



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:34 PM UTC

PDB ID : 5XTI / pdb_00005xti
EMDB ID : EMD-6776
Title : Cryo-EM architecture of human respiratory chain megacomplex-I2III2IV2
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 17.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

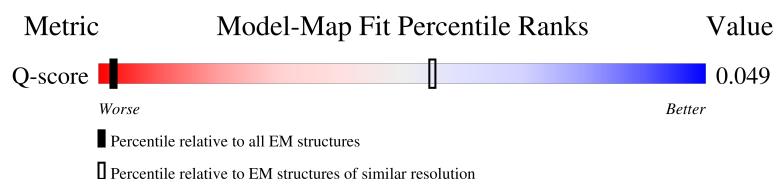
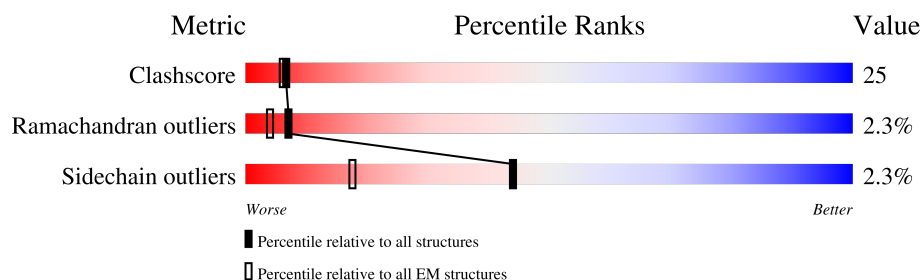
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.40 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.



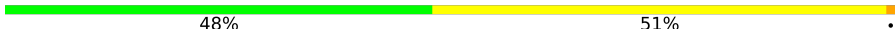
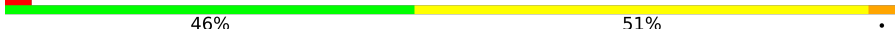
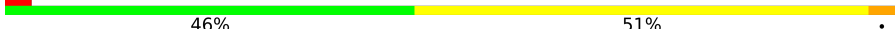
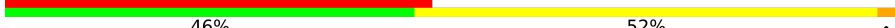
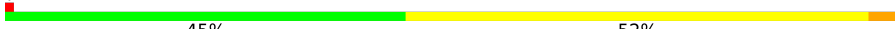
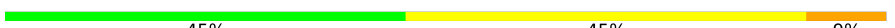
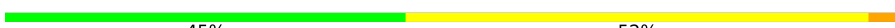
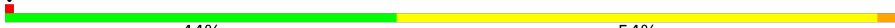
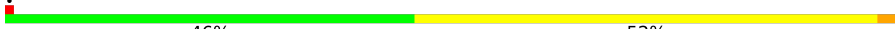
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	31 (16.90 - 17.60)

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

Mol	Chain	Length	Quality of chain
1	A	431	22% 48% 50% .
1	BA	431	48% 49% .
2	B	176	48% 50% .
2	BB	176	47% 51% .

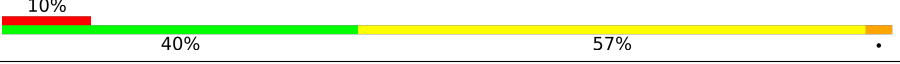
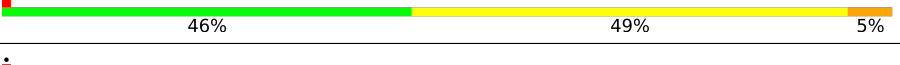
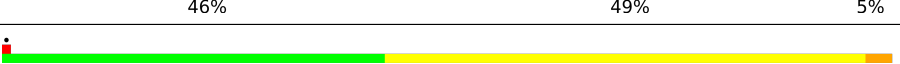
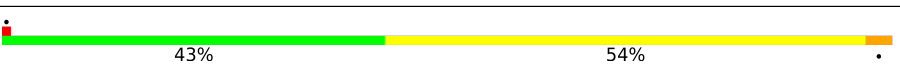
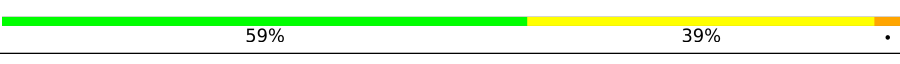
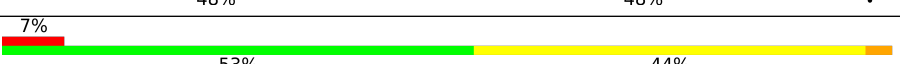
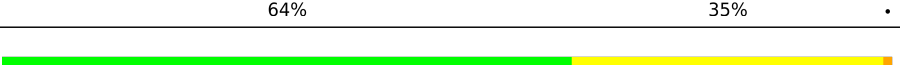
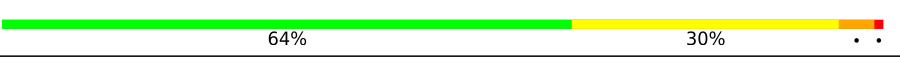
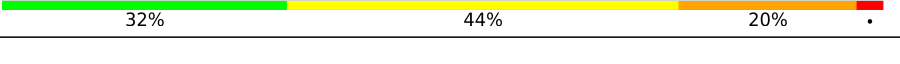
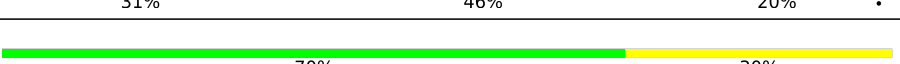
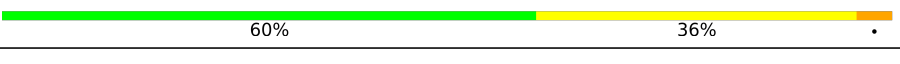
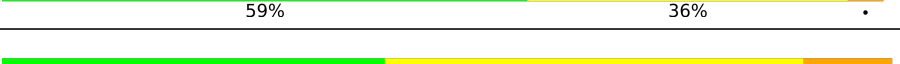
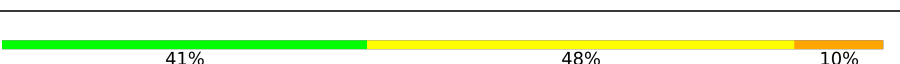
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Mol	Chain	Length	Quality of chain
3	BC	156	
3	C	156	
4	BE	113	
4	E	113	
5	BF	83	
5	F	83	
6	BG	85	
6	BX	85	
6	G	85	
6	X	85	
7	BH	112	
7	H	112	
8	BI	110	
8	I	110	
9	BJ	337	
9	J	337	
10	BK	33	
10	K	33	
11	BL	118	
11	L	118	
12	BM	687	
12	M	687	
13	BN	143	
13	N	143	
14	BO	212	

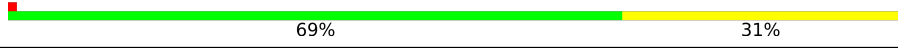
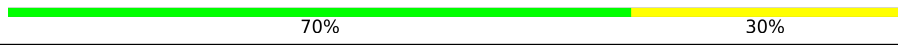
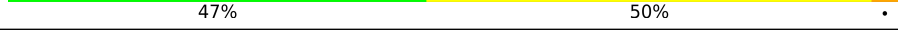
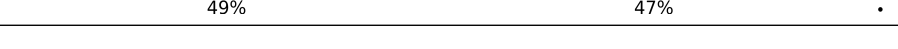
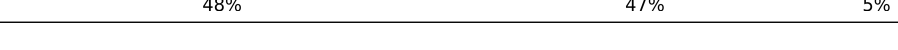
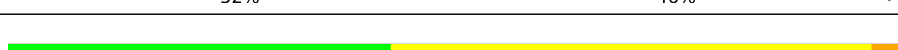
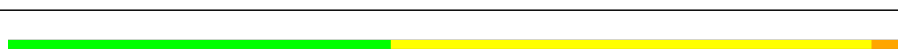
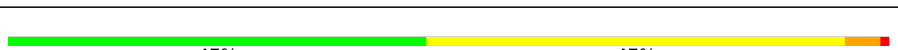
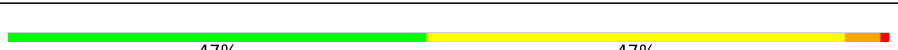
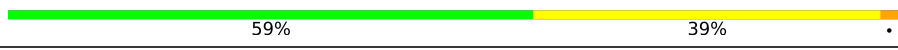
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Mol	Chain	Length	Quality of chain
14	O	212	
15	BP	208	
15	P	208	
16	BQ	430	
16	Q	430	
17	BS	70	
17	S	70	
18	BT	95	
18	T	95	
19	BU	83	
19	U	83	
20	BV	140	
20	V	140	
21	BW	138	
21	W	138	
22	BY	59	
22	Y	59	
23	BZ	80	
23	Z	80	
24	Ba	138	
24	a	138	
25	Bb	124	
25	b	124	
26	Bc	153	
26	c	153	

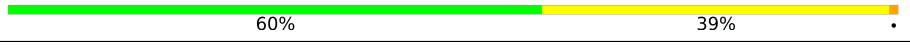
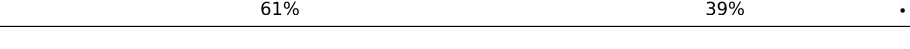
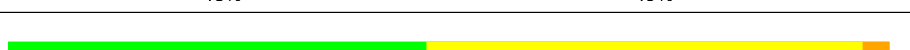
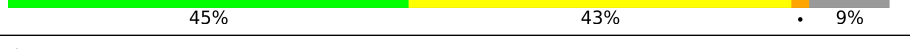
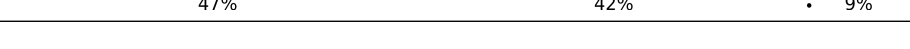
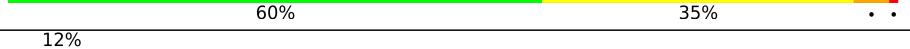
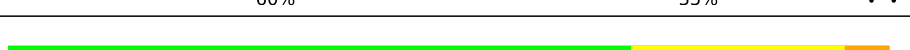
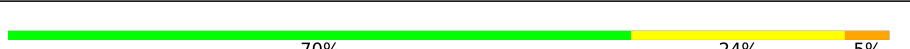
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Mol	Chain	Length	Quality of chain
27	Bd	171	
27	d	171	
28	Be	97	
28	e	97	
29	Bf	47	
29	f	47	
30	Bg	119	
30	g	119	
31	Bh	104	
31	h	104	
32	Bi	347	
32	i	347	
33	Bj	115	
33	j	115	
34	Bk	97	
34	k	97	
35	Bl	603	
35	l	603	
36	Bm	174	
36	m	174	
37	Bn	56	
37	n	56	
38	Bo	128	
38	o	128	
39	Bp	172	

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Mol	Chain	Length	Quality of chain
39	p	172	
40	Br	459	
40	r	459	
41	Bs	318	
41	s	318	
42	Bu	169	
42	u	169	
43	Bv	122	
43	v	122	
44	Bw	320	
44	w	320	
45	Bx	514	
45	x	514	
46	By	227	
46	y	227	
47	Bz	261	
47	z	261	
48	0	144	
48	B0	144	
49	1	109	
49	B1	109	
50	2	98	
50	B2	98	
51	3	84	
51	B3	84	

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Mol	Chain	Length	Quality of chain
52	4	75	
52	B4	75	
53	5	73	
53	B5	73	
54	6	56	
54	B6	56	
55	7	49	
55	B7	49	
56	8	47	
56	B8	47	
57	9	43	
57	B9	43	
58	AA	81	
58	AN	81	
59	AB	57	
59	AO	57	
60	AC	196	
60	AP	196	
61	AD	62	
61	AQ	62	
62	AE	74	
62	AR	74	
63	AF	106	
63	AS	106	
64	AG	51	

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Mol	Chain	Length	Quality of chain
64	AT	51	
65	AH	241	
65	AU	241	
66	AJ	378	
66	AV	378	
67	AK	419	
67	AW	419	
68	AL	446	
68	AY	446	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	SF4	A	501	-	-	X	-
69	SF4	B	302	-	-	X	-
69	SF4	BA	501	-	-	X	-
69	SF4	BB	302	-	-	X	-
69	SF4	BM	801	-	-	X	-
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
70	FMN	BA	502	-	-	X	-
71	PLX	Bb	201	-	-	X	-
71	PLX	b	201	-	-	X	-
73	NDP	BJ	401	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	301	-	-	X	-
74	FES	BO	301	-	-	X	-
74	FES	O	301	-	-	X	-
75	CDL	AG	101	-	-	X	-
75	CDL	AL	502	-	-	X	-
76	PEE	AH	401	-	-	X	-
76	PEE	AL	503	-	-	X	-
76	PEE	AU	401	-	-	X	-
76	PEE	AV	403	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
76	PEE	AY	502	-	-	X	-
76	PEE	BV	202	-	-	X	-
76	PEE	Bl	701	-	-	X	-
76	PEE	V	202	-	-	X	-
76	PEE	l	701	-	-	X	-

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 196753 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		
1	BA	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		
2	BB	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		
3	BC	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		
4	BE	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		
5	BF	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		
6	BG	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	BX	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		
7	BH	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		
8	BI	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	BJ	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		
10	BK	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		
11	BL	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		
12	BM	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		
13	BN	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		
14	BO	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		
15	BP	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		
16	BQ	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		
17	BS	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		
18	BT	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		
19	BU	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		
20	BV	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		
21	BW	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		
22	BY	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		
23	BZ	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		
24	Ba	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		
25	Bb	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		
26	Bc	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		
27	Bd	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		
28	Be	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		
29	Bf	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		
30	Bg	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		
31	Bh	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		
32	Bi	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		
33	Bj	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bk	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		
35	Bl	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		
36	Bm	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		
37	Bn	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1063	684	191	186	2		
38	Bo	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		
39	Bp	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		
40	Br	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		
41	Bs	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		
42	Bu	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		
43	Bv	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		
44	Bw	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		
45	Bx	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		
46	By	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		
47	Bz	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		
48	B0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		
50	B2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		
51	B3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		
52	B4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		
53	B5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		
54	B6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		
55	B7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		
56	B8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		
57	B9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AG	51	Total	C	N	O	0	0
			425	287	72	66		
64	AT	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

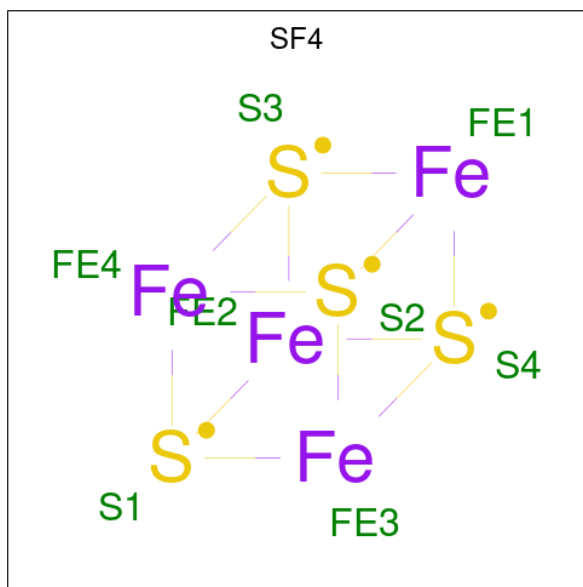
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

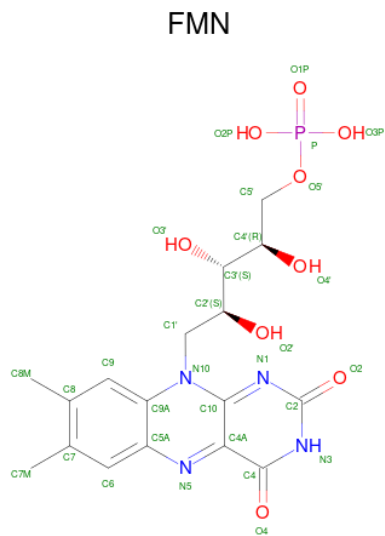
Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3442	2160	602	660	20		
68	AY	446	Total	C	N	O	S	0	0
			3428	2147	601	660	20		

- Molecule 69 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



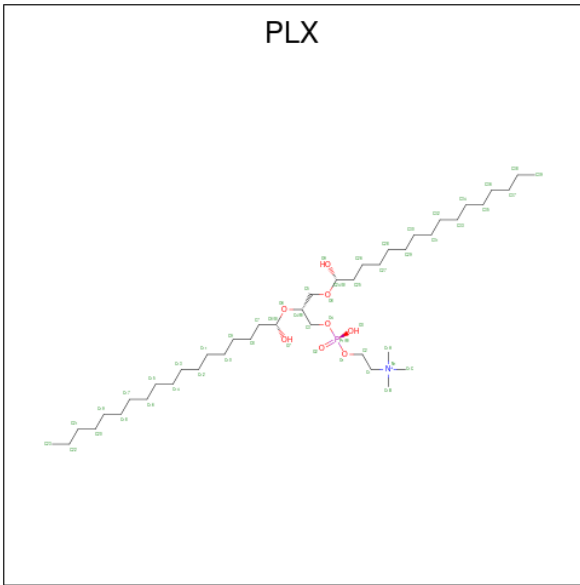
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	
69	BA	1	Total	Fe	S	0
			8	4	4	
69	BB	1	Total	Fe	S	0
			8	4	4	
69	BB	1	Total	Fe	S	0
			8	4	4	
69	BC	1	Total	Fe	S	0
			8	4	4	
69	BM	1	Total	Fe	S	0
			8	4	4	
69	BM	1	Total	Fe	S	0
			8	4	4	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
70	A	1	Total 31	C 17	N 4	O 9	P 1	0
70	BA	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 71 is (9R,11S)-9-([{(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total 52	C 42	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
71	U	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AL	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AN	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AQ	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AT	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	BB	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	BU	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	BV	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Bb	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Bg	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Bg	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Bg	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Br	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	Br	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).

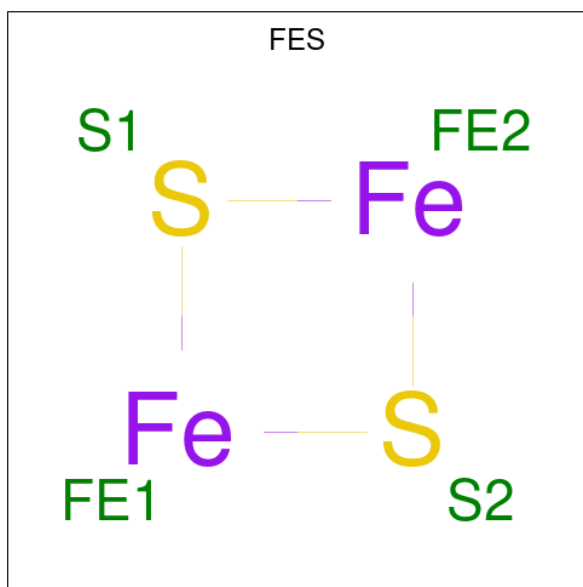


- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



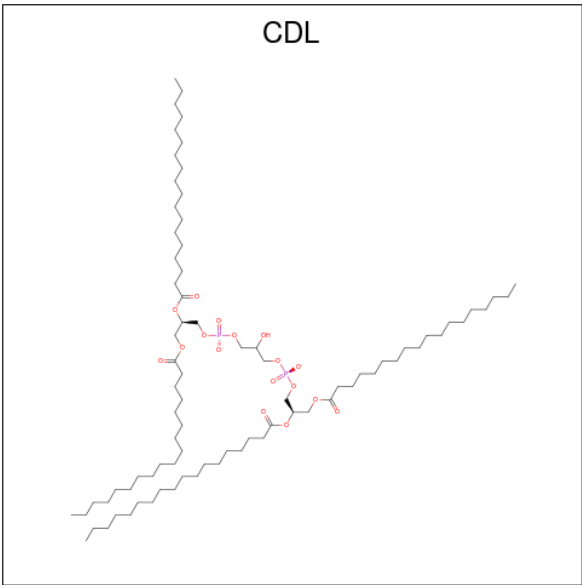
Mol	Chain	Residues	Atoms					AltConf
73	J	1	Total	C	N	O	P	0
			48	21	7	17	3	
73	BJ	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	
74	BM	1	Total	Fe	S	0
			4	2	2	
74	BO	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



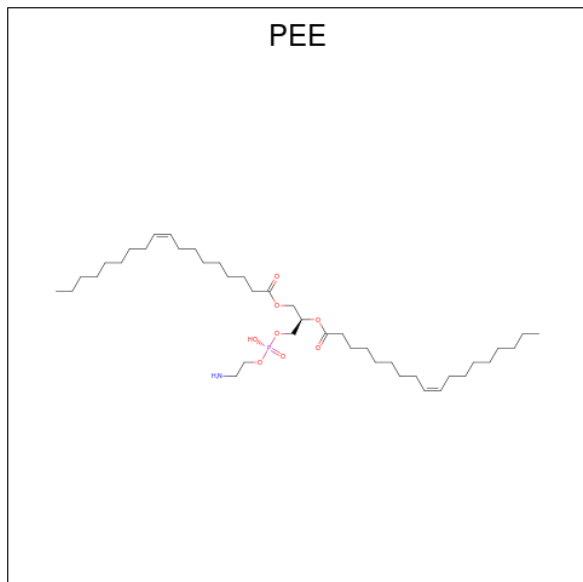
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total	C	O	P	0
			64	45	17	2	
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AL	1	Total	C	O	P	0
			64	45	17	2	
75	AN	1	Total	C	O	P	0
			64	45	17	2	
75	AU	1	Total	C	O	P	0
			64	45	17	2	
75	AY	1	Total	C	O	P	0
			64	45	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	BV	1	Total	C	O	P	0
			63	44	17	2	
75	Bi	1	Total	C	O	P	0
			64	45	17	2	
75	Bl	1	Total	C	O	P	0
			64	45	17	2	
75	Bl	1	Total	C	O	P	0
			64	45	17	2	
75	Bn	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 76 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	l	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	AH	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	BV	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	BW	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	Bl	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	Bl	1	Total	C	N	O	P	0
			51	41	1	8	1	

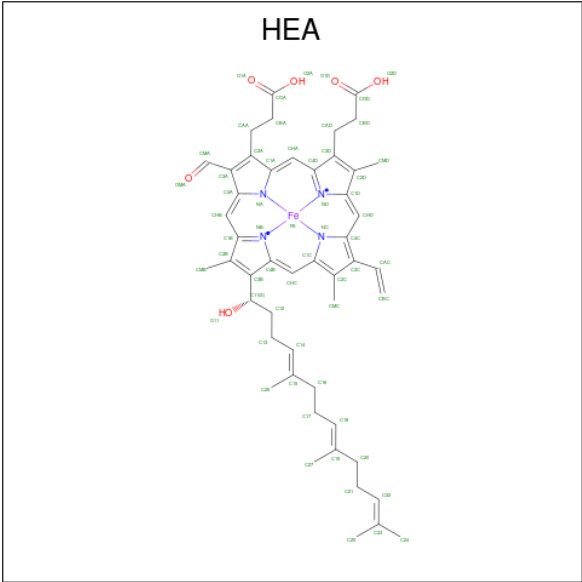
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	x	1	Total	Cu	0
			1	1	
77	y	2	Total	Cu	0
			2	2	
77	Bx	1	Total	Cu	0
			1	1	
77	By	2	Total	Cu	0
			2	2	

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	x	1	Total	Mg	0
			1	1	
78	Bx	1	Total	Mg	0
			1	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

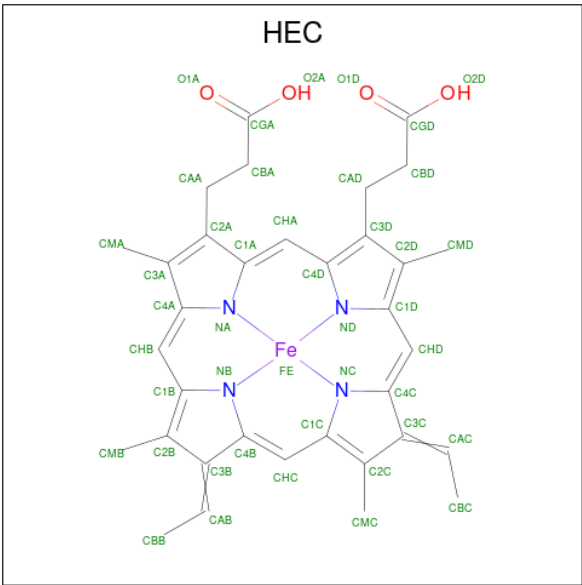


Mol	Chain	Residues	Atoms					AltConf
79	x	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	x	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	Bx	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	Bx	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

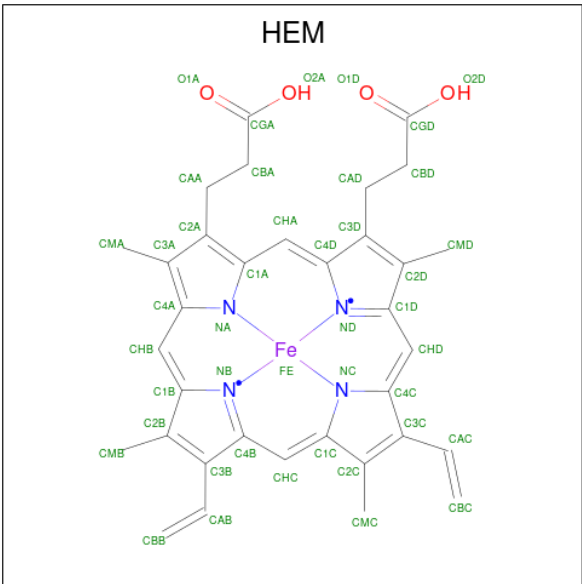
Mol	Chain	Residues	Atoms		AltConf
80	2	1	Total	Zn	0
			1	1	
80	B2	1	Total	Zn	0
			1	1	

- Molecule 81 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
81	AH	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	AU	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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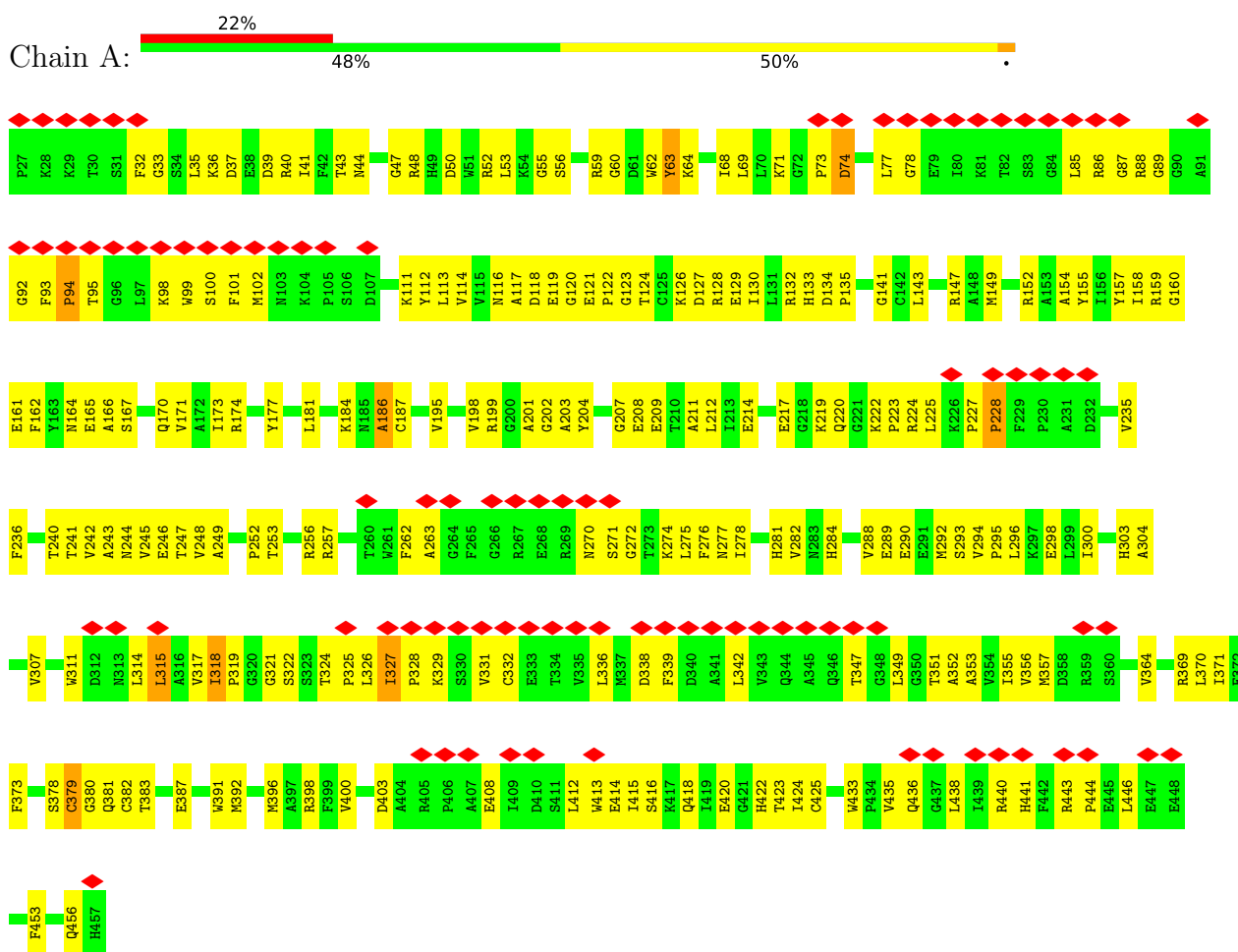
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Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0

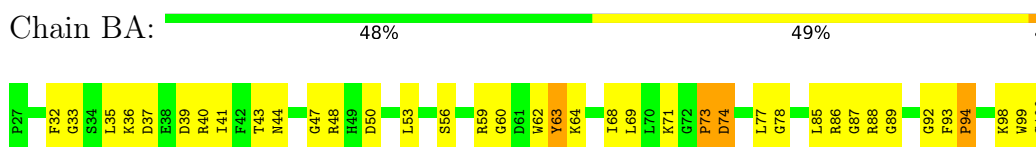
3 Residue-property plots

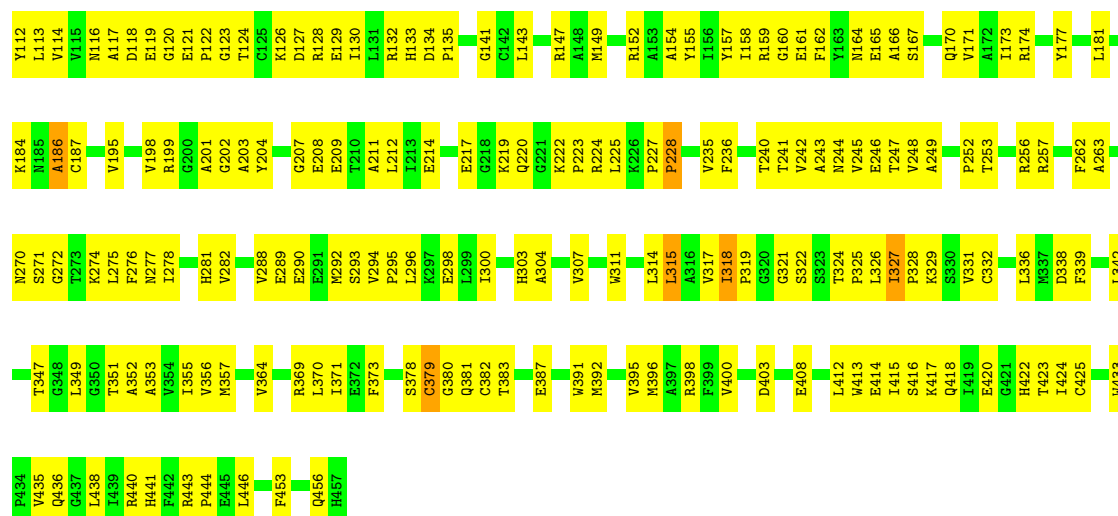
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

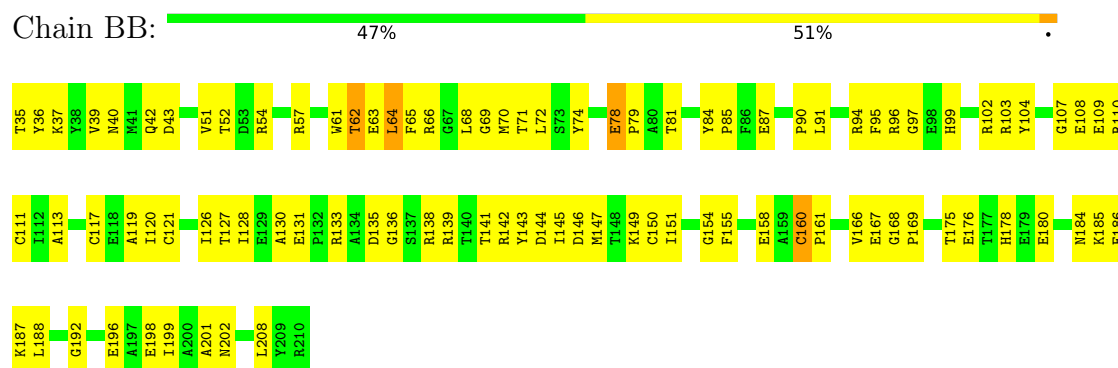




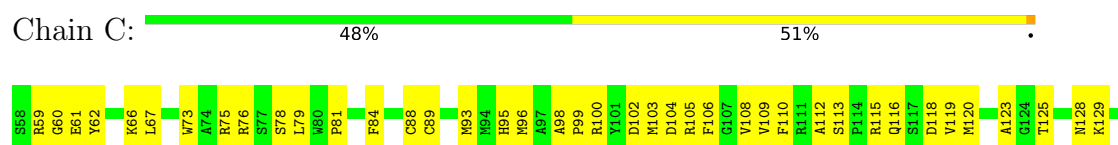
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

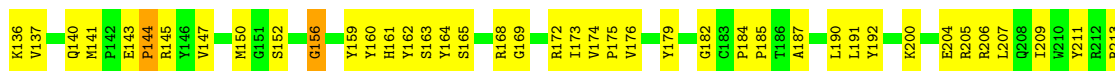


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

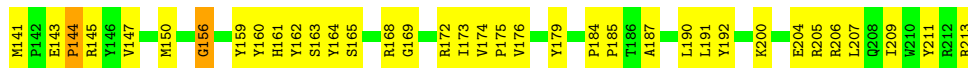


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

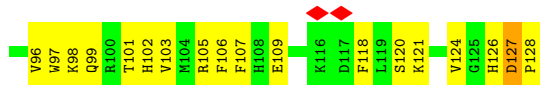
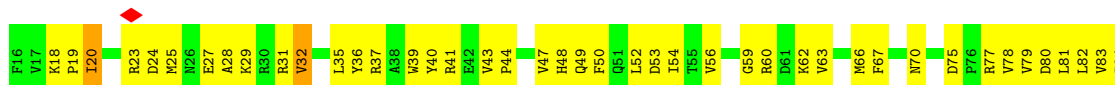




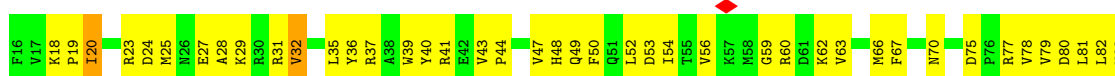
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



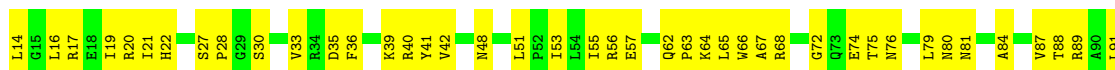
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

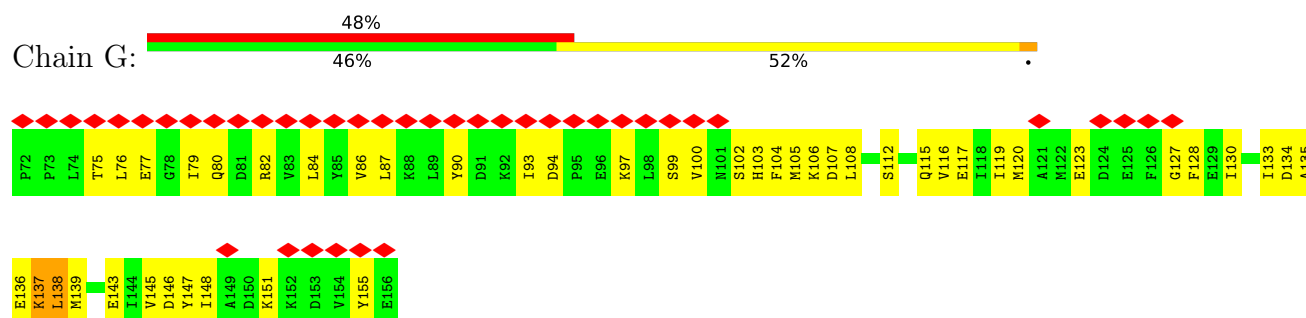


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

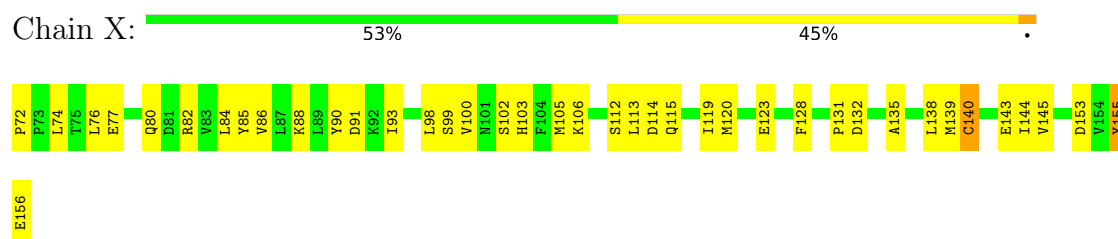




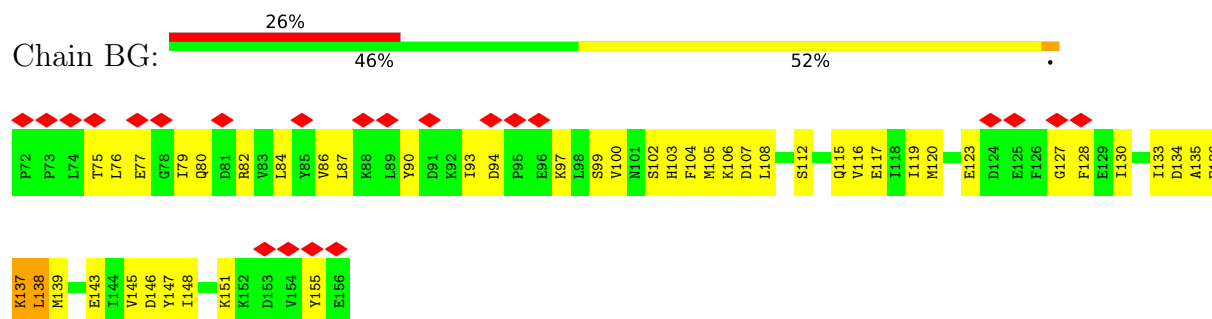
- Molecule 6: Acyl carrier protein, mitochondrial



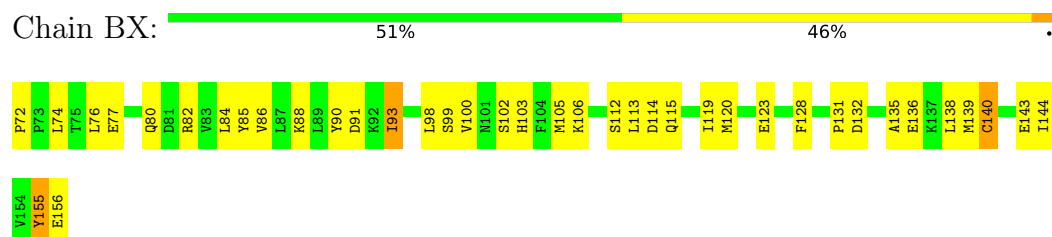
- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial

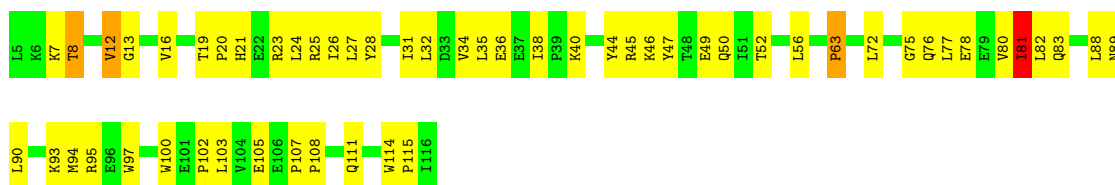


- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5





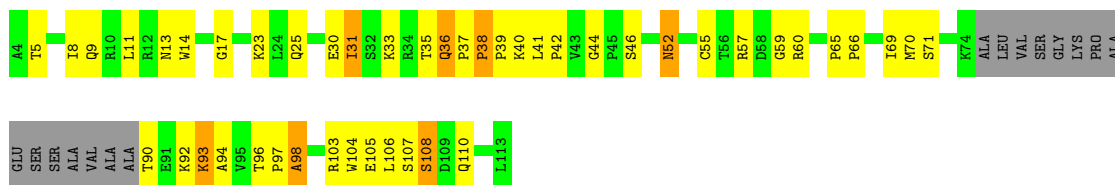
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

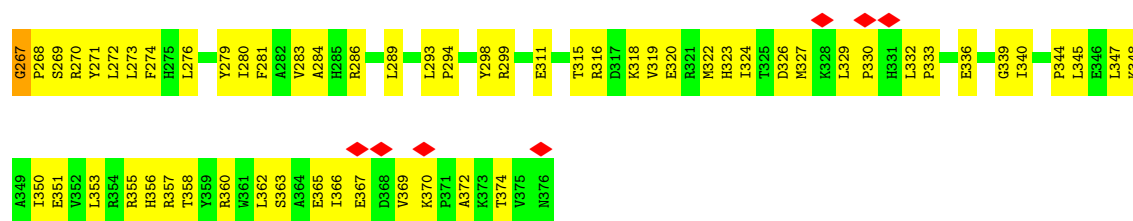
Chain BH: 50% 46% ..



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

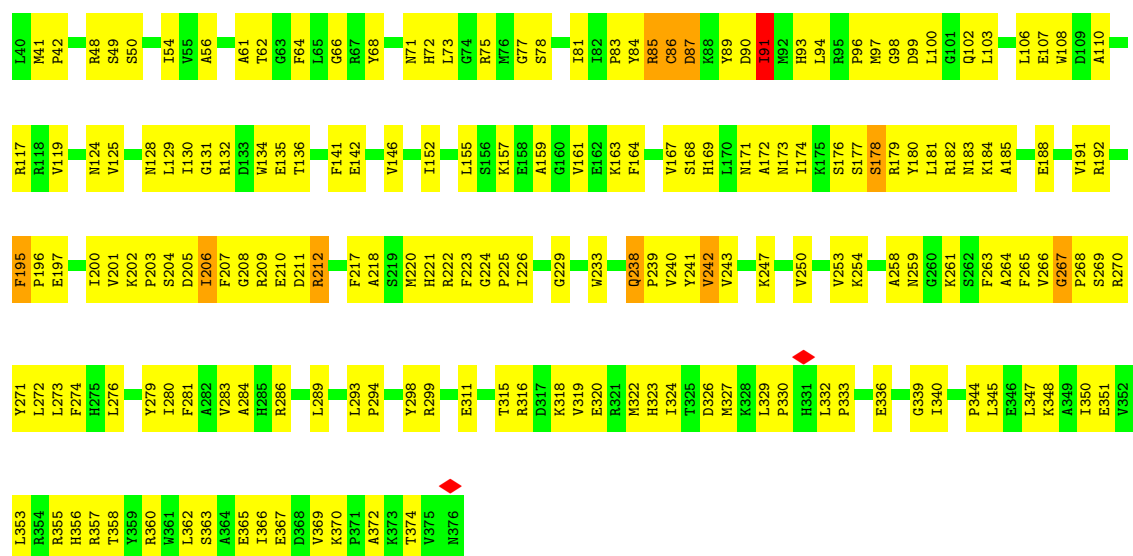
Chain I: 45% 35% 6% 14%

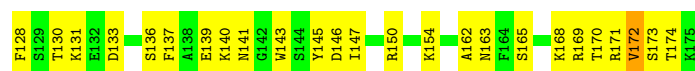




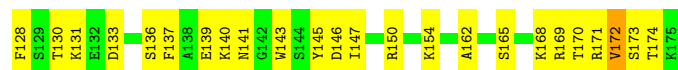
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain BJ: 45% 52%

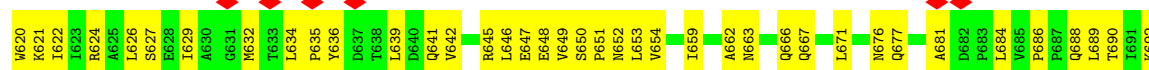
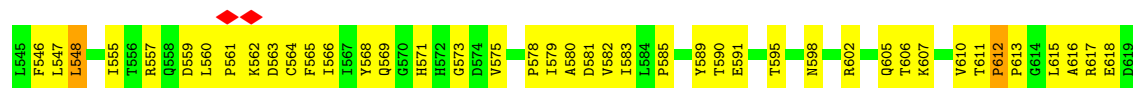
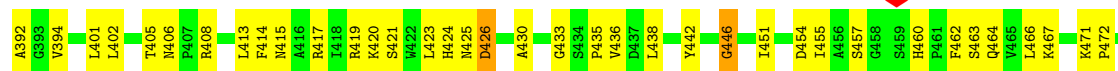
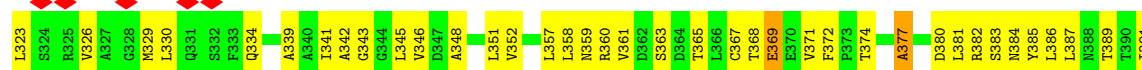


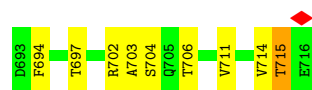


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



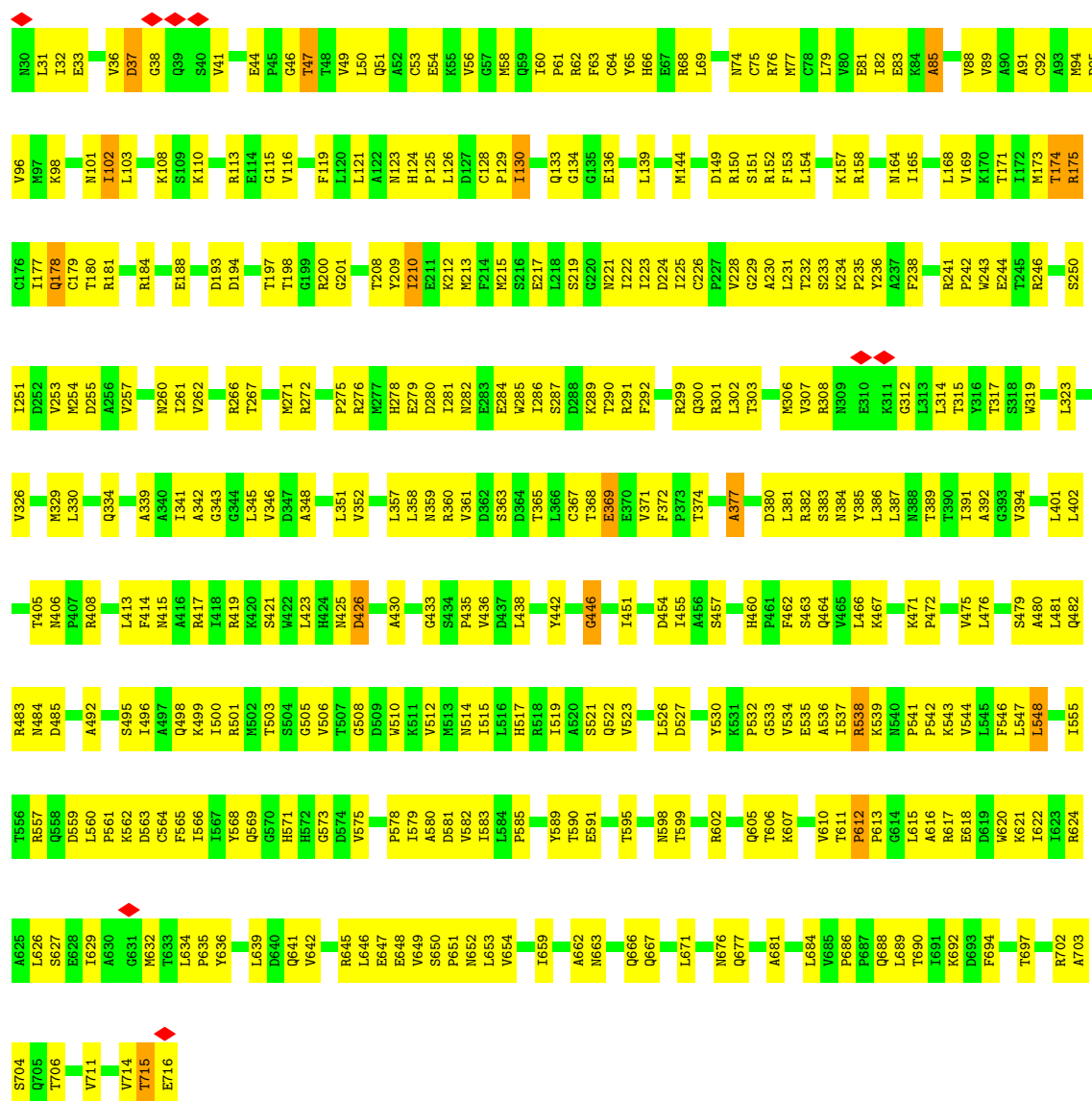
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain BM: 46% 52%



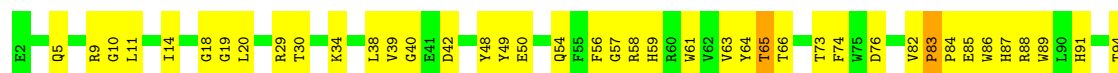
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N: 59% 38%

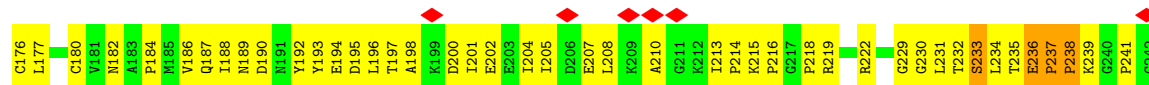
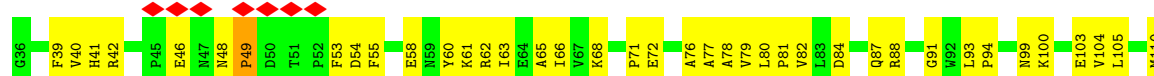




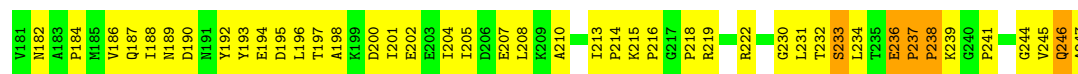
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



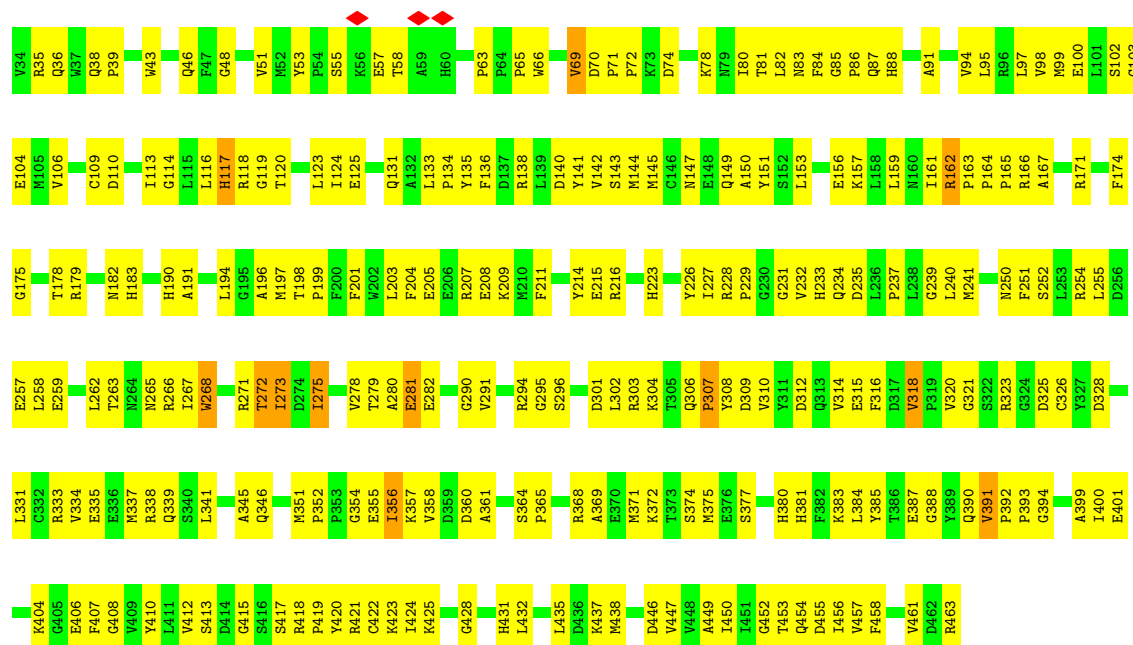
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



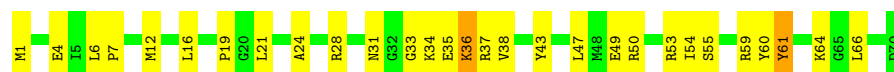




- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

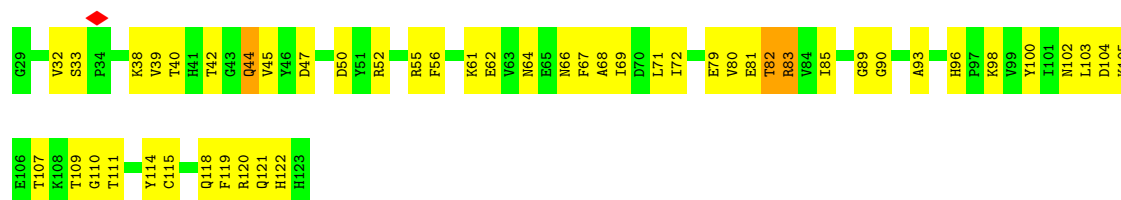


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

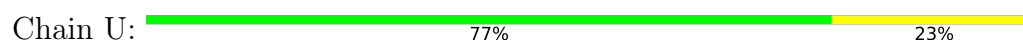


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

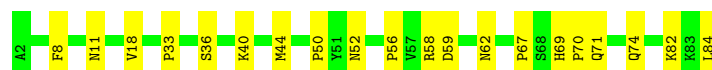
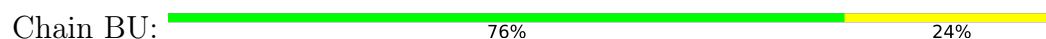




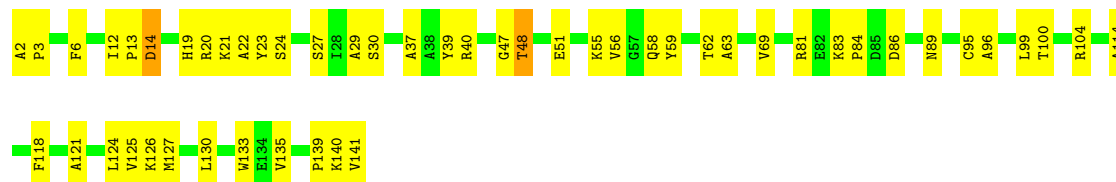
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



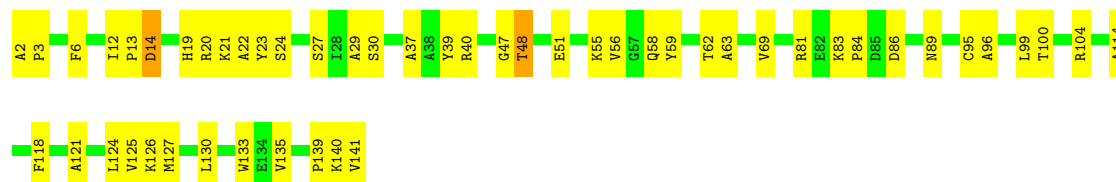
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

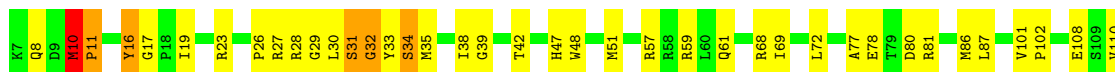


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13





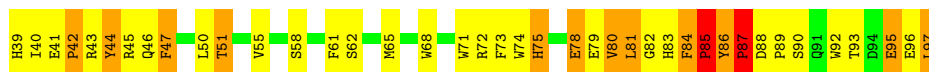
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

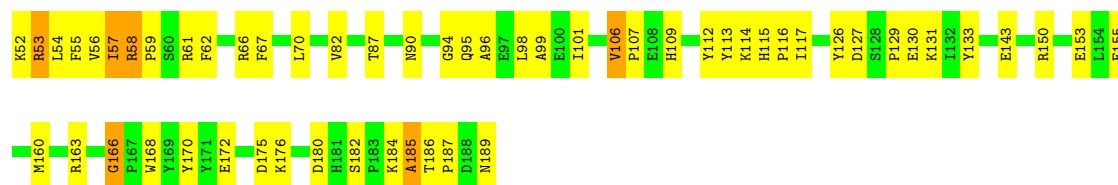


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

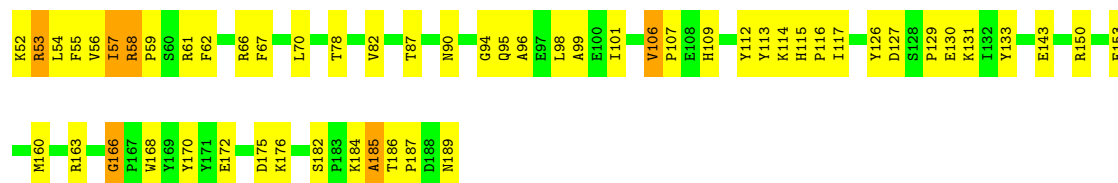


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

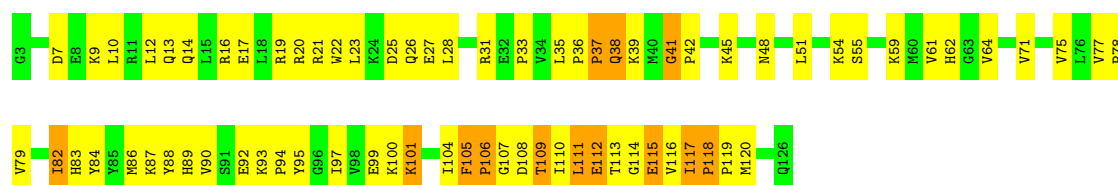




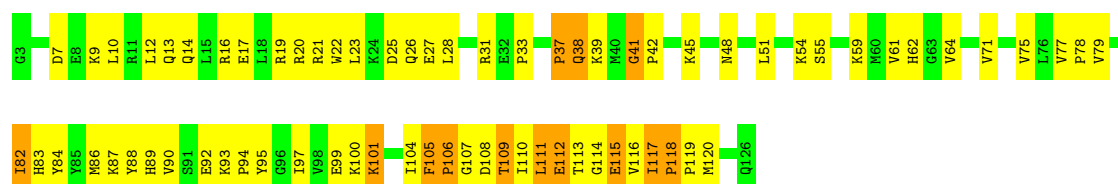
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



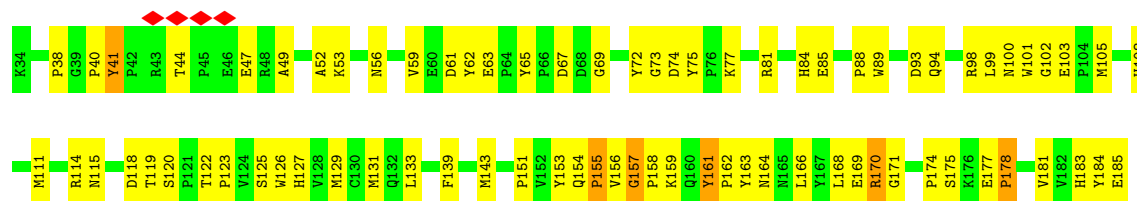
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

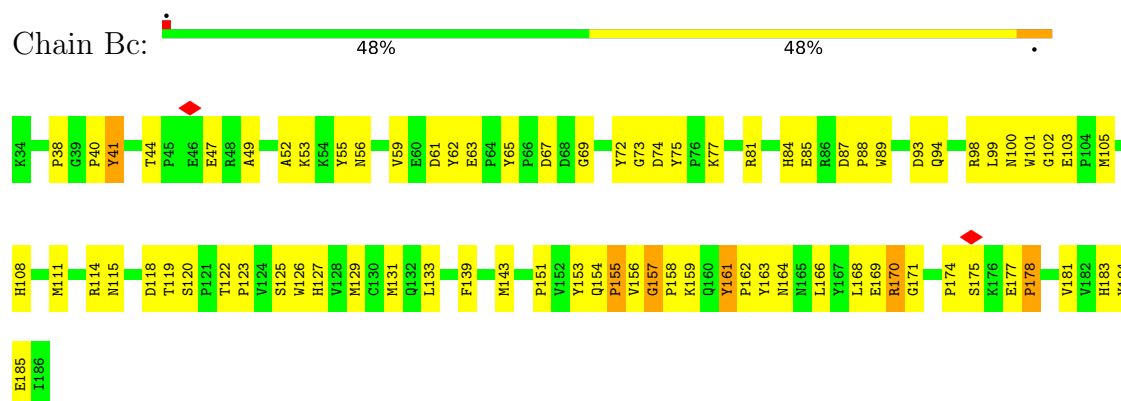


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

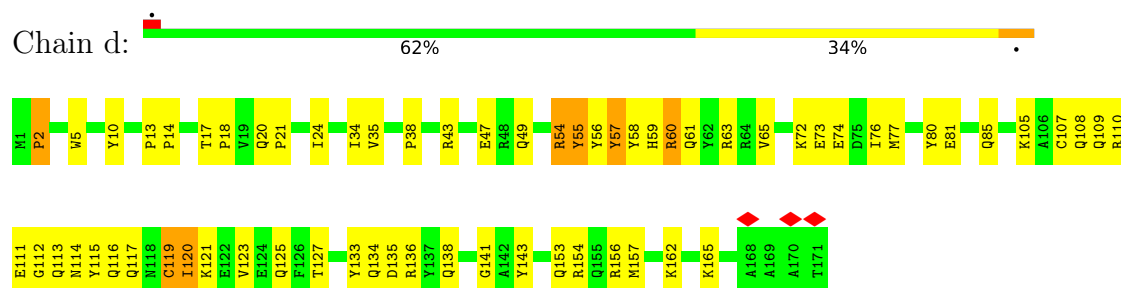


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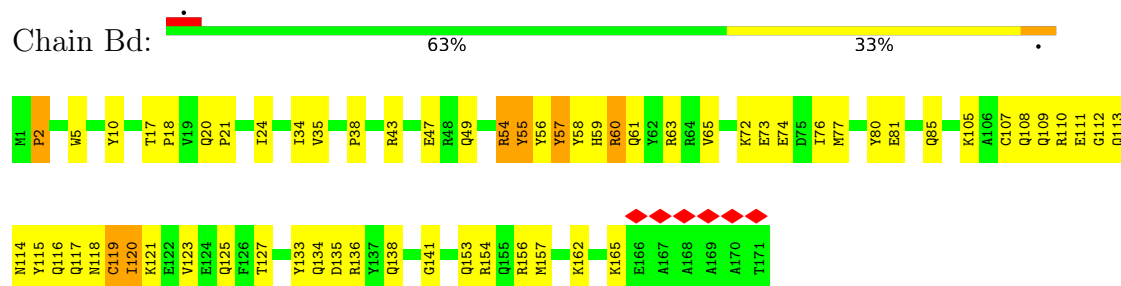
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



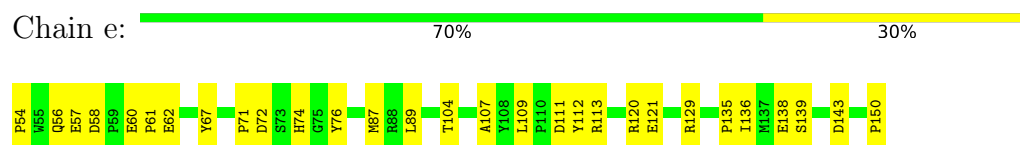
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



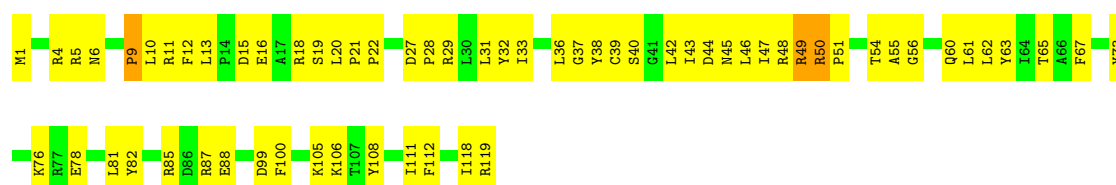
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



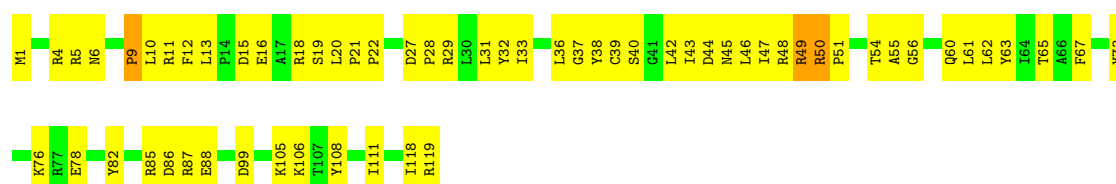
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



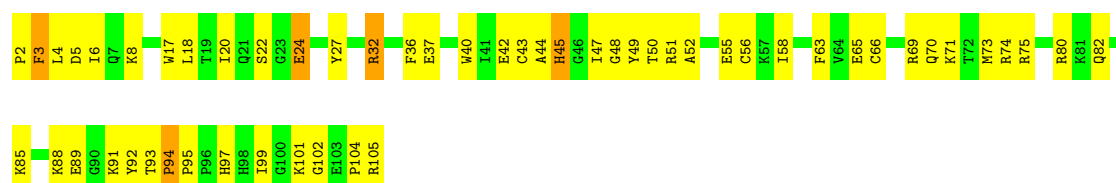
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



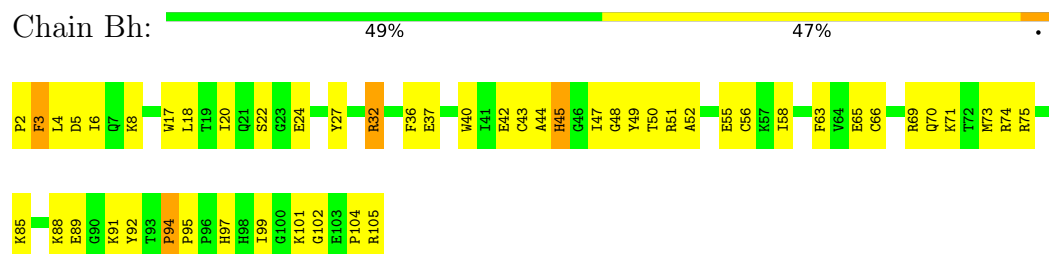
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



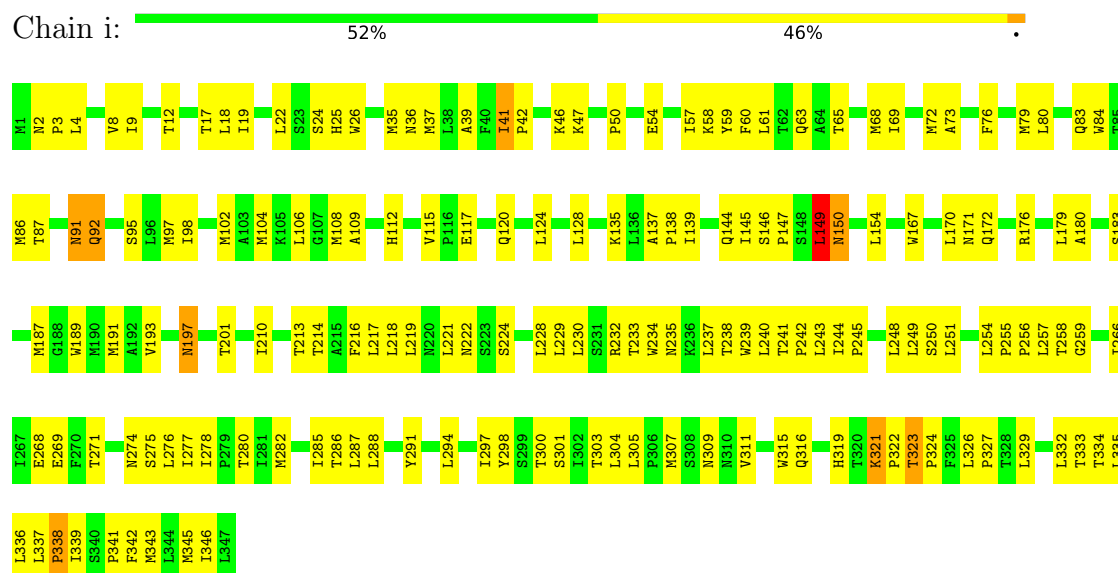
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



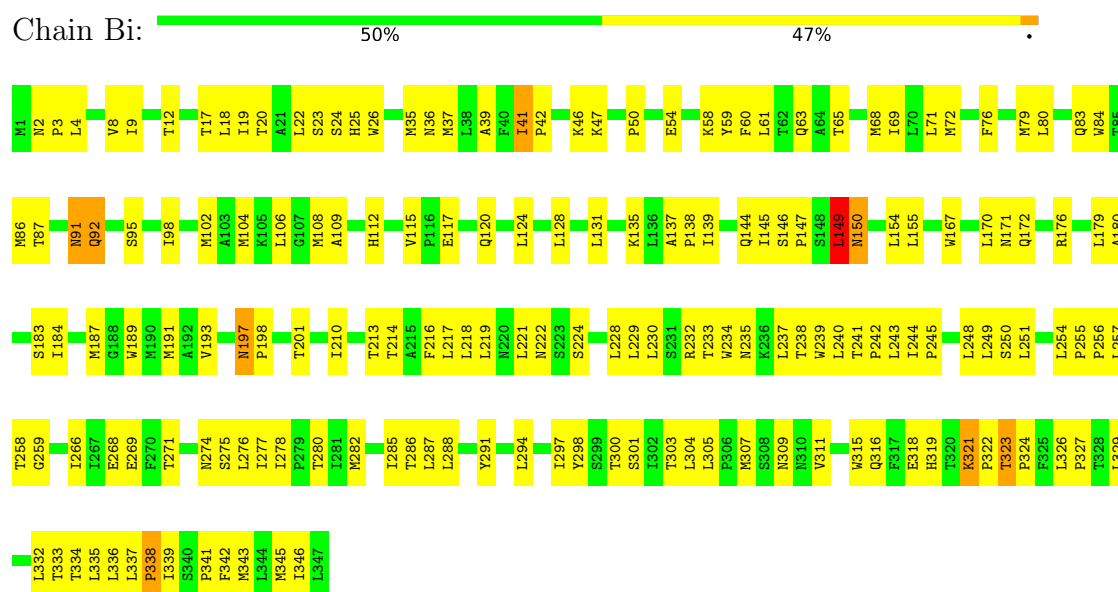
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



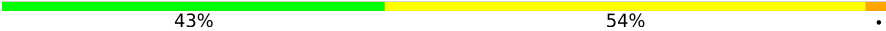
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

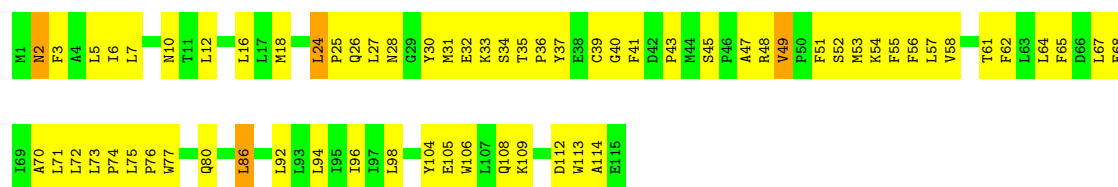


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

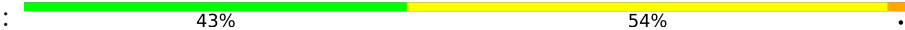


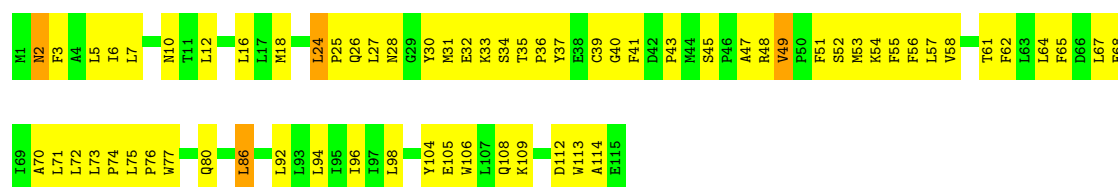
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 

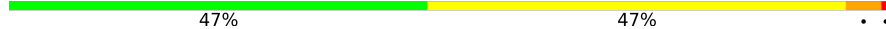


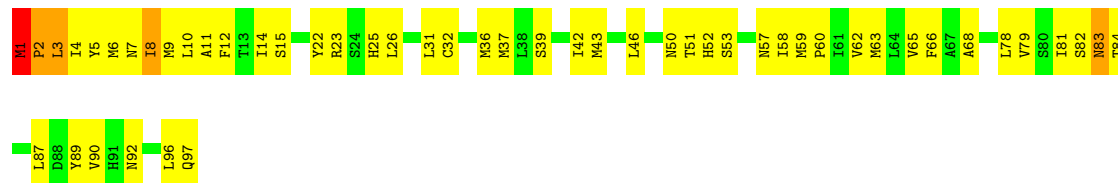
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain Bj: 



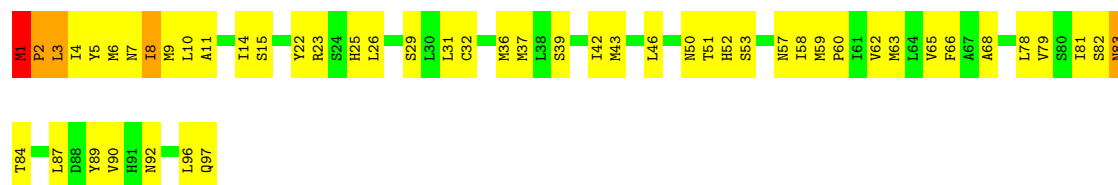
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 



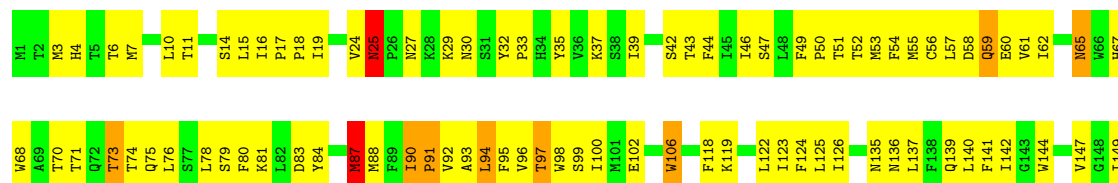
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

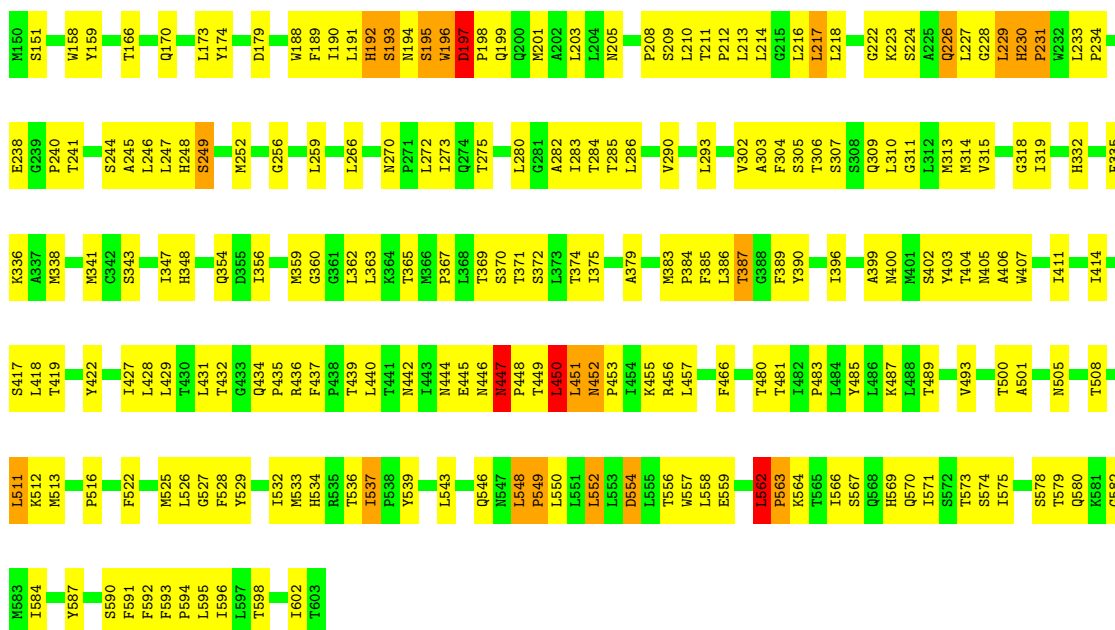
Chain Bk: 



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

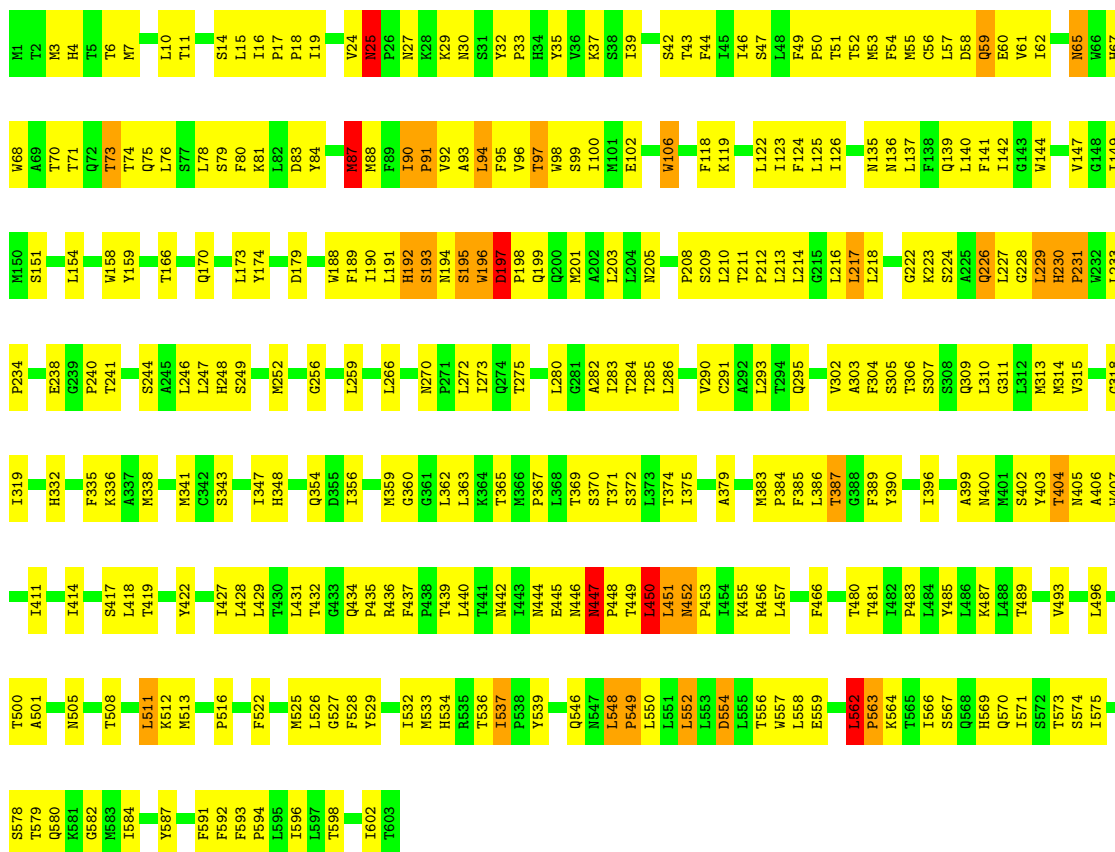
Chain l: 



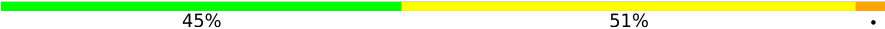


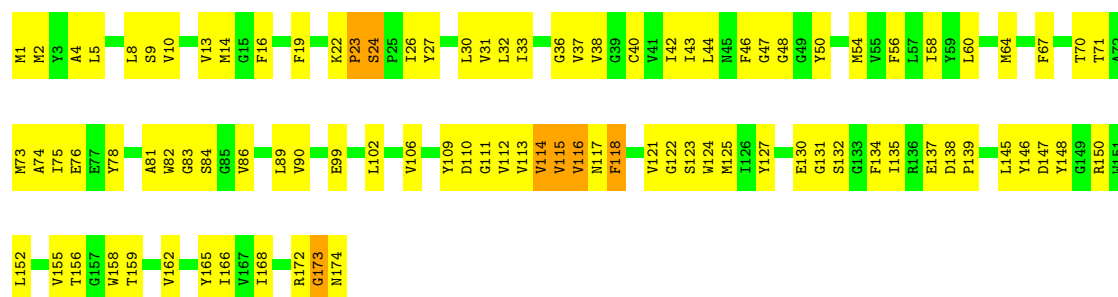
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain B1: 49% 45% 5% •



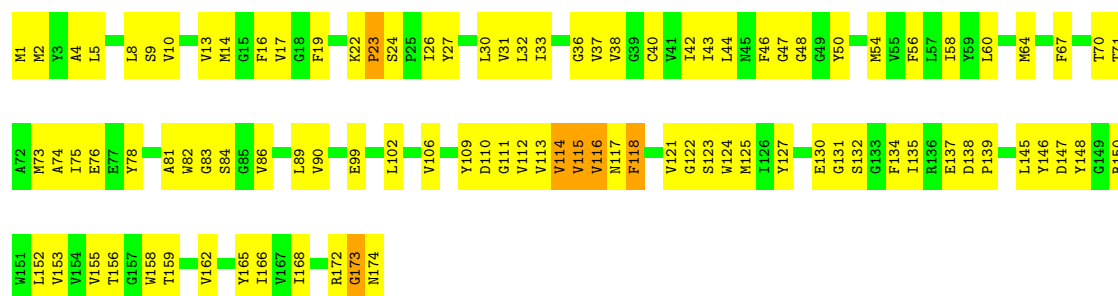
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  45% 51%



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain Bm:  44% 52%



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  59% 39%



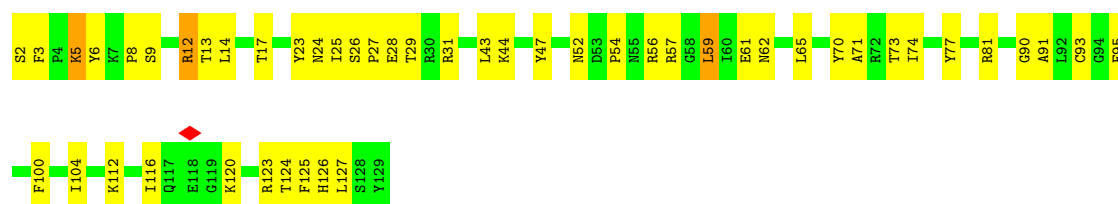
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain Bn:  59% 39%



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  62% 36%



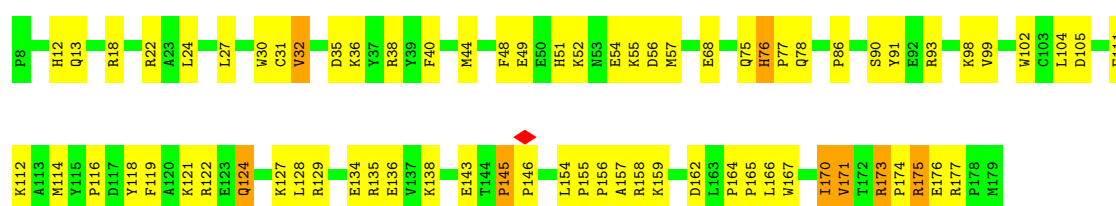
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain Bo: 



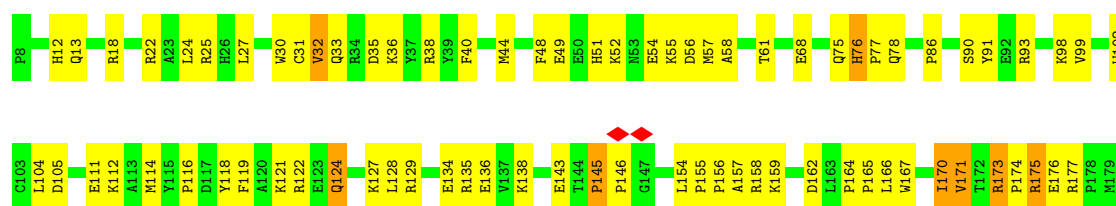
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 



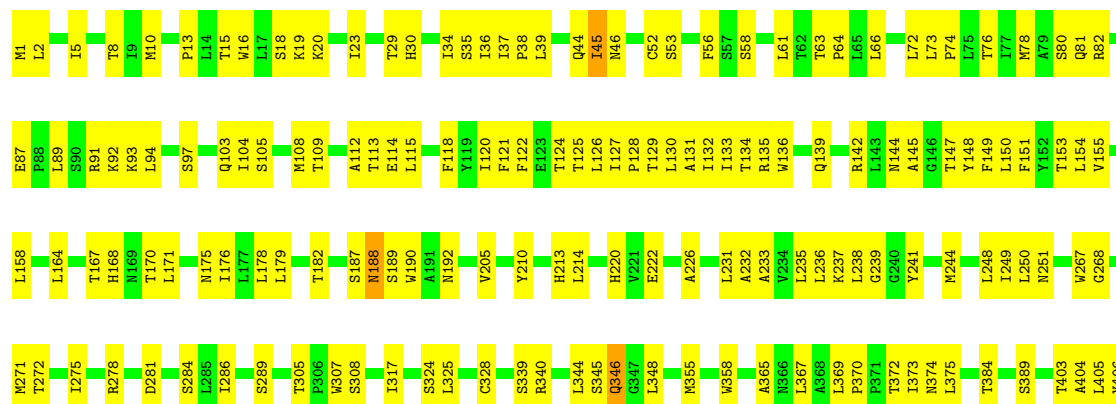
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

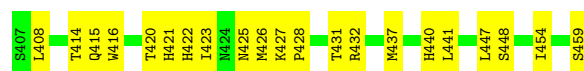
Chain Bp: 



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

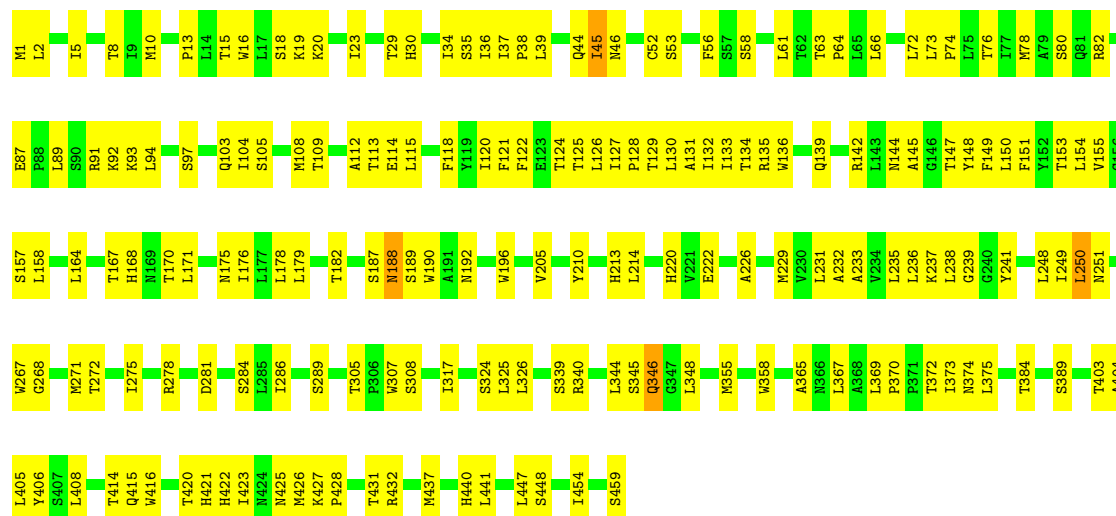
Chain r: 





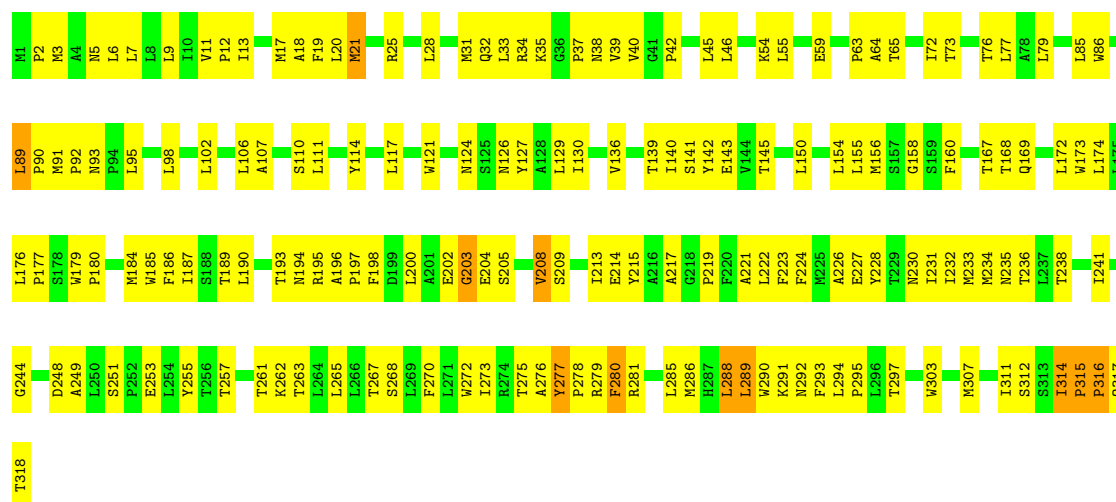
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain Br: 60% 39%



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

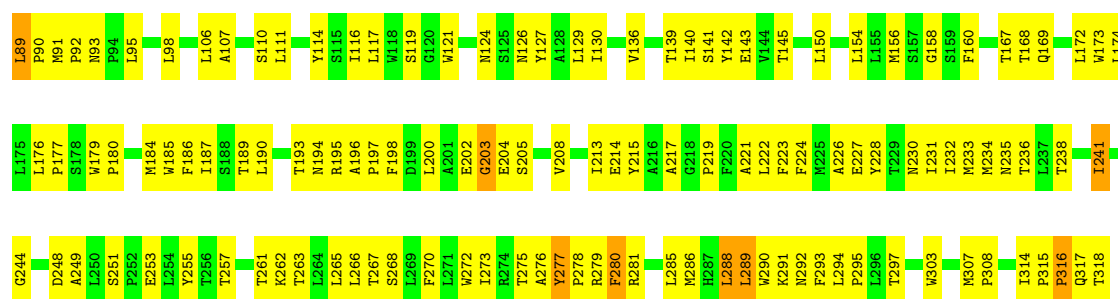
Chain s: 47% 49%



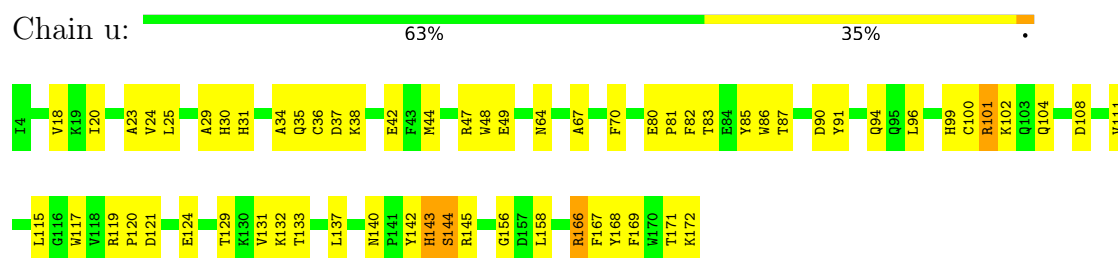
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain Bs: 48% 49%

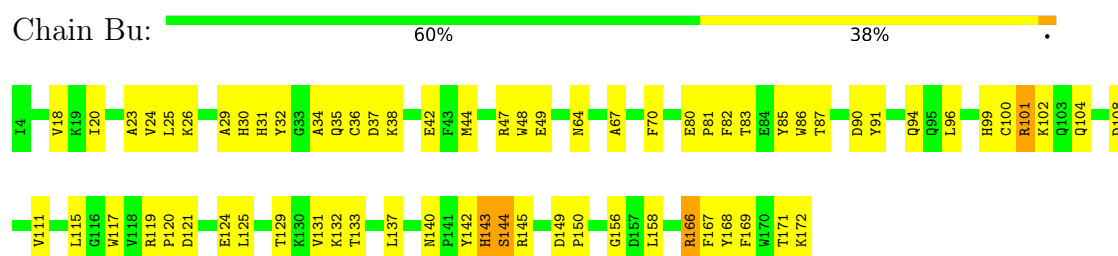




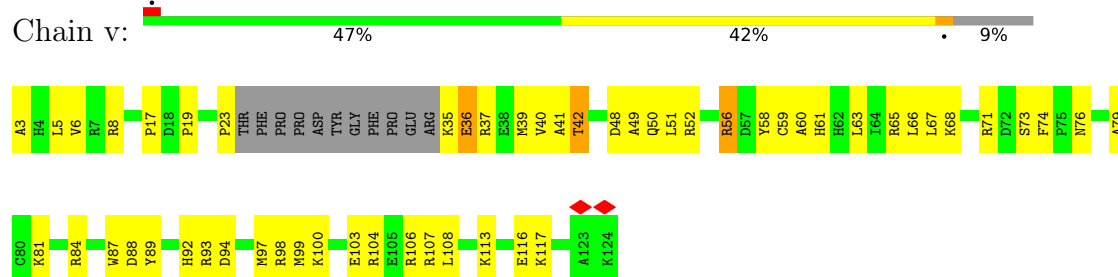
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



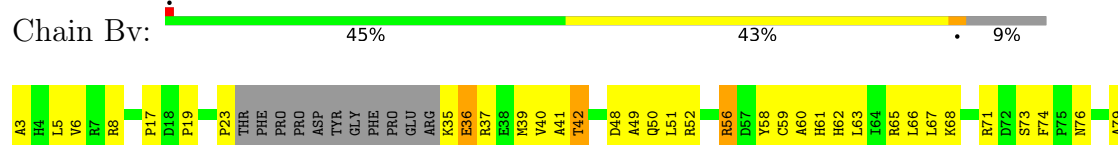
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

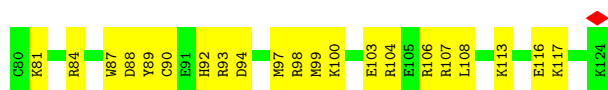


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



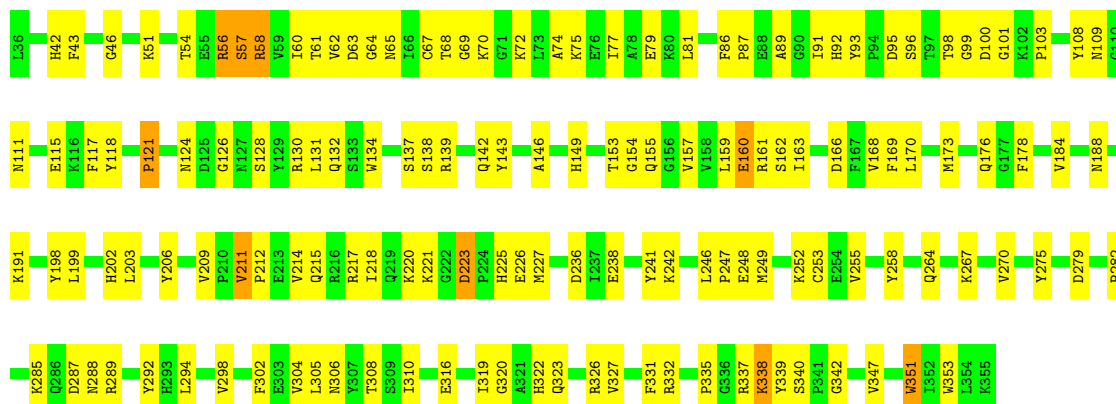
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





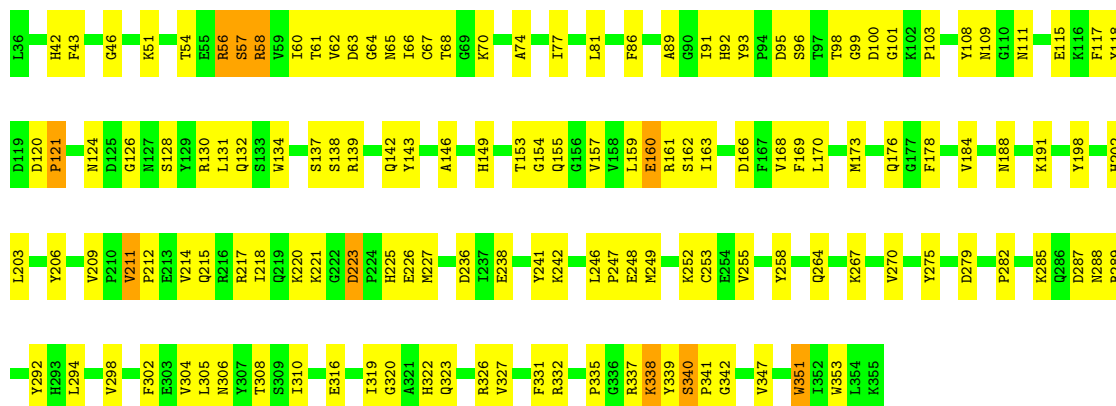
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 55% 42%



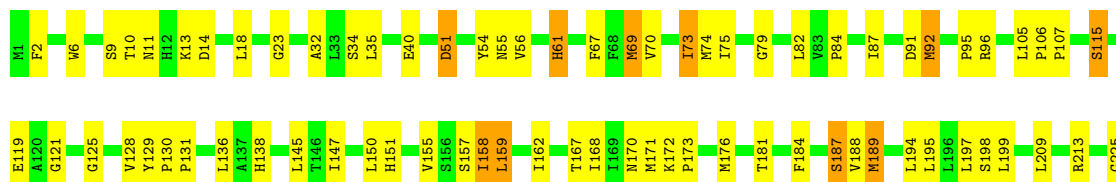
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

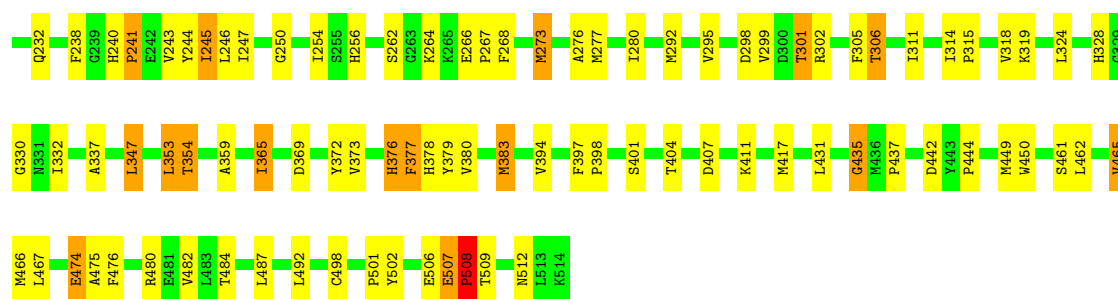
Chain Bw: 56% 41%



- Molecule 45: Cytochrome c oxidase subunit 1

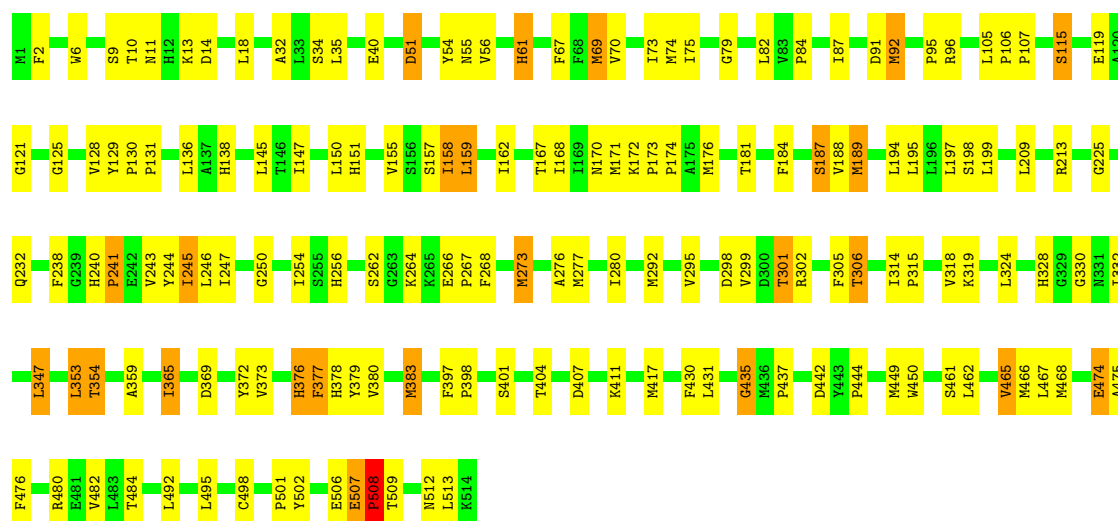
Chain x: 68% 26% 5%





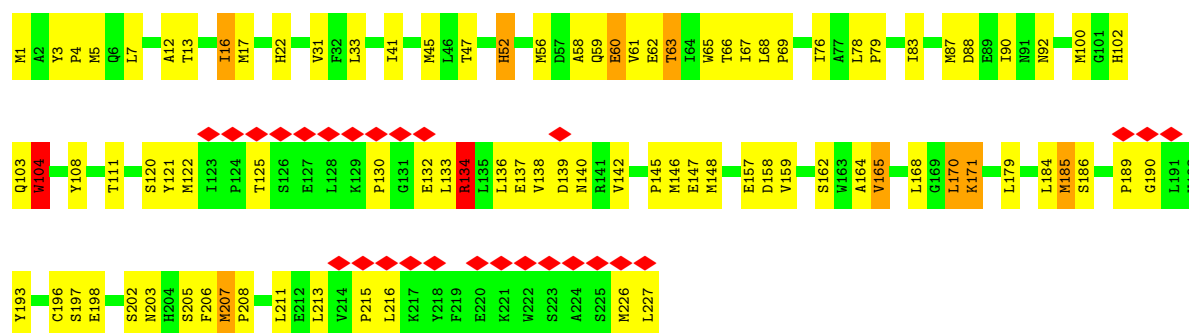
• Molecule 45: Cytochrome c oxidase subunit 1

Chain Bx: 68% 27% 5%



• Molecule 46: Cytochrome c oxidase subunit 2

Chain y: 12% 60% 35%



• Molecule 46: Cytochrome c oxidase subunit 2

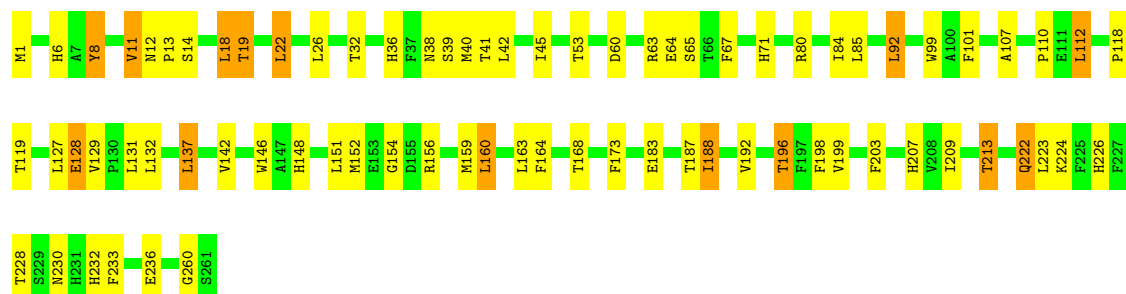
Chain By: 60% 35%





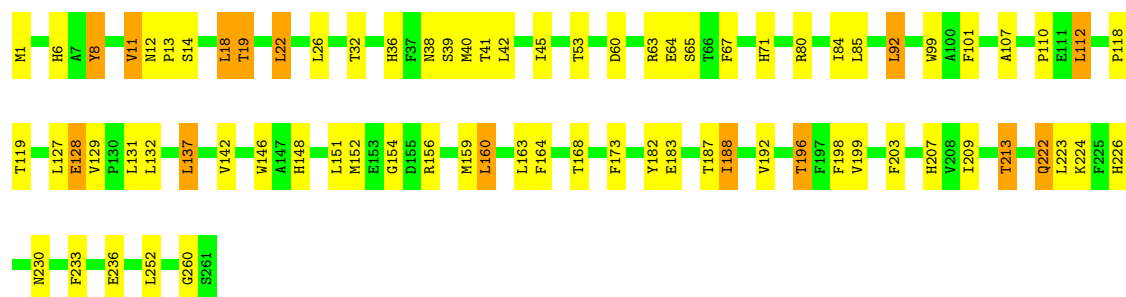
• Molecule 47: Cytochrome c oxidase subunit 3

Chain z: 70% 24% 5%



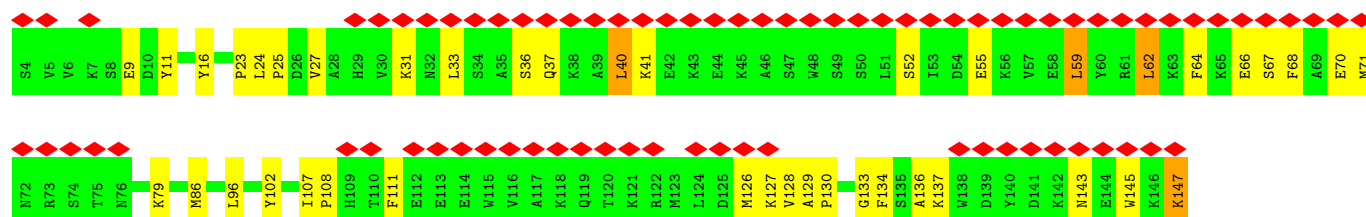
• Molecule 47: Cytochrome c oxidase subunit 3

Chain Bz: 70% 24% 5%



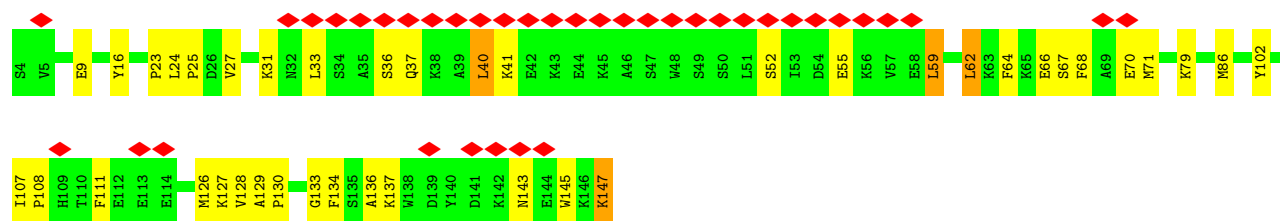
• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain 0: 54% 71% 26%

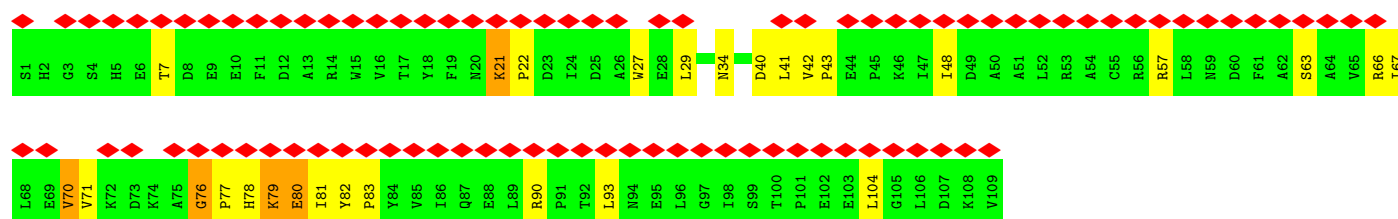
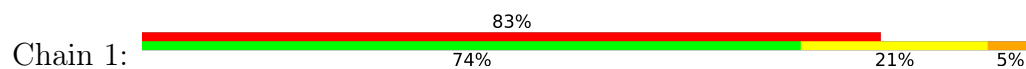


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

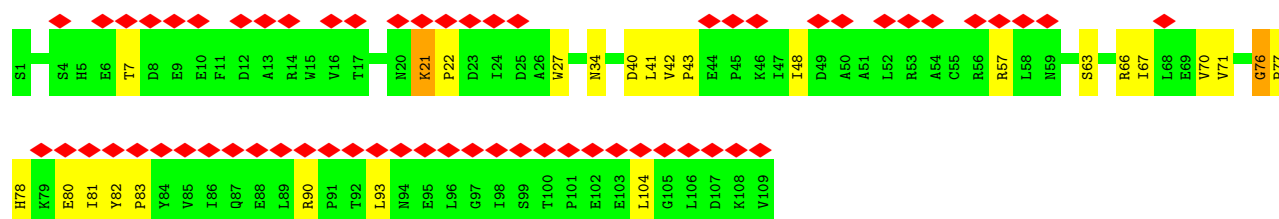
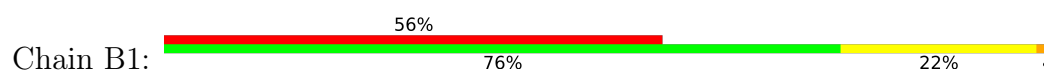
Chain B0: 26% 72% 25%



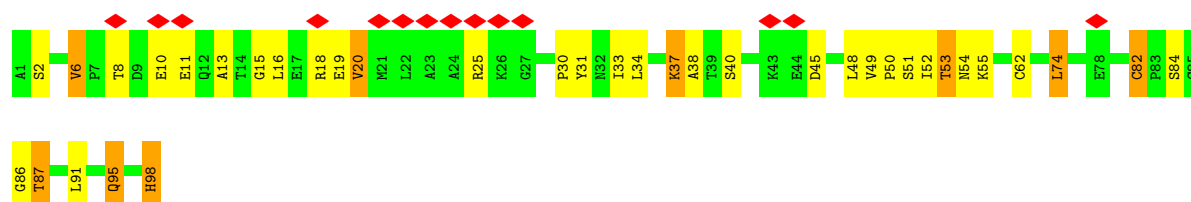
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



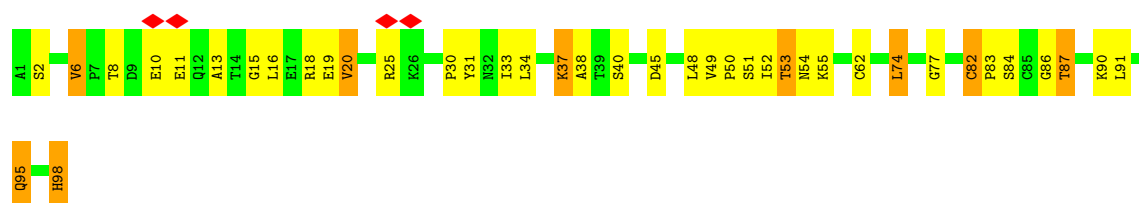
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



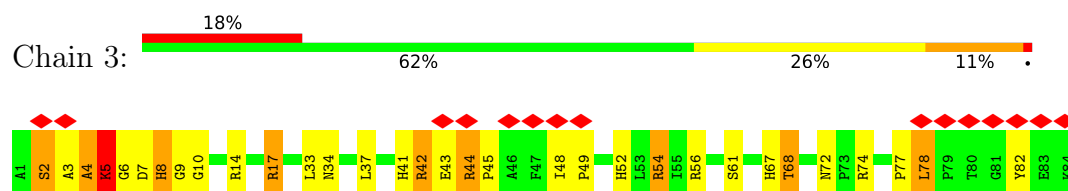
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



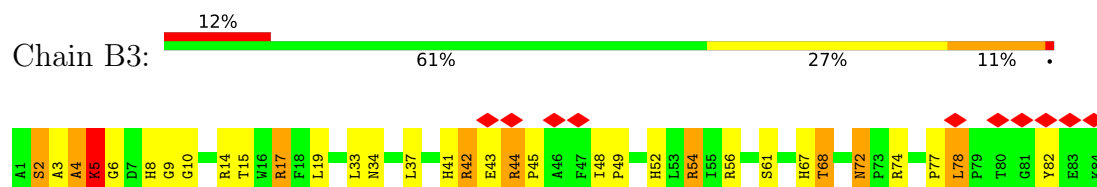
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



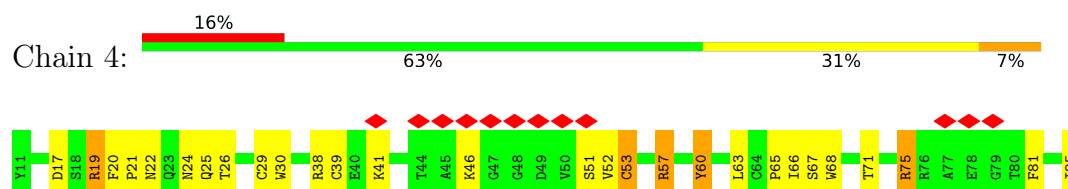
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



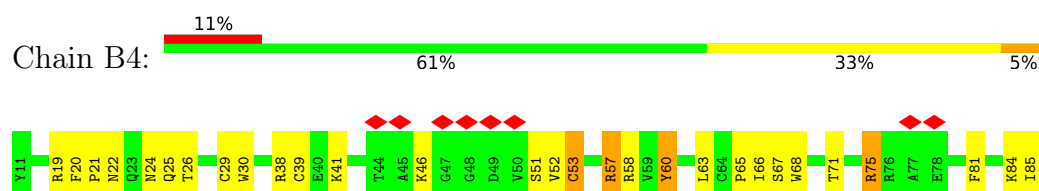
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



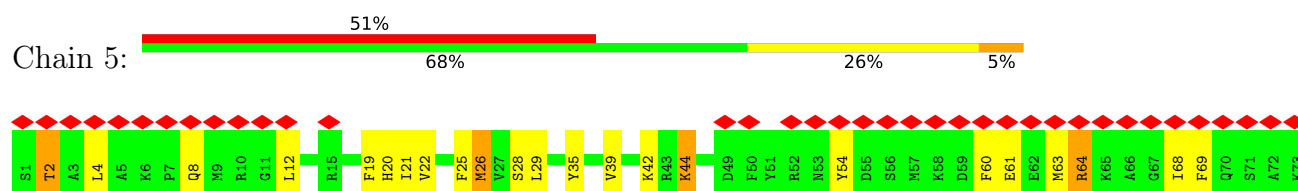
- Molecule 52: Cytochrome c oxidase subunit 6B1



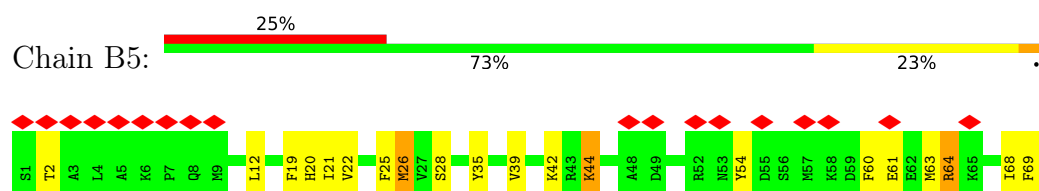
- Molecule 52: Cytochrome c oxidase subunit 6B1



- Molecule 53: Cytochrome c oxidase subunit 6C



- Molecule 53: Cytochrome c oxidase subunit 6C



- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial

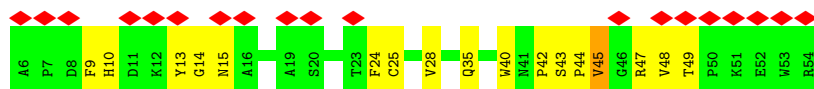




- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



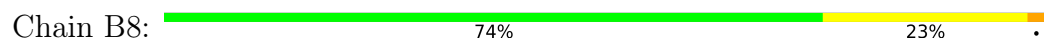
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



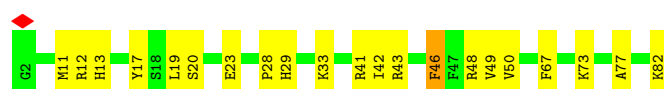
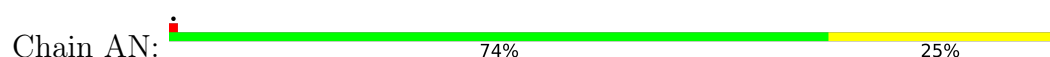
- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 58: Cytochrome b-c1 complex subunit 8



- Molecule 58: Cytochrome b-c1 complex subunit 8



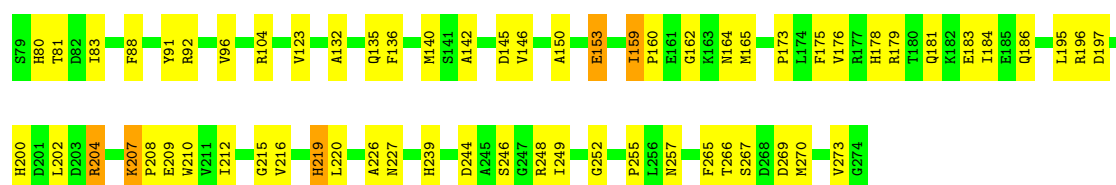
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



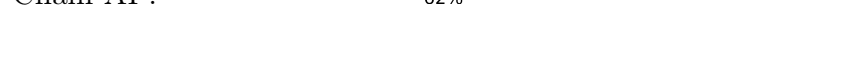
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

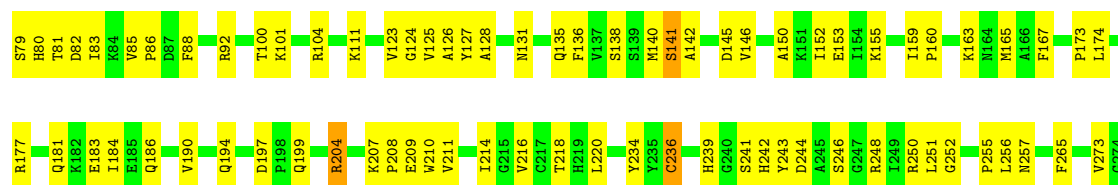


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

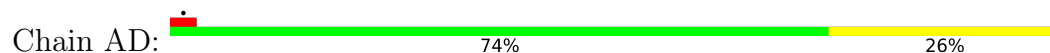


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

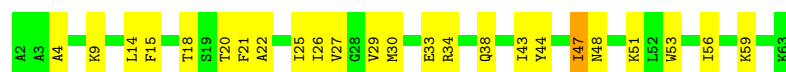




- Molecule 61: Cytochrome b-c1 complex subunit 9



- Molecule 61: Cytochrome b-c1 complex subunit 9



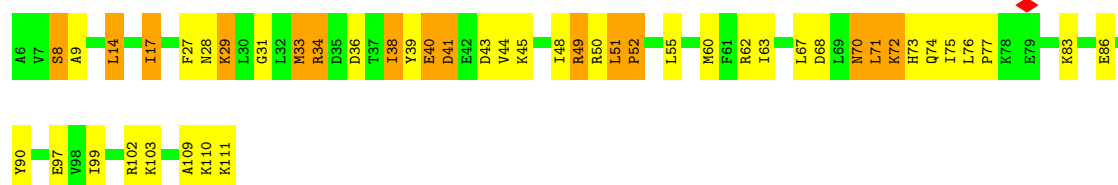
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

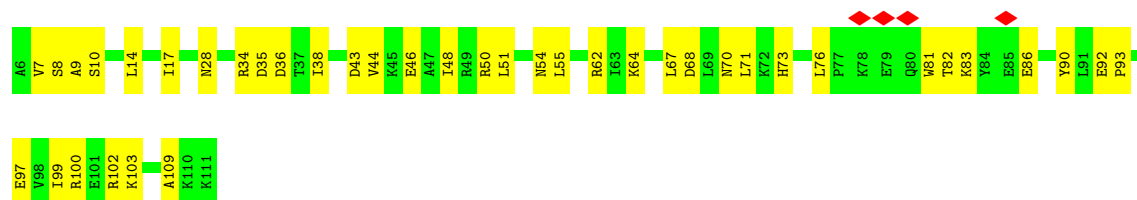


- Molecule 63: Cytochrome b-c1 complex subunit 7



- Molecule 63: Cytochrome b-c1 complex subunit 7





- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AG: 73% 25% .



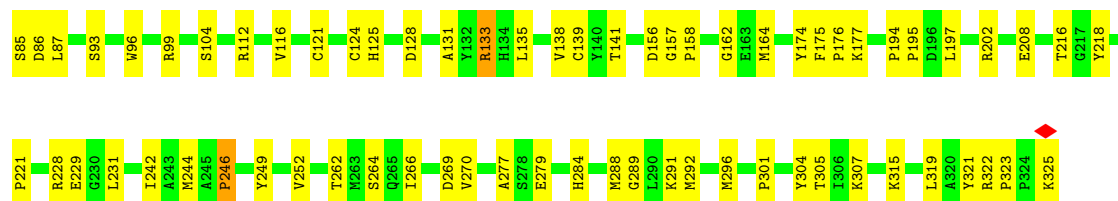
- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AT: 65% 29% 6% .



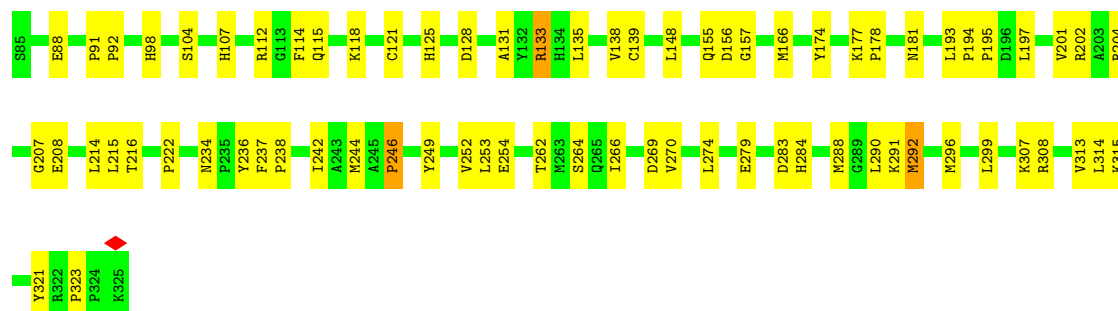
- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AH: 72% 27% .



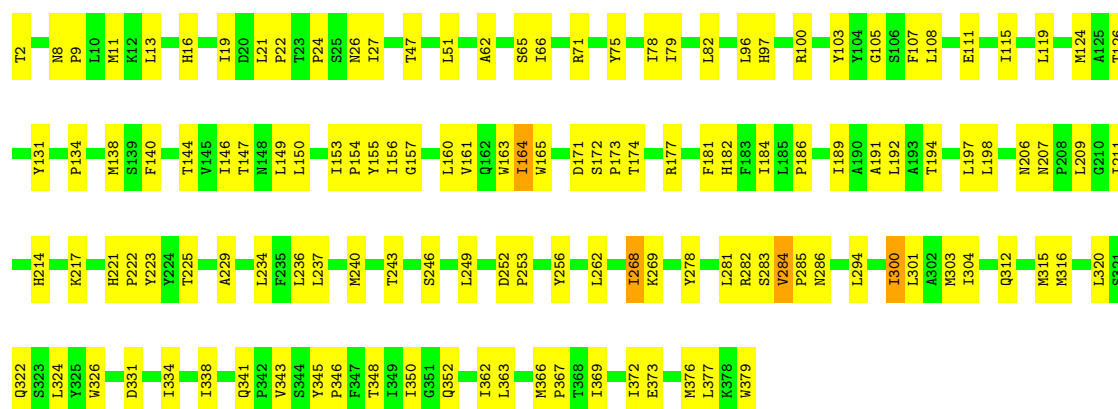
- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AU: 70% 29% .



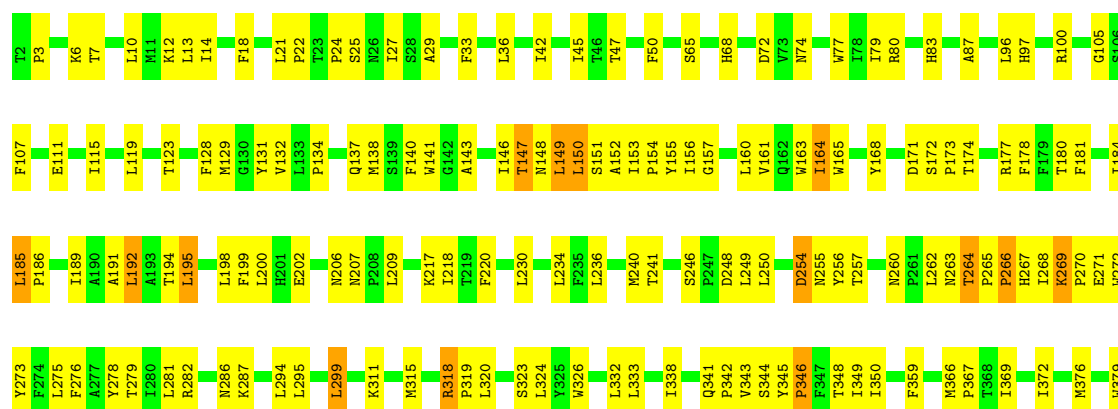
- Molecule 66: Cytochrome b

Chain AJ: 65% 34% .



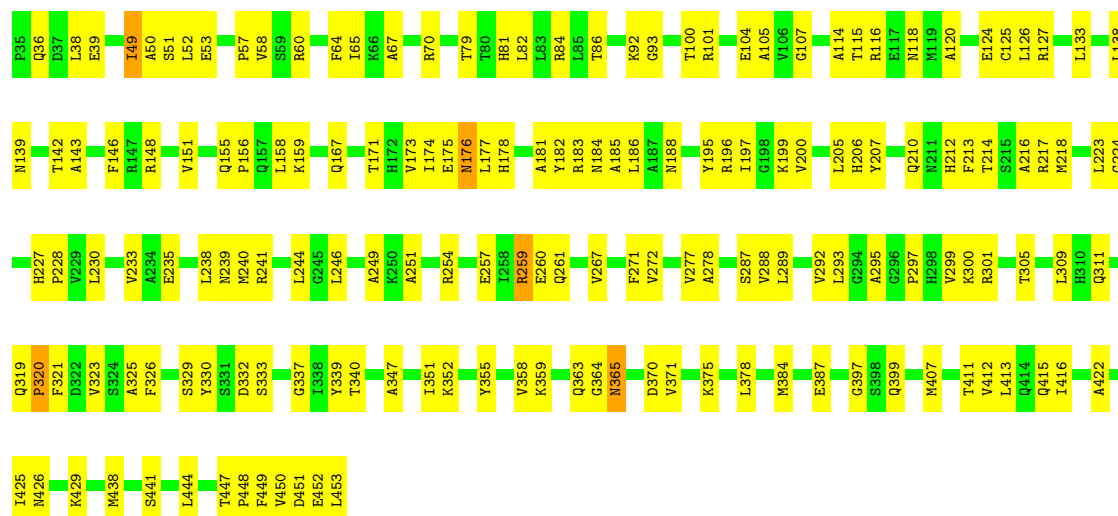
• Molecule 66: Cytochrome b

Chain AV: 59% 38% .



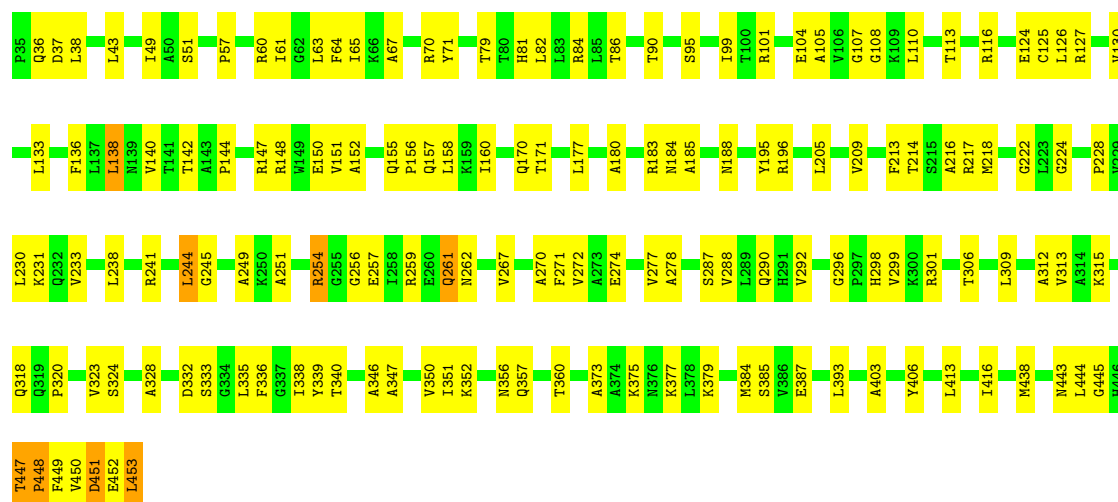
• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AK: 60% 38% .



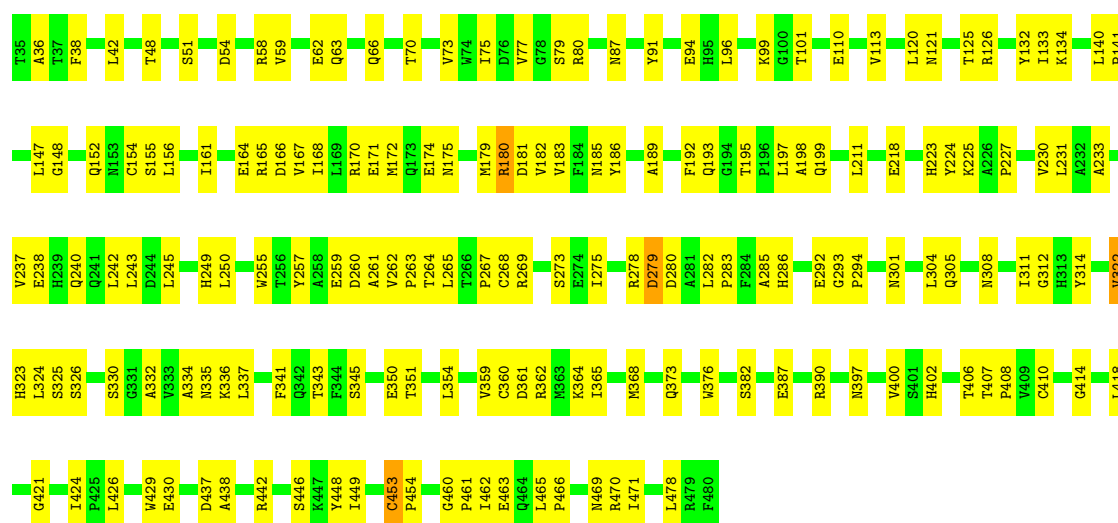
• Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AW:  64% 34% .



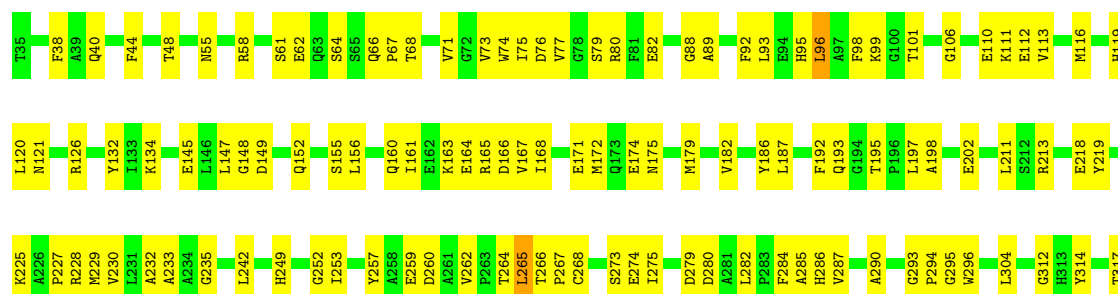
• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AL:  61% 38% .



• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AY:  59% 38% .



Y318	G319	V322	H323	L324	S325	S326	S330	G331	A332	V333	A334	R335	K336	L337	F341	Y348	A349	E350	T351	L354	G355	V359	C360	D361	R362	R363	K364	M368	Q373	M377	S382	E387	R390	G391	K392	R396	N397	V400	T406	T407	P408	D412	I413
G414	R415	S416	L417	L418	T419	Y420	G421	R422	R423	T424	P425	E428	W429	D437	A438	Y448	I449	Y450	D451	Q452	C453	G458	Y459	G460	P461	I462	E463	Q464	L465	P466	D467	Y468	I471	R472	S473	W477	L478	R479	F480				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8600	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 ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0056	Depositor
Map size ($\text{\AA}$)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, HEM, ZN, HEC, PEE, MG, SF4, CU, 8Q1, FMN, PLX, HEA, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/3398	0.87	6/4590 (0.1%)
1	BA	0.39	0/3398	0.87	6/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
2	BB	0.59	0/1452	0.96	9/1964 (0.5%)
3	BC	0.74	0/1280	0.93	3/1732 (0.2%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	BE	0.44	0/993	0.92	3/1335 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	BF	0.37	0/682	0.87	0/922
5	F	0.37	0/682	0.87	0/922
6	BG	0.40	0/684	0.83	0/926
6	BX	0.71	0/698	0.89	0/942
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	BH	0.45	0/941	0.87	2/1275 (0.2%)
7	H	0.45	0/941	0.86	2/1275 (0.2%)
8	BI	0.45	0/788	1.10	7/1066 (0.7%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	BJ	0.44	0/2785	0.91	13/3771 (0.3%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	BK	0.30	0/282	0.74	0/381
10	K	0.30	0/282	0.74	0/381
11	BL	0.42	0/987	0.83	1/1331 (0.1%)
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	BM	0.43	0/5362	0.87	11/7266 (0.2%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	BN	0.44	0/1236	0.91	7/1681 (0.4%)
13	N	0.44	0/1236	0.91	6/1681 (0.4%)
14	BO	0.40	0/1682	0.87	4/2289 (0.2%)
14	O	0.40	0/1682	0.87	4/2289 (0.2%)
15	BP	0.48	0/1780	0.94	5/2424 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BQ	0.55	0/3552	1.01	14/4815 (0.3%)
16	Q	0.55	0/3552	1.01	14/4815 (0.3%)
17	BS	0.81	0/583	0.94	1/785 (0.1%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	BT	0.38	0/755	0.79	0/1017
18	T	0.37	0/755	0.79	0/1017
19	BU	0.69	0/670	1.05	4/920 (0.4%)
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	BV	0.64	0/1065	0.89	4/1450 (0.3%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	BW	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
21	W	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
22	BY	0.61	0/559	1.16	7/763 (0.9%)
22	Y	0.62	0/559	1.16	7/763 (0.9%)
23	BZ	0.56	0/669	0.82	0/899
23	Z	0.56	0/669	0.81	0/899
24	Ba	0.85	0/1209	0.98	6/1639 (0.4%)
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	Bb	0.71	4/1095 (0.4%)	1.08	6/1480 (0.4%)
25	b	0.71	4/1095 (0.4%)	1.08	6/1480 (0.4%)
26	Bc	0.69	0/1287	0.99	10/1761 (0.6%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	Bd	0.79	0/1445	0.97	3/1945 (0.2%)
27	d	0.79	0/1445	0.97	3/1945 (0.2%)
28	Be	0.76	0/835	0.95	2/1134 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	Bf	0.66	0/418	0.87	1/566 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	Bg	0.78	0/1035	0.97	4/1398 (0.3%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	Bh	0.79	0/884	0.98	3/1182 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)
32	Bi	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	Bj	0.76	0/945	1.01	3/1292 (0.2%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	Bk	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	Bl	0.84	6/4840 (0.1%)	1.04	29/6611 (0.4%)
35	l	0.84	6/4840 (0.1%)	1.04	29/6611 (0.4%)
36	Bm	0.82	0/1346	0.99	6/1832 (0.3%)
36	m	0.82	0/1346	0.99	6/1832 (0.3%)
37	Bn	0.63	0/484	0.99	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	n	0.63	0/484	0.99	0/652
38	Bo	0.71	0/1093	0.89	0/1479
38	o	0.71	0/1090	0.89	0/1475
39	Bp	0.70	0/1549	1.01	11/2098 (0.5%)
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	Br	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	Bs	0.83	0/2580	1.09	15/3539 (0.4%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	Bu	0.70	0/1433	0.96	2/1937 (0.1%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	Bv	0.64	0/934	1.00	4/1241 (0.3%)
43	v	0.64	0/934	1.00	4/1241 (0.3%)
44	Bw	0.54	1/2533 (0.0%)	0.91	7/3440 (0.2%)
44	w	0.54	1/2533 (0.0%)	0.91	9/3440 (0.3%)
45	Bx	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
45	x	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
46	By	0.78	0/1868	1.12	11/2544 (0.4%)
46	y	0.78	0/1868	1.12	11/2544 (0.4%)
47	Bz	0.75	0/2211	1.02	7/3023 (0.2%)
47	z	0.75	0/2211	1.02	7/3023 (0.2%)
48	0	0.68	0/1229	0.96	3/1658 (0.2%)
48	B0	0.68	0/1229	0.96	3/1658 (0.2%)
49	1	0.64	0/898	1.03	6/1218 (0.5%)
49	B1	0.64	0/898	1.02	6/1218 (0.5%)
50	2	0.72	0/765	1.13	3/1038 (0.3%)
50	B2	0.72	0/765	1.14	3/1038 (0.3%)
51	3	0.69	0/699	1.10	6/950 (0.6%)
51	B3	0.69	0/699	1.10	6/950 (0.6%)
52	4	0.67	0/648	1.17	5/877 (0.6%)
52	B4	0.67	0/648	1.17	5/877 (0.6%)
53	5	0.71	0/611	0.94	2/810 (0.2%)
53	B5	0.71	0/611	0.94	2/810 (0.2%)
54	6	0.70	0/451	1.04	3/610 (0.5%)
54	B6	0.70	0/451	1.04	3/610 (0.5%)
55	7	0.76	0/398	1.01	1/546 (0.2%)
55	B7	0.76	0/398	1.01	1/546 (0.2%)
56	8	0.78	0/399	0.97	2/534 (0.4%)
56	B8	0.78	0/399	0.97	2/534 (0.4%)
57	9	0.69	0/345	0.99	1/470 (0.2%)
57	B9	0.69	0/345	0.99	1/470 (0.2%)
58	AA	0.44	0/715	0.83	1/964 (0.1%)
58	AN	0.37	0/707	0.86	2/953 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
59	AB	0.37	0/421	0.91	0/574
59	AO	0.40	0/417	0.98	0/569
60	AC	0.32	0/1554	0.81	6/2104 (0.3%)
60	AP	0.30	0/1554	0.84	6/2104 (0.3%)
61	AD	0.30	0/521	0.63	0/699
61	AQ	0.31	0/521	0.68	0/699
62	AE	0.48	1/587 (0.2%)	0.84	2/789 (0.3%)
62	AR	0.37	0/587	0.77	2/789 (0.3%)
63	AF	0.61	2/942 (0.2%)	0.85	3/1263 (0.2%)
63	AS	0.34	0/942	0.66	0/1263
64	AG	0.38	0/442	0.82	4/608 (0.7%)
64	AT	0.40	0/442	0.80	1/608 (0.2%)
65	AH	0.35	0/1983	0.84	6/2691 (0.2%)
65	AU	0.35	0/1983	0.79	4/2691 (0.1%)
66	AJ	0.42	2/3108 (0.1%)	0.82	7/4254 (0.2%)
66	AV	0.46	4/3108 (0.1%)	0.86	11/4254 (0.3%)
67	AK	0.37	0/3217	0.79	0/4361
67	AW	0.39	2/3220 (0.1%)	0.81	4/4365 (0.1%)
68	AL	0.37	0/3514	0.82	8/4769 (0.2%)
68	AY	0.40	2/3499 (0.1%)	0.83	6/4750 (0.1%)
All	All	0.65	57/197905 (0.0%)	0.96	719/268649 (0.3%)

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
44	Bw	0	1
44	w	0	1
All	All	0	2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.62	1.50	1.54
32	Bi	278	ILE	CA-CB	-7.56	1.50	1.54
45	x	61	HIS	CG-CD2	7.46	1.44	1.35
45	Bx	61	HIS	CG-CD2	7.45	1.44	1.35
45	Bx	378	HIS	ND1-CE1	7.40	1.40	1.32
45	x	378	HIS	ND1-CE1	7.34	1.39	1.32
62	AE	28	ASP	C-N	7.20	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	x	378	HIS	CE1-NE2	-6.53	1.26	1.32
45	Bx	378	HIS	CE1-NE2	-6.53	1.26	1.32
25	Bb	117	ILE	C-N	6.49	1.41	1.33
25	b	117	ILE	C-N	6.45	1.41	1.33
45	x	69	MET	SD-CE	-6.26	1.64	1.79
45	Bx	69	MET	SD-CE	-6.24	1.64	1.79
21	W	117	VAL	CA-CB	-6.06	1.49	1.54
21	BW	117	VAL	CA-CB	-5.97	1.49	1.54
40	Br	37	ILE	CA-CB	-5.93	1.51	1.54
40	r	37	ILE	CA-CB	-5.84	1.51	1.54
25	Bb	105	PHE	C-N	5.84	1.41	1.33
25	b	105	PHE	C-N	5.79	1.41	1.33
63	AF	51	LEU	C-N	5.79	1.41	1.33
44	w	211	VAL	CA-CB	5.74	1.57	1.54
45	Bx	61	HIS	ND1-CE1	5.74	1.38	1.32
45	x	61	HIS	ND1-CE1	5.71	1.38	1.32
67	AW	447	THR	C-N	5.66	1.41	1.33
68	AY	424	ILE	C-N	5.64	1.41	1.33
44	Bw	211	VAL	CA-CB	5.63	1.57	1.54
45	x	376	HIS	ND1-CE1	5.56	1.38	1.32
66	AJ	153	ILE	C-N	5.55	1.40	1.34
45	Bx	376	HIS	ND1-CE1	5.54	1.38	1.32
67	AW	448	PRO	N-CD	5.35	1.55	1.47
45	x	378	HIS	CG-CD2	5.33	1.41	1.35
45	Bx	378	HIS	CG-CD2	5.32	1.41	1.35
66	AJ	154	PRO	N-CD	5.31	1.55	1.47
66	AV	154	PRO	N-CD	5.30	1.55	1.47
25	b	118	PRO	N-CD	5.28	1.55	1.47
34	k	2	PRO	N-CD	5.28	1.55	1.47
34	Bk	2	PRO	N-CD	5.26	1.55	1.47
25	Bb	118	PRO	N-CD	5.21	1.55	1.47
66	AV	153	ILE	C-N	5.20	1.40	1.34
35	Bl	230	HIS	C-N	5.19	1.41	1.34
68	AY	425	PRO	N-CD	5.19	1.55	1.47
35	l	230	HIS	C-N	5.17	1.41	1.34
35	Bl	90	ILE	C-N	5.16	1.41	1.34
35	Bl	552	LEU	CA-C	-5.15	1.50	1.52
35	l	90	ILE	C-N	5.12	1.41	1.34
66	AV	345	TYR	C-N	5.12	1.41	1.34
35	l	91	PRO	N-CD	5.11	1.54	1.47
66	AV	346	PRO	N-CD	5.08	1.54	1.47
35	l	552	LEU	CA-C	-5.07	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Bl	231	PRO	N-CD	5.06	1.54	1.47
35	Bl	91	PRO	N-CD	5.06	1.54	1.47
63	AF	52	PRO	N-CD	5.05	1.54	1.47
35	l	231	PRO	N-CD	5.04	1.54	1.47
25	b	106	PRO	N-CD	5.03	1.54	1.47
35	l	197	ASP	C-N	5.02	1.40	1.34
25	Bb	106	PRO	N-CD	5.01	1.54	1.47
35	Bl	197	ASP	C-N	5.00	1.40	1.34

All (719) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	BW	31	SER	N-CA-C	-16.81	92.08	112.59
21	W	31	SER	N-CA-C	-16.81	92.09	112.59
21	W	10	MET	CA-C-N	-10.86	109.20	120.38
21	W	10	MET	C-N-CA	-10.86	109.20	120.38
21	BW	10	MET	CA-C-N	-10.85	109.21	120.38
21	BW	10	MET	C-N-CA	-10.85	109.21	120.38
8	I	38	PRO	CA-C-N	10.37	130.69	119.28
8	I	38	PRO	C-N-CA	10.37	130.69	119.28
8	BI	38	PRO	CA-C-N	10.35	130.66	119.28
8	BI	38	PRO	C-N-CA	10.35	130.66	119.28
45	Bx	376	HIS	ND1-CE1-NE2	10.32	118.72	108.40
45	x	376	HIS	ND1-CE1-NE2	10.29	118.69	108.40
16	BQ	162	ARG	CA-C-N	10.25	127.04	119.66
16	BQ	162	ARG	C-N-CA	10.25	127.04	119.66
16	Q	162	ARG	CA-C-N	10.23	127.03	119.66
16	Q	162	ARG	C-N-CA	10.23	127.03	119.66
16	Q	365	PRO	CA-C-N	9.99	129.94	119.85
16	Q	365	PRO	C-N-CA	9.99	129.94	119.85
16	BQ	365	PRO	CA-C-N	9.99	129.94	119.85
16	BQ	365	PRO	C-N-CA	9.99	129.94	119.85
41	s	314	ILE	CA-C-N	9.82	126.83	119.66
41	s	314	ILE	C-N-CA	9.82	126.83	119.66
41	Bs	314	ILE	CA-C-N	9.81	126.82	119.66
41	Bs	314	ILE	C-N-CA	9.81	126.82	119.66
4	E	18	LYS	CA-C-N	9.26	129.20	119.85
4	E	18	LYS	C-N-CA	9.26	129.20	119.85
4	BE	18	LYS	CA-C-N	9.21	129.27	119.78
4	BE	18	LYS	C-N-CA	9.21	129.27	119.78
52	4	52	VAL	N-CA-C	8.96	121.25	108.17
52	B4	52	VAL	N-CA-C	8.95	121.24	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	4	81	PHE	CA-C-N	8.80	128.45	119.56
52	4	81	PHE	C-N-CA	8.80	128.45	119.56
52	B4	81	PHE	CA-C-N	8.79	128.44	119.56
52	B4	81	PHE	C-N-CA	8.79	128.44	119.56
3	BC	60	GLY	N-CA-C	8.56	122.84	112.49
66	AV	264	THR	CA-C-N	8.55	125.90	119.66
66	AV	264	THR	C-N-CA	8.55	125.90	119.66
3	C	60	GLY	N-CA-C	8.52	122.80	112.49
32	Bi	323	THR	CA-C-N	8.51	147.41	127.00
32	Bi	323	THR	C-N-CA	8.51	147.41	127.00
32	i	323	THR	CA-C-N	8.50	147.39	127.00
32	i	323	THR	C-N-CA	8.50	147.39	127.00
22	BY	86	TYR	C-N-CD	8.48	139.25	120.60
22	Y	86	TYR	C-N-CD	8.45	139.18	120.60
22	BY	92	TRP	N-CA-C	-8.40	92.12	107.75
22	Y	92	TRP	N-CA-C	-8.39	92.15	107.75
22	Y	47	PHE	CA-C-N	8.22	128.25	119.78
22	Y	47	PHE	C-N-CA	8.22	128.25	119.78
22	BY	47	PHE	CA-C-N	8.22	128.24	119.78
22	BY	47	PHE	C-N-CA	8.22	128.24	119.78
13	N	82	VAL	CA-C-N	8.18	125.63	119.66
13	N	82	VAL	C-N-CA	8.18	125.63	119.66
45	x	82	LEU	N-CA-C	8.16	122.51	112.23
13	BN	82	VAL	CA-C-N	8.15	125.61	119.66
13	BN	82	VAL	C-N-CA	8.15	125.61	119.66
45	Bx	82	LEU	N-CA-C	8.14	122.49	112.23
27	Bd	119	CYS	N-CA-C	8.09	120.10	111.28
68	AY	421	GLY	N-CA-C	-8.09	99.67	112.61
56	8	20	ARG	N-CA-C	-8.06	102.57	111.36
45	x	378	HIS	ND1-CE1-NE2	8.06	116.46	108.40
56	B8	20	ARG	N-CA-C	-8.05	102.58	111.36
45	Bx	378	HIS	ND1-CE1-NE2	8.03	116.43	108.40
27	d	119	CYS	N-CA-C	8.03	120.04	111.28
9	J	311	GLU	CA-C-N	8.03	128.05	119.78
9	J	311	GLU	C-N-CA	8.03	128.05	119.78
9	BJ	311	GLU	CA-C-N	7.94	127.95	119.78
9	BJ	311	GLU	C-N-CA	7.94	127.95	119.78
60	AP	252	GLY	CA-C-N	7.90	127.97	119.28
60	AP	252	GLY	C-N-CA	7.90	127.97	119.28
32	i	255	PRO	N-CA-C	7.87	120.31	110.70
32	Bi	255	PRO	N-CA-C	7.84	120.27	110.70
27	d	2	PRO	N-CA-CB	7.78	111.42	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	x	56	VAL	N-CA-C	-7.77	103.23	110.53
45	Bx	56	VAL	N-CA-C	-7.77	103.23	110.53
45	x	435	GLY	N-CA-C	7.75	126.20	115.27
27	Bd	2	PRO	N-CA-CB	7.75	111.39	103.25
45	Bx	435	GLY	N-CA-C	7.73	126.17	115.27
60	AP	236	CYS	CA-C-N	7.59	127.63	119.28
60	AP	236	CYS	C-N-CA	7.59	127.63	119.28
43	v	17	PRO	N-CA-CB	7.48	110.40	103.15
16	BQ	318	VAL	N-CA-C	7.48	115.31	107.76
43	Bv	17	PRO	N-CA-CB	7.47	110.40	103.15
43	v	42	THR	CB-CA-C	-7.47	107.96	116.63
16	Q	318	VAL	N-CA-C	7.46	115.29	107.76
43	Bv	42	THR	CB-CA-C	-7.45	107.98	116.63
57	B9	27	LEU	N-CA-C	7.45	119.47	111.36
41	Bs	89	LEU	CA-C-N	7.42	129.11	119.84
41	Bs	89	LEU	C-N-CA	7.42	129.11	119.84
45	Bx	330	GLY	N-CA-C	7.41	120.48	112.33
41	s	89	LEU	CA-C-N	7.40	129.09	119.84
41	s	89	LEU	C-N-CA	7.40	129.09	119.84
57	9	27	LEU	N-CA-C	7.40	119.42	111.36
45	x	330	GLY	N-CA-C	7.39	120.46	112.33
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
32	Bi	323	THR	C-N-CD	-7.37	104.38	120.60
25	Bb	117	ILE	CA-C-N	-7.35	112.81	120.38
25	Bb	117	ILE	C-N-CA	-7.35	112.81	120.38
25	b	117	ILE	CA-C-N	-7.30	112.86	120.38
25	b	117	ILE	C-N-CA	-7.30	112.86	120.38
3	C	141	MET	CA-C-N	7.29	127.29	119.78
3	C	141	MET	C-N-CA	7.29	127.29	119.78
60	AP	159	ILE	CA-C-N	7.27	127.27	119.78
60	AP	159	ILE	C-N-CA	7.27	127.27	119.78
3	BC	141	MET	CA-C-N	7.26	127.26	119.78
3	BC	141	MET	C-N-CA	7.26	127.26	119.78
19	U	33	PRO	N-CA-C	7.24	119.53	110.70
19	BU	33	PRO	N-CA-C	7.23	119.53	110.70
49	1	76	GLY	CA-C-N	7.23	128.47	120.45
49	1	76	GLY	C-N-CA	7.23	128.47	120.45
45	x	9	SER	N-CA-C	7.22	119.89	110.43
45	Bx	9	SER	N-CA-C	7.22	119.89	110.43
41	Bs	277	TYR	CA-C-N	7.18	127.10	119.85
41	Bs	277	TYR	C-N-CA	7.18	127.10	119.85
45	Bx	376	HIS	CE1-NE2-CD2	-7.17	101.83	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	76	GLY	CA-C-N	7.16	128.39	120.45
49	B1	76	GLY	C-N-CA	7.16	128.39	120.45
41	s	277	TYR	CA-C-N	7.14	127.06	119.85
41	s	277	TYR	C-N-CA	7.14	127.06	119.85
39	Bp	173	ARG	CA-C-N	7.14	127.13	119.28
39	Bp	173	ARG	C-N-CA	7.14	127.13	119.28
45	Bx	332	ILE	N-CA-C	7.12	118.98	109.37
45	x	376	HIS	CE1-NE2-CD2	-7.12	101.88	109.00
45	x	332	ILE	N-CA-C	7.10	118.96	109.37
30	g	21	PRO	CA-C-N	7.10	124.77	119.66
30	g	21	PRO	C-N-CA	7.10	124.77	119.66
16	Q	351	MET	CA-C-N	7.09	124.84	119.66
16	Q	351	MET	C-N-CA	7.09	124.84	119.66
39	p	173	ARG	CA-C-N	7.09	127.08	119.28
39	p	173	ARG	C-N-CA	7.09	127.08	119.28
16	BQ	351	MET	CA-C-N	7.07	124.82	119.66
16	BQ	351	MET	C-N-CA	7.07	124.82	119.66
39	p	171	VAL	N-CA-C	7.06	117.86	110.72
30	Bg	21	PRO	CA-C-N	7.06	124.75	119.66
30	Bg	21	PRO	C-N-CA	7.06	124.75	119.66
49	l	42	VAL	N-CA-C	-7.05	99.73	108.05
49	B1	42	VAL	N-CA-C	-7.03	99.75	108.05
39	Bp	171	VAL	N-CA-C	7.02	117.81	110.72
45	x	130	PRO	N-CA-C	-7.00	102.15	110.70
35	l	537	ILE	CA-C-N	-7.00	111.58	119.28
35	l	537	ILE	C-N-CA	-7.00	111.58	119.28
14	O	237	PRO	N-CA-C	7.00	119.24	110.70
45	Bx	130	PRO	N-CA-C	-7.00	102.16	110.70
14	BO	237	PRO	N-CA-C	6.99	119.23	110.70
35	Bl	537	ILE	CA-C-N	-6.97	111.61	119.28
35	Bl	537	ILE	C-N-CA	-6.97	111.61	119.28
32	Bi	197	ASN	CA-C-N	6.96	126.93	119.28
32	Bi	197	ASN	C-N-CA	6.96	126.93	119.28
32	i	197	ASN	CA-C-N	6.94	126.92	119.28
32	i	197	ASN	C-N-CA	6.94	126.92	119.28
68	AL	424	ILE	CA-C-N	6.94	126.93	119.78
68	AL	424	ILE	C-N-CA	6.94	126.93	119.78
22	Y	93	THR	N-CA-C	6.93	120.05	108.20
22	BY	93	THR	N-CA-C	6.92	120.03	108.20
16	Q	356	ILE	N-CA-C	-6.90	105.81	112.29
16	BQ	356	ILE	N-CA-C	-6.89	105.81	112.29
9	BJ	224	GLY	CA-C-N	6.89	126.85	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	BJ	224	GLY	C-N-CA	6.89	126.85	120.03
1	BA	318	ILE	CA-C-N	6.88	126.87	119.78
1	BA	318	ILE	C-N-CA	6.88	126.87	119.78
47	Bz	36	HIS	N-CA-C	6.87	122.09	113.43
1	A	318	ILE	CA-C-N	6.87	126.85	119.78
1	A	318	ILE	C-N-CA	6.87	126.85	119.78
47	z	36	HIS	N-CA-C	6.86	122.08	113.43
31	Bh	94	PRO	CA-C-N	-6.86	113.32	120.38
31	Bh	94	PRO	C-N-CA	-6.86	113.32	120.38
31	h	94	PRO	CA-C-N	-6.84	113.34	120.38
31	h	94	PRO	C-N-CA	-6.84	113.34	120.38
45	x	125	GLY	N-CA-C	-6.82	104.23	112.48
35	Bl	24	VAL	CA-C-N	-6.81	115.36	122.85
35	Bl	24	VAL	C-N-CA	-6.81	115.36	122.85
62	AE	28	ASP	CA-C-N	-6.81	113.18	120.47
62	AE	28	ASP	C-N-CA	-6.81	113.18	120.47
1	BA	327	ILE	CA-C-N	6.81	126.79	119.78
1	BA	327	ILE	C-N-CA	6.81	126.79	119.78
9	J	224	GLY	CA-C-N	6.80	126.76	120.03
9	J	224	GLY	C-N-CA	6.80	126.76	120.03
60	AC	252	GLY	CA-C-N	6.80	126.76	119.28
60	AC	252	GLY	C-N-CA	6.80	126.76	119.28
35	l	24	VAL	CA-C-N	-6.80	115.37	122.85
35	l	24	VAL	C-N-CA	-6.80	115.37	122.85
26	c	157	GLY	CA-C-N	6.78	126.76	119.78
26	c	157	GLY	C-N-CA	6.78	126.76	119.78
51	3	5	LYS	N-CA-C	6.75	125.17	110.80
35	l	511	LEU	N-CA-C	6.74	118.56	108.31
51	B3	5	LYS	N-CA-C	6.74	125.16	110.80
45	Bx	507	GLU	N-CA-C	-6.74	97.90	109.15
48	B0	133	GLY	N-CA-C	6.74	129.15	113.18
48	0	133	GLY	N-CA-C	6.73	129.14	113.18
35	Bl	511	LEU	N-CA-C	6.73	118.55	108.31
45	x	507	GLU	N-CA-C	-6.73	97.91	109.15
49	1	21	LYS	CA-C-N	6.73	126.24	119.24
49	1	21	LYS	C-N-CA	6.73	126.24	119.24
26	Bc	157	GLY	CA-C-N	6.72	126.70	119.78
26	Bc	157	GLY	C-N-CA	6.72	126.70	119.78
1	A	327	ILE	CA-C-N	6.71	126.69	119.78
1	A	327	ILE	C-N-CA	6.71	126.69	119.78
25	Bb	105	PHE	CA-C-N	-6.70	112.86	119.76
25	Bb	105	PHE	C-N-CA	-6.70	112.86	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	v	23	PRO	N-CA-CB	6.70	110.37	103.00
25	b	105	PHE	CA-C-N	-6.69	112.86	119.76
25	b	105	PHE	C-N-CA	-6.69	112.86	119.76
26	c	72	TYR	N-CA-C	-6.69	100.14	110.10
26	Bc	72	TYR	N-CA-C	-6.69	100.14	110.10
43	Bv	23	PRO	N-CA-CB	6.69	110.35	103.00
49	B1	81	ILE	N-CA-C	6.66	116.79	110.53
49	1	81	ILE	N-CA-C	6.64	116.77	110.53
15	BP	166	TYR	N-CA-C	-6.62	104.06	111.28
15	P	166	TYR	N-CA-C	-6.62	104.06	111.28
68	AL	293	GLY	CA-C-N	6.62	126.60	119.78
68	AL	293	GLY	C-N-CA	6.62	126.60	119.78
2	B	168	GLY	CA-C-N	6.61	126.56	119.28
2	B	168	GLY	C-N-CA	6.61	126.56	119.28
16	Q	63	PRO	CA-C-N	6.60	124.48	119.66
16	Q	63	PRO	C-N-CA	6.60	124.48	119.66
35	B1	562	LEU	CA-C-N	-6.59	111.60	119.84
35	B1	562	LEU	C-N-CA	-6.59	111.60	119.84
2	BB	168	GLY	CA-C-N	6.59	126.53	119.28
2	BB	168	GLY	C-N-CA	6.59	126.53	119.28
35	l	562	LEU	CA-C-N	-6.59	111.61	119.84
35	l	562	LEU	C-N-CA	-6.59	111.61	119.84
67	AW	447	THR	CA-C-N	-6.58	113.20	119.85
67	AW	447	THR	C-N-CA	-6.58	113.20	119.85
17	S	61	TYR	N-CA-C	-6.57	104.12	111.28
45	Bx	61	HIS	CB-CG-CD2	-6.56	122.67	131.20
45	x	74	MET	N-CA-C	6.56	118.09	111.07
17	BS	61	TYR	N-CA-C	-6.56	104.13	111.28
22	BY	87	PRO	CA-N-CD	-6.55	102.33	111.50
45	x	61	HIS	CB-CG-CD2	-6.55	122.69	131.20
22	Y	87	PRO	CA-N-CD	-6.54	102.34	111.50
45	Bx	506	GLU	N-CA-C	-6.52	104.17	111.28
16	BQ	63	PRO	CA-C-N	6.51	124.42	119.66
16	BQ	63	PRO	C-N-CA	6.51	124.42	119.66
45	x	506	GLU	N-CA-C	-6.51	104.19	111.28
45	Bx	74	MET	N-CA-C	6.51	118.03	111.07
36	m	135	ILE	N-CA-C	6.50	117.48	108.12
66	AV	269	LYS	CA-C-N	6.50	126.47	119.78
66	AV	269	LYS	C-N-CA	6.50	126.47	119.78
35	B1	548	LEU	CA-C-N	-6.49	111.73	119.84
35	B1	548	LEU	C-N-CA	-6.49	111.73	119.84
36	Bm	135	ILE	N-CA-C	6.48	117.45	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	548	LEU	CA-C-N	-6.43	111.80	119.84
35	l	548	LEU	C-N-CA	-6.43	111.80	119.84
29	f	34	PRO	N-CA-C	6.40	118.50	110.70
44	Bw	211	VAL	CA-C-N	-6.39	111.96	119.05
44	Bw	211	VAL	C-N-CA	-6.39	111.96	119.05
44	w	211	VAL	CA-C-N	-6.38	111.97	119.05
44	w	211	VAL	C-N-CA	-6.38	111.97	119.05
45	x	61	HIS	ND1-CE1-NE2	6.37	114.77	108.40
29	Bf	34	PRO	N-CA-C	6.37	118.47	110.70
60	AC	159	ILE	CA-C-N	6.35	126.32	119.78
60	AC	159	ILE	C-N-CA	6.35	126.32	119.78
9	BJ	91	ILE	CB-CA-C	-6.35	104.89	112.19
39	Bp	78	GLN	CA-C-N	6.34	126.31	119.78
39	Bp	78	GLN	C-N-CA	6.34	126.31	119.78
45	Bx	61	HIS	ND1-CE1-NE2	6.34	114.74	108.40
9	J	91	ILE	CB-CA-C	-6.34	104.90	112.19
8	I	98	ALA	CA-C-N	-6.31	113.88	120.38
8	I	98	ALA	C-N-CA	-6.31	113.88	120.38
39	p	78	GLN	CA-C-N	6.31	126.28	119.78
39	p	78	GLN	C-N-CA	6.31	126.28	119.78
8	BI	98	ALA	CA-C-N	-6.28	113.91	120.38
8	BI	98	ALA	C-N-CA	-6.28	113.91	120.38
65	AU	91	PRO	CA-C-N	6.28	126.04	119.76
65	AU	91	PRO	C-N-CA	6.28	126.04	119.76
43	Bv	19	PRO	N-CA-CB	6.28	110.17	103.39
63	AF	51	LEU	CA-C-N	-6.27	113.52	119.85
63	AF	51	LEU	C-N-CA	-6.27	113.52	119.85
12	M	505	GLY	N-CA-C	-6.26	107.07	115.21
20	V	14	ASP	N-CA-C	6.26	117.77	111.07
15	P	119	VAL	CA-C-N	6.25	126.16	119.28
15	P	119	VAL	C-N-CA	6.25	126.16	119.28
9	BJ	238	GLN	CA-C-N	6.25	126.22	119.78
9	BJ	238	GLN	C-N-CA	6.25	126.22	119.78
43	v	19	PRO	N-CA-CB	6.25	110.14	103.39
12	BM	505	GLY	N-CA-C	-6.25	107.09	115.21
44	w	56	ARG	N-CA-C	-6.24	105.61	112.72
45	x	10	THR	N-CA-C	-6.24	103.86	112.03
45	Bx	10	THR	N-CA-C	-6.23	103.86	112.03
68	AY	424	ILE	CA-C-N	-6.23	113.34	119.76
68	AY	424	ILE	C-N-CA	-6.23	113.34	119.76
41	Bs	179	TRP	CA-C-N	-6.21	112.44	119.28
41	Bs	179	TRP	C-N-CA	-6.21	112.44	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	Bw	56	ARG	N-CA-C	-6.21	105.64	112.72
41	s	179	TRP	CA-C-N	-6.20	112.47	119.28
41	s	179	TRP	C-N-CA	-6.20	112.47	119.28
31	h	94	PRO	N-CA-C	6.19	118.25	110.70
51	3	2	SER	N-CA-C	6.19	119.44	109.79
9	J	238	GLN	CA-C-N	6.18	126.15	119.78
9	J	238	GLN	C-N-CA	6.18	126.15	119.78
20	BV	14	ASP	N-CA-C	6.17	117.68	111.07
51	B3	2	SER	N-CA-C	6.17	119.42	109.79
45	Bx	157	SER	N-CA-C	6.17	118.98	111.82
15	BP	119	VAL	CA-C-N	6.17	126.06	119.28
15	BP	119	VAL	C-N-CA	6.17	126.06	119.28
66	AV	359	PHE	N-CA-C	6.16	118.08	111.36
31	Bh	94	PRO	N-CA-C	6.16	118.22	110.70
45	x	157	SER	N-CA-C	6.16	118.96	111.82
51	B3	44	ARG	CA-C-N	6.14	126.16	119.90
51	B3	44	ARG	C-N-CA	6.14	126.16	119.90
45	Bx	170	ASN	N-CA-C	6.14	120.84	113.23
35	l	447	ASN	N-CA-C	6.13	116.02	108.11
51	3	44	ARG	CA-C-N	6.13	126.15	119.90
51	3	44	ARG	C-N-CA	6.13	126.15	119.90
26	Bc	155	PRO	CA-C-N	-6.12	116.90	123.08
26	Bc	155	PRO	C-N-CA	-6.12	116.90	123.08
35	Bl	447	ASN	N-CA-C	6.11	116.00	108.11
45	x	170	ASN	N-CA-C	6.10	120.80	113.23
26	c	155	PRO	CA-C-N	-6.10	116.92	123.08
26	c	155	PRO	C-N-CA	-6.10	116.92	123.08
12	M	175	ARG	N-CA-C	6.09	117.92	111.28
44	Bw	253	CYS	CB-CA-C	-6.09	109.53	116.54
66	AJ	341	GLN	CA-C-N	6.08	126.04	119.78
66	AJ	341	GLN	C-N-CA	6.08	126.04	119.78
12	BM	175	ARG	N-CA-C	6.08	117.91	111.28
16	Q	391	VAL	CA-C-N	-6.07	115.23	119.66
16	Q	391	VAL	C-N-CA	-6.07	115.23	119.66
9	J	86	CYS	N-CA-C	6.07	117.56	111.07
49	B1	21	LYS	CA-C-N	6.07	126.24	119.32
49	B1	21	LYS	C-N-CA	6.07	126.24	119.32
41	s	251	SER	CA-C-N	6.06	125.95	119.28
41	s	251	SER	C-N-CA	6.06	125.95	119.28
16	BQ	391	VAL	CA-C-N	-6.06	115.23	119.66
16	BQ	391	VAL	C-N-CA	-6.06	115.23	119.66
13	BN	64	TYR	N-CA-C	6.06	120.52	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	47	THR	N-CA-C	6.06	119.98	112.59
46	By	47	THR	N-CA-C	6.05	119.97	112.59
44	w	253	CYS	CB-CA-C	-6.05	109.58	116.54
9	BJ	86	CYS	N-CA-C	6.05	117.54	111.07
68	AL	453	CYS	CA-C-N	6.04	125.95	119.85
68	AL	453	CYS	C-N-CA	6.04	125.95	119.85
66	AV	345	TYR	CA-C-N	-6.04	112.34	119.05
66	AV	345	TYR	C-N-CA	-6.04	112.34	119.05
41	Bs	251	SER	CA-C-N	6.03	125.92	119.28
41	Bs	251	SER	C-N-CA	6.03	125.92	119.28
46	y	207	MET	CA-C-N	6.02	127.37	119.84
46	y	207	MET	C-N-CA	6.02	127.37	119.84
52	B4	63	LEU	N-CA-C	6.02	119.09	111.69
13	N	64	TYR	N-CA-C	6.01	120.46	113.18
52	4	63	LEU	N-CA-C	6.01	119.08	111.69
2	BB	160	CYS	CA-C-N	6.01	125.89	119.28
2	BB	160	CYS	C-N-CA	6.01	125.89	119.28
24	a	106	VAL	CA-C-N	6.01	125.92	119.85
24	a	106	VAL	C-N-CA	6.01	125.92	119.85
66	AV	153	ILE	CA-C-N	-6.00	112.73	118.97
66	AV	153	ILE	C-N-CA	-6.00	112.73	118.97
35	Bl	404	THR	N-CA-C	6.00	116.35	108.07
2	B	160	CYS	CA-C-N	5.98	125.86	119.28
2	B	160	CYS	C-N-CA	5.98	125.86	119.28
46	By	207	MET	CA-C-N	5.98	127.31	119.84
46	By	207	MET	C-N-CA	5.98	127.31	119.84
24	Ba	106	VAL	CA-C-N	5.97	125.88	119.85
24	Ba	106	VAL	C-N-CA	5.97	125.88	119.85
35	l	404	THR	N-CA-C	5.96	116.30	108.07
45	Bx	125	GLY	N-CA-C	-5.96	104.19	112.18
45	x	171	MET	N-CA-C	5.95	120.27	111.87
45	Bx	171	MET	N-CA-C	5.95	120.27	111.87
47	Bz	8	TYR	N-CA-C	5.95	118.21	110.53
47	z	8	TYR	N-CA-C	5.95	118.21	110.53
45	Bx	67	PHE	N-CA-C	5.92	119.69	112.23
39	p	155	PRO	CA-C-N	5.92	125.83	119.85
39	p	155	PRO	C-N-CA	5.92	125.83	119.85
21	W	118	PRO	CA-C-N	5.92	125.83	119.85
21	W	118	PRO	C-N-CA	5.92	125.83	119.85
39	Bp	155	PRO	CA-C-N	5.92	125.83	119.85
39	Bp	155	PRO	C-N-CA	5.92	125.83	119.85
46	By	134	ARG	N-CA-C	5.91	123.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	y	134	ARG	N-CA-C	5.91	123.39	110.80
47	Bz	198	PHE	N-CA-C	5.91	117.72	111.28
41	s	158	GLY	N-CA-C	5.91	121.72	114.69
58	AN	50	VAL	N-CA-C	5.90	119.44	112.35
65	AH	322	ARG	CA-C-N	5.90	123.97	119.66
65	AH	322	ARG	C-N-CA	5.90	123.97	119.66
45	x	67	PHE	N-CA-C	5.90	119.66	112.23
35	Bl	106	TRP	N-CA-C	5.89	117.78	111.36
41	Bs	158	GLY	N-CA-C	5.88	121.69	114.69
35	l	106	TRP	N-CA-C	5.88	117.77	111.36
64	AT	42	LEU	N-CA-C	5.88	117.69	111.28
41	s	315	PRO	CA-C-N	5.88	127.19	119.84
41	s	315	PRO	C-N-CA	5.88	127.19	119.84
47	z	198	PHE	N-CA-C	5.88	117.68	111.28
41	Bs	315	PRO	CA-C-N	5.87	127.18	119.84
41	Bs	315	PRO	C-N-CA	5.87	127.18	119.84
35	l	90	ILE	O-C-N	5.87	124.24	120.07
44	Bw	340	SER	N-CA-C	5.87	117.09	109.64
65	AU	246	PRO	CA-C-N	5.87	125.73	119.28
65	AU	246	PRO	C-N-CA	5.87	125.73	119.28
46	By	202	SER	N-CA-C	5.86	118.14	111.11
45	Bx	119	GLU	CB-CA-C	-5.85	109.81	116.54
35	Bl	90	ILE	O-C-N	5.85	124.22	120.07
21	BW	118	PRO	CA-C-N	5.85	125.80	119.78
21	BW	118	PRO	C-N-CA	5.85	125.80	119.78
44	w	340	SER	N-CA-C	5.84	117.06	109.64
65	AH	221	PRO	CA-C-N	5.84	125.80	119.78
65	AH	221	PRO	C-N-CA	5.84	125.80	119.78
21	BW	27	ARG	N-CA-C	-5.83	105.00	111.36
45	x	119	GLU	CB-CA-C	-5.83	109.84	116.54
46	y	202	SER	N-CA-C	5.82	118.09	111.11
21	W	27	ARG	N-CA-C	-5.81	105.03	111.36
46	By	190	GLY	N-CA-C	5.79	117.79	110.38
15	P	113	ASP	N-CA-C	5.79	117.91	108.76
35	Bl	87	MET	N-CA-C	5.79	117.39	111.14
13	N	65	THR	CB-CA-C	-5.78	108.91	115.79
35	l	87	MET	N-CA-C	5.78	117.38	111.14
15	BP	113	ASP	N-CA-C	5.78	117.89	108.76
46	y	190	GLY	N-CA-C	5.78	117.77	110.38
20	BV	22	ALA	N-CA-C	-5.77	105.07	111.36
2	B	64	LEU	N-CA-C	-5.77	104.90	111.07
22	Y	85	PRO	N-CA-C	5.77	124.35	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BY	85	PRO	N-CA-C	5.77	124.35	112.47
20	V	22	ALA	N-CA-C	-5.76	105.08	111.36
13	BN	65	THR	CB-CA-C	-5.76	108.94	115.79
8	BI	36	GLN	CA-C-N	5.76	123.86	119.66
8	BI	36	GLN	C-N-CA	5.76	123.86	119.66
45	x	129	TYR	CB-CA-C	-5.75	100.39	109.42
25	Bb	37	PRO	CA-N-CD	-5.75	103.95	112.00
2	BB	64	LEU	N-CA-C	-5.75	104.92	111.07
25	b	37	PRO	CA-N-CD	-5.74	103.96	112.00
1	A	318	ILE	N-CA-C	5.74	114.20	107.77
8	I	36	GLN	CA-C-N	5.74	123.85	119.66
8	I	36	GLN	C-N-CA	5.74	123.85	119.66
42	u	166	ARG	N-CA-C	-5.74	106.50	112.93
1	BA	318	ILE	N-CA-C	5.73	114.19	107.77
41	Bs	280	PHE	N-CA-C	5.73	118.47	111.82
33	Bj	45	SER	CA-C-N	5.73	125.63	119.85
33	Bj	45	SER	C-N-CA	5.73	125.63	119.85
41	s	21	MET	N-CA-C	-5.72	106.14	113.01
41	s	280	PHE	N-CA-C	5.72	118.45	111.82
45	Bx	129	TYR	CB-CA-C	-5.72	100.44	109.42
40	r	427	LYS	CA-C-N	5.71	125.66	119.78
40	r	427	LYS	C-N-CA	5.71	125.66	119.78
42	Bu	166	ARG	N-CA-C	-5.71	106.53	112.93
35	l	197	ASP	CA-C-N	-5.71	112.72	119.05
35	l	197	ASP	C-N-CA	-5.71	112.72	119.05
54	6	25	GLY	N-CA-C	5.70	118.92	110.60
41	Bs	21	MET	N-CA-C	-5.70	106.17	113.01
54	B6	25	GLY	N-CA-C	5.70	118.92	110.60
35	Bl	197	ASP	CA-C-N	-5.69	112.73	119.05
35	Bl	197	ASP	C-N-CA	-5.69	112.73	119.05
40	Br	427	LYS	CA-C-N	5.69	125.64	119.78
40	Br	427	LYS	C-N-CA	5.69	125.64	119.78
7	BH	81	ILE	N-CA-C	-5.69	104.98	110.72
33	j	45	SER	CA-C-N	5.69	125.59	119.85
33	j	45	SER	C-N-CA	5.69	125.59	119.85
8	BI	17	GLY	N-CA-C	-5.68	107.81	115.36
12	M	612	PRO	CA-C-N	5.68	125.52	119.28
12	M	612	PRO	C-N-CA	5.68	125.52	119.28
48	0	129	ALA	CA-C-N	5.66	126.92	119.84
48	0	129	ALA	C-N-CA	5.66	126.92	119.84
33	j	49	VAL	N-CA-C	5.66	114.50	108.95
8	I	17	GLY	N-CA-C	-5.66	107.83	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BM	612	PRO	CA-C-N	5.65	125.49	119.28
12	BM	612	PRO	C-N-CA	5.65	125.49	119.28
7	H	81	ILE	N-CA-C	-5.64	105.02	110.72
14	BO	236	GLU	CA-C-N	5.64	126.19	120.38
14	BO	236	GLU	C-N-CA	5.64	126.19	120.38
48	B0	129	ALA	CA-C-N	5.64	126.89	119.84
48	B0	129	ALA	C-N-CA	5.64	126.89	119.84
24	a	56	VAL	N-CA-C	5.64	117.86	111.88
33	Bj	49	VAL	N-CA-C	5.62	114.46	108.95
24	Ba	56	VAL	N-CA-C	5.62	117.84	111.88
35	Bl	450	LEU	N-CA-C	5.62	122.76	110.80
25	Bb	9	LYS	N-CA-C	-5.61	105.06	111.07
53	5	20	HIS	N-CA-C	5.61	118.16	111.71
50	2	82	CYS	CA-C-N	5.61	125.45	119.28
50	2	82	CYS	C-N-CA	5.61	125.45	119.28
16	BQ	272	THR	N-CA-C	5.61	120.39	113.50
46	By	104	TRP	N-CA-C	5.61	122.74	110.80
35	l	450	LEU	N-CA-C	5.60	122.73	110.80
53	B5	20	HIS	N-CA-C	5.60	118.15	111.71
50	B2	82	CYS	CA-C-N	5.59	125.43	119.28
50	B2	82	CYS	C-N-CA	5.59	125.43	119.28
46	y	104	TRP	N-CA-C	5.59	122.71	110.80
25	b	9	LYS	N-CA-C	-5.59	105.09	111.07
35	Bl	90	ILE	CA-C-N	-5.59	112.85	119.05
35	Bl	90	ILE	C-N-CA	-5.59	112.85	119.05
35	l	25	ASN	N-CA-C	5.58	118.24	108.75
14	O	236	GLU	CA-C-N	5.58	126.13	120.38
14	O	236	GLU	C-N-CA	5.58	126.13	120.38
35	l	90	ILE	CA-C-N	-5.58	112.86	119.05
35	l	90	ILE	C-N-CA	-5.58	112.86	119.05
16	Q	272	THR	N-CA-C	5.57	120.36	113.50
30	g	36	LEU	N-CA-C	-5.57	105.31	111.71
30	Bg	36	LEU	N-CA-C	-5.57	105.31	111.71
12	M	261	ILE	N-CA-C	5.56	116.68	108.45
12	BM	261	ILE	N-CA-C	5.56	116.67	108.45
26	c	120	SER	CA-C-N	5.55	125.50	119.78
26	c	120	SER	C-N-CA	5.55	125.50	119.78
68	AL	148	GLY	N-CA-C	-5.55	108.56	114.67
35	Bl	25	ASN	N-CA-C	5.55	118.19	108.75
32	Bi	149	LEU	N-CA-C	5.54	120.04	113.28
56	8	16	GLU	N-CA-C	5.53	117.39	111.36
24	Ba	166	GLY	CA-C-N	5.53	125.36	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Ba	166	GLY	C-N-CA	5.53	125.36	119.28
26	Bc	120	SER	CA-C-N	5.53	125.48	119.78
26	Bc	120	SER	C-N-CA	5.53	125.48	119.78
36	Bm	127	TYR	CB-CA-C	-5.53	110.18	116.54
56	B8	16	GLU	N-CA-C	5.53	117.39	111.36
32	i	149	LEU	N-CA-C	5.50	119.99	113.28
39	p	154	LEU	CA-C-N	5.50	123.62	119.66
39	p	154	LEU	C-N-CA	5.50	123.62	119.66
42	u	171	THR	N-CA-C	-5.50	106.61	113.38
68	AY	355	GLY	N-CA-C	5.49	118.47	110.63
42	Bu	171	THR	N-CA-C	-5.49	106.63	113.38
24	a	166	GLY	CA-C-N	5.48	125.31	119.28
24	a	166	GLY	C-N-CA	5.48	125.31	119.28
14	BO	233	SER	CB-CA-C	-5.48	109.77	117.23
14	O	233	SER	CB-CA-C	-5.48	109.78	117.23
47	z	188	ILE	CB-CA-C	-5.48	104.74	112.14
51	3	72	ASN	CA-C-N	5.47	125.82	119.47
51	3	72	ASN	C-N-CA	5.47	125.82	119.47
36	m	127	TYR	CB-CA-C	-5.47	110.25	116.54
47	Bz	188	ILE	CB-CA-C	-5.46	104.77	112.14
51	B3	72	ASN	CA-C-N	5.46	125.80	119.47
51	B3	72	ASN	C-N-CA	5.46	125.80	119.47
39	Bp	154	LEU	CA-C-N	5.45	123.59	119.66
39	Bp	154	LEU	C-N-CA	5.45	123.59	119.66
58	AN	50	VAL	CB-CA-C	-5.45	106.87	114.00
9	J	267	GLY	CA-C-N	5.43	125.26	119.28
9	J	267	GLY	C-N-CA	5.43	125.26	119.28
66	AJ	153	ILE	CA-C-N	-5.42	112.94	118.85
66	AJ	153	ILE	C-N-CA	-5.42	112.94	118.85
45	x	159	LEU	N-CA-C	-5.42	105.45	111.36
54	6	2	GLU	N-CA-C	5.42	122.34	110.80
9	BJ	267	GLY	CA-C-N	5.42	125.24	119.28
9	BJ	267	GLY	C-N-CA	5.42	125.24	119.28
54	B6	2	GLU	N-CA-C	5.42	122.33	110.80
12	M	85	ALA	CA-C-N	5.41	125.23	119.28
12	M	85	ALA	C-N-CA	5.41	125.23	119.28
67	AW	296	GLY	CA-C-N	5.41	125.35	119.78
67	AW	296	GLY	C-N-CA	5.41	125.35	119.78
26	Bc	126	TRP	N-CA-C	5.40	116.86	110.97
30	Bg	22	PRO	O-C-N	5.40	123.69	121.15
16	Q	281	GLU	N-CA-C	5.40	117.16	111.28
65	AH	246	PRO	CA-C-N	5.40	125.22	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	AH	246	PRO	C-N-CA	5.40	125.22	119.28
45	Bx	159	LEU	N-CA-C	-5.40	105.48	111.36
34	Bk	89	TYR	CB-CA-C	-5.39	109.37	115.79
26	c	161	TYR	CA-C-N	5.39	125.33	119.78
26	c	161	TYR	C-N-CA	5.39	125.33	119.78
26	c	126	TRP	N-CA-C	5.38	116.84	110.97
12	BM	85	ALA	CA-C-N	5.38	125.19	119.28
12	BM	85	ALA	C-N-CA	5.38	125.19	119.28
16	BQ	281	GLU	N-CA-C	5.38	117.14	111.28
45	Bx	245	ILE	N-CA-C	-5.37	104.33	111.05
45	x	245	ILE	N-CA-C	-5.37	104.34	111.05
26	Bc	161	TYR	CA-C-N	5.37	125.31	119.78
26	Bc	161	TYR	C-N-CA	5.37	125.31	119.78
2	B	78	GLU	CA-C-N	5.36	125.30	119.78
2	B	78	GLU	C-N-CA	5.36	125.30	119.78
34	k	89	TYR	CB-CA-C	-5.35	109.42	115.79
2	BB	78	GLU	CA-C-N	5.35	125.29	119.78
2	BB	78	GLU	C-N-CA	5.35	125.29	119.78
35	l	192	HIS	N-CA-C	5.34	117.18	111.36
30	g	22	PRO	O-C-N	5.33	123.66	121.15
66	AJ	284	VAL	CA-C-N	5.33	125.23	119.85
66	AJ	284	VAL	C-N-CA	5.33	125.23	119.85
45	x	305	PHE	N-CA-C	5.31	118.86	112.38
35	Bl	192	HIS	N-CA-C	5.31	117.15	111.36
47	z	99	TRP	N-CA-C	-5.31	105.39	111.07
35	Bl	270	ASN	CA-C-N	5.30	125.11	119.28
35	Bl	270	ASN	C-N-CA	5.30	125.11	119.28
2	B	43	ASP	CA-C-N	5.29	125.23	119.78
2	B	43	ASP	C-N-CA	5.29	125.23	119.78
2	BB	43	ASP	CA-C-N	5.29	125.23	119.78
2	BB	43	ASP	C-N-CA	5.29	125.23	119.78
35	l	230	HIS	CA-C-N	-5.29	113.17	119.05
35	l	230	HIS	C-N-CA	-5.29	113.17	119.05
45	x	6	TRP	N-CA-C	5.29	119.79	113.23
45	Bx	305	PHE	N-CA-C	5.28	118.83	112.38
45	Bx	6	TRP	N-CA-C	5.27	119.77	113.23
58	AA	50	VAL	N-CA-C	5.27	118.68	112.35
45	Bx	372	TYR	N-CA-C	-5.27	105.43	111.07
50	B2	38	ALA	N-CA-C	5.27	117.93	110.50
35	Bl	230	HIS	CA-C-N	-5.26	113.21	119.05
35	Bl	230	HIS	C-N-CA	-5.26	113.21	119.05
32	Bi	172	GLN	N-CA-C	5.26	117.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	270	ASN	CA-C-N	5.25	125.06	119.28
35	l	270	ASN	C-N-CA	5.25	125.06	119.28
45	x	372	TYR	N-CA-C	-5.25	105.45	111.07
47	Bz	99	TRP	N-CA-C	-5.25	105.45	111.07
7	H	12	VAL	N-CA-C	5.24	115.90	110.82
13	N	83	PRO	CA-C-N	5.24	125.04	119.28
13	N	83	PRO	C-N-CA	5.24	125.04	119.28
32	i	172	GLN	N-CA-C	5.24	117.44	110.53
35	l	16	ILE	CB-CA-C	-5.23	108.80	114.35
50	2	38	ALA	N-CA-C	5.23	117.88	110.50
13	BN	83	PRO	CA-C-N	5.23	125.03	119.28
13	BN	83	PRO	C-N-CA	5.23	125.03	119.28
35	Bl	16	ILE	CB-CA-C	-5.22	108.81	114.35
35	l	437	PHE	CA-C-N	5.21	125.15	119.78
35	l	437	PHE	C-N-CA	5.21	125.15	119.78
39	p	145	PRO	CA-C-N	5.21	125.01	119.28
39	p	145	PRO	C-N-CA	5.21	125.01	119.28
66	AV	318	ARG	CA-C-N	5.21	125.01	119.28
66	AV	318	ARG	C-N-CA	5.21	125.01	119.28
64	AG	7	GLY	CA-C-N	5.21	125.01	119.28
64	AG	7	GLY	C-N-CA	5.21	125.01	119.28
45	x	262	SER	N-CA-C	-5.21	106.61	113.17
12	M	102	ILE	N-CA-C	5.19	114.26	106.42
45	Bx	262	SER	N-CA-C	-5.19	106.63	113.17
12	BM	102	ILE	N-CA-C	5.19	114.26	106.42
27	d	120	ILE	N-CA-C	5.19	115.91	110.62
63	AF	70	ASN	N-CA-C	5.19	116.93	111.28
60	AC	207	LYS	CA-C-N	5.18	124.98	119.28
60	AC	207	LYS	C-N-CA	5.18	124.98	119.28
39	Bp	145	PRO	CA-C-N	5.18	124.98	119.28
39	Bp	145	PRO	C-N-CA	5.18	124.98	119.28
45	x	353	LEU	N-CA-C	-5.18	105.71	111.36
7	BH	12	VAL	N-CA-C	5.18	115.84	110.82
47	z	107	ALA	CA-C-N	5.18	125.98	119.98
47	z	107	ALA	C-N-CA	5.18	125.98	119.98
35	Bl	437	PHE	CA-C-N	5.17	125.11	119.78
35	Bl	437	PHE	C-N-CA	5.17	125.11	119.78
47	Bz	107	ALA	CA-C-N	5.17	125.98	119.98
47	Bz	107	ALA	C-N-CA	5.17	125.98	119.98
45	Bx	353	LEU	N-CA-C	-5.17	105.73	111.36
11	L	126	LEU	N-CA-C	5.17	116.60	107.61
34	k	1	MET	CA-C-N	-5.16	113.32	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	k	1	MET	C-N-CA	-5.16	113.32	119.05
45	x	377	PHE	N-CA-C	5.16	119.43	113.18
27	Bd	120	ILE	N-CA-C	5.16	115.88	110.62
44	Bw	223	ASP	CA-C-N	5.16	124.96	119.28
44	Bw	223	ASP	C-N-CA	5.16	124.96	119.28
4	BE	32	VAL	N-CA-C	5.15	115.36	110.42
4	E	32	VAL	N-CA-C	5.15	115.36	110.42
45	x	401	SER	N-CA-C	5.14	119.69	113.41
32	Bi	321	LYS	CA-C-N	5.14	124.94	119.28
32	Bi	321	LYS	C-N-CA	5.14	124.94	119.28
36	Bm	114	VAL	CA-C-N	5.14	131.23	121.97
36	Bm	114	VAL	C-N-CA	5.14	131.23	121.97
11	BL	126	LEU	N-CA-C	5.14	116.55	107.61
34	Bk	1	MET	CA-C-N	-5.13	113.35	119.05
34	Bk	1	MET	C-N-CA	-5.13	113.35	119.05
45	Bx	377	PHE	N-CA-C	5.13	119.39	113.18
46	y	165	VAL	CA-C-N	5.13	126.25	119.84
46	y	165	VAL	C-N-CA	5.13	126.25	119.84
36	Bm	137	GLU	N-CA-C	5.13	116.68	111.14
45	Bx	401	SER	N-CA-C	5.13	119.66	113.41
19	BU	62	ASN	CB-CA-C	-5.12	109.17	116.34
32	i	321	LYS	CA-C-N	5.12	124.92	119.28
32	i	321	LYS	C-N-CA	5.12	124.92	119.28
32	i	41	ILE	CB-CA-C	-5.12	107.29	114.00
36	m	114	VAL	CA-C-N	5.11	131.18	121.97
36	m	114	VAL	C-N-CA	5.11	131.18	121.97
68	AY	453	CYS	CA-C-N	5.11	125.03	119.76
68	AY	453	CYS	C-N-CA	5.11	125.03	119.76
19	U	62	ASN	CB-CA-C	-5.11	109.19	116.34
53	5	2	THR	N-CA-C	5.11	116.18	108.46
19	BU	36	SER	CA-C-N	5.11	124.90	119.28
19	BU	36	SER	C-N-CA	5.11	124.90	119.28
54	6	9	GLN	N-CA-C	-5.11	105.61	111.07
55	B7	35	GLN	N-CA-C	5.11	119.27	113.19
45	x	378	HIS	N-CA-C	-5.10	106.22	112.90
53	B5	2	THR	N-CA-C	5.09	116.15	108.46
36	m	137	GLU	N-CA-C	5.09	116.64	111.14
46	By	165	VAL	CA-C-N	5.09	126.20	119.84
46	By	165	VAL	C-N-CA	5.09	126.20	119.84
66	AJ	19	ILE	N-CA-C	5.09	115.81	110.62
24	a	106	VAL	N-CA-C	5.09	112.59	107.55
35	l	516	PRO	N-CA-C	5.09	119.08	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B4	22	ASN	N-CA-C	5.08	117.59	109.81
68	AL	421	GLY	N-CA-C	-5.08	103.12	112.62
32	Bi	41	ILE	CB-CA-C	-5.08	107.35	114.00
35	Bl	516	PRO	N-CA-C	5.08	119.06	111.14
64	AG	45	VAL	CA-C-N	5.08	124.86	119.28
64	AG	45	VAL	C-N-CA	5.08	124.86	119.28
24	Ba	106	VAL	N-CA-C	5.08	112.58	107.55
15	P	94	ILE	CB-CA-C	-5.07	107.35	114.00
19	U	36	SER	CA-C-N	5.07	124.86	119.28
19	U	36	SER	C-N-CA	5.07	124.86	119.28
44	w	223	ASP	CA-C-N	5.07	124.86	119.28
44	w	223	ASP	C-N-CA	5.07	124.86	119.28
20	BV	86	ASP	CA-C-N	5.07	124.73	119.56
20	BV	86	ASP	C-N-CA	5.07	124.73	119.56
12	BM	681	ALA	N-CA-C	5.07	114.84	108.45
45	Bx	378	HIS	N-CA-C	-5.07	106.26	112.90
45	x	2	PHE	N-CA-C	-5.06	105.65	111.07
15	BP	94	ILE	CB-CA-C	-5.06	107.37	114.00
9	BJ	242	VAL	N-CA-C	5.06	116.51	111.00
54	B6	9	GLN	N-CA-C	-5.06	105.66	111.07
28	e	58	ASP	CA-C-N	5.06	124.96	119.85
28	e	58	ASP	C-N-CA	5.06	124.96	119.85
52	4	22	ASN	N-CA-C	5.05	117.54	109.81
46	y	12	ALA	N-CA-C	5.05	117.48	109.96
55	7	35	GLN	N-CA-C	5.05	119.20	113.19
20	V	86	ASP	CA-C-N	5.05	124.71	119.56
20	V	86	ASP	C-N-CA	5.05	124.71	119.56
46	By	65	TRP	N-CA-C	5.05	119.15	113.15
13	BN	97	PRO	O-C-N	5.04	123.63	121.31
12	M	681	ALA	N-CA-C	5.04	114.80	108.45
62	AR	28	ASP	CA-C-N	5.04	124.83	119.28
62	AR	28	ASP	C-N-CA	5.04	124.83	119.28
46	y	65	TRP	N-CA-C	5.04	119.15	113.15
9	J	195	PHE	CA-C-N	5.04	124.82	119.28
9	J	195	PHE	C-N-CA	5.04	124.82	119.28
9	BJ	195	PHE	CA-C-N	5.04	124.82	119.28
9	BJ	195	PHE	C-N-CA	5.04	124.82	119.28
45	Bx	2	PHE	N-CA-C	-5.04	105.68	111.07
46	By	12	ALA	N-CA-C	5.04	117.46	109.96
21	BW	17	GLY	CA-C-N	5.03	124.97	119.78
21	BW	17	GLY	C-N-CA	5.03	124.97	119.78
9	J	242	VAL	N-CA-C	5.02	116.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Be	58	ASP	CA-C-N	5.02	124.95	119.78
28	Be	58	ASP	C-N-CA	5.02	124.95	119.78
2	B	67	GLY	N-CA-C	-5.02	106.71	112.73
21	W	17	GLY	CA-C-N	5.02	124.95	119.78
21	W	17	GLY	C-N-CA	5.02	124.95	119.78
45	x	487	LEU	N-CA-C	5.01	118.52	111.90
45	Bx	378	HIS	CB-CG-CD2	-5.01	124.68	131.20
45	Bx	73	ILE	N-CA-C	5.01	115.16	110.30
45	x	73	ILE	N-CA-C	5.01	115.16	110.30
12	BM	174	THR	CA-C-N	5.01	126.99	120.28
12	BM	174	THR	C-N-CA	5.01	126.99	120.28
36	Bm	173	GLY	N-CA-C	-5.00	107.77	115.73
1	A	315	LEU	N-CA-C	-5.00	108.92	114.62
36	m	173	GLY	N-CA-C	-5.00	107.78	115.73
44	w	199	LEU	CA-C-N	5.00	123.31	119.66
44	w	199	LEU	C-N-CA	5.00	123.31	119.66
1	BA	315	LEU	N-CA-C	-5.00	108.92	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	Bw	338	LYS	Peptide
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	214	0
1	BA	3322	0	3289	207	0
2	B	1420	0	1371	118	0
2	BB	1420	0	1371	123	0
3	BC	1249	0	1253	84	0
3	C	1249	0	1253	88	0
4	BE	968	0	982	64	0
4	E	968	0	982	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	670	0	679	38	0
5	F	670	0	679	37	0
6	BG	672	0	650	31	0
6	BX	686	0	676	36	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	BH	922	0	950	58	0
7	H	922	0	950	58	0
8	BI	769	0	788	47	0
8	I	769	0	788	47	0
9	BJ	2712	0	2757	234	0
9	J	2712	0	2757	234	0
10	BK	274	0	257	23	0
10	K	274	0	257	22	0
11	BL	964	0	962	63	0
11	L	964	0	962	63	0
12	BM	5274	0	5312	338	0
12	M	5274	0	5312	334	0
13	BN	1195	0	1155	50	0
13	N	1195	0	1155	49	0
14	BO	1643	0	1646	110	0
14	O	1643	0	1646	113	0
15	BP	1730	0	1685	116	0
15	P	1730	0	1685	115	0
16	BQ	3460	0	3419	309	0
16	Q	3460	0	3419	309	0
17	BS	568	0	567	43	0
17	S	568	0	567	44	0
18	BT	742	0	723	43	0
18	T	742	0	723	42	0
19	BU	647	0	653	16	0
19	U	647	0	653	15	0
20	BV	1038	0	1027	36	0
20	V	1038	0	1027	36	0
21	BW	1135	0	1129	62	0
21	W	1135	0	1129	62	0
22	BY	533	0	475	102	0
22	Y	533	0	475	99	0
23	BZ	648	0	627	19	0
23	Z	648	0	627	18	0
24	Ba	1174	0	1177	103	0
24	a	1174	0	1177	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Bb	1059	0	1079	123	0
25	b	1059	0	1079	126	0
26	Bc	1236	0	1092	87	0
26	c	1236	0	1092	82	0
27	Bd	1418	0	1375	119	0
27	d	1418	0	1375	118	0
28	Be	810	0	772	34	0
28	e	810	0	772	36	0
29	Bf	405	0	407	18	0
29	f	405	0	407	18	0
30	Bg	1004	0	1008	66	0
30	g	1004	0	1008	68	0
31	Bh	863	0	861	64	0
31	h	863	0	861	66	0
32	Bi	2735	0	2893	194	0
32	i	2735	0	2893	186	0
33	Bj	919	0	968	87	0
33	j	919	0	968	84	0
34	Bk	740	0	792	92	0
34	k	740	0	792	92	0
35	Bl	4717	0	4893	410	0
35	l	4717	0	4893	409	0
36	Bm	1313	0	1330	129	0
36	m	1313	0	1330	129	0
37	Bn	473	0	480	29	0
37	n	473	0	480	29	0
38	Bo	1066	0	1086	66	0
38	o	1063	0	1082	62	0
39	Bp	1495	0	1440	118	0
39	p	1495	0	1440	106	0
40	Br	3629	0	3825	162	0
40	r	3629	0	3825	161	0
41	Bs	2509	0	2617	168	0
41	s	2509	0	2617	168	0
42	Bu	1394	0	1367	64	0
42	u	1394	0	1367	60	0
43	Bv	921	0	892	91	0
43	v	921	0	892	89	0
44	Bw	2474	0	2304	120	0
44	w	2474	0	2304	119	0
45	Bx	4025	0	4003	88	0
45	x	4025	0	4003	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	By	1822	0	1834	73	0
46	y	1822	0	1834	72	0
47	Bz	2124	0	2042	52	0
47	z	2124	0	2042	52	0
48	0	1195	0	1183	33	0
48	B0	1195	0	1183	31	0
49	1	878	0	868	22	0
49	B1	878	0	868	23	0
50	2	748	0	728	23	0
50	B2	748	0	728	27	0
51	3	672	0	645	29	0
51	B3	672	0	645	29	0
52	4	628	0	582	21	0
52	B4	628	0	582	21	0
53	5	598	0	612	17	0
53	B5	598	0	612	14	0
54	6	441	0	439	28	0
54	B6	441	0	439	27	0
55	7	384	0	366	12	0
55	B7	384	0	366	12	0
56	8	386	0	388	8	0
56	B8	386	0	388	8	0
57	9	335	0	352	14	0
57	B9	335	0	352	13	0
58	AA	694	0	683	47	0
58	AN	687	0	676	30	0
59	AB	413	0	438	25	0
59	AO	409	0	432	24	0
60	AC	1521	0	1505	56	0
60	AP	1521	0	1505	64	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	23	0
62	AE	580	0	526	54	0
62	AR	580	0	526	33	0
63	AF	921	0	909	74	0
63	AS	921	0	910	30	0
64	AG	425	0	422	13	0
64	AT	425	0	422	30	0
65	AH	1924	0	1874	62	0
65	AU	1924	0	1874	80	0
66	AJ	3009	0	3065	114	0
66	AV	3009	0	3065	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	AK	3159	0	3130	160	0
67	AW	3162	0	3139	124	0
68	AL	3442	0	3357	174	0
68	AY	3428	0	3326	206	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	BA	8	0	0	6	0
69	BB	16	0	0	3	0
69	BC	8	0	0	0	0
69	BM	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	4	0
70	A	31	0	19	17	0
70	BA	31	0	19	16	0
71	AL	52	0	88	4	0
71	AN	52	0	88	10	0
71	AQ	52	0	88	9	0
71	AT	52	0	88	2	0
71	B	52	0	88	4	0
71	BB	52	0	88	4	0
71	BU	52	0	88	2	0
71	BV	52	0	88	4	0
71	Bb	52	0	88	35	0
71	Bg	156	0	264	14	0
71	Br	104	0	176	24	0
71	U	52	0	88	2	0
71	b	52	0	88	36	0
71	g	156	0	264	13	0
71	r	104	0	176	23	0
72	BE	35	0	0	4	0
72	Bp	35	0	0	13	0
72	E	35	0	0	4	0
72	p	35	0	0	12	0
73	BJ	48	0	26	26	0
73	J	48	0	26	26	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	BM	4	0	0	1	0
74	BO	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	AG	64	0	72	29	0
75	AH	64	0	72	8	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	24	0
75	AN	64	0	72	9	0
75	AU	64	0	72	11	0
75	AY	64	0	72	6	0
75	BV	63	0	68	6	0
75	Bi	64	0	72	2	0
75	Bl	128	0	144	5	0
75	Bn	64	0	72	10	0
75	V	63	0	68	8	0
75	i	64	0	72	2	0
75	l	128	0	144	4	0
75	n	64	0	72	10	0
76	AH	49	0	75	32	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	39	0
76	AU	41	0	56	24	0
76	AV	49	0	75	23	0
76	AY	49	0	75	21	0
76	BV	51	0	82	21	0
76	BW	51	0	82	20	0
76	Bl	100	0	157	67	0
76	V	51	0	82	22	0
76	W	51	0	82	20	0
76	l	100	0	157	66	0
77	Bx	1	0	0	0	0
77	By	2	0	0	0	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	Bx	1	0	0	0	0
78	x	1	0	0	0	0
79	Bx	120	0	108	4	0
79	x	120	0	108	4	0
80	2	1	0	0	0	0
80	B2	1	0	0	0	0
81	AH	43	0	32	5	0
81	AU	43	0	32	7	0
82	AJ	86	0	60	8	0
82	AV	86	0	60	13	0
All	All	196753	0	197037	9753	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 25.

All (9753) 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)
35:Bl:533:MET:CE	76:Bl:702:PEE:H36	1.25	1.65
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.64
35:l:533:MET:CE	76:l:702:PEE:H36	1.25	1.64
24:Ba:55:PHE:CE2	39:Bp:118:TYR:CE2	1.82	1.64
63:AF:29:LYS:CG	63:AF:75:ILE:HD11	1.16	1.63
68:AY:296:TRP:CD1	68:AY:419:THR:CG2	1.74	1.60
75:AJ:405:CDL:H112	76:AY:502:PEE:C45	1.18	1.57
63:AF:29:LYS:CD	63:AF:75:ILE:HD11	1.30	1.56
24:Ba:55:PHE:CE2	39:Bp:118:TYR:CD2	1.92	1.56
24:a:55:PHE:CE2	39:p:118:TYR:CD2	1.92	1.55
32:Bi:288:LEU:CD2	76:Bl:701:PEE:H58	1.37	1.53
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.53
35:Bl:37:LYS:HE2	35:Bl:98:TRP:CD1	1.40	1.53
32:i:288:LEU:CD2	76:l:701:PEE:H58	1.37	1.50
68:AY:296:TRP:CD1	68:AY:419:THR:HG23	0.99	1.49
68:AY:296:TRP:NE1	68:AY:419:THR:CG2	1.73	1.49
63:AF:29:LYS:HG2	63:AF:75:ILE:CD1	1.40	1.48
35:Bl:533:MET:HE1	76:Bl:702:PEE:C22	1.41	1.48
24:Ba:55:PHE:HE2	39:Bp:118:TYR:CE2	1.17	1.48
24:a:55:PHE:HE2	39:p:118:TYR:CE2	1.17	1.48
24:a:98:LEU:HB3	27:d:57:TYR:CE1	1.45	1.48
35:l:533:MET:HE1	76:l:702:PEE:C22	1.41	1.47
24:Ba:98:LEU:HB3	27:Bd:57:TYR:CE1	1.45	1.47
9:BJ:130:ILE:HG23	73:BJ:401:NDP:C8A	1.45	1.47
35:l:571:ILE:CD1	76:l:701:PEE:O5	1.64	1.45
12:M:134:GLY:HA2	69:M:801:SF4:S3	1.57	1.44
12:BM:134:GLY:HA2	69:BM:801:SF4:S3	1.57	1.44
60:AC:150:ALA:CB	66:AV:168:TYR:HE2	1.29	1.43
9:J:130:ILE:HG23	73:J:401:NDP:C8A	1.45	1.43
35:Bl:84:TYR:CD1	35:Bl:88:MET:HE2	1.54	1.42
35:Bl:571:ILE:CD1	76:Bl:701:PEE:O5	1.64	1.42
63:AF:29:LYS:CD	63:AF:75:ILE:CD1	1.97	1.42
58:AA:78:TYR:CB	62:AE:65:GLU:HG2	1.48	1.42
35:l:84:TYR:CD1	35:l:88:MET:HE2	1.54	1.41
58:AA:78:TYR:HB3	62:AE:65:GLU:CG	1.50	1.40
35:Bl:84:TYR:CE1	35:Bl:88:MET:CE	2.05	1.40
60:AC:150:ALA:CB	66:AV:168:TYR:CE2	2.05	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:84:TYR:CE1	35:l:88:MET:CE	2.05	1.39
68:AY:80:ARG:NH2	68:AY:265:LEU:HD23	1.33	1.38
63:AF:29:LYS:CG	63:AF:75:ILE:CD1	1.96	1.35
60:AC:150:ALA:HB3	66:AV:168:TYR:CE2	1.61	1.34
66:AV:10:LEU:HD21	76:AY:502:PEE:C27	1.60	1.32
9:BJ:171:ASN:O	9:BJ:181:LEU:HD21	1.23	1.32
16:BQ:262:LEU:HD22	16:BQ:268:TRP:CD1	1.64	1.31
68:AY:296:TRP:HE1	68:AY:419:THR:CB	1.42	1.31
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.31
75:AL:502:CDL:C57	76:AL:503:PEE:H63	1.61	1.31
66:AV:14:ILE:CD1	76:AY:502:PEE:H41	1.58	1.31
32:Bi:288:LEU:HD23	76:Bl:701:PEE:C36	1.60	1.30
32:i:288:LEU:HD23	76:l:701:PEE:C36	1.60	1.30
35:Bl:447:ASN:OD1	35:Bl:448:PRO:HD2	1.30	1.30
24:Ba:55:PHE:HE2	39:Bp:118:TYR:CD2	1.32	1.29
75:Aj:405:CDL:C11	76:AY:502:PEE:C45	2.08	1.29
67:AK:259:ARG:CG	67:AK:444:LEU:HD13	1.60	1.29
68:AY:296:TRP:NE1	68:AY:419:THR:OG1	1.64	1.29
35:l:84:TYR:CE1	35:l:88:MET:HE2	1.64	1.28
68:AY:80:ARG:HH22	68:AY:265:LEU:CD2	1.44	1.28
24:Ba:98:LEU:CB	27:Bd:57:TYR:HE1	1.46	1.28
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CE2	2.22	1.27
35:l:447:ASN:OD1	35:l:448:PRO:HD2	1.30	1.27
24:a:55:PHE:CD2	39:p:118:TYR:CE2	2.22	1.27
9:BJ:206:ILE:HA	9:BJ:240:VAL:O	1.35	1.27
58:AA:78:TYR:CD1	62:AE:65:GLU:HA	1.69	1.26
24:a:98:LEU:CB	27:d:57:TYR:HE1	1.46	1.26
16:BQ:82:LEU:O	16:BQ:98:VAL:HG13	1.25	1.26
16:Q:82:LEU:O	16:Q:98:VAL:HG13	1.24	1.24
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.24
65:AU:308:ARG:NH1	75:AU:403:CDL:O1	1.70	1.24
35:l:188:TRP:CE2	35:l:192:HIS:HD2	1.54	1.24
35:Bl:188:TRP:CE2	35:Bl:192:HIS:HD2	1.53	1.24
9:J:206:ILE:HA	9:J:240:VAL:O	1.34	1.23
35:Bl:84:TYR:CE1	35:Bl:88:MET:HE2	1.64	1.23
9:J:130:ILE:HG23	73:J:401:NDP:N7A	1.52	1.23
22:BY:84:PHE:CE2	35:Bl:483:PRO:HG3	1.74	1.23
76:AU:401:PEE:H17	66:AV:240:MET:CE	1.68	1.23
16:Q:271:ARG:NH1	41:s:281:ARG:HB2	1.52	1.23
22:Y:84:PHE:CE2	35:l:483:PRO:HG3	1.74	1.23
9:BJ:130:ILE:HG23	73:BJ:401:NDP:N7A	1.52	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:55:PHE:HE2	39:p:118:TYR:CD2	1.32	1.22
16:BQ:271:ARG:NH1	41:Bs:281:ARG:HB2	1.52	1.22
22:Y:87:PRO:HB3	43:v:103:GLU:OE2	1.38	1.20
35:Bl:37:LYS:CE	35:Bl:98:TRP:CD1	2.24	1.20
64:AT:42:LEU:O	64:AT:45:VAL:HG22	1.41	1.19
35:l:37:LYS:CE	35:l:98:TRP:CD1	2.24	1.19
68:AY:296:TRP:NE1	68:AY:419:THR:CB	2.03	1.19
76:AH:401:PEE:H18	66:Aj:240:MET:CE	1.70	1.19
22:BY:87:PRO:HB3	43:Bv:103:GLU:OE2	1.38	1.19
24:a:55:PHE:CD2	39:p:118:TYR:CZ	2.30	1.18
24:a:55:PHE:HD2	39:p:118:TYR:CZ	1.62	1.18
35:l:226:GLN:HE21	35:l:314:MET:CE	1.56	1.18
22:Y:72:ARG:NH1	35:l:390:TYR:OH	1.76	1.18
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CZ	2.30	1.18
9:J:206:ILE:O	9:J:211:ASP:OD2	1.61	1.18
9:BJ:206:ILE:O	9:BJ:211:ASP:OD2	1.61	1.18
22:BY:72:ARG:NH1	35:Bl:390:TYR:OH	1.76	1.18
75:AL:502:CDL:H572	76:AL:503:PEE:C40	1.73	1.18
35:Bl:84:TYR:CE1	35:Bl:88:MET:HE3	1.74	1.18
16:BQ:268:TRP:CZ3	16:BQ:272:THR:HG21	1.80	1.17
9:J:171:ASN:C	9:J:181:LEU:HD21	1.68	1.17
76:V:202:PEE:H70	76:l:701:PEE:C45	1.74	1.17
76:BV:202:PEE:H70	76:Bl:701:PEE:C45	1.75	1.17
35:Bl:226:GLN:HE21	35:Bl:314:MET:CE	1.56	1.17
76:V:202:PEE:C42	76:l:701:PEE:C45	2.23	1.17
9:BJ:171:ASN:C	9:BJ:181:LEU:HD21	1.69	1.17
35:l:84:TYR:CE1	35:l:88:MET:HE3	1.74	1.16
16:Q:268:TRP:CZ3	16:Q:272:THR:HG21	1.80	1.16
76:W:201:PEE:H75	41:s:77:LEU:CD2	1.75	1.16
1:A:93:PHE:CE2	1:A:98:LYS:HD3	1.80	1.16
32:i:291:TYR:CE2	76:l:701:PEE:C31	2.29	1.16
9:J:171:ASN:O	9:J:181:LEU:CD2	1.92	1.16
1:BA:93:PHE:CE2	1:BA:98:LYS:HD3	1.80	1.15
24:Ba:55:PHE:HD2	39:Bp:118:TYR:CZ	1.61	1.15
35:l:188:TRP:CE2	35:l:192:HIS:CD2	2.33	1.15
32:Bi:291:TYR:CE2	76:Bl:701:PEE:C31	2.29	1.15
35:Bl:188:TRP:CE2	35:Bl:192:HIS:CD2	2.33	1.15
39:p:167:TRP:O	39:p:171:VAL:HG23	1.47	1.15
35:Bl:533:MET:SD	76:Bl:702:PEE:H36	1.86	1.15
39:p:56:ASP:CB	68:AY:227:PRO:HG3	1.75	1.15
75:AG:101:CDL:HA62	75:AG:101:CDL:H332	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:98:PHE:CE2	68:AY:120:LEU:CD1	2.29	1.15
76:BV:202:PEE:C42	76:Bl:701:PEE:C45	2.23	1.15
76:BW:201:PEE:H75	41:Bs:77:LEU:CD2	1.75	1.15
35:l:533:MET:SD	76:l:702:PEE:H36	1.86	1.14
76:W:201:PEE:H75	41:s:77:LEU:HD21	1.19	1.14
4:E:25:MET:HB3	4:E:29:LYS:CE	1.77	1.14
9:BJ:171:ASN:O	9:BJ:181:LEU:CD2	1.92	1.14
39:Bp:167:TRP:O	39:Bp:171:VAL:HG23	1.47	1.14
63:AF:29:LYS:HD3	63:AF:75:ILE:CD1	1.64	1.14
66:AV:10:LEU:CD2	76:AY:502:PEE:H46	1.79	1.13
4:BE:25:MET:HB3	4:BE:29:LYS:CE	1.77	1.13
22:BY:84:PHE:CD1	22:BY:85:PRO:HD3	1.84	1.13
22:Y:84:PHE:CD1	22:Y:85:PRO:HD3	1.83	1.13
64:AT:40:LEU:HD12	64:AT:41:ILE:N	1.63	1.12
9:J:130:ILE:HG23	73:J:401:NDP:H8A	1.28	1.12
76:BW:201:PEE:H75	41:Bs:77:LEU:HD21	1.20	1.11
27:Bd:59:HIS:CE1	28:Be:120:ARG:HB3	1.84	1.11
58:AA:37:ASN:OD1	58:AA:40:ARG:NH2	1.83	1.11
75:AL:502:CDL:H571	76:AL:503:PEE:H63	1.12	1.11
27:d:59:HIS:CE1	28:e:120:ARG:HB3	1.84	1.11
9:BJ:130:ILE:HG23	73:BJ:401:NDP:H8A	1.28	1.11
35:l:84:TYR:CD1	35:l:88:MET:CE	2.30	1.10
68:AL:259:GLU:HB3	38:Bo:30:ARG:NE	1.66	1.10
4:BE:25:MET:HB3	4:BE:29:LYS:HE3	1.32	1.10
16:Q:78:LYS:NZ	33:j:48:ARG:HH21	1.49	1.10
24:a:96:ALA:HB3	27:d:55:TYR:HB2	1.33	1.10
25:b:110:ILE:HG23	25:b:111:LEU:HG	1.24	1.10
75:AL:502:CDL:C57	76:AL:503:PEE:H66	1.80	1.10
16:BQ:78:LYS:NZ	33:Bj:48:ARG:HH21	1.49	1.10
34:Bk:4:ILE:HD11	36:Bm:125:MET:SD	1.90	1.10
24:Ba:114:LYS:HB2	27:Bd:57:TYR:CE2	1.88	1.09
32:i:285:ILE:HG12	76:l:701:PEE:H75	1.35	1.09
34:k:4:ILE:HD11	36:m:125:MET:SD	1.91	1.09
35:Bl:84:TYR:HE1	35:Bl:88:MET:CE	1.50	1.09
22:Y:84:PHE:CZ	35:l:483:PRO:HG3	1.88	1.09
22:BY:84:PHE:CZ	35:Bl:483:PRO:HG3	1.88	1.09
24:a:98:LEU:CB	27:d:57:TYR:CE1	2.25	1.09
26:c:181:VAL:CB	43:v:37:ARG:HH21	1.66	1.09
35:l:37:LYS:CE	35:l:98:TRP:HD1	1.64	1.09
24:a:114:LYS:HB2	27:d:57:TYR:CE2	1.88	1.08
68:AL:218:GLU:OE2	38:Bo:27:PRO:HG2	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Bi:285:ILE:HG12	76:Bl:701:PEE:H75	1.35	1.08
35:l:54:PHE:CE1	35:l:58:ASP:OD1	2.06	1.08
68:AY:296:TRP:NE1	68:AY:419:THR:HG21	1.57	1.08
12:BM:134:GLY:CA	69:BM:801:SF4:S3	2.42	1.08
25:Bb:110:ILE:HG23	25:Bb:111:LEU:HG	1.24	1.07
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
75:AG:101:CDL:H712	75:AG:101:CDL:H531	1.32	1.07
26:Bc:181:VAL:CB	43:Bv:37:ARG:HH21	1.66	1.07
22:Y:71:TRP:CH2	22:Y:75:HIS:CD2	2.42	1.07
24:Ba:96:ALA:HB3	27:Bd:55:TYR:HB2	1.33	1.07
35:l:54:PHE:CZ	35:l:58:ASP:OD1	2.07	1.07
35:l:84:TYR:HE1	35:l:88:MET:CE	1.51	1.07
71:r:502:PLX:H332	71:r:502:PLX:H372	1.37	1.07
35:l:227:LEU:O	35:l:230:HIS:ND1	1.88	1.06
76:AL:503:PEE:H19	76:AL:503:PEE:H49	1.11	1.06
35:Bl:37:LYS:CE	35:Bl:98:TRP:HD1	1.64	1.06
35:Bl:54:PHE:CE1	35:Bl:58:ASP:OD1	2.06	1.06
71:Br:502:PLX:H332	71:Br:502:PLX:H372	1.37	1.06
12:M:134:GLY:CA	69:M:801:SF4:S3	2.42	1.06
22:BY:71:TRP:CH2	22:BY:75:HIS:CD2	2.42	1.06
60:AC:150:ALA:HB1	66:AV:168:TYR:CE2	1.80	1.06
35:Bl:54:PHE:CZ	35:Bl:58:ASP:OD1	2.07	1.06
35:Bl:227:LEU:O	35:Bl:230:HIS:ND1	1.88	1.06
58:AA:78:TYR:HE1	62:AE:64:GLU:O	1.36	1.06
24:Ba:98:LEU:CB	27:Bd:57:TYR:CE1	2.25	1.06
67:AK:259:ARG:HG3	67:AK:444:LEU:HD13	1.27	1.06
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.05
44:w:332:ARG:O	44:w:338:LYS:HA	1.55	1.05
58:AA:78:TYR:CE1	62:AE:64:GLU:O	2.09	1.05
65:AU:296:MET:CE	76:AU:401:PEE:H53	1.86	1.05
44:Bw:332:ARG:O	44:Bw:338:LYS:HA	1.55	1.05
62:AE:34:ARG:HD3	62:AE:78:ARG:NH2	1.71	1.05
27:Bd:105:LYS:CE	35:Bl:197:ASP:OD2	2.04	1.05
27:d:81:GLU:OE1	37:n:43:MET:HE3	1.57	1.05
68:AY:98:PHE:CE2	68:AY:120:LEU:HD13	1.87	1.05
34:k:7:ASN:HD21	36:m:9:SER:C	1.65	1.05
24:a:55:PHE:HD2	39:p:118:TYR:CE1	1.74	1.04
67:AK:259:ARG:HH21	67:AK:259:ARG:HB2	1.22	1.04
27:Bd:81:GLU:OE1	37:Bn:43:MET:HE3	1.57	1.04
27:d:105:LYS:CE	35:l:197:ASP:OD2	2.04	1.04
62:AR:34:ARG:HG3	62:AR:78:ARG:NH1	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:221:HIS:CE1	9:BJ:222:ARG:HG3	1.91	1.04
24:Ba:55:PHE:HD2	39:Bp:118:TYR:CE1	1.74	1.04
34:Bk:1:MET:N	34:Bk:1:MET:SD	2.30	1.04
35:Bl:84:TYR:HE1	35:Bl:88:MET:HE3	1.08	1.04
16:Q:82:LEU:O	16:Q:98:VAL:CG1	2.06	1.04
6:X:112:SER:CA	72:p:201:8Q1:O2	2.06	1.04
35:l:84:TYR:HE1	35:l:88:MET:HE3	1.08	1.04
27:d:105:LYS:NZ	35:l:197:ASP:OD2	1.91	1.03
63:AF:29:LYS:HG2	63:AF:75:ILE:CG1	1.87	1.03
76:AU:401:PEE:H17	66:AV:240:MET:HE1	1.05	1.03
35:Bl:84:TYR:CD1	35:Bl:88:MET:CE	2.30	1.03
39:Bp:170:ILE:HD12	39:Bp:170:ILE:H	1.24	1.03
6:BX:112:SER:CA	72:Bp:201:8Q1:O2	2.06	1.03
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	1.03
67:AK:438:MET:HE2	67:AK:450:VAL:HG13	1.39	1.03
35:l:571:ILE:HD11	76:l:701:PEE:C30	1.89	1.02
65:AU:288:MET:HB3	76:AU:401:PEE:O4	1.57	1.02
66:AV:14:ILE:HD12	76:AY:502:PEE:H41	1.41	1.02
35:Bl:25:ASN:O	35:Bl:25:ASN:ND2	1.91	1.02
35:Bl:97:THR:HG21	35:Bl:125:LEU:HD12	1.35	1.02
64:AG:38:TRP:CD1	75:AG:101:CDL:H511	1.94	1.02
34:Bk:7:ASN:HD21	36:Bm:9:SER:C	1.65	1.02
35:Bl:534:HIS:ND1	76:Bl:702:PEE:H14	1.74	1.02
9:J:176:SER:HA	9:J:182:ARG:HH21	1.24	1.02
35:l:97:THR:HG21	35:l:125:LEU:HD12	1.35	1.02
76:AH:401:PEE:H73	76:AH:401:PEE:H64	1.42	1.02
58:AN:43:ARG:NH1	71:AN:101:PLX:H1B2	1.71	1.02
16:BQ:82:LEU:O	16:BQ:98:VAL:CG1	2.06	1.02
27:Bd:105:LYS:NZ	35:Bl:197:ASP:OD2	1.91	1.02
22:Y:71:TRP:CH2	22:Y:75:HIS:HD2	1.76	1.02
4:BE:25:MET:CB	4:BE:29:LYS:HE3	1.89	1.02
24:a:96:ALA:CB	27:d:55:TYR:HB2	1.90	1.01
16:BQ:69:VAL:O	16:BQ:72:PRO:HD2	1.58	1.01
35:Bl:51:THR:HG21	35:Bl:91:PRO:HG2	1.42	1.01
16:Q:78:LYS:NZ	33:j:48:ARG:NH2	2.08	1.01
35:l:25:ASN:ND2	35:l:25:ASN:O	1.91	1.01
39:p:56:ASP:HB2	68:AY:227:PRO:CG	1.89	1.01
16:Q:69:VAL:O	16:Q:72:PRO:HD2	1.58	1.01
35:l:534:HIS:ND1	76:l:702:PEE:H14	1.74	1.01
39:p:48:PHE:HE1	72:p:201:8Q1:C8	1.73	1.01
75:AG:101:CDL:H712	75:AG:101:CDL:C53	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:176:SER:HA	9:BJ:182:ARG:HH21	1.24	1.01
24:Ba:96:ALA:CB	27:Bd:55:TYR:HB2	1.89	1.01
35:Bl:571:ILE:HD11	76:Bl:701:PEE:C30	1.89	1.01
39:Bp:48:PHE:HE1	72:Bp:201:8Q1:C8	1.73	1.01
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.25	1.01
34:k:1:MET:N	34:k:1:MET:SD	2.30	1.01
66:AJ:156:ILE:HG22	66:AJ:160:LEU:HB2	1.42	1.01
67:AK:257:GLU:OE2	67:AK:450:VAL:N	1.92	1.01
68:AL:259:GLU:HB3	38:Bo:30:ARG:HE	1.25	1.01
16:BQ:271:ARG:HH11	41:Bs:281:ARG:HB2	1.18	1.01
22:BY:71:TRP:CH2	22:BY:75:HIS:HD2	1.76	1.01
35:Bl:226:GLN:HG3	35:Bl:280:LEU:CD2	1.91	1.01
35:Bl:571:ILE:HD11	76:Bl:701:PEE:O5	0.84	1.01
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.00
65:AH:121:CYS:SG	81:AH:402:HEC:HBB2	2.01	1.00
9:J:130:ILE:CG2	73:J:401:NDP:N7A	2.24	1.00
76:Bl:701:PEE:H37	40:Br:155:VAL:HB	1.42	1.00
35:l:51:THR:HG21	35:l:91:PRO:HG2	1.42	1.00
62:AR:34:ARG:NH1	62:AR:78:ARG:HH12	1.59	1.00
16:BQ:262:LEU:HD22	16:BQ:268:TRP:HD1	1.23	1.00
35:Bl:533:MET:HE1	76:Bl:702:PEE:H35	1.44	1.00
35:Bl:222:GLY:CA	35:Bl:229:LEU:HD12	1.91	1.00
35:l:226:GLN:HG3	35:l:280:LEU:CD2	1.91	0.99
35:l:571:ILE:HD11	76:l:701:PEE:O5	0.84	0.99
1:BA:116:ASN:ND2	70:BA:502:FMN:C8	2.25	0.99
16:BQ:78:LYS:NZ	33:Bj:48:ARG:NH2	2.08	0.99
32:i:291:TYR:CE2	76:l:701:PEE:H48	1.95	0.99
32:Bi:291:TYR:CZ	76:Bl:701:PEE:H49	1.97	0.99
35:Bl:59:GLN:HE21	35:Bl:59:GLN:HA	1.23	0.99
35:Bl:193:SER:OG	35:Bl:205:ASN:ND2	1.95	0.99
32:i:291:TYR:CZ	76:l:701:PEE:H49	1.97	0.99
9:BJ:130:ILE:CG2	73:BJ:401:NDP:N7A	2.24	0.99
35:l:222:GLY:CA	35:l:229:LEU:HD12	1.91	0.99
76:Bl:701:PEE:H37	40:Br:155:VAL:CB	1.93	0.99
76:V:202:PEE:C25	76:V:202:PEE:H60	1.92	0.99
35:l:84:TYR:HD1	35:l:88:MET:HE2	1.20	0.99
76:l:701:PEE:H37	40:r:155:VAL:CB	1.93	0.99
62:AE:30:LEU:HD11	62:AE:34:ARG:HH21	1.26	0.99
67:AW:351:ILE:HD11	67:AW:448:PRO:HD2	1.44	0.99
34:k:7:ASN:HD22	36:m:9:SER:CB	1.75	0.99
35:l:59:GLN:HA	35:l:59:GLN:HE21	1.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Bl:701:PEE:H36	40:Br:155:VAL:HG11	1.44	0.99
1:A:116:ASN:ND2	70:A:502:FMN:C8	2.25	0.99
39:p:170:ILE:H	39:p:170:ILE:HD12	1.24	0.98
76:BV:202:PEE:C25	76:BV:202:PEE:H60	1.92	0.98
9:J:130:ILE:CG2	73:J:401:NDP:C8A	2.41	0.98
9:BJ:141:PHE:CE2	9:BJ:180:TYR:HA	1.98	0.98
25:Bb:107:GLY:N	25:Bb:115:GLU:OE1	1.96	0.98
62:AR:79:ASP:OD2	65:AU:236:TYR:OH	1.79	0.98
32:Bi:291:TYR:CE2	76:Bl:701:PEE:H48	1.95	0.98
34:Bk:7:ASN:HD22	36:Bm:9:SER:CB	1.75	0.98
25:b:107:GLY:N	25:b:115:GLU:OE1	1.96	0.98
16:Q:53:TYR:HE1	76:l:701:PEE:O1P	1.44	0.98
76:AH:401:PEE:C13	66:AJ:240:MET:CE	2.42	0.98
16:BQ:53:TYR:HE1	76:Bl:701:PEE:O1P	1.44	0.98
35:Bl:84:TYR:HD1	35:Bl:88:MET:HE2	1.20	0.98
66:AV:14:ILE:HD13	76:AY:502:PEE:H41	1.45	0.98
24:a:55:PHE:CD2	39:p:118:TYR:CD2	2.49	0.98
75:AG:101:CDL:HA62	75:AG:101:CDL:C33	1.94	0.98
9:J:141:PHE:CE2	9:J:180:TYR:HA	1.98	0.98
76:l:701:PEE:C22	40:r:155:VAL:HG11	1.94	0.98
9:BJ:130:ILE:CG2	73:BJ:401:NDP:C8A	2.41	0.98
9:BJ:217:PHE:HZ	9:BJ:322:MET:HE2	1.25	0.97
25:Bb:93:LYS:HE3	35:Bl:65:ASN:O	1.64	0.97
35:l:231:PRO:O	35:l:234:PRO:HD2	1.64	0.97
34:Bk:4:ILE:CD1	36:Bm:125:MET:SD	2.52	0.97
76:Bl:701:PEE:C22	40:Br:155:VAL:HG11	1.94	0.97
35:l:226:GLN:NE2	35:l:314:MET:CE	2.27	0.97
35:l:533:MET:HE1	76:l:702:PEE:H35	1.44	0.97
76:AL:503:PEE:H49	76:AL:503:PEE:C14	1.95	0.97
25:b:93:LYS:HE3	35:l:65:ASN:O	1.64	0.97
35:l:193:SER:OG	35:l:205:ASN:ND2	1.95	0.97
67:AK:259:ARG:CG	67:AK:444:LEU:CD1	2.42	0.97
76:AL:503:PEE:H50	76:AL:503:PEE:H16	1.45	0.97
68:AY:296:TRP:NE1	68:AY:419:THR:HG1	1.48	0.97
1:BA:93:PHE:HE2	1:BA:98:LYS:HD3	1.17	0.97
66:AV:10:LEU:CD2	76:AY:502:PEE:C27	2.36	0.97
34:Bk:1:MET:HB3	36:Bm:125:MET:HB2	1.43	0.97
75:AL:502:CDL:C57	76:AL:503:PEE:C38	2.43	0.97
76:AL:503:PEE:H16	76:AL:503:PEE:C32	1.95	0.97
34:k:1:MET:HB3	36:m:125:MET:HB2	1.43	0.97
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CD2	2.49	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:4:ILE:CD1	36:m:125:MET:SD	2.52	0.96
9:J:171:ASN:HB3	9:J:181:LEU:HD11	1.46	0.96
39:p:44:MET:HE1	72:p:201:8Q1:C10	1.94	0.96
3:BC:137:VAL:HG21	16:BQ:87:GLN:HE21	1.29	0.96
9:BJ:171:ASN:HB3	9:BJ:181:LEU:HD11	1.46	0.96
39:Bp:44:MET:HE1	72:Bp:201:8Q1:C10	1.94	0.96
64:AT:39:ARG:HA	64:AT:51:LYS:HE3	1.45	0.96
9:BJ:206:ILE:HB	9:BJ:242:VAL:HG22	1.47	0.96
1:A:116:ASN:HD22	70:A:502:FMN:C8M	1.78	0.96
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.96
76:l:701:PEE:H36	40:r:155:VAL:HG11	1.44	0.96
45:x:365:ILE:HD12	46:y:87:MET:HE1	1.48	0.96
76:l:701:PEE:H37	40:r:155:VAL:HB	1.42	0.96
39:p:48:PHE:CE1	72:p:201:8Q1:C8	2.48	0.96
39:p:56:ASP:HB2	68:AY:227:PRO:HG3	0.99	0.96
63:AF:67:LEU:HD23	66:AJ:209:LEU:HD12	1.47	0.96
32:i:291:TYR:CE2	76:l:701:PEE:H49	2.00	0.96
3:BC:204:GLU:OE2	3:BC:206:ARG:NH1	1.98	0.96
35:Bl:226:GLN:NE2	35:Bl:314:MET:CE	2.27	0.96
35:Bl:231:PRO:O	35:Bl:234:PRO:HD2	1.64	0.96
39:Bp:48:PHE:CE1	72:Bp:201:8Q1:C8	2.49	0.96
76:AL:503:PEE:H19	76:AL:503:PEE:C31	1.96	0.96
76:BV:202:PEE:H14	32:Bi:276:LEU:CD1	1.96	0.96
76:AU:401:PEE:C13	66:AV:240:MET:HE1	1.96	0.95
58:AN:43:ARG:NH1	71:AN:101:PLX:C1B	2.29	0.95
76:V:202:PEE:H14	32:i:276:LEU:CD1	1.96	0.95
26:c:122:THR:OG1	38:o:12:ARG:NH1	1.99	0.95
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.47	0.95
67:AK:259:ARG:HG3	67:AK:444:LEU:CD1	1.97	0.95
45:Bx:365:ILE:HD12	46:By:87:MET:HE1	1.48	0.95
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.95
1:BA:116:ASN:HD22	70:BA:502:FMN:C8M	1.78	0.95
68:AY:98:PHE:CD2	68:AY:120:LEU:HD11	2.01	0.94
71:Bb:201:PLX:O9	71:Br:502:PLX:H1C3	1.67	0.94
35:l:226:GLN:CG	35:l:280:LEU:HD21	1.98	0.94
26:Bc:122:THR:OG1	38:Bo:12:ARG:NH1	1.99	0.94
32:Bi:291:TYR:CE2	76:Bl:701:PEE:H49	2.01	0.94
35:Bl:74:THR:CG2	35:Bl:194:ASN:OD1	2.14	0.94
35:Bl:533:MET:CE	76:Bl:702:PEE:C22	2.16	0.94
25:b:88:TYR:CD1	71:b:201:PLX:H1C1	2.02	0.94
68:AL:227:PRO:HG3	39:Bp:56:ASP:HB2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:BV:202:PEE:H14	32:Bi:276:LEU:HD12	1.47	0.94
24:a:176:LYS:HE2	31:h:42:GLU:HG2	1.49	0.94
71:b:201:PLX:O9	71:r:502:PLX:H1C3	1.67	0.94
35:l:74:THR:CG2	35:l:194:ASN:OD1	2.14	0.94
58:AA:78:TYR:CD1	62:AE:65:GLU:CA	2.49	0.94
22:BY:83:HIS:O	22:BY:84:PHE:HB2	1.67	0.94
3:C:137:VAL:HG21	16:Q:87:GLN:HE21	1.29	0.94
14:O:177:LEU:N	74:O:301:FES:S1	2.39	0.94
16:Q:271:ARG:HH11	41:s:281:ARG:HB2	1.18	0.94
22:Y:86:TYR:OH	43:v:100:LYS:CE	2.15	0.94
60:AC:150:ALA:HB1	66:AV:168:TYR:CD2	2.02	0.94
67:AK:259:ARG:HB2	67:AK:259:ARG:NH2	1.82	0.94
66:AV:137:GLN:HE21	66:AV:141:TRP:HE1	1.10	0.94
16:BQ:271:ARG:NH1	41:Bs:281:ARG:CB	2.30	0.94
25:Bb:88:TYR:CD1	71:Bb:201:PLX:H1C1	2.02	0.94
68:AY:152:GLN:CD	68:AY:252:GLY:HA3	1.92	0.94
16:Q:78:LYS:HZ3	33:j:48:ARG:HH21	1.13	0.94
16:Q:271:ARG:NH1	41:s:281:ARG:CB	2.30	0.94
35:Bl:226:GLN:CG	35:Bl:280:LEU:HD21	1.98	0.94
14:BO:177:LEU:N	74:BO:301:FES:S1	2.39	0.93
76:V:202:PEE:H14	32:i:276:LEU:HD12	1.47	0.93
22:Y:83:HIS:O	22:Y:84:PHE:HB2	1.67	0.93
27:d:59:HIS:HE1	28:e:120:ARG:HB3	1.24	0.93
34:k:7:ASN:ND2	36:m:9:SER:CB	2.31	0.93
76:AH:401:PEE:H18	66:AJ:240:MET:HE1	1.49	0.93
76:AL:503:PEE:C31	76:AL:503:PEE:H26	1.97	0.93
68:AY:98:PHE:CD2	68:AY:120:LEU:CD1	2.52	0.93
22:BY:86:TYR:OH	43:Bv:100:LYS:CE	2.15	0.93
62:AE:34:ARG:HD3	62:AE:78:ARG:HH22	1.30	0.93
32:i:288:LEU:CD2	76:l:701:PEE:C36	2.32	0.93
4:E:25:MET:O	4:E:29:LYS:HG3	1.69	0.93
24:Ba:176:LYS:HE2	31:Bh:42:GLU:HG2	1.49	0.93
67:AK:259:ARG:HG2	67:AK:444:LEU:HD13	1.49	0.93
4:BE:25:MET:O	4:BE:29:LYS:HG3	1.69	0.93
45:x:449:MET:SD	46:y:5:MET:HE2	2.09	0.92
27:Bd:59:HIS:HE1	28:Be:120:ARG:HB3	1.24	0.92
32:Bi:288:LEU:CD2	76:Bl:701:PEE:C36	2.32	0.92
34:Bk:7:ASN:ND2	36:Bm:9:SER:CB	2.31	0.92
32:i:167:TRP:CZ3	35:l:573:THR:CB	2.52	0.92
45:Bx:449:MET:SD	46:By:5:MET:HE2	2.10	0.92
51:B3:5:LYS:HZ3	51:B3:6:GLY:H	0.93	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AC:150:ALA:HB3	66:AV:168:TYR:HE2	0.77	0.92
27:Bd:59:HIS:CE1	28:Be:120:ARG:CB	2.53	0.92
16:Q:78:LYS:HZ3	33:j:48:ARG:NH2	1.62	0.92
63:AF:29:LYS:HD2	63:AF:75:ILE:HD11	1.52	0.92
16:BQ:85:GLY:HA3	33:Bj:39:CYS:SG	2.08	0.92
16:BQ:271:ARG:HH11	41:Bs:281:ARG:CB	1.82	0.92
25:Bb:110:ILE:HG23	25:Bb:111:LEU:CG	1.99	0.92
32:Bi:167:TRP:CZ3	35:Bl:573:THR:CB	2.52	0.92
16:Q:85:GLY:HA3	33:j:39:CYS:SG	2.08	0.92
22:Y:87:PRO:CB	43:v:103:GLU:OE2	2.17	0.92
34:Bk:3:LEU:CD2	36:Bm:117:ASN:HD21	1.83	0.92
25:b:118:PRO:O	25:b:120:MET:HG2	1.69	0.92
76:AH:401:PEE:H66	76:AH:401:PEE:H28	1.50	0.92
62:AE:29:PRO:HD3	65:AH:262:THR:HG21	1.52	0.92
67:AK:257:GLU:OE2	67:AK:450:VAL:HG22	1.70	0.92
22:BY:87:PRO:CB	43:Bv:103:GLU:OE2	2.17	0.92
24:a:114:LYS:HB2	27:d:57:TYR:HE2	1.31	0.92
25:Bb:118:PRO:O	25:Bb:120:MET:HG2	1.68	0.91
16:BQ:78:LYS:HZ3	33:Bj:48:ARG:NH2	1.68	0.91
16:Q:271:ARG:HH11	41:s:281:ARG:CB	1.82	0.91
25:b:110:ILE:HG23	25:b:111:LEU:CG	1.99	0.91
27:d:105:LYS:HE2	35:l:197:ASP:OD2	1.70	0.91
68:AL:262:VAL:O	38:Bo:24:ASN:HA	1.70	0.91
65:AU:296:MET:HE1	76:AU:401:PEE:H53	1.51	0.91
16:BQ:78:LYS:HZ3	33:Bj:48:ARG:HH21	1.19	0.91
66:AV:149:LEU:HD21	66:AV:281:LEU:HD21	1.52	0.91
1:A:116:ASN:HD22	70:A:502:FMN:C8	1.82	0.91
27:d:59:HIS:CE1	28:e:120:ARG:CB	2.53	0.91
68:AY:424:ILE:HG23	68:AY:429:TRP:HE1	1.31	0.91
24:Ba:114:LYS:HB2	27:Bd:57:TYR:HE2	1.31	0.91
27:Bd:105:LYS:HE2	35:Bl:197:ASP:OD2	1.70	0.91
35:l:227:LEU:HD12	35:l:230:HIS:ND1	1.85	0.91
22:BY:79:GLU:O	35:Bl:487:LYS:HE3	1.70	0.91
35:l:226:GLN:HG3	35:l:280:LEU:HD21	1.53	0.91
66:AV:143:ALA:O	66:AV:147:THR:OG1	1.86	0.91
35:Bl:226:GLN:CG	35:Bl:280:LEU:CD2	2.49	0.91
67:AK:257:GLU:CG	67:AK:450:VAL:HG22	1.99	0.91
68:AY:99:LYS:O	68:AY:106:GLY:HA3	1.71	0.91
9:J:169:HIS:HD2	73:J:401:NDP:H5N	1.34	0.91
9:BJ:169:HIS:HD2	73:BJ:401:NDP:H5N	1.34	0.91
35:l:447:ASN:OD1	35:l:448:PRO:CD	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:260:ASP:OD2	39:Bp:12:HIS:N	2.03	0.90
35:l:37:LYS:HE3	35:l:102:GLU:HG3	1.53	0.90
32:i:291:TYR:HE2	76:l:701:PEE:H48	1.32	0.90
22:BY:96:GLU:OE2	26:Bc:185:GLU:O	1.89	0.90
34:k:7:ASN:ND2	36:m:9:SER:HB2	1.86	0.90
16:Q:400:ILE:HB	16:Q:407:PHE:HB3	1.54	0.90
22:Y:79:GLU:O	35:l:487:LYS:HE3	1.70	0.90
7:H:45:ARG:NH1	7:H:49:GLU:OE2	2.05	0.90
9:J:360:ARG:HA	36:m:78:TYR:CE1	2.07	0.90
35:l:533:MET:CE	76:l:702:PEE:C22	2.16	0.90
66:AV:14:ILE:CD1	76:AY:502:PEE:C25	2.49	0.90
34:Bk:7:ASN:ND2	36:Bm:9:SER:HB2	1.86	0.90
76:l:701:PEE:H37	40:r:155:VAL:CG1	2.02	0.90
34:k:3:LEU:CD2	36:m:117:ASN:HD21	1.83	0.90
35:l:51:THR:HG21	35:l:91:PRO:CG	2.02	0.90
1:BA:116:ASN:HD22	70:BA:502:FMN:C8	1.82	0.90
9:BJ:360:ARG:HA	36:Bm:78:TYR:CE1	2.07	0.90
16:BQ:400:ILE:HB	16:BQ:407:PHE:HB3	1.54	0.90
35:Bl:227:LEU:HD12	35:Bl:230:HIS:ND1	1.85	0.90
76:Bl:701:PEE:H37	40:Br:155:VAL:CG1	2.02	0.90
71:b:201:PLX:H1C3	71:b:201:PLX:C3	2.01	0.89
40:r:78:MET:O	40:r:432:ARG:NH1	2.05	0.89
51:3:5:LYS:HZ3	51:3:6:GLY:H	0.93	0.89
7:BH:45:ARG:NH1	7:BH:49:GLU:OE2	2.05	0.89
32:Bi:167:TRP:HZ3	35:Bl:570:GLN:HA	1.38	0.89
35:Bl:78:LEU:HD21	35:Bl:80:PHE:CE1	2.07	0.89
35:Bl:447:ASN:OD1	35:Bl:448:PRO:CD	2.19	0.89
26:c:169:GLU:OE2	43:v:56:ARG:NH2	2.05	0.89
32:Bi:291:TYR:HE2	76:Bl:701:PEE:H48	1.32	0.89
35:l:78:LEU:HD21	35:l:80:PHE:CE1	2.07	0.89
35:l:226:GLN:CG	35:l:280:LEU:CD2	2.49	0.89
9:BJ:141:PHE:CZ	9:BJ:180:TYR:HA	2.07	0.89
32:i:167:TRP:HZ3	35:l:570:GLN:HA	1.38	0.89
76:AH:401:PEE:H18	66:AJ:240:MET:SD	2.12	0.89
9:BJ:171:ASN:CB	9:BJ:181:LEU:HD11	2.02	0.89
9:BJ:212:ARG:HG2	9:BJ:212:ARG:HH11	1.37	0.89
26:Bc:169:GLU:OE2	43:Bv:56:ARG:NH2	2.05	0.89
35:Bl:51:THR:HG21	35:Bl:91:PRO:CG	2.02	0.89
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.89
9:J:212:ARG:HG2	9:J:212:ARG:HH11	1.37	0.89
22:Y:96:GLU:OE2	26:c:185:GLU:O	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:296:TRP:HE1	68:AY:419:THR:HG1	0.90	0.89
40:Br:78:MET:O	40:Br:432:ARG:NH1	2.05	0.89
27:d:60:ARG:HG2	27:d:60:ARG:HH11	1.36	0.89
75:AG:101:CDL:H712	75:AG:101:CDL:C52	2.03	0.89
9:BJ:83:PRO:HB2	9:BJ:108:TRP:NE1	1.88	0.89
71:Bb:201:PLX:C3	71:Bb:201:PLX:H1C3	2.01	0.89
9:J:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.89
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.88
27:d:110:ARG:HG2	27:d:110:ARG:HH11	1.38	0.88
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.88
47:z:112:LEU:HG	47:z:118:PRO:HB3	1.55	0.88
66:AV:137:GLN:HE21	66:AV:141:TRP:NE1	1.70	0.88
24:Ba:87:THR:HG22	71:Bb:201:PLX:C13	2.03	0.88
3:BC:100:ARG:HH21	16:BQ:208:GLU:HB3	1.39	0.88
25:Bb:110:ILE:C	25:Bb:111:LEU:HD23	1.98	0.88
35:Bl:193:SER:HB2	35:Bl:195:SER:OG	1.73	0.88
24:a:87:THR:HG22	71:b:201:PLX:C13	2.03	0.88
25:b:110:ILE:C	25:b:111:LEU:HD23	1.98	0.88
43:v:66:LEU:HD11	43:v:84:ARG:HD2	1.55	0.88
27:Bd:60:ARG:HG2	27:Bd:60:ARG:HH11	1.36	0.88
43:Bv:66:LEU:HD11	43:Bv:84:ARG:HD2	1.55	0.88
68:AY:296:TRP:CD1	68:AY:419:THR:HG21	1.91	0.88
68:AY:296:TRP:CE2	68:AY:419:THR:HG21	2.08	0.88
9:BJ:206:ILE:HB	9:BJ:242:VAL:CG2	2.04	0.88
34:Bk:2:PRO:HG2	36:Bm:115:VAL:HG21	1.56	0.88
35:Bl:37:LYS:HE3	35:Bl:102:GLU:HG3	1.53	0.88
3:C:137:VAL:CG2	16:Q:87:GLN:HE21	1.85	0.88
9:J:83:PRO:HB2	9:J:108:TRP:NE1	1.88	0.88
26:c:181:VAL:CB	43:v:37:ARG:NH2	2.37	0.88
35:l:193:SER:HB2	35:l:195:SER:OG	1.74	0.88
60:AC:150:ALA:CB	66:AV:168:TYR:CD2	2.55	0.88
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
47:Bz:112:LEU:HG	47:Bz:118:PRO:HB3	1.55	0.88
3:BC:137:VAL:CG2	16:BQ:87:GLN:HE21	1.86	0.87
22:Y:84:PHE:CG	22:Y:85:PRO:CD	2.58	0.87
27:d:59:HIS:CE1	28:e:120:ARG:CG	2.58	0.87
67:AW:450:VAL:HA	67:AW:453:LEU:CD1	2.03	0.87
27:Bd:59:HIS:CE1	28:Be:120:ARG:CG	2.58	0.87
34:k:2:PRO:HG2	36:m:115:VAL:HG21	1.56	0.87
35:l:88:MET:O	35:l:91:PRO:HD2	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:533:MET:SD	76:l:702:PEE:C22	2.62	0.87
76:BW:201:PEE:O2P	76:BW:201:PEE:N	2.08	0.87
41:Bs:185:TRP:HE1	41:Bs:238:THR:HG22	1.39	0.87
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.87
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.87
39:p:167:TRP:HE3	39:p:171:VAL:HG21	1.40	0.87
58:AN:43:ARG:HH12	71:AN:101:PLX:H1B2	1.34	0.87
76:W:201:PEE:O2P	76:W:201:PEE:N	2.08	0.87
32:i:224:SER:HB2	32:i:229:LEU:HB3	1.56	0.87
33:j:105:GLU:HG2	36:m:168:ILE:HD11	1.56	0.87
34:k:1:MET:HB2	34:k:4:ILE:CD1	2.04	0.87
35:l:533:MET:SD	76:l:702:PEE:H37	2.14	0.87
38:o:24:ASN:HA	68:AY:262:VAL:O	1.75	0.87
27:d:108:GLN:HG2	35:l:199:GLN:HB3	1.54	0.87
35:l:78:LEU:HD21	35:l:80:PHE:HE1	1.39	0.87
65:AU:296:MET:HE2	76:AU:401:PEE:H53	1.53	0.87
66:AV:10:LEU:HD21	76:AY:502:PEE:H46	0.88	0.87
16:BQ:194:LEU:HD12	16:BQ:268:TRP:CZ2	2.09	0.87
27:Bd:108:GLN:HG2	35:Bl:199:GLN:HB3	1.54	0.87
34:Bk:2:PRO:HG2	36:Bm:115:VAL:CG2	2.04	0.87
9:J:169:HIS:HD2	73:J:401:NDP:C5N	1.87	0.86
76:V:202:PEE:C43	76:l:701:PEE:C45	2.53	0.86
7:BH:102:PRO:HA	15:BP:70:PRO:HB2	1.57	0.86
22:Y:86:TYR:OH	43:v:100:LYS:CG	2.22	0.86
71:b:201:PLX:H102	71:b:201:PLX:H6	1.56	0.86
71:Bb:201:PLX:H102	71:Bb:201:PLX:H6	1.56	0.86
27:Bd:110:ARG:HG2	27:Bd:110:ARG:HH11	1.38	0.86
35:Bl:533:MET:SD	76:Bl:702:PEE:H37	2.15	0.86
22:Y:84:PHE:CD1	22:Y:85:PRO:CD	2.58	0.86
67:AK:438:MET:HB3	67:AK:450:VAL:CG1	2.05	0.86
68:AL:260:ASP:OD2	39:Bp:12:HIS:CB	2.23	0.86
22:BY:86:TYR:OH	43:Bv:100:LYS:CG	2.22	0.86
32:Bi:224:SER:HB2	32:Bi:229:LEU:HB3	1.56	0.86
34:k:2:PRO:HG2	36:m:115:VAL:CG2	2.05	0.86
58:AA:78:TYR:CE1	62:AE:65:GLU:HA	2.08	0.86
67:AK:257:GLU:CD	67:AK:450:VAL:HG22	1.99	0.86
76:BV:202:PEE:C43	76:Bl:701:PEE:C45	2.53	0.86
44:Bw:332:ARG:O	44:Bw:338:LYS:HG2	1.76	0.86
9:J:85:ARG:HG3	9:J:85:ARG:HH11	1.41	0.86
24:a:53:ARG:HD2	25:b:28:LEU:HD11	1.57	0.86
30:g:1:MET:HE2	30:g:85:ARG:HD3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:185:TRP:HE1	41:s:238:THR:HG22	1.39	0.86
44:w:332:ARG:O	44:w:338:LYS:HG2	1.76	0.86
9:BJ:176:SER:CA	9:BJ:182:ARG:HH21	1.88	0.86
25:Bb:110:ILE:O	25:Bb:111:LEU:HD23	1.75	0.86
26:Bc:181:VAL:CB	43:Bv:37:ARG:NH2	2.37	0.86
63:AF:71:LEU:HD23	63:AF:71:LEU:H	1.40	0.86
68:AY:152:GLN:NE2	68:AY:253:ILE:H	1.74	0.86
35:Bl:78:LEU:HD21	35:Bl:80:PHE:HE1	1.39	0.86
35:Bl:88:MET:O	35:Bl:91:PRO:HD2	1.74	0.86
12:M:130:ILE:HD13	18:T:114:TYR:CE1	2.11	0.86
9:BJ:169:HIS:HD2	73:BJ:401:NDP:C5N	1.87	0.86
9:J:176:SER:CA	9:J:182:ARG:HH21	1.89	0.86
22:BY:84:PHE:CG	22:BY:85:PRO:CD	2.57	0.86
30:Bg:1:MET:HE2	30:Bg:85:ARG:HD3	1.57	0.86
34:Bk:1:MET:HB2	34:Bk:4:ILE:CD1	2.04	0.86
39:Bp:167:TRP:HE3	39:Bp:171:VAL:HG21	1.40	0.86
24:a:96:ALA:HB3	27:d:55:TYR:CB	2.05	0.86
7:BH:36:GLU:HA	7:BH:45:ARG:HH21	1.38	0.86
9:BJ:85:ARG:HH11	9:BJ:85:ARG:HG3	1.41	0.86
12:BM:130:ILE:HD13	18:BT:114:TYR:CE1	2.10	0.86
24:Ba:96:ALA:HB3	27:Bd:55:TYR:CB	2.05	0.86
68:AY:412:ASP:O	68:AY:416:SER:HB2	1.76	0.86
12:BM:299:ARG:HG2	12:BM:300:GLN:H	1.41	0.86
44:Bw:99:GLY:HA3	44:Bw:337:ARG:HH12	1.40	0.86
24:Ba:53:ARG:HD2	25:Bb:28:LEU:HD11	1.57	0.85
46:By:78:LEU:HB2	46:By:79:PRO:HD3	1.58	0.85
46:y:78:LEU:HB2	46:y:79:PRO:HD3	1.58	0.85
63:AF:52:PRO:HG2	63:AF:55:LEU:HB2	1.57	0.85
66:AV:344:SER:O	66:AV:348:THR:HG23	1.76	0.85
1:BA:126:LYS:HB3	1:BA:277:ASN:HD21	1.40	0.85
27:Bd:111:GLU:OE2	27:Bd:119:CYS:N	2.10	0.85
67:AK:183:ARG:NH1	67:AW:451:ASP:OD2	2.08	0.85
66:AV:295:LEU:O	66:AV:299:LEU:HD22	1.77	0.85
67:AW:259:ARG:NH1	67:AW:449:PHE:CE1	2.44	0.85
1:BA:244:ASN:N	70:BA:502:FMN:O2P	2.09	0.85
33:Bj:105:GLU:HG2	36:Bm:168:ILE:HD11	1.56	0.85
4:E:70:ASN:OD1	72:E:201:8Q1:O4	1.95	0.85
44:w:99:GLY:HA3	44:w:337:ARG:HH12	1.40	0.85
62:AE:21:GLU:O	62:AE:25:GLU:N	2.09	0.85
22:BY:84:PHE:CD1	22:BY:85:PRO:CD	2.58	0.85
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:23:ARG:H	36:m:22:LYS:HE2	1.39	0.85
67:AK:438:MET:CB	67:AK:450:VAL:CG1	2.54	0.85
66:AV:137:GLN:NE2	66:AV:141:TRP:HE1	1.73	0.85
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.85
25:b:110:ILE:O	25:b:111:LEU:HD23	1.75	0.85
27:d:114:ASN:O	27:d:114:ASN:ND2	2.09	0.85
35:l:188:TRP:NE1	35:l:192:HIS:CD2	2.45	0.85
16:BQ:273:ILE:CD1	16:BQ:325:ASP:OD2	2.25	0.85
67:AW:257:GLU:OE2	67:AW:450:VAL:N	2.08	0.85
27:d:111:GLU:OE2	27:d:119:CYS:N	2.10	0.85
32:i:54:GLU:OE2	32:i:58:LYS:NZ	2.10	0.85
4:BE:25:MET:HB3	4:BE:29:LYS:HE2	1.55	0.85
27:Bd:114:ASN:O	27:Bd:114:ASN:ND2	2.09	0.85
35:Bl:533:MET:SD	76:Bl:702:PEE:C22	2.62	0.84
34:Bk:23:ARG:H	36:Bm:22:LYS:HE2	1.39	0.84
1:A:244:ASN:N	70:A:502:FMN:O2P	2.09	0.84
2:BB:81:THR:O	13:BN:58:ARG:NH2	2.09	0.84
45:Bx:187:SER:HB2	45:Bx:277:MET:HE1	1.60	0.84
51:B3:5:LYS:HZ3	51:B3:6:GLY:N	1.75	0.84
51:3:5:LYS:HZ3	51:3:6:GLY:N	1.73	0.84
62:AE:30:LEU:HD21	65:AH:216:THR:CG2	2.07	0.84
67:AW:449:PHE:N	67:AW:452:GLU:OE2	2.10	0.84
62:AR:34:ARG:NH1	62:AR:78:ARG:NH1	2.25	0.84
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.84
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.84
26:Bc:122:THR:HG1	38:Bo:12:ARG:HH12	1.24	0.84
59:AB:27:ARG:HE	67:AK:174:ILE:HD12	1.43	0.84
71:AL:501:PLX:H71	76:AL:503:PEE:H17	1.60	0.84
4:BE:70:ASN:OD1	72:BE:201:8Q1:O4	1.95	0.84
16:BQ:53:TYR:CE1	76:Bl:701:PEE:O1P	2.30	0.84
6:X:99:SER:HG	6:X:102:SER:HG	1.24	0.84
20:BV:84:PRO:O	20:BV:89:ASN:ND2	2.10	0.84
24:a:90:ASN:HD22	71:b:201:PLX:H122	1.43	0.84
45:x:187:SER:HB2	45:x:277:MET:HE1	1.60	0.83
63:AF:50:ARG:O	67:AW:148:ARG:NH2	2.11	0.83
30:g:49:ARG:HD3	44:w:339:TYR:HA	1.60	0.83
35:Bl:226:GLN:HG3	35:Bl:280:LEU:HD21	1.53	0.83
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.83
75:AG:101:CDL:H332	75:AG:101:CDL:CA6	2.06	0.83
75:AG:101:CDL:H731	75:AG:101:CDL:H542	1.60	0.83
76:AL:503:PEE:H16	76:AL:503:PEE:C31	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.83
9:BJ:206:ILE:CA	9:BJ:240:VAL:O	2.24	0.83
30:Bg:62:LEU:HD22	71:Bg:203:PLX:H91	1.61	0.83
16:Q:145:MET:HE1	16:Q:226:TYR:HB3	1.61	0.83
20:V:84:PRO:O	20:V:89:ASN:ND2	2.10	0.83
76:V:202:PEE:H74	76:l:701:PEE:C45	2.08	0.83
24:a:87:THR:HG22	71:b:201:PLX:H132	1.61	0.83
35:l:533:MET:HE1	76:l:702:PEE:H36	0.83	0.83
62:AR:79:ASP:HB3	65:AU:92:PRO:HG2	1.60	0.83
16:BQ:294:ARG:O	16:BQ:321:GLY:N	2.11	0.83
32:Bi:12:THR:HG21	36:Bm:162:VAL:HG21	1.60	0.83
35:Bl:188:TRP:NE1	35:Bl:192:HIS:CD2	2.45	0.83
16:Q:53:TYR:CE1	76:l:701:PEE:O1P	2.30	0.83
4:BE:101:THR:HG22	15:BP:218:ARG:HB2	1.60	0.83
76:BV:202:PEE:H74	76:Bl:701:PEE:C45	2.08	0.83
24:Ba:143:GLU:OE1	40:Br:175:ASN:ND2	2.11	0.83
68:AY:152:GLN:HE21	68:AY:253:ILE:H	1.25	0.83
39:p:124:GLN:O	39:p:128:LEU:HG	1.79	0.83
33:Bj:6:ILE:O	33:Bj:10:ASN:ND2	2.12	0.83
44:Bw:160:GLU:HG2	44:Bw:161:ARG:H	1.43	0.83
32:i:12:THR:HG21	36:m:162:VAL:HG21	1.60	0.82
58:AA:25:ARG:HG2	60:AC:91:TYR:O	1.79	0.82
76:AH:401:PEE:H64	76:AH:401:PEE:C43	2.08	0.82
16:BQ:145:MET:HE1	16:BQ:226:TYR:HB3	1.61	0.82
40:Br:365:ALA:O	40:Br:374:ASN:ND2	2.13	0.82
65:AH:291:LYS:HD2	76:AH:401:PEE:H8	1.62	0.82
41:Bs:17:MET:HE1	41:Bs:232:ILE:HD12	1.61	0.82
24:a:143:GLU:OE1	40:r:175:ASN:ND2	2.11	0.82
32:i:91:ASN:OD1	32:i:92:GLN:N	2.13	0.82
40:r:365:ALA:O	40:r:374:ASN:ND2	2.13	0.82
62:AE:34:ARG:CD	62:AE:78:ARG:NH2	2.42	0.82
24:Ba:87:THR:HG22	71:Bb:201:PLX:H132	1.61	0.82
32:Bi:54:GLU:OE2	32:Bi:58:LYS:NZ	2.10	0.82
71:Br:502:PLX:H372	71:Br:502:PLX:C33	2.09	0.82
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.82
68:AL:259:GLU:HB3	38:Bo:30:ARG:CZ	2.09	0.82
24:Ba:54:LEU:HD22	25:Bb:26:GLN:C	2.05	0.82
32:Bi:235:ASN:ND2	32:Bi:307:MET:SD	2.53	0.82
16:Q:87:GLN:O	16:Q:88:HIS:C	2.22	0.82
24:a:54:LEU:HD22	25:b:26:GLN:C	2.05	0.82
27:d:59:HIS:CE1	28:e:120:ARG:HG2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:152:GLN:NE2	68:AY:253:ILE:N	2.28	0.82
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.82
62:AR:86:LEU:O	62:AR:86:LEU:HD23	1.79	0.82
27:Bd:59:HIS:CE1	28:Be:120:ARG:HG2	2.14	0.82
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.82
30:g:62:LEU:HD22	71:g:203:PLX:H91	1.61	0.82
62:AE:29:PRO:CD	65:AH:262:THR:HG21	2.09	0.82
24:Ba:55:PHE:CE2	39:Bp:118:TYR:HE2	1.96	0.82
64:AT:39:ARG:HH21	64:AT:39:ARG:HG2	1.45	0.81
65:AU:307:LYS:NZ	75:AU:403:CDL:OA3	2.12	0.81
34:Bk:7:ASN:ND2	36:Bm:9:SER:C	2.38	0.81
35:Bl:224:SER:OG	35:Bl:256:GLY:HA3	1.80	0.81
22:Y:72:ARG:HH11	35:l:466:PHE:HD1	1.29	0.81
32:i:235:ASN:ND2	32:i:307:MET:SD	2.53	0.81
33:j:6:ILE:O	33:j:10:ASN:ND2	2.12	0.81
35:l:224:SER:OG	35:l:256:GLY:HA3	1.81	0.81
58:AA:78:TYR:CG	62:AE:65:GLU:HG2	2.15	0.81
62:AE:30:LEU:HD21	65:AH:216:THR:HG23	1.59	0.81
51:3:5:LYS:NZ	51:3:6:GLY:H	1.78	0.81
24:Ba:90:ASN:HD22	71:Bb:201:PLX:H122	1.43	0.81
35:Bl:533:MET:HE1	76:Bl:702:PEE:H36	0.83	0.81
16:Q:58:THR:HG23	35:l:580:GLN:HE21	1.46	0.81
35:Bl:222:GLY:HA2	35:Bl:229:LEU:HD12	1.63	0.81
39:Bp:124:GLN:O	39:Bp:128:LEU:HG	1.79	0.81
9:BJ:169:HIS:CD2	73:BJ:401:NDP:H5N	2.15	0.81
32:i:167:TRP:CZ3	35:l:570:GLN:HA	2.14	0.81
30:Bg:49:ARG:HD3	44:Bw:339:TYR:HA	1.61	0.81
65:AU:121:CYS:SG	81:AU:402:HEC:HBB2	2.21	0.81
26:Bc:93:ASP:OD1	38:Bo:44:LYS:NZ	2.13	0.81
32:Bi:167:TRP:CZ3	35:Bl:570:GLN:HA	2.15	0.81
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.13	0.81
38:o:27:PRO:CG	68:AY:218:GLU:OE2	2.28	0.81
44:w:160:GLU:HG2	44:w:161:ARG:H	1.43	0.81
60:AC:220:LEU:HB2	74:AC:301:FES:S2	2.21	0.81
66:AV:195:LEU:CD2	66:AV:199:PHE:HE2	1.94	0.81
5:BF:57:GLU:HB3	12:BM:662:ALA:H	1.45	0.81
35:Bl:188:TRP:CZ2	35:Bl:192:HIS:CD2	2.69	0.81
22:Y:74:TRP:CE3	22:Y:75:HIS:HA	2.16	0.81
71:AQ:101:PLX:H322	76:AY:502:PEE:H59	1.63	0.81
35:Bl:226:GLN:NE2	35:Bl:314:MET:SD	2.53	0.81
35:l:226:GLN:NE2	35:l:314:MET:SD	2.53	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:222:GLY:HA2	35:l:229:LEU:HD12	1.63	0.80
41:s:17:MET:HE1	41:s:232:ILE:HD12	1.61	0.80
44:w:332:ARG:O	44:w:338:LYS:CA	2.29	0.80
39:Bp:167:TRP:O	39:Bp:171:VAL:CG2	2.28	0.80
16:BQ:273:ILE:HD13	16:BQ:325:ASP:OD2	1.81	0.80
6:BX:112:SER:N	72:Bp:201:8Q1:O2	2.14	0.80
9:BJ:226:ILE:HD12	9:BJ:289:LEU:H	1.45	0.80
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.80
24:a:55:PHE:CD2	39:p:118:TYR:CE1	2.64	0.80
66:AV:326:TRP:CZ2	76:AV:403:PEE:H13	2.16	0.80
3:BC:156:GLY:HA2	3:BC:169:GLY:HA2	1.62	0.80
9:BJ:130:ILE:CG2	73:BJ:401:NDP:H8A	2.10	0.80
9:BJ:207:PHE:HA	9:BJ:211:ASP:OD2	1.82	0.80
76:Bl:701:PEE:C23	40:Br:155:VAL:HG11	2.12	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80
76:W:201:PEE:C44	41:s:77:LEU:HD21	2.09	0.80
26:c:159:LYS:HA	43:v:98:ARG:HH22	1.46	0.80
34:k:7:ASN:ND2	36:m:9:SER:C	2.39	0.80
52:B4:39:CYS:SG	52:B4:53:CYS:HB3	2.22	0.80
9:J:169:HIS:CD2	73:J:401:NDP:H5N	2.15	0.80
9:J:177:SER:HB2	9:J:320:GLU:HB3	1.64	0.80
22:BY:74:TRP:CE3	22:BY:75:HIS:HA	2.16	0.80
31:h:88:LYS:HG3	31:h:89:GLU:HG3	1.63	0.80
64:AT:35:ALA:HB1	76:AY:502:PEE:H75	1.63	0.80
32:Bi:91:ASN:OD1	32:Bi:92:GLN:N	2.13	0.80
35:Bl:4:HIS:CE1	35:Bl:87:MET:CE	2.65	0.80
35:Bl:188:TRP:NE1	35:Bl:192:HIS:HD2	1.78	0.80
22:BY:72:ARG:HH11	35:Bl:466:PHE:HD1	1.29	0.80
9:J:130:ILE:CG2	73:J:401:NDP:H8A	2.10	0.79
76:l:701:PEE:C23	40:r:155:VAL:HG11	2.11	0.79
38:o:24:ASN:CB	68:AY:264:THR:OG1	2.30	0.79
32:Bi:12:THR:HG22	36:Bm:158:TRP:HE1	1.47	0.79
39:Bp:13:GLN:NE2	72:Bp:201:8Q1:O3	2.15	0.79
35:l:188:TRP:CZ2	35:l:192:HIS:CD2	2.69	0.79
39:p:143:GLU:OE2	39:p:158:ARG:NH2	2.15	0.79
52:4:39:CYS:SG	52:4:53:CYS:CB	2.71	0.79
44:Bw:332:ARG:O	44:Bw:338:LYS:CA	2.29	0.79
2:B:133:ARG:HG3	2:B:135:ASP:H	1.47	0.79
27:d:111:GLU:OE1	27:d:115:TYR:HB2	1.82	0.79
27:Bd:111:GLU:OE1	27:Bd:115:TYR:HB2	1.82	0.79
39:Bp:143:GLU:OE2	39:Bp:158:ARG:NH2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:12:THR:HG22	36:m:158:TRP:HE1	1.47	0.79
32:i:50:PRO:HB3	34:k:84:THR:HG21	1.65	0.79
39:p:167:TRP:O	39:p:171:VAL:CG2	2.28	0.79
63:AF:34:ARG:HG2	63:AF:34:ARG:HH11	1.46	0.79
34:Bk:1:MET:HB2	34:Bk:4:ILE:HD12	1.63	0.79
9:J:86:CYS:O	9:J:87:ASP:HB2	1.83	0.79
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.79
6:X:112:SER:N	72:p:201:8Q1:O2	2.14	0.79
22:Y:86:TYR:OH	43:v:100:LYS:HE2	1.82	0.79
35:l:188:TRP:NE1	35:l:192:HIS:HD2	1.78	0.79
71:r:502:PLX:H372	71:r:502:PLX:C33	2.09	0.79
52:4:39:CYS:SG	52:4:53:CYS:HB3	2.22	0.79
75:AJ:405:CDL:H732	75:AJ:405:CDL:H351	1.65	0.79
3:BC:120:MET:HB3	3:BC:147:VAL:HG12	1.64	0.79
82:AV:401:HEM:HHD	82:AV:401:HEM:HBC2	1.65	0.79
9:BJ:355:ARG:HD2	33:Bj:31:MET:SD	2.23	0.79
26:Bc:159:LYS:HA	43:Bv:98:ARG:HH22	1.46	0.79
52:B4:39:CYS:SG	52:B4:53:CYS:CB	2.71	0.79
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.79
35:l:74:THR:HG22	35:l:194:ASN:OD1	1.83	0.79
16:BQ:70:ASP:O	16:BQ:74:ASP:OD1	2.00	0.79
35:Bl:142:ILE:HG12	40:Br:370:PRO:HB2	1.65	0.79
43:v:8:ARG:HH11	43:v:106:ARG:HH22	1.29	0.79
68:AY:74:TRP:O	68:AY:418:LEU:HD21	1.82	0.79
16:BQ:83:ASN:HA	16:BQ:98:VAL:HG22	1.65	0.79
32:Bi:339:ILE:HG22	32:Bi:342:PHE:HB3	1.65	0.79
12:M:68:ARG:HD2	12:M:285:TRP:HE1	1.48	0.79
34:k:1:MET:HB2	34:k:4:ILE:HD12	1.63	0.79
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.16	0.79
66:AJ:324:LEU:HD11	66:AJ:369:ILE:HD12	1.65	0.79
35:Bl:226:GLN:HE21	35:Bl:314:MET:HE1	1.48	0.79
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.65	0.79
32:i:339:ILE:HG22	32:i:342:PHE:HB3	1.65	0.79
5:BF:63:PRO:HB2	5:BF:79:LEU:HB2	1.65	0.79
11:BL:75:ARG:NH1	11:BL:119:ASP:OD2	2.16	0.79
9:J:176:SER:HA	9:J:182:ARG:NH2	1.99	0.78
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.65	0.78
71:b:201:PLX:H6	71:b:201:PLX:C10	2.13	0.78
35:l:4:HIS:CE1	35:l:87:MET:CE	2.65	0.78
71:r:502:PLX:H52	71:r:502:PLX:O3	1.82	0.78
63:AF:29:LYS:HD3	63:AF:75:ILE:HD13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:363:GLN:HB2	67:AK:365:ASN:OD1	1.83	0.78
9:BJ:177:SER:HB2	9:BJ:320:GLU:HB3	1.64	0.78
9:BJ:217:PHE:HZ	9:BJ:322:MET:CE	1.95	0.78
25:Bb:110:ILE:CG2	25:Bb:111:LEU:HG	2.11	0.78
32:Bi:50:PRO:HB3	34:Bk:84:THR:HG21	1.65	0.78
9:J:217:PHE:HZ	9:J:322:MET:CE	1.95	0.78
22:Y:74:TRP:HZ3	22:Y:75:HIS:HD1	1.29	0.78
34:k:3:LEU:HD23	36:m:117:ASN:HD21	1.48	0.78
52:4:39:CYS:HG	52:4:53:CYS:CB	1.96	0.78
67:AK:259:ARG:HG2	67:AK:444:LEU:CD1	2.08	0.78
2:BB:133:ARG:HG3	2:BB:135:ASP:H	1.47	0.78
9:BJ:176:SER:HA	9:BJ:182:ARG:NH2	1.98	0.78
6:BX:99:SER:HG	6:BX:102:SER:HG	1.27	0.78
71:Bb:201:PLX:H6	71:Bb:201:PLX:C10	2.13	0.78
36:Bm:111:GLY:HA2	36:Bm:116:VAL:HA	1.65	0.78
71:Br:502:PLX:H52	71:Br:502:PLX:O3	1.82	0.78
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.64	0.78
22:Y:86:TYR:OH	43:v:100:LYS:HG2	1.84	0.78
75:AG:101:CDL:H531	75:AG:101:CDL:H731	1.66	0.78
75:AG:101:CDL:H351	75:AG:101:CDL:H742	1.64	0.78
3:BC:59:ARG:HH22	3:BC:61:GLU:HB3	1.48	0.78
22:BY:86:TYR:OH	43:Bv:100:LYS:HG2	1.84	0.78
22:BY:90:SER:HA	43:Bv:107:ARG:NH1	1.98	0.78
34:Bk:97:GLN:HB2	35:Bl:579:THR:HG21	1.66	0.78
16:Q:268:TRP:CZ3	16:Q:272:THR:CG2	2.66	0.78
22:Y:90:SER:HA	43:v:107:ARG:NH1	1.98	0.78
62:AE:28:ASP:OD1	62:AE:30:LEU:N	2.15	0.78
68:AY:421:GLY:C	68:AY:422:ARG:HG3	2.06	0.78
32:Bi:167:TRP:CH2	35:Bl:570:GLN:HG3	2.19	0.78
35:Bl:74:THR:HG22	35:Bl:194:ASN:OD1	1.83	0.78
9:J:355:ARG:HD2	33:j:31:MET:SD	2.23	0.78
16:BQ:268:TRP:CZ3	16:BQ:272:THR:CG2	2.66	0.78
22:Y:84:PHE:CG	22:Y:85:PRO:HD2	2.19	0.78
35:l:227:LEU:O	35:l:227:LEU:HD12	1.82	0.78
65:AU:215:LEU:HD11	81:AU:402:HEC:HMB3	1.63	0.78
65:AU:315:LYS:HE3	75:AU:403:CDL:H1	1.66	0.78
9:BJ:270:ARG:NH2	9:BJ:326:ASP:O	2.16	0.78
12:BM:68:ARG:HD2	12:BM:285:TRP:HE1	1.48	0.78
22:BY:84:PHE:CG	22:BY:85:PRO:HD2	2.19	0.78
25:Bb:86:MET:O	25:Bb:90:VAL:HG23	1.83	0.78
35:Bl:227:LEU:O	35:Bl:227:LEU:HD12	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AR:78:ARG:O	62:AR:82:VAL:HG23	1.84	0.78
67:AW:277:VAL:HG13	67:AW:278:ALA:HB2	1.66	0.78
12:BM:647:GLU:HB2	12:BM:654:VAL:HG11	1.65	0.78
76:BW:201:PEE:C44	41:Bs:77:LEU:HD21	2.09	0.78
34:Bk:3:LEU:HD23	36:Bm:117:ASN:HD21	1.48	0.78
16:Q:70:ASP:O	16:Q:74:ASP:OD1	2.00	0.78
25:b:86:MET:O	25:b:90:VAL:HG23	1.83	0.78
71:b:201:PLX:C6	71:b:201:PLX:H111	2.14	0.78
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.65	0.78
9:BJ:206:ILE:HG12	73:BJ:401:NDP:N7N	1.99	0.78
16:BQ:194:LEU:CD1	16:BQ:268:TRP:CZ2	2.67	0.78
15:P:187:ILE:HG22	15:P:188:LEU:HG	1.66	0.78
24:a:54:LEU:CD2	25:b:27:GLU:HA	2.14	0.78
33:j:108:GLN:O	36:m:172:ARG:NH2	2.16	0.78
36:m:111:GLY:HA2	36:m:116:VAL:HA	1.65	0.78
66:AJ:262:LEU:HD22	60:AP:216:VAL:HG21	1.64	0.78
67:AK:438:MET:HB3	67:AK:450:VAL:HG11	1.65	0.78
16:BQ:58:THR:HG23	35:Bl:580:GLN:HE21	1.46	0.78
31:Bh:88:LYS:HG3	31:Bh:89:GLU:HG3	1.63	0.78
40:Br:355:MET:HE1	40:Br:437:MET:HE3	1.65	0.78
52:B4:39:CYS:HG	52:B4:53:CYS:CB	1.96	0.78
22:Y:96:GLU:O	22:Y:97:LEU:HD23	1.84	0.77
39:p:13:GLN:NE2	72:p:201:8Q1:O3	2.15	0.77
76:AH:401:PEE:H49	76:AH:401:PEE:H14	1.65	0.77
22:BY:81:LEU:HD22	43:Bv:92:HIS:CD2	2.18	0.77
22:BY:83:HIS:O	22:BY:84:PHE:CB	2.31	0.77
43:Bv:8:ARG:HH11	43:Bv:106:ARG:HH22	1.29	0.77
11:L:75:ARG:NH1	11:L:119:ASP:OD2	2.16	0.77
63:AF:34:ARG:NH1	66:AJ:379:TRP:HE1	1.82	0.77
22:BY:74:TRP:HZ3	22:BY:75:HIS:HD1	1.29	0.77
39:Bp:105:ASP:OD1	39:Bp:122:ARG:NH1	2.16	0.77
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.02	0.77
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77
22:Y:81:LEU:HD22	43:v:92:HIS:CD2	2.18	0.77
35:l:90:ILE:O	35:l:94:LEU:HD22	1.84	0.77
5:BF:42:VAL:HG21	12:BM:671:LEU:HD12	1.66	0.77
15:BP:187:ILE:HG22	15:BP:188:LEU:HG	1.66	0.77
34:k:97:GLN:HB2	35:l:579:THR:HG21	1.66	0.77
68:AL:73:VAL:HG23	68:AL:147:LEU:HD23	1.66	0.77
2:BB:68:LEU:HG	41:Bs:272:TRP:HE1	1.50	0.77
24:Ba:54:LEU:CD2	25:Bb:27:GLU:HA	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:167:TRP:CH2	35:l:570:GLN:HG3	2.19	0.77
68:AL:259:GLU:CB	38:Bo:30:ARG:HE	1.97	0.77
16:BQ:87:GLN:O	16:BQ:88:HIS:C	2.22	0.77
22:BY:86:TYR:OH	43:Bv:100:LYS:HE2	1.82	0.77
26:Bc:166:LEU:HD21	43:Bv:56:ARG:HG3	1.65	0.77
7:H:50:GLN:HE22	8:I:93:LYS:HA	1.50	0.77
25:b:110:ILE:CG2	25:b:111:LEU:HG	2.11	0.77
44:w:56:ARG:NH1	44:w:81:LEU:O	2.18	0.77
3:BC:59:ARG:NH2	3:BC:61:GLU:HB3	1.98	0.77
35:Bl:226:GLN:NE2	35:Bl:314:MET:HE3	1.99	0.77
44:Bw:64:GLY:O	44:Bw:161:ARG:NH2	2.17	0.77
44:Bw:98:THR:O	44:Bw:337:ARG:NH2	2.18	0.77
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.77
9:J:206:ILE:HG12	73:J:401:NDP:N7N	1.99	0.77
66:AV:148:ASN:O	66:AV:151:SER:HB3	1.84	0.77
37:Bn:55:VAL:HG12	37:Bn:56:THR:H	1.48	0.77
9:J:217:PHE:CB	9:J:280:ILE:HD13	2.15	0.77
39:p:57:MET:HG3	68:AY:257:TYR:CB	2.15	0.77
40:r:355:MET:HE1	40:r:437:MET:HE3	1.65	0.77
66:AJ:8:ASN:HD22	66:AJ:11:MET:HG2	1.50	0.77
66:AV:165:TRP:CZ3	66:AV:168:TYR:O	2.37	0.77
3:BC:105:ARG:HB3	41:Bs:39:VAL:HG23	1.67	0.77
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.77
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.65	0.77
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.17	0.77
26:c:166:LEU:HD21	43:v:56:ARG:HG3	1.65	0.77
34:k:23:ARG:N	36:m:22:LYS:HE2	2.00	0.77
52:4:75:ARG:HH11	52:4:75:ARG:HG2	1.48	0.77
58:AA:78:TYR:CE1	62:AE:64:GLU:C	2.62	0.77
16:BQ:78:LYS:CE	33:Bj:48:ARG:HH21	1.97	0.77
71:Bb:201:PLX:H111	71:Bb:201:PLX:C6	2.14	0.77
33:Bj:108:GLN:O	36:Bm:172:ARG:NH2	2.16	0.77
37:n:55:VAL:HG12	37:n:56:THR:H	1.48	0.77
59:AB:52:ARG:NH1	68:AL:343:THR:O	2.18	0.77
9:BJ:217:PHE:CB	9:BJ:280:ILE:HD13	2.15	0.77
16:BQ:140:ASP:OD2	16:BQ:143:SER:OG	2.02	0.77
52:B4:75:ARG:HG2	52:B4:75:ARG:HH11	1.48	0.77
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.76
76:V:202:PEE:H60	76:V:202:PEE:H41	1.67	0.76
22:Y:83:HIS:O	22:Y:84:PHE:CB	2.31	0.76
1:BA:64:LYS:NZ	14:BO:244:GLY:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BP:85:GLU:OE2	15:BP:142:ARG:NH1	2.19	0.76
35:Bl:54:PHE:CD1	35:Bl:58:ASP:HA	2.21	0.76
35:l:190:ILE:H	35:l:190:ILE:HD12	1.49	0.76
44:w:98:THR:O	44:w:337:ARG:NH2	2.18	0.76
63:AF:68:ASP:HA	63:AF:71:LEU:HD21	1.66	0.76
65:AU:125:HIS:NE2	81:AU:402:HEC:NC	2.33	0.76
68:AY:230:VAL:HG21	68:AY:418:LEU:CD1	2.15	0.76
33:Bj:6:ILE:HG13	41:Bs:6:LEU:HD11	1.68	0.76
35:Bl:90:ILE:O	35:Bl:94:LEU:HD22	1.84	0.76
36:Bm:115:VAL:O	36:Bm:117:ASN:N	2.19	0.76
9:BJ:86:CYS:O	9:BJ:87:ASP:HB2	1.83	0.76
16:BQ:384:LEU:HA	16:BQ:388:GLY:HA2	1.68	0.76
4:E:79:VAL:HG22	72:E:201:8Q1:C38	2.16	0.76
44:w:64:GLY:O	44:w:161:ARG:NH2	2.17	0.76
12:BM:223:ILE:HD13	12:BM:233:SER:HB3	1.65	0.76
35:Bl:228:GLY:C	35:Bl:229:LEU:HD23	2.11	0.76
39:Bp:27:LEU:HD11	39:Bp:44:MET:HG3	1.67	0.76
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
8:I:33:LYS:NZ	8:I:35:THR:O	2.18	0.76
27:d:63:ARG:NH1	37:n:44:LEU:O	2.18	0.76
63:AS:36:ASP:OD2	63:AS:62:ARG:NH1	2.19	0.76
8:BI:33:LYS:NZ	8:BI:35:THR:O	2.18	0.76
22:BY:84:PHE:CZ	35:Bl:483:PRO:CG	2.68	0.76
22:BY:96:GLU:O	22:BY:97:LEU:HD23	1.84	0.76
27:Bd:63:ARG:NH1	37:Bn:44:LEU:O	2.18	0.76
32:Bi:288:LEU:HD23	76:Bl:701:PEE:H58	0.77	0.76
35:l:54:PHE:CD1	35:l:58:ASP:HA	2.21	0.76
62:AR:34:ARG:HH11	62:AR:78:ARG:HH22	1.33	0.76
16:Q:78:LYS:CE	33:j:48:ARG:HH21	1.97	0.76
35:l:228:GLY:C	35:l:229:LEU:HD23	2.11	0.76
76:AH:401:PEE:C13	66:AJ:240:MET:HE2	2.14	0.76
68:AL:260:ASP:OD2	39:Bp:12:HIS:HB2	1.84	0.76
3:BC:143:GLU:OE1	9:BJ:89:TYR:OH	2.03	0.76
34:Bk:23:ARG:N	36:Bm:22:LYS:HE2	2.00	0.76
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.76
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.68	0.76
33:j:6:ILE:HG13	41:s:6:LEU:HD11	1.67	0.76
34:k:7:ASN:HD22	36:m:9:SER:HB2	1.47	0.76
39:p:54:GLU:OE2	72:p:201:8Q1:C38	2.34	0.76
44:w:60:ILE:HG13	44:w:203:LEU:HD11	1.68	0.76
58:AA:82:LYS:HE2	62:AE:60:ARG:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:54:ILE:HB	9:BJ:78:SER:HB2	1.68	0.76
12:BM:128:CYS:HB2	12:BM:129:PRO:HD3	1.68	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	0.76
32:i:288:LEU:HD23	76:l:701:PEE:H58	0.77	0.76
67:AK:438:MET:CB	67:AK:450:VAL:HG11	2.16	0.76
76:AL:503:PEE:H26	76:AL:503:PEE:H48	1.66	0.76
58:AN:41:ARG:NE	75:AN:102:CDL:OA4	2.19	0.76
4:BE:37:ARG:NH2	6:BG:123:GLU:OE2	2.19	0.76
9:BJ:77:GLY:O	9:BJ:102:GLN:NE2	2.19	0.76
35:Bl:190:ILE:HD12	35:Bl:190:ILE:H	1.49	0.76
26:c:155:PRO:HB3	43:v:5:LEU:HD22	1.67	0.76
35:l:226:GLN:NE2	35:l:314:MET:HE3	1.99	0.76
66:AJ:149:LEU:HD21	66:AJ:281:LEU:HD21	1.65	0.76
9:BJ:221:HIS:ND1	9:BJ:222:ARG:N	2.34	0.76
20:BV:40:ARG:HH22	20:BV:55:LYS:HD3	1.51	0.76
2:B:68:LEU:HG	41:s:272:TRP:HE1	1.50	0.75
12:M:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.75
62:AR:34:ARG:HH11	62:AR:78:ARG:HH12	1.34	0.75
26:Bc:155:PRO:HB3	43:Bv:5:LEU:HD22	1.67	0.75
5:F:42:VAL:HG21	12:M:671:LEU:HD12	1.66	0.75
22:Y:84:PHE:CZ	35:l:483:PRO:CG	2.68	0.75
59:AB:2:LEU:HD22	67:AK:278:ALA:HB1	1.68	0.75
44:Bw:60:ILE:HG13	44:Bw:203:LEU:HD11	1.68	0.75
12:M:543:LYS:HG3	12:M:565:PHE:HD2	1.51	0.75
40:r:114:GLU:HG3	42:u:169:PHE:HB3	1.68	0.75
76:BV:202:PEE:H60	76:BV:202:PEE:H41	1.67	0.75
22:BY:71:TRP:CZ2	22:BY:75:HIS:CD2	2.74	0.75
35:Bl:78:LEU:HG	35:Bl:139:GLN:NE2	2.02	0.75
44:Bw:56:ARG:NH1	44:Bw:81:LEU:O	2.18	0.75
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.19	0.75
9:J:54:ILE:HB	9:J:78:SER:HB2	1.68	0.75
71:b:201:PLX:H1C3	71:b:201:PLX:H32	1.68	0.75
75:AG:101:CDL:H521	75:AG:101:CDL:OB8	1.87	0.75
67:AW:450:VAL:HA	67:AW:453:LEU:HD12	1.67	0.75
63:AF:29:LYS:HD3	63:AF:75:ILE:HD12	1.65	0.75
7:BH:50:GLN:HE22	8:BI:93:LYS:HA	1.49	0.75
14:BO:182:ASN:ND2	14:BO:194:GLU:OE1	2.19	0.75
21:BW:31:SER:OG	21:BW:35:MET:CE	2.35	0.75
46:By:59:GLN:H	46:By:62:GLU:HG3	1.51	0.75
11:L:137:PHE:O	11:L:141:ASN:ND2	2.15	0.75
68:AL:70:THR:HG1	68:AL:410:CYS:HG	1.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:By:5:MET:HE3	55:B7:42:PRO:HA	1.67	0.75
3:C:105:ARG:HB3	41:s:39:VAL:HG23	1.67	0.75
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.19	0.75
60:AP:234:TYR:HB2	60:AP:243:TYR:HB2	1.69	0.75
67:AW:375:LYS:NZ	67:AW:416:ILE:O	2.18	0.75
19:BU:82:LYS:NZ	42:Bu:121:ASP:OD1	2.18	0.75
39:Bp:54:GLU:OE2	72:Bp:201:8Q1:C38	2.34	0.75
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	0.75
35:l:226:GLN:HE21	35:l:314:MET:HE1	1.48	0.75
39:p:27:LEU:HD11	39:p:44:MET:HG3	1.67	0.75
67:AW:384:MET:HE2	68:AY:134:LYS:HD3	1.68	0.75
12:BM:50:LEU:HB2	12:BM:92:CYS:HA	1.68	0.75
24:Ba:168:TRP:NE1	30:Bg:88:GLU:OE1	2.20	0.75
24:Ba:189:ASN:ND2	42:Bu:142:TYR:OH	2.20	0.75
27:Bd:154:ARG:NH2	30:Bg:108:TYR:O	2.19	0.75
12:M:128:CYS:HB2	12:M:129:PRO:HD3	1.68	0.75
22:Y:71:TRP:CZ2	22:Y:75:HIS:CD2	2.74	0.75
39:p:170:ILE:HD12	39:p:170:ILE:N	2.02	0.75
47:z:187:THR:HG21	51:3:68:THR:HG21	1.68	0.75
58:AN:67:PHE:HB2	66:AV:346:PRO:HG3	1.69	0.75
12:BM:506:VAL:HG12	12:BM:508:GLY:H	1.52	0.75
51:B3:5:LYS:NZ	51:B3:6:GLY:H	1.78	0.75
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.74
20:V:40:ARG:HH22	20:V:55:LYS:HD3	1.50	0.74
27:d:154:ARG:NH2	30:g:108:TYR:O	2.19	0.74
35:l:78:LEU:HG	35:l:139:GLN:NE2	2.02	0.74
36:m:115:VAL:O	36:m:117:ASN:N	2.19	0.74
38:o:27:PRO:HG2	68:AY:218:GLU:OE2	1.87	0.74
1:BA:116:ASN:HD22	70:BA:502:FMN:HM81	1.51	0.74
27:Bd:81:GLU:CD	37:Bn:43:MET:HE3	2.11	0.74
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.69	0.74
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	0.74
12:M:50:LEU:HB2	12:M:92:CYS:HA	1.68	0.74
21:W:31:SER:OG	21:W:35:MET:CE	2.35	0.74
67:AK:127:ARG:HB3	68:AL:36:ALA:HB1	1.69	0.74
75:AN:102:CDL:OA3	76:AV:403:PEE:H12	1.86	0.74
12:BM:54:GLU:OE2	12:BM:62:ARG:NH2	2.19	0.74
2:B:68:LEU:CG	41:s:272:TRP:HE1	1.99	0.74
9:J:221:HIS:ND1	9:J:222:ARG:N	2.34	0.74
24:a:163:ARG:NH2	30:g:99:ASP:OD2	2.20	0.74
24:a:168:TRP:NE1	30:g:88:GLU:OE1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:533:MET:SD	76:l:702:PEE:C23	2.75	0.74
46:y:184:LEU:HD11	46:y:211:LEU:HD21	1.69	0.74
75:AL:502:CDL:H572	76:AL:503:PEE:H66	0.84	0.74
66:AV:96:LEU:HD23	76:AV:403:PEE:H26	1.69	0.74
66:AV:195:LEU:CD2	66:AV:199:PHE:CE2	2.70	0.74
12:BM:58:MET:SD	15:BP:246:ARG:NH1	2.55	0.74
35:Bl:533:MET:SD	76:Bl:702:PEE:C23	2.75	0.74
46:By:184:LEU:HD11	46:By:211:LEU:HD21	1.69	0.74
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	0.74
16:Q:82:LEU:C	16:Q:98:VAL:HG13	2.10	0.74
46:y:5:MET:HE3	55:7:42:PRO:HA	1.68	0.74
75:AG:101:CDL:H731	75:AG:101:CDL:C54	2.18	0.74
67:AW:270:ALA:HB2	67:AW:339:TYR:HD1	1.52	0.74
4:BE:79:VAL:HG22	72:BE:201:8Q1:C38	2.16	0.74
22:BY:89:PRO:O	43:Bv:107:ARG:NH2	2.20	0.74
47:Bz:187:THR:HG21	51:B3:68:THR:HG21	1.69	0.74
35:l:4:HIS:NE2	35:l:87:MET:HE1	2.02	0.74
52:4:39:CYS:HG	52:4:53:CYS:HG	0.78	0.74
2:BB:68:LEU:CG	41:Bs:272:TRP:HE1	1.99	0.74
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CE1	2.64	0.74
35:Bl:59:GLN:HA	35:Bl:59:GLN:NE2	2.00	0.74
41:Bs:289:LEU:HA	41:Bs:293:PHE:HB3	1.70	0.74
68:AL:260:ASP:CG	39:Bp:12:HIS:HB2	2.13	0.74
6:BG:79:ILE:HG21	6:BG:148:ILE:HG21	1.70	0.74
15:BP:46:THR:O	16:BQ:162:ARG:N	2.16	0.74
40:Br:114:GLU:HG3	42:Bu:169:PHE:HB3	1.68	0.74
22:Y:45:ARG:HH21	35:l:439:THR:HG21	1.52	0.74
27:d:81:GLU:CD	37:n:43:MET:HE3	2.11	0.74
35:l:190:ILE:HD11	35:l:196:TRP:NE1	2.02	0.74
66:AV:165:TRP:CE3	66:AV:168:TYR:O	2.41	0.74
68:AY:152:GLN:NE2	68:AY:252:GLY:CA	2.50	0.74
3:BC:88:CYS:SG	16:BQ:223:HIS:NE2	2.60	0.74
16:BQ:262:LEU:CD2	16:BQ:268:TRP:CD1	2.60	0.74
71:Bb:201:PLX:H1C3	71:Bb:201:PLX:H32	1.68	0.74
35:l:135:ASN:OD1	35:l:198:PRO:HG3	1.88	0.74
35:l:512:LYS:HG3	54:6:16:ASN:CB	2.17	0.74
12:BM:128:CYS:HB2	12:BM:129:PRO:CD	2.18	0.74
24:Ba:163:ARG:NH2	30:Bg:99:ASP:OD2	2.20	0.74
35:Bl:190:ILE:HD11	35:Bl:196:TRP:NE1	2.02	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:129:LYS:H	14:O:168:LEU:HA	1.53	0.74
76:AH:401:PEE:C13	66:AJ:240:MET:HE1	2.12	0.74
26:Bc:123:PRO:HG3	39:Bp:75:GLN:HE21	1.52	0.74
44:Bw:319:ILE:HG23	44:Bw:323:GLN:HE21	1.53	0.74
62:AE:30:LEU:CD1	62:AE:34:ARG:HH21	2.00	0.74
67:AK:125:CYS:HB3	67:AK:133:LEU:HD22	1.70	0.74
1:BA:158:ILE:HG21	1:BA:166:ALA:HB2	1.69	0.74
12:BM:406:ASN:HB2	12:BM:438:LEU:HD21	1.68	0.74
16:BQ:125:GLU:HA	16:BQ:419:PRO:HG2	1.67	0.74
35:Bl:571:ILE:CG1	76:Bl:701:PEE:O5	2.36	0.74
9:J:83:PRO:HB2	9:J:108:TRP:HE1	1.53	0.73
24:a:189:ASN:ND2	42:u:142:TYR:OH	2.20	0.73
8:Bl:106:LEU:O	8:Bl:108:SER:N	2.19	0.73
11:BL:92:ASN:HB3	15:BP:238:PRO:HA	1.70	0.73
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	0.73
34:k:3:LEU:HD22	36:m:117:ASN:HD21	1.53	0.73
44:w:319:ILE:HG23	44:w:323:GLN:HE21	1.53	0.73
67:AK:300:LYS:HG2	67:AK:301:ARG:HG2	1.69	0.73
12:BM:198:THR:HG22	14:BO:39:PHE:HB3	1.70	0.73
21:BW:115:ARG:HH11	31:Bh:36:PHE:HD1	1.36	0.73
35:Bl:4:HIS:NE2	35:Bl:87:MET:HE1	2.02	0.73
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.73
22:Y:84:PHE:CG	22:Y:85:PRO:HD3	2.22	0.73
35:l:59:GLN:HA	35:l:59:GLN:NE2	2.00	0.73
67:AW:65:ILE:HG22	67:AW:67:ALA:H	1.53	0.73
11:BL:137:PHE:O	11:BL:141:ASN:ND2	2.15	0.73
12:BM:307:VAL:HG13	12:BM:582:VAL:HG22	1.69	0.73
35:Bl:135:ASN:OD1	35:Bl:198:PRO:HG3	1.88	0.73
35:Bl:512:LYS:HG3	54:B6:16:ASN:CB	2.17	0.73
16:Q:281:GLU:N	16:Q:281:GLU:OE1	2.22	0.73
76:V:202:PEE:H39	76:V:202:PEE:H32	1.70	0.73
25:b:109:THR:HB	25:b:113:THR:HA	1.70	0.73
68:AL:227:PRO:HG3	39:Bp:56:ASP:CB	2.18	0.73
59:AO:33:THR:HA	59:AO:38:PRO:HG3	1.69	0.73
68:AY:171:GLU:OE2	68:AY:175:ASN:ND2	2.21	0.73
68:AY:192:PHE:HB3	68:AY:195:THR:HB	1.70	0.73
68:AY:322:VAL:HG12	68:AY:323:HIS:H	1.54	0.73
12:BM:543:LYS:HG3	12:BM:565:PHE:HD2	1.50	0.73
16:BQ:82:LEU:C	16:BQ:98:VAL:HG13	2.10	0.73
1:A:174:ARG:HG3	10:K:91:LEU:HD21	1.69	0.73
25:b:10:LEU:HD22	39:p:156:PRO:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:O:23:PRO:O	49:1:66:ARG:HD3	1.89	0.73
1:BA:174:ARG:HG3	10:BK:91:LEU:HD21	1.69	0.73
4:BE:25:MET:C	4:BE:29:LYS:HG3	2.13	0.73
1:A:116:ASN:HD22	70:A:502:FMN:HM81	1.51	0.73
39:Bp:55:LYS:HE2	39:Bp:55:LYS:HA	1.70	0.73
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.73
68:AL:470:ARG:NH2	75:AL:502:CDL:OA4	2.22	0.73
61:AQ:30:MET:SD	64:AT:34:TRP:HB2	2.29	0.73
1:BA:98:LYS:HD2	1:BA:101:PHE:CE2	2.24	0.73
48:B0:23:PRO:O	49:B1:66:ARG:HD3	1.89	0.73
51:B3:54:ARG:HD3	51:B3:54:ARG:N	2.04	0.73
41:s:289:LEU:HA	41:s:293:PHE:HB3	1.70	0.73
46:y:59:GLN:H	46:y:62:GLU:HG3	1.51	0.73
67:AK:438:MET:CE	67:AK:450:VAL:HG13	2.16	0.73
9:BJ:132:ARG:NH2	73:BJ:401:NDP:O2B	2.22	0.73
15:BP:233:PHE:O	16:BQ:418:ARG:NH2	2.22	0.73
22:BY:86:TYR:HB3	22:BY:87:PRO:CA	2.19	0.73
35:Bl:170:GLN:NE2	76:Bl:702:PEE:O2P	2.22	0.73
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.73
9:J:174:ILE:HG13	9:J:182:ARG:HG3	1.70	0.73
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73
71:b:201:PLX:O3	71:b:201:PLX:O7	2.04	0.73
76:AL:503:PEE:H50	76:AL:503:PEE:C12	2.18	0.73
68:AY:152:GLN:OE1	68:AY:252:GLY:HA3	1.89	0.73
16:BQ:333:ARG:NH2	16:BQ:453:THR:O	2.21	0.73
22:Y:86:TYR:HB3	22:Y:87:PRO:CA	2.19	0.73
63:AF:34:ARG:HG2	63:AF:34:ARG:NH1	2.00	0.73
9:BJ:83:PRO:HB2	9:BJ:108:TRP:HE1	1.53	0.73
9:BJ:132:ARG:NH2	73:BJ:401:NDP:C2B	2.52	0.73
9:BJ:279:TYR:HB2	9:BJ:372:ALA:HB2	1.71	0.73
1:A:381:GLN:HG2	69:A:501:SF4:S2	2.29	0.72
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.54	0.72
25:b:106:PRO:HA	25:b:115:GLU:OE2	1.89	0.72
35:l:384:PRO:O	35:l:389:PHE:HB2	1.89	0.72
5:BF:17:ARG:HB2	5:BF:68:ARG:HE	1.54	0.72
14:BO:116:ALA:O	14:BO:124:ARG:NH1	2.21	0.72
35:Bl:71:THR:HG21	40:Br:307:TRP:HE1	1.54	0.72
39:Bp:170:ILE:HD12	39:Bp:170:ILE:N	2.02	0.72
76:V:202:PEE:C44	76:l:701:PEE:C45	2.66	0.72
26:c:123:PRO:HG3	39:p:75:GLN:HE21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:71:THR:HG21	40:r:307:TRP:HE1	1.54	0.72
12:BM:543:LYS:NZ	12:BM:563:ASP:OD2	2.23	0.72
14:BO:129:LYS:H	14:BO:168:LEU:HA	1.53	0.72
76:BV:202:PEE:C44	76:Bl:701:PEE:C45	2.66	0.72
76:BV:202:PEE:H39	76:BV:202:PEE:H32	1.70	0.72
22:BY:86:TYR:OH	43:Bv:100:LYS:HE3	1.89	0.72
33:Bj:25:PRO:O	33:Bj:27:LEU:N	2.23	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.72
35:l:546:GLN:OE1	40:r:278:ARG:NE	2.22	0.72
60:AP:155:LYS:HZ3	60:AP:273:VAL:HG21	1.52	0.72
65:AU:288:MET:CB	76:AU:401:PEE:O4	2.35	0.72
3:BC:129:LYS:NZ	16:BQ:113:ILE:O	2.23	0.72
9:J:132:ARG:NH2	73:J:401:NDP:C2B	2.52	0.72
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.72
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.22	0.72
76:l:701:PEE:H46	40:r:155:VAL:HG12	1.71	0.72
65:AU:290:LEU:HD23	65:AU:290:LEU:C	2.14	0.72
76:AU:401:PEE:H61	76:AU:401:PEE:H27	1.70	0.72
9:BJ:174:ILE:HG13	9:BJ:182:ARG:HG3	1.70	0.72
9:BJ:217:PHE:CZ	9:BJ:322:MET:HE2	2.17	0.72
22:BY:45:ARG:HH21	35:Bl:439:THR:HG21	1.52	0.72
25:Bb:10:LEU:HD22	39:Bp:156:PRO:HB2	1.71	0.72
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	0.72
12:M:198:THR:HG22	14:O:39:PHE:HB3	1.70	0.72
16:Q:345:ALA:HB2	21:W:19:ILE:HD11	1.70	0.72
51:3:54:ARG:HD3	51:3:54:ARG:N	2.04	0.72
63:AF:29:LYS:CD	63:AF:75:ILE:HD12	2.17	0.72
65:AU:308:ARG:HH11	75:AU:403:CDL:H1O1	1.38	0.72
3:BC:67:LEU:HD22	3:BC:207:LEU:HD21	1.70	0.72
34:Bk:3:LEU:HD22	36:Bm:117:ASN:HD21	1.53	0.72
35:Bl:451:LEU:H	35:Bl:453:PRO:HD2	1.54	0.72
48:B0:147:LYS:HA	48:B0:147:LYS:HE3	1.72	0.72
1:A:383:THR:HG22	12:M:75:CYS:HA	1.72	0.72
3:C:143:GLU:OE2	3:C:145:ARG:NH2	2.23	0.72
14:O:116:ALA:O	14:O:124:ARG:NH1	2.21	0.72
31:h:70:GLN:HG2	36:m:115:VAL:HG12	1.71	0.72
75:AJ:405:CDL:H742	75:AJ:405:CDL:C78	2.20	0.72
1:BA:383:THR:HG22	12:BM:75:CYS:HA	1.72	0.72
12:BM:63:PHE:O	12:BM:181:ARG:NH2	2.23	0.72
16:BQ:118:ARG:NH2	16:BQ:138:ARG:O	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:281:GLU:N	16:BQ:281:GLU:OE1	2.22	0.72
35:Bl:78:LEU:CD2	35:Bl:80:PHE:HE1	2.02	0.72
44:Bw:209:VAL:HG13	44:Bw:214:VAL:HG21	1.70	0.72
4:E:25:MET:O	4:E:29:LYS:CG	2.38	0.72
9:J:132:ARG:NH2	73:J:401:NDP:O2B	2.22	0.72
39:p:55:LYS:HE2	39:p:55:LYS:HA	1.70	0.72
2:BB:62:THR:HG22	21:BW:35:MET:HE1	1.71	0.72
18:BT:83:ARG:NH1	18:BT:102:ASN:OD1	2.22	0.72
22:BY:43:ARG:HG3	22:BY:46:GLN:HB2	1.72	0.72
35:Bl:100:ILE:HD12	35:Bl:246:LEU:HG	1.72	0.72
35:Bl:384:PRO:O	35:Bl:389:PHE:HB2	1.89	0.72
1:A:98:LYS:HD2	1:A:101:PHE:CE2	2.24	0.72
1:A:381:GLN:NE2	69:A:501:SF4:S3	2.63	0.72
12:M:374:THR:HB	12:M:377:ALA:HA	1.72	0.72
22:Y:86:TYR:HH	43:v:100:LYS:HE2	1.51	0.72
27:d:154:ARG:NH1	30:g:111:ILE:O	2.22	0.72
35:l:170:GLN:NE2	76:l:702:PEE:O2P	2.22	0.72
44:w:209:VAL:HG13	44:w:214:VAL:HG21	1.70	0.72
48:0:147:LYS:HE3	48:0:147:LYS:HA	1.72	0.72
9:BJ:212:ARG:NH2	73:BJ:401:NDP:O2N	2.22	0.72
12:BM:566:ILE:HG13	12:BM:580:ALA:HA	1.72	0.72
22:BY:84:PHE:CG	22:BY:85:PRO:HD3	2.22	0.72
27:Bd:154:ARG:NH1	30:Bg:111:ILE:O	2.22	0.72
68:AL:192:PHE:HB3	68:AL:195:THR:HB	1.72	0.72
4:BE:25:MET:O	4:BE:29:LYS:CG	2.38	0.72
24:Ba:54:LEU:HD22	25:Bb:26:GLN:O	1.90	0.72
25:Bb:109:THR:HB	25:Bb:113:THR:HA	1.70	0.72
32:i:167:TRP:CE3	35:l:573:THR:CB	2.72	0.72
33:j:67:LEU:HD21	34:k:68:ALA:HB3	1.72	0.72
35:l:450:LEU:C	35:l:450:LEU:HD22	2.15	0.72
39:p:56:ASP:CB	68:AY:227:PRO:CG	2.59	0.72
62:AE:34:ARG:CD	62:AE:78:ARG:HH22	2.03	0.72
67:AK:65:ILE:HG22	67:AK:67:ALA:H	1.54	0.72
1:BA:381:GLN:NE2	69:BA:501:SF4:S3	2.63	0.72
9:BJ:350:ILE:HD13	9:BJ:366:ILE:HG12	1.72	0.72
16:BQ:232:VAL:HG12	16:BQ:234:GLN:H	1.54	0.72
25:Bb:106:PRO:HA	25:Bb:115:GLU:OE2	1.89	0.72
32:i:298:TYR:O	32:i:303:THR:OG1	2.08	0.71
41:s:235:ASN:HD22	41:s:267:THR:HG22	1.55	0.71
65:AU:296:MET:HE2	76:AU:401:PEE:C33	2.19	0.71
3:BC:143:GLU:OE2	3:BC:145:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:345:ALA:HB2	21:BW:19:ILE:HD11	1.70	0.71
27:Bd:136:ARG:NH2	28:Be:138:GLU:O	2.23	0.71
16:Q:80:ILE:O	16:Q:81:THR:HG22	1.90	0.71
21:W:134:LEU:HD11	36:m:2:MET:HB2	1.72	0.71
22:Y:89:PRO:O	43:v:107:ARG:NH2	2.20	0.71
27:d:136:ARG:NH2	28:e:138:GLU:O	2.23	0.71
35:l:227:LEU:HD12	35:l:230:HIS:CE1	2.24	0.71
62:AR:34:ARG:HH11	62:AR:78:ARG:NH2	1.87	0.71
3:BC:137:VAL:HG21	16:BQ:87:GLN:NE2	2.05	0.71
21:BW:134:LEU:HD11	36:Bm:2:MET:HB2	1.72	0.71
35:l:100:ILE:HD12	35:l:246:LEU:HG	1.72	0.71
68:AY:195:THR:HG22	68:AY:197:LEU:H	1.55	0.71
1:BA:391:TRP:HH2	12:BM:153:PHE:HA	1.55	0.71
31:Bh:70:GLN:HG2	36:Bm:115:VAL:HG12	1.71	0.71
35:Bl:227:LEU:HD12	35:Bl:230:HIS:CE1	2.24	0.71
2:B:62:THR:HG22	21:W:35:MET:HE1	1.71	0.71
8:I:106:LEU:O	8:I:108:SER:N	2.19	0.71
9:J:212:ARG:NH2	73:J:401:NDP:O2N	2.22	0.71
12:M:557:ARG:NH1	12:M:579:ILE:O	2.24	0.71
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.22	0.71
35:l:571:ILE:CG1	76:l:701:PEE:O5	2.36	0.71
47:z:12:ASN:HD22	54:6:20:VAL:H	1.39	0.71
1:BA:219:LYS:HA	11:BL:174:THR:HG22	1.71	0.71
15:BP:55:HIS:NE2	15:BP:78:VAL:O	2.24	0.71
16:BQ:78:LYS:HZ1	33:Bj:48:ARG:NH2	1.88	0.71
27:Bd:73:GLU:HG2	30:Bg:111:ILE:HD11	1.72	0.71
32:Bi:167:TRP:CE3	35:Bl:573:THR:CB	2.72	0.71
76:Bl:701:PEE:H46	40:Br:155:VAL:HG12	1.71	0.71
6:X:91:ASP:OD1	23:Z:47:ARG:NH1	2.24	0.71
35:l:78:LEU:HG	35:l:139:GLN:HE22	1.55	0.71
35:l:78:LEU:CD2	35:l:80:PHE:HE1	2.02	0.71
76:l:701:PEE:H37	40:r:155:VAL:HG11	1.70	0.71
1:BA:327:ILE:HG23	1:BA:331:VAL:HG13	1.72	0.71
1:BA:381:GLN:HG2	69:BA:501:SF4:S2	2.29	0.71
12:BM:374:THR:HB	12:BM:377:ALA:HA	1.72	0.71
32:Bi:180:ALA:O	32:Bi:183:SER:OG	2.08	0.71
35:Bl:450:LEU:C	35:Bl:450:LEU:HD22	2.15	0.71
2:B:184:ASN:HD21	13:N:127:TYR:H	1.38	0.71
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	0.71
24:a:54:LEU:HD22	25:b:26:GLN:O	1.90	0.71
35:l:451:LEU:H	35:l:453:PRO:HD2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Be:76:TYR:O	40:Br:82:ARG:NH1	2.21	0.71
34:Bk:7:ASN:HD22	36:Bm:9:SER:HB2	1.47	0.71
1:A:116:ASN:O	1:A:245:VAL:HG23	1.91	0.71
22:Y:81:LEU:HD23	22:Y:81:LEU:C	2.15	0.71
33:j:25:PRO:O	33:j:27:LEU:N	2.23	0.71
45:x:176:MET:HE3	45:x:181:THR:HG22	1.71	0.71
61:AQ:22:ALA:HB2	71:AQ:101:PLX:H272	1.72	0.71
68:AY:417:LEU:HD23	68:AY:422:ARG:O	1.91	0.71
12:BM:121:LEU:HD21	12:BM:139:LEU:HD21	1.71	0.71
45:Bx:176:MET:HE3	45:Bx:181:THR:HG22	1.71	0.71
1:A:391:TRP:HH2	12:M:153:PHE:HA	1.55	0.71
5:F:39:LYS:HG3	5:F:40:ARG:H	1.56	0.71
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.71
12:M:63:PHE:O	12:M:181:ARG:NH2	2.23	0.71
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.71	0.71
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.71
27:d:73:GLU:HG2	30:g:111:ILE:HD11	1.72	0.71
39:p:104:LEU:HD21	39:p:119:PHE:HE1	1.55	0.71
63:AF:29:LYS:HG2	63:AF:75:ILE:HD13	1.67	0.71
63:AF:29:LYS:HB2	63:AF:29:LYS:NZ	2.05	0.71
68:AL:195:THR:HG22	68:AL:197:LEU:H	1.53	0.71
68:AL:280:ASP:HA	68:AL:461:PRO:HB3	1.71	0.71
68:AY:152:GLN:HE21	68:AY:253:ILE:N	1.88	0.71
21:BW:108:GLU:OE2	31:Bh:75:ARG:NH1	2.24	0.71
35:Bl:546:GLN:OE1	40:Br:278:ARG:NE	2.22	0.71
1:A:158:ILE:HB	1:A:199:ARG:HG2	1.73	0.71
1:A:327:ILE:HG23	1:A:331:VAL:HG13	1.72	0.71
28:e:76:TYR:O	40:r:82:ARG:NH1	2.21	0.71
64:AG:38:TRP:CD1	75:AG:101:CDL:C51	2.74	0.71
75:AG:101:CDL:H712	75:AG:101:CDL:H521	1.72	0.71
1:BA:158:ILE:HB	1:BA:199:ARG:HG2	1.73	0.71
33:Bj:67:LEU:HD21	34:Bk:68:ALA:HB3	1.72	0.71
16:Q:95:LEU:HD13	16:Q:97:LEU:HD23	1.73	0.71
21:W:115:ARG:HH11	31:h:36:PHE:HD1	1.36	0.71
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.72	0.71
40:r:44:GLN:O	40:r:46:ASN:N	2.24	0.71
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.24	0.71
58:AN:43:ARG:HH11	71:AN:101:PLX:H1B1	1.56	0.71
9:BJ:201:VAL:HG12	9:BJ:203:PRO:HD3	1.71	0.71
5:F:68:ARG:NH1	12:M:359:ASN:OD1	2.23	0.70
16:Q:432:LEU:HD12	16:Q:461:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AE:21:GLU:O	62:AE:24:GLU:N	2.24	0.70
62:AR:34:ARG:HH11	62:AR:78:ARG:NH1	1.88	0.70
9:BJ:176:SER:O	9:BJ:182:ARG:NH2	2.24	0.70
12:BM:557:ARG:NH1	12:BM:579:ILE:O	2.24	0.70
76:BV:202:PEE:H60	76:BV:202:PEE:H42	1.72	0.70
32:Bi:298:TYR:O	32:Bi:303:THR:OG1	2.08	0.70
35:Bl:567:SER:O	35:Bl:571:ILE:CD1	2.39	0.70
12:M:543:LYS:NZ	12:M:563:ASP:OD2	2.23	0.70
14:O:187:GLN:HE21	14:O:190:ASP:HA	1.56	0.70
68:AY:296:TRP:HD1	68:AY:419:THR:HG23	0.90	0.70
5:BF:68:ARG:NH1	12:BM:359:ASN:OD1	2.23	0.70
22:BY:81:LEU:HD23	22:BY:81:LEU:C	2.15	0.70
44:Bw:176:GLN:NE2	44:Bw:236:ASP:OD2	2.24	0.70
3:C:137:VAL:HG21	16:Q:87:GLN:NE2	2.05	0.70
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.72	0.70
12:M:566:ILE:HG13	12:M:580:ALA:HA	1.72	0.70
16:Q:232:VAL:HG12	16:Q:234:GLN:H	1.54	0.70
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.70
22:Y:86:TYR:OH	43:v:100:LYS:HE3	1.89	0.70
28:e:129:ARG:NH1	28:e:136:ILE:O	2.24	0.70
76:AH:401:PEE:H28	76:AH:401:PEE:C40	2.21	0.70
1:BA:116:ASN:O	1:BA:245:VAL:HG23	1.91	0.70
15:BP:93:VAL:HB	15:BP:154:GLU:HB2	1.73	0.70
6:BX:84:LEU:HD22	6:BX:98:LEU:HD21	1.74	0.70
35:Bl:10:LEU:HD22	35:Bl:46:ILE:HG21	1.72	0.70
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.70
18:T:83:ARG:NH1	18:T:102:ASN:OD1	2.22	0.70
45:x:11:ASN:HD22	45:x:14:ASP:H	1.39	0.70
63:AF:14:LEU:O	63:AF:17:ILE:HG13	1.91	0.70
67:AK:399:GLN:HE22	67:AK:407:MET:HB3	1.56	0.70
3:BC:105:ARG:HA	41:Bs:37:PRO:HA	1.72	0.70
35:Bl:78:LEU:HG	35:Bl:139:GLN:HE22	1.55	0.70
35:Bl:190:ILE:HG13	35:Bl:196:TRP:CD1	2.27	0.70
35:Bl:379:ALA:HA	35:Bl:386:LEU:HD11	1.73	0.70
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.70
15:P:93:VAL:HB	15:P:154:GLU:HB2	1.72	0.70
35:l:567:SER:O	35:l:571:ILE:CD1	2.39	0.70
59:AB:8:SER:OG	59:AB:26:LEU:O	2.09	0.70
66:AV:80:ARG:NH1	82:AV:401:HEM:O1A	2.25	0.70
66:AV:324:LEU:HD11	66:AV:369:ILE:HD12	1.72	0.70
76:BW:201:PEE:H24	76:BW:201:PEE:H53	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Be:129:ARG:NH1	28:Be:136:ILE:O	2.24	0.70
40:Br:44:GLN:O	40:Br:46:ASN:N	2.24	0.70
47:Bz:12:ASN:HD22	54:B6:20:VAL:H	1.39	0.70
35:l:78:LEU:CD2	35:l:80:PHE:CE1	2.74	0.70
63:AF:29:LYS:HG2	63:AF:75:ILE:HG12	1.70	0.70
67:AW:184:ASN:HB3	67:AW:251:ALA:HA	1.72	0.70
67:AW:261:GLN:NE2	67:AW:443:ASN:O	2.25	0.70
41:Bs:235:ASN:HD22	41:Bs:267:THR:HG22	1.55	0.70
12:M:144:MET:SD	16:Q:380:HIS:ND1	2.63	0.70
25:b:105:PHE:CE2	43:v:68:LYS:HA	2.27	0.70
34:k:2:PRO:CG	36:m:115:VAL:HG21	2.21	0.70
68:AY:48:THR:HG22	68:AY:62:GLU:HB2	1.73	0.70
11:BL:82:PRO:HG3	11:BL:98:LYS:HE3	1.73	0.70
6:BX:91:ASP:OD1	23:BZ:47:ARG:NH1	2.24	0.70
27:Bd:65:VAL:H	27:Bd:85:GLN:NE2	1.89	0.70
39:Bp:104:LEU:HD21	39:Bp:119:PHE:HE1	1.55	0.70
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.70
16:Q:48:GLY:HA2	32:i:228:LEU:HD11	1.74	0.70
76:V:202:PEE:H60	76:V:202:PEE:H42	1.72	0.70
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.70
71:r:502:PLX:H31	71:r:502:PLX:H72	1.73	0.70
4:BE:70:ASN:O	72:BE:201:8Q1:O40	2.10	0.70
9:BJ:85:ARG:HD2	9:BJ:85:ARG:O	1.92	0.70
12:BM:289:LYS:NZ	12:BM:694:PHE:O	2.25	0.70
35:Bl:341:MET:HE2	35:Bl:457:LEU:HD12	1.72	0.70
71:Br:502:PLX:H72	71:Br:502:PLX:H31	1.73	0.70
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.56	0.70
27:d:65:VAL:H	27:d:85:GLN:NE2	1.89	0.70
67:AK:438:MET:HB2	67:AK:450:VAL:CG1	2.22	0.70
66:AV:344:SER:OG	66:AV:346:PRO:HD2	1.91	0.70
67:AW:351:ILE:HD11	67:AW:448:PRO:CD	2.20	0.70
1:BA:124:THR:HG23	1:BA:126:LYS:HG2	1.72	0.70
1:BA:318:ILE:HG22	1:BA:326:LEU:HA	1.74	0.70
15:BP:134:SER:HG	15:BP:139:SER:HG	1.23	0.70
16:BQ:80:ILE:O	16:BQ:81:THR:HG22	1.91	0.70
22:BY:86:TYR:CB	22:BY:87:PRO:HA	2.22	0.70
12:M:476:LEU:HB3	12:M:515:ILE:HG22	1.74	0.70
21:W:31:SER:OG	21:W:35:MET:HE3	1.91	0.70
21:W:108:GLU:OE2	31:h:75:ARG:NH1	2.24	0.70
75:AG:101:CDL:H542	75:AG:101:CDL:C73	2.22	0.70
1:BA:211:ALA:HB2	1:BA:223:PRO:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:221:HIS:CE1	9:BJ:222:ARG:CG	2.72	0.70
12:BM:472:PRO:O	12:BM:510:TRP:NE1	2.25	0.70
16:BQ:95:LEU:HD13	16:BQ:97:LEU:HD23	1.73	0.70
16:BQ:282:GLU:OE2	16:BQ:437:LYS:NZ	2.22	0.70
25:Bb:105:PHE:CE2	43:Bv:68:LYS:HA	2.26	0.70
35:Bl:78:LEU:CD2	35:Bl:80:PHE:CE1	2.74	0.70
39:Bp:55:LYS:HE2	39:Bp:55:LYS:CA	2.21	0.70
35:l:10:LEU:HD22	35:l:46:ILE:HG21	1.72	0.69
66:AJ:156:ILE:CG2	66:AJ:160:LEU:HB2	2.18	0.69
12:BM:194:ASP:O	12:BM:208:THR:OG1	2.10	0.69
71:Bb:201:PLX:O3	71:Bb:201:PLX:O7	2.05	0.69
1:A:124:THR:HG23	1:A:126:LYS:HG2	1.72	0.69
4:E:70:ASN:O	72:E:201:8Q1:O40	2.10	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	0.69
9:J:247:LYS:HD2	9:J:340:ILE:HD12	1.74	0.69
35:l:190:ILE:HG13	35:l:196:TRP:CD1	2.27	0.69
75:AL:502:CDL:H772	76:AL:503:PEE:H70	1.73	0.69
68:AY:387:GLU:OE2	68:AY:390:ARG:NH2	2.23	0.69
9:BJ:233:TRP:HA	9:BJ:272:LEU:HD21	1.74	0.69
12:BM:595:THR:HA	12:BM:605:GLN:HA	1.74	0.69
34:Bk:2:PRO:CG	36:Bm:115:VAL:HG21	2.21	0.69
35:Bl:4:HIS:HE1	35:Bl:87:MET:HE3	1.57	0.69
35:Bl:135:ASN:HD21	35:Bl:199:GLN:HE22	1.39	0.69
46:By:13:THR:HB	46:By:168:LEU:HD23	1.74	0.69
75:AG:101:CDL:HA62	75:AG:101:CDL:C34	2.22	0.69
65:AU:202:ARG:NH1	65:AU:279:GLU:OE2	2.25	0.69
65:AU:292:MET:HE1	66:AV:241:THR:HG23	1.74	0.69
66:AV:295:LEU:O	66:AV:299:LEU:CD2	2.40	0.69
22:BY:86:TYR:HH	43:Bv:100:LYS:HE2	1.55	0.69
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.69
16:Q:241:MET:HG3	21:W:11:PRO:HB2	1.72	0.69
16:Q:282:GLU:OE2	16:Q:437:LYS:NZ	2.22	0.69
35:l:226:GLN:HG3	35:l:280:LEU:HD23	1.74	0.69
12:BM:476:LEU:HB3	12:BM:515:ILE:HG22	1.74	0.69
16:BQ:268:TRP:HZ3	16:BQ:272:THR:HG21	1.52	0.69
21:BW:31:SER:OG	21:BW:35:MET:HE3	1.91	0.69
34:Bk:66:PHE:HE1	36:Bm:159:THR:HG21	1.57	0.69
35:Bl:97:THR:HG21	35:Bl:125:LEU:CD1	2.20	0.69
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.69
22:Y:43:ARG:HG3	22:Y:46:GLN:HB2	1.72	0.69
30:g:15:ASP:HB2	30:g:18:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:29:LYS:CG	63:AF:75:ILE:HD13	2.16	0.69
66:AJ:300:ILE:O	66:AJ:303:MET:N	2.25	0.69
67:AK:257:GLU:CG	67:AK:450:VAL:CG2	2.70	0.69
66:AV:332:LEU:CD1	76:AV:403:PEE:H37	2.22	0.69
5:BF:39:LYS:HG3	5:BF:40:ARG:H	1.56	0.69
7:BH:12:VAL:HG13	16:BQ:280:ALA:H	1.57	0.69
38:Bo:23:TYR:OH	39:Bp:68:GLU:OE1	2.09	0.69
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.73	0.69
16:Q:85:GLY:HA3	33:j:39:CYS:CB	2.22	0.69
24:a:55:PHE:CE2	39:p:118:TYR:HE2	1.96	0.69
44:w:67:CYS:N	44:w:70:LYS:HD3	2.07	0.69
46:y:13:THR:HB	46:y:168:LEU:HD23	1.74	0.69
67:AK:183:ARG:HH21	67:AK:183:ARG:HG3	1.57	0.69
68:AY:145:GLU:HB2	68:AY:249:HIS:NE2	2.08	0.69
16:BQ:85:GLY:HA3	33:Bj:39:CYS:CB	2.22	0.69
20:BV:81:ARG:HG2	20:BV:83:LYS:HG3	1.75	0.69
44:Bw:67:CYS:N	44:Bw:70:LYS:HD3	2.07	0.69
3:C:105:ARG:HA	41:s:37:PRO:HA	1.72	0.69
14:O:137:THR:HG21	14:O:176:CYS:HB2	1.74	0.69
16:Q:190:HIS:HD2	16:Q:452:GLY:HA3	1.58	0.69
22:Y:86:TYR:HB3	22:Y:87:PRO:HA	1.75	0.69
35:l:338:MET:HE3	35:l:372:SER:HB2	1.74	0.69
39:p:170:ILE:H	39:p:170:ILE:CD1	2.02	0.69
76:AH:401:PEE:H15	66:AJ:240:MET:HE1	1.75	0.69
12:BM:613:PRO:HB2	13:BN:134:ILE:HD13	1.73	0.69
16:BQ:241:MET:HG3	21:BW:11:PRO:HB2	1.72	0.69
16:BQ:262:LEU:HD13	16:BQ:268:TRP:NE1	2.08	0.69
25:Bb:16:ARG:O	25:Bb:20:ARG:HG2	1.93	0.69
25:Bb:54:LYS:HG3	25:Bb:55:SER:H	1.58	0.69
25:Bb:94:PRO:HB3	27:Bd:5:TRP:HA	1.74	0.69
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
14:O:133:GLN:HB2	14:O:174:VAL:HG21	1.75	0.69
76:W:201:PEE:H75	41:s:77:LEU:HD23	1.75	0.69
76:W:201:PEE:H24	76:W:201:PEE:H53	1.73	0.69
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.09	0.69
39:p:55:LYS:HE2	39:p:55:LYS:CA	2.21	0.69
64:AT:24:TRP:CZ3	75:AY:501:CDL:H551	2.28	0.69
2:BB:120:ILE:HD11	16:BQ:385:TYR:HB3	1.74	0.69
9:BJ:202:LYS:HB2	9:BJ:264:ALA:HA	1.75	0.69
14:BO:54:ASP:OD1	14:BO:60:TYR:OH	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BO:137:THR:HG21	14:BO:176:CYS:HB2	1.74	0.69
16:BQ:190:HIS:HD2	16:BQ:452:GLY:HA3	1.58	0.69
16:BQ:432:LEU:HD12	16:BQ:461:VAL:HG11	1.73	0.69
22:BY:86:TYR:HB3	22:BY:87:PRO:HA	1.75	0.69
35:Bl:567:SER:O	35:Bl:571:ILE:HD12	1.92	0.69
22:Y:86:TYR:CB	22:Y:87:PRO:HA	2.22	0.69
35:l:4:HIS:CE1	35:l:87:MET:HE3	2.28	0.69
76:l:701:PEE:H36	40:r:155:VAL:CG1	2.21	0.69
47:z:156:ARG:HG3	47:z:156:ARG:HH11	1.56	0.69
14:BO:187:GLN:HE21	14:BO:190:ASP:HA	1.56	0.69
45:Bx:11:ASN:HD22	45:Bx:14:ASP:H	1.39	0.69
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.69
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.58	0.69
25:b:54:LYS:HG3	25:b:55:SER:H	1.58	0.69
36:m:121:VAL:O	36:m:123:SER:N	2.26	0.69
44:w:63:ASP:OD2	44:w:241:TYR:OH	2.11	0.69
60:AC:216:VAL:HG21	66:AV:262:LEU:HD22	1.74	0.69
66:AV:111:GLU:HG2	66:AV:199:PHE:CE1	2.28	0.69
7:BH:12:VAL:HG13	16:BQ:280:ALA:N	2.07	0.69
9:BJ:247:LYS:HD2	9:BJ:340:ILE:HD12	1.74	0.69
16:BQ:338:ARG:HH22	21:BW:23:ARG:HB3	1.58	0.69
45:Bx:69:MET:HE2	45:Bx:70:VAL:HG23	1.75	0.69
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.59	0.68
12:M:472:PRO:O	12:M:510:TRP:NE1	2.25	0.68
25:b:94:PRO:HB3	27:d:5:TRP:HA	1.73	0.68
35:l:379:ALA:HA	35:l:386:LEU:HD11	1.73	0.68
40:r:144:ASN:O	40:r:147:THR:OG1	2.10	0.68
44:w:132:GLN:HE22	44:w:169:PHE:HD2	1.41	0.68
3:C:128:ASN:ND2	3:C:164:TYR:O	2.24	0.68
9:J:233:TRP:HA	9:J:272:LEU:HD21	1.74	0.68
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	0.68
15:P:46:THR:O	16:Q:162:ARG:N	2.16	0.68
24:a:98:LEU:HA	27:d:57:TYR:CD1	2.28	0.68
25:b:16:ARG:O	25:b:20:ARG:HG2	1.93	0.68
35:l:222:GLY:HA3	35:l:229:LEU:HD12	1.74	0.68
41:s:265:LEU:O	41:s:268:SER:OG	2.10	0.68
63:AF:39:TYR:CD1	63:AF:40:GLU:N	2.61	0.68
1:BA:60:GLY:HA3	14:BO:241:PRO:HB3	1.74	0.68
1:BA:379:CYS:HA	12:BM:200:ARG:HB2	1.74	0.68
9:BJ:203:PRO:HA	9:BJ:265:PHE:HB2	1.75	0.68
33:Bj:30:TYR:HB2	33:Bj:33:LYS:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:4:HIS:CE1	35:Bl:87:MET:HE1	2.28	0.68
41:Bs:107:ALA:O	41:Bs:110:SER:OG	2.11	0.68
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.75	0.68
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.75	0.68
62:AE:30:LEU:HD12	62:AE:30:LEU:O	1.93	0.68
65:AU:288:MET:HE2	66:AV:77:TRP:HH2	1.58	0.68
2:BB:184:ASN:HD21	13:BN:127:TYR:H	1.39	0.68
16:BQ:48:GLY:HA2	32:Bi:228:LEU:HD11	1.74	0.68
16:BQ:271:ARG:NH1	41:Bs:281:ARG:CA	2.57	0.68
35:Bl:444:ASN:OD1	35:Bl:445:GLU:N	2.26	0.68
46:By:186:SER:HB3	46:By:213:LEU:HD22	1.76	0.68
47:Bz:156:ARG:HH11	47:Bz:156:ARG:HG3	1.56	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
12:M:173:MET:O	12:M:175:ARG:N	2.24	0.68
12:M:194:ASP:O	12:M:208:THR:OG1	2.11	0.68
16:Q:271:ARG:NH1	41:s:281:ARG:CA	2.57	0.68
35:l:567:SER:O	35:l:571:ILE:HD12	1.92	0.68
46:y:186:SER:HB3	46:y:213:LEU:HD22	1.76	0.68
65:AH:124:CYS:SG	81:AH:402:HEC:HBC2	2.33	0.68
67:AK:257:GLU:HG3	67:AK:450:VAL:CG2	2.23	0.68
4:BE:25:MET:HB2	4:BE:29:LYS:HE3	1.75	0.68
12:BM:299:ARG:HD3	12:BM:703:ALA:HB1	1.74	0.68
76:Bl:701:PEE:H36	40:Br:155:VAL:CG1	2.21	0.68
39:Bp:48:PHE:HE1	72:Bp:201:8Q1:C7	2.06	0.68
47:Bz:154:GLY:HA2	50:B2:6:VAL:HG22	1.75	0.68
7:H:12:VAL:HG13	16:Q:280:ALA:N	2.07	0.68
12:M:225:ILE:HD12	12:M:285:TRP:HH2	1.57	0.68
15:P:134:SER:HG	15:P:139:SER:HG	1.29	0.68
19:U:82:LYS:NZ	42:u:121:ASP:OD1	2.17	0.68
35:l:396:ILE:O	35:l:400:ASN:ND2	2.26	0.68
45:x:69:MET:HE2	45:x:70:VAL:HG23	1.75	0.68
67:AK:257:GLU:HG3	67:AK:450:VAL:HG22	1.73	0.68
63:AS:67:LEU:HD23	66:AV:209:LEU:HD12	1.75	0.68
65:AU:112:ARG:NH1	65:AU:269:ASP:OD2	2.26	0.68
4:BE:23:ARG:N	4:BE:27:GLU:OE1	2.24	0.68
25:Bb:14:GLN:HE22	39:Bp:157:ALA:HB3	1.56	0.68
32:i:180:ALA:O	32:i:183:SER:OG	2.08	0.68
68:AL:171:GLU:OE2	68:AL:175:ASN:ND2	2.26	0.68
66:AV:14:ILE:HD13	76:AY:502:PEE:C25	2.22	0.68
68:AY:152:GLN:HE21	68:AY:253:ILE:HG13	1.58	0.68
68:AY:285:ALA:HB3	68:AY:360:CYS:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:159:TYR:HE1	16:BQ:135:TYR:CZ	2.12	0.68
10:BK:99:PRO:HG2	14:BO:71:PRO:HB3	1.76	0.68
12:BM:124:HIS:HD2	16:BQ:375:MET:HE2	1.58	0.68
35:Bl:338:MET:HE3	35:Bl:372:SER:HB2	1.74	0.68
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.68
14:O:54:ASP:OD1	14:O:60:TYR:OH	2.11	0.68
27:d:49:GLN:OE1	27:d:49:GLN:N	2.27	0.68
33:j:30:TYR:HB2	33:j:33:LYS:HD2	1.75	0.68
34:k:66:PHE:HE1	36:m:159:THR:HG21	1.57	0.68
68:AL:262:VAL:HG11	39:Bp:58:ALA:HA	1.75	0.68
12:BM:225:ILE:HD12	12:BM:285:TRP:HH2	1.57	0.68
15:BP:157:VAL:HG21	15:BP:181:HIS:HD2	1.58	0.68
24:Ba:98:LEU:CB	27:Bd:57:TYR:CD1	2.77	0.68
24:Ba:98:LEU:HA	27:Bd:57:TYR:CD1	2.28	0.68
25:Bb:93:LYS:CE	35:Bl:65:ASN:O	2.41	0.68
35:Bl:141:PHE:HE2	40:Br:375:LEU:HD21	1.58	0.68
42:Bu:34:ALA:HB2	42:Bu:120:PRO:HD3	1.75	0.68
9:J:221:HIS:CE1	9:J:222:ARG:CG	2.72	0.68
10:K:99:PRO:HG2	14:O:71:PRO:HB3	1.76	0.68
16:Q:262:LEU:CD2	16:Q:268:TRP:CD1	2.60	0.68
35:l:4:HIS:CE1	35:l:87:MET:HE1	2.28	0.68
61:AD:48:ASN:HB2	61:AD:51:LYS:HD2	1.74	0.68
59:AO:35:PRO:HB3	67:AW:320:PRO:HA	1.75	0.68
60:AP:236:CYS:HB3	60:AP:241:SER:HB2	1.74	0.68
21:BW:86:MET:SD	21:BW:128:ARG:NH1	2.66	0.68
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CG	2.82	0.68
35:Bl:396:ILE:O	35:Bl:400:ASN:ND2	2.26	0.68
35:l:135:ASN:HD21	35:l:199:GLN:HE22	1.39	0.68
30:Bg:15:ASP:HB2	30:Bg:18:ARG:HH21	1.57	0.68
44:Bw:132:GLN:HE22	44:Bw:169:PHE:HD2	1.41	0.68
56:B8:19:TRP:HZ2	57:B9:14:GLU:HG2	1.59	0.68
18:T:79:GLU:HG2	18:T:120:ARG:HB3	1.76	0.68
20:V:81:ARG:HG2	20:V:83:LYS:HG3	1.75	0.68
24:a:55:PHE:HE2	39:p:118:TYR:HE2	1.26	0.68
66:AJ:338:ILE:HD11	66:AJ:350:ILE:HG22	1.76	0.68
3:BC:136:LYS:O	3:BC:140:GLN:HG3	1.94	0.68
24:Ba:98:LEU:HA	27:Bd:57:TYR:HD1	1.59	0.68
34:Bk:3:LEU:HD23	36:Bm:117:ASN:ND2	2.09	0.68
34:Bk:83:ASN:ND2	36:Bm:173:GLY:O	2.27	0.68
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.67
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:U:101:PLX:HO9	33:j:106:TRP:CD1	2.12	0.67
39:p:48:PHE:HE1	72:p:201:8Q1:C7	2.06	0.67
39:p:56:ASP:CG	68:AY:227:PRO:HG3	2.18	0.67
56:8:19:TRP:HZ2	57:9:14:GLU:HG2	1.59	0.67
67:AK:100:THR:HG21	68:AL:324:LEU:HB3	1.75	0.67
59:AO:18:THR:OG1	67:AW:110:LEU:O	2.11	0.67
62:AR:79:ASP:HB3	65:AU:92:PRO:CG	2.23	0.67
9:BJ:210:GLU:O	9:BJ:210:GLU:HG2	1.92	0.67
73:BJ:401:NDP:O2X	73:BJ:401:NDP:H1B	1.94	0.67
11:BL:58:LYS:NZ	11:BL:139:GLU:OE1	2.27	0.67
25:Bb:88:TYR:O	25:Bb:92:GLU:CB	2.42	0.67
34:Bk:51:THR:O	34:Bk:53:SER:N	2.28	0.67
21:W:86:MET:SD	21:W:128:ARG:NH1	2.66	0.67
24:a:98:LEU:HA	27:d:57:TYR:HD1	1.59	0.67
25:b:12:LEU:HB3	25:b:16:ARG:HH12	1.58	0.67
35:l:4:HIS:HE1	35:l:87:MET:HE3	1.57	0.67
35:l:97:THR:HG21	35:l:125:LEU:CD1	2.20	0.67
12:BM:466:LEU:HD23	12:BM:500:ILE:HD11	1.75	0.67
35:Bl:4:HIS:CE1	35:Bl:87:MET:HE3	2.28	0.67
36:Bm:121:VAL:O	36:Bm:123:SER:N	2.26	0.67
40:Br:15:THR:O	40:Br:93:LYS:NZ	2.24	0.67
16:Q:262:LEU:HD13	16:Q:268:TRP:NE1	2.08	0.67
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.67
25:b:51:LEU:HD11	25:b:62:HIS:CD2	2.30	0.67
35:l:444:ASN:OD1	35:l:445:GLU:N	2.26	0.67
42:u:34:ALA:HB2	42:u:120:PRO:HD3	1.75	0.67
58:AA:12:ARG:HG2	58:AA:13:HIS:ND1	2.10	0.67
75:AG:101:CDL:C53	75:AG:101:CDL:H731	2.24	0.67
76:AH:401:PEE:C12	66:AJ:240:MET:HE1	2.24	0.67
68:AL:261:ALA:HB1	38:Bo:25:ILE:O	1.95	0.67
70:BA:502:FMN:O4'	70:BA:502:FMN:H9	1.94	0.67
14:BO:133:GLN:HB2	14:BO:174:VAL:HG21	1.75	0.67
71:Bb:201:PLX:H6	71:Bb:201:PLX:H111	1.75	0.67
35:Bl:188:TRP:CD2	35:Bl:192:HIS:HD2	2.09	0.67
35:Bl:226:GLN:HG2	35:Bl:280:LEU:CD2	2.25	0.67
40:Br:369:LEU:O	40:Br:372:THR:OG1	2.12	0.67
49:B1:43:PRO:HB2	49:B1:48:ILE:HD11	1.76	0.67
9:J:210:GLU:O	9:J:210:GLU:HG2	1.93	0.67
16:Q:271:ARG:HD3	41:s:279:ARG:O	1.95	0.67
34:k:51:THR:O	34:k:53:SER:N	2.28	0.67
76:AJ:403:PEE:H25	76:AJ:403:PEE:H61	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:114:TRP:HE1	16:BQ:394:GLY:HA2	1.59	0.67
16:BQ:271:ARG:HD3	41:Bs:279:ARG:O	1.95	0.67
76:BW:201:PEE:H36	33:Bj:7:LEU:HD22	1.77	0.67
45:Bx:151:HIS:O	45:Bx:155:VAL:HG23	1.94	0.67
16:Q:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.67
22:Y:81:LEU:CD2	43:v:92:HIS:CD2	2.77	0.67
22:Y:84:PHE:CD2	22:Y:85:PRO:HD2	2.30	0.67
25:b:120:MET:SD	43:v:65:ARG:NH2	2.66	0.67
34:k:83:ASN:ND2	36:m:173:GLY:O	2.27	0.67
35:l:141:PHE:HE2	40:r:375:LEU:HD21	1.58	0.67
40:r:369:LEU:O	40:r:372:THR:OG1	2.12	0.67
45:x:151:HIS:O	45:x:155:VAL:HG23	1.95	0.67
47:z:154:GLY:HA2	50:2:6:VAL:HG22	1.75	0.67
59:AB:49:PHE:O	68:AL:180:ARG:NH1	2.26	0.67
1:BA:118:ASP:O	1:BA:159:ARG:HD2	1.95	0.67
9:BJ:173:ASN:HB2	9:BJ:327:MET:HE1	1.76	0.67
11:BL:89:SER:OG	15:BP:239:TRP:NE1	2.26	0.67
34:Bk:25:HIS:HA	34:Bk:90:VAL:HG13	1.77	0.67
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	0.67
2:B:111:CYS:O	2:B:139:ARG:NH2	2.28	0.67
26:c:62:TYR:OH	26:c:74:ASP:O	2.11	0.67
67:AW:57:PRO:HG2	68:AY:400:VAL:HG11	1.75	0.67
1:BA:381:GLN:HG3	1:BA:382:CYS:H	1.59	0.67
12:BM:144:MET:SD	16:BQ:380:HIS:ND1	2.63	0.67
26:Bc:122:THR:O	38:Bo:12:ARG:NH2	2.27	0.67
27:Bd:59:HIS:HE1	28:Be:120:ARG:CB	1.98	0.67
33:Bj:5:LEU:HD13	41:Bs:3:MET:HE1	1.77	0.67
7:H:114:TRP:HE1	16:Q:394:GLY:HA2	1.59	0.67
22:Y:90:SER:HA	43:v:107:ARG:HH12	1.59	0.67
25:b:88:TYR:O	25:b:92:GLU:CB	2.42	0.67
34:k:3:LEU:HD23	36:m:117:ASN:ND2	2.09	0.67
35:l:227:LEU:HD12	35:l:230:HIS:HD1	1.60	0.67
68:AL:80:ARG:NH1	68:AL:268:CYS:SG	2.67	0.67
3:BC:161:HIS:O	3:BC:168:ARG:NH2	2.28	0.67
35:Bl:447:ASN:CG	35:Bl:448:PRO:HD2	2.16	0.67
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.67
70:A:502:FMN:O4'	70:A:502:FMN:H9	1.94	0.67
3:C:159:TYR:HE1	16:Q:135:TYR:CZ	2.12	0.67
11:L:58:LYS:NZ	11:L:139:GLU:OE1	2.27	0.67
34:k:4:ILE:HD13	36:m:125:MET:SD	2.35	0.67
22:BY:81:LEU:CD2	43:Bv:92:HIS:CD2	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Bb:120:MET:SD	43:Bv:65:ARG:NH2	2.66	0.67
71:Bb:201:PLX:H6	71:Bb:201:PLX:C11	2.24	0.67
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.67
15:P:134:SER:OG	15:P:139:SER:OG	2.07	0.67
24:a:55:PHE:CD2	39:p:118:TYR:CG	2.82	0.67
24:a:98:LEU:CB	27:d:57:TYR:CD1	2.77	0.67
71:b:201:PLX:H6	71:b:201:PLX:H111	1.75	0.67
34:k:1:MET:HB2	34:k:4:ILE:HD13	1.77	0.67
63:AF:36:ASP:OD2	63:AF:62:ARG:NH1	2.28	0.67
2:BB:119:ALA:HA	15:BP:233:PHE:HE2	1.60	0.67
12:BM:300:GLN:HB2	13:BN:137:TRP:HA	1.77	0.67
24:Ba:58:ARG:HH21	24:Ba:61:ARG:HD2	1.60	0.67
25:Bb:12:LEU:HB3	25:Bb:16:ARG:HH12	1.58	0.67
25:Bb:115:GLU:HG2	25:Bb:116:VAL:N	2.10	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	0.67
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.67
45:x:298:ASP:HB2	45:x:301:THR:HG23	1.77	0.67
66:AV:150:LEU:HD23	66:AV:164:ILE:HD13	1.75	0.67
8:BI:66:PRO:HB3	15:BP:79:SER:HB3	1.77	0.67
9:BJ:171:ASN:O	9:BJ:181:LEU:CG	2.41	0.67
25:Bb:51:LEU:HD11	25:Bb:62:HIS:CD2	2.30	0.67
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.66
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.77	0.66
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.66
12:M:300:GLN:HB2	13:N:137:TRP:HA	1.77	0.66
41:s:85:LEU:HB3	41:s:233:MET:SD	2.34	0.66
63:AF:33:MET:HG3	63:AF:62:ARG:NH1	2.09	0.66
75:AG:101:CDL:H521	75:AG:101:CDL:CB7	2.26	0.66
68:AY:225:LYS:NZ	68:AY:257:TYR:HA	2.09	0.66
1:BA:43:THR:HG21	14:BO:239:LYS:HB2	1.76	0.66
1:BA:214:GLU:OE2	1:BA:224:ARG:NH1	2.24	0.66
16:BQ:35:ARG:NH1	28:Be:60:GLU:OE2	2.28	0.66
18:BT:79:GLU:HG2	18:BT:120:ARG:HB3	1.76	0.66
22:BY:84:PHE:CD2	22:BY:85:PRO:HD2	2.30	0.66
73:J:401:NDP:O2X	73:J:401:NDP:H1B	1.94	0.66
35:l:226:GLN:HG2	35:l:280:LEU:CD2	2.25	0.66
59:AB:16:SER:OG	59:AB:19:SER:O	2.12	0.66
16:BQ:251:PHE:HB2	16:BQ:254:ARG:HH21	1.59	0.66
25:Bb:114:GLY:O	25:Bb:115:GLU:HB3	1.95	0.66
10:K:100:SER:HA	14:O:72:GLU:HB3	1.77	0.66
33:j:5:LEU:HD13	41:s:3:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:25:HIS:HA	34:k:90:VAL:HG13	1.77	0.66
41:s:107:ALA:O	41:s:110:SER:OG	2.11	0.66
3:BC:137:VAL:CG2	16:BQ:87:GLN:NE2	2.59	0.66
10:BK:100:SER:HA	14:BO:72:GLU:HB3	1.77	0.66
18:BT:40:THR:OG1	18:BT:42:THR:O	2.14	0.66
32:Bi:12:THR:HG22	36:Bm:158:TRP:NE1	2.10	0.66
34:Bk:1:MET:HB2	34:Bk:4:ILE:HD13	1.77	0.66
41:Bs:85:LEU:HB3	41:Bs:233:MET:SD	2.34	0.66
47:Bz:209:ILE:O	47:Bz:213:THR:HG23	1.95	0.66
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.66
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	0.66
16:Q:338:ARG:HH22	21:W:23:ARG:HB3	1.58	0.66
76:W:201:PEE:H36	33:j:7:LEU:HD22	1.77	0.66
25:b:93:LYS:CE	35:l:65:ASN:O	2.41	0.66
30:g:27:ASP:OD2	30:g:29:ARG:NH1	2.29	0.66
3:BC:125:THR:HG21	16:BQ:118:ARG:HG2	1.77	0.66
21:BW:28:ARG:HG2	21:BW:28:ARG:O	1.93	0.66
41:Bs:200:LEU:HD12	41:Bs:285:LEU:HD11	1.77	0.66
3:C:161:HIS:O	3:C:168:ARG:NH2	2.28	0.66
9:J:132:ARG:NH2	73:J:401:NDP:H2B	2.11	0.66
9:J:173:ASN:HB2	9:J:327:MET:HE1	1.76	0.66
40:r:305:THR:O	40:r:308:SER:OG	2.12	0.66
64:AT:45:VAL:HG21	64:AT:48:ILE:HB	1.77	0.66
1:BA:89:GLY:HA2	1:BA:244:ASN:HD22	1.59	0.66
2:BB:111:CYS:O	2:BB:139:ARG:NH2	2.28	0.66
32:Bi:42:PRO:HG3	36:Bm:166:ILE:HG23	1.78	0.66
34:Bk:11:ALA:HB1	36:Bm:16:PHE:CD2	2.31	0.66
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.66
16:Q:271:ARG:HH11	41:s:281:ARG:CA	2.09	0.66
71:b:201:PLX:H6	71:b:201:PLX:C11	2.24	0.66
34:k:11:ALA:HB1	36:m:16:PHE:CD2	2.31	0.66
52:4:38:ARG:HG2	52:4:85:ILE:HG23	1.76	0.66
67:AK:176:ASN:ND2	67:AK:260:GLU:OE2	2.29	0.66
68:AL:257:TYR:HD2	68:AL:262:VAL:HG22	1.59	0.66
66:AV:326:TRP:HZ2	76:AV:403:PEE:H13	1.60	0.66
32:Bi:288:LEU:HD22	76:Bl:701:PEE:H58	1.69	0.66
40:Br:150:LEU:O	40:Br:153:THR:OG1	2.12	0.66
44:Bw:63:ASP:OD2	44:Bw:241:TYR:OH	2.11	0.66
44:Bw:188:ASN:HA	44:Bw:191:LYS:HE2	1.78	0.66
3:C:125:THR:HG21	16:Q:118:ARG:HG2	1.76	0.66
9:J:355:ARG:HB3	33:j:31:MET:SD	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:28:ARG:HG2	21:W:28:ARG:O	1.93	0.66
28:e:76:TYR:H	40:r:432:ARG:HD2	1.61	0.66
35:l:190:ILE:HG12	35:l:196:TRP:CE2	2.31	0.66
47:z:209:ILE:O	47:z:213:THR:HG23	1.95	0.66
9:BJ:48:ARG:NH1	9:BJ:98:GLY:O	2.29	0.66
71:BU:101:PLX:HO9	33:Bj:106:TRP:CD1	2.13	0.66
22:BY:90:SER:HA	43:Bv:107:ARG:HH12	1.59	0.66
52:B4:38:ARG:HG2	52:B4:85:ILE:HG23	1.76	0.66
2:B:119:ALA:HA	15:P:233:PHE:HE2	1.60	0.66
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.66
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.66
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.77	0.66
22:Y:81:LEU:HD12	43:v:88:ASP:HB3	1.78	0.66
24:a:58:ARG:HH21	24:a:61:ARG:HD2	1.60	0.66
26:c:122:THR:O	38:o:12:ARG:NH2	2.27	0.66
35:l:447:ASN:CG	35:l:448:PRO:HD2	2.16	0.66
41:s:200:LEU:HD12	41:s:285:LEU:HD11	1.78	0.66
65:AU:133:ARG:O	65:AU:135:LEU:N	2.29	0.66
1:BA:116:ASN:ND2	70:BA:502:FMN:C8M	2.52	0.66
25:Bb:110:ILE:HG23	25:Bb:111:LEU:CD2	2.26	0.66
27:Bd:108:GLN:NE2	35:Bl:203:LEU:HG	2.10	0.66
35:Bl:190:ILE:HG12	35:Bl:196:TRP:CE2	2.31	0.66
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.66
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.66
67:AK:60:ARG:HG3	67:AK:124:GLU:HG2	1.78	0.66
22:BY:85:PRO:HG2	43:Bv:99:MET:HE2	1.78	0.66
26:Bc:184:TYR:CB	43:Bv:37:ARG:HG3	2.25	0.66
27:Bd:49:GLN:OE1	27:Bd:49:GLN:N	2.27	0.66
28:Be:76:TYR:H	40:Br:432:ARG:HD2	1.61	0.66
44:Bw:58:ARG:NH1	44:Bw:279:ASP:O	2.29	0.66
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.66
12:M:618:GLU:OE2	12:M:620:TRP:NE1	2.29	0.66
32:i:12:THR:HG22	36:m:158:TRP:NE1	2.10	0.66
44:w:58:ARG:NH1	44:w:279:ASP:O	2.29	0.66
49:1:43:PRO:HB2	49:1:48:ILE:HD11	1.76	0.66
65:AH:277:ALA:O	66:AJ:71:ARG:NH2	2.29	0.66
59:AO:17:ALA:HA	68:AY:319:GLY:H	1.61	0.66
68:AY:152:GLN:CD	68:AY:252:GLY:CA	2.68	0.66
1:BA:364:VAL:HG12	1:BA:400:VAL:HG12	1.78	0.66
1:BA:379:CYS:SG	1:BA:380:GLY:N	2.68	0.66
1:BA:424:ILE:HG22	69:BA:501:SF4:S4	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:12:VAL:HG11	16:BQ:278:VAL:O	1.96	0.66
16:BQ:86:PRO:HG2	33:Bj:41:PHE:HE2	1.60	0.66
6:G:120:MET:HA	6:G:123:GLU:HG2	1.78	0.65
7:H:12:VAL:HG11	16:Q:278:VAL:O	1.96	0.65
8:I:66:PRO:HB3	15:P:79:SER:HB3	1.77	0.65
26:c:184:TYR:CB	43:v:37:ARG:HG3	2.25	0.65
33:j:3:PHE:HA	33:j:6:ILE:HD13	1.77	0.65
41:s:202:GLU:O	41:s:204:GLU:N	2.29	0.65
62:AE:34:ARG:HH22	65:AH:216:THR:HG22	1.61	0.65
63:AF:40:GLU:HG2	63:AF:45:LYS:HG3	1.77	0.65
67:AK:107:GLY:O	68:AL:397:ASN:ND2	2.28	0.65
67:AK:183:ARG:NH2	67:AK:254:ARG:HB3	2.11	0.65
58:AN:43:ARG:NH1	71:AN:101:PLX:H1B1	2.11	0.65
61:AQ:22:ALA:CB	71:AQ:101:PLX:H272	2.26	0.65
1:BA:98:LYS:HD2	1:BA:101:PHE:HE2	1.61	0.65
1:BA:295:PRO:HG2	1:BA:298:GLU:HB2	1.77	0.65
22:BY:81:LEU:HD12	43:Bv:88:ASP:HB3	1.78	0.65
24:Ba:94:GLY:O	24:Ba:96:ALA:N	2.30	0.65
26:Bc:62:TYR:OH	26:Bc:74:ASP:O	2.11	0.65
22:Y:79:GLU:O	22:Y:80:VAL:HG13	1.96	0.65
24:a:94:GLY:O	24:a:96:ALA:N	2.30	0.65
27:d:108:GLN:NE2	35:l:203:LEU:HG	2.10	0.65
48:0:24:LEU:H	49:1:34:ASN:HD21	1.44	0.65
67:AK:36:GLN:NE2	67:AK:39:GLU:OE2	2.29	0.65
67:AK:384:MET:HE2	68:AL:134:LYS:HD3	1.77	0.65
16:BQ:171:ARG:HH21	16:BQ:231:GLY:HA2	1.61	0.65
18:BT:39:VAL:HG12	18:BT:45:VAL:HB	1.79	0.65
33:Bj:36:PRO:HG2	33:Bj:43:PRO:HG3	1.77	0.65
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.77	0.65
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.78	0.65
9:J:319:VAL:O	9:J:323:HIS:ND1	2.28	0.65
16:Q:78:LYS:HZ1	33:j:48:ARG:NH2	1.93	0.65
17:S:53:ARG:NH2	31:h:105:ARG:HD3	2.12	0.65
18:T:39:VAL:HG12	18:T:45:VAL:HB	1.79	0.65
44:w:188:ASN:HA	44:w:191:LYS:HE2	1.78	0.65
47:z:101:PHE:HZ	47:z:260:GLY:HA3	1.61	0.65
66:AJ:66:ILE:HD11	66:AJ:134:PRO:HA	1.77	0.65
66:AJ:165:TRP:O	66:AJ:174:THR:OG1	2.14	0.65
76:AL:503:PEE:H49	76:AL:503:PEE:H26	1.78	0.65
66:AV:195:LEU:HD21	66:AV:199:PHE:HE2	1.60	0.65
1:BA:116:ASN:ND2	70:BA:502:FMN:C9	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:258:ALA:HA	9:BJ:261:LYS:HD2	1.78	0.65
22:BY:79:GLU:O	22:BY:80:VAL:HG13	1.96	0.65
27:Bd:110:ARG:HG2	27:Bd:110:ARG:NH1	2.11	0.65
32:Bi:170:LEU:HD12	35:Bl:574:SER:HB3	1.77	0.65
35:Bl:512:LYS:HG3	54:B6:16:ASN:HB3	1.78	0.65
41:Bs:185:TRP:NE1	41:Bs:238:THR:HG22	2.12	0.65
41:Bs:202:GLU:O	41:Bs:204:GLU:N	2.29	0.65
45:Bx:298:ASP:HB2	45:Bx:301:THR:HG23	1.77	0.65
25:b:114:GLY:O	25:b:115:GLU:HB3	1.95	0.65
25:b:115:GLU:HG2	25:b:116:VAL:N	2.10	0.65
41:s:169:GLN:HE21	41:s:174:LEU:H	1.42	0.65
68:AL:262:VAL:HG21	39:Bp:61:THR:CG2	2.27	0.65
68:AY:75:ILE:HG22	68:AY:77:VAL:H	1.61	0.65
6:BG:105:MET:HG3	6:BG:106:LYS:HG3	1.76	0.65
33:Bj:3:PHE:HA	33:Bj:6:ILE:HD13	1.77	0.65
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.65
25:b:105:PHE:CZ	43:v:67:LEU:HB2	2.31	0.65
32:i:170:LEU:HD12	35:l:574:SER:HB3	1.77	0.65
43:v:74:PHE:O	43:v:76:ASN:ND2	2.29	0.65
67:AK:407:MET:HE3	67:AK:411:THR:HG22	1.78	0.65
5:BF:33:VAL:HG22	5:BF:87:VAL:HG21	1.78	0.65
6:BG:120:MET:HA	6:BG:123:GLU:HG2	1.79	0.65
9:BJ:355:ARG:HB3	33:Bj:31:MET:SD	2.36	0.65
12:BM:169:VAL:HG12	12:BM:223:ILE:HD11	1.79	0.65
21:BW:68:ARG:HD3	36:Bm:134:PHE:CE1	2.32	0.65
25:Bb:105:PHE:CZ	43:Bv:67:LEU:HB2	2.31	0.65
35:Bl:359:MET:O	35:Bl:436:ARG:NH2	2.29	0.65
2:B:61:TRP:CH2	41:s:187:ILE:HD11	2.31	0.65
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.77	0.65
12:M:169:VAL:HG12	12:M:223:ILE:HD11	1.79	0.65
16:Q:80:ILE:O	16:Q:81:THR:CG2	2.45	0.65
27:d:108:GLN:NE2	35:l:199:GLN:O	2.29	0.65
35:l:188:TRP:CD2	35:l:192:HIS:HD2	2.09	0.65
75:AJ:405:CDL:C31	75:AJ:405:CDL:HB61	2.27	0.65
67:AK:183:ARG:HH21	67:AK:254:ARG:HB3	1.62	0.65
66:AV:332:LEU:HD11	76:AV:403:PEE:H37	1.79	0.65
67:AW:60:ARG:HG3	67:AW:124:GLU:HG2	1.78	0.65
16:BQ:80:ILE:C	16:BQ:81:THR:CG2	2.70	0.65
76:BW:201:PEE:H1	41:Bs:98:LEU:HD22	1.79	0.65
27:Bd:108:GLN:NE2	35:Bl:199:GLN:O	2.29	0.65
35:Bl:222:GLY:HA3	35:Bl:229:LEU:HD12	1.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Bs:169:GLN:HE21	41:Bs:174:LEU:H	1.42	0.65
44:Bw:249:MET:HB3	44:Bw:255:VAL:HG11	1.79	0.65
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.65
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.65
16:Q:35:ARG:NH1	28:e:60:GLU:OE2	2.28	0.65
25:b:110:ILE:HG23	25:b:111:LEU:CD2	2.26	0.65
35:l:453:PRO:HA	35:l:456:ARG:NH2	2.11	0.65
44:w:249:MET:HB3	44:w:255:VAL:HG11	1.79	0.65
68:AY:460:GLY:HA2	68:AY:462:ILE:HD12	1.79	0.65
2:BB:61:TRP:CH2	41:Bs:187:ILE:HD11	2.31	0.65
6:BG:145:VAL:HA	6:BG:148:ILE:HD12	1.77	0.65
12:BM:381:LEU:O	12:BM:383:SER:N	2.24	0.65
25:Bb:7:ASP:HB2	39:Bp:156:PRO:HG3	1.79	0.65
35:Bl:190:ILE:HD11	35:Bl:196:TRP:HE1	1.61	0.65
42:Bu:24:VAL:HG22	42:Bu:86:TRP:NE1	2.12	0.65
45:Bx:172:LYS:HB2	45:Bx:172:LYS:NZ	2.12	0.65
56:B8:45:LEU:HD21	57:B9:40:TYR:HA	1.78	0.65
2:B:51:VAL:HG22	2:B:54:ARG:HH11	1.62	0.65
15:P:173:MET:HE1	15:P:189:THR:HG23	1.78	0.65
25:b:38:GLN:OE1	25:b:39:LYS:N	2.28	0.65
25:b:88:TYR:CD1	71:b:201:PLX:C1C	2.79	0.65
58:AN:12:ARG:HG2	58:AN:13:HIS:ND1	2.12	0.65
76:AU:401:PEE:C19	76:AU:401:PEE:H64	2.27	0.65
9:BJ:206:ILE:CB	9:BJ:242:VAL:HG22	2.25	0.65
12:BM:36:VAL:O	12:BM:38:GLY:N	2.29	0.65
16:BQ:271:ARG:HH11	41:Bs:281:ARG:CA	2.09	0.65
25:Bb:38:GLN:OE1	25:Bb:39:LYS:N	2.28	0.65
30:Bg:27:ASP:OD2	30:Bg:29:ARG:NH1	2.29	0.65
40:Br:305:THR:O	40:Br:308:SER:OG	2.12	0.65
1:A:116:ASN:ND2	70:A:502:FMN:C9	2.59	0.65
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	0.65
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	0.65
32:i:42:PRO:HG3	36:m:166:ILE:HG23	1.78	0.65
32:i:291:TYR:CD2	76:l:701:PEE:H51	2.32	0.65
34:k:26:LEU:HD11	34:k:78:LEU:HD21	1.78	0.65
60:AC:162:GLY:O	60:AC:227:ASN:ND2	2.30	0.65
67:AK:375:LYS:NZ	67:AK:416:ILE:O	2.30	0.65
68:AL:280:ASP:O	68:AL:362:ARG:NH2	2.30	0.65
65:AU:296:MET:HE2	76:AU:401:PEE:H51	1.79	0.65
21:BW:39:GLY:O	21:BW:42:THR:OG1	2.15	0.65
6:BX:120:MET:HE1	39:Bp:24:LEU:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:226:GLN:HG3	35:Bl:280:LEU:HD23	1.74	0.65
47:Bz:101:PHE:HZ	47:Bz:260:GLY:HA3	1.61	0.65
48:B0:24:LEU:H	49:B1:34:ASN:HD21	1.43	0.65
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.65
14:O:87:GLN:O	14:O:91:GLY:N	2.22	0.65
16:Q:86:PRO:HG2	33:j:41:PHE:HE2	1.60	0.65
34:k:92:ASN:ND2	35:l:582:GLY:O	2.31	0.65
35:l:359:MET:O	35:l:436:ARG:NH2	2.29	0.65
76:l:701:PEE:C22	40:r:155:VAL:HG21	2.27	0.65
2:BB:126:ILE:O	15:BP:231:ARG:NH2	2.23	0.65
12:BM:180:THR:OG1	12:BM:184:ARG:NH1	2.29	0.65
46:By:120:SER:OG	46:By:138:VAL:HG21	1.97	0.65
47:Bz:160:LEU:HD13	47:Bz:222:GLN:HG2	1.78	0.65
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	0.64
2:B:52:THR:HG22	21:W:33:TYR:CE1	2.33	0.64
76:W:201:PEE:H1	41:s:98:LEU:HD22	1.79	0.64
42:u:24:VAL:HG22	42:u:86:TRP:NE1	2.12	0.64
67:AW:70:ARG:NH2	67:AW:332:ASP:OD2	2.22	0.64
68:AY:121:ASN:ND2	68:AY:132:TYR:OH	2.29	0.64
68:AY:326:SER:O	68:AY:330:SER:N	2.30	0.64
1:BA:244:ASN:OD1	1:BA:245:VAL:N	2.29	0.64
1:BA:414:GLU:OE1	12:BM:152:ARG:NH1	2.30	0.64
2:BB:57:ARG:O	16:BQ:266:ARG:NH2	2.30	0.64
2:BB:151:ILE:HG21	3:BC:159:TYR:HD2	1.62	0.64
3:BC:93:MET:HG2	3:BC:110:PHE:HZ	1.63	0.64
12:BM:266:ARG:HG2	12:BM:267:THR:HG23	1.79	0.64
15:BP:173:MET:HE1	15:BP:189:THR:HG23	1.78	0.64
17:BS:53:ARG:NH2	31:Bh:105:ARG:HD3	2.12	0.64
35:Bl:307:SER:HA	35:Bl:310:LEU:HD12	1.80	0.64
1:A:424:ILE:HG22	69:A:501:SF4:S4	2.36	0.64
7:H:72:LEU:HD22	7:H:77:LEU:HD13	1.78	0.64
12:M:500:ILE:O	12:M:503:THR:OG1	2.12	0.64
30:g:32:TYR:OH	32:i:335:LEU:O	2.13	0.64
31:h:91:LYS:HG3	31:h:92:TYR:H	1.62	0.64
76:l:701:PEE:H36	40:r:155:VAL:HG21	1.79	0.64
45:x:172:LYS:HB2	45:x:172:LYS:NZ	2.12	0.64
67:AK:230:LEU:HA	67:AK:233:VAL:HG22	1.78	0.64
67:AK:413:LEU:HA	67:AK:416:ILE:HG22	1.80	0.64
68:AL:75:ILE:HG22	68:AL:77:VAL:H	1.61	0.64
64:AT:42:LEU:O	64:AT:45:VAL:CG2	2.34	0.64
65:AU:288:MET:SD	76:AU:401:PEE:O4	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:444:LEU:HD23	67:AW:447:THR:HG21	1.79	0.64
68:AY:101:THR:HA	68:AY:155:SER:H	1.60	0.64
4:BE:25:MET:CB	4:BE:29:LYS:CE	2.59	0.64
16:BQ:80:ILE:O	16:BQ:81:THR:CG2	2.45	0.64
16:BQ:136:PHE:HB3	16:BQ:147:ASN:HB3	1.79	0.64
32:Bi:291:TYR:CD2	76:Bl:701:PEE:H51	2.32	0.64
40:Br:210:TYR:O	40:Br:213:HIS:ND1	2.31	0.64
43:Bv:74:PHE:O	43:Bv:76:ASN:ND2	2.29	0.64
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.78	0.64
12:M:381:LEU:O	12:M:383:SER:N	2.24	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CZ	2.32	0.64
35:l:512:LYS:HG3	54:6:16:ASN:HB3	1.78	0.64
41:s:228:TYR:HD1	41:s:231:ILE:HD12	1.63	0.64
44:w:160:GLU:HG2	44:w:161:ARG:N	2.13	0.64
63:AF:29:LYS:HB2	63:AF:29:LYS:HZ3	1.62	0.64
63:AS:97:GLU:OE1	63:AS:100:ARG:NH2	2.31	0.64
67:AW:449:PHE:HB2	67:AW:452:GLU:OE1	1.97	0.64
2:BB:52:THR:HG22	21:BW:33:TYR:CE1	2.33	0.64
4:BE:107:PHE:HB3	4:BE:109:GLU:HG3	1.78	0.64
10:BK:81:THR:HB	14:BO:88:ARG:HD2	1.79	0.64
35:Bl:453:PRO:HA	35:Bl:456:ARG:NH2	2.11	0.64
76:Bl:701:PEE:H36	40:Br:155:VAL:HG21	1.79	0.64
76:Bl:701:PEE:C22	40:Br:155:VAL:HG21	2.27	0.64
40:Br:144:ASN:O	40:Br:147:THR:OG1	2.10	0.64
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.64
16:Q:145:MET:H	16:Q:178:THR:HG21	1.63	0.64
25:b:7:ASP:HB2	39:p:156:PRO:HG3	1.79	0.64
26:c:159:LYS:HA	43:v:98:ARG:HH12	1.62	0.64
33:j:36:PRO:HG2	33:j:43:PRO:HG3	1.77	0.64
35:l:307:SER:HA	35:l:310:LEU:HD12	1.80	0.64
47:z:160:LEU:HD13	47:z:222:GLN:HG2	1.78	0.64
62:AR:29:PRO:HD2	65:AU:262:THR:HG21	1.79	0.64
62:AR:86:LEU:HD23	62:AR:86:LEU:C	2.21	0.64
64:AT:40:LEU:HD12	64:AT:40:LEU:C	2.21	0.64
68:AY:280:ASP:HA	68:AY:461:PRO:HB3	1.79	0.64
3:BC:128:ASN:ND2	3:BC:164:TYR:O	2.24	0.64
12:BM:618:GLU:OE2	12:BM:620:TRP:NE1	2.30	0.64
35:Bl:4:HIS:HE1	35:Bl:87:MET:CE	2.10	0.64
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	0.64
12:M:591:GLU:OE1	12:M:591:GLU:N	2.30	0.64
22:Y:85:PRO:HG2	43:v:99:MET:HE2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:24:ILE:HD11	23:Z:47:ARG:HG2	1.80	0.64
40:r:210:TYR:O	40:r:213:HIS:ND1	2.31	0.64
44:w:117:PHE:HB2	44:w:131:LEU:HD21	1.80	0.64
56:8:45:LEU:HD21	57:9:40:TYR:HA	1.78	0.64
65:AH:315:LYS:NZ	75:AH:403:CDL:OB3	2.21	0.64
67:AK:351:ILE:HD11	67:AK:448:PRO:CG	2.27	0.64
66:AV:22:PRO:HB3	66:AV:217:LYS:HB3	1.78	0.64
9:BJ:132:ARG:NH2	73:BJ:401:NDP:H2B	2.11	0.64
11:BL:81:VAL:HG11	11:BL:150:ARG:HA	1.78	0.64
12:BM:65:TYR:O	12:BM:181:ARG:NH2	2.29	0.64
75:BV:201:CDL:OA7	75:BV:201:CDL:O1	2.16	0.64
41:Bs:265:LEU:O	41:Bs:268:SER:OG	2.10	0.64
3:C:93:MET:HG2	3:C:110:PHE:HZ	1.63	0.64
16:Q:87:GLN:OE1	16:Q:87:GLN:N	2.26	0.64
18:T:40:THR:OG1	18:T:42:THR:O	2.14	0.64
35:l:190:ILE:HD11	35:l:196:TRP:HE1	1.61	0.64
35:l:405:ASN:OD1	35:l:406:ALA:N	2.31	0.64
42:u:31:HIS:CE1	42:u:119:ARG:HB3	2.33	0.64
2:BB:70:MET:HE2	16:BQ:257:GLU:HG2	1.79	0.64
7:BH:72:LEU:HD22	7:BH:77:LEU:HD13	1.78	0.64
9:BJ:319:VAL:O	9:BJ:323:HIS:ND1	2.28	0.64
24:Ba:95:GLN:HA	24:Ba:116:PRO:HD3	1.79	0.64
34:Bk:92:ASN:ND2	35:Bl:582:GLY:O	2.31	0.64
35:Bl:405:ASN:OD1	35:Bl:406:ALA:N	2.31	0.64
4:E:107:PHE:HB3	4:E:109:GLU:HG3	1.78	0.64
46:y:120:SER:OG	46:y:138:VAL:HG21	1.97	0.64
7:BH:32:LEU:HD23	7:BH:35:LEU:HD21	1.77	0.64
12:BM:692:LYS:HD2	12:BM:715:THR:HG22	1.80	0.64
39:Bp:170:ILE:H	39:Bp:170:ILE:CD1	2.02	0.64
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.64
2:B:70:MET:HE2	16:Q:257:GLU:HG2	1.79	0.64
14:O:245:VAL:O	14:O:247:ALA:N	2.31	0.64
40:r:150:LEU:HD21	40:r:154:LEU:HD12	1.79	0.64
76:AH:401:PEE:H49	76:AH:401:PEE:C11	2.27	0.64
75:AL:502:CDL:C58	76:AL:503:PEE:C38	2.76	0.64
32:Bi:245:PRO:HB3	32:Bi:297:ILE:HG12	1.80	0.64
35:Bl:332:HIS:HE1	35:Bl:336:LYS:HZ1	1.46	0.64
41:Bs:20:LEU:HD13	41:Bs:232:ILE:HD11	1.78	0.64
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.64
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.79	0.64
45:x:84:PRO:HG3	45:x:92:MET:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:195:LEU:HD23	45:x:245:ILE:HD13	1.79	0.64
58:AA:78:TYR:HE1	62:AE:64:GLU:C	1.99	0.64
67:AK:351:ILE:HD11	67:AK:448:PRO:CD	2.27	0.64
68:AL:96:LEU:HD23	68:AL:164:GLU:HG3	1.80	0.64
16:BQ:166:ARG:NH1	16:BQ:352:PRO:O	2.30	0.64
76:BV:202:PEE:H32	76:BV:202:PEE:C24	2.25	0.64
22:BY:73:PHE:HA	35:Bl:385:PHE:CE2	2.33	0.64
23:BZ:24:ILE:HD11	23:BZ:47:ARG:HG2	1.80	0.64
25:Bb:105:PHE:CE2	43:Bv:68:LYS:CA	2.81	0.64
35:Bl:226:GLN:OE1	35:Bl:226:GLN:HA	1.97	0.64
35:Bl:227:LEU:HD12	35:Bl:230:HIS:HD1	1.60	0.64
44:Bw:117:PHE:HB2	44:Bw:131:LEU:HD21	1.80	0.64
3:C:137:VAL:CG2	16:Q:87:GLN:NE2	2.59	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CE1	2.32	0.64
25:b:108:ASP:O	25:b:113:THR:HA	1.98	0.64
32:i:288:LEU:HD21	76:l:701:PEE:H64	1.80	0.64
40:r:15:THR:O	40:r:93:LYS:NZ	2.24	0.64
41:s:20:LEU:HD13	41:s:232:ILE:HD11	1.78	0.64
42:u:140:ASN:ND2	42:u:143:HIS:O	2.31	0.64
45:x:187:SER:CB	45:x:277:MET:HE1	2.28	0.64
66:AV:129:MET:HE1	66:AV:185:LEU:CD1	2.28	0.64
67:AW:299:VAL:HG13	68:AY:120:LEU:HD11	1.79	0.64
6:BG:80:GLN:HE22	6:BG:100:VAL:HG13	1.63	0.64
9:BJ:85:ARG:HH11	9:BJ:85:ARG:CG	2.09	0.64
16:BQ:84:PHE:HE2	16:BQ:91:ALA:HB2	1.63	0.64
23:BZ:32:ILE:HD12	39:Bp:35:ASP:OD1	1.98	0.64
26:Bc:94:GLN:O	26:Bc:98:ARG:N	2.30	0.64
41:Bs:228:TYR:HD1	41:Bs:231:ILE:HD12	1.63	0.64
45:Bx:195:LEU:HD23	45:Bx:245:ILE:HD13	1.79	0.64
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.63
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	0.63
16:Q:171:ARG:HH21	16:Q:231:GLY:HA2	1.62	0.63
22:Y:73:PHE:HA	35:l:385:PHE:CE2	2.33	0.63
32:i:197:ASN:HB3	32:i:269:GLU:OE1	1.97	0.63
8:Bi:23:LYS:NZ	16:BQ:252:SER:OG	2.31	0.63
12:BM:254:MET:HB2	12:BM:290:THR:HG22	1.78	0.63
16:BQ:145:MET:H	16:BQ:178:THR:HG21	1.63	0.63
25:Bb:88:TYR:CD1	71:Bb:201:PLX:C1C	2.79	0.63
30:Bg:32:TYR:OH	32:Bi:335:LEU:O	2.13	0.63
34:Bk:4:ILE:HD13	36:Bm:125:MET:SD	2.34	0.63
40:Br:150:LEU:HD21	40:Br:154:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bu:31:HIS:CE1	42:Bu:119:ARG:HB3	2.33	0.63
16:Q:80:ILE:C	16:Q:81:THR:CG2	2.70	0.63
16:Q:84:PHE:HE2	16:Q:91:ALA:HB2	1.63	0.63
16:Q:150:ALA:HB1	16:Q:400:ILE:HG13	1.80	0.63
75:V:201:CDL:OA7	75:V:201:CDL:O1	2.16	0.63
25:b:112:GLU:N	25:b:112:GLU:OE2	2.31	0.63
38:o:26:SER:O	38:o:29:THR:OG1	2.15	0.63
62:AE:26:LEU:O	62:AE:28:ASP:N	2.26	0.63
62:AE:27:VAL:O	62:AE:28:ASP:HB3	1.96	0.63
67:AK:185:ALA:HB3	67:AK:251:ALA:HB2	1.81	0.63
68:AL:262:VAL:HB	39:Bp:61:THR:HG21	1.79	0.63
12:BM:173:MET:C	12:BM:175:ARG:H	2.06	0.63
12:BM:326:VAL:HG23	12:BM:626:LEU:HD13	1.80	0.63
16:BQ:72:PRO:HB2	32:Bi:50:PRO:HG3	1.80	0.63
22:BY:96:GLU:O	22:BY:97:LEU:HB2	1.98	0.63
32:Bi:288:LEU:HD21	76:Bl:701:PEE:H64	1.80	0.63
35:Bl:501:ALA:O	35:Bl:505:ASN:ND2	2.29	0.63
38:Bo:26:SER:O	38:Bo:29:THR:OG1	2.15	0.63
12:M:254:MET:HB2	12:M:290:THR:HG22	1.78	0.63
12:M:543:LYS:HG3	12:M:565:PHE:CD2	2.33	0.63
16:Q:80:ILE:C	16:Q:81:THR:HG23	2.23	0.63
76:V:202:PEE:H32	76:V:202:PEE:C24	2.25	0.63
23:Z:32:ILE:HD12	39:p:35:ASP:OD1	1.98	0.63
27:d:59:HIS:HE1	28:e:120:ARG:CB	1.97	0.63
35:l:124:PHE:HE1	35:l:147:VAL:HG13	1.64	0.63
38:o:56:ARG:HH12	38:o:59:LEU:C	2.06	0.63
41:s:169:GLN:NE2	41:s:244:GLY:H	1.96	0.63
65:AH:262:THR:HG22	65:AH:264:SER:H	1.63	0.63
66:AV:200:LEU:HD13	82:AV:402:HEM:HAD2	1.79	0.63
67:AW:127:ARG:NH1	67:AW:224:GLY:O	2.32	0.63
67:AW:450:VAL:O	67:AW:453:LEU:HD13	1.98	0.63
1:BA:416:SER:HB3	1:BA:436:GLN:HE21	1.63	0.63
9:BJ:83:PRO:HB2	9:BJ:108:TRP:CD1	2.33	0.63
9:BJ:205:ASP:HB2	9:BJ:239:PRO:HA	1.79	0.63
26:Bc:163:TYR:OH	43:Bv:42:THR:O	2.11	0.63
34:Bk:26:LEU:HD11	34:Bk:78:LEU:HD21	1.78	0.63
35:Bl:67:HIS:CE1	35:Bl:75:GLN:HG3	2.33	0.63
41:Bs:169:GLN:NE2	41:Bs:244:GLY:H	1.96	0.63
45:Bx:187:SER:CB	45:Bx:277:MET:HE1	2.28	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	0.63
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:81:THR:HB	14:O:88:ARG:HD2	1.78	0.63
24:a:95:GLN:HA	24:a:116:PRO:HD3	1.79	0.63
76:l:701:PEE:H32	40:r:155:VAL:HG21	1.80	0.63
45:x:273:MET:HG3	45:x:319:LYS:HZ1	1.61	0.63
67:AK:70:ARG:NH2	67:AK:332:ASP:OD2	2.31	0.63
68:AL:387:GLU:OE2	68:AL:390:ARG:NH2	2.27	0.63
21:BW:68:ARG:HD3	36:Bm:134:PHE:CZ	2.32	0.63
24:Ba:96:ALA:CB	27:Bd:55:TYR:CB	2.70	0.63
26:Bc:159:LYS:HA	43:Bv:98:ARG:HH12	1.62	0.63
32:Bi:197:ASN:HB3	32:Bi:269:GLU:OE1	1.98	0.63
3:C:136:LYS:HD2	33:j:40:GLY:O	1.99	0.63
11:L:75:ARG:HH21	11:L:101:PHE:HB3	1.63	0.63
22:Y:74:TRP:HE3	22:Y:75:HIS:HA	1.61	0.63
35:l:216:LEU:HD22	35:l:259:LEU:HD21	1.80	0.63
41:s:185:TRP:NE1	41:s:238:THR:HG22	2.11	0.63
65:AH:202:ARG:HD2	65:AH:279:GLU:HG3	1.81	0.63
68:AL:48:THR:HG22	68:AL:62:GLU:HB2	1.78	0.63
14:BO:158:ILE:HD11	14:BO:164:THR:HB	1.81	0.63
25:Bb:108:ASP:O	25:Bb:113:THR:HA	1.98	0.63
38:Bo:56:ARG:HH12	38:Bo:59:LEU:C	2.06	0.63
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.63
35:l:229:LEU:HD23	35:l:229:LEU:N	2.13	0.63
60:AC:104:ARG:HH21	68:AL:292:GLU:HG3	1.64	0.63
62:AR:34:ARG:CZ	62:AR:78:ARG:HH12	2.11	0.63
14:BO:245:VAL:O	14:BO:247:ALA:N	2.31	0.63
35:Bl:537:ILE:HD11	76:Bl:702:PEE:H38	1.80	0.63
76:Bl:701:PEE:H32	40:Br:155:VAL:HG21	1.80	0.63
31:h:5:ASP:HB3	31:h:8:LYS:HB3	1.80	0.63
35:l:67:HIS:CE1	35:l:75:GLN:HG3	2.33	0.63
35:l:226:GLN:OE1	35:l:226:GLN:HA	1.97	0.63
40:r:150:LEU:O	40:r:153:THR:OG1	2.12	0.63
75:AG:101:CDL:H551	75:AG:101:CDL:H512	1.81	0.63
65:AH:202:ARG:NH2	66:AJ:256:TYR:OH	2.31	0.63
10:BK:98:GLN:HB3	14:BO:71:PRO:HA	1.80	0.63
16:BQ:150:ALA:HB1	16:BQ:400:ILE:HG13	1.80	0.63
25:Bb:112:GLU:OE2	25:Bb:112:GLU:N	2.31	0.63
40:Br:373:ILE:HG23	40:Br:448:SER:HA	1.81	0.63
48:B0:16:TYR:CE1	48:B0:25:PRO:HG3	2.34	0.63
1:A:207:GLY:O	70:A:502:FMN:C5A	2.47	0.63
12:M:65:TYR:O	12:M:181:ARG:NH2	2.29	0.63
12:M:282:ASN:HA	12:M:413:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:112:GLY:O	27:d:115:TYR:HB3	1.99	0.63
58:AA:49:VAL:HG21	76:AJ:403:PEE:O5	1.98	0.63
63:AF:28:ASN:OD1	63:AF:29:LYS:N	2.31	0.63
67:AK:422:ALA:O	67:AK:426:ASN:ND2	2.31	0.63
66:AV:138:MET:HB2	66:AV:255:ASN:HD21	1.62	0.63
1:BA:391:TRP:CH2	12:BM:153:PHE:HA	2.34	0.63
3:BC:136:LYS:HD2	33:Bj:40:GLY:O	1.99	0.63
12:BM:591:GLU:OE1	12:BM:591:GLU:N	2.30	0.63
16:BQ:273:ILE:HD13	16:BQ:325:ASP:CG	2.23	0.63
22:BY:74:TRP:HE3	22:BY:75:HIS:HA	1.61	0.63
42:Bu:30:HIS:CE1	42:Bu:119:ARG:HH11	2.17	0.63
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.33	0.63
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.46	0.63
11:L:111:LEU:HG	11:L:112:MET:HG2	1.80	0.63
24:a:127:ASP:HB3	24:a:131:LYS:HD3	1.80	0.63
32:i:245:PRO:HB3	32:i:297:ILE:HG12	1.80	0.63
35:l:4:HIS:HE1	35:l:87:MET:CE	2.10	0.63
43:v:8:ARG:HH11	43:v:106:ARG:NH2	1.97	0.63
48:0:16:TYR:CE1	48:0:25:PRO:HG3	2.34	0.63
52:4:57:ARG:HB3	52:4:57:ARG:HH11	1.64	0.63
75:AG:101:CDL:H531	75:AG:101:CDL:C71	2.19	0.63
67:AK:365:ASN:OD1	67:AK:365:ASN:N	2.31	0.63
2:BB:51:VAL:HG22	2:BB:54:ARG:HH11	1.62	0.63
2:BB:99:HIS:NE2	69:BB:302:SF4:S1	2.70	0.63
10:BK:82:TYR:HD2	14:BO:62:ARG:HH12	1.47	0.63
12:BM:543:LYS:HG3	12:BM:565:PHE:CD2	2.33	0.63
12:BM:546:PHE:HB2	12:BM:568:TYR:HA	1.81	0.63
26:Bc:159:LYS:HA	43:Bv:98:ARG:NH2	2.13	0.63
35:Bl:229:LEU:HD23	35:Bl:229:LEU:N	2.13	0.63
76:Bl:701:PEE:H37	40:Br:155:VAL:HG11	1.70	0.63
42:Bu:140:ASN:ND2	42:Bu:143:HIS:O	2.31	0.63
45:Bx:128:VAL:HG22	45:Bx:128:VAL:O	1.99	0.63
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
12:M:627:SER:OG	12:M:632:MET:O	2.17	0.62
16:Q:72:PRO:HB2	32:i:50:PRO:HG3	1.80	0.62
25:b:105:PHE:CE2	43:v:68:LYS:CA	2.81	0.62
34:k:82:SER:HB3	34:k:87:LEU:HD23	1.80	0.62
35:l:88:MET:O	35:l:92:VAL:HG23	1.98	0.62
43:v:40:VAL:HB	43:v:61:HIS:CE1	2.34	0.62
65:AU:296:MET:CE	76:AU:401:PEE:C33	2.71	0.62
1:BA:325:PRO:HG3	1:BA:433:TRP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:48:ARG:HH21	15:BP:211:ARG:HD2	1.64	0.62
9:BJ:141:PHE:CZ	9:BJ:180:TYR:HD1	2.17	0.62
43:Bv:40:VAL:HB	43:Bv:61:HIS:CE1	2.34	0.62
44:Bw:332:ARG:O	44:Bw:338:LYS:CG	2.45	0.62
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	0.62
25:b:88:TYR:HD1	25:b:92:GLU:OE2	1.82	0.62
33:j:77:TRP:NE1	41:s:318:THR:O	2.31	0.62
46:y:122:MET:HB2	46:y:208:PRO:HD2	1.81	0.62
61:AD:53:TRP:NE1	65:AH:139:CYS:O	2.32	0.62
65:AH:231:LEU:HD21	60:AP:239:HIS:HA	1.81	0.62
65:AU:242:ILE:HG12	65:AU:244:MET:H	1.64	0.62
66:AV:119:LEU:HD12	66:AV:192:LEU:HB3	1.81	0.62
11:BL:111:LEU:HG	11:BL:112:MET:HG2	1.80	0.62
16:BQ:38:GLN:HE21	32:Bi:304:LEU:HB2	1.64	0.62
71:Bb:201:PLX:H11	71:Bb:201:PLX:O4	1.99	0.62
31:Bh:91:LYS:HG3	31:Bh:92:TYR:H	1.62	0.62
35:Bl:216:LEU:HD22	35:Bl:259:LEU:HD21	1.80	0.62
35:Bl:303:ALA:O	35:Bl:306:THR:OG1	2.17	0.62
36:Bm:118:PHE:CD1	36:Bm:121:VAL:HB	2.34	0.62
36:Bm:147:ASP:OD1	36:Bm:148:TYR:N	2.30	0.62
11:L:128:PHE:HA	15:P:121:THR:HG22	1.81	0.62
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	0.62
14:O:158:ILE:HD11	14:O:164:THR:HB	1.81	0.62
16:Q:53:TYR:HE1	76:l:701:PEE:P	2.22	0.62
24:a:96:ALA:CB	27:d:55:TYR:CB	2.70	0.62
35:l:537:ILE:HD11	76:l:702:PEE:H38	1.80	0.62
65:AH:112:ARG:NH1	65:AH:269:ASP:OD2	2.31	0.62
82:AJ:401:HEM:HBC2	82:AJ:401:HEM:HMC1	1.80	0.62
66:AV:333:LEU:HD21	76:AV:403:PEE:C39	2.29	0.62
1:BA:88:ARG:O	1:BA:244:ASN:ND2	2.32	0.62
2:BB:64:LEU:O	2:BB:68:LEU:N	2.30	0.62
16:BQ:450:ILE:O	16:BQ:453:THR:OG1	2.07	0.62
25:Bb:42:PRO:HA	25:Bb:45:LYS:HB2	1.82	0.62
46:By:122:MET:HB2	46:By:208:PRO:HD2	1.81	0.62
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.62
36:m:56:PHE:CD2	41:s:107:ALA:HB1	2.35	0.62
36:m:116:VAL:O	36:m:118:PHE:N	2.31	0.62
59:AO:7:ARG:NH1	67:AW:287:SER:OG	2.32	0.62
67:AW:125:CYS:HB3	67:AW:133:LEU:HD22	1.81	0.62
5:BF:56:ARG:NH2	12:BM:527:ASP:O	2.29	0.62
35:Bl:124:PHE:HE1	35:Bl:147:VAL:HG13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:ND2	70:A:502:FMN:C8M	2.52	0.62
6:G:80:GLN:HE22	6:G:100:VAL:HG13	1.63	0.62
22:Y:96:GLU:O	22:Y:97:LEU:HB2	1.98	0.62
29:f:38:LYS:HB2	29:f:39:PRO:HD3	1.81	0.62
30:g:44:ASP:OD2	30:g:63:TYR:OH	2.16	0.62
31:h:49:TYR:HA	31:h:52:ALA:HB3	1.82	0.62
41:s:280:PHE:HE2	41:s:288:LEU:HD11	1.63	0.62
44:w:89:ALA:N	44:w:160:GLU:OE1	2.27	0.62
9:BJ:83:PRO:HB3	9:BJ:119:VAL:HG21	1.81	0.62
9:BJ:241:TYR:CE2	9:BJ:243:VAL:HB	2.35	0.62
9:BJ:272:LEU:HD23	9:BJ:274:PHE:H	1.65	0.62
12:BM:385:TYR:OH	12:BM:527:ASP:OD1	2.17	0.62
25:Bb:115:GLU:HG2	25:Bb:116:VAL:H	1.65	0.62
31:Bh:5:ASP:HB3	31:Bh:8:LYS:HB3	1.80	0.62
35:Bl:37:LYS:NZ	35:Bl:98:TRP:NE1	2.47	0.62
35:Bl:450:LEU:O	35:Bl:450:LEU:HD13	1.99	0.62
36:Bm:56:PHE:CD2	41:Bs:107:ALA:HB1	2.35	0.62
41:Bs:280:PHE:HE2	41:Bs:288:LEU:HD11	1.63	0.62
45:Bx:84:PRO:HG3	45:Bx:92:MET:HE3	1.80	0.62
1:A:74:ASP:O	1:A:78:GLY:N	2.27	0.62
2:B:99:HIS:NE2	69:B:302:SF4:S1	2.70	0.62
12:M:546:PHE:HB2	12:M:568:TYR:HA	1.81	0.62
16:Q:85:GLY:HA3	33:j:39:CYS:HG	1.63	0.62
32:i:72:MET:HE1	34:k:9:MET:HG2	1.81	0.62
32:i:271:THR:HG22	32:i:276:LEU:HD22	1.81	0.62
40:r:61:LEU:HD22	40:r:241:TYR:HD1	1.64	0.62
40:r:373:ILE:HG23	40:r:448:SER:HA	1.81	0.62
42:u:30:HIS:CE1	42:u:119:ARG:HH11	2.17	0.62
67:AW:299:VAL:HG21	68:AY:110:GLU:HG3	1.81	0.62
2:BB:36:TYR:HB3	8:BI:104:TRP:CE3	2.34	0.62
16:BQ:357:LYS:HE3	16:BQ:364:SER:HB2	1.81	0.62
24:Ba:127:ASP:HB3	24:Ba:131:LYS:HD3	1.80	0.62
35:Bl:88:MET:O	35:Bl:92:VAL:HG23	1.98	0.62
43:Bv:52:ARG:O	43:Bv:56:ARG:NH1	2.33	0.62
1:A:88:ARG:O	1:A:244:ASN:ND2	2.33	0.62
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.62
17:S:53:ARG:HB2	31:h:105:ARG:HH12	1.64	0.62
76:V:202:PEE:H71	76:l:701:PEE:C45	2.28	0.62
22:Y:81:LEU:HD23	22:Y:82:GLY:N	2.14	0.62
25:b:42:PRO:HA	25:b:45:LYS:HB2	1.82	0.62
35:l:450:LEU:O	35:l:450:LEU:HD13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:56:PHE:HD2	41:s:107:ALA:HB1	1.64	0.62
36:m:118:PHE:HE1	36:m:124:TRP:HE1	1.47	0.62
44:w:60:ILE:O	44:w:159:LEU:N	2.33	0.62
62:AR:34:ARG:HG3	62:AR:78:ARG:HH12	1.61	0.62
67:AW:313:VAL:HG21	67:AW:323:VAL:HG21	1.80	0.62
11:BL:75:ARG:HH21	11:BL:101:PHE:HB3	1.63	0.62
12:BM:282:ASN:HA	12:BM:413:LEU:HD23	1.81	0.62
12:BM:627:SER:OG	12:BM:632:MET:O	2.17	0.62
16:BQ:80:ILE:C	16:BQ:81:THR:HG23	2.23	0.62
16:BQ:85:GLY:HA3	33:Bj:39:CYS:HG	1.63	0.62
16:BQ:432:LEU:HG	16:BQ:456:ILE:HD13	1.81	0.62
17:BS:53:ARG:HB2	31:Bh:105:ARG:HH12	1.64	0.62
29:Bf:38:LYS:HB2	29:Bf:39:PRO:HD3	1.81	0.62
32:Bi:72:MET:HE1	34:Bk:9:MET:HG2	1.81	0.62
34:Bk:82:SER:HB3	34:Bk:87:LEU:HD23	1.80	0.62
36:Bm:118:PHE:HE1	36:Bm:124:TRP:HE1	1.48	0.62
57:B9:13:LYS:HD3	57:B9:13:LYS:H	1.65	0.62
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	0.62
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.62
15:P:83:GLU:HB3	15:P:142:ARG:HH12	1.65	0.62
16:Q:38:GLN:HE21	32:i:304:LEU:HB2	1.64	0.62
45:x:11:ASN:HD21	45:x:13:LYS:HB2	1.65	0.62
45:x:128:VAL:O	45:x:128:VAL:HG22	1.99	0.62
66:AJ:96:LEU:HD23	76:AJ:403:PEE:H26	1.82	0.62
67:AK:184:ASN:HB3	67:AK:251:ALA:HA	1.81	0.62
15:BP:190:ASP:CG	15:BP:191:TYR:H	2.08	0.62
27:Bd:112:GLY:O	27:Bd:115:TYR:HB3	1.99	0.62
36:Bm:56:PHE:HD2	41:Bs:107:ALA:HB1	1.64	0.62
40:Br:447:LEU:HD11	71:Br:502:PLX:H382	1.82	0.62
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
36:m:118:PHE:CD1	36:m:121:VAL:HB	2.34	0.62
44:w:332:ARG:O	44:w:338:LYS:CG	2.45	0.62
1:BA:85:LEU:HD21	1:BA:247:THR:HG23	1.80	0.62
17:BS:50:ARG:HA	31:Bh:105:ARG:CZ	2.30	0.62
76:BV:202:PEE:H71	76:Bl:701:PEE:C45	2.28	0.62
35:Bl:37:LYS:HZ3	35:Bl:98:TRP:NE1	1.97	0.62
71:Br:502:PLX:H31	71:Br:502:PLX:C7	2.30	0.62
45:Bx:11:ASN:HD21	45:Bx:13:LYS:HB2	1.65	0.62
12:M:467:LYS:HG3	12:M:503:THR:HB	1.80	0.62
43:v:52:ARG:O	43:v:56:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:9:13:LYS:HD3	57:9:13:LYS:H	1.65	0.62
68:AL:262:VAL:CB	39:Bp:61:THR:HG21	2.30	0.62
6:BG:76:LEU:HD21	6:BG:155:TYR:HA	1.82	0.62
9:BJ:212:ARG:HH11	9:BJ:212:ARG:CG	2.12	0.62
22:BY:81:LEU:HD23	22:BY:82:GLY:N	2.14	0.62
27:Bd:107:CYS:SG	27:Bd:119:CYS:HA	2.39	0.62
29:Bf:55:TRP:O	29:Bf:59:ILE:HG12	2.00	0.62
30:Bg:9:PRO:O	30:Bg:11:ARG:N	2.32	0.62
49:B1:82:TYR:HB3	49:B1:83:PRO:HD3	1.82	0.62
54:B6:3:ASN:HD22	54:B6:3:ASN:C	2.08	0.62
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	0.61
26:c:94:GLN:O	26:c:98:ARG:N	2.30	0.61
32:i:58:LYS:HE3	35:l:584:ILE:HG12	1.82	0.61
32:i:193:VAL:HG21	32:i:266:ILE:HG12	1.82	0.61
35:l:427:ILE:HG23	35:l:431:LEU:HD12	1.82	0.61
67:AK:295:ALA:HB2	67:AK:325:ALA:HB3	1.82	0.61
68:AL:322:VAL:HG12	68:AL:323:HIS:H	1.64	0.61
61:AQ:34:ARG:HH12	61:AQ:38:GLN:HB3	1.64	0.61
62:AR:34:ARG:HH11	62:AR:78:ARG:CZ	2.13	0.61
12:BM:339:ALA:HB3	12:BM:544:VAL:HG12	1.82	0.61
12:BM:467:LYS:HG3	12:BM:503:THR:HB	1.80	0.61
32:Bi:271:THR:HG22	32:Bi:276:LEU:HD22	1.81	0.61
33:Bj:77:TRP:NE1	41:Bs:318:THR:O	2.31	0.61
37:Bn:10:ASP:HB3	40:Br:19:LYS:HZ3	1.65	0.61
44:Bw:60:ILE:O	44:Bw:159:LEU:N	2.33	0.61
2:B:151:ILE:HG21	3:C:159:TYR:HD2	1.62	0.61
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.82	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
25:b:115:GLU:HG2	25:b:116:VAL:H	1.65	0.61
71:b:201:PLX:O4	71:b:201:PLX:H11	1.99	0.61
35:l:37:LYS:NZ	35:l:98:TRP:NE1	2.47	0.61
47:z:154:GLY:HA2	50:2:6:VAL:CG2	2.30	0.61
1:BA:207:GLY:O	70:BA:502:FMN:C5A	2.47	0.61
11:BL:109:ASN:ND2	11:BL:111:LEU:O	2.33	0.61
25:Bb:88:TYR:HD1	25:Bb:92:GLU:OE2	1.82	0.61
7:H:89:ASN:O	7:H:93:LYS:HG2	2.00	0.61
6:X:72:PRO:HG3	35:l:442:ASN:HD22	1.65	0.61
27:d:107:CYS:SG	27:d:119:CYS:HA	2.39	0.61
40:r:112:ALA:O	40:r:113:THR:OG1	2.14	0.61
40:r:447:LEU:HD11	71:r:502:PLX:H382	1.82	0.61
75:AL:502:CDL:H761	76:AL:503:PEE:H74	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:73:VAL:HG23	68:AY:147:LEU:HD23	1.83	0.61
68:AY:165:ARG:NH2	68:AY:211:LEU:O	2.24	0.61
13:BN:130:THR:N	18:BT:44:GLN:OE1	2.34	0.61
31:Bh:37:GLU:HB2	31:Bh:63:PHE:CE1	2.35	0.61
44:Bw:89:ALA:N	44:Bw:160:GLU:OE1	2.27	0.61
45:Bx:273:MET:HG3	45:Bx:319:LYS:HZ1	1.63	0.61
12:M:339:ALA:HB3	12:M:544:VAL:HG12	1.82	0.61
14:O:143:ARG:HB3	14:O:184:PRO:HD3	1.82	0.61
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	0.61
16:Q:51:VAL:HG13	32:i:171:ASN:OD1	2.00	0.61
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.81	0.61
24:a:55:PHE:CD2	39:p:118:TYR:CD1	2.88	0.61
29:f:55:TRP:O	29:f:59:ILE:HG12	2.00	0.61
33:j:32:GLU:O	33:j:37:TYR:OH	2.18	0.61
35:l:450:LEU:HD22	35:l:450:LEU:O	2.00	0.61
37:n:50:GLN:HG3	37:n:51:PRO:HD2	1.83	0.61
76:AJ:403:PEE:H61	76:AJ:403:PEE:H28	1.81	0.61
66:AV:83:HIS:NE2	82:AV:401:HEM:C4D	2.67	0.61
68:AY:98:PHE:CD2	68:AY:120:LEU:HD13	2.29	0.61
68:AY:152:GLN:NE2	68:AY:252:GLY:HA3	2.15	0.61
12:BM:500:ILE:O	12:BM:503:THR:OG1	2.12	0.61
16:BQ:179:ARG:CZ	16:BQ:303:ARG:HH21	2.13	0.61
34:Bk:10:LEU:HD12	36:Bm:102:LEU:HD12	1.82	0.61
1:A:339:PHE:HB3	1:A:349:LEU:HD13	1.81	0.61
12:M:69:LEU:HD21	12:M:184:ARG:HB2	1.83	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
25:b:12:LEU:HB3	25:b:16:ARG:NH1	2.15	0.61
26:c:159:LYS:HA	43:v:98:ARG:NH2	2.13	0.61
35:l:37:LYS:NZ	35:l:98:TRP:CD1	2.69	0.61
38:o:27:PRO:HG3	68:AY:218:GLU:OE2	2.01	0.61
71:r:502:PLX:H31	71:r:502:PLX:C7	2.30	0.61
54:6:3:ASN:C	54:6:3:ASN:HD22	2.08	0.61
58:AA:19:LEU:HD23	68:AL:273:SER:HB3	1.81	0.61
66:AV:206:ASN:OD1	66:AV:207:ASN:N	2.34	0.61
14:BO:40:VAL:HG13	14:BO:42:ARG:H	1.64	0.61
1:A:123:GLY:HA3	1:A:355:ILE:HD11	1.83	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.33	0.61
12:M:346:VAL:HB	12:M:548:LEU:HD13	1.82	0.61
15:P:154:GLU:HA	15:P:179:ALA:HB2	1.81	0.61
24:a:53:ARG:HH21	25:b:28:LEU:HD11	1.66	0.61
41:s:28:LEU:O	41:s:32:GLN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:16:ILE:HD12	46:y:17:MET:N	2.15	0.61
47:z:148:HIS:O	47:z:152:MET:HG3	2.01	0.61
75:AL:502:CDL:C58	76:AL:503:PEE:H63	2.29	0.61
12:BM:173:MET:O	12:BM:175:ARG:N	2.24	0.61
12:BM:387:LEU:HD12	12:BM:514:ASN:HB2	1.82	0.61
12:BM:483:ARG:O	12:BM:485:ASP:N	2.34	0.61
6:BX:72:PRO:HG3	35:Bl:442:ASN:HD22	1.65	0.61
47:Bz:6:HIS:HD2	47:Bz:8:TYR:H	1.49	0.61
50:B2:13:ALA:O	50:B2:18:ARG:HD2	2.00	0.61
52:B4:57:ARG:HB3	52:B4:57:ARG:HH11	1.64	0.61
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.81	0.61
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.81	0.61
44:w:67:CYS:H	44:w:70:LYS:HD3	1.65	0.61
45:x:92:MET:CE	45:x:167:THR:HG21	2.31	0.61
50:2:13:ALA:O	50:2:18:ARG:HD2	2.00	0.61
62:AR:30:LEU:HD13	62:AR:86:LEU:HD11	1.82	0.61
64:AT:38:TRP:CE3	64:AT:41:ILE:HD13	2.35	0.61
67:AW:116:ARG:NH1	67:AW:188:ASN:O	2.33	0.61
67:AW:357:GLN:O	67:AW:360:THR:OG1	2.17	0.61
67:AW:443:ASN:O	67:AW:444:LEU:HB2	1.99	0.61
68:AY:265:LEU:HD12	68:AY:265:LEU:N	2.15	0.61
1:BA:123:GLY:HA3	1:BA:355:ILE:HD11	1.83	0.61
16:BQ:428:GLY:HA2	16:BQ:431:HIS:HD2	1.66	0.61
32:Bi:37:MET:HE1	32:Bi:60:PHE:HA	1.82	0.61
40:Br:61:LEU:HD22	40:Br:241:TYR:HD1	1.64	0.61
40:Br:178:LEU:O	40:Br:182:THR:OG1	2.16	0.61
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.61
12:M:534:VAL:HG12	12:M:536:ALA:H	1.66	0.61
35:l:37:LYS:HZ3	35:l:98:TRP:NE1	1.99	0.61
36:m:83:GLY:HA2	36:m:89:LEU:HD21	1.83	0.61
36:m:147:ASP:OD1	36:m:148:TYR:N	2.30	0.61
66:AJ:282:ARG:HD2	66:AJ:343:VAL:HG22	1.83	0.61
1:BA:339:PHE:HB3	1:BA:349:LEU:HD13	1.81	0.61
16:BQ:87:GLN:OE1	16:BQ:87:GLN:N	2.27	0.61
41:Bs:28:LEU:O	41:Bs:32:GLN:HB2	2.01	0.61
45:Bx:92:MET:HE2	45:Bx:167:THR:HG21	1.82	0.61
1:A:263:ALA:HA	1:A:271:SER:HB3	1.83	0.61
2:B:74:TYR:HD2	41:s:33:LEU:HG	1.66	0.61
9:J:188:GLU:HG3	9:J:200:ILE:HG21	1.83	0.61
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.81	0.61
17:S:50:ARG:HA	31:h:105:ARG:CZ	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:27:SER:O	20:V:30:SER:OG	2.14	0.61
27:d:81:GLU:OE1	37:n:43:MET:CE	2.43	0.61
65:AU:135:LEU:HA	65:AU:138:VAL:HG12	1.82	0.61
1:BA:37:ASP:OD2	14:BO:236:GLU:N	2.30	0.61
11:BL:128:PHE:HA	15:BP:121:THR:HG22	1.81	0.61
12:BM:31:LEU:HD22	12:BM:44:GLU:HA	1.83	0.61
16:BQ:338:ARG:HH12	21:BW:23:ARG:HB3	1.64	0.61
24:Ba:55:PHE:CD2	39:Bp:118:TYR:CD1	2.88	0.61
35:Bl:450:LEU:HD22	35:Bl:450:LEU:O	2.00	0.61
47:Bz:154:GLY:HA2	50:B2:6:VAL:CG2	2.30	0.61
1:A:35:LEU:HD22	1:A:290:GLU:HA	1.83	0.61
3:C:184:PRO:HD3	16:Q:223:HIS:HD2	1.65	0.61
9:J:212:ARG:HH11	9:J:212:ARG:CG	2.12	0.61
12:M:177:ILE:HG13	12:M:179:CYS:SG	2.41	0.61
27:d:110:ARG:HG2	27:d:110:ARG:NH1	2.11	0.61
34:k:10:LEU:HD12	36:m:102:LEU:HD12	1.82	0.61
35:l:303:ALA:O	35:l:306:THR:OG1	2.17	0.61
46:y:226:MET:O	46:y:227:LEU:HB2	2.01	0.61
62:AE:30:LEU:HD21	65:AH:216:THR:HG21	1.83	0.61
75:AJ:404:CDL:HB62	66:AV:13:LEU:HD22	1.83	0.61
75:AL:502:CDL:OA9	76:AL:503:PEE:O5	2.19	0.61
65:AU:133:ARG:NH1	66:AV:72:ASP:OD1	2.32	0.61
66:AV:141:TRP:HB3	66:AV:268:ILE:HD11	1.82	0.61
68:AY:96:LEU:HA	68:AY:99:LYS:HG2	1.83	0.61
68:AY:424:ILE:HG23	68:AY:424:ILE:O	2.00	0.61
68:AY:460:GLY:HA2	68:AY:462:ILE:H	1.64	0.61
1:BA:398:ARG:NH1	1:BA:408:GLU:OE1	2.25	0.61
9:BJ:315:THR:HG23	9:BJ:318:LYS:H	1.66	0.61
12:BM:168:LEU:HD23	12:BM:292:PHE:HD2	1.66	0.61
12:BM:352:VAL:HG21	12:BM:646:LEU:HD21	1.82	0.61
15:BP:154:GLU:HA	15:BP:179:ALA:HB2	1.81	0.61
15:BP:204:LEU:HD11	16:BQ:123:LEU:HD23	1.83	0.61
16:BQ:412:VAL:HB	16:BQ:421:ARG:HB3	1.81	0.61
35:Bl:194:ASN:HB2	38:Bo:125:PHE:O	2.01	0.61
41:Bs:280:PHE:CE2	41:Bs:288:LEU:HD11	2.36	0.61
41:Bs:294:LEU:O	41:Bs:297:THR:OG1	2.15	0.61
44:Bw:160:GLU:HG2	44:Bw:161:ARG:N	2.13	0.61
45:Bx:92:MET:CE	45:Bx:167:THR:HG21	2.31	0.61
46:By:59:GLN:HA	46:By:62:GLU:HB2	1.83	0.61
47:Bz:119:THR:O	51:B3:52:HIS:HE1	1.84	0.61
3:C:136:LYS:HD2	33:j:40:GLY:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.34	0.60
9:J:241:TYR:CE2	9:J:243:VAL:HB	2.35	0.60
9:J:286:ARG:NH2	9:J:356:HIS:O	2.34	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	0.60
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.83	0.60
71:U:101:PLX:H252	33:j:106:TRP:CD1	2.36	0.60
21:W:29:GLY:O	21:W:32:GLY:N	2.34	0.60
21:W:111:PHE:HE2	21:W:117:VAL:HG11	1.66	0.60
76:W:201:PEE:H8	41:s:98:LEU:HD22	1.83	0.60
24:a:153:GLU:OE2	42:u:166:ARG:NH1	2.33	0.60
26:c:105:MET:HE2	38:o:65:LEU:HA	1.83	0.60
27:d:59:HIS:NE2	28:e:121:GLU:HG2	2.16	0.60
45:x:92:MET:HE2	45:x:167:THR:HG21	1.82	0.60
58:AA:78:TYR:HB3	62:AE:65:GLU:HG2	0.68	0.60
61:AD:48:ASN:HD22	65:AH:104:SER:HB3	1.66	0.60
67:AK:51:SER:HB2	67:AK:230:LEU:HD12	1.82	0.60
68:AL:218:GLU:OE2	38:Bo:27:PRO:CG	2.42	0.60
67:AW:151:VAL:HG12	67:AW:155:GLN:HE21	1.64	0.60
2:BB:72:LEU:HB2	41:Bs:272:TRP:CH2	2.36	0.60
71:BU:101:PLX:H252	33:Bj:106:TRP:CD1	2.36	0.60
21:BW:111:PHE:HE2	21:BW:117:VAL:HG11	1.66	0.60
22:BY:73:PHE:O	22:BY:73:PHE:HD1	1.84	0.60
24:Ba:153:GLU:OE2	42:Bu:166:ARG:NH1	2.33	0.60
27:Bd:59:HIS:NE2	28:Be:121:GLU:HG2	2.16	0.60
36:Bm:83:GLY:HA2	36:Bm:89:LEU:HD21	1.83	0.60
46:By:16:ILE:HD12	46:By:17:MET:N	2.15	0.60
57:B9:28:LEU:HB2	57:B9:29:PRO:HD3	1.83	0.60
2:B:72:LEU:HB2	41:s:272:TRP:CH2	2.36	0.60
11:L:75:ARG:HH11	11:L:104:ARG:HE	1.49	0.60
12:M:483:ARG:O	12:M:485:ASP:N	2.34	0.60
13:N:130:THR:N	18:T:44:GLN:OE1	2.34	0.60
76:V:202:PEE:C11	32:i:276:LEU:HD12	2.28	0.60
25:b:14:GLN:NE2	39:p:164:PRO:HD3	2.15	0.60
39:p:98:LYS:HE2	39:p:176:GLU:HA	1.83	0.60
58:AA:78:TYR:CG	62:AE:65:GLU:HA	2.33	0.60
68:AL:165:ARG:NH2	68:AL:211:LEU:O	2.32	0.60
67:AW:318:GLN:HB3	67:AW:320:PRO:HD2	1.83	0.60
1:BA:203:ALA:HA	12:BM:200:ARG:HH12	1.65	0.60
4:BE:37:ARG:HH21	4:BE:41:ARG:NH2	2.00	0.60
5:BF:63:PRO:HB2	5:BF:79:LEU:CB	2.32	0.60
12:BM:387:LEU:HA	12:BM:514:ASN:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BP:212:TYR:HA	15:BP:219:VAL:HA	1.83	0.60
33:Bj:32:GLU:O	33:Bj:37:TYR:OH	2.18	0.60
35:Bl:37:LYS:NZ	35:Bl:98:TRP:CD1	2.69	0.60
35:Bl:54:PHE:HD2	35:Bl:55:MET:HE2	1.65	0.60
44:Bw:67:CYS:H	44:Bw:70:LYS:HD3	1.65	0.60
12:M:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60
16:Q:338:ARG:HH12	21:W:23:ARG:HB3	1.65	0.60
31:h:37:GLU:HB2	31:h:63:PHE:CE1	2.35	0.60
33:j:55:PHE:O	33:j:58:VAL:HG12	2.01	0.60
41:s:280:PHE:CE2	41:s:288:LEU:HD11	2.36	0.60
49:1:82:TYR:HB3	49:1:83:PRO:HD3	1.82	0.60
60:AP:131:ASN:HD22	76:AU:401:PEE:H7	1.66	0.60
1:BA:282:VAL:HG21	1:BA:304:ALA:HB1	1.83	0.60
8:BI:52:ASN:OD1	8:BI:57:ARG:NE	2.34	0.60
12:BM:346:VAL:HB	12:BM:548:LEU:HD13	1.82	0.60
16:BQ:140:ASP:HB3	16:BQ:147:ASN:HD21	1.66	0.60
26:Bc:84:HIS:CE1	26:Bc:114:ARG:HA	2.37	0.60
30:Bg:44:ASP:OD2	30:Bg:63:TYR:OH	2.16	0.60
32:Bi:58:LYS:HE3	35:Bl:584:ILE:HG12	1.82	0.60
33:Bj:55:PHE:O	33:Bj:58:VAL:HG12	2.01	0.60
47:Bz:148:HIS:O	47:Bz:152:MET:HG3	2.01	0.60
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.60
9:J:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.60
47:z:6:HIS:HD2	47:z:8:TYR:H	1.49	0.60
65:AH:124:CYS:CB	81:AH:402:HEC:HBC2	2.31	0.60
67:AK:363:GLN:CB	67:AK:365:ASN:OD1	2.49	0.60
1:BA:161:GLU:O	14:BO:192:TYR:OH	2.18	0.60
2:BB:74:TYR:HD2	41:Bs:33:LEU:HG	1.66	0.60
2:BB:103:ARG:NH2	18:BT:66:ASN:O	2.35	0.60
3:BC:184:PRO:HD3	16:BQ:223:HIS:HD2	1.65	0.60
7:BH:89:ASN:O	7:BH:93:LYS:HG2	2.00	0.60
12:BM:177:ILE:HG13	12:BM:179:CYS:SG	2.40	0.60
16:BQ:53:TYR:HE1	76:Bl:701:PEE:P	2.22	0.60
76:BV:202:PEE:C11	32:Bi:276:LEU:HD12	2.28	0.60
24:Ba:87:THR:HG22	71:Bb:201:PLX:H131	1.81	0.60
31:Bh:49:TYR:HA	31:Bh:52:ALA:HB3	1.82	0.60
35:Bl:149:ILE:HD12	40:Br:369:LEU:HD21	1.83	0.60
40:Br:190:TRP:NE1	71:Br:501:PLX:H1A2	2.17	0.60
2:B:103:ARG:NH2	18:T:66:ASN:O	2.35	0.60
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:228:VAL:HG23	12:M:230:ALA:H	1.66	0.60
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	0.60
22:Y:73:PHE:O	22:Y:73:PHE:HD1	1.84	0.60
35:l:534:HIS:ND1	76:l:702:PEE:C11	2.59	0.60
59:AB:33:THR:HA	59:AB:38:PRO:HG3	1.82	0.60
68:AL:264:THR:H	38:Bo:24:ASN:HB3	1.65	0.60
63:AS:7:VAL:HB	63:AS:10:SER:HB2	1.84	0.60
65:AU:202:ARG:NH2	66:AV:256:TYR:OH	2.28	0.60
24:Ba:53:ARG:HH21	25:Bb:28:LEU:HD11	1.66	0.60
25:Bb:12:LEU:HB3	25:Bb:16:ARG:NH1	2.15	0.60
25:Bb:14:GLN:NE2	39:Bp:164:PRO:HD3	2.15	0.60
32:Bi:193:VAL:HG21	32:Bi:266:ILE:HG12	1.82	0.60
37:Bn:50:GLN:HG3	37:Bn:51:PRO:HD2	1.83	0.60
39:Bp:98:LYS:HE2	39:Bp:176:GLU:HA	1.84	0.60
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.60
32:i:37:MET:HE1	32:i:60:PHE:HA	1.82	0.60
44:w:149:HIS:O	44:w:153:THR:OG1	2.16	0.60
49:1:80:GLU:H	49:1:80:GLU:CD	2.10	0.60
9:BJ:171:ASN:HB2	9:BJ:181:LEU:HD11	1.84	0.60
12:BM:537:ILE:O	12:BM:539:LYS:N	2.33	0.60
13:BN:137:TRP:CH2	13:BN:140:PRO:HD3	2.36	0.60
76:BW:201:PEE:H8	41:Bs:98:LEU:HD22	1.83	0.60
23:BZ:25:GLU:HA	23:BZ:30:GLU:HG3	1.84	0.60
25:Bb:51:LEU:HD21	25:Bb:62:HIS:HB2	1.83	0.60
26:Bc:105:MET:HE2	38:Bo:65:LEU:HA	1.84	0.60
40:Br:164:LEU:O	40:Br:167:THR:OG1	2.18	0.60
9:J:171:ASN:HB2	9:J:181:LEU:HD11	1.84	0.60
12:M:387:LEU:HA	12:M:514:ASN:HB2	1.82	0.60
14:O:137:THR:OG1	14:O:176:CYS:N	2.34	0.60
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.66	0.60
24:a:176:LYS:HB2	31:h:45:HIS:CD2	2.36	0.60
27:d:54:ARG:HD3	27:d:56:TYR:CZ	2.37	0.60
27:d:134:GLN:NE2	38:o:123:ARG:O	2.35	0.60
39:p:56:ASP:CG	68:AY:227:PRO:CG	2.75	0.60
47:z:192:VAL:O	47:z:196:THR:HB	2.01	0.60
63:AF:34:ARG:HH11	63:AF:34:ARG:CG	2.13	0.60
60:AP:111:LYS:NZ	68:AY:451:ASP:O	2.32	0.60
67:AW:449:PHE:HB2	67:AW:452:GLU:CD	2.27	0.60
9:BJ:221:HIS:HE1	9:BJ:222:ARG:HG3	1.61	0.60
11:BL:75:ARG:HH11	11:BL:104:ARG:HE	1.49	0.60
12:BM:534:VAL:HG12	12:BM:536:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:51:VAL:HG13	32:Bi:171:ASN:OD1	2.00	0.60
32:Bi:58:LYS:NZ	34:Bk:92:ASN:OD1	2.35	0.60
4:E:99:GLN:HE21	33:j:41:PHE:HD1	1.50	0.60
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.60
9:J:208:GLY:H	9:J:211:ASP:HB2	1.66	0.60
12:M:345:LEU:HB2	12:M:548:LEU:HD21	1.84	0.60
15:P:212:TYR:HA	15:P:219:VAL:HA	1.83	0.60
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.60
20:V:40:ARG:HA	75:V:201:CDL:OB3	2.02	0.60
27:d:54:ARG:HD3	27:d:56:TYR:CE1	2.37	0.60
32:i:291:TYR:CE2	76:l:701:PEE:C32	2.85	0.60
35:l:54:PHE:HD2	35:l:55:MET:HE2	1.65	0.60
35:l:194:ASN:HB2	38:o:125:PHE:O	2.01	0.60
38:o:54:PRO:HA	39:p:129:ARG:HH21	1.67	0.60
40:r:30:HIS:O	40:r:34:ILE:HD12	2.01	0.60
64:AG:38:TRP:O	64:AG:42:LEU:HD12	2.02	0.60
62:AR:37:CYS:SG	62:AR:85:LYS:NZ	2.73	0.60
66:AV:181:PHE:HA	66:AV:184:ILE:HG22	1.83	0.60
1:BA:74:ASP:O	1:BA:78:GLY:N	2.27	0.60
1:BA:220:GLN:NE2	14:BO:114:GLU:O	2.35	0.60
14:BO:137:THR:OG1	14:BO:176:CYS:N	2.34	0.60
16:BQ:142:VAL:HG11	16:BQ:182:ASN:HA	1.84	0.60
20:BV:40:ARG:HA	75:BV:201:CDL:OB3	2.02	0.60
24:Ba:176:LYS:HB2	31:Bh:45:HIS:CD2	2.36	0.60
35:Bl:534:HIS:ND1	76:Bl:702:PEE:C11	2.59	0.60
40:Br:447:LEU:HD13	40:Br:454:ILE:HD11	1.83	0.60
44:Bw:287:ASP:OD1	44:Bw:288:ASN:N	2.34	0.60
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.60
22:Y:45:ARG:HG3	23:Z:52:ARG:HB2	1.84	0.60
27:d:60:ARG:HH11	27:d:60:ARG:CG	2.12	0.60
35:l:552:LEU:HD13	38:o:90:GLY:HA2	1.83	0.60
37:n:31:SER:O	37:n:34:ARG:HG2	2.02	0.60
67:AK:259:ARG:CD	67:AK:444:LEU:HD13	2.30	0.60
60:AP:79:SER:N	60:AP:82:ASP:OD2	2.35	0.60
60:AP:81:THR:HG21	68:AY:202:GLU:HB2	1.84	0.60
1:BA:412:LEU:HA	1:BA:415:ILE:HD12	1.84	0.60
12:BM:358:LEU:O	12:BM:363:SER:N	2.35	0.60
76:BW:201:PEE:H75	41:Bs:77:LEU:HD23	1.75	0.60
27:Bd:54:ARG:HD3	27:Bd:56:TYR:CZ	2.37	0.60
35:Bl:174:TYR:OH	76:Bl:702:PEE:H19	2.02	0.60
36:Bm:116:VAL:O	36:Bm:118:PHE:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bp:121:LYS:O	39:Bp:124:GLN:HG2	2.02	0.60
1:A:412:LEU:HA	1:A:415:ILE:HD12	1.84	0.60
2:B:64:LEU:O	2:B:68:LEU:N	2.30	0.60
9:J:217:PHE:HB2	9:J:280:ILE:HD13	1.83	0.60
9:J:329:LEU:HD13	9:J:332:LEU:HB2	1.84	0.60
26:c:84:HIS:CE1	26:c:114:ARG:HA	2.37	0.60
60:AC:132:ALA:HB2	76:AH:401:PEE:H24	1.84	0.60
68:AL:79:SER:HB3	68:AL:126:ARG:HA	1.84	0.60
59:AO:34:VAL:HB	59:AO:35:PRO:HD3	1.83	0.60
67:AW:274:GLU:OE2	67:AW:333:SER:OG	2.16	0.60
1:BA:263:ALA:HA	1:BA:271:SER:HB3	1.83	0.60
4:BE:127:ASP:HB3	4:BE:128:PRO:HD2	1.84	0.60
9:BJ:188:GLU:HG3	9:BJ:200:ILE:HG21	1.83	0.60
12:BM:228:VAL:HG23	12:BM:230:ALA:H	1.66	0.60
14:BO:143:ARG:HB3	14:BO:184:PRO:HD3	1.82	0.60
50:B2:62:CYS:SG	50:B2:84:SER:OG	2.60	0.60
24:a:87:THR:HG22	71:b:201:PLX:H131	1.81	0.59
25:b:51:LEU:HD21	25:b:62:HIS:HB2	1.83	0.59
33:j:7:LEU:HA	33:j:10:ASN:HD22	1.67	0.59
58:AA:40:ARG:HG3	58:AA:41:ARG:N	2.16	0.59
75:AG:101:CDL:H521	75:AG:101:CDL:C71	2.32	0.59
67:AK:183:ARG:HH21	67:AK:183:ARG:CG	2.14	0.59
68:AL:80:ARG:NE	68:AL:265:LEU:HD11	2.17	0.59
75:AL:502:CDL:H572	76:AL:503:PEE:C38	2.24	0.59
68:AY:89:ALA:O	68:AY:93:LEU:HG	2.02	0.59
1:BA:164:ASN:ND2	14:BO:190:ASP:O	2.34	0.59
15:BP:94:ILE:HG13	15:BP:154:GLU:HB3	1.82	0.59
27:Bd:54:ARG:HD3	27:Bd:56:TYR:CE1	2.37	0.59
32:Bi:291:TYR:CE2	76:Bl:701:PEE:C32	2.85	0.59
33:Bj:32:GLU:HA	33:Bj:35:THR:HG23	1.84	0.59
46:By:226:MET:O	46:By:227:LEU:HB2	2.01	0.59
5:F:63:PRO:HB2	5:F:79:LEU:CB	2.32	0.59
12:M:173:MET:C	12:M:175:ARG:N	2.60	0.59
12:M:519:ILE:HG12	12:M:521:SER:H	1.67	0.59
35:l:174:TYR:OH	76:l:702:PEE:H19	2.02	0.59
35:l:512:LYS:HD3	54:6:18:LEU:CD1	2.31	0.59
43:v:113:LYS:HE2	43:v:117:LYS:HE3	1.84	0.59
44:w:170:LEU:HD21	44:w:184:VAL:HG22	1.84	0.59
66:AJ:283:SER:O	66:AJ:352:GLN:NE2	2.33	0.59
63:AS:43:ASP:OD2	63:AS:102:ARG:NH1	2.35	0.59
66:AV:272:TRP:HA	66:AV:275:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:205:ARG:HG3	3:BC:205:ARG:O	2.02	0.59
12:BM:345:LEU:HB2	12:BM:548:LEU:HD21	1.84	0.59
12:BM:460:HIS:O	12:BM:463:SER:OG	2.13	0.59
15:BP:147:THR:HG21	15:BP:153:ILE:HB	1.85	0.59
6:BX:138:LEU:HD21	6:BX:144:ILE:HG12	1.83	0.59
35:Bl:227:LEU:CD1	35:Bl:230:HIS:CE1	2.86	0.59
35:Bl:227:LEU:HB2	35:Bl:284:THR:HG22	1.84	0.59
40:Br:126:LEU:O	40:Br:129:THR:OG1	2.19	0.59
1:A:93:PHE:HE2	1:A:98:LYS:CD	2.05	0.59
9:J:192:ARG:O	9:J:196:PRO:HA	2.02	0.59
25:b:100:LYS:HB2	35:l:60:GLU:HB2	1.85	0.59
32:i:145:ILE:HD12	32:i:149:LEU:HD11	1.84	0.59
35:l:149:ILE:HD12	40:r:369:LEU:HD21	1.83	0.59
46:y:59:GLN:HA	46:y:62:GLU:HB2	1.83	0.59
50:2:62:CYS:SG	50:2:84:SER:OG	2.60	0.59
68:AY:96:LEU:CD2	68:AY:161:ILE:CD1	2.80	0.59
1:BA:35:LEU:HD22	1:BA:290:GLU:HA	1.82	0.59
1:BA:209:GLU:HB3	70:BA:502:FMN:H3'	1.85	0.59
12:BM:69:LEU:HD21	12:BM:184:ARG:HB2	1.83	0.59
12:BM:460:HIS:CD2	12:BM:462:PHE:HB3	2.38	0.59
15:BP:83:GLU:HB3	15:BP:142:ARG:HH12	1.65	0.59
22:BY:45:ARG:HG3	23:BZ:52:ARG:HB2	1.84	0.59
24:Ba:52:LYS:O	24:Ba:53:ARG:HG2	2.03	0.59
27:Bd:134:GLN:NE2	38:Bo:123:ARG:O	2.35	0.59
35:Bl:27:ASN:HB3	35:Bl:29:LYS:HG2	1.84	0.59
35:Bl:427:ILE:HG23	35:Bl:431:LEU:HD12	1.82	0.59
35:Bl:512:LYS:HD3	54:B6:18:LEU:CD1	2.32	0.59
37:Bn:31:SER:O	37:Bn:34:ARG:HG2	2.02	0.59
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	0.59
7:H:77:LEU:O	7:H:80:VAL:HG12	2.01	0.59
13:N:34:LYS:HZ1	13:N:58:ARG:HG2	1.67	0.59
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.13	0.59
35:l:227:LEU:CD1	35:l:230:HIS:CE1	2.85	0.59
40:r:164:LEU:O	40:r:167:THR:OG1	2.18	0.59
46:y:145:PRO:CG	46:y:148:MET:HE2	2.33	0.59
76:AU:401:PEE:H17	66:AV:240:MET:HE2	1.76	0.59
1:BA:288:VAL:HG11	1:BA:303:HIS:CD2	2.38	0.59
2:BB:74:TYR:OH	16:BQ:257:GLU:OE1	2.20	0.59
7:BH:77:LEU:O	7:BH:80:VAL:HG12	2.02	0.59
9:BJ:329:LEU:HD13	9:BJ:332:LEU:HB2	1.84	0.59
12:BM:330:LEU:HD22	12:BM:626:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ba:55:PHE:HE2	39:Bp:118:TYR:HE2	1.26	0.59
31:Bh:44:ALA:HA	31:Bh:47:ILE:HD12	1.85	0.59
32:Bi:249:LEU:HB3	32:Bi:254:LEU:HD12	1.85	0.59
33:Bj:7:LEU:HA	33:Bj:10:ASN:HD22	1.67	0.59
34:Bk:3:LEU:CD2	36:Bm:117:ASN:ND2	2.60	0.59
41:Bs:172:LEU:HD21	41:Bs:176:LEU:HB2	1.84	0.59
44:Bw:65:ASN:HD22	44:Bw:209:VAL:HG21	1.67	0.59
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.59
9:J:172:ALA:O	9:J:185:ALA:HB2	2.03	0.59
12:M:460:HIS:CD2	12:M:462:PHE:HB3	2.38	0.59
13:N:137:TRP:CH2	13:N:140:PRO:HD3	2.36	0.59
17:S:53:ARG:HB2	31:h:105:ARG:NH1	2.18	0.59
35:l:37:LYS:CE	35:l:98:TRP:NE1	2.65	0.59
35:l:227:LEU:HB2	35:l:284:THR:HG22	1.84	0.59
40:r:210:TYR:HB2	40:r:268:GLY:HA3	1.85	0.59
40:r:447:LEU:HD13	40:r:454:ILE:HD11	1.83	0.59
58:AN:73:LYS:O	58:AN:77:ALA:N	2.35	0.59
62:AR:30:LEU:HD21	65:AU:216:THR:HG23	1.84	0.59
64:AT:14:VAL:O	64:AT:18:VAL:HG23	2.02	0.59
66:AV:200:LEU:CD1	82:AV:402:HEM:HAD2	2.32	0.59
66:AV:338:ILE:HD11	66:AV:350:ILE:HG22	1.84	0.59
3:BC:136:LYS:HD2	33:Bj:40:GLY:C	2.26	0.59
3:BC:173:ILE:HG22	3:BC:174:VAL:HG13	1.84	0.59
4:BE:99:GLN:HE21	33:Bj:41:PHE:HD1	1.50	0.59
23:BZ:66:VAL:HG22	35:Bl:363:LEU:HD22	1.85	0.59
32:Bi:8:VAL:HG11	36:Bm:165:TYR:CE2	2.37	0.59
32:Bi:24:SER:O	32:Bi:86:MET:HG2	2.02	0.59
35:Bl:552:LEU:HD13	38:Bo:90:GLY:HA2	1.83	0.59
39:Bp:55:LYS:HE2	39:Bp:55:LYS:N	2.17	0.59
56:B8:46:LYS:O	56:B8:47:LYS:HB2	2.02	0.59
3:C:205:ARG:HG3	3:C:205:ARG:O	2.02	0.59
9:J:226:ILE:HD12	9:J:289:LEU:N	2.16	0.59
40:r:190:TRP:NE1	71:r:501:PLX:H1A2	2.17	0.59
62:AE:33:VAL:HG11	62:AE:85:LYS:O	2.03	0.59
68:AY:225:LYS:HZ2	68:AY:257:TYR:HA	1.65	0.59
25:Bb:88:TYR:CG	71:Bb:201:PLX:C1C	2.86	0.59
43:Bv:8:ARG:HH11	43:Bv:106:ARG:NH2	1.97	0.59
47:Bz:192:VAL:O	47:Bz:196:THR:HB	2.01	0.59
52:B4:57:ARG:HG3	52:B4:60:TYR:CE2	2.38	0.59
1:A:220:GLN:NE2	14:O:114:GLU:O	2.34	0.59
14:O:48:ASN:HD22	14:O:94:PRO:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.30	0.59
25:b:88:TYR:CG	71:b:201:PLX:C1C	2.86	0.59
31:h:51:ARG:NH1	31:h:55:GLU:OE2	2.36	0.59
41:s:172:LEU:HD21	41:s:176:LEU:HB2	1.84	0.59
57:9:28:LEU:HB2	57:9:29:PRO:HD3	1.83	0.59
58:AA:71:LYS:HE2	65:AH:87:LEU:HD12	1.84	0.59
9:BJ:208:GLY:H	9:BJ:211:ASP:HB2	1.66	0.59
9:BJ:217:PHE:HB2	9:BJ:280:ILE:HD13	1.83	0.59
12:BM:36:VAL:HG11	12:BM:56:VAL:HG11	1.85	0.59
16:BQ:182:ASN:HD21	16:BQ:404:LYS:HE3	1.68	0.59
16:BQ:267:ILE:HG21	41:Bs:278:PRO:O	2.03	0.59
27:Bd:21:PRO:HG2	27:Bd:24:ILE:HD12	1.85	0.59
27:Bd:81:GLU:OE1	37:Bn:43:MET:CE	2.43	0.59
35:Bl:247:LEU:O	35:Bl:252:MET:HB3	2.03	0.59
44:Bw:304:VAL:HG23	44:Bw:305:LEU:HG	1.84	0.59
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	0.59
2:B:72:LEU:HB2	41:s:272:TRP:HH2	1.68	0.59
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.59
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.59
35:l:501:ALA:O	35:l:505:ASN:ND2	2.29	0.59
39:p:121:LYS:O	39:p:124:GLN:HG2	2.02	0.59
41:s:294:LEU:O	41:s:297:THR:OG1	2.15	0.59
44:w:124:ASN:HB3	44:w:316:GLU:HG2	1.85	0.59
47:z:119:THR:O	51:3:52:HIS:HE1	1.84	0.59
60:AC:96:VAL:O	68:AL:269:ARG:NH1	2.36	0.59
2:BB:187:LYS:HB2	13:BN:124:TYR:CE1	2.36	0.59
9:BJ:141:PHE:CZ	9:BJ:180:TYR:CA	2.84	0.59
9:BJ:226:ILE:HD12	9:BJ:289:LEU:N	2.16	0.59
17:BS:53:ARG:HB2	31:Bh:105:ARG:NH1	2.18	0.59
21:BW:29:GLY:O	21:BW:32:GLY:N	2.34	0.59
24:Ba:67:PHE:HD1	40:Br:431:THR:HG23	1.68	0.59
32:Bi:145:ILE:HD12	32:Bi:149:LEU:HD11	1.84	0.59
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.67	0.59
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.85	0.59
25:b:88:TYR:O	25:b:92:GLU:HB2	2.03	0.59
26:c:93:ASP:OD2	26:c:101:TRP:N	2.36	0.59
26:c:122:THR:HG1	38:o:12:ARG:HH12	1.44	0.59
32:i:8:VAL:HG11	36:m:165:TYR:CE2	2.37	0.59
32:i:245:PRO:HA	32:i:248:LEU:HD12	1.85	0.59
32:i:249:LEU:HB3	32:i:254:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:247:LEU:O	35:l:252:MET:HB3	2.03	0.59
37:n:10:ASP:HB3	40:r:19:LYS:HZ3	1.68	0.59
46:y:179:LEU:HD21	52:4:65:PRO:HD3	1.85	0.59
52:4:57:ARG:HG3	52:4:60:TYR:CE2	2.38	0.59
63:AF:67:LEU:CD2	66:AJ:209:LEU:HD12	2.28	0.59
66:AV:343:VAL:HG13	66:AV:348:THR:HG22	1.84	0.59
2:BB:186:GLU:OE2	18:BT:64:ASN:N	2.36	0.59
5:BF:88:THR:HA	5:BF:91:LEU:HD12	1.85	0.59
9:BJ:207:PHE:HE2	9:BJ:348:LYS:HB2	1.67	0.59
12:BM:251:ILE:HG22	12:BM:260:ASN:HA	1.85	0.59
12:BM:519:ILE:HG12	12:BM:521:SER:H	1.68	0.59
12:BM:624:ARG:NE	12:BM:636:TYR:O	2.36	0.59
13:BN:129:THR:HA	18:BT:44:GLN:HE22	1.67	0.59
16:BQ:438:MET:HE1	16:BQ:454:GLN:NE2	2.18	0.59
40:Br:30:HIS:O	40:Br:34:ILE:HD12	2.01	0.59
40:Br:210:TYR:HB2	40:Br:268:GLY:HA3	1.85	0.59
44:Bw:170:LEU:HD21	44:Bw:184:VAL:HG22	1.84	0.59
12:M:602:ARG:HE	12:M:659:ILE:HD11	1.67	0.59
25:b:79:VAL:HG11	27:d:35:VAL:HG11	1.84	0.59
25:b:100:LYS:O	25:b:101:LYS:HG2	2.01	0.59
27:d:21:PRO:HG2	27:d:24:ILE:HD12	1.85	0.59
35:l:27:ASN:HB3	35:l:29:LYS:HG2	1.84	0.59
44:w:65:ASN:HD22	44:w:209:VAL:HG21	1.67	0.59
82:AJ:401:HEM:HBB2	82:AJ:401:HEM:HMB1	1.84	0.59
1:BA:126:LYS:HB2	1:BA:275:LEU:HD22	1.85	0.59
12:BM:454:ASP:HB3	12:BM:460:HIS:HB2	1.85	0.59
31:Bh:51:ARG:NH1	31:Bh:55:GLU:OE2	2.36	0.59
32:Bi:245:PRO:HA	32:Bi:248:LEU:HD12	1.85	0.59
35:Bl:452:ASN:N	35:Bl:452:ASN:OD1	2.36	0.59
35:Bl:512:LYS:O	39:Bp:40:PHE:CZ	2.56	0.59
8:I:69:ILE:HB	15:P:76:VAL:HB	1.85	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
21:W:81:ARG:HH22	42:u:64:ASN:ND2	2.01	0.58
23:Z:25:GLU:HA	23:Z:30:GLU:HG3	1.84	0.58
35:l:88:MET:C	35:l:91:PRO:HD2	2.28	0.58
67:AK:177:LEU:HD21	67:AK:272:VAL:HG21	1.85	0.58
9:BJ:172:ALA:O	9:BJ:185:ALA:HB2	2.03	0.58
16:BQ:390:GLN:HE22	16:BQ:417:SER:HB3	1.68	0.58
20:BV:27:SER:O	20:BV:30:SER:OG	2.14	0.58
25:Bb:100:LYS:O	25:Bb:101:LYS:HG2	2.01	0.58
39:Bp:176:GLU:HG2	39:Bp:177:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bu:38:LYS:O	42:Bu:42:GLU:HB2	2.03	0.58
1:A:209:GLU:HB3	70:A:502:FMN:H3'	1.85	0.58
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.58
16:Q:390:GLN:HE22	16:Q:417:SER:HB3	1.68	0.58
16:Q:438:MET:HE1	16:Q:454:GLN:NE2	2.18	0.58
17:S:59:ARG:O	17:S:61:TYR:N	2.36	0.58
76:W:201:PEE:C44	41:s:77:LEU:CD2	2.67	0.58
23:Z:66:VAL:HG22	35:l:363:LEU:HD22	1.85	0.58
33:j:32:GLU:HA	33:j:35:THR:HG23	1.84	0.58
39:p:176:GLU:HG2	39:p:177:ARG:HG3	1.85	0.58
61:AD:34:ARG:NH1	61:AD:38:GLN:OE1	2.35	0.58
67:AK:323:VAL:HG13	67:AK:340:THR:HG22	1.85	0.58
63:AS:71:LEU:O	65:AU:315:LYS:NZ	2.35	0.58
68:AY:98:PHE:CZ	68:AY:120:LEU:HD13	2.36	0.58
4:BE:97:TRP:HH2	15:BP:185:ARG:HH11	1.49	0.58
6:BX:84:LEU:O	6:BX:88:LYS:HG2	2.03	0.58
25:Bb:88:TYR:CG	71:Bb:201:PLX:H1C1	2.38	0.58
25:Bb:100:LYS:HB2	35:Bl:60:GLU:HB2	1.84	0.58
31:Bh:94:PRO:HG2	31:Bh:95:PRO:HD3	1.85	0.58
35:Bl:456:ARG:HH21	35:Bl:456:ARG:CB	2.16	0.58
2:B:36:TYR:HB3	8:I:104:TRP:HE3	1.68	0.58
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.58
13:N:129:THR:HA	18:T:44:GLN:HE22	1.67	0.58
24:a:52:LYS:O	24:a:53:ARG:HG2	2.03	0.58
27:d:153:GLN:O	27:d:157:MET:HG2	2.03	0.58
33:j:54:LYS:HE3	33:j:113:TRP:CD1	2.38	0.58
35:l:452:ASN:OD1	35:l:452:ASN:N	2.36	0.58
39:p:55:LYS:HE2	39:p:55:LYS:N	2.16	0.58
39:p:112:LYS:HA	39:p:119:PHE:CE2	2.38	0.58
66:AV:311:LYS:HG3	66:AV:379:TRP:HE1	1.67	0.58
9:BJ:286:ARG:NH2	9:BJ:356:HIS:O	2.34	0.58
12:BM:650:SER:OG	12:BM:652:ASN:OD1	2.22	0.58
39:Bp:112:LYS:HA	39:Bp:119:PHE:CE2	2.38	0.58
49:B1:80:GLU:CD	49:B1:80:GLU:H	2.10	0.58
1:A:243:ALA:HA	70:A:502:FMN:O2P	2.04	0.58
4:E:97:TRP:HH2	15:P:185:ARG:HH11	1.49	0.58
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.58
20:V:40:ARG:HD3	20:V:59:TYR:HE2	1.68	0.58
21:W:39:GLY:O	21:W:42:THR:OG1	2.15	0.58
30:g:9:PRO:O	30:g:11:ARG:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:512:LYS:O	39:p:40:PHE:CZ	2.56	0.58
46:y:193:TYR:HE1	48:0:126:MET:HE1	1.68	0.58
56:8:46:LYS:O	56:8:47:LYS:HB2	2.03	0.58
68:AY:424:ILE:CG2	68:AY:429:TRP:HE1	2.09	0.58
12:BM:385:TYR:HB2	12:BM:517:HIS:HE2	1.69	0.58
17:BS:49:GLU:O	31:Bh:105:ARG:NH2	2.37	0.58
27:Bd:153:GLN:O	27:Bd:157:MET:HG2	2.03	0.58
37:Bn:56:THR:HG1	37:Bn:57:TRP:CD1	2.20	0.58
44:Bw:124:ASN:HB3	44:Bw:316:GLU:HG2	1.85	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58
9:J:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.58
12:M:454:ASP:HB3	12:M:460:HIS:HB2	1.85	0.58
12:M:501:ARG:NH1	12:M:666:GLN:HB2	2.18	0.58
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.58
16:Q:267:ILE:HG21	41:s:278:PRO:O	2.03	0.58
42:u:96:LEU:HD11	42:u:99:HIS:CD2	2.38	0.58
59:AB:37:THR:HA	68:AL:174:GLU:HG2	1.85	0.58
71:AL:501:PLX:H71	76:AL:503:PEE:C13	2.33	0.58
67:AW:449:PHE:HB2	67:AW:452:GLU:OE2	2.04	0.58
1:BA:93:PHE:HE2	1:BA:98:LYS:CD	2.05	0.58
4:BE:32:VAL:O	4:BE:35:LEU:HB3	2.03	0.58
4:BE:126:HIS:NE2	12:BM:612:PRO:O	2.37	0.58
8:BI:69:ILE:HB	15:BP:76:VAL:HB	1.85	0.58
12:BM:334:GLN:HB2	12:BM:361:VAL:HB	1.85	0.58
20:BV:40:ARG:HD3	20:BV:59:TYR:HE2	1.68	0.58
76:Bl:701:PEE:C23	40:Br:155:VAL:CB	2.77	0.58
38:Bo:54:PRO:HA	39:Bp:129:ARG:HH21	1.67	0.58
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	0.58
12:M:126:LEU:HD12	18:T:98:LYS:O	2.04	0.58
12:M:330:LEU:HD22	12:M:626:LEU:HD21	1.84	0.58
15:P:147:THR:HG21	15:P:153:ILE:HB	1.84	0.58
22:Y:86:TYR:OH	43:v:100:LYS:HG3	2.03	0.58
24:a:53:ARG:O	24:a:54:LEU:HD23	2.04	0.58
71:b:201:PLX:P1	71:b:201:PLX:H72	2.43	0.58
26:c:127:HIS:O	26:c:131:MET:HG2	2.04	0.58
33:j:2:ASN:O	33:j:5:LEU:HG	2.03	0.58
35:l:367:PRO:O	35:l:370:SER:OG	2.17	0.58
35:l:456:ARG:CB	35:l:456:ARG:HH21	2.17	0.58
44:w:304:VAL:HG23	44:w:305:LEU:HG	1.84	0.58
65:AU:288:MET:HE2	66:AV:77:TRP:CH2	2.39	0.58
68:AY:423:ARG:O	68:AY:424:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:243:ALA:HA	70:BA:502:FMN:O2P	2.04	0.58
3:BC:62:TYR:OH	3:BC:66:LYS:NZ	2.29	0.58
10:BK:89:LEU:HD11	14:BO:61:LYS:HE3	1.86	0.58
12:BM:257:VAL:HG11	12:BM:413:LEU:HD22	1.85	0.58
12:BM:501:ARG:NH1	12:BM:666:GLN:HB2	2.18	0.58
16:BQ:81:THR:HA	16:BQ:100:GLU:HA	1.86	0.58
71:Bb:201:PLX:P1	71:Bb:201:PLX:H72	2.44	0.58
32:Bi:316:GLN:NE2	44:Bw:95:ASP:OD1	2.33	0.58
35:Bl:453:PRO:HA	35:Bl:456:ARG:HH22	1.69	0.58
35:Bl:556:THR:OG1	35:Bl:557:TRP:N	2.37	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.58
17:S:49:GLU:O	31:h:105:ARG:NH2	2.37	0.58
32:i:58:LYS:NZ	34:k:92:ASN:OD1	2.35	0.58
37:n:10:ASP:HB3	40:r:19:LYS:NZ	2.19	0.58
40:r:126:LEU:O	40:r:129:THR:OG1	2.19	0.58
68:AL:262:VAL:CG2	39:Bp:61:THR:HG21	2.33	0.58
60:AP:183:GLU:HA	60:AP:186:GLN:HG2	1.86	0.58
61:AQ:48:ASN:HB2	61:AQ:51:LYS:HD2	1.85	0.58
7:BH:40:LYS:HD3	7:BH:45:ARG:NH1	2.18	0.58
9:BJ:192:ARG:O	9:BJ:196:PRO:HA	2.02	0.58
12:BM:602:ARG:HE	12:BM:659:ILE:HD11	1.67	0.58
33:Bj:54:LYS:HE3	33:Bj:113:TRP:CD1	2.38	0.58
2:B:198:GLU:OE1	13:N:88:ARG:HB2	2.04	0.58
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.84	0.58
4:E:32:VAL:O	4:E:35:LEU:HB3	2.03	0.58
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.58
25:b:105:PHE:CD2	43:v:68:LYS:HA	2.39	0.58
25:b:105:PHE:HE2	43:v:68:LYS:N	2.01	0.58
34:k:7:ASN:ND2	36:m:9:SER:OG	2.31	0.58
34:k:97:GLN:HG2	35:l:582:GLY:HA2	1.84	0.58
42:u:124:GLU:OE1	42:u:124:GLU:N	2.37	0.58
66:AJ:100:ARG:NH2	82:AJ:402:HEM:O2A	2.37	0.58
66:AV:333:LEU:HD21	76:AV:403:PEE:H62	1.86	0.58
82:AV:402:HEM:HBA1	82:AV:402:HEM:HHA	1.86	0.58
1:BA:307:VAL:HG11	1:BA:314:LEU:HD21	1.86	0.58
2:BB:72:LEU:HB2	41:Bs:272:TRP:HH2	1.68	0.58
8:BI:23:LYS:HD3	16:BQ:250:ASN:HA	1.85	0.58
9:BJ:84:TYR:CB	9:BJ:91:ILE:HD11	2.34	0.58
12:BM:173:MET:C	12:BM:175:ARG:N	2.60	0.58
16:BQ:251:PHE:HD2	16:BQ:341:LEU:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:412:VAL:HG12	16:BQ:420:TYR:HB3	1.86	0.58
25:Bb:88:TYR:O	25:Bb:92:GLU:HB2	2.03	0.58
25:Bb:105:PHE:CD2	43:Bv:68:LYS:HA	2.39	0.58
27:Bd:60:ARG:HG2	27:Bd:60:ARG:NH1	2.12	0.58
33:Bj:2:ASN:O	33:Bj:5:LEU:HG	2.03	0.58
35:Bl:88:MET:C	35:Bl:91:PRO:HD2	2.28	0.58
41:Bs:190:LEU:HD22	41:Bs:195:ARG:HG2	1.86	0.58
46:By:179:LEU:HD21	52:B4:65:PRO:HD3	1.85	0.58
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.58
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.58
12:M:210:ILE:HG23	12:M:212:LYS:H	1.69	0.58
41:s:190:LEU:HD22	41:s:195:ARG:HG2	1.86	0.58
60:AP:244:ASP:OD1	60:AP:248:ARG:N	2.36	0.58
65:AU:292:MET:HE1	66:AV:241:THR:CG2	2.33	0.58
9:BJ:181:LEU:HD23	9:BJ:181:LEU:O	2.03	0.58
12:BM:636:TYR:CE1	12:BM:642:VAL:HB	2.39	0.58
76:BW:201:PEE:H1	41:Bs:98:LEU:CD2	2.34	0.58
37:Bn:10:ASP:HB3	40:Br:19:LYS:NZ	2.19	0.58
43:Bv:113:LYS:HE2	43:Bv:117:LYS:HE3	1.84	0.58
46:By:193:TYR:HE1	48:B0:126:MET:HE1	1.68	0.58
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.58
2:B:186:GLU:OE2	18:T:64:ASN:N	2.36	0.58
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.85	0.58
12:M:177:ILE:HG13	12:M:177:ILE:O	2.04	0.58
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.58
12:M:636:TYR:CE1	12:M:642:VAL:HB	2.39	0.58
16:Q:81:THR:HA	16:Q:100:GLU:HA	1.86	0.58
26:c:169:GLU:O	26:c:169:GLU:HG2	2.03	0.58
71:g:203:PLX:H251	32:i:324:PRO:HB2	1.85	0.58
32:i:24:SER:O	32:i:86:MET:HG2	2.02	0.58
35:l:453:PRO:HA	35:l:456:ARG:HH22	1.69	0.58
71:r:502:PLX:H72	71:r:502:PLX:C3	2.31	0.58
45:x:184:PHE:H	45:x:256:HIS:HE1	1.52	0.58
68:AL:262:VAL:HG21	39:Bp:61:THR:HG21	1.85	0.58
60:AP:197:ASP:O	60:AP:257:ASN:ND2	2.37	0.58
65:AU:296:MET:HE2	76:AU:401:PEE:C32	2.34	0.58
66:AV:137:GLN:HE21	66:AV:141:TRP:CD1	2.22	0.58
2:BB:198:GLU:OE1	13:BN:88:ARG:HB2	2.04	0.58
3:BC:115:ARG:NH2	33:Bj:37:TYR:CD2	2.72	0.58
9:BJ:64:PHE:HD1	9:BJ:210:GLU:HB3	1.69	0.58
12:BM:126:LEU:HD12	18:BT:98:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Bx:404:THR:O	45:Bx:480:ARG:NH1	2.37	0.58
46:By:145:PRO:CG	46:By:148:MET:HE2	2.33	0.58
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.57
14:O:160:VAL:HA	14:O:171:LEU:HD23	1.86	0.57
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.57
19:U:67:PRO:HB3	19:U:74:GLN:HB2	1.86	0.57
31:h:44:ALA:HA	31:h:47:ILE:HD12	1.85	0.57
55:7:43:SER:OG	55:7:45:VAL:HG12	2.04	0.57
66:AJ:206:ASN:OD1	66:AJ:207:ASN:N	2.37	0.57
60:AP:104:ARG:NH2	68:AY:293:GLY:O	2.37	0.57
67:AW:217:ARG:HE	67:AW:245:GLY:HA3	1.69	0.57
2:BB:103:ARG:HH12	18:BT:68:ALA:HB2	1.69	0.57
9:BJ:204:SER:O	9:BJ:240:VAL:HG23	2.04	0.57
14:BO:48:ASN:HD22	14:BO:94:PRO:HA	1.68	0.57
20:BV:62:THR:HG22	20:BV:104:ARG:HE	1.69	0.57
26:Bc:93:ASP:OD2	26:Bc:101:TRP:N	2.36	0.57
32:Bi:237:LEU:HD13	32:Bi:240:LEU:HD12	1.86	0.57
35:Bl:37:LYS:CE	35:Bl:98:TRP:NE1	2.65	0.57
35:Bl:96:VAL:O	35:Bl:100:ILE:HG13	2.04	0.57
71:Br:502:PLX:H72	71:Br:502:PLX:C3	2.31	0.57
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.68	0.57
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	0.57
20:V:62:THR:HG22	20:V:104:ARG:HE	1.69	0.57
26:c:156:VAL:O	43:v:98:ARG:HG2	2.05	0.57
32:i:250:SER:O	32:i:259:GLY:HA3	2.04	0.57
45:x:404:THR:O	45:x:480:ARG:NH1	2.37	0.57
58:AA:78:TYR:CD1	62:AE:65:GLU:N	2.72	0.57
68:AL:134:LYS:NZ	68:AL:407:THR:OG1	2.38	0.57
68:AY:296:TRP:CD1	68:AY:419:THR:CB	2.67	0.57
2:BB:36:TYR:HB3	8:BI:104:TRP:HE3	1.68	0.57
3:BC:89:CYS:HB2	3:BC:123:ALA:HB1	1.85	0.57
12:BM:222:ILE:O	12:BM:225:ILE:HG22	2.04	0.57
21:BW:81:ARG:HH22	42:Bu:64:ASN:ND2	2.00	0.57
25:Bb:105:PHE:HE2	43:Bv:68:LYS:N	2.01	0.57
26:Bc:127:HIS:O	26:Bc:131:MET:HG2	2.04	0.57
26:Bc:156:VAL:O	43:Bv:98:ARG:HG2	2.04	0.57
44:Bw:332:ARG:O	44:Bw:338:LYS:CB	2.52	0.57
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.86	0.57
24:a:67:PHE:HD1	40:r:431:THR:HG23	1.68	0.57
25:b:88:TYR:CD1	25:b:92:GLU:OE2	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:88:TYR:CG	71:b:201:PLX:H1C1	2.38	0.57
71:g:203:PLX:H1A2	71:g:203:PLX:H72	1.87	0.57
31:h:94:PRO:HG2	31:h:95:PRO:HD3	1.85	0.57
32:i:277:ILE:O	32:i:280:THR:OG1	2.21	0.57
44:w:132:GLN:HG2	44:w:170:LEU:HD12	1.85	0.57
44:w:332:ARG:O	44:w:338:LYS:CB	2.52	0.57
63:AF:29:LYS:HD2	63:AF:75:ILE:CD1	2.17	0.57
13:BN:29:ARG:NH2	13:BN:65:THR:O	2.23	0.57
6:BX:99:SER:OG	6:BX:102:SER:OG	2.11	0.57
26:Bc:153:TYR:HB3	35:Bl:403:TYR:HD1	1.69	0.57
32:Bi:120:GLN:O	32:Bi:176:ARG:NH2	2.38	0.57
41:Bs:85:LEU:HD13	41:Bs:233:MET:HE1	1.85	0.57
47:Bz:203:PHE:O	47:Bz:207:HIS:HD2	1.88	0.57
55:B7:43:SER:OG	55:B7:45:VAL:HG12	2.04	0.57
1:A:123:GLY:N	14:O:180:CYS:SG	2.72	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
1:A:161:GLU:O	14:O:192:TYR:OH	2.18	0.57
1:A:307:VAL:HG11	1:A:314:LEU:HD21	1.86	0.57
2:B:208:LEU:HD22	8:I:39:PRO:HD2	1.85	0.57
3:C:67:LEU:HD22	3:C:207:LEU:CD2	2.34	0.57
9:J:204:SER:O	9:J:240:VAL:HG23	2.04	0.57
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	0.57
14:O:138:THR:HA	14:O:141:MET:HB3	1.85	0.57
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	1.86	0.57
21:W:47:HIS:CE1	41:s:307:MET:HE1	2.40	0.57
22:Y:39:HIS:ND1	22:Y:40:ILE:HG13	2.20	0.57
30:g:1:MET:SD	32:i:345:MET:HE1	2.44	0.57
71:g:201:PLX:H261	32:i:346:ILE:HG23	1.87	0.57
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.33	0.57
33:j:57:LEU:O	33:j:61:THR:HG23	2.04	0.57
37:n:56:THR:HG1	37:n:57:TRP:CD1	2.22	0.57
59:AB:27:ARG:NH1	67:AK:171:THR:HG22	2.19	0.57
58:AN:19:LEU:HD23	68:AY:273:SER:HB3	1.86	0.57
9:BJ:283:VAL:HG12	9:BJ:369:VAL:HG21	1.86	0.57
12:BM:210:ILE:HG23	12:BM:212:LYS:H	1.69	0.57
12:BM:226:CYS:HB2	12:BM:231:LEU:HD12	1.85	0.57
13:BN:34:LYS:HZ1	13:BN:58:ARG:HG2	1.70	0.57
25:Bb:79:VAL:HG11	27:Bd:35:VAL:HG11	1.84	0.57
27:Bd:135:ASP:HB3	27:Bd:156:ARG:NH2	2.19	0.57
71:Bg:201:PLX:H261	32:Bi:346:ILE:HG23	1.87	0.57
35:Bl:332:HIS:HE1	35:Bl:336:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Bo:17:THR:O	38:Bo:23:TYR:OH	2.21	0.57
44:Bw:149:HIS:O	44:Bw:153:THR:OG1	2.16	0.57
52:B4:75:ARG:HG2	52:B4:75:ARG:NH1	2.19	0.57
56:B8:41:ARG:HG3	57:B9:40:TYR:CE2	2.40	0.57
4:E:127:ASP:HB3	4:E:128:PRO:HD2	1.84	0.57
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.57
12:M:222:ILE:O	12:M:225:ILE:HG22	2.04	0.57
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.69	0.57
21:W:78:GLU:HB3	31:h:105:ARG:HB3	1.86	0.57
32:i:291:TYR:CZ	76:l:701:PEE:C31	2.71	0.57
33:j:72:LEU:HD21	33:j:94:LEU:HD22	1.86	0.57
41:s:169:GLN:NE2	41:s:174:LEU:H	2.02	0.57
58:AA:29:HIS:HD2	58:AA:33:LYS:HB2	1.69	0.57
1:BA:201:ALA:HB1	14:BO:121:MET:HB2	1.86	0.57
1:BA:319:PRO:O	1:BA:324:THR:OG1	2.23	0.57
12:BM:308:ARG:HA	12:BM:314:LEU:HA	1.86	0.57
16:BQ:251:PHE:HA	16:BQ:254:ARG:HE	1.69	0.57
16:BQ:306:GLN:O	16:BQ:308:TYR:N	2.38	0.57
21:BW:47:HIS:CE1	41:Bs:307:MET:HE1	2.40	0.57
21:BW:78:GLU:HB3	31:Bh:105:ARG:HB3	1.86	0.57
24:Ba:53:ARG:O	24:Ba:54:LEU:HD23	2.04	0.57
32:Bi:250:SER:O	32:Bi:259:GLY:HA3	2.04	0.57
34:Bk:2:PRO:HG2	36:Bm:115:VAL:HG23	1.86	0.57
34:Bk:37:MET:HE1	34:Bk:63:MET:HB3	1.86	0.57
16:Q:306:GLN:O	16:Q:308:TYR:N	2.38	0.57
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.45	0.57
76:W:201:PEE:H1	41:s:98:LEU:CD2	2.34	0.57
27:d:135:ASP:HB3	27:d:156:ARG:NH2	2.19	0.57
35:l:286:LEU:HD12	35:l:411:ILE:HG23	1.86	0.57
35:l:556:THR:OG1	35:l:557:TRP:N	2.37	0.57
40:r:178:LEU:O	40:r:182:THR:OG1	2.16	0.57
63:AF:97:GLU:OE2	67:AW:147:ARG:NH1	2.38	0.57
66:AJ:163:TRP:CD2	75:AJ:405:CDL:H331	2.39	0.57
66:AV:333:LEU:CD2	76:AV:403:PEE:H66	2.35	0.57
68:AY:145:GLU:CB	68:AY:249:HIS:NE2	2.68	0.57
68:AY:280:ASP:O	68:AY:362:ARG:NH2	2.37	0.57
1:BA:123:GLY:N	14:BO:180:CYS:SG	2.71	0.57
2:BB:37:LYS:O	16:BQ:320:VAL:N	2.37	0.57
2:BB:97:GLY:H	2:BB:167:GLU:HG3	1.70	0.57
6:BG:134:ASP:O	6:BG:138:LEU:N	2.38	0.57
8:BI:46:SER:OG	12:BM:150:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:141:PHE:CZ	9:BJ:180:TYR:CD1	2.92	0.57
16:BQ:94:VAL:HG11	16:BQ:458:PHE:HB3	1.87	0.57
32:Bi:258:THR:HG22	32:Bi:336:LEU:HB3	1.87	0.57
39:Bp:56:ASP:OD1	39:Bp:57:MET:N	2.38	0.57
40:Br:112:ALA:O	40:Br:113:THR:OG1	2.14	0.57
42:Bu:96:LEU:HD11	42:Bu:99:HIS:CD2	2.38	0.57
46:By:193:TYR:CE1	48:B0:126:MET:HE1	2.39	0.57
1:A:235:VAL:HG22	1:A:240:THR:HG21	1.87	0.57
2:B:97:GLY:H	2:B:167:GLU:HG3	1.70	0.57
8:I:36:GLN:HE22	16:Q:239:GLY:HA2	1.69	0.57
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.57
13:N:29:ARG:NH2	13:N:65:THR:O	2.23	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
6:X:132:ASP:OD2	39:p:18:ARG:HG2	2.05	0.57
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.87	0.57
35:l:96:VAL:O	35:l:100:ILE:HG13	2.04	0.57
35:l:332:HIS:HE1	35:l:336:LYS:NZ	2.02	0.57
67:AK:378:LEU:HB3	67:AK:416:ILE:HD11	1.87	0.57
68:AY:113:VAL:HG21	68:AY:120:LEU:HD23	1.87	0.57
3:BC:147:VAL:HG23	3:BC:176:VAL:HA	1.86	0.57
8:BI:36:GLN:HE22	16:BQ:239:GLY:HA2	1.69	0.57
9:BJ:176:SER:C	9:BJ:182:ARG:HH21	2.13	0.57
9:BJ:220:MET:HB2	9:BJ:281:PHE:HZ	1.68	0.57
14:BO:138:THR:HA	14:BO:141:MET:HB3	1.85	0.57
21:BW:111:PHE:HE1	31:Bh:65:GLU:OE1	1.88	0.57
25:Bb:105:PHE:HE2	43:Bv:68:LYS:HA	1.70	0.57
42:Bu:35:GLN:O	42:Bu:37:ASP:N	2.34	0.57
44:Bw:132:GLN:HG2	44:Bw:170:LEU:HD12	1.85	0.57
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.57
1:A:382:CYS:SG	69:A:501:SF4:S4	3.03	0.57
2:B:66:ARG:NH2	21:W:26:PRO:O	2.38	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
16:Q:84:PHE:CE2	16:Q:91:ALA:HB2	2.40	0.57
20:V:40:ARG:NH2	20:V:55:LYS:HD3	2.20	0.57
21:W:111:PHE:HE1	31:h:65:GLU:OE1	1.88	0.57
42:u:38:LYS:O	42:u:42:GLU:HB2	2.03	0.57
44:w:287:ASP:OD1	44:w:288:ASN:N	2.34	0.57
67:AK:57:PRO:O	67:AK:127:ARG:HG3	2.04	0.57
65:AU:98:HIS:NE2	65:AU:208:GLU:OE2	2.38	0.57
76:AY:502:PEE:H19	76:AY:502:PEE:O4	2.04	0.57
1:BA:438:LEU:HD21	1:BA:446:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:208:LEU:HD22	8:BI:39:PRO:HD2	1.85	0.57
3:BC:67:LEU:HD22	3:BC:207:LEU:CD2	2.34	0.57
9:BJ:358:THR:O	9:BJ:362:LEU:N	2.36	0.57
12:BM:47:THR:OG1	12:BM:51:GLN:OE1	2.23	0.57
16:BQ:251:PHE:CD2	16:BQ:341:LEU:HD21	2.40	0.57
20:BV:139:PRO:O	20:BV:141:VAL:N	2.38	0.57
26:Bc:169:GLU:HG2	26:Bc:169:GLU:O	2.02	0.57
33:Bj:57:LEU:O	33:Bj:61:THR:HG23	2.04	0.57
34:Bk:97:GLN:HG2	35:Bl:582:GLY:HA2	1.84	0.57
3:C:115:ARG:NH2	33:j:37:TYR:CD2	2.72	0.57
5:F:16:LEU:HD11	5:F:19:ILE:HB	1.87	0.57
22:Y:44:TYR:CD1	35:l:440:LEU:HB2	2.40	0.57
34:k:37:MET:HE1	34:k:63:MET:HB3	1.86	0.57
41:s:85:LEU:HD13	41:s:233:MET:HE1	1.85	0.57
45:x:95:PRO:HB2	47:z:11:VAL:HG13	1.87	0.57
56:8:41:ARG:HG3	57:9:40:TYR:CE2	2.40	0.57
59:AB:30:VAL:O	59:AB:33:THR:OG1	2.22	0.57
65:AH:242:ILE:HG12	65:AH:244:MET:H	1.70	0.57
68:AL:261:ALA:O	68:AL:263:PRO:HD3	2.04	0.57
68:AL:282:LEU:HB2	68:AL:461:PRO:HD3	1.86	0.57
68:AL:337:LEU:HB3	68:AL:368:MET:HG2	1.87	0.57
58:AN:41:ARG:HE	75:AN:102:CDL:PA1	2.28	0.57
60:AP:204:ARG:NH1	60:AP:246:SER:O	2.38	0.57
82:AV:402:HEM:HMB1	82:AV:402:HEM:HBB2	1.85	0.57
1:BA:342:LEU:HB3	1:BA:347:THR:HB	1.87	0.57
9:BJ:132:ARG:HD2	9:BJ:134:TRP:NE1	2.20	0.57
15:BP:94:ILE:N	15:BP:154:GLU:OE1	2.28	0.57
16:BQ:273:ILE:HD11	16:BQ:325:ASP:OD2	2.04	0.57
19:BU:67:PRO:HB3	19:BU:74:GLN:HB2	1.86	0.57
24:Ba:114:LYS:CB	27:Bd:57:TYR:CE2	2.76	0.57
30:Bg:1:MET:SD	32:Bi:345:MET:HE1	2.45	0.57
30:Bg:51:PRO:HG2	30:Bg:55:ALA:HB2	1.87	0.57
71:Bg:203:PLX:H251	32:Bi:324:PRO:HB2	1.85	0.57
34:Bk:8:ILE:HG21	34:Bk:43:MET:HB2	1.87	0.57
42:Bu:124:GLU:N	42:Bu:124:GLU:OE1	2.37	0.57
52:B4:71:THR:O	52:B4:75:ARG:HD3	2.05	0.57
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.57
2:B:103:ARG:HH12	18:T:68:ALA:HB2	1.69	0.57
20:V:139:PRO:O	20:V:141:VAL:N	2.38	0.57
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.57
25:b:88:TYR:O	25:b:92:GLU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:l:701:PEE:C23	40:r:155:VAL:CB	2.77	0.57
46:y:189:PRO:HD2	53:5:54:TYR:OH	2.05	0.57
60:AC:204:ARG:NH1	60:AC:248:ARG:HG3	2.19	0.57
11:BL:82:PRO:HD3	11:BL:98:LYS:HG2	1.87	0.57
12:BM:306:MET:HB3	12:BM:314:LEU:HD13	1.86	0.57
14:BO:160:VAL:HA	14:BO:171:LEU:HD23	1.86	0.57
22:BY:44:TYR:CD1	35:Bl:440:LEU:HB2	2.40	0.57
25:Bb:45:LYS:HA	25:Bb:48:ASN:HB2	1.87	0.57
25:Bb:88:TYR:CD1	25:Bb:92:GLU:OE2	2.57	0.57
35:Bl:564:LYS:O	35:Bl:567:SER:OG	2.23	0.57
3:C:89:CYS:HB2	3:C:123:ALA:HB1	1.85	0.56
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	0.56
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.56
9:J:141:PHE:CZ	9:J:180:TYR:CD1	2.93	0.56
12:M:476:LEU:HD11	12:M:480:ALA:HB3	1.87	0.56
12:M:624:ARG:NE	12:M:636:TYR:O	2.36	0.56
21:W:61:GLN:HE22	41:s:317:GLN:HA	1.69	0.56
25:b:111:LEU:O	25:b:112:GLU:HB2	2.04	0.56
34:k:2:PRO:HG2	36:m:115:VAL:HG23	1.86	0.56
35:l:508:THR:O	39:p:36:LYS:NZ	2.30	0.56
60:AC:83:ILE:HD12	68:AL:189:ALA:HB2	1.87	0.56
68:AL:337:LEU:C	68:AL:368:MET:HE2	2.29	0.56
63:AS:70:ASN:HD22	66:AV:209:LEU:HG	1.69	0.56
68:AY:96:LEU:HD23	68:AY:161:ILE:HD13	1.87	0.56
12:BM:50:LEU:N	12:BM:91:ALA:O	2.38	0.56
12:BM:591:GLU:HB3	12:BM:612:PRO:HD3	1.87	0.56
17:BS:59:ARG:O	17:BS:61:TYR:N	2.36	0.56
32:Bi:287:LEU:HD21	40:Br:158:LEU:HD11	1.87	0.56
34:Bk:7:ASN:ND2	36:Bm:9:SER:OG	2.31	0.56
39:Bp:30:TRP:CE2	39:Bp:76:HIS:HB2	2.40	0.56
41:Bs:280:PHE:O	41:Bs:281:ARG:HB3	2.05	0.56
6:G:134:ASP:O	6:G:138:LEU:N	2.38	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
12:M:221:ASN:HB3	12:M:285:TRP:CE3	2.40	0.56
16:Q:66:TRP:NE1	44:w:310:ILE:HD11	2.20	0.56
25:b:105:PHE:CE2	43:v:68:LYS:N	2.74	0.56
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.69	0.56
32:i:230:LEU:HD11	32:i:244:ILE:HG21	1.87	0.56
32:i:300:THR:OG1	32:i:301:SER:N	2.38	0.56
35:l:452:ASN:N	35:l:453:PRO:CD	2.68	0.56
76:l:702:PEE:O4	76:l:702:PEE:H7	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:40:VAL:H	43:v:61:HIS:HE1	1.53	0.56
46:y:145:PRO:HG3	46:y:148:MET:HE2	1.87	0.56
49:1:78:HIS:ND1	53:5:12:LEU:HD22	2.21	0.56
68:AY:74:TRP:CD2	68:AY:414:GLY:HA3	2.40	0.56
1:BA:227:PRO:HB3	12:BM:95:PRO:HD3	1.87	0.56
4:BE:118:PHE:HA	4:BE:121:LYS:HD3	1.86	0.56
9:BJ:49:SER:HB2	15:BP:225:GLU:HB3	1.87	0.56
16:BQ:84:PHE:CE2	16:BQ:91:ALA:HB2	2.40	0.56
16:BQ:326:CYS:SG	16:BQ:453:THR:HG22	2.44	0.56
21:BW:61:GLN:HE22	41:Bs:317:GLN:HA	1.68	0.56
25:Bb:88:TYR:O	25:Bb:92:GLU:HB3	2.05	0.56
25:Bb:105:PHE:CE2	43:Bv:68:LYS:N	2.74	0.56
25:Bb:111:LEU:O	25:Bb:112:GLU:HB2	2.05	0.56
40:Br:232:ALA:O	40:Br:237:LYS:NZ	2.38	0.56
1:A:438:LEU:HD21	1:A:446:LEU:HD21	1.86	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	0.56
12:M:358:LEU:O	12:M:363:SER:N	2.35	0.56
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.56
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.56
25:b:45:LYS:HA	25:b:48:ASN:HB2	1.87	0.56
27:d:59:HIS:ND1	28:e:120:ARG:HG2	2.21	0.56
30:g:47:ILE:HD12	32:i:327:PRO:HG3	1.88	0.56
32:i:237:LEU:HD13	32:i:240:LEU:HD12	1.86	0.56
34:k:66:PHE:CE1	36:m:159:THR:HG21	2.40	0.56
35:l:332:HIS:HE1	35:l:336:LYS:HZ1	1.54	0.56
36:m:16:PHE:HA	36:m:19:PHE:CE1	2.40	0.56
41:s:117:LEU:HD12	41:s:136:VAL:HG21	1.88	0.56
47:z:203:PHE:O	47:z:207:HIS:HD2	1.88	0.56
58:AA:19:LEU:HD11	60:AC:88:PHE:HB3	1.87	0.56
68:AL:470:ARG:HH22	75:AL:502:CDL:PA1	2.28	0.56
1:BA:119:GLU:HB3	1:BA:162:PHE:HE2	1.70	0.56
1:BA:159:ARG:NH1	14:BO:177:LEU:O	2.33	0.56
2:BB:66:ARG:NH2	21:BW:26:PRO:O	2.38	0.56
6:BG:97:LYS:HD3	6:BG:108:LEU:HG	1.86	0.56
9:BJ:117:ARG:HG2	9:BJ:155:LEU:HD22	1.86	0.56
12:BM:391:ILE:O	12:BM:417:ARG:NH2	2.38	0.56
21:BW:122:GLY:HA3	36:Bm:124:TRP:CE3	2.41	0.56
6:BX:132:ASP:OD2	39:Bp:18:ARG:HG2	2.05	0.56
30:Bg:47:ILE:HD12	32:Bi:327:PRO:HG3	1.88	0.56
33:Bj:72:LEU:HD21	33:Bj:94:LEU:HD22	1.86	0.56
35:Bl:310:LEU:HA	35:Bl:313:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:367:PRO:O	35:Bl:370:SER:OG	2.17	0.56
35:Bl:452:ASN:HB2	35:Bl:453:PRO:HD3	1.87	0.56
36:Bm:16:PHE:HD1	36:Bm:19:PHE:HE1	1.54	0.56
44:Bw:115:GLU:OE2	44:Bw:225:HIS:ND1	2.39	0.56
45:Bx:95:PRO:HB2	47:Bz:11:VAL:HG13	1.87	0.56
45:Bx:184:PHE:H	45:Bx:256:HIS:HE1	1.52	0.56
46:By:189:PRO:HD2	53:B5:54:TYR:OH	2.05	0.56
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.56
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	0.56
5:F:68:ARG:HD2	5:F:72:GLY:HA2	1.87	0.56
12:M:391:ILE:O	12:M:417:ARG:NH2	2.38	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
14:O:148:ILE:HG23	14:O:201:ILE:HD11	1.87	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
27:d:60:ARG:HG2	27:d:60:ARG:NH1	2.12	0.56
35:l:310:LEU:HA	35:l:313:MET:HE3	1.86	0.56
39:p:56:ASP:OD1	39:p:57:MET:N	2.38	0.56
45:x:69:MET:HE2	45:x:70:VAL:CG2	2.36	0.56
81:AH:402:HEC:HBC3	81:AH:402:HEC:HHD	1.87	0.56
1:BA:118:ASP:OD1	1:BA:120:GLY:N	2.35	0.56
8:BI:41:LEU:C	21:BW:8:GLN:HE22	2.13	0.56
22:BY:85:PRO:CG	43:Bv:99:MET:HE2	2.36	0.56
71:Bg:203:PLX:H1A2	71:Bg:203:PLX:H72	1.86	0.56
31:Bh:70:GLN:HG2	36:Bm:115:VAL:CG1	2.36	0.56
34:Bk:57:ASN:O	34:Bk:60:PRO:HD2	2.06	0.56
35:Bl:286:LEU:HD12	35:Bl:411:ILE:HG23	1.86	0.56
47:Bz:42:LEU:HD13	54:B6:45:TYR:CD2	2.41	0.56
12:M:402:LEU:HA	12:M:475:VAL:HB	1.88	0.56
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.70	0.56
31:h:48:GLY:O	31:h:50:THR:N	2.37	0.56
34:k:57:ASN:O	34:k:60:PRO:HD2	2.06	0.56
41:s:280:PHE:O	41:s:281:ARG:HB3	2.05	0.56
46:y:193:TYR:CE1	48:0:126:MET:HE1	2.39	0.56
51:3:5:LYS:HD2	51:3:6:GLY:N	2.21	0.56
63:AF:67:LEU:O	63:AF:71:LEU:HD23	2.05	0.56
66:AJ:24:PRO:HD2	66:AJ:27:ILE:HD11	1.87	0.56
66:AJ:100:ARG:HH22	82:AJ:402:HEM:HBD1	1.71	0.56
67:AK:399:GLN:NE2	67:AK:407:MET:HB3	2.20	0.56
68:AY:230:VAL:CG2	68:AY:418:LEU:HD11	2.36	0.56
8:BI:39:PRO:HB2	8:BI:41:LEU:HD12	1.87	0.56
9:BJ:84:TYR:O	9:BJ:107:GLU:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:217:GLU:HB2	12:BM:408:ARG:HH21	1.69	0.56
16:BQ:66:TRP:NE1	44:Bw:310:ILE:HD11	2.20	0.56
76:BW:201:PEE:C44	41:Bs:77:LEU:CD2	2.67	0.56
76:BW:201:PEE:H4	76:BW:201:PEE:P	2.26	0.56
35:Bl:35:TYR:CZ	35:Bl:39:ILE:HD11	2.40	0.56
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.56
62:AE:34:ARG:HD3	62:AE:78:ARG:CZ	2.35	0.56
66:AJ:316:MET:HA	66:AJ:322:GLN:NE2	2.21	0.56
67:AK:235:GLU:HA	67:AK:238:LEU:HD13	1.88	0.56
58:AN:19:LEU:HD11	60:AP:88:PHE:HB3	1.88	0.56
60:AP:123:VAL:HG13	61:AQ:29:VAL:HG22	1.88	0.56
60:AP:131:ASN:O	60:AP:135:GLN:HG2	2.05	0.56
1:BA:235:VAL:HG22	1:BA:240:THR:HG21	1.87	0.56
2:BB:87:GLU:HG2	13:BN:61:TRP:HB3	1.87	0.56
9:BJ:73:LEU:O	9:BJ:78:SER:OG	2.21	0.56
12:BM:193:ASP:OD2	14:BO:111:ARG:NH2	2.38	0.56
13:BN:57:GLY:H	13:BN:59:HIS:CE1	2.24	0.56
16:BQ:232:VAL:HB	16:BQ:356:ILE:HG22	1.88	0.56
24:Ba:98:LEU:CA	27:Bd:57:TYR:CE1	2.89	0.56
32:Bi:106:LEU:HD21	32:Bi:138:PRO:HB2	1.87	0.56
42:Bu:44:MET:HE3	42:Bu:48:TRP:CZ3	2.41	0.56
51:B3:5:LYS:HD2	51:B3:6:GLY:N	2.21	0.56
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.56
5:F:41:TYR:OH	12:M:380:ASP:OD2	2.20	0.56
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.56
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	0.56
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	0.56
12:M:308:ARG:HA	12:M:314:LEU:HA	1.86	0.56
32:i:287:LEU:HD21	40:r:158:LEU:HD11	1.87	0.56
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.40	0.56
59:AO:20:ARG:HD2	59:AO:51:SER:HB3	1.88	0.56
67:AW:272:VAL:HG11	67:AW:335:LEU:HB3	1.87	0.56
68:AY:80:ARG:NH2	68:AY:265:LEU:CD2	2.24	0.56
2:BB:151:ILE:HG21	3:BC:159:TYR:CD2	2.41	0.56
12:BM:402:LEU:HA	12:BM:475:VAL:HB	1.88	0.56
33:Bj:114:ALA:HB1	41:Bs:286:MET:HB2	1.87	0.56
34:Bk:1:MET:CB	34:Bk:4:ILE:HD13	2.36	0.56
36:Bm:81:ALA:HB3	36:Bm:84:SER:HB3	1.87	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.56
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:452:ASN:HB2	35:l:453:PRO:HD3	1.87	0.56
40:r:317:ILE:HD12	40:r:454:ILE:HG23	1.88	0.56
60:AC:153:GLU:HB3	60:AC:273:VAL:HB	1.88	0.56
81:AU:402:HEC:HBB3	81:AU:402:HEC:HHC	1.88	0.56
66:AV:138:MET:HE1	66:AV:268:ILE:HA	1.87	0.56
68:AY:160:GLN:NE2	68:AY:164:GLU:OE2	2.39	0.56
1:BA:222:LYS:HE2	1:BA:379:CYS:HB2	1.88	0.56
7:BH:16:VAL:HA	7:BH:78:GLU:OE2	2.06	0.56
12:BM:329:MET:HG3	12:BM:565:PHE:CE2	2.41	0.56
12:BM:476:LEU:HD11	12:BM:480:ALA:HB3	1.87	0.56
22:BY:39:HIS:ND1	22:BY:40:ILE:HG13	2.20	0.56
27:Bd:110:ARG:HH11	27:Bd:110:ARG:CG	2.14	0.56
35:Bl:452:ASN:N	35:Bl:453:PRO:CD	2.68	0.56
49:B1:78:HIS:ND1	53:B5:12:LEU:HD22	2.20	0.56
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.56
8:I:41:LEU:C	21:W:8:GLN:HE22	2.13	0.56
22:Y:73:PHE:HA	35:l:385:PHE:HE2	1.70	0.56
24:a:114:LYS:CB	27:d:57:TYR:CE2	2.77	0.56
27:d:108:GLN:HG2	35:l:199:GLN:CB	2.31	0.56
32:i:120:GLN:O	32:i:176:ARG:NH2	2.38	0.56
34:k:3:LEU:CD2	36:m:117:ASN:ND2	2.60	0.56
35:l:272:LEU:O	35:l:275:THR:OG1	2.18	0.56
35:l:407:TRP:NE1	35:l:411:ILE:HD11	2.21	0.56
41:s:186:PHE:O	41:s:189:THR:OG1	2.16	0.56
1:BA:48:ARG:HH12	14:BO:231:LEU:HD11	1.69	0.56
1:BA:159:ARG:HH22	14:BO:177:LEU:HA	1.70	0.56
1:BA:382:CYS:SG	69:BA:501:SF4:S4	3.03	0.56
2:BB:39:VAL:HG22	16:BQ:321:GLY:HA2	1.86	0.56
12:BM:221:ASN:HB3	12:BM:285:TRP:CE3	2.40	0.56
15:BP:85:GLU:HG3	15:BP:142:ARG:HB2	1.88	0.56
15:BP:213:ASP:OD1	15:BP:214:ASP:N	2.38	0.56
20:BV:40:ARG:NH2	20:BV:55:LYS:HD3	2.20	0.56
27:Bd:59:HIS:ND1	28:Be:120:ARG:HG2	2.21	0.56
38:Bo:8:PRO:HB3	38:Bo:14:LEU:HG	1.88	0.56
40:Br:317:ILE:HD12	40:Br:454:ILE:HG23	1.88	0.56
41:Bs:117:LEU:HD12	41:Bs:136:VAL:HG21	1.88	0.56
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.38	0.56
17:S:50:ARG:HA	31:h:105:ARG:NE	2.21	0.56
21:W:122:GLY:HA3	36:m:124:TRP:CE3	2.41	0.56
22:Y:84:PHE:CE2	35:l:483:PRO:CG	2.69	0.56
31:h:70:GLN:HG2	36:m:115:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:80:GLN:NE2	41:s:316:PRO:O	2.39	0.56
38:o:28:GLU:HA	38:o:31:ARG:HD3	1.88	0.56
40:r:1:MET:HG3	40:r:2:LEU:H	1.71	0.56
40:r:232:ALA:O	40:r:237:LYS:NZ	2.38	0.56
46:y:132:GLU:HB3	46:y:137:GLU:HG3	1.87	0.56
67:AK:351:ILE:HD11	67:AK:448:PRO:HD2	1.86	0.56
67:AK:438:MET:HB3	67:AK:450:VAL:HG13	1.86	0.56
68:AL:259:GLU:HB3	38:Bo:30:ARG:NH2	2.20	0.56
67:AW:259:ARG:NH2	67:AW:447:THR:OG1	2.39	0.56
5:BF:16:LEU:HB3	5:BF:51:LEU:HD13	1.88	0.56
9:BJ:168:SER:C	9:BJ:184:LYS:HE2	2.31	0.56
14:BO:148:ILE:HG23	14:BO:201:ILE:HD11	1.87	0.56
20:BV:3:PRO:HA	20:BV:6:PHE:HB3	1.88	0.56
21:BW:31:SER:OG	21:BW:35:MET:HE2	2.06	0.56
25:Bb:110:ILE:HG13	25:Bb:111:LEU:HD21	1.87	0.56
31:Bh:2:PRO:O	31:Bh:4:LEU:N	2.39	0.56
33:Bj:80:GLN:NE2	41:Bs:316:PRO:O	2.39	0.56
35:Bl:73:THR:OG1	35:Bl:74:THR:N	2.39	0.56
35:Bl:407:TRP:NE1	35:Bl:411:ILE:HD11	2.21	0.56
36:Bm:16:PHE:HA	36:Bm:19:PHE:CE1	2.40	0.56
41:Bs:169:GLN:NE2	41:Bs:174:LEU:H	2.02	0.56
1:A:381:GLN:CG	69:A:501:SF4:S2	2.94	0.55
7:H:16:VAL:HA	7:H:78:GLU:OE2	2.06	0.55
9:J:132:ARG:HD2	9:J:134:TRP:NE1	2.20	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
36:m:32:LEU:HD13	36:m:64:MET:HE1	1.88	0.55
37:n:30:LYS:NZ	75:n:101:CDL:HA31	2.22	0.55
60:AC:219:HIS:ND1	74:AC:301:FES:S1	2.74	0.55
63:AF:49:ARG:HA	63:AF:49:ARG:HE	1.71	0.55
5:BF:17:ARG:HB3	5:BF:68:ARG:HH21	1.71	0.55
9:BJ:94:LEU:HG	9:BJ:97:MET:SD	2.46	0.55
9:BJ:164:PHE:HE2	9:BJ:191:VAL:HG13	1.72	0.55
9:BJ:217:PHE:HB3	9:BJ:280:ILE:HD13	1.88	0.55
6:BX:84:LEU:HD11	6:BX:100:VAL:HG22	1.87	0.55
25:Bb:84:TYR:HE1	27:Bd:43:ARG:HD3	1.71	0.55
32:Bi:230:LEU:HD11	32:Bi:244:ILE:HG21	1.87	0.55
37:Bn:7:ILE:O	37:Bn:11:HIS:N	2.37	0.55
45:Bx:69:MET:HE2	45:Bx:70:VAL:CG2	2.36	0.55
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.55
1:A:418:GLN:O	1:A:422:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:16:LEU:HB3	5:F:51:LEU:HD13	1.88	0.55
12:M:50:LEU:N	12:M:91:ALA:O	2.38	0.55
12:M:128:CYS:N	12:M:129:PRO:HD2	2.21	0.55
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.41	0.55
15:P:235:LEU:HD22	16:Q:387:GLU:HG2	1.87	0.55
25:b:83:HIS:CD2	35:l:6:THR:HG21	2.42	0.55
31:h:74:ARG:HA	36:m:116:VAL:HG21	1.89	0.55
32:i:258:THR:HG22	32:i:336:LEU:HB3	1.87	0.55
32:i:288:LEU:HD22	76:l:701:PEE:H58	1.69	0.55
39:p:30:TRP:CE2	39:p:76:HIS:HB2	2.40	0.55
39:p:102:TRP:HZ2	40:r:422:HIS:HA	1.70	0.55
44:w:115:GLU:OE2	44:w:225:HIS:ND1	2.39	0.55
64:AG:17:TRP:NE1	68:AL:382:SER:OG	2.39	0.55
60:AP:100:THR:HG23	68:AY:266:THR:CG2	2.36	0.55
66:AV:111:GLU:HG2	66:AV:199:PHE:CD1	2.41	0.55
68:AY:98:PHE:CE2	68:AY:120:LEU:HD12	2.36	0.55
68:AY:152:GLN:NE2	68:AY:249:HIS:O	2.39	0.55
1:BA:418:GLN:O	1:BA:422:HIS:ND1	2.40	0.55
9:BJ:293:LEU:HD12	9:BJ:294:PRO:HD2	1.86	0.55
11:BL:61:ILE:HG21	15:BP:149:GLU:OE1	2.07	0.55
12:BM:177:ILE:HG13	12:BM:177:ILE:O	2.04	0.55
13:BN:84:PRO:HD3	13:BN:113:HIS:CD2	2.41	0.55
15:BP:235:LEU:HD22	16:BQ:387:GLU:HG2	1.87	0.55
16:BQ:390:GLN:OE1	16:BQ:417:SER:N	2.39	0.55
27:Bd:134:GLN:O	27:Bd:138:GLN:HB2	2.06	0.55
37:Bn:30:LYS:NZ	75:Bn:101:CDL:HA31	2.22	0.55
39:Bp:86:PRO:HA	39:Bp:91:TYR:CD1	2.41	0.55
46:By:132:GLU:HB3	46:By:137:GLU:HG3	1.87	0.55
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.55
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	0.55
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	0.55
9:J:212:ARG:HG2	9:J:212:ARG:NH1	2.15	0.55
11:L:82:PRO:HD3	11:L:98:LYS:HG2	1.87	0.55
12:M:408:ARG:HB3	12:M:415:ASN:ND2	2.21	0.55
15:P:85:GLU:HG3	15:P:142:ARG:HB2	1.88	0.55
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.55
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.39	0.55
27:d:134:GLN:O	27:d:138:GLN:HB2	2.06	0.55
30:g:46:LEU:HD11	32:i:239:TRP:HB3	1.88	0.55
31:h:2:PRO:O	31:h:4:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:AB:29:LEU:O	59:AB:31:GLN:N	2.38	0.55
65:AH:156:ASP:OD1	65:AH:157:GLY:N	2.37	0.55
66:AJ:51:LEU:HD13	82:AJ:401:HEM:HBD1	1.88	0.55
59:AO:27:ARG:NH1	67:AW:171:THR:HG22	2.21	0.55
66:AV:333:LEU:HD22	76:AV:403:PEE:H66	1.87	0.55
68:AY:145:GLU:HB3	68:AY:249:HIS:CE1	2.41	0.55
3:BC:172:ARG:NH1	15:BP:209:GLU:OE2	2.36	0.55
9:BJ:181:LEU:HD13	9:BJ:324:ILE:HD13	1.88	0.55
17:BS:50:ARG:HA	31:Bh:105:ARG:NE	2.21	0.55
20:BV:40:ARG:HD3	20:BV:59:TYR:CE2	2.41	0.55
29:Bf:72:ARG:HH11	30:Bg:19:SER:HB3	1.70	0.55
76:Bl:702:PEE:O4	76:Bl:702:PEE:H7	2.05	0.55
36:Bm:138:ASP:HB2	36:Bm:139:PRO:HD3	1.89	0.55
46:By:145:PRO:HG3	46:By:148:MET:HE2	1.87	0.55
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.55
13:N:57:GLY:H	13:N:59:HIS:CE1	2.24	0.55
76:V:202:PEE:H60	76:V:202:PEE:C24	2.37	0.55
21:W:31:SER:OG	21:W:35:MET:HE2	2.06	0.55
25:b:75:VAL:O	25:b:79:VAL:HG23	2.05	0.55
26:c:184:TYR:O	43:v:35:LYS:O	2.25	0.55
32:i:124:LEU:HD23	32:i:176:ARG:HD3	1.88	0.55
35:l:238:GLU:N	35:l:238:GLU:OE1	2.40	0.55
36:m:138:ASP:HB2	36:m:139:PRO:HD3	1.89	0.55
36:m:156:THR:O	36:m:159:THR:OG1	2.22	0.55
41:s:156:MET:HE1	41:s:177:PRO:HB2	1.88	0.55
47:z:42:LEU:HD13	54:6:45:TYR:CD2	2.41	0.55
75:AJ:405:CDL:OB7	75:AJ:405:CDL:HB62	2.05	0.55
61:AQ:48:ASN:HD22	65:AU:104:SER:HB3	1.72	0.55
5:BF:16:LEU:HD11	5:BF:19:ILE:HB	1.87	0.55
15:BP:51:ASN:HB2	15:BP:82:ASN:HD21	1.72	0.55
23:BZ:22:TRP:CE3	23:BZ:51:TRP:HA	2.40	0.55
26:Bc:56:ASN:ND2	38:Bo:43:LEU:HD11	2.22	0.55
32:Bi:167:TRP:HH2	35:Bl:570:GLN:HG3	1.70	0.55
33:Bj:92:LEU:O	33:Bj:96:ILE:HG12	2.06	0.55
35:Bl:238:GLU:OE1	35:Bl:238:GLU:N	2.40	0.55
4:E:36:TYR:HD1	4:E:67:PHE:CE2	2.25	0.55
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.55
20:V:40:ARG:HD3	20:V:59:TYR:CE2	2.41	0.55
25:b:84:TYR:HE1	27:d:43:ARG:HD3	1.71	0.55
33:j:114:ALA:HB1	41:s:286:MET:HB2	1.87	0.55
36:m:16:PHE:CD1	36:m:19:PHE:HE1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:23:PRO:O	36:m:24:SER:OG	2.23	0.55
60:AP:204:ARG:NH1	60:AP:248:ARG:HG3	2.21	0.55
67:AW:185:ALA:HB2	67:AW:249:ALA:HB1	1.89	0.55
67:AW:185:ALA:HB3	67:AW:251:ALA:HB2	1.88	0.55
1:BA:33:GLY:H	1:BA:294:VAL:HG12	1.72	0.55
2:BB:145:ILE:HG22	2:BB:188:LEU:HD11	1.89	0.55
8:BI:96:THR:OG1	8:BI:98:ALA:O	2.19	0.55
9:BJ:141:PHE:CE1	9:BJ:180:TYR:HD1	2.25	0.55
9:BJ:167:VAL:HA	9:BJ:201:VAL:HB	1.88	0.55
12:BM:128:CYS:N	12:BM:129:PRO:HD2	2.21	0.55
12:BM:510:TRP:CD1	12:BM:512:VAL:HG22	2.42	0.55
16:BQ:123:LEU:HB3	16:BQ:135:TYR:OH	2.05	0.55
22:BY:86:TYR:OH	43:Bv:100:LYS:HG3	2.03	0.55
25:Bb:105:PHE:HE2	43:Bv:68:LYS:CA	2.19	0.55
27:Bd:109:GLN:HG2	35:Bl:62:ILE:HD13	1.88	0.55
32:Bi:277:ILE:O	32:Bi:280:THR:OG1	2.21	0.55
41:Bs:156:MET:HE1	41:Bs:177:PRO:HB2	1.88	0.55
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.55
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.55
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.55
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.55
12:M:241:ARG:HG2	12:M:243:TRP:CZ2	2.42	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	0.55
76:V:202:PEE:H57	76:V:202:PEE:H40	1.87	0.55
23:Z:22:TRP:CE3	23:Z:51:TRP:HA	2.41	0.55
27:d:109:GLN:HG2	35:l:62:ILE:HD13	1.88	0.55
29:f:72:ARG:HH11	30:g:19:SER:HB3	1.70	0.55
32:i:232:ARG:NH2	44:w:306:ASN:OD1	2.29	0.55
35:l:35:TYR:CZ	35:l:39:ILE:HD11	2.40	0.55
39:p:86:PRO:HA	39:p:91:TYR:CD1	2.41	0.55
51:3:5:LYS:HD2	51:3:5:LYS:C	2.32	0.55
52:4:71:THR:O	52:4:75:ARG:HD3	2.05	0.55
53:5:63:MET:HB3	53:5:68:ILE:HD11	1.89	0.55
58:AA:78:TYR:O	58:AA:81:ASP:HB2	2.07	0.55
63:AF:41:ASP:N	63:AF:41:ASP:OD1	2.36	0.55
68:AY:76:ASP:HB3	68:AY:228:ARG:HG3	1.89	0.55
5:BF:80:ASN:OD1	5:BF:81:ASN:ND2	2.39	0.55
9:BJ:134:TRP:CZ3	9:BJ:136:THR:HA	2.41	0.55
12:BM:620:TRP:HE1	12:BM:639:LEU:HD13	1.71	0.55
24:Ba:59:PRO:HD3	39:Bp:99:VAL:HG21	1.89	0.55
32:Bi:288:LEU:HD21	76:Bl:701:PEE:H58	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Bm:16:PHE:CD1	36:Bm:19:PHE:HE1	2.25	0.55
12:M:124:HIS:ND1	12:M:125:PRO:HD2	2.22	0.55
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.42	0.55
12:M:598:ASN:HB3	12:M:602:ARG:HB3	1.89	0.55
20:V:3:PRO:HA	20:V:6:PHE:HB3	1.88	0.55
25:b:105:PHE:HE2	43:v:68:LYS:CA	2.19	0.55
34:k:1:MET:CB	34:k:4:ILE:HD13	2.36	0.55
35:l:37:LYS:HE2	35:l:98:TRP:HD1	0.69	0.55
35:l:102:GLU:OE1	35:l:453:PRO:HG3	2.07	0.55
1:BA:217:GLU:HB3	11:BL:171:ARG:HH22	1.72	0.55
1:BA:381:GLN:CG	69:BA:501:SF4:S2	2.94	0.55
4:BE:25:MET:HE3	4:BE:29:LYS:HE2	1.88	0.55
9:BJ:212:ARG:HG2	9:BJ:212:ARG:NH1	2.15	0.55
16:BQ:316:PHE:HB2	16:BQ:339:GLN:HE21	1.70	0.55
19:BU:67:PRO:HA	19:BU:74:GLN:OE1	2.07	0.55
31:Bh:74:ARG:HA	36:Bm:116:VAL:HG21	1.88	0.55
40:Br:91:ARG:HG2	40:Br:136:TRP:HH2	1.72	0.55
48:B0:108:PRO:HG2	48:B0:111:PHE:CE2	2.42	0.55
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.55
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.55
22:Y:74:TRP:HE3	22:Y:75:HIS:CA	2.19	0.55
24:a:98:LEU:CA	27:d:57:TYR:CE1	2.89	0.55
45:x:172:LYS:HB2	45:x:172:LYS:HZ2	1.71	0.55
47:z:222:GLN:HA	47:z:222:GLN:HE21	1.71	0.55
66:AJ:181:PHE:HA	66:AJ:184:ILE:HG22	1.88	0.55
60:AP:207:LYS:HD3	60:AP:265:PHE:HE2	1.71	0.55
66:AV:140:PHE:CD1	66:AV:140:PHE:C	2.85	0.55
5:BF:68:ARG:HD2	5:BF:72:GLY:HA2	1.87	0.55
11:BL:61:ILE:HB	11:BL:64:LEU:HB2	1.88	0.55
12:BM:481:LEU:HD11	12:BM:515:ILE:HD12	1.88	0.55
22:BY:73:PHE:HA	35:Bl:385:PHE:HE2	1.70	0.55
38:Bo:28:GLU:HA	38:Bo:31:ARG:HD3	1.88	0.55
40:Br:1:MET:HG3	40:Br:2:LEU:H	1.71	0.55
4:E:25:MET:HE3	4:E:29:LYS:HE2	1.88	0.55
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.55
15:P:55:HIS:CD2	15:P:78:VAL:HG12	2.42	0.55
19:U:67:PRO:HA	19:U:74:GLN:OE1	2.07	0.55
22:Y:74:TRP:CE3	22:Y:74:TRP:C	2.85	0.55
22:Y:85:PRO:CG	43:v:99:MET:HE2	2.36	0.55
23:Z:51:TRP:O	23:Z:53:TYR:N	2.37	0.55
25:b:105:PHE:HE2	43:v:67:LEU:C	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:11:ALA:HB1	36:m:16:PHE:HD2	1.71	0.55
44:w:138:SER:O	44:w:142:GLN:HG2	2.07	0.55
58:AN:43:ARG:HA	58:AN:46:PHE:HD2	1.72	0.55
63:AS:68:ASP:HA	63:AS:71:LEU:HD12	1.89	0.55
68:AY:161:ILE:O	68:AY:165:ARG:HG3	2.07	0.55
9:BJ:203:PRO:HG2	73:BJ:401:NDP:C5N	2.37	0.55
12:BM:68:ARG:NH2	12:BM:284:GLU:OE1	2.33	0.55
12:BM:408:ARG:HB3	12:BM:415:ASN:ND2	2.21	0.55
25:Bb:75:VAL:O	25:Bb:79:VAL:HG23	2.06	0.55
27:Bd:114:ASN:OD1	43:Bv:50:GLN:HG2	2.07	0.55
32:Bi:17:THR:OG1	32:Bi:36:ASN:ND2	2.39	0.55
40:Br:403:THR:HA	40:Br:406:TYR:CE2	2.42	0.55
42:Bu:115:LEU:HB3	42:Bu:117:TRP:CZ3	2.42	0.55
43:Bv:40:VAL:H	43:Bv:61:HIS:HE1	1.53	0.55
47:Bz:222:GLN:HE21	47:Bz:222:GLN:HA	1.72	0.55
53:B5:63:MET:HB3	53:B5:68:ILE:HD11	1.89	0.55
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.89	0.55
4:E:56:VAL:HG23	9:J:367:GLU:OE2	2.07	0.55
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.55
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.55
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	0.55
26:c:56:ASN:ND2	38:o:43:LEU:HD11	2.22	0.55
42:u:115:LEU:HB3	42:u:117:TRP:CZ3	2.42	0.55
66:AJ:119:LEU:HD11	66:AJ:192:LEU:HB3	1.89	0.55
66:AV:138:MET:HB2	66:AV:255:ASN:ND2	2.22	0.55
68:AY:152:GLN:HE22	68:AY:252:GLY:N	2.04	0.55
7:BH:111:GLN:NE2	15:BP:124:ASN:HB2	2.22	0.55
9:BJ:75:ARG:NH1	15:BP:215:GLU:OE2	2.34	0.55
25:Bb:110:ILE:HG13	25:Bb:111:LEU:CD2	2.37	0.55
27:Bd:115:TYR:C	27:Bd:115:TYR:CD1	2.85	0.55
32:Bi:217:LEU:HB3	32:Bi:326:LEU:HD12	1.89	0.55
40:Br:346:GLN:HB2	40:Br:420:THR:HG23	1.88	0.55
44:Bw:138:SER:O	44:Bw:142:GLN:HG2	2.07	0.55
2:B:37:LYS:O	16:Q:320:VAL:N	2.38	0.54
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.71	0.54
12:M:215:MET:HE1	12:M:714:VAL:HG23	1.90	0.54
25:b:110:ILE:HG13	25:b:111:LEU:HD21	1.87	0.54
30:g:51:PRO:HG2	30:g:55:ALA:HB2	1.87	0.54
33:j:24:LEU:H	33:j:25:PRO:HD2	1.72	0.54
40:r:134:THR:O	40:r:142:ARG:NE	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:127:TYR:HA	41:s:130:ILE:HD12	1.89	0.54
44:w:206:TYR:OH	44:w:238:GLU:OE2	2.25	0.54
48:0:108:PRO:HG2	48:0:111:PHE:CE2	2.42	0.54
68:AL:77:VAL:HG21	68:AL:223:HIS:HB3	1.89	0.54
76:AU:401:PEE:C19	76:AU:401:PEE:C39	2.86	0.54
4:BE:36:TYR:HD1	4:BE:67:PHE:CE2	2.25	0.54
4:BE:80:ASP:HA	4:BE:83:VAL:HG22	1.90	0.54
12:BM:380:ASP:OD1	12:BM:381:LEU:N	2.40	0.54
12:BM:389:THR:OG1	12:BM:514:ASN:ND2	2.40	0.54
12:BM:697:THR:O	12:BM:702:ARG:NH2	2.40	0.54
16:BQ:149:GLN:CD	16:BQ:171:ARG:HB3	2.32	0.54
22:BY:74:TRP:HE3	22:BY:75:HIS:CA	2.19	0.54
26:Bc:184:TYR:O	43:Bv:35:LYS:O	2.25	0.54
35:Bl:102:GLU:OE1	35:Bl:453:PRO:HG3	2.07	0.54
39:Bp:102:TRP:HZ2	40:Br:422:HIS:HA	1.70	0.54
50:B2:82:CYS:N	50:B2:86:GLY:O	2.40	0.54
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	0.54
12:M:380:ASP:OD1	12:M:381:LEU:N	2.40	0.54
23:Z:28:PRO:O	23:Z:31:THR:OG1	2.22	0.54
24:a:59:PRO:HD3	39:p:99:VAL:HG21	1.89	0.54
27:d:114:ASN:OD1	43:v:50:GLN:HG2	2.07	0.54
32:i:217:LEU:HB3	32:i:326:LEU:HD12	1.89	0.54
40:r:358:TRP:CE3	40:r:441:LEU:HD12	2.42	0.54
40:r:403:THR:HA	40:r:406:TYR:CE2	2.42	0.54
50:2:82:CYS:N	50:2:86:GLY:O	2.40	0.54
60:AP:220:LEU:HB2	74:AP:301:FES:S2	2.46	0.54
62:AR:34:ARG:CG	62:AR:78:ARG:NH1	2.61	0.54
62:AR:80:HIS:C	62:AR:80:HIS:CD2	2.86	0.54
68:AY:96:LEU:C	68:AY:96:LEU:HD12	2.32	0.54
68:AY:156:LEU:HB2	68:AY:213:ARG:HE	1.72	0.54
4:BE:66:MET:HE3	4:BE:106:PHE:HD1	1.71	0.54
12:BM:225:ILE:HD12	12:BM:285:TRP:CH2	2.39	0.54
12:BM:358:LEU:HB3	12:BM:363:SER:O	2.08	0.54
15:BP:107:GLN:HB3	15:BP:109:LYS:HE3	1.89	0.54
17:BS:54:ILE:HG13	31:Bh:105:ARG:HH11	1.72	0.54
76:BV:202:PEE:H57	76:BV:202:PEE:H40	1.87	0.54
25:Bb:87:LYS:HE3	27:Bd:43:ARG:HG2	1.89	0.54
1:A:33:GLY:H	1:A:294:VAL:HG12	1.72	0.54
2:B:71:THR:HG23	41:s:31:MET:CE	2.38	0.54
12:M:341:ILE:HD12	12:M:555:ILE:HG13	1.89	0.54
12:M:481:LEU:HD11	12:M:515:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:697:THR:O	12:M:702:ARG:NH2	2.40	0.54
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	0.54
20:V:47:GLY:O	20:V:48:THR:OG1	2.25	0.54
22:Y:81:LEU:CD1	43:v:88:ASP:HB3	2.37	0.54
24:a:98:LEU:HB3	27:d:57:TYR:HE1	0.54	0.54
32:i:167:TRP:HH2	35:l:570:GLN:HG3	1.70	0.54
36:m:81:ALA:HB3	36:m:84:SER:HB3	1.87	0.54
36:m:155:VAL:O	36:m:159:THR:HG23	2.08	0.54
38:o:17:THR:O	38:o:23:TYR:OH	2.21	0.54
40:r:73:LEU:HD12	40:r:103:GLN:HG2	1.89	0.54
59:AB:7:ARG:NH1	67:AK:287:SER:OG	2.25	0.54
67:AK:101:ARG:NH1	68:AL:325:SER:O	2.33	0.54
66:AV:326:TRP:CH2	76:AV:403:PEE:H51	2.42	0.54
6:BG:105:MET:HE2	6:BG:138:LEU:HD23	1.89	0.54
76:BV:202:PEE:H60	76:BV:202:PEE:C24	2.36	0.54
24:Ba:98:LEU:CA	27:Bd:57:TYR:CD1	2.91	0.54
25:Bb:78:PRO:O	25:Bb:82:ILE:HD12	2.08	0.54
27:Bd:108:GLN:HG2	35:Bl:199:GLN:CB	2.31	0.54
35:Bl:3:MET:O	35:Bl:7:MET:HG2	2.08	0.54
41:Bs:127:TYR:HA	41:Bs:130:ILE:HD12	1.89	0.54
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.54
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.89	0.54
4:E:75:ASP:HB3	4:E:78:VAL:HG23	1.89	0.54
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.23	0.54
13:N:94:THR:HG22	13:N:96:ASP:H	1.73	0.54
14:O:41:HIS:ND1	14:O:41:HIS:O	2.39	0.54
33:j:92:LEU:O	33:j:96:ILE:HG12	2.06	0.54
35:l:197:ASP:O	35:l:201:MET:HG3	2.08	0.54
35:l:293:LEU:HD23	35:l:422:TYR:HB3	1.90	0.54
35:l:306:THR:HA	35:l:336:LYS:HZ3	1.71	0.54
35:l:456:ARG:NH2	35:l:456:ARG:HB2	2.21	0.54
35:l:546:GLN:O	35:l:550:LEU:HB2	2.07	0.54
37:n:7:ILE:O	37:n:11:HIS:N	2.37	0.54
82:AJ:402:HEM:HMC2	82:AJ:402:HEM:HBC2	1.89	0.54
68:AL:465:LEU:HD12	68:AL:466:PRO:HD2	1.89	0.54
59:AO:45:LEU:HA	68:AY:284:PHE:HE2	1.71	0.54
1:BA:207:GLY:O	70:BA:502:FMN:C9A	2.56	0.54
11:BL:162:ALA:HA	11:BL:168:LYS:NZ	2.23	0.54
12:BM:308:ARG:HD2	12:BM:312:GLY:O	2.08	0.54
12:BM:565:PHE:HA	12:BM:581:ASP:OD2	2.08	0.54
13:BN:48:TYR:HB3	13:BN:89:TRP:CZ3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BY:74:TRP:CE3	22:BY:74:TRP:C	2.85	0.54
24:Ba:54:LEU:HD23	25:Bb:27:GLU:HA	1.90	0.54
24:Ba:90:ASN:ND2	71:Bb:201:PLX:H122	2.19	0.54
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.54
9:J:203:PRO:HG2	73:J:401:NDP:C5N	2.37	0.54
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	0.54
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.40	0.54
24:a:133:TYR:OH	27:d:81:GLU:HG2	2.08	0.54
25:b:105:PHE:HE2	43:v:68:LYS:HA	1.70	0.54
35:l:95:PHE:CD1	35:l:95:PHE:C	2.86	0.54
40:r:73:LEU:O	40:r:76:THR:OG1	2.18	0.54
46:y:111:THR:HG21	52:4:66:ILE:HD11	1.88	0.54
47:z:151:LEU:HB2	47:z:159:MET:HG3	1.89	0.54
59:AB:54:SER:HA	68:AL:402:HIS:CE1	2.43	0.54
66:AJ:229:ALA:HB1	71:AL:501:PLX:H131	1.89	0.54
75:AJ:405:CDL:C78	75:AJ:405:CDL:C74	2.86	0.54
68:AL:470:ARG:HH12	75:AL:502:CDL:HA31	1.72	0.54
75:AN:102:CDL:OB9	66:AV:29:ALA:HB3	2.08	0.54
1:BA:77:LEU:HD21	1:BA:100:SER:HA	1.90	0.54
1:BA:328:PRO:HG2	1:BA:441:HIS:CD2	2.43	0.54
4:BE:75:ASP:HB3	4:BE:78:VAL:HG23	1.89	0.54
14:BO:41:HIS:ND1	14:BO:41:HIS:O	2.40	0.54
22:BY:72:ARG:NH1	35:Bl:466:PHE:HD1	2.02	0.54
22:BY:86:TYR:HH	43:Bv:100:LYS:HG2	1.71	0.54
27:Bd:60:ARG:HH11	27:Bd:60:ARG:CG	2.12	0.54
40:Br:236:LEU:O	40:Br:239:GLY:N	2.40	0.54
41:Bs:145:THR:HG21	41:Bs:289:LEU:HD22	1.90	0.54
44:Bw:206:TYR:OH	44:Bw:238:GLU:OE2	2.25	0.54
50:B2:48:LEU:O	50:B2:50:PRO:HD3	2.08	0.54
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
6:G:105:MET:HE2	6:G:138:LEU:HD23	1.89	0.54
9:J:169:HIS:CD2	73:J:401:NDP:C5N	2.79	0.54
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.54
12:M:308:ARG:HD2	12:M:312:GLY:O	2.08	0.54
12:M:565:PHE:HA	12:M:581:ASP:OD2	2.08	0.54
15:P:94:ILE:N	15:P:154:GLU:OE1	2.28	0.54
16:Q:449:ALA:O	16:Q:453:THR:HG23	2.08	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CB	2.54	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CD2	2.54	0.54
32:i:106:LEU:HD21	32:i:138:PRO:HB2	1.87	0.54
36:m:16:PHE:HD1	36:m:19:PHE:HE1	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:5:LYS:HD2	60:AP:101:LYS:HZ3	1.71	0.54
40:r:91:ARG:HG2	40:r:136:TRP:HH2	1.72	0.54
44:w:61:THR:HG22	44:w:159:LEU:HD23	1.90	0.54
63:AF:27:PHE:CD1	63:AF:28:ASN:N	2.75	0.54
75:AL:502:CDL:H772	76:AL:503:PEE:C42	2.38	0.54
66:AV:165:TRP:O	66:AV:174:THR:OG1	2.23	0.54
1:BA:225:LEU:HG	1:BA:227:PRO:HD3	1.90	0.54
1:BA:278:ILE:HG12	1:BA:304:ALA:HB2	1.89	0.54
15:BP:55:HIS:CD2	15:BP:78:VAL:HG12	2.42	0.54
25:Bb:105:PHE:HE2	43:Bv:67:LEU:C	2.15	0.54
40:Br:414:THR:O	40:Br:415:GLN:NE2	2.41	0.54
71:Br:502:PLX:C33	71:Br:502:PLX:C37	2.85	0.54
49:B1:41:LEU:O	49:B1:41:LEU:HD12	2.08	0.54
1:A:207:GLY:O	70:A:502:FMN:C9A	2.56	0.54
5:F:17:ARG:HB3	5:F:68:ARG:HH21	1.71	0.54
9:J:176:SER:C	9:J:182:ARG:NH2	2.66	0.54
12:M:53:CYS:SG	12:M:102:ILE:HD12	2.48	0.54
15:P:107:GLN:HB3	15:P:109:LYS:HE3	1.89	0.54
16:Q:198:THR:HA	41:s:32:GLN:OE1	2.07	0.54
28:e:74:HIS:ND1	28:e:87:MET:HG3	2.23	0.54
35:l:293:LEU:HD11	35:l:418:LEU:HD22	1.90	0.54
35:l:564:LYS:O	35:l:567:SER:OG	2.23	0.54
76:AH:401:PEE:C40	76:AH:401:PEE:C18	2.85	0.54
67:AK:93:GLY:HA3	67:AK:139:ASN:HD21	1.72	0.54
1:BA:86:ARG:HA	1:BA:94:PRO:HA	1.88	0.54
2:BB:71:THR:HG23	41:Bs:31:MET:CE	2.38	0.54
2:BB:104:TYR:CE2	2:BB:110:ARG:HA	2.43	0.54
12:BM:53:CYS:SG	12:BM:102:ILE:HD12	2.48	0.54
16:BQ:291:VAL:HA	16:BQ:294:ARG:HB2	1.89	0.54
23:BZ:51:TRP:O	23:BZ:53:TYR:N	2.37	0.54
32:Bi:124:LEU:HD23	32:Bi:176:ARG:HD3	1.88	0.54
32:Bi:300:THR:OG1	32:Bi:301:SER:N	2.38	0.54
33:Bj:24:LEU:H	33:Bj:25:PRO:HD2	1.72	0.54
35:Bl:293:LEU:HD11	35:Bl:418:LEU:HD22	1.90	0.54
40:Br:73:LEU:HD12	40:Br:103:GLN:HG2	1.89	0.54
45:Bx:407:ASP:O	45:Bx:411:LYS:HG3	2.07	0.54
7:H:97:TRP:HB3	7:H:100:TRP:CH2	2.43	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.89	0.54
12:M:394:VAL:HG21	12:M:414:PHE:HE1	1.73	0.54
40:r:272:THR:HA	40:r:275:ILE:HD12	1.90	0.54
50:2:55:LYS:HA	50:2:74:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:304:TYR:HE1	75:AH:403:CDL:OA3	1.90	0.54
68:AL:66:GLN:NE2	68:AL:406:THR:OG1	2.41	0.54
68:AY:266:THR:O	68:AY:268:CYS:N	2.41	0.54
9:BJ:172:ALA:HA	9:BJ:181:LEU:CD2	2.38	0.54
9:BJ:176:SER:C	9:BJ:182:ARG:NH2	2.65	0.54
12:BM:124:HIS:ND1	12:BM:125:PRO:HD2	2.22	0.54
12:BM:241:ARG:HG2	12:BM:243:TRP:CZ2	2.42	0.54
13:BN:84:PRO:HA	13:BN:87:HIS:HB3	1.90	0.54
76:BW:201:PEE:C3	41:Bs:98:LEU:HD22	2.38	0.54
35:Bl:190:ILE:O	35:Bl:194:ASN:HA	2.08	0.54
36:Bm:48:GLY:HA2	36:Bm:138:ASP:OD2	2.08	0.54
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.54
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.54
2:B:61:TRP:O	2:B:63:GLU:N	2.41	0.54
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.54
12:M:519:ILE:HD13	12:M:522:GLN:HB2	1.90	0.54
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.54
15:P:186:ARG:NH2	15:P:193:PHE:O	2.40	0.54
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.54
21:W:31:SER:C	21:W:32:GLY:O	2.51	0.54
25:b:78:PRO:O	25:b:82:ILE:HD12	2.08	0.54
25:b:110:ILE:HG13	25:b:111:LEU:CD2	2.37	0.54
35:l:190:ILE:O	35:l:194:ASN:HA	2.08	0.54
40:r:346:GLN:HB2	40:r:420:THR:HG23	1.88	0.54
47:z:156:ARG:HG3	47:z:156:ARG:NH1	2.23	0.54
60:AC:164:ASN:OD1	60:AC:165:MET:N	2.41	0.54
68:AL:294:PRO:HG3	68:AL:448:TYR:CZ	2.43	0.54
75:AL:502:CDL:C58	76:AL:503:PEE:H62	2.37	0.54
60:AP:194:GLN:O	60:AP:250:ARG:NH1	2.41	0.54
11:BL:133:ASP:O	11:BL:136:SER:OG	2.21	0.54
12:BM:341:ILE:HD12	12:BM:555:ILE:HG13	1.89	0.54
16:BQ:449:ALA:O	16:BQ:453:THR:HG23	2.08	0.54
22:BY:81:LEU:HD22	43:Bv:92:HIS:HD2	1.70	0.54
24:Ba:133:TYR:OH	27:Bd:81:GLU:HG2	2.08	0.54
32:Bi:268:GLU:OE2	42:Bu:168:TYR:OH	2.24	0.54
34:Bk:11:ALA:HB1	36:Bm:16:PHE:HD2	1.72	0.54
35:Bl:456:ARG:NH2	35:Bl:456:ARG:HB2	2.21	0.54
40:Br:358:TRP:CE3	40:Br:441:LEU:HD12	2.42	0.54
47:Bz:151:LEU:HB2	47:Bz:159:MET:HG3	1.90	0.54
48:B0:67:SER:OG	48:B0:70:GLU:HG3	2.08	0.54
51:B3:5:LYS:HD2	51:B3:5:LYS:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.08	0.54
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.54
25:b:87:LYS:HE3	27:d:43:ARG:HG2	1.89	0.54
27:d:115:TYR:CD1	27:d:115:TYR:C	2.85	0.54
38:o:8:PRO:HB3	38:o:14:LEU:HG	1.88	0.54
45:x:407:ASP:O	45:x:411:LYS:HG3	2.07	0.54
60:AP:128:ALA:HB1	76:AU:401:PEE:H55	1.90	0.54
63:AS:55:LEU:HD21	63:AS:90:TYR:CD2	2.43	0.54
1:BA:41:ILE:HG23	1:BA:253:THR:HG21	1.90	0.54
1:BA:149:MET:HG3	1:BA:241:THR:HG21	1.89	0.54
2:BB:61:TRP:CD1	16:BQ:266:ARG:HH12	2.26	0.54
4:BE:50:PHE:HB2	4:BE:52:LEU:HD12	1.89	0.54
4:BE:56:VAL:HG23	9:BJ:367:GLU:OE2	2.07	0.54
4:BE:128:PRO:HB3	11:BL:104:ARG:HH22	1.73	0.54
7:BH:12:VAL:HG11	16:BQ:296:SER:HB2	1.90	0.54
9:BJ:89:TYR:CD1	9:BJ:89:TYR:C	2.85	0.54
9:BJ:344:PRO:HG2	9:BJ:347:LEU:HD13	1.89	0.54
12:BM:598:ASN:HB3	12:BM:602:ARG:HB3	1.89	0.54
22:BY:81:LEU:CD1	43:Bv:88:ASP:HB3	2.37	0.54
22:BY:96:GLU:O	22:BY:97:LEU:CB	2.54	0.54
25:Bb:83:HIS:CD2	35:Bl:6:THR:HG21	2.42	0.54
32:Bi:229:LEU:HD22	32:Bi:232:ARG:NH1	2.23	0.54
35:Bl:508:THR:O	39:Bp:36:LYS:NZ	2.30	0.54
36:Bm:32:LEU:HD13	36:Bm:64:MET:HE1	1.88	0.54
44:Bw:61:THR:HG22	44:Bw:159:LEU:HD23	1.90	0.54
4:E:66:MET:HE3	4:E:106:PHE:HD1	1.71	0.53
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.53
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	0.53
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.53
24:a:90:ASN:ND2	71:b:201:PLX:H122	2.19	0.53
35:l:98:TRP:CD1	35:l:98:TRP:C	2.86	0.53
76:l:701:PEE:C23	40:r:155:VAL:HB	2.29	0.53
36:m:48:GLY:HA2	36:m:138:ASP:OD2	2.08	0.53
40:r:414:THR:O	40:r:415:GLN:NE2	2.41	0.53
44:w:128:SER:O	44:w:131:LEU:HG	2.08	0.53
46:y:165:VAL:HB	46:y:170:LEU:HD12	1.90	0.53
50:2:48:LEU:O	50:2:50:PRO:HD3	2.08	0.53
63:AF:36:ASP:OD1	63:AF:90:TYR:OH	2.17	0.53
63:AF:72:LYS:O	63:AF:73:HIS:HB2	2.09	0.53
66:AJ:173:PRO:O	66:AJ:177:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AV:150:LEU:CD2	66:AV:164:ILE:HD13	2.37	0.53
68:AY:145:GLU:CB	68:AY:249:HIS:CE1	2.90	0.53
5:BF:41:TYR:OH	12:BM:380:ASP:OD2	2.20	0.53
12:BM:53:CYS:HB2	12:BM:60:ILE:HD11	1.90	0.53
16:BQ:265:ASN:OD1	16:BQ:266:ARG:N	2.42	0.53
27:Bd:76:ILE:O	27:Bd:80:TYR:N	2.41	0.53
34:Bk:15:SER:OG	34:Bk:36:MET:HG2	2.08	0.53
35:Bl:98:TRP:CD1	35:Bl:98:TRP:C	2.86	0.53
35:Bl:293:LEU:HD23	35:Bl:422:TYR:HB3	1.90	0.53
35:Bl:525:MET:HE2	39:Bp:77:PRO:HB3	1.91	0.53
46:By:111:THR:HG21	52:B4:66:ILE:HD11	1.89	0.53
1:A:118:ASP:OD1	1:A:120:GLY:N	2.35	0.53
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.90	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	0.53
12:M:225:ILE:HD12	12:M:285:TRP:CH2	2.39	0.53
15:P:113:ASP:HB3	15:P:115:THR:HG23	1.91	0.53
76:V:202:PEE:C24	76:V:202:PEE:H57	2.39	0.53
35:l:3:MET:O	35:l:7:MET:HG2	2.08	0.53
36:m:19:PHE:CZ	36:m:32:LEU:HD21	2.43	0.53
36:m:36:GLY:HA3	36:m:60:LEU:HD21	1.90	0.53
42:u:100:CYS:SG	42:u:101:ARG:N	2.78	0.53
48:0:52:SER:OG	48:0:55:GLU:HG3	2.08	0.53
51:3:2:SER:OG	51:3:3:ALA:N	2.41	0.53
75:AG:101:CDL:H331	66:AV:163:TRP:CD1	2.43	0.53
67:AK:289:LEU:O	67:AK:293:LEU:HD13	2.09	0.53
2:BB:61:TRP:HH2	41:Bs:187:ILE:HD11	1.73	0.53
3:BC:184:PRO:HD3	16:BQ:223:HIS:CD2	2.43	0.53
7:BH:97:TRP:HB3	7:BH:100:TRP:CH2	2.43	0.53
12:BM:343:GLY:HA3	12:BM:548:LEU:HB2	1.90	0.53
16:BQ:136:PHE:HE2	16:BQ:151:TYR:CD1	2.26	0.53
16:BQ:159:LEU:HD21	16:BQ:391:VAL:HA	1.90	0.53
16:BQ:198:THR:HA	41:Bs:32:GLN:OE1	2.07	0.53
17:BS:12:MET:HE1	41:Bs:20:LEU:HD12	1.91	0.53
22:BY:96:GLU:O	22:BY:97:LEU:CD2	2.54	0.53
27:Bd:57:TYR:HD1	27:Bd:57:TYR:O	1.91	0.53
27:Bd:73:GLU:HG3	30:Bg:106:LYS:O	2.08	0.53
30:Bg:46:LEU:HD11	32:Bi:239:TRP:HB3	1.88	0.53
34:Bk:66:PHE:CE1	36:Bm:159:THR:HG21	2.40	0.53
39:Bp:102:TRP:NE1	40:Br:426:MET:HE1	2.23	0.53
8:I:42:PRO:HB3	21:W:10:MET:HE1	1.90	0.53
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:104:TYR:CG	36:m:165:TYR:HE1	2.26	0.53
46:y:136:LEU:HB3	46:y:193:TYR:HD2	1.73	0.53
48:0:40:LEU:HD13	48:0:59:LEU:HD13	1.90	0.53
49:1:41:LEU:HD12	49:1:41:LEU:O	2.08	0.53
66:AJ:191:ALA:O	66:AJ:194:THR:OG1	2.20	0.53
68:AY:473:SER:HB3	76:AY:502:PEE:H10	1.90	0.53
2:BB:61:TRP:O	2:BB:63:GLU:N	2.41	0.53
9:BJ:172:ALA:HA	9:BJ:181:LEU:HD23	1.91	0.53
9:BJ:178:SER:OG	9:BJ:181:LEU:CB	2.57	0.53
12:BM:149:ASP:HB2	16:BQ:361:ALA:HB3	1.90	0.53
14:BO:87:GLN:O	14:BO:91:GLY:N	2.22	0.53
15:BP:160:PHE:C	15:BP:162:ALA:H	2.16	0.53
25:Bb:105:PHE:HD2	43:Bv:68:LYS:HG3	1.74	0.53
28:Be:74:HIS:ND1	28:Be:87:MET:HG3	2.23	0.53
35:Bl:546:GLN:O	35:Bl:550:LEU:HB2	2.07	0.53
41:Bs:228:TYR:CD1	41:Bs:231:ILE:HD12	2.43	0.53
46:By:165:VAL:HB	46:By:170:LEU:HD12	1.90	0.53
47:Bz:156:ARG:HG3	47:Bz:156:ARG:NH1	2.23	0.53
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.53
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.53
12:M:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
12:M:613:PRO:HB3	13:N:134:ILE:HG21	1.91	0.53
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.53
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.53
76:W:201:PEE:C3	41:s:98:LEU:HD22	2.38	0.53
24:a:54:LEU:HD23	25:b:27:GLU:HA	1.89	0.53
35:l:49:PHE:O	35:l:52:THR:OG1	2.22	0.53
41:s:145:THR:HG21	41:s:289:LEU:HD22	1.90	0.53
58:AA:12:ARG:HG2	58:AA:13:HIS:CE1	2.44	0.53
61:AD:60:TYR:HD2	65:AH:141:THR:HG21	1.73	0.53
67:AK:57:PRO:HG2	68:AL:400:VAL:HG11	1.91	0.53
67:AK:254:ARG:NH2	67:AW:257:GLU:OE1	2.41	0.53
67:AK:364:GLY:HA2	67:AK:425:ILE:HD12	1.89	0.53
60:AP:153:GLU:HB3	60:AP:273:VAL:HB	1.91	0.53
1:BA:111:LYS:O	1:BA:152:ARG:N	2.34	0.53
12:BM:319:TRP:HZ2	12:BM:615:LEU:O	1.92	0.53
16:BQ:191:ALA:HB1	16:BQ:196:ALA:HB3	1.89	0.53
19:BU:69:HIS:ND1	19:BU:70:PRO:HA	2.24	0.53
25:Bb:110:ILE:N	27:Bd:17:THR:O	2.41	0.53
30:Bg:27:ASP:OD1	42:Bu:172:LYS:NZ	2.42	0.53
35:Bl:51:THR:HG21	35:Bl:91:PRO:HG3	1.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:566:ILE:HA	35:Bl:569:HIS:HD2	1.73	0.53
36:Bm:19:PHE:CZ	36:Bm:32:LEU:HD21	2.43	0.53
45:Bx:398:PRO:O	45:Bx:498:CYS:HB3	2.09	0.53
2:B:61:TRP:CD1	16:Q:266:ARG:HH12	2.26	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
12:M:319:TRP:HZ2	12:M:615:LEU:O	1.92	0.53
17:S:54:ILE:HG13	31:h:105:ARG:HH11	1.72	0.53
19:U:69:HIS:ND1	19:U:70:PRO:HA	2.24	0.53
24:a:98:LEU:CA	27:d:57:TYR:CD1	2.91	0.53
30:g:27:ASP:OD1	42:u:172:LYS:NZ	2.42	0.53
34:k:4:ILE:O	34:k:8:ILE:HD13	2.09	0.53
35:l:244:SER:HA	35:l:248:HIS:HD2	1.73	0.53
41:s:195:ARG:NH1	41:s:270:PHE:HB3	2.24	0.53
42:u:83:THR:O	42:u:86:TRP:HB3	2.08	0.53
62:AE:21:GLU:O	62:AE:24:GLU:CA	2.57	0.53
75:AG:101:CDL:C54	75:AG:101:CDL:C73	2.85	0.53
76:AH:401:PEE:H66	76:AH:401:PEE:C18	2.30	0.53
67:AK:36:GLN:HG2	67:AK:53:GLU:HB3	1.90	0.53
67:AK:319:GLN:O	67:AK:321:PHE:N	2.41	0.53
75:AL:502:CDL:H572	76:AL:503:PEE:C39	2.38	0.53
66:AV:191:ALA:O	66:AV:194:THR:OG1	2.24	0.53
1:BA:141:GLY:HA2	1:BA:252:PRO:HD3	1.90	0.53
2:BB:68:LEU:O	2:BB:71:THR:HG22	2.07	0.53
9:BJ:298:TYR:CE2	9:BJ:319:VAL:HG22	2.44	0.53
12:BM:613:PRO:HB3	13:BN:134:ILE:HG21	1.91	0.53
13:BN:94:THR:HG22	13:BN:96:ASP:H	1.73	0.53
17:BS:37:ARG:O	21:BW:143:TYR:OH	2.27	0.53
76:BV:202:PEE:C24	76:BV:202:PEE:H57	2.39	0.53
27:Bd:156:ARG:NH1	28:Be:139:SER:O	2.37	0.53
34:Bk:4:ILE:O	34:Bk:8:ILE:HD13	2.09	0.53
35:Bl:95:PHE:CD1	35:Bl:95:PHE:C	2.86	0.53
35:Bl:226:GLN:HG2	35:Bl:280:LEU:HD21	1.84	0.53
46:By:203:ASN:HD22	46:By:206:PHE:HD2	1.55	0.53
1:A:68:ILE:HD11	1:A:256:ARG:HG2	1.91	0.53
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.53
16:Q:265:ASN:OD1	16:Q:266:ARG:N	2.41	0.53
20:V:124:LEU:HD23	20:V:127:MET:HE3	1.91	0.53
26:c:84:HIS:CD2	26:c:118:ASP:HB3	2.43	0.53
27:d:57:TYR:CD1	27:d:57:TYR:C	2.85	0.53
32:i:229:LEU:HD22	32:i:232:ARG:NH1	2.23	0.53
46:y:68:LEU:HB3	46:y:69:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AJ:405:CDL:H111	76:AY:502:PEE:C45	2.30	0.53
67:AK:217:ARG:HH21	67:AK:246:LEU:H	1.56	0.53
58:AN:20:SER:HB3	58:AN:23:GLU:HG2	1.91	0.53
61:AQ:51:LYS:O	65:AU:107:HIS:ND1	2.32	0.53
64:AT:19:PRO:HA	64:AT:22:TYR:HD2	1.74	0.53
67:AW:267:VAL:HG11	67:AW:347:ALA:HB2	1.90	0.53
9:BJ:141:PHE:CZ	9:BJ:180:TYR:CB	2.92	0.53
9:BJ:207:PHE:CZ	9:BJ:345:LEU:HA	2.44	0.53
12:BM:519:ILE:HD13	12:BM:522:GLN:HB2	1.90	0.53
16:BQ:55:SER:OG	35:Bl:580:GLN:NE2	2.42	0.53
16:BQ:404:LYS:HZ3	16:BQ:457:VAL:HB	1.74	0.53
22:BY:71:TRP:CE3	22:BY:71:TRP:C	2.87	0.53
23:BZ:49:GLU:OE2	39:Bp:38:ARG:NH2	2.33	0.53
32:Bi:291:TYR:HB2	40:Br:151:PHE:CZ	2.44	0.53
36:Bm:155:VAL:O	36:Bm:159:THR:HG23	2.08	0.53
41:Bs:195:ARG:NH1	41:Bs:270:PHE:HB3	2.24	0.53
42:Bu:111:VAL:HG12	42:Bu:117:TRP:O	2.09	0.53
1:A:86:ARG:NE	1:A:92:GLY:O	2.40	0.53
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.53
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.91	0.53
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.74	0.53
25:b:105:PHE:HD2	43:v:68:LYS:HG3	1.74	0.53
32:i:291:TYR:HB2	40:r:151:PHE:CZ	2.44	0.53
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.91	0.53
40:r:131:ALA:O	40:r:135:ARG:HB3	2.09	0.53
44:w:137:SER:O	44:w:139:ARG:N	2.37	0.53
45:x:268:PHE:CZ	46:y:58:ALA:HA	2.44	0.53
59:AO:5:ALA:HB1	67:AW:385:SER:HB2	1.90	0.53
63:AS:28:ASN:HD22	63:AS:82:THR:HB	1.73	0.53
1:BA:68:ILE:HD11	1:BA:256:ARG:HG2	1.91	0.53
1:BA:317:VAL:HG13	1:BA:356:VAL:HA	1.91	0.53
12:BM:168:LEU:HB3	12:BM:292:PHE:HE2	1.74	0.53
12:BM:351:LEU:HD23	12:BM:530:TYR:HE2	1.73	0.53
12:BM:394:VAL:HG21	12:BM:414:PHE:HE1	1.73	0.53
15:BP:238:PRO:O	15:BP:239:TRP:HB2	2.08	0.53
16:BQ:43:TRP:HZ3	32:Bi:305:LEU:HD21	1.74	0.53
21:BW:81:ARG:HH22	42:Bu:64:ASN:HD21	1.56	0.53
24:Ba:54:LEU:HD21	25:Bb:27:GLU:HA	1.90	0.53
32:Bi:239:TRP:HA	75:Bi:401:CDL:HB32	1.91	0.53
32:Bi:291:TYR:CZ	76:Bl:701:PEE:C31	2.71	0.53
40:Br:188:ASN:O	40:Br:189:SER:OG	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Bw:137:SER:O	44:Bw:139:ARG:N	2.37	0.53
44:Bw:149:HIS:CE1	44:Bw:155:GLN:HB3	2.43	0.53
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.90	0.53
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.53
6:G:75:THR:O	6:G:79:ILE:HG12	2.09	0.53
8:I:59:GLY:HA2	15:P:47:VAL:HG22	1.90	0.53
9:J:178:SER:OG	9:J:181:LEU:CB	2.57	0.53
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.53
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.53
16:Q:391:VAL:HG12	16:Q:392:PRO:O	2.08	0.53
16:Q:435:LEU:HA	16:Q:438:MET:HE3	1.91	0.53
23:Z:24:ILE:HG22	23:Z:30:GLU:HB2	1.90	0.53
25:b:39:LYS:HG3	25:b:41:GLY:H	1.74	0.53
26:c:159:LYS:HA	43:v:98:ARG:NH1	2.24	0.53
27:d:57:TYR:HD1	27:d:57:TYR:O	1.91	0.53
32:i:311:VAL:HG12	32:i:315:TRP:HE1	1.74	0.53
35:l:195:SER:O	35:l:196:TRP:HB2	2.08	0.53
40:r:236:LEU:O	40:r:239:GLY:N	2.40	0.53
44:w:58:ARG:HB3	44:w:202:HIS:CE1	2.44	0.53
46:y:203:ASN:HD22	46:y:206:PHE:HD2	1.55	0.53
68:AY:462:ILE:HG23	68:AY:465:LEU:HB3	1.91	0.53
1:BA:121:GLU:HA	1:BA:204:TYR:HE1	1.74	0.53
1:BA:236:PHE:HZ	14:BO:77:ALA:HB2	1.73	0.53
2:BB:37:LYS:N	16:BQ:318:VAL:O	2.37	0.53
11:BL:170:THR:O	11:BL:172:VAL:N	2.35	0.53
16:BQ:435:LEU:HA	16:BQ:438:MET:HE3	1.91	0.53
20:BV:124:LEU:HD23	20:BV:127:MET:HE3	1.91	0.53
26:Bc:159:LYS:HA	43:Bv:98:ARG:NH1	2.24	0.53
27:Bd:57:TYR:CD1	27:Bd:57:TYR:C	2.85	0.53
32:Bi:311:VAL:HG12	32:Bi:315:TRP:HE1	1.74	0.53
33:Bj:104:TYR:CG	36:Bm:165:TYR:HE1	2.26	0.53
34:Bk:87:LEU:HD11	36:Bm:73:MET:O	2.08	0.53
42:Bu:83:THR:O	42:Bu:86:TRP:HB3	2.08	0.53
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	0.53
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.53
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.53
17:S:12:MET:HE1	41:s:20:LEU:HD12	1.91	0.53
17:S:28:ARG:NH1	42:u:91:TYR:OH	2.42	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
27:d:73:GLU:HG3	30:g:106:LYS:O	2.08	0.53
34:k:62:VAL:HG21	36:m:152:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:102:TRP:NE1	40:r:426:MET:HE1	2.23	0.53
44:w:149:HIS:CE1	44:w:155:GLN:HB3	2.43	0.53
44:w:294:LEU:O	44:w:298:VAL:HG23	2.09	0.53
48:0:128:VAL:O	48:0:134:PHE:HB3	2.09	0.53
75:AG:101:CDL:H741	66:AV:156:ILE:HG23	1.91	0.53
67:AK:116:ARG:HH21	67:AK:175:GLU:HG3	1.74	0.53
75:AL:502:CDL:C76	76:AL:503:PEE:H74	2.38	0.53
59:AO:45:LEU:HD13	67:AW:160:ILE:HG23	1.91	0.53
60:AP:131:ASN:ND2	76:AU:401:PEE:H7	2.24	0.53
62:AR:37:CYS:SG	62:AR:85:LYS:CE	2.97	0.53
82:AV:402:HEM:HBC2	82:AV:402:HEM:HMC2	1.90	0.53
68:AY:79:SER:HB3	68:AY:126:ARG:HA	1.90	0.53
1:BA:154:ALA:HB3	1:BA:195:VAL:HG12	1.91	0.53
9:BJ:141:PHE:HZ	9:BJ:180:TYR:CD1	2.26	0.53
9:BJ:168:SER:O	73:BJ:401:NDP:H6N	2.08	0.53
9:BJ:221:HIS:HE1	9:BJ:222:ARG:CG	2.20	0.53
11:BL:120:PRO:HB2	15:BP:203:PRO:HG3	1.91	0.53
12:BM:278:HIS:CD2	12:BM:280:ASP:HB2	2.44	0.53
15:BP:186:ARG:NH2	15:BP:193:PHE:O	2.40	0.53
34:Bk:7:ASN:OD1	36:Bm:13:VAL:CG2	2.57	0.53
35:Bl:106:TRP:HB2	35:Bl:449:THR:OG1	2.09	0.53
35:Bl:144:TRP:NE1	35:Bl:179:ASP:OD1	2.42	0.53
48:B0:52:SER:OG	48:B0:55:GLU:HG3	2.08	0.53
1:A:116:ASN:HD22	70:A:502:FMN:C9	2.22	0.53
1:A:317:VAL:HG13	1:A:356:VAL:HA	1.91	0.53
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.53
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.53
15:P:235:LEU:HB3	16:Q:387:GLU:HG2	1.90	0.53
25:b:110:ILE:N	27:d:17:THR:O	2.41	0.53
32:i:222:ASN:HD21	32:i:233:THR:HG22	1.74	0.53
34:k:15:SER:OG	34:k:36:MET:HG2	2.08	0.53
35:l:302:VAL:O	35:l:305:SER:OG	2.24	0.53
35:l:512:LYS:HD3	54:6:18:LEU:HD11	1.91	0.53
46:y:102:HIS:O	46:y:104:TRP:N	2.42	0.53
48:0:23:PRO:HD2	49:1:34:ASN:HD22	1.74	0.53
48:0:67:SER:OG	48:0:70:GLU:HG3	2.08	0.53
58:AA:12:ARG:HA	68:AL:279:ASP:HA	1.90	0.53
62:AE:30:LEU:CD2	65:AH:216:THR:HG23	2.33	0.53
68:AL:255:TRP:CB	39:Bp:55:LYS:HB3	2.39	0.53
3:BC:140:GLN:NE2	33:Bj:40:GLY:HA2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BG:75:THR:O	6:BG:79:ILE:HG12	2.09	0.53
12:BM:76:ARG:HE	12:BM:79:LEU:HD21	1.74	0.53
12:BM:215:MET:HE1	12:BM:714:VAL:HG23	1.90	0.53
16:BQ:99:MET:HE2	16:BQ:109:CYS:SG	2.49	0.53
17:BS:12:MET:CE	41:Bs:20:LEU:HD12	2.39	0.53
21:BW:31:SER:C	21:BW:32:GLY:O	2.51	0.53
23:BZ:24:ILE:HG22	23:BZ:30:GLU:HB2	1.90	0.53
26:Bc:84:HIS:CD2	26:Bc:118:ASP:HB3	2.43	0.53
31:Bh:40:TRP:HH2	32:Bi:83:GLN:HE21	1.57	0.53
35:Bl:49:PHE:O	35:Bl:52:THR:OG1	2.22	0.53
35:Bl:244:SER:HA	35:Bl:248:HIS:HD2	1.73	0.53
48:B0:40:LEU:HD22	48:B0:59:LEU:HD13	1.91	0.53
51:B3:42:ARG:HH11	51:B3:42:ARG:HG3	1.74	0.53
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.45	0.52
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.91	0.52
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.52
4:E:24:ASP:OD1	4:E:25:MET:N	2.41	0.52
35:l:575:ILE:O	35:l:578:SER:OG	2.16	0.52
68:AY:134:LYS:NZ	68:AY:407:THR:OG1	2.42	0.52
6:BG:123:GLU:OE1	6:BG:130:ILE:N	2.39	0.52
18:BT:52:ARG:HB3	18:BT:55:ARG:HH12	1.74	0.52
24:Ba:98:LEU:HB3	27:Bd:57:TYR:HE1	0.54	0.52
24:Ba:112:TYR:HD1	27:Bd:58:TYR:O	1.92	0.52
35:Bl:197:ASP:O	35:Bl:201:MET:HG3	2.08	0.52
35:Bl:512:LYS:HD3	54:B6:18:LEU:HD11	1.91	0.52
35:Bl:512:LYS:O	39:Bp:40:PHE:HZ	1.91	0.52
41:Bs:226:ALA:O	41:Bs:230:ASN:ND2	2.40	0.52
46:By:102:HIS:O	46:By:104:TRP:N	2.42	0.52
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.52
3:C:140:GLN:NE2	33:j:40:GLY:HA2	2.23	0.52
9:J:168:SER:O	73:J:401:NDP:H6N	2.08	0.52
9:J:172:ALA:HA	9:J:181:LEU:CD2	2.38	0.52
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.52
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.52
12:M:82:ILE:HB	12:M:85:ALA:HB2	1.91	0.52
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.52
16:Q:99:MET:HE2	16:Q:109:CYS:SG	2.49	0.52
21:W:35:MET:HA	21:W:38:ILE:HD12	1.91	0.52
32:i:239:TRP:HA	75:i:401:CDL:HB32	1.91	0.52
34:k:87:LEU:HD11	36:m:73:MET:O	2.08	0.52
35:l:566:ILE:HA	35:l:569:HIS:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:145:ALA:HA	40:r:148:TYR:HB3	1.91	0.52
41:s:32:GLN:HB3	41:s:34:ARG:HG2	1.91	0.52
41:s:126:ASN:HA	41:s:129:LEU:HD12	1.91	0.52
60:AC:173:PRO:HB2	60:AC:215:GLY:HA3	1.90	0.52
68:AL:260:ASP:OD2	39:Bp:12:HIS:HB3	2.07	0.52
7:BH:31:ILE:HA	7:BH:34:VAL:HG12	1.90	0.52
8:BI:59:GLY:HA2	15:BP:47:VAL:HG22	1.90	0.52
12:BM:253:VAL:HG23	12:BM:345:LEU:HD22	1.91	0.52
12:BM:405:THR:HA	12:BM:686:PRO:HG3	1.90	0.52
15:BP:235:LEU:HB3	16:BQ:387:GLU:HG2	1.90	0.52
35:Bl:100:ILE:HD12	35:Bl:246:LEU:CG	2.39	0.52
40:Br:131:ALA:O	40:Br:135:ARG:HB3	2.09	0.52
40:Br:145:ALA:HA	40:Br:148:TYR:HB3	1.91	0.52
41:Bs:32:GLN:HB3	41:Bs:34:ARG:HG2	1.91	0.52
41:Bs:186:PHE:O	41:Bs:189:THR:OG1	2.16	0.52
45:Bx:225:GLY:HA3	47:Bz:112:LEU:HD13	1.92	0.52
46:By:68:LEU:HB3	46:By:69:PRO:HD3	1.91	0.52
50:B2:55:LYS:HA	50:B2:74:LEU:O	2.08	0.52
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	0.52
6:G:137:LYS:O	6:G:139:MET:N	2.42	0.52
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.52
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.52
22:Y:71:TRP:CE3	22:Y:71:TRP:C	2.87	0.52
25:b:95:TYR:HE2	27:d:10:TYR:CD1	2.27	0.52
32:i:268:GLU:OE2	42:u:168:TYR:OH	2.24	0.52
33:j:70:ALA:HB1	36:m:58:ILE:HD11	1.92	0.52
35:l:282:ALA:O	35:l:285:THR:OG1	2.27	0.52
36:m:106:VAL:HG11	36:m:117:ASN:HD22	1.74	0.52
44:w:65:ASN:O	44:w:68:THR:OG1	2.20	0.52
46:y:33:LEU:HD23	53:5:28:SER:HB2	1.91	0.52
48:0:40:LEU:HD22	48:0:59:LEU:HD13	1.91	0.52
51:3:8:HIS:O	51:3:10:GLY:N	2.42	0.52
68:AL:54:ASP:O	39:Bp:55:LYS:HG3	2.10	0.52
68:AL:311:ILE:O	68:AL:326:SER:OG	2.26	0.52
3:BC:75:ARG:NH2	3:BC:144:PRO:HG3	2.24	0.52
10:BK:92:SER:HB2	14:BO:68:LYS:HD2	1.90	0.52
12:BM:68:ARG:HD2	12:BM:285:TRP:NE1	2.21	0.52
36:Bm:50:TYR:O	36:Bm:54:MET:HG2	2.10	0.52
40:Br:286:ILE:O	40:Br:289:SER:OG	2.23	0.52
71:Br:501:PLX:H262	71:Br:501:PLX:H6	1.91	0.52
46:By:104:TRP:CG	46:By:203:ASN:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B0:40:LEU:HD13	48:B0:59:LEU:HD13	1.90	0.52
1:A:117:ALA:HB3	1:A:157:TYR:O	2.08	0.52
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.52
9:J:84:TYR:HB2	9:J:91:ILE:HD11	1.92	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.52
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	0.52
12:M:278:HIS:CD2	12:M:280:ASP:HB2	2.44	0.52
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.52
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.24	0.52
16:Q:338:ARG:NH2	21:W:23:ARG:HB3	2.24	0.52
22:Y:50:LEU:O	22:Y:51:THR:OG1	2.27	0.52
27:d:60:ARG:CG	27:d:60:ARG:NH1	2.73	0.52
35:l:100:ILE:HD12	35:l:246:LEU:CG	2.39	0.52
46:y:104:TRP:CG	46:y:203:ASN:HB2	2.44	0.52
50:2:8:THR:OG1	50:2:11:GLU:HG2	2.09	0.52
63:AF:36:ASP:OD1	63:AF:62:ARG:NH1	2.42	0.52
65:AU:125:HIS:HB3	65:AU:197:LEU:HD13	1.91	0.52
1:BA:208:GLU:OE1	1:BA:211:ALA:N	2.39	0.52
1:BA:293:SER:HB2	1:BA:336:LEU:HD23	1.91	0.52
9:BJ:64:PHE:CE1	9:BJ:68:TYR:HE2	2.27	0.52
16:BQ:391:VAL:HG12	16:BQ:392:PRO:O	2.08	0.52
22:BY:61:PHE:CE2	35:Bl:455:LYS:HG2	2.44	0.52
25:Bb:95:TYR:HE2	27:Bd:10:TYR:CD1	2.27	0.52
31:Bh:99:ILE:HD12	31:Bh:101:LYS:HD2	1.91	0.52
33:Bj:24:LEU:H	33:Bj:25:PRO:CD	2.22	0.52
71:Br:502:PLX:C7	71:Br:502:PLX:C3	2.88	0.52
41:Bs:139:THR:O	41:Bs:143:GLU:HG3	2.09	0.52
42:Bu:31:HIS:CE1	42:Bu:111:VAL:HG11	2.44	0.52
48:B0:128:VAL:O	48:B0:134:PHE:HB3	2.09	0.52
50:B2:51:SER:HB2	50:B2:91:LEU:HD11	1.90	0.52
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.92	0.52
6:G:147:TYR:O	6:G:151:LYS:N	2.43	0.52
9:J:64:PHE:CD1	9:J:210:GLU:HB3	2.44	0.52
12:M:61:PRO:HG2	12:M:113:ARG:HE	1.74	0.52
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.52
15:P:115:THR:HG22	16:Q:423:LYS:HD3	1.92	0.52
19:U:84:LEU:O	21:W:59:ARG:NH1	2.41	0.52
36:m:130:GLU:HG2	36:m:131:GLY:O	2.10	0.52
71:r:501:PLX:H262	71:r:501:PLX:H6	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AE:30:LEU:HD12	62:AE:30:LEU:C	2.35	0.52
63:AF:36:ASP:CG	63:AF:62:ARG:NH1	2.67	0.52
66:AV:97:HIS:CE1	66:AV:100:ARG:HH21	2.27	0.52
66:AV:254:ASP:O	66:AV:257:THR:OG1	2.28	0.52
66:AV:333:LEU:HD21	76:AV:403:PEE:C38	2.39	0.52
68:AY:364:LYS:HB2	68:AY:368:MET:HE3	1.90	0.52
1:BA:181:LEU:HA	1:BA:187:CYS:HB3	1.91	0.52
12:BM:610:VAL:O	12:BM:611:THR:OG1	2.25	0.52
17:BS:28:ARG:NH1	42:Bu:91:TYR:OH	2.42	0.52
35:Bl:567:SER:O	35:Bl:571:ILE:HD13	2.09	0.52
40:Br:73:LEU:O	40:Br:76:THR:OG1	2.18	0.52
45:Bx:302:ARG:O	45:Bx:306:THR:HG23	2.09	0.52
50:B2:8:THR:OG1	50:B2:11:GLU:HG2	2.09	0.52
51:B3:2:SER:OG	51:B3:3:ALA:N	2.41	0.52
51:B3:8:HIS:O	51:B3:10:GLY:N	2.42	0.52
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.52
9:J:172:ALA:HA	9:J:181:LEU:HD23	1.90	0.52
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	0.52
12:M:610:VAL:O	12:M:611:THR:OG1	2.25	0.52
16:Q:43:TRP:HZ3	32:i:305:LEU:HD21	1.74	0.52
16:Q:66:TRP:CE2	44:w:310:ILE:HD11	2.45	0.52
24:a:129:PRO:HG2	27:d:60:ARG:HH22	1.75	0.52
34:k:81:ILE:HG22	34:k:87:LEU:HA	1.92	0.52
36:m:50:TYR:O	36:m:54:MET:HG2	2.10	0.52
41:s:139:THR:O	41:s:143:GLU:HG3	2.09	0.52
42:u:111:VAL:HG12	42:u:117:TRP:O	2.09	0.52
44:w:98:THR:HG23	44:w:337:ARG:NH2	2.25	0.52
50:2:51:SER:HB2	50:2:91:LEU:HD11	1.90	0.52
67:AK:65:ILE:HG13	67:AK:218:MET:HG2	1.91	0.52
1:BA:170:GLN:HE21	10:BK:91:LEU:HD12	1.74	0.52
2:BB:79:PRO:HD2	17:BS:1:MET:SD	2.50	0.52
2:BB:90:PRO:HD2	3:BC:100:ARG:HH11	1.74	0.52
10:BK:77:HIS:CD2	14:BO:215:LYS:HE2	2.44	0.52
12:BM:188:GLU:O	12:BM:419:ARG:NE	2.40	0.52
32:Bi:222:ASN:HD21	32:Bi:233:THR:HG22	1.74	0.52
34:Bk:58:ILE:HG23	36:Bm:145:LEU:HD12	1.92	0.52
35:Bl:190:ILE:CG1	35:Bl:196:TRP:CD1	2.93	0.52
35:Bl:190:ILE:CG1	35:Bl:196:TRP:NE1	2.73	0.52
42:Bu:24:VAL:HG13	42:Bu:86:TRP:CD1	2.45	0.52
46:By:136:LEU:HB3	46:By:193:TYR:HD2	1.73	0.52
9:J:168:SER:HA	9:J:184:LYS:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	0.52
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.52
22:Y:61:PHE:CE2	35:l:455:LYS:HG2	2.44	0.52
24:a:87:THR:CG2	71:b:201:PLX:H131	2.40	0.52
24:a:112:TYR:HD1	27:d:58:TYR:O	1.92	0.52
31:h:99:ILE:HD12	31:h:101:LYS:HD2	1.91	0.52
32:i:243:LEU:HD21	75:i:401:CDL:H752	1.92	0.52
32:i:336:LEU:HD21	32:i:343:MET:SD	2.50	0.52
35:l:190:ILE:CG1	35:l:196:TRP:NE1	2.73	0.52
40:r:187:SER:O	40:r:192:ASN:ND2	2.43	0.52
45:x:398:PRO:O	45:x:498:CYS:HB3	2.09	0.52
66:AV:173:PRO:HB2	66:AV:177:ARG:HH12	1.74	0.52
1:BA:117:ALA:HB3	1:BA:157:TYR:O	2.08	0.52
7:BH:32:LEU:O	7:BH:36:GLU:HG3	2.10	0.52
9:BJ:64:PHE:CD1	9:BJ:210:GLU:HB3	2.44	0.52
9:BJ:223:PHE:O	9:BJ:225:PRO:HD2	2.09	0.52
12:BM:61:PRO:HG2	12:BM:113:ARG:HE	1.74	0.52
12:BM:89:VAL:HB	12:BM:94:MET:HG3	1.91	0.52
12:BM:308:ARG:NH1	12:BM:578:PRO:O	2.42	0.52
12:BM:634:LEU:HD23	12:BM:636:TYR:CZ	2.45	0.52
14:BO:152:ILE:HG21	14:BO:171:LEU:HD13	1.92	0.52
14:BO:204:ILE:O	14:BO:208:LEU:HG	2.08	0.52
16:BQ:66:TRP:CE2	44:Bw:310:ILE:HD11	2.45	0.52
16:BQ:338:ARG:NH2	21:BW:23:ARG:HB3	2.24	0.52
16:BQ:428:GLY:HA2	16:BQ:431:HIS:CD2	2.44	0.52
18:BT:56:PHE:CD1	18:BT:61:LYS:HB2	2.45	0.52
19:BU:84:LEU:O	21:BW:59:ARG:NH1	2.41	0.52
21:BW:33:TYR:CG	21:BW:34:SER:N	2.77	0.52
25:Bb:105:PHE:CD2	43:Bv:68:LYS:CB	2.93	0.52
35:Bl:227:LEU:HD12	35:Bl:227:LEU:C	2.35	0.52
36:Bm:130:GLU:HG2	36:Bm:131:GLY:O	2.10	0.52
36:Bm:156:THR:O	36:Bm:159:THR:OG1	2.22	0.52
40:Br:20:LYS:HA	40:Br:89:LEU:HD13	1.92	0.52
40:Br:272:THR:HA	40:Br:275:ILE:HD12	1.90	0.52
44:Bw:98:THR:HG23	44:Bw:337:ARG:NH2	2.25	0.52
2:B:37:LYS:N	16:Q:318:VAL:O	2.38	0.52
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.91	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.52
12:M:464:GLN:HE22	12:M:467:LYS:HE2	1.75	0.52
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.92	0.52
25:b:108:ASP:O	25:b:109:THR:HB	2.10	0.52
34:k:7:ASN:OD1	36:m:13:VAL:CG2	2.57	0.52
39:p:55:LYS:N	39:p:55:LYS:CE	2.73	0.52
47:z:18:LEU:HD22	47:z:22:LEU:HD22	1.92	0.52
61:AD:43:ILE:O	61:AD:47:ILE:HD12	2.10	0.52
65:AH:291:LYS:HD2	76:AH:401:PEE:C3	2.37	0.52
68:AL:285:ALA:HB3	68:AL:360:CYS:SG	2.50	0.52
66:AV:341:GLN:HB3	66:AV:342:PRO:HD2	1.90	0.52
68:AY:160:GLN:O	68:AY:164:GLU:HG2	2.09	0.52
1:BA:357:MET:HG2	14:BO:142:LEU:HD21	1.91	0.52
72:BE:201:8Q1:N36	72:BE:201:8Q1:C30	2.73	0.52
6:BG:137:LYS:O	6:BG:139:MET:N	2.42	0.52
6:BG:147:TYR:O	6:BG:151:LYS:N	2.43	0.52
7:BH:7:LYS:HG2	7:BH:8:THR:HG23	1.91	0.52
12:BM:308:ARG:HD3	12:BM:314:LEU:HB3	1.92	0.52
12:BM:573:GLY:HA3	13:BN:137:TRP:NE1	2.25	0.52
17:BS:34:LYS:NZ	42:Bu:90:ASP:HB3	2.25	0.52
25:Bb:105:PHE:HZ	43:Bv:67:LEU:CB	2.23	0.52
25:Bb:108:ASP:O	25:Bb:109:THR:HB	2.10	0.52
35:Bl:563:PRO:HG3	40:Br:148:TYR:OH	2.10	0.52
40:Br:187:SER:O	40:Br:192:ASN:ND2	2.43	0.52
41:Bs:126:ASN:HA	41:Bs:129:LEU:HD12	1.91	0.52
46:By:59:GLN:N	46:By:62:GLU:HG3	2.24	0.52
47:Bz:18:LEU:HD22	47:Bz:22:LEU:HD22	1.92	0.52
51:B3:5:LYS:HZ3	51:B3:5:LYS:HB3	1.74	0.52
2:B:61:TRP:HH2	41:s:187:ILE:HD11	1.72	0.52
2:B:79:PRO:HD2	17:S:1:MET:SD	2.50	0.52
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.90	0.52
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.52
11:L:120:PRO:HB2	15:P:203:PRO:HG3	1.91	0.52
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	0.52
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.52
21:W:33:TYR:CG	21:W:34:SER:N	2.77	0.52
35:l:73:THR:OG1	35:l:74:THR:N	2.39	0.52
35:l:144:TRP:NE1	35:l:179:ASP:OD1	2.42	0.52
41:s:228:TYR:CD1	41:s:231:ILE:HD12	2.43	0.52
44:w:198:TYR:OH	44:w:304:VAL:HG12	2.10	0.52
67:AK:352:LYS:HE2	67:AK:453:LEU:CB	2.40	0.52
66:AV:87:ALA:HB2	82:AV:401:HEM:HHB	1.92	0.52
66:AV:96:LEU:HD23	76:AV:403:PEE:C17	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:141:PHE:HE2	9:BJ:183:ASN:HB2	1.74	0.52
11:BL:61:ILE:HG22	11:BL:64:LEU:HD12	1.92	0.52
12:BM:77:MET:HA	12:BM:116:VAL:HG21	1.92	0.52
12:BM:82:ILE:HB	12:BM:85:ALA:HB2	1.91	0.52
16:BQ:228:ARG:CZ	16:BQ:233:HIS:HB2	2.40	0.52
23:BZ:28:PRO:O	23:BZ:31:THR:OG1	2.22	0.52
34:Bk:62:VAL:HG21	36:Bm:152:LEU:HD21	1.91	0.52
35:Bl:135:ASN:OD1	35:Bl:198:PRO:CG	2.57	0.52
44:Bw:128:SER:O	44:Bw:131:LEU:HG	2.08	0.52
48:B0:23:PRO:HD2	49:B1:34:ASN:HD22	1.74	0.52
49:B1:63:SER:O	49:B1:67:ILE:HG13	2.10	0.52
1:A:423:THR:OG1	69:A:501:SF4:S4	2.68	0.52
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.34	0.52
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.52
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.52
16:Q:55:SER:OG	35:l:580:GLN:NE2	2.42	0.52
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.45	0.52
18:T:83:ARG:NH1	18:T:103:LEU:H	2.08	0.52
25:b:105:PHE:CD2	43:v:68:LYS:CB	2.93	0.52
35:l:74:THR:HG23	35:l:194:ASN:OD1	2.08	0.52
38:o:91:ALA:HB2	71:AN:101:PLX:H151	1.92	0.52
40:r:20:LYS:HA	40:r:89:LEU:HD13	1.92	0.52
40:r:94:LEU:O	40:r:97:SER:OG	2.21	0.52
46:y:100:MET:CE	46:y:157:GLU:HG3	2.40	0.52
59:AB:31:GLN:NE2	67:AK:297:PRO:HA	2.24	0.52
66:AJ:281:LEU:HD11	66:AJ:294:LEU:HD22	1.90	0.52
1:BA:62:TRP:CE2	1:BA:181:LEU:HD13	2.44	0.52
7:BH:24:LEU:HD21	7:BH:81:ILE:HG22	1.92	0.52
14:BO:63:ILE:HA	14:BO:66:ILE:HD12	1.92	0.52
21:BW:35:MET:HA	21:BW:38:ILE:HD12	1.91	0.52
35:Bl:51:THR:CG2	35:Bl:91:PRO:CG	2.84	0.52
35:Bl:195:SER:O	35:Bl:196:TRP:HB2	2.08	0.52
40:Br:281:ASP:HB2	40:Br:284:SER:OG	2.10	0.52
40:Br:423:ILE:HD12	40:Br:425:ASN:H	1.75	0.52
44:Bw:294:LEU:O	44:Bw:298:VAL:HG23	2.09	0.52
3:C:209:ILE:HG21	9:J:86:CYS:O	2.11	0.51
6:G:123:GLU:OE1	6:G:130:ILE:N	2.39	0.51
9:J:223:PHE:O	9:J:225:PRO:HD2	2.09	0.51
11:L:61:ILE:HG12	11:L:140:LYS:O	2.10	0.51
14:O:129:LYS:HB3	14:O:168:LEU:HG	1.91	0.51
17:S:12:MET:CE	41:s:20:LEU:HD12	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:110:ARG:NH1	27:d:110:ARG:CG	2.73	0.51
31:h:40:TRP:HH2	32:i:83:GLN:HE21	1.57	0.51
32:i:17:THR:OG1	32:i:36:ASN:ND2	2.39	0.51
32:i:139:ILE:HD11	32:i:187:MET:HE1	1.92	0.51
35:l:592:PHE:CE2	35:l:596:ILE:HD11	2.45	0.51
40:r:281:ASP:HB2	40:r:284:SER:OG	2.10	0.51
41:s:173:TRP:CZ3	41:s:262:LYS:HE2	2.45	0.51
42:u:24:VAL:HG13	42:u:86:TRP:CD1	2.45	0.51
42:u:31:HIS:CE1	42:u:111:VAL:HG11	2.44	0.51
59:AB:26:LEU:HA	59:AB:27:ARG:C	2.35	0.51
62:AE:75:LEU:HD23	62:AE:78:ARG:HD3	1.92	0.51
67:AK:387:GLU:OE2	68:AL:406:THR:OG1	2.15	0.51
66:AV:47:THR:HG23	66:AV:79:ILE:HG23	1.93	0.51
1:BA:342:LEU:O	1:BA:347:THR:N	2.42	0.51
4:BE:24:ASP:OD1	4:BE:25:MET:N	2.41	0.51
11:BL:84:ARG:HG3	11:BL:90:GLY:O	2.10	0.51
12:BM:46:GLY:O	12:BM:96:VAL:HG22	2.09	0.51
16:BQ:85:GLY:H	16:BQ:88:HIS:HE2	1.58	0.51
6:BX:93:ILE:HG21	6:BX:98:LEU:HD12	1.91	0.51
22:BY:84:PHE:CE2	35:Bl:483:PRO:CG	2.69	0.51
25:Bb:39:LYS:HG3	25:Bb:41:GLY:H	1.74	0.51
31:Bh:32:ARG:NH2	34:Bk:50:ASN:O	2.42	0.51
32:Bi:139:ILE:HD11	32:Bi:187:MET:HE1	1.92	0.51
35:Bl:194:ASN:HD22	38:Bo:127:LEU:HD12	1.74	0.51
36:Bm:36:GLY:HA3	36:Bm:60:LEU:HD21	1.90	0.51
40:Br:271:MET:O	40:Br:275:ILE:HG13	2.11	0.51
43:Bv:56:ARG:O	43:Bv:60:ALA:HB2	2.10	0.51
44:Bw:58:ARG:HB3	44:Bw:202:HIS:CE1	2.44	0.51
45:Bx:268:PHE:CZ	46:By:58:ALA:HA	2.44	0.51
52:B4:60:TYR:CD1	52:B4:60:TYR:C	2.88	0.51
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.51
33:j:24:LEU:H	33:j:25:PRO:CD	2.22	0.51
35:l:15:LEU:O	35:l:18:PRO:HD2	2.11	0.51
35:l:135:ASN:OD1	35:l:198:PRO:CG	2.57	0.51
35:l:190:ILE:CG1	35:l:196:TRP:CD1	2.93	0.51
35:l:332:HIS:CE1	35:l:336:LYS:HG3	2.46	0.51
35:l:485:TYR:O	35:l:489:THR:HG23	2.10	0.51
35:l:567:SER:O	35:l:571:ILE:HD13	2.09	0.51
52:4:60:TYR:C	52:4:60:TYR:CD1	2.88	0.51
66:AJ:103:TYR:O	66:AJ:315:MET:HB2	2.10	0.51
67:AK:116:ARG:NH2	67:AK:175:GLU:HG3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:159:LYS:HG3	67:AK:197:ILE:HG21	1.92	0.51
67:AK:309:LEU:HD23	67:AK:323:VAL:HG12	1.92	0.51
66:AV:141:TRP:HZ2	66:AV:260:ASN:O	1.93	0.51
66:AV:151:SER:HB2	66:AV:161:VAL:HG21	1.92	0.51
6:BG:123:GLU:HB2	6:BG:128:PHE:O	2.09	0.51
15:BP:113:ASP:HB3	15:BP:115:THR:HG23	1.91	0.51
76:BV:202:PEE:H41	76:BV:202:PEE:C37	2.40	0.51
24:Ba:87:THR:CG2	71:Bb:201:PLX:H131	2.40	0.51
25:Bb:22:TRP:O	25:Bb:25:ASP:HB3	2.10	0.51
71:Bb:201:PLX:O3	71:Bb:201:PLX:H72	2.10	0.51
26:Bc:101:TRP:NE1	38:Bo:61:GLU:O	2.43	0.51
28:Be:87:MET:HE1	40:Br:431:THR:HG21	1.92	0.51
35:Bl:282:ALA:O	35:Bl:285:THR:OG1	2.27	0.51
35:Bl:332:HIS:CE1	35:Bl:336:LYS:HG3	2.46	0.51
36:Bm:106:VAL:HG11	36:Bm:117:ASN:HD22	1.74	0.51
41:Bs:167:THR:C	41:Bs:169:GLN:H	2.18	0.51
47:Bz:119:THR:O	51:B3:52:HIS:CE1	2.64	0.51
7:H:24:LEU:HD21	7:H:81:ILE:HG22	1.92	0.51
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	0.51
16:Q:304:LYS:HE3	16:Q:316:PHE:CE1	2.46	0.51
35:l:51:THR:HG21	35:l:91:PRO:HG3	1.86	0.51
35:l:100:ILE:CD1	35:l:246:LEU:HG	2.40	0.51
40:r:104:ILE:O	40:r:108:MET:HG2	2.10	0.51
45:x:302:ARG:O	45:x:306:THR:HG23	2.09	0.51
60:AC:80:HIS:CE1	68:AL:185:ASN:HD22	2.27	0.51
60:AC:244:ASP:OD1	60:AC:248:ARG:N	2.44	0.51
63:AF:70:ASN:HB3	66:AJ:26:ASN:HB2	1.91	0.51
82:AJ:402:HEM:HBB2	82:AJ:402:HEM:HMB1	1.92	0.51
68:AL:361:ASP:OD1	68:AL:362:ARG:N	2.42	0.51
64:AT:39:ARG:NH2	64:AT:39:ARG:CG	2.73	0.51
82:AV:401:HEM:HBB2	82:AV:401:HEM:HMB1	1.91	0.51
68:AY:152:GLN:NE2	68:AY:252:GLY:C	2.68	0.51
1:BA:86:ARG:NE	1:BA:92:GLY:O	2.41	0.51
1:BA:382:CYS:HA	12:BM:74:ASN:HA	1.91	0.51
5:BF:36:PHE:HB2	5:BF:84:ALA:HB1	1.92	0.51
7:BH:111:GLN:NE2	15:BP:122:ARG:HB3	2.26	0.51
8:BI:42:PRO:HB3	21:BW:10:MET:HE1	1.90	0.51
9:BJ:168:SER:HA	9:BJ:184:LYS:CE	2.40	0.51
15:BP:88:ILE:HG22	15:BP:89:HIS:O	2.09	0.51
16:BQ:39:PRO:HB3	16:BQ:43:TRP:CE3	2.45	0.51
16:BQ:381:HIS:O	16:BQ:385:TYR:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:BV:203:PLX:H151	38:Bo:91:ALA:HB2	1.92	0.51
22:BY:86:TYR:HB3	22:BY:87:PRO:CB	2.40	0.51
27:Bd:135:ASP:C	27:Bd:156:ARG:HH21	2.18	0.51
35:Bl:74:THR:HG23	35:Bl:194:ASN:OD1	2.08	0.51
40:Br:104:ILE:O	40:Br:108:MET:HG2	2.10	0.51
40:Br:130:LEU:HD11	40:Br:150:LEU:HD12	1.92	0.51
40:Br:134:THR:O	40:Br:142:ARG:NE	2.33	0.51
41:Bs:223:PHE:O	41:Bs:227:GLU:HG3	2.11	0.51
45:Bx:75:ILE:O	45:Bx:79:GLY:HA3	2.11	0.51
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.51
6:G:123:GLU:HB2	6:G:128:PHE:O	2.09	0.51
12:M:645:ARG:O	12:M:648:GLU:HG2	2.10	0.51
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.51
21:W:81:ARG:HH22	42:u:64:ASN:HD21	1.56	0.51
6:X:155:TYR:CD1	25:b:23:LEU:HB3	2.46	0.51
24:a:160:MET:HE2	24:a:168:TRP:HB2	1.93	0.51
35:l:563:PRO:HG3	40:r:148:TYR:OH	2.10	0.51
44:w:115:GLU:HA	44:w:118:TYR:HD2	1.76	0.51
46:y:1:MET:SD	46:y:133:LEU:CD1	2.99	0.51
49:1:63:SER:O	49:1:67:ILE:HG13	2.10	0.51
58:AA:78:TYR:CE1	62:AE:65:GLU:CA	2.87	0.51
67:AK:146:PHE:HD2	67:AK:206:HIS:CE1	2.28	0.51
58:AN:12:ARG:HG3	68:AY:279:ASP:HA	1.91	0.51
60:AP:242:HIS:HB2	60:AP:251:LEU:HB2	1.92	0.51
4:BE:81:LEU:HD23	11:BL:64:LEU:HD22	1.90	0.51
9:BJ:206:ILE:HB	9:BJ:242:VAL:HG23	1.90	0.51
18:BT:83:ARG:NH1	18:BT:103:LEU:H	2.08	0.51
32:Bi:336:LEU:HD21	32:Bi:343:MET:SD	2.50	0.51
36:Bm:114:VAL:O	36:Bm:115:VAL:HG13	2.11	0.51
41:Bs:173:TRP:CZ3	41:Bs:262:LYS:HE2	2.45	0.51
43:Bv:39:MET:SD	43:Bv:58:TYR:HD1	2.34	0.51
46:By:186:SER:CB	46:By:213:LEU:HD22	2.41	0.51
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.11	0.51
2:B:127:THR:HB	2:B:144:ASP:OD1	2.10	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
12:M:76:ARG:HE	12:M:79:LEU:HD21	1.75	0.51
12:M:124:HIS:CD2	16:Q:375:MET:HE2	2.42	0.51
12:M:385:TYR:O	12:M:517:HIS:NE2	2.43	0.51
13:N:18:GLY:O	13:N:20:LEU:N	2.44	0.51
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.51
16:Q:39:PRO:HB3	16:Q:43:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.51
18:T:52:ARG:HB3	18:T:55:ARG:HH12	1.74	0.51
22:Y:74:TRP:CE3	22:Y:75:HIS:CA	2.91	0.51
33:j:18:MET:SD	41:s:72:ILE:HA	2.50	0.51
35:l:419:THR:HA	35:l:422:TYR:CE2	2.45	0.51
71:r:502:PLX:C7	71:r:502:PLX:C3	2.87	0.51
41:s:154:LEU:HD13	41:s:160:PHE:CD1	2.46	0.51
41:s:195:ARG:HG3	41:s:197:PRO:HD2	1.93	0.51
45:x:225:GLY:HA3	47:z:112:LEU:HD13	1.92	0.51
45:x:250:GLY:O	45:x:254:ILE:HG12	2.11	0.51
51:3:42:ARG:HH11	51:3:42:ARG:HG3	1.74	0.51
62:AE:21:GLU:O	62:AE:24:GLU:CB	2.59	0.51
63:AF:63:ILE:HD13	66:AJ:211:ILE:HG21	1.93	0.51
64:AG:9:ARG:HD3	63:AS:109:ALA:O	2.10	0.51
67:AK:299:VAL:HG21	68:AL:110:GLU:HG3	1.91	0.51
68:AL:460:GLY:HA2	68:AL:462:ILE:HG13	1.92	0.51
63:AS:71:LEU:HD21	66:AV:25:SER:HB2	1.92	0.51
68:AY:96:LEU:CD2	68:AY:161:ILE:HD13	2.40	0.51
2:BB:107:GLY:HA3	18:BT:71:LEU:HD23	1.91	0.51
2:BB:138:ARG:NH1	12:BM:238:PHE:HA	2.26	0.51
3:BC:162:TYR:O	16:BQ:123:LEU:HD21	2.10	0.51
4:BE:50:PHE:HB2	4:BE:52:LEU:CD1	2.41	0.51
11:BL:169:ARG:NH1	12:BM:426:ASP:HA	2.25	0.51
12:BM:81:GLU:CD	12:BM:108:LYS:HB3	2.36	0.51
17:BS:24:ALA:HA	41:Bs:93:ASN:HD22	1.76	0.51
20:BV:58:GLN:O	20:BV:62:THR:HG23	2.10	0.51
31:Bh:80:ARG:NH1	36:Bm:121:VAL:HG22	2.26	0.51
32:Bi:128:LEU:HD11	32:Bi:213:THR:HG22	1.93	0.51
33:Bj:70:ALA:HB1	36:Bm:58:ILE:HD11	1.92	0.51
35:Bl:419:THR:HA	35:Bl:422:TYR:CE2	2.45	0.51
36:Bm:27:TYR:HB3	36:Bm:82:TRP:CZ2	2.46	0.51
37:Bn:40:ASN:ND2	37:Bn:56:THR:HG23	2.25	0.51
39:Bp:104:LEU:HD21	39:Bp:119:PHE:CE1	2.41	0.51
41:Bs:195:ARG:HG3	41:Bs:197:PRO:HD2	1.93	0.51
45:Bx:11:ASN:ND2	45:Bx:14:ASP:H	2.07	0.51
1:A:181:LEU:HA	1:A:187:CYS:HB3	1.92	0.51
11:L:107:TRP:HZ3	11:L:118:ALA:HB2	1.76	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
12:M:569:GLN:NE2	12:M:622:ILE:HD12	2.26	0.51
13:N:30:THR:HG21	13:N:63:VAL:HG22	1.91	0.51
15:P:168:ARG:NH1	15:P:185:ARG:HG3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:228:ARG:CZ	16:Q:233:HIS:HB2	2.40	0.51
16:Q:381:HIS:O	16:Q:385:TYR:HD2	1.93	0.51
17:S:34:LYS:NZ	42:u:90:ASP:HB3	2.25	0.51
18:T:56:PHE:CD1	18:T:61:LYS:HB2	2.45	0.51
25:b:61:VAL:HA	25:b:64:VAL:HG12	1.93	0.51
26:c:69:GLY:CA	38:o:81:ARG:H	2.23	0.51
34:k:7:ASN:OD1	36:m:13:VAL:HG23	2.10	0.51
35:l:106:TRP:HB2	35:l:449:THR:OG1	2.09	0.51
35:l:119:LYS:O	35:l:123:ILE:HG12	2.11	0.51
36:m:114:VAL:O	36:m:115:VAL:HG13	2.11	0.51
37:n:40:ASN:ND2	37:n:56:THR:HG23	2.25	0.51
41:s:13:ILE:HG23	41:s:17:MET:HE3	1.92	0.51
41:s:167:THR:C	41:s:169:GLN:H	2.19	0.51
41:s:230:ASN:O	41:s:234:MET:HG2	2.11	0.51
43:v:56:ARG:O	43:v:60:ALA:HB2	2.10	0.51
46:y:139:ASP:OD1	46:y:140:ASN:N	2.44	0.51
64:AG:16:ASN:ND2	68:AL:442:ARG:HH12	2.09	0.51
67:AK:185:ALA:HB2	67:AK:249:ALA:HB1	1.92	0.51
65:AU:315:LYS:HZ2	75:AU:403:CDL:HB22	1.74	0.51
67:AW:180:ALA:HA	67:AW:254:ARG:NH1	2.26	0.51
67:AW:214:THR:HG22	67:AW:216:ALA:H	1.75	0.51
2:BB:99:HIS:HE1	2:BB:150:CYS:SG	2.34	0.51
5:BF:65:LEU:HB2	5:BF:79:LEU:HD11	1.92	0.51
8:BI:25:GLN:OE1	16:BQ:254:ARG:HD3	2.10	0.51
9:BJ:178:SER:OG	9:BJ:181:LEU:HB3	2.11	0.51
9:BJ:212:ARG:CG	9:BJ:212:ARG:NH1	2.73	0.51
12:BM:314:LEU:HD11	13:BN:140:PRO:HD2	1.92	0.51
12:BM:385:TYR:HB2	12:BM:517:HIS:NE2	2.25	0.51
12:BM:430:ALA:HA	12:BM:442:TYR:HB2	1.93	0.51
12:BM:492:ALA:O	12:BM:495:SER:OG	2.21	0.51
12:BM:569:GLN:NE2	12:BM:622:ILE:HD12	2.26	0.51
13:BN:30:THR:HG21	13:BN:63:VAL:HG22	1.91	0.51
15:BP:168:ARG:NH1	15:BP:185:ARG:HG3	2.26	0.51
16:BQ:133:LEU:HD12	16:BQ:229:PRO:HD3	1.93	0.51
16:BQ:203:LEU:HD11	16:BQ:258:LEU:HD11	1.93	0.51
24:Ba:160:MET:HE2	24:Ba:168:TRP:HB2	1.93	0.51
25:Bb:105:PHE:CD2	43:Bv:68:LYS:HB2	2.45	0.51
25:Bb:105:PHE:HZ	43:Bv:67:LEU:HB2	1.75	0.51
32:Bi:244:ILE:HB	32:Bi:245:PRO:HD3	1.93	0.51
34:Bk:7:ASN:OD1	36:Bm:13:VAL:HG23	2.10	0.51
35:Bl:15:LEU:O	35:Bl:18:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:343:SER:O	35:Bl:347:ILE:HD12	2.11	0.51
39:Bp:55:LYS:N	39:Bp:55:LYS:CE	2.73	0.51
45:Bx:347:LEU:HG	45:Bx:383:MET:HE3	1.93	0.51
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.51
2:B:72:LEU:HA	41:s:31:MET:HE1	1.92	0.51
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.51
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.26	0.51
16:Q:203:LEU:HD11	16:Q:258:LEU:HD11	1.93	0.51
20:V:58:GLN:O	20:V:62:THR:HG23	2.10	0.51
25:b:86:MET:HA	25:b:89:HIS:HB3	1.92	0.51
25:b:105:PHE:CD2	43:v:68:LYS:HB2	2.45	0.51
27:d:111:GLU:HB3	27:d:115:TYR:CB	2.41	0.51
27:d:135:ASP:C	27:d:156:ARG:HH21	2.18	0.51
28:e:87:MET:HE1	40:r:431:THR:HG21	1.92	0.51
34:k:8:ILE:CD1	34:k:8:ILE:N	2.73	0.51
35:l:512:LYS:O	39:p:40:PHE:HZ	1.91	0.51
39:p:170:ILE:O	39:p:173:ARG:HG3	2.11	0.51
40:r:61:LEU:HD22	40:r:241:TYR:CD1	2.45	0.51
40:r:120:ILE:O	40:r:124:THR:HG23	2.11	0.51
46:y:186:SER:CB	46:y:213:LEU:HD22	2.41	0.51
62:AE:29:PRO:HD2	65:AH:262:THR:HG21	1.91	0.51
76:AU:401:PEE:H57	66:AV:236:LEU:HD13	1.92	0.51
68:AY:168:ILE:O	68:AY:172:MET:HG2	2.11	0.51
1:BA:113:LEU:HD23	1:BA:113:LEU:C	2.35	0.51
9:BJ:84:TYR:HB2	9:BJ:91:ILE:HD11	1.92	0.51
12:BM:385:TYR:O	12:BM:517:HIS:NE2	2.43	0.51
15:BP:115:THR:HG22	16:BQ:423:LYS:HD3	1.91	0.51
25:Bb:19:ARG:NH2	39:Bp:173:ARG:HB2	2.26	0.51
32:Bi:243:LEU:HD21	75:Bi:401:CDL:H752	1.92	0.51
35:Bl:87:MET:O	35:Bl:91:PRO:HD3	2.11	0.51
35:Bl:575:ILE:O	35:Bl:578:SER:OG	2.16	0.51
39:Bp:170:ILE:O	39:Bp:173:ARG:HG3	2.11	0.51
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.51
2:B:74:TYR:CD2	41:s:33:LEU:HG	2.45	0.51
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.51
3:C:112:ALA:O	3:C:113:SER:OG	2.29	0.51
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.51
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	0.51
17:S:24:ALA:HA	41:s:93:ASN:HD22	1.76	0.51
22:Y:81:LEU:HD22	43:v:92:HIS:HD2	1.70	0.51
24:a:54:LEU:HD21	25:b:27:GLU:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:19:ARG:NH2	39:p:173:ARG:HB2	2.26	0.51
25:b:105:PHE:HZ	43:v:67:LEU:CB	2.23	0.51
28:e:112:TYR:O	40:r:45:ILE:HG23	2.11	0.51
30:g:29:ARG:HH21	42:u:172:LYS:HB3	1.76	0.51
35:l:190:ILE:CD1	35:l:196:TRP:NE1	2.73	0.51
35:l:194:ASN:HD22	38:o:127:LEU:HD12	1.74	0.51
45:x:240:HIS:HB3	45:x:241:PRO:HD3	1.92	0.51
46:y:59:GLN:N	46:y:62:GLU:HG3	2.24	0.51
48:0:64:PHE:CE1	49:1:66:ARG:HD2	2.46	0.51
65:AH:135:LEU:HA	65:AH:138:VAL:HG12	1.91	0.51
66:AJ:97:HIS:HE1	66:AJ:100:ARG:HH21	1.58	0.51
75:AJ:405:CDL:HB61	75:AJ:405:CDL:H312	1.90	0.51
67:AK:183:ARG:NH2	67:AK:183:ARG:CG	2.73	0.51
68:AL:334:ALA:H	68:AL:336:LYS:H	1.58	0.51
2:BB:65:PHE:O	2:BB:69:GLY:N	2.41	0.51
2:BB:201:ALA:HB1	13:BN:88:ARG:NH1	2.26	0.51
5:BF:30:SER:OG	5:BF:63:PRO:HG3	2.11	0.51
5:BF:72:GLY:HA3	12:BM:359:ASN:HB3	1.92	0.51
6:BG:112:SER:O	6:BG:115:GLN:HB3	2.11	0.51
7:BH:83:GLN:HG2	15:BP:107:GLN:NE2	2.26	0.51
9:BJ:209:ARG:HD2	15:BP:217:LYS:HE2	1.93	0.51
11:BL:61:ILE:HG12	11:BL:140:LYS:O	2.10	0.51
6:BX:85:TYR:HE2	22:BY:45:ARG:NH1	2.09	0.51
22:BY:86:TYR:CB	22:BY:87:PRO:CA	2.85	0.51
71:Bg:202:PLX:H1C2	71:Bg:202:PLX:H31	1.93	0.51
34:Bk:8:ILE:N	34:Bk:8:ILE:CD1	2.73	0.51
35:Bl:119:LYS:O	35:Bl:123:ILE:HG12	2.11	0.51
35:Bl:593:PHE:HB2	35:Bl:594:PRO:HD3	1.93	0.51
42:Bu:142:TYR:O	42:Bu:144:SER:N	2.44	0.51
48:B0:64:PHE:CE1	49:B1:66:ARG:HD2	2.46	0.51
2:B:51:VAL:HG22	2:B:54:ARG:NH1	2.26	0.51
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	0.51
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.51
3:C:162:TYR:O	16:Q:123:LEU:HD21	2.10	0.51
5:F:30:SER:OG	5:F:63:PRO:HG3	2.11	0.51
11:L:61:ILE:HG22	11:L:64:LEU:HD12	1.92	0.51
15:P:74:GLN:HB2	15:P:87:CYS:HB2	1.93	0.51
32:i:37:MET:HE3	32:i:41:ILE:HD11	1.93	0.51
32:i:128:LEU:HD11	32:i:213:THR:HG22	1.93	0.51
32:i:309:ASN:OD1	44:w:319:ILE:HD11	2.11	0.51
35:l:593:PHE:HB2	35:l:594:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:24:VAL:HG22	42:u:86:TRP:HE1	1.76	0.51
44:w:149:HIS:HE1	44:w:155:GLN:HB3	1.76	0.51
63:AF:43:ASP:OD2	63:AF:102:ARG:NH1	2.44	0.51
68:AL:285:ALA:HB2	68:AL:461:PRO:O	2.11	0.51
67:AW:95:SER:O	67:AW:99:ILE:HD12	2.11	0.51
1:BA:164:ASN:HB3	10:BK:77:HIS:HB2	1.91	0.51
6:BG:143:GLU:HA	6:BG:146:ASP:HB3	1.92	0.51
9:BJ:142:GLU:OE2	9:BJ:146:VAL:HG21	2.11	0.51
11:BL:85:ASN:OD1	11:BL:87:MET:N	2.36	0.51
12:BM:506:VAL:HG12	12:BM:508:GLY:N	2.24	0.51
16:BQ:69:VAL:HG12	16:BQ:72:PRO:CD	2.41	0.51
16:BQ:394:GLY:O	16:BQ:413:SER:OG	2.23	0.51
24:Ba:129:PRO:HG2	27:Bd:60:ARG:HH22	1.75	0.51
33:Bj:18:MET:SD	41:Bs:72:ILE:HA	2.50	0.51
35:Bl:68:TRP:HB2	35:Bl:76:LEU:CD1	2.41	0.51
35:Bl:272:LEU:O	35:Bl:275:THR:OG1	2.18	0.51
41:Bs:230:ASN:O	41:Bs:234:MET:HG2	2.11	0.51
43:Bv:5:LEU:O	43:Bv:8:ARG:HG2	2.11	0.51
44:Bw:331:PHE:CZ	44:Bw:337:ARG:HB3	2.46	0.51
45:Bx:232:GLN:HB2	45:Bx:292:MET:HE3	1.93	0.51
45:Bx:240:HIS:HB3	45:Bx:241:PRO:HD3	1.92	0.51
46:By:100:MET:CE	46:By:157:GLU:HG3	2.40	0.51
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.51
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.51
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.51
35:l:68:TRP:HB2	35:l:76:LEU:CD1	2.41	0.51
35:l:136:ASN:OD1	35:l:137:LEU:N	2.44	0.51
40:r:130:LEU:HD11	40:r:150:LEU:HD12	1.92	0.51
41:s:180:PRO:O	41:s:184:MET:HG2	2.11	0.51
44:w:128:SER:OG	44:w:173:MET:SD	2.69	0.51
66:AJ:326:TRP:CH2	76:AJ:403:PEE:H50	2.46	0.51
65:AU:193:LEU:HD12	65:AU:194:PRO:HD2	1.93	0.51
66:AV:263:ASN:OD1	66:AV:264:THR:N	2.44	0.51
68:AY:182:VAL:HG12	68:AY:186:TYR:CE2	2.46	0.51
68:AY:304:LEU:HD13	68:AY:354:LEU:HD11	1.93	0.51
7:BH:114:TRP:NE1	16:BQ:394:GLY:HA2	2.25	0.51
9:BJ:54:ILE:HA	9:BJ:124:ASN:HD21	1.76	0.51
12:BM:124:HIS:CD2	16:BQ:375:MET:HE2	2.43	0.51
12:BM:213:MET:HG3	12:BM:215:MET:HG3	1.93	0.51
12:BM:464:GLN:HE22	12:BM:467:LYS:HE2	1.75	0.51
13:BN:34:LYS:NZ	13:BN:58:ARG:HG2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bf:55:TRP:CE2	30:Bg:65:THR:HG22	2.46	0.51
44:Bw:115:GLU:HA	44:Bw:118:TYR:HD2	1.76	0.51
46:By:1:MET:SD	46:By:133:LEU:CD1	2.99	0.51
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.47	0.50
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.50
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.50
22:Y:72:ARG:NH1	35:l:466:PHE:HD1	2.02	0.50
32:i:329:LEU:O	32:i:333:THR:HG23	2.11	0.50
34:k:58:ILE:HG23	36:m:145:LEU:HD12	1.92	0.50
35:l:87:MET:O	35:l:91:PRO:HD3	2.11	0.50
41:s:223:PHE:O	41:s:227:GLU:HG3	2.11	0.50
42:u:35:GLN:O	42:u:37:ASP:N	2.34	0.50
43:v:5:LEU:O	43:v:8:ARG:HG2	2.11	0.50
44:w:137:SER:C	44:w:139:ARG:H	2.19	0.50
44:w:331:PHE:CZ	44:w:337:ARG:HB3	2.46	0.50
45:x:145:LEU:HD21	47:z:32:THR:HG21	1.93	0.50
45:x:377:PHE:HA	45:x:380:VAL:HG22	1.93	0.50
63:AF:109:ALA:O	64:AT:9:ARG:HD3	2.11	0.50
67:AK:173:VAL:HG11	67:AK:339:TYR:HE1	1.77	0.50
66:AV:10:LEU:HD21	76:AY:502:PEE:H45	1.77	0.50
66:AV:282:ARG:NH1	66:AV:343:VAL:HG22	2.27	0.50
1:BA:300:ILE:HA	1:BA:304:ALA:HB3	1.93	0.50
2:BB:36:TYR:HD2	8:BI:104:TRP:HB2	1.77	0.50
2:BB:37:LYS:HE2	8:BI:110:GLN:O	2.11	0.50
2:BB:109:GLU:OE2	2:BB:139:ARG:HD2	2.10	0.50
2:BB:127:THR:HB	2:BB:144:ASP:OD1	2.10	0.50
13:BN:18:GLY:O	13:BN:20:LEU:N	2.44	0.50
16:BQ:145:MET:HB3	16:BQ:227:ILE:HD12	1.92	0.50
16:BQ:304:LYS:HE3	16:BQ:316:PHE:CE1	2.46	0.50
6:BX:88:LYS:HZ1	6:BX:98:LEU:HD22	1.76	0.50
6:BX:155:TYR:CD1	25:Bb:23:LEU:HB3	2.46	0.50
24:Ba:184:LYS:O	24:Ba:186:THR:N	2.45	0.50
28:Be:112:TYR:O	40:Br:45:ILE:HG23	2.11	0.50
32:Bi:309:ASN:OD1	44:Bw:319:ILE:HD11	2.11	0.50
35:Bl:592:PHE:CE2	35:Bl:596:ILE:HD11	2.45	0.50
41:Bs:13:ILE:HG23	41:Bs:17:MET:HE3	1.92	0.50
44:Bw:54:THR:C	44:Bw:56:ARG:H	2.19	0.50
46:By:33:LEU:HD23	53:B5:28:SER:HB2	1.91	0.50
46:By:139:ASP:OD1	46:By:140:ASN:N	2.44	0.50
1:A:112:TYR:CD1	1:A:155:TYR:HE2	2.30	0.50
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:E:201:8Q1:C30	72:E:201:8Q1:N36	2.73	0.50
6:G:112:SER:O	6:G:115:GLN:HB3	2.11	0.50
11:L:75:ARG:HH11	11:L:104:ARG:NE	2.09	0.50
12:M:372:PHE:CD1	12:M:481:LEU:HD13	2.46	0.50
16:Q:85:GLY:H	16:Q:88:HIS:HE2	1.58	0.50
16:Q:291:VAL:N	16:Q:294:ARG:HH21	2.09	0.50
16:Q:412:VAL:O	16:Q:420:TYR:N	2.43	0.50
20:V:39:TYR:HD2	75:V:201:CDL:H721	1.76	0.50
25:b:22:TRP:O	25:b:25:ASP:HB3	2.10	0.50
29:f:47:THR:HG22	71:g:203:PLX:H1A1	1.94	0.50
40:r:286:ILE:O	40:r:289:SER:OG	2.23	0.50
41:s:106:LEU:HD21	41:s:150:LEU:HD12	1.94	0.50
42:u:142:TYR:O	42:u:144:SER:N	2.44	0.50
58:AA:28:PRO:HB2	58:AA:29:HIS:CE1	2.46	0.50
75:AJ:405:CDL:H312	75:AJ:405:CDL:OB4	2.10	0.50
75:AL:502:CDL:H772	76:AL:503:PEE:C43	2.41	0.50
58:AN:42:ILE:HG22	58:AN:46:PHE:CE2	2.47	0.50
60:AP:239:HIS:HB2	74:AP:301:FES:S1	2.50	0.50
66:AV:149:LEU:HD21	66:AV:281:LEU:CD2	2.31	0.50
68:AY:424:ILE:HG23	68:AY:429:TRP:NE1	2.12	0.50
1:BA:152:ARG:HH12	10:BK:99:PRO:HB3	1.76	0.50
12:BM:645:ARG:O	12:BM:648:GLU:HG2	2.10	0.50
16:BQ:87:GLN:O	16:BQ:88:HIS:O	2.30	0.50
16:BQ:175:GLY:O	16:BQ:178:THR:OG1	2.29	0.50
22:BY:51:THR:HG21	35:Bl:446:ASN:HD21	1.76	0.50
22:BY:73:PHE:CD1	22:BY:73:PHE:C	2.88	0.50
32:Bi:232:ARG:NH2	44:Bw:306:ASN:OD1	2.29	0.50
35:Bl:100:ILE:CD1	35:Bl:246:LEU:HG	2.40	0.50
42:Bu:24:VAL:HG22	42:Bu:86:TRP:HE1	1.76	0.50
45:Bx:145:LEU:HD21	47:Bz:32:THR:HG21	1.93	0.50
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.50
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.50
4:E:50:PHE:HB2	4:E:52:LEU:CD1	2.40	0.50
16:Q:69:VAL:HG12	16:Q:72:PRO:CD	2.41	0.50
17:S:37:ARG:O	21:W:143:TYR:OH	2.27	0.50
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.88	0.50
32:i:234:TRP:O	32:i:238:THR:HG22	2.11	0.50
32:i:244:ILE:HB	32:i:245:PRO:HD3	1.93	0.50
36:m:67:PHE:O	36:m:71:THR:HG23	2.11	0.50
42:u:85:TYR:OH	42:u:104:GLN:NE2	2.45	0.50
45:x:11:ASN:ND2	45:x:14:ASP:H	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AH:402:HEC:HHC	81:AH:402:HEC:HBB3	1.92	0.50
66:AJ:131:TYR:O	66:AJ:134:PRO:HD2	2.11	0.50
68:AL:121:ASN:ND2	68:AL:132:TYR:OH	2.36	0.50
68:AL:437:ASP:OD1	68:AL:438:ALA:N	2.44	0.50
1:BA:116:ASN:HD22	70:BA:502:FMN:C9	2.22	0.50
1:BA:118:ASP:O	1:BA:119:GLU:C	2.54	0.50
12:BM:532:PRO:HB2	12:BM:534:VAL:HG23	1.93	0.50
14:BO:129:LYS:HB3	14:BO:168:LEU:HG	1.91	0.50
14:BO:135:CYS:O	14:BO:145:SER:OG	2.25	0.50
26:Bc:69:GLY:CA	38:Bo:81:ARG:H	2.23	0.50
31:Bh:99:ILE:HD12	31:Bh:101:LYS:HB2	1.93	0.50
35:Bl:485:TYR:O	35:Bl:489:THR:HG23	2.10	0.50
40:Br:113:THR:O	40:Br:176:ILE:HG13	2.12	0.50
44:Bw:128:SER:OG	44:Bw:173:MET:SD	2.69	0.50
44:Bw:198:TYR:OH	44:Bw:304:VAL:HG12	2.10	0.50
6:G:143:GLU:HA	6:G:146:ASP:HB3	1.92	0.50
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.50
12:M:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.50
13:N:40:GLY:HA3	13:N:48:TYR:HB2	1.92	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
25:b:92:GLU:HG2	25:b:93:LYS:HG3	1.93	0.50
28:e:56:GLN:HG2	44:w:320:GLY:HA3	1.93	0.50
35:l:42:SER:O	35:l:46:ILE:HG12	2.11	0.50
40:r:144:ASN:OD1	40:r:145:ALA:N	2.45	0.50
44:w:54:THR:C	44:w:56:ARG:H	2.19	0.50
45:x:75:ILE:O	45:x:79:GLY:HA3	2.11	0.50
51:3:44:ARG:HD2	51:3:74:ARG:O	2.11	0.50
58:AA:74:ASN:N	58:AA:75:PRO:HD2	2.27	0.50
63:AF:29:LYS:CB	63:AF:75:ILE:HD11	2.22	0.50
64:AG:39:ARG:HB2	75:AG:101:CDL:HB31	1.93	0.50
67:AK:92:LYS:HD2	67:AK:143:ALA:HB1	1.93	0.50
67:AK:378:LEU:HD13	67:AK:416:ILE:HD11	1.94	0.50
68:AL:470:ARG:NH1	75:AL:502:CDL:HA31	2.25	0.50
64:AT:40:LEU:HD12	64:AT:41:ILE:CA	2.36	0.50
67:AW:57:PRO:O	67:AW:127:ARG:HG3	2.11	0.50
2:BB:72:LEU:HA	41:Bs:31:MET:HE1	1.92	0.50
2:BB:108:GLU:OE1	18:BT:68:ALA:HB1	2.12	0.50
3:BC:137:VAL:HA	3:BC:140:GLN:CD	2.36	0.50
12:BM:302:LEU:N	12:BM:571:HIS:O	2.33	0.50
12:BM:372:PHE:CD1	12:BM:481:LEU:HD13	2.46	0.50
16:BQ:149:GLN:HG3	16:BQ:171:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ba:101:ILE:HG13	27:Bd:58:TYR:HB3	1.94	0.50
29:Bf:30:TYR:HD2	44:Bw:98:THR:HA	1.77	0.50
34:Bk:81:ILE:HG22	34:Bk:87:LEU:HA	1.92	0.50
38:Bo:6:TYR:OH	38:Bo:12:ARG:HG2	2.11	0.50
40:Br:355:MET:HA	40:Br:358:TRP:HD1	1.77	0.50
44:Bw:65:ASN:O	44:Bw:68:THR:OG1	2.20	0.50
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.50
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	0.50
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	0.50
9:J:159:ALA:HB3	9:J:161:VAL:HG23	1.93	0.50
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.50
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.50
31:h:6:ILE:HB	32:i:22:LEU:HD22	1.93	0.50
31:h:80:ARG:NH1	36:m:121:VAL:HG22	2.26	0.50
32:i:150:ASN:HD21	35:l:602:ILE:HD13	1.77	0.50
36:m:27:TYR:HB3	36:m:82:TRP:CZ2	2.46	0.50
37:n:50:GLN:OE1	37:n:51:PRO:HD2	2.11	0.50
44:w:248:GLU:OE1	44:w:252:LYS:NZ	2.45	0.50
45:x:184:PHE:H	45:x:256:HIS:CE1	2.29	0.50
46:y:136:LEU:HB3	46:y:193:TYR:CD2	2.46	0.50
58:AA:20:SER:HB3	58:AA:23:GLU:HG2	1.94	0.50
58:AN:29:HIS:ND1	58:AN:33:LYS:HB2	2.26	0.50
59:AO:28:PRO:HG3	67:AW:324:SER:OG	2.10	0.50
66:AV:186:PRO:HA	66:AV:189:ILE:HD12	1.94	0.50
68:AY:230:VAL:HG21	68:AY:418:LEU:HD11	1.92	0.50
1:BA:423:THR:OG1	69:BA:501:SF4:S4	2.68	0.50
3:BC:112:ALA:O	3:BC:113:SER:OG	2.29	0.50
7:BH:90:LEU:HD11	15:BP:99:PHE:HD1	1.76	0.50
15:BP:74:GLN:HB2	15:BP:87:CYS:HB2	1.93	0.50
71:BV:203:PLX:H201	38:Bo:95:PHE:CZ	2.47	0.50
6:BX:90:TYR:HD2	6:BX:93:ILE:HD12	1.77	0.50
23:BZ:29:LEU:HD23	39:Bp:35:ASP:OD1	2.12	0.50
26:Bc:123:PRO:HG3	39:Bp:75:GLN:NE2	2.25	0.50
32:Bi:234:TRP:O	32:Bi:238:THR:HG22	2.11	0.50
35:Bl:306:THR:HA	35:Bl:336:LYS:NZ	2.27	0.50
35:Bl:332:HIS:HA	35:Bl:335:PHE:CE2	2.46	0.50
41:Bs:106:LEU:HD21	41:Bs:150:LEU:HD12	1.94	0.50
44:Bw:139:ARG:HD2	44:Bw:166:ASP:OD2	2.12	0.50
45:Bx:40:GLU:HG2	45:Bx:54:TYR:CD1	2.46	0.50
45:Bx:250:GLY:O	45:Bx:254:ILE:HG12	2.11	0.50
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:53:ARG:HH21	31:h:105:ARG:HD3	1.77	0.50
24:a:101:ILE:HG13	27:d:58:TYR:HB3	1.94	0.50
33:j:28:ASN:HB2	33:j:30:TYR:CZ	2.47	0.50
35:l:37:LYS:HZ3	35:l:98:TRP:CD1	2.30	0.50
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.46	0.50
38:o:6:TYR:OH	38:o:12:ARG:HG2	2.11	0.50
41:s:303:TRP:NE1	41:s:307:MET:SD	2.85	0.50
44:w:218:ILE:HD11	44:w:226:GLU:HB3	1.93	0.50
65:AH:289:GLY:HA2	65:AH:292:MET:HG2	1.93	0.50
66:AV:96:LEU:CD2	76:AV:403:PEE:H26	2.40	0.50
67:AW:107:GLY:O	68:AY:397:ASN:ND2	2.41	0.50
68:AY:119:HIS:HB2	68:AY:134:LYS:HD2	1.93	0.50
1:BA:443:ARG:HB3	1:BA:444:PRO:HD3	1.94	0.50
2:BB:74:TYR:CD2	41:Bs:33:LEU:HG	2.45	0.50
4:BE:19:PRO:HA	4:BE:77:ARG:HD3	1.93	0.50
7:BH:107:PRO:HB2	7:BH:111:GLN:HB2	1.93	0.50
12:BM:50:LEU:HA	12:BM:60:ILE:HD13	1.93	0.50
16:BQ:291:VAL:N	16:BQ:294:ARG:HH21	2.09	0.50
16:BQ:360:ASP:O	16:BQ:364:SER:OG	2.29	0.50
6:BX:103:HIS:HB2	6:BX:106:LYS:HB3	1.94	0.50
25:Bb:86:MET:HA	25:Bb:89:HIS:HB3	1.92	0.50
29:Bf:47:THR:HG22	71:Bg:203:PLX:H1A1	1.94	0.50
32:Bi:137:ALA:HB3	32:Bi:138:PRO:HD3	1.93	0.50
35:Bl:594:PRO:O	35:Bl:598:THR:HG23	2.12	0.50
36:Bm:67:PHE:O	36:Bm:71:THR:HG23	2.11	0.50
37:Bn:50:GLN:OE1	37:Bn:51:PRO:HD2	2.11	0.50
40:Br:144:ASN:OD1	40:Br:145:ALA:N	2.45	0.50
44:Bw:218:ILE:HD11	44:Bw:226:GLU:HB3	1.93	0.50
44:Bw:248:GLU:OE1	44:Bw:252:LYS:NZ	2.45	0.50
46:By:136:LEU:HB3	46:By:193:TYR:CD2	2.46	0.50
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.50
1:A:118:ASP:O	1:A:159:ARG:CD	2.60	0.50
2:B:36:TYR:HD2	8:I:104:TRP:HB2	1.77	0.50
2:B:40:ASN:O	2:B:42:GLN:N	2.43	0.50
2:B:108:GLU:OE1	18:T:68:ALA:HB1	2.12	0.50
3:C:73:TRP:HD1	3:C:76:ARG:NH2	2.10	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.50
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.50
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	0.50
9:J:142:GLU:OE2	9:J:146:VAL:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:168:SER:N	9:J:201:VAL:O	2.40	0.50
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.77	0.50
12:M:61:PRO:HG2	12:M:113:ARG:NE	2.26	0.50
15:P:202:PHE:HB2	15:P:203:PRO:HD2	1.92	0.50
16:Q:85:GLY:CA	33:j:39:CYS:CB	2.90	0.50
16:Q:87:GLN:O	16:Q:88:HIS:O	2.30	0.50
17:S:34:LYS:HZ1	42:u:90:ASP:HB3	1.77	0.50
20:V:62:THR:HG22	20:V:104:ARG:NE	2.27	0.50
71:b:201:PLX:O3	71:b:201:PLX:H72	2.10	0.50
26:c:52:ALA:CB	26:c:59:VAL:HA	2.42	0.50
26:c:111:MET:HG3	40:r:278:ARG:HH12	1.77	0.50
29:f:30:TYR:HD2	44:w:98:THR:HA	1.77	0.50
29:f:55:TRP:CE2	30:g:65:THR:HG22	2.46	0.50
32:i:117:GLU:OE1	32:i:117:GLU:N	2.41	0.50
35:l:428:LEU:HD23	35:l:432:THR:HG21	1.93	0.50
40:r:127:ILE:HB	40:r:128:PRO:HD3	1.94	0.50
40:r:271:MET:O	40:r:275:ILE:HG13	2.11	0.50
40:r:423:ILE:HD12	40:r:425:ASN:H	1.75	0.50
50:2:37:LYS:N	50:2:37:LYS:HD3	2.27	0.50
67:AW:105:ALA:HA	68:AY:390:ARG:HG3	1.94	0.50
67:AW:288:VAL:O	67:AW:292:VAL:HG23	2.11	0.50
68:AY:119:HIS:HB2	68:AY:134:LYS:HB3	1.93	0.50
2:BB:51:VAL:HG22	2:BB:54:ARG:NH1	2.26	0.50
3:BC:209:ILE:HG21	9:BJ:86:CYS:O	2.11	0.50
4:BE:50:PHE:HE1	4:BE:96:VAL:HG13	1.76	0.50
9:BJ:64:PHE:HE2	9:BJ:242:VAL:HG21	1.77	0.50
12:BM:171:THR:HB	12:BM:173:MET:HE3	1.94	0.50
20:BV:12:ILE:HG22	20:BV:13:PRO:O	2.11	0.50
27:Bd:110:ARG:NH1	27:Bd:110:ARG:CG	2.73	0.50
27:Bd:111:GLU:HB3	27:Bd:115:TYR:CB	2.41	0.50
32:Bi:98:ILE:O	32:Bi:102:MET:HG2	2.12	0.50
75:Bn:101:CDL:HB62	42:Bu:172:LYS:HB2	1.93	0.50
41:Bs:154:LEU:HD13	41:Bs:160:PHE:CD1	2.46	0.50
44:Bw:121:PRO:HG2	44:Bw:178:PHE:HB3	1.93	0.50
1:A:116:ASN:HD21	70:A:502:FMN:C8	2.22	0.50
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.77	0.50
1:A:443:ARG:HB3	1:A:444:PRO:HD3	1.94	0.50
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	0.50
9:J:62:THR:HB	73:J:401:NDP:HO3A	1.76	0.50
9:J:179:ARG:HB3	9:J:179:ARG:NH1	2.27	0.50
9:J:365:GLU:N	9:J:365:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:133:ASP:O	11:L:136:SER:OG	2.20	0.50
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.50
12:M:213:MET:HG3	12:M:215:MET:HG3	1.93	0.50
12:M:381:LEU:HB2	12:M:384:ASN:OD1	2.12	0.50
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.50
16:Q:175:GLY:O	16:Q:178:THR:OG1	2.29	0.50
16:Q:424:ILE:O	16:Q:463:ARG:NE	2.45	0.50
6:X:88:LYS:HZ2	6:X:98:LEU:HD13	1.77	0.50
25:b:113:THR:OG1	25:b:114:GLY:N	2.44	0.50
30:g:38:TYR:CE2	30:g:42:LEU:HD11	2.47	0.50
31:h:101:LYS:C	31:h:104:PRO:HD2	2.37	0.50
32:i:98:ILE:O	32:i:102:MET:HG2	2.12	0.50
33:j:65:PHE:HA	33:j:68:GLU:HB2	1.93	0.50
43:v:39:MET:SD	43:v:58:TYR:HD1	2.34	0.50
60:AC:183:GLU:HA	60:AC:186:GLN:HG2	1.93	0.50
60:AP:160:PRO:HD2	60:AP:163:LYS:HD3	1.94	0.50
61:AQ:53:TRP:NE1	65:AU:139:CYS:O	2.45	0.50
63:AS:34:ARG:NH2	63:AS:92:GLU:OE2	2.45	0.50
66:AV:276:PHE:O	66:AV:279:THR:OG1	2.24	0.50
68:AY:437:ASP:OD1	68:AY:438:ALA:N	2.43	0.50
2:BB:68:LEU:CD1	41:Bs:272:TRP:HE1	2.25	0.50
9:BJ:62:THR:HB	73:BJ:401:NDP:HO3A	1.77	0.50
9:BJ:161:VAL:HG12	9:BJ:163:LYS:H	1.76	0.50
12:BM:151:SER:OG	16:BQ:374:SER:HB2	2.11	0.50
12:BM:381:LEU:HB2	12:BM:384:ASN:OD1	2.12	0.50
13:BN:40:GLY:HA3	13:BN:48:TYR:HB2	1.92	0.50
18:BT:80:VAL:HG12	18:BT:82:THR:H	1.76	0.50
18:BT:89:GLY:HA2	18:BT:115:CYS:SG	2.52	0.50
20:BV:39:TYR:HD2	75:BV:201:CDL:H721	1.76	0.50
25:Bb:61:VAL:HA	25:Bb:64:VAL:HG12	1.93	0.50
32:Bi:234:TRP:C	32:Bi:238:THR:HG22	2.37	0.50
32:Bi:329:LEU:O	32:Bi:333:THR:HG23	2.11	0.50
35:Bl:512:LYS:HB2	54:B6:16:ASN:HB2	1.94	0.50
40:Br:120:ILE:O	40:Br:124:THR:HG23	2.11	0.50
41:Bs:9:LEU:HD13	41:Bs:95:LEU:HD12	1.94	0.50
41:Bs:180:PRO:O	41:Bs:184:MET:HG2	2.11	0.50
41:Bs:303:TRP:NE1	41:Bs:307:MET:SD	2.85	0.50
1:A:300:ILE:HA	1:A:304:ALA:HB3	1.93	0.50
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.50
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.50
9:J:201:VAL:HG13	9:J:265:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:209:TYR:O	12:M:210:ILE:HG22	2.12	0.50
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.50
18:T:89:GLY:HA2	18:T:115:CYS:SG	2.52	0.50
20:V:12:ILE:HG22	20:V:13:PRO:O	2.11	0.50
21:W:33:TYR:O	21:W:34:SER:OG	2.27	0.50
32:i:315:TRP:HZ3	44:w:327:VAL:HG12	1.76	0.50
35:l:306:THR:HA	35:l:336:LYS:NZ	2.27	0.50
41:s:79:LEU:HD11	41:s:222:LEU:HD22	1.94	0.50
44:w:335:PRO:HA	44:w:338:LYS:HG3	1.94	0.50
46:y:78:LEU:HB2	46:y:79:PRO:CD	2.38	0.50
60:AC:132:ALA:CB	76:AH:401:PEE:H24	2.41	0.50
65:AH:125:HIS:HB3	65:AH:197:LEU:HD13	1.94	0.50
66:AJ:126:THR:O	66:AJ:182:HIS:ND1	2.45	0.50
67:AK:38:LEU:HB3	67:AK:52:LEU:HB2	1.94	0.50
67:AK:195:TYR:O	67:AK:199:LYS:NZ	2.30	0.50
67:AK:239:ASN:OD1	67:AK:240:MET:N	2.45	0.50
60:AP:100:THR:HG23	68:AY:266:THR:HB	1.94	0.50
60:AP:124:GLY:HA3	65:AU:299:LEU:HD21	1.94	0.50
64:AT:38:TRP:CD2	64:AT:41:ILE:HD13	2.47	0.50
66:AV:10:LEU:CD2	76:AY:502:PEE:H45	2.34	0.50
66:AV:281:LEU:HD11	66:AV:294:LEU:HD22	1.94	0.50
68:AY:152:GLN:NE2	68:AY:252:GLY:N	2.58	0.50
68:AY:230:VAL:HG21	68:AY:418:LEU:HD13	1.92	0.50
3:BC:79:LEU:HB2	3:BC:108:VAL:HG12	1.94	0.50
3:BC:100:ARG:NH2	16:BQ:208:GLU:HB3	2.18	0.50
7:BH:107:PRO:HD3	15:BP:74:GLN:HE22	1.76	0.50
12:BM:126:LEU:HD23	16:BQ:375:MET:SD	2.52	0.50
12:BM:209:TYR:O	12:BM:210:ILE:HG22	2.12	0.50
12:BM:299:ARG:HG2	12:BM:300:GLN:N	2.19	0.50
12:BM:307:VAL:HB	12:BM:317:THR:HG21	1.93	0.50
15:BP:74:GLN:HB2	15:BP:87:CYS:SG	2.52	0.50
16:BQ:262:LEU:HD22	16:BQ:268:TRP:NE1	2.18	0.50
22:BY:86:TYR:HB3	22:BY:87:PRO:HB3	1.93	0.50
28:Be:56:GLN:HG2	44:Bw:320:GLY:HA3	1.93	0.50
30:Bg:29:ARG:HH21	42:Bu:172:LYS:HB3	1.76	0.50
32:Bi:9:ILE:O	32:Bi:12:THR:OG1	2.30	0.50
32:Bi:37:MET:HE3	32:Bi:41:ILE:HD11	1.93	0.50
34:Bk:60:PRO:O	34:Bk:63:MET:HB2	2.12	0.50
36:Bm:33:ILE:HA	36:Bm:60:LEU:HD22	1.94	0.50
40:Br:94:LEU:O	40:Br:97:SER:OG	2.21	0.50
1:A:87:GLY:N	1:A:93:PHE:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:O	1:A:380:GLY:N	2.45	0.49
2:B:90:PRO:HD2	3:C:100:ARG:HH11	1.74	0.49
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.21	0.49
23:Z:29:LEU:HD23	39:p:35:ASP:OD1	2.12	0.49
24:a:184:LYS:O	24:a:186:THR:N	2.45	0.49
25:b:33:PRO:HD2	39:p:114:MET:O	2.12	0.49
32:i:234:TRP:C	32:i:238:THR:HG22	2.37	0.49
35:l:44:PHE:O	35:l:47:SER:OG	2.24	0.49
35:l:383:MET:SD	35:l:384:PRO:HD2	2.52	0.49
44:w:305:LEU:O	44:w:308:THR:HG22	2.12	0.49
67:AK:438:MET:HB2	67:AK:450:VAL:HG11	1.89	0.49
64:AT:40:LEU:C	64:AT:40:LEU:CD1	2.85	0.49
65:AU:155:GLN:HA	65:AU:166:MET:HA	1.94	0.49
67:AW:254:ARG:HG2	67:AW:256:GLY:H	1.77	0.49
67:AW:309:LEU:HD23	67:AW:323:VAL:HG12	1.93	0.49
67:AW:413:LEU:HA	67:AW:416:ILE:HG22	1.94	0.49
68:AY:164:GLU:O	68:AY:168:ILE:HG12	2.12	0.49
1:BA:71:LYS:HA	1:BA:147:ARG:HH21	1.77	0.49
1:BA:87:GLY:N	1:BA:93:PHE:O	2.44	0.49
1:BA:130:ILE:HD11	1:BA:275:LEU:HD21	1.94	0.49
1:BA:378:SER:O	1:BA:380:GLY:N	2.45	0.49
2:BB:175:THR:HA	13:BN:118:THR:HG21	1.94	0.49
3:BC:73:TRP:HD1	3:BC:76:ARG:NH2	2.10	0.49
12:BM:32:ILE:HG23	12:BM:98:LYS:HB2	1.93	0.49
15:BP:190:ASP:OD1	15:BP:191:TYR:N	2.45	0.49
15:BP:202:PHE:HB2	15:BP:203:PRO:HD2	1.92	0.49
16:BQ:143:SER:HB2	16:BQ:178:THR:HB	1.93	0.49
16:BQ:424:ILE:O	16:BQ:463:ARG:NE	2.45	0.49
21:BW:101:VAL:HG21	31:Bh:82:GLN:NE2	2.28	0.49
6:BX:77:GLU:HB2	23:BZ:13:LYS:HE2	1.93	0.49
25:Bb:108:ASP:CG	25:Bb:109:THR:H	2.20	0.49
32:Bi:150:ASN:HD21	35:Bl:602:ILE:HD13	1.76	0.49
32:Bi:274:ASN:O	32:Bi:275:SER:OG	2.30	0.49
33:Bj:28:ASN:HB2	33:Bj:30:TYR:CZ	2.47	0.49
35:Bl:136:ASN:OD1	35:Bl:137:LEU:N	2.44	0.49
35:Bl:428:LEU:HD23	35:Bl:432:THR:HG21	1.93	0.49
41:Bs:17:MET:CE	41:Bs:232:ILE:HD12	2.37	0.49
44:Bw:149:HIS:HE1	44:Bw:155:GLN:HB3	1.76	0.49
50:B2:37:LYS:HD3	50:B2:37:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:B3:5:LYS:NZ	51:B3:5:LYS:HB3	2.27	0.49
2:B:68:LEU:CD1	41:s:272:TRP:HE1	2.25	0.49
16:Q:149:GLN:HG3	16:Q:171:ARG:HD3	1.94	0.49
6:X:85:TYR:HE2	22:Y:45:ARG:NH1	2.09	0.49
35:l:343:SER:O	35:l:347:ILE:HD12	2.11	0.49
75:AG:101:CDL:H741	66:AV:156:ILE:CG2	2.43	0.49
65:AH:323:PRO:HB2	65:AH:325:LYS:HG2	1.93	0.49
66:AJ:62:ALA:O	66:AJ:65:SER:OG	2.22	0.49
67:AK:82:LEU:HD21	67:AK:151:VAL:HG13	1.94	0.49
66:AV:10:LEU:CD2	76:AY:502:PEE:C26	2.91	0.49
67:AW:444:LEU:HD23	67:AW:447:THR:CG2	2.42	0.49
68:AY:75:ILE:HG12	68:AY:229:MET:SD	2.52	0.49
5:BF:48:ASN:HD21	5:BF:53:ILE:HD11	1.77	0.49
7:BH:40:LYS:HA	7:BH:45:ARG:HD3	1.94	0.49
7:BH:115:PRO:O	15:BP:247:GLN:NE2	2.45	0.49
12:BM:128:CYS:CB	12:BM:129:PRO:CD	2.86	0.49
16:BQ:196:ALA:O	16:BQ:198:THR:N	2.41	0.49
26:Bc:52:ALA:CB	26:Bc:59:VAL:HA	2.42	0.49
32:Bi:92:GLN:O	32:Bi:95:SER:OG	2.21	0.49
40:Br:220:HIS:HE1	40:Br:232:ALA:HB2	1.77	0.49
45:Bx:266:GLU:HB2	45:Bx:267:PRO:HD2	1.94	0.49
1:A:318:ILE:HD11	1:A:355:ILE:HD13	1.94	0.49
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	0.49
12:M:171:THR:HB	12:M:173:MET:HE3	1.94	0.49
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.49
19:U:58:ARG:NH2	42:u:49:GLU:OE1	2.43	0.49
22:Y:86:TYR:HB3	22:Y:87:PRO:CB	2.40	0.49
24:a:115:HIS:HE1	24:a:117:ILE:HD12	1.77	0.49
71:b:201:PLX:H21	27:d:43:ARG:HH22	1.77	0.49
27:d:76:ILE:O	27:d:80:TYR:N	2.41	0.49
32:i:137:ALA:HB3	32:i:138:PRO:HD3	1.93	0.49
35:l:371:THR:O	35:l:374:THR:OG1	2.28	0.49
35:l:594:PRO:O	35:l:598:THR:HG23	2.12	0.49
38:o:95:PHE:CZ	71:AN:101:PLX:H201	2.47	0.49
40:r:220:HIS:CE1	40:r:232:ALA:HB2	2.47	0.49
44:w:121:PRO:HG2	44:w:178:PHE:HB3	1.93	0.49
45:x:508:PRO:HG3	47:z:6:HIS:HB3	1.94	0.49
47:z:119:THR:O	51:3:52:HIS:CE1	2.64	0.49
58:AA:11:MET:HE2	68:AL:278:ARG:HH11	1.77	0.49
65:AH:93:SER:HB2	65:AH:99:ARG:HH12	1.77	0.49
68:AL:257:TYR:CD2	68:AL:262:VAL:HG22	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AV:131:TYR:O	66:AV:134:PRO:HD2	2.13	0.49
66:AV:173:PRO:HB2	66:AV:177:ARG:NH1	2.27	0.49
1:BA:63:TYR:CE2	1:BA:64:LYS:HG3	2.47	0.49
1:BA:102:MET:SD	1:BA:149:MET:HB3	2.52	0.49
4:BE:49:GLN:HE21	4:BE:96:VAL:HG21	1.78	0.49
9:BJ:159:ALA:HB3	9:BJ:161:VAL:HG23	1.93	0.49
9:BJ:268:PRO:HG3	9:BJ:344:PRO:HA	1.94	0.49
12:BM:348:ALA:O	12:BM:352:VAL:HG23	2.12	0.49
15:BP:113:ASP:OD1	16:BQ:425:LYS:HD2	2.13	0.49
26:Bc:38:PRO:HG2	38:Bo:71:ALA:HB2	1.95	0.49
26:Bc:111:MET:HG3	40:Br:278:ARG:HH12	1.77	0.49
32:Bi:315:TRP:HZ3	44:Bw:327:VAL:HG12	1.76	0.49
33:Bj:65:PHE:HA	33:Bj:68:GLU:HB2	1.93	0.49
35:Bl:42:SER:O	35:Bl:46:ILE:HG12	2.11	0.49
35:Bl:47:SER:O	35:Bl:50:PRO:HD2	2.12	0.49
35:Bl:190:ILE:CD1	35:Bl:196:TRP:NE1	2.73	0.49
39:Bp:167:TRP:CE3	39:Bp:171:VAL:HG21	2.32	0.49
40:Br:61:LEU:HD22	40:Br:241:TYR:CD1	2.45	0.49
41:Bs:141:SER:HB2	41:Bs:290:TRP:HE1	1.77	0.49
46:By:13:THR:HG22	46:By:13:THR:O	2.12	0.49
51:B3:42:ARG:HD2	51:B3:42:ARG:O	2.13	0.49
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.49
4:E:50:PHE:HE1	4:E:96:VAL:HG13	1.76	0.49
7:H:46:LYS:HE3	8:I:90:THR:OG1	2.13	0.49
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.49
7:H:115:PRO:HG3	16:Q:393:PRO:HB2	1.95	0.49
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
16:Q:82:LEU:N	16:Q:99:MET:O	2.41	0.49
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	0.49
22:Y:86:TYR:HB3	22:Y:87:PRO:HB3	1.93	0.49
24:a:99:ALA:O	27:d:58:TYR:HD1	1.95	0.49
25:b:13:GLN:O	25:b:17:GLU:HG2	2.12	0.49
25:b:108:ASP:CG	25:b:109:THR:H	2.20	0.49
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.95	0.49
45:x:347:LEU:HG	45:x:383:MET:HE3	1.93	0.49
51:3:42:ARG:HD2	51:3:42:ARG:O	2.13	0.49
60:AC:123:VAL:HG13	61:AD:29:VAL:HG22	1.94	0.49
3:BC:140:GLN:HE22	33:Bj:40:GLY:HA2	1.78	0.49
12:BM:300:GLN:HA	13:BN:135:GLN:O	2.12	0.49
15:BP:172:ASP:OD2	15:BP:189:THR:OG1	2.23	0.49
25:Bb:33:PRO:HD2	39:Bp:114:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Bb:113:THR:OG1	25:Bb:114:GLY:N	2.44	0.49
71:Bb:201:PLX:H21	27:Bd:43:ARG:HH22	1.77	0.49
26:Bc:111:MET:HG3	40:Br:278:ARG:NH1	2.27	0.49
35:Bl:37:LYS:HE2	35:Bl:98:TRP:HD1	0.69	0.49
37:Bn:55:VAL:HG12	37:Bn:56:THR:N	2.24	0.49
41:Bs:79:LEU:HD11	41:Bs:222:LEU:HD22	1.94	0.49
45:Bx:184:PHE:H	45:Bx:256:HIS:CE1	2.29	0.49
46:By:90:ILE:HD12	46:By:90:ILE:H	1.77	0.49
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.28	0.49
10:K:104:GLU:OE1	10:K:104:GLU:N	2.46	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	0.49
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.49
21:W:101:VAL:HG21	31:h:82:GLN:NE2	2.28	0.49
22:Y:51:THR:HG21	35:l:446:ASN:HD21	1.76	0.49
25:b:77:VAL:HB	25:b:78:PRO:HD3	1.95	0.49
26:c:123:PRO:HG3	39:p:75:GLN:NE2	2.25	0.49
34:k:60:PRO:O	34:k:63:MET:HB2	2.12	0.49
39:p:55:LYS:CA	39:p:55:LYS:CE	2.89	0.49
41:s:17:MET:CE	41:s:232:ILE:HD12	2.37	0.49
45:x:40:GLU:HG2	45:x:54:TYR:CD1	2.46	0.49
46:y:90:ILE:H	46:y:90:ILE:HD12	1.77	0.49
67:AK:299:VAL:HG22	68:AL:120:LEU:HG	1.94	0.49
61:AQ:34:ARG:NH1	61:AQ:38:GLN:HB3	2.26	0.49
67:AW:101:ARG:NH1	68:AY:325:SER:O	2.44	0.49
1:BA:63:TYR:HD2	1:BA:256:ARG:HD2	1.76	0.49
1:BA:118:ASP:O	1:BA:159:ARG:CD	2.60	0.49
6:BG:99:SER:OG	6:BG:102:SER:OG	2.29	0.49
7:BH:46:LYS:HE3	8:BI:90:THR:OG1	2.13	0.49
8:BI:9:GLN:O	8:BI:13:ASN:ND2	2.40	0.49
11:BL:107:TRP:HZ3	11:BL:118:ALA:HB2	1.76	0.49
16:BQ:194:LEU:HD12	16:BQ:268:TRP:CE2	2.45	0.49
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.49
9:J:268:PRO:HG3	9:J:344:PRO:HA	1.94	0.49
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.49
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	0.49
14:O:193:TYR:HB3	14:O:196:LEU:HD11	1.94	0.49
22:Y:78:GLU:HG2	35:l:385:PHE:HE1	1.78	0.49
32:i:337:LEU:O	32:i:339:ILE:N	2.46	0.49
35:l:512:LYS:HB2	54:6:16:ASN:HB2	1.94	0.49
36:m:33:ILE:HA	36:m:60:LEU:HD22	1.94	0.49
41:s:226:ALA:O	41:s:230:ASN:ND2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:131:VAL:HG12	42:u:133:THR:HG23	1.95	0.49
46:y:13:THR:O	46:y:13:THR:HG22	2.12	0.49
67:AK:64:PHE:CE2	67:AK:397:GLY:HA3	2.48	0.49
68:AL:75:ILE:HG21	68:AL:224:TYR:HD1	1.77	0.49
68:AL:364:LYS:HB2	68:AL:368:MET:HE3	1.93	0.49
61:AQ:43:ILE:O	61:AQ:47:ILE:HD12	2.13	0.49
68:AY:187:LEU:HD11	68:AY:290:ALA:HB3	1.95	0.49
1:BA:112:TYR:CD1	1:BA:155:TYR:HE2	2.29	0.49
1:BA:274:LYS:HZ2	1:BA:352:ALA:HB3	1.77	0.49
1:BA:281:HIS:NE2	14:BO:142:LEU:O	2.38	0.49
7:BH:115:PRO:HG3	16:BQ:393:PRO:HB2	1.94	0.49
12:BM:61:PRO:HG2	12:BM:113:ARG:NE	2.26	0.49
19:BU:58:ARG:HH12	42:Bu:137:LEU:N	2.10	0.49
25:Bb:13:GLN:O	25:Bb:17:GLU:HG2	2.12	0.49
28:Be:107:ALA:O	71:Br:502:PLX:H1B3	2.13	0.49
30:Bg:38:TYR:CE2	30:Bg:42:LEU:HD11	2.47	0.49
35:Bl:70:THR:HG23	35:Bl:75:GLN:HB3	1.94	0.49
35:Bl:119:LYS:HD2	75:Bl:703:CDL:HB32	1.95	0.49
35:Bl:189:PHE:CD1	35:Bl:201:MET:HE3	2.48	0.49
43:Bv:49:ALA:O	43:Bv:51:LEU:N	2.46	0.49
44:Bw:137:SER:C	44:Bw:139:ARG:H	2.18	0.49
44:Bw:305:LEU:O	44:Bw:308:THR:HG22	2.12	0.49
45:Bx:87:ILE:O	45:Bx:173:PRO:HD3	2.13	0.49
45:Bx:172:LYS:HB2	45:Bx:172:LYS:HZ3	1.76	0.49
45:Bx:377:PHE:HA	45:Bx:380:VAL:HG22	1.93	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.94	0.49
9:J:238:GLN:NE2	9:J:267:GLY:O	2.43	0.49
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.49
16:Q:65:PRO:HG2	16:Q:69:VAL:HG22	1.94	0.49
16:Q:358:VAL:HG12	16:Q:360:ASP:H	1.78	0.49
20:V:37:ALA:HB1	20:V:56:VAL:HG22	1.95	0.49
26:c:69:GLY:HA3	38:o:81:ARG:O	2.13	0.49
30:g:4:ARG:NH1	30:g:6:ASN:HB3	2.28	0.49
31:h:99:ILE:HD12	31:h:101:LYS:HB2	1.93	0.49
32:i:41:ILE:HD11	32:i:60:PHE:HD1	1.78	0.49
40:r:113:THR:O	40:r:176:ILE:HG13	2.12	0.49
40:r:188:ASN:CG	40:r:189:SER:H	2.21	0.49
41:s:141:SER:HB2	41:s:290:TRP:HE1	1.77	0.49
45:x:87:ILE:O	45:x:173:PRO:HD3	2.13	0.49
45:x:197:LEU:O	47:z:92:LEU:HD22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:232:GLN:HB2	45:x:292:MET:HE3	1.93	0.49
46:y:59:GLN:O	46:y:62:GLU:HB2	2.13	0.49
58:AN:43:ARG:HH11	71:AN:101:PLX:C1B	2.09	0.49
65:AU:284:HIS:O	65:AU:288:MET:HG3	2.13	0.49
8:BI:11:LEU:O	8:BI:14:TRP:HB3	2.13	0.49
9:BJ:141:PHE:CZ	9:BJ:180:TYR:HB2	2.47	0.49
9:BJ:217:PHE:CZ	9:BJ:322:MET:CE	2.86	0.49
12:BM:66:HIS:HE1	12:BM:68:ARG:HG2	1.78	0.49
12:BM:124:HIS:CG	12:BM:125:PRO:HD2	2.48	0.49
13:BN:87:HIS:O	13:BN:91:HIS:HD2	1.96	0.49
14:BO:193:TYR:HB3	14:BO:196:LEU:HD11	1.94	0.49
16:BQ:323:ARG:N	16:BQ:328:ASP:OD2	2.46	0.49
25:Bb:39:LYS:O	25:Bb:42:PRO:HD2	2.13	0.49
26:Bc:69:GLY:HA3	38:Bo:81:ARG:O	2.12	0.49
31:Bh:6:ILE:HB	32:Bi:22:LEU:HD22	1.93	0.49
35:Bl:383:MET:SD	35:Bl:384:PRO:HD2	2.52	0.49
35:Bl:566:ILE:HA	35:Bl:569:HIS:CD2	2.47	0.49
45:Bx:508:PRO:HG3	47:Bz:6:HIS:HB3	1.94	0.49
46:By:186:SER:HB3	46:By:213:LEU:CD2	2.42	0.49
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.49
1:A:63:TYR:HD2	1:A:256:ARG:HD2	1.76	0.49
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.49
5:F:48:ASN:HD21	5:F:53:ILE:HD11	1.77	0.49
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.48	0.49
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.49
26:c:111:MET:HG3	40:r:278:ARG:NH1	2.27	0.49
71:g:202:PLX:H1C2	71:g:202:PLX:H31	1.93	0.49
35:l:47:SER:O	35:l:50:PRO:HD2	2.12	0.49
35:l:386:LEU:HD12	35:l:387:THR:N	2.28	0.49
35:l:566:ILE:HA	35:l:569:HIS:CD2	2.47	0.49
39:p:136:GLU:HG2	39:p:165:PRO:HA	1.94	0.49
41:s:9:LEU:HD13	41:s:95:LEU:HD12	1.94	0.49
43:v:113:LYS:HA	43:v:116:GLU:OE1	2.13	0.49
45:x:266:GLU:HB2	45:x:267:PRO:HD2	1.94	0.49
66:AJ:186:PRO:HA	66:AJ:189:ILE:HD12	1.94	0.49
76:AJ:403:PEE:H61	76:AJ:403:PEE:C17	2.42	0.49
68:AL:179:MET:O	68:AL:181:ASP:N	2.45	0.49
68:AL:186:TYR:CD1	68:AL:275:ILE:HG21	2.48	0.49
63:AS:54:ASN:OD1	63:AS:55:LEU:N	2.45	0.49
64:AT:39:ARG:HG2	64:AT:39:ARG:NH2	2.19	0.49
66:AV:246:SER:HB3	66:AV:249:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AY:424:ILE:HG13	68:AY:429:TRP:NE1	2.27	0.49
2:BB:78:GLU:HA	17:BS:1:MET:SD	2.53	0.49
5:BF:21:ILE:HG12	5:BF:55:ILE:HG12	1.93	0.49
9:BJ:152:ILE:HG22	9:BJ:164:PHE:HE1	1.77	0.49
9:BJ:365:GLU:N	9:BJ:365:GLU:OE1	2.45	0.49
16:BQ:65:PRO:HG2	16:BQ:69:VAL:HG22	1.94	0.49
20:BV:62:THR:HG22	20:BV:104:ARG:NE	2.27	0.49
24:Ba:99:ALA:O	27:Bd:58:TYR:HD1	1.95	0.49
25:Bb:92:GLU:HG2	25:Bb:93:LYS:HG3	1.94	0.49
71:Bb:201:PLX:O7	71:Bb:201:PLX:H31	2.13	0.49
30:Bg:4:ARG:NH1	30:Bg:6:ASN:HB3	2.28	0.49
34:Bk:1:MET:CB	34:Bk:4:ILE:CD1	2.86	0.49
40:Br:220:HIS:CE1	40:Br:232:ALA:HB2	2.47	0.49
45:Bx:168:ILE:HG21	45:Bx:189:MET:HG3	1.94	0.49
46:By:59:GLN:O	46:By:62:GLU:HB2	2.13	0.49
1:A:114:VAL:O	1:A:242:VAL:HA	2.13	0.49
2:B:78:GLU:HA	17:S:1:MET:SD	2.53	0.49
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.35	0.49
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.49
9:J:62:THR:HB	73:J:401:NDP:O2X	2.12	0.49
9:J:357:ARG:HG3	9:J:362:LEU:HA	1.94	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
13:N:11:LEU:HA	13:N:14:ILE:HD12	1.94	0.49
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.49
6:X:77:GLU:HB2	23:Z:13:LYS:HE2	1.93	0.49
71:b:201:PLX:O7	71:b:201:PLX:H31	2.13	0.49
30:g:27:ASP:OD1	30:g:28:PRO:HD2	2.13	0.49
31:h:22:SER:HB3	31:h:37:GLU:OE1	2.13	0.49
31:h:32:ARG:NH2	34:k:50:ASN:O	2.42	0.49
40:r:220:HIS:HE1	40:r:232:ALA:HB2	1.77	0.49
40:r:355:MET:HA	40:r:358:TRP:HD1	1.77	0.49
71:r:502:PLX:C33	71:r:502:PLX:C37	2.85	0.49
43:v:41:ALA:O	43:v:42:THR:OG1	2.31	0.49
45:x:168:ILE:HG21	45:x:189:MET:HG3	1.94	0.49
68:AL:308:ASN:HD21	68:AL:345:SER:HB3	1.77	0.49
75:AN:102:CDL:C58	76:AV:403:PEE:H52	2.42	0.49
66:AV:326:TRP:CH2	76:AV:403:PEE:H13	2.46	0.49
68:AY:101:THR:OG1	68:AY:149:ASP:OD1	2.31	0.49
9:BJ:179:ARG:HB3	9:BJ:179:ARG:NH1	2.27	0.49
9:BJ:250:VAL:O	9:BJ:254:LYS:HG2	2.13	0.49
11:BL:75:ARG:HH11	11:BL:104:ARG:NE	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:88:VAL:HG13	12:BM:108:LYS:HE2	1.94	0.49
13:BN:11:LEU:HA	13:BN:14:ILE:HD12	1.94	0.49
16:BQ:358:VAL:HG12	16:BQ:360:ASP:H	1.78	0.49
24:Ba:95:GLN:OE1	24:Ba:114:LYS:NZ	2.46	0.49
30:Bg:38:TYR:O	30:Bg:42:LEU:HG	2.13	0.49
35:Bl:75:GLN:O	35:Bl:75:GLN:HG2	2.13	0.49
35:Bl:500:THR:HG22	54:B6:33:ARG:HD2	1.95	0.49
41:Bs:65:THR:O	41:Bs:124:ASN:ND2	2.46	0.49
50:B2:49:VAL:HG21	50:B2:74:LEU:HD12	1.95	0.49
51:B3:42:ARG:NH1	51:B3:74:ARG:HH21	2.10	0.49
51:B3:44:ARG:HD2	51:B3:74:ARG:O	2.11	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
9:J:85:ARG:CG	9:J:85:ARG:NH1	2.72	0.49
11:L:115:ALA:O	15:P:228:GLN:N	2.44	0.49
17:S:50:ARG:CZ	17:S:54:ILE:HD11	2.43	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
26:c:108:HIS:HE1	35:l:546:GLN:HG2	1.77	0.49
28:e:107:ALA:O	71:r:502:PLX:H1B3	2.13	0.49
30:g:38:TYR:O	30:g:42:LEU:HG	2.13	0.49
32:i:167:TRP:HZ3	35:l:570:GLN:CA	2.20	0.49
38:o:8:PRO:HD3	38:o:14:LEU:HD21	1.95	0.49
44:w:217:ARG:HA	44:w:220:LYS:HD2	1.95	0.49
61:AD:16:ARG:NH1	68:AL:446:SER:OG	2.42	0.49
65:AU:288:MET:CG	76:AU:401:PEE:O4	2.60	0.49
66:AV:254:ASP:OD2	66:AV:267:HIS:NE2	2.46	0.49
67:AW:136:PHE:O	67:AW:140:VAL:HG23	2.13	0.49
67:AW:301:ARG:HD2	68:AY:95:HIS:CD2	2.48	0.49
9:BJ:62:THR:HB	73:BJ:401:NDP:O2X	2.13	0.49
9:BJ:64:PHE:CE2	9:BJ:242:VAL:HG21	2.48	0.49
9:BJ:350:ILE:HG21	9:BJ:366:ILE:HG12	1.95	0.49
12:BM:123:ASN:HA	12:BM:157:LYS:HG2	1.94	0.49
12:BM:302:LEU:HB3	12:BM:585:PRO:HB3	1.93	0.49
12:BM:711:VAL:HA	12:BM:714:VAL:HG12	1.94	0.49
14:BO:197:THR:H	14:BO:200:ASP:HB3	1.76	0.49
16:BQ:103:GLY:HA3	33:Bj:52:SER:HB3	1.95	0.49
20:BV:47:GLY:O	20:BV:48:THR:OG1	2.25	0.49
22:BY:78:GLU:HG2	35:Bl:385:PHE:HE1	1.78	0.49
27:Bd:34:ILE:HG13	27:Bd:35:VAL:HG13	1.95	0.49
31:Bh:101:LYS:C	31:Bh:104:PRO:HD2	2.37	0.49
41:Bs:169:GLN:NE2	41:Bs:241:ILE:O	2.42	0.49
42:Bu:85:TYR:OH	42:Bu:104:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bu:131:VAL:HG12	42:Bu:133:THR:HG23	1.95	0.49
44:Bw:109:ASN:HD21	44:Bw:111:ASN:HD22	1.61	0.49
44:Bw:323:GLN:O	44:Bw:326:ARG:HB3	2.13	0.49
46:By:16:ILE:HD12	46:By:17:MET:H	1.78	0.49
54:B6:8:LYS:NZ	54:B6:8:LYS:HB3	2.28	0.49
1:A:274:LYS:HB2	1:A:292:MET:SD	2.53	0.48
2:B:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.48
3:C:79:LEU:HB2	3:C:108:VAL:HG12	1.94	0.48
3:C:140:GLN:HE22	33:j:40:GLY:HA2	1.78	0.48
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.48
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	0.48
9:J:93:HIS:O	9:J:96:PRO:HD2	2.13	0.48
9:J:152:ILE:HG22	9:J:164:PHE:HE1	1.78	0.48
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.48
12:M:711:VAL:HA	12:M:714:VAL:HG12	1.94	0.48
13:N:129:THR:HA	18:T:44:GLN:NE2	2.28	0.48
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.48
18:T:80:VAL:HG12	18:T:82:THR:H	1.76	0.48
19:U:58:ARG:HH12	42:u:137:LEU:N	2.10	0.48
21:W:47:HIS:O	21:W:51:MET:HG3	2.13	0.48
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.48
71:b:201:PLX:C6	71:b:201:PLX:C11	2.85	0.48
32:i:115:VAL:HG12	32:i:180:ALA:HB1	1.95	0.48
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.95	0.48
33:j:71:LEU:O	36:m:146:TYR:OH	2.28	0.48
35:l:189:PHE:CD1	35:l:201:MET:HE3	2.48	0.48
44:w:139:ARG:HD2	44:w:166:ASP:OD2	2.12	0.48
51:3:42:ARG:NH1	51:3:74:ARG:HH21	2.10	0.48
67:AK:49:ILE:HG12	67:AK:50:ALA:N	2.26	0.48
62:AR:66:ASP:OD1	62:AR:67:CYS:N	2.44	0.48
65:AU:307:LYS:HE2	75:AU:403:CDL:CA3	2.43	0.48
68:AY:96:LEU:C	68:AY:96:LEU:CD1	2.86	0.48
1:BA:36:LYS:HB2	1:BA:39:ASP:CG	2.38	0.48
1:BA:116:ASN:HD21	70:BA:502:FMN:C8	2.22	0.48
1:BA:160:GLY:HA2	1:BA:199:ARG:NH1	2.27	0.48
12:BM:372:PHE:CE1	12:BM:481:LEU:HD13	2.48	0.48
32:Bi:41:ILE:HD11	32:Bi:60:PHE:HD1	1.77	0.48
36:Bm:118:PHE:HZ	36:Bm:124:TRP:HZ2	1.61	0.48
45:Bx:476:PHE:CD1	56:B8:15:VAL:HG21	2.48	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.48
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.48
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.48
16:Q:201:PHE:CB	41:s:32:GLN:HG3	2.43	0.48
28:e:89:LEU:HD13	40:r:29:THR:HG21	1.95	0.48
32:i:18:LEU:O	32:i:22:LEU:HG	2.13	0.48
32:i:334:THR:OG1	32:i:335:LEU:N	2.45	0.48
35:l:450:LEU:C	35:l:450:LEU:CD2	2.85	0.48
36:m:118:PHE:HZ	36:m:124:TRP:HZ2	1.61	0.48
41:s:311:ILE:O	41:s:312:SER:OG	2.28	0.48
51:3:5:LYS:HZ3	51:3:5:LYS:HB3	1.78	0.48
51:3:5:LYS:NZ	51:3:5:LYS:HB3	2.27	0.48
76:AH:401:PEE:H17	66:AJ:240:MET:HE2	1.93	0.48
68:AL:161:ILE:O	68:AL:165:ARG:HG3	2.12	0.48
65:AU:115:GLN:HA	65:AU:118:LYS:HE2	1.96	0.48
65:AU:242:ILE:HD13	65:AU:244:MET:HE2	1.95	0.48
66:AV:45:ILE:HA	82:AV:401:HEM:CMC	2.44	0.48
66:AV:286:ASN:OD1	66:AV:287:LYS:N	2.46	0.48
66:AV:366:MET:HB3	66:AV:367:PRO:HD3	1.95	0.48
68:AY:259:GLU:HG2	68:AY:259:GLU:O	2.12	0.48
1:BA:158:ILE:N	1:BA:198:VAL:O	2.47	0.48
2:BB:138:ARG:HG2	12:BM:238:PHE:CG	2.48	0.48
2:BB:198:GLU:OE2	2:BB:202:ASN:ND2	2.46	0.48
10:BK:104:GLU:OE1	10:BK:104:GLU:N	2.46	0.48
13:BN:129:THR:HA	18:BT:44:GLN:NE2	2.28	0.48
16:BQ:179:ARG:HG2	16:BQ:183:HIS:CD2	2.48	0.48
16:BQ:438:MET:HE1	16:BQ:454:GLN:HE22	1.78	0.48
20:BV:29:ALA:O	20:BV:63:ALA:HB1	2.14	0.48
6:BX:80:GLN:HG3	6:BX:145:VAL:HG11	1.95	0.48
22:BY:44:TYR:HD1	35:Bl:440:LEU:HB2	1.78	0.48
24:Ba:115:HIS:HE1	24:Ba:117:ILE:HD12	1.77	0.48
31:Bh:22:SER:HB3	31:Bh:37:GLU:OE1	2.13	0.48
32:Bi:115:VAL:HG12	32:Bi:180:ALA:HB1	1.95	0.48
34:Bk:83:ASN:HD21	36:Bm:174:ASN:HA	1.77	0.48
35:Bl:306:THR:HA	35:Bl:336:LYS:HZ3	1.77	0.48
40:Br:18:SER:OG	40:Br:23:ILE:HG12	2.13	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
9:J:130:ILE:HG21	73:J:401:NDP:N7A	2.23	0.48
12:M:92:CYS:SG	74:M:803:FES:S2	3.10	0.48
12:M:136:GLU:OE1	12:M:136:GLU:N	2.46	0.48
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.48
34:k:83:ASN:HD21	36:m:174:ASN:HA	1.78	0.48
35:l:591:PHE:O	35:l:594:PRO:HD2	2.13	0.48
75:n:101:CDL:HB62	42:u:172:LYS:HB2	1.93	0.48
39:p:104:LEU:HD21	39:p:119:PHE:CE1	2.41	0.48
40:r:5:ILE:O	40:r:8:THR:OG1	2.26	0.48
45:x:476:PHE:CD1	56:8:15:VAL:HG21	2.48	0.48
47:z:65:SER:HB3	47:z:71:HIS:CE1	2.49	0.48
50:2:49:VAL:HG21	50:2:74:LEU:HD12	1.95	0.48
58:AA:78:TYR:CD1	62:AE:64:GLU:C	2.91	0.48
63:AF:39:TYR:HD1	63:AF:40:GLU:H	1.60	0.48
68:AY:286:HIS:ND1	68:AY:359:VAL:HG22	2.29	0.48
1:BA:114:VAL:O	1:BA:242:VAL:HA	2.13	0.48
1:BA:256:ARG:O	14:BO:246:GLN:HB3	2.13	0.48
2:BB:113:ALA:HB1	2:BB:130:ALA:HB2	1.94	0.48
4:BE:20:ILE:H	4:BE:77:ARG:HG2	1.78	0.48
9:BJ:168:SER:N	9:BJ:201:VAL:O	2.40	0.48
16:BQ:334:VAL:O	16:BQ:338:ARG:HG2	2.12	0.48
16:BQ:338:ARG:NH1	21:BW:23:ARG:HB3	2.29	0.48
21:BW:141:MET:SD	36:Bm:47:GLY:HA2	2.53	0.48
25:Bb:105:PHE:CZ	43:Bv:67:LEU:CB	2.96	0.48
26:Bc:108:HIS:HE1	35:Bl:546:GLN:HG2	1.77	0.48
30:Bg:29:ARG:NH2	42:Bu:172:LYS:HD2	2.28	0.48
32:Bi:117:GLU:OE1	32:Bi:117:GLU:N	2.41	0.48
32:Bi:198:PRO:O	32:Bi:201:THR:OG1	2.23	0.48
35:Bl:188:TRP:CD2	35:Bl:212:PRO:HG3	2.48	0.48
35:Bl:190:ILE:CG1	35:Bl:196:TRP:CE2	2.96	0.48
35:Bl:286:LEU:HB2	35:Bl:411:ILE:HG23	1.95	0.48
41:Bs:42:PRO:HD2	41:Bs:45:LEU:HD12	1.95	0.48
41:Bs:253:GLU:O	41:Bs:257:THR:HG23	2.13	0.48
52:B4:24:ASN:ND2	52:B4:26:THR:H	2.11	0.48
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.48
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.48
9:J:250:VAL:O	9:J:254:LYS:HG2	2.13	0.48
12:M:68:ARG:NH2	12:M:284:GLU:OE1	2.33	0.48
12:M:69:LEU:HD22	12:M:181:ARG:HG3	1.95	0.48
12:M:383:SER:HA	12:M:386:LEU:HD12	1.96	0.48
12:M:636:TYR:HB2	12:M:641:GLN:HB3	1.95	0.48
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.48
25:b:89:HIS:C	25:b:89:HIS:CD2	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:105:PHE:HZ	43:v:67:LEU:HB2	1.75	0.48
27:d:34:ILE:HG13	27:d:35:VAL:HG13	1.95	0.48
34:k:81:ILE:CG2	34:k:87:LEU:HA	2.43	0.48
35:l:190:ILE:CG1	35:l:196:TRP:CE2	2.96	0.48
40:r:132:ILE:O	40:r:136:TRP:HB2	2.14	0.48
44:w:335:PRO:HA	44:w:338:LYS:NZ	2.29	0.48
45:x:115:SER:O	45:x:121:GLY:HA2	2.14	0.48
46:y:186:SER:HB3	46:y:213:LEU:CD2	2.42	0.48
47:z:42:LEU:HD13	54:6:45:TYR:HD2	1.77	0.48
58:AA:78:TYR:HB3	62:AE:65:GLU:CD	2.30	0.48
60:AC:136:PHE:CE2	76:AH:401:PEE:H34	2.48	0.48
60:AC:197:ASP:O	60:AC:257:ASN:ND2	2.45	0.48
67:AK:116:ARG:NH1	67:AK:188:ASN:O	2.46	0.48
68:AL:192:PHE:HB2	68:AL:198:ALA:HB2	1.95	0.48
68:AL:304:LEU:HD13	68:AL:354:LEU:HD11	1.95	0.48
2:BB:36:TYR:CD2	8:BI:104:TRP:HB2	2.48	0.48
9:BJ:201:VAL:HG13	9:BJ:265:PHE:CE2	2.47	0.48
12:BM:200:ARG:HH21	14:BO:120:THR:HG23	1.78	0.48
12:BM:266:ARG:NE	12:BM:271:MET:HE3	2.29	0.48
12:BM:704:SER:OG	12:BM:706:THR:HG22	2.14	0.48
14:BO:115:VAL:O	14:BO:119:TYR:HD2	1.96	0.48
16:BQ:136:PHE:CE2	16:BQ:151:TYR:HB2	2.49	0.48
26:Bc:174:PRO:O	26:Bc:175:SER:OG	2.26	0.48
28:Be:89:LEU:HD13	40:Br:29:THR:HG21	1.95	0.48
33:Bj:54:LYS:HB3	33:Bj:113:TRP:NE1	2.29	0.48
35:Bl:386:LEU:HD12	35:Bl:387:THR:N	2.28	0.48
38:Bo:8:PRO:HD3	38:Bo:14:LEU:HD21	1.95	0.48
39:Bp:136:GLU:HG2	39:Bp:165:PRO:HA	1.94	0.48
43:Bv:41:ALA:O	43:Bv:42:THR:OG1	2.31	0.48
54:B6:16:ASN:H	54:B6:16:ASN:ND2	2.12	0.48
1:A:132:ARG:HG2	1:A:165:GLU:OE1	2.13	0.48
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	0.48
11:L:98:LYS:HA	11:L:126:LEU:O	2.13	0.48
12:M:200:ARG:HH21	14:O:120:THR:HG23	1.78	0.48
26:c:159:LYS:CA	43:v:98:ARG:HH12	2.27	0.48
35:l:188:TRP:CD2	35:l:212:PRO:HG3	2.48	0.48
41:s:253:GLU:O	41:s:257:THR:HG23	2.13	0.48
44:w:258:TYR:CE1	44:w:267:LYS:HA	2.49	0.48
68:AL:113:VAL:HG11	68:AL:120:LEU:HD23	1.95	0.48
68:AL:168:ILE:O	68:AL:172:MET:HG2	2.12	0.48
65:AU:262:THR:HG22	65:AU:264:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:157:GLN:NE2	68:AY:317:THR:O	2.45	0.48
67:AW:230:LEU:HA	67:AW:233:VAL:HG22	1.94	0.48
4:BE:47:VAL:HG11	4:BE:56:VAL:HG22	1.95	0.48
8:BI:44:GLY:HA2	16:BQ:355:GLU:HG3	1.95	0.48
12:BM:392:ALA:HA	12:BM:417:ARG:HH22	1.78	0.48
12:BM:636:TYR:HB2	12:BM:641:GLN:HB3	1.95	0.48
14:BO:130:TYR:HA	14:BO:189:ASN:HD21	1.76	0.48
17:BS:50:ARG:CZ	17:BS:54:ILE:HD11	2.43	0.48
19:BU:52:ASN:HD21	31:Bh:27:TYR:C	2.20	0.48
20:BV:62:THR:HG22	20:BV:104:ARG:HD3	1.95	0.48
24:Ba:187:PRO:HB3	42:Bu:47:ARG:HG3	1.96	0.48
32:Bi:18:LEU:O	32:Bi:22:LEU:HG	2.14	0.48
35:Bl:548:LEU:HB2	35:Bl:549:PRO:HD3	1.95	0.48
76:Bl:701:PEE:C23	40:Br:155:VAL:HB	2.29	0.48
36:Bm:22:LYS:N	36:Bm:23:PRO:HD3	2.28	0.48
39:Bp:54:GLU:OE2	72:Bp:201:8Q1:C37	2.61	0.48
41:Bs:231:ILE:HG23	41:Bs:270:PHE:HD2	1.79	0.48
41:Bs:236:THR:HG22	41:Bs:263:THR:HG21	1.96	0.48
45:Bx:11:ASN:ND2	45:Bx:13:LYS:HB2	2.28	0.48
47:Bz:42:LEU:HD13	54:B6:45:TYR:HD2	1.77	0.48
4:E:20:ILE:H	4:E:77:ARG:HG2	1.78	0.48
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.48
9:J:350:ILE:HG21	9:J:366:ILE:HG12	1.95	0.48
12:M:564:CYS:O	12:M:566:ILE:HG12	2.14	0.48
24:a:126:TYR:OH	28:e:109:LEU:HD22	2.14	0.48
32:i:59:TYR:CZ	32:i:63:GLN:OE1	2.67	0.48
32:i:282:MET:O	32:i:286:THR:HG23	2.14	0.48
32:i:285:ILE:CG1	76:l:701:PEE:H75	2.25	0.48
33:j:54:LYS:HB3	33:j:113:TRP:NE1	2.29	0.48
34:k:97:GLN:HG2	35:l:587:TYR:OH	2.14	0.48
35:l:119:LYS:HD2	75:l:703:CDL:HB32	1.95	0.48
36:m:22:LYS:N	36:m:23:PRO:HD3	2.28	0.48
71:r:502:PLX:H52	71:r:502:PLX:P1	2.53	0.48
54:6:8:LYS:HB3	54:6:8:LYS:NZ	2.28	0.48
75:AJ:405:CDL:OA9	75:AJ:405:CDL:H332	2.10	0.48
67:AK:277:VAL:HG22	67:AK:278:ALA:HA	1.96	0.48
67:AK:305:THR:HA	67:AK:311:GLN:HE21	1.78	0.48
67:AK:438:MET:HB2	67:AK:450:VAL:HG12	1.94	0.48
68:AL:426:LEU:HA	68:AL:429:TRP:HD1	1.78	0.48
64:AT:9:ARG:HH22	71:AT:101:PLX:H1A1	1.79	0.48
4:BE:128:PRO:HG3	11:BL:74:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:111:GLN:HE22	15:BP:122:ARG:HB3	1.77	0.48
12:BM:381:LEU:C	12:BM:383:SER:H	2.16	0.48
12:BM:464:GLN:NE2	12:BM:467:LYS:HE2	2.27	0.48
16:BQ:85:GLY:CA	33:Bj:39:CYS:CB	2.90	0.48
16:BQ:301:ASP:OD1	16:BQ:302:LEU:N	2.47	0.48
6:BX:76:LEU:HD12	6:BX:156:GLU:HB2	1.94	0.48
24:Ba:160:MET:HE3	24:Ba:166:GLY:HA3	1.96	0.48
27:Bd:18:PRO:HG2	43:Bv:71:ARG:NH1	2.29	0.48
32:Bi:135:LYS:O	32:Bi:139:ILE:HG12	2.14	0.48
32:Bi:149:LEU:HD23	32:Bi:154:LEU:HD13	1.96	0.48
32:Bi:337:LEU:O	32:Bi:339:ILE:N	2.46	0.48
33:Bj:3:PHE:O	33:Bj:6:ILE:HB	2.14	0.48
35:Bl:527:GLY:C	35:Bl:529:TYR:H	2.22	0.48
75:Bl:704:CDL:OA9	75:Bl:704:CDL:O1	2.19	0.48
44:Bw:335:PRO:HA	44:Bw:338:LYS:NZ	2.29	0.48
46:By:4:PRO:HB2	55:B7:43:SER:HA	1.96	0.48
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.48
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.48
9:J:206:ILE:HB	9:J:242:VAL:HG23	1.90	0.48
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.48
12:M:704:SER:OG	12:M:706:THR:HG22	2.14	0.48
16:Q:301:ASP:OD1	16:Q:302:LEU:N	2.47	0.48
16:Q:338:ARG:NH1	21:W:23:ARG:HB3	2.29	0.48
16:Q:394:GLY:O	16:Q:413:SER:OG	2.23	0.48
20:V:29:ALA:O	20:V:63:ALA:HB1	2.14	0.48
20:V:96:ALA:HA	20:V:99:LEU:HD12	1.95	0.48
21:W:101:VAL:HG13	21:W:102:PRO:HD2	1.96	0.48
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
71:b:201:PLX:H111	71:b:201:PLX:C7	2.43	0.48
27:d:18:PRO:HG2	43:v:71:ARG:NH1	2.29	0.48
30:g:29:ARG:NH2	42:u:172:LYS:HD2	2.28	0.48
35:l:369:THR:O	35:l:372:SER:OG	2.27	0.48
40:r:18:SER:OG	40:r:23:ILE:HG12	2.13	0.48
41:s:205:SER:OG	41:s:279:ARG:NH1	2.47	0.48
63:AS:44:VAL:O	63:AS:48:ILE:HG12	2.14	0.48
64:AT:40:LEU:HD12	64:AT:41:ILE:H	1.64	0.48
65:AU:128:ASP:OD1	65:AU:177:LYS:NZ	2.47	0.48
66:AV:278:TYR:CE2	66:AV:282:ARG:HD2	2.49	0.48
1:BA:99:TRP:HH2	1:BA:248:VAL:HA	1.78	0.48
1:BA:318:ILE:HD11	1:BA:355:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:203:PRO:O	73:BJ:401:NDP:H5N	2.14	0.48
12:BM:262:VAL:HG23	12:BM:276:ARG:HB2	1.95	0.48
12:BM:383:SER:HA	12:BM:386:LEU:HD12	1.96	0.48
16:BQ:194:LEU:CD1	16:BQ:268:TRP:CE2	2.97	0.48
20:BV:96:ALA:HA	20:BV:99:LEU:HD12	1.95	0.48
6:BX:102:SER:O	6:BX:140:CYS:HA	2.14	0.48
25:Bb:77:VAL:HB	25:Bb:78:PRO:HD3	1.94	0.48
71:Bb:201:PLX:H111	71:Bb:201:PLX:C7	2.43	0.48
30:Bg:119:ARG:HD3	38:Bo:116:ILE:HD13	1.96	0.48
32:Bi:17:THR:HG23	32:Bi:137:ALA:HB2	1.96	0.48
32:Bi:334:THR:OG1	32:Bi:335:LEU:N	2.45	0.48
44:Bw:217:ARG:HA	44:Bw:220:LYS:HD2	1.94	0.48
47:Bz:65:SER:HB3	47:Bz:71:HIS:CE1	2.49	0.48
47:Bz:80:ARG:O	47:Bz:84:ILE:HG12	2.14	0.48
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	0.48
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.48
2:B:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.48
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	0.48
12:M:168:LEU:HD23	12:M:292:PHE:CD2	2.46	0.48
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	0.48
20:V:14:ASP:O	20:V:21:LYS:NZ	2.45	0.48
24:a:187:PRO:HB3	42:u:47:ARG:HG3	1.96	0.48
71:b:201:PLX:H72	71:b:201:PLX:O2	2.14	0.48
27:d:120:ILE:O	27:d:121:LYS:C	2.56	0.48
32:i:106:LEU:HB3	32:i:187:MET:HE2	1.95	0.48
33:j:109:LYS:HA	33:j:112:ASP:HB2	1.94	0.48
35:l:75:GLN:HG2	35:l:75:GLN:O	2.13	0.48
35:l:286:LEU:HB2	35:l:411:ILE:HG23	1.95	0.48
52:4:24:ASN:ND2	52:4:26:THR:H	2.11	0.48
63:AF:83:LYS:HB2	63:AF:86:GLU:HB2	1.95	0.48
67:AK:207:TYR:HA	67:AK:210:GLN:NE2	2.28	0.48
67:AK:259:ARG:HH12	67:AK:438:MET:CE	2.26	0.48
67:AK:299:VAL:HG13	68:AL:120:LEU:HD11	1.94	0.48
68:AL:75:ILE:HG21	68:AL:224:TYR:CD1	2.48	0.48
59:AO:26:LEU:HA	59:AO:27:ARG:O	2.14	0.48
60:AP:126:ALA:HA	76:AY:502:PEE:H61	1.94	0.48
60:AP:138:SER:O	66:AV:74:ASN:ND2	2.44	0.48
61:AQ:27:VAL:O	61:AQ:30:MET:HB2	2.13	0.48
67:AW:384:MET:SD	68:AY:68:THR:HG21	2.54	0.48
9:BJ:93:HIS:O	9:BJ:96:PRO:HD2	2.14	0.48
11:BL:95:LYS:NZ	15:BP:240:GLU:OE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:64:CYS:O	12:BM:184:ARG:NH2	2.46	0.48
12:BM:136:GLU:OE1	12:BM:136:GLU:N	2.46	0.48
13:BN:137:TRP:HH2	13:BN:140:PRO:HD3	1.75	0.48
15:BP:83:GLU:HB3	15:BP:142:ARG:NH1	2.29	0.48
26:Bc:63:GLU:O	26:Bc:77:LYS:N	2.43	0.48
40:Br:127:ILE:HB	40:Br:128:PRO:HD3	1.94	0.48
40:Br:132:ILE:O	40:Br:136:TRP:HB2	2.14	0.48
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
9:J:360:ARG:HA	36:m:78:TYR:CZ	2.47	0.48
13:N:87:HIS:O	13:N:91:HIS:HD2	1.96	0.48
16:Q:57:GLU:HB2	35:l:580:GLN:NE2	2.29	0.48
16:Q:103:GLY:HA3	33:j:52:SER:HB3	1.95	0.48
17:S:28:ARG:O	17:S:33:GLY:N	2.47	0.48
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.96	0.48
25:b:39:LYS:O	25:b:42:PRO:HD2	2.13	0.48
25:b:106:PRO:HG2	25:b:118:PRO:HD3	1.96	0.48
35:l:59:GLN:NE2	35:l:59:GLN:CA	2.73	0.48
35:l:70:THR:HG23	35:l:75:GLN:HB3	1.94	0.48
36:m:118:PHE:HD1	36:m:121:VAL:HB	1.79	0.48
41:s:126:ASN:O	41:s:130:ILE:HG13	2.14	0.48
63:AF:29:LYS:NZ	63:AF:29:LYS:CB	2.73	0.48
66:AJ:177:ARG:NH2	60:AP:140:MET:O	2.47	0.48
68:AL:101:THR:HA	68:AL:154:CYS:HA	1.95	0.48
68:AL:376:TRP:HB3	68:AL:449:ILE:HG21	1.95	0.48
68:AY:294:PRO:HG3	68:AY:448:TYR:CE1	2.48	0.48
1:BA:274:LYS:HB2	1:BA:292:MET:SD	2.53	0.48
2:BB:142:ARG:NH2	11:BL:112:MET:O	2.47	0.48
4:BE:52:LEU:HB3	4:BE:54:ILE:HG13	1.96	0.48
9:BJ:357:ARG:HG3	9:BJ:362:LEU:HA	1.95	0.48
11:BL:92:ASN:HB2	15:BP:239:TRP:H	1.77	0.48
13:BN:85:GLU:HG2	13:BN:86:TRP:N	2.29	0.48
14:BO:84:ASP:O	14:BO:88:ARG:N	2.47	0.48
16:BQ:82:LEU:N	16:BQ:99:MET:O	2.41	0.48
17:BS:35:GLU:HG2	17:BS:35:GLU:O	2.14	0.48
20:BV:37:ALA:HB1	20:BV:56:VAL:HG22	1.95	0.48
76:BV:202:PEE:H40	76:BV:202:PEE:C35	2.42	0.48
24:Ba:54:LEU:CD2	25:Bb:27:GLU:CA	2.89	0.48
32:Bi:59:TYR:CZ	32:Bi:63:GLN:OE1	2.67	0.48
35:Bl:159:TYR:HB2	40:Br:416:TRP:CG	2.49	0.48
35:Bl:347:ILE:HG12	35:Bl:354:GLN:HG2	1.95	0.48
35:Bl:558:LEU:HA	35:Bl:558:LEU:HD23	1.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:591:PHE:O	35:Bl:594:PRO:HD2	2.13	0.48
40:Br:188:ASN:CG	40:Br:189:SER:H	2.21	0.48
71:Br:502:PLX:H52	71:Br:502:PLX:P1	2.53	0.48
41:Bs:205:SER:OG	41:Bs:279:ARG:NH1	2.47	0.48
44:Bw:139:ARG:HH12	44:Bw:160:GLU:CD	2.21	0.48
44:Bw:335:PRO:HA	44:Bw:338:LYS:HG3	1.94	0.48
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.48
9:J:217:PHE:CZ	9:J:322:MET:CE	2.86	0.48
12:M:348:ALA:O	12:M:352:VAL:HG23	2.12	0.48
14:O:54:ASP:OD1	14:O:55:PHE:N	2.47	0.48
76:W:201:PEE:H4	76:W:201:PEE:P	2.31	0.48
6:X:99:SER:OG	6:X:102:SER:OG	2.11	0.48
24:a:95:GLN:OE1	24:a:114:LYS:NZ	2.46	0.48
25:b:109:THR:HG22	25:b:111:LEU:H	1.79	0.48
26:c:184:TYR:HA	43:v:36:GLU:C	2.39	0.48
32:i:17:THR:HG23	32:i:137:ALA:HB2	1.96	0.48
32:i:37:MET:CE	32:i:60:PHE:HA	2.44	0.48
32:i:237:LEU:HD22	32:i:240:LEU:HD12	1.96	0.48
33:j:3:PHE:O	33:j:6:ILE:HB	2.14	0.48
35:l:211:THR:HG21	75:l:704:CDL:HA4	1.96	0.48
35:l:213:LEU:HB3	35:l:273:ILE:HD13	1.96	0.48
39:p:54:GLU:OE2	72:p:201:8Q1:C37	2.61	0.48
41:s:65:THR:O	41:s:124:ASN:ND2	2.46	0.48
53:5:39:VAL:O	53:5:42:LYS:HE2	2.14	0.48
59:AB:34:VAL:HB	59:AB:35:PRO:HD3	1.95	0.48
64:AG:14:VAL:O	64:AG:18:VAL:HG23	2.14	0.48
65:AH:296:MET:HE3	66:AJ:237:LEU:HA	1.96	0.48
66:AJ:13:LEU:HD11	66:AV:198:LEU:HD11	1.95	0.48
67:AK:64:PHE:CE1	67:AK:120:ALA:HB1	2.49	0.48
67:AK:84:ARG:HH11	67:AK:114:ALA:HB3	1.79	0.48
68:AL:260:ASP:OD2	39:Bp:12:HIS:CA	2.61	0.48
60:AP:88:PHE:O	60:AP:92:ARG:HG3	2.13	0.48
62:AR:30:LEU:HD13	62:AR:86:LEU:CD1	2.44	0.48
64:AT:40:LEU:CD1	64:AT:41:ILE:N	2.56	0.48
66:AV:141:TRP:CZ2	66:AV:260:ASN:O	2.67	0.48
68:AY:296:TRP:HB3	68:AY:349:ALA:HA	1.96	0.48
9:BJ:360:ARG:HA	36:Bm:78:TYR:CZ	2.47	0.48
10:BK:96:MET:HE3	10:BK:97:PRO:HD2	1.96	0.48
16:BQ:46:GLN:NE2	76:Bl:701:PEE:H11	2.29	0.48
21:BW:47:HIS:O	21:BW:51:MET:HG3	2.13	0.48
25:Bb:106:PRO:HG2	25:Bb:118:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Bb:201:PLX:H72	71:Bb:201:PLX:O2	2.14	0.48
32:Bi:326:LEU:HB3	32:Bi:327:PRO:HD3	1.95	0.48
35:Bl:213:LEU:HB3	35:Bl:273:ILE:HD13	1.96	0.48
41:Bs:142:TYR:CE1	41:Bs:289:LEU:HD21	2.49	0.48
44:Bw:212:PRO:O	44:Bw:215:GLN:HB2	2.14	0.48
8:I:38:PRO:HA	8:I:39:PRO:HD3	1.58	0.47
9:J:197:GLU:OE1	9:J:197:GLU:N	2.45	0.47
9:J:203:PRO:O	73:J:401:NDP:H5N	2.14	0.47
10:K:89:LEU:HD13	14:O:65:ALA:HB2	1.95	0.47
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.96	0.47
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	0.47
16:Q:124:ILE:HG22	16:Q:419:PRO:HG3	1.96	0.47
16:Q:136:PHE:CE2	16:Q:151:TYR:HB2	2.49	0.47
16:Q:205:GLU:HG3	16:Q:209:LYS:NZ	2.29	0.47
16:Q:323:ARG:N	16:Q:328:ASP:OD2	2.46	0.47
76:V:202:PEE:H40	76:V:202:PEE:C35	2.42	0.47
25:b:42:PRO:HA	25:b:45:LYS:HD2	1.96	0.47
32:i:128:LEU:HD13	32:i:216:PHE:HD2	1.78	0.47
35:l:500:THR:HG22	54:6:33:ARG:HD2	1.95	0.47
41:s:42:PRO:HD2	41:s:45:LEU:HD12	1.95	0.47
41:s:236:THR:HG22	41:s:263:THR:HG21	1.96	0.47
44:w:139:ARG:HH12	44:w:160:GLU:CD	2.21	0.47
50:2:31:TYR:HE1	50:2:98:HIS:HE1	1.62	0.47
54:6:16:ASN:ND2	54:6:16:ASN:H	2.12	0.47
66:Aj:22:PRO:HB3	66:Aj:217:LYS:HB3	1.94	0.47
67:AK:267:VAL:HG21	67:AK:447:THR:HG21	1.96	0.47
76:AL:503:PEE:H26	76:AL:503:PEE:C33	2.44	0.47
67:AW:306:THR:OG1	68:AY:111:LYS:NZ	2.46	0.47
1:BA:132:ARG:HG2	1:BA:165:GLU:OE1	2.13	0.47
2:BB:40:ASN:C	2:BB:42:GLN:H	2.21	0.47
9:BJ:141:PHE:HE2	9:BJ:183:ASN:HD22	1.62	0.47
9:BJ:218:ALA:HB2	9:BJ:353:LEU:HD22	1.96	0.47
11:BL:75:ARG:NH2	11:BL:101:PHE:HB3	2.29	0.47
12:BM:365:THR:HG22	12:BM:537:ILE:HD11	1.95	0.47
14:BO:207:GLU:HA	14:BO:210:ALA:HB3	1.96	0.47
17:BS:53:ARG:HB2	31:Bh:105:ARG:NH2	2.29	0.47
32:Bi:319:HIS:CE1	44:Bw:302:PHE:HD2	2.32	0.47
33:Bj:67:LEU:HD23	34:Bk:65:VAL:HG13	1.95	0.47
36:Bm:118:PHE:HD1	36:Bm:121:VAL:HB	1.79	0.47
38:Bo:73:THR:OG1	38:Bo:74:ILE:N	2.47	0.47
45:Bx:197:LEU:O	47:Bz:92:LEU:HD22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
2:B:52:THR:CG2	21:W:33:TYR:CE1	2.97	0.47
4:E:25:MET:CB	4:E:29:LYS:CE	2.59	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.47
11:L:170:THR:O	11:L:172:VAL:N	2.35	0.47
12:M:365:THR:HG22	12:M:537:ILE:HD11	1.95	0.47
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.29	0.47
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.97	0.47
17:S:4:GLU:O	17:S:7:PRO:HD2	2.15	0.47
21:W:141:MET:SD	36:m:47:GLY:HA2	2.53	0.47
25:b:38:GLN:OE1	25:b:38:GLN:HA	2.14	0.47
32:i:135:LYS:O	32:i:139:ILE:HG12	2.14	0.47
32:i:319:HIS:CE1	44:w:302:PHE:CD2	3.02	0.47
33:j:86:LEU:HD21	36:m:150:ARG:HD3	1.96	0.47
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.96	0.47
35:l:527:GLY:C	35:l:529:TYR:H	2.22	0.47
44:w:212:PRO:O	44:w:215:GLN:HB2	2.14	0.47
47:z:80:ARG:O	47:z:84:ILE:HG12	2.14	0.47
47:z:173:PHE:CD1	47:z:173:PHE:C	2.92	0.47
76:AH:401:PEE:C11	76:AH:401:PEE:C30	2.92	0.47
75:AJ:405:CDL:H762	75:AJ:405:CDL:H132	1.95	0.47
67:AK:425:ILE:HG22	67:AK:429:LYS:HE2	1.95	0.47
60:AP:199:GLN:NE2	60:AP:204:ARG:HG2	2.29	0.47
68:AY:377:MET:HE2	68:AY:477:TRP:H	1.78	0.47
2:BB:151:ILE:HD13	3:BC:159:TYR:CD2	2.49	0.47
3:BC:96:MET:HG2	3:BC:103:MET:HB3	1.96	0.47
11:BL:98:LYS:HA	11:BL:126:LEU:O	2.13	0.47
12:BM:287:SER:HB3	12:BM:290:THR:HG23	1.97	0.47
14:BO:182:ASN:HD21	14:BO:218:PRO:HB3	1.79	0.47
17:BS:21:LEU:HD21	41:Bs:253:GLU:HA	1.97	0.47
19:BU:58:ARG:NH2	42:Bu:49:GLU:OE1	2.43	0.47
24:Ba:114:LYS:CA	27:Bd:57:TYR:CD2	2.97	0.47
32:Bi:106:LEU:HB3	32:Bi:187:MET:HE2	1.95	0.47
32:Bi:282:MET:O	32:Bi:286:THR:HG23	2.14	0.47
34:Bk:81:ILE:CG2	34:Bk:87:LEU:HA	2.43	0.47
35:Bl:360:GLY:HA3	35:Bl:435:PRO:HA	1.96	0.47
47:Bz:173:PHE:C	47:Bz:173:PHE:CD1	2.92	0.47
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.50	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.14	0.47
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.47
17:S:53:ARG:HB2	31:h:105:ARG:NH2	2.30	0.47
20:V:62:THR:HG22	20:V:104:ARG:HD3	1.95	0.47
26:c:153:TYR:HB3	35:l:403:TYR:CD1	2.48	0.47
32:i:332:LEU:HD22	32:i:336:LEU:HD12	1.97	0.47
33:j:67:LEU:HD23	34:k:65:VAL:HG13	1.95	0.47
34:k:37:MET:HE1	34:k:63:MET:HE3	1.96	0.47
35:l:548:LEU:HB2	35:l:549:PRO:HD3	1.95	0.47
37:n:55:VAL:HG12	37:n:56:THR:N	2.24	0.47
41:s:231:ILE:HG23	41:s:270:PHE:HD2	1.79	0.47
46:y:22:HIS:CE1	53:5:44:LYS:HD3	2.49	0.47
75:AJ:404:CDL:H152	75:AJ:404:CDL:H121	1.70	0.47
68:AL:164:GLU:O	68:AL:168:ILE:HG12	2.14	0.47
60:AP:136:PHE:HB3	66:AV:50:PHE:CE2	2.49	0.47
68:AY:98:PHE:N	68:AY:98:PHE:CD1	2.79	0.47
7:BH:34:VAL:HG23	7:BH:95:ARG:CZ	2.44	0.47
9:BJ:299:ARG:HE	9:BJ:316:ARG:HH11	1.62	0.47
12:BM:36:VAL:HG23	12:BM:41:VAL:HG21	1.96	0.47
16:BQ:156:GLU:OE2	16:BQ:163:PRO:HG3	2.15	0.47
16:BQ:205:GLU:HG3	16:BQ:209:LYS:NZ	2.29	0.47
18:BT:109:THR:HB	18:BT:118:GLN:HB3	1.95	0.47
20:BV:40:ARG:HG3	75:BV:201:CDL:HB22	1.96	0.47
24:Ba:168:TRP:CZ2	30:Bg:85:ARG:HG3	2.50	0.47
24:Ba:182:SER:O	24:Ba:184:LYS:HG3	2.15	0.47
26:Bc:184:TYR:HA	43:Bv:36:GLU:C	2.39	0.47
30:Bg:27:ASP:OD1	30:Bg:28:PRO:HD2	2.13	0.47
30:Bg:67:PHE:CE1	71:Bg:203:PLX:H172	2.49	0.47
32:Bi:319:HIS:CE1	44:Bw:302:PHE:CD2	3.02	0.47
33:Bj:109:LYS:HA	33:Bj:112:ASP:HB2	1.94	0.47
35:Bl:84:TYR:HD1	35:Bl:88:MET:CE	2.01	0.47
35:Bl:211:THR:HG21	75:Bl:704:CDL:HA4	1.96	0.47
35:Bl:559:GLU:O	35:Bl:564:LYS:HG2	2.15	0.47
43:Bv:113:LYS:HA	43:Bv:116:GLU:OE1	2.13	0.47
46:By:108:TYR:N	46:By:108:TYR:CD1	2.83	0.47
47:Bz:164:PHE:O	47:Bz:168:THR:HG23	2.14	0.47
3:C:106:PHE:CD1	41:s:39:VAL:HG21	2.49	0.47
4:E:128:PRO:HG3	11:L:74:THR:OG1	2.14	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.63	0.47
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.47
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	0.47
12:M:287:SER:HB3	12:M:290:THR:HG23	1.96	0.47
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.47
24:a:113:TYR:C	27:d:57:TYR:HD2	2.23	0.47
24:a:168:TRP:CZ2	30:g:85:ARG:HG3	2.50	0.47
27:d:20:GLN:OE1	43:v:71:ARG:NH1	2.48	0.47
75:n:101:CDL:H741	75:n:101:CDL:H711	1.60	0.47
39:p:157:ALA:HB2	39:p:164:PRO:N	2.30	0.47
40:r:44:GLN:O	40:r:46:ASN:ND2	2.47	0.47
68:AL:373:GLN:HE22	68:AL:471:ILE:HG23	1.80	0.47
59:AO:11:PHE:H	59:AO:27:ARG:CZ	2.27	0.47
64:AT:24:TRP:HZ3	75:AY:501:CDL:H551	1.79	0.47
65:AU:156:ASP:OD1	65:AU:157:GLY:N	2.43	0.47
66:AV:65:SER:O	66:AV:68:HIS:HB3	2.14	0.47
67:AW:259:ARG:NH1	67:AW:449:PHE:CZ	2.83	0.47
6:BG:133:ILE:O	6:BG:136:GLU:HB2	2.15	0.47
11:BL:115:ALA:O	15:BP:228:GLN:N	2.44	0.47
15:BP:201:ASP:OD1	15:BP:202:PHE:N	2.48	0.47
16:BQ:201:PHE:CB	41:Bs:32:GLN:HG3	2.43	0.47
17:BS:4:GLU:O	17:BS:7:PRO:HD2	2.15	0.47
24:Ba:55:PHE:CE2	39:Bp:118:TYR:CG	2.82	0.47
25:Bb:106:PRO:O	43:Bv:68:LYS:NZ	2.38	0.47
25:Bb:109:THR:HA	27:Bd:18:PRO:HA	1.97	0.47
29:Bf:28:LYS:HB3	29:Bf:31:VAL:HB	1.96	0.47
29:Bf:60:LYS:O	29:Bf:64:GLU:HG3	2.15	0.47
32:Bi:37:MET:CE	32:Bi:60:PHE:HA	2.44	0.47
32:Bi:128:LEU:HD13	32:Bi:216:PHE:HD2	1.78	0.47
35:Bl:302:VAL:O	35:Bl:305:SER:OG	2.24	0.47
35:Bl:450:LEU:C	35:Bl:450:LEU:CD2	2.85	0.47
40:Br:5:ILE:O	40:Br:8:THR:OG1	2.26	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
2:B:151:ILE:HD13	3:C:159:TYR:CD2	2.50	0.47
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.47
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.47
12:M:221:ASN:OD1	12:M:291:ARG:NH2	2.35	0.47
12:M:506:VAL:HG12	12:M:508:GLY:N	2.24	0.47
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.47
16:Q:46:GLN:NE2	76:l:701:PEE:H11	2.29	0.47
16:Q:57:GLU:HB2	35:l:580:GLN:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:110:GLY:N	18:T:119:PHE:O	2.28	0.47
19:U:52:ASN:ND2	31:h:27:TYR:O	2.42	0.47
24:a:114:LYS:N	27:d:57:TYR:HD2	2.12	0.47
30:g:32:TYR:HB2	75:n:101:CDL:H732	1.97	0.47
32:i:149:LEU:HD23	32:i:154:LEU:HD13	1.96	0.47
32:i:319:HIS:CE1	44:w:302:PHE:HD2	2.32	0.47
35:l:173:LEU:HD21	40:r:405:LEU:HD21	1.96	0.47
40:r:1:MET:HG3	40:r:2:LEU:N	2.29	0.47
41:s:142:TYR:CE1	41:s:289:LEU:HD21	2.49	0.47
46:y:83:ILE:O	46:y:87:MET:HG3	2.14	0.47
60:AC:164:ASN:HD21	60:AC:175:PHE:HB3	1.80	0.47
75:AJ:405:CDL:OB9	75:AJ:405:CDL:HA4	2.13	0.47
62:AR:86:LEU:C	62:AR:86:LEU:CD2	2.86	0.47
68:AY:80:ARG:HH12	68:AY:265:LEU:HB3	1.79	0.47
3:BC:113:SER:OG	3:BC:116:GLN:OE1	2.24	0.47
7:BH:32:LEU:HG	7:BH:52:THR:HG21	1.97	0.47
7:BH:108:PRO:HG2	7:BH:111:GLN:HG2	1.96	0.47
8:BI:97:PRO:HG3	15:BP:61:PHE:CG	2.49	0.47
9:BJ:221:HIS:ND1	9:BJ:221:HIS:C	2.73	0.47
12:BM:69:LEU:HD22	12:BM:181:ARG:HG3	1.95	0.47
12:BM:198:THR:HG23	14:BO:117:THR:HG21	1.97	0.47
14:BO:54:ASP:OD1	14:BO:55:PHE:N	2.47	0.47
17:BS:53:ARG:HB2	31:Bh:105:ARG:HH22	1.80	0.47
32:Bi:237:LEU:HD22	32:Bi:240:LEU:HD12	1.96	0.47
35:Bl:95:PHE:C	35:Bl:95:PHE:HD1	2.23	0.47
35:Bl:95:PHE:CZ	35:Bl:456:ARG:HG2	2.50	0.47
44:Bw:57:SER:OG	44:Bw:154:GLY:O	2.28	0.47
44:Bw:242:LYS:HA	44:Bw:246:LEU:HG	1.95	0.47
48:B0:68:PHE:HA	48:B0:71:MET:HG2	1.95	0.47
53:B5:39:VAL:O	53:B5:42:LYS:HE2	2.14	0.47
11:L:92:ASN:O	11:L:95:LYS:HG2	2.15	0.47
12:M:236:TYR:CZ	12:M:272:ARG:HD3	2.50	0.47
22:Y:41:GLU:HG2	35:l:442:ASN:HB2	1.96	0.47
24:a:168:TRP:HZ2	30:g:85:ARG:HG3	1.80	0.47
26:c:156:VAL:HG12	43:v:98:ARG:CD	2.44	0.47
30:g:20:LEU:HD21	42:u:158:LEU:HB3	1.96	0.47
31:h:18:LEU:HD21	34:k:59:MET:HE3	1.96	0.47
35:l:32:TYR:HB3	35:l:33:PRO:HD3	1.96	0.47
40:r:367:LEU:HD13	40:r:404:ALA:HA	1.97	0.47
45:x:172:LYS:HB3	45:x:176:MET:HE2	1.96	0.47
48:0:68:PHE:HA	48:0:71:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:277:VAL:HG11	67:AK:329:SER:HA	1.97	0.47
68:AL:96:LEU:HA	68:AL:99:LYS:HG2	1.96	0.47
2:BB:84:TYR:CE2	2:BB:85:PRO:HB3	2.49	0.47
5:BF:35:ASP:O	5:BF:39:LYS:HG2	2.14	0.47
9:BJ:220:MET:SD	9:BJ:223:PHE:CD2	3.08	0.47
12:BM:564:CYS:O	12:BM:566:ILE:HG12	2.14	0.47
13:BN:38:LEU:HD22	13:BN:50:GLU:HB2	1.96	0.47
13:BN:49:TYR:HD2	13:BN:61:TRP:CZ3	2.33	0.47
16:BQ:99:MET:HE1	16:BQ:447:VAL:HG21	1.97	0.47
6:BX:82:ARG:O	6:BX:86:VAL:HG23	2.15	0.47
24:Ba:113:TYR:C	27:Bd:57:TYR:HD2	2.23	0.47
27:Bd:20:GLN:OE1	43:Bv:71:ARG:NH1	2.48	0.47
28:Be:71:PRO:O	28:Be:72:ASP:HB2	2.15	0.47
29:Bf:28:LYS:HE2	44:Bw:100:ASP:HA	1.97	0.47
30:Bg:20:LEU:HD21	42:Bu:158:LEU:HB3	1.96	0.47
71:Bg:203:PLX:H72	71:Bg:203:PLX:H11	1.96	0.47
35:Bl:549:PRO:HG3	40:Br:271:MET:HE3	1.96	0.47
37:Bn:34:ARG:CZ	75:Bn:101:CDL:HB22	2.45	0.47
40:Br:44:GLN:O	40:Br:46:ASN:ND2	2.47	0.47
40:Br:80:SER:HB3	40:Br:226:ALA:HB2	1.97	0.47
45:Bx:115:SER:O	45:Bx:121:GLY:HA2	2.14	0.47
46:By:22:HIS:CE1	53:B5:44:LYS:HD3	2.49	0.47
46:By:63:THR:O	46:By:66:THR:HG22	2.15	0.47
1:A:174:ARG:HB2	10:K:91:LEU:HD11	1.96	0.47
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.47
1:A:370:LEU:O	1:A:373:PHE:HB3	2.14	0.47
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.47
4:E:52:LEU:HB3	4:E:54:ILE:HG13	1.96	0.47
5:F:22:HIS:HB2	5:F:64:LYS:HB3	1.97	0.47
5:F:35:ASP:O	5:F:39:LYS:HG2	2.14	0.47
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
8:I:33:LYS:NZ	8:I:36:GLN:HA	2.30	0.47
8:I:69:ILE:O	8:I:71:SER:N	2.48	0.47
9:J:41:MET:HE3	9:J:42:PRO:HD2	1.96	0.47
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.47
11:L:77:VAL:HG22	11:L:78:ARG:H	1.80	0.47
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.95	0.47
12:M:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.47
14:O:115:VAL:O	14:O:119:TYR:HD2	1.96	0.47
16:Q:156:GLU:OE2	16:Q:163:PRO:HG3	2.15	0.47
16:Q:438:MET:HE1	16:Q:454:GLN:HE22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:35:GLU:HG2	17:S:35:GLU:O	2.14	0.47
76:V:202:PEE:H41	76:V:202:PEE:C37	2.40	0.47
21:W:48:TRP:O	21:W:51:MET:HB2	2.15	0.47
24:a:114:LYS:CA	27:d:57:TYR:CD2	2.97	0.47
24:a:160:MET:HE3	24:a:166:GLY:HA3	1.96	0.47
25:b:111:LEU:HB2	25:b:112:GLU:OE1	2.14	0.47
29:f:60:LYS:O	29:f:64:GLU:HG3	2.14	0.47
30:g:119:ARG:HD3	38:o:116:ILE:HD13	1.96	0.47
34:k:2:PRO:CG	36:m:115:VAL:CG2	2.84	0.47
35:l:159:TYR:HB2	40:r:416:TRP:CG	2.49	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
35:l:347:ILE:HG12	35:l:354:GLN:HG2	1.96	0.47
35:l:559:GLU:O	35:l:564:LYS:HG2	2.15	0.47
40:r:80:SER:HB3	40:r:226:ALA:HB2	1.97	0.47
43:v:104:ARG:O	43:v:108:LEU:HG	2.15	0.47
44:w:109:ASN:HD21	44:w:111:ASN:HD22	1.61	0.47
44:w:124:ASN:O	44:w:126:GLY:N	2.41	0.47
44:w:242:LYS:HA	44:w:246:LEU:HG	1.96	0.47
45:x:397:PHE:HB3	45:x:398:PRO:HD3	1.95	0.47
46:y:4:PRO:HB2	55:7:43:SER:HA	1.96	0.47
46:y:63:THR:O	46:y:66:THR:HG22	2.15	0.47
47:z:137:LEU:HD12	47:z:137:LEU:HA	1.70	0.47
48:0:41:LYS:HD3	48:0:62:LEU:HD23	1.97	0.47
51:3:67:HIS:CD2	51:3:78:LEU:HD11	2.50	0.47
54:6:11:LEU:HD23	54:6:11:LEU:O	2.15	0.47
66:AJ:97:HIS:CE1	66:AJ:100:ARG:HH21	2.32	0.47
66:AJ:223:TYR:OH	68:AL:469:ASN:ND2	2.44	0.47
75:AJ:404:CDL:OB9	75:AJ:404:CDL:O1	2.33	0.47
68:AL:133:ILE:HG22	68:AL:134:LYS:H	1.80	0.47
61:AQ:56:ILE:O	61:AQ:59:LYS:HG2	2.14	0.47
61:AQ:56:ILE:HG23	61:AQ:59:LYS:HE3	1.96	0.47
64:AT:39:ARG:HH21	64:AT:39:ARG:CG	2.15	0.47
67:AW:387:GLU:OE2	68:AY:406:THR:OG1	2.19	0.47
68:AY:294:PRO:HG3	68:AY:448:TYR:CZ	2.50	0.47
1:BA:40:ARG:NH1	1:BA:289:GLU:O	2.40	0.47
1:BA:89:GLY:HA2	1:BA:244:ASN:ND2	2.28	0.47
1:BA:203:ALA:HB2	14:BO:119:TYR:CE1	2.49	0.47
3:BC:95:HIS:HE1	16:BQ:211:PHE:CE2	2.32	0.47
5:BF:22:HIS:HB2	5:BF:64:LYS:HB3	1.97	0.47
6:BG:104:PHE:CD1	6:BG:108:LEU:HD22	2.49	0.47
7:BH:28:TYR:HD1	7:BH:52:THR:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:130:ILE:HG21	73:BJ:401:NDP:N7A	2.23	0.47
13:BN:119:GLY:O	13:BN:120:THR:OG1	2.27	0.47
16:BQ:57:GLU:HB2	35:Bl:580:GLN:NE2	2.29	0.47
16:BQ:281:GLU:N	16:BQ:281:GLU:CD	2.73	0.47
17:BS:28:ARG:O	17:BS:33:GLY:N	2.47	0.47
17:BS:38:VAL:HG21	42:Bu:94:GLN:HG2	1.97	0.47
20:BV:2:ALA:O	20:BV:6:PHE:N	2.45	0.47
24:Ba:78:THR:OG1	28:Be:96:SER:O	2.24	0.47
24:Ba:82:VAL:HG11	28:Be:104:THR:HG21	1.96	0.47
24:Ba:168:TRP:HZ2	30:Bg:85:ARG:HG3	1.80	0.47
25:Bb:38:GLN:OE1	25:Bb:38:GLN:HA	2.14	0.47
25:Bb:108:ASP:CG	25:Bb:109:THR:N	2.73	0.47
26:Bc:44:THR:HB	26:Bc:47:GLU:HG2	1.97	0.47
26:Bc:156:VAL:HG12	43:Bv:98:ARG:CD	2.44	0.47
30:Bg:32:TYR:HB2	75:Bn:101:CDL:H732	1.97	0.47
31:Bh:18:LEU:HD21	34:Bk:59:MET:HE3	1.96	0.47
35:Bl:19:ILE:HD11	35:Bl:126:ILE:HD11	1.96	0.47
35:Bl:37:LYS:HZ3	35:Bl:98:TRP:CD1	2.30	0.47
35:Bl:173:LEU:HD21	40:Br:405:LEU:HD21	1.96	0.47
37:Bn:34:ARG:HH22	75:Bn:101:CDL:PA1	2.38	0.47
45:Bx:397:PHE:HB3	45:Bx:398:PRO:HD3	1.95	0.47
45:Bx:507:GLU:O	45:Bx:508:PRO:O	2.32	0.47
46:By:83:ILE:O	46:By:87:MET:HG3	2.14	0.47
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.97	0.47
10:K:96:MET:HE3	10:K:97:PRO:HD2	1.96	0.47
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
12:M:303:THR:O	12:M:615:LEU:HB2	2.15	0.47
12:M:360:ARG:NH1	12:M:635:PRO:HD3	2.29	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
17:S:50:ARG:HD3	31:h:105:ARG:HG2	1.97	0.47
76:W:201:PEE:N	76:W:201:PEE:P	2.87	0.47
71:g:203:PLX:H72	71:g:203:PLX:H11	1.96	0.47
35:l:194:ASN:ND2	38:o:127:LEU:HB2	2.29	0.47
35:l:227:LEU:HD12	35:l:227:LEU:C	2.35	0.47
37:n:34:ARG:CZ	75:n:101:CDL:HB22	2.45	0.47
44:w:57:SER:OG	44:w:154:GLY:O	2.28	0.47
45:x:507:GLU:O	45:x:508:PRO:O	2.32	0.47
48:0:33:LEU:HD22	48:0:37:GLN:HB3	1.97	0.47
58:AA:27:TYR:HE2	65:AH:305:THR:HG22	1.80	0.47
61:AD:38:GLN:NE2	64:AG:47:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:242:ILE:HD13	65:AH:244:MET:HE2	1.97	0.47
66:AJ:171:ASP:CG	66:AJ:172:SER:H	2.23	0.47
75:AU:403:CDL:HB62	75:AU:403:CDL:H732	1.96	0.47
66:AV:171:ASP:CG	66:AV:172:SER:H	2.23	0.47
76:AV:403:PEE:H65	76:AV:403:PEE:H71	1.49	0.47
1:BA:174:ARG:HB2	10:BK:91:LEU:HD11	1.96	0.47
1:BA:275:LEU:HA	1:BA:289:GLU:HA	1.97	0.47
1:BA:371:ILE:HD11	1:BA:435:VAL:HB	1.97	0.47
2:BB:94:ARG:NH2	16:BQ:237:PRO:HG3	2.30	0.47
3:BC:106:PHE:CD1	41:Bs:39:VAL:HG21	2.49	0.47
4:BE:36:TYR:HD1	4:BE:67:PHE:HE2	1.62	0.47
5:BF:68:ARG:HA	5:BF:74:GLU:HG2	1.96	0.47
9:BJ:41:MET:HB3	9:BJ:42:PRO:HD2	1.97	0.47
10:BK:89:LEU:HD13	14:BO:65:ALA:HB2	1.95	0.47
12:BM:221:ASN:OD1	12:BM:291:ARG:NH2	2.35	0.47
12:BM:546:PHE:HD2	12:BM:568:TYR:HD1	1.63	0.47
16:BQ:97:LEU:HA	16:BQ:110:ASP:O	2.15	0.47
24:Ba:126:TYR:OH	28:Be:109:LEU:HD22	2.14	0.47
34:Bk:97:GLN:HG2	35:Bl:587:TYR:OH	2.14	0.47
71:Br:502:PLX:H192	71:Br:502:PLX:H162	1.44	0.47
41:Bs:126:ASN:O	41:Bs:130:ILE:HG13	2.14	0.47
3:C:81:PRO:HA	3:C:119:VAL:O	2.15	0.47
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.50	0.47
9:J:238:GLN:HG3	9:J:269:SER:O	2.15	0.47
12:M:620:TRP:NE1	12:M:639:LEU:HD13	2.30	0.47
16:Q:216:ARG:HE	16:Q:240:LEU:HD23	1.80	0.47
19:U:52:ASN:HD21	31:h:27:TYR:C	2.20	0.47
26:c:63:GLU:O	26:c:77:LYS:N	2.43	0.47
27:d:141:GLY:HA3	30:g:118:ILE:HD12	1.97	0.47
29:f:47:THR:OG1	29:f:48:LEU:N	2.48	0.47
35:l:549:PRO:HG3	40:r:271:MET:HE3	1.96	0.47
37:n:34:ARG:HH22	75:n:101:CDL:PA1	2.38	0.47
38:o:2:SER:OG	38:o:3:PHE:N	2.48	0.47
40:r:35:SER:O	40:r:38:PRO:HD2	2.15	0.47
71:r:501:PLX:H182	71:r:501:PLX:H211	1.66	0.47
41:s:294:LEU:HB3	41:s:295:PRO:HD3	1.97	0.47
44:w:323:GLN:O	44:w:326:ARG:HB3	2.13	0.47
46:y:108:TYR:N	46:y:108:TYR:CD1	2.83	0.47
60:AC:207:LYS:HD3	60:AC:265:PHE:CE2	2.50	0.47
67:AK:305:THR:HA	67:AK:311:GLN:NE2	2.30	0.47
67:AW:63:LEU:HD21	67:AW:218:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:369:ARG:NH2	14:BO:175:GLU:OE2	2.33	0.47
1:BA:370:LEU:O	1:BA:373:PHE:HB3	2.14	0.47
2:BB:94:ARG:CZ	16:BQ:237:PRO:HG3	2.44	0.47
7:BH:35:LEU:HA	7:BH:38:ILE:HD12	1.96	0.47
9:BJ:99:ASP:O	9:BJ:102:GLN:HG2	2.14	0.47
12:BM:236:TYR:CZ	12:BM:272:ARG:HD3	2.49	0.47
12:BM:303:THR:O	12:BM:615:LEU:HB2	2.15	0.47
12:BM:535:GLU:O	12:BM:538:ARG:HG2	2.15	0.47
14:BO:78:ALA:O	14:BO:82:VAL:HG23	2.15	0.47
14:BO:138:THR:OG1	14:BO:139:PRO:HD3	2.15	0.47
15:BP:64:TYR:CE2	15:BP:68:ILE:HD11	2.50	0.47
16:BQ:57:GLU:HB2	35:Bl:580:GLN:CD	2.40	0.47
16:BQ:71:PRO:N	16:BQ:72:PRO:CD	2.78	0.47
16:BQ:412:VAL:O	16:BQ:420:TYR:N	2.43	0.47
17:BS:50:ARG:HD3	31:Bh:105:ARG:HG2	1.97	0.47
21:BW:48:TRP:O	21:BW:51:MET:HB2	2.15	0.47
22:BY:41:GLU:HG2	35:Bl:442:ASN:HB2	1.96	0.47
25:Bb:109:THR:HG22	25:Bb:111:LEU:H	1.79	0.47
25:Bb:111:LEU:HB2	25:Bb:112:GLU:OE1	2.14	0.47
27:Bd:65:VAL:HG11	27:Bd:81:GLU:HB3	1.96	0.47
30:Bg:33:ILE:HG22	30:Bg:67:PHE:HB3	1.97	0.47
35:Bl:194:ASN:ND2	38:Bo:127:LEU:HB2	2.29	0.47
35:Bl:315:VAL:O	35:Bl:318:GLY:N	2.48	0.47
40:Br:405:LEU:HD23	40:Br:405:LEU:HA	1.73	0.47
41:Bs:294:LEU:HB3	41:Bs:295:PRO:HD3	1.97	0.47
45:Bx:484:THR:HB	57:B9:2:THR:OG1	2.15	0.47
1:A:128:ARG:O	1:A:132:ARG:HG3	2.15	0.47
5:F:14:LEU:N	5:F:17:ARG:HH22	2.13	0.47
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
10:K:91:LEU:HA	10:K:94:PHE:HD2	1.79	0.47
13:N:49:TYR:HD2	13:N:61:TRP:CZ3	2.33	0.47
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.47
14:O:84:ASP:O	14:O:88:ARG:N	2.47	0.47
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.47
16:Q:71:PRO:N	16:Q:72:PRO:CD	2.78	0.47
18:T:109:THR:HB	18:T:118:GLN:HB3	1.95	0.47
28:e:71:PRO:O	28:e:72:ASP:HB2	2.15	0.47
32:i:241:THR:OG1	32:i:242:PRO:HD3	2.15	0.47
32:i:337:LEU:C	32:i:339:ILE:H	2.23	0.47
45:x:11:ASN:ND2	45:x:13:LYS:HB2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:0:23:PRO:HB3	49:1:70:VAL:CG2	2.45	0.47
67:AK:214:THR:HG22	67:AK:216:ALA:H	1.79	0.47
68:AL:183:VAL:HG21	68:AL:286:HIS:HD2	1.79	0.47
68:AL:260:ASP:CG	39:Bp:12:HIS:CB	2.81	0.47
76:AL:503:PEE:H16	76:AL:503:PEE:C30	2.44	0.47
60:AP:167:PHE:HB2	60:AP:174:LEU:HB3	1.97	0.47
2:BB:52:THR:CG2	21:BW:33:TYR:CE1	2.98	0.47
3:BC:81:PRO:HA	3:BC:119:VAL:O	2.15	0.47
9:BJ:91:ILE:HA	9:BJ:93:HIS:CE1	2.49	0.47
9:BJ:207:PHE:CE2	9:BJ:348:LYS:HB2	2.49	0.47
9:BJ:238:GLN:HG3	9:BJ:269:SER:O	2.15	0.47
21:BW:101:VAL:HG13	21:BW:102:PRO:HD2	1.96	0.47
24:Ba:66:ARG:NH1	28:Be:74:HIS:NE2	2.63	0.47
24:Ba:114:LYS:N	27:Bd:57:TYR:HD2	2.12	0.47
26:Bc:159:LYS:CA	43:Bv:98:ARG:HH12	2.27	0.47
27:Bd:20:GLN:NE2	35:Bl:57:LEU:HD21	2.30	0.47
27:Bd:120:ILE:O	27:Bd:121:LYS:C	2.56	0.47
27:Bd:133:TYR:O	27:Bd:136:ARG:N	2.48	0.47
33:Bj:86:LEU:HD21	36:Bm:150:ARG:HD3	1.96	0.47
40:Br:35:SER:O	40:Br:38:PRO:HD2	2.15	0.47
41:Bs:203:GLY:O	41:Bs:205:SER:N	2.43	0.47
44:Bw:46:GLY:HA2	44:Bw:51:LYS:HE3	1.97	0.47
48:B0:23:PRO:HB3	49:B1:70:VAL:CG2	2.45	0.47
54:B6:11:LEU:O	54:B6:11:LEU:HD23	2.15	0.47
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.96	0.46
11:L:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
12:M:299:ARG:O	12:M:301:ARG:HG2	2.15	0.46
12:M:535:GLU:O	12:M:538:ARG:HG2	2.15	0.46
12:M:546:PHE:CE2	12:M:566:ILE:HD12	2.50	0.46
14:O:233:SER:OG	14:O:234:LEU:N	2.47	0.46
16:Q:190:HIS:HD2	16:Q:452:GLY:CA	2.26	0.46
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.98	0.46
22:Y:72:ARG:NH1	35:l:390:TYR:CZ	2.79	0.46
25:b:105:PHE:CD2	43:v:68:LYS:CA	2.98	0.46
25:b:108:ASP:CG	25:b:109:THR:N	2.73	0.46
27:d:65:VAL:HG11	27:d:81:GLU:HB3	1.96	0.46
29:f:28:LYS:HE2	44:w:100:ASP:HA	1.97	0.46
41:s:73:THR:O	41:s:76:THR:OG1	2.19	0.46
43:v:49:ALA:O	43:v:51:LEU:N	2.46	0.46
44:w:93:TYR:O	44:w:96:SER:OG	2.25	0.46
45:x:306:THR:HB	45:x:359:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:45:LYS:HZ2	63:AF:45:LYS:HB3	1.80	0.46
65:AH:96:TRP:CZ3	65:AH:208:GLU:HG3	2.49	0.46
65:AH:133:ARG:O	65:AH:135:LEU:N	2.37	0.46
66:AJ:47:THR:HG23	66:AJ:79:ILE:HG23	1.96	0.46
66:AJ:82:LEU:HD23	66:AJ:243:THR:HG21	1.96	0.46
76:AJ:403:PEE:H61	76:AJ:403:PEE:C18	2.45	0.46
68:AL:125:THR:HG22	68:AL:126:ARG:H	1.81	0.46
68:AL:332:ALA:HA	68:AL:337:LEU:HB2	1.97	0.46
60:AP:136:PHE:HD1	66:AV:50:PHE:HD2	1.62	0.46
66:AV:111:GLU:O	66:AV:115:ILE:HG12	2.15	0.46
66:AV:195:LEU:HD22	66:AV:199:PHE:CE2	2.48	0.46
68:AY:166:ASP:OD1	68:AY:167:VAL:N	2.49	0.46
1:BA:69:LEU:HD11	1:BA:143:LEU:HD21	1.96	0.46
7:BH:18:ASN:O	7:BH:19:THR:OG1	2.31	0.46
9:BJ:41:MET:HE3	9:BJ:42:PRO:HD2	1.96	0.46
12:BM:64:CYS:SG	12:BM:75:CYS:HB3	2.56	0.46
12:BM:92:CYS:SG	74:BM:803:FES:S2	3.10	0.46
12:BM:360:ARG:NH1	12:BM:635:PRO:HD3	2.29	0.46
12:BM:602:ARG:NE	12:BM:659:ILE:HD11	2.30	0.46
16:BQ:131:GLN:O	16:BQ:134:PRO:HD2	2.16	0.46
17:BS:43:TYR:CZ	21:BW:68:ARG:HD2	2.51	0.46
25:Bb:104:ILE:HB	43:Bv:48:ASP:HB3	1.98	0.46
25:Bb:105:PHE:CD2	43:Bv:68:LYS:CA	2.98	0.46
32:Bi:71:LEU:HD23	32:Bi:71:LEU:HA	1.73	0.46
35:Bl:32:TYR:HB3	35:Bl:33:PRO:HD3	1.96	0.46
35:Bl:224:SER:OG	35:Bl:256:GLY:CA	2.59	0.46
40:Br:63:THR:OG1	40:Br:64:PRO:HD3	2.15	0.46
44:Bw:139:ARG:O	44:Bw:142:GLN:HB2	2.16	0.46
45:Bx:172:LYS:HB3	45:Bx:176:MET:HE2	1.96	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.51	0.46
1:A:321:GLY:HA2	1:A:353:ALA:HB3	1.97	0.46
6:G:84:LEU:HD23	6:G:87:LEU:HD12	1.97	0.46
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.46
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.81	0.46
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.46
20:V:40:ARG:HG3	75:V:201:CDL:HB22	1.96	0.46
29:f:31:VAL:O	29:f:34:PRO:HD2	2.15	0.46
32:i:256:PRO:HG2	32:i:257:LEU:HG	1.97	0.46
35:l:512:LYS:HG3	54:6:16:ASN:HB2	1.96	0.46
39:p:167:TRP:CE3	39:p:171:VAL:HG21	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:267:TRP:O	40:r:271:MET:HG2	2.15	0.46
71:r:502:PLX:H151	71:r:502:PLX:H122	1.83	0.46
59:AB:11:PHE:CD1	59:AB:24:GLY:HA3	2.50	0.46
59:AB:35:PRO:HB3	67:AK:320:PRO:HA	1.96	0.46
63:AF:70:ASN:HD22	66:AJ:209:LEU:HG	1.80	0.46
67:AK:178:HIS:HE1	67:AK:330:TYR:CE2	2.34	0.46
61:AQ:26:ILE:HD12	64:AT:27:VAL:HG13	1.98	0.46
63:AS:14:LEU:HA	63:AS:17:ILE:HG12	1.97	0.46
63:AS:93:PRO:O	63:AS:97:GLU:HG2	2.15	0.46
1:BA:119:GLU:O	1:BA:159:ARG:NH1	2.45	0.46
2:BB:91:LEU:HG	16:BQ:215:GLU:OE2	2.15	0.46
2:BB:133:ARG:NH1	2:BB:139:ARG:HG3	2.29	0.46
71:BB:303:PLX:H272	41:Bs:280:PHE:HZ	1.79	0.46
12:BM:299:ARG:O	12:BM:301:ARG:HG2	2.15	0.46
24:Ba:114:LYS:HA	27:Bd:57:TYR:CD2	2.50	0.46
25:Bb:111:LEU:HB2	25:Bb:112:GLU:CD	2.41	0.46
26:Bc:69:GLY:HA2	38:Bo:81:ARG:H	1.80	0.46
32:Bi:241:THR:OG1	32:Bi:242:PRO:HD3	2.15	0.46
32:Bi:256:PRO:HG2	32:Bi:257:LEU:HG	1.97	0.46
33:Bj:62:PHE:CG	41:Bs:140:ILE:HG23	2.50	0.46
75:Bn:101:CDL:H342	75:Bn:101:CDL:HA62	1.97	0.46
42:Bu:25:LEU:O	42:Bu:29:ALA:HB2	2.16	0.46
51:B3:67:HIS:CD2	51:B3:78:LEU:HD11	2.50	0.46
57:B9:1:ILE:O	57:B9:1:ILE:HG23	2.15	0.46
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.46
7:H:32:LEU:HA	7:H:35:LEU:HG	1.97	0.46
8:I:96:THR:OG1	8:I:98:ALA:O	2.19	0.46
12:M:64:CYS:SG	12:M:75:CYS:HB3	2.55	0.46
12:M:382:ARG:O	12:M:386:LEU:HG	2.16	0.46
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.46
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.16	0.46
22:Y:88:ASP:N	22:Y:89:PRO:CD	2.78	0.46
24:a:114:LYS:HA	27:d:57:TYR:CD2	2.50	0.46
27:d:120:ILE:O	27:d:123:VAL:N	2.48	0.46
27:d:121:LYS:O	27:d:125:GLN:HG3	2.15	0.46
27:d:133:TYR:O	27:d:136:ARG:N	2.48	0.46
30:g:33:ILE:HG22	30:g:67:PHE:HB3	1.97	0.46
30:g:67:PHE:CE1	71:g:203:PLX:H172	2.49	0.46
71:g:202:PLX:H1B3	71:g:202:PLX:H22	1.58	0.46
71:g:203:PLX:H101	71:g:203:PLX:H291	1.98	0.46
33:j:62:PHE:CG	41:s:140:ILE:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:95:PHE:C	35:l:95:PHE:HD1	2.22	0.46
38:o:95:PHE:CE1	71:AN:101:PLX:H221	2.51	0.46
71:r:502:PLX:H311	71:r:502:PLX:H282	1.76	0.46
42:u:25:LEU:O	42:u:29:ALA:HB2	2.16	0.46
45:x:273:MET:HG3	45:x:319:LYS:NZ	2.31	0.46
48:0:102:TYR:CD2	57:9:35:TYR:HE1	2.33	0.46
57:9:1:ILE:HG23	57:9:1:ILE:O	2.15	0.46
58:AA:12:ARG:NH1	68:AL:279:ASP:OD1	2.49	0.46
65:AH:249:TYR:O	65:AH:252:VAL:HG23	2.14	0.46
76:AH:401:PEE:C11	76:AH:401:PEE:C31	2.93	0.46
65:AU:88:GLU:HB3	65:AU:238:PRO:HA	1.97	0.46
1:BA:128:ARG:O	1:BA:132:ARG:HG3	2.15	0.46
7:BH:32:LEU:HA	7:BH:35:LEU:HG	1.97	0.46
9:BJ:85:ARG:CG	9:BJ:85:ARG:NH1	2.72	0.46
12:BM:168:LEU:HD23	12:BM:292:PHE:CD2	2.46	0.46
12:BM:292:PHE:HB3	12:BM:706:THR:HG21	1.96	0.46
13:BN:29:ARG:HH22	13:BN:65:THR:C	2.17	0.46
16:BQ:82:LEU:HD23	16:BQ:82:LEU:HA	1.77	0.46
16:BQ:97:LEU:HD12	16:BQ:97:LEU:O	2.15	0.46
16:BQ:408:GLY:HA3	16:BQ:425:LYS:HB3	1.98	0.46
6:BX:132:ASP:HA	6:BX:135:ALA:HB3	1.98	0.46
22:BY:87:PRO:HB3	43:Bv:103:GLU:CD	2.32	0.46
27:Bd:43:ARG:O	27:Bd:47:GLU:HG2	2.15	0.46
29:Bf:31:VAL:O	29:Bf:34:PRO:HD2	2.15	0.46
32:Bi:102:MET:HE3	32:Bi:138:PRO:HB3	1.98	0.46
32:Bi:332:LEU:HD22	32:Bi:336:LEU:HD12	1.96	0.46
35:Bl:140:LEU:O	35:Bl:144:TRP:HB2	2.15	0.46
35:Bl:533:MET:HE3	76:Bl:702:PEE:H32	1.97	0.46
40:Br:267:TRP:O	40:Br:271:MET:HG2	2.15	0.46
48:B0:41:LYS:HD3	48:B0:62:LEU:HD23	1.97	0.46
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
2:B:192:GLY:O	2:B:196:GLU:HB2	2.15	0.46
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	0.46
12:M:602:ARG:NE	12:M:659:ILE:HD11	2.30	0.46
13:N:38:LEU:HD22	13:N:50:GLU:HB2	1.96	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
17:S:53:ARG:HB2	31:h:105:ARG:HH22	1.80	0.46
22:Y:44:TYR:HD1	35:l:440:LEU:HB2	1.78	0.46
71:b:201:PLX:C3	71:b:201:PLX:C1C	2.86	0.46
26:c:101:TRP:NE1	38:o:61:GLU:O	2.43	0.46
26:c:177:GLU:O	26:c:178:PRO:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:73:THR:OG1	38:o:74:ILE:N	2.47	0.46
40:r:61:LEU:O	40:r:64:PRO:HD2	2.15	0.46
45:x:484:THR:HB	57:9:2:THR:OG1	2.15	0.46
46:y:1:MET:SD	46:y:133:LEU:HD11	2.56	0.46
47:z:128:GLU:HB3	47:z:129:VAL:H	1.56	0.46
47:z:164:PHE:O	47:z:168:THR:HG23	2.14	0.46
48:0:33:LEU:HD13	48:0:41:LYS:HG3	1.97	0.46
63:AF:51:LEU:HD22	63:AF:55:LEU:HB3	1.96	0.46
65:AH:321:TYR:CD2	65:AH:323:PRO:HD3	2.51	0.46
66:AJ:362:ILE:HG13	66:AJ:363:LEU:HD12	1.98	0.46
58:AN:67:PHE:HD1	66:AV:344:SER:HG	1.62	0.46
61:AQ:14:LEU:O	61:AQ:20:THR:OG1	2.33	0.46
63:AS:35:ASP:O	63:AS:38:ILE:HG22	2.15	0.46
63:AS:55:LEU:HD11	63:AS:90:TYR:HB2	1.97	0.46
65:AU:131:ALA:HA	65:AU:174:TYR:HA	1.97	0.46
65:AU:204:ARG:HE	81:AU:402:HEC:CGA	2.29	0.46
1:BA:276:PHE:CE2	1:BA:290:GLU:HB3	2.50	0.46
2:BB:104:TYR:N	2:BB:108:GLU:O	2.33	0.46
5:BF:36:PHE:CE1	5:BF:40:ARG:HB2	2.51	0.46
9:BJ:163:LYS:HE2	9:BJ:253:VAL:HA	1.97	0.46
11:BL:92:ASN:O	11:BL:95:LYS:HG2	2.15	0.46
12:BM:255:ASP:HB3	12:BM:257:VAL:HG23	1.98	0.46
12:BM:457:SER:O	12:BM:499:LYS:NZ	2.49	0.46
12:BM:546:PHE:CE2	12:BM:566:ILE:HD12	2.50	0.46
12:BM:692:LYS:HG3	12:BM:714:VAL:HG13	1.98	0.46
16:BQ:124:ILE:HG22	16:BQ:419:PRO:HG3	1.96	0.46
22:BY:81:LEU:HD11	43:Bv:89:TYR:HA	1.98	0.46
29:Bf:47:THR:O	29:Bf:51:THR:HG23	2.16	0.46
31:Bh:80:ARG:NH1	36:Bm:1:MET:SD	2.89	0.46
34:Bk:37:MET:HE1	34:Bk:63:MET:HE3	1.97	0.46
35:Bl:51:THR:CG2	35:Bl:91:PRO:HG2	2.30	0.46
37:Bn:42:SER:O	37:Bn:46:LYS:HB2	2.16	0.46
39:Bp:157:ALA:HB2	39:Bp:164:PRO:N	2.30	0.46
44:Bw:86:PHE:CE2	44:Bw:157:VAL:HG11	2.50	0.46
44:Bw:91:ILE:HG23	44:Bw:134:TRP:CD1	2.51	0.46
46:By:1:MET:SD	46:By:133:LEU:HD11	2.56	0.46
48:B0:108:PRO:HG2	48:B0:111:PHE:CD2	2.50	0.46
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	0.46
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	0.46
12:M:392:ALA:HA	12:M:417:ARG:HH22	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:241:MET:HE3	21:W:16:TYR:OH	2.15	0.46
24:a:170:TYR:HE2	24:a:172:GLU:HG2	1.80	0.46
25:b:111:LEU:HB2	25:b:112:GLU:CD	2.41	0.46
26:c:69:GLY:HA2	38:o:81:ARG:H	1.80	0.46
36:m:19:PHE:HB3	36:m:31:VAL:HB	1.98	0.46
45:x:435:GLY:O	45:x:437:PRO:HD3	2.16	0.46
76:AH:401:PEE:C30	76:AH:401:PEE:C10	2.93	0.46
67:AK:115:THR:HG23	67:AK:118:ASN:H	1.80	0.46
67:AK:183:ARG:NH2	67:AK:254:ARG:CB	2.78	0.46
68:AL:101:THR:HA	68:AL:155:SER:H	1.81	0.46
65:AU:104:SER:OG	65:AU:283:ASP:OD1	2.27	0.46
68:AY:465:LEU:HD12	68:AY:466:PRO:HD2	1.97	0.46
1:BA:177:TYR:CE2	10:BK:91:LEU:HD13	2.50	0.46
6:BG:84:LEU:HD23	6:BG:87:LEU:HD12	1.97	0.46
9:BJ:281:PHE:HA	9:BJ:284:ALA:HB3	1.97	0.46
11:BL:78:ARG:HA	11:BL:146:ASP:OD1	2.16	0.46
12:BM:164:ASN:OD1	12:BM:165:ILE:N	2.49	0.46
22:BY:88:ASP:N	22:BY:89:PRO:CD	2.78	0.46
25:Bb:89:HIS:CD2	25:Bb:89:HIS:C	2.90	0.46
28:Be:113:ARG:HH21	40:Br:459:SER:HB2	1.80	0.46
32:Bi:39:ALA:O	32:Bi:42:PRO:HD2	2.16	0.46
32:Bi:337:LEU:C	32:Bi:339:ILE:H	2.23	0.46
35:Bl:233:LEU:HB3	35:Bl:234:PRO:HD3	1.96	0.46
35:Bl:367:PRO:O	35:Bl:371:THR:HG23	2.16	0.46
45:Bx:306:THR:HB	45:Bx:359:ALA:O	2.15	0.46
46:By:78:LEU:HB2	46:By:79:PRO:CD	2.38	0.46
50:B2:40:SER:OG	50:B2:45:ASP:HB3	2.16	0.46
55:B7:9:PHE:HD1	55:B7:10:HIS:HD2	1.63	0.46
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	0.46
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46
6:G:133:ILE:O	6:G:136:GLU:HB2	2.15	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
9:J:221:HIS:ND1	9:J:221:HIS:C	2.73	0.46
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	0.46
9:J:281:PHE:HA	9:J:284:ALA:HB3	1.97	0.46
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.46
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.46
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.46
16:Q:205:GLU:O	16:Q:209:LYS:HG3	2.16	0.46
17:S:21:LEU:HD21	41:s:253:GLU:HA	1.96	0.46
21:W:115:ARG:NH1	31:h:36:PHE:HD1	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:156:ARG:NH1	28:e:139:SER:O	2.37	0.46
29:f:55:TRP:CZ2	30:g:65:THR:HG22	2.51	0.46
35:l:19:ILE:HD11	35:l:126:ILE:HD11	1.96	0.46
39:p:51:HIS:O	72:p:201:8Q1:C38	2.64	0.46
44:w:139:ARG:O	44:w:142:GLN:HB2	2.15	0.46
59:AB:53:GLU:O	68:AL:402:HIS:ND1	2.47	0.46
64:AG:16:ASN:CG	68:AL:442:ARG:HH12	2.23	0.46
68:AL:286:HIS:ND1	68:AL:359:VAL:HG22	2.31	0.46
66:AV:24:PRO:HD2	66:AV:27:ILE:HD11	1.97	0.46
66:AV:129:MET:HE1	66:AV:185:LEU:HD12	1.97	0.46
66:AV:343:VAL:CG1	66:AV:348:THR:HG22	2.46	0.46
1:BA:119:GLU:OE1	1:BA:127:ASP:HB2	2.14	0.46
1:BA:321:GLY:HA2	1:BA:353:ALA:HB3	1.97	0.46
4:BE:40:TYR:CE1	4:BE:60:ARG:HD3	2.51	0.46
10:BK:91:LEU:HA	10:BK:94:PHE:HD2	1.79	0.46
13:BN:83:PRO:HG2	13:BN:86:TRP:HB2	1.98	0.46
14:BO:58:GLU:O	14:BO:62:ARG:HG3	2.15	0.46
15:BP:186:ARG:NH2	15:BP:193:PHE:HB3	2.30	0.46
16:BQ:241:MET:HE3	21:BW:16:TYR:OH	2.15	0.46
21:BW:111:PHE:CD2	21:BW:117:VAL:HG21	2.51	0.46
27:Bd:141:GLY:HA3	30:Bg:118:ILE:HD12	1.97	0.46
29:Bf:47:THR:OG1	29:Bf:48:LEU:N	2.48	0.46
31:Bh:91:LYS:HG3	31:Bh:92:TYR:N	2.28	0.46
33:Bj:56:PHE:CE1	36:Bm:70:THR:HG21	2.51	0.46
35:Bl:371:THR:O	35:Bl:374:THR:OG1	2.28	0.46
35:Bl:512:LYS:HD3	54:B6:18:LEU:HD12	1.97	0.46
41:Bs:89:LEU:HA	41:Bs:90:PRO:HD3	1.65	0.46
41:Bs:248:ASP:OD1	41:Bs:249:ALA:N	2.49	0.46
43:Bv:50:GLN:O	43:Bv:56:ARG:NH1	2.41	0.46
43:Bv:104:ARG:O	43:Bv:108:LEU:HG	2.15	0.46
44:Bw:258:TYR:CE1	44:Bw:267:LYS:HA	2.49	0.46
1:A:319:PRO:HB2	1:A:347:THR:HG21	1.98	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	0.46
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	0.46
4:E:62:LYS:HE3	4:E:66:MET:HE2	1.98	0.46
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.96	0.46
12:M:589:TYR:CE2	12:M:590:THR:HG23	2.50	0.46
13:N:83:PRO:HG2	13:N:86:TRP:HB2	1.98	0.46
14:O:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.97	0.46
25:b:109:THR:HA	27:d:18:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:56:ASN:HD21	38:o:43:LEU:HD11	1.81	0.46
27:d:20:GLN:NE2	35:l:57:LEU:HD21	2.31	0.46
35:l:140:LEU:O	35:l:144:TRP:HB2	2.15	0.46
35:l:189:PHE:CG	35:l:201:MET:HE3	2.50	0.46
35:l:512:LYS:HD3	54:6:18:LEU:HD12	1.97	0.46
40:r:63:THR:OG1	40:r:64:PRO:HD3	2.15	0.46
46:y:58:ALA:O	46:y:60:GLU:HG3	2.16	0.46
60:AC:178:HIS:HD2	60:AC:209:GLU:O	1.99	0.46
62:AE:74:PHE:CZ	62:AE:78:ARG:HD2	2.51	0.46
64:AG:39:ARG:HE	64:AG:51:LYS:HD2	1.80	0.46
75:AG:101:CDL:H371	75:AG:101:CDL:H341	1.78	0.46
67:AK:370:ASP:OD1	67:AK:371:VAL:N	2.49	0.46
75:AL:502:CDL:HB62	75:AL:502:CDL:H712	1.75	0.46
64:AT:24:TRP:CH2	75:AY:501:CDL:H551	2.50	0.46
68:AY:152:GLN:HE22	68:AY:252:GLY:H	1.61	0.46
3:BC:147:VAL:CG2	3:BC:176:VAL:HA	2.46	0.46
9:BJ:229:GLY:HA2	9:BJ:293:LEU:O	2.15	0.46
11:BL:77:VAL:HG22	11:BL:78:ARG:H	1.80	0.46
15:BP:97:LEU:HA	15:BP:100:LEU:HD12	1.97	0.46
17:BS:53:ARG:HH21	31:Bh:105:ARG:HD3	1.77	0.46
20:BV:14:ASP:O	20:BV:21:LYS:NZ	2.45	0.46
26:Bc:41:TYR:CE1	26:Bc:67:ASP:HB3	2.51	0.46
26:Bc:177:GLU:O	26:Bc:178:PRO:C	2.59	0.46
29:Bf:34:PRO:O	29:Bf:38:LYS:HG3	2.16	0.46
29:Bf:55:TRP:CZ2	30:Bg:65:THR:HG22	2.51	0.46
35:Bl:189:PHE:CG	35:Bl:201:MET:HE3	2.50	0.46
36:Bm:10:VAL:O	36:Bm:14:MET:HG2	2.16	0.46
48:B0:33:LEU:HD13	48:B0:41:LYS:HG3	1.97	0.46
71:B:303:PLX:H272	41:s:280:PHE:HZ	1.80	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.50	0.46
3:C:113:SER:OG	3:C:116:GLN:OE1	2.24	0.46
4:E:40:TYR:OH	6:G:117:GLU:OE2	2.28	0.46
4:E:43:VAL:HB	4:E:44:PRO:HD3	1.98	0.46
12:M:37:ASP:HA	12:M:103:LEU:HD23	1.98	0.46
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	0.46
16:Q:82:LEU:HD23	16:Q:82:LEU:HA	1.78	0.46
24:a:182:SER:O	24:a:184:LYS:HG3	2.15	0.46
25:b:112:GLU:N	25:b:112:GLU:CD	2.74	0.46
35:l:399:ALA:O	35:l:402:SER:OG	2.33	0.46
37:n:42:SER:O	37:n:46:LYS:HB2	2.16	0.46
41:s:203:GLY:O	41:s:205:SER:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:248:ASP:OD1	41:s:249:ALA:N	2.49	0.46
44:w:86:PHE:CE2	44:w:157:VAL:HG11	2.50	0.46
46:y:185:MET:SD	46:y:185:MET:C	2.98	0.46
48:0:108:PRO:HG2	48:0:111:PHE:CD2	2.50	0.46
50:2:40:SER:OG	50:2:45:ASP:HB3	2.16	0.46
58:AA:41:ARG:NE	75:AA:101:CDL:OA4	2.34	0.46
58:AA:66:GLU:HG2	66:AJ:346:PRO:HB3	1.96	0.46
66:AJ:140:PHE:O	66:AJ:144:THR:OG1	2.26	0.46
67:AW:277:VAL:HA	67:AW:278:ALA:HA	1.73	0.46
67:AW:298:HIS:HE1	67:AW:377:LYS:HG2	1.81	0.46
67:AW:449:PHE:N	67:AW:452:GLU:CD	2.73	0.46
2:BB:151:ILE:HD13	3:BC:159:TYR:CE2	2.51	0.46
4:BE:99:GLN:NE2	33:Bj:41:PHE:CD1	2.82	0.46
5:BF:14:LEU:N	5:BF:17:ARG:HH22	2.13	0.46
9:BJ:141:PHE:CE2	9:BJ:183:ASN:ND2	2.83	0.46
12:BM:620:TRP:NE1	12:BM:639:LEU:HD13	2.30	0.46
14:BO:76:ALA:HA	14:BO:79:VAL:HG23	1.98	0.46
14:BO:200:ASP:O	14:BO:204:ILE:HG12	2.16	0.46
16:BQ:399:ALA:HB1	16:BQ:406:GLU:HG3	1.98	0.46
22:BY:74:TRP:CE3	22:BY:75:HIS:CA	2.91	0.46
22:BY:89:PRO:O	43:Bv:107:ARG:NH1	2.49	0.46
35:Bl:512:LYS:CB	54:B6:16:ASN:HB2	2.46	0.46
36:Bm:109:TYR:O	36:Bm:112:VAL:HG23	2.16	0.46
38:Bo:52:ASN:HD22	39:Bp:166:LEU:HG	1.81	0.46
40:Br:1:MET:HG3	40:Br:2:LEU:N	2.29	0.46
71:Br:501:PLX:H122	71:Br:501:PLX:H151	1.80	0.46
45:Bx:299:VAL:HA	45:Bx:302:ARG:NH1	2.31	0.46
45:Bx:449:MET:HE3	55:B7:40:TRP:HB3	1.98	0.46
48:B0:33:LEU:HD22	48:B0:37:GLN:HB3	1.97	0.46
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.46
9:J:163:LYS:HE2	9:J:253:VAL:HA	1.98	0.46
16:Q:159:LEU:O	16:Q:161:ILE:HG13	2.16	0.46
16:Q:281:GLU:N	16:Q:281:GLU:CD	2.73	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.46
32:i:102:MET:HE3	32:i:138:PRO:HB3	1.98	0.46
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.50	0.46
35:l:512:LYS:CB	54:6:16:ASN:HB2	2.46	0.46
35:l:533:MET:HE3	76:l:702:PEE:H32	1.97	0.46
38:o:52:ASN:HD22	39:p:166:LEU:HG	1.81	0.46
40:r:408:LEU:HA	40:r:408:LEU:HD23	1.70	0.46
44:w:46:GLY:HA2	44:w:51:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:91:ILE:HG23	44:w:134:TRP:CD1	2.51	0.46
46:y:16:ILE:HD12	46:y:17:MET:H	1.77	0.46
58:AA:74:ASN:OD1	58:AA:78:TYR:HE2	1.99	0.46
68:AL:75:ILE:HD13	68:AL:224:TYR:CD1	2.51	0.46
68:AL:166:ASP:OD1	68:AL:167:VAL:N	2.49	0.46
68:AL:373:GLN:NE2	68:AL:471:ILE:HG23	2.31	0.46
1:BA:311:TRP:CD1	1:BA:314:LEU:HD12	2.50	0.46
7:BH:114:TRP:CD2	7:BH:115:PRO:HA	2.51	0.46
11:BL:62:THR:HG23	11:BL:72:ILE:HD13	1.98	0.46
12:BM:589:TYR:CE2	12:BM:590:THR:HG23	2.50	0.46
12:BM:645:ARG:HG3	12:BM:648:GLU:OE2	2.16	0.46
15:BP:97:LEU:HD23	15:BP:100:LEU:HD12	1.97	0.46
16:BQ:216:ARG:HE	16:BQ:240:LEU:HD23	1.80	0.46
71:BV:203:PLX:H221	38:Bo:95:PHE:CE1	2.51	0.46
23:BZ:31:THR:O	23:BZ:34:LYS:HB3	2.16	0.46
25:Bb:112:GLU:N	25:Bb:112:GLU:CD	2.74	0.46
27:Bd:120:ILE:O	27:Bd:123:VAL:N	2.48	0.46
35:Bl:370:SER:O	35:Bl:374:THR:HG23	2.16	0.46
39:Bp:51:HIS:O	72:Bp:201:8Q1:C38	2.64	0.46
40:Br:367:LEU:HD13	40:Br:404:ALA:HA	1.97	0.46
46:By:185:MET:SD	46:By:185:MET:C	2.99	0.46
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.46
1:A:371:ILE:HD11	1:A:435:VAL:HB	1.97	0.46
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.46
71:B:303:PLX:H1B3	71:B:303:PLX:H21	1.76	0.46
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.46
12:M:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.46
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.46
14:O:58:GLU:O	14:O:62:ARG:HG3	2.15	0.46
16:Q:255:LEU:HD11	16:Q:337:MET:HG2	1.98	0.46
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.98	0.46
24:a:66:ARG:NH1	28:e:74:HIS:NE2	2.63	0.46
26:c:44:THR:HB	26:c:47:GLU:HG2	1.97	0.46
26:c:174:PRO:O	26:c:175:SER:OG	2.26	0.46
35:l:302:VAL:O	35:l:306:THR:HG23	2.16	0.46
35:l:367:PRO:O	35:l:371:THR:HG23	2.16	0.46
37:n:30:LYS:HZ3	75:n:101:CDL:HA31	1.80	0.46
41:s:89:LEU:HD12	41:s:91:MET:HE2	1.98	0.46
43:v:60:ALA:O	43:v:61:HIS:C	2.59	0.46
46:y:76:ILE:O	46:y:79:PRO:HD2	2.16	0.46
50:2:98:HIS:ND1	50:2:98:HIS:N	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:7:9:PHE:HD1	55:7:10:HIS:HD2	1.63	0.46
63:AF:38:ILE:HG12	63:AF:39:TYR:N	2.30	0.46
67:AK:259:ARG:HH21	67:AK:259:ARG:CB	2.10	0.46
59:AO:11:PHE:CD1	59:AO:27:ARG:HD2	2.51	0.46
59:AO:37:THR:N	68:AY:174:GLU:OE2	2.41	0.46
62:AR:62:HIS:ND1	62:AR:62:HIS:O	2.48	0.46
67:AW:138:LEU:O	67:AW:142:THR:OG1	2.25	0.46
71:BB:303:PLX:H332	71:BB:303:PLX:H301	1.79	0.46
3:BC:106:PHE:CE2	3:BC:191:LEU:HD11	2.51	0.46
4:BE:98:LYS:HG2	15:BP:191:TYR:HB3	1.96	0.46
8:BI:33:LYS:NZ	8:BI:36:GLN:HA	2.30	0.46
9:BJ:168:SER:HA	9:BJ:184:LYS:HE3	1.97	0.46
11:BL:109:ASN:OD1	11:BL:110:PRO:HD2	2.16	0.46
11:BL:121:LEU:HA	15:BP:203:PRO:HB3	1.97	0.46
11:BL:136:SER:O	11:BL:140:LYS:HG3	2.16	0.46
12:BM:455:ILE:HG12	12:BM:463:SER:HB3	1.98	0.46
14:BO:153:GLN:HG3	14:BO:158:ILE:O	2.15	0.46
16:BQ:255:LEU:HD11	16:BQ:337:MET:HG2	1.98	0.46
27:Bd:121:LYS:O	27:Bd:125:GLN:HG3	2.15	0.46
32:Bi:324:PRO:C	32:Bi:326:LEU:H	2.24	0.46
34:Bk:2:PRO:CG	36:Bm:115:VAL:CG2	2.84	0.46
35:Bl:302:VAL:O	35:Bl:306:THR:HG23	2.16	0.46
36:Bm:19:PHE:HB3	36:Bm:31:VAL:HB	1.98	0.46
38:Bo:52:ASN:O	39:Bp:129:ARG:NH2	2.49	0.46
40:Br:61:LEU:O	40:Br:64:PRO:HD2	2.15	0.46
71:Br:502:PLX:H151	71:Br:502:PLX:H122	1.83	0.46
46:By:59:GLN:CA	46:By:62:GLU:HB2	2.46	0.46
48:B0:102:TYR:CD2	57:B9:35:TYR:HE1	2.33	0.46
49:B1:70:VAL:HG12	49:B1:71:VAL:N	2.31	0.46
53:B5:19:PHE:CD1	53:B5:19:PHE:C	2.94	0.46
1:A:44:ASN:HD22	1:A:59:ARG:NH2	2.14	0.45
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.45
5:F:36:PHE:CE1	5:F:40:ARG:HB2	2.51	0.45
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.45
11:L:107:TRP:O	11:L:116:SER:HB2	2.16	0.45
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.45
12:M:421:SER:O	12:M:425:ASN:N	2.49	0.45
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.45
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.98	0.45
25:b:116:VAL:HG12	25:b:117:ILE:N	2.31	0.45
29:f:28:LYS:HB3	29:f:31:VAL:HB	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:34:PRO:O	29:f:38:LYS:HG3	2.16	0.45
37:n:27:LEU:HD12	40:r:2:LEU:HD21	1.99	0.45
75:n:101:CDL:H342	75:n:101:CDL:HA62	1.97	0.45
45:x:32:ALA:HB3	56:8:36:PRO:HG2	1.98	0.45
45:x:195:LEU:CD2	45:x:245:ILE:HD13	2.45	0.45
45:x:299:VAL:HA	45:x:302:ARG:NH1	2.31	0.45
47:z:42:LEU:HD12	47:z:42:LEU:HA	1.65	0.45
48:0:66:GLU:O	49:1:66:ARG:NH2	2.49	0.45
58:AA:16:SER:HA	65:AH:319:LEU:HA	1.98	0.45
60:AC:135:GLN:HG3	66:AJ:75:TYR:CD2	2.51	0.45
66:AJ:138:MET:HE1	66:AJ:268:ILE:HA	1.97	0.45
68:AL:326:SER:O	68:AL:330:SER:N	2.43	0.45
58:AN:67:PHE:CB	66:AV:346:PRO:HG3	2.42	0.45
60:AP:181:GLN:HA	60:AP:184:ILE:HD12	1.98	0.45
62:AR:71:LEU:HD22	65:AU:222:PRO:HG3	1.97	0.45
63:AS:76:LEU:O	63:AS:81:TRP:NE1	2.37	0.45
63:AS:83:LYS:HB2	63:AS:86:GLU:HB2	1.98	0.45
67:AW:38:LEU:HD21	67:AW:406:TYR:CD1	2.51	0.45
1:BA:202:GLY:O	12:BM:200:ARG:NH2	2.42	0.45
1:BA:319:PRO:HB2	1:BA:347:THR:HG21	1.98	0.45
3:BC:168:ARG:HG3	3:BC:172:ARG:NH1	2.31	0.45
9:BJ:238:GLN:NE2	9:BJ:267:GLY:O	2.43	0.45
11:BL:69:GLU:HB2	11:BL:73:LYS:NZ	2.30	0.45
12:BM:382:ARG:O	12:BM:386:LEU:HG	2.16	0.45
16:BQ:140:ASP:HB3	16:BQ:147:ASN:ND2	2.28	0.45
18:BT:68:ALA:O	18:BT:72:ILE:HG13	2.16	0.45
20:BV:121:ALA:O	20:BV:125:VAL:HG23	2.15	0.45
21:BW:77:ALA:O	21:BW:80:ASP:HB3	2.16	0.45
24:Ba:170:TYR:HE2	24:Ba:172:GLU:HG2	1.80	0.45
25:Bb:42:PRO:HA	25:Bb:45:LYS:HD2	1.97	0.45
25:Bb:88:TYR:CG	71:Bb:201:PLX:H1C2	2.51	0.45
25:Bb:106:PRO:HA	25:Bb:115:GLU:CD	2.41	0.45
71:Bb:201:PLX:C3	71:Bb:201:PLX:C1C	2.86	0.45
26:Bc:153:TYR:HB3	35:Bl:403:TYR:CD1	2.48	0.45
71:Bg:203:PLX:H291	71:Bg:203:PLX:H101	1.98	0.45
37:Bn:27:LEU:HD12	40:Br:2:LEU:HD21	1.98	0.45
40:Br:58:SER:HB2	40:Br:63:THR:HG22	1.97	0.45
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.81	0.45
1:A:129:GLU:OE1	1:A:132:ARG:NH1	2.49	0.45
1:A:379:CYS:O	12:M:201:GLY:N	2.49	0.45
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.45
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.45
7:H:35:LEU:O	7:H:45:ARG:NE	2.43	0.45
8:I:30:GLU:HG2	8:I:31:ILE:N	2.32	0.45
9:J:207:PHE:CE2	9:J:348:LYS:HB2	2.49	0.45
9:J:220:MET:O	9:J:223:PHE:HB2	2.16	0.45
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.45
12:M:692:LYS:HG3	12:M:714:VAL:HG13	1.98	0.45
16:Q:97:LEU:HD12	16:Q:97:LEU:O	2.15	0.45
16:Q:259:GLU:O	16:Q:263:THR:OG1	2.34	0.45
16:Q:446:ASP:O	16:Q:450:ILE:HG13	2.16	0.45
19:U:18:VAL:HG11	41:s:292:ASN:O	2.17	0.45
27:d:43:ARG:O	27:d:47:GLU:HG2	2.15	0.45
29:f:32:ARG:O	29:f:35:PRO:HD2	2.16	0.45
31:h:36:PHE:HD2	31:h:66:CYS:HB2	1.82	0.45
32:i:25:HIS:CE1	32:i:84:TRP:CE3	3.05	0.45
32:i:251:LEU:HD23	32:i:251:LEU:HA	1.82	0.45
33:j:56:PHE:CE1	36:m:70:THR:HG21	2.51	0.45
35:l:166:THR:CG2	76:l:702:PEE:H2	2.46	0.45
35:l:241:THR:O	35:l:244:SER:OG	2.32	0.45
35:l:315:VAL:O	35:l:318:GLY:N	2.48	0.45
36:m:109:TYR:O	36:m:112:VAL:HG23	2.16	0.45
36:m:130:GLU:OE1	36:m:130:GLU:N	2.39	0.45
40:r:58:SER:HB2	40:r:63:THR:HG22	1.97	0.45
43:v:50:GLN:O	43:v:56:ARG:NH1	2.41	0.45
60:AC:164:ASN:HB3	60:AC:226:ALA:HB1	1.98	0.45
58:AN:28:PRO:HB2	58:AN:29:HIS:CD2	2.50	0.45
59:AO:43:LEU:HD11	68:AY:179:MET:HG3	1.97	0.45
60:AP:177:ARG:HB3	60:AP:211:VAL:HG13	1.97	0.45
63:AS:51:LEU:HD22	63:AS:55:LEU:HD22	1.99	0.45
66:AV:7:THR:O	66:AV:12:LYS:HE3	2.17	0.45
66:AV:150:LEU:HD23	66:AV:164:ILE:CD1	2.43	0.45
1:BA:44:ASN:HD22	1:BA:59:ARG:NH2	2.14	0.45
3:BC:161:HIS:CE1	3:BC:168:ARG:HD2	2.51	0.45
12:BM:566:ILE:HD11	12:BM:579:ILE:HG22	1.99	0.45
12:BM:616:ALA:O	12:BM:617:ARG:NH1	2.44	0.45
22:BY:81:LEU:HD12	43:Bv:88:ASP:CB	2.45	0.45
29:Bf:32:ARG:O	29:Bf:35:PRO:HD2	2.16	0.45
30:Bg:48:ARG:O	30:Bg:50:ARG:HG3	2.16	0.45
31:Bh:48:GLY:O	31:Bh:50:THR:N	2.37	0.45
32:Bi:46:LYS:O	32:Bi:47:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Bi:335:LEU:O	32:Bi:338:PRO:HD2	2.16	0.45
34:Bk:42:ILE:O	34:Bk:46:LEU:HG	2.17	0.45
35:Bl:30:ASN:O	35:Bl:33:PRO:HD2	2.17	0.45
42:Bu:23:ALA:HB1	42:Bu:90:ASP:OD1	2.16	0.45
43:Bv:60:ALA:O	43:Bv:61:HIS:C	2.59	0.45
45:Bx:431:LEU:HD21	45:Bx:450:TRP:HB2	1.98	0.45
48:B0:66:GLU:O	49:B1:66:ARG:NH2	2.49	0.45
2:B:151:ILE:HD13	3:C:159:TYR:CE2	2.51	0.45
14:O:196:LEU:HD21	14:O:204:ILE:HG13	1.98	0.45
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.98	0.45
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	0.45
25:b:89:HIS:CE1	25:b:97:ILE:HG13	2.51	0.45
25:b:106:PRO:HA	25:b:115:GLU:CD	2.41	0.45
32:i:4:LEU:HG	44:w:43:PHE:HE2	1.82	0.45
32:i:146:SER:O	32:i:149:LEU:HD13	2.16	0.45
35:l:30:ASN:O	35:l:33:PRO:HD2	2.17	0.45
36:m:10:VAL:O	36:m:14:MET:HG2	2.16	0.45
37:n:7:ILE:HG23	37:n:11:HIS:HB2	1.99	0.45
38:o:52:ASN:O	39:p:129:ARG:NH2	2.49	0.45
40:r:73:LEU:HB3	40:r:74:PRO:HD3	1.97	0.45
50:2:33:ILE:HG22	50:2:34:LEU:HD12	1.98	0.45
60:AC:179:ARG:NE	60:AC:208:PRO:O	2.43	0.45
66:AJ:221:HIS:HB3	66:AJ:222:PRO:HD3	1.97	0.45
67:AK:257:GLU:HG3	67:AK:450:VAL:HG21	1.99	0.45
66:AV:25:SER:HB3	66:AV:218:ILE:HD12	1.98	0.45
67:AW:444:LEU:HA	67:AW:447:THR:HG23	1.99	0.45
68:AY:412:ASP:O	68:AY:416:SER:CB	2.56	0.45
8:BI:69:ILE:O	8:BI:71:SER:N	2.48	0.45
9:BJ:220:MET:SD	9:BJ:223:PHE:HD2	2.39	0.45
9:BJ:319:VAL:C	9:BJ:323:HIS:HD1	2.22	0.45
12:BM:37:ASP:HA	12:BM:103:LEU:HD23	1.98	0.45
14:BO:218:PRO:HG2	14:BO:222:ARG:O	2.16	0.45
16:BQ:205:GLU:O	16:BQ:209:LYS:HG3	2.16	0.45
16:BQ:259:GLU:O	16:BQ:263:THR:OG1	2.34	0.45
16:BQ:315:GLU:HB2	16:BQ:346:GLN:HE22	1.80	0.45
16:BQ:390:GLN:NE2	16:BQ:417:SER:HB3	2.29	0.45
20:BV:69:VAL:HG21	20:BV:100:THR:HG21	1.98	0.45
32:Bi:146:SER:O	32:Bi:149:LEU:HD13	2.16	0.45
32:Bi:285:ILE:CG1	76:Bl:701:PEE:H75	2.25	0.45
36:Bm:2:MET:N	36:Bm:123:SER:OG	2.50	0.45
36:Bm:130:GLU:OE1	36:Bm:130:GLU:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bn:101:CDL:H341	75:Bn:101:CDL:H312	1.56	0.45
40:Br:73:LEU:HB3	40:Br:74:PRO:HD3	1.97	0.45
40:Br:325:LEU:HD12	40:Br:440:HIS:HB3	1.98	0.45
45:Bx:32:ALA:HB3	56:B8:36:PRO:HG2	1.98	0.45
45:Bx:273:MET:HG3	45:Bx:319:LYS:NZ	2.31	0.45
45:Bx:513:LEU:HD12	45:Bx:513:LEU:HA	1.64	0.45
46:By:58:ALA:O	46:By:60:GLU:HG3	2.16	0.45
50:B2:31:TYR:HE1	50:B2:98:HIS:CE1	2.34	0.45
50:B2:31:TYR:HE1	50:B2:98:HIS:HE1	1.62	0.45
52:B4:58:ARG:HD2	52:B4:58:ARG:HA	1.73	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.45
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	0.45
16:Q:94:VAL:HG21	16:Q:458:PHE:HB2	1.99	0.45
17:S:38:VAL:HG21	42:u:94:GLN:HG2	1.97	0.45
20:V:69:VAL:HG21	20:V:100:THR:HG21	1.98	0.45
21:W:57:ARG:CZ	41:s:168:THR:HG22	2.47	0.45
22:Y:81:LEU:HD11	43:v:89:TYR:HA	1.98	0.45
23:Z:31:THR:O	23:Z:34:LYS:HB3	2.16	0.45
26:c:101:TRP:CD1	38:o:62:ASN:ND2	2.84	0.45
30:g:32:TYR:CD2	32:i:339:ILE:HD11	2.51	0.45
32:i:39:ALA:O	32:i:42:PRO:HD2	2.16	0.45
34:k:22:TYR:O	34:k:22:TYR:CG	2.70	0.45
36:m:13:VAL:HG11	36:m:99:GLU:HG2	1.99	0.45
36:m:118:PHE:HZ	36:m:124:TRP:CZ2	2.34	0.45
37:n:50:GLN:CG	37:n:51:PRO:HD2	2.46	0.45
40:r:1:MET:HE1	40:r:53:SER:HB3	1.98	0.45
40:r:325:LEU:HD12	40:r:440:HIS:HB3	1.98	0.45
71:r:501:PLX:H251	71:r:501:PLX:H282	1.77	0.45
41:s:234:MET:O	41:s:238:THR:HG23	2.17	0.45
41:s:257:THR:O	41:s:261:THR:HG23	2.17	0.45
44:w:168:VAL:HG11	44:w:241:TYR:HA	1.97	0.45
63:AF:71:LEU:HD23	63:AF:71:LEU:N	2.20	0.45
67:AK:148:ARG:NH1	63:AS:50:ARG:O	2.50	0.45
68:AL:125:THR:HG22	68:AL:126:ARG:N	2.31	0.45
67:AW:450:VAL:HA	67:AW:453:LEU:HD13	1.94	0.45
68:AY:148:GLY:O	68:AY:152:GLN:N	2.42	0.45
7:BH:50:GLN:NE2	8:BI:93:LYS:HD2	2.32	0.45
11:BL:107:TRP:O	11:BL:116:SER:HB2	2.16	0.45
12:BM:157:LYS:HB2	18:BT:100:TYR:CD2	2.52	0.45
12:BM:219:SER:O	12:BM:222:ILE:HG12	2.16	0.45
14:BO:233:SER:OG	14:BO:234:LEU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BP:163:ALA:O	15:BP:167:GLU:HB2	2.17	0.45
16:BQ:113:ILE:HG12	16:BQ:114:GLY:H	1.80	0.45
16:BQ:446:ASP:O	16:BQ:450:ILE:HG13	2.16	0.45
18:BT:110:GLY:N	18:BT:119:PHE:O	2.28	0.45
22:BY:73:PHE:HD1	22:BY:73:PHE:C	2.24	0.45
71:Bg:203:PLX:H332	71:Bg:203:PLX:H302	1.80	0.45
35:Bl:286:LEU:O	35:Bl:290:VAL:HG23	2.17	0.45
38:Bo:17:THR:HG21	39:Bp:22:ARG:HH12	1.82	0.45
71:Br:501:PLX:H101	71:Br:501:PLX:H132	1.59	0.45
44:Bw:332:ARG:C	44:Bw:338:LYS:HA	2.36	0.45
45:Bx:147:ILE:HD11	45:Bx:209:LEU:HD23	1.98	0.45
46:By:41:ILE:O	46:By:45:MET:HG2	2.16	0.45
3:C:156:GLY:HA2	3:C:169:GLY:CA	2.41	0.45
9:J:220:MET:SD	9:J:223:PHE:HD2	2.39	0.45
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.45
16:Q:304:LYS:HE3	16:Q:316:PHE:CZ	2.52	0.45
17:S:16:LEU:O	17:S:19:PRO:HD2	2.16	0.45
17:S:43:TYR:CZ	21:W:68:ARG:HD2	2.50	0.45
17:S:47:LEU:HA	17:S:50:ARG:HB3	1.98	0.45
18:T:52:ARG:HB3	18:T:55:ARG:NH1	2.31	0.45
18:T:68:ALA:O	18:T:72:ILE:HG13	2.16	0.45
21:W:77:ALA:O	21:W:80:ASP:HB3	2.16	0.45
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.45
22:Y:74:TRP:HE3	22:Y:75:HIS:N	2.15	0.45
24:a:175:ASP:OD1	24:a:176:LYS:N	2.49	0.45
29:f:47:THR:O	29:f:51:THR:HG23	2.16	0.45
32:i:46:LYS:O	32:i:47:LYS:HB2	2.16	0.45
35:l:51:THR:CG2	35:l:91:PRO:CG	2.84	0.45
35:l:319:ILE:HG22	35:l:319:ILE:O	2.17	0.45
40:r:66:LEU:HD23	40:r:66:LEU:HA	1.76	0.45
45:x:240:HIS:O	45:x:243:VAL:HG22	2.16	0.45
53:5:42:LYS:HE2	53:5:42:LYS:HB3	1.83	0.45
63:AF:28:ASN:O	63:AF:31:GLY:N	2.42	0.45
68:AL:113:VAL:HG21	68:AL:120:LEU:HD23	1.99	0.45
4:BE:53:ASP:OD2	9:BJ:351:GLU:HB3	2.17	0.45
7:BH:28:TYR:CD2	7:BH:56:LEU:HD13	2.52	0.45
12:BM:221:ASN:HB3	12:BM:285:TRP:HE3	1.82	0.45
12:BM:405:THR:OG1	12:BM:479:SER:OG	2.28	0.45
14:BO:205:ILE:HA	14:BO:208:LEU:HD12	1.98	0.45
15:BP:124:ASN:HB3	15:BP:146:TYR:HB2	1.98	0.45
16:BQ:304:LYS:HE3	16:BQ:316:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:316:PHE:HD1	16:BQ:339:GLN:NE2	2.14	0.45
17:BS:47:LEU:HA	17:BS:50:ARG:HB3	1.98	0.45
22:BY:74:TRP:HE3	22:BY:75:HIS:N	2.15	0.45
35:Bl:567:SER:C	35:Bl:571:ILE:HD13	2.42	0.45
51:B3:42:ARG:HG3	51:B3:42:ARG:NH1	2.32	0.45
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.81	0.45
7:H:31:ILE:HG12	7:H:88:LEU:HA	1.99	0.45
12:M:221:ASN:HB3	12:M:285:TRP:HE3	1.82	0.45
12:M:457:SER:O	12:M:499:LYS:NZ	2.49	0.45
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
14:O:80:LEU:HB2	14:O:81:PRO:HD3	1.99	0.45
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	0.45
16:Q:70:ASP:N	16:Q:71:PRO:CD	2.80	0.45
16:Q:265:ASN:OD1	16:Q:267:ILE:HD12	2.17	0.45
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	0.45
17:S:53:ARG:HB3	31:h:102:GLY:HA2	1.99	0.45
30:g:48:ARG:O	30:g:50:ARG:HG3	2.16	0.45
32:i:9:ILE:O	32:i:12:THR:OG1	2.30	0.45
34:k:42:ILE:O	34:k:46:LEU:HG	2.17	0.45
35:l:79:SER:OG	35:l:135:ASN:HB3	2.16	0.45
36:m:32:LEU:HB3	36:m:64:MET:HE3	1.99	0.45
44:w:58:ARG:HB3	44:w:202:HIS:HE1	1.82	0.45
44:w:99:GLY:HA3	44:w:337:ARG:NH1	2.20	0.45
45:x:147:ILE:HD11	45:x:209:LEU:HD23	1.98	0.45
45:x:240:HIS:NE2	45:x:244:TYR:CE2	2.81	0.45
46:y:59:GLN:CA	46:y:62:GLU:HB2	2.46	0.45
48:0:79:LYS:NZ	55:7:15:ASN:HD21	2.15	0.45
75:AG:101:CDL:C52	75:AG:101:CDL:C71	2.86	0.45
66:AV:333:LEU:CD2	76:AV:403:PEE:C40	2.94	0.45
68:AY:377:MET:HE1	68:AY:450:TYR:CE1	2.51	0.45
2:BB:90:PRO:HG2	13:BN:56:PHE:CE2	2.52	0.45
8:BI:30:GLU:HG2	8:BI:31:ILE:N	2.32	0.45
22:BY:72:ARG:NH1	35:Bl:390:TYR:CZ	2.79	0.45
30:Bg:39:CYS:O	30:Bg:43:ILE:HG13	2.17	0.45
71:Bg:202:PLX:H1B3	71:Bg:202:PLX:H22	1.58	0.45
32:Bi:4:LEU:HG	44:Bw:43:PHE:HE2	1.82	0.45
33:Bj:75:LEU:N	33:Bj:76:PRO:HD2	2.32	0.45
35:Bl:166:THR:CG2	76:Bl:702:PEE:H2	2.46	0.45
76:Bl:701:PEE:H36	40:Br:155:VAL:CG2	2.46	0.45
36:Bm:118:PHE:HZ	36:Bm:124:TRP:CZ2	2.34	0.45
37:Bn:50:GLN:CG	37:Bn:51:PRO:HD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bp:173:ARG:HA	39:Bp:174:PRO:HD3	1.83	0.45
40:Br:1:MET:HE1	40:Br:53:SER:HB3	1.98	0.45
71:Br:502:PLX:H311	71:Br:502:PLX:H282	1.75	0.45
41:Bs:257:THR:O	41:Bs:261:THR:HG23	2.17	0.45
45:Bx:435:GLY:O	45:Bx:437:PRO:HD3	2.16	0.45
46:By:162:SER:HB2	46:By:198:GLU:HB2	1.99	0.45
4:E:120:SER:O	4:E:124:VAL:HG23	2.17	0.45
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.45
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.45
12:M:446:GLY:N	12:M:451:ILE:HD11	2.32	0.45
12:M:566:ILE:HD11	12:M:579:ILE:HG22	1.99	0.45
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.45
20:V:40:ARG:HE	75:V:201:CDL:CA2	2.30	0.45
20:V:121:ALA:O	20:V:125:VAL:HG23	2.15	0.45
24:a:54:LEU:CD2	25:b:27:GLU:CA	2.89	0.45
28:e:113:ARG:HH21	40:r:459:SER:HB2	1.80	0.45
32:i:324:PRO:C	32:i:326:LEU:H	2.24	0.45
33:j:49:VAL:HG12	36:m:75:ILE:H	1.82	0.45
35:l:304:PHE:HZ	35:l:526:LEU:HD22	1.82	0.45
35:l:370:SER:O	35:l:374:THR:HG23	2.16	0.45
37:n:40:ASN:HD22	37:n:56:THR:HG23	1.82	0.45
37:n:43:MET:HE3	37:n:43:MET:HB2	1.87	0.45
56:8:35:ALA:HB3	56:8:36:PRO:HD3	1.99	0.45
63:AF:34:ARG:HH11	66:AJ:379:TRP:HE1	1.60	0.45
66:AJ:246:SER:HB3	66:AJ:249:LEU:HD23	1.98	0.45
68:AL:126:ARG:NH1	68:AL:199:GLN:O	2.50	0.45
68:AL:225:LYS:HD2	68:AL:257:TYR:CE1	2.52	0.45
62:AR:75:LEU:HD23	62:AR:75:LEU:HA	1.80	0.45
65:AU:313:VAL:HG13	65:AU:314:LEU:HD12	1.97	0.45
68:AY:192:PHE:HB2	68:AY:198:ALA:HB2	1.98	0.45
1:BA:379:CYS:O	12:BM:201:GLY:N	2.49	0.45
2:BB:40:ASN:O	2:BB:42:GLN:N	2.43	0.45
2:BB:160:CYS:O	16:BQ:368:ARG:NH1	2.41	0.45
4:BE:62:LYS:HE3	4:BE:66:MET:HE2	1.98	0.45
12:BM:197:THR:O	14:BO:114:GLU:HG2	2.17	0.45
12:BM:275:PRO:HB3	12:BM:286:ILE:HB	1.98	0.45
12:BM:421:SER:O	12:BM:425:ASN:N	2.49	0.45
14:BO:236:GLU:HA	14:BO:237:PRO:HD2	1.78	0.45
15:BP:164:ASN:HA	15:BP:181:HIS:HE2	1.82	0.45
21:BW:30:LEU:C	21:BW:32:GLY:H	2.21	0.45
26:Bc:55:TYR:OH	26:Bc:74:ASP:OD2	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Bc:101:TRP:CD1	38:Bo:62:ASN:ND2	2.84	0.45
27:Bd:59:HIS:HD2	28:Be:121:GLU:OE2	1.99	0.45
71:Bg:201:PLX:H1B1	31:Bh:2:PRO:HG2	1.99	0.45
35:Bl:304:PHE:HZ	35:Bl:526:LEU:HD22	1.81	0.45
50:B2:33:ILE:HG22	50:B2:34:LEU:HD12	1.98	0.45
52:B4:57:ARG:HB3	52:B4:57:ARG:NH1	2.31	0.45
1:A:208:GLU:OE1	1:A:211:ALA:N	2.38	0.45
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.45
7:H:28:TYR:CD2	7:H:56:LEU:HD13	2.52	0.45
9:J:212:ARG:CG	9:J:212:ARG:NH1	2.72	0.45
11:L:136:SER:O	11:L:140:LYS:HG3	2.17	0.45
12:M:37:ASP:OD1	12:M:38:GLY:N	2.41	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.99	0.45
17:S:7:PRO:O	17:S:10:SER:OG	2.23	0.45
21:W:111:PHE:CD2	21:W:117:VAL:HG21	2.51	0.45
22:Y:73:PHE:HD1	22:Y:73:PHE:C	2.24	0.45
26:c:168:LEU:HD12	26:c:169:GLU:HB3	1.98	0.45
71:g:201:PLX:H1B1	31:h:2:PRO:HG2	1.99	0.45
32:i:92:GLN:O	32:i:95:SER:OG	2.21	0.45
32:i:335:LEU:O	32:i:338:PRO:HD2	2.16	0.45
35:l:222:GLY:N	35:l:229:LEU:HD12	2.31	0.45
35:l:481:THR:HG22	43:v:92:HIS:CD2	2.52	0.45
35:l:567:SER:C	35:l:571:ILE:HD13	2.42	0.45
39:p:12:HIS:N	68:AY:260:ASP:OD2	2.45	0.45
41:s:40:VAL:CG1	41:s:46:LEU:HB2	2.47	0.45
49:1:78:HIS:CE1	53:5:12:LEU:HD22	2.52	0.45
66:AJ:366:MET:HB3	66:AJ:367:PRO:HD3	1.98	0.45
67:AK:155:GLN:NE2	67:AK:200:VAL:O	2.50	0.45
68:AL:63:GLN:HE22	68:AL:238:GLU:HA	1.81	0.45
75:AL:502:CDL:H511	76:AL:503:PEE:H67	1.98	0.45
76:AL:503:PEE:H19	76:AL:503:PEE:C30	2.47	0.45
59:AO:36:ALA:HB3	67:AW:320:PRO:HB3	1.97	0.45
60:AP:136:PHE:HB3	66:AV:50:PHE:HE2	1.81	0.45
66:AV:18:PHE:O	66:AV:220:PHE:HB3	2.17	0.45
66:AV:129:MET:CE	66:AV:185:LEU:CD1	2.95	0.45
67:AW:323:VAL:HG22	67:AW:340:THR:HG22	1.99	0.45
68:AY:421:GLY:O	68:AY:422:ARG:HG3	2.16	0.45
1:BA:86:ARG:HB3	1:BA:92:GLY:O	2.16	0.45
1:BA:201:ALA:O	14:BO:119:TYR:HB3	2.17	0.45
2:BB:138:ARG:HD3	12:BM:130:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:192:GLY:O	2:BB:196:GLU:HB2	2.16	0.45
4:BE:35:LEU:HD11	4:BE:39:TRP:HE1	1.81	0.45
4:BE:59:GLY:O	4:BE:63:VAL:HG23	2.16	0.45
6:BG:77:GLU:OE1	6:BG:77:GLU:N	2.38	0.45
9:BJ:99:ASP:H	9:BJ:102:GLN:HB2	1.82	0.45
15:BP:214:ASP:O	15:BP:217:LYS:HD2	2.16	0.45
19:BU:18:VAL:HG11	41:Bs:292:ASN:O	2.17	0.45
6:BX:140:CYS:HB2	6:BX:143:GLU:CD	2.41	0.45
25:Bb:89:HIS:CE1	25:Bb:97:ILE:HG13	2.51	0.45
25:Bb:90:VAL:HG22	25:Bb:97:ILE:HD12	1.98	0.45
71:Bb:201:PLX:H171	71:Bb:201:PLX:H141	1.68	0.45
29:Bf:32:ARG:C	29:Bf:35:PRO:HD2	2.42	0.45
32:Bi:58:LYS:HZ1	34:Bk:92:ASN:CG	2.23	0.45
33:Bj:49:VAL:HG12	36:Bm:75:ILE:H	1.82	0.45
35:Bl:414:ILE:O	35:Bl:417:SER:OG	2.29	0.45
76:Bl:701:PEE:H33	76:Bl:701:PEE:H27	1.62	0.45
41:Bs:142:TYR:CD2	41:Bs:289:LEU:HD11	2.52	0.45
44:Bw:211:VAL:HG13	44:Bw:212:PRO:HD3	1.98	0.45
44:Bw:238:GLU:O	44:Bw:242:LYS:HG3	2.17	0.45
45:Bx:195:LEU:CD2	45:Bx:245:ILE:HD13	2.45	0.45
47:Bz:137:LEU:HD12	47:Bz:137:LEU:HA	1.70	0.45
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.45
71:B:303:PLX:H332	71:B:303:PLX:H301	1.80	0.45
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	0.45
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.45
12:M:157:LYS:HB2	18:T:100:TYR:CD2	2.52	0.45
12:M:358:LEU:HD22	12:M:363:SER:HB2	1.99	0.45
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	0.45
16:Q:136:PHE:CD2	16:Q:151:TYR:HB2	2.52	0.45
76:V:202:PEE:H60	76:V:202:PEE:H40	1.99	0.45
30:g:45:ASN:HD21	30:g:60:GLN:HE21	1.65	0.45
32:i:2:ASN:HD21	32:i:4:LEU:HB2	1.81	0.45
33:j:75:LEU:N	33:j:76:PRO:HD2	2.32	0.45
35:l:194:ASN:ND2	38:o:127:LEU:HD12	2.32	0.45
36:m:2:MET:N	36:m:123:SER:OG	2.50	0.45
40:r:56:PHE:HZ	40:r:108:MET:HE1	1.82	0.45
40:r:405:LEU:HA	40:r:405:LEU:HD23	1.73	0.45
42:u:23:ALA:HB1	42:u:90:ASP:OD1	2.16	0.45
44:w:246:LEU:HB2	44:w:247:PRO:HD3	1.99	0.45
46:y:60:GLU:CD	46:y:61:VAL:H	2.24	0.45
46:y:162:SER:HB2	46:y:198:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3:42:ARG:HG3	51:3:42:ARG:NH1	2.32	0.45
59:AB:41:PRO:HB2	67:AK:167:GLN:NE2	2.31	0.45
59:AB:46:LYS:HD2	59:AB:49:PHE:CZ	2.52	0.45
60:AC:80:HIS:CE1	68:AL:182:VAL:HG22	2.52	0.45
60:AC:140:MET:HA	66:AV:177:ARG:HH21	1.81	0.45
60:AC:195:LEU:HD13	60:AC:248:ARG:HD2	1.99	0.45
62:AE:53:CYS:O	62:AE:57:VAL:HG23	2.17	0.45
65:AH:288:MET:SD	76:AH:401:PEE:O4	2.75	0.45
65:AU:201:VAL:O	65:AU:207:GLY:HA2	2.17	0.45
65:AU:214:LEU:O	65:AU:234:ASN:ND2	2.44	0.45
65:AU:253:LEU:HD23	65:AU:254:GLU:N	2.32	0.45
67:AW:104:GLU:OE1	68:AY:325:SER:HA	2.17	0.45
1:BA:225:LEU:HB2	1:BA:424:ILE:HD11	1.99	0.45
4:BE:28:ALA:HA	4:BE:31:ARG:HG3	1.99	0.45
4:BE:120:SER:O	4:BE:124:VAL:HG23	2.17	0.45
11:BL:69:GLU:HB2	11:BL:73:LYS:HZ2	1.81	0.45
12:BM:371:VAL:HG12	12:BM:533:GLY:O	2.17	0.45
16:BQ:70:ASP:N	16:BQ:71:PRO:CD	2.80	0.45
16:BQ:136:PHE:CD2	16:BQ:151:TYR:HB2	2.52	0.45
16:BQ:159:LEU:O	16:BQ:161:ILE:HG13	2.16	0.45
16:BQ:190:HIS:HD2	16:BQ:452:GLY:CA	2.26	0.45
18:BT:52:ARG:HB3	18:BT:55:ARG:NH1	2.31	0.45
18:BT:81:GLU:HA	18:BT:122:HIS:O	2.17	0.45
76:BW:201:PEE:H28	76:BW:201:PEE:H22	1.50	0.45
30:Bg:32:TYR:CD2	32:Bi:339:ILE:HD11	2.51	0.45
30:Bg:45:ASN:HD21	30:Bg:60:GLN:HE21	1.65	0.45
32:Bi:146:SER:OG	32:Bi:147:PRO:HD3	2.17	0.45
35:Bl:79:SER:OG	35:Bl:135:ASN:HB3	2.16	0.45
35:Bl:552:LEU:O	35:Bl:556:THR:OG1	2.29	0.45
37:Bn:7:ILE:HG23	37:Bn:11:HIS:HB2	1.98	0.45
41:Bs:40:VAL:CG1	41:Bs:46:LEU:HB2	2.47	0.45
45:Bx:158:ILE:O	45:Bx:162:ILE:HG13	2.17	0.45
46:By:121:TYR:C	46:By:138:VAL:HG23	2.42	0.45
50:B2:98:HIS:ND1	50:B2:98:HIS:N	2.64	0.45
2:B:91:LEU:HD23	2:B:95:PHE:CD2	2.52	0.45
3:C:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.45
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.45
12:M:455:ILE:HG12	12:M:463:SER:HB3	1.98	0.45
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	0.45
14:O:198:ALA:HA	14:O:201:ILE:HD12	1.99	0.45
14:O:207:GLU:HG2	14:O:213:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:236:GLU:HA	14:O:237:PRO:HD2	1.78	0.45
22:Y:78:GLU:CG	35:l:385:PHE:HE1	2.30	0.45
23:Z:49:GLU:OE2	39:p:38:ARG:NH2	2.33	0.45
25:b:88:TYR:CG	71:b:201:PLX:H1C2	2.51	0.45
26:c:41:TYR:CE1	26:c:67:ASP:HB3	2.51	0.45
29:f:32:ARG:C	29:f:35:PRO:HD2	2.42	0.45
30:g:87:ARG:HD2	42:u:156:GLY:C	2.42	0.45
32:i:288:LEU:HD21	76:l:701:PEE:H58	1.70	0.45
35:l:33:PRO:HA	35:l:118:PHE:HD2	1.82	0.45
35:l:95:PHE:HZ	35:l:456:ARG:HG2	1.82	0.45
42:u:100:CYS:O	42:u:102:LYS:N	2.50	0.45
45:x:158:ILE:O	45:x:162:ILE:HG13	2.17	0.45
46:y:121:TYR:C	46:y:138:VAL:HG23	2.42	0.45
50:2:31:TYR:HE1	50:2:98:HIS:CE1	2.34	0.45
61:AD:27:VAL:O	61:AD:30:MET:HB2	2.17	0.45
66:AJ:105:GLY:HA2	66:AJ:107:PHE:CE2	2.52	0.45
68:AL:279:ASP:OD2	68:AL:282:LEU:HG	2.17	0.45
68:AL:294:PRO:HB2	68:AL:301:ASN:HD21	1.82	0.45
63:AS:99:ILE:O	63:AS:103:LYS:HG2	2.17	0.45
66:AV:160:LEU:O	66:AV:164:ILE:HD12	2.17	0.45
68:AY:296:TRP:HB2	68:AY:348:TYR:C	2.42	0.45
9:BJ:197:GLU:OE1	9:BJ:197:GLU:N	2.45	0.45
12:BM:323:LEU:HG	12:BM:629:ILE:HD12	1.98	0.45
12:BM:446:GLY:N	12:BM:451:ILE:HD11	2.32	0.45
12:BM:471:LYS:HB3	12:BM:510:TRP:CH2	2.52	0.45
12:BM:612:PRO:HB3	12:BM:616:ALA:HB3	1.99	0.45
12:BM:688:GLN:O	12:BM:690:THR:N	2.50	0.45
13:BN:5:GLN:O	13:BN:9:ARG:HG2	2.17	0.45
15:BP:63:GLU:O	15:BP:67:GLU:HG3	2.17	0.45
15:BP:109:LYS:O	15:BP:110:SER:OG	2.31	0.45
16:BQ:86:PRO:CG	33:Bj:41:PHE:HE2	2.29	0.45
16:BQ:94:VAL:HG21	16:BQ:458:PHE:HB2	1.99	0.45
16:BQ:147:ASN:O	16:BQ:150:ALA:HB3	2.17	0.45
16:BQ:235:ASP:OD1	16:BQ:356:ILE:HD12	2.17	0.45
75:BV:201:CDL:H541	75:BV:201:CDL:H572	1.46	0.45
26:Bc:166:LEU:HB2	26:Bc:170:ARG:NH2	2.32	0.45
32:Bi:218:LEU:HD23	32:Bi:218:LEU:HA	1.81	0.45
33:Bj:53:MET:HG3	34:Bk:79:VAL:HG13	1.99	0.45
34:Bk:59:MET:HB2	34:Bk:60:PRO:HD3	1.99	0.45
35:Bl:33:PRO:HA	35:Bl:118:PHE:HD2	1.82	0.45
40:Br:408:LEU:HD23	40:Br:408:LEU:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bu:82:PHE:CE2	42:Bu:86:TRP:HD1	2.35	0.45
44:Bw:168:VAL:HG11	44:Bw:241:TYR:HA	1.97	0.45
45:Bx:240:HIS:O	45:Bx:243:VAL:HG22	2.16	0.45
46:By:76:ILE:O	46:By:79:PRO:HD2	2.16	0.45
54:B6:31:LEU:HD23	54:B6:31:LEU:HA	1.83	0.45
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	0.44
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.44
1:A:317:VAL:HG22	1:A:356:VAL:HA	1.99	0.44
3:C:88:CYS:SG	16:Q:223:HIS:CE1	3.10	0.44
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	0.44
11:L:75:ARG:NH2	11:L:101:PHE:HB3	2.29	0.44
12:M:134:GLY:HA3	69:M:801:SF4:S3	2.52	0.44
18:T:81:GLU:HA	18:T:122:HIS:O	2.17	0.44
24:a:106:VAL:HA	24:a:107:PRO:HD2	1.82	0.44
31:h:82:GLN:HA	31:h:85:LYS:HE3	1.99	0.44
32:i:146:SER:OG	32:i:147:PRO:HD3	2.17	0.44
35:l:208:PRO:HG2	35:l:266:LEU:HB3	1.99	0.44
35:l:286:LEU:O	35:l:290:VAL:HG23	2.17	0.44
35:l:356:ILE:CG2	35:l:429:LEU:HB3	2.48	0.44
76:l:701:PEE:H36	40:r:155:VAL:CG2	2.46	0.44
40:r:145:ALA:HB3	40:r:222:GLU:OE2	2.17	0.44
42:u:82:PHE:CE2	42:u:86:TRP:HD1	2.35	0.44
44:w:108:TYR:HD1	44:w:327:VAL:HG13	1.82	0.44
45:x:51:ASP:O	45:x:55:ASN:HB2	2.18	0.44
66:Aj:16:HIS:O	66:Aj:21:LEU:HB3	2.16	0.44
68:AL:259:GLU:CB	38:Bo:30:ARG:NE	2.56	0.44
58:AN:41:ARG:HH21	75:AN:102:CDL:H1	1.81	0.44
65:AU:114:PHE:CE2	65:AU:148:LEU:HD21	2.52	0.44
67:AW:49:ILE:HD11	67:AW:230:LEU:HB3	1.98	0.44
68:AY:112:GLU:HG3	68:AY:116:MET:HE2	2.00	0.44
1:BA:53:LEU:O	1:BA:56:SER:OG	2.24	0.44
1:BA:63:TYR:HE2	1:BA:64:LYS:NZ	2.15	0.44
3:BC:140:GLN:HG2	33:Bj:37:TYR:CG	2.51	0.44
3:BC:156:GLY:HA2	3:BC:169:GLY:CA	2.41	0.44
4:BE:43:VAL:HB	4:BE:44:PRO:HD3	1.98	0.44
6:BG:123:GLU:O	6:BG:127:GLY:N	2.50	0.44
7:BH:31:ILE:HG12	7:BH:88:LEU:HA	1.99	0.44
9:BJ:220:MET:O	9:BJ:223:PHE:HB2	2.16	0.44
12:BM:278:HIS:NE2	12:BM:280:ASP:HB2	2.32	0.44
14:BO:145:SER:O	14:BO:148:ILE:HB	2.18	0.44
14:BO:207:GLU:HG2	14:BO:213:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BO:236:GLU:C	14:BO:238:PRO:HD2	2.41	0.44
15:BP:167:GLU:HG2	15:BP:181:HIS:CD2	2.52	0.44
15:BP:170:ILE:HG23	15:BP:174:PHE:CD2	2.52	0.44
16:BQ:149:GLN:NE2	16:BQ:309:ASP:OD2	2.49	0.44
16:BQ:271:ARG:NH1	41:Bs:281:ARG:HA	2.31	0.44
17:BS:16:LEU:O	17:BS:19:PRO:HD2	2.16	0.44
76:BW:201:PEE:N	76:BW:201:PEE:P	2.87	0.44
35:Bl:18:PRO:HG3	35:Bl:39:ILE:HD12	1.98	0.44
36:Bm:32:LEU:HB3	36:Bm:64:MET:HE3	1.99	0.44
71:Br:501:PLX:H182	71:Br:501:PLX:H211	1.67	0.44
41:Bs:277:TYR:HA	41:Bs:278:PRO:HD2	1.69	0.44
44:Bw:246:LEU:HB2	44:Bw:247:PRO:HD3	1.99	0.44
45:Bx:51:ASP:O	45:Bx:55:ASN:HB2	2.18	0.44
45:Bx:379:TYR:CE2	45:Bx:383:MET:HE2	2.52	0.44
46:By:60:GLU:CD	46:By:61:VAL:H	2.24	0.44
47:Bz:183:GLU:O	51:B3:42:ARG:NH2	2.50	0.44
1:A:99:TRP:HA	1:A:149:MET:HE1	2.00	0.44
1:A:225:LEU:HB2	1:A:424:ILE:HD11	1.99	0.44
1:A:392:MET:O	1:A:396:MET:HG2	2.16	0.44
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	0.44
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.44
9:J:178:SER:OG	9:J:181:LEU:HB2	2.17	0.44
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.44
13:N:5:GLN:O	13:N:9:ARG:HG2	2.18	0.44
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.44
16:Q:147:ASN:O	16:Q:150:ALA:HB3	2.17	0.44
16:Q:316:PHE:HD1	16:Q:339:GLN:NE2	2.14	0.44
21:W:120:LEU:HG	31:h:69:ARG:NH1	2.32	0.44
32:i:218:LEU:HA	32:i:218:LEU:HD23	1.81	0.44
34:k:59:MET:HB2	34:k:60:PRO:HD3	1.99	0.44
35:l:434:GLN:HB3	35:l:435:PRO:HD2	1.99	0.44
41:s:288:LEU:O	41:s:293:PHE:N	2.50	0.44
45:x:431:LEU:HD21	45:x:450:TRP:HB2	1.98	0.44
46:y:41:ILE:O	46:y:45:MET:HG2	2.16	0.44
47:z:183:GLU:O	51:3:42:ARG:NH2	2.50	0.44
61:AD:34:ARG:NH1	61:AD:38:GLN:HB3	2.32	0.44
63:AF:44:VAL:O	63:AF:48:ILE:HG12	2.17	0.44
66:AJ:8:ASN:HB3	66:AJ:11:MET:HB2	2.00	0.44
66:AJ:198:LEU:CD1	75:AJ:404:CDL:H332	2.48	0.44
76:AL:503:PEE:H49	76:AL:503:PEE:C17	2.44	0.44
1:BA:392:MET:O	1:BA:396:MET:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:94:ARG:HE	16:BQ:234:GLN:NE2	2.15	0.44
3:BC:163:SER:H	3:BC:168:ARG:HH22	1.64	0.44
12:BM:358:LEU:HD22	12:BM:363:SER:HB2	1.99	0.44
12:BM:385:TYR:HE1	12:BM:523:VAL:HG23	1.82	0.44
16:BQ:145:MET:HG3	16:BQ:174:PHE:HB3	1.99	0.44
21:BW:57:ARG:CZ	41:Bs:168:THR:HG22	2.47	0.44
21:BW:111:PHE:CE2	21:BW:117:VAL:HG11	2.49	0.44
22:BY:50:LEU:O	22:BY:51:THR:OG1	2.27	0.44
26:Bc:168:LEU:HD12	26:Bc:169:GLU:HB3	1.98	0.44
32:Bi:2:ASN:HD21	32:Bi:4:LEU:HB2	1.81	0.44
32:Bi:25:HIS:CE1	32:Bi:84:TRP:CE3	3.05	0.44
32:Bi:291:TYR:CE2	76:Bl:701:PEE:H51	2.52	0.44
33:Bj:34:SER:HB2	41:Bs:63:PRO:HA	1.99	0.44
34:Bk:22:TYR:CG	34:Bk:22:TYR:O	2.69	0.44
35:Bl:222:GLY:N	35:Bl:229:LEU:HD12	2.31	0.44
35:Bl:319:ILE:O	35:Bl:319:ILE:HG22	2.17	0.44
35:Bl:356:ILE:CG2	35:Bl:429:LEU:HB3	2.48	0.44
39:Bp:55:LYS:CA	39:Bp:55:LYS:CE	2.89	0.44
41:Bs:73:THR:O	41:Bs:76:THR:OG1	2.20	0.44
49:B1:78:HIS:CE1	53:B5:12:LEU:HD22	2.52	0.44
1:A:121:GLU:HA	1:A:122:PRO:HD3	1.87	0.44
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.44
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.44
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.44
12:M:371:VAL:HG12	12:M:533:GLY:O	2.17	0.44
12:M:645:ARG:HG3	12:M:648:GLU:OE2	2.16	0.44
12:M:688:GLN:O	12:M:690:THR:N	2.50	0.44
13:N:83:PRO:HA	13:N:84:PRO:HD3	1.87	0.44
75:V:201:CDL:H552	75:V:201:CDL:H522	1.69	0.44
22:Y:42:PRO:HD2	23:Z:14:MET:HG3	1.98	0.44
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.44
27:d:59:HIS:HD2	28:e:121:GLU:OE2	1.99	0.44
28:e:57:GLU:HB2	44:w:323:GLN:HB3	2.00	0.44
32:i:291:TYR:CE2	76:l:701:PEE:H51	2.52	0.44
40:r:13:PRO:HA	40:r:16:TRP:HB2	1.98	0.44
40:r:339:SER:O	40:r:340:ARG:HB2	2.17	0.44
44:w:351:TRP:HA	44:w:353:TRP:CZ3	2.52	0.44
63:AF:70:ASN:ND2	66:AJ:209:LEU:HG	2.33	0.44
65:AH:218:TYR:OH	65:AH:244:MET:HE3	2.17	0.44
75:AH:403:CDL:O1	75:AH:403:CDL:OB8	2.35	0.44
66:AV:315:MET:SD	66:AV:318:ARG:NH2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:173:ILE:HG22	1:BA:177:TYR:CE2	2.52	0.44
9:BJ:168:SER:CA	9:BJ:184:LYS:HE3	2.47	0.44
12:BM:133:GLN:HA	12:BM:136:GLU:OE2	2.17	0.44
13:BN:48:TYR:HB3	13:BN:89:TRP:HZ3	1.81	0.44
14:BO:195:ASP:HB2	14:BO:219:ARG:H	1.83	0.44
16:BQ:265:ASN:OD1	16:BQ:267:ILE:HD12	2.17	0.44
19:BU:52:ASN:ND2	31:Bh:27:TYR:O	2.42	0.44
76:BV:202:PEE:H60	76:BV:202:PEE:H40	1.99	0.44
21:BW:120:LEU:HG	31:Bh:69:ARG:NH1	2.32	0.44
25:Bb:116:VAL:HG12	25:Bb:117:ILE:N	2.31	0.44
26:Bc:56:ASN:HD21	38:Bo:43:LEU:HD11	1.81	0.44
26:Bc:108:HIS:CE1	35:Bl:546:GLN:HG2	2.53	0.44
28:Be:57:GLU:HB2	44:Bw:323:GLN:HB3	2.00	0.44
35:Bl:81:LYS:HD3	35:Bl:83:ASP:OD2	2.18	0.44
35:Bl:98:TRP:CD1	35:Bl:98:TRP:O	2.71	0.44
37:Bn:30:LYS:HZ2	75:Bn:101:CDL:HA31	1.82	0.44
41:Bs:234:MET:O	41:Bs:238:THR:HG23	2.17	0.44
42:Bu:18:VAL:HG12	42:Bu:20:ILE:H	1.83	0.44
79:Bx:604:HEA:O11	79:Bx:604:HEA:HHC	2.17	0.44
4:E:35:LEU:HD11	4:E:39:TRP:HE1	1.81	0.44
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.44
12:M:254:MET:CB	12:M:290:THR:HG22	2.46	0.44
12:M:510:TRP:HD1	12:M:512:VAL:HG22	1.82	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.17	0.44
15:P:163:ALA:O	15:P:167:GLU:HB2	2.17	0.44
15:P:170:ILE:HG23	15:P:174:PHE:CD2	2.52	0.44
16:Q:369:ALA:HA	18:T:93:ALA:HB2	1.99	0.44
71:b:201:PLX:C2	27:d:43:ARG:HH22	2.31	0.44
26:c:108:HIS:CE1	35:l:546:GLN:HG2	2.53	0.44
30:g:39:CYS:O	30:g:43:ILE:HG13	2.17	0.44
31:h:91:LYS:HG3	31:h:92:TYR:N	2.28	0.44
33:j:34:SER:HB2	41:s:64:ALA:H	1.82	0.44
35:l:98:TRP:CD1	35:l:98:TRP:O	2.71	0.44
35:l:456:ARG:HH21	35:l:456:ARG:HB2	1.82	0.44
40:r:154:LEU:HD23	40:r:154:LEU:HA	1.83	0.44
44:w:79:GLU:OE1	44:w:79:GLU:N	2.43	0.44
47:z:19:THR:CG2	47:z:53:THR:OG1	2.66	0.44
49:1:70:VAL:HG12	49:1:71:VAL:N	2.31	0.44
65:AH:304:TYR:CE1	75:AH:403:CDL:OA3	2.70	0.44
66:AJ:155:TYR:HE2	64:AT:38:TRP:CZ2	2.35	0.44
66:AJ:372:ILE:O	66:AJ:376:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:57:PRO:HG2	68:AL:400:VAL:CG1	2.47	0.44
67:AK:126:LEU:HB3	68:AL:38:PHE:CZ	2.52	0.44
67:AK:158:LEU:HB2	67:AK:197:ILE:HG23	1.99	0.44
65:AU:291:LYS:HE3	76:AU:401:PEE:O1P	2.18	0.44
68:AY:64:SER:HB3	68:AY:235:GLY:HA2	1.99	0.44
68:AY:66:GLN:OE1	68:AY:67:PRO:HD2	2.16	0.44
2:BB:69:GLY:O	2:BB:72:LEU:HB3	2.17	0.44
4:BE:50:PHE:CD2	4:BE:103:VAL:HG21	2.52	0.44
9:BJ:178:SER:OG	9:BJ:181:LEU:HB2	2.17	0.44
12:BM:385:TYR:HB2	12:BM:517:HIS:CE1	2.53	0.44
14:BO:196:LEU:HD21	14:BO:204:ILE:HG13	1.98	0.44
16:BQ:372:LYS:HD2	18:BT:93:ALA:HA	2.00	0.44
24:Ba:175:ASP:OD1	24:Ba:176:LYS:N	2.49	0.44
71:Bb:201:PLX:C6	71:Bb:201:PLX:C11	2.85	0.44
26:Bc:101:TRP:CD1	38:Bo:47:TYR:CD1	3.06	0.44
32:Bi:309:ASN:HD21	44:Bw:130:ARG:HD3	1.82	0.44
35:Bl:194:ASN:ND2	38:Bo:127:LEU:HD12	2.32	0.44
35:Bl:227:LEU:HD22	35:Bl:283:ILE:HG22	2.00	0.44
36:Bm:13:VAL:HG11	36:Bm:99:GLU:HG2	1.99	0.44
40:Br:56:PHE:HZ	40:Br:108:MET:HE1	1.82	0.44
40:Br:145:ALA:HB3	40:Br:222:GLU:OE2	2.17	0.44
45:Bx:70:VAL:HG11	45:Bx:246:LEU:HD22	1.99	0.44
54:B6:30:ILE:HG13	54:B6:31:LEU:N	2.33	0.44
3:C:140:GLN:HG2	33:j:37:TYR:CG	2.51	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
9:J:283:VAL:O	9:J:357:ARG:NH2	2.51	0.44
16:Q:55:SER:N	16:Q:58:THR:OG1	2.50	0.44
16:Q:372:LYS:HD2	18:T:93:ALA:HA	2.00	0.44
21:W:30:LEU:C	21:W:32:GLY:H	2.21	0.44
30:g:78:GLU:OE1	32:i:342:PHE:HD1	2.01	0.44
32:i:258:THR:CG2	32:i:336:LEU:HB3	2.48	0.44
33:j:53:MET:HG3	34:k:79:VAL:HG13	1.99	0.44
35:l:227:LEU:HD22	35:l:283:ILE:HG22	2.00	0.44
44:w:217:ARG:O	44:w:221:LYS:HG2	2.18	0.44
45:x:449:MET:HE3	55:7:40:TRP:HB3	1.98	0.44
79:x:604:HEA:O11	79:x:604:HEA:HHC	2.17	0.44
53:5:21:ILE:HD12	53:5:21:ILE:HA	1.81	0.44
54:6:2:GLU:CG	54:6:3:ASN:H	2.30	0.44
62:AR:34:ARG:NH1	62:AR:78:ARG:CZ	2.76	0.44
62:AR:43:CYS:SG	62:AR:78:ARG:HA	2.57	0.44
67:AW:323:VAL:HG13	67:AW:340:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:328:ALA:HB3	67:AW:335:LEU:HB2	1.99	0.44
68:AY:92:PHE:O	68:AY:92:PHE:HD1	2.00	0.44
7:BH:12:VAL:HG13	7:BH:13:GLY:N	2.33	0.44
9:BJ:72:HIS:O	9:BJ:75:ARG:HG2	2.18	0.44
12:BM:546:PHE:CZ	12:BM:566:ILE:HD12	2.52	0.44
28:Be:115:LYS:O	28:Be:118:SER:OG	2.30	0.44
30:Bg:82:TYR:OH	32:Bi:341:PRO:O	2.35	0.44
38:Bo:6:TYR:HE1	38:Bo:12:ARG:NH2	2.15	0.44
40:Br:13:PRO:HA	40:Br:16:TRP:HB2	1.99	0.44
40:Br:237:LYS:N	40:Br:237:LYS:HD2	2.33	0.44
41:Bs:7:LEU:HD23	41:Bs:7:LEU:HA	1.78	0.44
41:Bs:288:LEU:O	41:Bs:293:PHE:N	2.50	0.44
44:Bw:108:TYR:HD1	44:Bw:327:VAL:HG13	1.82	0.44
44:Bw:217:ARG:O	44:Bw:221:LYS:HG2	2.18	0.44
44:Bw:351:TRP:HA	44:Bw:353:TRP:CZ3	2.52	0.44
51:B3:3:ALA:O	51:B3:4:ALA:HB2	2.17	0.44
56:B8:35:ALA:HB3	56:B8:36:PRO:HD3	1.99	0.44
2:B:131:GLU:OE1	2:B:141:THR:HG21	2.18	0.44
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.44
5:F:65:LEU:O	5:F:76:ASN:HA	2.18	0.44
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.44
9:J:329:LEU:HD12	9:J:329:LEU:O	2.17	0.44
10:K:78:ASP:HA	14:O:215:LYS:HD3	1.99	0.44
12:M:306:MET:HA	12:M:315:THR:O	2.18	0.44
12:M:307:VAL:HG22	12:M:582:VAL:HG13	1.99	0.44
16:Q:235:ASP:OD1	16:Q:356:ILE:HD12	2.17	0.44
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.44
26:c:166:LEU:HB2	26:c:170:ARG:NH2	2.33	0.44
32:i:8:VAL:O	32:i:12:THR:HG23	2.18	0.44
35:l:18:PRO:HG3	35:l:39:ILE:HD12	1.99	0.44
40:r:36:ILE:O	40:r:39:LEU:HB3	2.18	0.44
40:r:237:LYS:HD2	40:r:237:LYS:N	2.33	0.44
44:w:238:GLU:O	44:w:242:LYS:HG3	2.17	0.44
48:0:40:LEU:HD22	48:0:59:LEU:CD1	2.47	0.44
76:AH:401:PEE:C12	66:AJ:240:MET:CE	2.91	0.44
66:AJ:278:TYR:O	66:AJ:281:LEU:HB2	2.17	0.44
63:AS:71:LEU:HD21	66:AV:25:SER:CB	2.48	0.44
66:AV:265:PRO:HA	66:AV:266:PRO:HD3	1.79	0.44
67:AW:152:ALA:HA	67:AW:155:GLN:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:312:ALA:HA	67:AW:315:LYS:HE3	1.98	0.44
68:AY:337:LEU:C	68:AY:368:MET:HE2	2.41	0.44
1:BA:88:ARG:C	1:BA:244:ASN:HD22	2.26	0.44
1:BA:129:GLU:OE1	1:BA:132:ARG:NH1	2.49	0.44
2:BB:91:LEU:HD23	2:BB:95:PHE:CD2	2.52	0.44
2:BB:127:THR:HA	15:BP:231:ARG:HH12	1.81	0.44
8:BI:55:CYS:HB3	12:BM:110:LYS:HE3	1.98	0.44
9:BJ:283:VAL:O	9:BJ:357:ARG:NH2	2.51	0.44
15:BP:55:HIS:HD2	15:BP:79:SER:O	2.01	0.44
16:BQ:162:ARG:HA	16:BQ:163:PRO:HD3	1.80	0.44
16:BQ:201:PHE:HB2	41:Bs:32:GLN:HG3	1.99	0.44
22:BY:42:PRO:HD2	23:BZ:14:MET:HG3	1.99	0.44
22:BY:85:PRO:O	22:BY:86:TYR:CD1	2.71	0.44
30:Bg:78:GLU:OE1	32:Bi:342:PHE:HD1	2.01	0.44
32:Bi:232:ARG:NH1	44:Bw:306:ASN:O	2.50	0.44
35:Bl:481:THR:HG22	43:Bv:92:HIS:CD2	2.52	0.44
41:Bs:89:LEU:HD12	41:Bs:91:MET:HE2	1.98	0.44
43:Bv:63:LEU:O	43:Bv:67:LEU:HG	2.18	0.44
44:Bw:86:PHE:HD2	44:Bw:159:LEU:HD13	1.83	0.44
57:B9:37:LEU:HD23	57:B9:37:LEU:HA	1.84	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
1:A:274:LYS:NZ	1:A:351:THR:O	2.51	0.44
3:C:150:MET:HE3	3:C:185:PRO:HG2	2.00	0.44
4:E:99:GLN:NE2	33:j:41:PHE:CD1	2.82	0.44
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.44
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
15:P:109:LYS:O	15:P:110:SER:OG	2.31	0.44
76:W:201:PEE:C2	41:s:98:LEU:HD22	2.47	0.44
32:i:309:ASN:HD21	44:w:130:ARG:HD3	1.82	0.44
33:j:48:ARG:HD2	33:j:49:VAL:H	1.83	0.44
71:r:501:PLX:H122	71:r:501:PLX:H151	1.80	0.44
41:s:142:TYR:CD2	41:s:289:LEU:HD11	2.52	0.44
42:u:18:VAL:HG12	42:u:20:ILE:H	1.83	0.44
44:w:92:HIS:HB3	44:w:103:PRO:HB3	1.99	0.44
44:w:211:VAL:HG13	44:w:212:PRO:HD3	1.98	0.44
44:w:270:VAL:O	44:w:275:TYR:N	2.47	0.44
54:6:3:ASN:ND2	54:6:5:VAL:HG13	2.33	0.44
67:AK:105:ALA:HA	68:AL:390:ARG:HG3	2.00	0.44
67:AK:155:GLN:N	67:AK:156:PRO:HD2	2.33	0.44
68:AL:152:GLN:NE2	68:AL:249:HIS:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:286:HIS:CE1	68:AL:359:VAL:HG22	2.52	0.44
67:AW:228:PRO:O	67:AW:231:LYS:HB2	2.18	0.44
1:BA:440:ARG:HE	1:BA:441:HIS:CE1	2.35	0.44
7:BH:23:ARG:HH22	7:BH:27:LEU:HD21	1.83	0.44
12:BM:37:ASP:OD1	12:BM:38:GLY:N	2.41	0.44
12:BM:158:ARG:HH21	12:BM:178:GLN:HE22	1.64	0.44
14:BO:104:VAL:HG12	14:BO:105:LEU:HD12	2.00	0.44
14:BO:198:ALA:HA	14:BO:201:ILE:HD12	1.99	0.44
17:BS:53:ARG:HB3	31:Bh:102:GLY:HA2	1.99	0.44
17:BS:54:ILE:HG13	31:Bh:105:ARG:NH1	2.32	0.44
20:BV:40:ARG:HE	75:BV:201:CDL:CA2	2.30	0.44
6:BX:123:GLU:HB2	6:BX:128:PHE:O	2.18	0.44
37:Bn:39:ARG:HB2	37:Bn:57:TRP:CZ2	2.53	0.44
40:Br:36:ILE:O	40:Br:39:LEU:HB3	2.18	0.44
42:Bu:100:CYS:SG	42:Bu:101:ARG:N	2.78	0.44
47:Bz:128:GLU:HB3	47:Bz:129:VAL:H	1.55	0.44
48:B0:40:LEU:HD22	48:B0:59:LEU:CD1	2.47	0.44
53:B5:61:GLU:OE1	53:B5:64:ARG:NH1	2.51	0.44
53:B5:68:ILE:HG13	53:B5:69:PHE:N	2.33	0.44
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.44
2:B:166:VAL:HG11	2:B:199:ILE:HG23	2.00	0.44
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.44
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	0.44
9:J:141:PHE:CD2	9:J:183:ASN:ND2	2.86	0.44
11:L:72:ILE:HA	11:L:143:TRP:NE1	2.33	0.44
12:M:278:HIS:NE2	12:M:280:ASP:HB2	2.33	0.44
15:P:90:PRO:O	15:P:93:VAL:HG23	2.18	0.44
21:W:111:PHE:CE2	21:W:117:VAL:HG11	2.49	0.44
22:Y:85:PRO:O	22:Y:86:TYR:CD1	2.71	0.44
24:a:185:ALA:O	42:u:48:TRP:HZ2	2.01	0.44
25:b:71:VAL:O	25:b:75:VAL:HB	2.18	0.44
25:b:90:VAL:HG22	25:b:97:ILE:HD12	1.98	0.44
71:b:201:PLX:H1C3	71:b:201:PLX:H31	1.94	0.44
26:c:133:LEU:HD13	35:l:532:ILE:HD12	2.00	0.44
26:c:139:PHE:O	26:c:143:MET:HG2	2.18	0.44
26:c:163:TYR:OH	43:v:42:THR:O	2.11	0.44
34:k:87:LEU:HD13	36:m:74:ALA:HB2	2.00	0.44
38:o:6:TYR:CD2	38:o:14:LEU:HD23	2.52	0.44
38:o:17:THR:HG21	39:p:22:ARG:HH12	1.82	0.44
39:p:30:TRP:O	39:p:32:VAL:HG23	2.18	0.44
40:r:72:LEU:O	40:r:76:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:63:LEU:O	43:v:67:LEU:HG	2.18	0.44
45:x:379:TYR:CE2	45:x:383:MET:HE2	2.52	0.44
46:y:1:MET:SD	46:y:133:LEU:HD13	2.58	0.44
47:z:41:THR:O	47:z:45:ILE:HG13	2.18	0.44
47:z:63:ARG:HA	47:z:67:PHE:CD2	2.53	0.44
53:5:61:GLU:OE1	53:5:64:ARG:NH1	2.51	0.44
68:AL:267:PRO:HA	68:AL:350:GLU:OE1	2.18	0.44
67:AW:61:ILE:HG22	67:AW:222:GLY:HA2	1.99	0.44
67:AW:81:HIS:CD2	67:AW:158:LEU:HD22	2.53	0.44
67:AW:452:GLU:HG2	67:AW:453:LEU:N	2.31	0.44
68:AY:82:GLU:OE2	68:AY:219:TYR:OH	2.28	0.44
1:BA:47:GLY:HA2	1:BA:133:HIS:HB3	2.00	0.44
1:BA:317:VAL:HG22	1:BA:356:VAL:HA	1.99	0.44
2:BB:35:THR:N	8:BI:105:GLU:O	2.51	0.44
2:BB:81:THR:HG23	41:Bs:35:LYS:H	1.83	0.44
4:BE:40:TYR:OH	6:BG:117:GLU:OE2	2.28	0.44
7:BH:13:GLY:HA2	16:BQ:279:THR:HG22	2.00	0.44
9:BJ:71:ASN:ND2	15:BP:214:ASP:HB3	2.33	0.44
9:BJ:220:MET:HA	9:BJ:223:PHE:CD2	2.53	0.44
12:BM:66:HIS:CE1	12:BM:68:ARG:HG2	2.53	0.44
14:BO:80:LEU:HB2	14:BO:81:PRO:HD3	1.99	0.44
14:BO:147:SER:HA	14:BO:150:GLU:OE1	2.18	0.44
16:BQ:391:VAL:O	16:BQ:415:GLY:HA2	2.18	0.44
17:BS:31:ASN:HD21	17:BS:36:LYS:HD3	1.83	0.44
26:Bc:139:PHE:O	26:Bc:143:MET:HG2	2.18	0.44
30:Bg:87:ARG:HD2	42:Bu:156:GLY:C	2.42	0.44
32:Bi:79:MET:SD	34:Bk:43:MET:HE1	2.58	0.44
33:Bj:71:LEU:O	36:Bm:146:TYR:OH	2.28	0.44
34:Bk:8:ILE:N	34:Bk:8:ILE:HD12	2.33	0.44
35:Bl:59:GLN:NE2	35:Bl:59:GLN:CA	2.73	0.44
40:Br:72:LEU:O	40:Br:76:THR:HG23	2.18	0.44
41:Bs:215:TYR:HD1	41:Bs:219:PRO:HB2	1.83	0.44
54:B6:2:GLU:CG	54:B6:3:ASN:H	2.30	0.44
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	0.44
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.44
1:A:440:ARG:HE	1:A:441:HIS:CE1	2.35	0.44
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.44
6:G:77:GLU:OE1	6:G:77:GLU:N	2.38	0.44
6:G:87:LEU:HA	6:G:90:TYR:HB3	2.00	0.44
7:H:12:VAL:HG13	7:H:13:GLY:N	2.33	0.44
7:H:23:ARG:O	7:H:26:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:236:GLU:HB3	14:O:238:PRO:HD2	2.00	0.44
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	0.44
22:Y:86:TYR:HH	43:v:100:LYS:HG2	1.79	0.44
25:b:111:LEU:C	25:b:112:GLU:CD	2.85	0.44
26:c:102:GLY:HA3	38:o:43:LEU:HD13	2.00	0.44
32:i:79:MET:SD	34:k:43:MET:HE1	2.58	0.44
33:j:64:LEU:O	33:j:68:GLU:HG2	2.18	0.44
35:l:51:THR:CG2	35:l:91:PRO:HG2	2.30	0.44
35:l:533:MET:CE	76:l:702:PEE:H32	2.48	0.44
35:l:548:LEU:O	35:l:552:LEU:HB2	2.18	0.44
41:s:90:PRO:HB2	41:s:92:PRO:O	2.18	0.44
54:6:36:MET:O	54:6:40:LEU:HG	2.18	0.44
59:AB:1:MET:SD	67:AK:412:VAL:HG13	2.58	0.44
60:AC:132:ALA:HB1	76:AH:401:PEE:H27	2.00	0.44
68:AL:42:LEU:HD11	68:AL:430:GLU:OE1	2.17	0.44
68:AL:140:LEU:HD21	68:AL:237:VAL:HG13	1.99	0.44
68:AL:282:LEU:HA	68:AL:283:PRO:HD3	1.89	0.44
75:AN:102:CDL:H172	75:AN:102:CDL:H142	1.77	0.44
60:AP:150:ALA:C	60:AP:152:ILE:H	2.24	0.44
65:AU:249:TYR:O	65:AU:252:VAL:HG23	2.17	0.44
66:AV:155:TYR:O	66:AV:155:TYR:CD1	2.70	0.44
66:AV:333:LEU:HD21	76:AV:403:PEE:C40	2.48	0.44
68:AY:333:VAL:HG13	68:AY:336:LYS:HD2	1.99	0.44
1:BA:274:LYS:NZ	1:BA:351:THR:O	2.51	0.44
3:BC:150:MET:HE3	3:BC:185:PRO:HG2	2.00	0.44
4:BE:39:TRP:O	4:BE:43:VAL:HG23	2.18	0.44
8:BI:60:ARG:HD3	16:BQ:159:LEU:HD22	1.99	0.44
9:BJ:329:LEU:HD12	9:BJ:329:LEU:O	2.17	0.44
12:BM:498:GLN:HE22	12:BM:501:ARG:HD2	1.82	0.44
15:BP:90:PRO:O	15:BP:93:VAL:HG23	2.18	0.44
16:BQ:55:SER:N	16:BQ:58:THR:OG1	2.50	0.44
16:BQ:106:VAL:HG11	16:BQ:109:CYS:HB2	2.00	0.44
17:BS:53:ARG:HH21	31:Bh:105:ARG:HA	1.83	0.44
76:BW:201:PEE:C2	41:Bs:98:LEU:HD22	2.47	0.44
24:Ba:150:ARG:NH1	40:Br:168:HIS:CE1	2.86	0.44
32:Bi:8:VAL:O	32:Bi:12:THR:HG23	2.18	0.44
32:Bi:321:LYS:HA	32:Bi:322:PRO:HD3	1.80	0.44
34:Bk:46:LEU:HD22	36:Bm:46:PHE:CD2	2.53	0.44
35:Bl:95:PHE:HZ	35:Bl:456:ARG:HG2	1.83	0.44
39:Bp:54:GLU:N	39:Bp:54:GLU:OE1	2.51	0.44
41:Bs:224:PHE:CZ	41:Bs:228:TYR:HE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Bw:58:ARG:HB3	44:Bw:202:HIS:HE1	1.82	0.44
44:Bw:92:HIS:HB3	44:Bw:103:PRO:HB3	1.99	0.44
44:Bw:93:TYR:O	44:Bw:96:SER:OG	2.25	0.44
48:B0:79:LYS:NZ	55:B7:15:ASN:HD21	2.15	0.44
1:A:88:ARG:C	1:A:244:ASN:HD22	2.26	0.43
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.00	0.43
9:J:108:TRP:HZ3	9:J:110:ALA:HA	1.82	0.43
9:J:124:ASN:OD1	9:J:125:VAL:N	2.51	0.43
9:J:167:VAL:HG22	9:J:201:VAL:HB	2.00	0.43
9:J:319:VAL:C	9:J:323:HIS:HD1	2.22	0.43
11:L:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.43
12:M:639:LEU:O	12:M:642:VAL:HG12	2.18	0.43
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.43
14:O:195:ASP:HB2	14:O:219:ARG:H	1.83	0.43
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.49	0.43
16:Q:271:ARG:NH1	41:s:281:ARG:HA	2.31	0.43
17:S:53:ARG:HH21	31:h:105:ARG:HA	1.83	0.43
18:T:67:PHE:O	18:T:71:LEU:HD13	2.17	0.43
24:a:54:LEU:HD23	24:a:54:LEU:HA	1.81	0.43
24:a:150:ARG:NH1	40:r:168:HIS:CE1	2.86	0.43
26:c:101:TRP:CD1	38:o:47:TYR:CD1	3.06	0.43
26:c:161:TYR:HA	26:c:162:PRO:HD3	1.84	0.43
27:d:57:TYR:CD1	27:d:57:TYR:O	2.70	0.43
32:i:298:TYR:HE2	40:r:147:THR:HG23	1.83	0.43
35:l:224:SER:OG	35:l:256:GLY:CA	2.59	0.43
38:o:9:SER:OG	38:o:12:ARG:HB3	2.18	0.43
71:r:502:PLX:H361	71:r:502:PLX:H392	1.64	0.43
44:w:86:PHE:HA	44:w:87:PRO:HD2	1.85	0.43
45:x:70:VAL:HG11	45:x:246:LEU:HD22	2.00	0.43
53:5:68:ILE:HG13	53:5:69:PHE:N	2.33	0.43
61:AD:25:ILE:O	61:AD:29:VAL:HG23	2.18	0.43
65:AH:301:PRO:O	65:AH:305:THR:HG23	2.17	0.43
68:AL:294:PRO:HB2	68:AL:301:ASN:ND2	2.33	0.43
58:AN:17:TYR:HD1	68:AY:275:ILE:HG12	1.83	0.43
65:AU:290:LEU:C	65:AU:290:LEU:CD2	2.86	0.43
66:AV:123:THR:HG22	66:AV:189:ILE:HD13	2.00	0.43
1:BA:99:TRP:HA	1:BA:149:MET:HE1	2.00	0.43
1:BA:167:SER:O	1:BA:171:VAL:HG23	2.18	0.43
2:BB:131:GLU:OE1	2:BB:141:THR:HG21	2.18	0.43
5:BF:67:ALA:HB3	5:BF:75:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:125:VAL:HG12	9:BJ:163:LYS:HB2	2.00	0.43
9:BJ:141:PHE:CD2	9:BJ:183:ASN:ND2	2.86	0.43
9:BJ:169:HIS:CD2	73:BJ:401:NDP:C5N	2.79	0.43
10:BK:86:ASP:O	10:BK:90:GLU:HG3	2.18	0.43
11:BL:77:VAL:HG22	11:BL:78:ARG:N	2.33	0.43
12:BM:306:MET:HA	12:BM:315:THR:O	2.18	0.43
12:BM:323:LEU:HA	12:BM:326:VAL:HG22	1.99	0.43
22:BY:65:MET:SD	35:Bl:375:ILE:HG12	2.58	0.43
24:Ba:185:ALA:O	42:Bu:48:TRP:HZ2	2.01	0.43
26:Bc:102:GLY:HA3	38:Bo:43:LEU:HD13	2.00	0.43
27:Bd:57:TYR:CD1	27:Bd:57:TYR:O	2.70	0.43
31:Bh:36:PHE:HD2	31:Bh:66:CYS:HB2	1.82	0.43
33:Bj:34:SER:HB2	41:Bs:64:ALA:H	1.82	0.43
34:Bk:87:LEU:HD13	36:Bm:74:ALA:HB2	2.00	0.43
35:Bl:533:MET:CE	76:Bl:702:PEE:H32	2.48	0.43
39:Bp:25:ARG:HA	39:Bp:25:ARG:HD3	1.80	0.43
39:Bp:44:MET:CE	72:Bp:201:8Q1:C10	2.83	0.43
41:Bs:195:ARG:O	41:Bs:198:PHE:N	2.52	0.43
42:Bu:80:GLU:N	42:Bu:81:PRO:HD2	2.33	0.43
47:Bz:148:HIS:CE1	47:Bz:152:MET:HE3	2.53	0.43
47:Bz:223:LEU:HA	47:Bz:223:LEU:HD23	1.79	0.43
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.43
8:I:36:GLN:HA	8:I:37:PRO:HD3	1.88	0.43
12:M:133:GLN:HA	12:M:136:GLU:OE2	2.17	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	0.43
14:O:104:VAL:HG12	14:O:105:LEU:HD12	2.00	0.43
15:P:227:ALA:O	15:P:229:GLU:N	2.47	0.43
16:Q:145:MET:HG3	16:Q:174:PHE:HB3	1.99	0.43
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.43
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.66	0.43
26:c:52:ALA:HB2	26:c:62:TYR:HB2	1.99	0.43
27:d:111:GLU:OE1	27:d:119:CYS:HB2	2.18	0.43
31:h:3:PHE:HB2	32:i:144:GLN:HE21	1.83	0.43
35:l:227:LEU:HA	35:l:230:HIS:HB3	2.00	0.43
36:m:26:ILE:HD13	41:s:121:TRP:CE2	2.54	0.43
44:w:86:PHE:HD2	44:w:159:LEU:HD13	1.83	0.43
53:5:19:PHE:CD1	53:5:19:PHE:C	2.94	0.43
59:AB:26:LEU:HG	59:AB:28:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:158:PRO:HG3	65:AU:181:ASN:HD22	1.82	0.43
67:AK:127:ARG:NH1	67:AK:224:GLY:O	2.49	0.43
67:AK:227:HIS:N	67:AK:228:PRO:HD2	2.33	0.43
68:AL:322:VAL:HG12	68:AL:323:HIS:N	2.32	0.43
68:AL:414:GLY:O	68:AL:418:LEU:HD13	2.18	0.43
59:AO:46:LYS:HG2	59:AO:47:ARG:O	2.18	0.43
60:AP:127:TYR:HE1	61:AQ:33:GLU:HG2	1.83	0.43
75:AY:501:CDL:H122	75:AY:501:CDL:H151	1.87	0.43
1:BA:152:ARG:NH1	10:BK:99:PRO:HB3	2.33	0.43
2:BB:128:ILE:HG12	2:BB:143:TYR:HD1	1.83	0.43
3:BC:88:CYS:SG	16:BQ:223:HIS:CE1	3.10	0.43
3:BC:160:TYR:HE1	16:BQ:120:THR:HG22	1.81	0.43
5:BF:65:LEU:O	5:BF:76:ASN:HA	2.18	0.43
8:BI:5:THR:HB	8:BI:8:ILE:HD12	2.00	0.43
8:BI:37:PRO:HA	8:BI:38:PRO:HD3	1.81	0.43
11:BL:72:ILE:HA	11:BL:143:TRP:CD1	2.53	0.43
11:BL:72:ILE:HA	11:BL:143:TRP:NE1	2.33	0.43
12:BM:307:VAL:HG22	12:BM:582:VAL:HG13	1.99	0.43
12:BM:342:ALA:HA	12:BM:547:LEU:HB2	2.00	0.43
12:BM:342:ALA:O	12:BM:369:GLU:HG2	2.18	0.43
15:BP:227:ALA:O	15:BP:229:GLU:N	2.47	0.43
18:BT:67:PHE:O	18:BT:71:LEU:HD13	2.17	0.43
21:BW:115:ARG:NH1	31:Bh:36:PHE:HD1	2.09	0.43
26:Bc:52:ALA:HB2	26:Bc:62:TYR:HB2	1.99	0.43
27:Bd:111:GLU:OE1	27:Bd:119:CYS:HB2	2.18	0.43
32:Bi:258:THR:CG2	32:Bi:336:LEU:HB3	2.48	0.43
38:Bo:100:PHE:CZ	38:Bo:104:ILE:HD11	2.53	0.43
70:A:502:FMN:H4'	70:A:502:FMN:H1'2	1.63	0.43
73:J:401:NDP:O2X	73:J:401:NDP:O3B	2.33	0.43
12:M:385:TYR:HB2	12:M:517:HIS:CE1	2.53	0.43
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43
15:P:164:ASN:HA	15:P:181:HIS:HE2	1.82	0.43
17:S:43:TYR:CE2	21:W:68:ARG:HD2	2.53	0.43
20:V:62:THR:HG22	20:V:104:ARG:CD	2.49	0.43
25:b:35:LEU:HA	25:b:36:PRO:HD2	1.90	0.43
25:b:79:VAL:HG22	35:l:10:LEU:CD1	2.48	0.43
31:h:56:CYS:HA	42:u:145:ARG:NH1	2.33	0.43
38:o:6:TYR:HE1	38:o:12:ARG:NH2	2.15	0.43
41:s:92:PRO:HB3	41:s:255:TYR:CD2	2.53	0.43
41:s:195:ARG:O	41:s:198:PHE:N	2.52	0.43
41:s:224:PHE:CZ	41:s:228:TYR:HE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:z:223:LEU:HD23	47:z:223:LEU:HA	1.79	0.43
48:0:37:GLN:O	48:0:41:LYS:HG2	2.18	0.43
53:5:26:MET:N	53:5:26:MET:SD	2.91	0.43
62:AE:40:LEU:O	62:AE:44:VAL:HG23	2.19	0.43
61:AQ:44:TYR:HB2	65:AU:290:LEU:HD13	2.01	0.43
61:AQ:53:TRP:HA	61:AQ:56:ILE:HB	1.99	0.43
67:AW:79:THR:HG23	67:AW:205:LEU:HD23	2.00	0.43
67:AW:262:ASN:O	67:AW:443:ASN:HA	2.18	0.43
1:BA:157:TYR:HB2	1:BA:212:LEU:HD21	1.99	0.43
3:BC:211:TYR:CD1	3:BC:211:TYR:C	2.96	0.43
9:BJ:61:ALA:HA	9:BJ:66:GLY:HA3	2.00	0.43
12:BM:229:GLY:O	12:BM:232:THR:HG23	2.18	0.43
12:BM:646:LEU:HD13	12:BM:653:LEU:HB3	2.00	0.43
15:BP:188:LEU:HD22	16:BQ:117:HIS:HB2	2.00	0.43
20:BV:51:GLU:HB3	20:BV:55:LYS:NZ	2.34	0.43
25:Bb:79:VAL:HG22	35:Bl:10:LEU:CD1	2.48	0.43
71:Bb:201:PLX:H1C3	71:Bb:201:PLX:H31	1.94	0.43
32:Bi:251:LEU:HA	32:Bi:251:LEU:HD23	1.82	0.43
33:Bj:48:ARG:HD2	33:Bj:49:VAL:H	1.83	0.43
35:Bl:226:GLN:HG2	35:Bl:280:LEU:HD22	2.00	0.43
35:Bl:280:LEU:O	35:Bl:284:THR:HG23	2.19	0.43
37:Bn:40:ASN:HD22	37:Bn:56:THR:HG23	1.82	0.43
38:Bo:6:TYR:CD2	38:Bo:14:LEU:HD23	2.52	0.43
41:Bs:92:PRO:HB3	41:Bs:255:TYR:CD2	2.53	0.43
46:By:63:THR:HA	46:By:66:THR:HG22	2.00	0.43
46:By:148:MET:HE3	46:By:148:MET:HB3	1.77	0.43
49:B1:43:PRO:HB2	49:B1:48:ILE:CD1	2.48	0.43
1:A:53:LEU:O	1:A:56:SER:OG	2.24	0.43
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.43
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.43
6:G:138:LEU:O	6:G:143:GLU:HB2	2.18	0.43
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	0.43
12:M:612:PRO:HB3	12:M:616:ALA:HB3	1.99	0.43
15:P:55:HIS:HD2	15:P:79:SER:O	2.01	0.43
17:S:54:ILE:HG13	31:h:105:ARG:NH1	2.32	0.43
30:g:15:ASP:OD1	30:g:16:GLU:N	2.52	0.43
32:i:294:LEU:HD23	32:i:294:LEU:HA	1.74	0.43
34:k:32:CYS:O	34:k:36:MET:HG3	2.18	0.43
35:l:209:SER:O	35:l:212:PRO:HD2	2.19	0.43
36:m:106:VAL:HG11	36:m:117:ASN:ND2	2.34	0.43
39:p:104:LEU:HD22	39:p:122:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:80:GLU:N	42:u:81:PRO:HD2	2.33	0.43
42:u:121:ASP:HB3	42:u:124:GLU:OE2	2.18	0.43
44:w:332:ARG:C	44:w:338:LYS:HA	2.36	0.43
46:y:52:HIS:CD2	49:1:40:ASP:HB2	2.54	0.43
47:z:148:HIS:CE1	47:z:152:MET:HE3	2.53	0.43
52:4:75:ARG:HG2	52:4:75:ARG:NH1	2.19	0.43
60:AC:200:HIS:O	60:AC:204:ARG:HG3	2.18	0.43
65:AH:307:LYS:NZ	75:AH:403:CDL:OA4	2.42	0.43
75:AJ:405:CDL:H341	75:AJ:405:CDL:H371	1.67	0.43
67:AK:293:LEU:HD21	67:AK:358:VAL:HG22	2.00	0.43
64:AT:17:TRP:NE1	68:AY:382:SER:OG	2.41	0.43
66:AV:155:TYR:CD1	66:AV:155:TYR:C	2.94	0.43
66:AV:326:TRP:CZ2	76:AV:403:PEE:O5	2.72	0.43
2:BB:84:TYR:OH	3:BC:192:TYR:HB2	2.19	0.43
2:BB:166:VAL:HG11	2:BB:199:ILE:HG23	2.00	0.43
4:BE:80:ASP:OD1	4:BE:81:LEU:N	2.52	0.43
6:BG:138:LEU:O	6:BG:143:GLU:HB2	2.18	0.43
7:BH:23:ARG:O	7:BH:26:ILE:HB	2.18	0.43
9:BJ:273:LEU:O	9:BJ:276:LEU:HB3	2.17	0.43
10:BK:78:ASP:HA	14:BO:215:LYS:HD3	2.00	0.43
12:BM:200:ARG:HB3	14:BO:118:PHE:CD1	2.54	0.43
12:BM:221:ASN:HB3	12:BM:285:TRP:CZ3	2.53	0.43
14:BO:132:ILE:O	14:BO:172:ILE:HG22	2.18	0.43
20:BV:62:THR:HG22	20:BV:104:ARG:CD	2.49	0.43
6:BX:105:MET:HE2	6:BX:139:MET:HE3	2.01	0.43
22:BY:78:GLU:CG	35:Bl:385:PHE:HE1	2.30	0.43
28:Be:54:PRO:O	28:Be:56:GLN:HG3	2.18	0.43
32:Bi:298:TYR:HE2	40:Br:147:THR:HG23	1.83	0.43
35:Bl:37:LYS:HE3	35:Bl:102:GLU:CG	2.37	0.43
35:Bl:209:SER:O	35:Bl:212:PRO:HD2	2.19	0.43
35:Bl:548:LEU:O	35:Bl:552:LEU:HB2	2.18	0.43
36:Bm:56:PHE:CZ	41:Bs:111:LEU:HD11	2.54	0.43
41:Bs:90:PRO:HB2	41:Bs:92:PRO:O	2.18	0.43
47:Bz:41:THR:O	47:Bz:45:ILE:HG13	2.18	0.43
47:Bz:60:ASP:O	47:Bz:64:GLU:HG3	2.18	0.43
49:B1:27:TRP:CH2	50:B2:86:GLY:HA2	2.54	0.43
53:B5:26:MET:N	53:B5:26:MET:SD	2.91	0.43
1:A:418:GLN:CD	12:M:115:GLY:HA2	2.44	0.43
2:B:69:GLY:O	2:B:72:LEU:HB3	2.17	0.43
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.43
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:123:GLU:O	6:G:127:GLY:N	2.50	0.43
10:K:86:ASP:O	10:K:90:GLU:HG3	2.18	0.43
12:M:221:ASN:HB3	12:M:285:TRP:CZ3	2.53	0.43
12:M:229:GLY:O	12:M:232:THR:HG23	2.18	0.43
15:P:55:HIS:NE2	15:P:78:VAL:HG12	2.34	0.43
16:Q:201:PHE:HB2	41:s:32:GLN:HG3	1.99	0.43
21:W:58:ARG:HD3	21:W:58:ARG:HA	1.86	0.43
26:c:61:ASP:O	26:c:63:GLU:HG3	2.19	0.43
29:f:28:LYS:HE3	44:w:101:GLY:H	1.83	0.43
32:i:274:ASN:O	32:i:275:SER:OG	2.30	0.43
33:j:106:TRP:HZ3	41:s:291:LYS:HA	1.84	0.43
35:l:226:GLN:HG2	35:l:280:LEU:HD21	1.84	0.43
37:n:39:ARG:HB2	37:n:57:TRP:CZ2	2.53	0.43
40:r:105:SER:O	40:r:109:THR:HG23	2.18	0.43
40:r:328:CYS:HG	40:r:440:HIS:HE2	1.63	0.43
40:r:345:SER:O	40:r:348:LEU:HG	2.18	0.43
41:s:231:ILE:HG23	41:s:270:PHE:CD2	2.53	0.43
45:x:247:ILE:HB	79:x:604:HEA:HBC1	2.01	0.43
45:x:377:PHE:CD2	79:x:604:HEA:HAD1	2.54	0.43
47:z:19:THR:HG22	47:z:53:THR:OG1	2.18	0.43
47:z:60:ASP:O	47:z:64:GLU:HG3	2.18	0.43
51:3:3:ALA:O	51:3:4:ALA:HB2	2.17	0.43
51:3:54:ARG:N	51:3:54:ARG:CD	2.80	0.43
52:4:57:ARG:HB3	52:4:57:ARG:NH1	2.31	0.43
55:7:44:PRO:HA	55:7:47:ARG:NH1	2.34	0.43
60:AC:239:HIS:HB2	74:AC:301:FES:S1	2.59	0.43
65:AH:131:ALA:HA	65:AH:174:TYR:HA	2.00	0.43
66:AJ:197:LEU:HD22	75:AJ:404:CDL:H162	2.01	0.43
68:AL:360:CYS:HB3	68:AL:368:MET:SD	2.59	0.43
65:AU:202:ARG:NH2	66:AV:248:ASP:OD1	2.51	0.43
1:BA:282:VAL:HA	1:BA:307:VAL:HA	2.01	0.43
3:BC:88:CYS:HB3	16:BQ:141:TYR:CG	2.54	0.43
9:BJ:83:PRO:HA	9:BJ:106:LEU:O	2.18	0.43
9:BJ:124:ASN:OD1	9:BJ:125:VAL:N	2.51	0.43
11:BL:170:THR:HG22	12:BM:423:LEU:O	2.18	0.43
15:BP:210:LEU:HA	15:BP:221:ALA:HA	2.01	0.43
16:BQ:164:PRO:HA	16:BQ:165:PRO:HD3	1.83	0.43
18:BT:102:ASN:HD21	18:BT:104:ASP:HB2	1.84	0.43
20:BV:19:HIS:CD2	20:BV:20:ARG:HG3	2.54	0.43
26:Bc:61:ASP:O	26:Bc:63:GLU:HG3	2.19	0.43
29:Bf:28:LYS:HE3	44:Bw:101:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bh:3:PHE:HB2	32:Bi:144:GLN:HE21	1.83	0.43
31:Bh:56:CYS:HA	42:Bu:145:ARG:NH1	2.33	0.43
35:Bl:369:THR:O	35:Bl:372:SER:OG	2.27	0.43
35:Bl:399:ALA:O	35:Bl:402:SER:OG	2.33	0.43
35:Bl:548:LEU:HD22	38:Bo:93:CYS:HB3	2.01	0.43
76:Bl:701:PEE:H65	76:Bl:701:PEE:H71	1.79	0.43
36:Bm:43:ILE:HG22	36:Bm:48:GLY:HA3	2.00	0.43
41:Bs:59:GLU:OE1	41:Bs:59:GLU:N	2.52	0.43
41:Bs:142:TYR:CE2	41:Bs:289:LEU:HD11	2.54	0.43
41:Bs:231:ILE:HG23	41:Bs:270:PHE:CD2	2.54	0.43
42:Bu:100:CYS:O	42:Bu:102:LYS:N	2.50	0.43
46:By:1:MET:SD	46:By:133:LEU:HD13	2.58	0.43
47:Bz:19:THR:CG2	47:Bz:53:THR:OG1	2.66	0.43
54:B6:3:ASN:ND2	54:B6:5:VAL:HG13	2.33	0.43
54:B6:36:MET:O	54:B6:40:LEU:HG	2.18	0.43
55:B7:44:PRO:HA	55:B7:47:ARG:NH1	2.34	0.43
1:A:270:ASN:CG	1:A:338:ASP:HB2	2.44	0.43
1:A:282:VAL:HA	1:A:307:VAL:HA	2.01	0.43
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	0.43
9:J:273:LEU:O	9:J:276:LEU:HB3	2.17	0.43
12:M:420:LYS:O	12:M:424:HIS:ND1	2.34	0.43
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.43
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.43
16:Q:316:PHE:HD1	16:Q:339:GLN:HE21	1.67	0.43
6:X:105:MET:HE2	6:X:139:MET:HE3	2.00	0.43
22:Y:58:SER:HB2	35:l:371:THR:HG21	2.01	0.43
32:i:234:TRP:HH2	32:i:305:LEU:HB2	1.84	0.43
35:l:151:SER:HA	35:l:247:LEU:HD13	2.01	0.43
40:r:109:THR:HG22	40:r:121:PHE:HB2	2.00	0.43
44:w:137:SER:C	44:w:139:ARG:N	2.77	0.43
45:x:131:PRO:HB2	46:y:159:VAL:HA	2.00	0.43
50:2:53:THR:HG22	50:2:54:ASN:OD1	2.19	0.43
58:AA:74:ASN:OD1	58:AA:78:TYR:CE2	2.71	0.43
60:AC:246:SER:HG	60:AC:248:ARG:HE	1.64	0.43
63:AF:51:LEU:CD2	63:AF:55:LEU:HD13	2.49	0.43
75:AH:403:CDL:H122	66:AJ:234:LEU:HD12	2.01	0.43
68:AL:332:ALA:O	68:AL:337:LEU:N	2.43	0.43
75:AN:102:CDL:C58	76:AV:403:PEE:C33	2.96	0.43
59:AO:28:PRO:O	67:AW:170:GLN:NE2	2.52	0.43
60:AP:82:ASP:OD1	60:AP:83:ILE:N	2.51	0.43
60:AP:214:ILE:HG22	60:AP:216:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:244:ASP:OD2	60:AP:248:ARG:HB2	2.19	0.43
65:AU:177:LYS:HA	65:AU:178:PRO:HD3	1.87	0.43
66:AV:33:PHE:HA	66:AV:36:LEU:HD12	2.01	0.43
67:AW:373:ALA:O	67:AW:377:LYS:HG3	2.19	0.43
68:AY:479:ARG:HH11	75:AY:501:CDL:HB62	1.82	0.43
7:BH:35:LEU:O	7:BH:45:ARG:NE	2.43	0.43
9:BJ:108:TRP:HZ3	9:BJ:110:ALA:HA	1.82	0.43
9:BJ:131:GLY:HA3	73:BJ:401:NDP:O3D	2.19	0.43
12:BM:134:GLY:HA3	69:BM:801:SF4:S3	2.52	0.43
12:BM:243:TRP:CD1	12:BM:244:GLU:HG3	2.54	0.43
12:BM:501:ARG:HH12	12:BM:666:GLN:HB2	1.82	0.43
18:BT:96:HIS:NE2	18:BT:115:CYS:SG	2.90	0.43
6:BX:90:TYR:OH	6:BX:114:ASP:OD1	2.36	0.43
24:Ba:98:LEU:HB2	27:Bd:57:TYR:CE1	2.40	0.43
32:Bi:76:PHE:CZ	32:Bi:80:LEU:HD11	2.54	0.43
33:Bj:64:LEU:O	33:Bj:68:GLU:HG2	2.18	0.43
34:Bk:32:CYS:O	34:Bk:36:MET:HG3	2.18	0.43
35:Bl:512:LYS:HG3	54:B6:16:ASN:HB2	1.96	0.43
36:Bm:26:ILE:HD13	41:Bs:121:TRP:CE2	2.54	0.43
36:Bm:33:ILE:O	36:Bm:37:VAL:HG23	2.19	0.43
38:Bo:9:SER:OG	38:Bo:12:ARG:HB3	2.18	0.43
40:Br:66:LEU:HD23	40:Br:66:LEU:HA	1.76	0.43
40:Br:339:SER:O	40:Br:340:ARG:HB2	2.16	0.43
44:Bw:124:ASN:O	44:Bw:126:GLY:N	2.41	0.43
44:Bw:137:SER:C	44:Bw:139:ARG:N	2.77	0.43
45:Bx:495:LEU:HD23	45:Bx:495:LEU:HA	1.68	0.43
49:B1:90:ARG:HD3	49:B1:90:ARG:HA	1.78	0.43
2:B:140:THR:OG1	2:B:185:LYS:NZ	2.28	0.43
3:C:211:TYR:CD1	3:C:211:TYR:C	2.97	0.43
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	0.43
8:I:37:PRO:HA	8:I:38:PRO:HD3	1.81	0.43
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	0.43
11:L:102:ASP:OD1	11:L:102:ASP:N	2.50	0.43
11:L:162:ALA:HA	11:L:168:LYS:HZ1	1.84	0.43
13:N:73:THR:HG22	13:N:74:PHE:N	2.34	0.43
14:O:132:ILE:O	14:O:172:ILE:HG22	2.18	0.43
15:P:157:VAL:HG21	15:P:181:HIS:CD2	2.46	0.43
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	2.01	0.43
16:Q:391:VAL:O	16:Q:415:GLY:HA2	2.18	0.43
26:c:41:TYR:CZ	26:c:67:ASP:HB3	2.54	0.43
28:e:87:MET:HE3	28:e:87:MET:HB3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:32:TYR:CE2	32:i:339:ILE:HD11	2.54	0.43
30:g:61:LEU:O	30:g:65:THR:HG23	2.19	0.43
33:j:68:GLU:HG3	33:j:98:LEU:HD21	2.01	0.43
34:k:51:THR:O	34:k:51:THR:OG1	2.28	0.43
35:l:68:TRP:HB2	35:l:76:LEU:HD12	2.01	0.43
40:r:45:ILE:O	40:r:45:ILE:HG22	2.19	0.43
63:AF:39:TYR:CD1	63:AF:39:TYR:C	2.95	0.43
67:AK:60:ARG:HB3	67:AK:223:LEU:HD12	2.00	0.43
68:AL:133:ILE:HG22	68:AL:134:LYS:N	2.34	0.43
68:AL:233:ALA:HB1	68:AL:237:VAL:HG21	2.01	0.43
68:AL:453:CYS:HA	68:AL:454:PRO:HD2	1.88	0.43
1:BA:134:ASP:N	1:BA:135:PRO:HD3	2.34	0.43
1:BA:270:ASN:CG	1:BA:338:ASP:HB2	2.44	0.43
2:BB:169:PRO:HG3	2:BB:198:GLU:HG2	2.00	0.43
4:BE:118:PHE:HZ	12:BM:621:LYS:HG3	1.83	0.43
8:BI:40:LYS:HG2	21:BW:8:GLN:HA	2.00	0.43
9:BJ:81:ILE:HG22	9:BJ:83:PRO:HD3	2.00	0.43
12:BM:136:GLU:HB3	12:BM:242:PRO:HG2	2.00	0.43
12:BM:307:VAL:HA	12:BM:582:VAL:HA	2.01	0.43
12:BM:542:PRO:HB2	12:BM:543:LYS:HD3	2.01	0.43
12:BM:639:LEU:O	12:BM:642:VAL:HG12	2.18	0.43
12:BM:651:PRO:O	12:BM:654:VAL:HG22	2.19	0.43
13:BN:106:ARG:O	13:BN:109:ILE:HG12	2.19	0.43
15:BP:55:HIS:NE2	15:BP:78:VAL:HG12	2.33	0.43
16:BQ:174:PHE:HD1	16:BQ:214:TYR:HE1	1.66	0.43
18:BT:79:GLU:OE1	18:BT:122:HIS:HB3	2.19	0.43
76:BW:201:PEE:H60	36:Bm:56:PHE:HZ	1.84	0.43
30:Bg:46:LEU:CD1	32:Bi:239:TRP:HB3	2.49	0.43
34:Bk:39:SER:HB3	36:Bm:16:PHE:HE2	1.84	0.43
35:Bl:208:PRO:HG2	35:Bl:266:LEU:HB3	1.99	0.43
45:Bx:377:PHE:CD2	79:Bx:604:HEA:HAD1	2.54	0.43
51:B3:5:LYS:CD	51:B3:6:GLY:N	2.82	0.43
56:B8:41:ARG:HD2	57:B9:40:TYR:CZ	2.54	0.43
1:A:122:PRO:HB2	1:A:322:SER:HB2	2.01	0.43
9:J:83:PRO:HA	9:J:106:LEU:O	2.18	0.43
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.43
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.43
15:P:210:LEU:HA	15:P:221:ALA:HA	2.01	0.43
17:S:31:ASN:HD21	17:S:36:LYS:HD3	1.82	0.43
25:b:105:PHE:CZ	43:v:67:LEU:CB	2.96	0.43
30:g:51:PRO:HB2	30:g:54:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:34:SER:HB2	41:s:63:PRO:HA	2.00	0.43
34:k:8:ILE:N	34:k:8:ILE:HD12	2.33	0.43
34:k:46:LEU:HD22	36:m:46:PHE:CD2	2.53	0.43
34:k:97:GLN:CD	35:l:587:TYR:HE1	2.27	0.43
36:m:33:ILE:O	36:m:37:VAL:HG23	2.19	0.43
37:n:28:ASP:OD1	40:r:2:LEU:HB3	2.19	0.43
38:o:100:PHE:CZ	38:o:104:ILE:HD11	2.53	0.43
39:p:54:GLU:OE1	39:p:54:GLU:N	2.51	0.43
40:r:87:GLU:O	40:r:92:LYS:HE3	2.18	0.43
71:r:501:PLX:H22	71:r:501:PLX:H1B3	1.57	0.43
41:s:142:TYR:CE2	41:s:289:LEU:HD11	2.54	0.43
41:s:150:LEU:O	41:s:154:LEU:HG	2.19	0.43
47:z:110:PRO:HB3	52:4:30:TRP:CD2	2.54	0.43
63:AF:34:ARG:NH1	66:AJ:379:TRP:NE1	2.60	0.43
65:AH:175:PHE:HA	65:AH:176:PRO:HD3	1.84	0.43
67:AK:65:ILE:HG21	67:AK:213:PHE:HD1	1.83	0.43
68:AL:121:ASN:HB3	68:AL:132:TYR:CZ	2.54	0.43
68:AL:240:GLN:HE22	68:AL:243:LEU:HD23	1.84	0.43
65:AU:197:LEU:HD23	65:AU:274:LEU:HD21	1.99	0.43
67:AW:108:GLY:HA2	68:AY:397:ASN:ND2	2.33	0.43
1:BA:123:GLY:CA	1:BA:355:ILE:HD11	2.48	0.43
6:BG:87:LEU:HA	6:BG:90:TYR:HB3	2.00	0.43
6:BG:116:VAL:HA	6:BG:119:ILE:HG22	2.01	0.43
8:BI:97:PRO:HG3	15:BP:61:PHE:CD1	2.52	0.43
11:BL:102:ASP:OD1	11:BL:102:ASP:N	2.50	0.43
16:BQ:39:PRO:HD2	32:Bi:304:LEU:O	2.19	0.43
16:BQ:140:ASP:CG	16:BQ:143:SER:HG	2.22	0.43
24:Ba:150:ARG:NH1	40:Br:168:HIS:HE1	2.16	0.43
26:Bc:41:TYR:CZ	26:Bc:67:ASP:HB3	2.54	0.43
33:Bj:64:LEU:HD23	33:Bj:64:LEU:HA	1.81	0.43
35:Bl:227:LEU:HA	35:Bl:230:HIS:HB3	2.00	0.43
40:Br:109:THR:HG22	40:Br:121:PHE:HB2	2.00	0.43
41:Bs:266:LEU:HD23	41:Bs:266:LEU:HA	1.73	0.43
42:Bu:121:ASP:HB3	42:Bu:124:GLU:OE2	2.18	0.43
45:Bx:131:PRO:HB2	46:By:159:VAL:HA	2.00	0.43
47:Bz:63:ARG:HA	47:Bz:67:PHE:CD2	2.53	0.43
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.43
1:A:222:LYS:HA	1:A:223:PRO:HD3	1.84	0.43
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.43
2:B:133:ARG:NH2	18:T:69:ILE:HG13	2.34	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.43
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
16:Q:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	0.43
17:S:12:MET:HE1	41:s:19:PHE:C	2.43	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
24:a:62:PHE:HB2	39:p:111:GLU:OE2	2.19	0.43
30:g:51:PRO:HG2	30:g:55:ALA:CA	2.49	0.43
31:h:58:ILE:HD12	42:u:145:ARG:NH2	2.34	0.43
35:l:81:LYS:HD3	35:l:83:ASP:OD2	2.18	0.43
35:l:587:TYR:O	35:l:590:SER:OG	2.27	0.43
36:m:43:ILE:HG22	36:m:48:GLY:HA3	2.00	0.43
39:p:56:ASP:HA	68:AY:227:PRO:CD	2.49	0.43
40:r:339:SER:HB2	40:r:344:LEU:HD12	2.00	0.43
55:7:9:PHE:CD1	55:7:9:PHE:C	2.97	0.43
62:AE:34:ARG:NH2	65:AH:216:THR:HG22	2.33	0.43
65:AH:288:MET:HE1	66:AJ:78:ILE:HD11	2.00	0.43
66:AJ:331:ASP:HA	66:AJ:334:ILE:HD12	2.00	0.43
68:AL:58:ARG:HB2	68:AL:230:VAL:HG22	2.01	0.43
68:AL:259:GLU:CG	38:Bo:30:ARG:HE	2.31	0.43
68:AL:262:VAL:HG21	39:Bp:61:THR:HG23	1.99	0.43
66:AV:206:ASN:H	82:AV:402:HEM:CGD	2.31	0.43
68:AY:88:GLY:O	68:AY:92:PHE:HB2	2.19	0.43
2:BB:61:TRP:HB2	2:BB:65:PHE:HE2	1.82	0.43
2:BB:158:GLU:O	16:BQ:368:ARG:NH2	2.52	0.43
6:BG:115:GLN:NE2	6:BG:135:ALA:HB1	2.34	0.43
9:BJ:293:LEU:HD23	9:BJ:298:TYR:HD1	1.84	0.43
14:BO:163:THR:HG22	14:BO:170:THR:HG22	2.01	0.43
16:BQ:144:MET:HA	16:BQ:147:ASN:HD22	1.84	0.43
16:BQ:369:ALA:HA	18:BT:93:ALA:HB2	1.99	0.43
16:BQ:392:PRO:HA	16:BQ:393:PRO:HD3	1.90	0.43
21:BW:110:VAL:HG11	31:Bh:71:LYS:HB2	2.01	0.43
23:BZ:65:ASP:O	23:BZ:69:LYS:HB2	2.19	0.43
24:Ba:62:PHE:HB2	39:Bp:111:GLU:OE2	2.19	0.43
25:Bb:71:VAL:O	25:Bb:75:VAL:HB	2.18	0.43
25:Bb:111:LEU:C	25:Bb:112:GLU:CD	2.85	0.43
71:Bb:201:PLX:C2	27:Bd:43:ARG:HH22	2.31	0.43
32:Bi:20:THR:O	32:Bi:23:SER:OG	2.34	0.43
32:Bi:256:PRO:HB3	40:Br:124:THR:HG22	2.01	0.43
39:Bp:30:TRP:O	39:Bp:32:VAL:HG23	2.18	0.43
40:Br:122:PHE:CE1	40:Br:238:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Br:339:SER:HB2	40:Br:344:LEU:HD12	2.00	0.43
41:Bs:18:ALA:O	41:Bs:21:MET:HG2	2.19	0.43
43:Bv:93:ARG:O	43:Bv:97:MET:HG2	2.18	0.43
44:Bw:163:ILE:HD12	44:Bw:166:ASP:OD2	2.19	0.43
45:Bx:106:PRO:HB2	45:Bx:107:PRO:HD3	2.01	0.43
45:Bx:247:ILE:HB	79:Bx:604:HEA:HBC1	2.01	0.43
50:B2:53:THR:HG22	50:B2:54:ASN:OD1	2.19	0.43
54:B6:11:LEU:HD23	54:B6:11:LEU:C	2.44	0.43
2:B:78:GLU:HG3	17:S:1:MET:SD	2.59	0.43
2:B:99:HIS:ND1	2:B:147:MET:HE1	2.34	0.43
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.43
2:B:158:GLU:O	16:Q:368:ARG:NH2	2.52	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.43
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.43
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.43
12:M:153:PHE:C	12:M:154:LEU:HD12	2.44	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.43
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	0.43
16:Q:119:GLY:H	16:Q:463:ARG:C	2.27	0.43
16:Q:199:PRO:HB3	16:Q:258:LEU:HD21	2.01	0.43
19:U:40:LYS:O	19:U:44:MET:HG2	2.18	0.43
20:V:51:GLU:HB3	20:V:55:LYS:NZ	2.33	0.43
76:W:201:PEE:H60	36:m:56:PHE:HZ	1.84	0.43
24:a:57:ILE:HA	39:p:104:LEU:HD12	2.01	0.43
35:l:67:HIS:ND1	35:l:75:GLN:HG3	2.33	0.43
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.65	0.43
42:u:67:ALA:O	42:u:70:PHE:HB3	2.19	0.43
43:v:79:ALA:C	43:v:81:LYS:H	2.26	0.43
43:v:93:ARG:O	43:v:97:MET:HG2	2.18	0.43
45:x:106:PRO:HB2	45:x:107:PRO:HD3	2.01	0.43
46:y:162:SER:HB3	46:y:197:SER:C	2.44	0.43
48:0:126:MET:HG3	48:0:128:VAL:HG23	2.00	0.43
58:AA:27:TYR:CE2	65:AH:305:THR:HG22	2.53	0.43
60:AC:145:ASP:OD1	60:AC:146:VAL:N	2.51	0.43
60:AC:159:ILE:HA	60:AC:160:PRO:HD3	1.85	0.43
62:AE:78:ARG:O	62:AE:82:VAL:HG23	2.19	0.43
65:AH:291:LYS:CD	76:AH:401:PEE:H8	2.42	0.43
67:AK:326:PHE:HB3	67:AK:337:GLY:O	2.19	0.43
68:AL:231:LEU:HD22	68:AL:250:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:350:GLU:HG2	68:AL:351:THR:HG23	2.00	0.43
76:AL:503:PEE:H25	76:AL:503:PEE:H53	2.01	0.43
5:BF:57:GLU:HB3	12:BM:662:ALA:N	2.24	0.43
7:BH:21:HIS:NE2	7:BH:63:PRO:O	2.52	0.43
12:BM:559:ASP:OD1	12:BM:560:LEU:N	2.51	0.43
13:BN:83:PRO:HA	13:BN:84:PRO:HD3	1.87	0.43
16:BQ:199:PRO:HB3	16:BQ:258:LEU:HD21	2.01	0.43
19:BU:40:LYS:O	19:BU:44:MET:HG2	2.19	0.43
30:Bg:61:LEU:O	30:Bg:65:THR:HG23	2.19	0.43
30:Bg:87:ARG:HD2	42:Bu:156:GLY:O	2.19	0.43
31:Bh:94:PRO:O	31:Bh:97:HIS:N	2.52	0.43
33:Bj:68:GLU:HG3	33:Bj:98:LEU:HD21	2.01	0.43
34:Bk:31:LEU:HA	34:Bk:31:LEU:HD23	1.75	0.43
34:Bk:97:GLN:CD	35:Bl:587:TYR:HE1	2.27	0.43
35:Bl:151:SER:HA	35:Bl:247:LEU:HD13	2.01	0.43
35:Bl:241:THR:O	35:Bl:244:SER:OG	2.32	0.43
35:Bl:434:GLN:HB3	35:Bl:435:PRO:HD2	1.99	0.43
39:Bp:104:LEU:HD22	39:Bp:122:ARG:NH2	2.34	0.43
40:Br:87:GLU:O	40:Br:92:LYS:HE3	2.18	0.43
40:Br:105:SER:O	40:Br:109:THR:HG23	2.18	0.43
44:Bw:270:VAL:O	44:Bw:275:TYR:N	2.47	0.43
46:By:52:HIS:CD2	49:B1:40:ASP:HB2	2.54	0.43
46:By:162:SER:HB3	46:By:197:SER:C	2.44	0.43
49:B1:21:LYS:HA	49:B1:22:PRO:HD2	1.84	0.43
52:B4:84:LYS:HD2	52:B4:84:LYS:HA	1.83	0.43
7:H:44:TYR:CD2	7:H:94:MET:HE2	2.54	0.42
8:I:40:LYS:HG2	21:W:8:GLN:HA	2.00	0.42
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.42
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.42
17:S:53:ARG:HB2	31:h:105:ARG:CZ	2.49	0.42
18:T:102:ASN:HD21	18:T:104:ASP:HB2	1.84	0.42
21:W:110:VAL:HG11	31:h:71:LYS:HB2	2.01	0.42
22:Y:40:ILE:HD11	35:l:446:ASN:ND2	2.34	0.42
23:Z:65:ASP:O	23:Z:69:LYS:HB2	2.19	0.42
26:c:44:THR:HB	26:c:47:GLU:CG	2.49	0.42
71:g:203:PLX:H22	71:g:203:PLX:H1B3	1.74	0.42
31:h:73:MET:HG2	36:m:124:TRP:CH2	2.54	0.42
32:i:214:THR:HG22	32:i:329:LEU:HB3	2.01	0.42
32:i:321:LYS:HA	32:i:322:PRO:HD3	1.80	0.42
35:l:511:LEU:HB3	35:l:512:LYS:H	1.58	0.42
36:m:56:PHE:CZ	41:s:111:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:6:31:LEU:HD23	54:6:31:LEU:HA	1.83	0.42
65:AH:162:GLY:C	65:AH:164:MET:H	2.26	0.42
66:AJ:156:ILE:HG21	66:AJ:160:LEU:HD13	2.00	0.42
67:AK:407:MET:HE2	67:AK:412:VAL:HA	2.01	0.42
58:AN:13:HIS:H	68:AY:279:ASP:H	1.67	0.42
65:AU:292:MET:CE	66:AV:241:THR:CG2	2.96	0.42
66:AV:149:LEU:O	66:AV:152:ALA:HB3	2.19	0.42
1:BA:257:ARG:HH12	14:BO:239:LYS:NZ	2.17	0.42
1:BA:314:LEU:O	1:BA:315:LEU:HD12	2.19	0.42
1:BA:403:ASP:HA	1:BA:453:PHE:CE2	2.54	0.42
2:BB:78:GLU:HG3	17:BS:1:MET:SD	2.59	0.42
5:BF:87:VAL:O	5:BF:91:LEU:HG	2.18	0.42
6:BG:93:ILE:HG12	6:BG:94:ASP:O	2.19	0.42
9:BJ:56:ALA:HA	9:BJ:125:VAL:HG23	2.01	0.42
9:BJ:180:TYR:O	9:BJ:184:LYS:HG3	2.19	0.42
12:BM:433:GLY:HA3	12:BM:684:LEU:HD23	2.01	0.42
12:BM:589:TYR:O	12:BM:606:THR:HG21	2.19	0.42
12:BM:711:VAL:O	12:BM:715:THR:HG23	2.19	0.42
15:BP:188:LEU:HA	16:BQ:114:GLY:HA3	2.00	0.42
16:BQ:295:GLY:HA2	16:BQ:321:GLY:HA3	2.01	0.42
17:BS:6:LEU:HD23	17:BS:6:LEU:HA	1.86	0.42
17:BS:12:MET:HE1	41:Bs:19:PHE:C	2.43	0.42
17:BS:53:ARG:HB2	31:Bh:105:ARG:CZ	2.49	0.42
24:Ba:170:TYR:CD1	30:Bg:5:ARG:HD3	2.54	0.42
27:Bd:74:GLU:HB2	30:Bg:105:LYS:HD2	2.01	0.42
31:Bh:73:MET:HG2	36:Bm:124:TRP:CH2	2.54	0.42
32:Bi:237:LEU:HB3	32:Bi:240:LEU:HB2	2.00	0.42
33:Bj:70:ALA:HA	33:Bj:73:LEU:HD13	2.01	0.42
34:Bk:7:ASN:ND2	36:Bm:9:SER:CA	2.82	0.42
35:Bl:67:HIS:ND1	35:Bl:75:GLN:HG3	2.33	0.42
37:Bn:28:ASP:OD1	40:Br:2:LEU:HB3	2.19	0.42
39:Bp:48:PHE:HE1	72:Bp:201:8Q1:C6	2.32	0.42
39:Bp:174:PRO:O	39:Bp:175:ARG:HB3	2.19	0.42
40:Br:115:LEU:O	40:Br:118:PHE:HB3	2.19	0.42
44:Bw:332:ARG:HD3	44:Bw:332:ARG:HA	1.61	0.42
46:By:98:LYS:HE3	46:By:98:LYS:HB2	1.80	0.42
48:B0:37:GLN:O	48:B0:41:LYS:HG2	2.18	0.42
48:B0:126:MET:HG3	48:B0:128:VAL:HG23	2.00	0.42
1:A:403:ASP:HA	1:A:453:PHE:CE2	2.54	0.42
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.42
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
11:L:77:VAL:HG22	11:L:78:ARG:N	2.33	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
12:M:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.42
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	0.42
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.42
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	1.91	0.42
76:V:202:PEE:H38	76:V:202:PEE:H43	1.79	0.42
32:i:256:PRO:HB3	40:r:124:THR:HG22	2.01	0.42
35:l:210:LEU:HD21	35:l:214:LEU:HD13	2.00	0.42
35:l:280:LEU:O	35:l:284:THR:HG23	2.19	0.42
36:m:27:TYR:HA	36:m:30:LEU:HD12	2.01	0.42
40:r:355:MET:HA	40:r:358:TRP:CD1	2.54	0.42
46:y:3:TYR:CD1	46:y:3:TYR:N	2.87	0.42
51:3:5:LYS:CD	51:3:6:GLY:N	2.81	0.42
54:6:3:ASN:C	54:6:3:ASN:ND2	2.77	0.42
54:6:30:ILE:HG13	54:6:31:LEU:N	2.33	0.42
56:8:41:ARG:HD2	57:9:40:TYR:CZ	2.54	0.42
67:AK:138:LEU:O	67:AK:142:THR:N	2.52	0.42
76:AL:503:PEE:H1	76:AL:503:PEE:H13	1.74	0.42
58:AN:48:ARG:HE	66:AV:319:PRO:HB3	1.84	0.42
58:AN:82:LYS:HE2	62:AR:65:GLU:HB2	2.01	0.42
60:AP:125:VAL:CG2	71:AQ:101:PLX:H141	2.49	0.42
81:AU:402:HEC:HBC3	81:AU:402:HEC:HHD	2.01	0.42
66:AV:14:ILE:HD11	76:AY:502:PEE:H41	1.80	0.42
1:BA:227:PRO:HB2	1:BA:228:PRO:HD3	2.01	0.42
1:BA:418:GLN:CD	12:BM:115:GLY:HA2	2.44	0.42
2:BB:96:ARG:HB3	2:BB:167:GLU:HG2	2.01	0.42
2:BB:117:CYS:HB2	69:BB:301:SF4:S1	2.59	0.42
2:BB:178:HIS:HB2	3:BC:179:TYR:CZ	2.53	0.42
4:BE:43:VAL:O	4:BE:47:VAL:HG23	2.19	0.42
5:BF:27:SER:HA	5:BF:28:PRO:HD3	1.93	0.42
8:BI:42:PRO:HG3	16:BQ:354:GLY:O	2.19	0.42
9:BJ:204:SER:OG	9:BJ:240:VAL:HG23	2.18	0.42
11:BL:79:ILE:HD12	11:BL:145:TYR:CD2	2.54	0.42
14:BO:46:GLU:C	14:BO:49:PRO:HD3	2.44	0.42
24:Ba:112:TYR:CD1	27:Bd:58:TYR:O	2.72	0.42
30:Bg:15:ASP:OD1	30:Bg:16:GLU:N	2.52	0.42
30:Bg:51:PRO:HG2	30:Bg:55:ALA:CA	2.49	0.42
32:Bi:234:TRP:HH2	32:Bi:305:LEU:HB2	1.83	0.42
34:Bk:10:LEU:CD1	36:Bm:102:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Bm:27:TYR:HA	36:Bm:30:LEU:HD12	2.01	0.42
39:Bp:48:PHE:CZ	72:Bp:201:8Q1:C8	2.99	0.42
1:A:159:ARG:HD3	1:A:162:PHE:CE2	2.55	0.42
2:B:175:THR:HB	2:B:180:GLU:OE1	2.19	0.42
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.42
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.42
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.42
9:J:179:ARG:HB3	9:J:179:ARG:HH11	1.84	0.42
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.42
11:L:79:ILE:HD12	11:L:145:TYR:CD2	2.54	0.42
14:O:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
15:P:188:LEU:HA	16:Q:114:GLY:HA3	2.00	0.42
22:Y:81:LEU:HD12	43:v:88:ASP:CB	2.45	0.42
24:a:112:TYR:CD1	27:d:58:TYR:O	2.72	0.42
27:d:74:GLU:HB2	30:g:105:LYS:HD2	2.01	0.42
30:g:46:LEU:CD1	32:i:239:TRP:HB3	2.49	0.42
71:g:202:PLX:H101	71:g:202:PLX:H132	1.44	0.42
32:i:2:ASN:HA	32:i:3:PRO:HD2	1.86	0.42
75:l:703:CDL:HA61	75:l:703:CDL:H1	2.02	0.42
36:m:40:CYS:O	36:m:44:LEU:HG	2.20	0.42
36:m:86:VAL:O	36:m:90:VAL:HG23	2.19	0.42
39:p:49:GLU:O	39:p:52:LYS:HG2	2.19	0.42
39:p:90:SER:HB2	39:p:93:ARG:HE	1.84	0.42
41:s:18:ALA:O	41:s:21:MET:HG2	2.19	0.42
41:s:154:LEU:HD23	41:s:154:LEU:HA	1.73	0.42
60:AC:246:SER:OG	60:AC:248:ARG:NE	2.47	0.42
63:AF:110:LYS:HG3	63:AF:111:LYS:HG3	2.02	0.42
67:AK:178:HIS:HE1	67:AK:330:TYR:HE2	1.66	0.42
67:AK:195:TYR:CE2	67:AK:196:ARG:HG2	2.54	0.42
67:AK:260:GLU:OE1	67:AK:441:SER:OG	2.31	0.42
68:AL:233:ALA:HB3	68:AL:242:LEU:HD22	2.01	0.42
76:AL:503:PEE:C33	76:AL:503:PEE:C17	2.97	0.42
61:AQ:18:THR:HG22	68:AY:480:PHE:OXT	2.19	0.42
62:AR:34:ARG:NH1	62:AR:78:ARG:NH2	2.63	0.42
75:AU:403:CDL:H112	66:AV:234:LEU:HD12	2.00	0.42
66:AV:156:ILE:HG22	66:AV:160:LEU:HB2	2.01	0.42
1:BA:220:GLN:NE2	14:BO:114:GLU:HB3	2.34	0.42
2:BB:99:HIS:ND1	2:BB:147:MET:HE1	2.34	0.42
2:BB:166:VAL:HG11	2:BB:199:ILE:CG2	2.49	0.42
3:BC:163:SER:HB3	16:BQ:123:LEU:HD11	2.00	0.42
3:BC:175:PRO:HB3	9:BJ:96:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:187:ALA:O	3:BC:190:LEU:HB3	2.20	0.42
7:BH:83:GLN:HG2	15:BP:107:GLN:HE21	1.84	0.42
9:BJ:168:SER:O	9:BJ:203:PRO:HD2	2.18	0.42
12:BM:341:ILE:HD13	12:BM:367:CYS:SG	2.59	0.42
14:BO:164:THR:HG23	14:BO:167:LYS:N	2.34	0.42
15:BP:200:LYS:HE2	16:BQ:420:TYR:CE1	2.55	0.42
15:BP:202:PHE:HB2	15:BP:207:TYR:CE2	2.55	0.42
16:BQ:267:ILE:HB	41:Bs:278:PRO:HG2	2.01	0.42
17:BS:43:TYR:CE2	21:BW:68:ARG:HD2	2.53	0.42
30:Bg:27:ASP:O	30:Bg:31:LEU:HG	2.19	0.42
32:Bi:214:THR:HG22	32:Bi:329:LEU:HB3	2.01	0.42
33:Bj:51:PHE:CG	33:Bj:52:SER:N	2.88	0.42
35:Bl:149:ILE:HD12	40:Br:369:LEU:HD11	2.01	0.42
36:Bm:106:VAL:HG11	36:Bm:117:ASN:ND2	2.34	0.42
39:Bp:90:SER:HB2	39:Bp:93:ARG:HE	1.84	0.42
47:Bz:19:THR:HG22	47:Bz:53:THR:OG1	2.18	0.42
1:A:369:ARG:HH22	14:O:175:GLU:CD	2.25	0.42
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.42
5:F:62:GLN:HE21	5:F:64:LYS:NZ	2.17	0.42
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
16:Q:70:ASP:HB2	16:Q:71:PRO:HD3	2.02	0.42
20:V:133:TRP:CG	76:V:202:PEE:H7	2.54	0.42
22:Y:74:TRP:CZ3	22:Y:75:HIS:HA	2.53	0.42
25:b:119:PRO:HB2	43:v:40:VAL:HG13	2.01	0.42
26:c:73:GLY:C	26:c:75:TYR:H	2.28	0.42
30:g:87:ARG:HD2	42:u:156:GLY:O	2.19	0.42
31:h:74:ARG:HG2	36:m:116:VAL:HG13	2.02	0.42
32:i:2:ASN:ND2	32:i:4:LEU:HB2	2.35	0.42
32:i:69:ILE:HD12	32:i:104:MET:HE1	2.01	0.42
32:i:76:PHE:CZ	32:i:80:LEU:HD11	2.54	0.42
33:j:51:PHE:CG	33:j:52:SER:N	2.88	0.42
35:l:217:LEU:O	35:l:217:LEU:HD23	2.19	0.42
36:m:32:LEU:HA	36:m:32:LEU:HD23	1.77	0.42
36:m:33:ILE:HD11	41:s:114:TYR:CE1	2.55	0.42
41:s:215:TYR:HD1	41:s:219:PRO:HB2	1.83	0.42
46:y:63:THR:HA	46:y:66:THR:HG22	2.00	0.42
49:1:21:LYS:O	49:1:57:ARG:NH1	2.53	0.42
49:1:93:LEU:HD23	49:1:93:LEU:HA	1.88	0.42
50:2:86:GLY:O	50:2:87:THR:O	2.37	0.42
63:AF:34:ARG:HD2	66:AJ:377:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:131:ALA:HB3	65:AH:133:ARG:HG2	2.00	0.42
66:AJ:214:HIS:ND1	66:AJ:217:LYS:NZ	2.68	0.42
66:AJ:312:GLN:HG3	66:AJ:379:TRP:HH2	1.84	0.42
71:AN:101:PLX:H141	71:AN:101:PLX:H332	2.01	0.42
63:AS:36:ASP:OD1	63:AS:90:TYR:OH	2.37	0.42
65:AU:292:MET:CE	66:AV:241:THR:HG22	2.49	0.42
75:AU:403:CDL:OA6	66:AV:230:LEU:HD23	2.19	0.42
75:AU:403:CDL:H742	75:AU:403:CDL:H711	1.77	0.42
68:AY:58:ARG:HH11	68:AY:230:VAL:HG22	1.85	0.42
68:AY:71:VAL:HG22	68:AY:233:ALA:HB2	2.02	0.42
1:BA:262:PHE:CZ	1:BA:272:GLY:HA3	2.54	0.42
4:BE:53:ASP:HA	9:BJ:366:ILE:HD11	2.00	0.42
7:BH:44:TYR:CD2	7:BH:94:MET:HE2	2.54	0.42
12:BM:153:PHE:C	12:BM:154:LEU:HD12	2.44	0.42
12:BM:510:TRP:HD1	12:BM:512:VAL:HG22	1.82	0.42
13:BN:66:THR:HG23	13:BN:74:PHE:H	1.85	0.42
14:BO:236:GLU:HB3	14:BO:238:PRO:HD2	2.00	0.42
71:BV:203:PLX:H141	71:BV:203:PLX:H332	2.01	0.42
76:BW:201:PEE:H36	33:Bj:7:LEU:CD2	2.47	0.42
22:BY:40:ILE:HD11	35:Bl:446:ASN:ND2	2.34	0.42
26:Bc:81:ARG:HD3	26:Bc:85:GLU:OE1	2.20	0.42
30:Bg:32:TYR:CE2	32:Bi:339:ILE:HD11	2.54	0.42
30:Bg:51:PRO:HB2	30:Bg:54:THR:OG1	2.19	0.42
31:Bh:82:GLN:HA	31:Bh:85:LYS:HE3	1.99	0.42
33:Bj:30:TYR:HB2	33:Bj:33:LYS:CD	2.47	0.42
40:Br:10:MET:O	40:Br:13:PRO:HD2	2.20	0.42
40:Br:45:ILE:HG22	40:Br:45:ILE:O	2.19	0.42
40:Br:179:LEU:O	40:Br:248:LEU:HD13	2.19	0.42
41:Bs:86:TRP:HH2	41:Bs:232:ILE:HG22	1.85	0.42
43:Bv:79:ALA:C	43:Bv:81:LYS:H	2.26	0.42
46:By:122:MET:HB2	46:By:208:PRO:CD	2.47	0.42
55:B7:9:PHE:CD1	55:B7:9:PHE:C	2.97	0.42
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.42
1:A:184:LYS:C	1:A:186:ALA:H	2.27	0.42
2:B:96:ARG:HB3	2:B:167:GLU:HG2	2.01	0.42
2:B:117:CYS:HB2	69:B:301:SF4:S1	2.60	0.42
3:C:213:ARG:O	3:C:213:ARG:HG2	2.20	0.42
11:L:130:THR:O	11:L:133:ASP:HB3	2.19	0.42
12:M:342:ALA:O	12:M:369:GLU:HG2	2.19	0.42
12:M:542:PRO:HB2	12:M:543:LYS:HD3	2.01	0.42
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:46:GLU:C	14:O:49:PRO:HD3	2.44	0.42
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.42
18:T:83:ARG:HH12	18:T:103:LEU:H	1.68	0.42
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.52	0.42
24:a:66:ARG:O	24:a:70:LEU:HG	2.19	0.42
24:a:150:ARG:NH1	40:r:168:HIS:HE1	2.16	0.42
39:p:173:ARG:HA	39:p:174:PRO:HD3	1.83	0.42
40:r:10:MET:O	40:r:13:PRO:HD2	2.20	0.42
40:r:115:LEU:O	40:r:118:PHE:HB3	2.19	0.42
40:r:122:PHE:CE1	40:r:238:LEU:HD21	2.54	0.42
71:r:502:PLX:H1B2	71:r:502:PLX:H22	1.53	0.42
44:w:163:ILE:HD12	44:w:166:ASP:OD2	2.19	0.42
49:l:27:TRP:CH2	50:2:86:GLY:HA2	2.54	0.42
53:5:35:TYR:O	53:5:39:VAL:HB	2.19	0.42
54:6:11:LEU:HD23	54:6:11:LEU:C	2.44	0.42
58:AA:3:ARG:HH12	66:AJ:217:LYS:CE	2.32	0.42
60:AC:200:HIS:HE1	60:AC:202:LEU:HB3	1.84	0.42
62:AE:34:ARG:HE	62:AE:34:ARG:HB2	1.62	0.42
66:AJ:8:ASN:OD1	66:AJ:9:PRO:HD2	2.19	0.42
68:AL:87:ASN:HD21	68:AL:199:GLN:HB2	1.85	0.42
60:AP:80:HIS:CD2	60:AP:81:THR:HG23	2.54	0.42
67:AW:346:ALA:O	67:AW:350:VAL:HG23	2.19	0.42
67:AW:379:LYS:HG2	67:AW:413:LEU:HG	2.00	0.42
67:AW:443:ASN:OD1	67:AW:445:GLY:N	2.43	0.42
6:BG:103:HIS:N	6:BG:107:ASP:HB2	2.35	0.42
9:BJ:50:SER:O	9:BJ:77:GLY:HA3	2.20	0.42
9:BJ:329:LEU:HD22	9:BJ:332:LEU:HD12	2.01	0.42
11:BL:130:THR:O	11:BL:133:ASP:HB3	2.19	0.42
12:BM:153:PHE:O	12:BM:154:LEU:HD12	2.19	0.42
14:BO:213:ILE:HG22	14:BO:214:PRO:O	2.20	0.42
15:BP:171:TRP:CZ3	15:BP:177:PHE:HA	2.54	0.42
16:BQ:70:ASP:HB2	16:BQ:71:PRO:HD3	2.02	0.42
16:BQ:167:ALA:O	16:BQ:171:ARG:HG3	2.19	0.42
6:BX:155:TYR:O	6:BX:155:TYR:CD2	2.73	0.42
26:Bc:100:ASN:HB2	26:Bc:103:GLU:HG3	2.02	0.42
27:Bd:60:ARG:NH1	27:Bd:60:ARG:CG	2.73	0.42
32:Bi:197:ASN:HD22	32:Bi:269:GLU:CD	2.27	0.42
35:Bl:93:ALA:O	35:Bl:97:THR:OG1	2.38	0.42
36:Bm:33:ILE:HD11	41:Bs:114:TYR:CE1	2.55	0.42
42:Bu:104:GLN:HB3	42:Bu:108:ASP:OD2	2.20	0.42
47:Bz:80:ARG:HG2	47:Bz:233:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B0:127:LYS:O	48:B0:130:PRO:HD3	2.20	0.42
49:B1:76:GLY:HA3	49:B1:77:PRO:HD2	1.85	0.42
53:B5:35:TYR:O	53:B5:39:VAL:HB	2.19	0.42
2:B:81:THR:HG23	41:s:35:LYS:H	1.83	0.42
3:C:150:MET:SD	3:C:190:LEU:HD13	2.60	0.42
9:J:283:VAL:HG13	9:J:369:VAL:HG11	2.02	0.42
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.42
15:P:171:TRP:CZ3	15:P:177:PHE:HA	2.54	0.42
16:Q:116:LEU:O	16:Q:118:ARG:HG3	2.19	0.42
16:Q:150:ALA:CB	16:Q:400:ILE:HG13	2.49	0.42
16:Q:236:LEU:HA	16:Q:237:PRO:HD3	1.93	0.42
16:Q:267:ILE:HB	41:s:278:PRO:HG2	2.02	0.42
16:Q:338:ARG:O	16:Q:341:LEU:HB2	2.19	0.42
19:U:69:HIS:CE1	19:U:70:PRO:HA	2.54	0.42
20:V:2:ALA:O	20:V:6:PHE:N	2.45	0.42
25:b:51:LEU:HD22	25:b:59:LYS:HA	2.01	0.42
26:c:81:ARG:HD3	26:c:85:GLU:OE1	2.20	0.42
26:c:154:GLN:C	26:c:156:VAL:HG23	2.44	0.42
27:d:143:TYR:OH	40:r:244:MET:O	2.33	0.42
28:e:54:PRO:O	28:e:56:GLN:HG3	2.18	0.42
31:h:56:CYS:HA	42:u:145:ARG:HH12	1.84	0.42
32:i:109:ALA:CB	32:i:112:HIS:HD2	2.33	0.42
32:i:237:LEU:HB3	32:i:240:LEU:HB2	2.00	0.42
33:j:49:VAL:CG1	36:m:75:ILE:H	2.32	0.42
33:j:70:ALA:HA	33:j:73:LEU:HD13	2.01	0.42
35:l:149:ILE:HD12	40:r:369:LEU:HD11	2.01	0.42
35:l:226:GLN:HG2	35:l:280:LEU:HD22	2.00	0.42
46:y:146:MET:SD	46:y:189:PRO:HB3	2.60	0.42
53:5:21:ILE:O	53:5:25:PHE:HD2	2.02	0.42
60:AC:176:VAL:HG22	60:AC:212:ILE:HG12	2.02	0.42
60:AC:181:GLN:HA	60:AC:184:ILE:HD12	2.01	0.42
61:AD:39:GLY:O	61:AD:43:ILE:HG12	2.19	0.42
66:AJ:163:TRP:CG	75:AJ:405:CDL:H331	2.55	0.42
66:AJ:300:ILE:H	66:AJ:300:ILE:HG13	1.57	0.42
66:AJ:316:MET:HB3	76:AJ:403:PEE:O2P	2.20	0.42
67:AK:82:LEU:O	67:AK:86:THR:HG23	2.20	0.42
68:AL:54:ASP:O	39:Bp:55:LYS:CG	2.68	0.42
60:AP:100:THR:HG23	68:AY:266:THR:HG21	2.01	0.42
67:AW:155:GLN:N	67:AW:156:PRO:HD2	2.35	0.42
68:AY:295:GLY:HA2	68:AY:351:THR:O	2.19	0.42
68:AY:392:LYS:O	68:AY:396:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:160:CYS:HA	2:BB:161:PRO:HD2	1.83	0.42
3:BC:213:ARG:O	3:BC:213:ARG:HG2	2.20	0.42
5:BF:62:GLN:HE21	5:BF:64:LYS:NZ	2.17	0.42
7:BH:47:TYR:OH	8:BI:92:LYS:HG3	2.20	0.42
9:BJ:336:GLU:C	9:BJ:339:GLY:H	2.28	0.42
11:BL:86:ASN:ND2	12:BM:224:ASP:OD2	2.53	0.42
12:BM:560:LEU:HA	12:BM:561:PRO:HD2	1.91	0.42
12:BM:573:GLY:HA3	13:BN:137:TRP:CD1	2.54	0.42
13:BN:73:THR:HG22	13:BN:74:PHE:N	2.34	0.42
15:BP:129:VAL:HG22	15:BP:144:LYS:HB3	2.01	0.42
16:BQ:235:ASP:HA	16:BQ:356:ILE:HD12	2.02	0.42
16:BQ:275:ILE:HD13	16:BQ:446:ASP:OD1	2.20	0.42
16:BQ:371:MET:HE1	16:BQ:381:HIS:CE1	2.55	0.42
19:BU:69:HIS:CE1	19:BU:70:PRO:HA	2.54	0.42
20:BV:95:CYS:O	20:BV:99:LEU:HG	2.19	0.42
76:BW:201:PEE:H53	76:BW:201:PEE:C16	2.46	0.42
6:BX:131:PRO:HG3	26:Bc:89:TRP:CE3	2.55	0.42
6:BX:138:LEU:CD2	6:BX:144:ILE:HG12	2.47	0.42
22:BY:74:TRP:C	22:BY:74:TRP:CD2	2.97	0.42
22:BY:95:GLU:CD	22:BY:95:GLU:N	2.77	0.42
26:Bc:133:LEU:HD13	35:Bl:532:ILE:HD12	2.00	0.42
27:Bd:24:ILE:HD11	35:Bl:56:CYS:HB3	2.02	0.42
35:Bl:222:GLY:HA2	35:Bl:229:LEU:CD1	2.43	0.42
35:Bl:310:LEU:HD23	35:Bl:313:MET:HE3	2.01	0.42
36:Bm:86:VAL:O	36:Bm:90:VAL:HG23	2.19	0.42
40:Br:345:SER:O	40:Br:348:LEU:HG	2.18	0.42
42:Bu:67:ALA:O	42:Bu:70:PHE:HB3	2.19	0.42
43:Bv:5:LEU:HG	43:Bv:6:VAL:N	2.34	0.42
43:Bv:62:HIS:CD2	43:Bv:90:CYS:HG	2.37	0.42
50:B2:86:GLY:O	50:B2:87:THR:O	2.37	0.42
51:B3:77:PRO:HA	51:B3:82:TYR:HA	2.01	0.42
52:B4:24:ASN:HD22	52:B4:25:GLN:N	2.18	0.42
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.01	0.42
4:E:102:HIS:HA	4:E:105:ARG:HG3	2.02	0.42
9:J:56:ALA:HA	9:J:125:VAL:HG23	2.01	0.42
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.42
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.42
9:J:128:ASN:O	9:J:129:LEU:HD12	2.20	0.42
9:J:131:GLY:HA3	73:J:401:NDP:O3D	2.19	0.42
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.42
16:Q:39:PRO:HD2	32:i:304:LEU:O	2.19	0.42
16:Q:341:LEU:HD23	16:Q:341:LEU:HA	1.88	0.42
16:Q:368:ARG:HA	16:Q:371:MET:HG2	2.01	0.42
22:Y:95:GLU:CD	22:Y:95:GLU:N	2.77	0.42
71:b:201:PLX:C10	71:b:201:PLX:C6	2.86	0.42
26:c:94:GLN:OE1	26:c:99:LEU:HB2	2.20	0.42
26:c:101:TRP:CD1	38:o:62:ASN:HD22	2.38	0.42
26:c:159:LYS:HA	43:v:98:ARG:CZ	2.50	0.42
33:j:12:LEU:O	33:j:16:LEU:HB2	2.20	0.42
76:l:701:PEE:H51	76:l:701:PEE:H56	1.56	0.42
41:s:11:VAL:N	41:s:12:PRO:HD2	2.34	0.42
41:s:155:LEU:HD23	41:s:155:LEU:HA	1.81	0.42
44:w:143:TYR:OH	44:w:162:SER:HB2	2.20	0.42
45:x:462:LEU:O	45:x:466:MET:HG3	2.20	0.42
47:z:40:MET:O	47:z:41:THR:C	2.62	0.42
51:3:77:PRO:HA	51:3:82:TYR:HA	2.01	0.42
63:AF:99:ILE:O	63:AF:103:LYS:HG2	2.19	0.42
66:AJ:111:GLU:O	66:AJ:115:ILE:HG12	2.20	0.42
66:AJ:147:THR:HG22	66:AJ:161:VAL:HG13	2.02	0.42
68:AL:407:THR:HB	68:AL:408:PRO:HD3	2.02	0.42
75:AL:502:CDL:C77	76:AL:503:PEE:H70	2.47	0.42
66:AV:177:ARG:O	66:AV:180:THR:OG1	2.36	0.42
67:AW:214:THR:HG21	67:AW:244:LEU:N	2.34	0.42
68:AY:284:PHE:C	68:AY:461:PRO:HD2	2.45	0.42
1:BA:413:TRP:HZ3	1:BA:436:GLN:HB3	1.84	0.42
9:BJ:240:VAL:HG22	9:BJ:266:VAL:C	2.45	0.42
9:BJ:271:TYR:HE1	9:BJ:374:THR:HB	1.85	0.42
12:BM:254:MET:CB	12:BM:290:THR:HG22	2.46	0.42
12:BM:560:LEU:HD12	12:BM:561:PRO:HD2	2.02	0.42
13:BN:10:GLY:O	13:BN:14:ILE:HG13	2.20	0.42
14:BO:108:PRO:HA	14:BO:109:PRO:HD3	1.78	0.42
14:BO:143:ARG:CB	14:BO:184:PRO:HD3	2.47	0.42
14:BO:176:CYS:HA	74:BO:301:FES:S1	2.60	0.42
16:BQ:410:TYR:O	16:BQ:422:CYS:HA	2.19	0.42
18:BT:52:ARG:O	18:BT:55:ARG:HG2	2.20	0.42
20:BV:126:LYS:HE3	20:BV:130:LEU:HD11	2.02	0.42
22:BY:55:VAL:O	22:BY:58:SER:OG	2.33	0.42
23:BZ:18:ASP:OD1	23:BZ:19:TYR:N	2.52	0.42
32:Bi:26:TRP:HD1	32:Bi:84:TRP:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Bj:12:LEU:O	33:Bj:16:LEU:HB2	2.20	0.42
35:Bl:210:LEU:HD21	35:Bl:214:LEU:HD13	2.01	0.42
75:Bl:703:CDL:H1	75:Bl:703:CDL:HA61	2.02	0.42
36:Bm:5:LEU:HD23	36:Bm:8:LEU:HD12	2.02	0.42
39:Bp:145:PRO:HA	39:Bp:146:PRO:HD3	1.84	0.42
45:Bx:462:LEU:O	45:Bx:466:MET:HG3	2.20	0.42
45:Bx:468:MET:HE2	45:Bx:468:MET:HB3	1.90	0.42
46:By:3:TYR:CD1	46:By:3:TYR:N	2.87	0.42
47:Bz:110:PRO:HB3	52:B4:30:TRP:CD2	2.54	0.42
1:A:453:PHE:O	1:A:456:GLN:HG2	2.20	0.42
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.42
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.42
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.42
12:M:405:THR:OG1	12:M:479:SER:OG	2.28	0.42
12:M:436:VAL:HG21	12:M:686:PRO:HG2	2.02	0.42
12:M:543:LYS:N	12:M:543:LYS:HD2	2.35	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.42
13:N:10:GLY:O	13:N:14:ILE:HG13	2.20	0.42
15:P:48:ARG:HA	15:P:49:PRO:HD3	1.94	0.42
15:P:240:GLU:OE1	15:P:246:ARG:NE	2.51	0.42
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.54	0.42
20:V:23:TYR:O	20:V:24:SER:HB2	2.20	0.42
22:Y:55:VAL:O	22:Y:58:SER:OG	2.33	0.42
24:a:101:ILE:HG13	27:d:58:TYR:CB	2.49	0.42
25:b:117:ILE:HG23	25:b:118:PRO:HD2	2.01	0.42
71:b:201:PLX:H171	71:b:201:PLX:H141	1.69	0.42
26:c:125:SER:O	26:c:129:MET:HG3	2.20	0.42
30:g:82:TYR:OH	32:i:341:PRO:O	2.35	0.42
31:h:80:ARG:NH1	36:m:1:MET:SD	2.89	0.42
32:i:19:ILE:HD12	32:i:35:MET:HE1	2.02	0.42
35:l:37:LYS:HE3	35:l:102:GLU:CG	2.37	0.42
35:l:536:THR:OG1	35:l:537:ILE:N	2.53	0.42
71:r:501:PLX:H101	71:r:501:PLX:H132	1.59	0.42
41:s:59:GLU:OE1	41:s:59:GLU:N	2.52	0.42
41:s:314:ILE:HA	41:s:315:PRO:HD3	1.82	0.42
42:u:104:GLN:HB3	42:u:108:ASP:OD2	2.20	0.42
43:v:59:CYS:O	43:v:87:TRP:HZ3	2.03	0.42
79:x:603:HEA:HHC	79:x:603:HEA:H122	2.02	0.42
52:4:24:ASN:HD22	52:4:25:GLN:N	2.18	0.42
58:AA:78:TYR:CD1	62:AE:65:GLU:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AJ:9:PRO:HG2	66:AV:199:PHE:CE1	2.55	0.42
67:AK:81:HIS:CD2	67:AK:158:LEU:HD22	2.55	0.42
67:AK:355:TYR:CE2	67:AK:359:LYS:HD2	2.54	0.42
58:AN:11:MET:SD	63:AS:64:LYS:HD2	2.60	0.42
67:AW:51:SER:HB2	67:AW:230:LEU:HD12	2.02	0.42
67:AW:271:PHE:CZ	67:AW:338:ILE:HB	2.55	0.42
1:BA:159:ARG:HD3	1:BA:162:PHE:CE2	2.55	0.42
1:BA:329:LYS:HA	1:BA:332:CYS:HB3	2.02	0.42
2:BB:133:ARG:NH2	18:BT:69:ILE:HG13	2.34	0.42
4:BE:126:HIS:HD2	12:BM:612:PRO:HD2	1.84	0.42
7:BH:81:ILE:HG13	7:BH:82:LEU:N	2.34	0.42
9:BJ:167:VAL:HG22	9:BJ:201:VAL:HB	2.00	0.42
9:BJ:179:ARG:HB3	9:BJ:179:ARG:HH11	1.84	0.42
12:BM:492:ALA:O	12:BM:496:ILE:HG13	2.19	0.42
17:BS:53:ARG:CZ	31:Bh:105:ARG:NH2	2.83	0.42
20:BV:23:TYR:O	20:BV:24:SER:HB2	2.20	0.42
20:BV:133:TRP:CG	76:BV:202:PEE:H7	2.54	0.42
25:Bb:117:ILE:HG23	25:Bb:118:PRO:HD2	2.01	0.42
26:Bc:44:THR:HB	26:Bc:47:GLU:CG	2.49	0.42
28:Be:62:GLU:OE2	38:Bo:57:ARG:NH2	2.53	0.42
32:Bi:179:LEU:HD23	32:Bi:179:LEU:HA	1.81	0.42
33:Bj:49:VAL:CG1	36:Bm:75:ILE:H	2.32	0.42
35:Bl:174:TYR:OH	35:Bl:534:HIS:HE1	2.03	0.42
35:Bl:511:LEU:HB3	35:Bl:512:LYS:H	1.57	0.42
40:Br:248:LEU:HD12	40:Br:249:ILE:N	2.35	0.42
44:Bw:143:TYR:OH	44:Bw:162:SER:HB2	2.20	0.42
45:Bx:501:PRO:O	45:Bx:502:TYR:C	2.63	0.42
79:Bx:603:HEA:HHC	79:Bx:603:HEA:H122	2.02	0.42
49:B1:21:LYS:O	49:B1:57:ARG:NH1	2.53	0.42
50:B2:82:CYS:HA	50:B2:83:PRO:HD3	1.90	0.42
52:B4:20:PHE:N	52:B4:21:PRO:HD3	2.35	0.42
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	0.42
70:A:502:FMN:H9	70:A:502:FMN:H1'2	1.76	0.42
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.42
3:C:156:GLY:O	3:C:161:HIS:ND1	2.52	0.42
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.19	0.42
12:M:646:LEU:HD13	12:M:653:LEU:HB3	2.00	0.42
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	0.42
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.42
15:P:97:LEU:HD11	15:P:130:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:202:PHE:HB2	15:P:207:TYR:CE2	2.55	0.42
18:T:79:GLU:OE1	18:T:122:HIS:HB3	2.19	0.42
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.42
22:Y:74:TRP:C	22:Y:74:TRP:CD2	2.97	0.42
22:Y:89:PRO:O	43:v:107:ARG:NH1	2.49	0.42
24:a:53:ARG:HH21	25:b:28:LEU:CD1	2.33	0.42
26:c:100:ASN:HB2	26:c:103:GLU:HG3	2.02	0.42
26:c:119:THR:HB	38:o:13:THR:HG23	2.02	0.42
26:c:183:HIS:CB	43:v:37:ARG:HA	2.50	0.42
30:g:37:GLY:O	30:g:40:SER:OG	2.28	0.42
34:k:3:LEU:HD22	36:m:117:ASN:ND2	2.30	0.42
34:k:10:LEU:CD1	36:m:102:LEU:HD12	2.49	0.42
34:k:97:GLN:N	35:l:579:THR:OG1	2.40	0.42
35:l:122:LEU:HD23	35:l:122:LEU:HA	1.85	0.42
35:l:548:LEU:HD22	38:o:93:CYS:HB3	2.01	0.42
37:n:16:LEU:HD21	40:r:10:MET:HE3	2.02	0.42
37:n:51:PRO:O	37:n:53:GLU:HG3	2.20	0.42
40:r:308:SER:HB3	40:r:384:THR:HG21	2.01	0.42
46:y:193:TYR:N	46:y:193:TYR:CD1	2.88	0.42
48:0:102:TYR:HD2	57:9:35:TYR:HE1	1.68	0.42
60:AC:266:THR:OG1	60:AC:267:SER:N	2.53	0.42
65:AU:266:ILE:O	65:AU:270:VAL:HG23	2.20	0.42
66:AV:271:GLU:HG3	66:AV:273:TYR:CZ	2.55	0.42
66:AV:333:LEU:HD11	76:AV:403:PEE:H62	2.02	0.42
67:AW:82:LEU:O	67:AW:86:THR:HG23	2.19	0.42
68:AY:407:THR:HB	68:AY:408:PRO:HD3	2.01	0.42
1:BA:73:PRO:HB2	1:BA:74:ASP:H	1.58	0.42
4:BE:78:VAL:O	4:BE:82:LEU:HD13	2.20	0.42
9:BJ:263:PHE:CE1	9:BJ:333:PRO:HG2	2.55	0.42
10:BK:101:SER:OG	10:BK:102:GLY:N	2.53	0.42
12:BM:33:GLU:O	12:BM:98:LYS:HA	2.20	0.42
12:BM:715:THR:OG1	12:BM:716:GLU:N	2.53	0.42
16:BQ:116:LEU:HD11	16:BQ:141:TYR:OH	2.20	0.42
16:BQ:371:MET:HA	16:BQ:377:SER:OG	2.20	0.42
18:BT:47:ASP:N	18:BT:50:ASP:OD2	2.47	0.42
21:BW:57:ARG:NH2	41:Bs:316:PRO:HG3	2.35	0.42
22:BY:58:SER:HB2	35:Bl:371:THR:HG21	2.01	0.42
26:Bc:154:GLN:C	26:Bc:156:VAL:HG23	2.44	0.42
28:Be:87:MET:HB3	28:Be:87:MET:HE3	1.78	0.42
31:Bh:56:CYS:HA	42:Bu:145:ARG:HH12	1.84	0.42
31:Bh:58:ILE:HD12	42:Bu:145:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Bi:79:MET:HE3	34:Bk:5:TYR:CD2	2.55	0.42
35:Bl:122:LEU:HA	35:Bl:122:LEU:HD23	1.85	0.42
37:Bn:16:LEU:HD21	40:Br:10:MET:HE3	2.02	0.42
40:Br:170:THR:OG1	40:Br:171:LEU:N	2.53	0.42
40:Br:326:LEU:HA	40:Br:326:LEU:HD23	1.85	0.42
44:Bw:340:SER:HA	44:Bw:341:PRO:HD3	1.91	0.42
45:Bx:240:HIS:NE2	45:Bx:244:TYR:CE2	2.81	0.42
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.42
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.42
3:C:78:SER:O	41:s:54:LYS:NZ	2.51	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.19	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
11:L:170:THR:HG22	12:M:423:LEU:O	2.18	0.42
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.42
15:P:148:ASP:HB2	15:P:151:THR:HG23	2.02	0.42
18:T:96:HIS:NE2	18:T:115:CYS:SG	2.90	0.42
24:a:109:HIS:O	24:a:112:TYR:HD2	2.03	0.42
27:d:134:GLN:OE1	38:o:124:THR:HA	2.20	0.42
32:i:120:GLN:HA	32:i:176:ARG:HE	1.85	0.42
32:i:287:LEU:HD11	40:r:158:LEU:HD12	2.02	0.42
32:i:307:MET:O	44:w:319:ILE:HD12	2.20	0.42
33:j:92:LEU:HD23	33:j:92:LEU:HA	1.89	0.42
35:l:414:ILE:O	35:l:417:SER:OG	2.29	0.42
36:m:114:VAL:O	36:m:115:VAL:HG22	2.20	0.42
39:p:55:LYS:HG3	68:AY:55:ASN:HA	2.01	0.42
40:r:344:LEU:O	40:r:420:THR:HG21	2.20	0.42
47:z:80:ARG:HG2	47:z:233:PHE:CE1	2.54	0.42
47:z:146:TRP:NE1	51:3:17:ARG:HB2	2.35	0.42
57:9:19:LEU:HD23	57:9:19:LEU:C	2.45	0.42
61:AD:30:MET:SD	64:AG:34:TRP:HB2	2.60	0.42
63:AF:39:TYR:CE2	66:AJ:108:LEU:HD13	2.55	0.42
63:AF:63:ILE:HD13	66:AJ:211:ILE:CG2	2.50	0.42
76:AH:401:PEE:H61	66:AJ:236:LEU:HD13	2.01	0.42
66:AJ:9:PRO:HB3	66:AV:202:GLU:OE1	2.20	0.42
67:AK:347:ALA:O	67:AK:351:ILE:HG12	2.20	0.42
68:AL:51:SER:HB2	68:AL:59:VAL:HB	2.01	0.42
67:AW:43:LEU:HD13	67:AW:238:LEU:HD11	2.01	0.42
1:BA:63:TYR:CD2	1:BA:64:LYS:HG3	2.55	0.42
1:BA:113:LEU:HD23	1:BA:114:VAL:N	2.35	0.42
2:BB:184:ASN:ND2	13:BN:126:PRO:HA	2.35	0.42
3:BC:156:GLY:O	3:BC:161:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:102:HIS:HA	4:BE:105:ARG:HG3	2.02	0.42
8:BI:60:ARG:HD2	16:BQ:390:GLN:O	2.19	0.42
9:BJ:128:ASN:O	9:BJ:129:LEU:HD12	2.20	0.42
9:BJ:152:ILE:HG22	9:BJ:164:PHE:CE1	2.55	0.42
9:BJ:201:VAL:HG13	9:BJ:265:PHE:CD2	2.55	0.42
14:BO:53:PHE:HE2	14:BO:55:PHE:CE1	2.38	0.42
15:BP:157:VAL:HG21	15:BP:181:HIS:CD2	2.46	0.42
16:BQ:119:GLY:H	16:BQ:463:ARG:C	2.27	0.42
16:BQ:338:ARG:O	16:BQ:341:LEU:HB2	2.19	0.42
6:BX:105:MET:CE	6:BX:139:MET:HG3	2.50	0.42
6:BX:115:GLN:HE21	6:BX:119:ILE:HD11	1.84	0.42
24:Ba:57:ILE:HA	39:Bp:104:LEU:HD12	2.01	0.42
26:Bc:159:LYS:HA	43:Bv:98:ARG:CZ	2.50	0.42
31:Bh:6:ILE:HD12	32:Bi:22:LEU:HD21	2.01	0.42
31:Bh:74:ARG:HG2	36:Bm:116:VAL:HG13	2.02	0.42
32:Bi:2:ASN:ND2	32:Bi:4:LEU:HB2	2.35	0.42
32:Bi:109:ALA:CB	32:Bi:112:HIS:HD2	2.33	0.42
33:Bj:71:LEU:O	33:Bj:74:PRO:HD2	2.20	0.42
34:Bk:14:ILE:HD13	36:Bm:17:VAL:HG22	2.02	0.42
35:Bl:14:SER:O	35:Bl:17:PRO:HD2	2.20	0.42
35:Bl:106:TRP:CZ2	35:Bl:348:HIS:HD2	2.38	0.42
35:Bl:197:ASP:O	35:Bl:201:MET:CG	2.68	0.42
35:Bl:217:LEU:HD23	35:Bl:217:LEU:O	2.19	0.42
35:Bl:550:LEU:HA	35:Bl:554:ASP:HB3	2.01	0.42
39:Bp:49:GLU:O	39:Bp:52:LYS:HG2	2.19	0.42
71:Br:501:PLX:H22	71:Br:501:PLX:H1B3	1.57	0.42
71:Br:501:PLX:H251	71:Br:501:PLX:H282	1.77	0.42
41:Bs:11:VAL:N	41:Bs:12:PRO:HD2	2.34	0.42
43:Bv:59:CYS:HB2	43:Bv:94:ASP:OD2	2.20	0.42
51:B3:42:ARG:NH1	51:B3:74:ARG:NH2	2.68	0.42
57:B9:19:LEU:HD23	57:B9:19:LEU:C	2.45	0.42
1:A:244:ASN:ND2	70:A:502:FMN:HM82	2.36	0.41
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	0.41
3:C:79:LEU:O	3:C:108:VAL:HA	2.20	0.41
3:C:187:ALA:O	3:C:190:LEU:HB3	2.20	0.41
6:G:103:HIS:N	6:G:107:ASP:HB2	2.35	0.41
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.41
9:J:201:VAL:HG13	9:J:265:PHE:CD2	2.55	0.41
9:J:329:LEU:HD22	9:J:332:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:49:VAL:HG23	12:M:94:MET:O	2.20	0.41
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.41
12:M:357:LEU:O	12:M:361:VAL:HG22	2.20	0.41
12:M:711:VAL:O	12:M:715:THR:HG23	2.19	0.41
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.41
16:Q:271:ARG:HH11	41:s:281:ARG:N	2.18	0.41
16:Q:371:MET:HA	16:Q:377:SER:OG	2.20	0.41
25:b:106:PRO:O	43:v:68:LYS:NZ	2.38	0.41
28:e:62:GLU:OE2	38:o:57:ARG:NH2	2.53	0.41
32:i:91:ASN:CG	32:i:92:GLN:H	2.13	0.41
34:k:3:LEU:O	34:k:3:LEU:HD13	2.20	0.41
34:k:10:LEU:O	34:k:14:ILE:HG13	2.20	0.41
35:l:7:MET:O	35:l:11:THR:HG23	2.20	0.41
35:l:14:SER:O	35:l:17:PRO:HD2	2.20	0.41
35:l:93:ALA:O	35:l:97:THR:OG1	2.38	0.41
35:l:595:LEU:O	35:l:598:THR:OG1	2.31	0.41
75:n:101:CDL:H712	75:n:101:CDL:H512	2.01	0.41
41:s:86:TRP:HH2	41:s:232:ILE:HG22	1.85	0.41
43:v:5:LEU:HG	43:v:6:VAL:N	2.34	0.41
45:x:365:ILE:HD12	46:y:87:MET:CE	2.34	0.41
49:1:21:LYS:HA	49:1:22:PRO:HD2	1.84	0.41
52:4:57:ARG:HA	52:4:60:TYR:CD2	2.55	0.41
63:AF:8:SER:OG	63:AF:9:ALA:N	2.53	0.41
68:AL:156:LEU:HB3	68:AL:161:ILE:HD11	2.01	0.41
60:AP:145:ASP:OD1	60:AP:146:VAL:N	2.53	0.41
60:AP:207:LYS:HE3	60:AP:209:GLU:OE2	2.20	0.41
67:AW:90:THR:HG22	67:AW:150:GLU:OE1	2.19	0.41
68:AY:274:GLU:OE2	68:AY:468:TYR:HB2	2.20	0.41
2:BB:128:ILE:HG12	2:BB:143:TYR:CD1	2.55	0.41
7:BH:19:THR:N	7:BH:20:PRO:HD3	2.35	0.41
8:BI:36:GLN:HA	8:BI:37:PRO:HD3	1.88	0.41
10:BK:82:TYR:HB3	14:BO:62:ARG:HH22	1.84	0.41
11:BL:78:ARG:HD2	12:BM:607:LYS:HE2	2.02	0.41
12:BM:436:VAL:HG21	12:BM:686:PRO:HG2	2.02	0.41
12:BM:541:PRO:HA	12:BM:542:PRO:HD2	1.77	0.41
12:BM:543:LYS:N	12:BM:543:LYS:HD2	2.35	0.41
14:BO:100:LYS:O	14:BO:104:VAL:HG23	2.20	0.41
15:BP:97:LEU:HD11	15:BP:130:TYR:CE2	2.54	0.41
25:Bb:51:LEU:HD22	25:Bb:59:LYS:HA	2.01	0.41
26:Bc:73:GLY:C	26:Bc:75:TYR:H	2.28	0.41
26:Bc:94:GLN:OE1	26:Bc:99:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bh:17:TRP:CZ3	31:Bh:18:LEU:HB2	2.55	0.41
32:Bi:68:MET:HG3	34:Bk:36:MET:HE3	2.02	0.41
32:Bi:108:MET:SD	32:Bi:191:MET:HG3	2.60	0.41
32:Bi:210:ILE:O	32:Bi:214:THR:HG23	2.20	0.41
35:Bl:68:TRP:HB2	35:Bl:76:LEU:HD12	2.01	0.41
36:Bm:114:VAL:O	36:Bm:115:VAL:HG22	2.20	0.41
75:Bn:101:CDL:H512	75:Bn:101:CDL:H712	2.01	0.41
40:Br:154:LEU:HD23	40:Br:154:LEU:HA	1.83	0.41
40:Br:308:SER:HB3	40:Br:384:THR:HG21	2.01	0.41
40:Br:344:LEU:O	40:Br:420:THR:HG21	2.20	0.41
40:Br:454:ILE:HD13	40:Br:454:ILE:HG21	1.86	0.41
41:Bs:150:LEU:O	41:Bs:154:LEU:HG	2.19	0.41
41:Bs:193:THR:O	41:Bs:194:ASN:HB2	2.20	0.41
42:Bu:83:THR:O	42:Bu:87:THR:HG23	2.20	0.41
47:Bz:224:LYS:NZ	47:Bz:226:HIS:HE2	2.18	0.41
1:A:32:PHE:HB3	1:A:294:VAL:HA	2.02	0.41
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.41
2:B:166:VAL:HG11	2:B:199:ILE:CG2	2.49	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
12:M:33:GLU:O	12:M:98:LYS:HA	2.20	0.41
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.41
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.41
20:V:95:CYS:O	20:V:99:LEU:HG	2.19	0.41
6:X:131:PRO:HG3	26:c:89:TRP:CE3	2.55	0.41
26:c:151:PRO:O	26:c:153:TYR:HD1	2.03	0.41
30:g:27:ASP:O	30:g:31:LEU:HG	2.19	0.41
32:i:210:ILE:O	32:i:214:THR:HG23	2.20	0.41
32:i:339:ILE:HD13	32:i:339:ILE:HG21	1.82	0.41
34:k:12:PHE:O	34:k:15:SER:OG	2.25	0.41
34:k:39:SER:HB3	36:m:16:PHE:HE2	1.84	0.41
35:l:197:ASP:O	35:l:201:MET:CG	2.68	0.41
35:l:310:LEU:HD23	35:l:313:MET:HE3	2.01	0.41
35:l:536:THR:O	35:l:539:TYR:HB3	2.20	0.41
36:m:5:LEU:HD23	36:m:8:LEU:HD12	2.02	0.41
40:r:91:ARG:HG2	40:r:136:TRP:CH2	2.54	0.41
40:r:170:THR:OG1	40:r:171:LEU:N	2.53	0.41
40:r:374:ASN:OD1	40:r:374:ASN:N	2.52	0.41
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.41
44:w:68:THR:OG1	44:w:69:GLY:N	2.54	0.41
48:0:137:LYS:O	48:0:145:TRP:HE3	2.03	0.41
55:7:13:TYR:O	55:7:14:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:128:ASP:OD1	65:AH:177:LYS:HE2	2.20	0.41
67:AK:239:ASN:OD1	67:AK:240:MET:HG2	2.20	0.41
67:AK:330:TYR:HB2	67:AK:333:SER:O	2.20	0.41
58:AN:49:VAL:HG21	76:AV:403:PEE:H7	2.02	0.41
60:AP:218:THR:HG21	60:AP:256:LEU:HD12	2.02	0.41
61:AQ:15:PHE:O	71:AQ:101:PLX:H1A1	2.20	0.41
66:AV:269:LYS:HA	66:AV:270:PRO:HD2	1.83	0.41
66:AV:346:PRO:O	66:AV:349:ILE:HG22	2.19	0.41
67:AW:209:VAL:HG13	67:AW:213:PHE:CD2	2.55	0.41
68:AY:287:VAL:HG12	68:AY:458:GLY:HA2	2.01	0.41
1:BA:222:LYS:NZ	12:BM:197:THR:HG21	2.35	0.41
1:BA:223:PRO:HB2	1:BA:425:CYS:SG	2.60	0.41
1:BA:453:PHE:O	1:BA:456:GLN:HG2	2.20	0.41
2:BB:96:ARG:HD2	2:BB:154:GLY:HA3	2.02	0.41
71:BB:303:PLX:H21	71:BB:303:PLX:H1B3	1.77	0.41
4:BE:48:HIS:HE1	9:BJ:363:SER:O	2.02	0.41
8:BI:94:ALA:HB1	15:BP:105:ASN:HD21	1.84	0.41
9:BJ:171:ASN:O	9:BJ:181:LEU:HG	2.18	0.41
9:BJ:283:VAL:HG13	9:BJ:369:VAL:HG11	2.02	0.41
15:BP:61:PHE:O	15:BP:64:TYR:HB3	2.20	0.41
15:BP:96:VAL:O	15:BP:100:LEU:HG	2.20	0.41
16:BQ:190:HIS:CE1	16:BQ:268:TRP:CH2	3.08	0.41
16:BQ:307:PRO:HB2	16:BQ:312:ASP:HB3	2.00	0.41
18:BT:80:VAL:O	18:BT:121:GLN:HA	2.20	0.41
22:BY:74:TRP:CZ3	22:BY:75:HIS:HA	2.53	0.41
71:Bb:201:PLX:C6	71:Bb:201:PLX:P1	3.09	0.41
26:Bc:163:TYR:HB3	26:Bc:168:LEU:HD21	2.02	0.41
27:Bd:76:ILE:HG22	27:Bd:77:MET:HE2	2.02	0.41
33:Bj:106:TRP:HZ3	41:Bs:291:LYS:HA	1.84	0.41
34:Bk:26:LEU:O	34:Bk:29:SER:OG	2.32	0.41
35:Bl:272:LEU:HD11	75:Bl:704:CDL:HB61	2.02	0.41
35:Bl:404:THR:HB	35:Bl:405:ASN:H	1.66	0.41
40:Br:374:ASN:N	40:Br:374:ASN:OD1	2.52	0.41
44:Bw:62:VAL:HG21	44:Bw:74:ALA:HB2	2.02	0.41
45:Bx:474:GLU:HG3	45:Bx:475:ALA:N	2.35	0.41
46:By:193:TYR:N	46:By:193:TYR:CD1	2.88	0.41
48:B0:86:MET:O	55:B7:25:CYS:HB2	2.20	0.41
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
3:C:104:ASP:OD2	41:s:37:PRO:HD3	2.20	0.41
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.41
7:H:50:GLN:HE22	8:I:93:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:271:TYR:HE1	9:J:374:THR:HB	1.85	0.41
11:L:131:LYS:HD2	11:L:147:ILE:HG23	2.02	0.41
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.81	0.41
12:M:560:LEU:HD12	12:M:561:PRO:HD2	2.02	0.41
16:Q:275:ILE:HD13	16:Q:446:ASP:OD1	2.20	0.41
17:S:53:ARG:CZ	31:h:105:ARG:NH2	2.83	0.41
17:S:55:SER:C	17:S:64:LYS:HZ1	2.28	0.41
71:b:201:PLX:P1	71:b:201:PLX:O6	2.79	0.41
32:i:79:MET:HE3	34:k:5:TYR:CD2	2.55	0.41
32:i:86:MET:HE2	32:i:144:GLN:OE1	2.21	0.41
32:i:221:LEU:HD23	32:i:221:LEU:HA	1.84	0.41
33:j:30:TYR:HB2	33:j:33:LYS:CD	2.47	0.41
35:l:272:LEU:HD11	75:l:704:CDL:HB61	2.02	0.41
35:l:564:LYS:HG3	38:o:77:TYR:OH	2.21	0.41
39:p:31:CYS:HB3	39:p:36:LYS:HD2	2.02	0.41
40:r:179:LEU:O	40:r:248:LEU:HD13	2.19	0.41
48:0:127:LYS:O	48:0:130:PRO:HD3	2.20	0.41
49:1:76:GLY:HA3	49:1:77:PRO:HD2	1.85	0.41
51:3:42:ARG:NH1	51:3:74:ARG:NH2	2.68	0.41
59:AB:50:LEU:HD23	59:AB:51:SER:O	2.19	0.41
62:AE:21:GLU:HA	62:AE:24:GLU:CB	2.49	0.41
63:AF:14:LEU:HD23	63:AF:14:LEU:HA	1.84	0.41
65:AH:266:ILE:O	65:AH:270:VAL:HG23	2.20	0.41
76:AH:401:PEE:C30	76:AH:401:PEE:H13	2.50	0.41
66:AJ:146:ILE:HA	66:AJ:149:LEU:HD13	2.02	0.41
67:AK:449:PHE:CE2	67:AW:183:ARG:HB3	2.54	0.41
75:AU:403:CDL:O1	75:AU:403:CDL:HB61	2.20	0.41
67:AW:257:GLU:HG2	67:AW:450:VAL:HB	2.02	0.41
1:BA:184:LYS:C	1:BA:186:ALA:H	2.27	0.41
1:BA:249:ALA:O	1:BA:252:PRO:HD2	2.21	0.41
3:BC:79:LEU:O	3:BC:108:VAL:HA	2.21	0.41
3:BC:109:VAL:HG21	41:Bs:25:ARG:HH12	1.85	0.41
3:BC:150:MET:SD	3:BC:190:LEU:HD13	2.60	0.41
9:BJ:157:LYS:HA	9:BJ:195:PHE:HE1	1.84	0.41
11:BL:131:LYS:HD2	11:BL:147:ILE:CG2	2.49	0.41
12:BM:319:TRP:HH2	12:BM:617:ARG:NE	2.18	0.41
12:BM:357:LEU:O	12:BM:361:VAL:HG22	2.20	0.41
14:BO:156:LEU:HD13	14:BO:158:ILE:HD12	2.03	0.41
17:BS:47:LEU:O	17:BS:50:ARG:HB3	2.20	0.41
22:BY:73:PHE:O	22:BY:73:PHE:CD1	2.71	0.41
24:Ba:66:ARG:O	24:Ba:70:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ba:101:ILE:HG13	27:Bd:58:TYR:CB	2.49	0.41
25:Bb:117:ILE:CG2	25:Bb:118:PRO:HD2	2.50	0.41
26:Bc:101:TRP:CD1	38:Bo:62:ASN:HD22	2.38	0.41
32:Bi:189:TRP:HE1	32:Bi:286:THR:HG21	1.85	0.41
36:Bm:40:CYS:O	36:Bm:44:LEU:HG	2.19	0.41
38:Bo:56:ARG:O	38:Bo:58:GLY:N	2.50	0.41
45:Bx:198:SER:HB2	45:Bx:238:PHE:HA	2.03	0.41
46:By:146:MET:SD	46:By:189:PRO:HB3	2.60	0.41
47:Bz:252:LEU:HD23	47:Bz:252:LEU:HA	1.90	0.41
52:B4:57:ARG:HA	52:B4:60:TYR:CD2	2.55	0.41
2:B:96:ARG:HD2	2:B:154:GLY:HA3	2.03	0.41
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.55	0.41
3:C:118:ASP:CG	3:C:119:VAL:H	2.28	0.41
7:H:75:GLY:CA	8:I:103:ARG:HH11	2.34	0.41
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.84	0.41
9:J:240:VAL:HG22	9:J:266:VAL:C	2.45	0.41
9:J:255:ASP:HA	9:J:256:PRO:HD2	1.91	0.41
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.41
14:O:176:CYS:HA	74:O:301:FES:S1	2.60	0.41
15:P:190:ASP:CG	15:P:191:TYR:N	2.77	0.41
16:Q:310:VAL:O	16:Q:314:VAL:HG23	2.21	0.41
26:c:65:TYR:CE2	26:c:77:LYS:HG3	2.55	0.41
26:c:157:GLY:HA2	26:c:158:PRO:HD3	1.76	0.41
27:d:162:LYS:O	27:d:165:LYS:HB3	2.20	0.41
32:i:68:MET:HG3	34:k:36:MET:HE3	2.02	0.41
32:i:124:LEU:HD13	32:i:219:LEU:HG	2.02	0.41
32:i:189:TRP:HE1	32:i:286:THR:HG21	1.85	0.41
35:l:106:TRP:CZ2	35:l:348:HIS:HD2	2.38	0.41
45:x:354:THR:HG21	45:x:376:HIS:HA	2.03	0.41
45:x:474:GLU:HG3	45:x:475:ALA:N	2.35	0.41
46:y:122:MET:HB2	46:y:208:PRO:CD	2.47	0.41
48:0:11:TYR:CD1	48:0:11:TYR:C	2.99	0.41
49:1:79:LYS:HE2	49:1:79:LYS:HB2	1.92	0.41
51:3:44:ARG:HA	51:3:45:PRO:HD2	1.76	0.41
75:AG:101:CDL:H562	75:AG:101:CDL:H532	1.94	0.41
65:AH:112:ARG:O	65:AH:116:VAL:HG23	2.21	0.41
66:AJ:320:LEU:HB2	66:AJ:373:GLU:OE2	2.20	0.41
67:AK:104:GLU:OE1	68:AL:325:SER:HA	2.20	0.41
68:AL:478:LEU:HD11	76:AL:503:PEE:H2	2.03	0.41
58:AN:19:LEU:HD11	60:AP:88:PHE:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:186:GLN:O	60:AP:190:VAL:HG23	2.20	0.41
67:AW:64:PHE:HZ	67:AW:393:LEU:HD23	1.86	0.41
67:AW:195:TYR:CE2	67:AW:196:ARG:HG2	2.55	0.41
68:AY:40:GLN:HB3	68:AY:44:PHE:HE2	1.84	0.41
68:AY:282:LEU:HB2	68:AY:461:PRO:HD3	2.03	0.41
68:AY:425:PRO:O	68:AY:428:GLU:N	2.52	0.41
2:BB:175:THR:HB	2:BB:180:GLU:OE1	2.19	0.41
7:BH:75:GLY:CA	8:BI:103:ARG:HH11	2.34	0.41
9:BJ:98:GLY:HA3	9:BJ:103:LEU:HG	2.01	0.41
12:BM:209:TYR:H	14:BO:110:MET:HE1	1.86	0.41
13:BN:34:LYS:NZ	13:BN:54:GLN:HG2	2.36	0.41
15:BP:81:PHE:HE1	16:BQ:157:LYS:O	2.03	0.41
16:BQ:116:LEU:O	16:BQ:118:ARG:HG3	2.19	0.41
21:BW:72:LEU:HA	21:BW:72:LEU:HD23	1.84	0.41
26:Bc:49:ALA:O	26:Bc:53:LYS:HG2	2.21	0.41
26:Bc:151:PRO:O	26:Bc:153:TYR:HD1	2.03	0.41
30:Bg:11:ARG:O	30:Bg:13:LEU:N	2.54	0.41
30:Bg:44:ASP:OD1	32:Bi:327:PRO:HG2	2.20	0.41
32:Bi:72:MET:CE	34:Bk:9:MET:HG2	2.49	0.41
32:Bi:120:GLN:HA	32:Bi:176:ARG:HE	1.85	0.41
35:Bl:158:TRP:CH2	35:Bl:240:PRO:HB3	2.55	0.41
35:Bl:305:SER:O	35:Bl:309:GLN:HG2	2.20	0.41
41:Bs:116:ILE:O	41:Bs:119:SER:OG	2.34	0.41
45:Bx:430:PHE:O	45:Bx:431:LEU:C	2.64	0.41
50:B2:10:GLU:HG2	50:B2:25:ARG:HH22	1.86	0.41
50:B2:49:VAL:O	50:B2:91:LEU:HD12	2.21	0.41
51:B3:44:ARG:HA	51:B3:45:PRO:HD2	1.76	0.41
52:B4:65:PRO:HG2	52:B4:68:TRP:CG	2.56	0.41
53:B5:21:ILE:O	53:B5:25:PHE:HD2	2.02	0.41
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	0.41
3:C:59:ARG:HH22	3:C:61:GLU:CB	2.25	0.41
9:J:263:PHE:CE1	9:J:333:PRO:HG2	2.55	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.41
12:M:557:ARG:HE	12:M:579:ILE:HG23	1.86	0.41
12:M:598:ASN:HD22	12:M:602:ARG:NH1	2.19	0.41
16:Q:190:HIS:CE1	16:Q:268:TRP:CH2	3.08	0.41
16:Q:331:LEU:O	16:Q:335:GLU:HG3	2.20	0.41
75:V:201:CDL:H572	75:V:201:CDL:H541	1.46	0.41
76:W:201:PEE:H51	76:W:201:PEE:H56	1.33	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.41
22:Y:81:LEU:HB3	35:l:480:THR:OG1	2.20	0.41
24:a:129:PRO:CG	27:d:60:ARG:HH22	2.33	0.41
24:a:170:TYR:CD1	30:g:5:ARG:HD3	2.54	0.41
32:i:26:TRP:HD1	32:i:84:TRP:O	2.02	0.41
35:l:188:TRP:O	35:l:192:HIS:HB2	2.20	0.41
35:l:245:ALA:O	35:l:249:SER:OG	2.32	0.41
35:l:452:ASN:N	35:l:453:PRO:HD2	2.36	0.41
35:l:550:LEU:HA	35:l:554:ASP:HB3	2.01	0.41
35:l:558:LEU:HB3	40:r:214:LEU:HD11	2.02	0.41
75:n:101:CDL:H341	75:n:101:CDL:H312	1.56	0.41
39:p:145:PRO:HA	39:p:146:PRO:HD3	1.84	0.41
40:r:121:PHE:O	40:r:125:THR:HG23	2.20	0.41
41:s:7:LEU:HA	41:s:7:LEU:HD23	1.78	0.41
42:u:24:VAL:CG2	42:u:86:TRP:HE1	2.34	0.41
44:w:93:TYR:CZ	44:w:142:GLN:OE1	2.73	0.41
45:x:198:SER:HB2	45:x:238:PHE:HA	2.03	0.41
45:x:398:PRO:HB3	45:x:482:VAL:HG21	2.03	0.41
47:z:224:LYS:NZ	47:z:226:HIS:HE2	2.18	0.41
54:6:12:PHE:O	54:6:23:LYS:HE2	2.21	0.41
58:AA:42:ILE:HG23	75:AA:101:CDL:H121	2.02	0.41
61:AD:11:TYR:HA	61:AD:15:PHE:HB2	2.02	0.41
63:AF:27:PHE:HD1	63:AF:28:ASN:N	2.17	0.41
65:AH:194:PRO:HA	65:AH:195:PRO:HD3	1.86	0.41
66:AJ:284:VAL:HA	66:AJ:285:PRO:HD2	1.91	0.41
67:AK:58:VAL:HG23	68:AL:400:VAL:HG11	2.03	0.41
67:AK:67:ALA:HB2	67:AK:212:HIS:HB3	2.02	0.41
68:AL:360:CYS:SG	68:AL:365:ILE:HG12	2.60	0.41
58:AN:17:TYR:CD1	68:AY:275:ILE:HG12	2.55	0.41
59:AO:29:LEU:O	59:AO:31:GLN:N	2.42	0.41
60:AP:141:SER:OG	60:AP:142:ALA:N	2.51	0.41
61:AQ:4:ALA:HB3	61:AQ:9:LYS:HE3	2.02	0.41
65:AU:114:PHE:HE2	65:AU:148:LEU:HD21	1.83	0.41
65:AU:201:VAL:HG13	65:AU:208:GLU:N	2.36	0.41
76:AU:401:PEE:H55	76:AU:401:PEE:H49	1.82	0.41
66:AV:21:LEU:HA	66:AV:22:PRO:HD3	1.93	0.41
66:AV:171:ASP:OD1	66:AV:172:SER:N	2.50	0.41
67:AW:290:GLN:HB3	67:AW:336:PHE:HE1	1.85	0.41
68:AY:74:TRP:CG	68:AY:414:GLY:HA3	2.54	0.41
68:AY:225:LYS:O	68:AY:228:ARG:HB3	2.20	0.41
1:BA:122:PRO:HB2	1:BA:322:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:140:GLN:HG2	33:Bj:37:TYR:CD1	2.56	0.41
11:BL:131:LYS:HD2	11:BL:147:ILE:HG23	2.03	0.41
16:BQ:35:ARG:HH21	44:Bw:322:HIS:HB3	1.86	0.41
16:BQ:233:HIS:CD2	16:BQ:234:GLN:HB2	2.55	0.41
16:BQ:271:ARG:HH11	41:Bs:281:ARG:N	2.18	0.41
16:BQ:290:GLY:C	16:BQ:294:ARG:HE	2.28	0.41
6:BX:132:ASP:O	6:BX:136:GLU:N	2.49	0.41
26:Bc:87:ASP:HA	26:Bc:88:PRO:HD2	1.87	0.41
26:Bc:125:SER:O	26:Bc:129:MET:HG3	2.20	0.41
27:Bd:107:CYS:HG	27:Bd:119:CYS:CB	2.33	0.41
30:Bg:37:GLY:HA2	30:Bg:67:PHE:CE2	2.56	0.41
32:Bi:167:TRP:HZ3	35:Bl:570:GLN:CA	2.20	0.41
34:Bk:10:LEU:O	34:Bk:14:ILE:HG13	2.20	0.41
40:Br:229:MET:HE2	40:Br:229:MET:HB3	1.90	0.41
43:Bv:59:CYS:O	43:Bv:87:TRP:HZ3	2.03	0.41
44:Bw:93:TYR:CZ	44:Bw:142:GLN:OE1	2.73	0.41
48:B0:130:PRO:O	48:B0:136:ALA:HB2	2.21	0.41
49:B1:93:LEU:HD23	49:B1:93:LEU:HA	1.88	0.41
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.41
3:C:109:VAL:HG21	41:s:25:ARG:HH12	1.85	0.41
9:J:171:ASN:O	9:J:181:LEU:HG	2.18	0.41
9:J:336:GLU:C	9:J:339:GLY:H	2.28	0.41
12:M:342:ALA:HB3	12:M:368:THR:HA	2.02	0.41
16:Q:233:HIS:CD2	16:Q:234:GLN:HB2	2.55	0.41
16:Q:255:LEU:HD23	16:Q:255:LEU:HA	1.91	0.41
20:V:126:LYS:HE3	20:V:130:LEU:HD11	2.02	0.41
75:V:201:CDL:H722	75:V:201:CDL:H752	1.75	0.41
22:Y:94:ASP:HB3	22:Y:95:GLU:H	1.71	0.41
24:a:130:GLU:HA	37:n:45:PHE:CD2	2.56	0.41
25:b:117:ILE:CG2	25:b:118:PRO:HD2	2.50	0.41
26:c:49:ALA:O	26:c:53:LYS:HG2	2.20	0.41
26:c:88:PRO:HB2	39:p:86:PRO:HG2	2.03	0.41
31:h:17:TRP:CZ3	31:h:18:LEU:HB2	2.55	0.41
32:i:108:MET:SD	32:i:191:MET:HG3	2.60	0.41
35:l:174:TYR:OH	35:l:534:HIS:HE1	2.03	0.41
35:l:396:ILE:HG22	35:l:400:ASN:HD21	1.85	0.41
36:m:16:PHE:CD1	36:m:19:PHE:CE1	3.07	0.41
36:m:38:VAL:O	36:m:42:ILE:HG13	2.21	0.41
39:p:48:PHE:HE1	72:p:201:8Q1:C6	2.33	0.41
39:p:135:ARG:HD3	39:p:162:ASP:OD1	2.21	0.41
39:p:174:PRO:O	39:p:175:ARG:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:289:LEU:HA	41:s:289:LEU:HD23	1.82	0.41
43:v:59:CYS:HB2	43:v:94:ASP:OD2	2.20	0.41
45:x:128:VAL:O	45:x:128:VAL:CG2	2.68	0.41
47:z:12:ASN:ND2	54:6:20:VAL:H	2.14	0.41
52:4:20:PHE:N	52:4:21:PRO:HD3	2.35	0.41
55:7:24:PHE:CE1	55:7:28:VAL:HG21	2.56	0.41
60:AC:196:ARG:HB3	60:AC:249:ILE:HG23	2.01	0.41
60:AC:200:HIS:CE1	60:AC:202:LEU:HB3	2.55	0.41
63:AF:51:LEU:C	67:AW:148:ARG:HH22	2.29	0.41
66:AJ:138:MET:HE1	66:AJ:269:LYS:H	1.86	0.41
66:AJ:160:LEU:O	66:AJ:164:ILE:HD12	2.20	0.41
66:AJ:198:LEU:HD12	75:AJ:404:CDL:H311	2.02	0.41
64:AT:9:ARG:HH22	71:AT:101:PLX:C1A	2.33	0.41
66:AV:320:LEU:O	66:AV:323:SER:OG	2.30	0.41
68:AY:322:VAL:HG12	68:AY:323:HIS:N	2.27	0.41
68:AY:331:GLY:O	68:AY:337:LEU:HD12	2.21	0.41
5:BF:16:LEU:HD12	5:BF:68:ARG:O	2.21	0.41
73:BJ:401:NDP:O3B	73:BJ:401:NDP:P2B	2.79	0.41
12:BM:522:GLN:HE21	12:BM:526:LEU:HG	1.85	0.41
14:BO:87:GLN:OE1	14:BO:122:TYR:HA	2.21	0.41
14:BO:186:VAL:HG12	14:BO:188:ILE:HG13	2.03	0.41
14:BO:198:ALA:O	14:BO:202:GLU:HG2	2.21	0.41
16:BQ:255:LEU:HD23	16:BQ:255:LEU:HA	1.91	0.41
16:BQ:331:LEU:O	16:BQ:335:GLU:HG3	2.20	0.41
26:Bc:183:HIS:CB	43:Bv:37:ARG:HA	2.50	0.41
27:Bd:72:LYS:HE3	30:Bg:105:LYS:O	2.20	0.41
30:Bg:37:GLY:O	30:Bg:40:SER:OG	2.28	0.41
35:Bl:558:LEU:HB3	40:Br:214:LEU:HD11	2.02	0.41
38:Bo:112:LYS:NZ	40:Br:389:SER:HA	2.36	0.41
39:Bp:31:CYS:HB3	39:Bp:36:LYS:HD2	2.02	0.41
39:Bp:134:GLU:O	39:Bp:138:LYS:HG3	2.21	0.41
39:Bp:158:ARG:O	39:Bp:159:LYS:HB2	2.21	0.41
44:Bw:99:GLY:HA3	44:Bw:337:ARG:NH1	2.20	0.41
45:Bx:264:LYS:NZ	46:By:56:MET:HE2	2.35	0.41
46:By:100:MET:HE3	46:By:157:GLU:HG3	2.02	0.41
47:Bz:154:GLY:CA	50:B2:6:VAL:HG22	2.47	0.41
1:A:223:PRO:HB2	1:A:425:CYS:SG	2.60	0.41
3:C:106:PHE:HB2	3:C:108:VAL:HG22	2.03	0.41
7:H:45:ARG:O	7:H:49:GLU:HG3	2.21	0.41
73:J:401:NDP:O3B	73:J:401:NDP:P2B	2.79	0.41
11:L:88:GLN:NE2	12:M:136:GLU:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.35	0.41
16:Q:35:ARG:HH21	44:w:322:HIS:HB3	1.86	0.41
16:Q:333:ARG:HE	16:Q:455:ASP:CG	2.29	0.41
16:Q:371:MET:HE1	16:Q:381:HIS:CE1	2.55	0.41
18:T:32:VAL:HG22	18:T:38:LYS:HE3	2.03	0.41
18:T:40:THR:OG1	18:T:44:GLN:HG2	2.20	0.41
27:d:24:ILE:HD11	35:l:56:CYS:HB3	2.02	0.41
27:d:76:ILE:HG22	27:d:77:MET:HE2	2.02	0.41
30:g:44:ASP:OD1	32:i:327:PRO:HG2	2.20	0.41
30:g:73:TYR:O	30:g:76:LYS:HB3	2.21	0.41
31:h:6:ILE:HD12	32:i:22:LEU:HD21	2.01	0.41
39:p:134:GLU:O	39:p:138:LYS:HG3	2.21	0.41
40:r:89:LEU:O	40:r:93:LYS:HG3	2.20	0.41
41:s:275:THR:OG1	41:s:276:ALA:N	2.53	0.41
45:x:264:LYS:NZ	46:y:56:MET:HE2	2.35	0.41
45:x:337:ALA:HB2	45:x:394:VAL:HG23	2.03	0.41
46:y:5:MET:CE	55:7:42:PRO:HA	2.45	0.41
50:2:16:LEU:O	50:2:20:VAL:HG13	2.21	0.41
75:AA:101:CDL:H562	75:AA:101:CDL:H141	2.03	0.41
60:AC:88:PHE:O	60:AC:92:ARG:HG3	2.20	0.41
62:AE:20:GLU:O	62:AE:24:GLU:N	2.48	0.41
65:AH:284:HIS:CG	65:AH:288:MET:HE2	2.56	0.41
66:AJ:2:THR:HG21	68:AL:335:ASN:HD22	1.86	0.41
67:AK:159:LYS:HG2	67:AK:197:ILE:HD13	2.03	0.41
68:AL:141:PRO:HA	68:AL:245:LEU:HD13	2.03	0.41
75:AN:102:CDL:OB4	63:AS:73:HIS:CE1	2.73	0.41
60:AP:85:VAL:HA	60:AP:86:PRO:HD2	1.93	0.41
63:AS:8:SER:OG	63:AS:9:ALA:N	2.51	0.41
66:AV:249:LEU:CD1	66:AV:250:LEU:HD12	2.50	0.41
67:AW:125:CYS:SG	67:AW:130:VAL:HG22	2.60	0.41
68:AY:314:TYR:HB3	68:AY:341:PHE:CE1	2.56	0.41
68:AY:337:LEU:O	68:AY:368:MET:HE2	2.21	0.41
1:BA:122:PRO:HA	14:BO:176:CYS:SG	2.61	0.41
7:BH:50:GLN:HE22	8:BI:93:LYS:HD2	1.85	0.41
16:BQ:150:ALA:CB	16:BQ:400:ILE:HG13	2.49	0.41
16:BQ:368:ARG:HA	16:BQ:371:MET:HG2	2.01	0.41
18:BT:32:VAL:HG22	18:BT:38:LYS:HE3	2.02	0.41
19:BU:50:PRO:HB2	21:BW:69:ILE:HD11	2.03	0.41
21:BW:86:MET:HG2	21:BW:128:ARG:HH22	1.86	0.41
24:Ba:129:PRO:CG	27:Bd:60:ARG:HH22	2.33	0.41
25:Bb:99:GLU:HG2	35:Bl:61:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Bc:38:PRO:HD2	38:Bo:70:TYR:CD2	2.56	0.41
27:Bd:134:GLN:OE1	38:Bo:124:THR:HA	2.20	0.41
30:Bg:15:ASP:HB2	30:Bg:18:ARG:NH2	2.29	0.41
34:Bk:3:LEU:O	34:Bk:3:LEU:HD13	2.20	0.41
35:Bl:396:ILE:HG22	35:Bl:400:ASN:HD21	1.85	0.41
36:Bm:32:LEU:HA	36:Bm:32:LEU:HD23	1.77	0.41
38:Bo:124:THR:C	38:Bo:126:HIS:H	2.29	0.41
39:Bp:135:ARG:HD3	39:Bp:162:ASP:OD1	2.21	0.41
40:Br:130:LEU:O	40:Br:134:THR:OG1	2.25	0.41
40:Br:153:THR:O	40:Br:157:SER:N	2.54	0.41
40:Br:231:LEU:HA	40:Br:235:LEU:HD12	2.03	0.41
41:Bs:195:ARG:HG3	41:Bs:196:ALA:H	1.86	0.41
44:Bw:86:PHE:HE2	44:Bw:146:ALA:HB2	1.86	0.41
44:Bw:289:ARG:O	44:Bw:292:TYR:HB3	2.21	0.41
45:Bx:398:PRO:HB3	45:Bx:482:VAL:HG21	2.03	0.41
47:Bz:40:MET:O	47:Bz:41:THR:C	2.62	0.41
49:B1:104:LEU:HD23	49:B1:104:LEU:HA	1.88	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
1:A:314:LEU:O	1:A:315:LEU:HD12	2.19	0.41
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
3:C:140:GLN:HG2	33:j:37:TYR:CD1	2.56	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
5:F:89:ARG:HD2	5:F:92:GLU:OE2	2.21	0.41
8:I:65:PRO:HD3	15:P:245:TYR:CE2	2.56	0.41
12:M:646:LEU:O	12:M:651:PRO:HA	2.21	0.41
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41
16:Q:80:ILE:HG22	16:Q:81:THR:N	2.35	0.41
19:U:8:PHE:O	19:U:11:ASN:HB3	2.21	0.41
20:V:114:ALA:HB1	20:V:118:PHE:CE2	2.56	0.41
21:W:57:ARG:NH2	41:s:316:PRO:HG3	2.35	0.41
22:Y:62:SER:O	22:Y:65:MET:HB3	2.21	0.41
22:Y:73:PHE:O	22:Y:73:PHE:CD1	2.71	0.41
25:b:31:ARG:HH12	39:p:116:PRO:HG2	1.85	0.41
27:d:72:LYS:HE3	30:g:105:LYS:O	2.20	0.41
28:e:143:ASP:N	28:e:143:ASP:OD1	2.53	0.41
30:g:15:ASP:HB2	30:g:18:ARG:NH2	2.29	0.41
30:g:45:ASN:HD21	30:g:60:GLN:NE2	2.19	0.41
30:g:81:LEU:HD23	30:g:81:LEU:HA	1.85	0.41
31:h:94:PRO:O	31:h:97:HIS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:193:VAL:HB	32:i:201:THR:HG22	2.02	0.41
35:l:522:PHE:HA	35:l:528:PHE:CE2	2.56	0.41
38:o:6:TYR:HE2	38:o:14:LEU:HA	1.85	0.41
38:o:23:TYR:O	38:o:25:ILE:HG12	2.21	0.41
40:r:231:LEU:HA	40:r:235:LEU:HD12	2.03	0.41
44:w:223:ASP:O	44:w:227:MET:HG3	2.21	0.41
46:y:100:MET:HE3	46:y:157:GLU:HG3	2.02	0.41
62:AE:28:ASP:OD2	65:AH:262:THR:CG2	2.69	0.41
63:AF:17:ILE:H	63:AF:17:ILE:HG12	1.60	0.41
75:AH:403:CDL:H362	75:AH:403:CDL:H332	1.93	0.41
66:AJ:221:HIS:HA	66:AJ:225:THR:HG23	2.02	0.41
66:AJ:300:ILE:O	66:AJ:301:LEU:C	2.63	0.41
67:AK:452:GLU:O	67:AK:452:GLU:HG3	2.20	0.41
68:AL:314:TYR:HB3	68:AL:341:PHE:CZ	2.55	0.41
59:AO:13:PRO:HB2	67:AW:84:ARG:HH12	1.86	0.41
65:AU:290:LEU:HD23	65:AU:290:LEU:O	2.19	0.41
67:AW:352:LYS:O	67:AW:356:ASN:ND2	2.54	0.41
68:AY:373:GLN:NE2	68:AY:471:ILE:HG23	2.35	0.41
1:BA:244:ASN:ND2	70:BA:502:FMN:HM82	2.36	0.41
70:BA:502:FMN:H4'	70:BA:502:FMN:H1'2	1.63	0.41
2:BB:176:GLU:OE1	3:BC:200:LYS:HD2	2.20	0.41
3:BC:104:ASP:OD2	41:Bs:37:PRO:HD3	2.20	0.41
9:BJ:209:ARG:HD2	15:BP:217:LYS:CE	2.50	0.41
12:BM:49:VAL:HG23	12:BM:94:MET:O	2.20	0.41
12:BM:236:TYR:CE1	12:BM:272:ARG:HB3	2.55	0.41
12:BM:483:ARG:O	12:BM:483:ARG:HG3	2.21	0.41
15:BP:148:ASP:HB2	15:BP:151:THR:HG23	2.02	0.41
16:BQ:303:ARG:HG3	16:BQ:401:GLU:HG3	2.03	0.41
18:BT:33:SER:HB3	18:BT:45:VAL:HG21	2.03	0.41
19:BU:8:PHE:O	19:BU:11:ASN:HB3	2.21	0.41
21:BW:87:LEU:HD23	21:BW:87:LEU:HA	1.91	0.41
24:Ba:130:GLU:HA	37:Bn:45:PHE:CD2	2.56	0.41
25:Bb:111:LEU:C	25:Bb:113:THR:N	2.78	0.41
26:Bc:154:GLN:HE22	43:Bv:3:ALA:HB2	1.86	0.41
30:Bg:29:ARG:NH2	42:Bu:172:LYS:HB3	2.36	0.41
30:Bg:73:TYR:O	30:Bg:76:LYS:HB3	2.21	0.41
71:Bg:202:PLX:H101	71:Bg:202:PLX:H132	1.44	0.41
32:Bi:124:LEU:HD13	32:Bi:219:LEU:HG	2.03	0.41
32:Bi:294:LEU:HA	32:Bi:294:LEU:HD23	1.74	0.41
33:Bj:75:LEU:HD23	33:Bj:75:LEU:HA	1.91	0.41
33:Bj:94:LEU:HD12	36:Bm:153:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:7:MET:O	35:Bl:11:THR:HG23	2.20	0.41
35:Bl:154:LEU:HD23	35:Bl:154:LEU:HA	1.85	0.41
71:Br:501:PLX:H301	71:Br:501:PLX:H271	1.66	0.41
42:Bu:125:LEU:HD23	42:Bu:125:LEU:HA	1.87	0.41
44:Bw:120:ASP:HA	44:Bw:121:PRO:HD3	1.84	0.41
44:Bw:223:ASP:O	44:Bw:227:MET:HG3	2.20	0.41
45:Bx:168:ILE:CG2	45:Bx:189:MET:HG3	2.51	0.41
45:Bx:240:HIS:O	45:Bx:241:PRO:C	2.64	0.41
45:Bx:442:ASP:OD2	46:By:134:ARG:NH2	2.54	0.41
54:B6:3:ASN:C	54:B6:3:ASN:ND2	2.77	0.41
54:B6:5:VAL:O	54:B6:9:GLN:HG3	2.21	0.41
57:B9:35:TYR:HD2	57:B9:36:HIS:CE1	2.39	0.41
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.41
1:A:86:ARG:C	1:A:95:THR:HG23	2.46	0.41
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
2:B:143:TYR:HB3	2:B:185:LYS:HB2	2.03	0.41
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.41
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.41
71:B:303:PLX:H112	71:B:303:PLX:H81	1.68	0.41
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	0.41
9:J:231:LEU:HB3	9:J:232:GLY:H	1.69	0.41
11:L:123:ASN:HB3	15:P:232:LYS:HD2	2.02	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
12:M:209:TYR:H	14:O:110:MET:HE1	1.86	0.41
12:M:645:ARG:O	12:M:649:VAL:HG12	2.21	0.41
14:O:164:THR:CG2	14:O:168:LEU:H	2.34	0.41
14:O:168:LEU:HD22	14:O:169:PHE:CE2	2.56	0.41
14:O:186:VAL:HG12	14:O:188:ILE:HG13	2.03	0.41
15:P:186:ARG:HD3	15:P:189:THR:O	2.21	0.41
16:Q:55:SER:O	16:Q:58:THR:OG1	2.37	0.41
16:Q:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
16:Q:235:ASP:HA	16:Q:356:ILE:HD12	2.01	0.41
17:S:37:ARG:NH1	17:S:51:ASP:OD2	2.51	0.41
19:U:59:ASP:OD2	42:u:132:LYS:HG3	2.21	0.41
21:W:57:ARG:NH2	41:s:168:THR:HG22	2.36	0.41
21:W:93:GLU:OE1	31:h:93:THR:HG21	2.21	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.86	0.41
24:a:170:TYR:CD2	30:g:5:ARG:HB3	2.56	0.41
25:b:33:PRO:HG2	39:p:116:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:88:TYR:HB2	71:b:201:PLX:C1B	2.51	0.41
71:b:201:PLX:C6	71:b:201:PLX:P1	3.08	0.41
26:c:38:PRO:HD2	38:o:70:TYR:CD2	2.56	0.41
26:c:49:ALA:HA	26:c:59:VAL:HG13	2.03	0.41
27:d:35:VAL:C	27:d:38:PRO:HD2	2.46	0.41
28:e:138:GLU:OE1	28:e:138:GLU:N	2.42	0.41
28:e:150:PRO:HD3	30:g:112:PHE:CD1	2.56	0.41
30:g:37:GLY:HA2	30:g:67:PHE:CE2	2.56	0.41
32:i:179:LEU:HD23	32:i:179:LEU:HA	1.81	0.41
33:j:54:LYS:HB3	33:j:113:TRP:HE1	1.85	0.41
33:j:71:LEU:O	33:j:74:PRO:HD2	2.20	0.41
35:l:37:LYS:NZ	35:l:98:TRP:HE1	2.18	0.41
35:l:158:TRP:CH2	35:l:240:PRO:HB3	2.55	0.41
35:l:305:SER:O	35:l:309:GLN:HG2	2.20	0.41
35:l:558:LEU:HD23	35:l:558:LEU:HA	1.71	0.41
36:m:118:PHE:CE1	36:m:121:VAL:HB	2.56	0.41
38:o:112:LYS:NZ	40:r:389:SER:HA	2.36	0.41
40:r:248:LEU:HD12	40:r:249:ILE:N	2.35	0.41
44:w:62:VAL:HG21	44:w:74:ALA:HB2	2.02	0.41
45:x:168:ILE:CG2	45:x:189:MET:HG3	2.51	0.41
45:x:311:ILE:HG21	45:x:311:ILE:HD13	1.74	0.41
45:x:501:PRO:O	45:x:502:TYR:C	2.63	0.41
46:y:164:ALA:HB2	46:y:171:LYS:HD3	2.03	0.41
47:z:6:HIS:CD2	47:z:8:TYR:HB2	2.55	0.41
50:2:10:GLU:HG2	50:2:25:ARG:HH22	1.86	0.41
51:3:5:LYS:HB3	51:3:6:GLY:H	1.67	0.41
54:6:5:VAL:O	54:6:9:GLN:HG3	2.21	0.41
60:AC:209:GLU:HG2	60:AC:210:TRP:CD1	2.56	0.41
66:AJ:186:PRO:HG2	82:AJ:401:HEM:HHC	2.03	0.41
66:AJ:348:THR:O	66:AJ:352:GLN:HG2	2.21	0.41
67:AK:407:MET:HE1	67:AK:415:GLN:OE1	2.21	0.41
68:AL:70:THR:OG1	68:AL:410:CYS:SG	2.50	0.41
68:AL:462:ILE:HG23	68:AL:465:LEU:HB3	2.03	0.41
63:AS:46:GLU:OE2	63:AS:50:ARG:NH2	2.54	0.41
66:AV:87:ALA:HB2	82:AV:401:HEM:CHB	2.50	0.41
66:AV:146:ILE:O	66:AV:149:LEU:HB2	2.21	0.41
68:AY:61:SER:HB2	68:AY:242:LEU:HD23	2.03	0.41
1:BA:222:LYS:HA	1:BA:223:PRO:HD3	1.84	0.41
1:BA:296:LEU:HD22	1:BA:332:CYS:SG	2.61	0.41
2:BB:57:ARG:HG2	2:BB:62:THR:OG1	2.21	0.41
2:BB:68:LEU:HD11	41:Bs:272:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:120:ILE:O	2:BB:121:CYS:C	2.64	0.41
2:BB:133:ARG:C	2:BB:136:GLY:H	2.29	0.41
2:BB:143:TYR:HB3	2:BB:185:LYS:HB2	2.03	0.41
8:BI:38:PRO:HA	8:BI:39:PRO:HD3	1.58	0.41
9:BJ:130:ILE:HA	73:BJ:401:NDP:H8A	2.03	0.41
12:BM:130:ILE:H	12:BM:130:ILE:HG12	1.69	0.41
12:BM:246:ARG:NH2	15:BP:229:GLU:OE2	2.54	0.41
14:BO:99:ASN:O	14:BO:103:GLU:HG3	2.21	0.41
16:BQ:149:GLN:OE1	16:BQ:171:ARG:HB3	2.20	0.41
16:BQ:204:PHE:CE1	16:BQ:207:ARG:HD3	2.56	0.41
16:BQ:310:VAL:O	16:BQ:314:VAL:HG23	2.21	0.41
18:BT:40:THR:OG1	18:BT:44:GLN:HG2	2.20	0.41
19:BU:59:ASP:OD2	42:Bu:132:LYS:HG3	2.21	0.41
76:BW:201:PEE:H51	76:BW:201:PEE:H56	1.33	0.41
6:BX:152:LYS:HA	6:BX:152:LYS:HD2	1.89	0.41
22:BY:68:TRP:CZ3	35:Bl:386:LEU:HA	2.56	0.41
24:Ba:96:ALA:CB	27:Bd:55:TYR:H	2.34	0.41
24:Ba:106:VAL:HA	24:Ba:107:PRO:HD2	1.82	0.41
24:Ba:109:HIS:O	24:Ba:112:TYR:HD2	2.03	0.41
25:Bb:31:ARG:HH12	39:Bp:116:PRO:HG2	1.85	0.41
25:Bb:110:ILE:HD12	25:Bb:110:ILE:HA	1.89	0.41
26:Bc:65:TYR:CE2	26:Bc:77:LYS:HG3	2.55	0.41
26:Bc:119:THR:HB	38:Bo:13:THR:HG23	2.02	0.41
26:Bc:168:LEU:HD12	26:Bc:169:GLU:N	2.36	0.41
27:Bd:162:LYS:O	27:Bd:165:LYS:HB3	2.20	0.41
29:Bf:34:PRO:HG3	44:Bw:342:GLY:HA2	2.03	0.41
32:Bi:287:LEU:HD11	40:Br:158:LEU:HD12	2.02	0.41
34:Bk:3:LEU:CD1	34:Bk:3:LEU:C	2.94	0.41
34:Bk:31:LEU:HD21	36:Bm:67:PHE:CE2	2.56	0.41
35:Bl:188:TRP:O	35:Bl:192:HIS:HB2	2.20	0.41
35:Bl:456:ARG:NH2	35:Bl:456:ARG:CB	2.79	0.41
35:Bl:536:THR:OG1	35:Bl:537:ILE:N	2.53	0.41
35:Bl:562:LEU:O	35:Bl:566:ILE:HD12	2.21	0.41
35:Bl:564:LYS:HG3	38:Bo:77:TYR:OH	2.21	0.41
36:Bm:38:VAL:O	36:Bm:42:ILE:HG13	2.21	0.41
37:Bn:51:PRO:O	37:Bn:53:GLU:HG3	2.20	0.41
39:Bp:31:CYS:O	39:Bp:33:GLN:N	2.54	0.41
39:Bp:124:GLN:HA	39:Bp:127:LYS:NZ	2.36	0.41
39:Bp:158:ARG:O	39:Bp:162:ASP:HB2	2.21	0.41
40:Br:89:LEU:O	40:Br:93:LYS:HG3	2.20	0.41
40:Br:121:PHE:O	40:Br:125:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Bs:55:LEU:HD13	41:Bs:221:ALA:HB2	2.01	0.41
41:Bs:173:TRP:HZ3	41:Bs:262:LYS:HE2	1.85	0.41
41:Bs:273:ILE:HG23	41:Bs:277:TYR:HD2	1.86	0.41
41:Bs:275:THR:OG1	41:Bs:276:ALA:N	2.53	0.41
42:Bu:24:VAL:CG2	42:Bu:86:TRP:HE1	2.34	0.41
46:By:5:MET:CE	55:B7:42:PRO:HA	2.44	0.41
48:B0:137:LYS:O	48:B0:145:TRP:HE3	2.03	0.41
55:B7:13:TYR:O	55:B7:14:GLY:C	2.63	0.41
1:A:202:GLY:O	12:M:200:ARG:NH2	2.42	0.41
1:A:382:CYS:HA	12:M:75:CYS:H	1.86	0.41
5:F:16:LEU:HD12	5:F:68:ARG:O	2.21	0.41
6:G:82:ARG:O	6:G:86:VAL:HG23	2.21	0.41
9:J:62:THR:HG21	73:J:401:NDP:O1X	2.21	0.41
12:M:130:ILE:H	12:M:130:ILE:HG12	1.69	0.41
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.41
16:Q:290:GLY:C	16:Q:294:ARG:HE	2.28	0.41
76:W:201:PEE:H22	76:W:201:PEE:H28	1.50	0.41
25:b:111:LEU:C	25:b:113:THR:N	2.78	0.41
26:c:162:PRO:O	26:c:166:LEU:HD12	2.21	0.41
27:d:107:CYS:HG	27:d:119:CYS:CB	2.34	0.41
28:e:67:TYR:CE2	40:r:428:PRO:HG2	2.56	0.41
35:l:543:LEU:HD23	35:l:543:LEU:HA	1.93	0.41
38:o:27:PRO:HG2	68:AY:218:GLU:CD	2.45	0.41
41:s:2:PRO:O	41:s:5:ASN:HB2	2.20	0.41
44:w:42:HIS:O	44:w:46:GLY:N	2.54	0.41
45:x:276:ALA:O	45:x:280:ILE:HG13	2.21	0.41
48:0:96:LEU:HD23	48:0:96:LEU:HA	1.94	0.41
48:0:130:PRO:O	48:0:136:ALA:HB2	2.21	0.41
53:5:29:LEU:HD23	53:5:29:LEU:HA	1.85	0.41
57:9:13:LYS:HD3	57:9:13:LYS:N	2.35	0.41
57:9:37:LEU:HD23	57:9:37:LEU:HA	1.84	0.41
75:AH:403:CDL:H311	75:AH:403:CDL:H341	1.79	0.41
66:AJ:252:ASP:HA	66:AJ:253:PRO:HD2	1.84	0.41
66:AJ:316:MET:HA	66:AJ:322:GLN:HE21	1.86	0.41
67:AK:79:THR:HG23	67:AK:205:LEU:HD23	2.02	0.41
67:AK:181:ALA:O	67:AK:254:ARG:N	2.41	0.41
68:AL:294:PRO:HG3	68:AL:448:TYR:CE1	2.56	0.41
59:AO:14:VAL:HA	67:AW:113:THR:HA	2.01	0.41
66:AV:349:ILE:HG23	66:AV:350:ILE:N	2.36	0.41
67:AW:177:LEU:HD21	67:AW:272:VAL:HG21	2.02	0.41
67:AW:205:LEU:O	67:AW:209:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:261:GLN:H	67:AW:444:LEU:HD12	1.85	0.41
2:BB:155:PHE:HB2	69:BB:302:SF4:S2	2.61	0.41
4:BE:84:ILE:HD13	15:BP:177:PHE:CE1	2.56	0.41
5:BF:20:ARG:CG	5:BF:66:TRP:HB2	2.51	0.41
5:BF:22:HIS:ND1	5:BF:64:LYS:HD2	2.36	0.41
5:BF:89:ARG:HD2	5:BF:92:GLU:OE2	2.21	0.41
12:BM:568:TYR:HB2	12:BM:580:ALA:CB	2.51	0.41
13:BN:117:VAL:HG11	13:BN:122:GLU:HB2	2.02	0.41
16:BQ:80:ILE:HG22	16:BQ:81:THR:N	2.35	0.41
17:BS:43:TYR:HB2	36:Bm:132:SER:O	2.21	0.41
20:BV:139:PRO:O	20:BV:141:VAL:HG23	2.21	0.41
6:BX:113:LEU:HD12	6:BX:114:ASP:N	2.36	0.41
22:BY:75:HIS:HA	22:BY:75:HIS:HD1	1.82	0.41
25:Bb:119:PRO:HB2	43:Bv:40:VAL:HG13	2.01	0.41
26:Bc:49:ALA:HA	26:Bc:59:VAL:HG13	2.03	0.41
26:Bc:161:TYR:HA	26:Bc:162:PRO:HD3	1.84	0.41
26:Bc:162:PRO:O	26:Bc:166:LEU:HD12	2.21	0.41
27:Bd:35:VAL:C	27:Bd:38:PRO:HD2	2.46	0.41
71:Bg:203:PLX:H1B3	71:Bg:203:PLX:H22	1.74	0.41
32:Bi:61:LEU:O	32:Bi:65:THR:HG23	2.21	0.41
33:Bj:36:PRO:HA	41:Bs:214:GLU:OE2	2.21	0.41
34:Bk:46:LEU:HD22	36:Bm:46:PHE:CE2	2.56	0.41
34:Bk:97:GLN:N	35:Bl:579:THR:OG1	2.40	0.41
35:Bl:33:PRO:HA	35:Bl:118:PHE:CD2	2.56	0.41
35:Bl:417:SER:HB3	35:Bl:493:VAL:CG1	2.51	0.41
35:Bl:493:VAL:O	35:Bl:496:LEU:HB3	2.21	0.41
36:Bm:64:MET:HB2	41:Bs:114:TYR:OH	2.21	0.41
37:Bn:43:MET:HE3	37:Bn:43:MET:HB2	1.86	0.41
41:Bs:59:GLU:HA	41:Bs:60:PRO:HD3	1.93	0.41
41:Bs:195:ARG:HG3	41:Bs:196:ALA:N	2.36	0.41
42:Bu:29:ALA:HA	42:Bu:32:TYR:HB3	2.03	0.41
44:Bw:42:HIS:O	44:Bw:46:GLY:N	2.54	0.41
45:Bx:173:PRO:HA	45:Bx:174:PRO:HD3	1.96	0.41
45:Bx:461:SER:O	45:Bx:465:VAL:HG13	2.20	0.41
46:By:164:ALA:HB2	46:By:171:LYS:HD3	2.03	0.41
47:Bz:6:HIS:CD2	47:Bz:8:TYR:HB2	2.56	0.41
47:Bz:146:TRP:CE2	51:B3:17:ARG:HB2	2.56	0.41
50:B2:16:LEU:O	50:B2:20:VAL:HG13	2.21	0.41
54:B6:12:PHE:O	54:B6:23:LYS:HE2	2.21	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.40
2:B:120:ILE:O	2:B:121:CYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40
12:M:522:GLN:HE21	12:M:526:LEU:HG	1.85	0.40
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.40
14:O:99:ASN:O	14:O:103:GLU:HG3	2.21	0.40
16:Q:153:LEU:O	16:Q:157:LYS:HG3	2.21	0.40
16:Q:303:ARG:HG3	16:Q:401:GLU:HG3	2.03	0.40
16:Q:316:PHE:HB2	16:Q:339:GLN:CG	2.51	0.40
76:W:201:PEE:H53	76:W:201:PEE:C16	2.46	0.40
76:W:201:PEE:H36	33:j:7:LEU:CD2	2.47	0.40
22:Y:47:PHE:HE2	22:Y:50:LEU:HD11	1.87	0.40
24:a:180:ASP:HB3	31:h:24:GLU:HG3	2.02	0.40
25:b:115:GLU:CG	25:b:116:VAL:N	2.82	0.40
28:e:74:HIS:HB3	28:e:87:MET:SD	2.62	0.40
29:f:34:PRO:HG3	44:w:342:GLY:HA2	2.03	0.40
32:i:73:ALA:HA	32:i:97:MET:HE3	2.03	0.40
34:k:46:LEU:HD23	34:k:46:LEU:HA	1.88	0.40
35:l:3:MET:CE	35:l:53:MET:HE3	2.51	0.40
35:l:311:GLY:O	35:l:315:VAL:HG23	2.21	0.40
40:r:80:SER:O	40:r:81:GLN:C	2.64	0.40
41:s:193:THR:O	41:s:194:ASN:HB2	2.20	0.40
41:s:195:ARG:HG3	41:s:196:ALA:H	1.86	0.40
41:s:195:ARG:HG3	41:s:196:ALA:N	2.36	0.40
41:s:273:ILE:HG23	41:s:277:TYR:HD2	1.86	0.40
45:x:314:ILE:HB	45:x:315:PRO:CD	2.51	0.40
48:0:86:MET:O	55:7:25:CYS:HB2	2.20	0.40
50:2:30:PRO:HG2	50:2:31:TYR:CD1	2.56	0.40
52:4:17:ASP:OD1	52:4:19:ARG:HG2	2.22	0.40
63:AF:76:LEU:HD12	63:AF:77:PRO:HD2	2.02	0.40
65:AH:85:SER:OG	65:AH:86:ASP:N	2.52	0.40
65:AH:228:ARG:NH1	65:AH:229:GLU:HB3	2.36	0.40
66:AJ:345:TYR:N	66:AJ:346:PRO:HD2	2.36	0.40
71:AQ:101:PLX:H261	75:AY:501:CDL:H552	2.03	0.40
67:AW:67:ALA:HA	67:AW:71:TYR:CD2	2.56	0.40
67:AW:299:VAL:HG22	68:AY:120:LEU:HG	2.03	0.40
68:AY:74:TRP:CZ3	68:AY:232:ALA:HB3	2.56	0.40
3:BC:140:GLN:HA	33:Bj:37:TYR:CE2	2.57	0.40
7:BH:21:HIS:O	7:BH:25:ARG:HG3	2.22	0.40
9:BJ:62:THR:HG21	73:BJ:401:NDP:O1X	2.21	0.40
12:BM:342:ALA:HB3	12:BM:368:THR:HA	2.03	0.40
12:BM:382:ARG:NE	12:BM:527:ASP:OD1	2.54	0.40
12:BM:517:HIS:HB2	12:BM:599:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:645:ARG:O	12:BM:649:VAL:HG12	2.21	0.40
13:BN:39:VAL:HG12	13:BN:40:GLY:O	2.21	0.40
21:BW:57:ARG:NH2	41:Bs:168:THR:HG22	2.36	0.40
22:BY:62:SER:O	22:BY:65:MET:HB3	2.21	0.40
22:BY:81:LEU:HB3	35:Bl:480:THR:OG1	2.20	0.40
23:BZ:61:VAL:HB	35:Bl:432:THR:O	2.21	0.40
25:Bb:111:LEU:C	25:Bb:113:THR:H	2.27	0.40
71:Bb:201:PLX:P1	71:Bb:201:PLX:O6	2.79	0.40
26:Bc:88:PRO:HB2	39:Bp:86:PRO:HG2	2.03	0.40
26:Bc:157:GLY:HA2	26:Bc:158:PRO:HD3	1.76	0.40
30:Bg:29:ARG:O	30:Bg:33:ILE:HG13	2.21	0.40
30:Bg:51:PRO:HG2	30:Bg:55:ALA:CB	2.50	0.40
30:Bg:86:ASP:CG	42:Bu:166:ARG:HH22	2.27	0.40
32:Bi:86:MET:HE2	32:Bi:144:GLN:OE1	2.20	0.40
32:Bi:112:HIS:HB2	32:Bi:184:ILE:HD13	2.03	0.40
32:Bi:224:SER:HB2	32:Bi:229:LEU:CB	2.39	0.40
32:Bi:271:THR:HG22	32:Bi:276:LEU:CD2	2.50	0.40
32:Bi:339:ILE:HG22	32:Bi:342:PHE:CB	2.42	0.40
35:Bl:3:MET:CE	35:Bl:53:MET:HE3	2.51	0.40
35:Bl:39:ILE:O	35:Bl:43:THR:HG23	2.21	0.40
35:Bl:44:PHE:O	35:Bl:47:SER:OG	2.24	0.40
75:Bn:101:CDL:H711	75:Bn:101:CDL:H741	1.60	0.40
38:Bo:6:TYR:HE2	38:Bo:14:LEU:HA	1.85	0.40
40:Br:133:ILE:O	40:Br:142:ARG:HD2	2.21	0.40
40:Br:196:TRP:NE1	40:Br:250:LEU:HD13	2.36	0.40
45:Bx:354:THR:HG21	45:Bx:376:HIS:HA	2.03	0.40
47:Bz:182:TYR:O	51:B3:72:ASN:HB2	2.21	0.40
48:B0:102:TYR:HD2	57:B9:35:TYR:HE1	1.68	0.40
50:B2:30:PRO:HG2	50:B2:31:TYR:CD1	2.57	0.40
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	0.40
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.40
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.40
2:B:103:ARG:HH21	18:T:64:ASN:HD21	1.69	0.40
5:F:14:LEU:N	5:F:17:ARG:HH12	2.20	0.40
7:H:21:HIS:O	7:H:25:ARG:HG3	2.22	0.40
12:M:128:CYS:HA	69:M:801:SF4:S4	2.62	0.40
12:M:198:THR:CG2	14:O:117:THR:HG21	2.52	0.40
14:O:156:LEU:HD13	14:O:158:ILE:HD12	2.03	0.40
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.40
16:Q:169:TRP:C	16:Q:351:MET:HE2	2.46	0.40
16:Q:241:MET:HB3	21:W:16:TYR:OH	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:331:LEU:HA	16:Q:331:LEU:HD23	1.84	0.40
17:S:47:LEU:O	17:S:50:ARG:HB3	2.20	0.40
18:T:41:HIS:HB3	18:T:67:PHE:CE1	2.57	0.40
18:T:52:ARG:O	18:T:55:ARG:HG2	2.20	0.40
18:T:80:VAL:O	18:T:121:GLN:HA	2.20	0.40
24:a:98:LEU:HB2	27:d:57:TYR:CE1	2.40	0.40
25:b:99:GLU:HG2	35:l:61:VAL:HG22	2.03	0.40
30:g:11:ARG:O	30:g:13:LEU:N	2.54	0.40
32:i:61:LEU:O	32:i:65:THR:HG23	2.21	0.40
34:k:1:MET:CB	34:k:4:ILE:CD1	2.86	0.40
34:k:3:LEU:C	34:k:3:LEU:CD1	2.94	0.40
34:k:7:ASN:ND2	36:m:9:SER:CA	2.83	0.40
35:l:449:THR:O	35:l:451:LEU:N	2.55	0.40
35:l:562:LEU:O	35:l:566:ILE:HD12	2.21	0.40
38:o:124:THR:C	38:o:126:HIS:H	2.29	0.40
39:p:158:ARG:O	39:p:162:ASP:HB2	2.21	0.40
39:p:158:ARG:O	39:p:159:LYS:HB2	2.21	0.40
40:r:130:LEU:HD21	40:r:149:PHE:HD2	1.86	0.40
41:s:208:VAL:O	41:s:209:SER:OG	2.35	0.40
41:s:277:TYR:HA	41:s:278:PRO:HD2	1.69	0.40
44:w:86:PHE:HE2	44:w:146:ALA:HB2	1.86	0.40
44:w:163:ILE:HD12	44:w:163:ILE:HA	1.98	0.40
45:x:23:GLY:HA3	45:x:73:ILE:HG13	2.03	0.40
45:x:461:SER:O	45:x:465:VAL:HG13	2.21	0.40
46:y:196:CYS:HB2	46:y:207:MET:HG3	2.04	0.40
47:z:146:TRP:CE2	51:3:17:ARG:HB2	2.56	0.40
47:z:228:THR:O	47:z:232:HIS:HD2	2.04	0.40
52:4:65:PRO:HG2	52:4:68:TRP:CG	2.56	0.40
54:6:21:HIS:CD2	54:6:22:LEU:HG	2.57	0.40
57:9:35:TYR:HD2	57:9:36:HIS:CE1	2.39	0.40
58:AA:17:TYR:CD1	68:AL:275:ILE:HG12	2.56	0.40
58:AA:78:TYR:CD1	62:AE:65:GLU:CG	3.04	0.40
66:AJ:301:LEU:HA	66:AJ:304:ILE:HD12	2.03	0.40
68:AL:170:ARG:O	68:AL:174:GLU:HG3	2.20	0.40
60:AP:125:VAL:HG21	71:AQ:101:PLX:H141	2.03	0.40
71:AQ:101:PLX:H271	71:AQ:101:PLX:H24	1.83	0.40
66:AV:3:PRO:HG2	66:AV:6:LYS:HG2	2.03	0.40
66:AV:128:PHE:O	66:AV:132:VAL:HG23	2.22	0.40
67:AW:36:GLN:HG3	67:AW:37:ASP:O	2.21	0.40
67:AW:438:MET:HB2	67:AW:450:VAL:HG23	2.03	0.40
68:AY:163:LYS:O	68:AY:167:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:387:GLU:HG2	12:BM:119:PHE:O	2.20	0.40
1:BA:391:TRP:O	1:BA:395:VAL:HG23	2.22	0.40
2:BB:146:ASP:OD2	2:BB:149:LYS:HE2	2.21	0.40
3:BC:137:VAL:HA	3:BC:140:GLN:OE1	2.20	0.40
9:BJ:202:LYS:N	9:BJ:263:PHE:O	2.54	0.40
11:BL:117:THR:OG1	15:BP:229:GLU:HB2	2.22	0.40
11:BL:123:ASN:HB3	15:BP:232:LYS:HD2	2.02	0.40
12:BM:198:THR:CG2	14:BO:117:THR:HG21	2.52	0.40
12:BM:234:LYS:N	12:BM:235:PRO:HD2	2.36	0.40
14:BO:168:LEU:HD22	14:BO:169:PHE:CE2	2.56	0.40
15:BP:52:ASP:O	15:BP:56:LYS:HG3	2.22	0.40
16:BQ:316:PHE:HB2	16:BQ:339:GLN:CG	2.51	0.40
16:BQ:333:ARG:HE	16:BQ:455:ASP:CG	2.29	0.40
17:BS:66:LEU:HD11	42:Bu:82:PHE:CD2	2.56	0.40
19:BU:56:PRO:HB3	42:Bu:129:THR:OG1	2.20	0.40
23:BZ:16:LEU:HA	23:BZ:17:PRO:HD3	1.95	0.40
24:Ba:54:LEU:HD23	24:Ba:54:LEU:HA	1.81	0.40
24:Ba:115:HIS:CG	24:Ba:116:PRO:HD2	2.56	0.40
24:Ba:170:TYR:CD2	30:Bg:5:ARG:HB3	2.56	0.40
32:Bi:131:LEU:HA	32:Bi:131:LEU:HD23	1.85	0.40
32:Bi:193:VAL:HB	32:Bi:201:THR:HG22	2.02	0.40
32:Bi:318:GLU:OE2	44:Bw:341:PRO:HD3	2.21	0.40
35:Bl:311:GLY:O	35:Bl:315:VAL:HG23	2.21	0.40
35:Bl:512:LYS:CG	54:B6:16:ASN:HB2	2.51	0.40
35:Bl:536:THR:O	35:Bl:539:TYR:HB3	2.20	0.40
71:Br:502:PLX:H1B2	71:Br:502:PLX:H22	1.53	0.40
42:Bu:26:LYS:HB2	42:Bu:26:LYS:HE3	1.89	0.40
44:Bw:77:ILE:HG23	44:Bw:81:LEU:HD13	2.02	0.40
46:By:215:PRO:HD3	53:B5:60:PHE:CD1	2.57	0.40
47:Bz:42:LEU:HD12	47:Bz:42:LEU:HA	1.65	0.40
50:B2:19:GLU:HB3	50:B2:98:HIS:CE1	2.57	0.40
55:B7:24:PHE:CE1	55:B7:28:VAL:HG21	2.56	0.40
1:A:382:CYS:SG	1:A:424:ILE:HG22	2.62	0.40
2:B:186:GLU:HG2	18:T:62:GLU:O	2.21	0.40
4:E:78:VAL:O	4:E:82:LEU:HD13	2.20	0.40
9:J:168:SER:CA	9:J:184:LYS:CE	2.99	0.40
9:J:336:GLU:OE1	9:J:336:GLU:N	2.55	0.40
11:L:163:ASN:O	11:L:171:ARG:N	2.55	0.40
12:M:483:ARG:O	12:M:483:ARG:HG3	2.21	0.40
15:P:61:PHE:O	15:P:64:TYR:HB3	2.20	0.40
16:Q:71:PRO:HB2	16:Q:72:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:85:ILE:O	18:T:100:TYR:HA	2.22	0.40
30:g:29:ARG:NH2	42:u:172:LYS:HB3	2.36	0.40
32:i:146:SER:HA	32:i:149:LEU:HD13	2.04	0.40
32:i:342:PHE:CD2	32:i:343:MET:HE2	2.57	0.40
33:j:36:PRO:HA	41:s:214:GLU:OE2	2.21	0.40
33:j:57:LEU:HD23	33:j:57:LEU:HA	1.89	0.40
34:k:31:LEU:HD21	36:m:67:PHE:CE2	2.56	0.40
35:l:33:PRO:HA	35:l:118:PHE:CD2	2.56	0.40
35:l:39:ILE:O	35:l:43:THR:HG23	2.22	0.40
40:r:233:ALA:HB2	40:r:324:SER:HB3	2.04	0.40
44:w:72:LYS:HD2	44:w:75:LYS:HD2	2.03	0.40
45:x:34:SER:HB3	45:x:61:HIS:CE1	2.57	0.40
45:x:240:HIS:O	45:x:241:PRO:C	2.64	0.40
46:y:215:PRO:HD3	53:5:60:PHE:CD1	2.57	0.40
47:z:233:PHE:HA	47:z:236:GLU:HG3	2.03	0.40
49:1:104:LEU:HD23	49:1:104:LEU:HA	1.88	0.40
50:2:19:GLU:HB3	50:2:98:HIS:CE1	2.57	0.40
75:AJ:405:CDL:H142	75:AJ:405:CDL:C38	2.52	0.40
67:AK:182:TYR:CD2	67:AK:186:LEU:HB2	2.57	0.40
67:AK:271:PHE:CE2	67:AK:351:ILE:HD12	2.57	0.40
59:AO:20:ARG:NH2	59:AO:48:PRO:HG2	2.36	0.40
60:AP:209:GLU:HG2	60:AP:210:TRP:CD1	2.56	0.40
66:AV:372:ILE:O	66:AV:376:MET:HG2	2.22	0.40
68:AY:61:SER:HA	68:AY:233:ALA:O	2.21	0.40
68:AY:334:ALA:H	68:AY:336:LYS:H	1.68	0.40
68:AY:423:ARG:O	68:AY:424:ILE:CB	2.70	0.40
1:BA:32:PHE:HB3	1:BA:294:VAL:HA	2.02	0.40
3:BC:81:PRO:HA	3:BC:119:VAL:HG13	2.03	0.40
6:BG:82:ARG:O	6:BG:86:VAL:HG23	2.21	0.40
9:BJ:329:LEU:HD13	9:BJ:332:LEU:HD12	2.03	0.40
11:BL:154:LYS:HG2	12:BM:279:GLU:HG3	2.02	0.40
11:BL:162:ALA:HA	11:BL:168:LYS:HZ1	1.87	0.40
12:BM:314:LEU:HD22	12:BM:583:ILE:HD12	2.02	0.40
12:BM:598:ASN:HD22	12:BM:602:ARG:NH1	2.19	0.40
16:BQ:153:LEU:O	16:BQ:157:LYS:HG3	2.21	0.40
16:BQ:383:LYS:HA	16:BQ:383:LYS:HD2	1.87	0.40
17:BS:55:SER:C	17:BS:64:LYS:HZ1	2.28	0.40
20:BV:114:ALA:HB1	20:BV:118:PHE:CE2	2.56	0.40
22:BY:47:PHE:HE2	22:BY:50:LEU:HD11	1.87	0.40
22:BY:61:PHE:CZ	35:Bl:455:LYS:HG2	2.56	0.40
24:Ba:96:ALA:HB2	27:Bd:55:TYR:HB2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Bb:88:TYR:HB2	71:Bb:201:PLX:C1B	2.51	0.40
28:Be:74:HIS:HB3	28:Be:87:MET:SD	2.62	0.40
32:Bi:2:ASN:HA	32:Bi:3:PRO:HD2	1.87	0.40
32:Bi:19:ILE:HD12	32:Bi:35:MET:HE1	2.02	0.40
33:Bj:47:ALA:HB1	41:Bs:129:LEU:HD11	2.03	0.40
33:Bj:54:LYS:HB3	33:Bj:113:TRP:HE1	1.85	0.40
35:Bl:291:CYS:O	35:Bl:295:GLN:HG2	2.22	0.40
35:Bl:522:PHE:HA	35:Bl:528:PHE:CE2	2.56	0.40
38:Bo:23:TYR:O	38:Bo:25:ILE:HG12	2.21	0.40
40:Br:130:LEU:HD21	40:Br:149:PHE:HD2	1.86	0.40
45:Bx:276:ALA:O	45:Bx:280:ILE:HG13	2.21	0.40
54:B6:21:HIS:CD2	54:B6:22:LEU:HG	2.57	0.40
1:A:93:PHE:HA	1:A:94:PRO:HD3	1.97	0.40
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.57	0.40
2:B:99:HIS:NE2	2:B:167:GLU:OE1	2.55	0.40
2:B:155:PHE:HB2	69:B:302:SF4:S2	2.61	0.40
3:C:152:SER:N	3:C:182:GLY:O	2.54	0.40
5:F:22:HIS:ND1	5:F:64:LYS:HD2	2.36	0.40
9:J:202:LYS:N	9:J:263:PHE:O	2.54	0.40
12:M:401:LEU:HD13	12:M:462:PHE:CE2	2.56	0.40
14:O:198:ALA:O	14:O:202:GLU:HG2	2.21	0.40
16:Q:198:THR:HG21	41:s:275:THR:HB	2.03	0.40
17:S:43:TYR:HB2	36:m:132:SER:O	2.21	0.40
19:U:56:PRO:HB3	42:u:129:THR:OG1	2.20	0.40
23:Z:52:ARG:HH11	23:Z:53:TYR:HE1	1.70	0.40
30:g:29:ARG:O	30:g:33:ILE:HG13	2.22	0.40
32:i:57:ILE:HD11	34:k:81:ILE:HD11	2.04	0.40
33:j:47:ALA:HB1	41:s:129:LEU:HD11	2.03	0.40
35:l:362:LEU:HA	35:l:365:THR:OG1	2.22	0.40
35:l:417:SER:HB3	35:l:493:VAL:CG1	2.51	0.40
36:m:64:MET:HB2	41:s:114:TYR:OH	2.21	0.40
36:m:102:LEU:HD23	36:m:102:LEU:HA	1.86	0.40
39:p:48:PHE:CZ	72:p:201:8Q1:C8	2.99	0.40
39:p:124:GLN:HA	39:p:127:LYS:NZ	2.36	0.40
40:r:235:LEU:O	40:r:238:LEU:HB3	2.22	0.40
41:s:102:LEU:HD23	41:s:102:LEU:HA	1.87	0.40
42:u:83:THR:O	42:u:87:THR:HG23	2.20	0.40
44:w:289:ARG:O	44:w:292:TYR:HB3	2.21	0.40
58:AA:28:PRO:HB2	58:AA:29:HIS:ND1	2.37	0.40
64:AG:45:VAL:HG21	64:AG:48:ILE:HB	2.02	0.40
68:AL:91:TYR:O	68:AL:94:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:301:ASN:O	68:AL:305:GLN:HG2	2.21	0.40
65:AU:194:PRO:HA	65:AU:195:PRO:HD3	1.85	0.40
65:AU:237:PHE:CZ	81:AU:402:HEC:O2D	2.75	0.40
66:AV:105:GLY:HA2	66:AV:107:PHE:CE2	2.56	0.40
66:AV:132:VAL:HG11	66:AV:178:PHE:CD2	2.57	0.40
68:AY:377:MET:HE2	68:AY:477:TRP:N	2.37	0.40
2:BB:84:TYR:CD1	2:BB:85:PRO:HA	2.56	0.40
2:BB:103:ARG:HH21	18:BT:64:ASN:HD21	1.69	0.40
71:BB:303:PLX:H112	71:BB:303:PLX:H81	1.68	0.40
5:BF:66:TRP:CZ2	12:BM:648:GLU:HB2	2.57	0.40
8:BI:65:PRO:HD3	15:BP:245:TYR:CE2	2.56	0.40
9:BJ:168:SER:CA	9:BJ:184:LYS:CE	2.99	0.40
12:BM:646:LEU:O	12:BM:651:PRO:HA	2.21	0.40
15:BP:77:GLN:HB2	15:BP:85:GLU:HB2	2.03	0.40
15:BP:114:LEU:HG	15:BP:130:TYR:CE1	2.57	0.40
16:BQ:120:THR:O	16:BQ:124:ILE:HG13	2.22	0.40
16:BQ:182:ASN:ND2	16:BQ:404:LYS:HE3	2.35	0.40
16:BQ:316:PHE:HD1	16:BQ:339:GLN:HE21	1.67	0.40
16:BQ:393:PRO:HG3	16:BQ:415:GLY:HA3	2.04	0.40
21:BW:111:PHE:CE2	21:BW:117:VAL:HG21	2.56	0.40
26:Bc:153:TYR:CB	35:Bl:403:TYR:HD1	2.35	0.40
27:Bd:123:VAL:O	27:Bd:127:THR:HG23	2.21	0.40
30:Bg:45:ASN:HD21	30:Bg:60:GLN:NE2	2.19	0.40
32:Bi:155:LEU:HD23	32:Bi:155:LEU:HA	1.94	0.40
32:Bi:221:LEU:HA	32:Bi:221:LEU:HD23	1.84	0.40
32:Bi:307:MET:O	44:Bw:319:ILE:HD12	2.20	0.40
32:Bi:339:ILE:O	32:Bi:342:PHE:HB3	2.22	0.40
35:Bl:244:SER:HA	35:Bl:248:HIS:CD2	2.56	0.40
35:Bl:362:LEU:HA	35:Bl:365:THR:OG1	2.21	0.40
36:Bm:118:PHE:CE1	36:Bm:121:VAL:HB	2.56	0.40
40:Br:233:ALA:HB2	40:Br:324:SER:HB3	2.04	0.40
42:Bu:149:ASP:HA	42:Bu:150:PRO:HD3	1.88	0.40
44:Bw:139:ARG:HA	44:Bw:142:GLN:CG	2.52	0.40
45:Bx:244:TYR:HD1	45:Bx:244:TYR:HA	1.81	0.40
46:By:168:LEU:HD13	46:By:184:LEU:HG	2.04	0.40
47:Bz:146:TRP:NE1	51:B3:17:ARG:HB2	2.35	0.40
50:B2:77:GLY:O	50:B2:90:LYS:NZ	2.54	0.40
1:A:159:ARG:HH21	1:A:161:GLU:HG2	1.87	0.40
2:B:90:PRO:O	2:B:91:LEU:HD12	2.21	0.40
12:M:234:LYS:N	12:M:235:PRO:HD2	2.36	0.40
15:P:56:LYS:O	15:P:59:SER:OG	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:33:SER:HB3	18:T:45:VAL:HG21	2.03	0.40
20:V:139:PRO:O	20:V:141:VAL:HG23	2.21	0.40
21:W:43:LEU:HD23	21:W:43:LEU:HA	1.91	0.40
21:W:81:ARG:NH2	42:u:64:ASN:HD21	2.19	0.40
22:Y:61:PHE:CZ	35:l:455:LYS:HG2	2.56	0.40
24:a:96:ALA:CB	27:d:55:TYR:H	2.34	0.40
24:a:155:GLU:HG2	30:g:100:PHE:HE1	1.86	0.40
25:b:111:LEU:C	25:b:113:THR:H	2.27	0.40
26:c:154:GLN:HE22	43:v:3:ALA:HB2	1.86	0.40
27:d:13:PRO:HA	27:d:14:PRO:HD3	1.95	0.40
27:d:123:VAL:O	27:d:127:THR:HG23	2.21	0.40
28:e:62:GLU:CD	38:o:57:ARG:HH12	2.30	0.40
30:g:51:PRO:HG2	30:g:55:ALA:CB	2.50	0.40
32:i:232:ARG:NH1	44:w:306:ASN:O	2.50	0.40
34:k:31:LEU:HD23	34:k:31:LEU:HA	1.75	0.40
35:l:49:PHE:HB2	35:l:50:PRO:HD3	2.03	0.40
35:l:70:THR:HA	35:l:75:GLN:HB2	2.04	0.40
35:l:450:LEU:O	35:l:450:LEU:CG	2.70	0.40
35:l:452:ASN:CB	35:l:453:PRO:HD3	2.51	0.40
35:l:512:LYS:CG	54:6:16:ASN:HB2	2.51	0.40
40:r:133:ILE:O	40:r:142:ARG:HD2	2.21	0.40
44:w:77:ILE:HG23	44:w:81:LEU:HD13	2.03	0.40
45:x:442:ASP:OD2	46:y:134:ARG:NH2	2.54	0.40
47:z:160:LEU:HD12	47:z:160:LEU:HA	1.94	0.40
59:AB:9:GLY:HA2	67:AK:326:PHE:CE1	2.57	0.40
60:AC:80:HIS:CD2	60:AC:80:HIS:C	2.99	0.40
60:AC:81:THR:O	60:AC:83:ILE:N	2.48	0.40
60:AC:248:ARG:HG2	60:AC:257:ASN:ND2	2.36	0.40
60:AC:269:ASP:OD1	60:AC:270:MET:HG2	2.22	0.40
63:AF:49:ARG:HE	63:AF:49:ARG:CA	2.34	0.40
76:AH:401:PEE:H70	71:AL:501:PLX:H212	2.03	0.40
66:AJ:312:GLN:HG3	66:AJ:379:TRP:CH2	2.57	0.40
67:AK:257:GLU:OE2	67:AK:450:VAL:CG2	2.56	0.40
67:AK:277:VAL:HA	67:AK:278:ALA:HA	1.99	0.40
67:AK:288:VAL:O	67:AK:292:VAL:HG23	2.21	0.40
60:AP:125:VAL:HG21	71:AQ:101:PLX:H122	2.03	0.40
60:AP:163:LYS:NZ	60:AP:165:MET:HB2	2.36	0.40
60:AP:173:PRO:HD2	60:AP:216:VAL:HG23	2.03	0.40
60:AP:184:ILE:HD13	60:AP:208:PRO:HB2	2.04	0.40
60:AP:248:ARG:HG2	60:AP:257:ASN:ND2	2.35	0.40
61:AQ:21:PHE:CE2	61:AQ:25:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:AT:38:TRP:CD1	64:AT:40:LEU:HG	2.56	0.40
65:AU:237:PHE:CD1	65:AU:238:PRO:HD2	2.57	0.40
65:AU:321:TYR:CD2	65:AU:323:PRO:HD3	2.56	0.40
67:AW:126:LEU:HB3	68:AY:38:PHE:HZ	1.86	0.40
1:BA:126:LYS:HZ3	1:BA:246:GLU:HG3	1.86	0.40
1:BA:288:VAL:HG21	1:BA:303:HIS:CD2	2.57	0.40
1:BA:314:LEU:O	1:BA:329:LYS:HD2	2.21	0.40
1:BA:417:LYS:HA	1:BA:417:LYS:HD2	1.89	0.40
2:BB:62:THR:OG1	2:BB:63:GLU:N	2.53	0.40
2:BB:68:LEU:HD11	41:Bs:272:TRP:HE1	1.87	0.40
2:BB:90:PRO:O	2:BB:91:LEU:HD12	2.22	0.40
2:BB:102:ARG:HB2	2:BB:196:GLU:OE2	2.21	0.40
2:BB:169:PRO:HG3	2:BB:198:GLU:CG	2.51	0.40
2:BB:186:GLU:HG2	18:BT:62:GLU:O	2.21	0.40
3:BC:172:ARG:HH12	15:BP:209:GLU:CD	2.27	0.40
7:BH:45:ARG:O	7:BH:49:GLU:HG3	2.21	0.40
9:BJ:86:CYS:HB2	9:BJ:90:ASP:OD2	2.22	0.40
11:BL:88:GLN:NE2	12:BM:136:GLU:O	2.29	0.40
12:BM:83:GLU:HB2	12:BM:101:ASN:HB3	2.02	0.40
12:BM:401:LEU:HD13	12:BM:462:PHE:CE2	2.56	0.40
14:BO:118:PHE:HD2	14:BO:119:TYR:CE2	2.40	0.40
15:BP:100:LEU:O	15:BP:108:PHE:HD2	2.05	0.40
16:BQ:71:PRO:HB2	16:BQ:72:PRO:HD3	2.03	0.40
18:BT:85:ILE:O	18:BT:100:TYR:HA	2.22	0.40
18:BT:105:LYS:HB3	18:BT:107:THR:HG22	2.04	0.40
18:BT:111:THR:HA	18:BT:118:GLN:HA	2.04	0.40
21:BW:61:GLN:NE2	41:Bs:317:GLN:HA	2.36	0.40
22:BY:45:ARG:HG2	22:BY:45:ARG:O	2.22	0.40
27:Bd:111:GLU:OE2	27:Bd:118:ASN:CB	2.70	0.40
28:Be:67:TYR:CE2	40:Br:428:PRO:HG2	2.56	0.40
32:Bi:69:ILE:HD12	32:Bi:104:MET:HE1	2.01	0.40
35:Bl:173:LEU:HA	35:Bl:173:LEU:HD23	1.73	0.40
36:Bm:16:PHE:CD1	36:Bm:19:PHE:CE1	3.07	0.40
41:Bs:2:PRO:O	41:Bs:5:ASN:HB2	2.20	0.40
41:Bs:307:MET:N	41:Bs:308:PRO:HD2	2.37	0.40
44:Bw:65:ASN:OD1	44:Bw:66:ILE:N	2.55	0.40
45:Bx:34:SER:HB3	45:Bx:61:HIS:CE1	2.57	0.40
45:Bx:314:ILE:HB	45:Bx:315:PRO:CD	2.50	0.40
47:Bz:233:PHE:HA	47:Bz:236:GLU:HG3	2.03	0.40
51:B3:15:THR:O	51:B3:19:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	30
1	BA	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	30
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	59
2	BB	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	59
3	BC	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	21
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	21
4	BE	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	BF	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	BG	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	27
6	BX	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	16
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	27
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	16
7	BH	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	17
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	17
8	BI	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	12
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	12
9	BJ	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	30
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	30
10	BK	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
11	BL	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	21
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	21
12	BM	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	21
13	BN	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	16
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	16
14	BO	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	21
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	21
15	BP	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	15
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	15
16	BQ	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	38
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	38
17	BS	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	23
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	23
18	BT	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	17
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	17
19	BU	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	44
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	44
20	BV	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	29
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	29
21	BW	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	20
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	20
22	BY	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
23	BZ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	Ba	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	29
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	29
25	Bb	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	18
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	18
26	Bc	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	17
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	17
27	Bd	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	59
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Be	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	21
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	21
29	Bf	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	29
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	29
30	Bg	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	15
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	15
31	Bh	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	13
31	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	13
32	Bi	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
33	Bj	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	25
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	25
34	Bk	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	21
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	21
35	Bl	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	36
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	36
36	Bm	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	14
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	14
37	Bn	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	20
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	20
38	Bo	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	21
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	21
39	Bp	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	Br	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	31
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	31
41	Bs	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	24
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	24
42	Bu	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	23
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	23
43	Bv	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	24
44	Bw	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	24
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	24
45	Bx	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
46	By	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
47	Bz	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
48	B0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
49	B1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
50	B2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
51	B3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	40
52	B4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	40
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
53	B5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	20
54	B6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	20
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
55	B7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
56	B8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
57	B9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	26
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	15
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	6
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	25
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8	40
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	4	24
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	40
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	12	49
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16	54
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	54
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16	54
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16	54
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	10	44
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	10	44
68	AL	444/446 (100%)	403 (91%)	35 (8%)	6 (1%)	9	40
68	AY	444/446 (100%)	414 (93%)	22 (5%)	8 (2%)	6	34
All	All	23880/24216 (99%)	21833 (91%)	1487 (6%)	560 (2%)	7	28

All (560) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE

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Mol	Chain	Res	Type
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE
24	a	58	ARG
26	c	115	ASN
26	c	178	PRO
27	d	2	PRO
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
45	x	328	HIS
45	x	508	PRO
50	2	2	SER
50	2	87	THR
50	2	95	GLN
51	3	4	ALA
51	3	9	GLY
52	4	46	LYS
54	6	2	GLU
66	AJ	268	ILE
67	AK	241	ARG
59	AO	23	ALA
60	AP	141	SER

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Mol	Chain	Res	Type
68	AY	424	ILE
1	BA	63	TYR
1	BA	73	PRO
1	BA	379	CYS
2	BB	62	THR
12	BM	37	ASP
12	BM	47	THR
12	BM	178	GLN
12	BM	210	ILE
12	BM	369	GLU
13	BN	115	PHE
14	BO	232	THR
14	BO	246	GLN
15	BP	167	GLU
17	BS	60	TYR
18	BT	82	THR
19	BU	71	GLN
21	BW	34	SER
6	BX	155	TYR
22	BY	84	PHE
24	Ba	58	ARG
26	Bc	115	ASN
26	Bc	178	PRO
27	Bd	2	PRO
31	Bh	20	ILE
32	Bi	91	ASN
32	Bi	323	THR
33	Bj	24	LEU
33	Bj	26	GLN
34	Bk	52	HIS
35	Bl	450	LEU
36	Bm	115	VAL
36	Bm	116	VAL
36	Bm	118	PHE
37	Bn	55	VAL
40	Br	52	CYS
40	Br	346	GLN
44	Bw	57	SER
44	Bw	282	PRO
44	Bw	347	VAL
45	Bx	328	HIS
45	Bx	508	PRO

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Mol	Chain	Res	Type
50	B2	2	SER
50	B2	87	THR
50	B2	95	GLN
51	B3	4	ALA
51	B3	9	GLY
52	B4	46	LYS
54	B6	2	GLU
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE

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Mol	Chain	Res	Type
31	h	24	GLU
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS
51	3	5	LYS
60	AC	153	GLU
60	AC	255	PRO
66	AJ	157	GLY
67	AK	176	ASN
59	AO	38	PRO
60	AP	255	PRO
66	AV	157	GLY
66	AV	254	ASP
66	AV	266	PRO
67	AW	244	LEU
68	AY	312	GLY
68	AY	322	VAL
3	BC	84	PHE
3	BC	165	SER
4	BE	20	ILE
4	BE	127	ASP
6	BG	138	LEU
7	BH	105	GLU
8	BI	31	ILE
8	BI	93	LYS
8	BI	107	SER
9	BJ	87	ASP
11	BL	173	SER
12	BM	250	SER

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Mol	Chain	Res	Type
12	BM	482	GLN
12	BM	484	ASN
12	BM	562	LYS
12	BM	663	ASN
12	BM	676	ASN
13	BN	19	GLY
13	BN	76	ASP
14	BO	49	PRO
14	BO	160	VAL
16	BQ	104	GLU
16	BQ	117	HIS
18	BT	44	GLN
20	BV	135	VAL
20	BV	140	LYS
21	BW	11	PRO
22	BY	44	TYR
22	BY	51	THR
24	Ba	57	ILE
24	Ba	185	ALA
25	Bb	101	LYS
26	Bc	170	ARG
30	Bg	9	PRO
31	Bh	3	PHE
31	Bh	24	GLU
31	Bh	43	CYS
33	Bj	2	ASN
35	Bl	73	THR
36	Bm	122	GLY
37	Bn	52	SER
40	Br	45	ILE
40	Br	188	ASN
40	Br	250	LEU
40	Br	421	HIS
41	Bs	203	GLY
41	Bs	213	ILE
41	Bs	217	ALA
41	Bs	316	PRO
43	Bv	56	ARG
44	Bw	264	GLN
44	Bw	285	LYS
51	B3	5	LYS
1	A	74	ASP

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Mol	Chain	Res	Type
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS

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Mol	Chain	Res	Type
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
46	y	104	TRP
51	3	61	SER
58	AA	13	HIS
58	AA	29	HIS
59	AB	38	PRO
63	AF	8	SER
65	AH	133	ARG
67	AK	244	LEU
68	AL	180	ARG
68	AL	312	GLY
68	AL	322	VAL
58	AN	46	PHE
59	AO	51	SER
67	AW	241	ARG
67	AW	261	GLN
68	AY	382	SER
1	BA	74	ASP
7	BH	8	THR
7	BH	63	PRO
8	BI	52	ASN
9	BJ	135	GLU
9	BJ	178	SER
10	BK	101	SER
11	BL	165	SER
12	BM	538	ARG
12	BM	677	GLN
12	BM	689	LEU
12	BM	715	THR
13	BN	113	HIS
14	BO	238	PRO
15	BP	44	ARG
15	BP	179	ALA
15	BP	214	ASP
15	BP	229	GLU

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Mol	Chain	Res	Type
16	BQ	36	GLN
16	BQ	197	MET
18	BT	83	ARG
6	BX	140	CYS
22	BY	85	PRO
25	Bb	37	PRO
25	Bb	109	THR
26	Bc	164	ASN
28	Be	61	PRO
28	Be	111	ASP
30	Bg	10	LEU
30	Bg	12	PHE
30	Bg	50	ARG
32	Bi	87	THR
34	Bk	83	ASN
34	Bk	96	LEU
35	Bl	65	ASN
35	Bl	451	LEU
35	Bl	549	PRO
35	Bl	554	ASP
35	Bl	563	PRO
36	Bm	4	ALA
36	Bm	76	GLU
36	Bm	110	ASP
38	Bo	5	LYS
38	Bo	12	ARG
40	Br	139	GLN
41	Bs	38	ASN
42	Bu	36	CYS
42	Bu	101	ARG
42	Bu	143	HIS
43	Bv	73	SER
44	Bw	351	TRP
46	By	104	TRP
51	B3	61	SER
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN
8	I	108	SER
9	J	100	LEU
9	J	330	PRO

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Mol	Chain	Res	Type
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU
45	x	51	ASP
59	AB	51	SER
60	AC	142	ALA
60	AC	204	ARG
60	AC	219	HIS
62	AE	86	LEU

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Mol	Chain	Res	Type
67	AK	261	GLN
68	AL	193	GLN
62	AR	28	ASP
65	AU	133	ARG
67	AW	144	PRO
67	AW	403	ALA
68	AY	193	GLN
68	AY	461	PRO
1	BA	50	ASP
1	BA	186	ALA
3	BC	156	GLY
7	BH	76	GLN
8	BI	108	SER
9	BJ	100	LEU
9	BJ	330	PRO
9	BJ	370	LYS
10	BK	78	ASP
11	BL	172	VAL
12	BM	377	ALA
12	BM	426	ASP
13	BN	42	ASP
13	BN	130	THR
14	BO	216	PRO
14	BO	230	GLY
15	BP	175	GLY
15	BP	246	ARG
17	BS	36	LYS
21	BW	16	TYR
6	BX	74	LEU
22	BY	42	PRO
22	BY	87	PRO
25	Bb	115	GLU
26	Bc	40	PRO
26	Bc	41	TYR
30	Bg	49	ARG
30	Bg	56	GLY
31	Bh	32	ARG
31	Bh	45	HIS
32	Bi	150	ASN
35	Bl	249	SER
35	Bl	387	THR
35	Bl	562	LEU

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Mol	Chain	Res	Type
38	Bo	59	LEU
38	Bo	120	LYS
39	Bp	76	HIS
40	Br	251	ASN
41	Bs	208	VAL
41	Bs	288	LEU
41	Bs	289	LEU
42	Bu	167	PHE
43	Bv	36	GLU
45	Bx	51	ASP
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
46	y	103	GLN
54	6	3	ASN
59	AB	40	GLN
62	AE	28	ASP
68	AL	463	GLU
59	AO	27	ARG
59	AO	40	GLN
60	AP	204	ARG
65	AU	246	PRO
68	AY	463	GLU

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Mol	Chain	Res	Type
1	BA	228	PRO
1	BA	420	GLU
7	BH	103	LEU
9	BJ	259	ASN
12	BM	281	ILE
12	BM	548	LEU
12	BM	667	GLN
15	BP	110	SER
15	BP	202	PHE
15	BP	239	TRP
15	BP	245	TYR
16	BQ	102	SER
20	BV	48	THR
6	BX	153	ASP
26	Bc	171	GLY
32	Bi	92	GLN
36	Bm	113	VAL
39	Bp	175	ARG
42	Bu	144	SER
44	Bw	58	ARG
44	Bw	121	PRO
44	Bw	160	GLU
46	By	103	GLN
54	B6	3	ASN
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
45	x	91	ASP
46	y	158	ASP
51	3	49	PRO
65	AH	246	PRO
66	AJ	286	ASN
68	AL	279	ASP

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Mol	Chain	Res	Type
3	BC	102	ASP
6	BG	137	LYS
8	BI	70	MET
11	BL	96	LYS
12	BM	446	GLY
13	BN	135	GLN
18	BT	90	GLY
25	Bb	41	GLY
29	Bf	39	PRO
36	Bm	24	SER
39	Bp	32	VAL
40	Br	205	VAL
45	Bx	91	ASP
46	By	158	ASP
51	B3	49	PRO
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
12	BM	435	PRO
21	BW	10	MET
41	Bs	241	ILE
1	A	94	PRO
12	M	575	VAL
21	W	32	GLY
36	m	23	PRO
50	2	15	GLY
59	AO	30	VAL
1	BA	94	PRO
12	BM	575	VAL
36	Bm	23	PRO
50	B2	15	GLY
3	C	144	PRO
16	Q	307	PRO
3	BC	144	PRO
16	BQ	307	PRO
21	BW	32	GLY
16	Q	69	VAL
67	AK	320	PRO
68	AY	267	PRO
16	BQ	69	VAL
10	K	102	GLY
32	i	338	PRO

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Mol	Chain	Res	Type
10	BK	102	GLY
32	Bi	338	PRO
28	e	135	PRO
28	Be	135	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
1	BA	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
2	BB	151/151 (100%)	151 (100%)	0	100	100
3	BC	132/132 (100%)	132 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	BE	106/106 (100%)	106 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
5	BF	74/74 (100%)	74 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	BG	74/79 (94%)	74 (100%)	0	100	100
6	BX	78/79 (99%)	77 (99%)	1 (1%)	61	74
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	BH	100/100 (100%)	99 (99%)	1 (1%)	68	78
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	78
8	BI	87/96 (91%)	87 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	BJ	292/292 (100%)	288 (99%)	4 (1%)	59	72
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	BK	32/32 (100%)	32 (100%)	0	100	100
10	K	32/32 (100%)	32 (100%)	0	100	100
11	BL	107/107 (100%)	107 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	BM	576/577 (100%)	574 (100%)	2 (0%)	86	86
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	86
13	BN	129/129 (100%)	129 (100%)	0	100	100
13	N	129/129 (100%)	129 (100%)	0	100	100
14	BO	181/181 (100%)	181 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	BP	190/190 (100%)	190 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	BQ	371/371 (100%)	368 (99%)	3 (1%)	73	80
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	80
17	BS	59/59 (100%)	59 (100%)	0	100	100
17	S	59/59 (100%)	59 (100%)	0	100	100
18	BT	79/79 (100%)	79 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	BU	72/72 (100%)	72 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	BV	102/102 (100%)	102 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	BW	119/119 (100%)	119 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	BY	57/57 (100%)	50 (88%)	7 (12%)	4	17
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	17
23	BZ	62/63 (98%)	62 (100%)	0	100	100
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	Ba	124/124 (100%)	123 (99%)	1 (1%)	73	80
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	80
25	Bb	118/118 (100%)	113 (96%)	5 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	b	118/118 (100%)	113 (96%)	5 (4%)	26	48
26	Bc	124/137 (90%)	124 (100%)	0	100	100
26	c	124/137 (90%)	124 (100%)	0	100	100
27	Bd	145/154 (94%)	137 (94%)	8 (6%)	19	41
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	41
28	Be	90/90 (100%)	90 (100%)	0	100	100
28	e	90/90 (100%)	90 (100%)	0	100	100
29	Bf	43/43 (100%)	43 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	Bg	105/105 (100%)	105 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	Bh	90/90 (100%)	90 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	Bi	314/314 (100%)	313 (100%)	1 (0%)	86	86
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	86
33	Bj	102/103 (99%)	101 (99%)	1 (1%)	68	78
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	78
34	Bk	85/85 (100%)	81 (95%)	4 (5%)	23	45
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	45
35	Bl	531/532 (100%)	511 (96%)	20 (4%)	29	50
35	l	531/532 (100%)	511 (96%)	20 (4%)	29	50
36	Bm	137/137 (100%)	137 (100%)	0	100	100
36	m	137/137 (100%)	137 (100%)	0	100	100
37	Bn	53/53 (100%)	53 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	Bo	114/114 (100%)	114 (100%)	0	100	100
38	o	113/114 (99%)	113 (100%)	0	100	100
39	Bp	157/157 (100%)	155 (99%)	2 (1%)	61	74
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	74
40	Br	416/416 (100%)	416 (100%)	0	100	100
40	r	416/416 (100%)	416 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Bs	278/278 (100%)	278 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	Bu	153/153 (100%)	153 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	Bv	89/111 (80%)	89 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	Bw	249/288 (86%)	249 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	Bx	427/427 (100%)	387 (91%)	40 (9%)	8	26
45	x	427/427 (100%)	387 (91%)	40 (9%)	8	26
46	By	211/211 (100%)	191 (90%)	20 (10%)	8	25
46	y	211/211 (100%)	192 (91%)	19 (9%)	9	27
47	Bz	226/226 (100%)	199 (88%)	27 (12%)	5	18
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	18
48	0	128/128 (100%)	118 (92%)	10 (8%)	11	32
48	B0	128/128 (100%)	118 (92%)	10 (8%)	11	32
49	1	95/95 (100%)	89 (94%)	6 (6%)	16	37
49	B1	95/95 (100%)	94 (99%)	1 (1%)	65	76
50	2	81/81 (100%)	73 (90%)	8 (10%)	7	24
50	B2	81/81 (100%)	73 (90%)	8 (10%)	7	24
51	3	68/68 (100%)	52 (76%)	16 (24%)	1	5
51	B3	68/68 (100%)	55 (81%)	13 (19%)	1	8
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	14
52	B4	67/67 (100%)	58 (87%)	9 (13%)	4	14
53	5	58/58 (100%)	51 (88%)	7 (12%)	5	17
53	B5	58/58 (100%)	54 (93%)	4 (7%)	14	36
54	6	47/47 (100%)	41 (87%)	6 (13%)	4	15
54	B6	47/47 (100%)	44 (94%)	3 (6%)	16	37
55	7	39/39 (100%)	36 (92%)	3 (8%)	12	32
55	B7	39/39 (100%)	36 (92%)	3 (8%)	12	32
56	8	40/40 (100%)	37 (92%)	3 (8%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	B8	40/40 (100%)	37 (92%)	3 (8%)	12	33
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	31
57	B9	37/37 (100%)	34 (92%)	3 (8%)	11	31
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	31
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	51 (98%)	1 (2%)	50	67
62	AE	61/71 (86%)	59 (97%)	2 (3%)	33	55
62	AR	61/71 (86%)	58 (95%)	3 (5%)	22	43
63	AF	95/95 (100%)	82 (86%)	13 (14%)	3	14
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	23	44
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	81	83
66	AJ	330/330 (100%)	326 (99%)	4 (1%)	63	75
66	AV	330/330 (100%)	321 (97%)	9 (3%)	39	61
67	AK	334/335 (100%)	330 (99%)	4 (1%)	63	75
67	AW	335/335 (100%)	331 (99%)	4 (1%)	63	75
68	AL	365/367 (100%)	365 (100%)	0	100	100
68	AY	362/367 (99%)	356 (98%)	6 (2%)	53	69
All	All	20773/21008 (99%)	20298 (98%)	475 (2%)	44	64

All (475) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	81	ILE
9	J	85	ARG
9	J	91	ILE

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Mol	Chain	Res	Type
9	J	206	ILE
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
16	Q	275	ILE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	87	PRO
22	Y	95	GLU
22	Y	97	LEU
24	a	53	ARG
25	b	21	ARG
25	b	38	GLN
25	b	82	ILE
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
32	i	149	LEU
33	j	86	LEU
34	k	1	MET
34	k	3	LEU
34	k	6	MET
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	94	LEU
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER

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Mol	Chain	Res	Type
35	l	195	SER
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	229	LEU
35	l	447	ASN
35	l	450	LEU
35	l	452	ASN
35	l	513	MET
39	p	124	GLN
39	p	170	ILE
45	x	18	LEU
45	x	35	LEU
45	x	92	MET
45	x	96	ARG
45	x	105	LEU
45	x	115	SER
45	x	136	LEU
45	x	138	HIS
45	x	150	LEU
45	x	158	ILE
45	x	159	LEU
45	x	187	SER
45	x	188	VAL
45	x	189	MET
45	x	194	LEU
45	x	199	LEU
45	x	213	ARG
45	x	241	PRO
45	x	273	MET
45	x	295	VAL
45	x	301	THR
45	x	306	THR
45	x	318	VAL
45	x	324	LEU
45	x	347	LEU
45	x	353	LEU
45	x	354	THR
45	x	365	ILE

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Mol	Chain	Res	Type
45	x	369	ASP
45	x	373	VAL
45	x	383	MET
45	x	417	MET
45	x	444	PRO
45	x	465	VAL
45	x	467	LEU
45	x	474	GLU
45	x	492	LEU
45	x	508	PRO
45	x	509	THR
45	x	512	ASN
46	y	7	LEU
46	y	16	ILE
46	y	31	VAL
46	y	52	HIS
46	y	60	GLU
46	y	63	THR
46	y	67	ILE
46	y	88	ASP
46	y	92	ASN
46	y	125	THR
46	y	130	PRO
46	y	134	ARG
46	y	142	VAL
46	y	147	GLU
46	y	170	LEU
46	y	171	LYS
46	y	185	MET
46	y	205	SER
46	y	216	LEU
47	z	1	MET
47	z	11	VAL
47	z	13	PRO
47	z	14	SER
47	z	18	LEU
47	z	19	THR
47	z	22	LEU
47	z	26	LEU
47	z	38	ASN
47	z	39	SER
47	z	85	LEU

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Mol	Chain	Res	Type
47	z	92	LEU
47	z	112	LEU
47	z	127	LEU
47	z	128	GLU
47	z	131	LEU
47	z	132	LEU
47	z	137	LEU
47	z	142	VAL
47	z	160	LEU
47	z	163	LEU
47	z	188	ILE
47	z	196	THR
47	z	199	VAL
47	z	213	THR
47	z	222	GLN
47	z	230	ASN
48	0	9	GLU
48	0	27	VAL
48	0	31	LYS
48	0	36	SER
48	0	40	LEU
48	0	59	LEU
48	0	62	LEU
48	0	107	ILE
48	0	143	ASN
48	0	147	LYS
49	1	7	THR
49	1	29	LEU
49	1	70	VAL
49	1	79	LYS
49	1	80	GLU
49	1	90	ARG
50	2	6	VAL
50	2	20	VAL
50	2	37	LYS
50	2	52	ILE
50	2	53	THR
50	2	74	LEU
50	2	95	GLN
50	2	98	HIS
51	3	5	LYS
51	3	7	ASP

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Mol	Chain	Res	Type
51	3	8	HIS
51	3	14	ARG
51	3	17	ARG
51	3	33	LEU
51	3	34	ASN
51	3	37	LEU
51	3	41	HIS
51	3	42	ARG
51	3	43	GLU
51	3	48	ILE
51	3	54	ARG
51	3	56	ARG
51	3	68	THR
51	3	78	LEU
52	4	19	ARG
52	4	29	CYS
52	4	41	LYS
52	4	51	SER
52	4	53	CYS
52	4	57	ARG
52	4	60	TYR
52	4	67	SER
52	4	75	ARG
53	5	2	THR
53	5	4	LEU
53	5	8	GLN
53	5	22	VAL
53	5	26	MET
53	5	44	LYS
53	5	64	ARG
54	6	2	GLU
54	6	5	VAL
54	6	8	LYS
54	6	16	ASN
54	6	23	LYS
54	6	27	THR
55	7	45	VAL
55	7	48	VAL
55	7	49	THR
56	8	15	VAL
56	8	22	LEU
56	8	26	THR

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Mol	Chain	Res	Type
57	9	13	LYS
57	9	24	LEU
57	9	42	LYS
58	AA	25	ARG
58	AA	40	ARG
58	AA	48	ARG
58	AA	61	THR
58	AA	64	THR
58	AA	66	GLU
62	AE	28	ASP
62	AE	30	LEU
63	AF	14	LEU
63	AF	17	ILE
63	AF	29	LYS
63	AF	33	MET
63	AF	34	ARG
63	AF	38	ILE
63	AF	40	GLU
63	AF	41	ASP
63	AF	49	ARG
63	AF	60	MET
63	AF	71	LEU
63	AF	72	LYS
63	AF	74	GLN
66	AJ	124	MET
66	AJ	150	LEU
66	AJ	164	ILE
66	AJ	300	ILE
67	AK	49	ILE
67	AK	259	ARG
67	AK	365	ASN
67	AK	451	ASP
61	AQ	47	ILE
62	AR	30	LEU
62	AR	78	ARG
62	AR	81	CYS
64	AT	39	ARG
64	AT	40	LEU
65	AU	292	MET
66	AV	42	ILE
66	AV	147	THR
66	AV	149	LEU

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Mol	Chain	Res	Type
66	AV	150	LEU
66	AV	164	ILE
66	AV	185	LEU
66	AV	192	LEU
66	AV	195	LEU
66	AV	299	LEU
67	AW	138	LEU
67	AW	254	ARG
67	AW	451	ASP
67	AW	453	LEU
68	AY	96	LEU
68	AY	265	LEU
68	AY	418	LEU
68	AY	422	ARG
68	AY	423	ARG
68	AY	462	ILE
7	BH	81	ILE
9	BJ	85	ARG
9	BJ	91	ILE
9	BJ	206	ILE
9	BJ	212	ARG
12	BM	130	ILE
12	BM	174	THR
16	BQ	268	TRP
16	BQ	273	ILE
16	BQ	275	ILE
6	BX	93	ILE
22	BY	75	HIS
22	BY	78	GLU
22	BY	80	VAL
22	BY	81	LEU
22	BY	87	PRO
22	BY	95	GLU
22	BY	97	LEU
24	Ba	53	ARG
25	Bb	21	ARG
25	Bb	38	GLN
25	Bb	82	ILE
25	Bb	111	LEU
25	Bb	112	GLU
27	Bd	54	ARG
27	Bd	55	TYR

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Mol	Chain	Res	Type
27	Bd	57	TYR
27	Bd	60	ARG
27	Bd	61	GLN
27	Bd	113	GLN
27	Bd	116	GLN
27	Bd	117	GLN
32	Bi	149	LEU
33	Bj	86	LEU
34	Bk	1	MET
34	Bk	3	LEU
34	Bk	6	MET
34	Bk	8	ILE
35	Bl	25	ASN
35	Bl	59	GLN
35	Bl	87	MET
35	Bl	94	LEU
35	Bl	97	THR
35	Bl	99	SER
35	Bl	191	LEU
35	Bl	193	SER
35	Bl	195	SER
35	Bl	196	TRP
35	Bl	197	ASP
35	Bl	217	LEU
35	Bl	218	LEU
35	Bl	223	LYS
35	Bl	226	GLN
35	Bl	229	LEU
35	Bl	447	ASN
35	Bl	450	LEU
35	Bl	452	ASN
35	Bl	513	MET
39	Bp	124	GLN
39	Bp	170	ILE
45	Bx	18	LEU
45	Bx	35	LEU
45	Bx	92	MET
45	Bx	96	ARG
45	Bx	105	LEU
45	Bx	115	SER
45	Bx	136	LEU
45	Bx	138	HIS

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Mol	Chain	Res	Type
45	Bx	150	LEU
45	Bx	158	ILE
45	Bx	159	LEU
45	Bx	187	SER
45	Bx	188	VAL
45	Bx	189	MET
45	Bx	194	LEU
45	Bx	199	LEU
45	Bx	213	ARG
45	Bx	241	PRO
45	Bx	273	MET
45	Bx	295	VAL
45	Bx	301	THR
45	Bx	306	THR
45	Bx	318	VAL
45	Bx	324	LEU
45	Bx	347	LEU
45	Bx	353	LEU
45	Bx	354	THR
45	Bx	365	ILE
45	Bx	369	ASP
45	Bx	373	VAL
45	Bx	383	MET
45	Bx	417	MET
45	Bx	444	PRO
45	Bx	465	VAL
45	Bx	467	LEU
45	Bx	474	GLU
45	Bx	492	LEU
45	Bx	508	PRO
45	Bx	509	THR
45	Bx	512	ASN
46	By	7	LEU
46	By	16	ILE
46	By	31	VAL
46	By	33	LEU
46	By	52	HIS
46	By	60	GLU
46	By	63	THR
46	By	67	ILE
46	By	88	ASP
46	By	92	ASN

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Mol	Chain	Res	Type
46	By	125	THR
46	By	130	PRO
46	By	134	ARG
46	By	142	VAL
46	By	147	GLU
46	By	170	LEU
46	By	171	LYS
46	By	185	MET
46	By	205	SER
46	By	216	LEU
47	Bz	1	MET
47	Bz	11	VAL
47	Bz	13	PRO
47	Bz	14	SER
47	Bz	18	LEU
47	Bz	19	THR
47	Bz	22	LEU
47	Bz	26	LEU
47	Bz	38	ASN
47	Bz	39	SER
47	Bz	85	LEU
47	Bz	92	LEU
47	Bz	112	LEU
47	Bz	127	LEU
47	Bz	128	GLU
47	Bz	131	LEU
47	Bz	132	LEU
47	Bz	137	LEU
47	Bz	142	VAL
47	Bz	160	LEU
47	Bz	163	LEU
47	Bz	188	ILE
47	Bz	196	THR
47	Bz	199	VAL
47	Bz	213	THR
47	Bz	222	GLN
47	Bz	230	ASN
48	B0	9	GLU
48	B0	27	VAL
48	B0	31	LYS
48	B0	36	SER
48	B0	40	LEU

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Mol	Chain	Res	Type
48	B0	59	LEU
48	B0	62	LEU
48	B0	107	ILE
48	B0	143	ASN
48	B0	147	LYS
49	B1	7	THR
50	B2	6	VAL
50	B2	20	VAL
50	B2	37	LYS
50	B2	52	ILE
50	B2	53	THR
50	B2	74	LEU
50	B2	95	GLN
50	B2	98	HIS
51	B3	14	ARG
51	B3	17	ARG
51	B3	33	LEU
51	B3	34	ASN
51	B3	37	LEU
51	B3	41	HIS
51	B3	42	ARG
51	B3	43	GLU
51	B3	48	ILE
51	B3	54	ARG
51	B3	56	ARG
51	B3	68	THR
51	B3	78	LEU
52	B4	19	ARG
52	B4	29	CYS
52	B4	41	LYS
52	B4	51	SER
52	B4	53	CYS
52	B4	57	ARG
52	B4	60	TYR
52	B4	67	SER
52	B4	75	ARG
53	B5	22	VAL
53	B5	26	MET
53	B5	44	LYS
53	B5	64	ARG
54	B6	16	ASN
54	B6	23	LYS

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Mol	Chain	Res	Type
54	B6	27	THR
55	B7	45	VAL
55	B7	48	VAL
55	B7	49	THR
56	B8	15	VAL
56	B8	22	LEU
56	B8	26	THR
57	B9	13	LYS
57	B9	24	LEU
57	B9	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (482) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	HIS
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
1	A	270	ASN
1	A	284	HIS
1	A	313	ASN
1	A	376	HIS
1	A	441	HIS
2	B	184	ASN
3	C	72	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
4	E	108	HIS
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	142	GLN
7	H	50	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
9	J	71	ASN

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Mol	Chain	Res	Type
9	J	93	HIS
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	86	ASN
12	M	142	GLN
12	M	425	ASN
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	663	ASN
12	M	666	GLN
12	M	669	ASN
13	N	72	ASN
13	N	91	HIS
13	N	113	HIS
14	O	69	ASN
14	O	187	GLN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
16	Q	38	GLN
16	Q	60	HIS
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	S	44	HIS
18	T	64	ASN
20	V	44	ASN
21	W	8	GLN
21	W	61	GLN

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Mol	Chain	Res	Type
21	W	112	HIS
21	W	135	HIS
6	X	142	GLN
22	Y	75	HIS
23	Z	33	GLN
24	a	90	ASN
24	a	109	HIS
24	a	115	HIS
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
26	c	56	ASN
26	c	84	HIS
26	c	127	HIS
26	c	154	GLN
26	c	165	ASN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	108	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
28	e	140	ASN
30	g	45	ASN
30	g	58	HIS
30	g	96	HIS
32	i	78	ASN
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
35	l	113	ASN
35	l	192	HIS
35	l	199	GLN

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Mol	Chain	Res	Type
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	320	ASN
35	l	323	HIS
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	117	ASN
37	n	40	ASN
38	o	52	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	21	HIS
40	r	46	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	97	ASN
41	s	169	GLN
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS
42	u	104	GLN
42	u	140	ASN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS

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Mol	Chain	Res	Type
43	v	85	HIS
43	v	92	HIS
44	w	92	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	GLN
44	w	323	GLN
45	x	4	ASN
45	x	11	ASN
45	x	12	HIS
45	x	55	ASN
45	x	99	ASN
45	x	170	ASN
45	x	256	HIS
45	x	360	ASN
45	x	368	HIS
45	x	413	HIS
45	x	503	HIS
45	x	512	ASN
46	y	52	HIS
46	y	102	HIS
46	y	195	GLN
46	y	203	ASN
47	z	3	HIS
47	z	6	HIS
47	z	12	ASN
47	z	133	ASN
47	z	148	HIS
47	z	158	HIS
47	z	204	HIS
47	z	207	HIS
47	z	222	GLN
47	z	232	HIS
48	0	109	HIS
49	1	34	ASN
50	2	66	ASN
51	3	51	HIS
51	3	52	HIS
52	4	23	GLN
52	4	24	ASN
52	4	25	GLN

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Mol	Chain	Res	Type
52	4	28	ASN
52	4	32	ASN
52	4	37	HIS
54	6	3	ASN
54	6	16	ASN
54	6	21	HIS
55	7	10	HIS
55	7	15	ASN
55	7	35	GLN
55	7	41	ASN
56	8	42	HIS
57	9	39	ASN
58	AA	29	HIS
59	AB	31	GLN
60	AC	80	HIS
63	AF	23	ASN
63	AF	73	HIS
64	AG	16	ASN
65	AH	107	HIS
65	AH	205	HIS
65	AH	265	GLN
66	AJ	8	ASN
66	AJ	16	HIS
66	AJ	54	HIS
66	AJ	97	HIS
66	AJ	137	GLN
66	AJ	260	ASN
66	AJ	308	HIS
66	AJ	313	GLN
66	AJ	322	GLN
67	AK	139	ASN
67	AK	155	GLN
67	AK	167	GLN
67	AK	178	HIS
67	AK	206	HIS
67	AK	290	GLN
67	AK	291	HIS
67	AK	310	HIS
67	AK	311	GLN
67	AK	399	GLN
68	AL	66	GLN
68	AL	87	ASN

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Mol	Chain	Res	Type
68	AL	207	ASN
68	AL	239	HIS
68	AL	240	GLN
68	AL	301	ASN
68	AL	308	ASN
68	AL	335	ASN
68	AL	452	GLN
60	AP	178	HIS
60	AP	199	GLN
61	AQ	38	GLN
62	AR	80	HIS
63	AS	23	ASN
63	AS	28	ASN
63	AS	70	ASN
63	AS	73	HIS
64	AT	16	ASN
66	AV	32	ASN
66	AV	97	HIS
66	AV	137	GLN
66	AV	255	ASN
66	AV	341	GLN
67	AW	81	HIS
67	AW	155	GLN
67	AW	176	ASN
67	AW	206	HIS
67	AW	227	HIS
67	AW	284	ASN
67	AW	298	HIS
67	AW	310	HIS
67	AW	311	GLN
67	AW	357	GLN
67	AW	421	ASN
67	AW	426	ASN
67	AW	446	HIS
68	AY	87	ASN
68	AY	152	GLN
68	AY	223	HIS
68	AY	301	ASN
68	AY	342	GLN
68	AY	375	GLN
68	AY	469	ASN
1	BA	44	ASN

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Mol	Chain	Res	Type
1	BA	49	HIS
1	BA	116	ASN
1	BA	164	ASN
1	BA	170	GLN
1	BA	270	ASN
1	BA	284	HIS
1	BA	313	ASN
1	BA	376	HIS
1	BA	441	HIS
2	BB	184	ASN
3	BC	72	ASN
3	BC	95	HIS
4	BE	48	HIS
4	BE	49	GLN
4	BE	51	GLN
4	BE	70	ASN
4	BE	108	HIS
5	BF	62	GLN
5	BF	81	ASN
5	BF	93	ASN
6	BG	80	GLN
6	BG	142	GLN
7	BH	50	GLN
7	BH	76	GLN
7	BH	83	GLN
7	BH	111	GLN
9	BJ	71	ASN
9	BJ	93	HIS
9	BJ	102	GLN
9	BJ	183	ASN
10	BK	77	HIS
11	BL	86	ASN
12	BM	425	ASN
12	BM	444	HIS
12	BM	460	HIS
12	BM	464	GLN
12	BM	498	GLN
12	BM	514	ASN
12	BM	569	GLN
12	BM	663	ASN
12	BM	666	GLN
12	BM	669	ASN

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Mol	Chain	Res	Type
13	BN	72	ASN
13	BN	91	HIS
13	BN	113	HIS
13	BN	123	GLN
14	BO	69	ASN
14	BO	189	ASN
14	BO	191	ASN
15	BP	74	GLN
15	BP	82	ASN
15	BP	105	ASN
16	BQ	38	GLN
16	BQ	147	ASN
16	BQ	182	ASN
16	BQ	183	HIS
16	BQ	190	HIS
16	BQ	233	HIS
16	BQ	234	GLN
16	BQ	339	GLN
16	BQ	431	HIS
16	BQ	442	HIS
16	BQ	454	GLN
17	BS	44	HIS
18	BT	64	ASN
20	BV	44	ASN
21	BW	8	GLN
21	BW	61	GLN
21	BW	112	HIS
21	BW	135	HIS
6	BX	142	GLN
22	BY	75	HIS
23	BZ	33	GLN
24	Ba	90	ASN
24	Ba	115	HIS
24	Ba	189	ASN
25	Bb	14	GLN
25	Bb	83	HIS
25	Bb	89	HIS
26	Bc	56	ASN
26	Bc	84	HIS
26	Bc	127	HIS
26	Bc	154	GLN
26	Bc	165	ASN

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Mol	Chain	Res	Type
27	Bd	59	HIS
27	Bd	61	GLN
27	Bd	85	GLN
27	Bd	108	GLN
27	Bd	113	GLN
27	Bd	116	GLN
27	Bd	117	GLN
28	Be	140	ASN
30	Bg	45	ASN
30	Bg	58	HIS
30	Bg	96	HIS
32	Bi	78	ASN
32	Bi	83	GLN
32	Bi	112	HIS
32	Bi	150	ASN
32	Bi	186	HIS
32	Bi	222	ASN
33	Bj	10	ASN
34	Bk	7	ASN
34	Bk	94	ASN
35	Bl	4	HIS
35	Bl	59	GLN
35	Bl	192	HIS
35	Bl	199	GLN
35	Bl	205	ASN
35	Bl	226	GLN
35	Bl	248	HIS
35	Bl	274	GLN
35	Bl	296	ASN
35	Bl	323	HIS
35	Bl	332	HIS
35	Bl	348	HIS
35	Bl	394	HIS
35	Bl	400	ASN
35	Bl	442	ASN
35	Bl	446	ASN
35	Bl	534	HIS
35	Bl	569	HIS
35	Bl	580	GLN
36	Bm	117	ASN
37	Bn	40	ASN
38	Bo	52	ASN

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Mol	Chain	Res	Type
38	Bo	62	ASN
38	Bo	126	HIS
39	Bp	75	GLN
40	Br	21	HIS
40	Br	46	ASN
40	Br	168	HIS
40	Br	390	ASN
40	Br	415	GLN
40	Br	425	ASN
41	Bs	93	ASN
41	Bs	97	ASN
41	Bs	169	GLN
41	Bs	235	ASN
42	Bu	30	HIS
42	Bu	31	HIS
42	Bu	64	ASN
42	Bu	77	HIS
42	Bu	99	HIS
42	Bu	104	GLN
42	Bu	140	ASN
42	Bu	143	HIS
43	Bv	43	GLN
43	Bv	61	HIS
43	Bv	85	HIS
43	Bv	92	HIS
44	Bw	92	HIS
44	Bw	111	ASN
44	Bw	132	GLN
44	Bw	149	HIS
44	Bw	257	GLN
45	Bx	4	ASN
45	Bx	11	ASN
45	Bx	12	HIS
45	Bx	55	ASN
45	Bx	99	ASN
45	Bx	170	ASN
45	Bx	178	GLN
45	Bx	256	HIS
45	Bx	360	ASN
45	Bx	368	HIS
45	Bx	413	HIS
45	Bx	503	HIS

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Mol	Chain	Res	Type
45	Bx	512	ASN
46	By	52	HIS
46	By	91	ASN
46	By	102	HIS
46	By	195	GLN
46	By	203	ASN
47	Bz	3	HIS
47	Bz	6	HIS
47	Bz	12	ASN
47	Bz	133	ASN
47	Bz	148	HIS
47	Bz	158	HIS
47	Bz	207	HIS
47	Bz	222	GLN
47	Bz	232	HIS
48	B0	109	HIS
49	B1	34	ASN
50	B2	66	ASN
51	B3	51	HIS
51	B3	52	HIS
52	B4	23	GLN
52	B4	24	ASN
52	B4	25	GLN
52	B4	28	ASN
52	B4	32	ASN
52	B4	37	HIS
54	B6	3	ASN
54	B6	16	ASN
54	B6	21	HIS
55	B7	10	HIS
55	B7	15	ASN
55	B7	35	GLN
55	B7	41	ASN
57	B9	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 10 are monoatomic - leaving 90 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	8Q1	p	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
74	FES	AP	301	60	0,4,4	-	-	-		
75	CDL	AA	101	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	5 (7%)
72	8Q1	BE	201	-	32,34,34	1.58	6 (18%)	39,43,43	1.42	7 (17%)
71	PLX	b	201	-	51,51,51	0.55	0	53,59,59	0.64	0
71	PLX	Bg	202	-	51,51,51	0.76	1 (1%)	53,59,59	0.62	1 (1%)
75	CDL	Bn	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
71	PLX	AN	101	-	51,51,51	0.80	1 (1%)	53,59,59	0.61	1 (1%)
79	HEA	Bx	603	45	67,67,67	1.20	4 (5%)	81,103,103	1.33	10 (12%)
71	PLX	AQ	101	-	51,51,51	0.79	1 (1%)	53,59,59	0.63	2 (3%)
71	PLX	BU	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
69	SF4	BM	802	12	0,12,12	-	-	-		
71	PLX	U	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
74	FES	M	803	-	0,4,4	-	-	-		
69	SF4	C	301	3	0,12,12	-	-	-		
69	SF4	M	802	12	0,12,12	-	-	-		
69	SF4	BC	301	3	0,12,12	-	-	-		
69	SF4	BB	302	2	0,12,12	-	-	-		
75	CDL	Bl	703	-	63,63,99	1.22	5 (7%)	69,75,111	1.09	4 (5%)
76	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
70	FMN	BA	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	9 (18%)
74	FES	BM	803	-	0,4,4	-	-	-		
75	CDL	AH	403	-	63,63,99	1.27	5 (7%)	69,75,111	1.05	4 (5%)
69	SF4	M	801	12	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.24	5 (7%)
75	CDL	n	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
71	PLX	Br	502	-	51,51,51	0.62	0	53,59,59	0.67	1 (1%)
82	HEM	AJ	401	66	50,50,50	1.81	9 (18%)	67,82,82	1.19	2 (2%)
69	SF4	B	301	2	0,12,12	-	-	-	-	-
75	CDL	AJ	404	-	63,63,99	1.26	5 (7%)	69,75,111	1.04	4 (5%)
79	HEA	x	604	45	67,67,67	1.20	7 (10%)	81,103,103	1.35	11 (13%)
76	PEE	W	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
69	SF4	BM	801	12	0,12,12	-	-	-	-	-
72	8Q1	E	201	-	32,34,34	1.57	6 (18%)	39,43,43	1.42	7 (17%)
75	CDL	l	704	-	63,63,99	1.27	5 (7%)	69,75,111	1.02	4 (5%)
76	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
75	CDL	AU	403	-	63,63,99	1.26	6 (9%)	69,75,111	1.06	4 (5%)
73	NDP	BJ	401	-	51,52,52	1.15	6 (11%)	71,80,80	1.57	10 (14%)
71	PLX	g	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
75	CDL	AN	102	-	63,63,99	1.25	5 (7%)	69,75,111	1.04	4 (5%)
76	PEE	AH	401	-	48,48,50	1.37	4 (8%)	51,53,55	0.97	2 (3%)
76	PEE	Bl	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
74	FES	BO	301	14	0,4,4	-	-	-	-	-
82	HEM	AV	402	66	50,50,50	1.79	8 (16%)	67,82,82	1.25	6 (8%)
76	PEE	AU	401	-	40,40,50	1.47	4 (10%)	43,45,55	0.95	2 (4%)
75	CDL	l	703	-	63,63,99	1.22	5 (7%)	69,75,111	1.09	4 (5%)
71	PLX	g	202	-	51,51,51	0.76	1 (1%)	53,59,59	0.62	1 (1%)
75	CDL	V	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
71	PLX	r	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
76	PEE	l	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
74	FES	AC	301	60	0,4,4	-	-	-	-	-
79	HEA	x	603	45	67,67,67	1.20	4 (5%)	81,103,103	1.34	11 (13%)
75	CDL	i	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
71	PLX	AL	501	-	51,51,51	0.80	1 (1%)	53,59,59	0.64	1 (1%)
74	FES	O	301	14	0,4,4	-	-	-	-	-
71	PLX	g	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.59	1 (1%)
71	PLX	Bb	201	-	51,51,51	0.55	0	53,59,59	0.64	0
82	HEM	AV	401	66	50,50,50	1.82	9 (18%)	67,82,82	1.21	3 (4%)
71	PLX	Bg	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
76	PEE	AJ	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.00	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	AY	501	-	63,63,99	1.26	5 (7%)	69,75,111	1.03	4 (5%)
76	PEE	AY	502	-	48,48,50	1.41	4 (8%)	51,53,55	0.97	2 (3%)
76	PEE	AV	403	-	48,48,50	1.36	4 (8%)	51,53,55	1.05	2 (3%)
75	CDL	Bl	704	-	63,63,99	1.28	5 (7%)	69,75,111	1.02	4 (5%)
71	PLX	Bg	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.60	1 (1%)
76	PEE	BV	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
73	NDP	J	401	-	51,52,52	1.15	5 (9%)	71,80,80	1.56	10 (14%)
70	FMN	A	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	8 (16%)
71	PLX	r	502	-	51,51,51	0.62	0	53,59,59	0.66	1 (1%)
71	PLX	BB	303	-	51,51,51	0.80	1 (1%)	53,59,59	0.69	1 (1%)
82	HEM	AJ	402	66	50,50,50	1.82	8 (16%)	67,82,82	1.23	6 (8%)
69	SF4	BA	501	1	0,12,12	-	-	-	-	-
69	SF4	A	501	1	0,12,12	-	-	-	-	-
76	PEE	Bl	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
75	CDL	AL	502	-	63,63,99	1.26	5 (7%)	69,75,111	1.07	4 (5%)
75	CDL	BV	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
81	HEC	AU	402	65	46,50,50	1.84	5 (10%)	58,82,82	1.84	4 (6%)
69	SF4	BB	301	2	0,12,12	-	-	-	-	-
71	PLX	B	303	-	51,51,51	0.80	1 (1%)	53,59,59	0.69	1 (1%)
76	PEE	BW	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
71	PLX	AT	101	-	51,51,51	0.78	1 (1%)	53,59,59	0.61	1 (1%)
79	HEA	Bx	604	45	67,67,67	1.20	7 (10%)	81,103,103	1.35	11 (13%)
75	CDL	Bi	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
81	HEC	AH	402	65	46,50,50	1.82	5 (10%)	58,82,82	1.86	5 (8%)
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.18	6 (8%)
71	PLX	Br	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
76	PEE	AL	503	-	48,48,50	1.39	4 (8%)	51,53,55	0.94	2 (3%)
72	8Q1	Bp	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
69	SF4	B	302	2	0,12,12	-	-	-	-	-
71	PLX	BV	203	-	51,51,51	0.80	1 (1%)	53,59,59	0.61	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	8Q1	p	201	-	-	21/41/41/41	-
74	FES	AP	301	60	-	-	0/1/1/1
75	CDL	AA	101	-	-	35/74/74/110	-
72	8Q1	BE	201	-	-	18/41/41/41	-
71	PLX	b	201	-	-	26/55/55/55	-
71	PLX	Bg	202	-	-	26/55/55/55	-
75	CDL	Bn	101	-	-	32/74/74/110	-
71	PLX	AN	101	-	-	26/55/55/55	-
71	PLX	BV	203	-	-	26/55/55/55	-
79	HEA	Bx	603	45	-	7/36/76/76	-
71	PLX	AQ	101	-	-	24/55/55/55	-
71	PLX	BU	101	-	-	22/55/55/55	-
69	SF4	BM	802	12	-	-	0/6/5/5
71	PLX	U	101	-	-	22/55/55/55	-
74	FES	M	803	-	-	-	0/1/1/1
69	SF4	C	301	3	-	-	0/6/5/5
69	SF4	M	802	12	-	-	0/6/5/5
69	SF4	BC	301	3	-	-	0/6/5/5
69	SF4	BB	302	2	-	-	0/6/5/5
75	CDL	Bl	703	-	-	36/74/74/110	-
76	PEE	l	701	-	-	31/52/52/54	-
70	FMN	BA	502	-	-	7/18/18/18	0/3/3/3
74	FES	BM	803	-	-	-	0/1/1/1
75	CDL	AH	403	-	-	41/74/74/110	-
69	SF4	M	801	12	-	-	0/6/5/5
75	CDL	AJ	405	-	-	25/74/74/110	-
75	CDL	n	101	-	-	32/74/74/110	-
71	PLX	Br	502	-	-	36/55/55/55	-
82	HEM	AJ	401	66	-	1/14/54/54	-
69	SF4	B	301	2	-	-	0/6/5/5
75	CDL	AJ	404	-	-	31/74/74/110	-
79	HEA	x	604	45	-	7/36/76/76	-
76	PEE	W	201	-	-	29/54/54/54	-
69	SF4	BM	801	12	-	-	0/6/5/5
72	8Q1	E	201	-	-	18/41/41/41	-
75	CDL	l	704	-	-	42/74/74/110	-
76	PEE	V	202	-	-	26/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	AU	403	-	-	46/74/74/110	-
73	NDP	BJ	401	-	-	15/34/77/77	0/5/5/5
71	PLX	g	201	-	-	24/55/55/55	-
75	CDL	AN	102	-	-	39/74/74/110	-
76	PEE	AH	401	-	-	25/52/52/54	-
76	PEE	Bl	701	-	-	31/52/52/54	-
74	FES	BO	301	14	-	-	0/1/1/1
82	HEM	AV	402	66	-	4/14/54/54	-
76	PEE	AU	401	-	-	17/44/44/54	-
75	CDL	l	703	-	-	36/74/74/110	-
71	PLX	g	202	-	-	26/55/55/55	-
75	CDL	V	201	-	-	40/69/69/110	-
71	PLX	r	501	-	-	27/55/55/55	-
76	PEE	l	702	-	-	26/54/54/54	-
74	FES	AC	301	60	-	-	0/1/1/1
79	HEA	x	603	45	-	7/36/76/76	-
75	CDL	i	401	-	-	39/74/74/110	-
71	PLX	AL	501	-	-	23/55/55/55	-
74	FES	O	301	14	-	-	0/1/1/1
71	PLX	g	203	-	-	22/55/55/55	-
71	PLX	Bb	201	-	-	26/55/55/55	-
82	HEM	AV	401	66	-	5/14/54/54	-
71	PLX	Bg	201	-	-	24/55/55/55	-
76	PEE	AJ	403	-	-	18/52/52/54	-
75	CDL	AY	501	-	-	35/74/74/110	-
76	PEE	AY	502	-	-	18/52/52/54	-
76	PEE	AV	403	-	-	29/52/52/54	-
75	CDL	Bl	704	-	-	42/74/74/110	-
71	PLX	Bg	203	-	-	22/55/55/55	-
76	PEE	BV	202	-	-	26/54/54/54	-
73	NDP	J	401	-	-	15/34/77/77	0/5/5/5
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
71	PLX	r	502	-	-	36/55/55/55	-
71	PLX	BB	303	-	-	22/55/55/55	-
82	HEM	AJ	402	66	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SF4	BA	501	1	-	-	0/6/5/5
76	PEE	Bl	702	-	-	27/54/54/54	-
69	SF4	A	501	1	-	-	0/6/5/5
75	CDL	AL	502	-	-	42/74/74/110	-
75	CDL	BV	201	-	-	40/69/69/110	-
81	HEC	AU	402	65	-	4/14/54/54	-
69	SF4	BB	301	2	-	-	0/6/5/5
71	PLX	B	303	-	-	22/55/55/55	-
71	PLX	AT	101	-	-	22/55/55/55	-
79	HEA	Bx	604	45	-	7/36/76/76	-
75	CDL	Bi	401	-	-	39/74/74/110	-
81	HEC	AH	402	65	-	6/14/54/54	-
75	CDL	AG	101	-	-	37/74/74/110	-
71	PLX	Br	501	-	-	27/55/55/55	-
76	PEE	AL	503	-	-	21/52/52/54	-
72	8Q1	Bp	201	-	-	19/41/41/41	-
69	SF4	B	302	2	-	-	0/6/5/5
76	PEE	BW	201	-	-	29/54/54/54	-

All (288) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	C3D-C2D	7.74	1.53	1.36
82	AJ	401	HEM	C3D-C2D	7.74	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.69	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.61	1.53	1.36
81	AU	402	HEC	CAB-C3B	6.22	1.55	1.35
81	AH	402	HEC	CAC-C3C	6.15	1.55	1.35
81	AH	402	HEC	CAB-C3B	6.11	1.54	1.35
81	AU	402	HEC	CAC-C3C	6.10	1.54	1.35
81	AU	402	HEC	C3D-C2D	5.70	1.53	1.38
81	AH	402	HEC	C3D-C2D	5.66	1.53	1.38
72	Bp	201	8Q1	C39-N41	5.05	1.45	1.33
72	p	201	8Q1	C39-N41	5.01	1.45	1.33
72	p	201	8Q1	C34-N36	4.96	1.45	1.33
72	Bp	201	8Q1	C34-N36	4.94	1.45	1.33
72	E	201	8Q1	C34-N36	4.89	1.45	1.33
72	BE	201	8Q1	C34-N36	4.88	1.45	1.33
82	AV	401	HEM	FE-ND	4.81	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	BE	201	8Q1	C39-N41	4.71	1.44	1.33
72	E	201	8Q1	C39-N41	4.69	1.44	1.33
70	A	502	FMN	C9A-C5A	4.56	1.48	1.41
70	BA	502	FMN	C9A-C5A	4.55	1.48	1.41
76	AY	502	PEE	C39-C38	4.41	1.56	1.31
76	AU	401	PEE	C39-C38	4.38	1.56	1.31
76	AL	503	PEE	C39-C38	4.35	1.56	1.31
76	AV	403	PEE	C39-C38	4.35	1.56	1.31
75	Bl	704	CDL	OB8-CB7	4.35	1.46	1.33
76	AJ	403	PEE	C39-C38	4.34	1.56	1.31
75	l	704	CDL	OB8-CB7	4.34	1.46	1.33
75	AH	403	CDL	OA6-CA5	4.34	1.46	1.34
75	AL	502	CDL	OA6-CA5	4.33	1.46	1.34
76	AH	401	PEE	C39-C38	4.33	1.56	1.31
75	AH	403	CDL	OB8-CB7	4.33	1.46	1.33
76	AY	502	PEE	C18-C19	4.31	1.56	1.31
75	AJ	405	CDL	OA8-CA7	4.31	1.45	1.33
76	AH	401	PEE	C18-C19	4.30	1.56	1.31
75	AG	101	CDL	OB8-CB7	4.30	1.45	1.33
75	Bn	101	CDL	OA6-CA5	4.30	1.46	1.34
75	AU	403	CDL	OA6-CA5	4.29	1.46	1.34
76	AL	503	PEE	C18-C19	4.29	1.56	1.31
75	AY	501	CDL	OA6-CA5	4.29	1.46	1.34
75	n	101	CDL	OA6-CA5	4.28	1.46	1.34
75	l	703	CDL	OA6-CA5	4.28	1.46	1.34
76	Bl	701	PEE	C39-C38	4.27	1.55	1.31
76	l	701	PEE	C39-C38	4.27	1.55	1.31
75	BV	201	CDL	OA6-CA5	4.26	1.46	1.34
75	AJ	404	CDL	OA6-CA5	4.26	1.46	1.34
75	AU	403	CDL	OB8-CB7	4.26	1.45	1.33
75	V	201	CDL	OA6-CA5	4.25	1.46	1.34
75	Bl	703	CDL	OA6-CA5	4.24	1.46	1.34
76	AL	503	PEE	O3-C30	4.24	1.45	1.33
76	AJ	403	PEE	C18-C19	4.24	1.55	1.31
75	AG	101	CDL	OA8-CA7	4.23	1.45	1.33
75	AG	101	CDL	OA6-CA5	4.23	1.46	1.34
76	AV	403	PEE	C18-C19	4.23	1.55	1.31
75	l	703	CDL	OB8-CB7	4.23	1.45	1.33
76	Bl	701	PEE	C18-C19	4.23	1.55	1.31
76	l	701	PEE	C18-C19	4.23	1.55	1.31
75	Bl	703	CDL	OB8-CB7	4.23	1.45	1.33
75	BV	201	CDL	OB8-CB7	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AL	502	CDL	OB8-CB7	4.22	1.45	1.33
75	AJ	404	CDL	OB8-CB7	4.22	1.45	1.33
75	AY	501	CDL	OB8-CB7	4.22	1.45	1.33
75	V	201	CDL	OB8-CB7	4.21	1.45	1.33
76	AY	502	PEE	O3-C30	4.20	1.45	1.33
76	AH	401	PEE	O3-C30	4.19	1.45	1.33
75	AA	101	CDL	OB8-CB7	4.19	1.45	1.33
75	AA	101	CDL	OA6-CA5	4.18	1.46	1.34
75	Bl	704	CDL	OA6-CA5	4.18	1.46	1.34
75	AJ	405	CDL	OB8-CB7	4.18	1.45	1.33
79	Bx	603	HEA	C11-C3B	-4.16	1.46	1.51
76	AU	401	PEE	C19-C18	4.15	1.55	1.29
75	l	704	CDL	OA8-CA7	4.15	1.45	1.33
76	l	701	PEE	O3-C30	4.15	1.45	1.33
75	Bl	704	CDL	OA8-CA7	4.15	1.45	1.33
75	AN	102	CDL	OB8-CB7	4.14	1.45	1.33
76	Bl	701	PEE	O3-C30	4.14	1.45	1.33
76	AV	403	PEE	O3-C30	4.14	1.45	1.33
75	n	101	CDL	OB8-CB7	4.13	1.45	1.33
75	l	704	CDL	OA6-CA5	4.13	1.45	1.34
75	AN	102	CDL	OA6-CA5	4.12	1.45	1.34
82	AJ	402	HEM	FE-ND	4.12	2.07	1.94
82	AJ	401	HEM	FE-NB	4.12	2.07	1.94
76	AU	401	PEE	O3-C30	4.12	1.45	1.33
79	x	603	HEA	C11-C3B	-4.12	1.46	1.51
75	AJ	405	CDL	OB6-CB5	4.11	1.45	1.34
75	Bn	101	CDL	OB8-CB7	4.09	1.45	1.33
75	i	401	CDL	OB8-CB7	4.09	1.45	1.33
73	BJ	401	NDP	C5A-C4A	4.07	1.46	1.39
75	Bi	401	CDL	OB8-CB7	4.07	1.45	1.33
73	J	401	NDP	C5A-C4A	4.06	1.46	1.39
75	AG	101	CDL	OB6-CB5	4.03	1.45	1.34
75	Bi	401	CDL	OA6-CA5	4.01	1.45	1.34
75	AJ	405	CDL	OA6-CA5	4.00	1.45	1.34
75	i	401	CDL	OA6-CA5	3.99	1.45	1.34
75	AJ	404	CDL	OA8-CA7	3.99	1.45	1.33
76	AJ	403	PEE	O3-C30	3.98	1.44	1.33
75	AY	501	CDL	OA8-CA7	3.97	1.44	1.33
75	AU	403	CDL	OA8-CA7	3.95	1.44	1.33
82	AJ	401	HEM	FE-ND	3.93	2.07	1.94
75	AH	403	CDL	OA8-CA7	3.93	1.44	1.33
75	Bn	101	CDL	OA8-CA7	3.93	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AN	102	CDL	OA8-CA7	3.93	1.44	1.33
75	n	101	CDL	OA8-CA7	3.93	1.44	1.33
75	AA	101	CDL	OA8-CA7	3.91	1.44	1.33
75	AL	502	CDL	OA8-CA7	3.89	1.44	1.33
82	AV	402	HEM	FE-ND	3.88	2.06	1.94
76	V	202	PEE	C18-C19	3.87	1.53	1.31
76	Bl	702	PEE	C18-C19	3.86	1.53	1.31
76	l	702	PEE	C18-C19	3.86	1.53	1.31
76	BV	202	PEE	C18-C19	3.85	1.53	1.31
75	Bl	703	CDL	OA8-CA7	3.85	1.44	1.33
75	l	703	CDL	OA8-CA7	3.84	1.44	1.33
76	W	201	PEE	C18-C19	3.83	1.53	1.31
76	BW	201	PEE	C18-C19	3.83	1.53	1.31
76	V	202	PEE	C39-C38	3.80	1.53	1.31
76	BV	202	PEE	C39-C38	3.79	1.53	1.31
76	Bl	702	PEE	C39-C38	3.77	1.53	1.31
76	BW	201	PEE	C39-C38	3.76	1.53	1.31
76	l	702	PEE	C39-C38	3.76	1.53	1.31
76	W	201	PEE	C39-C38	3.76	1.53	1.31
75	Bi	401	CDL	OA8-CA7	3.72	1.44	1.33
75	i	401	CDL	OA8-CA7	3.70	1.44	1.33
79	Bx	604	HEA	CMA-C3A	-3.67	1.37	1.45
79	x	604	HEA	CMA-C3A	-3.60	1.37	1.45
82	AJ	402	HEM	FE-NC	3.53	2.06	1.95
76	AY	502	PEE	O2-C10	3.47	1.44	1.34
76	AL	503	PEE	O2-C10	3.44	1.44	1.34
75	Bl	704	CDL	OB6-CB5	3.35	1.43	1.34
76	Bl	701	PEE	O2-C10	3.35	1.43	1.34
75	l	704	CDL	OB6-CB5	3.34	1.43	1.34
76	l	701	PEE	O2-C10	3.32	1.43	1.34
75	AY	501	CDL	OB6-CB5	3.29	1.43	1.34
75	Bn	101	CDL	OB6-CB5	3.27	1.43	1.34
75	n	101	CDL	OB6-CB5	3.27	1.43	1.34
75	AJ	404	CDL	OB6-CB5	3.23	1.43	1.34
75	AN	102	CDL	OB6-CB5	3.23	1.43	1.34
75	AH	403	CDL	OB6-CB5	3.22	1.43	1.34
76	AJ	403	PEE	O2-C10	3.21	1.43	1.34
75	Bl	703	CDL	OB6-CB5	3.21	1.43	1.34
82	AJ	402	HEM	FE-NA	3.21	2.05	1.95
75	l	703	CDL	OB6-CB5	3.20	1.43	1.34
76	AU	401	PEE	O2-C10	3.20	1.43	1.34
75	AA	101	CDL	OB6-CB5	3.19	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AU	403	CDL	OB6-CB5	3.18	1.43	1.34
76	AV	403	PEE	O2-C10	3.16	1.43	1.34
70	BA	502	FMN	C8-C7	3.14	1.48	1.40
70	A	502	FMN	C8-C7	3.14	1.48	1.40
75	V	201	CDL	OB6-CB5	3.13	1.43	1.34
71	BB	303	PLX	O6-C4	-3.11	1.40	1.44
75	AL	502	CDL	OB6-CB5	3.11	1.43	1.34
76	AH	401	PEE	O2-C10	3.10	1.43	1.34
75	i	401	CDL	OB6-CB5	3.10	1.43	1.34
71	B	303	PLX	O6-C4	-3.09	1.40	1.44
75	BV	201	CDL	OB6-CB5	3.09	1.43	1.34
82	AV	402	HEM	FE-NC	3.07	2.05	1.95
82	AJ	402	HEM	CAB-C3B	3.06	1.55	1.47
75	BV	201	CDL	OA8-CA7	3.06	1.45	1.33
75	Bi	401	CDL	OB6-CB5	3.06	1.42	1.34
71	g	203	PLX	O6-C4	-3.06	1.40	1.44
75	V	201	CDL	OA8-CA7	3.05	1.45	1.33
82	AV	401	HEM	CAB-C3B	3.05	1.55	1.47
82	AV	402	HEM	CAC-C3C	3.05	1.55	1.47
71	Bg	203	PLX	O6-C4	-3.03	1.40	1.44
79	x	604	HEA	FE-NA	3.03	2.05	1.95
82	AJ	401	HEM	CAB-C3B	3.02	1.55	1.47
70	A	502	FMN	C4-N3	-3.02	1.33	1.38
82	AJ	401	HEM	CAC-C3C	3.00	1.55	1.47
79	Bx	604	HEA	FE-NA	2.99	2.05	1.95
70	BA	502	FMN	C4-N3	-2.99	1.33	1.38
82	AV	402	HEM	CAB-C3B	2.98	1.55	1.47
73	BJ	401	NDP	C5A-N7A	-2.98	1.33	1.39
73	J	401	NDP	C5A-N7A	-2.97	1.33	1.39
75	n	101	CDL	OB6-CB4	-2.95	1.39	1.46
82	AJ	402	HEM	FE-NB	2.93	2.03	1.94
75	Bn	101	CDL	OB6-CB4	-2.93	1.39	1.46
82	AV	401	HEM	FE-NC	2.91	2.04	1.95
82	AJ	402	HEM	CAC-C3C	2.89	1.55	1.47
71	Bg	201	PLX	O6-C4	-2.87	1.40	1.44
71	AN	101	PLX	O6-C4	-2.86	1.40	1.44
82	AV	401	HEM	FE-NA	2.86	2.04	1.95
82	AV	402	HEM	FE-NA	2.85	2.04	1.95
82	AV	402	HEM	FE-NB	2.84	2.03	1.94
71	BV	203	PLX	O6-C4	-2.84	1.41	1.44
71	g	201	PLX	O6-C4	-2.83	1.41	1.44
71	AL	501	PLX	O6-C4	-2.83	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	AL	502	CDL	OB6-CB4	-2.82	1.40	1.46
75	AH	403	CDL	OB6-CB4	-2.81	1.40	1.46
75	V	201	CDL	OB6-CB4	-2.81	1.40	1.46
82	AV	401	HEM	CAC-C3C	2.80	1.54	1.47
75	AA	101	CDL	OB6-CB4	-2.78	1.40	1.46
75	BV	201	CDL	OB6-CB4	-2.78	1.40	1.46
71	U	101	PLX	O6-C4	-2.72	1.41	1.44
71	AQ	101	PLX	O6-C4	-2.71	1.41	1.44
79	x	603	HEA	C1A-C2A	-2.70	1.40	1.45
79	Bx	603	HEA	C1A-C2A	-2.70	1.40	1.45
75	AN	102	CDL	OB6-CB4	-2.70	1.40	1.46
75	i	401	CDL	OB6-CB4	-2.68	1.40	1.46
75	AJ	404	CDL	OB6-CB4	-2.68	1.40	1.46
75	Bi	401	CDL	OB6-CB4	-2.67	1.40	1.46
75	AU	403	CDL	OB6-CB4	-2.67	1.40	1.46
71	BU	101	PLX	O6-C4	-2.67	1.41	1.44
75	AY	501	CDL	OB6-CB4	-2.65	1.40	1.46
82	AJ	401	HEM	FE-NA	2.64	2.03	1.95
72	p	201	8Q1	O35-C34	-2.61	1.18	1.23
82	AV	401	HEM	FE-NB	2.61	2.02	1.94
79	x	604	HEA	C1D-C2D	2.56	1.49	1.44
72	E	201	8Q1	O35-C34	-2.56	1.18	1.23
72	Bp	201	8Q1	O35-C34	-2.56	1.18	1.23
72	BE	201	8Q1	O35-C34	-2.55	1.18	1.23
79	Bx	603	HEA	CMA-C3A	-2.55	1.39	1.45
71	AT	101	PLX	O6-C4	-2.55	1.41	1.44
71	Bg	202	PLX	O6-C4	-2.54	1.41	1.44
79	x	604	HEA	C1D-ND	-2.54	1.35	1.40
71	r	501	PLX	O6-C4	-2.53	1.41	1.44
79	Bx	604	HEA	C1D-ND	-2.53	1.35	1.40
71	g	202	PLX	O6-C4	-2.53	1.41	1.44
79	x	603	HEA	CMA-C3A	-2.53	1.39	1.45
75	Bl	704	CDL	OB6-CB4	-2.52	1.40	1.46
75	l	704	CDL	OB6-CB4	-2.51	1.40	1.46
79	Bx	604	HEA	C1D-C2D	2.50	1.49	1.44
75	l	703	CDL	OB6-CB4	-2.50	1.40	1.46
71	Br	501	PLX	O6-C4	-2.49	1.41	1.44
75	Bl	703	CDL	OB6-CB4	-2.49	1.40	1.46
79	Bx	604	HEA	C3A-C2A	-2.46	1.31	1.37
79	x	604	HEA	C3A-C2A	-2.45	1.31	1.37
70	BA	502	FMN	C5A-N5	-2.43	1.35	1.39
76	BV	202	PEE	O2-C2	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	Bp	201	8Q1	O40-C39	-2.41	1.18	1.23
76	BV	202	PEE	O2-C10	2.40	1.41	1.34
76	l	702	PEE	O2-C10	2.40	1.41	1.34
76	V	202	PEE	O2-C2	-2.40	1.41	1.46
76	V	202	PEE	O2-C10	2.40	1.41	1.34
76	l	702	PEE	O2-C2	-2.39	1.41	1.46
76	Bl	702	PEE	O2-C10	2.39	1.41	1.34
76	Bl	702	PEE	O2-C2	-2.39	1.41	1.46
72	BE	201	8Q1	O40-C39	-2.39	1.18	1.23
70	A	502	FMN	C5A-N5	-2.38	1.35	1.39
72	E	201	8Q1	C1-S44	2.37	1.81	1.76
72	E	201	8Q1	O40-C39	-2.36	1.18	1.23
72	BE	201	8Q1	C1-S44	2.36	1.81	1.76
72	p	201	8Q1	O40-C39	-2.36	1.18	1.23
79	Bx	603	HEA	C3A-C4A	-2.35	1.41	1.46
76	l	702	PEE	O3-C30	2.34	1.40	1.33
76	W	201	PEE	O2-C2	-2.33	1.41	1.46
76	BW	201	PEE	O2-C2	-2.33	1.41	1.46
76	Bl	702	PEE	O3-C30	2.33	1.40	1.33
79	Bx	604	HEA	CMD-C2D	2.33	1.55	1.50
79	x	603	HEA	C3A-C4A	-2.31	1.42	1.46
79	x	604	HEA	CMD-C2D	2.30	1.55	1.50
81	AU	402	HEC	C3C-C2C	-2.28	1.33	1.41
76	Bl	702	PEE	O3-C3	-2.27	1.40	1.45
76	BV	202	PEE	O3-C3	-2.27	1.40	1.45
72	Bp	201	8Q1	C1-S44	2.27	1.81	1.76
76	V	202	PEE	O3-C30	2.26	1.39	1.33
76	V	202	PEE	O3-C3	-2.26	1.40	1.45
72	BE	201	8Q1	C6-C1	2.25	1.53	1.50
76	l	702	PEE	O3-C3	-2.25	1.40	1.45
76	BW	201	PEE	O3-C30	2.24	1.39	1.33
72	E	201	8Q1	C6-C1	2.23	1.53	1.50
72	p	201	8Q1	C1-S44	2.23	1.81	1.76
76	BV	202	PEE	O3-C30	2.23	1.39	1.33
76	W	201	PEE	O3-C3	-2.22	1.40	1.45
76	W	201	PEE	O3-C30	2.22	1.39	1.33
73	J	401	NDP	C5A-C6A	2.21	1.47	1.41
76	BW	201	PEE	O2-C10	2.21	1.40	1.34
76	W	201	PEE	O2-C10	2.20	1.40	1.34
70	A	502	FMN	C2-N3	-2.20	1.34	1.39
76	BW	201	PEE	O3-C3	-2.20	1.40	1.45
73	BJ	401	NDP	C5A-C6A	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AU	402	HEC	C3B-C2B	-2.19	1.33	1.41
82	AJ	401	HEM	C2A-C3A	-2.16	1.33	1.38
81	AH	402	HEC	C3B-C2B	-2.15	1.33	1.41
81	AH	402	HEC	C3C-C2C	-2.15	1.33	1.41
82	AV	401	HEM	C3C-C2C	-2.15	1.32	1.37
70	BA	502	FMN	C2-N3	-2.14	1.34	1.39
82	AJ	401	HEM	FE-NC	2.11	2.02	1.95
79	Bx	604	HEA	FE-NC	2.08	2.02	1.95
73	BJ	401	NDP	C4A-N9A	-2.07	1.33	1.37
73	BJ	401	NDP	C8A-N9A	-2.07	1.34	1.37
75	AU	403	CDL	C11-CA5	2.06	1.56	1.50
73	J	401	NDP	C8A-N9A	-2.05	1.34	1.37
79	x	604	HEA	FE-NC	2.05	2.01	1.95
82	AV	402	HEM	CMB-C2B	2.04	1.55	1.50
82	AV	401	HEM	C2A-C3A	-2.04	1.33	1.38
82	AJ	401	HEM	CMB-C2B	2.03	1.54	1.50
73	J	401	NDP	C4A-N9A	-2.03	1.33	1.37
82	AJ	402	HEM	C2A-C3A	-2.02	1.33	1.38
73	BJ	401	NDP	C8A-N7A	2.01	1.35	1.31

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	CBC-CAC-C3C	-8.69	110.07	127.43
81	AH	402	HEC	CBC-CAC-C3C	-7.92	111.60	127.43
81	AH	402	HEC	CBB-CAB-C3B	-7.83	111.78	127.43
81	AU	402	HEC	CBB-CAB-C3B	-7.08	113.28	127.43
72	p	201	8Q1	C6-C1-S44	5.92	120.45	113.40
72	Bp	201	8Q1	C6-C1-S44	5.90	120.44	113.40
73	BJ	401	NDP	C5A-C4A-N3A	-5.86	118.65	126.72
73	J	401	NDP	C5A-C4A-N3A	-5.83	118.69	126.72
82	AV	402	HEM	C4D-ND-C1D	5.28	111.46	105.21
82	AJ	401	HEM	C4D-ND-C1D	5.26	111.43	105.21
82	AJ	402	HEM	C4D-ND-C1D	5.16	111.32	105.21
73	BJ	401	NDP	N3A-C4A-N9A	4.79	135.32	127.17
73	J	401	NDP	N3A-C4A-N9A	4.78	135.29	127.17
82	AV	401	HEM	C4D-ND-C1D	4.54	110.59	105.21
72	E	201	8Q1	C6-C1-S44	4.52	118.78	113.40
72	BE	201	8Q1	C6-C1-S44	4.49	118.75	113.40
76	l	702	PEE	O2-C10-C11	4.37	120.94	111.48
76	Bl	702	PEE	O2-C10-C11	4.37	120.92	111.48
75	AJ	405	CDL	OB6-CB5-C51	4.30	120.79	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	AY	502	PEE	O2-C10-C11	4.30	120.79	111.48
75	AL	502	CDL	OA6-CA5-C11	4.24	120.66	111.48
75	AG	101	CDL	OB6-CB5-C51	4.21	120.59	111.48
75	AY	501	CDL	OA6-CA5-C11	4.21	120.58	111.48
75	l	703	CDL	OA6-CA5-C11	4.19	120.55	111.48
75	Bl	703	CDL	OA6-CA5-C11	4.18	120.53	111.48
79	x	603	HEA	C17-C18-C19	-4.17	118.08	127.62
79	Bx	603	HEA	C17-C18-C19	-4.17	118.09	127.62
75	AH	403	CDL	OA6-CA5-C11	4.15	120.47	111.48
75	AU	403	CDL	OA6-CA5-C11	4.15	120.46	111.48
75	i	401	CDL	OA6-CA5-C11	4.13	120.42	111.48
75	AJ	404	CDL	OA6-CA5-C11	4.12	120.39	111.48
75	Bi	401	CDL	OA6-CA5-C11	4.12	120.39	111.48
75	BV	201	CDL	OB6-CB5-C51	4.10	120.35	111.48
75	V	201	CDL	OB6-CB5-C51	4.10	120.35	111.48
75	l	704	CDL	OA6-CA5-C11	4.09	120.33	111.48
75	n	101	CDL	OB6-CB5-C51	4.07	120.29	111.48
75	Bn	101	CDL	OB6-CB5-C51	4.07	120.29	111.48
75	Bl	704	CDL	OA6-CA5-C11	4.07	120.29	111.48
75	AA	101	CDL	OA6-CA5-C11	4.07	120.28	111.48
75	AU	403	CDL	OB6-CB5-C51	4.04	120.22	111.48
75	AJ	404	CDL	OB6-CB5-C51	4.03	120.19	111.48
76	AJ	403	PEE	O2-C10-C11	4.02	120.18	111.48
76	Bl	701	PEE	O2-C10-C11	4.00	120.13	111.48
75	AA	101	CDL	OB6-CB5-C51	3.98	120.10	111.48
76	l	701	PEE	O2-C10-C11	3.98	120.09	111.48
75	l	703	CDL	OB6-CB5-C51	3.98	120.08	111.48
75	Bl	703	CDL	OB6-CB5-C51	3.96	120.06	111.48
75	AN	102	CDL	OA6-CA5-C11	3.95	120.03	111.48
75	n	101	CDL	OA6-CA5-C11	3.94	120.01	111.48
75	Bn	101	CDL	OA6-CA5-C11	3.94	120.01	111.48
75	Bl	704	CDL	OB6-CB5-C51	3.93	119.99	111.48
75	l	704	CDL	OB6-CB5-C51	3.93	119.98	111.48
75	AH	403	CDL	OB6-CB5-C51	3.92	119.96	111.48
76	AV	403	PEE	O2-C10-C11	3.91	119.94	111.48
75	AY	501	CDL	OB6-CB5-C51	3.89	119.91	111.48
73	BJ	401	NDP	C2A-N3A-C4A	3.89	121.33	111.83
73	J	401	NDP	C2A-N3A-C4A	3.86	121.26	111.83
75	AN	102	CDL	OB6-CB5-C51	3.86	119.82	111.48
75	AL	502	CDL	OB6-CB5-C51	3.85	119.81	111.48
73	BJ	401	NDP	N3A-C2A-N1A	-3.85	122.76	128.58
73	J	401	NDP	N3A-C2A-N1A	-3.78	122.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	p	201	8Q1	O4-C1-C6	-3.74	119.66	123.98
76	BW	201	PEE	O2-C10-C11	3.71	119.50	111.48
72	Bp	201	8Q1	O4-C1-C6	-3.70	119.71	123.98
76	W	201	PEE	O2-C10-C11	3.69	119.47	111.48
81	AH	402	HEC	C4D-ND-C1D	3.64	111.75	105.82
76	BV	202	PEE	O2-C10-C11	3.62	119.32	111.48
76	V	202	PEE	O2-C10-C11	3.60	119.28	111.48
75	AG	101	CDL	OA6-CA5-C11	3.59	119.25	111.48
76	AH	401	PEE	O2-C10-C11	3.55	119.16	111.48
75	AJ	405	CDL	OA6-CA5-C11	3.55	119.15	111.48
76	AL	503	PEE	O2-C10-C11	3.53	119.11	111.48
81	AU	402	HEC	C4D-ND-C1D	3.50	111.53	105.82
75	Bi	401	CDL	OB6-CB5-C51	3.49	119.04	111.48
75	i	401	CDL	OB6-CB5-C51	3.49	119.02	111.48
75	V	201	CDL	OA6-CA5-C11	3.45	118.95	111.48
75	BV	201	CDL	OA6-CA5-C11	3.44	118.92	111.48
75	AJ	405	CDL	OB8-CB7-C71	3.37	122.11	111.83
79	Bx	603	HEA	C13-C14-C15	-3.28	120.11	127.62
79	x	603	HEA	C13-C14-C15	-3.27	120.14	127.62
73	BJ	401	NDP	C4A-C5A-N7A	-3.26	106.86	110.58
73	J	401	NDP	C4A-C5A-N7A	-3.24	106.88	110.58
79	Bx	604	HEA	CHA-C1A-NA	-3.23	120.93	124.45
79	x	604	HEA	CHA-C1A-NA	-3.22	120.95	124.45
76	AU	401	PEE	O2-C10-C11	3.22	118.44	111.48
76	AV	403	PEE	O3-C30-C31	3.17	121.52	111.83
75	l	703	CDL	OA8-CA7-C31	3.10	121.28	111.83
75	Bl	703	CDL	OA8-CA7-C31	3.09	121.26	111.83
75	AA	101	CDL	OA8-CA7-C31	3.08	121.22	111.83
79	x	603	HEA	C1B-C2B-C3B	3.06	110.33	106.80
79	Bx	603	HEA	C1B-C2B-C3B	3.00	110.27	106.80
75	AG	101	CDL	CB4-OB6-CB5	-3.00	110.62	117.80
72	E	201	8Q1	C43-S44-C1	2.96	110.60	101.84
76	V	202	PEE	O3-C30-C31	2.95	120.84	111.83
76	BV	202	PEE	O3-C30-C31	2.95	120.84	111.83
76	Bl	702	PEE	O3-C30-C31	2.95	120.84	111.83
72	BE	201	8Q1	C43-S44-C1	2.95	110.56	101.84
72	E	201	8Q1	C32-C34-N36	2.95	122.08	116.48
76	l	702	PEE	O3-C30-C31	2.94	120.80	111.83
72	BE	201	8Q1	C32-C34-N36	2.93	122.05	116.48
70	A	502	FMN	C4-C4A-N5	2.93	122.25	118.21
70	BA	502	FMN	C4-C4A-N5	2.92	122.24	118.21
72	Bp	201	8Q1	C43-S44-C1	2.87	110.33	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	p	201	8Q1	C43-S44-C1	2.87	110.32	101.84
75	i	401	CDL	OB8-CB7-C71	2.86	120.56	111.83
75	Bn	101	CDL	OA8-CA7-C31	2.85	120.54	111.83
75	n	101	CDL	OA8-CA7-C31	2.85	120.53	111.83
75	Bi	401	CDL	OB8-CB7-C71	2.85	120.51	111.83
75	AG	101	CDL	OB8-CB7-C71	2.84	120.51	111.83
75	AL	502	CDL	OA8-CA7-C31	2.83	120.47	111.83
75	l	704	CDL	OA8-CA7-C31	2.82	120.43	111.83
75	Bl	704	CDL	OA8-CA7-C31	2.82	120.43	111.83
75	AJ	405	CDL	OA8-CA7-C31	2.81	120.41	111.83
73	BJ	401	NDP	C4A-N9A-C8A	2.81	108.68	105.74
75	l	703	CDL	OB8-CB7-C71	2.80	120.38	111.83
75	AL	502	CDL	OB8-CB7-C71	2.80	120.36	111.83
75	Bn	101	CDL	OB8-CB7-C71	2.80	120.36	111.83
76	W	201	PEE	O3-C30-C31	2.79	120.35	111.83
75	Bl	703	CDL	OB8-CB7-C71	2.79	120.35	111.83
75	n	101	CDL	OB8-CB7-C71	2.79	120.35	111.83
75	AN	102	CDL	OA8-CA7-C31	2.79	120.34	111.83
76	BW	201	PEE	O3-C30-C31	2.78	120.33	111.83
75	l	704	CDL	OB8-CB7-C71	2.78	120.32	111.83
75	Bl	704	CDL	OB8-CB7-C71	2.77	120.30	111.83
73	J	401	NDP	C4A-N9A-C8A	2.77	108.65	105.74
75	AU	403	CDL	OA8-CA7-C31	2.77	120.28	111.83
75	AH	403	CDL	OB8-CB7-C71	2.77	120.27	111.83
75	AJ	404	CDL	OA8-CA7-C31	2.76	120.25	111.83
76	AH	401	PEE	O3-C30-C31	2.75	120.23	111.83
75	AA	101	CDL	OB8-CB7-C71	2.70	120.07	111.83
75	AU	403	CDL	OB8-CB7-C71	2.69	120.03	111.83
75	AG	101	CDL	OA8-CA7-C31	2.67	119.97	111.83
75	V	201	CDL	OB8-CB7-C71	2.64	119.89	111.83
75	BV	201	CDL	OB8-CB7-C71	2.63	119.87	111.83
75	AJ	404	CDL	OB8-CB7-C71	2.63	119.86	111.83
75	AY	501	CDL	OA8-CA7-C31	2.63	119.84	111.83
75	AN	102	CDL	OB8-CB7-C71	2.62	119.82	111.83
73	BJ	401	NDP	C5A-N7A-C8A	2.62	107.57	103.45
73	J	401	NDP	C5A-N7A-C8A	2.61	107.56	103.45
75	AY	501	CDL	OB8-CB7-C71	2.61	119.81	111.83
75	AH	403	CDL	OA8-CA7-C31	2.60	119.75	111.83
76	AL	503	PEE	O3-C30-C31	2.57	119.69	111.83
72	E	201	8Q1	O4-C1-C6	-2.57	121.01	123.98
79	Bx	604	HEA	CMD-C2D-C1D	2.57	129.04	125.03
72	BE	201	8Q1	O4-C1-C6	-2.56	121.02	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	A	502	FMN	C4A-C10-N1	-2.56	118.32	124.59
79	x	604	HEA	CMD-C2D-C1D	2.55	129.02	125.03
70	BA	502	FMN	C4A-C10-N1	-2.55	118.34	124.59
75	Bi	401	CDL	OA8-CA7-C31	2.51	119.50	111.83
71	AT	101	PLX	C1C-N1-C1	2.51	119.90	109.91
75	i	401	CDL	OA8-CA7-C31	2.51	119.50	111.83
76	AJ	403	PEE	O3-C30-C31	2.49	119.44	111.83
70	A	502	FMN	C4A-C10-N10	2.47	120.01	116.48
79	x	603	HEA	C17-C16-C15	-2.46	105.02	113.19
70	BA	502	FMN	C4A-C10-N10	2.46	120.00	116.48
79	Bx	603	HEA	C17-C16-C15	-2.44	105.09	113.19
71	B	303	PLX	C1C-N1-C1	2.44	119.59	109.91
79	x	604	HEA	C4A-C3A-C2A	2.43	108.92	106.81
79	Bx	604	HEA	C4A-C3A-C2A	2.43	108.92	106.81
81	AU	402	HEC	C2A-C1A-NA	-2.43	107.98	110.32
79	Bx	604	HEA	C12-C11-C3B	2.43	115.92	112.12
71	BB	303	PLX	C1C-N1-C1	2.42	119.54	109.91
82	AV	401	HEM	CAD-CBD-CGD	-2.42	107.25	113.67
71	AL	501	PLX	C1C-N1-C1	2.42	119.53	109.91
81	AH	402	HEC	C2A-C1A-NA	-2.41	107.99	110.32
79	x	604	HEA	C1D-C2D-C3D	-2.41	104.44	106.98
79	x	604	HEA	C12-C11-C3B	2.41	115.89	112.12
79	Bx	604	HEA	C1D-C2D-C3D	-2.40	104.45	106.98
70	BA	502	FMN	C4'-C3'-C2'	-2.40	109.58	113.57
76	AU	401	PEE	O3-C30-C31	2.40	119.14	111.83
71	AN	101	PLX	C1C-N1-C1	2.40	119.44	109.91
72	Bp	201	8Q1	C38-C39-N41	2.40	120.71	116.34
71	BV	203	PLX	C1C-N1-C1	2.40	119.43	109.91
72	p	201	8Q1	C38-C39-N41	2.39	120.70	116.34
72	E	201	8Q1	C42-N41-C39	-2.39	118.37	122.82
76	l	701	PEE	O3-C30-C31	2.39	119.11	111.83
76	AY	502	PEE	O3-C30-C31	2.38	119.10	111.83
72	BE	201	8Q1	C42-N41-C39	-2.37	118.41	122.82
71	BU	101	PLX	C1C-N1-C1	2.37	119.32	109.91
76	Bl	701	PEE	O3-C30-C31	2.37	119.05	111.83
71	U	101	PLX	C1C-N1-C1	2.36	119.30	109.91
70	A	502	FMN	C4'-C3'-C2'	-2.36	109.64	113.57
79	x	604	HEA	C13-C14-C15	-2.35	122.24	127.62
82	AV	402	HEM	CAD-C3D-C4D	2.35	128.79	124.70
71	Bg	203	PLX	C1C-N1-C1	2.34	119.21	109.91
79	Bx	604	HEA	C13-C14-C15	-2.34	122.28	127.62
71	g	203	PLX	C1C-N1-C1	2.33	119.17	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	BA	502	FMN	C4-N3-C2	-2.33	121.51	125.64
70	A	502	FMN	O2-C2-N1	-2.32	117.94	121.80
79	x	603	HEA	CAD-C3D-C4D	2.32	128.74	124.70
72	E	201	8Q1	C37-N36-C34	-2.32	118.38	122.55
70	A	502	FMN	C4-N3-C2	-2.32	121.52	125.64
79	x	604	HEA	CMB-C2B-C3B	-2.32	125.79	130.28
79	Bx	603	HEA	CAD-C3D-C4D	2.32	128.74	124.70
72	BE	201	8Q1	C37-N36-C34	-2.31	118.39	122.55
79	Bx	604	HEA	C25-C23-C24	2.29	119.86	114.59
79	Bx	603	HEA	C3C-C4C-NC	2.29	111.72	109.80
79	Bx	604	HEA	CMB-C2B-C3B	-2.28	125.86	130.28
71	Bg	201	PLX	C1C-N1-C1	2.28	118.96	109.91
70	BA	502	FMN	O2-C2-N1	-2.28	118.02	121.80
71	g	201	PLX	C1C-N1-C1	2.27	118.94	109.91
79	x	603	HEA	C4B-C3B-C2B	-2.27	103.62	107.44
82	AJ	402	HEM	CAD-C3D-C4D	2.27	128.65	124.70
79	x	603	HEA	C3C-C4C-NC	2.26	111.71	109.80
79	x	604	HEA	C25-C23-C24	2.26	119.79	114.59
71	Bg	202	PLX	C1C-N1-C1	2.26	118.89	109.91
71	g	202	PLX	C1C-N1-C1	2.26	118.89	109.91
75	AJ	405	CDL	OB8-CB7-OB9	-2.25	118.00	123.63
79	Bx	603	HEA	C4B-C3B-C2B	-2.23	103.68	107.44
72	Bp	201	8Q1	O4-C1-S44	-2.23	119.85	122.68
72	p	201	8Q1	O4-C1-S44	-2.20	119.88	122.68
79	x	604	HEA	C26-C15-C16	2.20	119.04	115.23
71	Br	502	PLX	C2-C1-N1	-2.20	108.77	115.82
71	r	502	PLX	C2-C1-N1	-2.19	108.79	115.82
79	x	604	HEA	CAA-C2A-C1A	2.19	129.30	124.85
72	E	201	8Q1	O35-C34-N36	-2.18	118.36	122.98
79	Bx	604	HEA	CAA-C2A-C1A	2.18	129.29	124.85
73	BJ	401	NDP	C3D-C2D-C1D	2.18	105.59	101.46
73	J	401	NDP	C3D-C2D-C1D	2.17	105.58	101.46
72	BE	201	8Q1	O35-C34-N36	-2.17	118.38	122.98
79	Bx	604	HEA	C26-C15-C16	2.17	119.00	115.23
79	x	603	HEA	C12-C13-C14	-2.17	106.46	112.16
79	Bx	603	HEA	C12-C13-C14	-2.17	106.46	112.16
73	BJ	401	NDP	N9A-C8A-N7A	-2.17	110.86	113.94
82	AJ	402	HEM	C1B-NB-C4B	2.16	107.76	105.21
73	J	401	NDP	N9A-C8A-N7A	-2.14	110.89	113.94
71	AQ	101	PLX	C2-C1-N1	-2.13	108.99	115.82
71	r	501	PLX	C1C-N1-C1	2.13	118.37	109.91
71	Br	501	PLX	C1C-N1-C1	2.13	118.37	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	A	502	FMN	C4A-C4-N3	2.13	118.67	113.25
71	BU	101	PLX	C5-C4-C3	-2.12	106.83	111.78
70	BA	502	FMN	C4A-C4-N3	2.12	118.64	113.25
75	AG	101	CDL	OB6-CB5-OB7	-2.12	118.75	123.70
71	U	101	PLX	C5-C4-C3	-2.12	106.85	111.78
75	i	401	CDL	OA6-CA5-OA7	-2.10	118.78	123.70
79	x	603	HEA	C20-C19-C18	2.10	125.89	121.17
75	Bi	401	CDL	OA6-CA5-OA7	-2.10	118.80	123.70
79	Bx	603	HEA	C20-C19-C18	2.10	125.87	121.17
72	p	201	8Q1	C32-C34-N36	2.09	120.45	116.48
71	AQ	101	PLX	C1C-N1-C1	2.09	118.21	109.91
82	AJ	402	HEM	C3B-C2B-C1B	2.09	107.98	106.41
79	Bx	604	HEA	CBD-CAD-C3D	2.09	118.30	112.53
82	AV	402	HEM	CAA-C2A-C1A	2.08	129.00	124.94
72	Bp	201	8Q1	C32-C34-N36	2.07	120.42	116.48
70	BA	502	FMN	C5A-C9A-N10	2.07	119.84	117.97
79	x	604	HEA	CBD-CAD-C3D	2.06	118.24	112.53
82	AJ	402	HEM	C2A-C1A-NA	-2.06	107.87	110.15
82	AV	401	HEM	C1B-NB-C4B	2.05	107.64	105.21
82	AJ	402	HEM	CHD-C1D-ND	2.05	126.62	124.42
82	AV	402	HEM	C1B-NB-C4B	2.04	107.63	105.21
73	BJ	401	NDP	C6A-C5A-N7A	2.04	136.03	132.09
82	AV	402	HEM	C3B-C2B-C1B	2.04	107.94	106.41
73	J	401	NDP	C6A-C5A-N7A	2.04	136.02	132.09
79	x	603	HEA	C27-C19-C18	-2.03	118.40	123.63
82	AJ	401	HEM	CHC-C1C-NC	2.03	126.66	124.45
79	Bx	603	HEA	C27-C19-C18	-2.03	118.42	123.63
82	AV	402	HEM	C2A-C1A-NA	-2.03	107.91	110.15
70	A	502	FMN	C5A-C9A-N10	2.02	119.80	117.97
75	AA	101	CDL	CB4-OB6-CB5	-2.02	112.96	117.80
81	AH	402	HEC	CHA-C1A-C2A	2.02	128.05	124.86
79	x	603	HEA	OMA-CMA-C3A	-2.00	121.10	125.62
70	BA	502	FMN	C10-N1-C2	2.00	121.19	116.85

There are no chirality outliers.

All (1763) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
70	BA	502	FMN	C1'-C2'-C3'-O3'
70	BA	502	FMN	C1'-C2'-C3'-C4'
70	BA	502	FMN	C3'-C4'-C5'-O5'
70	BA	502	FMN	O4'-C4'-C5'-O5'
71	B	303	PLX	C2-O1-P1-O4
71	B	303	PLX	C2-O1-P1-O2
71	B	303	PLX	N1-C1-C2-O1
71	U	101	PLX	O7-C6-C7-C8
71	U	101	PLX	O7-C6-O6-C4
71	U	101	PLX	C3-O4-P1-O1
71	U	101	PLX	C3-O4-P1-O2
71	U	101	PLX	N1-C1-C2-O1
71	U	101	PLX	O9-C24-C25-C26
71	b	201	PLX	O7-C6-O6-C4
71	b	201	PLX	C3-O4-P1-O1
71	b	201	PLX	N1-C1-C2-O1
71	b	201	PLX	O9-C24-O8-C5
71	g	201	PLX	O7-C6-C7-C8
71	g	201	PLX	O7-C6-O6-C4
71	g	201	PLX	C3-C4-O6-C6
71	g	201	PLX	C3-O4-P1-O1
71	g	201	PLX	C3-O4-P1-O3
71	g	202	PLX	C2-O1-P1-O4
71	g	202	PLX	C2-O1-P1-O2
71	g	202	PLX	C2-O1-P1-O3
71	g	202	PLX	O9-C24-O8-C5
71	g	203	PLX	O7-C6-O6-C4
71	g	203	PLX	C2-O1-P1-O4
71	g	203	PLX	C2-O1-P1-O2
71	g	203	PLX	C25-C24-O8-C5
71	r	501	PLX	C3-O4-P1-O1
71	r	501	PLX	C3-O4-P1-O2
71	r	501	PLX	C3-O4-P1-O3
71	r	501	PLX	O8-C24-C25-C26
71	r	502	PLX	C7-C6-O6-C4
71	r	502	PLX	C3-O4-P1-O1
71	r	502	PLX	C3-O4-P1-O2
71	r	502	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O4
71	r	502	PLX	C2-O1-P1-O2
71	r	502	PLX	N1-C1-C2-O1
71	r	502	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
71	AL	501	PLX	O7-C6-C7-C8
71	AN	101	PLX	O7-C6-C7-C8
71	AN	101	PLX	N1-C1-C2-O1
71	AN	101	PLX	O9-C24-C25-C26
71	AQ	101	PLX	O7-C6-O6-C4
71	AQ	101	PLX	O6-C4-C5-O8
71	AQ	101	PLX	N1-C1-C2-O1
71	AQ	101	PLX	C25-C24-O8-C5
71	AQ	101	PLX	O9-C24-C25-C26
71	AT	101	PLX	C2-O1-P1-O4
71	AT	101	PLX	O9-C24-O8-C5
71	BB	303	PLX	C2-O1-P1-O4
71	BB	303	PLX	C2-O1-P1-O2
71	BB	303	PLX	N1-C1-C2-O1
71	BU	101	PLX	O7-C6-C7-C8
71	BU	101	PLX	O7-C6-O6-C4
71	BU	101	PLX	C3-O4-P1-O1
71	BU	101	PLX	C3-O4-P1-O2
71	BU	101	PLX	N1-C1-C2-O1
71	BU	101	PLX	O9-C24-C25-C26
71	BV	203	PLX	O7-C6-C7-C8
71	BV	203	PLX	N1-C1-C2-O1
71	BV	203	PLX	O9-C24-C25-C26
71	Bb	201	PLX	O7-C6-O6-C4
71	Bb	201	PLX	C3-O4-P1-O1
71	Bb	201	PLX	N1-C1-C2-O1
71	Bb	201	PLX	O9-C24-O8-C5
71	Bg	201	PLX	O7-C6-C7-C8
71	Bg	201	PLX	O7-C6-O6-C4
71	Bg	201	PLX	C3-C4-O6-C6
71	Bg	201	PLX	C3-O4-P1-O1
71	Bg	201	PLX	C3-O4-P1-O3
71	Bg	202	PLX	C2-O1-P1-O4
71	Bg	202	PLX	C2-O1-P1-O2
71	Bg	202	PLX	C2-O1-P1-O3
71	Bg	202	PLX	O9-C24-O8-C5
71	Bg	203	PLX	O7-C6-O6-C4
71	Bg	203	PLX	C2-O1-P1-O4
71	Bg	203	PLX	C2-O1-P1-O2
71	Bg	203	PLX	C25-C24-O8-C5
71	Br	501	PLX	C3-O4-P1-O1
71	Br	501	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
71	Br	501	PLX	C3-O4-P1-O3
71	Br	501	PLX	O8-C24-C25-C26
71	Br	502	PLX	C7-C6-O6-C4
71	Br	502	PLX	C3-O4-P1-O1
71	Br	502	PLX	C3-O4-P1-O2
71	Br	502	PLX	C3-O4-P1-O3
71	Br	502	PLX	C2-O1-P1-O4
71	Br	502	PLX	C2-O1-P1-O2
71	Br	502	PLX	N1-C1-C2-O1
71	Br	502	PLX	O9-C24-C25-C26
72	E	201	8Q1	C1-C6-C7-C8
72	E	201	8Q1	O4-C1-S44-C43
72	E	201	8Q1	C6-C1-S44-C43
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	C29-C32-C34-O35
72	E	201	8Q1	C42-C43-S44-C1
72	E	201	8Q1	C28-O27-P24-O3
72	E	201	8Q1	C28-O27-P24-O2
72	E	201	8Q1	C28-O27-P24-O1
72	p	201	8Q1	C1-C6-C7-C8
72	p	201	8Q1	O4-C1-S44-C43
72	p	201	8Q1	C6-C1-S44-C43
72	p	201	8Q1	C28-C29-C32-C34
72	p	201	8Q1	C28-C29-C32-O33
72	p	201	8Q1	C30-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-O33
72	p	201	8Q1	C28-O27-P24-O2
72	p	201	8Q1	C28-O27-P24-O1
72	BE	201	8Q1	C1-C6-C7-C8
72	BE	201	8Q1	O4-C1-S44-C43
72	BE	201	8Q1	C6-C1-S44-C43
72	BE	201	8Q1	C29-C32-C34-N36
72	BE	201	8Q1	C29-C32-C34-O35
72	BE	201	8Q1	C42-C43-S44-C1
72	BE	201	8Q1	C28-O27-P24-O3
72	BE	201	8Q1	C28-O27-P24-O2
72	BE	201	8Q1	C28-O27-P24-O1
72	Bp	201	8Q1	C1-C6-C7-C8
72	Bp	201	8Q1	O4-C1-S44-C43
72	Bp	201	8Q1	C6-C1-S44-C43
72	Bp	201	8Q1	C28-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
72	Bp	201	8Q1	C28-C29-C32-O33
72	Bp	201	8Q1	C30-C29-C32-C34
72	Bp	201	8Q1	C31-C29-C32-C34
72	Bp	201	8Q1	C31-C29-C32-O33
72	Bp	201	8Q1	C28-O27-P24-O2
72	Bp	201	8Q1	C28-O27-P24-O1
73	J	401	NDP	C5B-O5B-PA-O1A
73	J	401	NDP	C5B-O5B-PA-O3
73	J	401	NDP	C5D-O5D-PN-O1N
73	BJ	401	NDP	C5B-O5B-PA-O1A
73	BJ	401	NDP	C5B-O5B-PA-O3
73	BJ	401	NDP	C5D-O5D-PN-O1N
75	V	201	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CA2-OA2-PA1-OA3
75	V	201	CDL	CA2-OA2-PA1-OA4
75	V	201	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	CA3-OA5-PA1-OA2
75	V	201	CDL	CA3-OA5-PA1-OA3
75	V	201	CDL	CA3-OA5-PA1-OA4
75	V	201	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	CB3-OB5-PB2-OB2
75	V	201	CDL	CB3-OB5-PB2-OB4
75	V	201	CDL	C51-CB5-OB6-CB4
75	i	401	CDL	O1-C1-CA2-OA2
75	i	401	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	CA2-OA2-PA1-OA3
75	i	401	CDL	CA2-OA2-PA1-OA4
75	i	401	CDL	CA2-OA2-PA1-OA5
75	i	401	CDL	CA3-OA5-PA1-OA2
75	i	401	CDL	CA3-OA5-PA1-OA3
75	i	401	CDL	CA3-OA5-PA1-OA4
75	i	401	CDL	OA6-CA4-CA6-OA8
75	i	401	CDL	CB2-OB2-PB2-OB4
75	i	401	CDL	CB2-OB2-PB2-OB5
75	i	401	CDL	CB3-OB5-PB2-OB3
75	i	401	CDL	CB3-OB5-PB2-OB4
75	l	703	CDL	CA2-OA2-PA1-OA3
75	l	703	CDL	CA2-OA2-PA1-OA5
75	l	703	CDL	CB3-OB5-PB2-OB2
75	l	703	CDL	CB3-OB5-PB2-OB4
75	l	703	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	CA2-OA2-PA1-OA4
75	l	704	CDL	CA2-OA2-PA1-OA5
75	l	704	CDL	CA3-OA5-PA1-OA2
75	l	704	CDL	CA3-OA5-PA1-OA4
75	l	704	CDL	C11-CA5-OA6-CA4
75	l	704	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CA2-OA2-PA1-OA3
75	n	101	CDL	CA2-OA2-PA1-OA4
75	n	101	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	C11-CA5-OA6-CA4
75	n	101	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CB2-OB2-PB2-OB4
75	n	101	CDL	CB2-OB2-PB2-OB5
75	n	101	CDL	C51-CB5-OB6-CB4
75	AA	101	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	CB2-OB2-PB2-OB4
75	AA	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CA2-OA2-PA1-OA5
75	AG	101	CDL	OA9-CA7-OA8-CA6
75	AG	101	CDL	CB2-OB2-PB2-OB4
75	AG	101	CDL	CB2-OB2-PB2-OB5
75	AH	403	CDL	CA2-OA2-PA1-OA3
75	AH	403	CDL	CA2-OA2-PA1-OA4
75	AH	403	CDL	CA2-OA2-PA1-OA5
75	AH	403	CDL	CA3-OA5-PA1-OA2
75	AH	403	CDL	C11-CA5-OA6-CA4
75	AH	403	CDL	CB3-OB5-PB2-OB2
75	AH	403	CDL	CB3-OB5-PB2-OB3
75	AH	403	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	CA3-OA5-PA1-OA2
75	AJ	404	CDL	CA3-OA5-PA1-OA3
75	AJ	404	CDL	CA3-OA5-PA1-OA4
75	AJ	404	CDL	C11-CA5-OA6-CA4
75	AJ	404	CDL	CB3-OB5-PB2-OB2
75	AJ	404	CDL	CB3-OB5-PB2-OB3
75	AJ	404	CDL	CB3-OB5-PB2-OB4
75	AJ	405	CDL	CA3-OA5-PA1-OA2
75	AJ	405	CDL	CA3-OA5-PA1-OA4
75	AJ	405	CDL	C51-CB5-OB6-CB4
75	AL	502	CDL	O1-C1-CA2-OA2
75	AL	502	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	AL	502	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	C11-CA5-OA6-CA4
75	AL	502	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CB2-OB2-PB2-OB4
75	AL	502	CDL	CB2-OB2-PB2-OB5
75	AL	502	CDL	C71-CB7-OB8-CB6
75	AN	102	CDL	CA3-OA5-PA1-OA2
75	AN	102	CDL	CA3-OA5-PA1-OA3
75	AN	102	CDL	OA7-CA5-OA6-CA4
75	AN	102	CDL	C11-CA5-OA6-CA4
75	AN	102	CDL	CB2-OB2-PB2-OB4
75	AN	102	CDL	CB2-OB2-PB2-OB5
75	AU	403	CDL	CA3-OA5-PA1-OA2
75	AU	403	CDL	CA3-OA5-PA1-OA3
75	AU	403	CDL	C11-CA5-OA6-CA4
75	AU	403	CDL	CB3-OB5-PB2-OB3
75	AU	403	CDL	OB7-CB5-OB6-CB4
75	AY	501	CDL	CB2-C1-CA2-OA2
75	AY	501	CDL	CA3-OA5-PA1-OA2
75	AY	501	CDL	CA3-OA5-PA1-OA4
75	AY	501	CDL	C11-CA5-OA6-CA4
75	BV	201	CDL	CB2-C1-CA2-OA2
75	BV	201	CDL	CA2-OA2-PA1-OA3
75	BV	201	CDL	CA2-OA2-PA1-OA4
75	BV	201	CDL	CA2-OA2-PA1-OA5
75	BV	201	CDL	CA3-OA5-PA1-OA2
75	BV	201	CDL	CA3-OA5-PA1-OA3
75	BV	201	CDL	CA3-OA5-PA1-OA4
75	BV	201	CDL	OA9-CA7-OA8-CA6
75	BV	201	CDL	CB3-OB5-PB2-OB2
75	BV	201	CDL	CB3-OB5-PB2-OB4
75	BV	201	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	O1-C1-CA2-OA2
75	Bi	401	CDL	CB2-C1-CA2-OA2
75	Bi	401	CDL	CA2-OA2-PA1-OA3
75	Bi	401	CDL	CA2-OA2-PA1-OA4
75	Bi	401	CDL	CA2-OA2-PA1-OA5
75	Bi	401	CDL	CA3-OA5-PA1-OA2
75	Bi	401	CDL	CA3-OA5-PA1-OA3
75	Bi	401	CDL	CA3-OA5-PA1-OA4
75	Bi	401	CDL	OA6-CA4-CA6-OA8
75	Bi	401	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
75	Bi	401	CDL	CB2-OB2-PB2-OB5
75	Bi	401	CDL	CB3-OB5-PB2-OB3
75	Bi	401	CDL	CB3-OB5-PB2-OB4
75	Bl	703	CDL	CA2-OA2-PA1-OA3
75	Bl	703	CDL	CA2-OA2-PA1-OA5
75	Bl	703	CDL	CB3-OB5-PB2-OB2
75	Bl	703	CDL	CB3-OB5-PB2-OB4
75	Bl	703	CDL	OB7-CB5-OB6-CB4
75	Bl	704	CDL	CA2-OA2-PA1-OA3
75	Bl	704	CDL	CA2-OA2-PA1-OA4
75	Bl	704	CDL	CA2-OA2-PA1-OA5
75	Bl	704	CDL	CA3-OA5-PA1-OA2
75	Bl	704	CDL	CA3-OA5-PA1-OA4
75	Bl	704	CDL	C11-CA5-OA6-CA4
75	Bl	704	CDL	CB2-OB2-PB2-OB3
75	Bn	101	CDL	CA2-OA2-PA1-OA3
75	Bn	101	CDL	CA2-OA2-PA1-OA4
75	Bn	101	CDL	CA2-OA2-PA1-OA5
75	Bn	101	CDL	OA7-CA5-OA6-CA4
75	Bn	101	CDL	C11-CA5-OA6-CA4
75	Bn	101	CDL	CB2-OB2-PB2-OB3
75	Bn	101	CDL	CB2-OB2-PB2-OB4
75	Bn	101	CDL	CB2-OB2-PB2-OB5
75	Bn	101	CDL	C51-CB5-OB6-CB4
76	V	202	PEE	C2-C1-O3P-P
76	V	202	PEE	C1-O3P-P-O4P
76	V	202	PEE	O4P-C4-C5-N
76	W	201	PEE	C4-O4P-P-O3P
76	W	201	PEE	C4-O4P-P-O1P
76	l	701	PEE	C11-C10-O2-C2
76	l	701	PEE	C4-O4P-P-O2P
76	l	701	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C4-O4P-P-O2P
76	AJ	403	PEE	C37-C38-C39-C40
76	AL	503	PEE	C11-C10-O2-C2
76	AL	503	PEE	O4-C10-O2-C2
76	AU	401	PEE	C11-C10-O2-C2
76	AU	401	PEE	C1-O3P-P-O2P
76	AU	401	PEE	C1-O3P-P-O1P
76	AU	401	PEE	C4-O4P-P-O3P
76	AU	401	PEE	C4-O4P-P-O2P
76	AV	403	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
76	AV	403	PEE	O4P-C4-C5-N
76	AV	403	PEE	C39-C40-C41-C42
76	AY	502	PEE	C1-O3P-P-O2P
76	AY	502	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C4-O4P-P-O2P
76	AY	502	PEE	C4-O4P-P-O1P
76	BV	202	PEE	C2-C1-O3P-P
76	BV	202	PEE	C1-O3P-P-O4P
76	BV	202	PEE	O4P-C4-C5-N
76	BW	201	PEE	C4-O4P-P-O3P
76	BW	201	PEE	C4-O4P-P-O1P
76	Bl	701	PEE	C11-C10-O2-C2
76	Bl	701	PEE	C4-O4P-P-O2P
76	Bl	701	PEE	C4-O4P-P-O1P
79	x	603	HEA	C2A-C3A-CMA-OMA
79	x	603	HEA	C4A-C3A-CMA-OMA
79	x	604	HEA	C2A-C3A-CMA-OMA
79	x	604	HEA	C4A-C3A-CMA-OMA
79	Bx	603	HEA	C2A-C3A-CMA-OMA
79	Bx	603	HEA	C4A-C3A-CMA-OMA
79	Bx	604	HEA	C2A-C3A-CMA-OMA
79	Bx	604	HEA	C4A-C3A-CMA-OMA
81	AH	402	HEC	C2B-C3B-CAB-CBB
81	AH	402	HEC	C4B-C3B-CAB-CBB
81	AH	402	HEC	C2C-C3C-CAC-CBC
81	AH	402	HEC	C4C-C3C-CAC-CBC
81	AU	402	HEC	C2B-C3B-CAB-CBB
81	AU	402	HEC	C4B-C3B-CAB-CBB
81	AU	402	HEC	C2C-C3C-CAC-CBC
81	AU	402	HEC	C4C-C3C-CAC-CBC
82	AV	402	HEM	C1A-C2A-CAA-CBA
75	AL	502	CDL	OB9-CB7-OB8-CB6
75	l	704	CDL	OA9-CA7-OA8-CA6
75	l	704	CDL	OB9-CB7-OB8-CB6
75	n	101	CDL	OA9-CA7-OA8-CA6
75	AA	101	CDL	OB9-CB7-OB8-CB6
75	AN	102	CDL	OB9-CB7-OB8-CB6
75	AU	403	CDL	OB9-CB7-OB8-CB6
75	Bl	704	CDL	OA9-CA7-OA8-CA6
75	Bl	704	CDL	OB9-CB7-OB8-CB6
75	Bn	101	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	OA7-CA5-OA6-CA4
75	AJ	405	CDL	OB7-CB5-OB6-CB4
75	AL	502	CDL	OA7-CA5-OA6-CA4
75	AU	403	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OB7-CB5-OB6-CB4
75	BV	201	CDL	OB7-CB5-OB6-CB4
75	Bl	704	CDL	OA7-CA5-OA6-CA4
75	Bn	101	CDL	OB7-CB5-OB6-CB4
76	l	701	PEE	O4-C10-O2-C2
76	AU	401	PEE	O4-C10-O2-C2
76	Bl	701	PEE	O4-C10-O2-C2
75	l	704	CDL	C31-CA7-OA8-CA6
75	l	704	CDL	C71-CB7-OB8-CB6
75	n	101	CDL	C31-CA7-OA8-CA6
75	n	101	CDL	C71-CB7-OB8-CB6
75	AG	101	CDL	C31-CA7-OA8-CA6
75	AN	102	CDL	C71-CB7-OB8-CB6
75	AU	403	CDL	C71-CB7-OB8-CB6
75	Bl	704	CDL	C31-CA7-OA8-CA6
75	Bl	704	CDL	C71-CB7-OB8-CB6
75	Bn	101	CDL	C31-CA7-OA8-CA6
75	Bn	101	CDL	C71-CB7-OB8-CB6
75	l	703	CDL	C51-CB5-OB6-CB4
75	AH	403	CDL	C51-CB5-OB6-CB4
75	AU	403	CDL	C51-CB5-OB6-CB4
75	AY	501	CDL	C51-CB5-OB6-CB4
75	Bl	703	CDL	C51-CB5-OB6-CB4
72	E	201	8Q1	C38-C39-N41-C42
72	BE	201	8Q1	C38-C39-N41-C42
75	AA	101	CDL	C71-CB7-OB8-CB6
75	AH	403	CDL	C71-CB7-OB8-CB6
75	AJ	405	CDL	C31-CA7-OA8-CA6
75	AL	502	CDL	C31-CA7-OA8-CA6
76	l	701	PEE	C37-C38-C39-C40
76	l	702	PEE	C37-C38-C39-C40
76	Bl	701	PEE	C37-C38-C39-C40
76	Bl	702	PEE	C37-C38-C39-C40
75	n	101	CDL	OB9-CB7-OB8-CB6
75	Bn	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
76	l	702	PEE	O5-C30-O3-C3
76	Bl	702	PEE	O5-C30-O3-C3
75	AH	403	CDL	OA7-CA5-OA6-CA4
71	AL	501	PLX	C2-C1-N1-C1C
75	l	703	CDL	O1-C1-CA2-OA2
75	l	704	CDL	O1-C1-CA2-OA2
75	AG	101	CDL	O1-C1-CB2-OB2
75	AY	501	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	O1-C1-CB2-OB2
75	Bl	703	CDL	O1-C1-CA2-OA2
75	Bl	704	CDL	O1-C1-CA2-OA2
75	AU	403	CDL	C31-CA7-OA8-CA6
75	AH	403	CDL	OB9-CB7-OB8-CB6
75	i	401	CDL	C11-CA5-OA6-CA4
75	AA	101	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	C11-CA5-OA6-CA4
76	l	702	PEE	C31-C30-O3-C3
76	Bl	702	PEE	C31-C30-O3-C3
75	AJ	405	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	OA9-CA7-OA8-CA6
75	AU	403	CDL	OA9-CA7-OA8-CA6
79	x	603	HEA	C15-C16-C17-C18
79	Bx	603	HEA	C15-C16-C17-C18
71	b	201	PLX	C4-C3-O4-P1
71	Bb	201	PLX	C4-C3-O4-P1
72	E	201	8Q1	O40-C39-N41-C42
72	BE	201	8Q1	O40-C39-N41-C42
76	W	201	PEE	C17-C18-C19-C20
76	BW	201	PEE	C17-C18-C19-C20
76	AU	401	PEE	C31-C32-C33-C34
76	l	701	PEE	C32-C33-C34-C35
76	Bl	701	PEE	C32-C33-C34-C35
73	J	401	NDP	C1B-C2B-O2B-P2B
73	BJ	401	NDP	C1B-C2B-O2B-P2B
75	l	703	CDL	CB2-C1-CA2-OA2
75	AA	101	CDL	CA2-C1-CB2-OB2
75	AJ	404	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CA2-C1-CB2-OB2
75	Bl	703	CDL	CB2-C1-CA2-OA2
75	AH	403	CDL	C31-CA7-OA8-CA6
75	AY	501	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
76	W	201	PEE	C31-C30-O3-C3
76	BW	201	PEE	C31-C30-O3-C3
71	r	501	PLX	C10-C11-C12-C13
71	Bg	203	PLX	C26-C27-C28-C29
71	Br	501	PLX	C10-C11-C12-C13
71	g	203	PLX	C26-C27-C28-C29
75	AH	403	CDL	C31-C32-C33-C34
76	V	202	PEE	C20-C21-C22-C23
76	W	201	PEE	C21-C22-C23-C24
76	BV	202	PEE	C20-C21-C22-C23
76	BW	201	PEE	C21-C22-C23-C24
71	Br	502	PLX	C16-C17-C18-C19
71	r	502	PLX	C16-C17-C18-C19
76	W	201	PEE	C32-C33-C34-C35
76	BW	201	PEE	C32-C33-C34-C35
75	V	201	CDL	O1-C1-CA2-OA2
75	l	703	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	O1-C1-CA2-OA2
75	AJ	404	CDL	O1-C1-CA2-OA2
75	BV	201	CDL	O1-C1-CA2-OA2
75	Bl	703	CDL	O1-C1-CB2-OB2
71	b	201	PLX	C14-C15-C16-C17
71	g	203	PLX	C30-C31-C32-C33
71	r	502	PLX	C30-C31-C32-C33
71	Bb	201	PLX	C14-C15-C16-C17
71	Bg	203	PLX	C30-C31-C32-C33
71	Br	502	PLX	C30-C31-C32-C33
75	AJ	405	CDL	C71-C72-C73-C74
75	AY	501	CDL	C12-C13-C14-C15
76	W	201	PEE	O5-C30-O3-C3
76	BW	201	PEE	O5-C30-O3-C3
71	g	202	PLX	C10-C11-C12-C13
71	Bg	202	PLX	C10-C11-C12-C13
75	AY	501	CDL	CB5-C51-C52-C53
75	AH	403	CDL	OA9-CA7-OA8-CA6
82	AV	402	HEM	C3A-C2A-CAA-CBA
75	i	401	CDL	OA7-CA5-OA6-CA4
75	Bi	401	CDL	OA7-CA5-OA6-CA4
75	l	703	CDL	OB5-CB3-CB4-OB6
75	Bl	703	CDL	OB5-CB3-CB4-OB6
71	AT	101	PLX	O6-C4-C5-O8
71	r	502	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
71	Br	502	PLX	C12-C13-C14-C15
75	i	401	CDL	C31-C32-C33-C34
75	Bi	401	CDL	C31-C32-C33-C34
76	l	702	PEE	C17-C18-C19-C20
76	AH	401	PEE	C37-C38-C39-C40
76	Bl	702	PEE	C17-C18-C19-C20
76	W	201	PEE	C15-C16-C17-C18
76	BW	201	PEE	C15-C16-C17-C18
76	Bl	702	PEE	C10-C11-C12-C13
75	l	703	CDL	C73-C74-C75-C76
75	Bl	703	CDL	C73-C74-C75-C76
75	AA	101	CDL	OB7-CB5-OB6-CB4
75	i	401	CDL	CA5-C11-C12-C13
75	l	704	CDL	CB5-C51-C52-C53
75	n	101	CDL	CA7-C31-C32-C33
75	AH	403	CDL	CB5-C51-C52-C53
75	AN	102	CDL	CA5-C11-C12-C13
75	AY	501	CDL	CA7-C31-C32-C33
75	Bi	401	CDL	CA5-C11-C12-C13
75	Bl	704	CDL	CB5-C51-C52-C53
75	Bn	101	CDL	CA7-C31-C32-C33
76	l	702	PEE	C10-C11-C12-C13
76	AV	403	PEE	C10-C11-C12-C13
82	AJ	401	HEM	C3D-CAD-CBD-CGD
82	AV	401	HEM	C3D-CAD-CBD-CGD
75	AJ	404	CDL	CA7-C31-C32-C33
75	AL	502	CDL	CA5-C11-C12-C13
75	AU	403	CDL	CA5-C11-C12-C13
76	V	202	PEE	C10-C11-C12-C13
76	BV	202	PEE	C10-C11-C12-C13
75	V	201	CDL	C54-C55-C56-C57
75	BV	201	CDL	C54-C55-C56-C57
76	W	201	PEE	C12-C13-C14-C15
76	l	701	PEE	C34-C35-C36-C37
76	BW	201	PEE	C12-C13-C14-C15
76	Bl	701	PEE	C34-C35-C36-C37
71	r	501	PLX	C12-C13-C14-C15
71	Br	501	PLX	C12-C13-C14-C15
75	AL	502	CDL	O1-C1-CB2-OB2
75	i	401	CDL	C31-CA7-OA8-CA6
75	Bi	401	CDL	C31-CA7-OA8-CA6
75	AY	501	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
75	AG	101	CDL	CB7-C71-C72-C73
71	AN	101	PLX	C13-C14-C15-C16
71	BV	203	PLX	C13-C14-C15-C16
76	V	202	PEE	C17-C18-C19-C20
76	l	701	PEE	C17-C18-C19-C20
76	BV	202	PEE	C17-C18-C19-C20
76	Bl	701	PEE	C17-C18-C19-C20
76	l	701	PEE	C30-C31-C32-C33
75	AY	501	CDL	C71-CB7-OB8-CB6
76	V	202	PEE	C31-C30-O3-C3
76	BV	202	PEE	C31-C30-O3-C3
75	AN	102	CDL	C71-C72-C73-C74
75	AA	101	CDL	CB7-C71-C72-C73
75	AJ	405	CDL	CB7-C71-C72-C73
73	J	401	NDP	C3B-C2B-O2B-P2B
73	BJ	401	NDP	C3B-C2B-O2B-P2B
71	r	501	PLX	C27-C28-C29-C30
75	AL	502	CDL	C52-C53-C54-C55
76	Bl	701	PEE	C30-C31-C32-C33
75	l	703	CDL	CA2-C1-CB2-OB2
75	AG	101	CDL	CA2-C1-CB2-OB2
75	AY	501	CDL	CA2-C1-CB2-OB2
75	Bl	703	CDL	CA2-C1-CB2-OB2
75	l	703	CDL	C71-CB7-OB8-CB6
75	Bl	703	CDL	C71-CB7-OB8-CB6
71	Br	501	PLX	C27-C28-C29-C30
71	AL	501	PLX	C2-C1-N1-C1A
76	AL	503	PEE	C30-C31-C32-C33
76	l	701	PEE	C39-C40-C41-C42
76	Bl	701	PEE	C39-C40-C41-C42
71	B	303	PLX	O6-C6-C7-C8
71	U	101	PLX	O6-C6-C7-C8
71	g	203	PLX	O8-C24-C25-C26
71	AQ	101	PLX	O8-C24-C25-C26
71	BB	303	PLX	O6-C6-C7-C8
71	BU	101	PLX	O6-C6-C7-C8
71	Bg	203	PLX	O8-C24-C25-C26
75	l	704	CDL	C51-CB5-OB6-CB4
75	AG	101	CDL	C51-CB5-OB6-CB4
75	Bl	704	CDL	C51-CB5-OB6-CB4
75	l	704	CDL	OB7-CB5-OB6-CB4
75	AG	101	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	Bl	704	CDL	OB7-CB5-OB6-CB4
75	n	101	CDL	C31-C32-C33-C34
75	Bn	101	CDL	C31-C32-C33-C34
82	AJ	402	HEM	C1A-C2A-CAA-CBA
75	AJ	404	CDL	C1-CB2-OB2-PB2
75	AN	102	CDL	C14-C15-C16-C17
75	AH	403	CDL	C33-C34-C35-C36
75	AL	502	CDL	CA6-CA4-OA6-CA5
71	AL	501	PLX	C12-C13-C14-C15
75	AY	501	CDL	OA5-CA3-CA4-OA6
75	AN	102	CDL	CB4-CB6-OB8-CB7
71	AL	501	PLX	C2-C1-N1-C1B
75	n	101	CDL	C13-C14-C15-C16
75	Bn	101	CDL	C13-C14-C15-C16
71	B	303	PLX	C27-C28-C29-C30
71	g	201	PLX	C13-C14-C15-C16
71	g	201	PLX	C7-C8-C9-C10
71	g	203	PLX	C29-C30-C31-C32
71	g	203	PLX	C34-C35-C36-C37
71	BB	303	PLX	C27-C28-C29-C30
71	Bg	201	PLX	C13-C14-C15-C16
71	Bg	203	PLX	C29-C30-C31-C32
71	Bg	203	PLX	C34-C35-C36-C37
75	AJ	405	CDL	C12-C13-C14-C15
75	AY	501	CDL	C32-C33-C34-C35
76	l	701	PEE	C22-C23-C24-C25
76	AY	502	PEE	C11-C12-C13-C14
76	BW	201	PEE	C14-C15-C16-C17
76	Bl	701	PEE	C22-C23-C24-C25
76	W	201	PEE	C37-C38-C39-C40
76	BW	201	PEE	C37-C38-C39-C40
71	g	202	PLX	C7-C8-C9-C10
71	AQ	101	PLX	C19-C20-C21-C22
71	AQ	101	PLX	C12-C13-C14-C15
71	AT	101	PLX	C7-C8-C9-C10
71	Bg	201	PLX	C7-C8-C9-C10
71	Bg	202	PLX	C7-C8-C9-C10
75	n	101	CDL	C12-C13-C14-C15
75	AG	101	CDL	C33-C34-C35-C36
75	Bn	101	CDL	C12-C13-C14-C15
76	W	201	PEE	C14-C15-C16-C17
76	V	202	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
76	BV	202	PEE	O5-C30-O3-C3
71	B	303	PLX	O7-C6-C7-C8
71	g	203	PLX	O9-C24-C25-C26
71	r	501	PLX	O9-C24-C25-C26
71	AT	101	PLX	O9-C24-C25-C26
71	BB	303	PLX	O7-C6-C7-C8
71	Bg	203	PLX	O9-C24-C25-C26
71	Br	501	PLX	O9-C24-C25-C26
71	AQ	101	PLX	C10-C11-C12-C13
71	AT	101	PLX	C9-C10-C11-C12
75	l	704	CDL	C31-C32-C33-C34
75	AU	403	CDL	C13-C14-C15-C16
75	Bl	704	CDL	C31-C32-C33-C34
76	l	702	PEE	C20-C21-C22-C23
76	AJ	403	PEE	C20-C21-C22-C23
76	Bl	701	PEE	C21-C22-C23-C24
76	Bl	702	PEE	C20-C21-C22-C23
72	p	201	8Q1	C11-C12-C13-C14
72	Bp	201	8Q1	C11-C12-C13-C14
76	l	701	PEE	C21-C22-C23-C24
75	n	101	CDL	CB5-C51-C52-C53
75	AA	101	CDL	CA5-C11-C12-C13
75	Bn	101	CDL	CB5-C51-C52-C53
76	l	702	PEE	C33-C34-C35-C36
76	Bl	702	PEE	C33-C34-C35-C36
75	i	401	CDL	OA9-CA7-OA8-CA6
75	AY	501	CDL	OB9-CB7-OB8-CB6
75	Bi	401	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	C51-CB5-OB6-CB4
75	l	704	CDL	C51-C52-C53-C54
75	Bl	704	CDL	C51-C52-C53-C54
71	U	101	PLX	C33-C34-C35-C36
71	AL	501	PLX	C15-C16-C17-C18
71	BU	101	PLX	C33-C34-C35-C36
75	AA	101	CDL	C31-C32-C33-C34
75	BV	201	CDL	C71-C72-C73-C74
75	l	703	CDL	CB7-C71-C72-C73
75	l	704	CDL	CA7-C31-C32-C33
75	l	704	CDL	CB7-C71-C72-C73
75	Bl	703	CDL	CB7-C71-C72-C73
75	Bl	704	CDL	CA7-C31-C32-C33
75	Bl	704	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
73	J	401	NDP	C3B-C4B-C5B-O5B
73	BJ	401	NDP	C3B-C4B-C5B-O5B
71	U	101	PLX	C19-C20-C21-C22
71	g	202	PLX	C14-C15-C16-C17
71	AQ	101	PLX	C34-C35-C36-C37
71	BU	101	PLX	C19-C20-C21-C22
75	V	201	CDL	C71-C72-C73-C74
75	AA	101	CDL	C51-C52-C53-C54
75	AL	502	CDL	C51-C52-C53-C54
76	AH	401	PEE	C21-C22-C23-C24
76	AL	503	PEE	C32-C33-C34-C35
71	r	501	PLX	C13-C14-C15-C16
71	Br	501	PLX	C13-C14-C15-C16
75	AG	101	CDL	C14-C15-C16-C17
75	AU	403	CDL	C54-C55-C56-C57
76	AJ	403	PEE	C13-C14-C15-C16
76	AJ	403	PEE	C11-C12-C13-C14
71	Bg	202	PLX	C14-C15-C16-C17
76	V	202	PEE	C12-C13-C14-C15
76	BV	202	PEE	C12-C13-C14-C15
75	AG	101	CDL	CA5-C11-C12-C13
75	l	703	CDL	OB9-CB7-OB8-CB6
75	Bl	703	CDL	OB9-CB7-OB8-CB6
71	AN	101	PLX	C25-C26-C27-C28
71	BV	203	PLX	C25-C26-C27-C28
75	AJ	405	CDL	C33-C34-C35-C36
75	AY	501	CDL	C14-C15-C16-C17
76	AU	401	PEE	C11-C12-C13-C14
75	l	703	CDL	C31-CA7-OA8-CA6
75	Bl	703	CDL	C31-CA7-OA8-CA6
71	r	502	PLX	C11-C12-C13-C14
71	Br	502	PLX	C11-C12-C13-C14
72	p	201	8Q1	C6-C7-C8-C9
72	Bp	201	8Q1	C6-C7-C8-C9
76	V	202	PEE	C40-C41-C42-C43
76	l	702	PEE	C21-C22-C23-C24
76	BV	202	PEE	C40-C41-C42-C43
76	Bl	702	PEE	C21-C22-C23-C24
75	AL	502	CDL	CA7-C31-C32-C33
75	AU	403	CDL	CB7-C71-C72-C73
71	U	101	PLX	C12-C13-C14-C15
71	U	101	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
71	U	101	PLX	C35-C36-C37-C38
71	b	201	PLX	C16-C17-C18-C19
71	r	502	PLX	C14-C15-C16-C17
71	r	502	PLX	C10-C11-C12-C13
71	AL	501	PLX	C13-C14-C15-C16
71	BU	101	PLX	C12-C13-C14-C15
71	BU	101	PLX	C10-C11-C12-C13
71	BU	101	PLX	C35-C36-C37-C38
71	Bb	201	PLX	C16-C17-C18-C19
71	Br	502	PLX	C14-C15-C16-C17
71	Br	502	PLX	C10-C11-C12-C13
75	l	703	CDL	C11-C12-C13-C14
75	Bl	703	CDL	C11-C12-C13-C14
76	AY	502	PEE	C22-C23-C24-C25
71	b	201	PLX	C27-C28-C29-C30
71	g	203	PLX	C15-C16-C17-C18
71	AN	101	PLX	C32-C33-C34-C35
71	BV	203	PLX	C32-C33-C34-C35
71	Bb	201	PLX	C27-C28-C29-C30
71	Bg	203	PLX	C15-C16-C17-C18
71	Br	502	PLX	C32-C33-C34-C35
71	B	303	PLX	C28-C29-C30-C31
71	r	502	PLX	C32-C33-C34-C35
71	BB	303	PLX	C28-C29-C30-C31
75	AG	101	CDL	C72-C73-C74-C75
71	r	502	PLX	C25-C26-C27-C28
71	AN	101	PLX	C10-C11-C12-C13
71	BV	203	PLX	C10-C11-C12-C13
71	Bg	203	PLX	C17-C18-C19-C20
75	AY	501	CDL	C33-C34-C35-C36
75	V	201	CDL	C11-CA5-OA6-CA4
75	BV	201	CDL	C11-CA5-OA6-CA4
76	AH	401	PEE	C11-C10-O2-C2
76	AV	403	PEE	C35-C36-C37-C38
76	AL	503	PEE	C37-C38-C39-C40
71	Br	502	PLX	C25-C26-C27-C28
75	AL	502	CDL	C32-C33-C34-C35
76	AJ	403	PEE	C32-C33-C34-C35
71	g	203	PLX	C17-C18-C19-C20
76	l	702	PEE	C40-C41-C42-C43
75	n	101	CDL	CB7-C71-C72-C73
75	Bn	101	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	C29-C30-C31-C32
71	Bb	201	PLX	C29-C30-C31-C32
75	i	401	CDL	C13-C14-C15-C16
75	l	704	CDL	C32-C33-C34-C35
75	AU	403	CDL	C31-C32-C33-C34
75	Bi	401	CDL	C13-C14-C15-C16
75	Bl	704	CDL	C32-C33-C34-C35
76	Bl	702	PEE	C40-C41-C42-C43
71	AL	501	PLX	C10-C11-C12-C13
75	V	201	CDL	OA7-CA5-OA6-CA4
75	BV	201	CDL	OA7-CA5-OA6-CA4
71	BB	303	PLX	C9-C10-C11-C12
76	l	702	PEE	C34-C35-C36-C37
76	AH	401	PEE	C22-C23-C24-C25
76	Bl	702	PEE	C34-C35-C36-C37
71	U	101	PLX	C9-C10-C11-C12
71	b	201	PLX	C18-C19-C20-C21
71	g	201	PLX	C16-C17-C18-C19
71	g	203	PLX	C7-C8-C9-C10
71	r	501	PLX	C7-C8-C9-C10
71	r	502	PLX	C9-C10-C11-C12
71	BU	101	PLX	C9-C10-C11-C12
71	Bb	201	PLX	C18-C19-C20-C21
71	Bg	201	PLX	C16-C17-C18-C19
71	Bg	203	PLX	C14-C15-C16-C17
71	Bg	203	PLX	C7-C8-C9-C10
71	Br	501	PLX	C7-C8-C9-C10
71	Br	502	PLX	C9-C10-C11-C12
72	E	201	8Q1	C12-C13-C14-C15
72	BE	201	8Q1	C12-C13-C14-C15
75	i	401	CDL	C11-C12-C13-C14
75	AU	403	CDL	C53-C54-C55-C56
75	Bi	401	CDL	C11-C12-C13-C14
76	AH	401	PEE	C11-C12-C13-C14
75	Bi	401	CDL	C71-CB7-OB8-CB6
75	n	101	CDL	C55-C56-C57-C58
75	Bn	101	CDL	C55-C56-C57-C58
71	B	303	PLX	C9-C10-C11-C12
71	U	101	PLX	C7-C8-C9-C10
71	g	203	PLX	C14-C15-C16-C17
71	BU	101	PLX	C7-C8-C9-C10
76	BV	202	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
76	V	202	PEE	C14-C15-C16-C17
71	b	201	PLX	C25-C26-C27-C28
71	Bg	201	PLX	C10-C11-C12-C13
76	AJ	403	PEE	C22-C23-C24-C25
76	AL	503	PEE	C11-C12-C13-C14
71	g	201	PLX	C10-C11-C12-C13
71	Bb	201	PLX	C25-C26-C27-C28
75	l	703	CDL	C51-C52-C53-C54
75	AJ	404	CDL	C14-C15-C16-C17
75	Bl	703	CDL	C51-C52-C53-C54
75	i	401	CDL	C71-CB7-OB8-CB6
75	i	401	CDL	C51-CB5-OB6-CB4
75	Bi	401	CDL	C51-CB5-OB6-CB4
76	AV	403	PEE	C11-C10-O2-C2
75	V	201	CDL	CB5-C51-C52-C53
75	i	401	CDL	CB5-C51-C52-C53
75	BV	201	CDL	CB5-C51-C52-C53
76	AL	503	PEE	C10-C11-C12-C13
76	AV	403	PEE	C30-C31-C32-C33
75	AL	502	CDL	OB7-CB5-OB6-CB4
76	AV	403	PEE	O4-C10-O2-C2
71	AN	101	PLX	C11-C12-C13-C14
71	BV	203	PLX	C11-C12-C13-C14
75	AG	101	CDL	C31-C32-C33-C34
76	AY	502	PEE	C19-C20-C21-C22
76	BW	201	PEE	C23-C24-C25-C26
71	r	502	PLX	C20-C21-C22-C23
71	Br	502	PLX	C20-C21-C22-C23
71	Br	502	PLX	C36-C37-C38-C39
75	Bi	401	CDL	CB5-C51-C52-C53
71	r	502	PLX	C36-C37-C38-C39
76	W	201	PEE	C23-C24-C25-C26
71	AQ	101	PLX	C15-C16-C17-C18
71	g	201	PLX	C32-C33-C34-C35
75	n	101	CDL	C51-C52-C53-C54
75	Bn	101	CDL	C51-C52-C53-C54
71	g	202	PLX	C9-C10-C11-C12
71	Bg	201	PLX	C32-C33-C34-C35
71	Bg	202	PLX	C9-C10-C11-C12
75	AG	101	CDL	C73-C74-C75-C76
75	AG	101	CDL	C52-C53-C54-C55
75	l	703	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
75	Bl	703	CDL	OA9-CA7-OA8-CA6
75	AJ	405	CDL	CB5-C51-C52-C53
75	Bi	401	CDL	C73-C74-C75-C76
75	AL	502	CDL	OA5-CA3-CA4-OA6
75	AL	502	CDL	OB5-CB3-CB4-OB6
75	i	401	CDL	C73-C74-C75-C76
76	V	202	PEE	C31-C32-C33-C34
76	l	701	PEE	C20-C21-C22-C23
76	AL	503	PEE	C34-C35-C36-C37
76	BV	202	PEE	C31-C32-C33-C34
76	Bl	701	PEE	C20-C21-C22-C23
71	r	502	PLX	C26-C27-C28-C29
71	BB	303	PLX	C12-C13-C14-C15
71	Br	502	PLX	C26-C27-C28-C29
71	B	303	PLX	C12-C13-C14-C15
71	g	203	PLX	C10-C11-C12-C13
71	Bg	203	PLX	C10-C11-C12-C13
75	AU	403	CDL	C14-C15-C16-C17
76	V	202	PEE	C34-C35-C36-C37
76	AV	403	PEE	C32-C33-C34-C35
76	BV	202	PEE	C34-C35-C36-C37
71	AL	501	PLX	O6-C4-C5-O8
76	l	701	PEE	C15-C16-C17-C18
76	l	702	PEE	C19-C20-C21-C22
76	Bl	701	PEE	C15-C16-C17-C18
76	Bl	702	PEE	C19-C20-C21-C22
76	l	702	PEE	C31-C32-C33-C34
76	Bl	702	PEE	C31-C32-C33-C34
75	l	703	CDL	C33-C34-C35-C36
75	Bl	703	CDL	C33-C34-C35-C36
71	g	202	PLX	C11-C12-C13-C14
71	AT	101	PLX	C11-C12-C13-C14
71	Bg	202	PLX	C11-C12-C13-C14
76	AH	401	PEE	C32-C33-C34-C35
76	l	701	PEE	C16-C17-C18-C19
76	Bl	701	PEE	C16-C17-C18-C19
75	i	401	CDL	C32-C33-C34-C35
75	i	401	CDL	C34-C35-C36-C37
75	AH	403	CDL	C32-C33-C34-C35
75	Bi	401	CDL	C34-C35-C36-C37
76	AH	401	PEE	C2-C1-O3P-P
72	p	201	8Q1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
72	Bp	201	8Q1	C7-C8-C9-C10
75	Bi	401	CDL	C32-C33-C34-C35
71	r	501	PLX	C35-C36-C37-C38
71	Br	501	PLX	C35-C36-C37-C38
76	V	202	PEE	C43-C44-C45-C46
75	l	704	CDL	CB2-C1-CA2-OA2
75	Bl	704	CDL	CB2-C1-CA2-OA2
71	b	201	PLX	C30-C31-C32-C33
71	Bb	201	PLX	C30-C31-C32-C33
75	AA	101	CDL	C12-C13-C14-C15
75	AJ	404	CDL	C11-C12-C13-C14
75	AJ	405	CDL	C52-C53-C54-C55
75	AY	501	CDL	C13-C14-C15-C16
76	W	201	PEE	C43-C44-C45-C46
76	l	701	PEE	C41-C42-C43-C44
76	BV	202	PEE	C43-C44-C45-C46
76	BW	201	PEE	C43-C44-C45-C46
76	Bl	701	PEE	C13-C14-C15-C16
76	Bl	701	PEE	C41-C42-C43-C44
71	AQ	101	PLX	C13-C14-C15-C16
75	n	101	CDL	C71-C72-C73-C74
75	Bn	101	CDL	C71-C72-C73-C74
76	l	701	PEE	C13-C14-C15-C16
71	AQ	101	PLX	C18-C19-C20-C21
75	V	201	CDL	C14-C15-C16-C17
75	BV	201	CDL	C14-C15-C16-C17
76	AL	503	PEE	C12-C13-C14-C15
71	b	201	PLX	C32-C33-C34-C35
71	Bb	201	PLX	C32-C33-C34-C35
71	Bg	203	PLX	C35-C36-C37-C38
75	AG	101	CDL	CA7-C31-C32-C33
71	g	203	PLX	C35-C36-C37-C38
72	p	201	8Q1	C12-C13-C14-C15
72	Bp	201	8Q1	C12-C13-C14-C15
76	AV	403	PEE	C41-C42-C43-C44
71	r	501	PLX	C26-C27-C28-C29
71	Br	501	PLX	C26-C27-C28-C29
75	AA	101	CDL	C33-C34-C35-C36
76	V	202	PEE	C19-C20-C21-C22
76	W	201	PEE	C19-C20-C21-C22
76	BV	202	PEE	C19-C20-C21-C22
76	BW	201	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
71	AL	501	PLX	O4-C3-C4-C5
75	l	704	CDL	OB5-CB3-CB4-CB6
75	Bl	704	CDL	OB5-CB3-CB4-CB6
76	l	701	PEE	O3P-C1-C2-C3
76	AJ	403	PEE	O3P-C1-C2-C3
76	Bl	701	PEE	O3P-C1-C2-C3
70	A	502	FMN	O2'-C2'-C3'-O3'
70	BA	502	FMN	O2'-C2'-C3'-O3'
76	AH	401	PEE	O4-C10-O2-C2
75	AN	102	CDL	C31-C32-C33-C34
76	W	201	PEE	C41-C42-C43-C44
76	AV	403	PEE	C12-C13-C14-C15
76	AU	401	PEE	C33-C34-C35-C36
73	J	401	NDP	O4B-C4B-C5B-O5B
73	BJ	401	NDP	O4B-C4B-C5B-O5B
71	r	502	PLX	C7-C8-C9-C10
71	Br	502	PLX	C7-C8-C9-C10
76	BW	201	PEE	C41-C42-C43-C44
76	Bl	701	PEE	C23-C24-C25-C26
75	i	401	CDL	OB9-CB7-OB8-CB6
75	Bi	401	CDL	OB9-CB7-OB8-CB6
71	U	101	PLX	O8-C24-C25-C26
71	BU	101	PLX	O8-C24-C25-C26
76	l	701	PEE	C23-C24-C25-C26
70	A	502	FMN	O2'-C2'-C3'-C4'
70	BA	502	FMN	O2'-C2'-C3'-C4'
71	AL	501	PLX	C7-C8-C9-C10
71	AT	101	PLX	C33-C34-C35-C36
71	AT	101	PLX	C32-C33-C34-C35
75	AJ	404	CDL	C15-C16-C17-C18
71	r	501	PLX	C3-C4-C5-O8
71	Br	501	PLX	C3-C4-C5-O8
75	l	703	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CA3-CA4-CA6-OA8
75	AJ	405	CDL	CB3-CB4-CB6-OB8
75	AL	502	CDL	CA3-CA4-CA6-OA8
75	AL	502	CDL	CB3-CB4-CB6-OB8
75	AN	102	CDL	CB3-CB4-CB6-OB8
75	AU	403	CDL	CA3-CA4-CA6-OA8
75	Bl	703	CDL	CA3-CA4-CA6-OA8
76	AV	403	PEE	C1-C2-C3-O3
76	AY	502	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
76	AV	403	PEE	C19-C20-C21-C22
76	AV	403	PEE	C15-C16-C17-C18
75	n	101	CDL	C33-C34-C35-C36
72	p	201	8Q1	C13-C14-C15-C16
72	Bp	201	8Q1	C13-C14-C15-C16
71	g	202	PLX	C26-C27-C28-C29
71	Bg	202	PLX	C26-C27-C28-C29
75	AL	502	CDL	C14-C15-C16-C17
75	Bn	101	CDL	C33-C34-C35-C36
75	AG	101	CDL	C34-C35-C36-C37
76	AV	403	PEE	C40-C41-C42-C43
71	r	502	PLX	C35-C36-C37-C38
71	AQ	101	PLX	C26-C27-C28-C29
71	Br	502	PLX	C35-C36-C37-C38
76	l	701	PEE	C2-C1-O3P-P
76	Bl	701	PEE	C2-C1-O3P-P
75	i	401	CDL	OB7-CB5-OB6-CB4
75	Bi	401	CDL	OB7-CB5-OB6-CB4
76	AU	401	PEE	C34-C35-C36-C37
71	B	303	PLX	C29-C30-C31-C32
71	BB	303	PLX	C29-C30-C31-C32
75	AH	403	CDL	C53-C54-C55-C56
71	B	303	PLX	C11-C10-C9-C8
71	AT	101	PLX	C34-C35-C36-C37
71	BB	303	PLX	C11-C10-C9-C8
75	AJ	405	CDL	C55-C56-C57-C58
71	r	501	PLX	C9-C10-C11-C12
71	Br	501	PLX	C9-C10-C11-C12
75	AG	101	CDL	C71-CB7-OB8-CB6
75	AJ	404	CDL	CA3-CA4-OA6-CA5
75	AJ	405	CDL	CB6-CB4-OB6-CB5
71	b	201	PLX	C11-C12-C13-C14
71	Bb	201	PLX	C11-C12-C13-C14
76	AJ	403	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C39-C40-C41-C42
76	AU	401	PEE	C15-C16-C17-C18
71	B	303	PLX	C15-C16-C17-C18
71	g	202	PLX	C11-C10-C9-C8
71	AQ	101	PLX	C7-C8-C9-C10
71	BB	303	PLX	C15-C16-C17-C18
71	Bg	202	PLX	C11-C10-C9-C8
71	Br	502	PLX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	C13-C14-C15-C16
75	n	101	CDL	C34-C35-C36-C37
75	AU	403	CDL	C73-C74-C75-C76
75	Bl	704	CDL	C13-C14-C15-C16
75	Bn	101	CDL	C34-C35-C36-C37
76	l	701	PEE	C40-C41-C42-C43
76	AV	403	PEE	C33-C34-C35-C36
76	Bl	701	PEE	C40-C41-C42-C43
71	r	502	PLX	C17-C18-C19-C20
75	AJ	405	CDL	CA7-C31-C32-C33
75	AY	501	CDL	CB7-C71-C72-C73
75	AL	502	CDL	C31-C32-C33-C34
75	V	201	CDL	OA5-CA3-CA4-OA6
75	BV	201	CDL	OA5-CA3-CA4-OA6
71	r	502	PLX	C15-C16-C17-C18
71	AQ	101	PLX	C36-C37-C38-C39
71	r	501	PLX	C18-C19-C20-C21
71	Br	501	PLX	C18-C19-C20-C21
71	Br	502	PLX	C15-C16-C17-C18
71	AT	101	PLX	C18-C19-C20-C21
76	AL	503	PEE	C21-C22-C23-C24
76	l	702	PEE	C42-C43-C44-C45
76	Bl	702	PEE	C42-C43-C44-C45
75	V	201	CDL	C12-C13-C14-C15
75	BV	201	CDL	C12-C13-C14-C15
76	W	201	PEE	C33-C34-C35-C36
76	BW	201	PEE	C33-C34-C35-C36
76	AY	502	PEE	C42-C43-C44-C45
71	AT	101	PLX	C13-C14-C15-C16
76	W	201	PEE	O2-C2-C3-O3
76	BW	201	PEE	O2-C2-C3-O3
75	AG	101	CDL	C75-C76-C77-C78
75	AN	102	CDL	C55-C56-C57-C58
75	Bi	401	CDL	C35-C36-C37-C38
76	l	701	PEE	C42-C43-C44-C45
76	Bl	701	PEE	C42-C43-C44-C45
75	AL	502	CDL	C13-C14-C15-C16
76	AY	502	PEE	C33-C34-C35-C36
76	BV	202	PEE	C41-C42-C43-C44
75	i	401	CDL	C35-C36-C37-C38
76	V	202	PEE	C41-C42-C43-C44
71	g	201	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
76	AJ	403	PEE	C41-C42-C43-C44
75	AH	403	CDL	C55-C56-C57-C58
76	l	702	PEE	C44-C45-C46-C47
76	Bl	702	PEE	C44-C45-C46-C47
71	Bg	201	PLX	C26-C27-C28-C29
75	AU	403	CDL	C15-C16-C17-C18
72	p	201	8Q1	C30-C29-C32-O33
72	Bp	201	8Q1	C30-C29-C32-O33
71	AL	501	PLX	C34-C35-C36-C37
76	l	702	PEE	C12-C13-C14-C15
76	Bl	702	PEE	C12-C13-C14-C15
75	AY	501	CDL	C15-C16-C17-C18
76	W	201	PEE	C44-C45-C46-C47
76	BW	201	PEE	C44-C45-C46-C47
75	AJ	404	CDL	C74-C75-C76-C77
71	b	201	PLX	C20-C21-C22-C23
71	Bb	201	PLX	C20-C21-C22-C23
75	AU	403	CDL	CB5-C51-C52-C53
71	r	502	PLX	O7-C6-C7-C8
71	Br	502	PLX	O7-C6-C7-C8
75	AJ	404	CDL	CA5-C11-C12-C13
75	AA	101	CDL	C71-C72-C73-C74
71	AN	101	PLX	C7-C8-C9-C10
71	BV	203	PLX	C7-C8-C9-C10
71	AQ	101	PLX	C31-C32-C33-C34
71	U	101	PLX	C11-C10-C9-C8
71	BU	101	PLX	C11-C10-C9-C8
75	AN	102	CDL	C15-C16-C17-C18
71	AQ	101	PLX	C9-C10-C11-C12
71	U	101	PLX	C26-C27-C28-C29
71	BU	101	PLX	C26-C27-C28-C29
75	l	703	CDL	OB5-CB3-CB4-CB6
75	AL	502	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OB5-CB3-CB4-CB6
75	Bl	703	CDL	OB5-CB3-CB4-CB6
76	BW	201	PEE	O3P-C1-C2-C3
76	l	702	PEE	C11-C10-O2-C2
75	AJ	405	CDL	C32-C33-C34-C35
75	l	703	CDL	C75-C76-C77-C78
75	Bl	703	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
75	AH	403	CDL	C32-C31-CA7-OA8
76	AH	401	PEE	C30-C31-C32-C33
76	AH	401	PEE	C34-C35-C36-C37
75	AH	403	CDL	C15-C16-C17-C18
76	AH	401	PEE	C24-C25-C26-C27
75	V	201	CDL	C72-C73-C74-C75
75	BV	201	CDL	C72-C73-C74-C75
71	g	201	PLX	C27-C28-C29-C30
75	AJ	404	CDL	C73-C74-C75-C76
75	i	401	CDL	C52-C51-CB5-OB6
71	Bg	201	PLX	C27-C28-C29-C30
71	AN	101	PLX	C16-C17-C18-C19
76	AV	403	PEE	C13-C14-C15-C16
71	BV	203	PLX	C16-C17-C18-C19
75	Bi	401	CDL	C52-C51-CB5-OB6
75	AG	101	CDL	OB9-CB7-OB8-CB6
76	W	201	PEE	C34-C35-C36-C37
76	BW	201	PEE	C34-C35-C36-C37
76	Bl	702	PEE	C11-C10-O2-C2
71	AN	101	PLX	C12-C13-C14-C15
71	BV	203	PLX	C12-C13-C14-C15
71	AL	501	PLX	C3-C4-C5-O8
71	AQ	101	PLX	C3-C4-C5-O8
71	AT	101	PLX	C3-C4-C5-O8
75	V	201	CDL	CB3-CB4-CB6-OB8
75	i	401	CDL	CA3-CA4-CA6-OA8
75	BV	201	CDL	CB3-CB4-CB6-OB8
75	Bi	401	CDL	CA3-CA4-CA6-OA8
76	W	201	PEE	C1-C2-C3-O3
76	BW	201	PEE	C1-C2-C3-O3
71	Bg	201	PLX	C17-C18-C19-C20
71	b	201	PLX	C36-C37-C38-C39
71	Bb	201	PLX	C36-C37-C38-C39
75	AA	101	CDL	C75-C76-C77-C78
71	g	201	PLX	C17-C18-C19-C20
75	AJ	404	CDL	C12-C13-C14-C15
75	BV	201	CDL	C52-C53-C54-C55
71	B	303	PLX	C30-C31-C32-C33
71	r	501	PLX	C25-C26-C27-C28
75	V	201	CDL	C52-C53-C54-C55
76	AH	401	PEE	C20-C21-C22-C23
71	AN	101	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
71	BB	303	PLX	C30-C31-C32-C33
71	BV	203	PLX	C31-C32-C33-C34
71	Br	501	PLX	C25-C26-C27-C28
71	U	101	PLX	C28-C29-C30-C31
71	b	201	PLX	C11-C10-C9-C8
71	Bb	201	PLX	C11-C10-C9-C8
71	U	101	PLX	C27-C28-C29-C30
71	BU	101	PLX	C27-C28-C29-C30
71	BU	101	PLX	C28-C29-C30-C31
75	l	704	CDL	OA5-CA3-CA4-OA6
75	AN	102	CDL	OA5-CA3-CA4-OA6
75	Bl	704	CDL	OA5-CA3-CA4-OA6
76	AJ	403	PEE	O3P-C1-C2-O2
71	b	201	PLX	C13-C14-C15-C16
71	Bb	201	PLX	C13-C14-C15-C16
75	AA	101	CDL	C1-CB2-OB2-PB2
75	AA	101	CDL	CB4-CB3-OB5-PB2
75	AH	403	CDL	C1-CA2-OA2-PA1
75	AN	102	CDL	CB4-CB3-OB5-PB2
76	AJ	403	PEE	C40-C41-C42-C43
75	l	703	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OB6-CB4-CB6-OB8
75	AH	403	CDL	OB6-CB4-CB6-OB8
75	AL	502	CDL	OA6-CA4-CA6-OA8
75	AL	502	CDL	OB6-CB4-CB6-OB8
75	AU	403	CDL	OA6-CA4-CA6-OA8
75	Bl	703	CDL	OA6-CA4-CA6-OA8
71	r	502	PLX	C27-C28-C29-C30
71	Br	502	PLX	C27-C28-C29-C30
72	BE	201	8Q1	C7-C8-C9-C10
72	Bp	201	8Q1	C10-C11-C12-C13
76	AV	403	PEE	C22-C23-C24-C25
72	E	201	8Q1	C7-C8-C9-C10
72	p	201	8Q1	C10-C11-C12-C13
71	r	501	PLX	C28-C29-C30-C31
71	AQ	101	PLX	C14-C15-C16-C17
71	Br	501	PLX	C28-C29-C30-C31
75	AH	403	CDL	C52-C53-C54-C55
75	BV	201	CDL	C53-C54-C55-C56
76	W	201	PEE	C13-C14-C15-C16
76	BW	201	PEE	C13-C14-C15-C16
75	V	201	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	C35-C36-C37-C38
71	Bb	201	PLX	C35-C36-C37-C38
75	AJ	404	CDL	C71-C72-C73-C74
71	AL	501	PLX	C32-C33-C34-C35
71	AN	101	PLX	C26-C27-C28-C29
71	BV	203	PLX	C26-C27-C28-C29
76	AL	503	PEE	C14-C15-C16-C17
75	AJ	404	CDL	C31-C32-C33-C34
76	AV	403	PEE	C16-C17-C18-C19
71	AL	501	PLX	C6-C7-C8-C9
76	W	201	PEE	C11-C10-O2-C2
76	BW	201	PEE	C11-C10-O2-C2
81	AH	402	HEC	C1A-C2A-CAA-CBA
75	V	201	CDL	C12-C11-CA5-OA6
75	BV	201	CDL	C12-C11-CA5-OA6
75	V	201	CDL	OB5-CB3-CB4-CB6
75	AA	101	CDL	OA5-CA3-CA4-CA6
75	AJ	404	CDL	OB5-CB3-CB4-CB6
75	AN	102	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OB5-CB3-CB4-CB6
75	BV	201	CDL	OB5-CB3-CB4-CB6
76	W	201	PEE	O3P-C1-C2-C3
75	AA	101	CDL	C35-C36-C37-C38
75	AU	403	CDL	C55-C56-C57-C58
75	AG	101	CDL	C74-C75-C76-C77
75	AN	102	CDL	C52-C53-C54-C55
75	l	704	CDL	C73-C74-C75-C76
76	AV	403	PEE	C34-C35-C36-C37
75	Bl	704	CDL	C73-C74-C75-C76
71	g	201	PLX	C20-C21-C22-C23
71	Bg	201	PLX	C20-C21-C22-C23
71	r	501	PLX	C19-C20-C21-C22
71	Br	501	PLX	C19-C20-C21-C22
75	AU	403	CDL	C74-C75-C76-C77
76	AV	403	PEE	C20-C21-C22-C23
75	AJ	405	CDL	CA6-CA4-OA6-CA5
75	AU	403	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CB3-CB4-OB6-CB5
75	AL	502	CDL	C53-C54-C55-C56
76	AH	401	PEE	C15-C16-C17-C18
71	B	303	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
71	BB	303	PLX	C11-C12-C13-C14
76	AY	502	PEE	C14-C15-C16-C17
75	l	703	CDL	C15-C16-C17-C18
75	Bl	703	CDL	C15-C16-C17-C18
76	AV	403	PEE	C11-C12-C13-C14
76	W	201	PEE	O4-C10-O2-C2
76	Bl	702	PEE	O4-C10-O2-C2
71	g	202	PLX	O4-C3-C4-O6
71	AL	501	PLX	O4-C3-C4-O6
71	AQ	101	PLX	O4-C3-C4-O6
71	Bg	202	PLX	O4-C3-C4-O6
75	V	201	CDL	OB5-CB3-CB4-OB6
75	l	703	CDL	OA5-CA3-CA4-OA6
75	AJ	404	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OA5-CA3-CA4-OA6
75	BV	201	CDL	OB5-CB3-CB4-OB6
75	Bl	703	CDL	OA5-CA3-CA4-OA6
71	g	201	PLX	C3-C4-C5-O8
71	Bg	201	PLX	C3-C4-C5-O8
75	AA	101	CDL	CA3-CA4-CA6-OA8
75	AA	101	CDL	CB3-CB4-CB6-OB8
75	AN	102	CDL	CA3-CA4-CA6-OA8
75	AY	501	CDL	CA3-CA4-CA6-OA8
75	n	101	CDL	CA5-C11-C12-C13
82	AV	401	HEM	C4C-C3C-CAC-CBC
71	g	202	PLX	C30-C31-C32-C33
71	Bg	202	PLX	C30-C31-C32-C33
71	b	201	PLX	C1-C2-O1-P1
71	g	203	PLX	C1-C2-O1-P1
71	AT	101	PLX	C1-C2-O1-P1
71	Bb	201	PLX	C1-C2-O1-P1
71	Bg	203	PLX	C1-C2-O1-P1
76	AH	401	PEE	C5-C4-O4P-P
75	Bn	101	CDL	CA5-C11-C12-C13
76	AH	401	PEE	C17-C18-C19-C20
76	AV	403	PEE	C17-C18-C19-C20
71	B	303	PLX	C32-C33-C34-C35
71	BB	303	PLX	C32-C33-C34-C35
75	AU	403	CDL	C71-C72-C73-C74
76	l	701	PEE	C31-C32-C33-C34
71	b	201	PLX	O6-C4-C5-O8
71	r	501	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
71	Bb	201	PLX	O6-C4-C5-O8
71	Br	501	PLX	O6-C4-C5-O8
75	V	201	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	OB6-CB4-CB6-OB8
75	AA	101	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OB6-CB4-CB6-OB8
75	AN	102	CDL	OA6-CA4-CA6-OA8
75	BV	201	CDL	OA6-CA4-CA6-OA8
75	BV	201	CDL	OB6-CB4-CB6-OB8
76	AH	401	PEE	C39-C40-C41-C42
75	AG	101	CDL	C11-C12-C13-C14
76	l	702	PEE	O4-C10-O2-C2
76	BW	201	PEE	O4-C10-O2-C2
76	AL	503	PEE	C31-C32-C33-C34
76	Bl	701	PEE	C31-C32-C33-C34
71	AT	101	PLX	C26-C27-C28-C29
71	Br	501	PLX	C30-C31-C32-C33
71	r	502	PLX	C24-C25-C26-C27
71	Br	502	PLX	C24-C25-C26-C27
71	r	501	PLX	C30-C31-C32-C33
76	BV	202	PEE	C33-C34-C35-C36
76	V	202	PEE	C33-C34-C35-C36
76	V	202	PEE	C32-C33-C34-C35
76	BV	202	PEE	C32-C33-C34-C35
75	BV	201	CDL	C75-C76-C77-C78
71	AL	501	PLX	N1-C1-C2-O1
75	V	201	CDL	C75-C76-C77-C78
72	BE	201	8Q1	C6-C7-C8-C9
72	E	201	8Q1	C6-C7-C8-C9
75	Bl	704	CDL	C12-C13-C14-C15
75	AH	403	CDL	C12-C13-C14-C15
75	l	704	CDL	C12-C13-C14-C15
71	g	202	PLX	O7-C6-C7-C8
71	Bg	202	PLX	O7-C6-C7-C8
71	U	101	PLX	C25-C24-O8-C5
71	r	501	PLX	C25-C24-O8-C5
71	BU	101	PLX	C25-C24-O8-C5
71	Br	501	PLX	C25-C24-O8-C5
72	E	201	8Q1	O33-C32-C34-O35
72	BE	201	8Q1	O33-C32-C34-O35

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Mol	Chain	Res	Type	Atoms
75	AJ	404	CDL	C33-C34-C35-C36
71	r	502	PLX	C34-C35-C36-C37
71	Bg	201	PLX	C35-C36-C37-C38
71	Br	502	PLX	C34-C35-C36-C37
71	g	201	PLX	C35-C36-C37-C38
76	Bl	702	PEE	C11-C12-C13-C14
71	g	202	PLX	O4-C3-C4-C5
71	AQ	101	PLX	O4-C3-C4-C5
71	Bg	202	PLX	O4-C3-C4-C5
75	V	201	CDL	OA5-CA3-CA4-CA6
75	l	703	CDL	OA5-CA3-CA4-CA6
75	l	704	CDL	OA5-CA3-CA4-CA6
75	AL	502	CDL	OB5-CB3-CB4-CB6
75	BV	201	CDL	OA5-CA3-CA4-CA6
75	Bl	703	CDL	OA5-CA3-CA4-CA6
75	Bl	704	CDL	OA5-CA3-CA4-CA6
75	AA	101	CDL	C32-C31-CA7-OA8
76	l	702	PEE	C11-C12-C13-C14
76	AJ	403	PEE	O4-C10-O2-C2
72	E	201	8Q1	O27-C28-C29-C30
72	p	201	8Q1	O27-C28-C29-C31
72	BE	201	8Q1	O27-C28-C29-C30
72	Bp	201	8Q1	O27-C28-C29-C31
75	n	101	CDL	C11-C12-C13-C14
75	Bn	101	CDL	C11-C12-C13-C14
76	W	201	PEE	C31-C32-C33-C34
76	BW	201	PEE	C31-C32-C33-C34
71	r	501	PLX	C31-C32-C33-C34
71	Br	501	PLX	C31-C32-C33-C34
75	AL	502	CDL	C11-C12-C13-C14
75	AH	403	CDL	C1-CB2-OB2-PB2
75	AJ	404	CDL	CA4-CA3-OA5-PA1
75	AN	102	CDL	C1-CB2-OB2-PB2
75	AU	403	CDL	C1-CB2-OB2-PB2
76	l	701	PEE	C24-C25-C26-C27
75	n	101	CDL	C35-C36-C37-C38
76	Bl	701	PEE	C24-C25-C26-C27
71	r	502	PLX	O8-C24-C25-C26
71	BV	203	PLX	O6-C6-C7-C8
71	Br	502	PLX	O8-C24-C25-C26
75	l	704	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
75	AY	501	CDL	OB5-CB3-CB4-OB6
75	Bl	704	CDL	OB5-CB3-CB4-OB6
76	l	701	PEE	O3P-C1-C2-O2
76	Bl	701	PEE	O3P-C1-C2-O2
75	Bn	101	CDL	C35-C36-C37-C38
71	r	501	PLX	C15-C16-C17-C18
76	AJ	403	PEE	C11-C10-O2-C2
71	Br	501	PLX	C15-C16-C17-C18
75	AL	502	CDL	C33-C34-C35-C36
71	Bg	203	PLX	C19-C20-C21-C22
71	AN	101	PLX	C19-C20-C21-C22
71	BV	203	PLX	C19-C20-C21-C22
75	V	201	CDL	C74-C75-C76-C77
75	BV	201	CDL	C74-C75-C76-C77
71	g	203	PLX	O6-C4-C5-O8
71	r	502	PLX	O6-C4-C5-O8
71	Bg	203	PLX	O6-C4-C5-O8
71	Br	502	PLX	O6-C4-C5-O8
75	l	704	CDL	OA6-CA4-CA6-OA8
75	AH	403	CDL	OA6-CA4-CA6-OA8
75	AY	501	CDL	OA6-CA4-CA6-OA8
75	Bl	704	CDL	OA6-CA4-CA6-OA8
76	AV	403	PEE	O2-C2-C3-O3
71	g	203	PLX	C19-C20-C21-C22
75	AU	403	CDL	CA2-C1-CB2-OB2
71	g	203	PLX	C3-C4-C5-O8
71	r	502	PLX	C3-C4-C5-O8
71	Bg	203	PLX	C3-C4-C5-O8
75	AG	101	CDL	CA3-CA4-CA6-OA8
76	AY	502	PEE	C38-C39-C40-C41
71	AL	501	PLX	C19-C20-C21-C22
75	AJ	404	CDL	C55-C56-C57-C58
71	AN	101	PLX	C14-C15-C16-C17
76	AH	401	PEE	C14-C15-C16-C17
71	BV	203	PLX	C14-C15-C16-C17
71	b	201	PLX	C3-O4-P1-O2
71	g	202	PLX	C3-C4-O6-C6
71	g	202	PLX	C5-C4-O6-C6
71	g	202	PLX	C3-O4-P1-O1
71	g	202	PLX	C3-O4-P1-O2
71	g	202	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
71	AN	101	PLX	C3-O4-P1-O2
71	AQ	101	PLX	C3-O4-P1-O3
71	AT	101	PLX	C3-O4-P1-O1
71	AT	101	PLX	C2-O1-P1-O3
71	BV	203	PLX	C3-O4-P1-O2
71	Bb	201	PLX	C3-O4-P1-O2
71	Bg	202	PLX	C3-C4-O6-C6
71	Bg	202	PLX	C5-C4-O6-C6
71	Bg	202	PLX	C3-O4-P1-O1
71	Bg	202	PLX	C3-O4-P1-O2
71	Bg	202	PLX	C3-O4-P1-O3
71	Br	502	PLX	C2-O1-P1-O3
73	J	401	NDP	C5B-O5B-PA-O2A
73	J	401	NDP	C5D-O5D-PN-O3
73	J	401	NDP	C5D-O5D-PN-O2N
73	BJ	401	NDP	C5B-O5B-PA-O2A
73	BJ	401	NDP	C5D-O5D-PN-O3
73	BJ	401	NDP	C5D-O5D-PN-O2N
75	i	401	CDL	CB2-OB2-PB2-OB3
75	i	401	CDL	CB3-OB5-PB2-OB2
75	l	703	CDL	CA2-OA2-PA1-OA4
75	l	704	CDL	CA3-OA5-PA1-OA3
75	l	704	CDL	CB3-OB5-PB2-OB3
75	n	101	CDL	CA3-OA5-PA1-OA3
75	AA	101	CDL	CA3-OA5-PA1-OA3
75	AA	101	CDL	CB2-OB2-PB2-OB3
75	AG	101	CDL	CA2-OA2-PA1-OA3
75	AG	101	CDL	CB2-OB2-PB2-OB3
75	AJ	405	CDL	CA2-OA2-PA1-OA3
75	AL	502	CDL	CA2-OA2-PA1-OA5
75	AL	502	CDL	CB3-OB5-PB2-OB2
75	AL	502	CDL	CB3-OB5-PB2-OB3
75	AL	502	CDL	CB3-OB5-PB2-OB4
75	AN	102	CDL	CA2-OA2-PA1-OA3
75	AN	102	CDL	CA2-OA2-PA1-OA5
75	AN	102	CDL	CB2-OB2-PB2-OB3
75	AU	403	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA2-OA2-PA1-OA3
75	Bi	401	CDL	CB2-OB2-PB2-OB3
75	Bi	401	CDL	CB3-OB5-PB2-OB2
75	Bl	703	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	Bl	704	CDL	CA3-OA5-PA1-OA3
75	Bl	704	CDL	CB3-OB5-PB2-OB3
75	Bn	101	CDL	CA3-OA5-PA1-OA3
76	V	202	PEE	C1-O3P-P-O1P
76	l	701	PEE	C4-O4P-P-O3P
76	l	701	PEE	O4P-C4-C5-N
76	l	702	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C1-O3P-P-O1P
76	AH	401	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C4-O4P-P-O1P
76	AU	401	PEE	C1-O3P-P-O4P
76	AU	401	PEE	C4-O4P-P-O1P
76	AV	403	PEE	C1-O3P-P-O1P
76	AV	403	PEE	C1-O3P-P-O4P
76	AY	502	PEE	C1-O3P-P-O1P
76	AY	502	PEE	C1-O3P-P-O4P
76	AY	502	PEE	O4P-C4-C5-N
76	BV	202	PEE	C1-O3P-P-O1P
76	Bl	701	PEE	C4-O4P-P-O3P
76	Bl	701	PEE	O4P-C4-C5-N
76	Bl	702	PEE	C4-O4P-P-O1P
71	g	203	PLX	C4-C3-O4-P1
71	r	501	PLX	C4-C3-O4-P1
71	r	502	PLX	C4-C3-O4-P1
71	Bg	203	PLX	C4-C3-O4-P1
71	Br	501	PLX	C4-C3-O4-P1
71	Br	502	PLX	C4-C3-O4-P1
75	l	704	CDL	CA4-CA3-OA5-PA1
75	AA	101	CDL	C1-CA2-OA2-PA1
75	AH	403	CDL	CA4-CA3-OA5-PA1
75	AN	102	CDL	C1-CA2-OA2-PA1
75	Bl	704	CDL	CA4-CA3-OA5-PA1
76	W	201	PEE	C10-C11-C12-C13
76	BW	201	PEE	C10-C11-C12-C13
71	U	101	PLX	C36-C37-C38-C39
71	BU	101	PLX	C36-C37-C38-C39
75	V	201	CDL	CA3-CA4-OA6-CA5
75	l	703	CDL	CB6-CB4-OB6-CB5
75	l	704	CDL	CA6-CA4-OA6-CA5
75	AH	403	CDL	CA3-CA4-OA6-CA5
75	BV	201	CDL	CA3-CA4-OA6-CA5
75	Bl	703	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
75	Bl	704	CDL	CA6-CA4-OA6-CA5
76	l	701	PEE	C3-C2-O2-C10
76	l	702	PEE	C3-C2-O2-C10
76	Bl	701	PEE	C3-C2-O2-C10
76	Bl	702	PEE	C3-C2-O2-C10
75	AJ	404	CDL	C13-C14-C15-C16
71	B	303	PLX	C20-C21-C22-C23
75	l	704	CDL	C15-C16-C17-C18
75	Bl	704	CDL	C15-C16-C17-C18
71	BB	303	PLX	C20-C21-C22-C23
75	AN	102	CDL	CA2-C1-CB2-OB2
75	AA	101	CDL	OA5-CA3-CA4-OA6
75	AH	403	CDL	C54-C55-C56-C57
76	AL	503	PEE	C33-C34-C35-C36
71	r	502	PLX	C11-C10-C9-C8
75	Bn	101	CDL	C73-C74-C75-C76
75	n	101	CDL	C73-C74-C75-C76
71	Br	502	PLX	C11-C10-C9-C8
75	AH	403	CDL	C13-C14-C15-C16
75	AN	102	CDL	OB6-CB4-CB6-OB8
71	Bg	201	PLX	C14-C15-C16-C17
71	g	201	PLX	C14-C15-C16-C17
76	V	202	PEE	C11-C10-O2-C2
76	BV	202	PEE	C11-C10-O2-C2
75	BV	201	CDL	C55-C56-C57-C58
76	V	202	PEE	C35-C36-C37-C38
76	BV	202	PEE	C35-C36-C37-C38
75	Bi	401	CDL	C32-C31-CA7-OA8
75	V	201	CDL	C55-C56-C57-C58
71	Br	502	PLX	C3-C4-C5-O8
75	AG	101	CDL	CB3-CB4-CB6-OB8
75	i	401	CDL	C32-C31-CA7-OA8
75	n	101	CDL	C53-C54-C55-C56
75	Bn	101	CDL	C53-C54-C55-C56
75	Bn	101	CDL	C15-C16-C17-C18
71	B	303	PLX	C6-C7-C8-C9
71	g	201	PLX	C24-C25-C26-C27
71	AN	101	PLX	C6-C7-C8-C9
71	BB	303	PLX	C6-C7-C8-C9
71	BV	203	PLX	C6-C7-C8-C9
71	Bg	201	PLX	C24-C25-C26-C27
75	n	101	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
75	V	201	CDL	CB7-C71-C72-C73
75	BV	201	CDL	CB7-C71-C72-C73
71	Br	501	PLX	C11-C10-C9-C8
71	r	501	PLX	O7-C6-C7-C8
71	Br	501	PLX	O7-C6-C7-C8
71	g	201	PLX	O6-C6-C7-C8
71	AN	101	PLX	O6-C6-C7-C8
71	Bg	201	PLX	O6-C6-C7-C8
76	BV	202	PEE	C23-C24-C25-C26
82	AV	402	HEM	C4D-C3D-CAD-CBD
71	r	501	PLX	C11-C10-C9-C8
76	AH	401	PEE	C31-C32-C33-C34
75	AA	101	CDL	CB2-C1-CA2-OA2
76	V	202	PEE	C23-C24-C25-C26
75	Bl	703	CDL	CA7-C31-C32-C33
75	l	703	CDL	CA7-C31-C32-C33
71	BV	203	PLX	C29-C30-C31-C32
82	AJ	402	HEM	C3A-C2A-CAA-CBA
71	AN	101	PLX	C29-C30-C31-C32
75	AJ	405	CDL	C34-C35-C36-C37
71	b	201	PLX	C28-C29-C30-C31
71	Bb	201	PLX	C28-C29-C30-C31
75	AH	403	CDL	O1-C1-CB2-OB2
76	AY	502	PEE	C40-C41-C42-C43
76	AV	403	PEE	C31-C32-C33-C34
81	AH	402	HEC	C3A-C2A-CAA-CBA
75	AG	101	CDL	C51-C52-C53-C54
75	l	703	CDL	C34-C35-C36-C37
75	Bl	703	CDL	C34-C35-C36-C37
75	AJ	405	CDL	C14-C15-C16-C17
71	g	202	PLX	C15-C16-C17-C18
71	Bg	202	PLX	C15-C16-C17-C18
76	V	202	PEE	O4-C10-O2-C2
76	BV	202	PEE	O4-C10-O2-C2
73	J	401	NDP	O4D-C1D-N1N-C6N
73	BJ	401	NDP	O4D-C1D-N1N-C6N
75	AL	502	CDL	C54-C55-C56-C57
76	Bl	702	PEE	C23-C24-C25-C26
76	l	702	PEE	C23-C24-C25-C26
75	l	704	CDL	C1-CB2-OB2-PB2
75	Bl	704	CDL	C1-CB2-OB2-PB2
75	AJ	405	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
76	AJ	403	PEE	C15-C16-C17-C18
76	AL	503	PEE	C19-C20-C21-C22
71	AN	101	PLX	C3-C4-C5-O8
71	BV	203	PLX	C3-C4-C5-O8
72	E	201	8Q1	O33-C32-C34-N36
72	BE	201	8Q1	O33-C32-C34-N36
75	AN	102	CDL	C32-C33-C34-C35
71	g	201	PLX	C19-C20-C21-C22
71	Bg	201	PLX	C19-C20-C21-C22
75	AY	501	CDL	C52-C53-C54-C55
75	AU	403	CDL	CB3-CB4-OB6-CB5
75	AN	102	CDL	CB5-C51-C52-C53
71	g	201	PLX	C25-C26-C27-C28
71	Bg	201	PLX	C25-C26-C27-C28
79	x	604	HEA	CAD-CBD-CGD-O1D
79	Bx	604	HEA	CAD-CBD-CGD-O1D
82	AV	401	HEM	C1A-C2A-CAA-CBA
75	BV	201	CDL	C11-C12-C13-C14
75	i	401	CDL	C1-CB2-OB2-PB2
75	i	401	CDL	CB4-CB3-OB5-PB2
75	AJ	404	CDL	CB4-CB3-OB5-PB2
75	AU	403	CDL	CB4-CB3-OB5-PB2
75	Bi	401	CDL	C1-CB2-OB2-PB2
75	Bi	401	CDL	CB4-CB3-OB5-PB2
75	V	201	CDL	C11-C12-C13-C14
75	AG	101	CDL	C71-C72-C73-C74
76	W	201	PEE	C11-C12-C13-C14
76	BW	201	PEE	C11-C12-C13-C14
79	x	603	HEA	CAD-CBD-CGD-O1D
79	Bx	603	HEA	CAD-CBD-CGD-O1D
79	Bx	604	HEA	CAD-CBD-CGD-O2D
82	AV	401	HEM	C2A-CAA-CBA-CGA
71	g	201	PLX	O6-C4-C5-O8
71	Bg	201	PLX	O6-C4-C5-O8
75	AA	101	CDL	OB6-CB4-CB6-OB8
79	x	604	HEA	CAD-CBD-CGD-O2D
76	V	202	PEE	C21-C22-C23-C24
76	BV	202	PEE	C21-C22-C23-C24
75	i	401	CDL	C72-C71-CB7-OB8
75	Bi	401	CDL	C72-C71-CB7-OB8
71	AL	501	PLX	O6-C6-C7-C8
75	AN	102	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
75	AH	403	CDL	C51-C52-C53-C54
75	AG	101	CDL	C1-CA2-OA2-PA1
75	AH	403	CDL	C14-C15-C16-C17
71	AN	101	PLX	C24-C25-C26-C27
71	BV	203	PLX	C24-C25-C26-C27
75	AH	403	CDL	C32-C31-CA7-OA9
75	l	703	CDL	CB5-C51-C52-C53
75	Bl	703	CDL	CB5-C51-C52-C53
82	AV	402	HEM	C2D-C3D-CAD-CBD
71	AN	101	PLX	C33-C34-C35-C36
71	BV	203	PLX	C33-C34-C35-C36
75	l	704	CDL	CA3-CA4-CA6-OA8
75	Bl	704	CDL	CA3-CA4-CA6-OA8
75	AN	102	CDL	OA9-CA7-OA8-CA6
71	B	303	PLX	O9-C24-C25-C26
71	BB	303	PLX	O9-C24-C25-C26
73	J	401	NDP	C2D-C1D-N1N-C6N
73	BJ	401	NDP	C2D-C1D-N1N-C6N
71	g	201	PLX	O4-C3-C4-O6
71	Bg	201	PLX	O4-C3-C4-O6
79	Bx	603	HEA	CAD-CBD-CGD-O2D
75	i	401	CDL	C52-C51-CB5-OB7
75	Bi	401	CDL	C52-C51-CB5-OB7
71	BB	303	PLX	C7-C8-C9-C10
71	Br	502	PLX	C28-C29-C30-C31
76	AL	503	PEE	C40-C41-C42-C43
76	AV	403	PEE	C14-C15-C16-C17
79	x	603	HEA	CAD-CBD-CGD-O2D
71	B	303	PLX	C7-C8-C9-C10
71	r	502	PLX	C28-C29-C30-C31
75	AN	102	CDL	C53-C54-C55-C56
75	AY	501	CDL	C72-C71-CB7-OB8
76	AJ	403	PEE	C36-C37-C38-C39
75	l	703	CDL	CA4-CA3-OA5-PA1
75	Bl	703	CDL	CA4-CA3-OA5-PA1
75	V	201	CDL	C73-C74-C75-C76
75	BV	201	CDL	C73-C74-C75-C76
75	AN	102	CDL	C35-C36-C37-C38
71	g	202	PLX	C16-C17-C18-C19
71	Bg	202	PLX	C16-C17-C18-C19
71	AQ	101	PLX	C4-C5-O8-C24
72	p	201	8Q1	C28-O27-P24-O3

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Mol	Chain	Res	Type	Atoms
76	AL	503	PEE	C16-C17-C18-C19
76	AY	502	PEE	C36-C37-C38-C39
76	AU	401	PEE	C30-C31-C32-C33
76	W	201	PEE	C1-C2-O2-C10
76	BW	201	PEE	C1-C2-O2-C10
76	AU	401	PEE	C38-C39-C40-C41
76	AV	403	PEE	C36-C37-C38-C39
76	W	201	PEE	C35-C36-C37-C38
76	BW	201	PEE	C35-C36-C37-C38
75	AU	403	CDL	C34-C35-C36-C37
75	AU	403	CDL	O1-C1-CA2-OA2
75	AU	403	CDL	O1-C1-CB2-OB2
71	Bg	202	PLX	C27-C28-C29-C30
76	AL	503	PEE	C23-C24-C25-C26
76	AU	401	PEE	C14-C15-C16-C17
71	AT	101	PLX	C30-C31-C32-C33
71	g	202	PLX	C27-C28-C29-C30
79	x	603	HEA	CAA-CBA-CGA-O1A
79	Bx	603	HEA	CAA-CBA-CGA-O1A
76	AH	401	PEE	O3P-C1-C2-O2
76	AJ	403	PEE	C19-C20-C21-C22
71	b	201	PLX	C3-C4-C5-O8
71	Bb	201	PLX	C3-C4-C5-O8
75	V	201	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CB3-CB4-CB6-OB8
75	AJ	405	CDL	CA3-CA4-CA6-OA8
75	BV	201	CDL	CA3-CA4-CA6-OA8
76	AU	401	PEE	C42-C43-C44-C45
75	AH	403	CDL	C73-C74-C75-C76
79	x	604	HEA	CAA-CBA-CGA-O2A
79	Bx	604	HEA	CAA-CBA-CGA-O2A
75	AH	403	CDL	CB7-C71-C72-C73
76	l	701	PEE	C38-C39-C40-C41
76	Bl	701	PEE	C38-C39-C40-C41
71	B	303	PLX	C14-C15-C16-C17
71	BB	303	PLX	C14-C15-C16-C17
76	AH	401	PEE	C40-C41-C42-C43
71	BV	203	PLX	C35-C36-C37-C38
71	AN	101	PLX	C35-C36-C37-C38
75	AA	101	CDL	C15-C16-C17-C18
75	Bl	704	CDL	C32-C31-CA7-OA8
71	Br	502	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
75	l	703	CDL	C32-C31-CA7-OA8
75	l	704	CDL	C32-C31-CA7-OA8
75	Bl	703	CDL	C32-C31-CA7-OA8
71	r	502	PLX	C33-C34-C35-C36
71	AT	101	PLX	C10-C11-C12-C13
79	x	604	HEA	CAA-CBA-CGA-O1A
79	Bx	604	HEA	CAA-CBA-CGA-O1A
75	AJ	404	CDL	C52-C51-CB5-OB6
76	AH	401	PEE	C36-C37-C38-C39
75	l	704	CDL	C35-C36-C37-C38
75	Bl	704	CDL	C35-C36-C37-C38
76	BV	202	PEE	C30-C31-C32-C33
75	AG	101	CDL	C32-C31-CA7-OA8
76	V	202	PEE	C30-C31-C32-C33
71	AL	501	PLX	C29-C30-C31-C32
75	AN	102	CDL	C12-C11-CA5-OA6
71	AL	501	PLX	C11-C12-C13-C14
71	b	201	PLX	C24-C25-C26-C27
71	Bb	201	PLX	C24-C25-C26-C27
75	AU	403	CDL	CB3-CB4-CB6-OB8
76	l	702	PEE	C1-C2-C3-O3
76	Bl	702	PEE	C1-C2-C3-O3
71	b	201	PLX	C25-C24-O8-C5
71	g	202	PLX	C25-C24-O8-C5
71	AT	101	PLX	C25-C24-O8-C5
71	Bb	201	PLX	C25-C24-O8-C5
71	Bg	202	PLX	C25-C24-O8-C5
79	x	604	HEA	C26-C15-C16-C17
79	Bx	604	HEA	C26-C15-C16-C17
75	AU	403	CDL	OB6-CB4-CB6-OB8
75	AA	101	CDL	C32-C33-C34-C35
76	l	702	PEE	C18-C19-C20-C21
76	Bl	702	PEE	C18-C19-C20-C21
71	BV	203	PLX	C17-C18-C19-C20
71	AN	101	PLX	C17-C18-C19-C20
76	Bl	702	PEE	C22-C23-C24-C25
76	l	702	PEE	C22-C23-C24-C25
70	A	502	FMN	N10-C1'-C2'-O2'
70	BA	502	FMN	N10-C1'-C2'-O2'
72	E	201	8Q1	O27-C28-C29-C31
72	p	201	8Q1	O27-C28-C29-C30
72	BE	201	8Q1	O27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
75	Bl	703	CDL	C32-C33-C34-C35
71	AT	101	PLX	C25-C26-C27-C28
75	l	703	CDL	C32-C33-C34-C35
76	AL	503	PEE	O2-C10-C11-C12
76	AL	503	PEE	C41-C42-C43-C44
75	AG	101	CDL	C15-C16-C17-C18
73	J	401	NDP	O4D-C4D-C5D-O5D
73	J	401	NDP	C3D-C4D-C5D-O5D
73	BJ	401	NDP	O4D-C4D-C5D-O5D
73	BJ	401	NDP	C3D-C4D-C5D-O5D
71	AL	501	PLX	C33-C34-C35-C36
75	V	201	CDL	C12-C11-CA5-OA7
75	BV	201	CDL	C12-C11-CA5-OA7
76	l	701	PEE	C33-C34-C35-C36
71	B	303	PLX	C4-C3-O4-P1
71	BB	303	PLX	C4-C3-O4-P1
75	AU	403	CDL	C1-CA2-OA2-PA1
75	AU	403	CDL	C75-C76-C77-C78
71	g	202	PLX	C6-C7-C8-C9
71	g	202	PLX	C24-C25-C26-C27
71	Bg	202	PLX	C6-C7-C8-C9
71	Bg	202	PLX	C24-C25-C26-C27
75	l	703	CDL	C32-C31-CA7-OA9
75	Bl	703	CDL	C32-C31-CA7-OA9
76	Bl	701	PEE	C33-C34-C35-C36
76	l	702	PEE	C41-C42-C43-C44
76	AY	502	PEE	C21-C22-C23-C24
76	Bl	702	PEE	C41-C42-C43-C44
75	AN	102	CDL	C12-C11-CA5-OA7
76	V	202	PEE	C39-C40-C41-C42
76	BV	202	PEE	C39-C40-C41-C42
75	AG	101	CDL	C52-C51-CB5-OB6
75	AU	403	CDL	C72-C71-CB7-OB8
75	AN	102	CDL	O1-C1-CB2-OB2
71	r	501	PLX	C14-C15-C16-C17
71	AN	101	PLX	C15-C16-C17-C18
71	Br	501	PLX	C14-C15-C16-C17
75	AG	101	CDL	C32-C31-CA7-OA9
75	AN	102	CDL	C72-C71-CB7-OB8
71	B	303	PLX	O9-C24-O8-C5
71	U	101	PLX	O9-C24-O8-C5
71	AL	501	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
71	BB	303	PLX	O9-C24-O8-C5
71	BU	101	PLX	O9-C24-O8-C5
76	l	701	PEE	C11-C12-C13-C14
71	BV	203	PLX	C15-C16-C17-C18
75	AY	501	CDL	C51-C52-C53-C54
76	Bl	701	PEE	C11-C12-C13-C14
75	AA	101	CDL	C12-C11-CA5-OA6
79	x	603	HEA	CAA-CBA-CGA-O2A
79	Bx	603	HEA	CAA-CBA-CGA-O2A
75	AJ	404	CDL	C52-C51-CB5-OB7
71	g	201	PLX	C4-C5-O8-C24
71	Bg	201	PLX	C4-C5-O8-C24
76	Bl	702	PEE	O2-C2-C3-O3
71	AT	101	PLX	C17-C18-C19-C20
82	AV	401	HEM	CAA-CBA-CGA-O2A
75	l	704	CDL	C32-C31-CA7-OA9
75	Bl	704	CDL	C32-C31-CA7-OA9
72	p	201	8Q1	O33-C32-C34-N36
72	Bp	201	8Q1	O33-C32-C34-N36
76	Bl	702	PEE	C32-C33-C34-C35
76	l	702	PEE	C32-C33-C34-C35
75	Bl	704	CDL	C74-C75-C76-C77
75	l	704	CDL	C74-C75-C76-C77
71	g	203	PLX	C36-C37-C38-C39
71	Bg	203	PLX	C36-C37-C38-C39
75	AA	101	CDL	C52-C51-CB5-OB6
71	AN	101	PLX	C34-C35-C36-C37
73	J	401	NDP	O4D-C1D-N1N-C2N
73	BJ	401	NDP	O4D-C1D-N1N-C2N
75	l	704	CDL	C52-C51-CB5-OB6
76	AL	503	PEE	O3-C30-C31-C32
75	AU	403	CDL	C72-C71-CB7-OB9
76	AL	503	PEE	O4-C10-C11-C12
76	AJ	403	PEE	C10-C11-C12-C13
71	BV	203	PLX	C34-C35-C36-C37
75	AH	403	CDL	C12-C11-CA5-OA6
75	Bl	704	CDL	C52-C51-CB5-OB6

There are no ring outliers.

86 monomers are involved in 860 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	p	201	8Q1	12	0
74	AP	301	FES	2	0
75	AA	101	CDL	3	0
72	BE	201	8Q1	4	0
71	b	201	PLX	36	0
71	Bg	202	PLX	3	0
75	Bn	101	CDL	10	0
71	AN	101	PLX	10	0
79	Bx	603	HEA	1	0
71	AQ	101	PLX	9	0
71	BU	101	PLX	2	0
71	U	101	PLX	2	0
74	M	803	FES	1	0
69	BB	302	SF4	2	0
75	Bl	703	CDL	2	0
76	l	701	PEE	48	0
70	BA	502	FMN	16	0
74	BM	803	FES	1	0
75	AH	403	CDL	8	0
69	M	801	SF4	4	0
75	AJ	405	CDL	17	0
75	n	101	CDL	10	0
71	Br	502	PLX	16	0
82	AJ	401	HEM	4	0
69	B	301	SF4	1	0
75	AJ	404	CDL	6	0
79	x	604	HEA	3	0
76	W	201	PEE	20	0
69	BM	801	SF4	3	0
72	E	201	8Q1	4	0
75	l	704	CDL	2	0
76	V	202	PEE	22	0
75	AU	403	CDL	11	0
73	BJ	401	NDP	26	0
71	g	201	PLX	2	0
75	AN	102	CDL	9	0
76	AH	401	PEE	32	0
76	Bl	701	PEE	49	0
74	BO	301	FES	2	0
82	AV	402	HEM	6	0
76	AU	401	PEE	24	0
75	l	703	CDL	2	0
71	g	202	PLX	3	0

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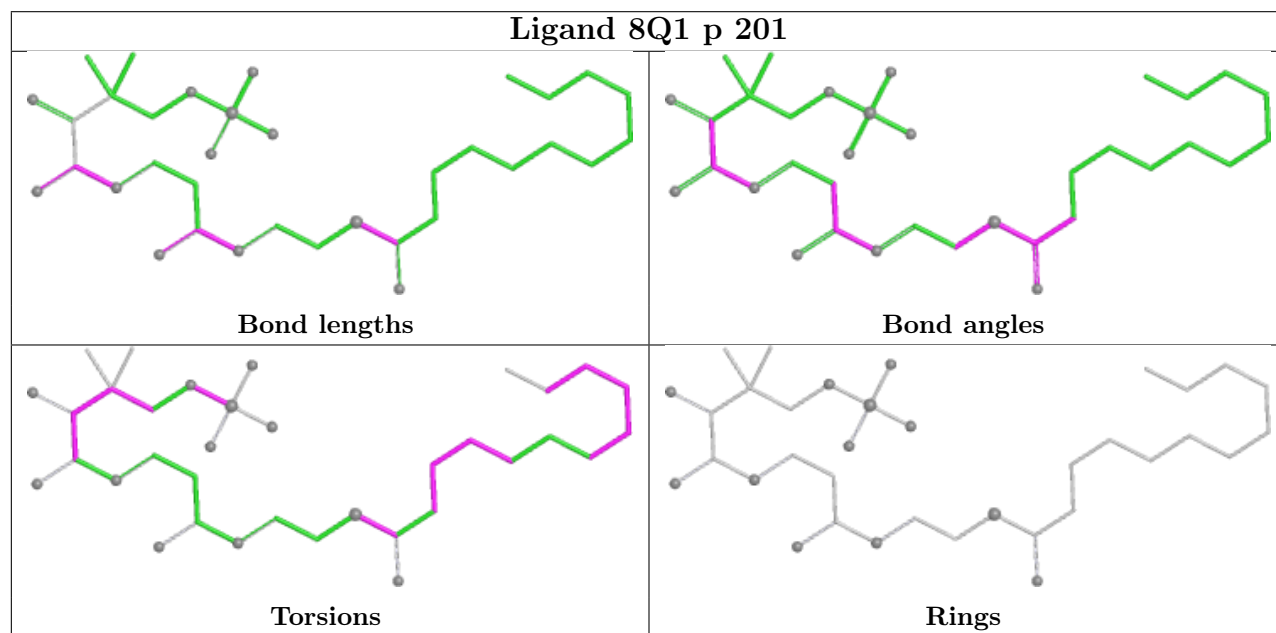
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	V	201	CDL	8	0
71	r	501	PLX	7	0
76	l	702	PEE	18	0
74	AC	301	FES	3	0
79	x	603	HEA	1	0
75	i	401	CDL	2	0
71	AL	501	PLX	4	0
74	O	301	FES	2	0
71	g	203	PLX	8	0
71	Bb	201	PLX	35	0
82	AV	401	HEM	7	0
71	Bg	201	PLX	2	0
76	AJ	403	PEE	8	0
75	AY	501	CDL	6	0
76	AY	502	PEE	21	0
76	AV	403	PEE	23	0
75	Bl	704	CDL	3	0
71	Bg	203	PLX	9	0
76	BV	202	PEE	21	0
73	J	401	NDP	26	0
70	A	502	FMN	17	0
71	r	502	PLX	16	0
71	BB	303	PLX	4	0
82	AJ	402	HEM	4	0
69	BA	501	SF4	6	0
69	A	501	SF4	6	0
76	Bl	702	PEE	18	0
75	AL	502	CDL	24	0
75	BV	201	CDL	6	0
81	AU	402	HEC	7	0
69	BB	301	SF4	1	0
71	B	303	PLX	4	0
76	BW	201	PEE	20	0
71	AT	101	PLX	2	0
79	Bx	604	HEA	3	0
75	Bi	401	CDL	2	0
81	AH	402	HEC	5	0
75	AG	101	CDL	29	0
71	Br	501	PLX	8	0
76	AL	503	PEE	39	0
72	Bp	201	8Q1	13	0
69	B	302	SF4	2	0

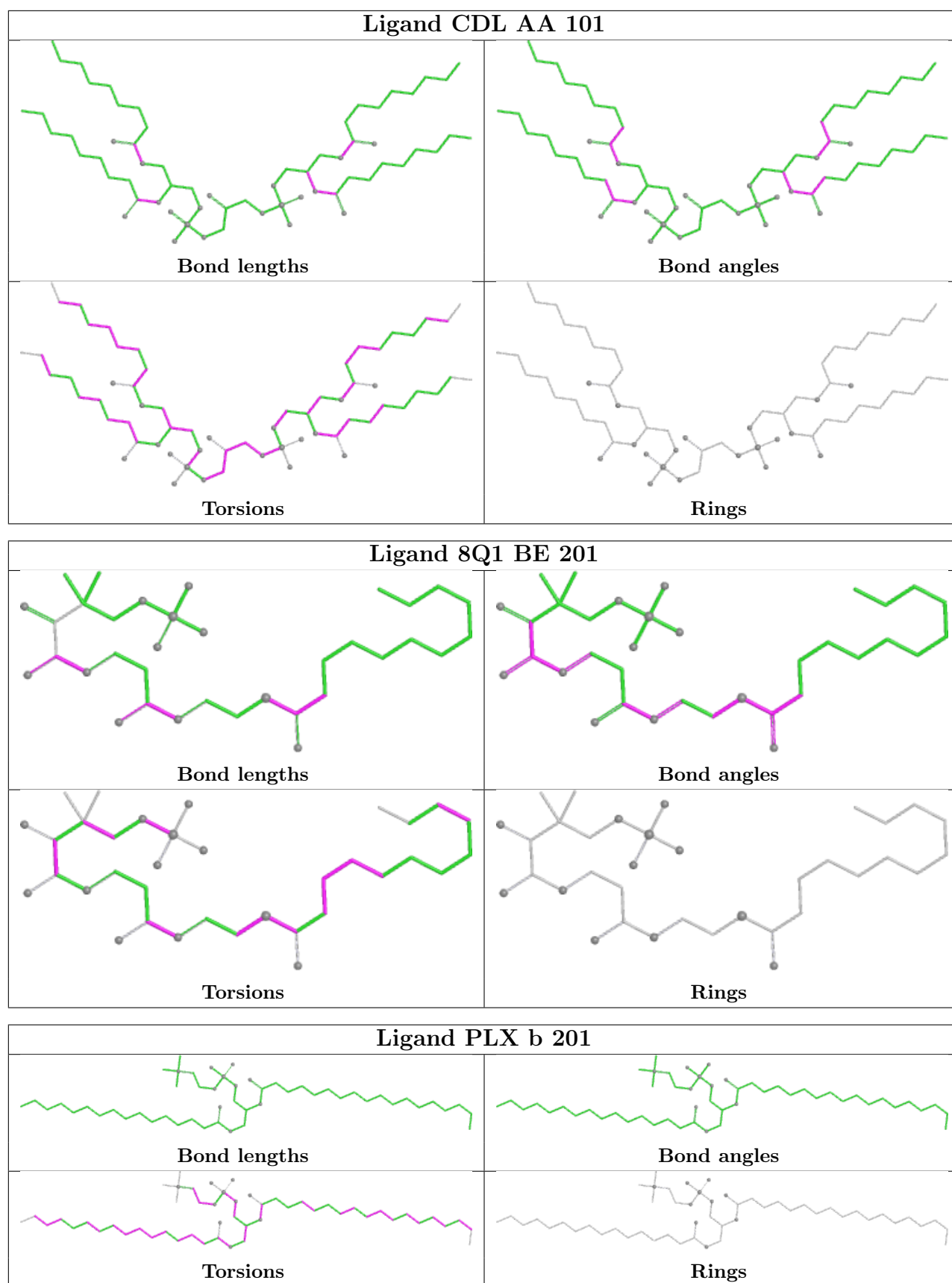
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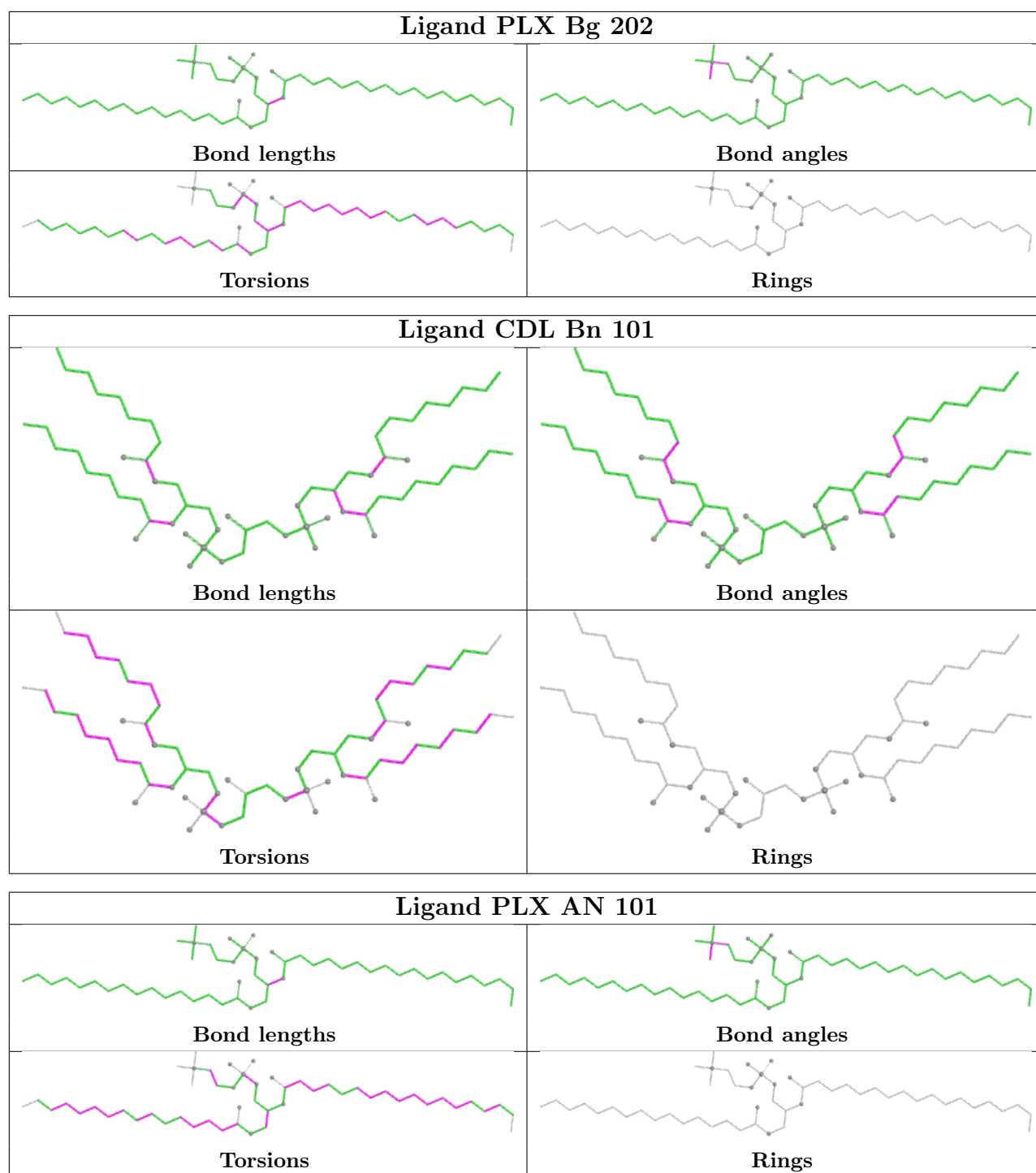
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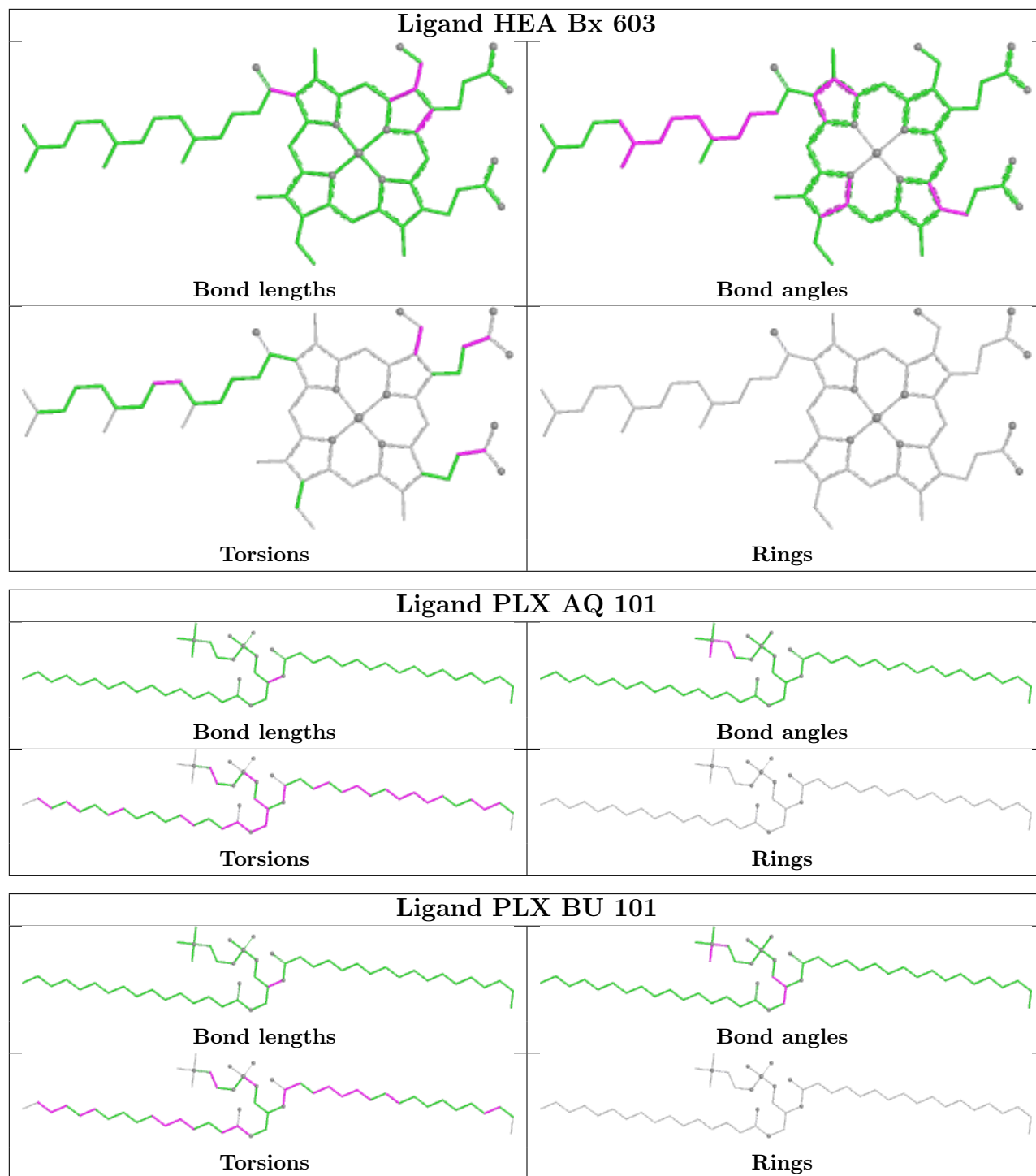
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	BV	203	PLX	4	0

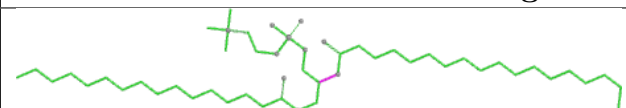
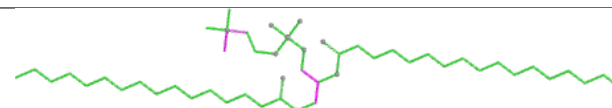
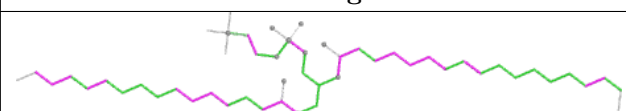
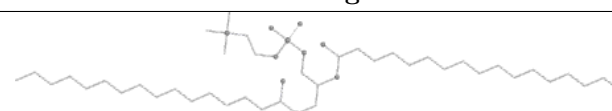
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

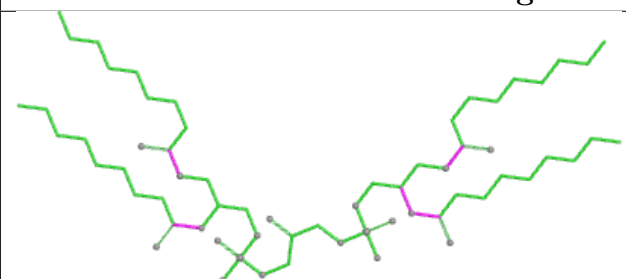
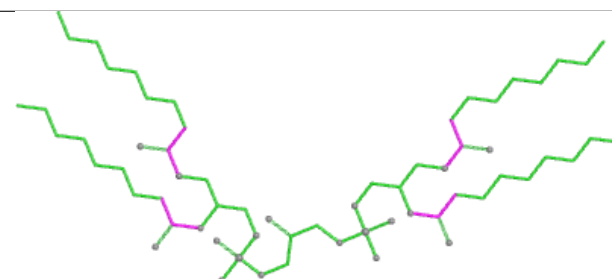
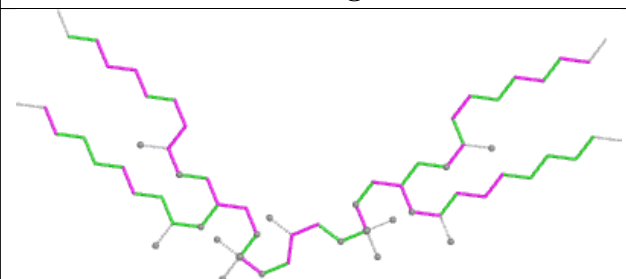
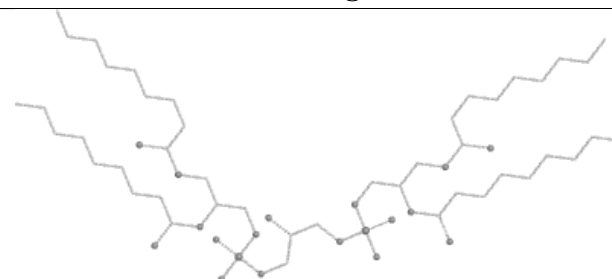


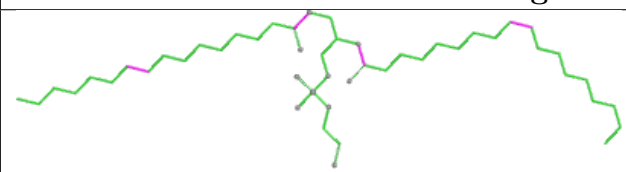
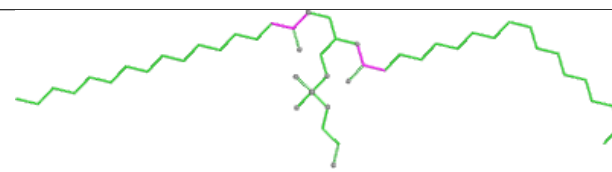
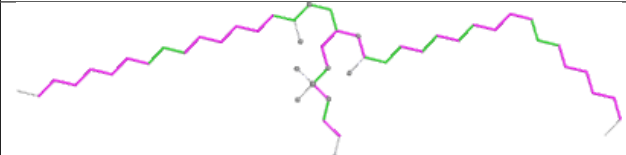
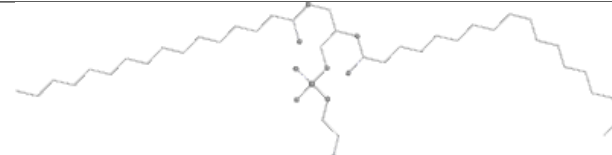




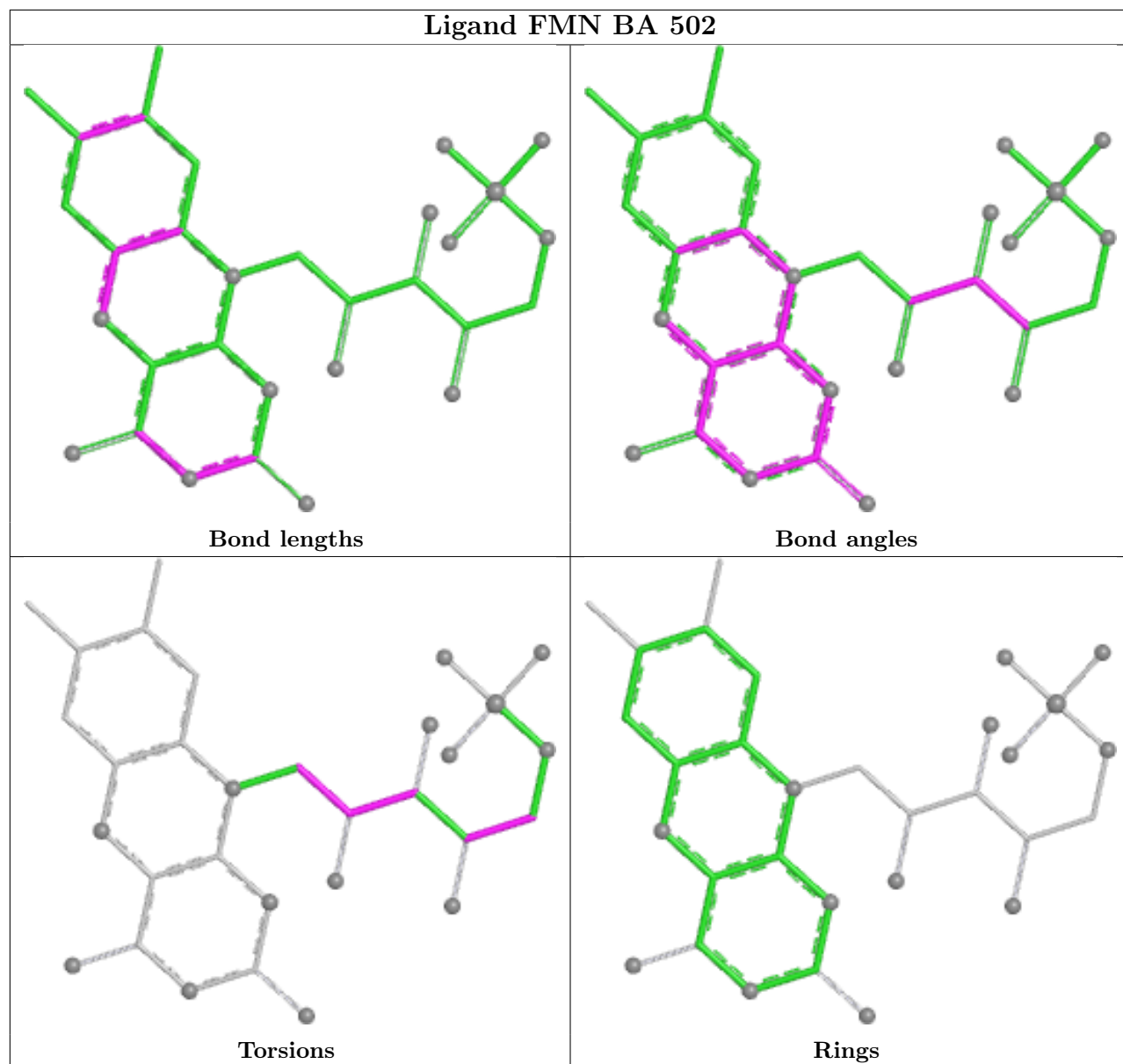


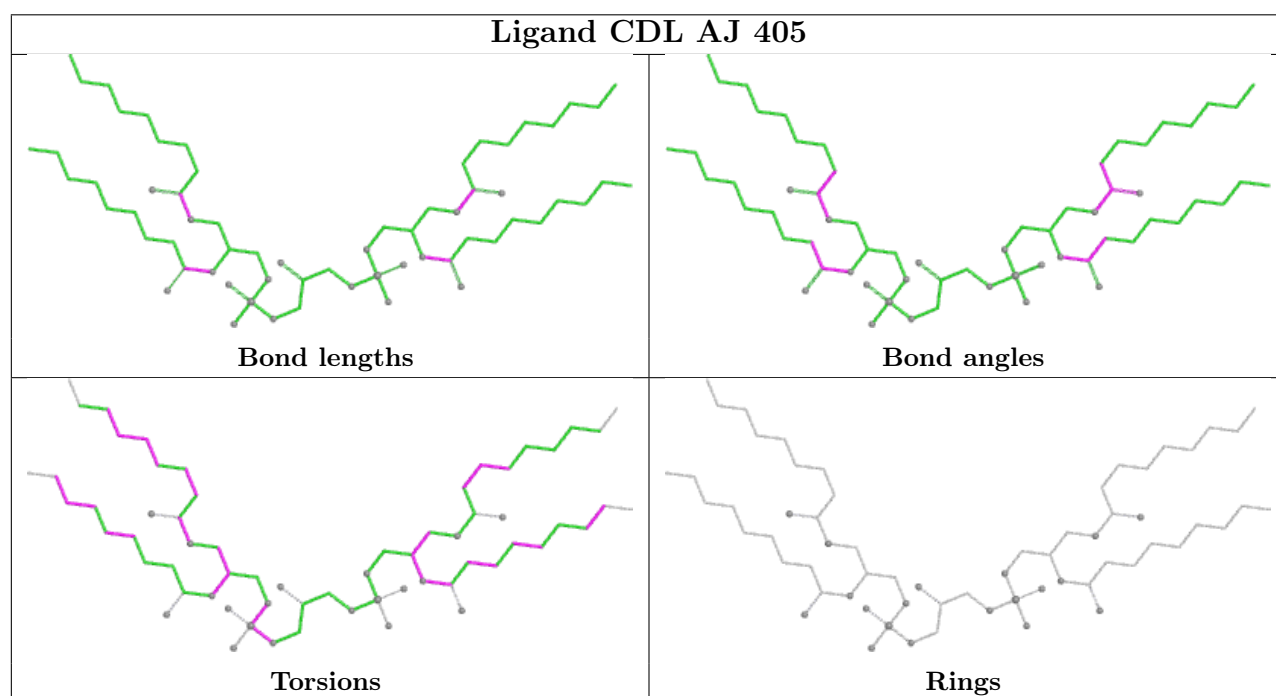
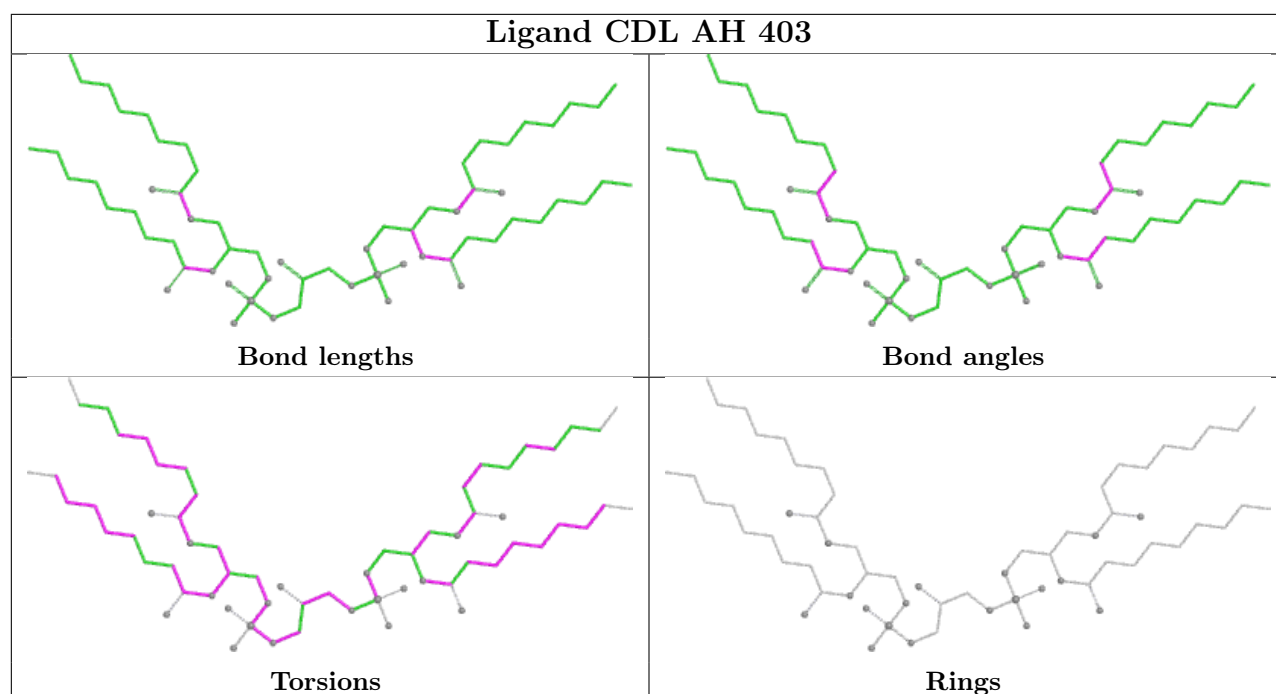
Ligand PLX U 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

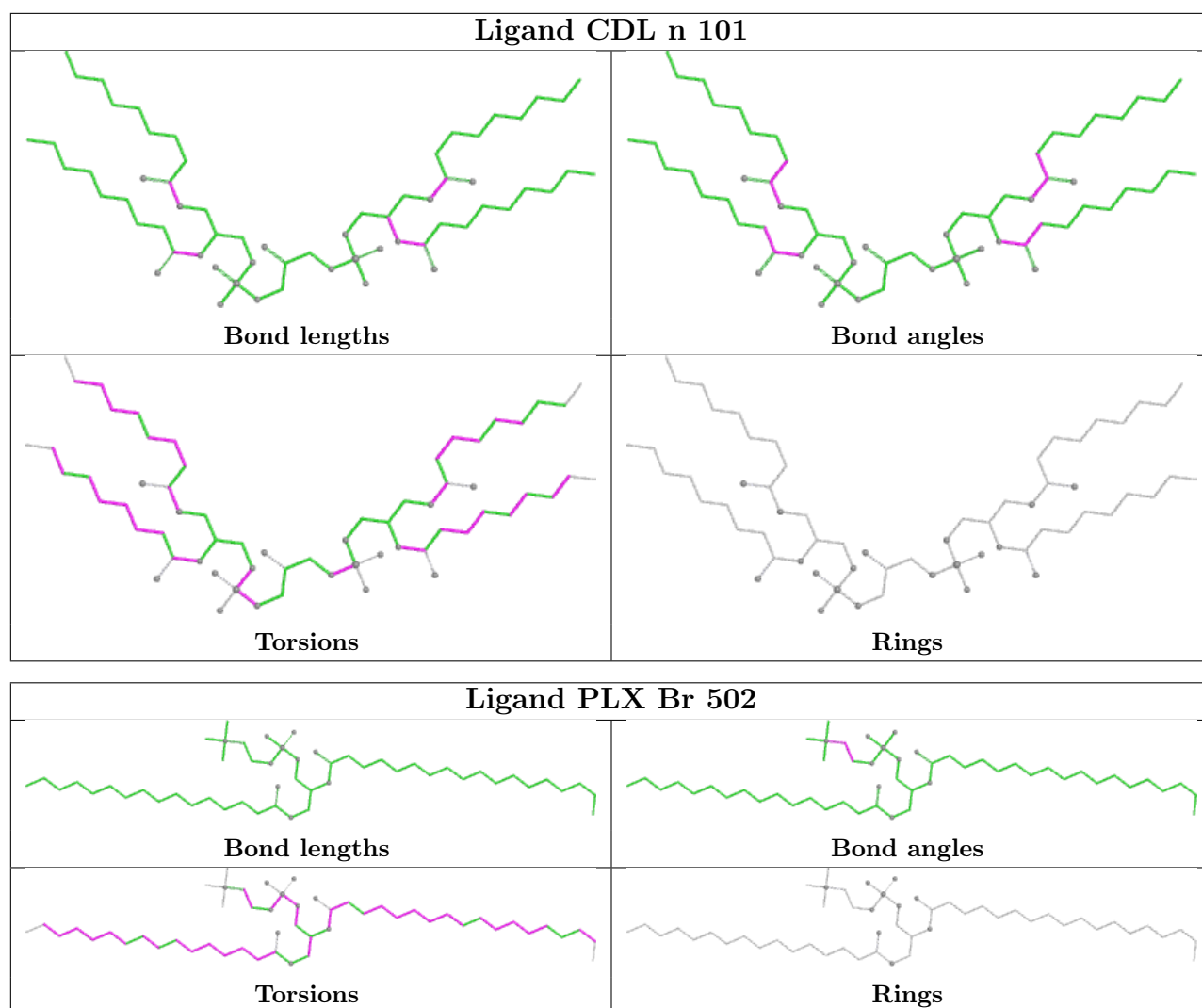
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE l 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

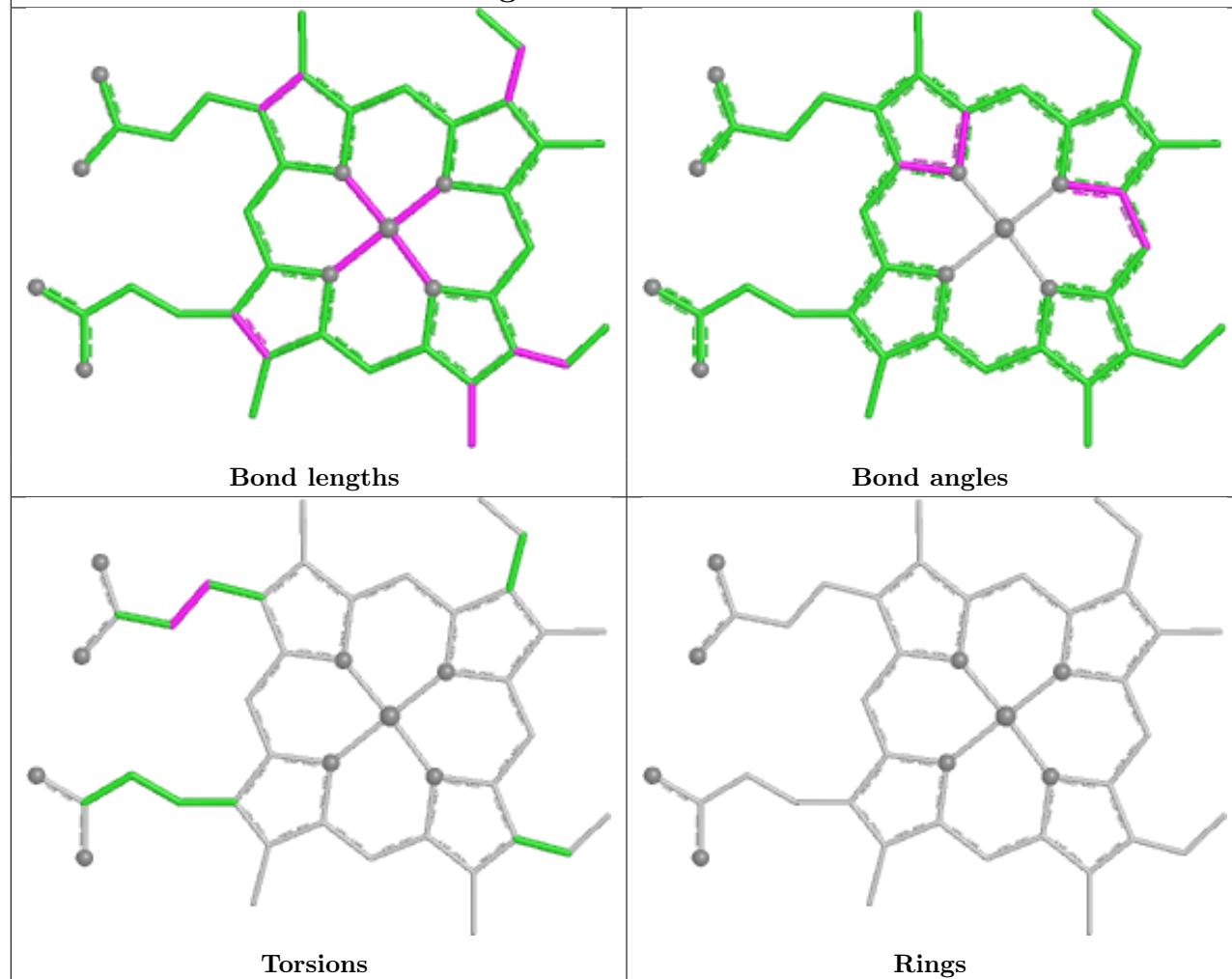
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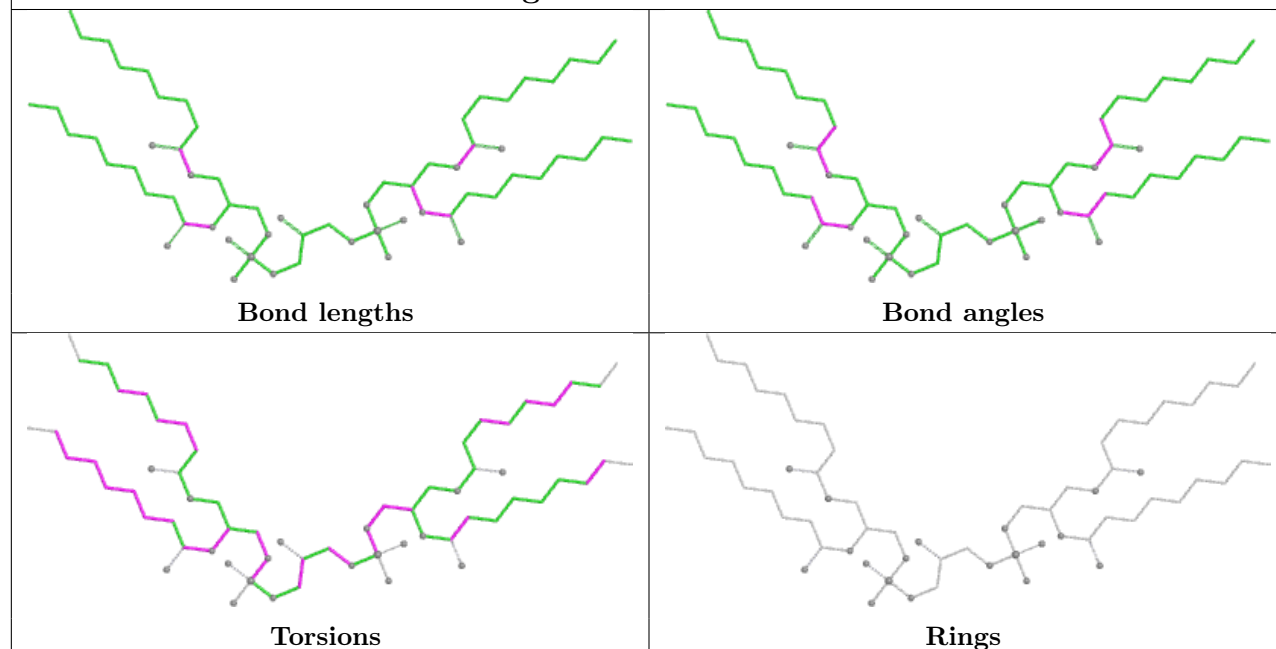


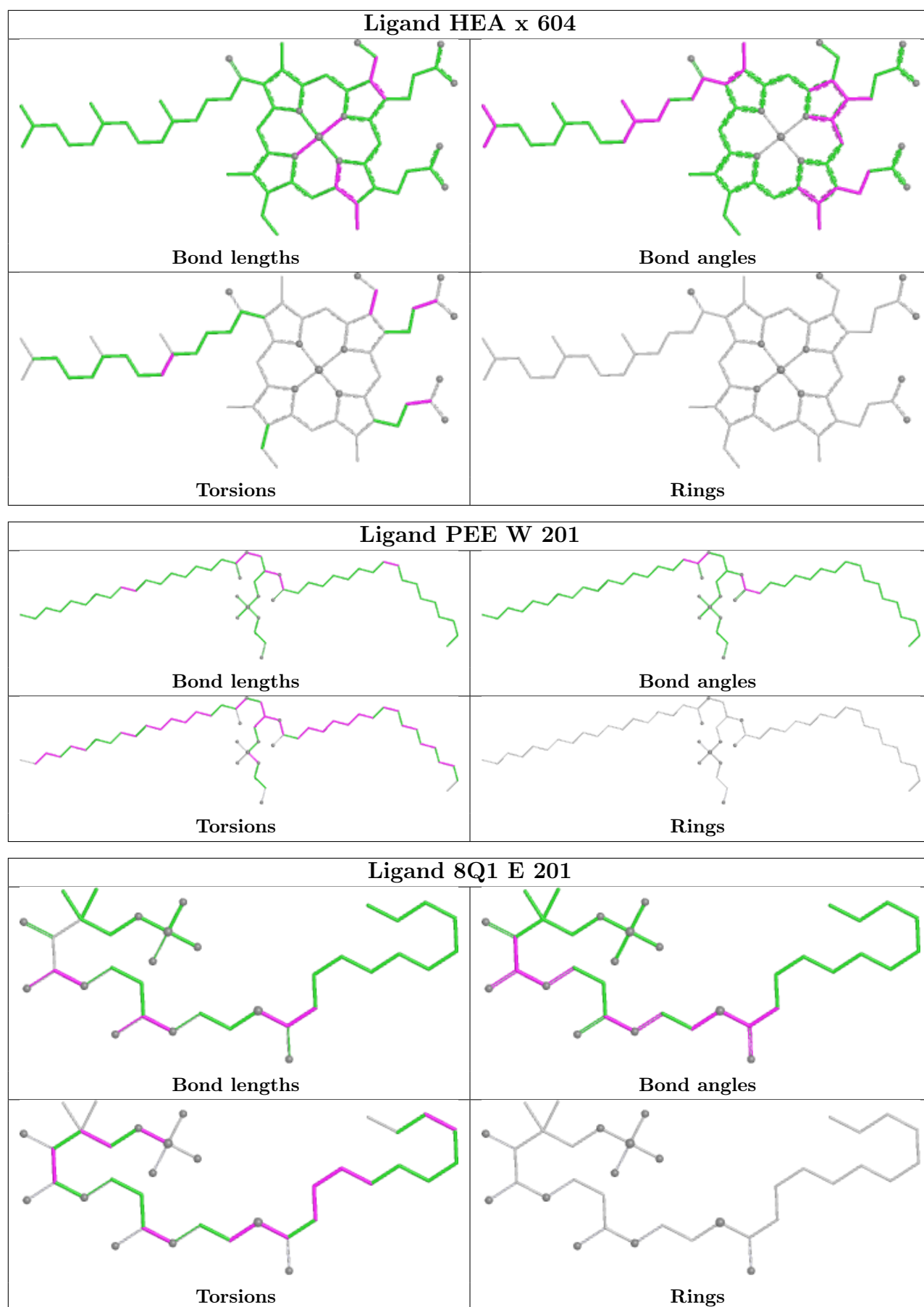


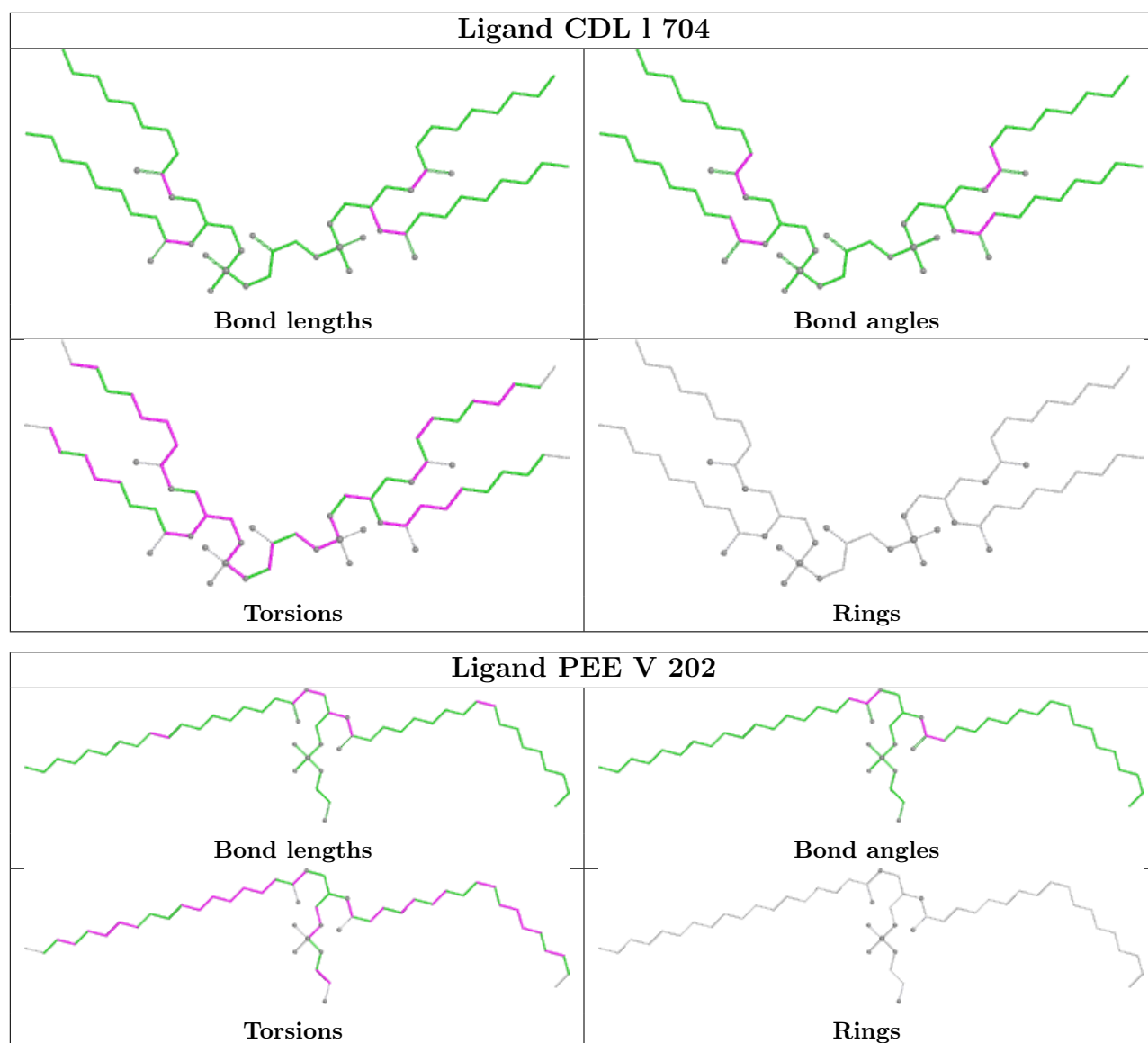
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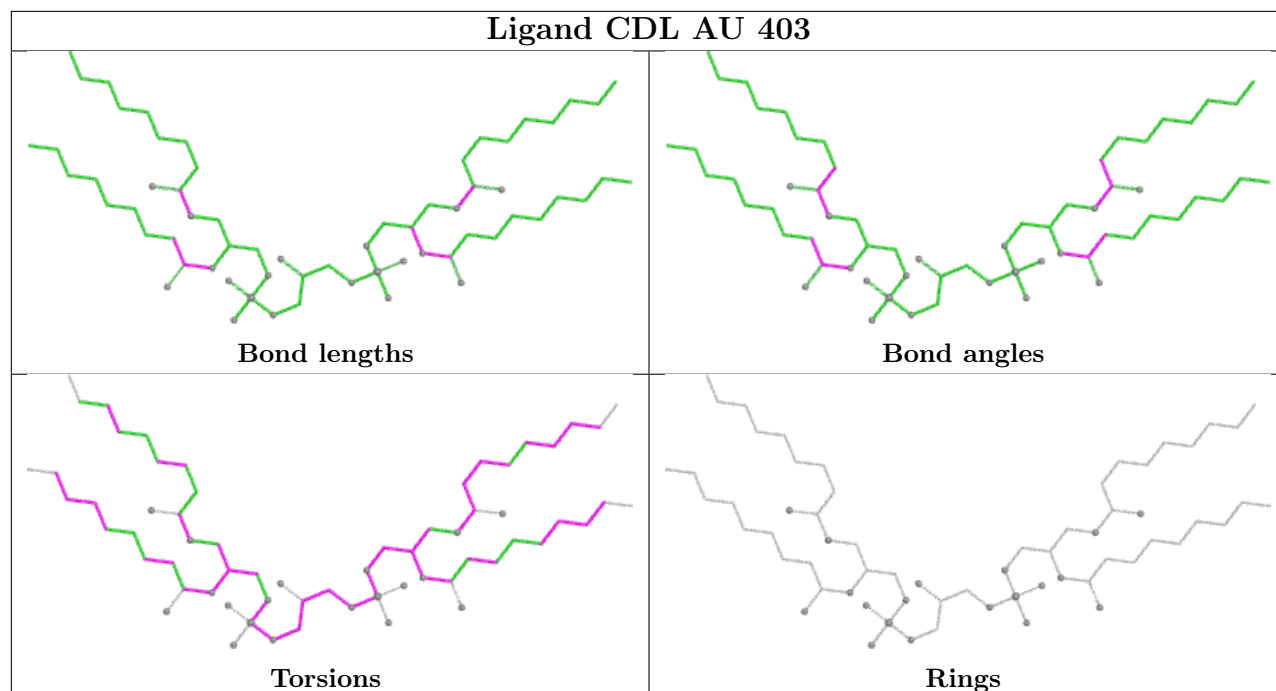
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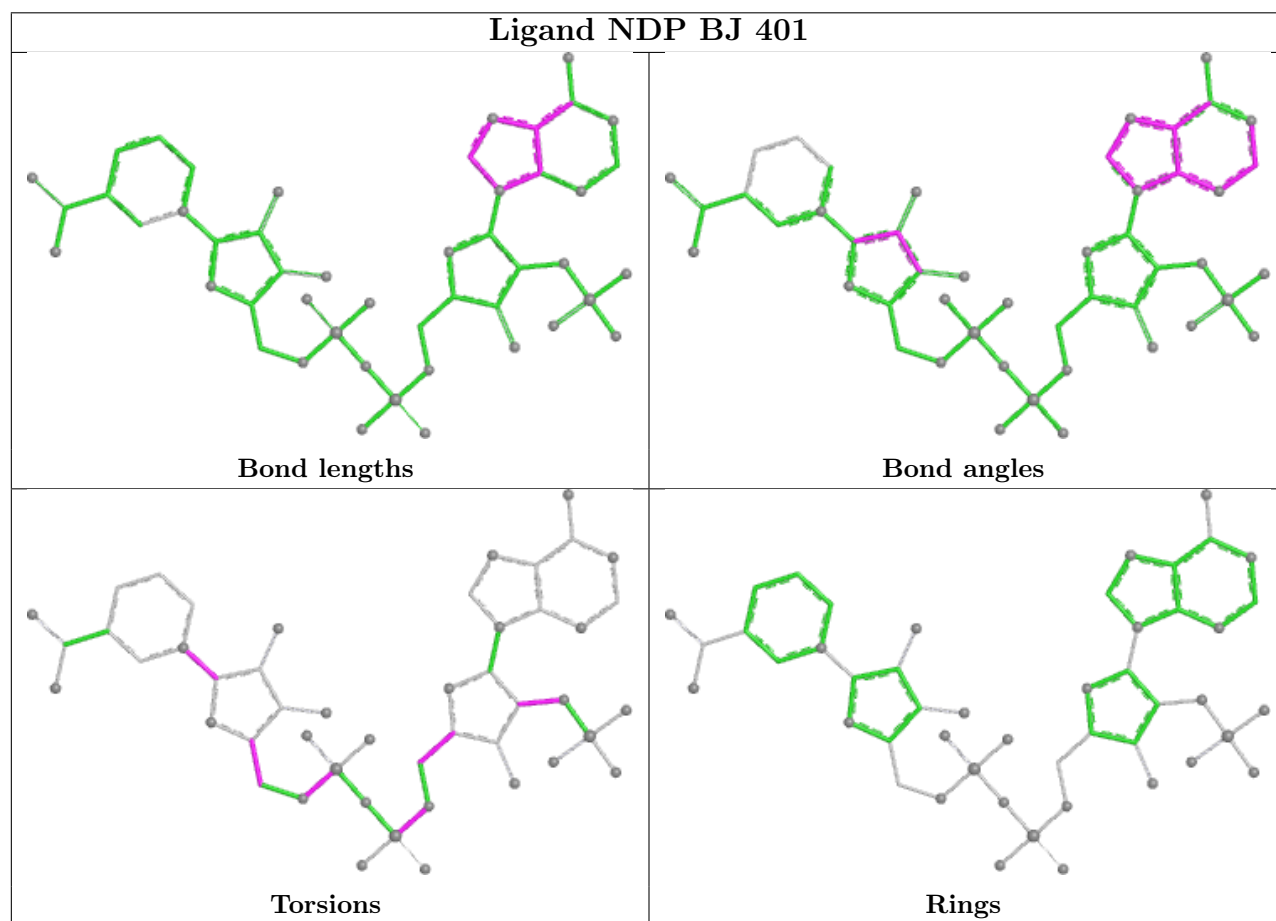


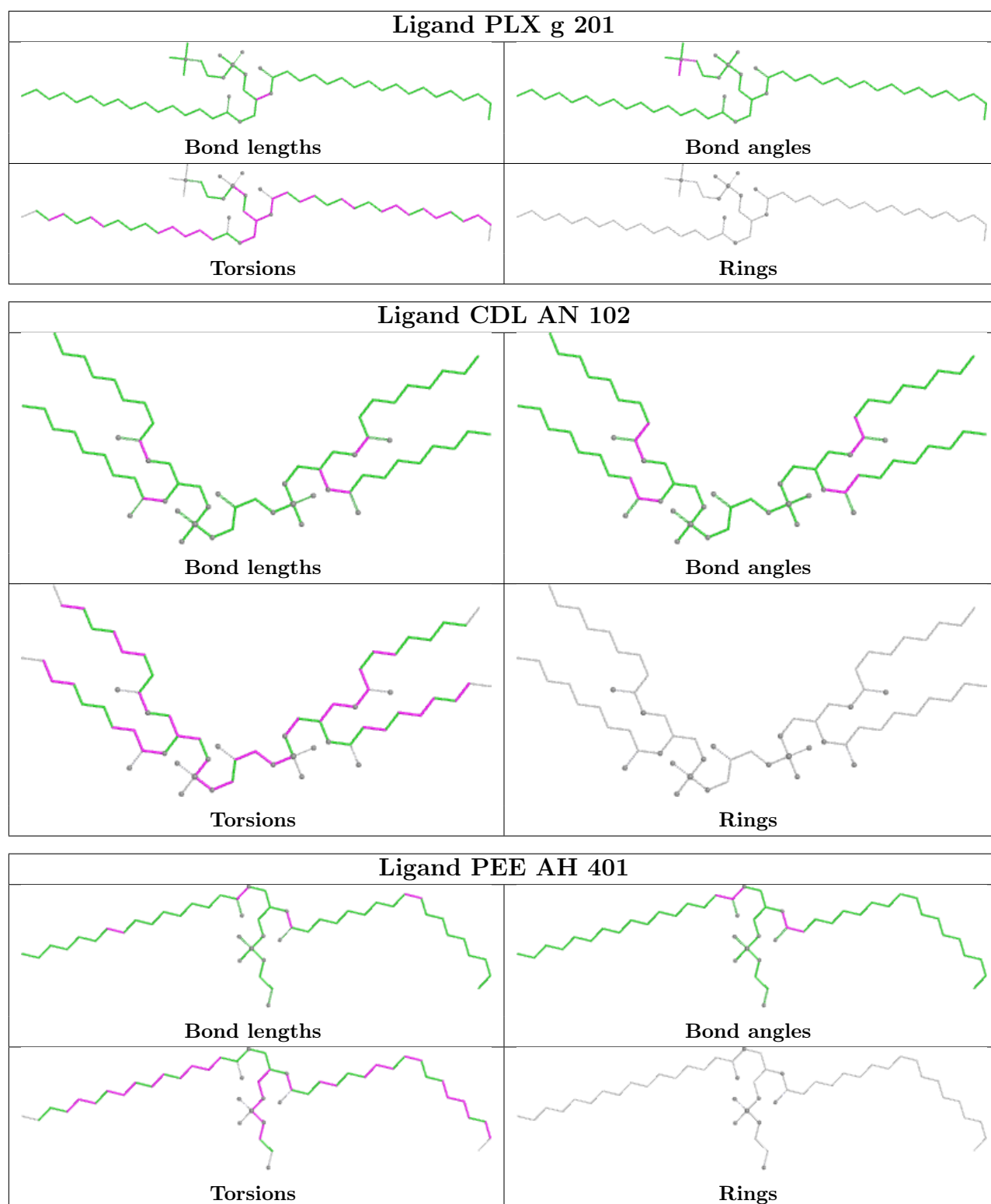


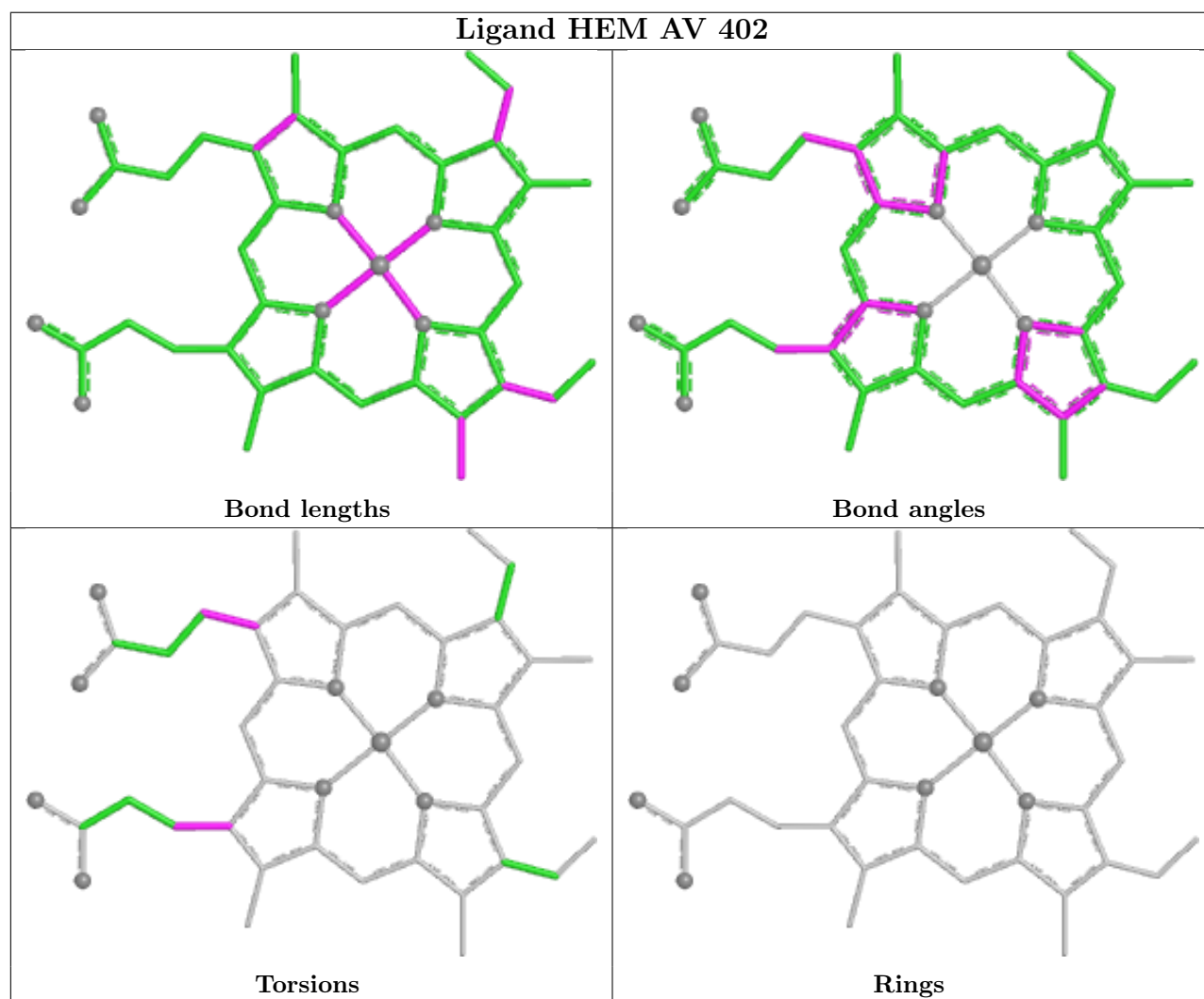
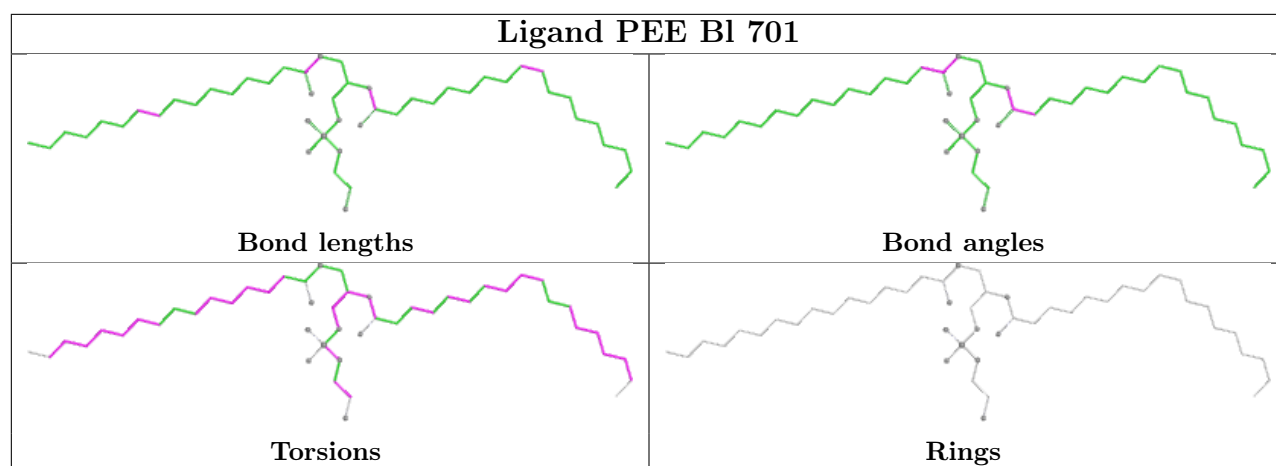
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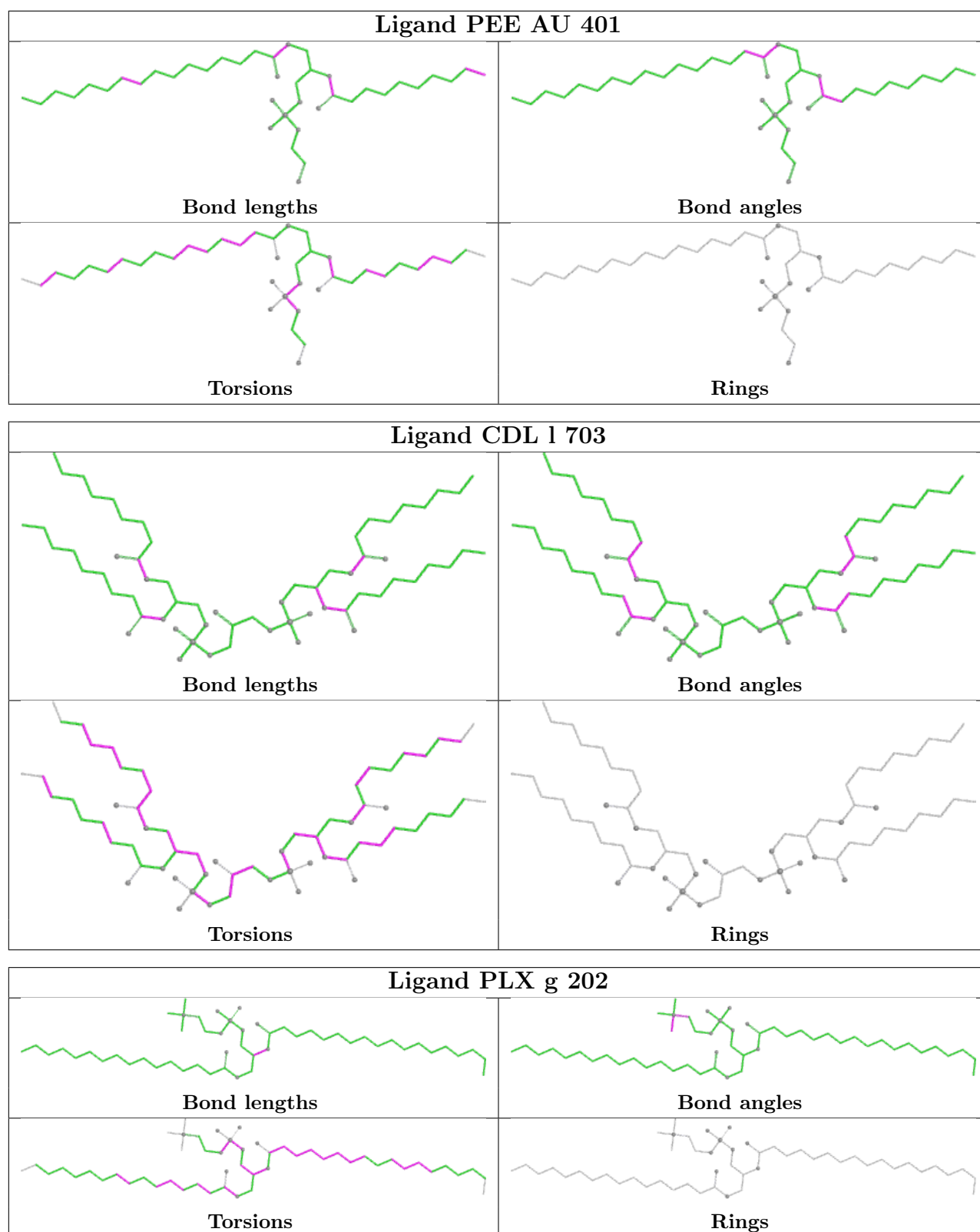


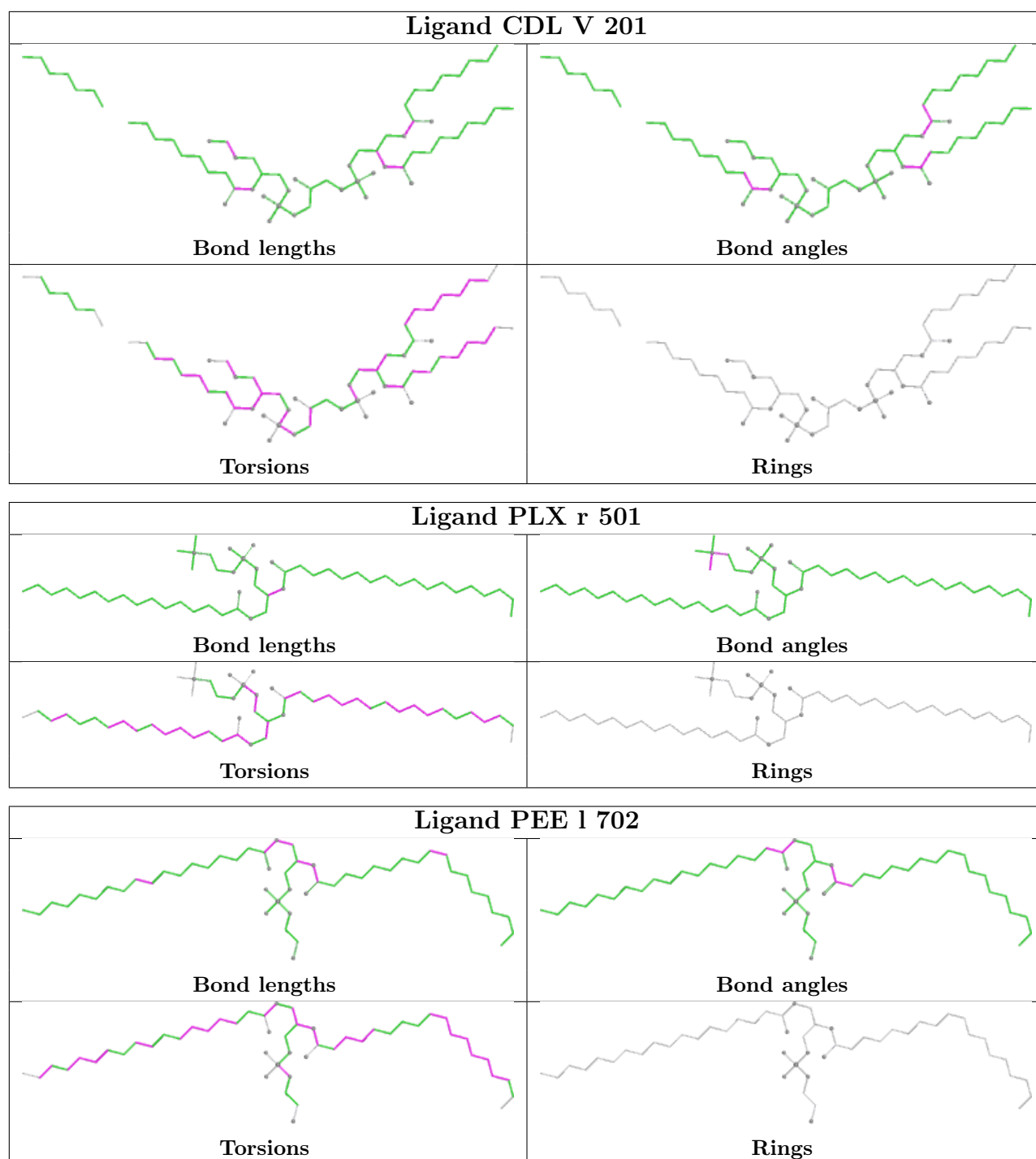
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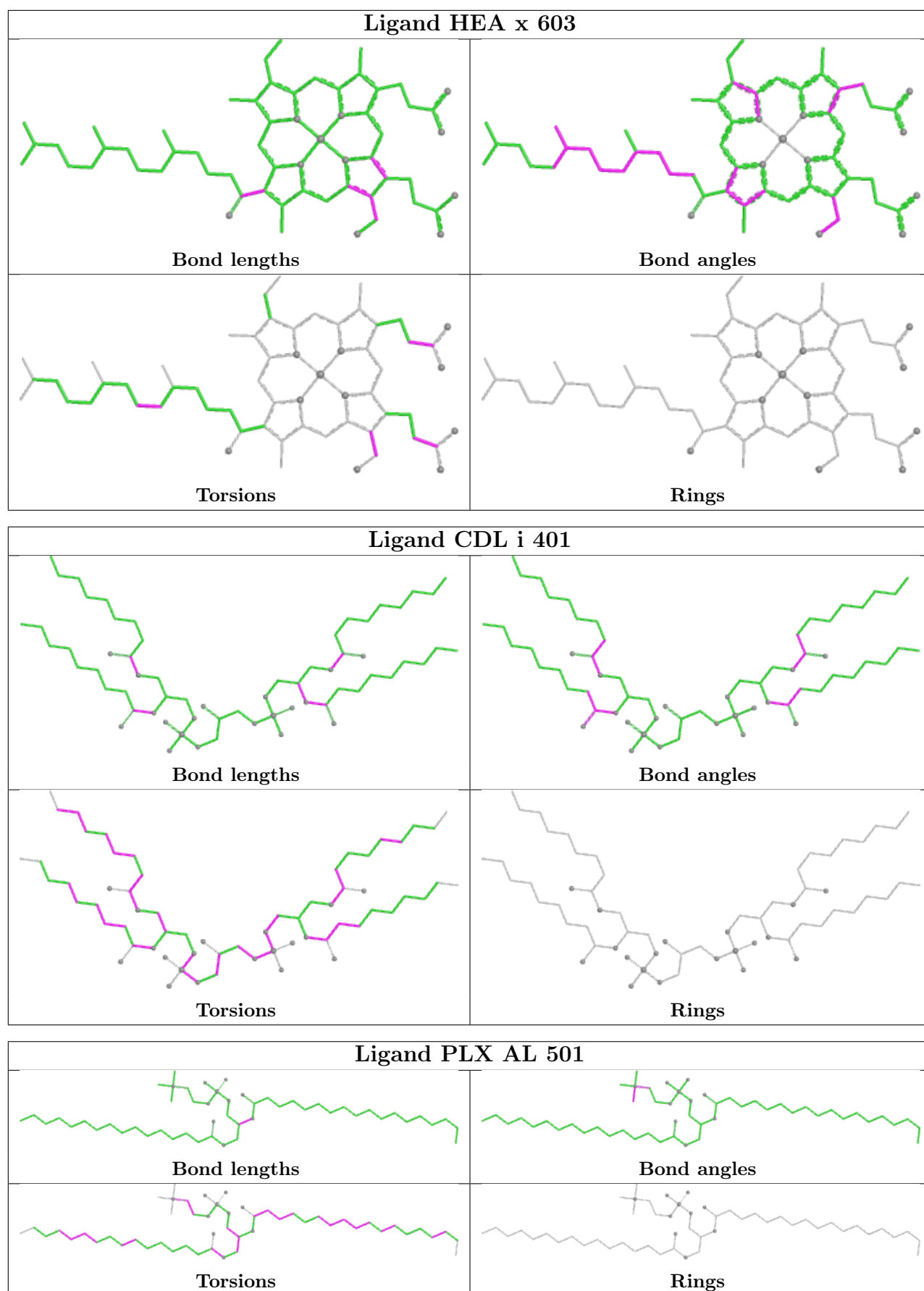




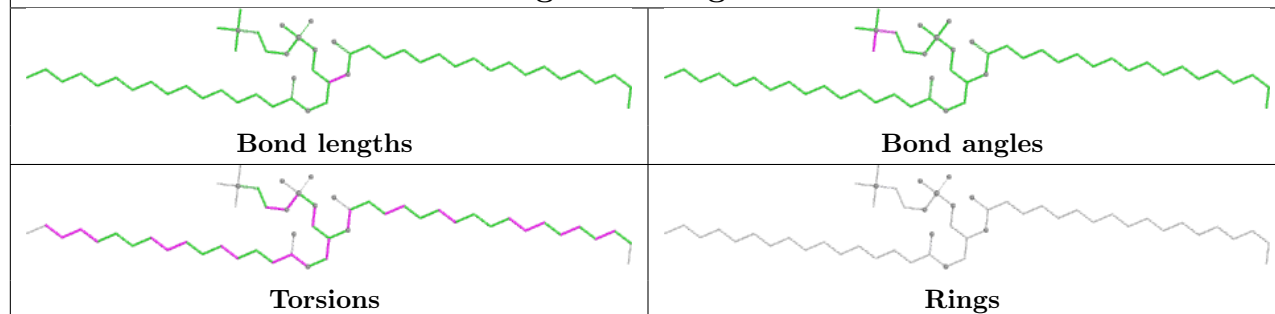




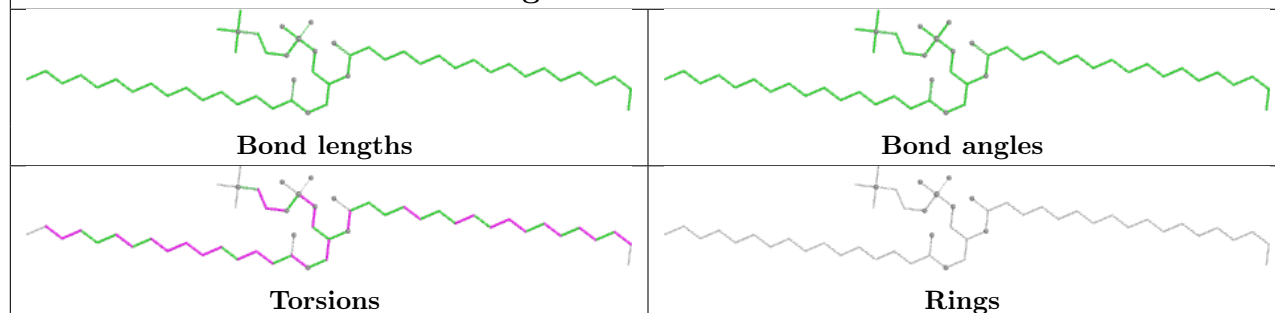




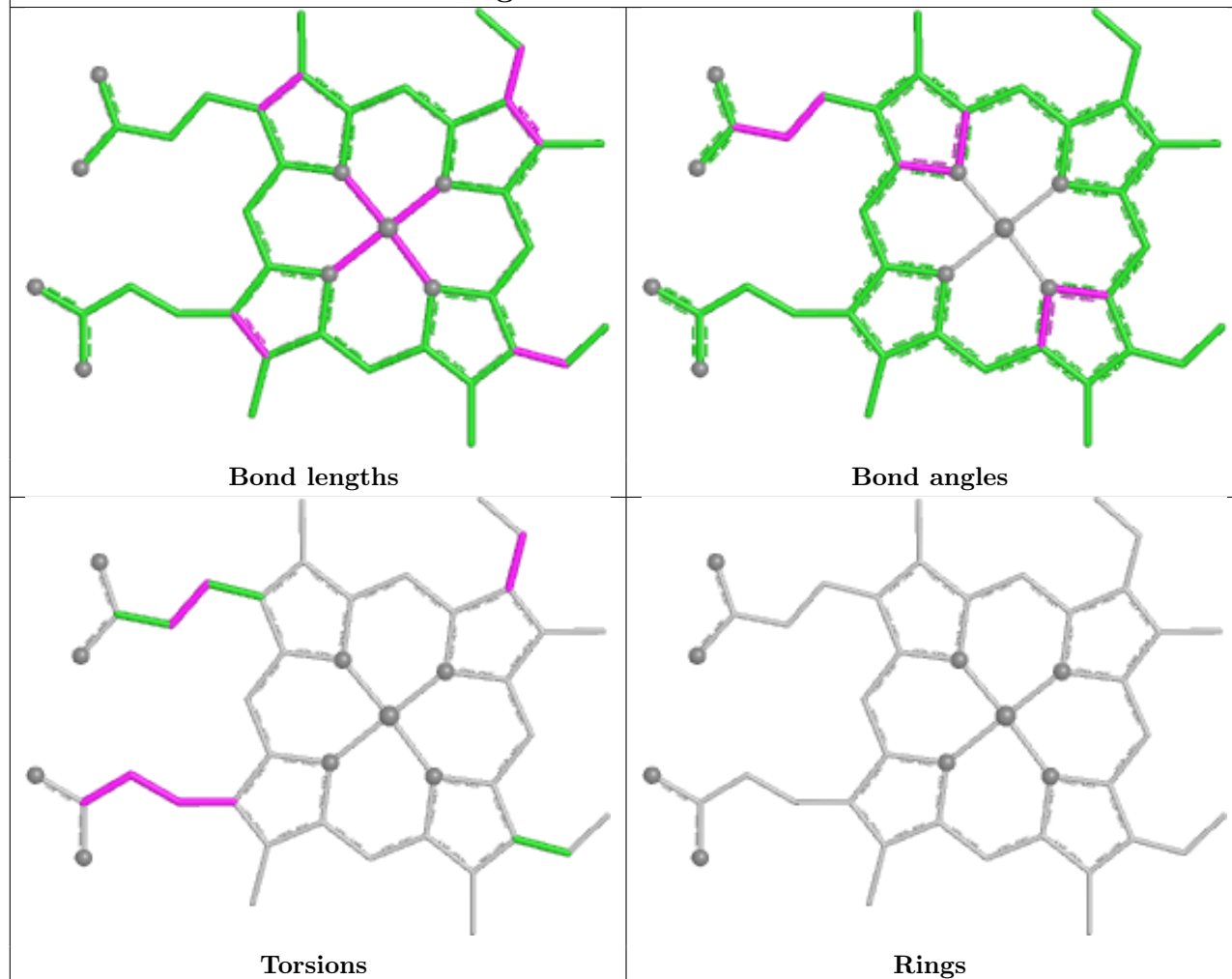
Ligand PLX g 203

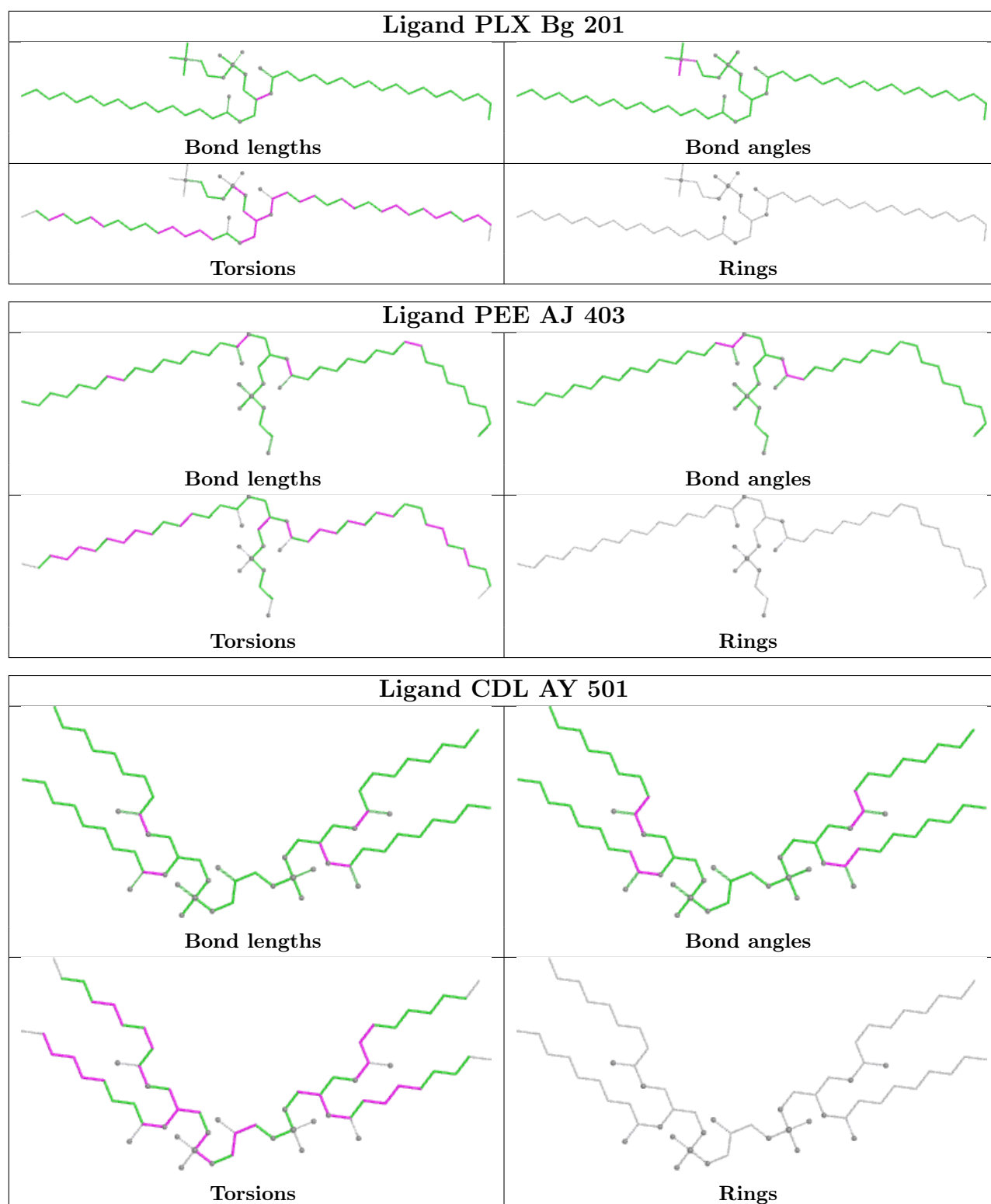


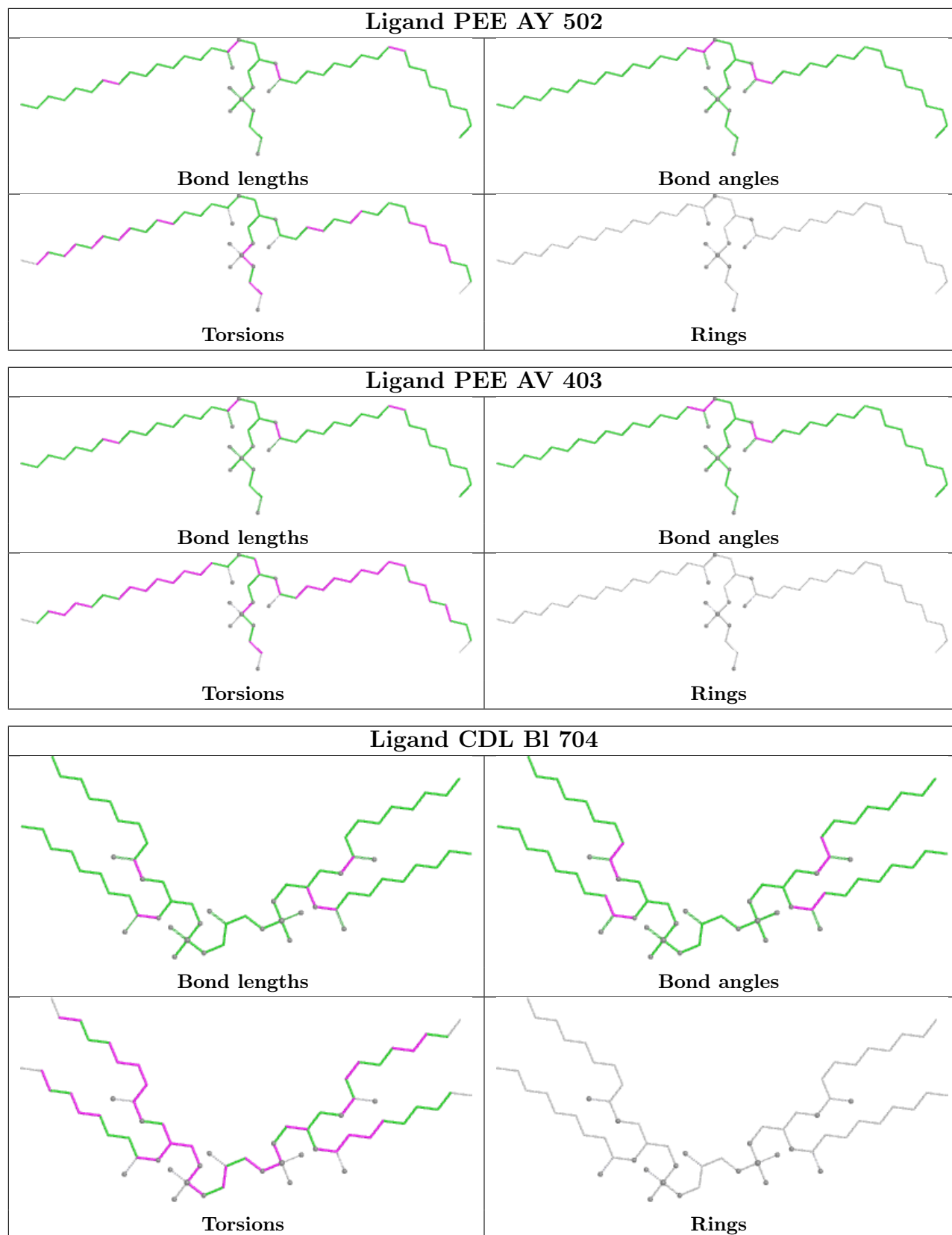
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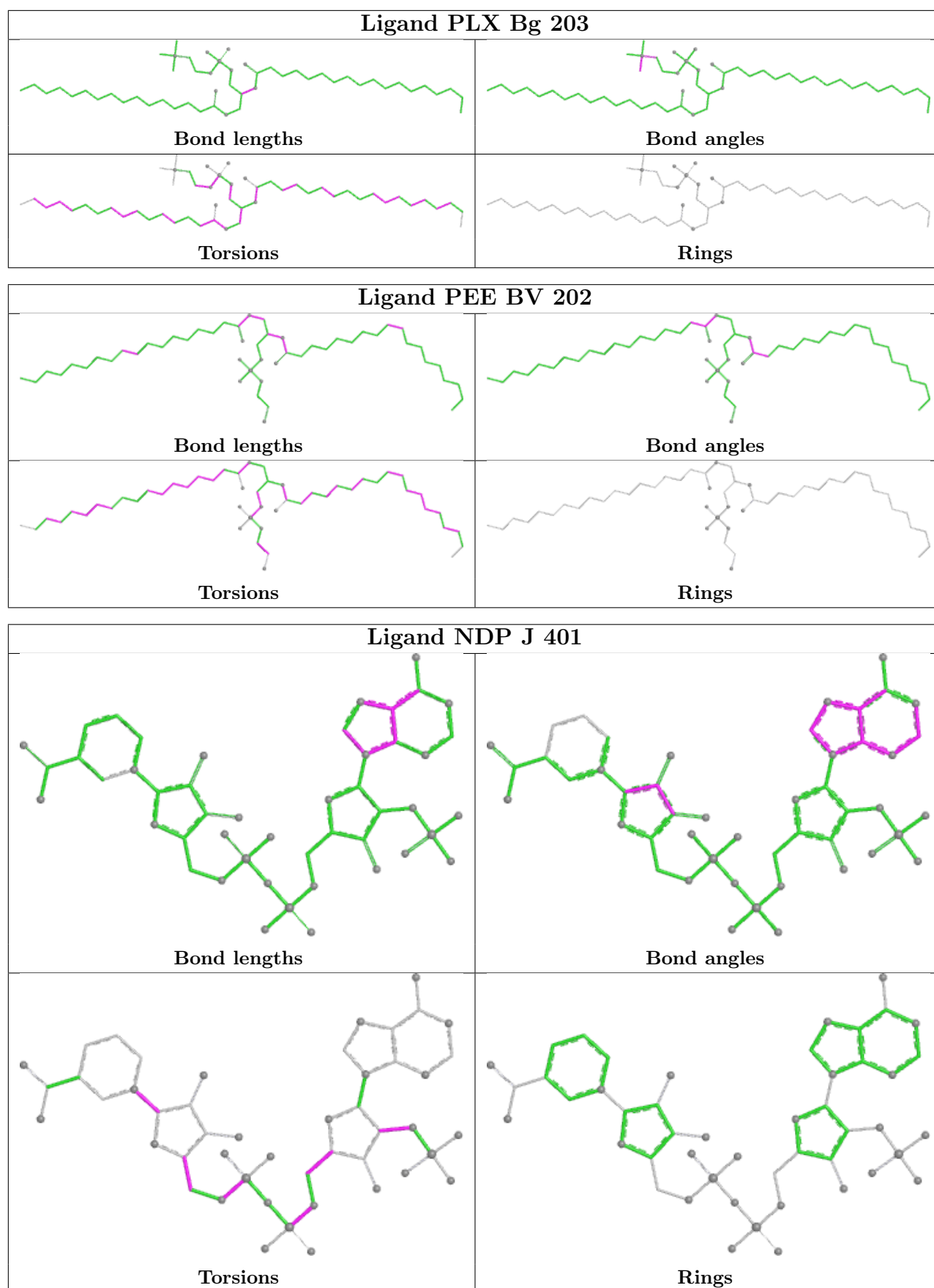


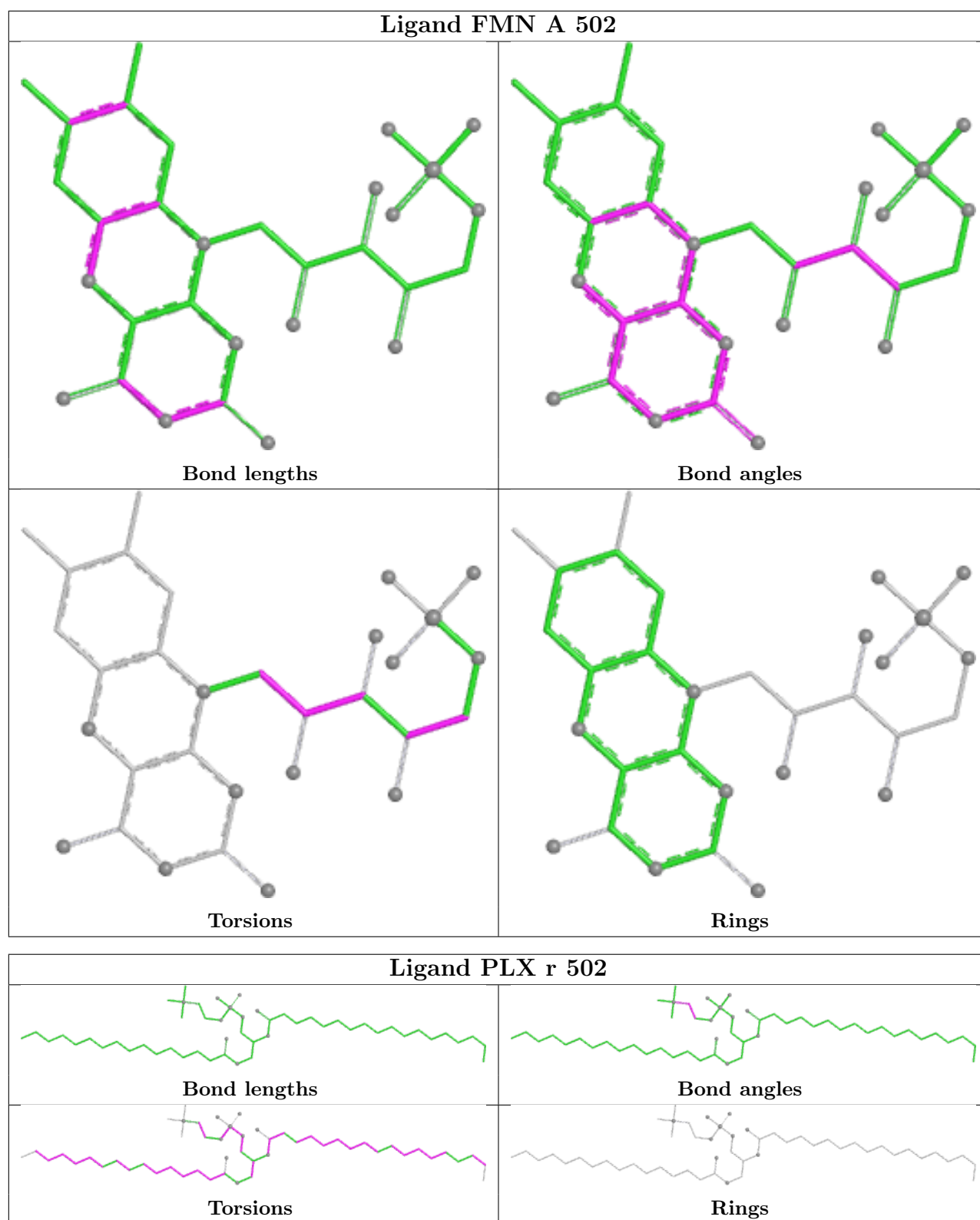
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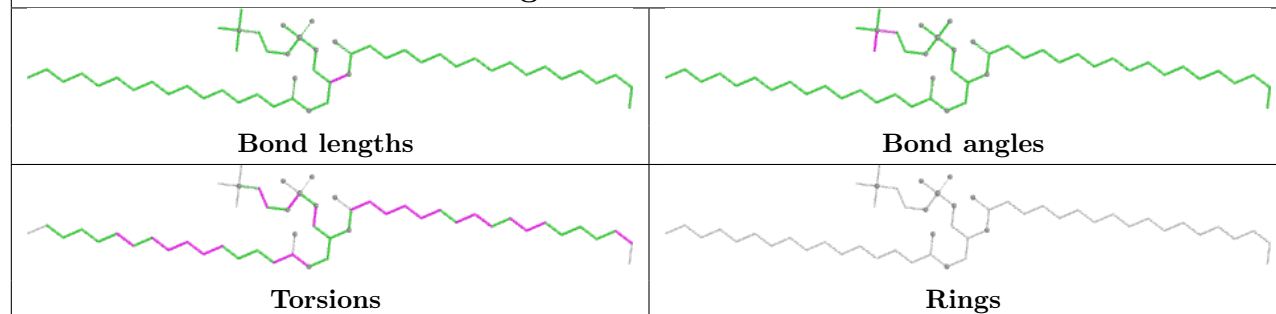
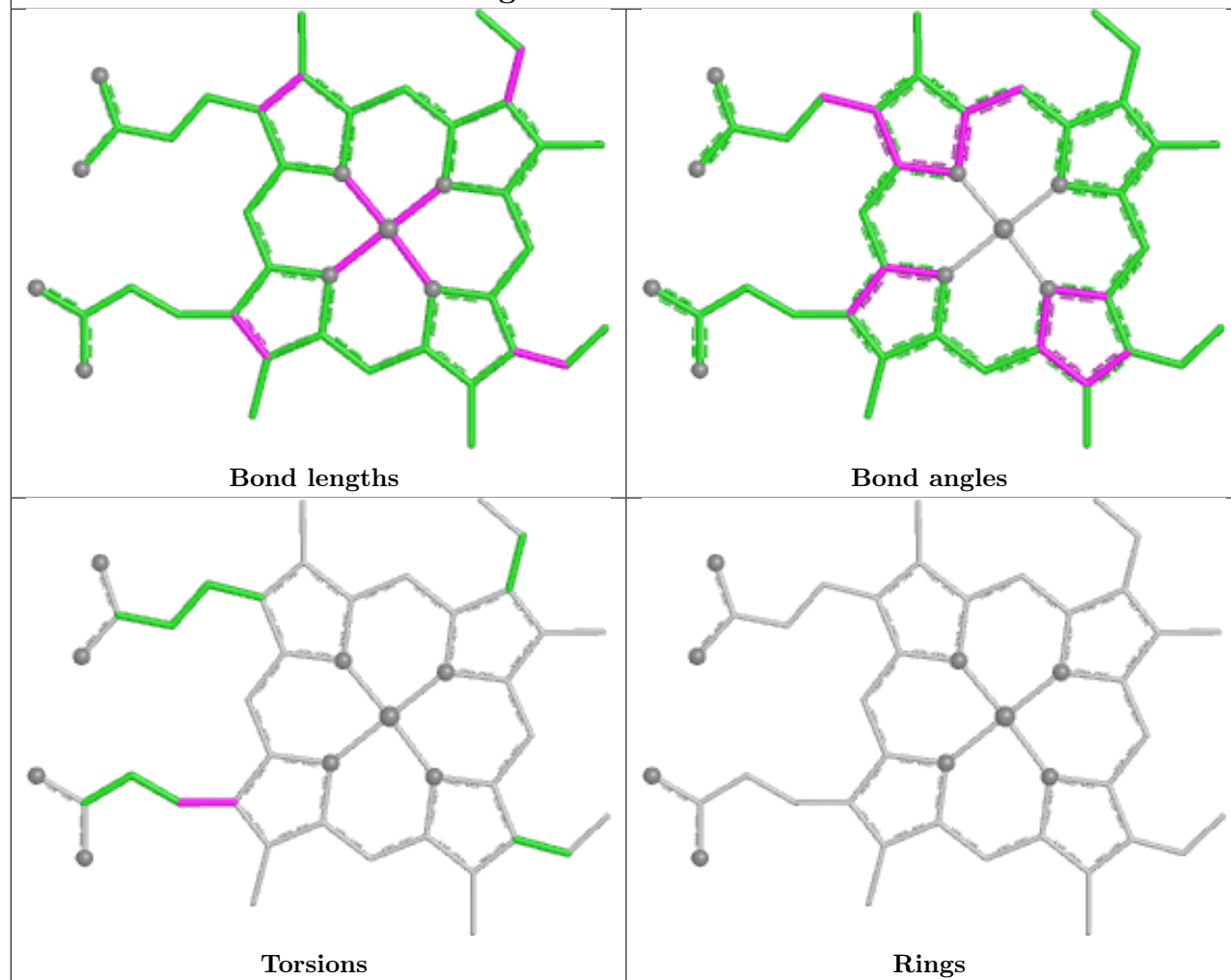


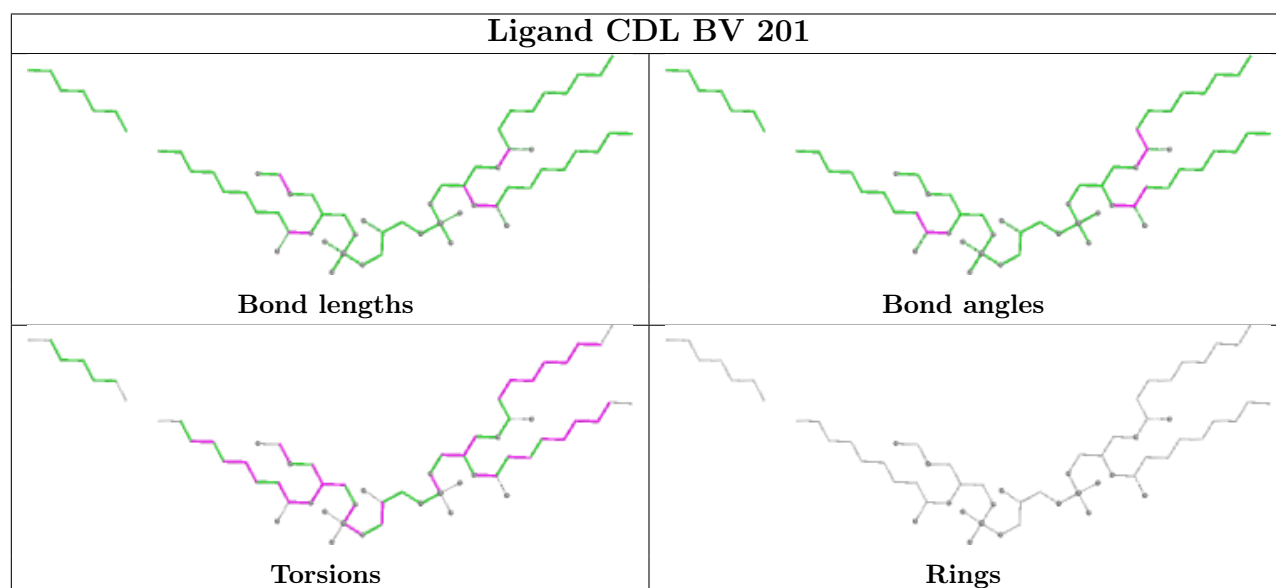
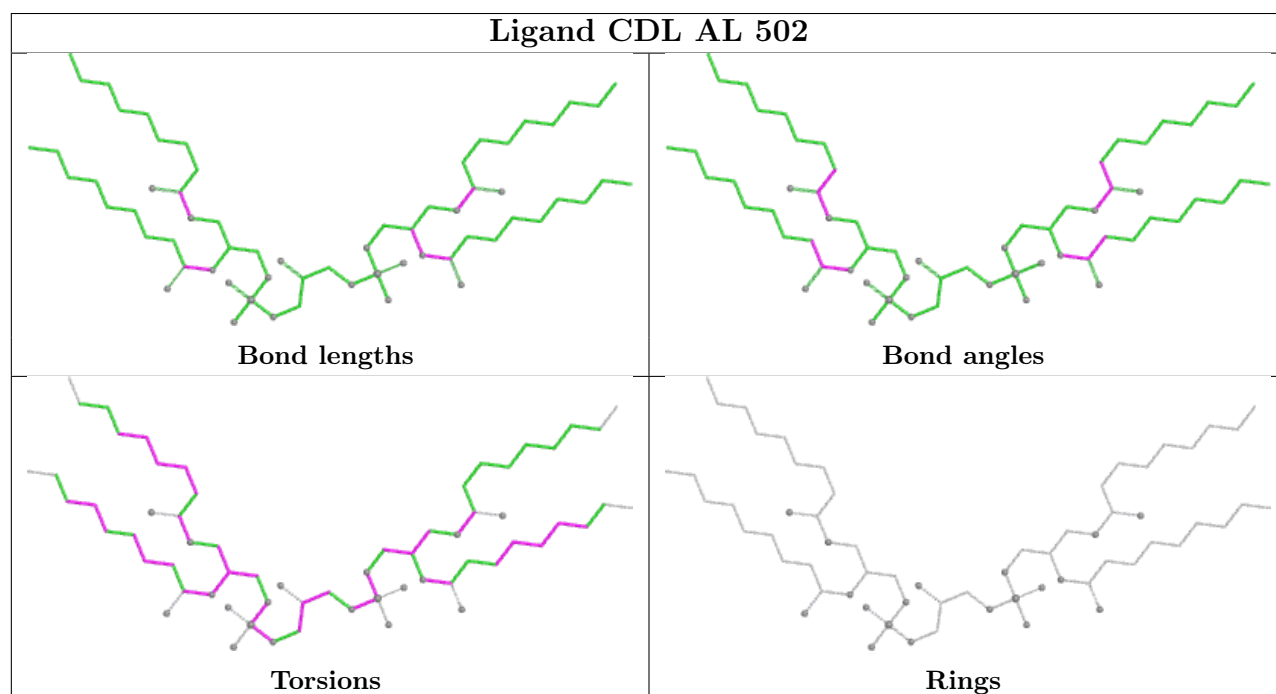
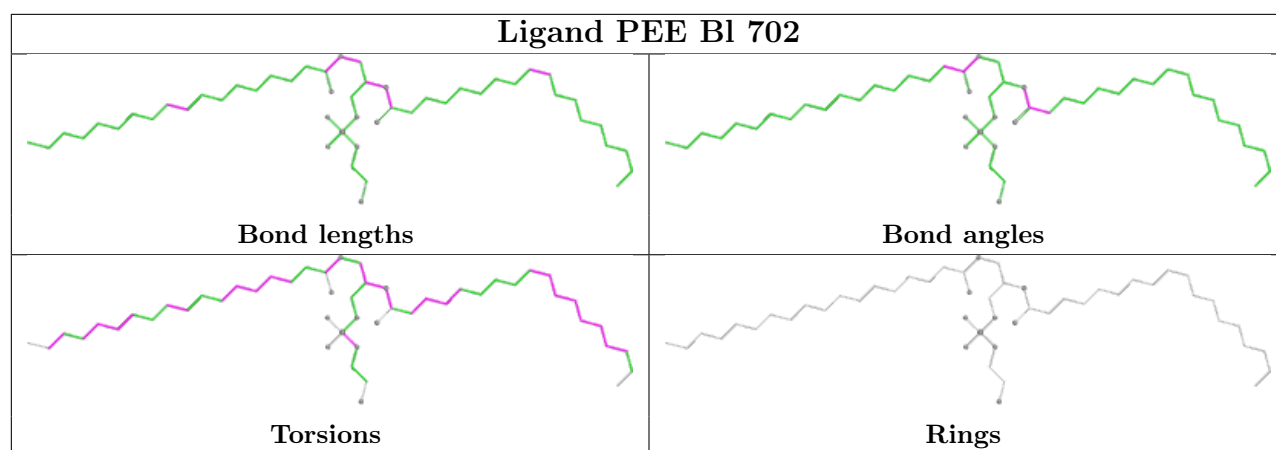




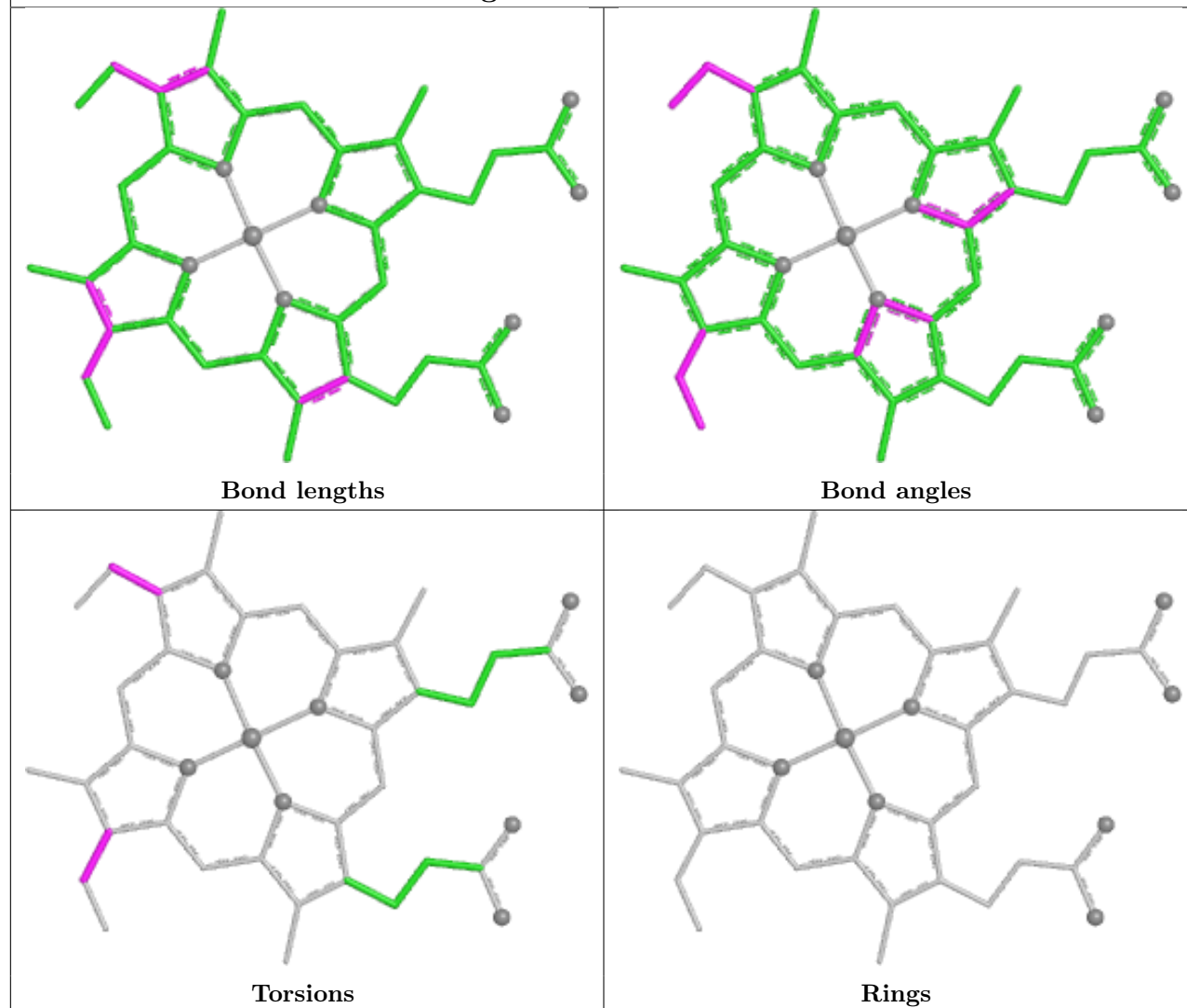




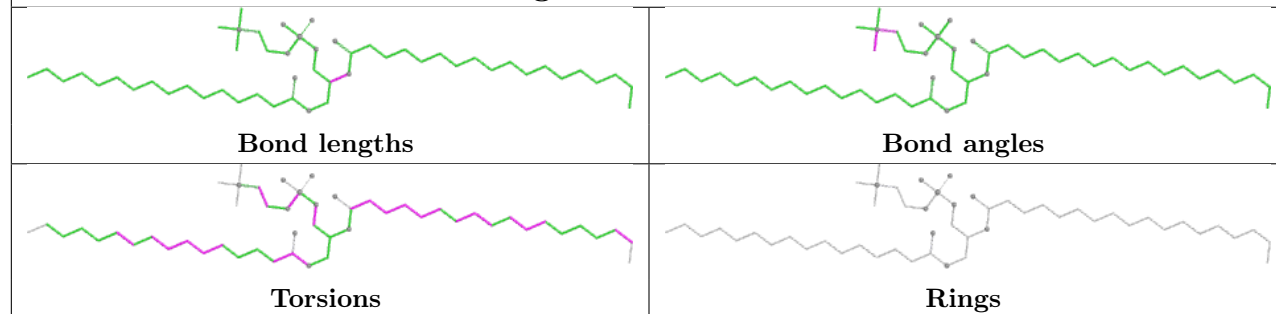
Ligand PLX BB 303**Ligand HEM AJ 402**

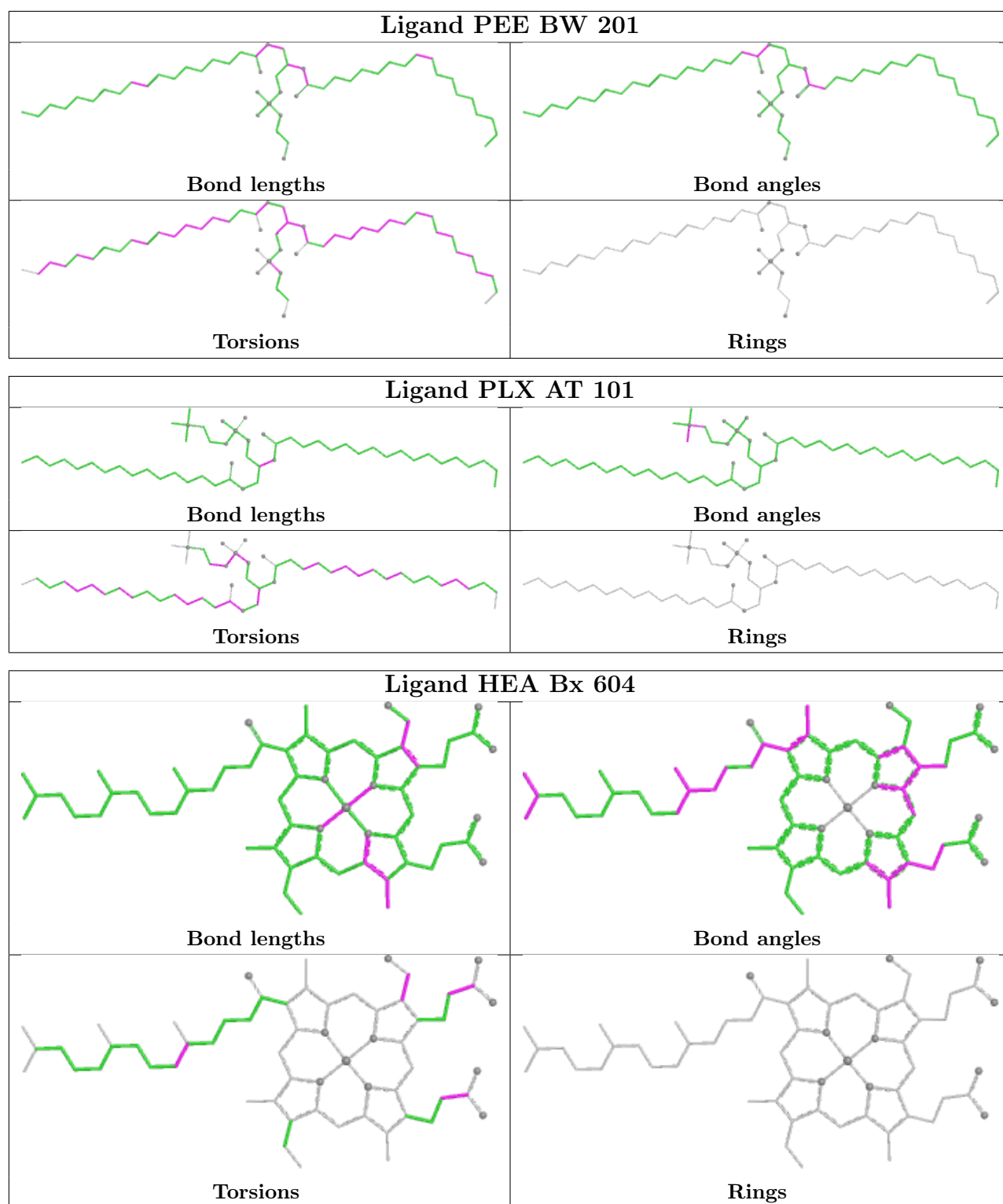


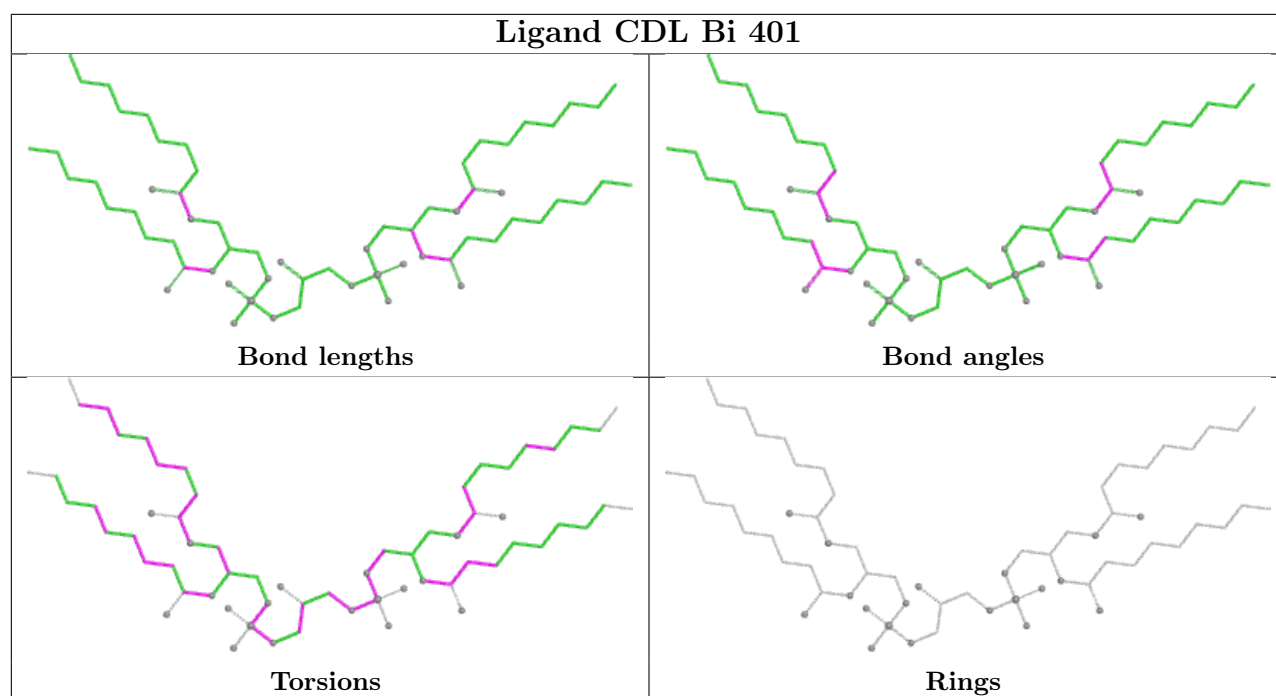
Ligand HEC AU 402



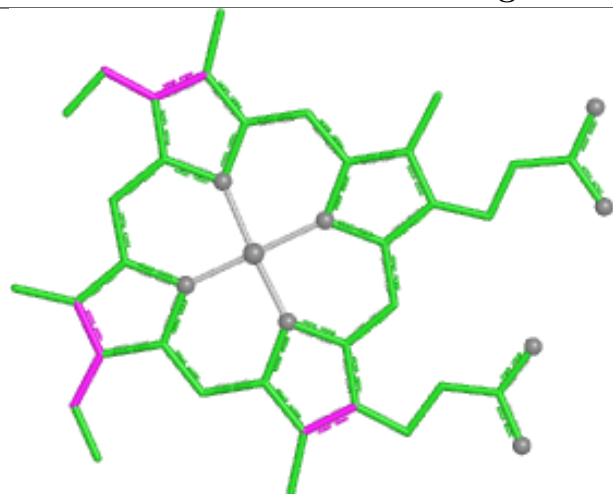
Ligand PLX B 303



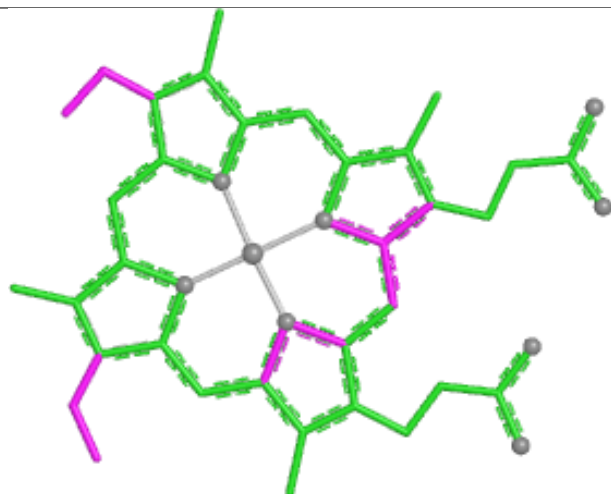




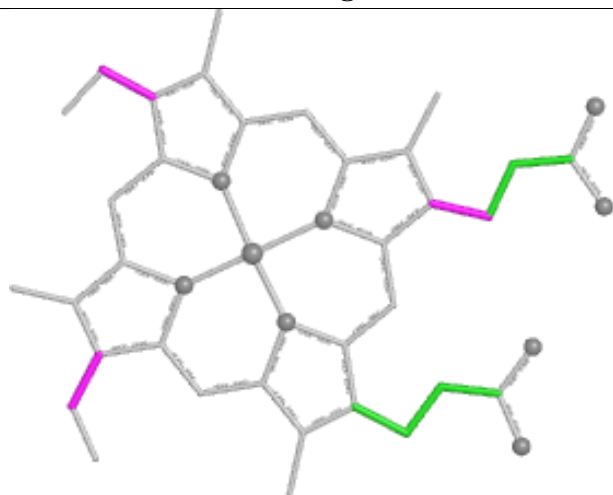
Ligand HEC AH 402



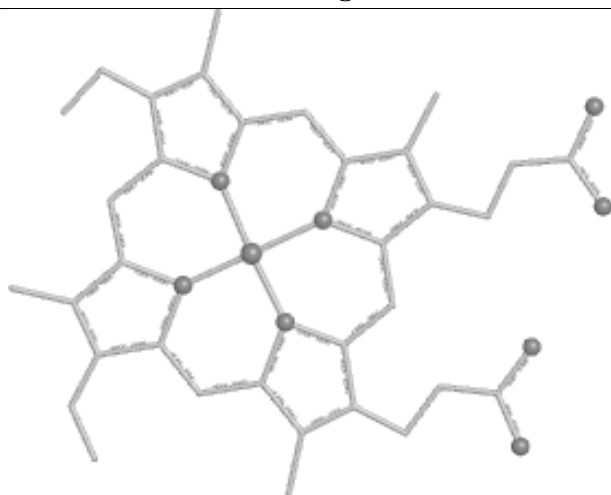
Bond lengths



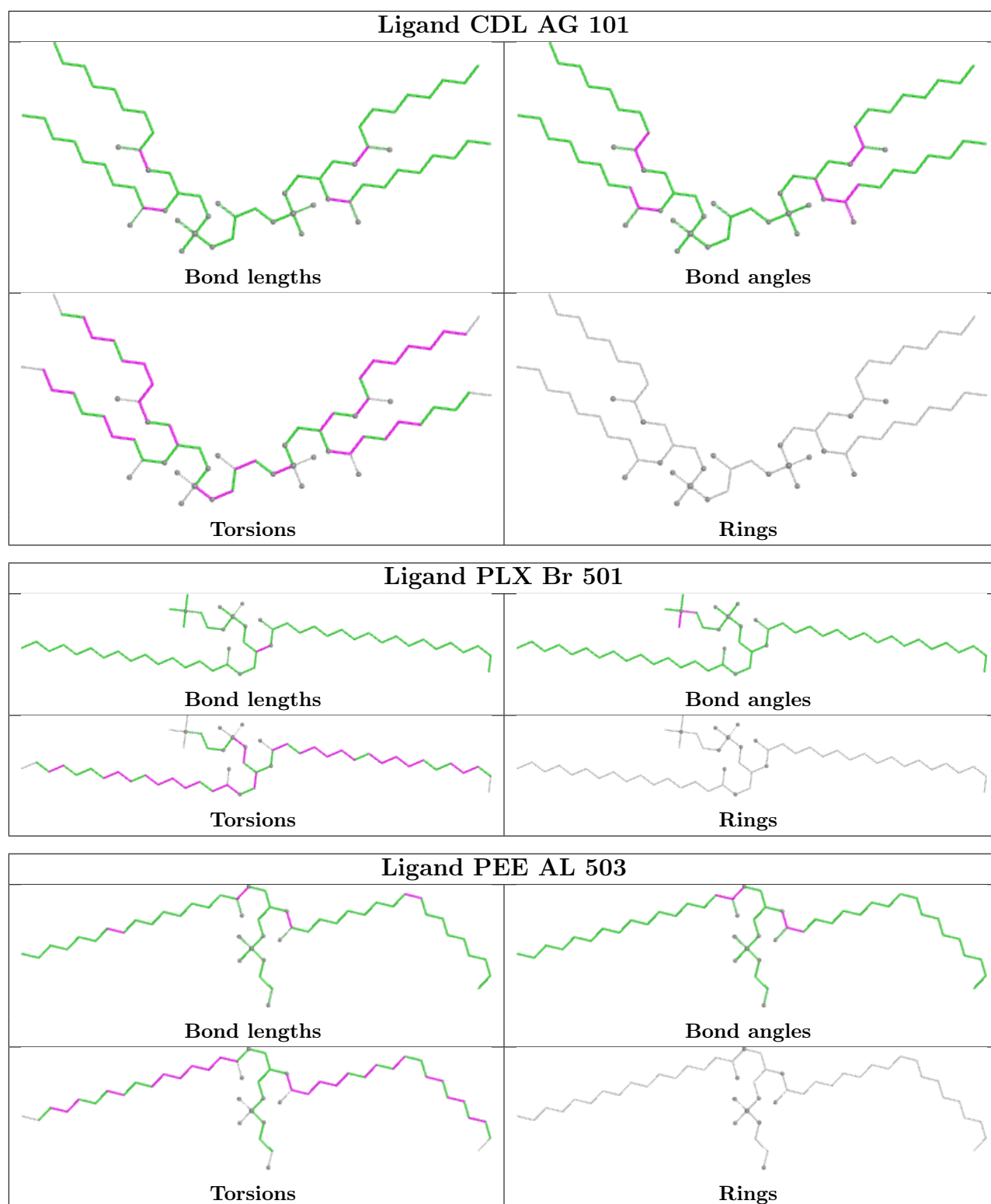
Bond angles

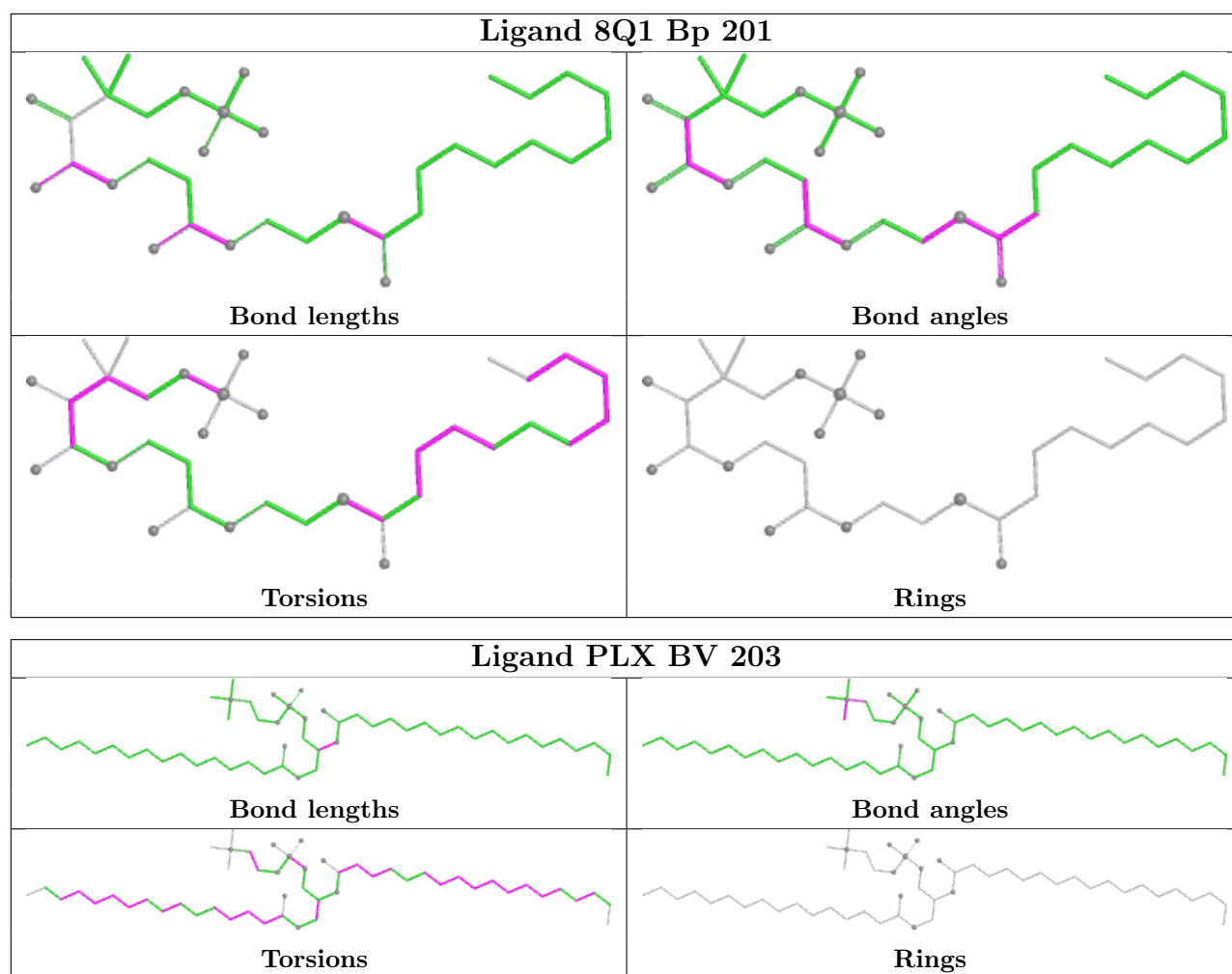


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

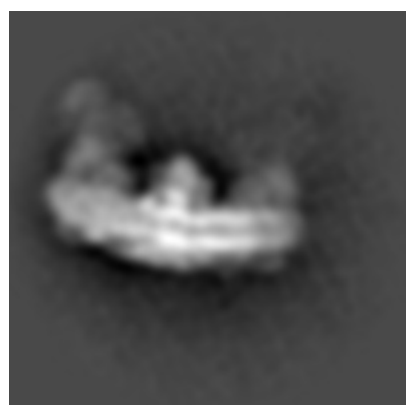
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6776. These allow visual inspection of the internal detail of the map and identification of artifacts.

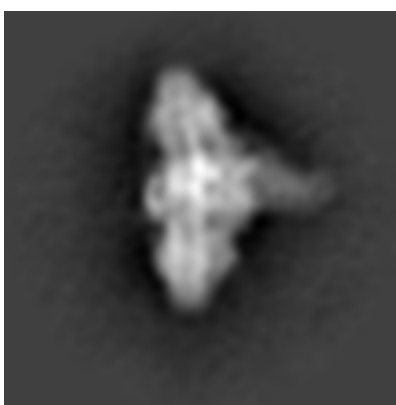
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

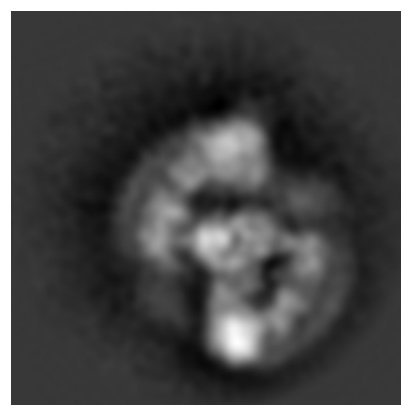
6.1.1 Primary map



X



Y



Z

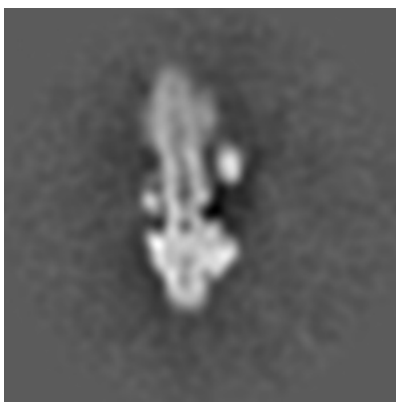
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

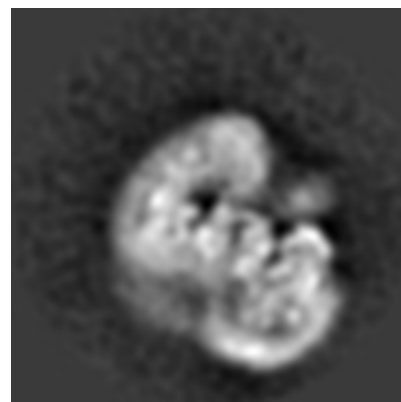
6.2.1 Primary map



X Index: 240



Y Index: 240

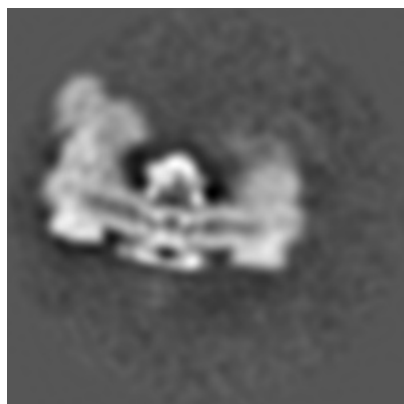


Z Index: 240

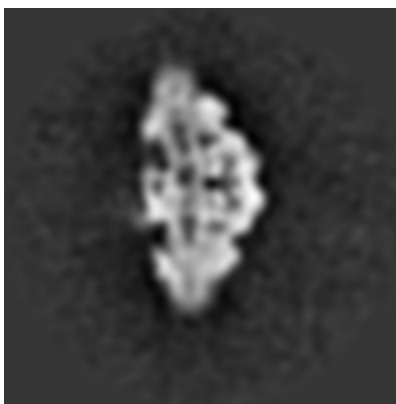
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

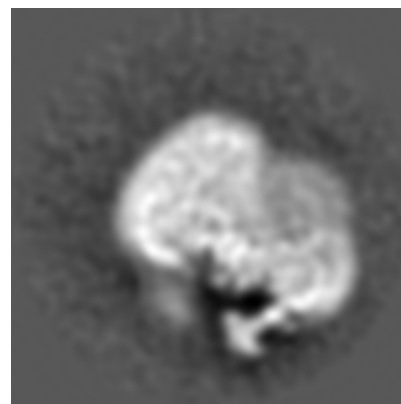
6.3.1 Primary map



X Index: 266



Y Index: 204

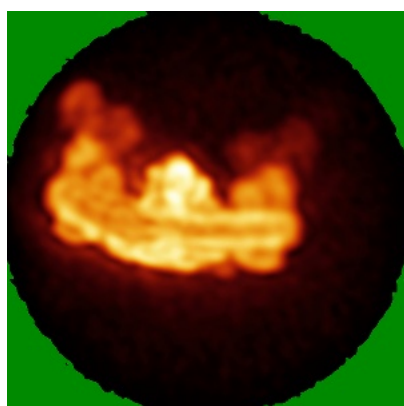


Z Index: 202

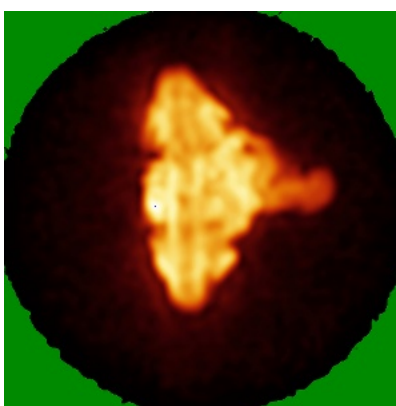
The images above show the largest variance slices of the map in three orthogonal directions.

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

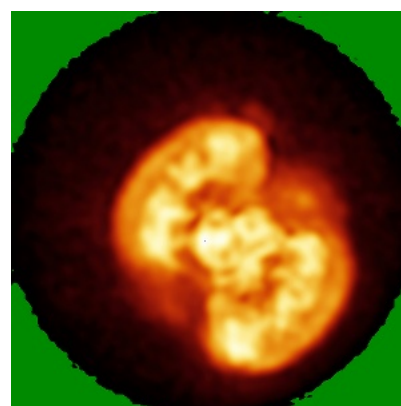
6.4.1 Primary map



X



Y

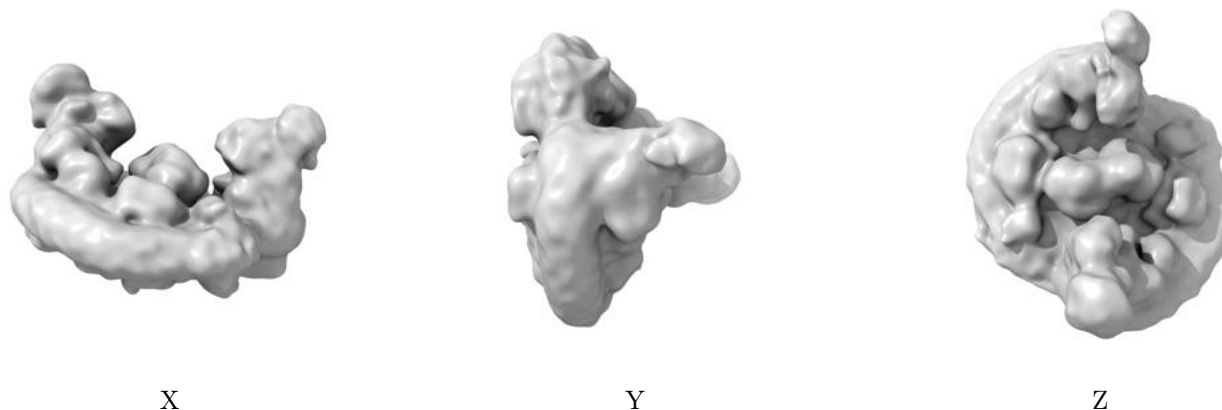


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

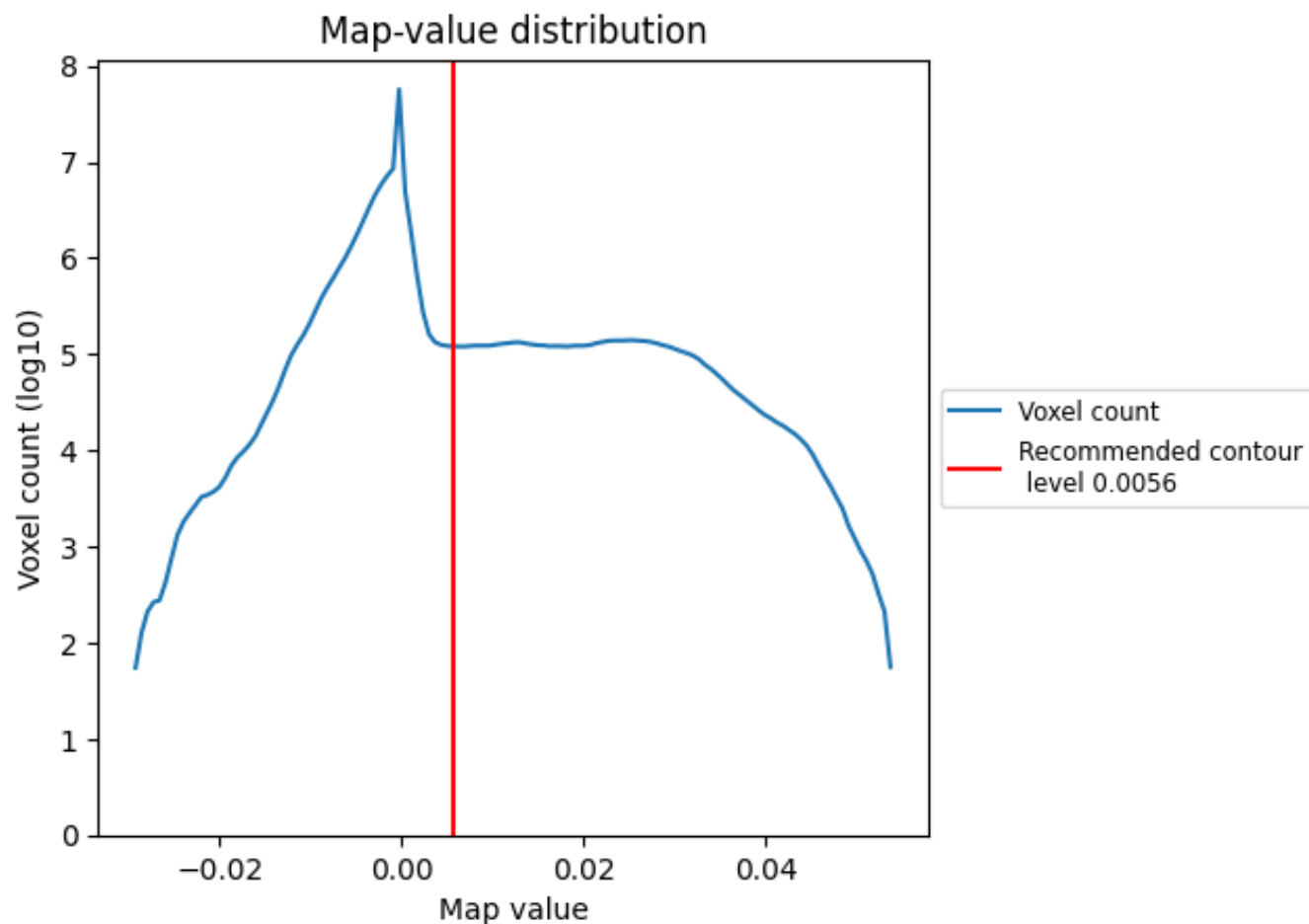
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

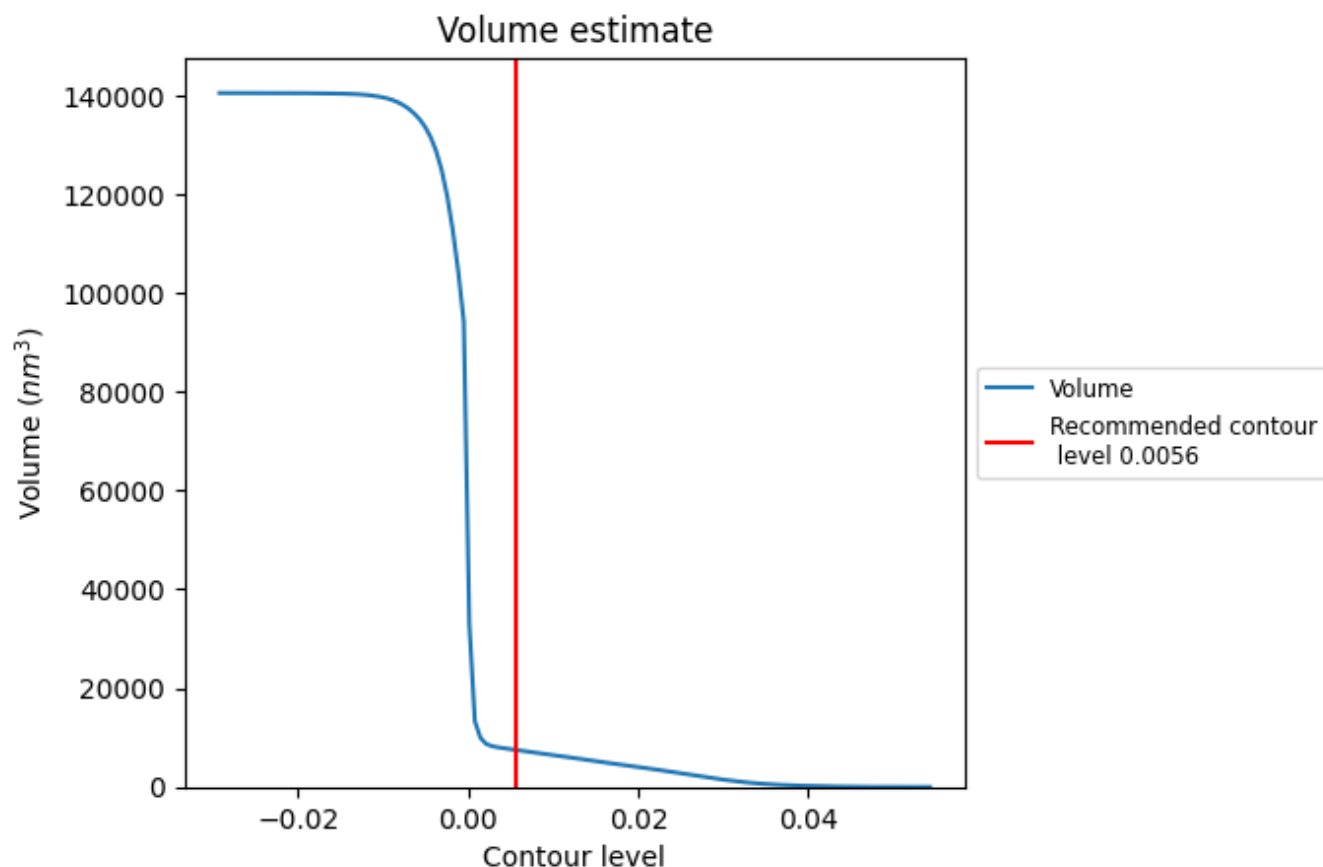
This section contains the results of statistical analysis of the map.

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.

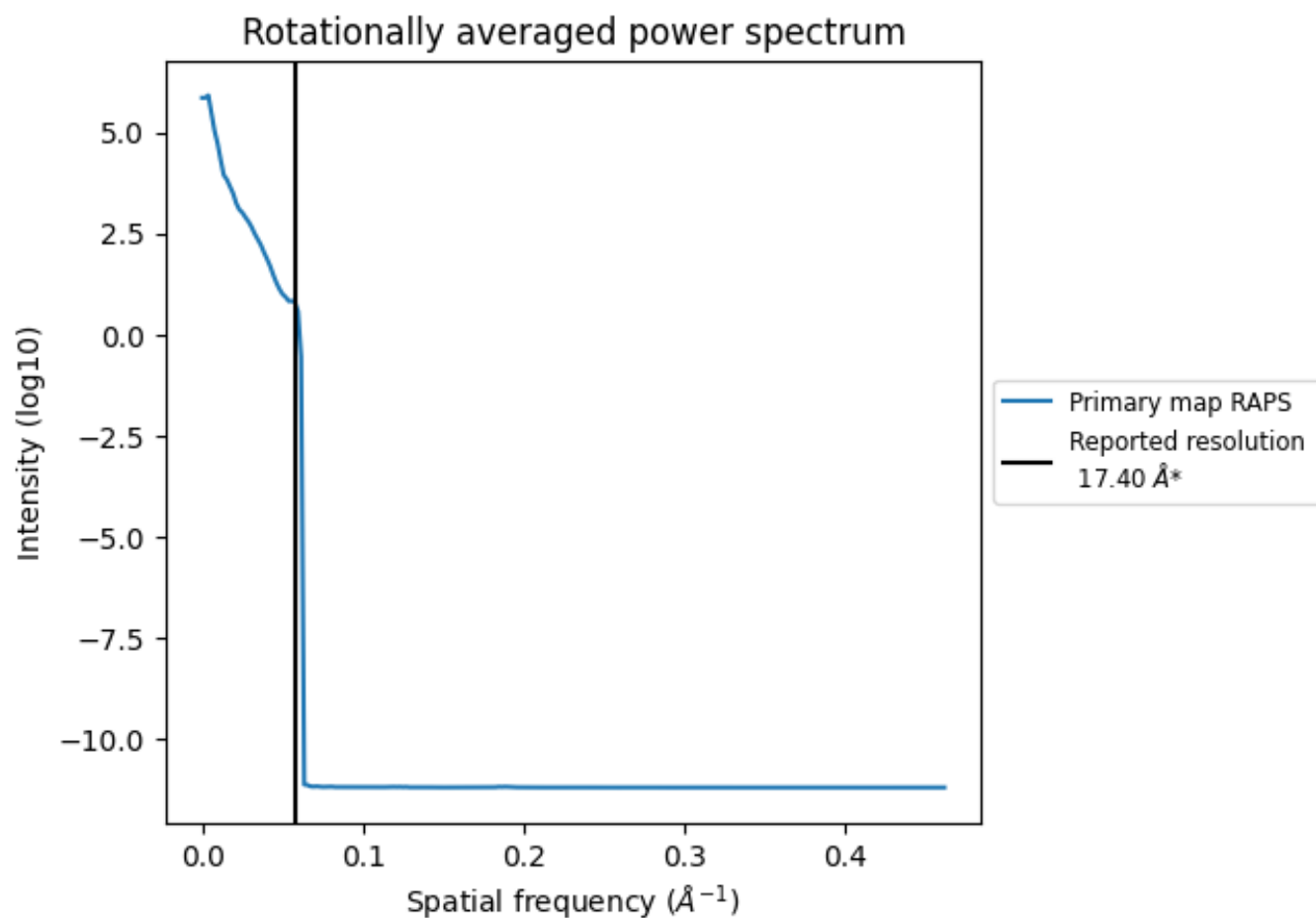
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7506 nm^3 ; this corresponds to an approximate mass of 6780 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 0.057 $\text{\AA}^{-1}$

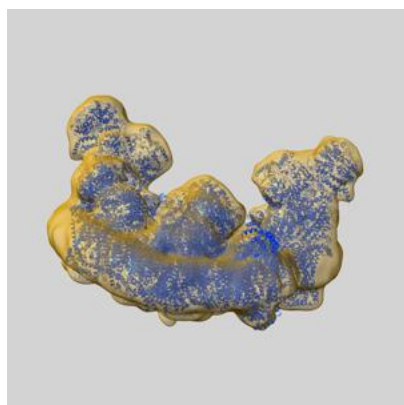
8 Fourier-Shell correlation ⓘ

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

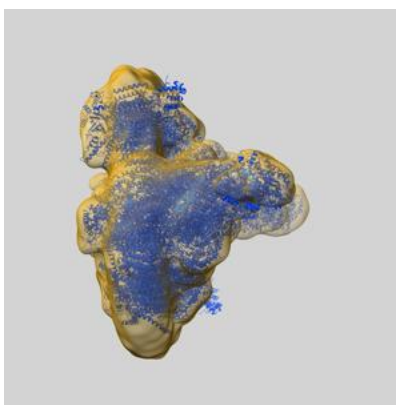
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6776 and PDB model 5XTI. Per-residue inclusion information can be found in section [3](#) on page [35](#).

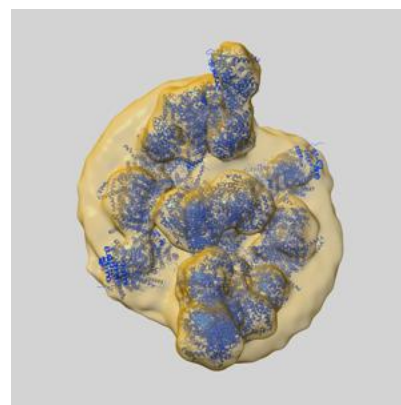
9.1 Map-model overlay [i](#)



X



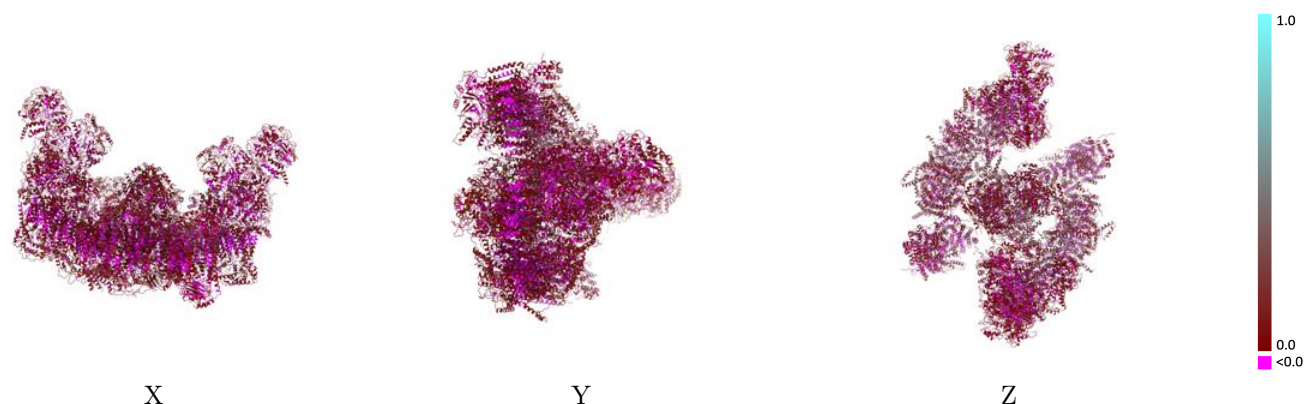
Y



Z

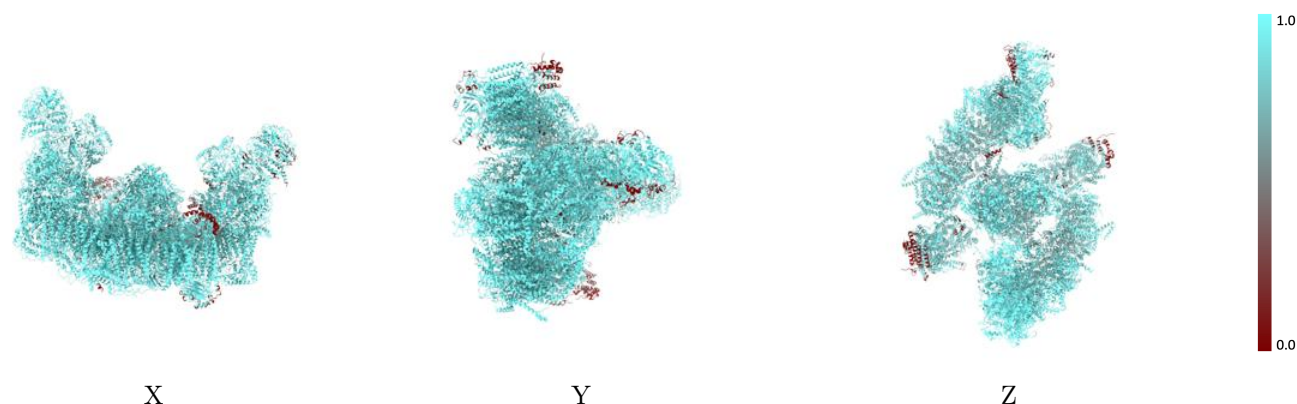
The images above show the 3D surface view of the map at the recommended contour level 0.0056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



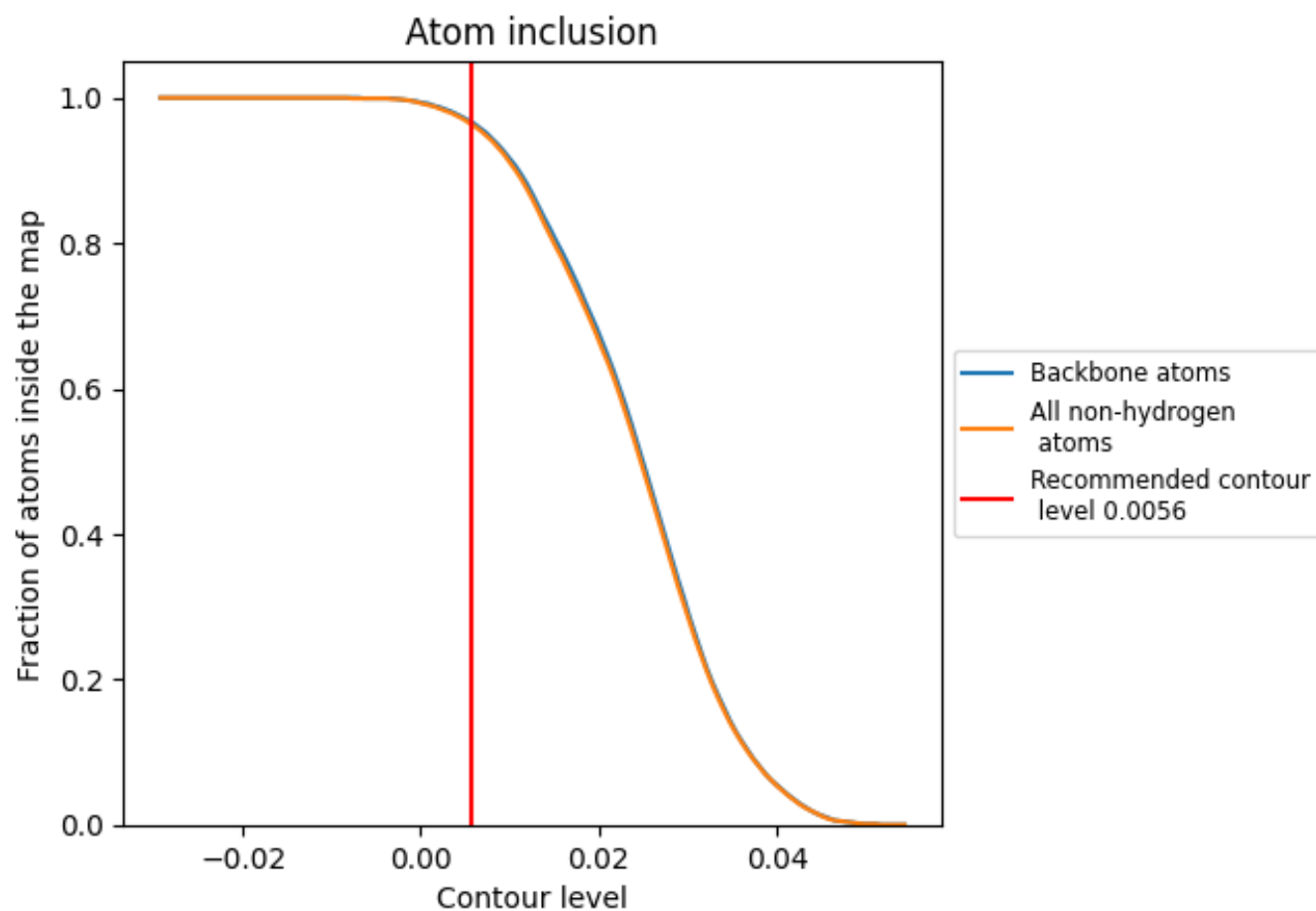
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0056).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.0490
0	 0.4390	 0.0310
1	 0.1490	 0.0480
2	 0.8350	 0.0570
3	 0.8150	 0.0140
4	 0.8660	 0.0570
5	 0.4740	 0.0160
6	 0.9610	 0.0080
7	 0.5870	 0.0110
8	 1.0000	 0.0130
9	 0.8980	 0.0270
A	 0.7550	 0.0440
AA	 0.9860	 0.0800
AB	 1.0000	 -0.0640
AC	 0.9950	 0.0580
AD	 0.9660	 0.1020
AE	 0.9980	 0.0910
AF	 0.9830	 0.0910
AG	 0.9940	 0.0930
AH	 0.9960	 0.0670
AJ	 0.9990	 0.0520
AK	 0.9990	 0.0770
AL	 0.9960	 0.0590
AN	 0.9950	 0.0710
AO	 1.0000	 -0.0730
AP	 0.9900	 0.0620
AQ	 0.9860	 0.0800
AR	 1.0000	 0.0990
AS	 0.9460	 0.0730
AT	 1.0000	 0.0850
AU	 0.9960	 0.0700
AV	 0.9980	 0.0540
AW	 0.9990	 0.0750
AY	 0.9980	 0.0610
B	 1.0000	 0.0610



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Chain	Atom inclusion	Q-score
B0	 0.7250	 0.0280
B1	 0.4010	 0.0380
B2	 0.9040	 0.0640
B3	 0.8590	 0.0230
B4	 0.8980	 0.0540
B5	 0.7100	 0.0380
B6	 0.8980	 0.0250
B7	 0.9280	 0.0540
B8	 0.9920	 0.0530
B9	 0.9370	 0.0260
BA	 0.9940	 0.0540
BB	 1.0000	 0.0520
BC	 1.0000	 0.0320
BE	 0.9470	 0.0410
BF	 0.9970	 0.0800
BG	 0.7100	 0.0790
BH	 0.9990	 0.0570
BI	 0.9930	 0.0470
BJ	 0.9800	 0.0510
BK	 1.0000	 0.0830
BL	 0.9860	 0.0100
BM	 0.9860	 0.0460
BN	 0.9850	 0.0570
BO	 0.9960	 0.0580
BP	 0.9890	 0.0530
BQ	 0.9890	 0.0240
BS	 1.0000	 0.0600
BT	 0.9780	 0.0630
BU	 0.9990	 0.0510
BV	 0.9990	 0.0900
BW	 0.9950	 0.0800
BX	 0.9880	 0.0580
BY	 1.0000	 0.1000
BZ	 1.0000	 0.0880
Ba	 0.9970	 0.0780
Bb	 1.0000	 0.0850
Bc	 0.9750	 0.0800
Bd	 0.9720	 0.1000
Be	 0.9850	 0.0430
Bf	 0.9980	 0.0650
Bg	 0.9950	 0.0640
Bh	 0.9980	 0.0780

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Chain	Atom inclusion	Q-score
Bi	 1.0000	 0.0420
Bj	 1.0000	 -0.0070
Bk	 1.0000	 0.0160
Bl	 1.0000	 0.0250
Bm	 1.0000	 0.0300
Bn	 0.9910	 0.0680
Bo	 0.9890	 0.0680
Bp	 0.9900	 0.0740
Br	 0.9990	 0.0200
Bs	 1.0000	 0.0340
Bu	 0.9930	 0.0710
Bv	 0.9880	 0.1100
Bw	 0.9960	 0.0650
Bx	 1.0000	 0.0300
By	 0.9770	 0.0100
Bz	 1.0000	 0.0450
C	 1.0000	 0.0540
E	 0.9510	 0.0410
F	 0.9710	 0.0720
G	 0.4850	 0.0550
H	 0.9990	 0.0500
I	 0.9870	 0.0350
J	 0.9730	 0.0400
K	 0.9780	 0.0470
L	 0.9840	 -0.0060
M	 0.9240	 0.0390
N	 0.9740	 0.0270
O	 0.8670	 0.0510
P	 0.9880	 0.0530
Q	 0.9920	 0.0310
S	 1.0000	 0.0550
T	 0.9060	 0.0120
U	 1.0000	 0.0630
V	 0.9990	 0.0830
W	 0.9990	 0.0710
X	 1.0000	 0.0630
Y	 1.0000	 0.0930
Z	 1.0000	 0.0890
a	 0.9970	 0.0830
b	 1.0000	 0.0860
c	 0.9760	 0.0760
d	 0.9880	 0.1000

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Chain	Atom inclusion	Q-score
e	 1.0000	 0.0470
f	 1.0000	 0.0610
g	 0.9970	 0.0540
h	 1.0000	 0.0700
i	 1.0000	 0.0490
j	 1.0000	 -0.0020
k	 1.0000	 0.0210
l	 1.0000	 0.0240
m	 1.0000	 0.0370
n	 0.9870	 0.0570
o	 0.9870	 0.0480
p	 0.9950	 0.0570
r	 0.9990	 0.0240
s	 1.0000	 0.0240
u	 0.9970	 0.0630
v	 0.9850	 0.1040
w	 0.9990	 0.0660
x	 0.9990	 0.0280
y	 0.8650	 0.0330
z	 1.0000	 0.0310