:HD11	2.00	0.43
52:u:49:ASN:H	52:u:49:ASN:HD22	1.63	0.43
53:a:378:LYS:O	53:a:379:ASP:HB2	2.18	0.43
58:q:134:ALA:CB	65:h:72:ARG:HH11	2.32	0.43
58:q:149:LYS:CD	69:v:40:ALA:CA	2.83	0.43
58:q:186:GLU:HB3	58:q:243:LEU:HD22	1.97	0.43
58:q:437:HIS:HE1	58:q:472:GLU:O	1.99	0.43
4:DA:409:HIS:CE1	4:DA:411:GLU:HB2	2.53	0.43
4:DA:1052:ARG:O	4:DA:1052:ARG:CG	2.66	0.43
9:PA:872:MET:O	9:PA:879:VAL:HA	2.18	0.43
10:DB:766:LEU:HA	10:DB:807:THR:HG21	2.00	0.43
15:PB:544:PHE:CE1	15:PB:590:LEU:HD11	2.54	0.43
28:Dc:101:VAL:HG22	31:Df:127:LEU:HA	2.00	0.43
30:De:332:ILE:HA	30:De:336:HIS:HD2	1.84	0.43
30:DE:476:VAL:HB	30:DE:782:HIS:HB2	2.01	0.43
38:DH:116:ARG:HG2	33:DJ:126:TYR:OH	2.19	0.43
43:HF:36:GLN:CG	43:HF:37:ASP:N	2.80	0.43
44:HI:111:PRO:HD2	55:f:63:MET:CG	2.47	0.43
45:HJ:98:GLU:OE2	45:HJ:98:GLU:CA	2.66	0.43
45:HJ:102:ARG:NH1	45:HJ:102:ARG:CG	2.80	0.43
50:n:210:PRO:HD2	50:n:211:GLN:HE21	1.83	0.43
50:n:909:GLN:HB2	50:n:913:HIS:O	2.18	0.43
50:n:938:ASP:HB2	50:n:1171:ALA:CB	2.47	0.43
53:a:467:MET:HE3	53:a:475:VAL:HG11	2.00	0.43
53:a:489:CYS:SG	53:a:514:LYS:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:d:156:SER:CA	54:d:161:VAL:CG1	2.95	0.43
56:i:109:LEU:HD22	56:i:117:GLN:HE22	1.84	0.43
62:e:79:GLN:O	62:e:82:GLN:HG2	2.18	0.43
62:e:95:PHE:CZ	63:l:37:GLY:HA3	2.54	0.43
63:l:166:LEU:HD22	69:v:123:ILE:HD12	2.01	0.43
65:h:149:ASN:O	65:h:153:LYS:HG2	2.19	0.43
72:x:433:GLU:C	72:x:433:GLU:CD	2.86	0.43
4:DA:474:ASP:N	4:DA:474:ASP:OD1	2.52	0.43
15:PB:752:TYR:O	22:PJ:1:MET:N	2.51	0.43
21:PI:104:ALA:O	21:PI:105:GLU:HG2	2.18	0.43
30:DE:790:LEU:HD13	38:DH:146:ILE:HG12	2.01	0.43
31:DF:105:TYR:O	33:DJ:217:PHE:CD1	2.70	0.43
32:DI:23:LEU:HD22	32:DI:28:ILE:HD12	2.01	0.43
39:HD:300:ALA:HB1	45:HJ:166:PRO:CA	2.36	0.43
42:HH:133:THR:HB	42:HH:160:THR:HG21	2.00	0.43
44:HI:13:GLU:OE2	44:HI:15:LEU:HB2	2.19	0.43
44:HI:47:HIS:HA	44:HI:52:LYS:CG	2.44	0.43
44:HI:247:VAL:O	44:HI:247:VAL:HG13	2.17	0.43
45:HJ:85:MET:HE3	45:HJ:85:MET:C	2.44	0.43
45:HJ:138:LYS:HE3	45:HJ:138:LYS:HB3	1.86	0.43
48:g:175:LEU:HD21	56:i:132:LEU:CD1	2.43	0.43
50:n:166:TYR:OH	57:m:70:PRO:C	2.62	0.43
50:n:554:MET:HE3	50:n:554:MET:HB2	1.88	0.43
50:n:909:GLN:OE1	60:b:114:ASP:OD1	2.36	0.43
52:u:77:PRO:HG2	59:z:596:TYR:OH	2.17	0.43
53:a:373:CYS:O	53:a:439:GLN:HA	2.19	0.43
53:a:420:LEU:HD22	53:a:504:ILE:CG1	2.49	0.43
54:d:42:ARG:NH2	56:i:93:LYS:N	2.66	0.43
56:i:104:MET:HE3	56:i:104:MET:HB3	1.84	0.43
61:c:238:VAL:HG22	61:c:292:LEU:HD22	1.99	0.43
64:o:625:VAL:HG23	64:o:634:PHE:HZ	1.84	0.43
71:w:952:LEU:HD23	71:w:952:LEU:HA	1.80	0.43
77:NY:-82:DG:H2"	77:NY:-81:DG:C8	2.54	0.43
7:HA:49:THR:HG23	7:HA:50:VAL:N	2.34	0.43
7:HA:576:GLU:OE2	13:HB:308:ASN:ND2	2.49	0.43
9:PA:786:ALA:O	9:PA:787:VAL:HG23	2.18	0.43
11:EB:88:ARG:O	11:EB:91:ARG:HB2	2.19	0.43
16:HC:380:THR:HG23	16:HC:380:THR:O	2.19	0.43
28:Dc:24:ASP:CB	33:Dj:192:LYS:HD2	2.48	0.43
31:Df:11:ASN:OD1	31:Df:48:LYS:NZ	2.51	0.43
31:Df:223:TYR:CD2	31:Df:255:MET:HE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DE:696:TRP:HH2	30:DE:703:MET:SD	2.25	0.43
31:DF:327:TRP:CD1	31:DF:327:TRP:C	2.97	0.43
31:DF:336:LEU:O	31:DF:339:GLN:HG3	2.19	0.43
32:DI:21:GLN:HE22	32:DI:24:LYS:HE2	1.84	0.43
32:DI:35:VAL:HG12	32:DI:39:MET:HE2	1.99	0.43
39:HD:116:ASP:OD1	39:HD:117:ASN:N	2.51	0.43
39:HD:283:LEU:O	39:HD:284:ALA:C	2.59	0.43
42:HH:193:VAL:HG11	42:HH:283:ARG:CD	2.49	0.43
44:HI:75:ILE:HD12	44:HI:75:ILE:HA	1.83	0.43
44:HI:169:TYR:CG	44:HI:190:TYR:CZ	3.06	0.43
44:HI:245:ASP:N	44:HI:245:ASP:OD1	2.51	0.43
46:PD:66:ASN:HD21	69:v:13:THR:HG21	1.83	0.43
50:n:201:HIS:CE1	52:u:122:LEU:HD12	2.54	0.43
53:a:107:MET:O	53:a:107:MET:SD	2.77	0.43
54:d:131:LYS:HB2	54:d:131:LYS:HE2	1.35	0.43
58:q:166:ARG:CG	58:q:166:ARG:NH1	2.79	0.43
58:q:475:VAL:HG22	58:q:495:LEU:HB2	2.01	0.43
58:q:646:LEU:HD21	63:l:115:ILE:CD1	2.49	0.43
62:e:73:ILE:O	62:e:77:VAL:HG13	2.18	0.43
66:k:30:THR:HA	66:k:33:LEU:HD12	2.01	0.43
66:k:104:LEU:HD23	66:k:104:LEU:HA	1.75	0.43
68:t:11:VAL:HG11	68:t:17:VAL:HA	2.00	0.43
71:w:782:MET:HE3	71:w:782:MET:HB2	1.90	0.43
72:x:577:ALA:O	72:x:581:ILE:HG13	2.18	0.43
77:NY:-160:DG:H2''	77:NY:-159:DG:O5'	2.18	0.43
1:X:21:DC:N4	2:Y:-21:DG:H1	2.08	0.43
5:EA:139:LEU:CG	47:PG:151:ARG:HB3	2.29	0.43
15:PB:854:ILE:O	15:PB:907:VAL:HG21	2.18	0.43
16:HC:261:PHE:CZ	16:HC:265:LEU:HD21	2.54	0.43
31:Df:55:LEU:HD13	32:Di:28:ILE:HG12	2.01	0.43
34:Dk:179:MET:HB3	34:Dk:180:PRO:HD2	2.01	0.43
30:DE:731:MET:HE3	30:DE:731:MET:HB3	1.91	0.43
31:DF:82:PRO:CD	31:DF:96:PHE:HA	2.47	0.43
31:DF:283:MET:HE1	31:DF:308:VAL:HG12	2.00	0.43
31:DF:402:ARG:O	31:DF:406:VAL:HG13	2.19	0.43
42:HH:409:THR:O	42:HH:413:LEU:HD13	2.19	0.43
44:HI:297:ASN:HB3	44:HI:299:PRO:HD2	2.00	0.43
46:PD:107:THR:HG23	46:PD:110:GLU:H	1.83	0.43
50:n:169:LEU:N	57:m:104:HIS:CE1	2.81	0.43
50:n:808:LEU:O	50:n:821:SER:HA	2.18	0.43
52:u:73:ILE:C	52:u:75:SER:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:259:ILE:H	53:a:259:ILE:CD1	2.22	0.43
56:i:88:ASN:C	56:i:88:ASN:OD1	2.62	0.43
56:i:133:GLN:O	56:i:136:LYS:HB3	2.18	0.43
58:q:19:VAL:HG22	58:q:22:VAL:HG22	2.01	0.43
58:q:264:GLN:H	58:q:264:GLN:HG3	1.57	0.43
58:q:431:ILE:HD13	58:q:431:ILE:HA	1.75	0.43
59:z:485:ILE:H	59:z:485:ILE:HG13	1.67	0.43
60:b:175:HIS:CD2	61:c:113:TRP:CZ2	3.07	0.43
62:e:146:ILE:C	62:e:148:VAL:N	2.72	0.43
66:k:109:ARG:NH1	66:k:109:ARG:HB2	2.34	0.43
68:t:196:LEU:HD22	68:t:196:LEU:HA	1.85	0.43
71:w:273:VAL:HG21	71:w:286:MET:HE1	1.99	0.43
72:x:187:SER:O	72:x:190:THR:OG1	2.35	0.43
73:y:226:LEU:HD12	73:y:227:VAL:N	2.34	0.43
4:DA:1053:PHE:HB2	4:DA:1057:GLU:HB2	2.00	0.43
5:EA:142:ASN:HB3	47:PG:158:PHE:CD2	2.48	0.43
7:HA:168:VAL:O	7:HA:168:VAL:HG13	2.19	0.43
9:PA:1171:ALA:N	9:PA:1215:GLU:O	2.47	0.43
9:PA:1213:ARG:NH2	9:PA:1215:GLU:OE2	2.51	0.43
11:EB:73:TYR:O	11:EB:74:LYS:HG2	2.18	0.43
11:EB:103:LEU:HD22	11:EB:108:HIS:CB	2.49	0.43
15:PB:218:THR:O	15:PB:218:THR:HG23	2.18	0.43
15:PB:239:MET:HB2	15:PB:372:LEU:HD21	2.01	0.43
15:PB:565:THR:HG21	15:PB:580:PRO:HG3	2.01	0.43
15:PB:752:TYR:CE1	15:PB:809:VAL:HG23	2.52	0.43
20:PH:91:VAL:HG22	20:PH:144:LEU:HD22	1.98	0.43
32:Di:16:ALA:HB2	32:Di:40:LEU:HD11	2.00	0.43
35:Dl:113:VAL:O	35:Dl:113:VAL:HG22	2.17	0.43
30:DE:564:ASP:OD1	30:DE:564:ASP:N	2.51	0.43
31:DF:26:MET:HE2	32:DI:48:THR:HG22	2.01	0.43
31:DF:82:PRO:HD2	31:DF:96:PHE:HA	2.01	0.43
41:HG:369:VAL:HG13	41:HG:370:ASP:N	2.33	0.43
42:HH:532:LEU:CD2	42:HH:716:VAL:HG13	2.49	0.43
44:HI:162:PHE:CD1	44:HI:162:PHE:N	2.86	0.43
50:n:954:TYR:OH	50:n:1169:TRP:HA	2.19	0.43
52:u:78:SER:C	52:u:80:GLU:H	2.26	0.43
53:a:384:ASP:N	53:a:384:ASP:OD1	2.52	0.43
55:f:127:GLN:HE22	69:v:62:HIS:HD2	1.66	0.43
62:e:132:HIS:CE1	63:l:163:LEU:HD11	2.54	0.43
68:t:21:VAL:HG22	68:t:138:ILE:HD11	2.01	0.43
68:t:194:MET:HE3	68:t:194:MET:HB3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:p:569:LEU:HD12	70:p:572:PRO:HB3	2.01	0.43
2:Y:27:DT:H72	2:Y:28:DT:C7	2.49	0.43
4:DA:484:ILE:HD13	31:Df:309:MET:HG2	2.00	0.43
7:HA:67:VAL:O	7:HA:67:VAL:HG23	2.19	0.43
13:HB:303:ILE:HG22	13:HB:307:PHE:CE2	2.54	0.43
15:PB:719:SER:OG	15:PB:720:PRO:HD3	2.18	0.43
15:PB:1128:ALA:HB1	15:PB:1135:TYR:HD1	1.84	0.43
31:DF:85:GLY:C	33:DJ:212:LYS:HG2	2.43	0.43
38:DH:132:LYS:HA	38:DH:132:LYS:HD2	1.69	0.43
32:DI:32:GLU:HB3	32:DI:35:VAL:HG23	2.00	0.43
39:HD:295:ARG:NH2	39:HD:295:ARG:HG2	2.33	0.43
48:g:140:GLU:HG2	52:u:93:LEU:HD21	2.01	0.43
49:j:82:LYS:HZ3	51:s:96:PHE:HD1	1.61	0.43
50:n:166:TYR:CE2	57:m:71:GLN:HA	2.29	0.43
50:n:273:PHE:CD2	55:f:181:LEU:HD13	2.54	0.43
50:n:274:ILE:CG1	55:f:181:LEU:HD22	2.49	0.43
50:n:482:VAL:HG13	50:n:489:ILE:HD11	2.01	0.43
54:d:163:ALA:HA	57:m:105:TRP:CE2	2.53	0.43
56:i:118:LEU:C	56:i:118:LEU:CD2	2.91	0.43
58:q:36:MET:SD	58:q:37:SER:N	2.92	0.43
58:q:171:VAL:HG21	66:k:17:ILE:HG22	1.83	0.43
58:q:245:VAL:HG22	58:q:291:TRP:HB3	2.01	0.43
59:z:489:TYR:HA	59:z:492:ARG:HD2	2.00	0.43
63:l:92:LEU:HA	63:l:95:VAL:HG22	1.99	0.43
64:o:694:ASP:HB2	64:o:705:HIS:HB2	2.00	0.43
68:t:197:PHE:HA	68:t:200:ILE:HD11	2.00	0.43
69:v:41:LYS:HB3	69:v:41:LYS:HE2	1.79	0.43
69:v:131:GLU:CG	69:v:135:TYR:HE2	2.31	0.43
70:p:216:ALA:HA	70:p:229:ALA:O	2.19	0.43
70:p:398:SER:O	70:p:400:GLN:N	2.51	0.43
71:w:470:ASN:OD1	71:w:470:ASN:N	2.52	0.43
71:w:758:LYS:HA	71:w:758:LYS:HD3	1.81	0.43
72:x:11:LEU:HD22	72:x:15:LYS:HG3	2.01	0.43
77:NY:-96:DG:H2"	77:NY:-95:DG:C8	2.54	0.43
7:HA:143:ARG:NH1	7:HA:159:GLU:OE1	2.48	0.42
9:PA:154:CYS:SG	9:PA:155:GLU:N	2.92	0.42
9:PA:883:ILE:O	9:PA:883:ILE:HG22	2.19	0.42
10:DB:653:LEU:HG	10:DB:684:ILE:HG13	2.00	0.42
11:EB:145:VAL:HG21	11:EB:151:LEU:HB2	2.01	0.42
16:HC:58:ARG:HD2	40:HE:229:TRP:CZ3	2.54	0.42
32:Di:78:ARG:HD3	32:Di:78:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:67:THR:O	31:DF:68:THR:C	2.62	0.42
31:DF:336:LEU:HD23	31:DF:336:LEU:HA	1.84	0.42
39:HD:280:PRO:HB2	39:HD:281:GLN:OE1	2.19	0.42
43:HF:24:ASP:OD1	43:HF:24:ASP:C	2.61	0.42
44:HI:24:ALA:CA	44:HI:44:LYS:HB2	2.47	0.42
44:HI:102:ILE:O	44:HI:102:ILE:CG2	2.67	0.42
46:PD:64:THR:HG22	47:PG:103:PRO:HD3	2.01	0.42
50:n:199:LEU:CD1	50:n:222:VAL:HG13	2.48	0.42
50:n:1185:LEU:HD11	50:n:1207:LEU:HB2	2.01	0.42
53:a:383:PRO:CG	72:x:92:LEU:CD2	2.95	0.42
53:a:468:ASP:OD1	53:a:468:ASP:O	2.36	0.42
53:a:503:SER:O	53:a:506:VAL:HB	2.19	0.42
60:b:71:LEU:HD23	60:b:71:LEU:HA	1.87	0.42
61:c:114:SER:O	61:c:117:LEU:HG	2.19	0.42
71:w:236:ALA:HB2	71:w:663:PRO:HG3	2.00	0.42
71:w:356:LEU:HD21	71:w:372:LEU:HD11	2.01	0.42
71:w:389:LEU:HA	71:w:392:PHE:HD2	1.84	0.42
4:DA:571:GLU:CD	4:DA:571:GLU:N	2.74	0.42
4:DA:1068:ARG:HD2	4:DA:1068:ARG:O	2.18	0.42
5:EA:157:CYS:O	5:EA:158:HIS:HB2	2.18	0.42
5:EA:174:ARG:HG2	39:HD:37:LEU:HD21	2.00	0.42
10:DB:216:SER:OG	10:DB:217:ASN:N	2.52	0.42
10:DB:431:LEU:H	10:DB:431:LEU:CD2	2.32	0.42
11:EB:168:LEU:HD22	11:EB:199:LYS:HB2	2.01	0.42
15:PB:871:VAL:O	15:PB:871:VAL:HG13	2.18	0.42
16:HC:70:ALA:HB1	16:HC:74:TRP:CZ2	2.54	0.42
28:Dc:21:LEU:HD11	28:Dc:23:TRP:CD1	2.53	0.42
31:DF:104:LEU:CB	33:DJ:217:PHE:HE2	2.12	0.42
32:DI:82:SER:HB3	32:DI:83:PHE:H	1.70	0.42
35:DL:69:GLU:O	35:DL:70:VAL:C	2.62	0.42
35:DL:120:LEU:O	35:DL:125:ASN:N	2.52	0.42
42:HH:184:VAL:HG13	42:HH:185:ILE:N	2.33	0.42
45:HJ:3:HIS:C	45:HJ:5:SER:N	2.77	0.42
45:HJ:182:GLU:O	45:HJ:182:GLU:OE2	2.37	0.42
50:n:273:PHE:CE2	55:f:185:ARG:CD	2.88	0.42
50:n:857:GLU:O	50:n:861:LYS:HG2	2.19	0.42
53:a:111:GLU:OE2	53:a:111:GLU:O	2.37	0.42
53:a:231:LEU:O	53:a:241:ILE:HB	2.19	0.42
58:q:460:ILE:HD12	58:q:529:MET:HE2	1.98	0.42
64:o:719:PRO:N	64:o:720:PRO:HD2	2.34	0.42
67:r:57:VAL:HG13	67:r:69:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:p:194:LYS:HG3	70:p:198:GLN:HB3	2.00	0.42
71:w:237:ILE:HG21	71:w:285:ASN:HB3	2.01	0.42
72:x:269:MET:O	72:x:273:MET:HG2	2.20	0.42
5:EA:105:TYR:N	5:EA:105:TYR:CD1	2.88	0.42
7:HA:338:GLU:HG2	39:HD:68:VAL:HG11	2.00	0.42
9:PA:511:THR:HG21	15:PB:1105:GLU:OE1	2.19	0.42
9:PA:706:ILE:O	9:PA:710:LYS:HG2	2.19	0.42
9:PA:1234:LYS:NZ	9:PA:1297:THR:O	2.52	0.42
9:PA:1281:ASP:O	9:PA:1285:LEU:HD13	2.19	0.42
10:DB:431:LEU:CD2	10:DB:431:LEU:N	2.82	0.42
10:DB:839:MET:HE1	10:DB:843:LEU:HD13	2.00	0.42
13:HB:374:LEU:HD12	13:HB:374:LEU:C	2.45	0.42
13:HB:496:ASN:HB3	13:HB:536:LEU:HD11	2.01	0.42
15:PB:1162:LEU:HB3	15:PB:1167:ILE:HB	2.00	0.42
27:DO:1:MET:C	29:DD:1000:ARG:HD2	2.44	0.42
32:Di:45:ARG:HG3	33:Dj:212:LYS:HB3	2.01	0.42
30:DE:377:LEU:HD21	30:DE:422:PRO:HG2	2.00	0.42
31:DF:312:ILE:HG22	31:DF:313:VAL:CG1	2.49	0.42
38:DH:57:SER:N	33:DJ:197:MET:SD	2.92	0.42
35:DL:111:LEU:N	35:DL:114:LYS:HZ1	2.16	0.42
39:HD:85:ARG:CZ	39:HD:140:LEU:HG	2.38	0.42
42:HH:532:LEU:HD23	42:HH:532:LEU:O	2.19	0.42
44:HI:160:LYS:HG2	44:HI:167:ARG:HH22	1.84	0.42
44:HI:185:PHE:HE2	44:HI:237:TRP:CH2	2.37	0.42
48:g:140:GLU:OE2	59:z:556:GLN:HG2	2.19	0.42
50:n:541:LYS:HG3	50:n:549:TYR:CZ	2.54	0.42
51:s:105:LEU:HB3	51:s:117:ASP:OD1	2.20	0.42
53:a:500:ARG:HA	53:a:500:ARG:HD2	1.65	0.42
54:d:115:LYS:HE2	54:d:115:LYS:O	2.18	0.42
55:f:145:TYR:CG	65:h:43:PRO:HD3	2.52	0.42
56:i:135:TYR:HA	56:i:138:LEU:HB2	2.00	0.42
64:o:619:GLN:NE2	64:o:623:ASP:OD1	2.38	0.42
66:k:70:LEU:HG	69:v:82:LEU:HD21	1.98	0.42
68:t:197:PHE:O	68:t:200:ILE:HG12	2.20	0.42
70:p:35:LEU:HD22	70:p:49:MET:HA	2.00	0.42
7:HA:345:ARG:NH2	39:HD:64:GLU:OE1	2.52	0.42
7:HA:661:ALA:HA	7:HA:664:VAL:HG12	2.01	0.42
9:PA:560:VAL:HG21	9:PA:586:TRP:HB2	2.02	0.42
9:PA:1338:THR:OG1	9:PA:1340:GLY:O	2.36	0.42
15:PB:399:LEU:HB3	15:PB:453:TRP:CZ2	2.55	0.42
18:PE:13:ILE:HD12	18:PE:13:ILE:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DQ:18:ILE:HD11	26:DQ:46:TRP:CH2	2.54	0.42
31:Df:432:ALA:HB1	31:Df:462:GLN:CB	2.49	0.42
29:DD:1084:LEU:HB3	32:DI:99:ARG:HH21	1.84	0.42
30:DE:460:SER:HB3	31:DF:135:TRP:CZ3	2.55	0.42
31:DF:14:LEU:CD2	32:DI:19:MET:CE	2.88	0.42
35:DL:122:ARG:HA	35:DL:122:ARG:HD2	1.87	0.42
39:HD:287:TYR:CZ	44:HI:189:MET:SD	3.11	0.42
44:HI:37:ILE:H	44:HI:37:ILE:CD1	2.32	0.42
50:n:237:MET:CE	58:q:45:GLN:HG2	2.48	0.42
53:a:66:GLN:HE21	53:a:66:GLN:HB3	1.47	0.42
53:a:461:SER:N	72:x:7:LYS:HD3	2.35	0.42
54:d:164:PRO:CD	54:d:167:TRP:HB2	2.45	0.42
55:f:134:MET:HE3	55:f:134:MET:HB3	1.86	0.42
56:i:94:PHE:O	56:i:94:PHE:HD1	2.01	0.42
58:q:152:SER:HB2	69:v:58:ASN:CB	2.50	0.42
67:r:74:ARG:HD3	67:r:83:TRP:CZ2	2.54	0.42
68:t:91:PHE:O	68:t:95:MET:HG2	2.20	0.42
68:t:134:SER:O	68:t:134:SER:OG	2.37	0.42
68:t:145:GLY:N	68:t:146:PRO:HD2	2.33	0.42
70:p:523:SER:OG	70:p:524:THR:N	2.52	0.42
3:BA:127:ARG:NH1	15:PB:435:ILE:O	2.51	0.42
6:FA:153:ARG:O	6:FA:177:MET:HE1	2.19	0.42
9:PA:106:VAL:O	9:PA:110:VAL:HG12	2.19	0.42
9:PA:575:PRO:HG3	9:PA:594:LEU:HD11	2.01	0.42
10:DB:594:SER:OG	10:DB:595:LYS:N	2.52	0.42
10:DB:887:ARG:NH2	10:DB:917:ASP:OD2	2.49	0.42
11:EB:148:LYS:CD	11:EB:184:ALA:HB3	2.49	0.42
28:Dc:124:ILE:HD11	31:Df:133:ALA:HB1	2.00	0.42
30:De:667:GLY:O	30:De:692:ARG:NH2	2.52	0.42
30:DE:485:ILE:HD12	31:DF:131:LEU:HD21	2.02	0.42
31:DF:138:ILE:HG13	38:DH:159:TYR:CE2	2.46	0.42
31:DF:433:PRO:O	31:DF:437:LYS:N	2.33	0.42
39:HD:254:GLU:CD	39:HD:254:GLU:O	2.62	0.42
40:HE:257:CYS:HB2	40:HE:258:HIS:CD2	2.54	0.42
44:HI:67:GLN:HE22	45:HJ:157:HIS:HA	1.83	0.42
45:HJ:107:THR:O	45:HJ:108:CYS:C	2.58	0.42
45:HJ:201:THR:C	45:HJ:203:ALA:N	2.78	0.42
53:a:67:LYS:HD3	53:a:70:LYS:HE2	2.00	0.42
54:d:45:ILE:CD1	56:i:73:ILE:HG13	2.32	0.42
60:b:187:GLY:O	62:e:53:GLU:OE2	2.38	0.42
69:v:131:GLU:O	69:v:135:TYR:CD2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:w:1046:ASP:N	71:w:1046:ASP:OD1	2.52	0.42
72:x:101:MET:HE1	72:x:131:LEU:HD11	2.01	0.42
72:x:273:MET:HE1	72:x:818:LEU:HB2	2.01	0.42
73:y:40:LEU:HD12	73:y:40:LEU:N	2.35	0.42
76:NX:85:DC:H2"	76:NX:86:DC:C6	2.54	0.42
4:DA:344:GLY:O	4:DA:347:ARG:HB3	2.19	0.42
4:DA:401:ASN:H	4:DA:401:ASN:ND2	2.16	0.42
4:DA:1061:ARG:HD3	4:DA:1061:ARG:HA	1.63	0.42
9:PA:893:GLU:OE1	18:PE:197:SER:OG	2.33	0.42
9:PA:1430:CYS:O	9:PA:1435:THR:OG1	2.38	0.42
15:PB:446:TYR:CE1	15:PB:450:THR:HG21	2.55	0.42
24:PL:32:ASP:OD1	24:PL:32:ASP:N	2.50	0.42
30:De:774:MET:HE2	30:De:774:MET:HB2	1.90	0.42
34:Dk:179:MET:HB3	34:Dk:180:PRO:CD	2.50	0.42
35:Dl:139:TYR:HD2	36:Dm:73:MET:HE3	1.84	0.42
29:DD:1078:LEU:HD23	35:DL:83:MET:HE1	1.84	0.42
36:Dm:68:MET:HE3	36:Dm:68:MET:HB3	1.95	0.42
37:DG:181:TRP:O	37:DG:181:TRP:CD2	2.72	0.42
38:DH:110:TYR:CE1	38:DH:113:ARG:NH1	2.87	0.42
39:HD:85:ARG:NH2	39:HD:139:LYS:HB3	2.34	0.42
39:HD:294:HIS:O	39:HD:295:ARG:C	2.62	0.42
39:HD:301:PHE:CE1	45:HJ:170:PHE:CE1	3.08	0.42
44:HI:71:HIS:HB3	44:HI:74:ILE:HG13	2.00	0.42
44:HI:276:PHE:CD1	44:HI:276:PHE:N	2.87	0.42
50:n:178:ILE:HD11	57:m:84:PHE:HB2	2.01	0.42
50:n:266:VAL:CG2	55:f:177:VAL:HG13	2.49	0.42
50:n:945:ASP:OD1	50:n:945:ASP:N	2.53	0.42
53:a:87:GLN:HE21	53:a:87:GLN:HB2	1.64	0.42
53:a:257:VAL:HG23	53:a:305:LEU:HD23	2.02	0.42
53:a:407:ILE:HD13	53:a:407:ILE:N	2.34	0.42
56:i:89:ALA:O	56:i:93:LYS:HG3	2.19	0.42
58:q:95:TRP:CZ3	65:h:33:LEU:HD21	2.48	0.42
58:q:146:LEU:HD22	58:q:150:LYS:HG3	2.00	0.42
58:q:226:LYS:HD3	58:q:226:LYS:H	1.85	0.42
62:e:146:ILE:CG2	62:e:147:ASN:N	2.52	0.42
63:l:167:ILE:CD1	69:v:123:ILE:HG22	2.48	0.42
71:w:427:CYS:O	71:w:431:HIS:ND1	2.40	0.42
72:x:68:ILE:HD11	72:x:78:VAL:HG11	2.01	0.42
1:X:17:DC:OP1	42:HH:472:ARG:HG3	2.19	0.42
5:EA:105:TYR:CE2	11:EB:236:TYR:HB3	2.54	0.42
7:HA:557:ILE:HG22	7:HA:561:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:PA:668:PHE:CZ	9:PA:672:ILE:HD11	2.54	0.42
9:PA:1129:ASN:O	9:PA:1130:ILE:C	2.63	0.42
9:PA:1795:PRO:HG2	54:d:169:PRO:HB3	1.98	0.42
10:DB:492:MET:HE3	10:DB:492:MET:HB2	1.85	0.42
13:HB:524:HIS:NE2	13:HB:528:MET:SD	2.93	0.42
15:PB:994:GLY:O	22:PJ:31:GLU:HB2	2.20	0.42
28:Dc:94:HIS:CD2	31:Df:122:LEU:HD22	2.55	0.42
30:De:504:LEU:HD22	30:De:575:PHE:HZ	1.85	0.42
31:Df:320:ARG:HH11	31:Df:320:ARG:HB2	1.83	0.42
29:DD:885:ILE:HA	29:DD:888:LYS:HE3	2.02	0.42
31:DF:14:LEU:CD2	32:DI:19:MET:HE1	2.40	0.42
38:DH:116:ARG:HD3	33:DJ:126:TYR:HE1	1.82	0.42
38:DH:127:GLN:N	38:DH:128:PRO:HD2	2.34	0.42
44:HI:60:LEU:HD12	44:HI:60:LEU:HA	1.86	0.42
44:HI:141:ASN:O	44:HI:143:LEU:N	2.53	0.42
50:n:133:ALA:HB2	52:u:23:ILE:HG22	2.02	0.42
50:n:152:PHE:C	50:n:154:ILE:H	2.26	0.42
50:n:459:HIS:CE1	58:q:316:VAL:HG22	2.54	0.42
50:n:907:LEU:HD11	60:b:118:LEU:CB	2.40	0.42
50:n:908:PRO:HG3	60:b:121:ARG:NH2	2.34	0.42
50:n:921:MET:HE2	50:n:1215:ILE:CD1	2.41	0.42
51:s:105:LEU:HD23	51:s:105:LEU:HA	1.78	0.42
53:a:321:LEU:HD21	53:a:407:ILE:CB	2.50	0.42
54:d:45:ILE:HG12	56:i:73:ILE:CB	2.49	0.42
54:d:64:GLN:NE2	54:d:68:LEU:CD1	2.82	0.42
58:q:366:ASP:OD1	58:q:366:ASP:N	2.50	0.42
58:q:523:ASP:HA	58:q:563:ILE:HD12	2.02	0.42
71:w:1131:LEU:HA	71:w:1131:LEU:HD13	1.87	0.42
77:NY:-143:DG:H2''	77:NY:-142:DG:C8	2.55	0.42
77:NY:-94:DG:H2''	77:NY:-93:DG:C8	2.55	0.42
77:NY:-73:DG:H2'	77:NY:-72:DG:C8	2.54	0.42
4:DA:397:LEU:HD22	31:Df:360:THR:HG22	2.00	0.42
4:DA:925:ASP:OD1	4:DA:925:ASP:N	2.51	0.42
7:HA:323:ILE:O	7:HA:378:ARG:NH1	2.53	0.42
10:DB:622:ASP:CB	43:HF:36:GLN:HG3	2.49	0.42
31:Df:219:GLU:H	31:Df:219:GLU:CD	2.21	0.42
31:Df:428:LEU:HD13	31:Df:458:LEU:CB	2.50	0.42
30:DE:464:TYR:CG	31:DF:133:ALA:HB2	2.54	0.42
30:DE:645:GLY:N	30:DE:675:LEU:HD11	2.34	0.42
30:DE:651:VAL:HG21	30:DE:686:THR:HG21	2.01	0.42
31:DF:43:VAL:HG23	32:DI:46:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:249:ASP:HB3	31:DF:252:LEU:HB2	2.02	0.42
31:DF:270:ASN:HD22	31:DF:270:ASN:HA	1.62	0.42
38:DH:61:LEU:HD11	33:DJ:200:LEU:HD21	2.02	0.42
35:DL:62:LYS:HD3	35:DL:62:LYS:C	2.44	0.42
39:HD:23:VAL:HG12	39:HD:59:ARG:HB2	2.01	0.42
39:HD:288:THR:O	39:HD:289:SER:C	2.62	0.42
40:HE:175:MET:HE3	40:HE:179:ASN:ND2	2.35	0.42
42:HH:193:VAL:HG11	42:HH:283:ARG:HD3	2.01	0.42
44:HI:151:LEU:C	44:HI:151:LEU:CD2	2.93	0.42
44:HI:192:VAL:O	44:HI:192:VAL:CG1	2.66	0.42
45:HJ:3:HIS:C	45:HJ:5:SER:H	2.26	0.42
49:j:83:GLU:HB3	49:j:87:ARG:HH12	1.84	0.42
49:j:89:LEU:HD23	49:j:89:LEU:HA	1.88	0.42
50:n:94:GLN:HA	50:n:97:VAL:HG12	2.02	0.42
50:n:114:LYS:HB3	51:s:89:LEU:HD11	2.02	0.42
50:n:250:LEU:CG	50:n:275:HIS:CB	2.94	0.42
50:n:553:GLU:OE2	50:n:569:TYR:OH	2.37	0.42
50:n:707:ASP:CA	64:o:684:ARG:NH2	2.83	0.42
50:n:1283:LYS:HB2	50:n:1283:LYS:HE2	1.85	0.42
52:u:7:GLN:HG3	59:z:594:LEU:HB2	2.02	0.42
52:u:78:SER:H	59:z:562:GLY:C	2.28	0.42
53:a:161:TYR:C	53:a:163:LEU:H	2.27	0.42
53:a:383:PRO:CG	72:x:92:LEU:HD22	2.35	0.42
53:a:424:CYS:CA	53:a:505:PRO:HG3	2.48	0.42
53:a:466:VAL:CG2	72:x:54:PRO:HG3	2.47	0.42
53:a:501:CYS:O	53:a:502:MET:HB2	2.19	0.42
55:f:127:GLN:NE2	69:v:62:HIS:HD2	2.17	0.42
58:q:203:ILE:HG13	58:q:203:ILE:O	2.18	0.42
64:o:772:LEU:HA	64:o:775:THR:HG22	2.02	0.42
65:h:151:LEU:HG	69:v:37:ILE:HB	2.01	0.42
69:v:45:GLU:CD	69:v:45:GLU:C	2.88	0.42
71:w:1090:CYS:SG	71:w:1091:ASP:N	2.88	0.42
4:DA:511:LEU:HD12	4:DA:511:LEU:N	2.31	0.42
4:DA:645:LYS:HD2	4:DA:645:LYS:HA	1.76	0.42
4:DA:727:THR:HG23	4:DA:727:THR:O	2.19	0.42
6:FA:50:ASP:OD1	6:FA:53:ASN:ND2	2.52	0.42
7:HA:111:SER:N	7:HA:211:TYR:OH	2.52	0.42
10:DB:562:GLY:O	10:DB:581:ILE:HG12	2.19	0.42
31:Df:447:ALA:CB	31:Df:456:GLY:HA3	2.49	0.42
34:Dk:130:PRO:HD3	36:Dm:35:GLU:HG2	2.02	0.42
34:Dk:182:LEU:HD23	34:Dk:182:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DF:320:ARG:NE	31:DF:415:ILE:HD12	2.35	0.42
39:HD:32:GLU:OE1	39:HD:32:GLU:N	2.47	0.42
39:HD:255:THR:OG1	39:HD:256:TYR:N	2.53	0.42
44:HI:208:LEU:HD23	44:HI:208:LEU:HA	1.77	0.42
50:n:916:LEU:HD12	50:n:917:ALA:H	1.85	0.42
53:a:361:MET:HE3	53:a:376:LEU:HB2	2.02	0.42
53:a:493:PHE:HE2	53:a:514:LYS:HB2	1.85	0.42
54:d:42:ARG:HH21	56:i:93:LYS:N	2.18	0.42
55:f:24:LEU:HD22	55:f:24:LEU:HA	1.79	0.42
55:f:78:LEU:CD1	65:h:81:LEU:HD23	2.42	0.42
55:f:111:LEU:HD22	58:q:127:LEU:CD1	2.49	0.42
58:q:544:MET:HE2	58:q:544:MET:HB3	1.84	0.42
59:z:597:VAL:HG11	59:z:599:LEU:HD12	2.02	0.42
66:k:8:ASN:OD1	66:k:8:ASN:N	2.52	0.42
68:t:3:VAL:HG22	68:t:150:ALA:CB	2.50	0.42
68:t:79:PHE:C	68:t:80:GLU:HG3	2.44	0.42
70:p:182:VAL:HG21	70:p:228:VAL:HG21	2.01	0.42
71:w:314:ARG:NH1	71:w:326:THR:OG1	2.48	0.42
6:FA:47:LEU:HD11	6:FA:98:TRP:HB3	2.01	0.42
7:HA:109:LEU:HD11	7:HA:199:ILE:HD11	2.01	0.42
7:HA:249:VAL:HG21	7:HA:403:PHE:HB2	2.00	0.42
12:FB:58:LEU:CD1	12:FB:62:LEU:HD23	2.49	0.42
15:PB:905:ASP:OD1	15:PB:924:ARG:NH1	2.49	0.42
16:HC:118:LEU:HD11	40:HE:50:PHE:CZ	2.55	0.42
23:PK:64:PRO:HG3	23:PK:72:ILE:HD12	2.02	0.42
26:DQ:330:ASP:OD2	29:DD:1011:ALA:CB	2.68	0.42
31:Df:238:LYS:HG2	38:DH:197:THR:HB	2.02	0.42
31:DF:396:LEU:HA	31:DF:399:GLU:OE1	2.20	0.42
31:DF:401:GLU:C	31:DF:401:GLU:CD	2.87	0.42
32:DI:50:ILE:HG22	32:DI:71:VAL:HG13	2.02	0.42
32:DI:78:ARG:O	32:DI:82:SER:HB2	2.20	0.42
44:HI:266:ASP:HA	44:HI:269:LEU:CB	2.49	0.42
45:HJ:288:ASN:ND2	45:HJ:288:ASN:O	2.53	0.42
46:PD:60:VAL:HG22	47:PG:103:PRO:HG3	2.02	0.42
49:j:82:LYS:HD3	51:s:96:PHE:CD1	2.55	0.42
50:n:212:LEU:HD22	50:n:226:VAL:HA	2.02	0.42
50:n:586:LEU:HD23	50:n:587:LEU:HD22	2.02	0.42
50:n:909:GLN:NE2	60:b:114:ASP:OD1	2.53	0.42
53:a:457:PRO:HB3	53:a:512:ARG:HD2	2.00	0.42
54:d:115:LYS:O	54:d:115:LYS:HD3	2.20	0.42
54:d:126:TYR:CD1	54:d:126:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:129:PRO:HB3	65:h:74:GLN:CG	2.49	0.42
60:b:87:ASN:HA	60:b:90:ASN:HB2	2.00	0.42
62:e:129:VAL:CG1	66:k:114:MET:HE2	2.48	0.42
64:o:729:TYR:C	64:o:731:ALA:H	2.28	0.42
65:h:137:GLN:OE1	65:h:137:GLN:HA	2.20	0.42
65:h:151:LEU:CG	69:v:37:ILE:HB	2.50	0.42
66:k:33:LEU:CA	66:k:36:SER:OG	2.63	0.42
67:r:47:GLU:CD	67:r:47:GLU:H	2.26	0.42
70:p:56:GLN:O	70:p:59:THR:OG1	2.35	0.42
70:p:168:LEU:HD12	70:p:168:LEU:HA	1.92	0.42
71:w:60:ILE:HA	71:w:63:ILE:HD12	2.01	0.42
71:w:248:LEU:HD23	71:w:248:LEU:HA	1.83	0.42
71:w:363:ARG:HD2	71:w:365:LEU:HD11	2.01	0.42
5:EA:17:LEU:HD22	5:EA:194:THR:CB	2.50	0.41
5:EA:26:TYR:HD1	11:EB:220:TRP:CZ2	2.37	0.41
6:FA:15:VAL:HG12	6:FA:16:VAL:N	2.34	0.41
7:HA:56:ILE:HG21	7:HA:70:LEU:HD22	2.01	0.41
9:PA:672:ILE:HG23	9:PA:676:ILE:HD13	2.02	0.41
10:DB:464:ILE:HG12	10:DB:513:LYS:HE2	2.02	0.41
10:DB:544:LEU:HD22	10:DB:625:LEU:HD22	2.02	0.41
12:FB:31:TRP:CD1	12:FB:62:LEU:HD21	2.55	0.41
16:HC:359:ILE:HG22	16:HC:360:THR:N	2.35	0.41
21:PI:41:ASN:OD1	21:PI:41:ASN:C	2.63	0.41
31:Df:104:LEU:HD22	33:Dj:216:TYR:HB2	2.02	0.41
29:DD:1001:GLN:O	29:DD:1002:ARG:C	2.62	0.41
44:HI:200:GLY:HA3	44:HI:276:PHE:HE1	1.84	0.41
44:HI:235:GLU:O	44:HI:236:GLN:C	2.63	0.41
48:g:126:TYR:C	48:g:130:GLN:H	2.28	0.41
50:n:154:ILE:CB	50:n:155:PRO:HD3	2.43	0.41
50:n:376:PRO:HD2	50:n:377:PRO:HD3	2.01	0.41
50:n:382:ASP:O	50:n:386:VAL:HG22	2.20	0.41
50:n:647:MET:HG2	50:n:651:ASN:HD21	1.85	0.41
51:s:108:PHE:O	51:s:109:LEU:C	2.63	0.41
53:a:109:TYR:C	53:a:109:TYR:CD1	2.98	0.41
56:i:65:PHE:HD1	56:i:99:LYS:CD	2.33	0.41
58:q:188:LEU:HD13	69:v:87:ILE:CG1	2.46	0.41
60:b:157:TYR:N	60:b:158:PRO:HD2	2.35	0.41
61:c:180:LEU:HD12	61:c:181:SER:H	1.84	0.41
65:h:68:THR:HB	65:h:69:PRO:HD2	2.02	0.41
67:r:196:LEU:HA	67:r:196:LEU:HD23	1.77	0.41
68:t:122:PHE:CE2	68:t:156:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:p:174:LYS:HG3	73:y:84:CYS:HB3	2.01	0.41
70:p:273:ARG:HD2	70:p:273:ARG:HA	1.83	0.41
71:w:8:ILE:O	71:w:12:VAL:HG23	2.20	0.41
72:x:42:LEU:HD12	72:x:42:LEU:HA	1.94	0.41
72:x:707:ILE:HD12	72:x:707:ILE:HA	1.88	0.41
76:NX:20:DC:H1'	76:NX:21:DC:N3	2.35	0.41
76:NX:136:DC:H2''	76:NX:137:DC:C5	2.55	0.41
4:DA:825:ILE:HD12	4:DA:830:ILE:HD11	2.01	0.41
7:HA:618:VAL:HG11	7:HA:664:VAL:HA	2.03	0.41
9:PA:219:GLU:OE1	11:EB:227:SER:HA	2.20	0.41
10:DB:176:HIS:HE1	10:DB:310:ASP:H	1.68	0.41
10:DB:622:ASP:CG	43:HF:36:GLN:HG3	2.44	0.41
11:EB:99:LEU:HD12	11:EB:124:LEU:HD11	2.01	0.41
16:HC:96:TRP:HB3	16:HC:110:LEU:HD23	2.02	0.41
18:PE:106:VAL:HG12	18:PE:107:GLN:N	2.33	0.41
35:DI:129:PRO:HB2	36:Dm:56:ILE:HG23	2.01	0.41
31:DF:219:GLU:OE1	38:DH:156:PRO:HB2	2.21	0.41
39:HD:284:ALA:C	39:HD:286:GLY:H	2.28	0.41
42:HH:559:ILE:HG22	42:HH:561:PHE:CE1	2.55	0.41
44:HI:257:LEU:H	44:HI:257:LEU:HG	1.61	0.41
50:n:104:LYS:HZ2	51:s:108:PHE:CA	2.28	0.41
50:n:751:ASN:OD1	50:n:752:LEU:N	2.52	0.41
53:a:204:LEU:HD23	53:a:204:LEU:HA	1.89	0.41
58:q:451:LEU:HD22	58:q:451:LEU:HA	1.85	0.41
60:b:159:GLN:O	60:b:163:VAL:HG13	2.20	0.41
66:k:75:THR:C	66:k:77:GLN:N	2.78	0.41
67:r:18:MET:SD	67:r:176:PRO:HA	2.59	0.41
67:r:53:ASP:HB3	67:r:73:ARG:NE	2.35	0.41
67:r:141:MET:HA	67:r:173:VAL:HG22	2.01	0.41
69:v:35:GLU:OE2	69:v:64:ARG:NH2	2.53	0.41
69:v:35:GLU:HB3	69:v:64:ARG:HD2	2.02	0.41
71:w:213:ARG:HA	71:w:213:ARG:HD3	1.95	0.41
3:BA:195:PHE:CZ	3:BA:199:LEU:HD11	2.55	0.41
4:DA:342:ARG:O	4:DA:347:ARG:HB2	2.20	0.41
9:PA:544:ALA:CB	9:PA:680:LEU:HD13	2.50	0.41
9:PA:567:LEU:HB2	9:PA:570:TRP:HB2	2.01	0.41
9:PA:1166:LEU:HA	9:PA:1298:LEU:HD11	2.02	0.41
10:DB:984:PRO:HG2	10:DB:987:LEU:HD22	2.02	0.41
15:PB:718:GLN:CD	15:PB:976:MET:HE3	2.45	0.41
17:PC:36:ARG:HD3	23:PK:41:THR:OG1	2.20	0.41
32:Di:57:TYR:HE1	35:DI:118:LEU:CD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DE:704:VAL:HA	30:DE:759:ILE:HD11	2.01	0.41
31:DF:279:LEU:HD22	31:DF:330:ARG:CZ	2.51	0.41
38:DH:53:ALA:CB	33:DJ:195:LEU:HB3	2.50	0.41
39:HD:85:ARG:HH12	39:HD:140:LEU:H	1.66	0.41
39:HD:290:SER:O	39:HD:291:LEU:C	2.63	0.41
39:HD:295:ARG:O	39:HD:296:ALA:C	2.61	0.41
40:HE:175:MET:HE3	40:HE:179:ASN:CG	2.45	0.41
40:HE:217:VAL:HG23	40:HE:217:VAL:O	2.20	0.41
40:HE:255:CYS:HB2	40:HE:276:CYS:N	2.35	0.41
42:HH:535:THR:HG23	42:HH:627:SER:HB2	2.02	0.41
45:HJ:15:SER:N	45:HJ:18:GLN:OE1	2.42	0.41
45:HJ:97:MET:H	45:HJ:97:MET:HG2	1.66	0.41
50:n:220:GLY:C	50:n:221:ARG:HG3	2.46	0.41
52:u:115:LEU:CB	54:d:121:LEU:HD11	2.26	0.41
58:q:102:LEU:HD13	65:h:29:PHE:CD2	2.54	0.41
60:b:64:ILE:HD13	60:b:64:ILE:HA	1.79	0.41
61:c:16:GLN:HB3	61:c:73:LEU:HD21	2.02	0.41
61:c:70:LEU:HD12	61:c:70:LEU:HA	1.82	0.41
64:o:763:LEU:HD11	64:o:775:THR:HG21	2.02	0.41
66:k:64:SER:HB2	66:k:68:ARG:NH2	2.35	0.41
71:w:805:GLN:HE22	71:w:809:ARG:HE	1.68	0.41
72:x:269:MET:HE2	72:x:269:MET:HB2	1.76	0.41
72:x:687:PHE:CD1	72:x:687:PHE:N	2.88	0.41
7:HA:225:LEU:O	7:HA:227:ARG:NH1	2.53	0.41
10:DB:957:MET:O	10:DB:968:ARG:NH1	2.53	0.41
15:PB:1107:LEU:O	15:PB:1111:SER:OG	2.30	0.41
16:HC:51:LEU:HD23	40:HE:237:GLN:CD	2.45	0.41
30:De:270:ASP:OD1	30:De:271:GLN:NE2	2.42	0.41
30:De:636:HIS:CD2	30:De:638:ASN:H	2.36	0.41
31:Df:20:LYS:HE2	31:Df:20:LYS:HB3	1.83	0.41
41:HG:333:GLU:O	41:HG:333:GLU:HG2	2.21	0.41
45:HJ:54:MET:HE3	45:HJ:54:MET:HB3	1.88	0.41
45:HJ:186:ILE:HD13	45:HJ:186:ILE:N	2.21	0.41
48:g:127:ARG:HH22	52:u:9:GLN:CD	2.29	0.41
50:n:287:LYS:HA	50:n:287:LYS:HD2	1.87	0.41
50:n:1354:THR:HA	50:n:1364:LEU:O	2.20	0.41
53:a:462:LEU:HB2	72:x:49:GLN:HA	2.02	0.41
55:f:114:VAL:O	55:f:118:ARG:HG2	2.21	0.41
60:b:116:LEU:HD23	60:b:116:LEU:HA	1.79	0.41
65:h:191:LEU:HD23	65:h:191:LEU:HA	1.89	0.41
66:k:106:ASP:HA	66:k:109:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:x:561:LEU:O	72:x:608:ASN:ND2	2.51	0.41
72:x:794:ASP:HB3	72:x:797:LYS:HB2	2.02	0.41
72:x:821:TYR:HE2	72:x:946:PHE:HE2	1.67	0.41
8:NE:734:ARG:O	8:NE:735:ALA:CB	2.68	0.41
4:DA:847:LYS:HE2	4:DA:847:LYS:HB3	1.77	0.41
4:DA:954:ALA:HA	37:DG:149:ARG:HH22	1.85	0.41
7:HA:56:ILE:HD12	7:HA:230:VAL:HG11	2.02	0.41
9:PA:497:ASP:OD1	9:PA:497:ASP:C	2.63	0.41
9:PA:549:THR:O	9:PA:549:THR:HG22	2.19	0.41
9:PA:910:LYS:N	9:PA:911:PRO:CD	2.84	0.41
9:PA:1437:ASP:O	9:PA:1441:GLU:HG2	2.20	0.41
9:PA:1443:ALA:HB2	15:PB:1167:ILE:HG23	2.01	0.41
10:DB:831:GLU:OE1	10:DB:835:ARG:NH2	2.52	0.41
27:DO:11:LEU:HD23	27:DO:44:ILE:HD12	2.02	0.41
30:De:467:LEU:HD23	30:De:467:LEU:HA	1.93	0.41
29:DD:949:GLN:O	29:DD:952:GLN:HB2	2.20	0.41
30:DE:747:LEU:N	30:DE:747:LEU:HD13	2.35	0.41
31:DF:289:LEU:HD23	31:DF:289:LEU:HA	1.94	0.41
32:DI:35:VAL:CG1	32:DI:39:MET:HE2	2.50	0.41
43:HF:21:LEU:O	43:HF:24:ASP:OD1	2.38	0.41
44:HI:135:HIS:CD2	44:HI:137:ASP:H	2.34	0.41
46:PD:58:SER:OG	47:PG:35:GLU:OE2	2.35	0.41
50:n:394:HIS:CD2	50:n:399:LYS:HD2	2.56	0.41
50:n:944:PHE:O	50:n:945:ASP:C	2.64	0.41
53:a:351:ASP:O	53:a:351:ASP:CG	2.63	0.41
55:f:50:VAL:HG11	55:f:56:THR:HB	2.03	0.41
58:q:644:SER:HB2	62:e:97:GLN:N	2.35	0.41
66:k:106:ASP:HA	66:k:109:ARG:NE	2.36	0.41
70:p:558:SER:O	70:p:562:SER:N	2.53	0.41
71:w:916:ASP:OD1	71:w:916:ASP:N	2.53	0.41
72:x:183:LEU:HD21	72:x:974:SER:HB3	2.03	0.41
76:NX:135:DC:H4'	76:NX:136:DC:OP1	2.20	0.41
77:NY:-67:DG:H2''	77:NY:-66:DG:C8	2.55	0.41
4:DA:1055:VAL:HG13	4:DA:1056:ALA:H	1.85	0.41
5:EA:28:ILE:HG13	5:EA:29:GLU:N	2.36	0.41
5:EA:139:LEU:HD23	47:PG:151:ARG:HB3	1.77	0.41
7:HA:46:THR:HG22	7:HA:670:GLY:HA3	2.03	0.41
8:NA:534:ARG:O	8:NA:535:ALA:HB2	2.20	0.41
9:PA:876:ASP:OD2	9:PA:880:ARG:NH2	2.53	0.41
9:PA:1666:PRO:HB2	9:PA:1667:THR:H	1.62	0.41
9:PA:1793:THR:H	65:h:102:HIS:CE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:PC:72:PRO:HG3	22:PJ:13:ILE:HD11	2.03	0.41
30:DE:236:LEU:HD21	30:DE:317:LEU:HB2	2.03	0.41
30:DE:589:TRP:HH2	31:DF:57:PHE:CE1	2.37	0.41
30:DE:695:LEU:O	30:DE:704:VAL:HB	2.20	0.41
39:HD:13:LYS:N	39:HD:13:LYS:HD3	2.36	0.41
39:HD:259:HIS:ND1	39:HD:259:HIS:N	2.68	0.41
39:HD:295:ARG:CZ	45:HJ:165:ARG:HH21	2.25	0.41
44:HI:250:LYS:HB3	44:HI:252:PHE:CZ	2.55	0.41
44:HI:293:LYS:HA	44:HI:293:LYS:HD3	1.92	0.41
45:HJ:25:ASP:OD1	45:HJ:25:ASP:C	2.63	0.41
45:HJ:27:ASN:OD1	45:HJ:27:ASN:C	2.63	0.41
48:g:123:ILE:HA	48:g:126:TYR:HB2	2.03	0.41
50:n:573:VAL:HG21	50:n:583:ALA:HB1	2.02	0.41
50:n:689:PRO:O	50:n:690:CYS:HB2	2.21	0.41
50:n:713:GLN:O	50:n:719:THR:HB	2.20	0.41
50:n:853:HIS:O	50:n:857:GLU:HG2	2.21	0.41
50:n:870:GLN:HG3	64:o:655:THR:HG21	2.03	0.41
54:d:79:LEU:HD12	54:d:79:LEU:HA	1.76	0.41
58:q:160:LEU:HD23	58:q:160:LEU:HA	1.81	0.41
61:c:207:LEU:HD12	61:c:207:LEU:HA	1.91	0.41
62:e:133:LEU:HD12	66:k:115:LEU:CD1	2.51	0.41
65:h:113:PRO:HB2	65:h:117:VAL:CG2	2.50	0.41
71:w:301:GLU:HG3	71:w:347:ALA:HB1	2.03	0.41
71:w:442:LYS:HE2	71:w:442:LYS:HB3	1.88	0.41
71:w:684:ASN:HD22	71:w:723:THR:HG21	1.85	0.41
71:w:1200:TYR:HD1	72:x:287:LYS:HD3	1.85	0.41
72:x:101:MET:HB3	72:x:101:MET:HE2	1.87	0.41
4:DA:482:ASP:N	4:DA:482:ASP:OD1	2.54	0.41
4:DA:620:LEU:HD11	4:DA:766:ARG:HD3	2.02	0.41
9:PA:1007:ILE:HD12	9:PA:1007:ILE:HA	1.89	0.41
11:EB:76:GLY:N	12:FB:192:GLU:OE2	2.53	0.41
11:EB:103:LEU:HD22	11:EB:108:HIS:HB3	2.02	0.41
16:HC:223:ALA:HA	16:HC:226:ARG:HG2	2.02	0.41
25:DP:258:MET:N	25:DP:315:ALA:O	2.54	0.41
31:Df:216:LEU:HD21	31:Df:254:GLN:O	2.21	0.41
30:DE:452:ARG:O	30:DE:453:LEU:C	2.63	0.41
31:DF:85:GLY:C	33:DJ:212:LYS:CG	2.93	0.41
32:DI:19:MET:CE	32:DI:40:LEU:HD23	2.51	0.41
40:HE:42:MET:HE3	40:HE:108:ASN:HA	2.02	0.41
41:HG:186:ILE:HG12	41:HG:211:LEU:HD12	2.03	0.41
44:HI:96:THR:HB	44:HI:97:ASP:H	1.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:HJ:167:PHE:O	45:HJ:168:GLU:C	2.62	0.41
50:n:121:PHE:HD2	51:s:83:LEU:HD21	1.81	0.41
50:n:907:LEU:HD21	60:b:118:LEU:CA	2.50	0.41
50:n:922:TYR:HH	50:n:1214:VAL:HG12	1.85	0.41
53:a:62:LEU:HD22	54:d:48:LEU:HD21	2.03	0.41
53:a:359:HIS:HD2	53:a:361:MET:H	1.68	0.41
55:f:34:SER:C	55:f:36:ARG:N	2.78	0.41
55:f:96:ALA:HA	58:q:130:VAL:HG11	2.03	0.41
58:q:35:SER:CB	58:q:42:ARG:HH22	2.30	0.41
58:q:36:MET:O	58:q:39:ASN:N	2.54	0.41
58:q:339:LEU:HD11	58:q:439:PHE:CD2	2.51	0.41
62:e:102:LEU:HD23	62:e:106:LYS:HE3	2.03	0.41
64:o:697:HIS:HB2	64:o:698:CYS:H	1.78	0.41
64:o:764:PRO:HA	71:w:15:THR:HG21	2.01	0.41
68:t:1:MET:HG2	68:t:186:PRO:HD3	2.01	0.41
70:p:146:HIS:NE2	70:p:160:SER:OG	2.49	0.41
70:p:590:VAL:HG11	70:p:695:LYS:HE3	2.02	0.41
70:p:678:ALA:HA	70:p:724:LEU:HD23	2.03	0.41
70:p:703:GLU:CD	70:p:703:GLU:N	2.79	0.41
72:x:303:LEU:HD13	72:x:303:LEU:HA	1.87	0.41
72:x:466:ARG:NH2	72:x:512:ILE:O	2.53	0.41
72:x:687:PHE:H	72:x:687:PHE:HD1	1.67	0.41
73:y:131:MET:HE2	73:y:131:MET:HB3	1.99	0.41
5:EA:171:LYS:HZ1	39:HD:41:ARG:CD	2.33	0.41
9:PA:847:LEU:HD21	15:PB:720:PRO:HB3	2.02	0.41
9:PA:1420:ASN:O	9:PA:1429:LYS:NZ	2.53	0.41
10:DB:835:ARG:CZ	38:DH:184:ARG:HH11	2.33	0.41
11:EB:83:ASN:OD1	12:FB:188:PHE:CZ	2.74	0.41
31:DF:66:LEU:HB3	32:DI:32:GLU:OE2	2.21	0.41
31:DF:75:LEU:HG	31:DF:84:TYR:OH	2.21	0.41
31:DF:233:GLY:CA	31:DF:239:ARG:HE	2.34	0.41
37:DG:74:MET:HE1	37:DG:136:ILE:HD12	2.03	0.41
39:HD:84:LYS:CB	39:HD:136:ASN:HD21	2.33	0.41
39:HD:281:GLN:NE2	39:HD:281:GLN:CA	2.79	0.41
44:HI:17:PHE:C	44:HI:17:PHE:CD1	2.96	0.41
44:HI:56:ASN:HD22	44:HI:56:ASN:HA	1.68	0.41
45:HJ:181:LEU:HD22	45:HJ:181:LEU:C	2.46	0.41
50:n:281:ARG:HG2	55:f:190:PRO:HA	2.02	0.41
50:n:297:HIS:HA	50:n:300:CYS:SG	2.61	0.41
53:a:498:VAL:CG2	53:a:507:THR:HG22	2.51	0.41
55:f:114:VAL:HG12	55:f:115:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:q:102:LEU:HD13	65:h:29:PHE:HD2	1.85	0.41
58:q:596:PHE:HE2	63:l:112:GLU:CG	2.34	0.41
62:e:55:CYS:SG	63:l:52:PHE:HZ	2.43	0.41
65:h:151:LEU:HD11	69:v:37:ILE:C	2.45	0.41
70:p:252:LYS:HD3	70:p:252:LYS:HA	1.85	0.41
71:w:786:PRO:HA	71:w:787:PRO:HD3	1.82	0.41
4:DA:405:VAL:HG23	4:DA:410:TRP:HZ2	1.86	0.41
5:EA:17:LEU:HD22	5:EA:194:THR:OG1	2.21	0.41
5:EA:21:VAL:HG23	5:EA:22:ILE:N	2.36	0.41
5:EA:185:GLU:HG3	5:EA:186:PRO:HD3	2.02	0.41
7:HA:12:PHE:CE2	7:HA:14:TYR:HB2	2.56	0.41
7:HA:383:LEU:HD21	7:HA:388:ILE:HD11	2.02	0.41
9:PA:353:ASN:O	9:PA:357:LYS:HG3	2.21	0.41
9:PA:1643:TYR:CZ	57:m:93:CYS:CB	3.04	0.41
10:DB:100:GLN:O	10:DB:101:ARG:NH1	2.46	0.41
10:DB:218:GLY:HA2	10:DB:238:LEU:HD13	2.03	0.41
10:DB:367:GLU:OE2	10:DB:371:LYS:NZ	2.39	0.41
11:EB:85:MET:HE2	11:EB:139:PHE:H	1.86	0.41
12:FB:186:MET:SD	29:DD:995:GLU:CD	3.04	0.41
12:FB:224:ASN:ND2	12:FB:234:GLU:OE2	2.53	0.41
15:PB:516:GLU:OE1	15:PB:516:GLU:N	2.54	0.41
16:HC:58:ARG:CD	40:HE:229:TRP:CE3	3.04	0.41
16:HC:146:PRO:HA	16:HC:149:ASP:OD2	2.21	0.41
17:PC:62:GLU:OE1	17:PC:62:GLU:N	2.52	0.41
26:DQ:19:GLU:O	26:DQ:22:ILE:HG12	2.21	0.41
26:DQ:330:ASP:OD2	29:DD:1011:ALA:HB1	2.21	0.41
31:Df:83:LEU:HD11	32:Di:42:PHE:HB2	2.03	0.41
31:Df:402:ARG:HH22	31:Df:403:ILE:HD12	1.85	0.41
35:Dl:128:ILE:HA	35:Dl:129:PRO:HD3	1.93	0.41
31:DF:231:CYS:HB3	31:DF:285:MET:HE2	2.02	0.41
31:DF:368:THR:O	31:DF:369:PRO:C	2.64	0.41
31:DF:370:TRP:CH2	31:DF:402:ARG:HB3	2.56	0.41
38:DH:114:SER:C	38:DH:116:ARG:N	2.76	0.41
39:HD:297:LEU:O	39:HD:298:GLN:C	2.61	0.41
42:HH:364:LEU:HD23	42:HH:410:TYR:CD1	2.56	0.41
44:HI:20:GLU:CD	44:HI:20:GLU:N	2.79	0.41
44:HI:139:LYS:O	44:HI:140:PRO:C	2.64	0.41
44:HI:148:ASN:N	44:HI:148:ASN:OD1	2.53	0.41
44:HI:261:PHE:CZ	44:HI:272:ILE:HG21	2.55	0.41
44:HI:279:ASN:C	44:HI:281:CYS:N	2.74	0.41
45:HJ:158:LEU:HD12	45:HJ:158:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g:127:ARG:HD3	48:g:130:GLN:CG	2.51	0.41
49:j:82:LYS:HE3	51:s:101:VAL:HB	2.02	0.41
50:n:152:PHE:CE1	54:d:149:ILE:HG23	2.56	0.41
50:n:205:THR:HA	54:d:108:GLN:HE22	1.85	0.41
50:n:237:MET:HE2	58:q:45:GLN:CG	2.51	0.41
50:n:310:SER:O	50:n:313:LEU:HG	2.21	0.41
50:n:311:GLN:O	50:n:315:LEU:HG	2.20	0.41
50:n:707:ASP:OD1	50:n:708:CYS:N	2.53	0.41
52:u:49:ASN:ND2	52:u:49:ASN:N	2.67	0.41
53:a:211:LEU:HD11	53:a:220:MET:SD	2.61	0.41
53:a:228:PRO:CB	53:a:502:MET:HB2	2.40	0.41
53:a:427:ARG:HE	53:a:427:ARG:HB3	1.50	0.41
54:d:42:ARG:HH22	56:i:93:LYS:CG	2.32	0.41
54:d:49:ALA:HB3	56:i:76:MET:SD	2.41	0.41
54:d:182:MET:HE3	54:d:182:MET:HB3	1.79	0.41
57:m:103:LEU:HD23	57:m:103:LEU:HA	1.95	0.41
58:q:20:HIS:HB3	58:q:31:LEU:HB2	2.01	0.41
58:q:89:GLN:OE1	58:q:90:PRO:HD2	2.16	0.41
58:q:395:PRO:HA	67:r:53:ASP:OD1	2.20	0.41
58:q:430:LYS:HG2	58:q:471:TYR:OH	2.21	0.41
68:t:204:GLN:CA	68:t:204:GLN:HE21	2.33	0.41
71:w:1183:TRP:HE1	71:w:1190:LEU:HD13	1.85	0.41
72:x:436:LEU:HD23	72:x:436:LEU:HA	1.79	0.41
72:x:901:LEU:HD23	72:x:901:LEU:HA	1.91	0.41
1:X:22:DC:H42	2:Y:-22:DG:H1	1.68	0.41
7:HA:604:VAL:O	7:HA:608:ILE:HG22	2.21	0.41
9:PA:457:ILE:HD11	9:PA:515:ILE:HG23	2.03	0.41
9:PA:1022:ILE:N	9:PA:1034:GLN:OE1	2.45	0.41
10:DB:639:LYS:NZ	10:DB:641:GLU:OE2	2.42	0.41
13:HB:422:LEU:HD21	40:HE:224:LEU:HB3	2.02	0.41
15:PB:794:VAL:HG22	15:PB:967:ILE:HG22	2.02	0.41
19:PF:71:LEU:HG	47:PG:62:GLY:O	2.21	0.41
31:Df:244:GLN:O	31:Df:248:THR:OG1	2.34	0.41
30:DE:239:LEU:HB3	30:DE:307:LEU:HD21	2.03	0.41
31:DF:118:ILE:HD12	31:DF:118:ILE:O	2.21	0.41
31:DF:215:GLU:H	31:DF:215:GLU:CD	2.29	0.41
31:DF:392:ILE:O	31:DF:392:ILE:CG2	2.69	0.41
38:DH:40:VAL:HG11	33:DJ:130:ILE:HG12	2.03	0.41
38:DH:111:ALA:CB	33:DJ:119:PHE:CZ	3.03	0.41
39:HD:85:ARG:NH1	39:HD:140:LEU:N	2.68	0.41
39:HD:287:TYR:CG	44:HI:189:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:HI:17:PHE:C	44:HI:17:PHE:HD1	2.29	0.41
45:HJ:239:LYS:N	45:HJ:239:LYS:HE3	2.36	0.41
50:n:505:CYS:HB3	50:n:641:LEU:HD21	2.03	0.41
50:n:731:LEU:HD12	50:n:800:VAL:HG11	2.03	0.41
50:n:794:LEU:HA	50:n:797:PHE:HB3	2.02	0.41
50:n:932:GLY:CA	50:n:1179:HIS:NE2	2.83	0.41
50:n:944:PHE:CD2	60:b:101:ARG:NH2	2.89	0.41
53:a:63:GLU:O	53:a:67:LYS:HB2	2.21	0.41
53:a:337:ALA:CB	53:a:338:PRO:CD	2.89	0.41
55:f:16:VAL:CG1	55:f:104:VAL:HA	2.50	0.41
59:z:543:LEU:HD12	59:z:543:LEU:HA	1.87	0.41
65:h:116:GLU:O	65:h:120:GLN:HG2	2.20	0.41
70:p:284:LYS:HB3	70:p:356:LEU:HD11	2.03	0.41
71:w:844:ASN:HA	71:w:847:ILE:HG22	2.02	0.41
7:HA:195:ALA:O	7:HA:199:ILE:HG12	2.21	0.40
9:PA:478:PRO:HD2	23:PK:67:LEU:HD13	2.03	0.40
9:PA:869:GLU:OE2	15:PB:1091:ARG:NH1	2.47	0.40
10:DB:490:SER:O	10:DB:491:HIS:C	2.62	0.40
13:HB:407:ILE:HD12	40:HE:22:TRP:CB	2.51	0.40
16:HC:415:GLN:HB3	16:HC:439:ARG:HD3	2.03	0.40
27:DO:44:ILE:O	27:DO:48:LEU:HD13	2.21	0.40
30:De:238:GLN:H	30:De:238:GLN:HG2	1.64	0.40
31:Df:254:GLN:O	31:Df:254:GLN:HG3	2.21	0.40
31:Df:409:GLY:HA2	31:Df:410:PRO:HD2	1.96	0.40
31:DF:374:TYR:CE1	31:DF:422:HIS:HB3	2.56	0.40
39:HD:84:LYS:HB3	39:HD:136:ASN:ND2	2.36	0.40
39:HD:264:GLU:HB2	39:HD:269:LEU:HB2	2.01	0.40
39:HD:268:ARG:H	39:HD:268:ARG:HD3	1.87	0.40
44:HI:185:PHE:HE2	44:HI:237:TRP:HH2	1.68	0.40
44:HI:266:ASP:HA	44:HI:269:LEU:HB2	2.01	0.40
45:HJ:43:ASN:CG	45:HJ:43:ASN:O	2.62	0.40
45:HJ:97:MET:HB3	45:HJ:97:MET:HE3	1.82	0.40
50:n:548:TYR:CE2	50:n:652:MET:CE	3.03	0.40
50:n:552:VAL:HG22	50:n:568:TYR:HD1	1.86	0.40
50:n:678:PHE:CZ	58:q:583:ARG:HB2	2.56	0.40
50:n:793:HIS:HD2	50:n:794:LEU:HG	1.86	0.40
50:n:1210:PHE:HD1	50:n:1211:LEU:HD23	1.85	0.40
51:s:142:ASN:HB2	51:s:143:PRO:HD2	2.03	0.40
53:a:59:VAL:CG1	54:d:51:SER:OG	2.53	0.40
53:a:70:LYS:N	56:i:70:HIS:HE1	2.20	0.40
53:a:161:TYR:C	53:a:163:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:437:LEU:HD23	53:a:437:LEU:HA	1.63	0.40
55:f:77:ILE:HG13	55:f:78:LEU:N	2.37	0.40
56:i:140:MET:SD	56:i:140:MET:N	2.93	0.40
58:q:495:LEU:HD22	58:q:504:VAL:HG22	2.03	0.40
63:l:160:MET:CE	69:v:134:TYR:CD2	3.04	0.40
65:h:32:LYS:NZ	65:h:40:LEU:HD11	2.36	0.40
66:k:77:GLN:NE2	67:r:192:GLN:HB2	2.36	0.40
70:p:564:LEU:H	70:p:564:LEU:HG	1.77	0.40
71:w:727:TRP:HB2	71:w:732:LEU:HD13	2.02	0.40
72:x:363:LEU:HA	72:x:363:LEU:HD23	1.81	0.40
74:NC:842:SER:C	74:NC:844:GLY:N	2.79	0.40
76:NX:18:DC:H42	77:NY:-17:DG:H1	1.69	0.40
3:BA:282:ASP:OD1	3:BA:283:VAL:N	2.55	0.40
4:DA:725:CYS:SG	4:DA:734:LEU:HD12	2.61	0.40
4:DA:899:LYS:HE3	4:DA:899:LYS:HB2	1.82	0.40
7:HA:345:ARG:NH1	39:HD:1:MET:HG3	2.36	0.40
9:PA:1137:PRO:HB2	9:PA:1341:VAL:HG13	2.03	0.40
9:PA:1430:CYS:SG	9:PA:1435:THR:HG23	2.61	0.40
10:DB:55:PRO:HB3	10:DB:60:LEU:HD22	2.03	0.40
10:DB:267:HIS:HB3	10:DB:277:LEU:HD11	2.03	0.40
10:DB:463:ARG:HD2	10:DB:515:ILE:HG22	2.03	0.40
10:DB:487:LYS:O	10:DB:487:LYS:CG	2.67	0.40
15:PB:771:GLU:O	22:PJ:55:LEU:HD21	2.21	0.40
16:HC:62:LEU:O	16:HC:115:ARG:NH2	2.54	0.40
16:HC:124:GLY:H	40:HE:100:LYS:NZ	2.20	0.40
19:PF:71:LEU:HD13	19:PF:71:LEU:HA	1.93	0.40
30:DE:359:LEU:HD12	30:DE:359:LEU:C	2.46	0.40
31:DF:316:GLN:NE2	31:DF:320:ARG:CA	2.84	0.40
31:DF:350:ASN:O	31:DF:354:ARG:NH1	2.54	0.40
38:DH:153:PHE:HA	38:DH:154:PRO:HD3	1.97	0.40
42:HH:128:SER:O	42:HH:334:ARG:NH2	2.51	0.40
42:HH:340:LEU:CD2	42:HH:491:ALA:HB2	2.52	0.40
42:HH:474:ASP:N	42:HH:474:ASP:OD1	2.54	0.40
44:HI:141:ASN:OD1	44:HI:141:ASN:N	2.53	0.40
45:HJ:111:LEU:O	45:HJ:115:VAL:HG12	2.21	0.40
46:PD:70:ARG:HG2	69:v:20:LYS:HE3	2.02	0.40
46:PD:76:ASN:O	46:PD:79:THR:OG1	2.38	0.40
50:n:231:GLU:CB	50:n:253:LEU:HD21	2.51	0.40
50:n:634:MET:HE2	58:q:519:GLN:CD	2.45	0.40
53:a:221:ASN:HB3	53:a:254:ASN:ND2	2.35	0.40
53:a:336:TYR:CG	53:a:391:THR:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a:402:GLY:O	53:a:405:PRO:HD2	2.20	0.40
54:d:115:LYS:HE2	54:d:115:LYS:C	2.46	0.40
55:f:57:LEU:HB3	55:f:58:GLU:H	1.50	0.40
61:c:214:VAL:HG22	61:c:243:THR:HG23	2.03	0.40
62:e:136:LEU:HD11	66:k:107:VAL:CG1	2.50	0.40
63:l:36:ILE:O	63:l:40:THR:HG23	2.21	0.40
63:l:166:LEU:HD22	69:v:123:ILE:HD13	2.04	0.40
64:o:689:PHE:CG	64:o:773:LEU:HD13	2.57	0.40
70:p:50:ASP:OD1	70:p:50:ASP:N	2.43	0.40
70:p:306:VAL:HG23	70:p:399:LEU:HD13	2.02	0.40
70:p:444:VAL:HG22	70:p:452:LEU:HD11	2.02	0.40
70:p:518:LEU:HA	70:p:521:VAL:HG22	2.03	0.40
70:p:813:THR:OG1	70:p:814:THR:N	2.54	0.40
1:X:1:DC:H2"	1:X:2:DG:C8	2.56	0.40
4:DA:728:SER:HA	4:DA:729:PRO:HD3	1.97	0.40
6:FA:167:ARG:NE	15:PB:307:GLU:OE2	2.46	0.40
9:PA:1645:PRO:HB2	9:PA:1646:THR:H	1.66	0.40
10:DB:684:ILE:HD13	10:DB:684:ILE:HA	1.95	0.40
10:DB:749:LEU:HA	10:DB:752:THR:HG22	2.02	0.40
10:DB:987:LEU:HG	10:DB:988:PRO:HD2	2.03	0.40
12:FB:179:ASP:OD1	12:FB:179:ASP:N	2.54	0.40
15:PB:573:TRP:NE1	15:PB:575:GLY:O	2.51	0.40
15:PB:647:GLU:O	15:PB:648:TYR:CG	2.74	0.40
15:PB:954:MET:HE3	15:PB:963:PRO:O	2.22	0.40
16:HC:58:ARG:HD2	40:HE:229:TRP:HE3	1.84	0.40
18:PE:2:ASP:OD1	18:PE:4:GLU:N	2.54	0.40
24:PL:22:CYS:SG	24:PL:24:THR:OG1	2.69	0.40
26:DQ:32:ASP:OD2	27:DO:32:LEU:HD13	2.21	0.40
31:DF:396:LEU:HA	31:DF:399:GLU:CD	2.46	0.40
35:DL:128:ILE:O	35:DL:128:ILE:HG22	2.19	0.40
39:HD:56:SER:O	39:HD:57:ASN:C	2.65	0.40
41:HG:115:GLU:N	41:HG:115:GLU:OE1	2.54	0.40
44:HI:110:THR:HA	55:f:63:MET:HG3	2.04	0.40
44:HI:195:ASP:O	44:HI:199:VAL:HG23	2.22	0.40
45:HJ:175:LYS:CA	45:HJ:175:LYS:NZ	2.77	0.40
50:n:129:PHE:O	50:n:132:THR:OG1	2.37	0.40
50:n:743:ARG:HB3	50:n:805:TYR:CE2	2.56	0.40
52:u:78:SER:C	52:u:80:GLU:N	2.79	0.40
52:u:115:LEU:HA	54:d:121:LEU:HD12	1.96	0.40
53:a:109:TYR:HE1	53:a:150:PHE:CZ	2.36	0.40
53:a:380:ALA:HB3	53:a:444:PRO:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:f:64:VAL:HG21	55:f:88:SER:HA	2.04	0.40
56:i:65:PHE:CE1	56:i:99:LYS:CG	3.03	0.40
58:q:139:GLN:C	58:q:139:GLN:CD	2.89	0.40
58:q:147:ILE:HD12	58:q:147:ILE:HA	1.80	0.40
58:q:566:ALA:HB1	58:q:583:ARG:HD3	2.03	0.40
60:b:60:TYR:OH	61:c:70:LEU:O	2.36	0.40
70:p:738:LEU:HD23	70:p:738:LEU:HA	1.91	0.40
74:NG:1017:VAL:O	74:NG:1018:SER:CB	2.69	0.40
4:DA:345:PRO:HD2	4:DA:500:LEU:HD13	2.02	0.40
4:DA:410:TRP:HB3	31:DF:306:PRO:HD3	2.02	0.40
4:DA:646:LYS:HD3	4:DA:646:LYS:HA	1.97	0.40
7:HA:531:VAL:HG12	7:HA:532:PRO:O	2.22	0.40
9:PA:486:LEU:HB3	9:PA:538:VAL:HG21	2.03	0.40
9:PA:509:LEU:HD12	19:PF:71:LEU:HD13	2.03	0.40
12:FB:57:THR:O	12:FB:57:THR:HG23	2.21	0.40
12:FB:123:ASN:OD1	12:FB:123:ASN:N	2.54	0.40
17:PC:185:GLU:OE2	17:PC:206:SER:OG	2.36	0.40
28:Dc:105:ASN:OD1	28:Dc:105:ASN:N	2.55	0.40
31:DF:277:ALA:O	31:DF:278:LEU:C	2.64	0.40
35:DL:120:LEU:HD23	35:DL:126:MET:HG3	2.03	0.40
40:HE:31:GLN:OE1	40:HE:36:LYS:NZ	2.42	0.40
40:HE:272:LEU:CD2	41:HG:318:LEU:HD12	2.51	0.40
42:HH:532:LEU:HD22	42:HH:716:VAL:HG13	2.04	0.40
44:HI:87:ILE:HD11	45:HJ:148:LEU:HD22	2.04	0.40
48:g:104:LYS:O	48:g:108:LYS:N	2.47	0.40
48:g:127:ARG:HD3	48:g:130:GLN:CB	2.51	0.40
50:n:274:ILE:HG13	55:f:181:LEU:HD21	2.02	0.40
50:n:524:ASN:C	50:n:526:SER:H	2.29	0.40
52:u:4:ARG:HG3	59:z:594:LEU:O	2.21	0.40
52:u:115:LEU:HD12	54:d:121:LEU:CD1	2.51	0.40
53:a:211:LEU:HD12	53:a:212:THR:N	2.37	0.40
53:a:445:LEU:N	53:a:445:LEU:HD23	2.36	0.40
53:a:453:SER:O	72:x:14:TRP:CZ2	2.74	0.40
53:a:462:LEU:HD12	72:x:49:GLN:HB3	1.98	0.40
54:d:109:GLN:HA	54:d:112:LYS:CE	2.52	0.40
55:f:78:LEU:HD21	65:h:81:LEU:HD23	2.04	0.40
56:i:110:SER:CB	56:i:111:PRO:CD	2.99	0.40
58:q:188:LEU:CA	69:v:87:ILE:HD11	2.39	0.40
59:z:583:ASP:HB2	59:z:590:ARG:HG2	2.03	0.40
70:p:15:LEU:HD12	70:p:15:LEU:HA	1.81	0.40
70:p:679:THR:OG1	70:p:722:SER:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:w:1005:LEU:HD23	71:w:1005:LEU:HA	1.91	0.40
72:x:102:ASP:HB2	72:x:164:ARG:HE	1.86	0.40
73:y:84:CYS:SG	73:y:85:HIS:N	2.94	0.40
4:DA:475:LEU:HD13	4:DA:475:LEU:O	2.21	0.40
4:DA:485:ILE:O	4:DA:485:ILE:HG23	2.21	0.40
5:EA:139:LEU:HD11	47:PG:151:ARG:HD2	0.47	0.40
5:EA:181:ASN:HD21	39:HD:9:CYS:CA	2.24	0.40
7:HA:101:LYS:C	7:HA:102:LEU:HD12	2.46	0.40
7:HA:145:GLN:HG2	7:HA:150:THR:HG22	2.03	0.40
9:PA:57:LEU:O	9:PA:261:ARG:NH2	2.54	0.40
9:PA:564:LEU:HD23	9:PA:567:LEU:HD12	2.04	0.40
13:HB:303:ILE:HG22	13:HB:307:PHE:HE2	1.86	0.40
15:PB:428:ASP:OD1	15:PB:429:PHE:N	2.52	0.40
17:PC:183:ALA:HB3	17:PC:232:ASN:HB3	2.04	0.40
20:PH:136:GLU:O	20:PH:139:SER:OG	2.31	0.40
41:HG:379:LEU:O	41:HG:379:LEU:HD23	2.21	0.40
42:HH:530:ARG:O	42:HH:534:TYR:CD2	2.75	0.40
45:HJ:243:THR:O	45:HJ:244:CYS:C	2.65	0.40
45:HJ:285:LEU:O	45:HJ:286:ALA:HB3	2.21	0.40
48:g:125:GLU:CA	48:g:128:PRO:HD3	2.52	0.40
50:n:838:VAL:HG23	50:n:838:VAL:O	2.21	0.40
50:n:957:PRO:HG2	50:n:1210:PHE:CZ	2.25	0.40
53:a:59:VAL:HA	53:a:62:LEU:HB2	2.03	0.40
53:a:388:LEU:CD2	53:a:447:GLU:HG3	2.46	0.40
53:a:398:PHE:O	53:a:398:PHE:CG	2.74	0.40
54:d:107:ILE:HG12	56:i:132:LEU:HD21	2.04	0.40
54:d:121:LEU:HD23	54:d:121:LEU:HA	1.79	0.40
55:f:118:ARG:CB	58:q:108:GLU:OE2	2.70	0.40
57:m:124:GLN:NE2	59:z:590:ARG:HB2	2.35	0.40
58:q:154:ALA:HB2	66:k:35:LEU:HD22	2.02	0.40
58:q:646:LEU:CD2	63:l:115:ILE:HD11	2.51	0.40
60:b:168:ILE:HD12	60:b:168:ILE:HA	1.96	0.40
65:h:8:LEU:HG	65:h:69:PRO:HG3	2.04	0.40
65:h:51:LEU:O	65:h:52:LEU:C	2.64	0.40
68:t:156:LEU:O	68:t:157:LEU:C	2.64	0.40
70:p:730:ASP:OD1	70:p:730:ASP:N	2.41	0.40
71:w:711:TRP:CD1	71:w:711:TRP:H	2.39	0.40
72:x:7:LYS:HB3	72:x:49:GLN:HE22	1.86	0.40
72:x:301:GLU:N	72:x:301:GLU:CD	2.80	0.40
72:x:492:LEU:HD23	72:x:492:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BA	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
4	DA	542/1872 (29%)	524 (97%)	15 (3%)	3 (1%)	21	58
5	EA	185/439 (42%)	183 (99%)	1 (0%)	1 (0%)	24	63
6	FA	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
7	HA	710/760 (93%)	682 (96%)	28 (4%)	0	100	100
8	NA	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	6	30
8	NE	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	6	30
9	PA	1457/1970 (74%)	1406 (96%)	47 (3%)	4 (0%)	36	72
10	DB	959/1199 (80%)	910 (95%)	49 (5%)	0	100	100
11	EB	169/291 (58%)	164 (97%)	5 (3%)	0	100	100
12	FB	218/249 (88%)	213 (98%)	4 (2%)	1 (0%)	24	63
13	HB	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
14	NB	78/103 (76%)	78 (100%)	0	0	100	100
14	NF	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	2	19
15	PB	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
16	HC	380/462 (82%)	363 (96%)	17 (4%)	0	100	100
17	PC	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
18	PE	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
19	PF	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
20	PH	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
21	PI	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
22	PJ	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
23	PK	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
24	PL	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
25	DP	177/339 (52%)	175 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DQ	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
27	DO	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
28	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
29	DD	153/1085 (14%)	146 (95%)	5 (3%)	2 (1%)	9	40
29	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
30	DE	540/800 (68%)	505 (94%)	33 (6%)	2 (0%)	30	67
30	De	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
31	DF	404/677 (60%)	376 (93%)	21 (5%)	7 (2%)	7	34
31	Df	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	36	72
32	DI	118/264 (45%)	113 (96%)	3 (2%)	2 (2%)	7	34
32	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
33	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
33	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
34	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
35	DL	72/161 (45%)	62 (86%)	6 (8%)	4 (6%)	1	14
35	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
36	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
37	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
38	DH	207/310 (67%)	190 (92%)	13 (6%)	4 (2%)	6	31
39	HD	304/309 (98%)	267 (88%)	27 (9%)	10 (3%)	3	20
40	HE	259/308 (84%)	252 (97%)	7 (3%)	0	100	100
41	HG	341/395 (86%)	329 (96%)	12 (4%)	0	100	100
42	HH	601/782 (77%)	575 (96%)	26 (4%)	0	100	100
43	HF	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
44	HI	297/346 (86%)	267 (90%)	18 (6%)	12 (4%)	2	17
45	HJ	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	11	45
46	PD	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
47	PG	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
48	g	104/233 (45%)	99 (95%)	4 (4%)	1 (1%)	12	47
49	j	120/135 (89%)	117 (98%)	1 (1%)	2 (2%)	7	34
50	n	993/1454 (68%)	894 (90%)	80 (8%)	19 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	s	91/244 (37%)	82 (90%)	7 (8%)	2 (2%)	5	28
52	u	113/144 (78%)	105 (93%)	5 (4%)	3 (3%)	4	24
53	a	430/1581 (27%)	386 (90%)	39 (9%)	5 (1%)	10	42
54	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	9	40
55	f	163/246 (66%)	149 (91%)	12 (7%)	2 (1%)	10	42
56	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	23
57	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
58	q	543/651 (83%)	484 (89%)	52 (10%)	7 (1%)	9	40
59	z	93/600 (16%)	84 (90%)	6 (6%)	3 (3%)	3	21
60	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	50
61	c	255/311 (82%)	241 (94%)	14 (6%)	0	100	100
62	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	30
63	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
64	o	152/788 (19%)	136 (90%)	12 (8%)	4 (3%)	4	25
65	h	188/268 (70%)	165 (88%)	15 (8%)	8 (4%)	2	17
66	k	110/117 (94%)	96 (87%)	12 (11%)	2 (2%)	6	32
67	r	190/208 (91%)	180 (95%)	6 (3%)	4 (2%)	5	29
68	t	189/212 (89%)	169 (89%)	16 (8%)	4 (2%)	5	29
69	v	132/200 (66%)	116 (88%)	10 (8%)	6 (4%)	2	16
70	p	756/841 (90%)	704 (93%)	50 (7%)	2 (0%)	36	72
71	w	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	36	72
72	x	877/989 (89%)	828 (94%)	44 (5%)	5 (1%)	21	58
73	y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	24	63
74	NC	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	3	22
74	NG	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	3	23
75	ND	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	11	45
75	NH	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	11	45
All	All	22102/36357 (61%)	20865 (94%)	1075 (5%)	162 (1%)	20	55

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DA	498	PRO

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Mol	Chain	Res	Type
4	DA	1158	SER
8	NA	534	ARG
9	PA	1666	PRO
12	FB	229	HIS
29	DD	876	ALA
30	DE	452	ARG
31	DF	68	THR
31	DF	69	SER
31	DF	442	PRO
38	DH	115	GLN
38	DH	141	PRO
35	DL	73	ASN
39	HD	54	ARG
39	HD	214	LYS
39	HD	220	PRO
39	HD	237	PRO
49	j	31	PRO
50	n	154	ILE
50	n	363	GLU
50	n	1351	PRO
50	n	1355	PRO
53	a	502	MET
54	d	187	LEU
55	f	53	GLN
58	q	131	SER
65	h	100	PHE
65	h	130	ARG
65	h	167	ARG
65	h	168	PRO
68	t	173	PRO
69	v	91	PHE
70	p	705	PRO
72	x	15	LYS
72	x	567	MET
8	NE	636	LYS
74	NG	1017	VAL
74	NC	841	THR
75	ND	1301	GLY
75	NH	1501	GLY
9	PA	1645	PRO
9	PA	1663	SER
29	DD	898	VAL

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Mol	Chain	Res	Type
30	DE	704	VAL
38	DH	129	VAL
35	DL	111	LEU
35	DL	114	LYS
39	HD	233	ILE
39	HD	234	SER
44	HI	96	THR
44	HI	108	VAL
44	HI	192	VAL
44	HI	236	GLN
44	HI	239	ASP
44	HI	310	PRO
50	n	169	LEU
50	n	254	VAL
50	n	1343	PRO
52	u	32	PRO
52	u	76	LEU
53	a	164	PRO
53	a	334	PRO
56	i	108	HIS
56	i	138	LEU
58	q	399	PRO
62	e	146	ILE
64	o	714	ASP
65	h	37	TYR
65	h	131	ILE
68	t	99	LYS
69	v	40	ALA
69	v	41	LYS
69	v	42	ILE
69	v	139	SER
70	p	727	PRO
71	w	1196	CYS
72	x	444	SER
72	x	564	SER
74	NC	843	HIS
31	DF	321	PRO
39	HD	56	SER
39	HD	289	SER
44	HI	106	SER
44	HI	277	LEU
45	HJ	237	MET

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Mol	Chain	Res	Type
50	n	150	PRO
50	n	153	ALA
50	n	1237	PRO
51	s	129	SER
52	u	84	ALA
53	a	487	LEU
54	d	170	GLY
58	q	91	SER
58	q	458	PRO
64	o	709	LYS
67	r	156	ASN
69	v	38	LYS
71	w	1203	MET
74	NC	840	THR
5	EA	153	ARG
31	DF	66	LEU
38	DH	137	GLY
32	DI	62	LYS
44	HI	264	ALA
45	HJ	286	ALA
49	j	34	GLN
50	n	165	SER
50	n	265	LEU
50	n	1255	PRO
51	s	105	LEU
53	a	208	VAL
58	q	127	LEU
58	q	134	ALA
59	z	533	PRO
60	b	100	GLN
62	e	147	ASN
67	r	113	ASN
68	t	172	ALA
72	x	566	GLU
73	y	226	LEU
14	NF	220	LYS
14	NF	301	GLY
74	NG	1042	SER
8	NA	438	PRO
31	DF	64	GLN
31	DF	440	PRO
39	HD	225	THR

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Mol	Chain	Res	Type
39	HD	265	MET
45	HJ	16	GLU
48	g	127	ARG
50	n	264	ALA
50	n	286	GLU
50	n	524	ASN
50	n	1352	PRO
55	f	55	LEU
59	z	540	LEU
64	o	721	LEU
66	k	79	HIS
66	k	81	GLY
68	t	129	VAL
71	w	32	ASP
74	NG	1018	SER
4	DA	506	ASP
31	Df	411	VAL
35	DL	72	PRO
44	HI	82	GLY
44	HI	212	PHE
50	n	164	GLY
58	q	89	GLN
65	h	188	GLY
71	w	1194	THR
8	NE	734	ARG
14	NF	219	ARG
59	z	537	PRO
67	r	94	GLY
67	r	153	VAL
50	n	528	HIS
9	PA	1648	PRO
44	HI	186	GLY
64	o	716	PRO
65	h	99	VAL
32	DI	85	SER

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	
3	BA	215/268 (80%)	215 (100%)	0	100	100
4	DA	495/1665 (30%)	461 (93%)	34 (7%)	14	36
5	EA	169/373 (45%)	167 (99%)	2 (1%)	63	74
6	FA	121/448 (27%)	121 (100%)	0	100	100
7	HA	624/664 (94%)	624 (100%)	0	100	100
9	PA	1302/1749 (74%)	1296 (100%)	6 (0%)	81	82
10	DB	876/1083 (81%)	861 (98%)	15 (2%)	53	68
11	EB	154/261 (59%)	154 (100%)	0	100	100
12	FB	196/218 (90%)	196 (100%)	0	100	100
13	HB	241/484 (50%)	241 (100%)	0	100	100
15	PB	994/1027 (97%)	994 (100%)	0	100	100
16	HC	342/399 (86%)	342 (100%)	0	100	100
17	PC	234/252 (93%)	234 (100%)	0	100	100
18	PE	191/192 (100%)	191 (100%)	0	100	100
19	PF	69/111 (62%)	68 (99%)	1 (1%)	59	72
20	PH	129/131 (98%)	129 (100%)	0	100	100
21	PI	103/112 (92%)	103 (100%)	0	100	100
22	PJ	53/56 (95%)	53 (100%)	0	100	100
23	PK	104/106 (98%)	104 (100%)	0	100	100
24	PL	41/55 (74%)	41 (100%)	0	100	100
25	DP	154/293 (53%)	154 (100%)	0	100	100
26	DQ	105/324 (32%)	105 (100%)	0	100	100
27	DO	90/98 (92%)	90 (100%)	0	100	100
28	Dc	113/833 (14%)	111 (98%)	2 (2%)	51	67
29	DD	144/815 (18%)	132 (92%)	12 (8%)	10	30
29	Dd	146/815 (18%)	146 (100%)	0	100	100
30	DE	478/657 (73%)	465 (97%)	13 (3%)	39	60
30	De	475/657 (72%)	473 (100%)	2 (0%)	84	83
31	DF	324/574 (56%)	295 (91%)	29 (9%)	9	28
31	Df	322/574 (56%)	312 (97%)	10 (3%)	35	56
32	DI	106/235 (45%)	97 (92%)	9 (8%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Di	107/235 (46%)	107 (100%)	0	100	100
33	DJ	79/154 (51%)	77 (98%)	2 (2%)	42	62
33	Dj	83/154 (54%)	83 (100%)	0	100	100
34	Dk	87/182 (48%)	87 (100%)	0	100	100
35	DL	69/141 (49%)	58 (84%)	11 (16%)	2	12
35	DI	98/141 (70%)	98 (100%)	0	100	100
36	Dm	80/106 (76%)	79 (99%)	1 (1%)	61	72
37	DG	133/322 (41%)	125 (94%)	8 (6%)	17	39
38	DH	181/270 (67%)	170 (94%)	11 (6%)	17	39
39	HD	251/283 (89%)	233 (93%)	18 (7%)	13	35
40	HE	234/272 (86%)	229 (98%)	5 (2%)	47	65
41	HG	311/352 (88%)	311 (100%)	0	100	100
42	HH	536/688 (78%)	535 (100%)	1 (0%)	87	86
43	HF	59/64 (92%)	59 (100%)	0	100	100
44	HI	258/298 (87%)	181 (70%)	77 (30%)	0	2
45	HJ	252/296 (85%)	173 (69%)	79 (31%)	0	2
46	PD	118/126 (94%)	117 (99%)	1 (1%)	73	78
47	PG	152/153 (99%)	151 (99%)	1 (1%)	76	80
48	g	102/216 (47%)	93 (91%)	9 (9%)	9	29
49	j	66/124 (53%)	65 (98%)	1 (2%)	57	71
50	n	807/1271 (64%)	785 (97%)	22 (3%)	39	60
51	s	83/208 (40%)	74 (89%)	9 (11%)	6	21
52	u	95/119 (80%)	91 (96%)	4 (4%)	26	48
53	a	393/1391 (28%)	316 (80%)	77 (20%)	1	8
54	d	139/230 (60%)	93 (67%)	46 (33%)	0	2
55	f	149/223 (67%)	131 (88%)	18 (12%)	5	18
56	i	71/133 (53%)	61 (86%)	10 (14%)	3	14
57	m	102/115 (89%)	101 (99%)	1 (1%)	68	76
58	q	491/577 (85%)	407 (83%)	84 (17%)	2	11
59	z	89/512 (17%)	74 (83%)	15 (17%)	2	11
60	b	102/163 (63%)	91 (89%)	11 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	c	238/280 (85%)	227 (95%)	11 (5%)	24	46
62	e	94/152 (62%)	94 (100%)	0	100	100
63	l	116/155 (75%)	116 (100%)	0	100	100
64	o	141/697 (20%)	136 (96%)	5 (4%)	32	53
65	h	161/225 (72%)	123 (76%)	38 (24%)	1	5
66	k	94/98 (96%)	43 (46%)	51 (54%)	0	0
67	r	169/183 (92%)	140 (83%)	29 (17%)	2	11
68	t	166/178 (93%)	124 (75%)	42 (25%)	0	4
69	v	122/173 (70%)	76 (62%)	46 (38%)	0	1
70	p	681/736 (92%)	671 (98%)	10 (2%)	57	71
71	w	1203/1232 (98%)	1198 (100%)	5 (0%)	84	83
72	x	789/864 (91%)	779 (99%)	10 (1%)	61	72
73	y	175/601 (29%)	171 (98%)	4 (2%)	44	63
All	All	19036/30622 (62%)	18128 (95%)	908 (5%)	24	45

All (908) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	DA	353	LEU
4	DA	357	GLU
4	DA	396	LEU
4	DA	397	LEU
4	DA	401	ASN
4	DA	403	LEU
4	DA	404	MET
4	DA	405	VAL
4	DA	470	ILE
4	DA	474	ASP
4	DA	482	ASP
4	DA	484	ILE
4	DA	485	ILE
4	DA	491	MET
4	DA	496	GLU
4	DA	500	LEU
4	DA	502	LEU
4	DA	511	LEU
4	DA	574	TYR

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Mol	Chain	Res	Type
4	DA	639	LEU
4	DA	661	GLU
4	DA	667	THR
4	DA	711	ASP
4	DA	727	THR
4	DA	730	PHE
4	DA	828	GLU
4	DA	925	ASP
4	DA	943	LYS
4	DA	970	ASN
4	DA	1052	ARG
4	DA	1058	HIS
4	DA	1062	TYR
4	DA	1165	LEU
4	DA	1203	GLU
5	EA	106	LYS
5	EA	185	GLU
9	PA	1643	TYR
9	PA	1646	THR
9	PA	1647	SER
9	PA	1663	SER
9	PA	1678	TYR
9	PA	1794	SER
10	DB	21	GLU
10	DB	71	ARG
10	DB	140	GLU
10	DB	184	ASN
10	DB	262	MET
10	DB	266	THR
10	DB	293	GLU
10	DB	431	LEU
10	DB	559	LYS
10	DB	603	LYS
10	DB	640	VAL
10	DB	746	SER
10	DB	771	VAL
10	DB	818	THR
10	DB	987	LEU
19	PF	71	LEU
28	Dc	24	ASP
28	Dc	106	VAL
30	De	546	VAL

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Mol	Chain	Res	Type
30	De	579	VAL
31	Df	215	GLU
31	Df	253	TYR
31	Df	261	THR
31	Df	272	VAL
31	Df	322	ASP
31	Df	323	VAL
31	Df	326	HIS
31	Df	356	THR
31	Df	366	GLU
31	Df	421	ASP
29	DD	873	LEU
29	DD	888	LYS
29	DD	891	ILE
29	DD	894	LEU
29	DD	897	ASP
29	DD	898	VAL
29	DD	924	LYS
29	DD	953	ILE
29	DD	955	LYS
29	DD	958	LYS
29	DD	1006	LEU
29	DD	1009	LEU
36	Dm	31	LEU
30	DE	432	LEU
30	DE	433	LYS
30	DE	450	ARG
30	DE	451	VAL
30	DE	507	VAL
30	DE	513	LEU
30	DE	515	LEU
30	DE	519	GLU
30	DE	521	ASP
30	DE	702	LEU
30	DE	745	GLU
30	DE	746	ASP
30	DE	747	LEU
31	DF	55	LEU
31	DF	60	MET
31	DF	62	LYS
31	DF	64	GLN
31	DF	66	LEU

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Mol	Chain	Res	Type
31	DF	111	GLU
31	DF	114	LEU
31	DF	118	ILE
31	DF	120	THR
31	DF	129	VAL
31	DF	209	LYS
31	DF	261	THR
31	DF	269	VAL
31	DF	271	VAL
31	DF	280	ILE
31	DF	295	LEU
31	DF	301	VAL
31	DF	312	ILE
31	DF	317	LEU
31	DF	319	LEU
31	DF	320	ARG
31	DF	339	GLN
31	DF	348	THR
31	DF	354	ARG
31	DF	391	LEU
31	DF	397	GLN
31	DF	406	VAL
31	DF	415	ILE
31	DF	427	LEU
37	DG	41	ASP
37	DG	129	LYS
37	DG	131	ILE
37	DG	143	VAL
37	DG	161	ASP
37	DG	181	TRP
37	DG	182	GLU
37	DG	183	ILE
38	DH	50	PHE
38	DH	116	ARG
38	DH	132	LYS
38	DH	135	THR
38	DH	155	ASP
38	DH	159	TYR
38	DH	160	ILE
38	DH	161	LYS
38	DH	164	THR
38	DH	167	GLU

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Mol	Chain	Res	Type
38	DH	169	VAL
32	DI	31	TYR
32	DI	32	GLU
32	DI	35	VAL
32	DI	60	HIS
32	DI	63	LYS
32	DI	69	ASP
32	DI	73	LEU
32	DI	82	SER
32	DI	83	PHE
33	DJ	192	LYS
33	DJ	194	THR
35	DL	59	THR
35	DL	60	LYS
35	DL	61	LYS
35	DL	62	LYS
35	DL	63	LEU
35	DL	64	GLN
35	DL	70	VAL
35	DL	87	ILE
35	DL	110	THR
35	DL	111	LEU
35	DL	128	ILE
39	HD	11	THR
39	HD	28	HIS
39	HD	29	THR
39	HD	212	LEU
39	HD	251	LEU
39	HD	252	GLN
39	HD	254	GLU
39	HD	263	LEU
39	HD	268	ARG
39	HD	272	LEU
39	HD	275	VAL
39	HD	276	ARG
39	HD	287	TYR
39	HD	288	THR
39	HD	293	CYS
39	HD	295	ARG
39	HD	304	LEU
39	HD	305	PHE
40	HE	62	SER

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Mol	Chain	Res	Type
40	HE	64	ILE
40	HE	222	SER
40	HE	257	CYS
40	HE	258	HIS
42	HH	266	GLN
44	HI	13	GLU
44	HI	15	LEU
44	HI	20	GLU
44	HI	23	PHE
44	HI	30	ARG
44	HI	32	LYS
44	HI	33	ASN
44	HI	34	THR
44	HI	36	GLN
44	HI	38	VAL
44	HI	45	LEU
44	HI	47	HIS
44	HI	48	ARG
44	HI	52	LYS
44	HI	55	ILE
44	HI	56	ASN
44	HI	57	ARG
44	HI	58	THR
44	HI	60	LEU
44	HI	63	ILE
44	HI	64	LYS
44	HI	66	LEU
44	HI	67	GLN
44	HI	69	LEU
44	HI	74	ILE
44	HI	75	ILE
44	HI	83	HIS
44	HI	84	LYS
44	HI	86	ASN
44	HI	88	SER
44	HI	96	THR
44	HI	101	ILE
44	HI	102	ILE
44	HI	107	LEU
44	HI	108	VAL
44	HI	110	THR
44	HI	115	LYS

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Mol	Chain	Res	Type
44	HI	125	LEU
44	HI	131	HIS
44	HI	132	TRP
44	HI	139	LYS
44	HI	141	ASN
44	HI	143	LEU
44	HI	153	LEU
44	HI	160	LYS
44	HI	162	PHE
44	HI	164	SER
44	HI	169	TYR
44	HI	170	THR
44	HI	173	VAL
44	HI	177	TRP
44	HI	189	MET
44	HI	205	GLU
44	HI	206	LEU
44	HI	209	ARG
44	HI	210	VAL
44	HI	213	LEU
44	HI	223	THR
44	HI	225	ILE
44	HI	237	TRP
44	HI	241	CYS
44	HI	245	ASP
44	HI	249	PHE
44	HI	257	LEU
44	HI	258	HIS
44	HI	259	HIS
44	HI	260	ILE
44	HI	261	PHE
44	HI	267	ASP
44	HI	268	LEU
44	HI	272	ILE
44	HI	276	PHE
44	HI	280	PRO
44	HI	284	ILE
44	HI	285	THR
44	HI	288	GLN
44	HI	292	MET
45	HJ	3	HIS
45	HJ	7	GLN

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Mol	Chain	Res	Type
45	HJ	8	LYS
45	HJ	10	HIS
45	HJ	11	TRP
45	HJ	12	THR
45	HJ	14	SER
45	HJ	15	SER
45	HJ	21	ARG
45	HJ	28	ARG
45	HJ	32	CYS
45	HJ	33	LYS
45	HJ	37	ASN
45	HJ	41	LEU
45	HJ	44	ASP
45	HJ	55	THR
45	HJ	56	LEU
45	HJ	60	TYR
45	HJ	65	LEU
45	HJ	84	CYS
45	HJ	85	MET
45	HJ	92	LEU
45	HJ	93	ASN
45	HJ	94	ASN
45	HJ	96	VAL
45	HJ	97	MET
45	HJ	98	GLU
45	HJ	102	ARG
45	HJ	104	ILE
45	HJ	106	LEU
45	HJ	107	THR
45	HJ	108	CYS
45	HJ	111	LEU
45	HJ	113	CYS
45	HJ	114	LYS
45	HJ	115	VAL
45	HJ	129	LEU
45	HJ	134	LEU
45	HJ	136	GLN
45	HJ	140	LEU
45	HJ	141	GLU
45	HJ	143	ILE
45	HJ	145	GLU
45	HJ	148	LEU

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Mol	Chain	Res	Type
45	HJ	149	LEU
45	HJ	150	LEU
45	HJ	151	ILE
45	HJ	153	GLN
45	HJ	154	LEU
45	HJ	158	LEU
45	HJ	160	VAL
45	HJ	165	ARG
45	HJ	166	PRO
45	HJ	171	LEU
45	HJ	172	ILE
45	HJ	174	LEU
45	HJ	175	LYS
45	HJ	180	ILE
45	HJ	181	LEU
45	HJ	182	GLU
45	HJ	186	ILE
45	HJ	189	LYS
45	HJ	192	ASP
45	HJ	200	LEU
45	HJ	208	THR
45	HJ	211	GLN
45	HJ	226	ILE
45	HJ	227	THR
45	HJ	229	GLU
45	HJ	231	TYR
45	HJ	232	LEU
45	HJ	239	LYS
45	HJ	245	LEU
45	HJ	252	MET
45	HJ	262	TYR
45	HJ	266	ARG
45	HJ	277	LEU
45	HJ	279	ARG
45	HJ	288	ASN
46	PD	137	LYS
47	PG	59	ILE
48	g	72	PHE
48	g	126	TYR
48	g	130	GLN
48	g	137	VAL
48	g	143	LYS

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Mol	Chain	Res	Type
48	g	154	GLN
48	g	159	ARG
48	g	166	ASN
48	g	171	LEU
49	j	82	LYS
50	n	154	ILE
50	n	159	ASP
50	n	166	TYR
50	n	168	ARG
50	n	169	LEU
50	n	212	LEU
50	n	226	VAL
50	n	227	GLU
50	n	252	ILE
50	n	253	LEU
50	n	254	VAL
50	n	255	GLU
50	n	261	ASP
50	n	265	LEU
50	n	266	VAL
50	n	267	HIS
50	n	283	PHE
50	n	289	LEU
50	n	363	GLU
50	n	371	GLN
50	n	528	HIS
50	n	589	GLN
51	s	90	GLU
51	s	93	TYR
51	s	105	LEU
51	s	109	LEU
51	s	112	LEU
51	s	116	ILE
51	s	127	LEU
51	s	131	ILE
51	s	137	LEU
52	u	49	ASN
52	u	73	ILE
52	u	76	LEU
52	u	79	GLU
53	a	58	LEU
53	a	62	LEU

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Mol	Chain	Res	Type
53	a	64	THR
53	a	66	GLN
53	a	70	LYS
53	a	71	VAL
53	a	72	THR
53	a	74	LEU
53	a	77	MET
53	a	78	THR
53	a	80	ARG
53	a	82	GLU
53	a	83	SER
53	a	86	ARG
53	a	87	GLN
53	a	93	HIS
53	a	106	ASP
53	a	107	MET
53	a	108	PHE
53	a	109	TYR
53	a	111	GLU
53	a	128	HIS
53	a	131	ASN
53	a	133	VAL
53	a	135	CYS
53	a	145	LYS
53	a	148	ASP
53	a	160	LEU
53	a	162	ASN
53	a	167	ASN
53	a	168	LYS
53	a	173	MET
53	a	201	ASP
53	a	214	ARG
53	a	226	VAL
53	a	232	LEU
53	a	246	ASN
53	a	253	MET
53	a	254	ASN
53	a	258	THR
53	a	259	ILE
53	a	267	LYS
53	a	278	HIS
53	a	297	VAL

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Mol	Chain	Res	Type
53	a	305	LEU
53	a	309	GLN
53	a	324	CYS
53	a	325	THR
53	a	327	ILE
53	a	329	LEU
53	a	332	THR
53	a	333	GLN
53	a	335	THR
53	a	339	LEU
53	a	348	LEU
53	a	357	LEU
53	a	367	LEU
53	a	373	CYS
53	a	376	LEU
53	a	384	ASP
53	a	388	LEU
53	a	391	THR
53	a	400	HIS
53	a	414	GLN
53	a	421	ILE
53	a	427	ARG
53	a	430	LEU
53	a	432	GLU
53	a	433	ASP
53	a	437	LEU
53	a	438	LEU
53	a	441	GLU
53	a	443	CYS
53	a	501	CYS
53	a	502	MET
53	a	504	ILE
53	a	509	ARG
54	d	28	GLU
54	d	30	LEU
54	d	51	SER
54	d	62	GLU
54	d	63	ASN
54	d	64	GLN
54	d	66	LEU
54	d	67	GLU
54	d	69	LEU

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Mol	Chain	Res	Type
54	d	70	ILE
54	d	71	HIS
54	d	72	ARG
54	d	73	ASP
54	d	78	GLU
54	d	79	LEU
54	d	80	MET
54	d	81	LYS
54	d	82	LEU
54	d	85	ASN
54	d	92	GLU
54	d	93	MET
54	d	98	LYS
54	d	101	GLU
54	d	106	ASP
54	d	107	ILE
54	d	108	GLN
54	d	110	LEU
54	d	114	LEU
54	d	115	LYS
54	d	116	GLU
54	d	119	GLN
54	d	121	LEU
54	d	126	TYR
54	d	127	GLN
54	d	129	LYS
54	d	130	GLU
54	d	131	LYS
54	d	132	LEU
54	d	133	LYS
54	d	135	ILE
54	d	173	ARG
54	d	181	GLU
54	d	184	SER
54	d	186	LEU
54	d	187	LEU
54	d	189	GLN
55	f	16	VAL
55	f	19	SER
55	f	20	TRP
55	f	24	LEU
55	f	30	LEU

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Mol	Chain	Res	Type
55	f	41	TYR
55	f	50	VAL
55	f	52	MET
55	f	53	GLN
55	f	56	THR
55	f	57	LEU
55	f	60	LEU
55	f	64	VAL
55	f	66	ILE
55	f	114	VAL
55	f	117	SER
55	f	120	LEU
55	f	192	PHE
56	i	86	ASP
56	i	87	LEU
56	i	88	ASN
56	i	90	LEU
56	i	95	GLN
56	i	100	LEU
56	i	112	GLU
56	i	122	ARG
56	i	136	LYS
56	i	140	MET
57	m	59	LYS
58	q	1	MET
58	q	2	SER
58	q	7	VAL
58	q	16	GLU
58	q	19	VAL
58	q	22	VAL
58	q	28	GLU
58	q	29	THR
58	q	31	LEU
58	q	34	LEU
58	q	36	MET
58	q	91	SER
58	q	92	LEU
58	q	93	TRP
58	q	95	TRP
58	q	98	VAL
58	q	100	ASN
58	q	103	ARG

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Mol	Chain	Res	Type
58	q	107	THR
58	q	109	MET
58	q	110	CYS
58	q	111	VAL
58	q	112	LEU
58	q	115	VAL
58	q	116	LEU
58	q	118	ILE
58	q	120	ARG
58	q	122	LYS
58	q	123	LYS
58	q	124	PHE
58	q	125	MET
58	q	128	ASP
58	q	130	VAL
58	q	131	SER
58	q	132	GLN
58	q	133	ASP
58	q	135	LEU
58	q	138	LYS
58	q	139	GLN
58	q	143	THR
58	q	144	LEU
58	q	145	GLN
58	q	146	LEU
58	q	147	ILE
58	q	149	LYS
58	q	153	LEU
58	q	159	ILE
58	q	161	LEU
58	q	165	GLU
58	q	166	ARG
58	q	168	THR
58	q	169	LYS
58	q	171	VAL
58	q	172	THR
58	q	184	ASN
58	q	185	SER
58	q	187	LEU
58	q	188	LEU
58	q	226	LYS
58	q	262	GLN

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Mol	Chain	Res	Type
58	q	263	LYS
58	q	264	GLN
58	q	400	PHE
58	q	428	LEU
58	q	430	LYS
58	q	431	ILE
58	q	432	ILE
58	q	434	GLN
58	q	438	ILE
58	q	440	LEU
58	q	441	ARG
58	q	442	SER
58	q	443	ARG
58	q	447	THR
58	q	448	ILE
58	q	451	LEU
58	q	518	GLU
58	q	629	LYS
58	q	631	GLU
58	q	634	ASN
58	q	646	LEU
58	q	647	SER
58	q	649	CYS
58	q	651	LEU
59	z	492	ARG
59	z	528	LEU
59	z	530	VAL
59	z	540	LEU
59	z	551	ASP
59	z	564	ASN
59	z	567	GLN
59	z	572	ASN
59	z	579	CYS
59	z	582	LEU
59	z	585	HIS
59	z	591	LEU
59	z	594	LEU
59	z	598	CYS
59	z	599	LEU
60	b	57	VAL
60	b	74	LEU
60	b	82	LEU

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Mol	Chain	Res	Type
60	b	92	GLN
60	b	99	ILE
60	b	103	ASP
60	b	122	LEU
60	b	126	CYS
60	b	127	LEU
60	b	132	ASP
60	b	168	ILE
61	c	36	LYS
61	c	44	THR
61	c	45	LEU
61	c	72	ARG
61	c	73	LEU
61	c	77	VAL
61	c	274	ILE
61	c	275	LYS
61	c	276	LEU
61	c	300	ARG
61	c	301	THR
64	o	635	ASN
64	o	697	HIS
64	o	704	VAL
64	o	715	LEU
64	o	721	LEU
65	h	7	GLN
65	h	15	LEU
65	h	16	LEU
65	h	17	SER
65	h	18	GLN
65	h	19	VAL
65	h	22	LEU
65	h	23	LYS
65	h	30	ILE
65	h	32	LYS
65	h	33	LEU
65	h	34	GLU
65	h	37	TYR
65	h	39	ARG
65	h	40	LEU
65	h	49	PHE
65	h	51	LEU
65	h	52	LEU

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Mol	Chain	Res	Type
65	h	66	GLU
65	h	75	VAL
65	h	76	ILE
65	h	77	ILE
65	h	79	LEU
65	h	100	PHE
65	h	101	SER
65	h	102	HIS
65	h	110	ARG
65	h	111	THR
65	h	112	LYS
65	h	117	VAL
65	h	130	ARG
65	h	131	ILE
65	h	143	LEU
65	h	170	LYS
65	h	185	VAL
65	h	187	PHE
65	h	189	LYS
65	h	192	SER
66	k	8	ASN
66	k	10	ARG
66	k	11	LEU
66	k	12	ARG
66	k	14	LEU
66	k	15	GLU
66	k	18	GLU
66	k	19	ARG
66	k	21	ILE
66	k	25	LEU
66	k	26	GLN
66	k	32	ILE
66	k	33	LEU
66	k	34	GLU
66	k	35	LEU
66	k	36	SER
66	k	37	LYS
66	k	40	THR
66	k	42	GLU
66	k	43	ARG
66	k	44	LEU
66	k	45	LEU

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Mol	Chain	Res	Type
66	k	48	GLN
66	k	53	THR
66	k	56	VAL
66	k	57	GLN
66	k	58	HIS
66	k	60	GLU
66	k	64	SER
66	k	67	ILE
66	k	70	LEU
66	k	72	GLN
66	k	73	VAL
66	k	82	SER
66	k	83	SER
66	k	86	SER
66	k	87	ARG
66	k	88	LYS
66	k	90	CYS
66	k	91	GLN
66	k	92	MET
66	k	94	LEU
66	k	96	ARG
66	k	97	VAL
66	k	101	ARG
66	k	102	LEU
66	k	103	LYS
66	k	104	LEU
66	k	107	VAL
66	k	109	ARG
66	k	114	MET
67	r	16	ILE
67	r	17	ASN
67	r	18	MET
67	r	32	LEU
67	r	35	LEU
67	r	42	LEU
67	r	47	GLU
67	r	49	GLU
67	r	53	ASP
67	r	56	MET
67	r	60	LEU
67	r	73	ARG
67	r	85	LEU

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Mol	Chain	Res	Type
67	r	88	LEU
67	r	93	MET
67	r	101	LEU
67	r	107	ASP
67	r	124	ARG
67	r	143	ILE
67	r	152	LEU
67	r	156	ASN
67	r	168	LEU
67	r	179	GLN
67	r	187	LYS
67	r	197	VAL
67	r	200	GLU
67	r	201	LYS
67	r	202	ILE
67	r	206	ARG
68	t	1	MET
68	t	9	MET
68	t	16	SER
68	t	17	VAL
68	t	21	VAL
68	t	23	LEU
68	t	24	LEU
68	t	28	LEU
68	t	34	GLU
68	t	43	CYS
68	t	47	HIS
68	t	61	LYS
68	t	62	LEU
68	t	66	MET
68	t	67	HIS
68	t	70	GLU
68	t	78	LEU
68	t	79	PHE
68	t	80	GLU
68	t	81	ASN
68	t	84	CYS
68	t	85	LEU
68	t	98	LEU
68	t	99	LYS
68	t	101	PHE
68	t	103	GLN

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Mol	Chain	Res	Type
68	t	106	LYS
68	t	109	LYS
68	t	110	ILE
68	t	124	VAL
68	t	138	ILE
68	t	148	VAL
68	t	149	VAL
68	t	156	LEU
68	t	162	GLN
68	t	173	PRO
68	t	179	ARG
68	t	183	VAL
68	t	193	TYR
68	t	196	LEU
68	t	200	ILE
68	t	204	GLN
69	v	14	LEU
69	v	15	LEU
69	v	22	LEU
69	v	26	ILE
69	v	37	ILE
69	v	38	LYS
69	v	39	THR
69	v	41	LYS
69	v	43	GLU
69	v	45	GLU
69	v	47	GLN
69	v	50	ARG
69	v	52	THR
69	v	55	GLU
69	v	56	GLN
69	v	58	ASN
69	v	60	GLU
69	v	61	MET
69	v	62	HIS
69	v	63	VAL
69	v	69	VAL
69	v	81	ASP
69	v	82	LEU
69	v	86	LEU
69	v	87	ILE
69	v	88	LEU

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Mol	Chain	Res	Type
69	v	98	ILE
69	v	103	GLN
69	v	105	LEU
69	v	108	LEU
69	v	110	GLU
69	v	112	CYS
69	v	114	ARG
69	v	115	LYS
69	v	116	LEU
69	v	117	ILE
69	v	118	THR
69	v	119	LEU
69	v	120	ARG
69	v	123	ILE
69	v	125	ILE
69	v	130	LEU
69	v	131	GLU
69	v	132	GLU
69	v	133	GLU
69	v	138	SER
70	p	13	MET
70	p	162	VAL
70	p	170	LEU
70	p	228	VAL
70	p	289	ASP
70	p	401	THR
70	p	443	LEU
70	p	564	LEU
70	p	699	CYS
70	p	726	ILE
71	w	205	VAL
71	w	723	THR
71	w	726	ASN
71	w	1130	VAL
71	w	1134	GLN
72	x	4	VAL
72	x	11	LEU
72	x	52	ILE
72	x	118	ILE
72	x	239	THR
72	x	300	THR
72	x	443	LEU

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Mol	Chain	Res	Type
72	x	477	TYR
72	x	803	ASP
72	x	897	LEU
73	y	194	LEU
73	y	220	MET
73	y	224	ARG
73	y	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (368) such sidechains are listed below:

Mol	Chain	Res	Type
3	BA	116	ASN
4	DA	401	ASN
4	DA	407	GLN
4	DA	409	HIS
4	DA	630	GLN
4	DA	702	ASN
4	DA	755	HIS
4	DA	802	HIS
4	DA	860	ASN
4	DA	896	GLN
4	DA	1073	GLN
5	EA	142	ASN
7	HA	201	HIS
7	HA	560	ASN
7	HA	645	GLN
9	PA	700	GLN
9	PA	731	ASN
9	PA	905	ASN
9	PA	1032	GLN
9	PA	1310	HIS
10	DB	30	HIS
10	DB	36	ASN
10	DB	123	ASN
10	DB	137	HIS
10	DB	160	HIS
10	DB	176	HIS
10	DB	183	GLN
10	DB	235	HIS
10	DB	272	GLN
10	DB	348	GLN
10	DB	432	HIS

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Mol	Chain	Res	Type
10	DB	439	HIS
10	DB	450	GLN
10	DB	509	ASN
10	DB	577	HIS
10	DB	644	GLN
10	DB	652	GLN
10	DB	662	GLN
10	DB	663	GLN
10	DB	750	GLN
10	DB	813	ASN
10	DB	864	ASN
10	DB	908	GLN
10	DB	912	ASN
10	DB	963	HIS
11	EB	188	GLN
11	EB	217	GLN
12	FB	64	ASN
12	FB	152	ASN
12	FB	229	HIS
13	HB	420	GLN
13	HB	537	HIS
15	PB	90	GLN
15	PB	145	GLN
15	PB	420	GLN
15	PB	582	GLN
15	PB	631	GLN
15	PB	913	GLN
15	PB	1101	GLN
16	HC	211	GLN
16	HC	218	GLN
16	HC	390	GLN
17	PC	66	HIS
17	PC	260	GLN
17	PC	265	HIS
18	PE	92	GLN
21	PI	91	HIS
21	PI	98	GLN
23	PK	55	GLN
25	DP	229	GLN
25	DP	278	GLN
27	DO	35	GLN
27	DO	77	ASN

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Mol	Chain	Res	Type
28	Dc	19	GLN
28	Dc	27	GLN
28	Dc	50	HIS
29	Dd	912	ASN
30	De	223	HIS
30	De	256	HIS
30	De	320	HIS
30	De	368	ASN
30	De	420	ASN
30	De	424	GLN
30	De	660	ASN
30	De	733	ASN
31	Df	30	GLN
31	Df	37	GLN
31	Df	119	ASN
31	Df	134	HIS
31	Df	325	ASN
31	Df	350	ASN
32	Di	38	GLN
34	Dk	186	HIS
34	Dk	205	HIS
35	Dl	73	ASN
35	Dl	105	HIS
35	Dl	119	HIS
29	DD	875	GLN
29	DD	912	ASN
29	DD	936	GLN
36	Dm	107	ASN
30	DE	254	ASN
30	DE	268	HIS
30	DE	290	HIS
30	DE	326	ASN
30	DE	327	ASN
30	DE	351	GLN
30	DE	509	GLN
30	DE	573	GLN
30	DE	616	HIS
30	DE	636	HIS
30	DE	640	ASN
30	DE	733	ASN
31	DF	37	GLN
31	DF	79	ASN

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Mol	Chain	Res	Type
31	DF	119	ASN
31	DF	214	HIS
31	DF	270	ASN
31	DF	273	GLN
31	DF	275	ASN
31	DF	316	GLN
31	DF	326	HIS
37	DG	10	HIS
37	DG	48	HIS
37	DG	142	ASN
38	DH	145	HIS
32	DI	21	GLN
32	DI	38	GLN
32	DI	81	GLN
32	DI	98	GLN
33	DJ	160	GLN
33	DJ	173	HIS
35	DL	73	ASN
35	DL	86	GLN
35	DL	117	GLN
35	DL	123	GLN
39	HD	24	ASN
39	HD	45	ASN
39	HD	136	ASN
39	HD	249	GLN
39	HD	298	GLN
40	HE	9	ASN
40	HE	65	GLN
41	HG	227	HIS
41	HG	293	GLN
41	HG	317	HIS
42	HH	498	ASN
42	HH	598	HIS
43	HF	36	GLN
43	HF	51	ASN
44	HI	56	ASN
44	HI	67	GLN
44	HI	83	HIS
44	HI	135	HIS
44	HI	166	ASN
45	HJ	7	GLN
45	HJ	10	HIS

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Mol	Chain	Res	Type
45	HJ	37	ASN
45	HJ	100	HIS
45	HJ	211	GLN
45	HJ	275	GLN
45	HJ	288	ASN
46	PD	38	HIS
46	PD	66	ASN
46	PD	141	GLN
47	PG	28	GLN
47	PG	60	GLN
47	PG	124	ASN
48	g	120	HIS
48	g	130	GLN
49	j	92	ASN
50	n	201	HIS
50	n	211	GLN
50	n	267	HIS
50	n	330	HIS
50	n	410	HIS
50	n	411	GLN
50	n	459	HIS
50	n	507	GLN
50	n	532	ASN
50	n	668	HIS
50	n	669	GLN
50	n	672	GLN
50	n	698	GLN
50	n	841	ASN
50	n	848	HIS
50	n	880	ASN
50	n	883	ASN
50	n	909	GLN
50	n	1225	GLN
51	s	82	ASN
51	s	122	HIS
52	u	27	GLN
52	u	49	ASN
52	u	56	GLN
52	u	86	GLN
52	u	97	ASN
53	a	57	HIS
53	a	87	GLN

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Mol	Chain	Res	Type
53	a	127	HIS
53	a	131	ASN
53	a	146	ASN
53	a	221	ASN
53	a	254	ASN
53	a	333	GLN
53	a	359	HIS
53	a	370	GLN
53	a	377	ASN
53	a	399	GLN
53	a	413	HIS
53	a	459	ASN
54	d	63	ASN
54	d	64	GLN
54	d	71	HIS
54	d	85	ASN
54	d	90	HIS
54	d	94	GLN
54	d	108	GLN
54	d	111	GLN
54	d	113	GLN
54	d	119	GLN
54	d	127	GLN
54	d	189	GLN
54	d	191	ASN
55	f	84	GLN
55	f	107	GLN
55	f	127	GLN
56	i	70	HIS
56	i	85	GLN
56	i	108	HIS
56	i	113	GLN
56	i	117	GLN
57	m	35	ASN
57	m	80	GLN
57	m	106	GLN
57	m	116	GLN
58	q	139	GLN
58	q	142	GLN
58	q	262	GLN
58	q	310	GLN
58	q	321	GLN

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Mol	Chain	Res	Type
58	q	334	GLN
58	q	347	HIS
58	q	394	HIS
58	q	402	HIS
58	q	411	GLN
58	q	434	GLN
58	q	437	HIS
58	q	461	GLN
58	q	463	HIS
58	q	492	GLN
58	q	496	ASN
58	q	506	HIS
58	q	533	GLN
58	q	539	GLN
58	q	547	GLN
58	q	565	ASN
58	q	595	GLN
58	q	611	GLN
58	q	626	GLN
59	z	483	ASN
59	z	527	GLN
59	z	549	GLN
59	z	567	GLN
59	z	585	HIS
59	z	592	ASN
60	b	66	GLN
60	b	87	ASN
60	b	129	GLN
60	b	136	HIS
61	c	10	ASN
61	c	41	ASN
61	c	64	ASN
61	c	160	GLN
61	c	237	GLN
61	c	245	HIS
61	c	306	HIS
62	e	97	GLN
62	e	132	HIS
63	l	72	GLN
63	l	102	ASN
64	o	692	ASN
64	o	701	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
64	o	753	HIS
65	h	18	GLN
65	h	55	GLN
65	h	60	ASN
65	h	102	HIS
65	h	123	GLN
65	h	169	ASN
65	h	171	GLN
66	k	41	ASN
66	k	77	GLN
66	k	79	HIS
66	k	91	GLN
67	r	99	HIS
67	r	156	ASN
68	t	8	GLN
68	t	103	GLN
68	t	178	ASN
68	t	180	HIS
68	t	204	GLN
69	v	16	GLN
69	v	32	ASN
69	v	62	HIS
69	v	103	GLN
70	p	63	HIS
70	p	225	ASN
70	p	272	ASN
70	p	400	GLN
70	p	435	GLN
70	p	570	ASN
70	p	598	ASN
70	p	619	GLN
70	p	683	GLN
70	p	723	GLN
70	p	746	GLN
70	p	751	GLN
70	p	781	HIS
71	w	158	GLN
71	w	203	ASN
71	w	239	ASN
71	w	295	GLN
71	w	357	HIS
71	w	358	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	w	378	GLN
71	w	421	HIS
71	w	433	ASN
71	w	438	ASN
71	w	513	ASN
71	w	596	HIS
71	w	616	GLN
71	w	618	HIS
71	w	638	GLN
71	w	726	ASN
71	w	783	GLN
71	w	822	HIS
71	w	841	GLN
71	w	851	ASN
71	w	874	HIS
71	w	923	ASN
71	w	972	HIS
71	w	1037	ASN
71	w	1040	GLN
71	w	1059	ASN
71	w	1124	ASN
71	w	1320	ASN
72	x	8	GLN
72	x	49	GLN
72	x	179	HIS
72	x	214	GLN
72	x	217	GLN
72	x	335	ASN
72	x	356	ASN
72	x	361	ASN
72	x	380	ASN
72	x	402	ASN
72	x	404	GLN
72	x	472	ASN
72	x	502	HIS
72	x	544	HIS
72	x	679	GLN
72	x	737	HIS
72	x	799	HIS
73	y	72	ASN
73	y	85	HIS
73	y	134	GLN

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Mol	Chain	Res	Type
73	y	179	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	7	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	7	-	-	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

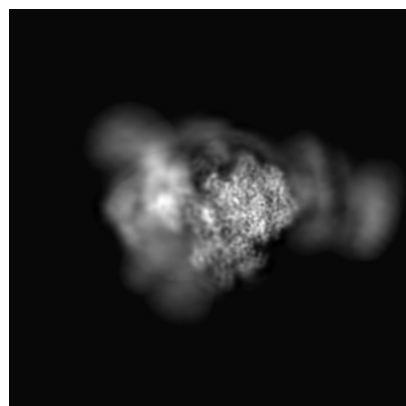
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34359. These allow visual inspection of the internal detail of the map and identification of artifacts.

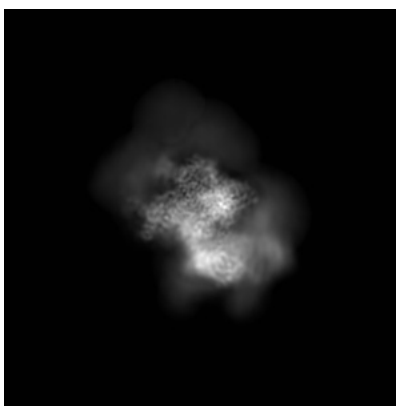
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

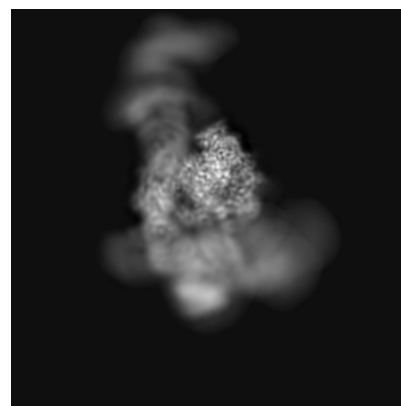
6.1.1 Primary map



X

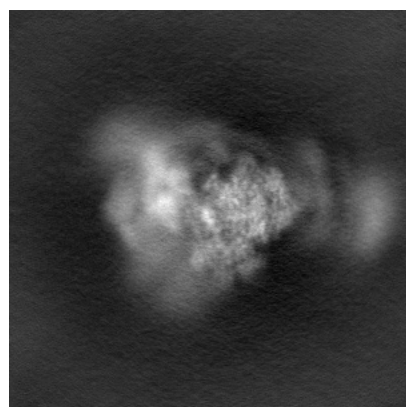


Y

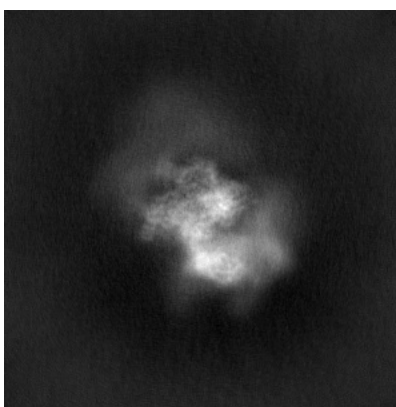


Z

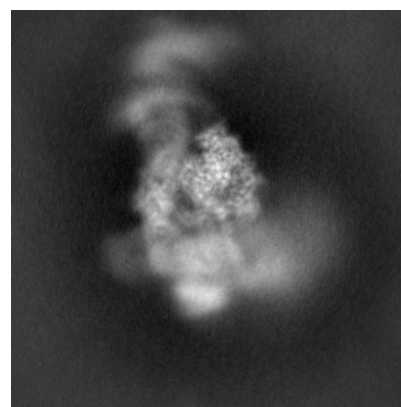
6.1.2 Raw map



X



Y

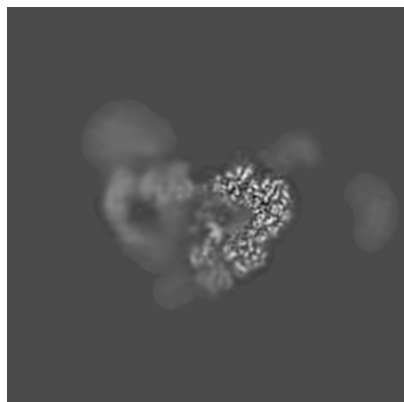


Z

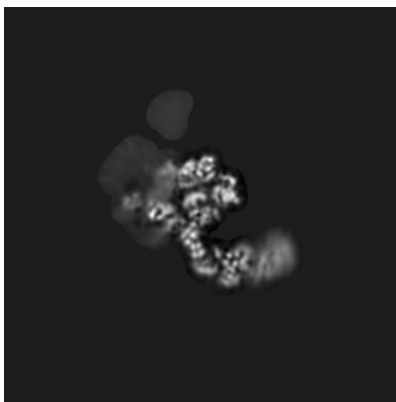
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

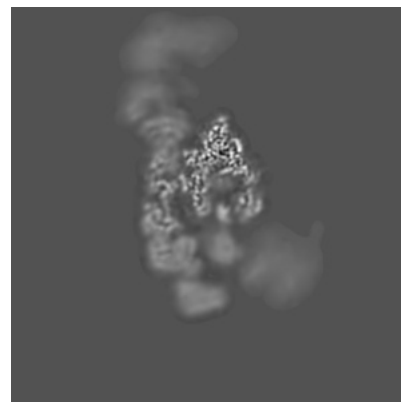
6.2.1 Primary map



X Index: 210

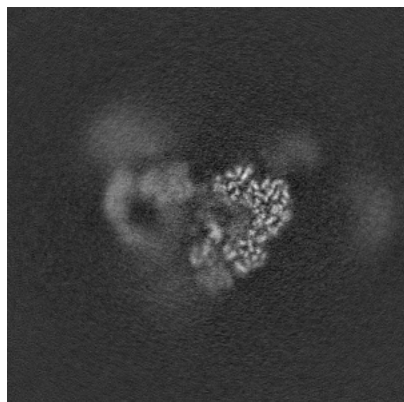


Y Index: 210

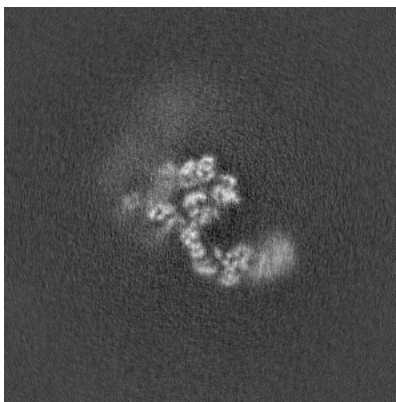


Z Index: 210

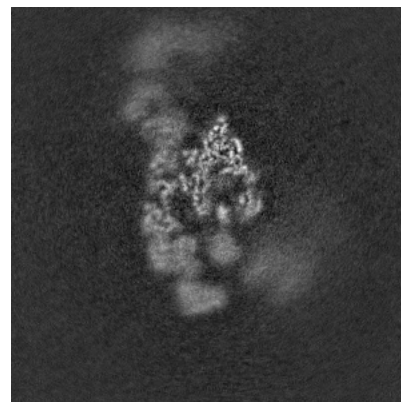
6.2.2 Raw map



X Index: 210



Y Index: 210

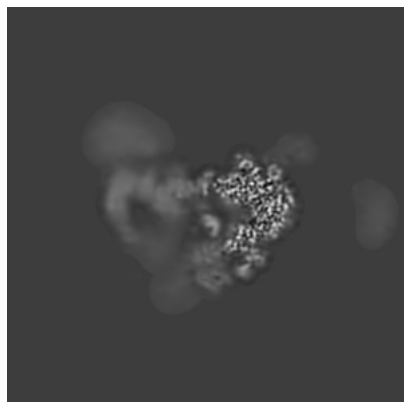


Z Index: 210

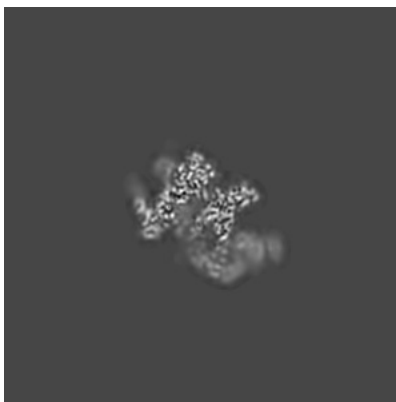
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

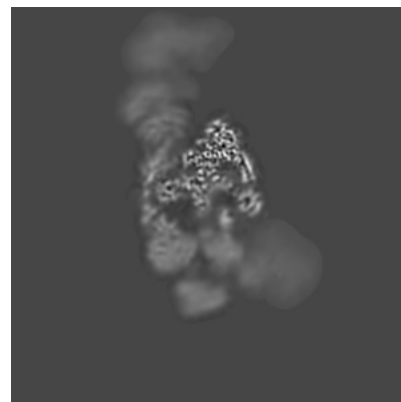
6.3.1 Primary map



X Index: 215

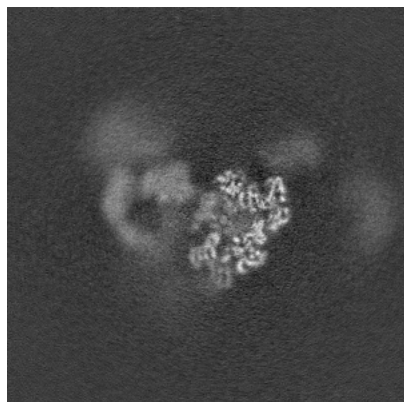


Y Index: 246

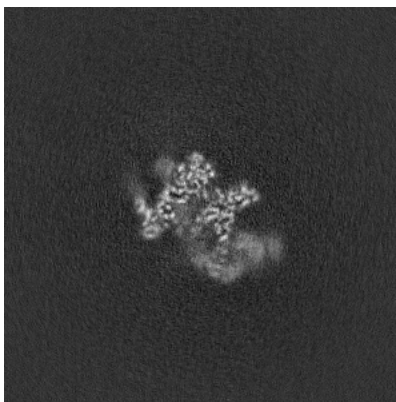


Z Index: 216

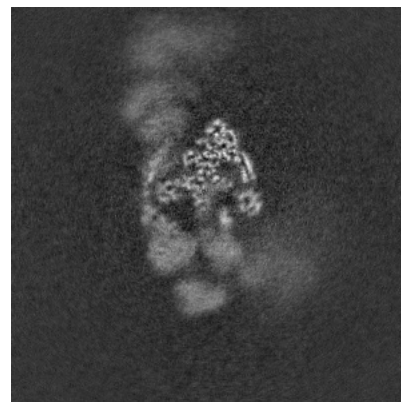
6.3.2 Raw map



X Index: 206



Y Index: 246

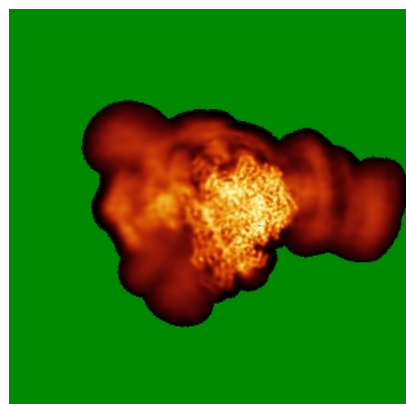


Z Index: 216

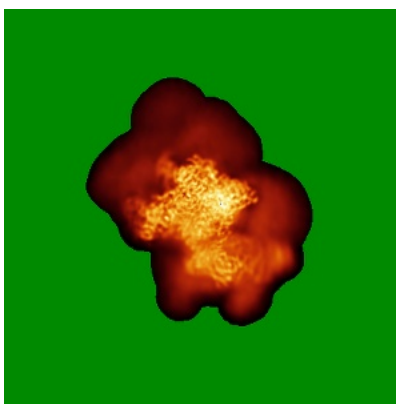
The images above show the largest variance slices of the map in three orthogonal directions.

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

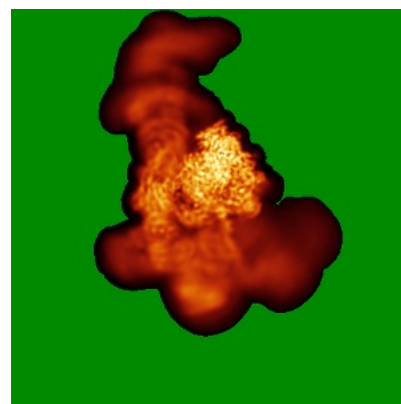
6.4.1 Primary map



X

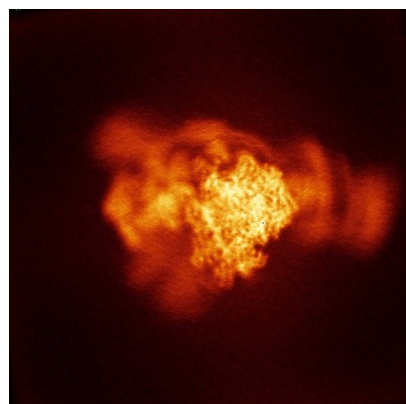


Y

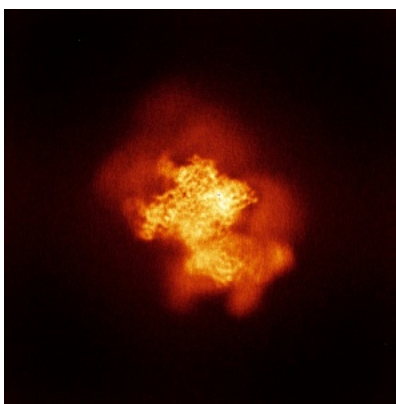


Z

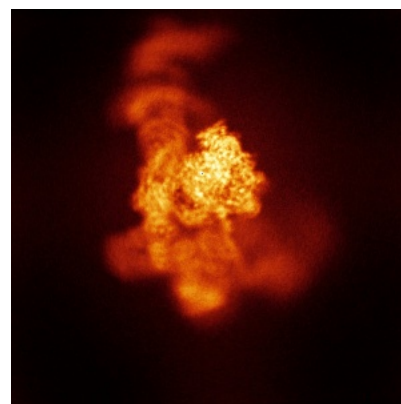
6.4.2 Raw map



X



Y

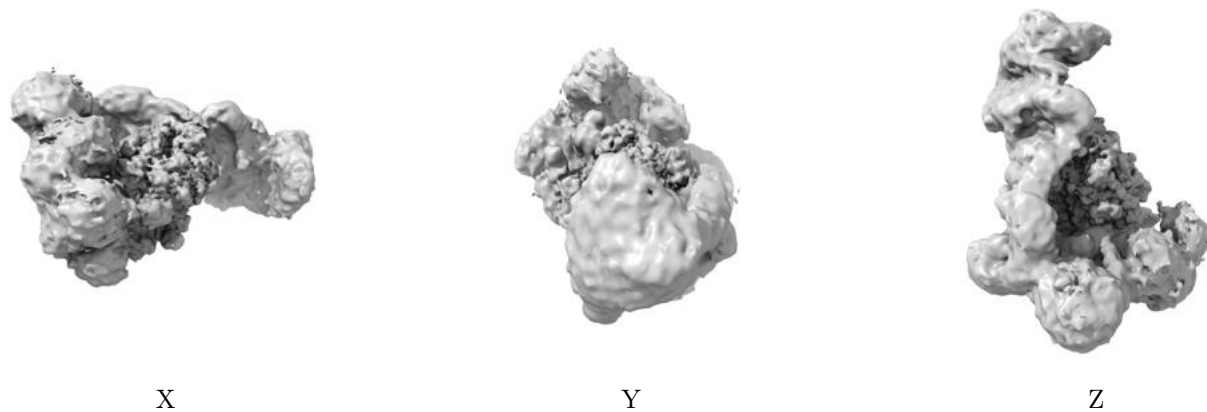


Z

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

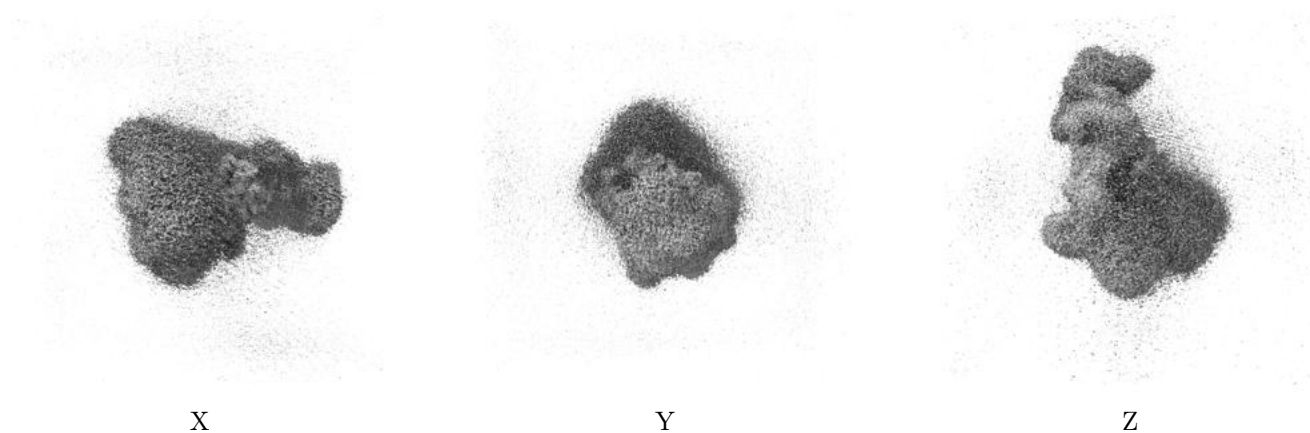
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

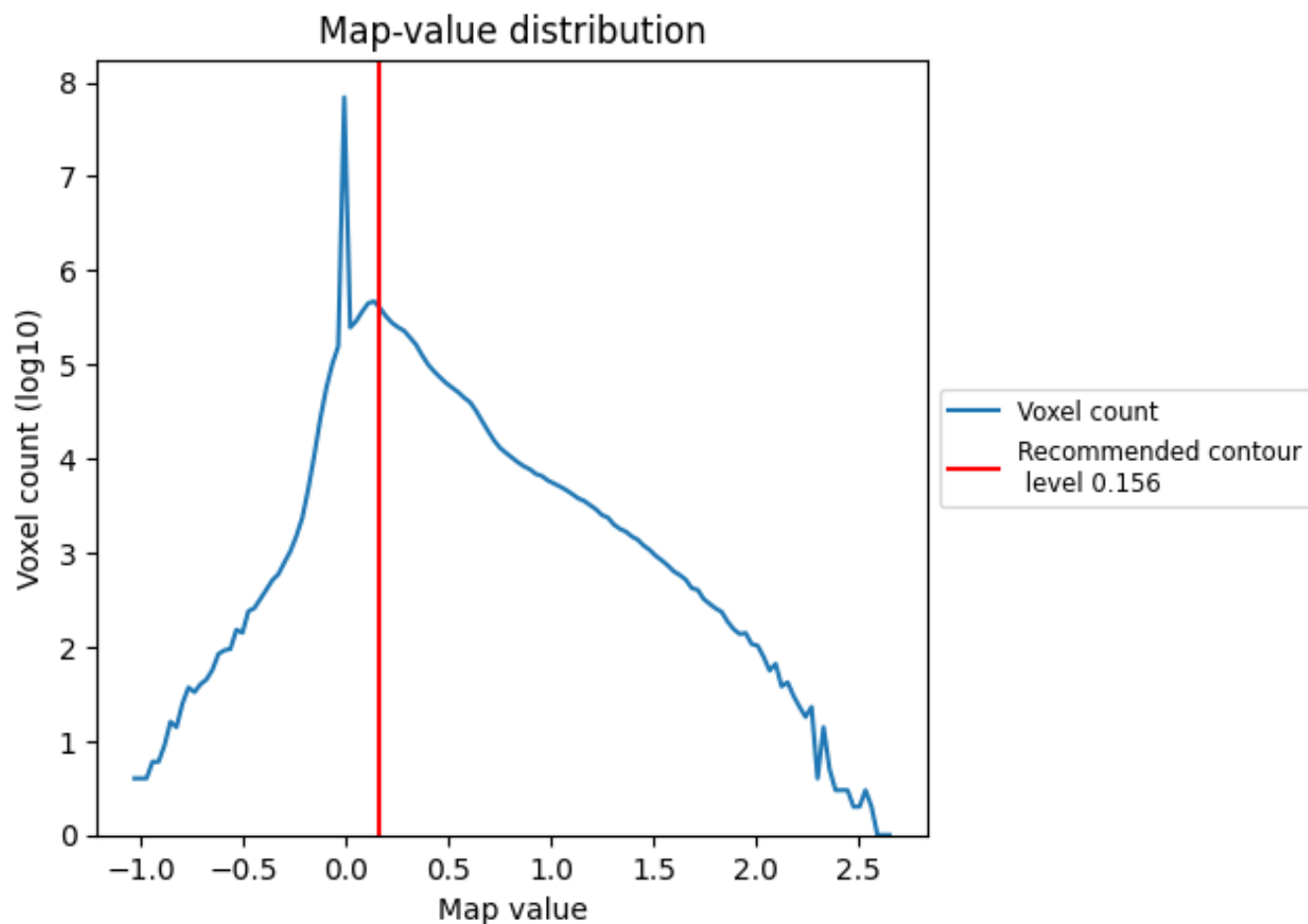
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

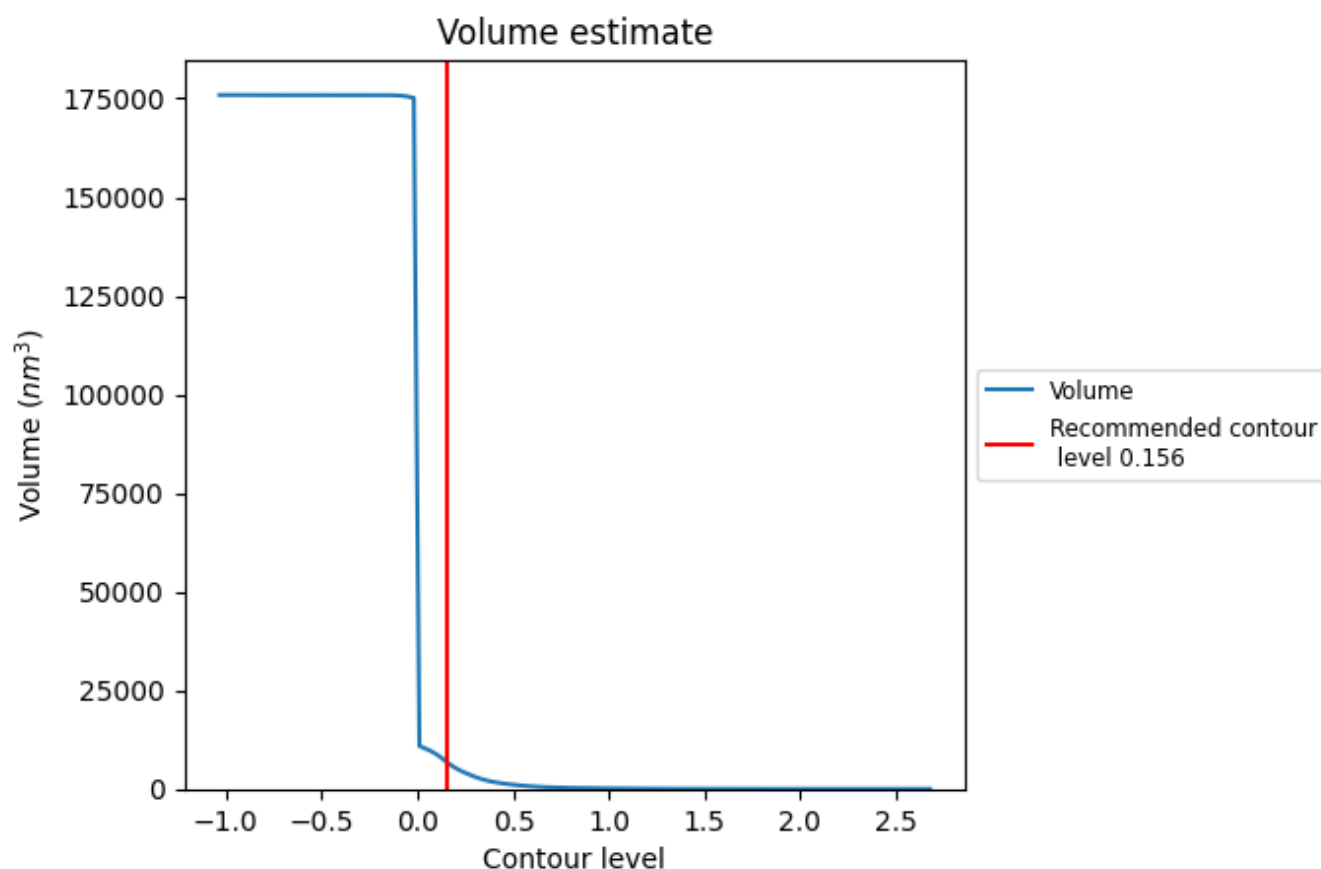
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

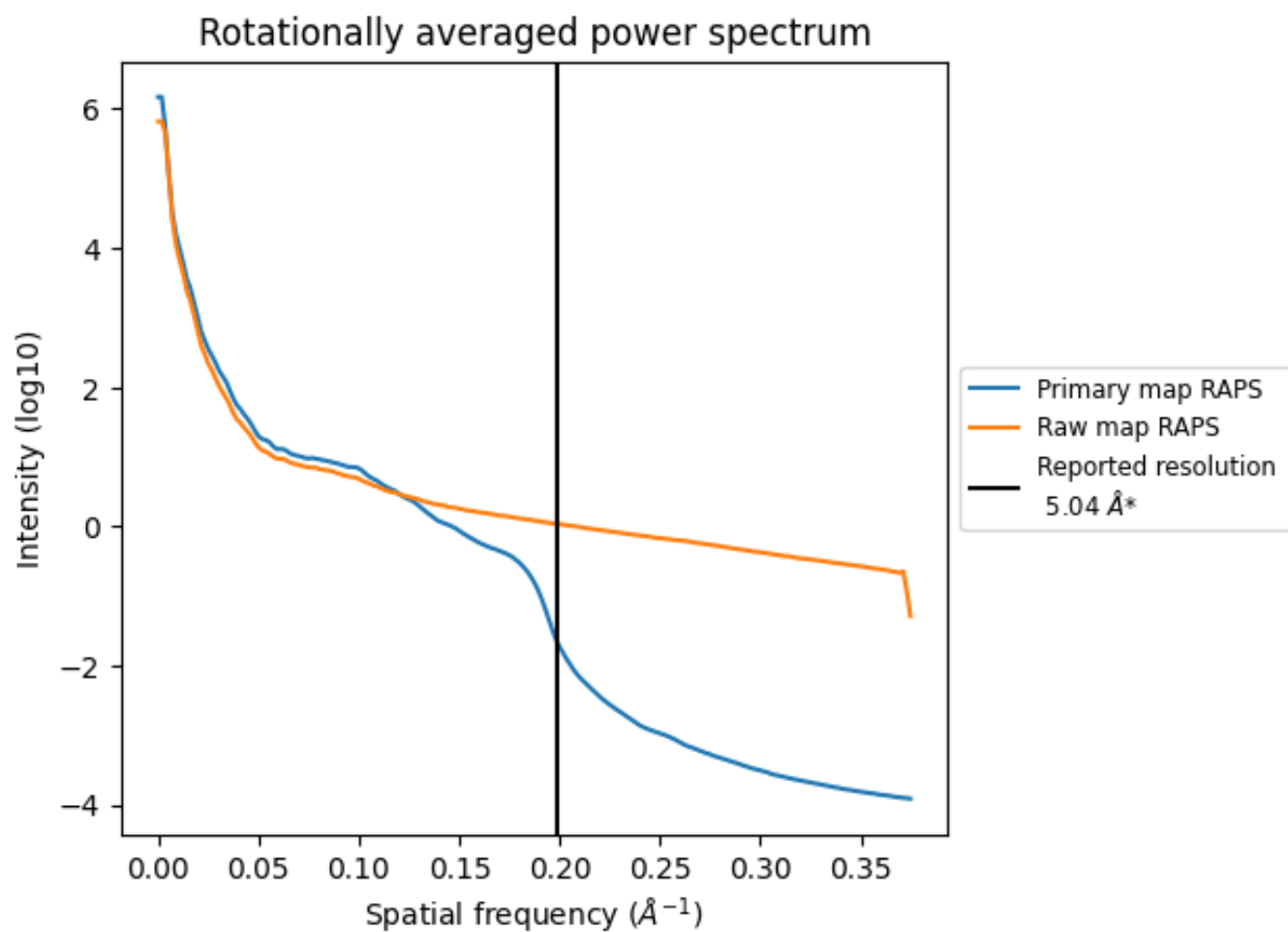
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6707 nm^3 ; this corresponds to an approximate mass of 6058 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 ⓘ

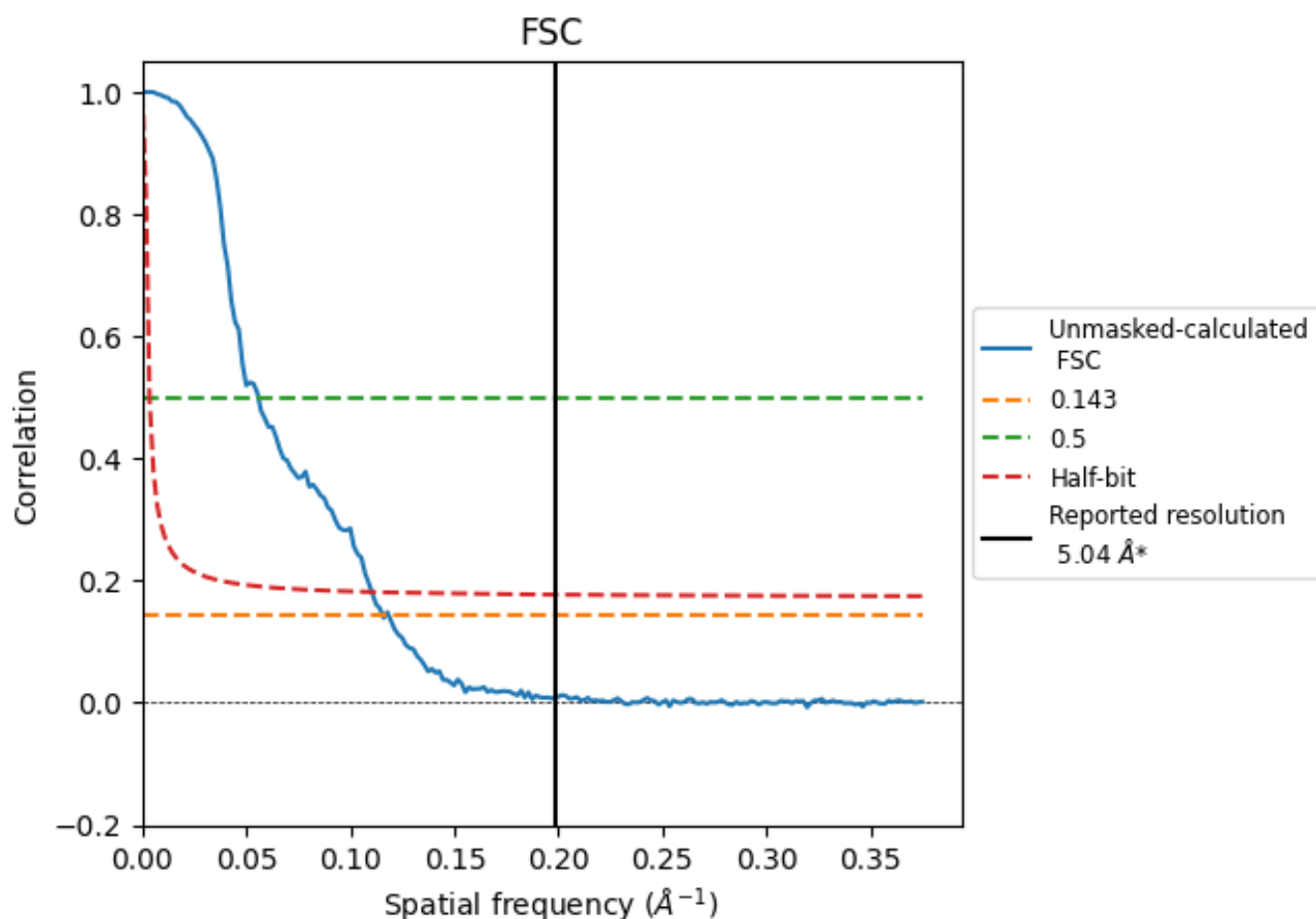


*Reported resolution corresponds to spatial frequency of 0.198 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.198 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

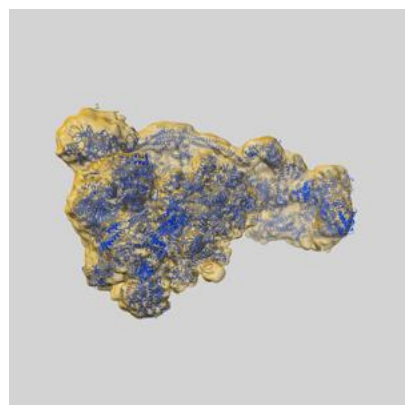
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.66	17.92	9.07

*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 8.66 differs from the reported value 5.04 by more than 10 %

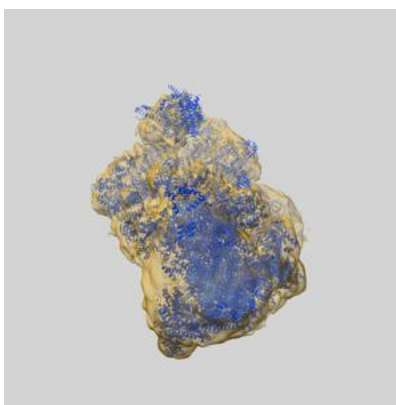
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34359 and PDB model 8GXQ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

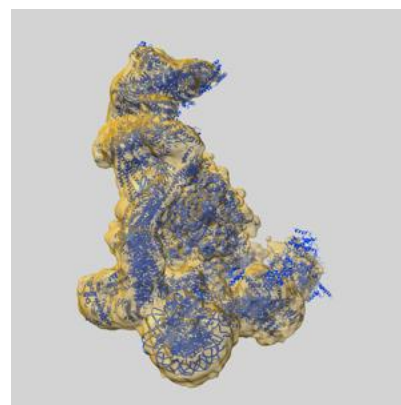
9.1 Map-model overlay [i](#)



X



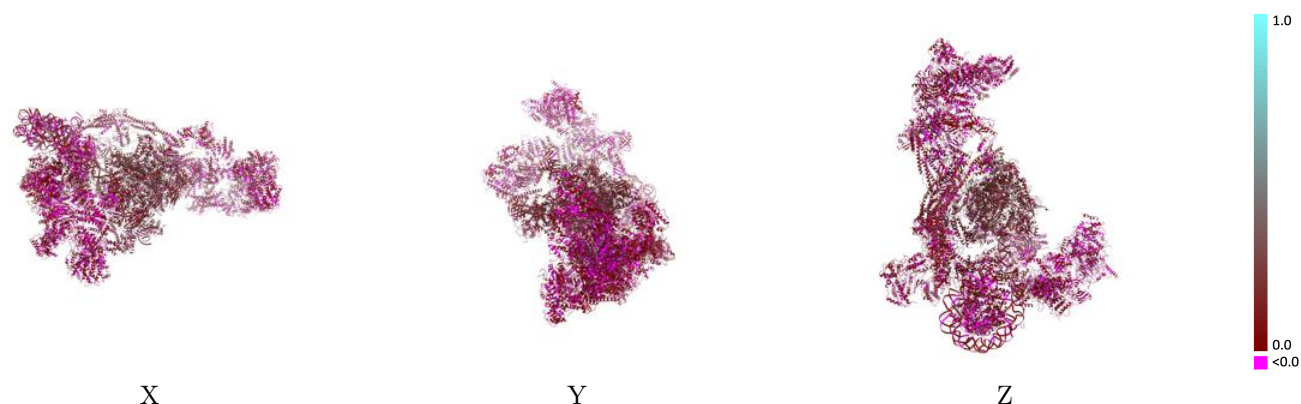
Y



Z

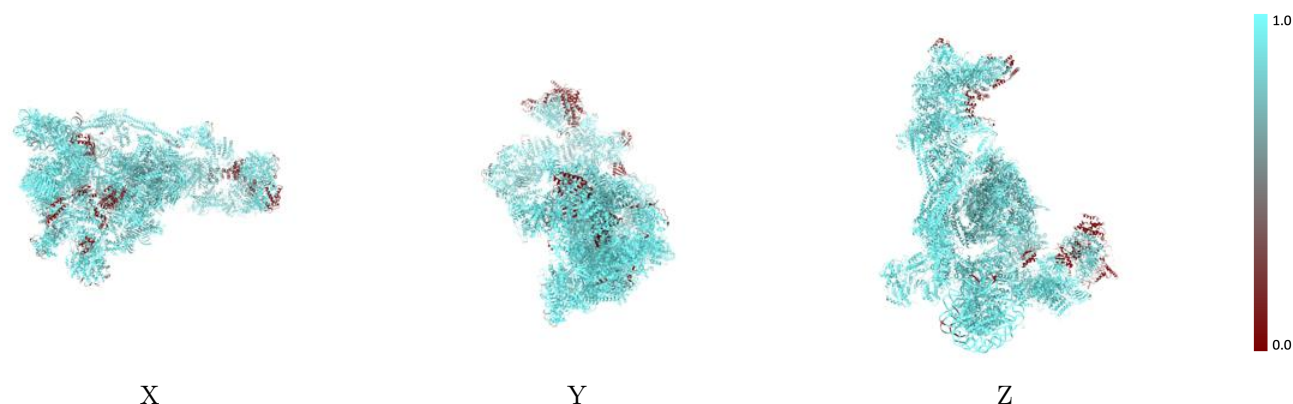
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



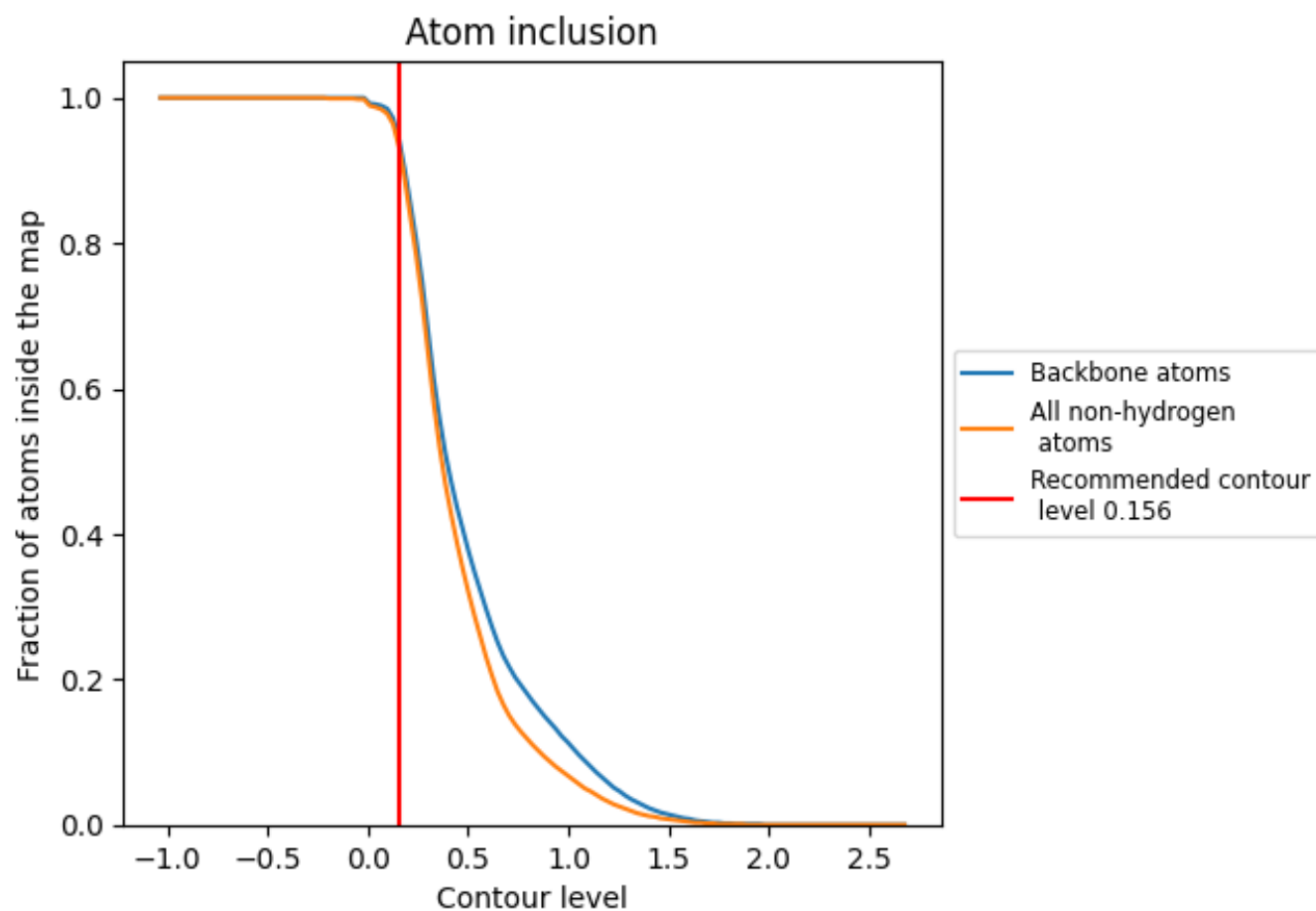
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.0840
BA	 0.9710	 0.1780
DA	 0.8720	 0.0300
DB	 0.9940	 0.0440
DD	 0.9020	 0.0440
DE	 0.9790	 0.0430
DF	 0.9610	 0.0410
DG	 0.5770	 0.0150
DH	 0.9980	 0.0490
DI	 0.9200	 0.0360
DJ	 0.9960	 0.0450
DL	 0.8450	 0.0330
DO	 0.9730	 0.1060
DP	 0.9830	 0.1390
DQ	 0.9680	 0.1190
Dc	 0.6200	 0.0290
Dd	 0.3480	 0.0030
De	 0.6780	 0.0240
Df	 0.8640	 0.0370
Di	 0.8370	 0.0200
Dj	 0.6600	 0.0400
Dk	 0.2270	 0.0000
DI	 0.6640	 0.0310
Dm	 0.2120	 0.0050
EA	 0.9500	 0.1120
EB	 0.9900	 0.1230
FA	 0.9870	 0.1360
FB	 0.9860	 0.1460
HA	 0.9980	 0.1150
HB	 0.9980	 0.0670
HC	 0.9970	 0.0860
HD	 0.9870	 0.1130
HE	 0.9980	 0.0490
HF	 1.0000	 0.0790
HG	 0.9990	 0.0690



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Chain	Atom inclusion	Q-score
HH	 0.9940	 0.0730
HI	 0.9980	 0.0630
HJ	 0.9830	 0.0630
NA	 0.9800	 0.0770
NB	 1.0000	 0.0420
NC	 0.9840	 0.0110
ND	 0.9700	 0.0500
NE	 0.9940	 0.0710
NF	 1.0000	 0.0330
NG	 1.0000	 0.0430
NH	 1.0000	 0.0020
NX	 0.9070	 0.0340
NY	 0.9400	 0.0460
PA	 0.9560	 0.1830
PB	 0.9530	 0.2030
PC	 0.9630	 0.2080
PD	 0.9630	 0.1720
PE	 0.9790	 0.1790
PF	 0.9290	 0.2020
PG	 0.9720	 0.1580
PH	 0.9600	 0.1920
PI	 0.9780	 0.1840
PJ	 0.9540	 0.1870
PK	 0.9450	 0.2030
PL	 0.9800	 0.2110
X	 1.0000	 0.1830
Y	 0.9990	 0.1940
a	 0.9250	 0.0510
b	 0.9970	 0.0400
c	 0.9890	 0.0500
d	 0.9730	 0.0590
e	 0.9990	 0.0910
f	 0.9990	 0.1300
g	 1.0000	 0.1080
h	 0.9880	 0.1470
i	 0.8660	 0.0960
j	 1.0000	 0.0750
k	 0.9880	 0.1390
l	 1.0000	 0.0690
m	 1.0000	 0.0690
n	 0.9880	 0.0610
o	 0.9970	 0.0280

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Chain	Atom inclusion	Q-score
p	 0.9960	 0.0430
q	 0.9970	 0.0780
r	 0.9950	 0.1020
s	 1.0000	 0.0400
t	 0.9870	 0.0680
u	 1.0000	 0.0900
v	 0.9840	 0.1110
w	 0.7510	 0.0240
x	 0.9500	 0.0400
y	 0.9750	 0.0310
z	 0.9480	 0.0340