



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 27, 2017 – 06:44 PM EST

PDB ID : 5XTH  
EMDB ID: : EMD-6775  
Title : Cryo-EM structure of human respiratory supercomplex I1III2IV1  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : unknown  
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

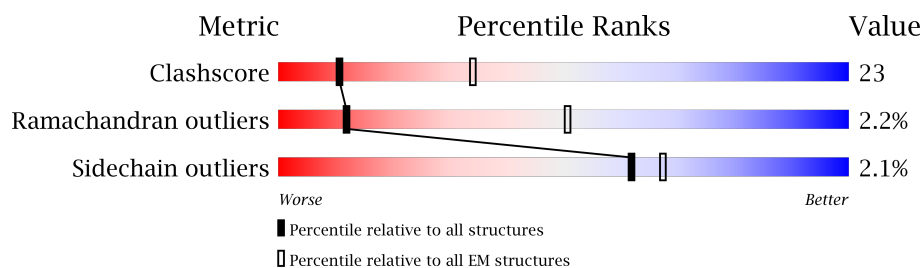
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.






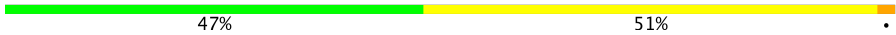

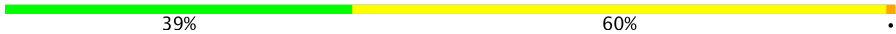







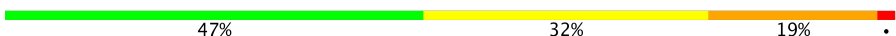

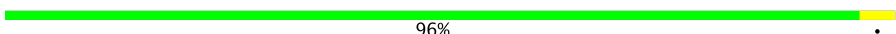

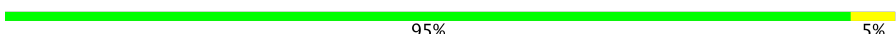
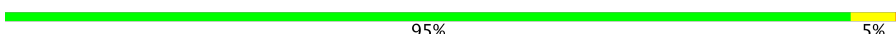
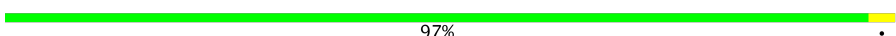
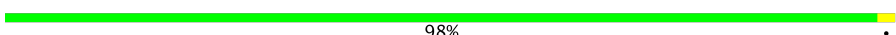
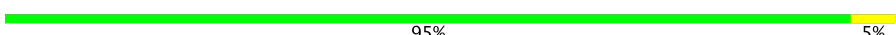
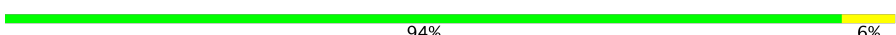
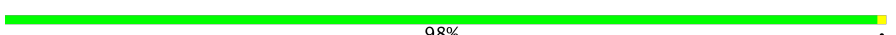

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	431	48% 51% .
2	B	176	49% 51% .
3	C	156	56% 42% .
4	E	113	49% 49% .
5	F	83	51% 49%
6	G	85	47% 51% .
6	X	85	58% 40% .
7	H	112	53% 46% .
8	I	110	46% 36% . 14%




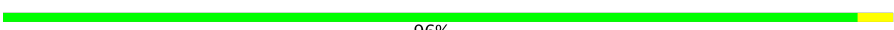
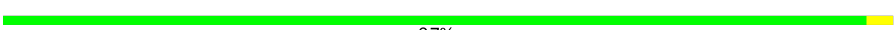





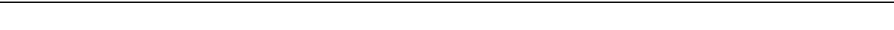

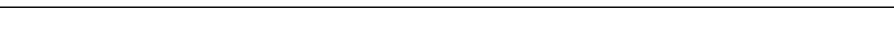
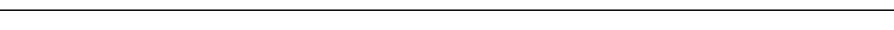











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Mol	Chain	Length	Quality of chain
9	J	337	 47%51%
10	K	33	 45%45%9%
11	L	118	 44%55%
12	M	687	 47%51%
13	N	143	 59%38%
14	O	212	 39%60%
15	P	208	 49%48%
16	Q	430	 48%50%
17	S	70	 71%27%
18	T	95	 54%43%
19	U	83	 84%16%
20	V	140	 66%34%
21	W	138	 76%21%
22	Y	59	 47%32%19%
23	Z	80	 79%21%
24	a	138	 96%
25	b	124	 90%10%
26	c	153	 95%5%
27	d	171	 95%5%
28	e	97	 97%
29	f	47	 98%
30	g	119	 95%5%
31	h	104	 94%6%
32	i	347	 98%
33	j	115	 97%






















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Mol	Chain	Length	Quality of chain
34	k	97	 93% 6% .
35	l	603	 94% 5% .
36	m	174	 94% 6% .
37	n	56	 96% .
38	o	128	 97% .
39	p	172	 98% .
40	r	459	 98% .
41	s	318	 97% .
42	u	169	 97% .
43	v	122	 86% 5% 9%
44	w	320	 97% .
45	x	514	 92% 8%
46	y	227	 90% 10%
47	z	261	 90% 10%
48	0	144	 74% 23% .
49	1	109	 81% 17% .
50	2	98	 66% 28% 6%
51	3	84	 61% 32% 6% .
52	4	75	 69% 24% 7%
53	5	73	 79% 18% .
54	6	56	 70% 21% 5% .
55	7	49	 76% 24%
56	8	47	 81% 19%
57	9	43	 74% 23% .
58	AA	81	 65% 27% 7%

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Mol	Chain	Length	Quality of chain
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	
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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	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	-
76	PEE	AY	502	-	-	X	-
79	HEA	x	603	X	-	-	-
79	HEA	x	604	X	-	-	-

## 2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 115642 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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
			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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		
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		

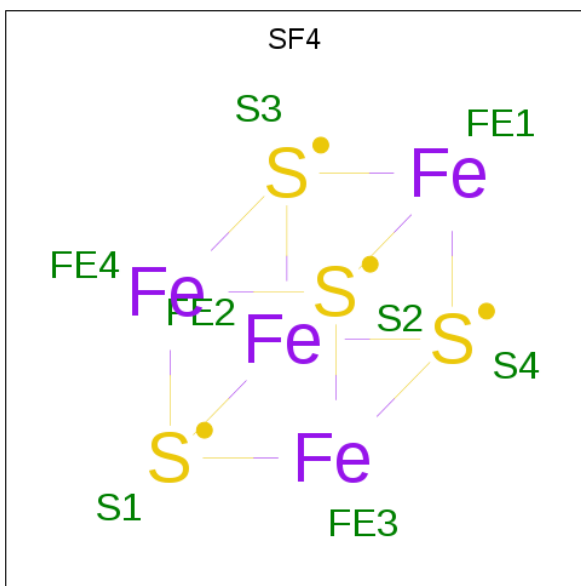
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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.

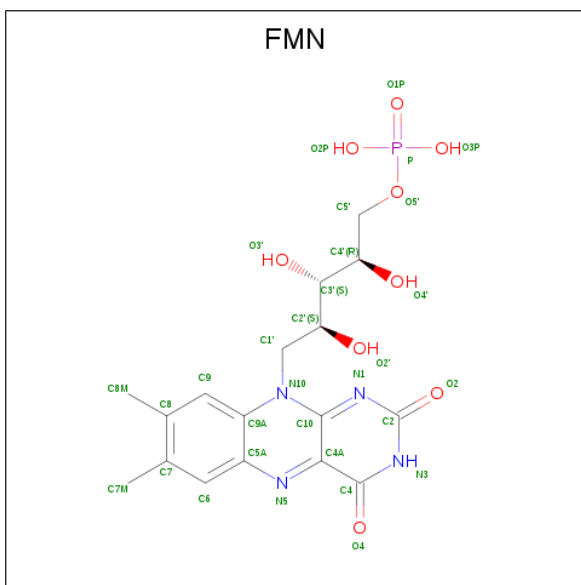
Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
68	AY	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 69 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



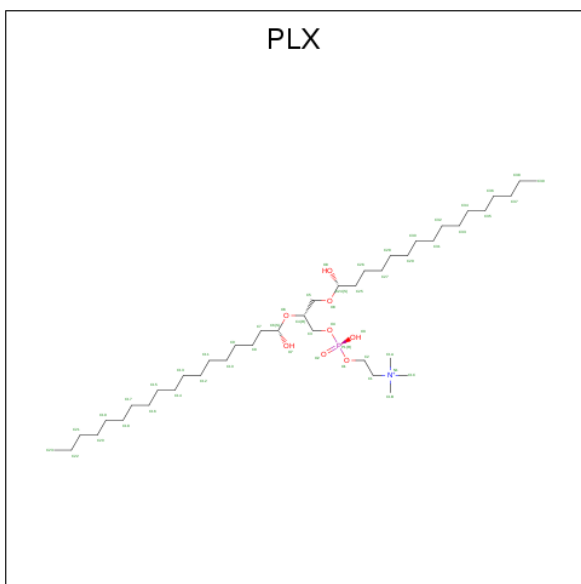
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			16	8	8	
69	B	1	Total	Fe	S	0
			16	8	8	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			16	8	8	
69	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



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

- 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 (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



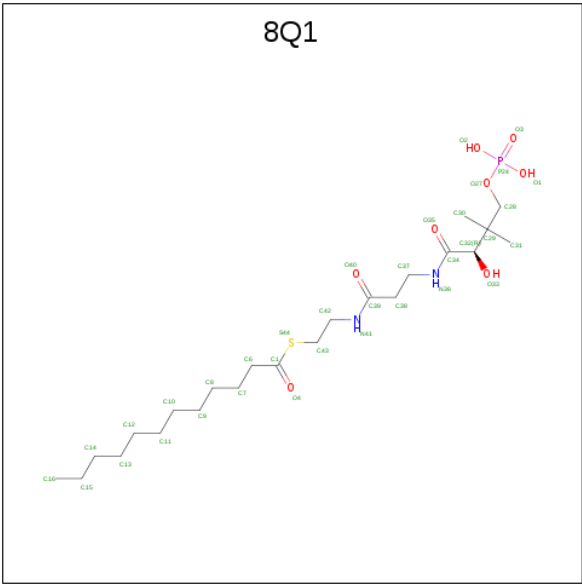
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total 52	C 42	N 1	O 8	P 1	0
71	U	1	Total 52	C 42	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
71	V	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
			156	126	3	24	3	
71	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
71	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
71	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
71	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
71	AL	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	

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS).



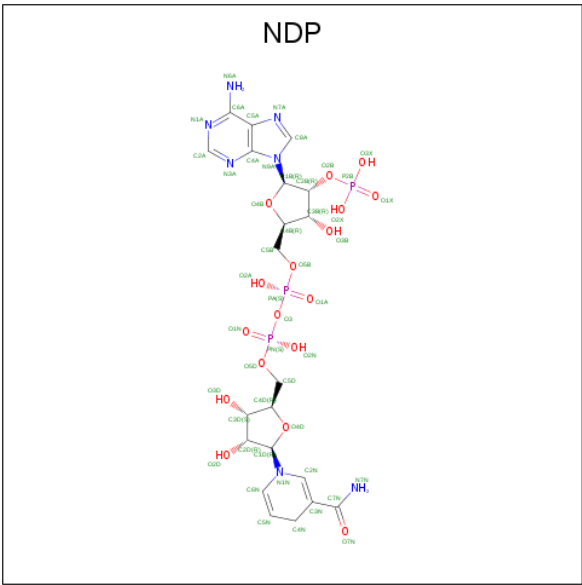
Mol	Chain	Residues	Atoms						AltConf
72	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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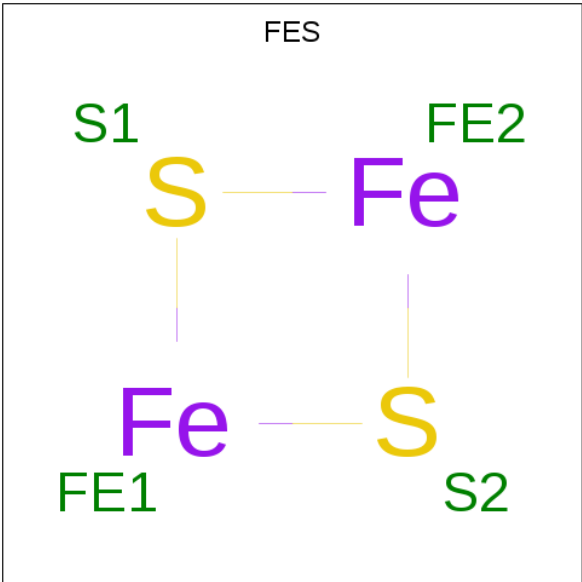
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
72	p	1	35	23	2	8	1	1	0

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



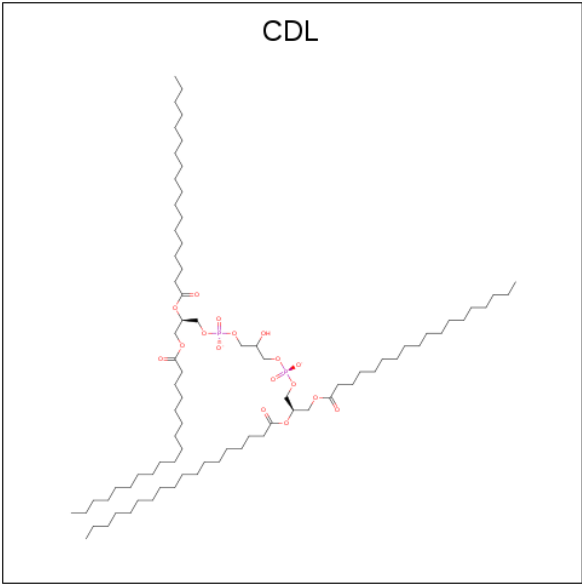
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	J	1	48	21	7	17	3	0

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



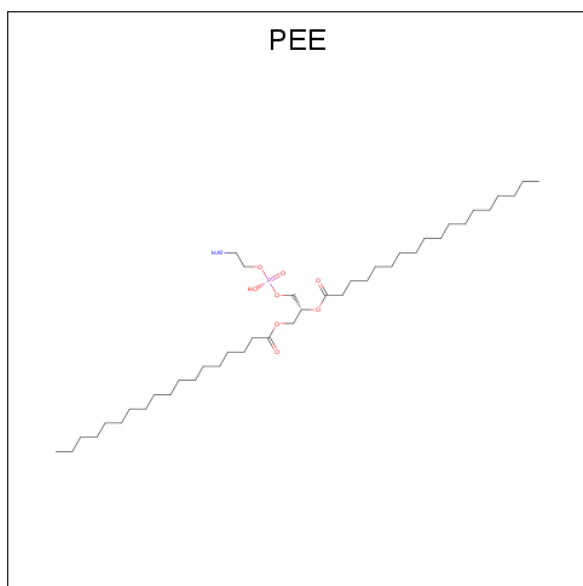
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			128	90	34	4	
75	l	1	Total	C	O	P	0
			128	90	34	4	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total	C	O	P	0
			64	45	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	AJ	1	Total	C	O	P	0
			128	90	34	4	
75	AJ	1	Total	C	O	P	0
			128	90	34	4	
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	

- Molecule 76 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



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
			100	80	2	16	2	
76	l	1	Total	C	N	O	P	0
			100	80	2	16	2	
76	AH	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	
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	

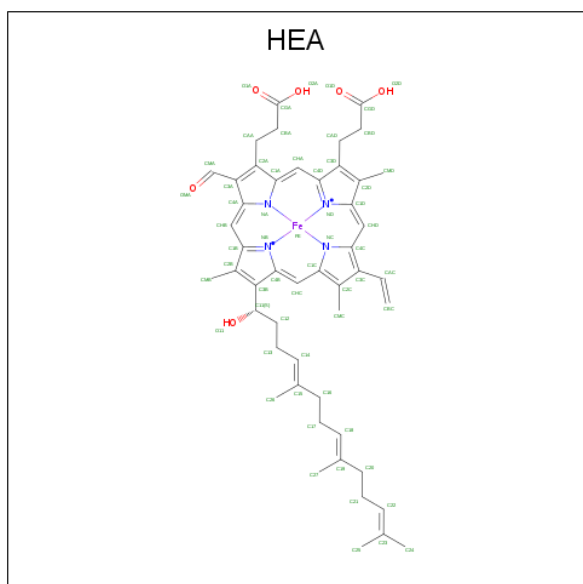
- Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



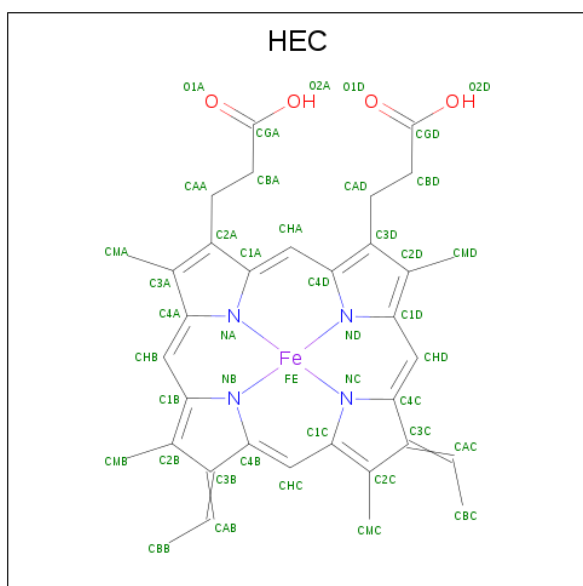


Mol	Chain	Residues	Atoms					AltConf
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

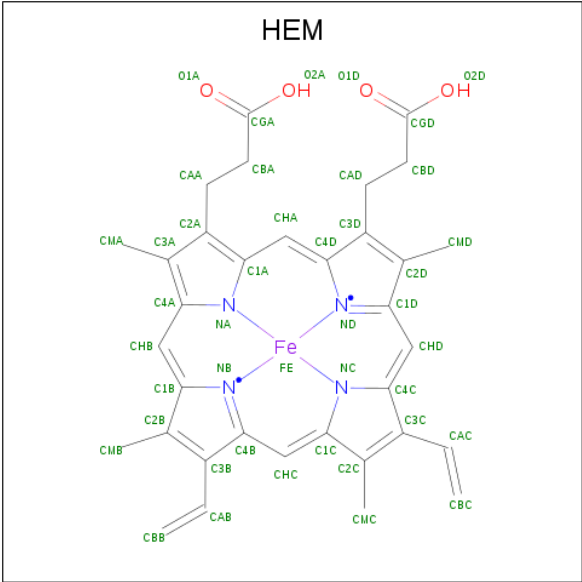
Mol	Chain	Residues	Atoms		AltConf
80	2	1	Total	Zn	0
			1	1	

- Molecule 81 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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 (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

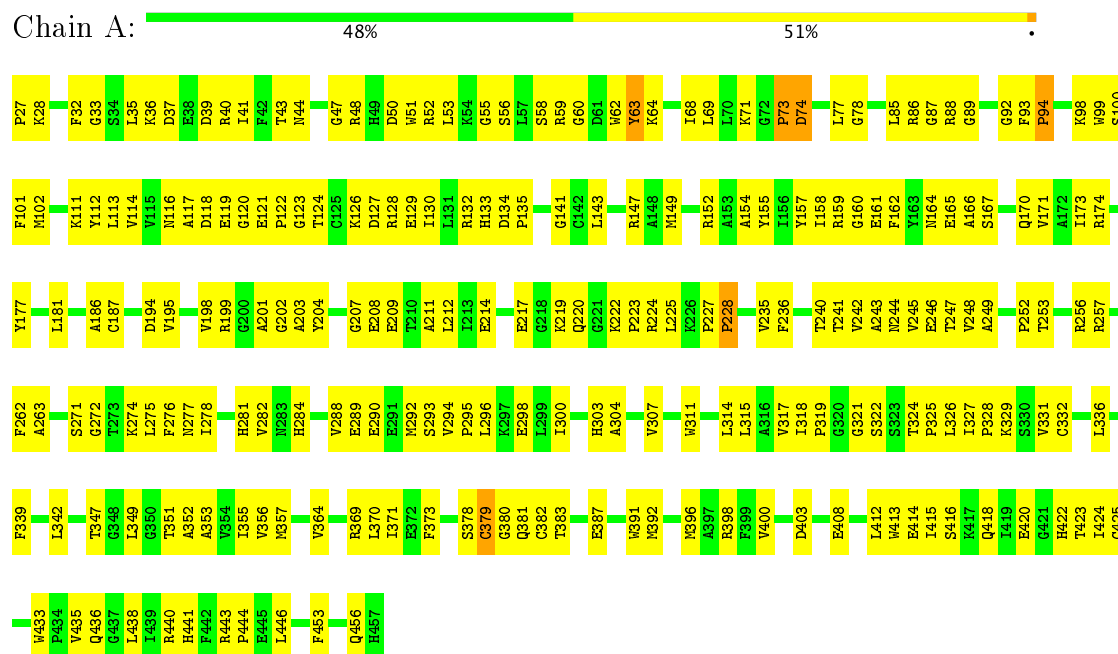


Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AJ	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AV	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
82	AV	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

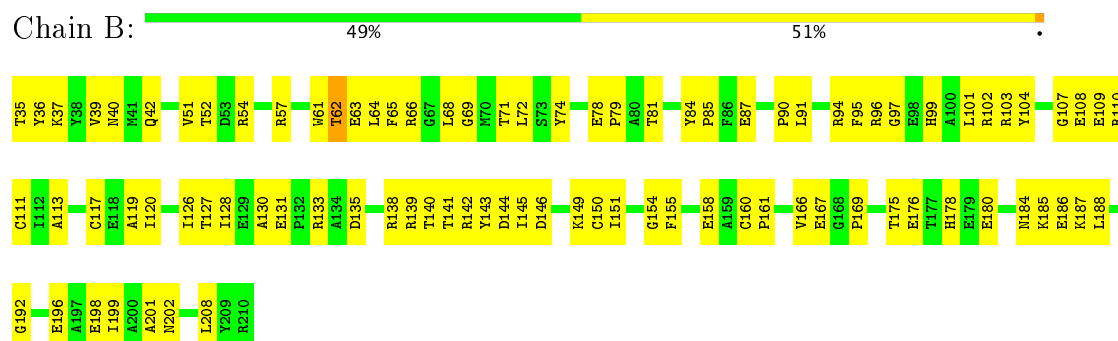
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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

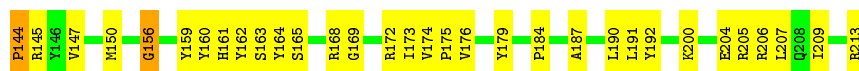


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

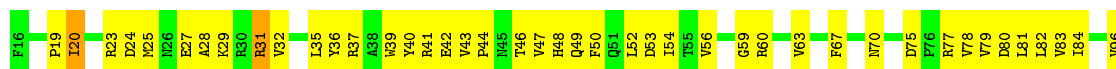


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

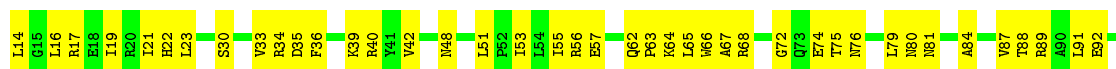




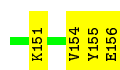
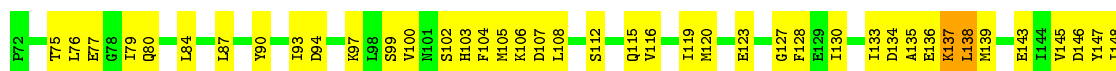
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



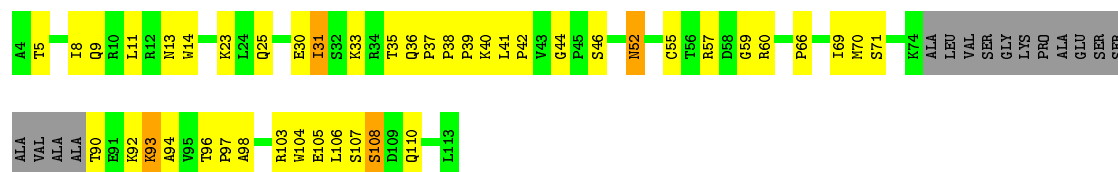
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5





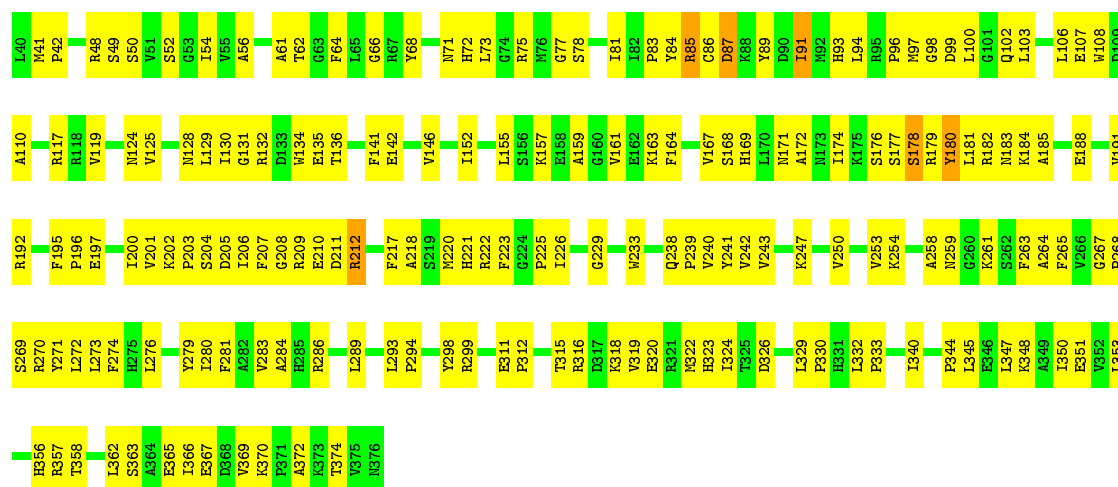
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 46% 36% 14%



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

Chain J: 47% 51%



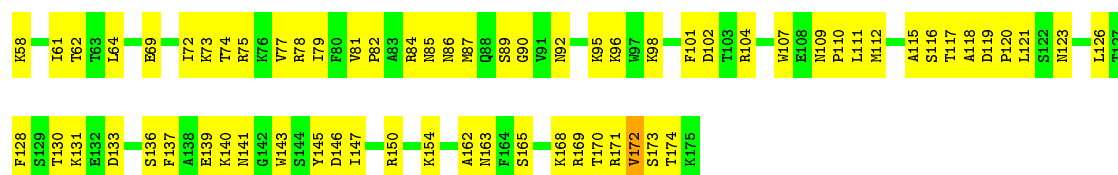
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 45% 45% 9%

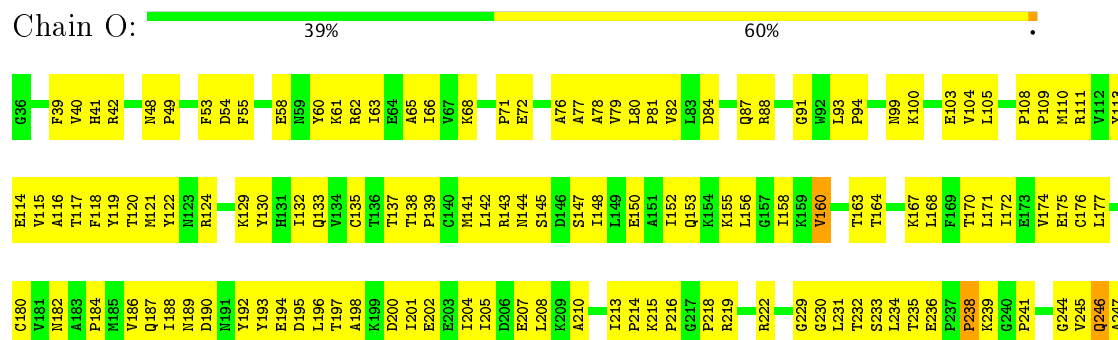
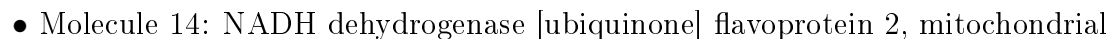
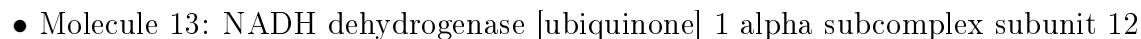


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

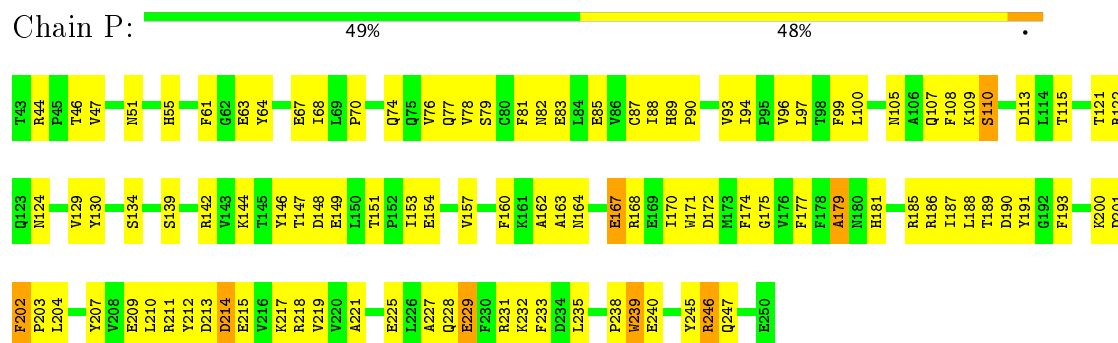
Chain L: 44% 55%



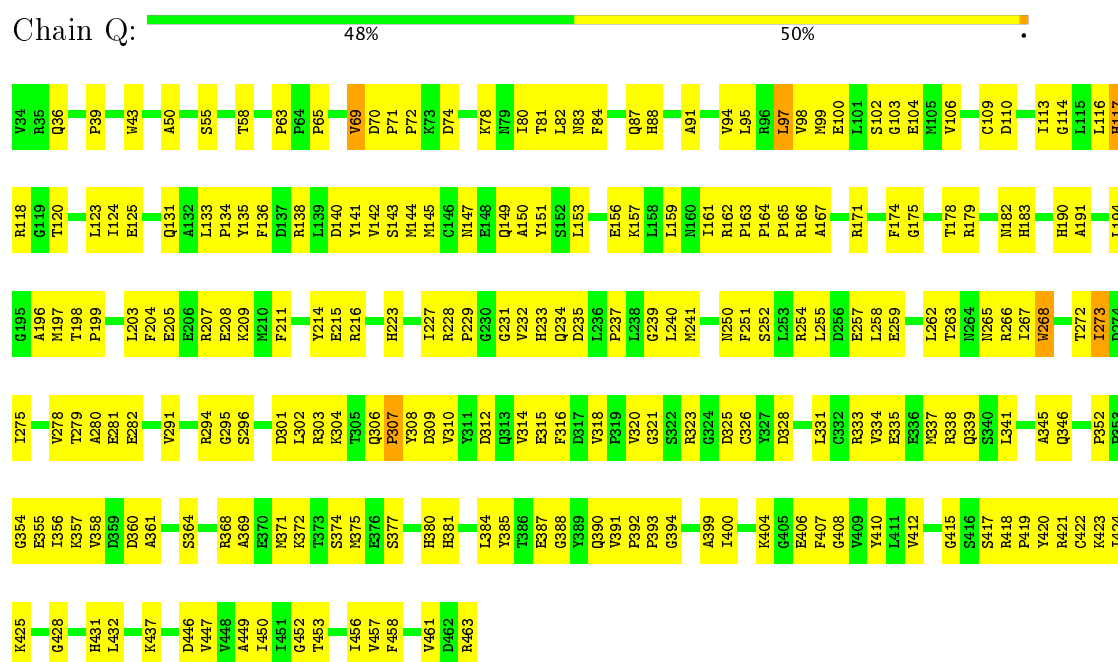
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



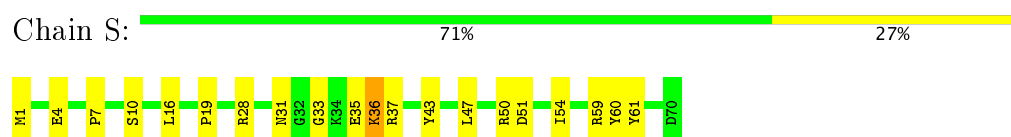
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



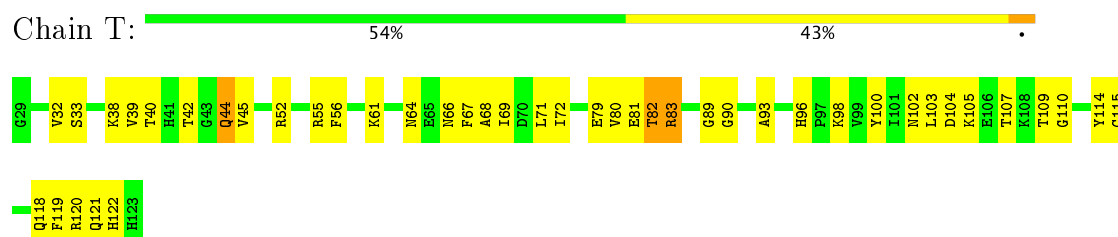
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial




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



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



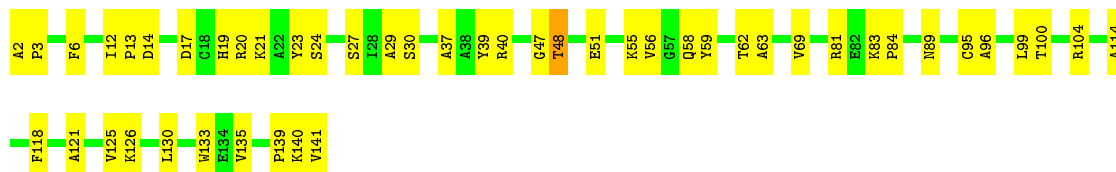
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  84% 16%




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

Chain V:  66% 34%



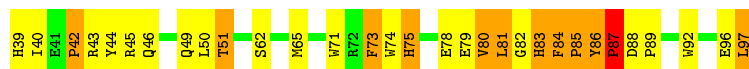
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  76% 21%




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

Chain Y:  47% 32% 19%



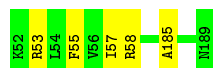
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  79% 21%




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

Chain a:  96%



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

Chain b:  90% 10%





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

Chain c: 95% 5%



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

Chain d: 95% 5%



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

Chain e: 97% .



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

Chain f: 98% .



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

Chain g: 95% 5%



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

Chain h: 94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 98% .



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 97%



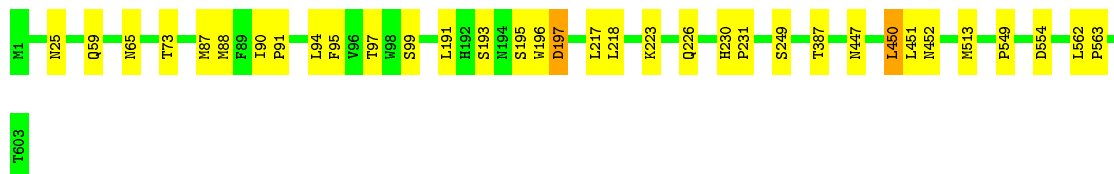
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 93%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 94%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m: 94%



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

Chain n: 96%



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

Chain o: 97%



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

Chain p: 98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



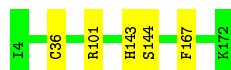
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97%



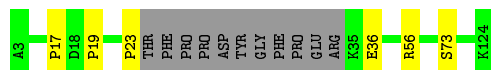
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97%



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

Chain v: 86% 5% 9%



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

Chain w: 97%




- Molecule 45: Cytochrome c oxidase subunit 1

Chain x: 92% 8%




- Molecule 46: Cytochrome c oxidase subunit 2

Chain y:  90% 10%



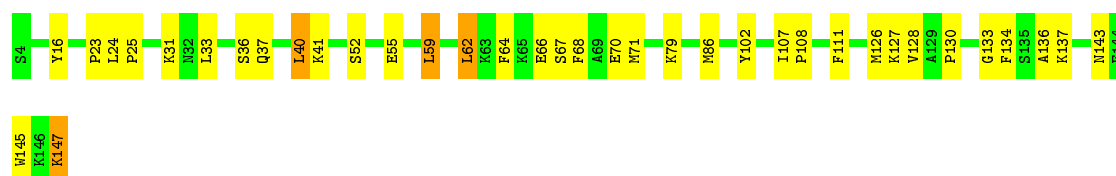
- Molecule 47: Cytochrome c oxidase subunit 3

Chain z:  90% 10%




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

Chain 0:  74% 23% .



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

Chain 1:  81% 17% .



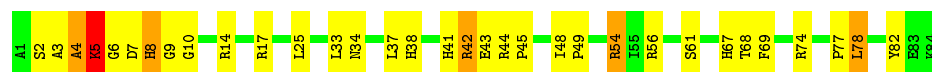
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 2:  66% 28% 6%



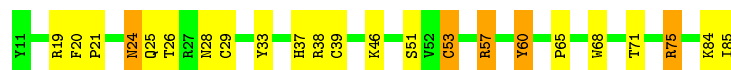
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 3:  61% 32% 6% .

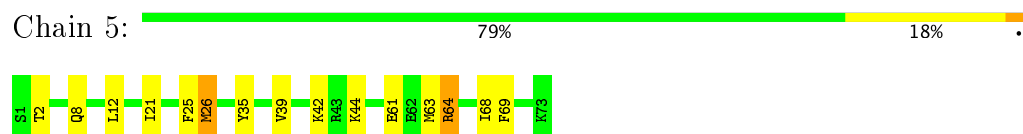


- Molecule 52: Cytochrome c oxidase subunit 6B1

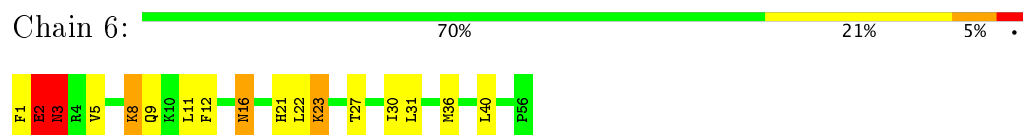
Chain 4:  69% 24% 7%



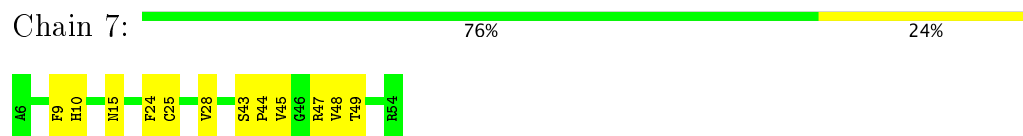
- Molecule 53: Cytochrome c oxidase subunit 6C



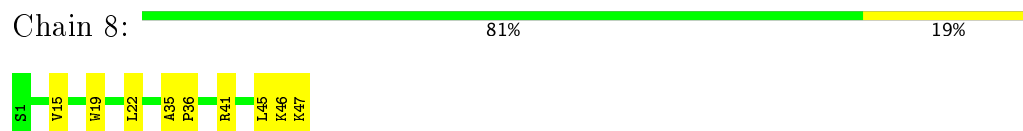
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



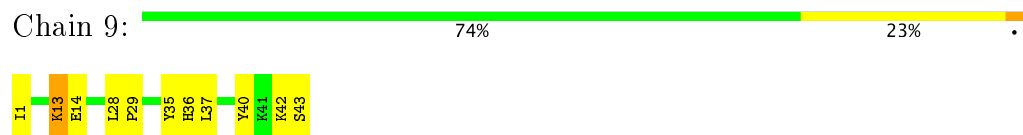
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



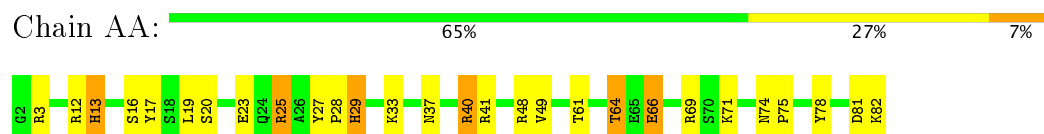
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



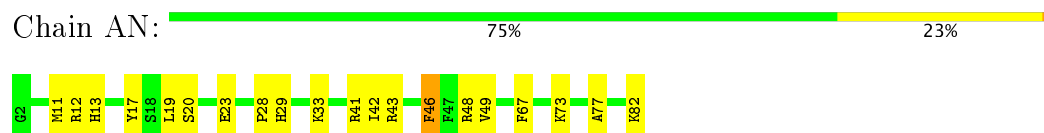
- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 58: Cytochrome b-c1 complex subunit 8

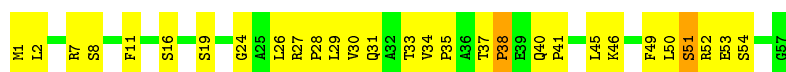


- Molecule 58: Cytochrome b-c1 complex subunit 8



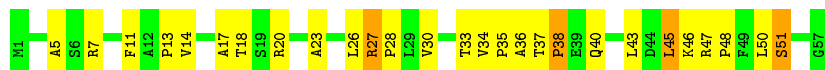
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial





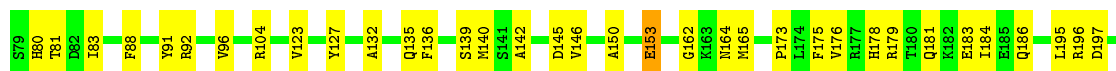
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AO: 53% 40% 7%



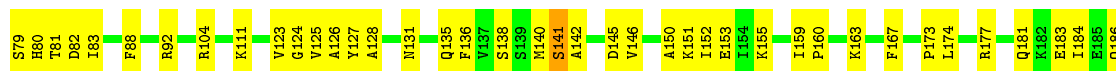
- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AC: 70% 28% 2%



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

Chain AP: 64% 35% 1%



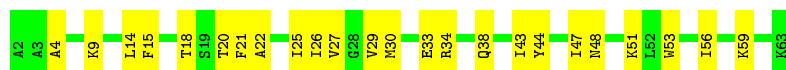
- Molecule 61: Cytochrome b-c1 complex subunit 9

Chain AD: 76% 24% 0%



- Molecule 61: Cytochrome b-c1 complex subunit 9

Chain AQ: 61% 39% 0%




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

Chain AE: 69% 28% 3%



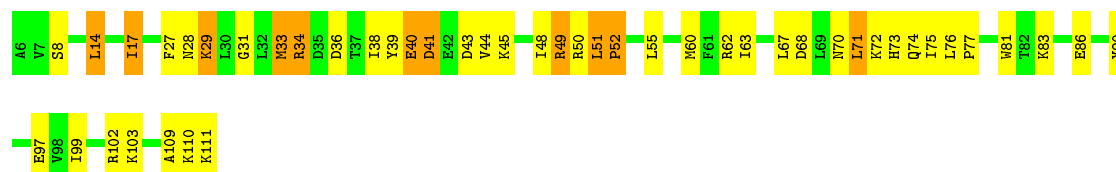
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AR:  74% 24% .



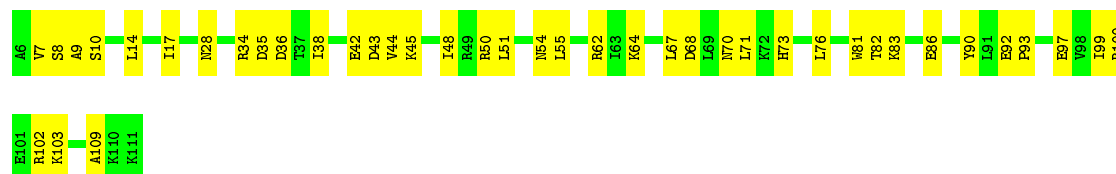
- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AF:  56% 34% 10%




- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AS:  61% 39%



- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AG:  73% 27%




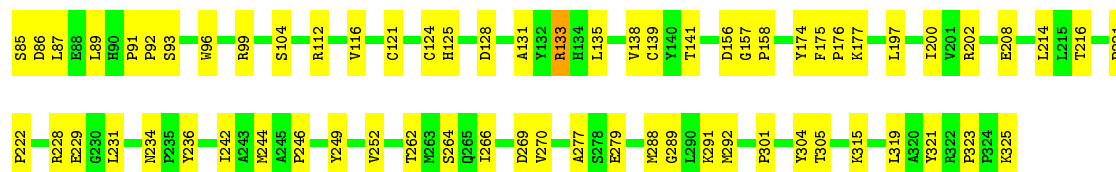
- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AT:  65% 31% .

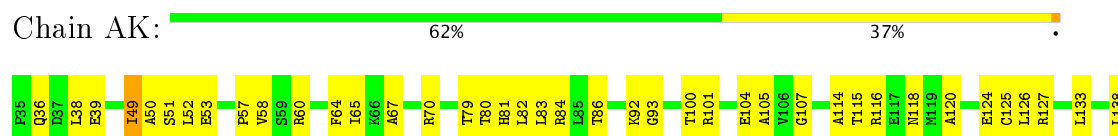


- Molecule 65: Cytochrome c1, heme protein, mitochondrial

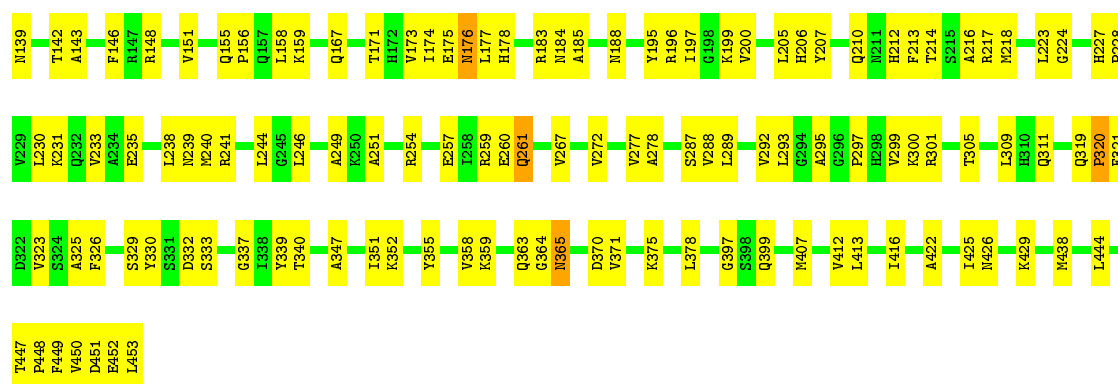
Chain AH:  73% 27%



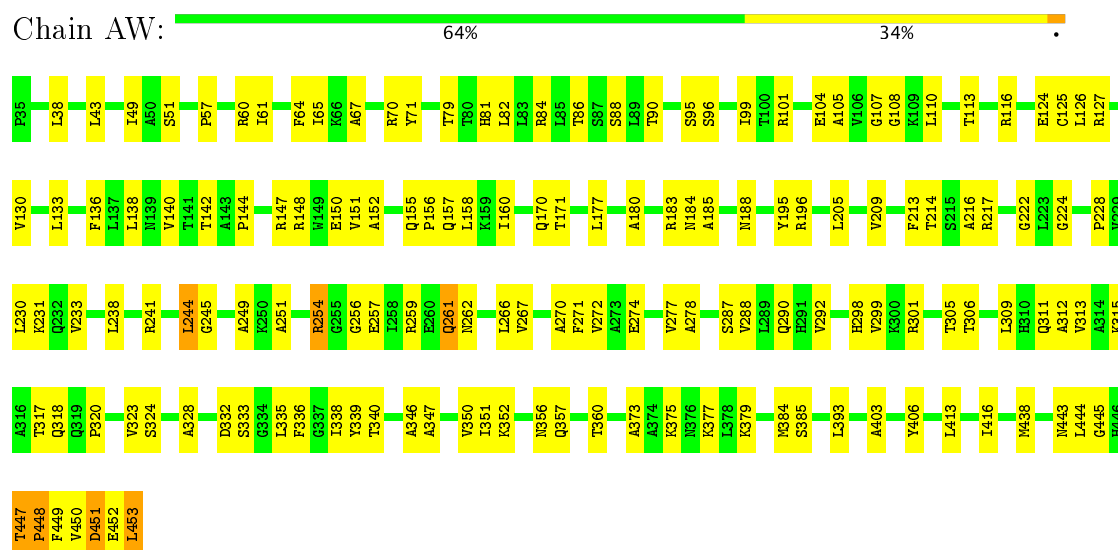
- Molecule 65: Cytochrome c1, heme protein, mitochondrial



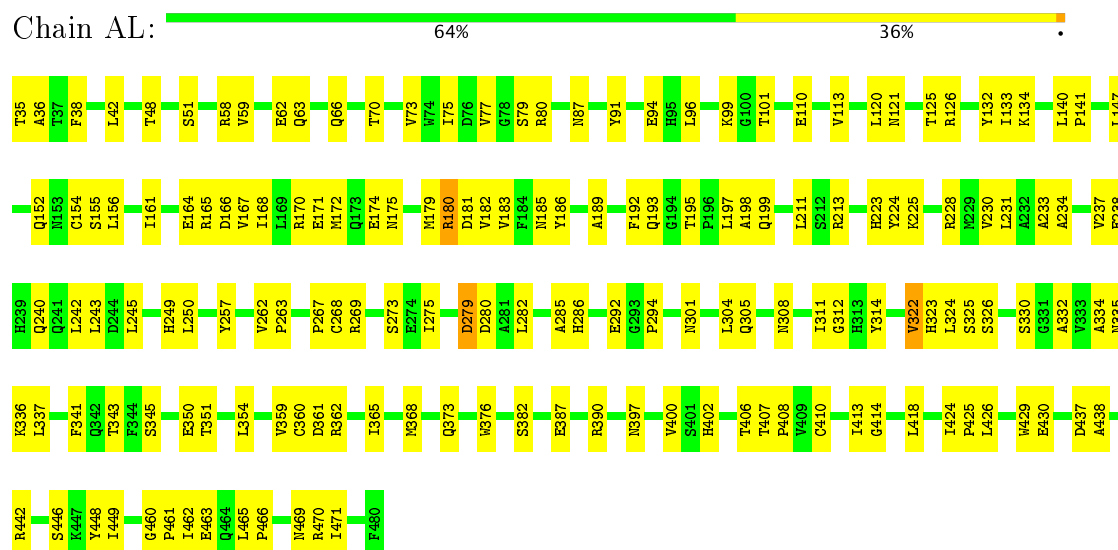




- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

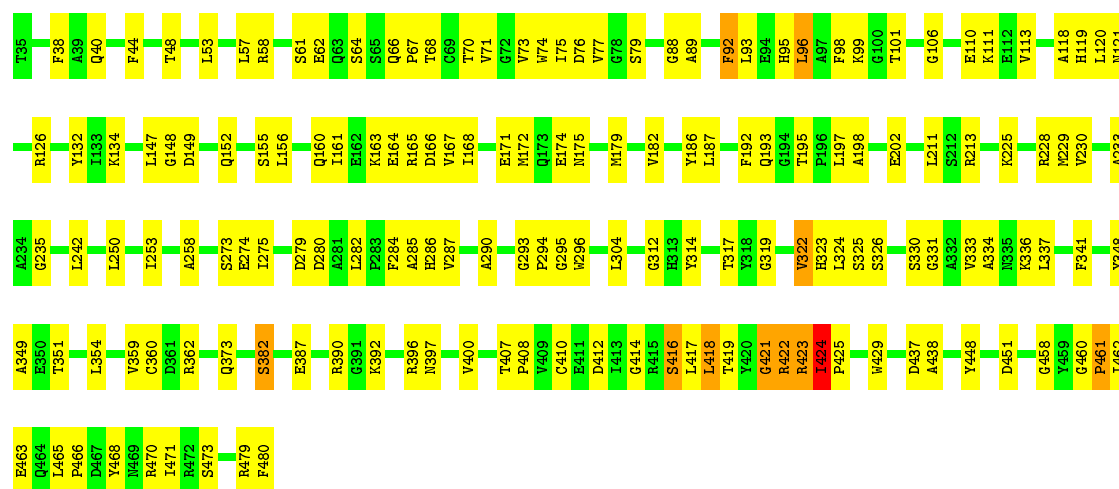


- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial



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

Chain AY:  64% 33%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.30	0/3398	0.49	0/4590
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.32	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
2	B	0.50	0/1452	0.57	0/1964
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.68	1/1579 (0.1%)
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.59	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
3	C	0.58	0/1280	0.57	0/1732
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	2/4840 (0.0%)	0.70	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	p	0.59	0/1549	0.59	0/2098
4	E	0.34	0/993	0.53	0/1335
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.49	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
45	x	0.60	0/4164	0.76	1/5688 (0.0%)
46	y	0.58	0/1868	0.80	0/2544
47	z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658 (0.1%)
49	1	0.50	0/898	0.66	0/1218
5	F	0.28	0/682	0.53	0/922
50	2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950 (0.1%)
52	4	0.55	0/648	0.73	0/877
53	5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953
59	AB	0.23	0/421	0.60	1/574 (0.2%)
59	AO	0.25	0/417	0.61	1/569 (0.2%)
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.23	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789 (0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	1/942 (0.1%)	0.52	1/1263 (0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
66	AV	0.34	2/3108 (0.1%)	0.54	2/4254 (0.0%)
67	AK	0.27	0/3217	0.49	0/4361
67	AW	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
68	AL	0.27	0/3527	0.47	0/4788
68	AY	0.29	1/3527 (0.0%)	0.50	2/4788 (0.0%)
7	H	0.34	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.35	0/2785	0.52	0/3771
All	All	0.47	10/115987 (0.0%)	0.60	35/157444 (0.0%)

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	w	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AW	448	PRO	N-CD	5.34	1.55	1.47
66	AJ	154	PRO	N-CD	5.22	1.55	1.47
66	AV	154	PRO	N-CD	5.22	1.55	1.47
34	k	2	PRO	N-CD	5.17	1.55	1.47
25	b	118	PRO	N-CD	5.17	1.55	1.47
68	AY	425	PRO	N-CD	5.08	1.54	1.47
35	l	91	PRO	N-CD	5.03	1.54	1.47
35	l	231	PRO	N-CD	5.02	1.54	1.47
63	AF	52	PRO	N-CD	5.02	1.54	1.47
66	AV	346	PRO	N-CD	5.01	1.54	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	Y	92	TRP	N-CA-C	-6.99	92.12	111.00
27	d	2	PRO	N-CA-CB	6.77	111.43	103.30
22	Y	87	PRO	CA-N-CD	-6.56	102.31	111.50
48	0	133	GLY	N-CA-C	6.43	129.17	113.10
25	b	36	PRO	C-N-CD	6.20	141.41	128.40
62	AE	28	ASP	C-N-CD	6.15	141.31	128.40
32	i	323	THR	C-N-CA	6.05	147.42	122.00
43	v	17	PRO	N-CA-CB	5.92	110.40	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	v	23	PRO	N-CA-CB	5.88	110.35	103.30
35	l	197	ASP	C-N-CD	5.87	140.72	128.40
66	AV	345	TYR	C-N-CD	5.82	140.62	128.40
25	b	105	PHE	C-N-CD	5.79	140.57	128.40
66	AV	153	ILE	C-N-CD	5.77	140.52	128.40
34	k	1	MET	C-N-CD	5.75	140.48	128.40
66	AJ	153	ILE	C-N-CD	5.74	140.45	128.40
43	v	19	PRO	N-CA-CB	5.72	110.16	103.30
35	l	90	ILE	C-N-CD	5.71	140.40	128.40
68	AY	424	ILE	C-N-CD	5.67	140.32	128.40
25	b	117	ILE	C-N-CD	5.67	140.31	128.40
35	l	230	HIS	C-N-CD	5.67	140.31	128.40
63	AF	51	LEU	C-N-CD	5.66	140.29	128.40
16	Q	97	LEU	CA-CB-CG	5.64	128.27	115.30
67	AW	447	THR	C-N-CD	5.63	140.22	128.40
59	AB	45	LEU	CA-CB-CG	5.47	127.88	115.30
33	j	98	LEU	CB-CG-CD2	-5.41	101.81	111.00
25	b	37	PRO	CA-N-CD	-5.39	103.95	111.50
68	AY	421	GLY	N-CA-C	-5.38	99.64	113.10
59	AO	45	LEU	CA-CB-CG	5.31	127.50	115.30
51	3	5	LYS	N-CA-C	5.24	125.15	111.00
45	x	435	GLY	N-CA-C	5.22	126.16	113.10
22	Y	86	TYR	C-N-CD	5.14	139.20	128.40
40	r	408	LEU	CA-CB-CG	-5.10	103.57	115.30
40	r	238	LEU	CB-CG-CD2	-5.09	102.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	209	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1420	0	1371	104	0
3	C	1249	0	1253	67	0
4	E	968	0	982	62	0
5	F	670	0	679	36	0
6	G	672	0	650	31	0
6	X	686	0	676	23	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	236	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	326	0
13	N	1195	0	1155	48	0
14	O	1643	0	1646	113	0
15	P	1730	0	1685	116	0
16	Q	3460	0	3419	253	0
17	S	568	0	567	17	0
18	T	742	0	723	39	0
19	U	647	0	653	9	0
20	V	1038	0	1027	35	0
21	W	1135	0	1129	38	0
22	Y	533	0	475	45	0
23	Z	648	0	627	13	0
24	a	1174	0	1177	0	0
25	b	1059	0	1079	0	0
26	c	1236	0	1092	0	0
27	d	1418	0	1375	0	0
28	e	810	0	772	0	0
29	f	405	0	407	0	0
30	g	1004	0	1008	0	0
31	h	863	0	861	0	0
32	i	2735	0	2893	0	0
33	j	919	0	968	0	0
34	k	740	0	792	0	0
35	l	4717	0	4893	0	0
36	m	1313	0	1330	0	0
37	n	473	0	480	0	0
38	o	1066	0	1086	0	0
39	p	1495	0	1440	0	0
40	r	3629	0	3825	0	0
41	s	2509	0	2617	0	0
42	u	1394	0	1367	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	921	0	892	0	0
44	w	2474	0	2304	0	0
45	x	4025	0	4003	0	0
46	y	1822	0	1834	0	0
47	z	2124	0	2042	0	0
48	0	1195	0	1183	30	0
49	1	878	0	868	17	0
50	2	748	0	728	22	0
51	3	672	0	645	24	0
52	4	628	0	582	18	0
53	5	598	0	612	11	0
54	6	441	0	439	12	0
55	7	384	0	366	6	0
56	8	386	0	388	6	0
57	9	335	0	352	11	0
58	AA	694	0	683	46	0
58	AN	687	0	676	25	0
59	AB	413	0	438	25	0
59	AO	409	0	432	26	0
60	AC	1521	0	1505	54	0
60	AP	1521	0	1505	62	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	24	0
62	AE	580	0	526	51	0
62	AR	580	0	526	34	0
63	AF	921	0	909	71	0
63	AS	921	0	910	30	0
64	AG	425	0	422	15	0
64	AT	425	0	422	31	0
65	AH	1924	0	1874	58	0
65	AU	1924	0	1874	82	0
66	AJ	3009	0	3065	107	0
66	AV	3009	0	3065	169	0
67	AK	3159	0	3130	152	0
67	AW	3162	0	3139	127	0
68	AL	3453	0	3370	140	0
68	AY	3453	0	3368	157	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	3	0
70	A	31	0	19	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	AL	52	0	88	3	0
71	AQ	52	0	88	7	0
71	AT	52	0	88	3	0
71	B	52	0	88	1	0
71	U	52	0	88	1	0
71	V	52	0	88	2	0
71	b	52	0	88	0	0
71	g	156	0	264	0	0
71	r	104	0	176	0	0
72	E	35	0	0	4	0
72	p	35	0	0	0	0
73	J	48	0	26	27	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	1	0
75	AG	64	0	72	29	0
75	AH	64	0	72	6	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	23	0
75	AN	64	0	72	8	0
75	AU	64	0	72	12	0
75	AY	64	0	72	4	0
75	V	63	0	68	8	0
75	i	64	0	72	0	0
75	l	128	0	144	0	0
75	n	64	0	72	0	0
76	AH	49	0	75	30	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	38	0
76	AU	41	0	56	25	0
76	AV	49	0	75	21	0
76	AY	49	0	75	22	0
76	V	51	0	82	12	0
76	W	51	0	82	5	0
76	l	100	0	157	0	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	x	1	0	0	0	0
79	x	120	0	108	0	0
80	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	AH	43	0	32	5	0
81	AU	43	0	32	7	0
82	AJ	86	0	60	7	0
82	AV	86	0	60	13	0
All	All	115642	0	115742	3308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (3308) 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)
68:AY:296:TRP:CD1	68:AY:419:THR:CG2	1.74	1.60
63:AF:29:LYS:CD	63:AF:75:ILE:HD11	1.31	1.58
75:AJ:405:CDL:H112	76:AY:502:PEE:C45	1.18	1.56
63:AF:29:LYS:CG	63:AF:75:ILE:HD11	1.16	1.55
68:AY:296:TRP:CD1	68:AY:419:THR:HG23	0.99	1.52
63:AF:29:LYS:HG2	63:AF:75:ILE:CD1	1.40	1.49
9:J:130:ILE:HG23	73:J:401:NDP:C8A	1.45	1.46
60:AC:150:ALA:CB	66:AV:168:TYR:HE2	1.29	1.44
68:AY:296:TRP:NE1	68:AY:419:THR:CG2	1.73	1.43
12:M:134:GLY:HA2	69:M:801:SF4:S3	1.57	1.41
58:AA:78:TYR:CB	62:AE:65:GLU:HG2	1.48	1.41
63:AF:29:LYS:CD	63:AF:75:ILE:CD1	1.97	1.41
63:AF:29:LYS:CG	63:AF:75:ILE:CD1	1.96	1.40
58:AA:78:TYR:HB3	62:AE:65:GLU:CG	1.50	1.39
60:AC:150:ALA:CB	66:AV:168:TYR:CE2	2.05	1.38
66:AV:14:ILE:CD1	76:AY:502:PEE:H41	1.58	1.33
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
67:AK:259:ARG:CG	67:AK:444:LEU:HD13	1.60	1.31
68:AY:296:TRP:HE1	68:AY:419:THR:CB	1.42	1.31
60:AC:150:ALA:HB3	66:AV:168:TYR:CE2	1.61	1.31
66:AV:10:LEU:HD21	76:AY:502:PEE:C27	1.59	1.30
75:AJ:405:CDL:C11	76:AY:502:PEE:C45	2.08	1.29
75:AL:502:CDL:C57	76:AL:503:PEE:H63	1.61	1.29
9:J:206:ILE:HA	9:J:240:VAL:O	1.34	1.27
16:Q:82:LEU:O	16:Q:98:VAL:HG13	1.24	1.27
58:AA:78:TYR:CD1	62:AE:65:GLU:HA	1.69	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.25
65:AU:308:ARG:NH1	75:AU:403:CDL:O1	1.70	1.24
9:J:130:ILE:HG23	73:J:401:NDP:N7A	1.52	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:AU:401:PEE:H17	66:AV:240:MET:CE	1.68	1.22
76:AH:401:PEE:H18	66:AJ:240:MET:CE	1.70	1.21
63:AF:29:LYS:HD3	63:AF:75:ILE:CD1	1.64	1.19
9:J:206:ILE:O	9:J:211:ASP:OD2	1.61	1.19
9:J:171:ASN:O	9:J:181:LEU:CD2	1.92	1.18
75:AL:502:CDL:H572	76:AL:503:PEE:C40	1.73	1.17
68:AY:98:PHE:CE2	68:AY:120:LEU:CD1	2.29	1.16
64:AT:42:LEU:O	64:AT:45:VAL:HG22	1.41	1.15
16:Q:268:TRP:CZ3	16:Q:272:THR:HG21	1.80	1.15
1:A:93:PHE:CE2	1:A:98:LYS:HD3	1.80	1.14
68:AY:296:TRP:NE1	68:AY:419:THR:HG21	1.57	1.14
22:Y:84:PHE:CD1	22:Y:85:PRO:HD3	1.84	1.13
9:J:171:ASN:C	9:J:181:LEU:HD21	1.68	1.13
67:AK:259:ARG:HG3	67:AK:444:LEU:HD13	1.27	1.13
4:E:25:MET:HB3	4:E:29:LYS:CE	1.77	1.13
68:AY:296:TRP:NE1	68:AY:419:THR:CB	2.03	1.13
66:AV:10:LEU:CD2	76:AY:502:PEE:H46	1.79	1.12
58:AA:37:ASN:OD1	58:AA:40:ARG:NH2	1.83	1.11
64:AT:40:LEU:HD12	64:AT:41:ILE:N	1.63	1.11
76:AU:401:PEE:H17	66:AV:240:MET:HE1	1.23	1.11
75:AG:101:CDL:H332	75:AG:101:CDL:HA62	1.25	1.10
60:AC:150:ALA:HB1	66:AV:168:TYR:CE2	1.80	1.10
75:AL:502:CDL:C57	76:AL:503:PEE:H66	1.80	1.10
76:AL:503:PEE:H49	76:AL:503:PEE:H19	1.11	1.10
75:AL:502:CDL:H571	76:AL:503:PEE:H63	1.12	1.10
68:AY:98:PHE:CE2	68:AY:120:LEU:HD13	1.87	1.10
9:J:130:ILE:HG23	73:J:401:NDP:H8A	1.28	1.08
67:AK:438:MET:HE2	67:AK:450:VAL:HG13	1.36	1.08
22:Y:71:TRP:CH2	22:Y:75:HIS:CD2	2.42	1.08
9:J:48:ARG:HH21	16:Q:78:LYS:NZ	43.60	1.07
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
12:M:134:GLY:CA	69:M:801:SF4:S3	2.42	1.07
75:AG:101:CDL:H712	75:AG:101:CDL:H531	1.32	1.06
58:AA:78:TYR:HE1	62:AE:64:GLU:O	1.36	1.06
65:AU:296:MET:HE1	76:AU:401:PEE:H53	1.33	1.05
58:AA:78:TYR:CE1	62:AE:64:GLU:O	2.09	1.04
62:AR:34:ARG:HG3	62:AR:78:ARG:NH1	1.72	1.04
62:AE:34:ARG:HD3	62:AE:78:ARG:NH2	1.71	1.04
63:AF:29:LYS:HG2	63:AF:75:ILE:CG1	1.87	1.04
22:Y:71:TRP:CH2	22:Y:75:HIS:HD2	1.76	1.04
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AU:288:MET:HB3	76:AU:401:PEE:O4	1.57	1.03
65:AU:296:MET:CE	76:AU:401:PEE:H53	1.86	1.03
16:Q:69:VAL:O	16:Q:72:PRO:HD2	1.58	1.03
16:Q:82:LEU:O	16:Q:98:VAL:CG1	2.06	1.03
67:AK:259:ARG:HB2	67:AK:259:ARG:HH21	1.22	1.03
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.03
66:AV:14:ILE:HD12	76:AY:502:PEE:H41	1.41	1.03
66:AV:10:LEU:CD2	76:AY:502:PEE:C27	2.36	1.02
75:AG:101:CDL:H712	75:AG:101:CDL:C53	1.90	1.02
64:AG:38:TRP:CD1	75:AG:101:CDL:H511	1.94	1.01
9:J:130:ILE:CG2	73:J:401:NDP:N7A	2.24	1.01
9:J:48:ARG:NH2	16:Q:78:LYS:NZ	43.78	1.01
15:P:170:ILE:HD12	15:P:170:ILE:H	3.73	1.01
62:AR:34:ARG:NH1	62:AR:78:ARG:HH12	1.59	1.00
67:AK:257:GLU:OE2	67:AK:450:VAL:N	1.92	1.00
62:AR:79:ASP:OD2	65:AU:236:TYR:OH	1.79	1.00
65:AH:121:CYS:SG	81:AH:402:HEC:HBB2	2.01	0.99
9:J:130:ILE:CG2	73:J:401:NDP:C8A	2.41	0.99
9:J:141:PHE:CE2	9:J:180:TYR:HA	1.98	0.99
9:J:176:SER:HA	9:J:182:ARG:HH21	1.24	0.99
76:AL:503:PEE:H16	76:AL:503:PEE:H50	1.45	0.99
64:AT:39:ARG:HA	64:AT:51:LYS:HE3	1.45	0.99
76:V:202:PEE:H60	76:V:202:PEE:C25	1.92	0.99
62:AE:30:LEU:HD11	62:AE:34:ARG:HH21	1.26	0.98
1:A:116:ASN:ND2	70:A:502:FMN:C8	2.25	0.98
76:AH:401:PEE:H73	76:AH:401:PEE:H64	1.42	0.98
67:AW:351:ILE:HD11	67:AW:448:PRO:HD2	1.44	0.98
66:AJ:156:ILE:HG22	66:AJ:160:LEU:HB2	1.42	0.98
9:J:171:ASN:HB3	9:J:181:LEU:HD11	1.46	0.98
75:AG:101:CDL:C33	75:AG:101:CDL:HA62	1.94	0.97
76:AH:401:PEE:C13	66:AJ:240:MET:CE	2.42	0.97
76:AH:401:PEE:H18	66:AJ:240:MET:HE1	1.47	0.97
67:AK:259:ARG:CG	67:AK:444:LEU:CD1	2.42	0.97
75:AL:502:CDL:C57	76:AL:503:PEE:C38	2.43	0.97
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.96
66:AV:14:ILE:HD13	76:AY:502:PEE:H41	1.45	0.96
6:X:99:SER:HG	6:X:102:SER:HG	1.09	0.96
76:AL:503:PEE:H16	76:AL:503:PEE:C32	1.95	0.96
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	0.95
68:AY:424:ILE:HG23	68:AY:429:TRP:HE1	1.31	0.95
3:C:137:VAL:HG21	16:Q:87:GLN:HE21	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:67:LEU:HD23	66:AJ:209:LEU:HD12	1.47	0.95
67:AK:259:ARG:HB2	67:AK:259:ARG:NH2	1.82	0.95
68:AY:98:PHE:CD2	68:AY:120:LEU:HD11	2.01	0.95
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.47	0.95
76:AL:503:PEE:H49	76:AL:503:PEE:C14	1.95	0.94
1:A:116:ASN:HD22	70:A:502:FMN:C8M	1.78	0.94
76:AL:503:PEE:H19	76:AL:503:PEE:C31	1.96	0.94
60:AC:150:ALA:HB1	66:AV:168:TYR:CD2	2.02	0.94
67:AK:259:ARG:HG3	67:AK:444:LEU:CD1	1.97	0.94
58:AA:78:TYR:CD1	62:AE:65:GLU:CA	2.49	0.94
76:AL:503:PEE:H26	76:AL:503:PEE:C31	1.97	0.94
14:O:177:LEU:N	74:O:301:FES:S1	2.39	0.94
66:AV:137:GLN:HE21	66:AV:141:TRP:HE1	1.10	0.93
67:AK:257:GLU:CG	67:AK:450:VAL:HG22	1.99	0.93
67:AK:259:ARG:HG2	67:AK:444:LEU:HD13	1.49	0.93
60:AC:150:ALA:HB3	66:AV:168:TYR:HE2	0.77	0.93
68:AY:98:PHE:CD2	68:AY:120:LEU:CD1	2.52	0.93
76:AH:401:PEE:H28	76:AH:401:PEE:H66	1.50	0.92
1:A:116:ASN:HD22	70:A:502:FMN:C8	1.82	0.92
62:AE:29:PRO:HD3	65:AH:262:THR:HG21	1.52	0.92
22:Y:83:HIS:O	22:Y:84:PHE:HB2	1.67	0.92
51:3:5:LYS:HZ3	51:3:6:GLY:H	0.93	0.91
9:J:48:ARG:NH2	16:Q:78:LYS:HZ3	44.46	0.91
66:AV:143:ALA:O	66:AV:147:THR:OG1	1.86	0.91
4:E:25:MET:O	4:E:29:LYS:HG3	1.69	0.91
9:J:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.90
62:AE:34:ARG:HD3	62:AE:78:ARG:HH22	1.30	0.90
7:H:45:ARG:NH1	7:H:49:GLU:OE2	2.05	0.90
9:J:169:HIS:HD2	73:J:401:NDP:H5N	1.33	0.90
67:AK:257:GLU:OE2	67:AK:450:VAL:HG22	1.70	0.90
67:AW:450:VAL:HA	67:AW:453:LEU:CD1	2.03	0.89
66:AV:149:LEU:HD21	66:AV:281:LEU:HD21	1.52	0.89
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.89
66:AV:14:ILE:CD1	76:AY:502:PEE:C25	2.49	0.89
63:AF:29:LYS:HD2	63:AF:75:ILE:HD11	1.52	0.89
68:AY:99:LYS:O	68:AY:106:GLY:HA3	1.71	0.89
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
9:J:83:PRO:HB2	9:J:108:TRP:NE1	1.88	0.88
3:C:137:VAL:CG2	16:Q:87:GLN:HE21	1.86	0.88
76:AH:401:PEE:H18	66:AJ:240:MET:SD	2.12	0.88
16:Q:400:ILE:HB	16:Q:407:PHE:HB3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
60:AC:150:ALA:CB	66:AV:168:TYR:CD2	2.55	0.88
68:AY:296:TRP:CE2	68:AY:419:THR:HG21	2.08	0.88
58:AA:78:TYR:CE1	62:AE:65:GLU:HA	2.08	0.87
22:Y:84:PHE:CG	22:Y:85:PRO:CD	2.57	0.87
75:AG:101:CDL:C52	75:AG:101:CDL:H712	2.03	0.87
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.87
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.87
12:M:130:ILE:HD13	18:T:114:TYR:CE1	2.11	0.86
76:AU:401:PEE:H17	66:AV:240:MET:HE2	1.58	0.86
9:J:212:ARG:HH11	9:J:212:ARG:HG2	1.37	0.86
67:AK:438:MET:HB3	67:AK:450:VAL:CG1	2.05	0.86
67:AK:183:ARG:NH1	67:AW:451:ASP:OD2	2.08	0.86
66:AV:137:GLN:NE2	66:AV:141:TRP:HE1	1.73	0.86
22:Y:84:PHE:CD1	22:Y:85:PRO:CD	2.58	0.86
9:J:169:HIS:HD2	73:J:401:NDP:C5N	1.87	0.86
51:3:5:LYS:HZ3	51:3:6:GLY:N	1.73	0.86
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.86
76:W:201:PEE:O2P	76:W:201:PEE:N	2.08	0.86
67:AK:438:MET:CB	67:AK:450:VAL:CG1	2.54	0.85
66:AV:10:LEU:HD21	76:AY:502:PEE:H46	0.88	0.85
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.85
62:AE:21:GLU:O	62:AE:25:GLU:N	2.09	0.85
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.85
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.85
66:AV:295:LEU:O	66:AV:299:LEU:HD22	1.77	0.85
68:AY:296:TRP:CD1	68:AY:419:THR:HG21	1.91	0.85
63:AF:71:LEU:HD23	63:AF:71:LEU:H	1.40	0.85
62:AE:30:LEU:HD21	65:AH:216:THR:CG2	2.07	0.85
1:A:244:ASN:N	70:A:502:FMN:O2P	2.09	0.84
67:AW:259:ARG:NH1	67:AW:449:PHE:CE1	2.44	0.84
68:AY:412:ASP:O	68:AY:416:SER:HB2	1.76	0.84
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.84
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.84
9:J:48:ARG:HH21	16:Q:78:LYS:HZ3	44.29	0.84
9:J:176:SER:CA	9:J:182:ARG:HH21	1.89	0.84
63:AF:52:PRO:HG2	63:AF:55:LEU:HB2	1.58	0.84
66:AV:344:SER:O	66:AV:348:THR:HG23	1.76	0.84
62:AE:30:LEU:HD21	65:AH:216:THR:HG23	1.59	0.84
9:J:85:ARG:HH11	9:J:85:ARG:HG3	1.41	0.84
20:V:84:PRO:O	20:V:89:ASN:ND2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:50:ARG:O	67:AW:148:ARG:NH2	2.11	0.83
4:E:70:ASN:OD1	72:E:201:8Q1:O4	1.95	0.83
62:AR:34:ARG:NH1	62:AR:78:ARG:NH1	2.25	0.83
75:AG:101:CDL:H731	75:AG:101:CDL:H542	1.60	0.83
59:AB:27:ARG:HE	67:AK:174:ILE:HD12	1.43	0.83
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.83
75:AG:101:CDL:CA6	75:AG:101:CDL:H332	2.06	0.83
58:AA:25:ARG:HG2	60:AC:91:TYR:O	1.79	0.82
76:AH:401:PEE:C43	76:AH:401:PEE:H64	2.08	0.82
76:AH:401:PEE:C13	66:AJ:240:MET:HE1	2.09	0.82
76:AL:503:PEE:H16	76:AL:503:PEE:C31	2.08	0.82
62:AR:86:LEU:O	62:AR:86:LEU:HD23	1.79	0.82
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.82
67:AW:449:PHE:N	67:AW:452:GLU:OE2	2.10	0.82
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.82
62:AR:79:ASP:HB3	65:AU:92:PRO:HG2	1.60	0.82
67:AW:257:GLU:OE2	67:AW:450:VAL:N	2.09	0.82
9:J:169:HIS:CD2	73:J:401:NDP:H5N	2.15	0.82
71:AL:501:PLX:H71	76:AL:503:PEE:H17	1.60	0.82
65:AH:291:LYS:HD2	76:AH:401:PEE:H8	1.62	0.81
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.81
62:AE:29:PRO:CD	65:AH:262:THR:HG21	2.09	0.81
67:AK:259:ARG:HG2	67:AK:444:LEU:CD1	2.08	0.81
65:AU:307:LYS:NZ	75:AU:403:CDL:OA3	2.12	0.81
63:AF:34:ARG:HG2	63:AF:34:ARG:HH11	1.46	0.81
60:AC:220:LEU:HB2	74:AC:301:FES:S2	2.21	0.81
67:AK:257:GLU:CD	67:AK:450:VAL:HG22	1.99	0.81
64:AT:39:ARG:HG2	64:AT:39:ARG:HH21	1.45	0.81
62:AE:34:ARG:CD	62:AE:78:ARG:NH2	2.42	0.81
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.81
71:AQ:101:PLX:H322	76:AY:502:PEE:H59	1.63	0.81
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.81
66:AV:326:TRP:CZ2	76:AV:403:PEE:H13	2.16	0.80
65:AU:121:CYS:SG	81:AU:402:HEC:HBB2	2.21	0.80
62:AE:28:ASP:OD1	62:AE:30:LEU:N	2.15	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80
22:Y:74:TRP:HZ3	22:Y:75:HIS:HD1	1.29	0.80
58:AA:78:TYR:CG	62:AE:65:GLU:HG2	2.15	0.80
66:AV:195:LEU:CD2	66:AV:199:PHE:HE2	1.94	0.80
66:AJ:262:LEU:HD22	60:AP:216:VAL:HG21	1.64	0.79
68:AY:74:TRP:O	68:AY:418:LEU:HD21	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:74:TRP:CE3	22:Y:75:HIS:HA	2.16	0.79
52:4:39:CYS:SG	52:4:53:CYS:CB	2.71	0.79
52:4:75:ARG:HH11	52:4:75:ARG:HG2	1.48	0.79
9:J:217:PHE:HZ	9:J:322:MET:CE	1.95	0.79
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.79
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.79
52:4:39:CYS:SG	52:4:53:CYS:HB3	2.22	0.79
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.47	0.79
82:AV:401:HEM:HBC2	82:AV:401:HEM:HHD	1.64	0.79
16:Q:70:ASP:O	16:Q:74:ASP:OD1	2.00	0.79
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.79
9:J:177:SER:HB2	9:J:320:GLU:HB3	1.64	0.79
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.64	0.79
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.79
75:AG:101:CDL:H351	75:AG:101:CDL:H742	1.64	0.78
2:B:133:ARG:HG3	2:B:135:ASP:H	1.47	0.78
58:AA:82:LYS:HE2	62:AE:60:ARG:HD3	1.66	0.78
75:AJ:405:CDL:H732	75:AJ:405:CDL:H351	1.65	0.78
65:AU:315:LYS:HE3	75:AU:403:CDL:H1	1.66	0.78
64:AT:35:ALA:HB1	76:AY:502:PEE:H75	1.63	0.78
9:J:206:ILE:HG12	73:J:401:NDP:N7N	1.99	0.78
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.65	0.78
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.02	0.78
67:AK:363:GLN:HB2	67:AK:365:ASN:OD1	1.83	0.78
63:AF:34:ARG:NH1	66:AJ:379:TRP:HE1	1.82	0.78
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.78
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.65	0.78
51:3:5:LYS:NZ	51:3:6:GLY:H	1.78	0.78
75:AG:101:CDL:H531	75:AG:101:CDL:H731	1.66	0.78
66:AJ:149:LEU:HD21	66:AJ:281:LEU:HD21	1.65	0.78
66:AV:165:TRP:CZ3	66:AV:168:TYR:O	2.37	0.78
9:J:86:CYS:O	9:J:87:ASP:HB2	1.83	0.78
67:AK:438:MET:HB3	67:AK:450:VAL:HG11	1.66	0.78
66:AV:148:ASN:O	66:AV:151:SER:HB3	1.84	0.78
9:J:176:SER:HA	9:J:182:ARG:NH2	1.98	0.78
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.65	0.78
16:Q:87:GLN:O	16:Q:88:HIS:C	2.22	0.78
22:Y:83:HIS:O	22:Y:84:PHE:CB	2.31	0.78
22:Y:84:PHE:CG	22:Y:85:PRO:HD2	2.19	0.77
8:I:33:LYS:NZ	8:I:35:THR:O	2.18	0.77
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:70:THR:HG1	68:AL:410:CYS:HG	1.33	0.77
9:J:217:PHE:CB	9:J:280:ILE:HD13	2.15	0.77
15:P:187:ILE:HG22	15:P:188:LEU:HG	1.66	0.77
9:J:48:ARG:HH21	16:Q:78:LYS:CE	43.01	0.77
22:Y:96:GLU:O	22:Y:97:LEU:HD23	1.84	0.77
76:AL:503:PEE:H26	76:AL:503:PEE:H48	1.66	0.77
62:AR:34:ARG:HH11	62:AR:78:ARG:HH22	1.33	0.77
68:AY:230:VAL:HG21	68:AY:418:LEU:CD1	2.15	0.77
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.77
76:AH:401:PEE:H49	76:AH:401:PEE:H14	1.65	0.77
66:AJ:324:LEU:HD11	66:AJ:369:ILE:HD12	1.65	0.77
62:AR:78:ARG:O	62:AR:82:VAL:HG23	1.84	0.77
67:AW:375:LYS:NZ	67:AW:416:ILE:O	2.18	0.77
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.77
63:AF:29:LYS:HD3	63:AF:75:ILE:HD13	1.64	0.77
16:Q:268:TRP:CZ3	16:Q:272:THR:CG2	2.66	0.77
67:AW:277:VAL:HG13	67:AW:278:ALA:HB2	1.66	0.76
63:AF:68:ASP:HA	63:AF:71:LEU:HD21	1.66	0.76
12:M:68:ARG:HD2	12:M:285:TRP:HE1	1.48	0.76
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.76
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
58:AN:41:ARG:NE	75:AN:101:CDL:OA4	2.19	0.76
9:J:130:ILE:CG2	73:J:401:NDP:H8A	2.10	0.76
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.19	0.76
67:AW:450:VAL:HA	67:AW:453:LEU:HD12	1.67	0.76
4:E:79:VAL:HG22	72:E:201:8Q1:C38	2.16	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	0.76
7:H:50:GLN:HE22	8:I:93:LYS:HA	1.50	0.76
5:F:42:VAL:HG21	12:M:671:LEU:HD12	1.66	0.76
63:AS:36:ASP:OD2	63:AS:62:ARG:NH1	2.19	0.75
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.19	0.75
12:M:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.75
65:AU:125:HIS:NE2	81:AU:402:HEC:NC	2.33	0.75
62:AE:30:LEU:CD1	62:AE:34:ARG:HH21	2.00	0.75
9:J:221:HIS:ND1	9:J:222:ARG:N	2.34	0.75
12:M:543:LYS:HG3	12:M:565:PHE:HD2	1.50	0.75
68:AL:73:VAL:HG23	68:AL:147:LEU:HD23	1.66	0.75
11:L:75:ARG:NH1	11:L:119:ASP:OD2	2.16	0.75
59:AB:52:ARG:NH1	68:AL:343:THR:O	2.18	0.75
67:AK:300:LYS:HG2	67:AK:301:ARG:HG2	1.69	0.75
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:128:CYS:HB2	12:M:129:PRO:HD3	1.68	0.75
20:V:40:ARG:HH22	20:V:55:LYS:HD3	1.50	0.75
1:A:174:ARG:HG3	10:K:91:LEU:HD21	1.69	0.75
60:AP:234:TYR:HB2	60:AP:243:TYR:HB2	1.69	0.75
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	0.75
21:W:31:SER:OG	21:W:35:MET:CE	2.35	0.75
75:AL:502:CDL:H572	76:AL:503:PEE:H66	0.84	0.74
59:AO:33:THR:HA	59:AO:38:PRO:HG3	1.69	0.74
22:Y:71:TRP:CZ2	22:Y:75:HIS:CD2	2.74	0.74
59:AB:2:LEU:HD22	67:AK:278:ALA:HB1	1.67	0.74
9:J:54:ILE:HB	9:J:78:SER:HB2	1.68	0.74
75:AG:101:CDL:H521	75:AG:101:CDL:OB8	1.87	0.74
58:AN:67:PHE:HB2	66:AV:346:PRO:HG3	1.69	0.74
66:AV:195:LEU:CD2	66:AV:199:PHE:CE2	2.70	0.74
67:AW:270:ALA:HB2	67:AW:339:TYR:HD1	1.52	0.74
22:Y:84:PHE:CG	22:Y:85:PRO:HD3	2.22	0.74
68:AY:421:GLY:C	68:AY:422:ARG:HG3	2.06	0.74
67:AK:127:ARG:HB3	68:AL:36:ALA:HB1	1.68	0.74
68:AY:192:PHE:HB3	68:AY:195:THR:HB	1.70	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	0.74
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.68	0.74
63:AF:29:LYS:CG	63:AF:75:ILE:HD13	2.16	0.74
75:AN:101:CDL:OA3	76:AV:403:PEE:H12	1.86	0.74
66:AJ:8:ASN:HD22	66:AJ:11:MET:HG2	1.50	0.74
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.74
76:V:202:PEE:H41	76:V:202:PEE:H60	1.67	0.74
76:AH:401:PEE:C13	66:AJ:240:MET:HE2	2.18	0.74
12:M:50:LEU:HB2	12:M:92:CYS:HA	1.68	0.74
15:P:170:ILE:HD12	15:P:170:ILE:N	4.19	0.74
68:AY:171:GLU:OE2	68:AY:175:ASN:ND2	2.21	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.74
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	0.74
16:Q:262:LEU:CD2	16:Q:268:TRP:CD1	2.60	0.74
66:AV:165:TRP:CE3	66:AV:168:TYR:O	2.41	0.74
76:AU:401:PEE:C13	66:AV:240:MET:HE1	2.12	0.73
9:J:174:ILE:HG13	9:J:182:ARG:HG3	1.70	0.73
63:AF:34:ARG:NH1	63:AF:34:ARG:HG2	2.00	0.73
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	0.73
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.73
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HD2	1:A:101:PHE:CE2	2.24	0.73
61:AQ:30:MET:SD	64:AT:34:TRP:HB2	2.29	0.73
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	0.73
67:AK:438:MET:CB	67:AK:450:VAL:HG11	2.16	0.73
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.73
58:AA:78:TYR:CE1	62:AE:64:GLU:C	2.62	0.73
67:AW:65:ILE:HG22	67:AW:67:ALA:H	1.53	0.73
76:V:202:PEE:H39	76:V:202:PEE:H32	1.70	0.73
9:J:132:ARG:NH2	73:J:401:NDP:C2B	2.52	0.73
16:Q:345:ALA:HB2	21:W:19:ILE:HD11	1.70	0.73
63:AF:29:LYS:HG2	63:AF:75:ILE:HG12	1.70	0.73
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.22	0.73
18:T:83:ARG:NH1	18:T:102:ASN:OD1	2.22	0.73
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.69	0.73
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.71	0.72
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.72
12:M:198:THR:HG22	14:O:39:PHE:HB3	1.70	0.72
51:3:54:ARG:HD3	51:3:54:ARG:N	2.04	0.72
67:AK:438:MET:CE	67:AK:450:VAL:HG13	2.16	0.72
9:J:132:ARG:NH2	73:J:401:NDP:O2B	2.22	0.72
16:Q:232:VAL:HG12	16:Q:234:GLN:H	1.54	0.72
48:O:23:PRO:O	49:1:66:ARG:HD3	1.89	0.72
68:AL:280:ASP:HA	68:AL:461:PRO:HB3	1.71	0.72
65:AU:288:MET:CB	76:AU:401:PEE:O4	2.35	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
63:AF:29:LYS:HG2	63:AF:75:ILE:HD11	1.02	0.72
67:AK:125:CYS:HB3	67:AK:133:LEU:HD22	1.70	0.72
66:AV:96:LEU:HD23	76:AV:403:PEE:H26	1.69	0.72
9:J:83:PRO:HB2	9:J:108:TRP:HE1	1.53	0.72
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	0.72
63:AF:29:LYS:HB2	63:AF:29:LYS:HZ3	1.54	0.72
76:AU:401:PEE:H61	76:AU:401:PEE:H27	1.70	0.72
14:O:116:ALA:O	14:O:124:ARG:NH1	2.21	0.72
1:A:381:GLN:HG2	69:A:501:SF4:S2	2.29	0.72
67:AK:65:ILE:HG22	67:AK:67:ALA:H	1.54	0.72
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.54	0.72
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.22	0.72
48:O:147:LYS:HA	48:O:147:LYS:HE3	1.72	0.72
75:AJ:405:CDL:C78	75:AJ:405:CDL:H742	2.20	0.72
68:AL:195:THR:HG22	68:AL:197:LEU:H	1.53	0.72
62:AR:34:ARG:HH11	62:AR:78:ARG:NH2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:GLU:OE2	3:C:145:ARG:NH2	2.23	0.72
9:J:212:ARG:NH2	73:J:401:NDP:O2N	2.22	0.72
75:AG:101:CDL:H731	75:AG:101:CDL:C54	2.18	0.72
68:AY:296:TRP:HD1	68:AY:419:THR:HG23	0.90	0.72
16:Q:282:GLU:OE2	16:Q:437:LYS:NZ	2.22	0.72
67:AW:184:ASN:HB3	67:AW:251:ALA:HA	1.72	0.72
22:Y:43:ARG:HG3	22:Y:46:GLN:HB2	1.72	0.72
12:M:543:LYS:NZ	12:M:563:ASP:OD2	2.23	0.72
16:Q:241:MET:HG3	21:W:11:PRO:HB2	1.72	0.72
11:L:137:PHE:O	11:L:141:ASN:ND2	2.15	0.71
1:A:391:TRP:HH2	12:M:153:PHE:HA	1.55	0.71
15:P:134:SER:HG	15:P:139:SER:HG	1.24	0.71
1:A:124:THR:HG23	1:A:126:LYS:HG2	1.72	0.71
1:A:327:ILE:HG23	1:A:331:VAL:HG13	1.72	0.71
68:AY:322:VAL:HG12	68:AY:323:HIS:H	1.53	0.71
5:F:68:ARG:NH1	12:M:359:ASN:OD1	2.23	0.71
76:V:202:PEE:H60	76:V:202:PEE:H42	1.73	0.71
12:M:374:THR:HB	12:M:377:ALA:HA	1.72	0.71
22:Y:86:TYR:HB3	22:Y:87:PRO:CA	2.19	0.71
75:AG:101:CDL:H521	75:AG:101:CDL:H712	1.72	0.71
61:AQ:22:ALA:HB2	71:AQ:101:PLX:H272	1.72	0.71
16:Q:95:LEU:HD13	16:Q:97:LEU:HD23	1.73	0.71
1:A:381:GLN:NE2	69:A:501:SF4:S3	2.63	0.71
62:AR:34:ARG:HH11	62:AR:78:ARG:NH1	1.88	0.71
9:J:221:HIS:CE1	9:J:222:ARG:CG	2.72	0.71
14:O:129:LYS:H	14:O:168:LEU:HA	1.53	0.71
68:AL:470:ARG:NH2	75:AL:502:CDL:OA4	2.22	0.71
12:M:63:PHE:O	12:M:181:ARG:NH2	2.23	0.71
14:O:187:GLN:HE21	14:O:190:ASP:HA	1.56	0.71
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.71
16:Q:80:ILE:O	16:Q:81:THR:HG22	1.90	0.71
63:AF:29:LYS:HD3	63:AF:75:ILE:HD12	1.65	0.71
12:M:566:ILE:HG13	12:M:580:ALA:HA	1.72	0.71
8:I:106:LEU:O	8:I:108:SER:N	2.19	0.71
1:A:116:ASN:ND2	70:A:502:FMN:C8M	2.52	0.71
67:AW:351:ILE:HD11	67:AW:448:PRO:CD	2.20	0.71
16:Q:432:LEU:HD12	16:Q:461:VAL:HG11	1.73	0.71
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.71
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.73	0.71
63:AF:29:LYS:HB2	63:AF:29:LYS:NZ	2.05	0.70
15:P:170:ILE:CD1	15:P:170:ILE:H	3.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:29:LYS:CD	63:AF:75:ILE:HD12	2.17	0.70
68:AY:48:THR:HG22	68:AY:62:GLU:HB2	1.73	0.70
16:Q:281:GLU:OE1	16:Q:281:GLU:N	2.22	0.70
1:A:158:ILE:HB	1:A:199:ARG:HG2	1.73	0.70
68:AL:192:PHE:HB3	68:AL:195:THR:HB	1.72	0.70
65:AU:296:MET:HE2	76:AU:401:PEE:H53	1.73	0.70
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.73	0.70
62:AE:21:GLU:O	62:AE:24:GLU:N	2.24	0.70
62:AR:34:ARG:HH11	62:AR:78:ARG:HH12	1.34	0.70
68:AY:417:LEU:HD23	68:AY:422:ARG:O	1.91	0.70
61:AD:48:ASN:HB2	61:AD:51:LYS:HD2	1.74	0.70
65:AU:296:MET:HE1	76:AU:401:PEE:C33	2.18	0.70
66:AV:324:LEU:HD11	66:AV:369:ILE:HD12	1.72	0.70
66:AV:344:SER:OG	66:AV:346:PRO:HD2	1.91	0.70
4:E:70:ASN:O	72:E:201:8Q1:O40	2.10	0.70
5:F:39:LYS:HG3	5:F:40:ARG:H	1.56	0.70
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.70
1:A:383:THR:HG22	12:M:75:CYS:HA	1.72	0.70
76:AH:401:PEE:H28	76:AH:401:PEE:C40	2.21	0.70
4:E:25:MET:O	4:E:29:LYS:CG	2.38	0.70
12:M:557:ARG:NH1	12:M:579:ILE:O	2.24	0.70
6:X:91:ASP:OD1	23:Z:47:ARG:NH1	2.24	0.70
66:AJ:300:ILE:O	66:AJ:303:MET:N	2.25	0.70
1:A:116:ASN:O	1:A:245:VAL:HG23	1.91	0.70
15:P:93:VAL:HB	15:P:154:GLU:HB2	1.72	0.70
21:W:31:SER:OG	21:W:35:MET:HE2	1.92	0.70
76:AH:401:PEE:C12	66:AJ:240:MET:HE1	2.22	0.70
67:AW:261:GLN:NE2	67:AW:443:ASN:O	2.25	0.70
68:AY:195:THR:HG22	68:AY:197:LEU:H	1.55	0.70
2:B:184:ASN:HD21	13:N:127:TYR:H	1.39	0.70
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.70
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.70
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.69
75:AL:502:CDL:H772	76:AL:503:PEE:H70	1.73	0.69
76:AH:401:PEE:H15	66:AJ:240:MET:HE1	1.74	0.69
67:AK:257:GLU:CG	67:AK:450:VAL:CG2	2.70	0.69
67:AW:57:PRO:HG2	68:AY:400:VAL:HG11	1.74	0.69
9:J:210:GLU:HG2	9:J:210:GLU:O	1.92	0.69
9:J:233:TRP:HA	9:J:272:LEU:HD21	1.74	0.69
15:P:46:THR:O	16:Q:162:ARG:N	2.16	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
22:Y:86:TYR:CB	22:Y:87:PRO:HA	2.22	0.69
59:AB:8:SER:OG	59:AB:26:LEU:O	2.09	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.25	0.69
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.69
62:AE:34:ARG:CD	62:AE:78:ARG:HH22	2.03	0.69
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.69
63:AF:14:LEU:O	63:AF:17:ILE:HG13	1.92	0.69
76:AL:503:PEE:C12	76:AL:503:PEE:H50	2.18	0.69
60:AC:216:VAL:HG21	66:AV:262:LEU:HD22	1.74	0.69
66:AV:80:ARG:NH1	82:AV:401:HEM:O1A	2.25	0.69
9:J:48:ARG:NH2	16:Q:78:LYS:HZ1	43.17	0.69
52:4:39:CYS:HG	52:4:53:CYS:CB	2.05	0.69
65:AU:202:ARG:NH1	65:AU:279:GLU:OE2	2.25	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
64:AG:38:TRP:CD1	75:AG:101:CDL:C51	2.74	0.69
66:AV:332:LEU:CD1	76:AV:403:PEE:H37	2.22	0.69
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.69
75:AG:101:CDL:C73	75:AG:101:CDL:H542	2.22	0.69
68:AL:171:GLU:OE2	68:AL:175:ASN:ND2	2.26	0.69
66:AV:295:LEU:O	66:AV:299:LEU:CD2	2.40	0.69
76:W:201:PEE:H24	76:W:201:PEE:H53	1.73	0.69
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.74	0.69
66:AJ:156:ILE:CG2	66:AJ:160:LEU:HB2	2.18	0.69
63:AF:39:TYR:CD1	63:AF:40:GLU:N	2.61	0.69
75:AG:101:CDL:C34	75:AG:101:CDL:HA62	2.22	0.69
59:AO:35:PRO:HB3	67:AW:320:PRO:HA	1.75	0.69
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.69
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.69
12:M:144:MET:SD	16:Q:380:HIS:ND1	2.63	0.69
12:M:225:ILE:HD12	12:M:285:TRP:HH2	1.57	0.69
65:AH:124:CYS:SG	81:AH:402:HEC:HBC2	2.33	0.68
67:AK:399:GLN:HE22	67:AK:407:MET:HB3	1.56	0.68
67:AK:438:MET:HB2	67:AK:450:VAL:CG1	2.22	0.68
7:H:12:VAL:HG13	16:Q:280:ALA:N	2.07	0.68
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.58	0.68
16:Q:190:HIS:HD2	16:Q:452:GLY:HA3	1.58	0.68
21:W:28:ARG:HG2	21:W:28:ARG:O	1.93	0.68
63:AS:67:LEU:HD23	66:AV:209:LEU:HD12	1.75	0.68
62:AE:30:LEU:O	62:AE:30:LEU:HD12	1.93	0.68
66:AV:150:LEU:HD23	66:AV:164:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.68
18:T:79:GLU:HG2	18:T:120:ARG:HB3	1.76	0.68
67:AK:100:THR:HG21	68:AL:324:LEU:HB3	1.75	0.68
67:AK:257:GLU:HG3	67:AK:450:VAL:CG2	2.23	0.68
3:C:159:TYR:HE1	16:Q:135:TYR:CZ	2.12	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
14:O:137:THR:HG21	14:O:176:CYS:HB2	1.74	0.68
67:AK:183:ARG:HG3	67:AK:183:ARG:HH21	1.57	0.68
16:Q:262:LEU:HD13	16:Q:268:TRP:NE1	2.08	0.68
20:V:81:ARG:HG2	20:V:83:LYS:HG3	1.75	0.68
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.68
64:AT:24:TRP:CZ3	75:AY:501:CDL:H551	2.28	0.68
9:J:247:LYS:HD2	9:J:340:ILE:HD12	1.74	0.68
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.75	0.68
70:A:502:FMN:H9	70:A:502:FMN:O4'	1.94	0.68
1:A:63:TYR:HE2	1:A:64:LYS:HZ2	1.40	0.68
68:AY:285:ALA:HB3	68:AY:360:CYS:HB2	1.76	0.68
3:C:128:ASN:ND2	3:C:164:TYR:O	2.24	0.68
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	0.68
22:Y:86:TYR:HB3	22:Y:87:PRO:HA	1.75	0.68
62:AR:79:ASP:HB3	65:AU:92:PRO:CG	2.23	0.68
73:J:401:NDP:O2X	73:J:401:NDP:H1B	1.94	0.68
52:4:38:ARG:HG2	52:4:85:ILE:HG23	1.77	0.67
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.67
68:AY:165:ARG:NH2	68:AY:211:LEU:O	2.24	0.67
66:AJ:66:ILE:HD11	66:AJ:134:PRO:HA	1.77	0.67
60:AP:236:CYS:HB3	60:AP:241:SER:HB2	1.74	0.67
65:AU:290:LEU:C	65:AU:290:LEU:HD23	2.14	0.67
66:AV:111:GLU:HG2	66:AV:199:PHE:CE1	2.28	0.67
12:M:194:ASP:O	12:M:208:THR:OG1	2.10	0.67
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.67
65:AU:112:ARG:NH1	65:AU:269:ASP:OD2	2.26	0.67
12:M:476:LEU:HB3	12:M:515:ILE:HG22	1.74	0.67
16:Q:87:GLN:N	16:Q:87:GLN:OE1	2.26	0.67
16:Q:82:LEU:C	16:Q:98:VAL:HG13	2.10	0.67
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.67
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.77	0.67
7:H:114:TRP:HE1	16:Q:394:GLY:HA2	1.59	0.67
12:M:381:LEU:O	12:M:383:SER:N	2.24	0.67
12:M:500:ILE:O	12:M:503:THR:OG1	2.12	0.67
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:29:LYS:HD2	63:AF:75:ILE:CD1	2.17	0.67
59:AO:18:THR:OG1	67:AW:110:LEU:O	2.11	0.67
2:B:119:ALA:HA	15:P:233:PHE:HE2	1.60	0.67
58:AA:12:ARG:HG2	58:AA:13:HIS:ND1	2.10	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	0.67
16:Q:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.67
22:Y:84:PHE:CD2	22:Y:85:PRO:HD2	2.30	0.67
56:8:19:TRP:HZ2	57:9:14:GLU:HG2	1.59	0.67
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.77	0.67
66:AJ:338:ILE:HD11	66:AJ:350:ILE:HG22	1.76	0.67
76:AJ:403:PEE:H61	76:AJ:403:PEE:H25	1.77	0.67
10:K:100:SER:HA	14:O:72:GLU:HB3	1.77	0.67
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.67
59:AB:49:PHE:O	68:AL:180:ARG:NH1	2.26	0.67
3:C:137:VAL:HG21	16:Q:87:GLN:NE2	2.05	0.67
12:M:173:MET:O	12:M:175:ARG:N	2.24	0.67
14:O:133:GLN:HB2	14:O:174:VAL:HG21	1.75	0.67
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.59	0.67
68:AL:80:ARG:NH1	68:AL:268:CYS:SG	2.67	0.67
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.77	0.67
11:L:58:LYS:NZ	11:L:139:GLU:OE1	2.27	0.67
10:K:99:PRO:HG2	14:O:71:PRO:HB3	1.76	0.67
14:O:54:ASP:OD1	14:O:60:TYR:OH	2.11	0.67
59:AB:16:SER:OG	59:AB:19:SER:O	2.12	0.66
63:AF:33:MET:HG3	63:AF:62:ARG:NH1	2.09	0.66
75:AG:101:CDL:H731	75:AG:101:CDL:C53	2.24	0.66
67:AK:107:GLY:O	68:AL:397:ASN:ND2	2.28	0.66
68:AL:257:TYR:HD2	68:AL:262:VAL:HG22	1.59	0.66
68:AY:101:THR:HA	68:AY:155:SER:H	1.60	0.66
2:B:111:CYS:O	2:B:139:ARG:NH2	2.28	0.66
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	0.66
68:AY:387:GLU:OE2	68:AY:390:ARG:NH2	2.23	0.66
66:AV:195:LEU:HD21	66:AV:199:PHE:HE2	1.60	0.66
21:W:86:MET:SD	21:W:128:ARG:NH1	2.66	0.66
3:C:125:THR:HG21	16:Q:118:ARG:HG2	1.76	0.66
3:C:161:HIS:O	3:C:168:ARG:NH2	2.28	0.66
16:Q:338:ARG:HH22	21:W:23:ARG:HB3	1.58	0.66
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	0.66
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:ND2	70:A:502:FMN:C9	2.59	0.66
1:A:74:ASP:O	1:A:78:GLY:N	2.27	0.66
62:AE:34:ARG:HH22	65:AH:216:THR:HG22	1.61	0.66
75:AG:101:CDL:H531	75:AG:101:CDL:C71	2.19	0.66
67:AK:176:ASN:ND2	67:AK:260:GLU:OE2	2.29	0.66
64:AT:45:VAL:HG21	64:AT:48:ILE:HB	1.77	0.66
67:AW:60:ARG:HG3	67:AW:124:GLU:HG2	1.78	0.66
2:B:62:THR:HG22	21:W:35:MET:HE1	1.78	0.66
67:AK:183:ARG:NH2	67:AK:254:ARG:HB3	2.11	0.66
4:E:107:PHE:HB3	4:E:109:GLU:HG3	1.78	0.66
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.78	0.66
12:M:254:MET:HB2	12:M:290:THR:HG22	1.78	0.66
75:AG:101:CDL:H521	75:AG:101:CDL:CB7	2.26	0.66
68:AY:121:ASN:ND2	68:AY:132:TYR:OH	2.29	0.66
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.66
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.66
12:M:300:GLN:HB2	13:N:137:TRP:HA	1.78	0.66
22:Y:81:LEU:HD23	22:Y:81:LEU:C	2.15	0.66
62:AE:27:VAL:O	62:AE:28:ASP:HB3	1.96	0.65
66:AJ:165:TRP:O	66:AJ:174:THR:OG1	2.14	0.65
67:AK:351:ILE:HD11	67:AK:448:PRO:CG	2.27	0.65
58:AN:12:ARG:HG2	58:AN:13:HIS:ND1	2.12	0.65
67:AW:299:VAL:HG13	68:AY:120:LEU:HD11	1.79	0.65
67:AW:449:PHE:HB2	67:AW:452:GLU:OE1	1.97	0.65
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.65
63:AF:36:ASP:OD2	63:AF:62:ARG:NH1	2.28	0.65
67:AK:36:GLN:NE2	67:AK:39:GLU:OE2	2.29	0.65
68:AL:280:ASP:O	68:AL:362:ARG:NH2	2.30	0.65
61:AQ:22:ALA:CB	71:AQ:101:PLX:H272	2.26	0.65
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.65
9:J:132:ARG:NH2	73:J:401:NDP:H2B	2.11	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.65
49:I:43:PRO:HB2	49:I:48:ILE:HD11	1.76	0.65
60:AC:162:GLY:O	60:AC:227:ASN:ND2	2.30	0.65
67:AK:230:LEU:HA	67:AK:233:VAL:HG22	1.78	0.65
7:H:12:VAL:HG11	16:Q:278:VAL:O	1.96	0.65
16:Q:80:ILE:O	16:Q:81:THR:CG2	2.45	0.65
56:8:45:LEU:HD21	57:9:40:TYR:HA	1.78	0.65
1:A:424:ILE:HG22	69:A:501:SF4:S4	2.36	0.65
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.65
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:257:GLU:HG3	67:AK:450:VAL:HG22	1.73	0.65
76:AU:401:PEE:C19	76:AU:401:PEE:H64	2.27	0.65
7:H:72:LEU:HD22	7:H:77:LEU:HD13	1.78	0.65
8:I:66:PRO:HB3	15:P:79:SER:HB3	1.77	0.65
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.78	0.65
68:AL:48:THR:HG22	68:AL:62:GLU:HB2	1.78	0.65
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	0.65
12:M:65:TYR:O	12:M:181:ARG:NH2	2.29	0.65
12:M:169:VAL:HG12	12:M:223:ILE:HD11	1.79	0.65
18:T:40:THR:OG1	18:T:42:THR:O	2.14	0.65
76:AH:401:PEE:C11	76:AH:401:PEE:H49	2.27	0.64
82:AJ:401:HEM:HBC2	82:AJ:401:HEM:HMC1	1.80	0.64
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.64
22:Y:79:GLU:O	22:Y:80:VAL:HG13	1.96	0.64
11:L:111:LEU:HG	11:L:112:MET:HG2	1.80	0.64
67:AK:351:ILE:HD11	67:AK:448:PRO:CD	2.27	0.64
58:AN:12:ARG:HG2	58:AN:13:HIS:HD1	1.62	0.64
62:AR:29:PRO:HD2	65:AU:262:THR:HG21	1.79	0.64
3:C:93:MET:HG2	3:C:110:PHE:HZ	1.62	0.64
67:AK:183:ARG:HH21	67:AK:254:ARG:HB3	1.62	0.64
67:AK:365:ASN:OD1	67:AK:365:ASN:N	2.31	0.64
64:AT:42:LEU:O	64:AT:45:VAL:CG2	2.34	0.64
66:AV:22:PRO:HB3	66:AV:217:LYS:HB3	1.78	0.64
2:B:51:VAL:HG22	2:B:54:ARG:HH11	1.62	0.64
2:B:151:ILE:HG21	3:C:159:TYR:HD2	1.62	0.64
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.64
12:M:618:GLU:OE2	12:M:620:TRP:NE1	2.30	0.64
18:T:39:VAL:HG12	18:T:45:VAL:HB	1.79	0.64
67:AK:422:ALA:O	67:AK:426:ASN:ND2	2.31	0.64
75:AL:502:CDL:C58	76:AL:503:PEE:C38	2.76	0.64
65:AU:202:ARG:NH2	66:AV:256:TYR:OH	2.28	0.64
2:B:52:THR:HG22	21:W:33:TYR:CE1	2.33	0.64
75:AJ:405:CDL:HB61	75:AJ:405:CDL:C31	2.27	0.64
10:K:81:THR:HB	14:O:88:ARG:HD2	1.79	0.64
12:M:543:LYS:HG3	12:M:565:PHE:CD2	2.33	0.64
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.64
63:AF:40:GLU:HG2	63:AF:45:LYS:HG3	1.77	0.64
67:AK:60:ARG:HG3	67:AK:124:GLU:HG2	1.78	0.64
68:AL:75:ILE:HG22	68:AL:77:VAL:H	1.61	0.64
68:AY:75:ILE:HG22	68:AY:77:VAL:H	1.61	0.64
12:M:591:GLU:N	12:M:591:GLU:OE1	2.30	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
58:AA:49:VAL:HG21	76:AJ:403:PEE:O5	1.98	0.64
65:AH:202:ARG:NH2	66:AJ:256:TYR:OH	2.31	0.64
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.64
20:V:27:SER:O	20:V:30:SER:OG	2.14	0.64
62:AR:34:ARG:CZ	62:AR:78:ARG:HH12	2.11	0.63
68:AY:424:ILE:CG2	68:AY:429:TRP:HE1	2.09	0.63
68:AY:460:GLY:HA2	68:AY:462:ILE:HD12	1.79	0.63
6:G:120:MET:HA	6:G:123:GLU:HG2	1.78	0.63
16:Q:145:MET:H	16:Q:178:THR:HG21	1.63	0.63
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.63
65:AU:288:MET:SD	76:AU:401:PEE:O4	2.55	0.63
67:AW:313:VAL:HG21	67:AW:323:VAL:HG21	1.80	0.63
14:O:245:VAL:O	14:O:247:ALA:N	2.31	0.63
48:O:24:LEU:H	49:1:34:ASN:HD21	1.44	0.63
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.63
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.63
67:AK:413:LEU:HA	67:AK:416:ILE:HG22	1.79	0.63
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	0.63
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	0.63
16:Q:171:ARG:HH21	16:Q:231:GLY:HA2	1.61	0.63
65:AH:262:THR:HG22	65:AH:264:SER:H	1.63	0.63
76:AJ:403:PEE:H61	76:AJ:403:PEE:H28	1.81	0.63
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	0.63
76:V:202:PEE:C24	76:V:202:PEE:H32	2.25	0.63
66:AV:326:TRP:HZ2	76:AV:403:PEE:H13	1.60	0.63
66:AV:333:LEU:HD21	76:AV:403:PEE:C39	2.29	0.63
59:AO:7:ARG:NH1	67:AW:287:SER:OG	2.32	0.63
12:M:467:LYS:HG3	12:M:503:THR:HB	1.80	0.63
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.63
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.63
16:Q:84:PHE:HE2	16:Q:91:ALA:HB2	1.63	0.63
22:Y:74:TRP:HE3	22:Y:75:HIS:HA	1.62	0.63
1:A:207:GLY:O	70:A:502:FMN:C5A	2.47	0.63
62:AR:34:ARG:HG3	62:AR:78:ARG:HH12	1.61	0.63
63:AS:97:GLU:OE1	63:AS:100:ARG:NH2	2.31	0.63
66:AV:200:LEU:HD13	82:AV:402:HEM:HAD2	1.79	0.63
67:AW:450:VAL:O	67:AW:453:LEU:HD13	1.98	0.63
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.80	0.63
67:AK:185:ALA:HB3	67:AK:251:ALA:HB2	1.81	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AF:28:ASN:OD1	63:AF:29:LYS:N	2.31	0.63
68:AL:322:VAL:HG12	68:AL:323:HIS:H	1.64	0.63
67:AW:151:VAL:HG12	67:AW:155:GLN:HE21	1.64	0.63
2:B:99:HIS:NE2	69:B:302:SF4:S1	2.70	0.63
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	0.63
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.81	0.63
68:AY:280:ASP:HA	68:AY:461:PRO:HB3	1.79	0.62
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.47	0.62
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.81	0.62
3:C:137:VAL:CG2	16:Q:87:GLN:NE2	2.59	0.62
57:9:13:LYS:HD3	57:9:13:LYS:H	1.65	0.62
67:AK:70:ARG:NH2	67:AK:332:ASP:OD2	2.31	0.62
58:AA:19:LEU:HD23	68:AL:273:SER:HB3	1.81	0.62
61:AD:53:TRP:NE1	65:AH:139:CYS:O	2.32	0.62
66:AV:138:MET:HB2	66:AV:255:ASN:HD21	1.62	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
48:0:16:TYR:CE1	48:0:25:PRO:HG3	2.34	0.62
75:AG:101:CDL:H512	75:AG:101:CDL:H551	1.81	0.62
66:AV:332:LEU:HD11	76:AV:403:PEE:H37	1.79	0.62
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.62
11:L:75:ARG:HH21	11:L:101:PHE:HB3	1.63	0.62
14:O:158:ILE:HD11	14:O:164:THR:HB	1.81	0.62
65:AH:202:ARG:HD2	65:AH:279:GLU:HG3	1.81	0.62
67:AW:443:ASN:O	67:AW:444:LEU:HB2	2.00	0.62
16:Q:150:ALA:HB1	16:Q:400:ILE:HG13	1.80	0.62
22:Y:96:GLU:O	22:Y:97:LEU:HB2	1.98	0.62
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.81	0.62
65:AH:112:ARG:NH1	65:AH:269:ASP:OD2	2.31	0.62
6:G:80:GLN:HE22	6:G:100:VAL:HG13	1.63	0.62
49:1:82:TYR:HB3	49:1:83:PRO:HD3	1.82	0.62
62:AE:26:LEU:O	62:AE:28:ASP:N	2.27	0.62
68:AL:228:ARG:HH22	68:AL:263:PRO:HG2	1.65	0.62
68:AY:424:ILE:HG23	68:AY:424:ILE:O	2.00	0.62
9:J:241:TYR:CE2	9:J:243:VAL:HB	2.35	0.62
13:N:29:ARG:NH2	13:N:65:THR:O	2.23	0.62
9:J:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.62
23:Z:24:ILE:HD11	23:Z:47:ARG:HG2	1.80	0.62
68:AL:70:THR:OG1	68:AL:410:CYS:SG	2.50	0.62
12:M:627:SER:OG	12:M:632:MET:O	2.17	0.62
15:P:83:GLU:HB3	15:P:142:ARG:HH12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:231:LEU:HD21	60:AP:239:HIS:HA	1.81	0.62
67:AK:184:ASN:HB3	67:AK:251:ALA:HA	1.81	0.62
75:AL:502:CDL:C58	76:AL:503:PEE:H63	2.29	0.62
66:AV:119:LEU:HD12	66:AV:192:LEU:HB3	1.81	0.62
1:A:116:ASN:HD22	70:A:502:FMN:HM83	1.63	0.62
67:AW:299:VAL:HG21	68:AY:110:GLU:HG3	1.81	0.62
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	0.62
15:P:154:GLU:HA	15:P:179:ALA:HB2	1.81	0.62
67:AK:295:ALA:HB2	67:AK:325:ALA:HB3	1.82	0.61
62:AR:30:LEU:HD13	62:AR:86:LEU:HD11	1.82	0.61
67:AW:127:ARG:NH1	67:AW:224:GLY:O	2.32	0.61
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.33	0.61
12:M:282:ASN:HA	12:M:413:LEU:HD23	1.81	0.61
14:O:143:ARG:HB3	14:O:184:PRO:HD3	1.82	0.61
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.81	0.61
65:AU:308:ARG:HH11	75:AU:403:CDL:H1O1	1.46	0.61
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.61
12:M:387:LEU:HA	12:M:514:ASN:HB2	1.82	0.61
12:M:546:PHE:HB2	12:M:568:TYR:HA	1.81	0.61
50:2:13:ALA:O	50:2:18:ARG:HD2	2.00	0.61
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.61
67:AK:51:SER:HB2	67:AK:230:LEU:HD12	1.82	0.61
68:AL:96:LEU:HD23	68:AL:164:GLU:HG3	1.80	0.61
61:AQ:34:ARG:HH12	61:AQ:38:GLN:HB3	1.64	0.61
66:AV:141:TRP:HB3	66:AV:268:ILE:HD11	1.82	0.61
67:AW:125:CYS:HB3	67:AW:133:LEU:HD22	1.81	0.61
52:4:57:ARG:HH11	52:4:57:ARG:HB3	1.64	0.61
65:AU:296:MET:CE	76:AU:401:PEE:C33	2.71	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.33	0.61
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.30	0.61
63:AF:34:ARG:CG	63:AF:34:ARG:HH11	2.13	0.61
66:AJ:96:LEU:HD23	76:AJ:403:PEE:H26	1.82	0.61
65:AU:133:ARG:O	65:AU:135:LEU:N	2.29	0.61
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
22:Y:81:LEU:HD23	22:Y:82:GLY:N	2.14	0.61
67:AW:116:ARG:NH1	67:AW:188:ASN:O	2.33	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.61
7:H:89:ASN:O	7:H:93:LYS:HG2	2.00	0.61
12:M:177:ILE:HG13	12:M:179:CYS:SG	2.40	0.61
12:M:346:VAL:HB	12:M:548:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
1:A:161:GLU:O	14:O:192:TYR:OH	2.18	0.61
1:A:88:ARG:O	1:A:244:ASN:ND2	2.32	0.61
64:AT:38:TRP:CE3	64:AT:41:ILE:HD13	2.35	0.61
3:C:184:PRO:HD3	16:Q:223:HIS:HD2	1.65	0.61
9:J:286:ARG:NH2	9:J:356:HIS:O	2.34	0.61
12:M:534:VAL:HG12	12:M:536:ALA:H	1.66	0.61
13:N:130:THR:N	18:T:44:GLN:OE1	2.34	0.61
9:J:226:ILE:HD12	9:J:289:LEU:N	2.16	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
62:AE:30:LEU:HD21	65:AH:216:THR:HG21	1.83	0.61
61:AD:48:ASN:HD22	65:AH:104:SER:HB3	1.66	0.61
76:AL:503:PEE:H49	76:AL:503:PEE:H26	1.78	0.61
11:L:75:ARG:HH11	11:L:104:ARG:HE	1.49	0.61
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.61
1:A:339:PHE:HB3	1:A:349:LEU:HD13	1.81	0.61
65:AH:315:LYS:NZ	75:AH:403:CDL:OB3	2.21	0.61
75:AL:502:CDL:H572	76:AL:503:PEE:C38	2.24	0.61
62:AR:34:ARG:HH11	62:AR:78:ARG:CZ	2.13	0.61
62:AR:86:LEU:HD23	62:AR:86:LEU:C	2.21	0.61
65:AU:135:LEU:HA	65:AU:138:VAL:HG12	1.82	0.61
65:AU:242:ILE:HG12	65:AU:244:MET:H	1.64	0.61
67:AW:318:GLN:HB3	67:AW:320:PRO:HD2	1.83	0.61
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.61
14:O:137:THR:OG1	14:O:176:CYS:N	2.34	0.61
15:P:212:TYR:HA	15:P:219:VAL:HA	1.83	0.61
75:V:201:CDL:OA7	75:V:201:CDL:O1	2.16	0.61
75:AJ:404:CDL:HB62	66:AV:13:LEU:HD22	1.83	0.60
67:AK:183:ARG:CG	67:AK:183:ARG:HH21	2.14	0.60
75:AL:502:CDL:OA9	76:AL:503:PEE:O5	2.19	0.60
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.60
22:Y:73:PHE:O	22:Y:73:PHE:HD1	1.84	0.60
60:AC:104:ARG:HH21	68:AL:292:GLU:HG3	1.64	0.60
67:AK:363:GLN:CB	67:AK:365:ASN:OD1	2.49	0.60
68:AL:165:ARG:NH2	68:AL:211:LEU:O	2.32	0.60
2:B:103:ARG:NH2	18:T:66:ASN:O	2.35	0.60
9:J:319:VAL:O	9:J:323:HIS:ND1	2.28	0.60
11:L:128:PHE:HA	15:P:121:THR:HG22	1.82	0.60
12:M:339:ALA:HB3	12:M:544:VAL:HG12	1.82	0.60
12:M:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
11:L:89:SER:HG	15:P:239:TRP:HE1	1.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:111:PHE:HE2	21:W:117:VAL:HG11	1.66	0.60
58:AA:78:TYR:HB3	62:AE:65:GLU:HG2	0.68	0.60
65:AH:124:CYS:CB	81:AH:402:HEC:HBC2	2.31	0.60
66:AV:206:ASN:OD1	66:AV:207:ASN:N	2.34	0.60
66:AV:272:TRP:HA	66:AV:275:LEU:HG	1.84	0.60
66:AV:83:HIS:NE2	82:AV:401:HEM:C4D	2.67	0.60
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.34	0.60
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	0.60
21:W:39:GLY:O	21:W:42:THR:OG1	2.15	0.60
57:9:28:LEU:HB2	57:9:29:PRO:HD3	1.83	0.60
3:C:205:ARG:O	3:C:205:ARG:HG3	2.02	0.60
12:M:483:ARG:O	12:M:485:ASP:N	2.33	0.60
14:O:87:GLN:O	14:O:91:GLY:N	2.22	0.60
58:AN:73:LYS:O	58:AN:77:ALA:N	2.35	0.60
12:M:228:VAL:HG23	12:M:230:ALA:H	1.66	0.60
12:M:345:LEU:HB2	12:M:548:LEU:HD21	1.84	0.60
67:AK:101:ARG:NH1	68:AL:325:SER:O	2.33	0.60
68:AY:98:PHE:CZ	68:AY:120:LEU:HD13	2.36	0.60
68:AY:460:GLY:HA2	68:AY:462:ILE:H	1.65	0.60
64:AT:14:VAL:O	64:AT:18:VAL:HG23	2.02	0.60
66:AV:200:LEU:CD1	82:AV:402:HEM:HAD2	2.32	0.60
7:H:77:LEU:O	7:H:80:VAL:HG12	2.01	0.60
9:J:208:GLY:H	9:J:211:ASP:HB2	1.66	0.60
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	0.60
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	0.60
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.13	0.60
16:Q:80:ILE:C	16:Q:81:THR:CG2	2.70	0.60
16:Q:338:ARG:HH12	21:W:23:ARG:HB3	1.65	0.60
63:AS:71:LEU:O	65:AU:315:LYS:NZ	2.35	0.60
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	0.60
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60
9:J:188:GLU:HG3	9:J:200:ILE:HG21	1.83	0.60
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.60
58:AA:71:LYS:HE2	65:AH:87:LEU:HD12	1.84	0.60
63:AF:29:LYS:CB	63:AF:75:ILE:HD11	2.22	0.60
66:AJ:282:ARG:HD2	66:AJ:343:VAL:HG22	1.83	0.60
64:AT:39:ARG:HH21	64:AT:39:ARG:CG	2.15	0.60
68:AY:73:VAL:HG23	68:AY:147:LEU:HD23	1.83	0.60
4:E:97:TRP:HH2	15:P:185:ARG:HH11	1.49	0.60
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:602:ARG:HE	12:M:659:ILE:HD11	1.67	0.60
13:N:137:TRP:CH2	13:N:140:PRO:HD3	2.36	0.60
75:AL:502:CDL:H761	76:AL:503:PEE:H74	1.82	0.60
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.82	0.60
13:N:129:THR:HA	18:T:44:GLN:HE22	1.67	0.60
50:2:62:CYS:SG	50:2:84:SER:OG	2.60	0.59
59:AB:33:THR:HA	59:AB:38:PRO:HG3	1.82	0.59
75:AG:101:CDL:H521	75:AG:101:CDL:C71	2.32	0.59
59:AO:34:VAL:HB	59:AO:35:PRO:HD3	1.83	0.59
66:AV:181:PHE:HA	66:AV:184:ILE:HG22	1.83	0.59
68:AY:96:LEU:HA	68:AY:99:LYS:HG2	1.83	0.59
9:J:217:PHE:HB2	9:J:280:ILE:HD13	1.83	0.59
12:M:460:HIS:CD2	12:M:462:PHE:HB3	2.38	0.59
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.66	0.59
1:A:412:LEU:HA	1:A:415:ILE:HD12	1.84	0.59
64:AG:38:TRP:O	64:AG:42:LEU:HD12	2.02	0.59
66:AV:311:LYS:HG3	66:AV:379:TRP:HE1	1.67	0.59
68:AY:89:ALA:O	68:AY:93:LEU:HG	2.02	0.59
12:M:69:LEU:HD21	12:M:184:ARG:HB2	1.83	0.59
1:A:263:ALA:HA	1:A:271:SER:HB3	1.83	0.59
59:AB:7:ARG:NH1	67:AK:287:SER:OG	2.25	0.59
68:AL:79:SER:HB3	68:AL:126:ARG:HA	1.84	0.59
61:AQ:48:ASN:HB2	61:AQ:51:LYS:HD2	1.85	0.59
68:AY:96:LEU:CD2	68:AY:161:ILE:CD1	2.80	0.59
68:AY:326:SER:O	68:AY:330:SER:N	2.30	0.59
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.59
1:A:35:LEU:HD22	1:A:290:GLU:HA	1.82	0.59
58:AA:40:ARG:HG3	58:AA:41:ARG:N	2.16	0.59
61:AD:34:ARG:NH1	61:AD:38:GLN:OE1	2.35	0.59
58:AA:78:TYR:CG	62:AE:65:GLU:HA	2.33	0.59
60:AP:131:ASN:HD22	76:AU:401:PEE:H7	1.66	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.67	0.59
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.83	0.59
21:W:29:GLY:O	21:W:32:GLY:N	2.34	0.59
2:B:208:LEU:HD22	8:I:39:PRO:HD2	1.85	0.59
2:B:64:LEU:O	2:B:68:LEU:N	2.30	0.59
12:M:519:ILE:HG12	12:M:521:SER:H	1.68	0.59
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.59
22:Y:45:ARG:HG3	23:Z:52:ARG:HB2	1.84	0.59
1:A:123:GLY:HA3	1:A:355:ILE:HD11	1.82	0.59
59:AB:37:THR:HA	68:AL:174:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:79:SER:N	60:AP:82:ASP:OD2	2.35	0.59
63:AS:43:ASP:OD2	63:AS:102:ARG:NH1	2.35	0.59
64:AT:40:LEU:C	64:AT:40:LEU:HD12	2.21	0.59
62:AR:30:LEU:HD21	65:AU:216:THR:HG23	1.84	0.59
9:J:172:ALA:O	9:J:185:ALA:HB2	2.03	0.59
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.59
20:V:40:ARG:HA	75:V:201:CDL:OB3	2.02	0.59
68:AY:98:PHE:CD2	68:AY:120:LEU:HD13	2.29	0.59
4:E:127:ASP:HB3	4:E:128:PRO:HD2	1.84	0.59
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
68:AL:387:GLU:OE2	68:AL:390:ARG:NH2	2.27	0.59
1:A:220:GLN:NE2	14:O:114:GLU:O	2.35	0.59
56:8:46:LYS:O	56:8:47:LYS:HB2	2.03	0.59
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	0.59
62:AE:33:VAL:HG11	62:AE:85:LYS:O	2.03	0.59
60:AP:81:THR:HG21	68:AY:202:GLU:HB2	1.84	0.59
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.85	0.59
12:M:624:ARG:NE	12:M:636:TYR:O	2.36	0.59
52:4:57:ARG:HG3	52:4:60:TYR:CE2	2.38	0.58
66:AV:338:ILE:HD11	66:AV:350:ILE:HG22	1.84	0.58
3:C:89:CYS:HB2	3:C:123:ALA:HB1	1.85	0.58
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.58
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
12:M:126:LEU:HD12	18:T:98:LYS:O	2.03	0.58
23:Z:25:GLU:HA	23:Z:30:GLU:HG3	1.84	0.58
60:AC:96:VAL:O	68:AL:269:ARG:NH1	2.36	0.58
60:AP:244:ASP:OD1	60:AP:248:ARG:N	2.36	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58
14:O:138:THR:HA	14:O:141:MET:HB3	1.85	0.58
63:AS:7:VAL:HB	63:AS:10:SER:HB2	1.84	0.58
9:J:192:ARG:O	9:J:196:PRO:HA	2.02	0.58
9:J:212:ARG:HG2	9:J:212:ARG:NH1	2.15	0.58
14:O:48:ASN:HD22	14:O:94:PRO:HA	1.68	0.58
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.58
2:B:186:GLU:OE2	18:T:64:ASN:N	2.36	0.58
60:AC:132:ALA:HB2	76:AH:401:PEE:H24	1.84	0.58
15:P:147:THR:HG21	15:P:153:ILE:HB	1.84	0.58
55:7:43:SER:OG	55:7:45:VAL:HG12	2.04	0.58
82:AV:402:HEM:HMB1	82:AV:402:HEM:HBB2	1.85	0.58
4:E:32:VAL:O	4:E:35:LEU:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	0.58
1:A:93:PHE:HE2	1:A:98:LYS:CD	2.05	0.58
67:AK:323:VAL:HG13	67:AK:340:THR:HG22	1.85	0.58
66:AV:333:LEU:HD21	76:AV:403:PEE:H62	1.86	0.58
12:M:330:LEU:HD22	12:M:626:LEU:HD21	1.84	0.58
66:AJ:283:SER:O	66:AJ:352:GLN:NE2	2.33	0.58
2:B:198:GLU:OE1	13:N:88:ARG:HB2	2.04	0.58
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.58
12:M:308:ARG:HA	12:M:314:LEU:HA	1.86	0.58
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.69	0.58
16:Q:80:ILE:C	16:Q:81:THR:HG23	2.23	0.58
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
67:AK:57:PRO:O	67:AK:127:ARG:HG3	2.04	0.58
68:AY:98:PHE:CE2	68:AY:120:LEU:HD12	2.36	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.85	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58
1:A:307:VAL:HG11	1:A:314:LEU:HD21	1.86	0.58
58:AA:29:HIS:HD2	58:AA:33:LYS:HB2	1.69	0.58
67:AK:438:MET:HB3	67:AK:450:VAL:HG13	1.86	0.58
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.58
8:I:69:ILE:HB	15:P:76:VAL:HB	1.85	0.58
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.58
66:AJ:100:ARG:NH2	82:AJ:402:HEM:O2A	2.37	0.58
82:AV:402:HEM:HHA	82:AV:402:HEM:HBA1	1.86	0.58
67:AW:70:ARG:NH2	67:AW:332:ASP:OD2	2.21	0.58
67:AW:357:GLN:O	67:AW:360:THR:OG1	2.17	0.58
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	0.58
12:M:501:ARG:NH1	12:M:666:GLN:HB2	2.18	0.58
1:A:118:ASP:OD1	1:A:120:GLY:N	2.35	0.57
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.57
60:AC:204:ARG:NH1	60:AC:248:ARG:HG3	2.19	0.57
63:AF:41:ASP:OD1	63:AF:41:ASP:N	2.36	0.57
60:AP:183:GLU:HA	60:AP:186:GLN:HG2	1.86	0.57
65:AU:296:MET:HE2	76:AU:401:PEE:H51	1.86	0.57
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.57
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	1.86	0.57
1:A:243:ALA:HA	70:A:502:FMN:O2P	2.04	0.57
1:A:438:LEU:HD21	1:A:446:LEU:HD21	1.86	0.57
66:AJ:163:TRP:CD2	75:AJ:405:CDL:H331	2.39	0.57
67:AK:177:LEU:HD21	67:AK:272:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AR:37:CYS:SG	62:AR:85:LYS:NZ	2.73	0.57
2:B:36:TYR:HB3	8:I:104:TRP:HE3	1.68	0.57
9:J:212:ARG:HH11	9:J:212:ARG:CG	2.12	0.57
12:M:210:ILE:HG23	12:M:212:LYS:H	1.69	0.57
12:M:222:ILE:O	12:M:225:ILE:HG22	2.04	0.57
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.57
14:O:160:VAL:HA	14:O:171:LEU:HD23	1.86	0.57
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
19:U:67:PRO:HB3	19:U:74:GLN:HB2	1.86	0.57
52:4:75:ARG:NH1	52:4:75:ARG:HG2	2.19	0.57
59:AB:27:ARG:NH1	67:AK:171:THR:HG22	2.19	0.57
68:AL:282:LEU:HB2	68:AL:461:PRO:HD3	1.86	0.57
66:AV:14:ILE:HD13	76:AY:502:PEE:C25	2.22	0.57
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.84	0.57
3:C:67:LEU:HD22	3:C:207:LEU:CD2	2.34	0.57
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.57
9:J:204:SER:O	9:J:240:VAL:HG23	2.04	0.57
12:M:177:ILE:O	12:M:177:ILE:HG13	2.04	0.57
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.57
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.57
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.57
66:AV:343:VAL:HG13	66:AV:348:THR:HG22	1.84	0.57
5:F:63:PRO:HB2	5:F:79:LEU:CB	2.31	0.57
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.57
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.57
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
58:AA:78:TYR:CD1	62:AE:65:GLU:N	2.73	0.57
66:AV:333:LEU:CD2	76:AV:403:PEE:H66	2.35	0.57
68:AY:113:VAL:HG21	68:AY:120:LEU:HD23	1.87	0.57
6:G:134:ASP:O	6:G:138:LEU:N	2.38	0.57
9:J:329:LEU:HD13	9:J:332:LEU:HB2	1.84	0.57
20:V:40:ARG:HD3	20:V:59:TYR:HE2	1.68	0.57
1:A:209:GLU:HB3	70:A:502:FMN:H3'	1.84	0.57
68:AL:134:LYS:NZ	68:AL:407:THR:OG1	2.38	0.57
71:AL:501:PLX:H71	76:AL:503:PEE:C13	2.33	0.57
60:AP:104:ARG:NH2	68:AY:293:GLY:O	2.37	0.57
68:AY:423:ARG:O	68:AY:424:ILE:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:NH2	21:W:26:PRO:O	2.38	0.57
8:I:36:GLN:HE22	16:Q:239:GLY:HA2	1.69	0.57
12:M:636:TYR:CE1	12:M:642:VAL:HB	2.39	0.57
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.57
63:AF:97:GLU:OE2	67:AW:147:ARG:NH1	2.38	0.57
67:AW:217:ARG:HE	67:AW:245:GLY:HA3	1.69	0.57
2:B:97:GLY:H	2:B:167:GLU:HG3	1.70	0.57
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.57
12:M:358:LEU:O	12:M:363:SER:N	2.35	0.57
16:Q:81:THR:HA	16:Q:100:GLU:HA	1.86	0.57
22:Y:39:HIS:ND1	22:Y:40:ILE:HG13	2.20	0.57
1:A:382:CYS:SG	69:A:501:SF4:S4	3.03	0.57
67:AW:274:GLU:OE2	67:AW:333:SER:OG	2.16	0.57
14:O:148:ILE:HG23	14:O:201:ILE:HD11	1.87	0.57
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.57
63:AF:36:ASP:OD1	63:AF:90:TYR:OH	2.17	0.57
66:AJ:206:ASN:OD1	66:AJ:207:ASN:N	2.37	0.57
76:AY:502:PEE:O4	76:AY:502:PEE:H19	2.04	0.57
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.68	0.57
9:J:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.57
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.57
16:Q:306:GLN:O	16:Q:308:TYR:N	2.38	0.57
1:A:235:VAL:HG22	1:A:240:THR:HG21	1.87	0.57
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.57
76:AH:401:PEE:H66	76:AH:401:PEE:C18	2.30	0.57
67:AK:378:LEU:HB3	67:AK:416:ILE:HD11	1.87	0.57
63:AS:70:ASN:HD22	66:AV:209:LEU:HG	1.69	0.57
67:AW:449:PHE:HB2	67:AW:452:GLU:OE2	2.04	0.57
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.57
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	0.57
12:M:391:ILE:O	12:M:417:ARG:NH2	2.38	0.57
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.57
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.38	0.56
16:Q:390:GLN:HE22	16:Q:417:SER:HB3	1.68	0.56
20:V:139:PRO:O	20:V:141:VAL:N	2.38	0.56
49:1:78:HIS:ND1	53:5:12:LEU:HD22	2.21	0.56
65:AH:156:ASP:OD1	65:AH:157:GLY:N	2.37	0.56
67:AK:195:TYR:O	67:AK:199:LYS:NZ	2.30	0.56
68:AY:280:ASP:O	68:AY:362:ARG:NH2	2.37	0.56
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:V:202:PEE:H40	76:V:202:PEE:H57	1.87	0.56
56:8:41:ARG:HG3	57:9:40:TYR:CE2	2.40	0.56
67:AK:259:ARG:CD	67:AK:444:LEU:HD13	2.30	0.56
60:AP:197:ASP:O	60:AP:257:ASN:ND2	2.37	0.56
60:AP:204:ARG:NH1	60:AP:246:SER:O	2.38	0.56
66:AV:333:LEU:HD22	76:AV:403:PEE:H66	1.87	0.56
68:AY:96:LEU:HD23	68:AY:161:ILE:HD13	1.87	0.56
12:M:454:ASP:HB3	12:M:460:HIS:HB2	1.85	0.56
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.44	0.56
21:W:31:SER:OG	21:W:35:MET:HE3	2.05	0.56
65:AH:242:ILE:HG12	65:AH:244:MET:H	1.70	0.56
66:AJ:24:PRO:HD2	66:AJ:27:ILE:HD11	1.87	0.56
58:AN:19:LEU:HD23	68:AY:273:SER:HB3	1.86	0.56
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	0.56
16:Q:84:PHE:CE2	16:Q:91:ALA:HB2	2.40	0.56
17:S:59:ARG:O	17:S:61:TYR:N	2.36	0.56
23:Z:51:TRP:O	23:Z:53:TYR:N	2.37	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
66:AJ:51:LEU:HD13	82:AJ:401:HEM:HBD1	1.88	0.56
58:AN:41:ARG:HE	75:AN:101:CDL:PA1	2.28	0.56
65:AU:133:ARG:NH1	66:AV:72:ASP:OD1	2.32	0.56
5:F:16:LEU:HD11	5:F:19:ILE:HB	1.87	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
12:M:225:ILE:HD12	12:M:285:TRP:CH2	2.39	0.56
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.56
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.56
23:Z:22:TRP:CE3	23:Z:51:TRP:HA	2.40	0.56
54:6:3:ASN:HD22	54:6:3:ASN:C	2.08	0.56
66:AJ:100:ARG:HH22	82:AJ:402:HEM:HBD1	1.71	0.56
67:AK:351:ILE:HD11	67:AK:448:PRO:HD2	1.86	0.56
68:AL:470:ARG:HH22	75:AL:502:CDL:PA1	2.28	0.56
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.56
9:J:141:PHE:CZ	9:J:180:TYR:CD1	2.93	0.56
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.86	0.56
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
20:V:62:THR:HG22	20:V:104:ARG:HE	1.69	0.56
20:V:40:ARG:NH2	20:V:55:LYS:HD3	2.20	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.56
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:337:LEU:HB3	68:AL:368:MET:HG2	1.87	0.56
58:AN:19:LEU:HD11	60:AP:88:PHE:HB3	1.88	0.56
65:AU:315:LYS:HZ2	75:AU:403:CDL:HB22	1.71	0.56
81:AU:402:HEC:HHC	81:AU:402:HEC:HBB3	1.88	0.56
67:AW:272:VAL:HG11	67:AW:335:LEU:HB3	1.87	0.56
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.39	0.56
63:AF:67:LEU:O	63:AF:71:LEU:HD23	2.05	0.56
67:AW:185:ALA:HB3	67:AW:251:ALA:HB2	1.88	0.56
68:AY:74:TRP:CD2	68:AY:414:GLY:HA3	2.40	0.56
5:F:16:LEU:HB3	5:F:51:LEU:HD13	1.88	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
51:3:5:LYS:HD2	51:3:6:GLY:N	2.21	0.56
59:AO:20:ARG:HD2	59:AO:51:SER:HB3	1.88	0.56
66:AV:111:GLU:HG2	66:AV:199:PHE:CD1	2.41	0.56
67:AW:259:ARG:NH2	67:AW:447:THR:OG1	2.38	0.56
12:M:221:ASN:HB3	12:M:285:TRP:CE3	2.40	0.56
75:AJ:405:CDL:HB62	75:AJ:405:CDL:OB7	2.05	0.56
64:AG:17:TRP:NE1	68:AL:382:SER:OG	2.39	0.56
64:AT:40:LEU:HD12	64:AT:41:ILE:H	1.64	0.56
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	0.56
11:L:82:PRO:HD3	11:L:98:LYS:HG2	1.87	0.56
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	0.56
52:4:71:THR:O	52:4:75:ARG:HD3	2.05	0.56
60:AP:123:VAL:HG13	61:AQ:29:VAL:HG22	1.88	0.56
66:AV:165:TRP:O	66:AV:174:THR:OG1	2.23	0.56
5:F:17:ARG:HB3	5:F:68:ARG:HH21	1.71	0.56
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.56
67:AK:399:GLN:NE2	67:AK:407:MET:HB3	2.20	0.55
9:J:132:ARG:HD2	9:J:134:TRP:NE1	2.20	0.55
12:M:476:LEU:HD11	12:M:480:ALA:HB3	1.87	0.55
60:AC:83:ILE:HD12	68:AL:189:ALA:HB2	1.87	0.55
66:AJ:181:PHE:HA	66:AJ:184:ILE:HG22	1.88	0.55
82:AJ:401:HEM:HMB2	82:AJ:401:HEM:HBB2	1.88	0.55
67:AK:235:GLU:HA	67:AK:238:LEU:HD13	1.88	0.55
60:AP:155:LYS:HZ3	60:AP:273:VAL:HG21	1.70	0.55
68:AY:424:ILE:HG23	68:AY:429:TRP:NE1	2.12	0.55
2:B:103:ARG:HH12	18:T:68:ALA:HB2	1.69	0.55
12:M:481:LEU:HD11	12:M:515:ILE:HD12	1.88	0.55
12:M:598:ASN:HB3	12:M:602:ARG:HB3	1.89	0.55
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.55
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.55
60:AP:131:ASN:O	60:AP:135:GLN:HG2	2.05	0.55
60:AP:220:LEU:HB2	74:AP:301:FES:S2	2.46	0.55
68:AY:230:VAL:CG2	68:AY:418:LEU:HD11	2.36	0.55
11:L:133:ASP:O	11:L:136:SER:OG	2.20	0.55
14:O:41:HIS:O	14:O:41:HIS:ND1	2.40	0.55
76:V:202:PEE:C24	76:V:202:PEE:H60	2.36	0.55
20:V:3:PRO:HA	20:V:6:PHE:HB3	1.88	0.55
1:A:381:GLN:CG	69:A:501:SF4:S2	2.94	0.55
63:AF:29:LYS:HG2	63:AF:75:ILE:HD13	1.67	0.55
66:AJ:316:MET:HA	66:AJ:322:GLN:NE2	2.21	0.55
59:AO:27:ARG:NH1	67:AW:171:THR:HG22	2.21	0.55
68:AY:160:GLN:NE2	68:AY:164:GLU:OE2	2.39	0.55
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.89	0.55
4:E:75:ASP:HB3	4:E:78:VAL:HG23	1.89	0.55
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.55
12:M:128:CYS:N	12:M:129:PRO:HD2	2.21	0.55
12:M:408:ARG:HB3	12:M:415:ASN:ND2	2.21	0.55
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.55
1:A:116:ASN:ND2	70:A:502:FMN:HM83	2.20	0.55
62:AE:30:LEU:CD2	65:AH:216:THR:HG23	2.33	0.55
81:AH:402:HEC:HHD	81:AH:402:HEC:HBC3	1.87	0.55
67:AK:375:LYS:NZ	67:AK:416:ILE:O	2.30	0.55
4:E:36:TYR:HD1	4:E:67:PHE:CE2	2.25	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
12:M:50:LEU:N	12:M:91:ALA:O	2.38	0.55
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.55
19:U:67:PRO:HA	19:U:74:GLN:OE1	2.07	0.55
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.55
65:AH:304:TYR:HE1	75:AH:403:CDL:OA3	1.90	0.55
67:AK:93:GLY:HA3	67:AK:139:ASN:HD21	1.72	0.55
60:AP:204:ARG:NH1	60:AP:248:ARG:HG3	2.21	0.55
68:AY:152:GLN:HE21	68:AY:253:ILE:HG13	1.72	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.23	0.55
20:V:40:ARG:HD3	20:V:59:TYR:CE2	2.42	0.55
22:Y:74:TRP:HE3	22:Y:75:HIS:CA	2.19	0.55
1:A:418:GLN:O	1:A:422:HIS:ND1	2.39	0.55
63:AF:49:ARG:HA	63:AF:49:ARG:HE	1.71	0.55
66:AJ:119:LEU:HD11	66:AJ:192:LEU:HB3	1.89	0.55
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.55
15:P:235:LEU:HD22	16:Q:387:GLU:HG2	1.87	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	0.55
63:AS:68:ASP:HA	63:AS:71:LEU:HD12	1.89	0.55
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
9:J:171:ASN:HB2	9:J:181:LEU:HD11	1.84	0.55
12:M:124:HIS:ND1	12:M:125:PRO:HD2	2.22	0.55
48:O:108:PRO:HG2	48:O:111:PHE:CE2	2.42	0.55
50:2:82:CYS:N	50:2:86:GLY:O	2.40	0.55
68:AL:470:ARG:HH12	75:AL:502:CDL:HA31	1.72	0.55
58:AN:43:ARG:HA	58:AN:46:PHE:HD2	1.72	0.55
61:AQ:48:ASN:HD22	65:AU:104:SER:HB3	1.72	0.55
5:F:68:ARG:HD2	5:F:72:GLY:HA2	1.87	0.55
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.55
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.41	0.55
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.55
13:N:57:GLY:H	13:N:59:HIS:CE1	2.24	0.55
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	0.55
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.55
66:AV:138:MET:HB2	66:AV:255:ASN:ND2	2.22	0.55
68:AY:161:ILE:O	68:AY:165:ARG:HG3	2.07	0.55
7:H:16:VAL:HA	7:H:78:GLU:OE2	2.06	0.55
63:AF:27:PHE:CD1	63:AF:28:ASN:N	2.75	0.54
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.23	0.54
58:AA:19:LEU:HD11	60:AC:88:PHE:HB3	1.87	0.54
66:AV:10:LEU:CD2	76:AY:502:PEE:H45	2.34	0.54
75:AG:101:CDL:H331	66:AV:163:TRP:CD1	2.43	0.54
67:AW:449:PHE:HB2	67:AW:452:GLU:CD	2.27	0.54
68:AY:156:LEU:HB2	68:AY:213:ARG:HE	1.73	0.54
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	0.54
12:M:241:ARG:HG2	12:M:243:TRP:CZ2	2.42	0.54
12:M:380:ASP:OD1	12:M:381:LEU:N	2.40	0.54
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.42	0.54
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	0.54
58:AA:12:ARG:HA	68:AL:279:ASP:HA	1.89	0.54
58:AA:78:TYR:O	58:AA:81:ASP:HB2	2.07	0.54
76:AU:401:PEE:C19	76:AU:401:PEE:C39	2.86	0.54
68:AY:76:ASP:HB3	68:AY:228:ARG:HG3	1.89	0.54
4:E:56:VAL:HG23	9:J:367:GLU:OE2	2.07	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.72	0.54
12:M:308:ARG:HD2	12:M:312:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:341:ILE:HD12	12:M:555:ILE:HG13	1.89	0.54
12:M:697:THR:O	12:M:702:ARG:NH2	2.40	0.54
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
1:A:207:GLY:O	70:A:502:FMN:C9A	2.56	0.54
60:AC:153:GLU:HB3	60:AC:273:VAL:HB	1.88	0.54
60:AC:173:PRO:HB2	60:AC:215:GLY:HA3	1.90	0.54
68:AL:465:LEU:HD12	68:AL:466:PRO:HD2	1.89	0.54
60:AP:207:LYS:HD3	60:AP:265:PHE:HE2	1.71	0.54
65:AU:98:HIS:NE2	65:AU:208:GLU:OE2	2.38	0.54
66:AV:326:TRP:CH2	76:AV:403:PEE:H51	2.42	0.54
68:AY:79:SER:HB3	68:AY:126:ARG:HA	1.90	0.54
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.54
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.54
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.54
49:1:80:GLU:H	49:1:80:GLU:CD	2.10	0.54
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.90	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.89	0.54
15:P:107:GLN:HB3	15:P:109:LYS:HE3	1.89	0.54
15:P:55:HIS:CD2	15:P:78:VAL:HG12	2.42	0.54
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CB	2.54	0.54
48:O:52:SER:OG	48:O:55:GLU:HG3	2.08	0.54
1:A:33:GLY:H	1:A:294:VAL:HG12	1.72	0.54
67:AK:364:GLY:HA2	67:AK:425:ILE:HD12	1.89	0.54
68:AL:311:ILE:O	68:AL:326:SER:OG	2.26	0.54
75:AL:502:CDL:H772	76:AL:503:PEE:C42	2.38	0.54
66:AV:150:LEU:CD2	66:AV:164:ILE:HD13	2.37	0.54
9:J:172:ALA:HA	9:J:181:LEU:CD2	2.38	0.54
9:J:203:PRO:HG2	73:J:401:NDP:C5N	2.37	0.54
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.40	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CD2	2.54	0.54
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.54
75:AL:502:CDL:C58	76:AL:503:PEE:H62	2.37	0.54
59:AO:45:LEU:HA	68:AY:284:PHE:HE2	1.71	0.54
67:AW:185:ALA:HB2	67:AW:249:ALA:HB1	1.89	0.54
9:J:168:SER:O	73:J:401:NDP:H6N	2.08	0.54
49:1:41:LEU:HD12	49:1:41:LEU:O	2.08	0.54
59:AB:29:LEU:O	59:AB:31:GLN:N	2.38	0.54
75:AJ:405:CDL:C78	75:AJ:405:CDL:C74	2.86	0.54
65:AU:292:MET:HE1	66:AV:241:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.54
11:L:170:THR:O	11:L:172:VAL:N	2.35	0.54
63:AF:67:LEU:CD2	66:AJ:209:LEU:HD12	2.28	0.54
68:AL:294:PRO:HG3	68:AL:448:TYR:CZ	2.43	0.54
59:AO:5:ALA:HB1	67:AW:385:SER:HB2	1.90	0.54
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.54
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	0.54
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	0.54
15:P:85:GLU:HG3	15:P:142:ARG:HB2	1.88	0.54
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.54
15:P:235:LEU:HB3	16:Q:387:GLU:HG2	1.90	0.54
50:2:51:SER:HB2	50:2:91:LEU:HD11	1.90	0.54
51:3:2:SER:OG	51:3:3:ALA:N	2.41	0.54
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.90	0.54
60:AC:164:ASN:OD1	60:AC:165:MET:N	2.41	0.54
82:AJ:402:HEM:HMC2	82:AJ:402:HEM:HBC2	1.89	0.54
68:AL:77:VAL:HG21	68:AL:223:HIS:HB3	1.89	0.54
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.54
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.07	0.54
12:M:402:LEU:HA	12:M:475:VAL:HB	1.88	0.54
15:P:94:ILE:N	15:P:154:GLU:OE1	2.28	0.54
16:Q:391:VAL:HG12	16:Q:392:PRO:O	2.09	0.54
63:AF:29:LYS:CD	63:AF:75:ILE:HD13	2.21	0.53
63:AS:28:ASN:HD22	63:AS:82:THR:HB	1.73	0.53
82:AV:401:HEM:HBB2	82:AV:401:HEM:HMB1	1.91	0.53
12:M:173:MET:C	12:M:175:ARG:N	2.60	0.53
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.53
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.53
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
53:5:63:MET:HB3	53:5:68:ILE:HD11	1.89	0.53
62:AE:21:GLU:O	62:AE:24:GLU:CA	2.57	0.53
67:AK:36:GLN:HG2	67:AK:53:GLU:HB3	1.90	0.53
68:AL:66:GLN:NE2	68:AL:406:THR:OG1	2.41	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
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.53
50:2:55:LYS:HA	50:2:74:LEU:O	2.08	0.53
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.53
67:AK:217:ARG:HH21	67:AK:246:LEU:H	1.56	0.53
59:AB:31:GLN:NE2	67:AK:297:PRO:HA	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:AL:121:ASN:ND2	68:AL:132:TYR:OH	2.36	0.53
63:AS:55:LEU:HD21	63:AS:90:TYR:CD2	2.43	0.53
66:AV:341:GLN:HB3	66:AV:342:PRO:HD2	1.91	0.53
68:AY:296:TRP:NE1	68:AY:419:THR:OG1	1.64	0.53
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.53
50:2:48:LEU:O	50:2:50:PRO:HD3	2.08	0.53
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.53
58:AA:12:ARG:HG2	58:AA:13:HIS:CE1	2.43	0.53
66:AJ:229:ALA:HB1	71:AL:501:PLX:H131	1.89	0.53
67:AW:267:VAL:HG11	67:AW:347:ALA:HB2	1.90	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.53
12:M:53:CYS:SG	12:M:102:ILE:HD12	2.48	0.53
12:M:82:ILE:HB	12:M:85:ALA:HB2	1.91	0.53
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.53
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	0.53
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.53
16:Q:265:ASN:OD1	16:Q:266:ARG:N	2.42	0.53
16:Q:449:ALA:O	16:Q:453:THR:HG23	2.08	0.53
76:V:202:PEE:C24	76:V:202:PEE:H57	2.39	0.53
23:Z:24:ILE:HG22	23:Z:30:GLU:HB2	1.90	0.53
61:AD:60:TYR:HD2	65:AH:141:THR:HG21	1.73	0.53
58:AN:12:ARG:HG3	68:AY:279:ASP:HA	1.91	0.53
75:AN:101:CDL:OB9	66:AV:29:ALA:HB3	2.08	0.53
82:AV:402:HEM:HBC2	82:AV:402:HEM:HMC2	1.90	0.53
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	0.53
12:M:565:PHE:HA	12:M:581:ASP:OD2	2.08	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
63:AF:70:ASN:HB3	66:AJ:26:ASN:HB2	1.91	0.53
67:AK:116:ARG:HH21	67:AK:175:GLU:HG3	1.74	0.53
67:AK:319:GLN:O	67:AK:321:PHE:N	2.41	0.53
2:B:61:TRP:O	2:B:63:GLU:N	2.41	0.53
9:J:172:ALA:HA	9:J:181:LEU:HD23	1.91	0.53
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.53
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.21	0.53
14:O:129:LYS:HB3	14:O:168:LEU:HG	1.91	0.53
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.36	0.53
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AJ:405:CDL:HB61	75:AJ:405:CDL:H312	1.90	0.53
59:AB:54:SER:HA	68:AL:402:HIS:CE1	2.43	0.53
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.53
4:E:24:ASP:OD1	4:E:25:MET:N	2.41	0.53
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.89	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
13:N:94:THR:HG22	13:N:96:ASP:H	1.73	0.53
1:A:117:ALA:HB3	1:A:157:TYR:O	2.08	0.53
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.53
63:AF:72:LYS:O	63:AF:73:HIS:HB2	2.09	0.53
67:AK:289:LEU:O	67:AK:293:LEU:HD13	2.09	0.53
66:AV:149:LEU:HD21	66:AV:281:LEU:CD2	2.31	0.53
59:AO:45:LEU:HD13	67:AW:160:ILE:HG23	1.91	0.53
67:AK:254:ARG:NH2	67:AW:257:GLU:OE1	2.41	0.53
6:G:75:THR:O	6:G:79:ILE:HG12	2.09	0.53
12:M:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
12:M:394:VAL:HG21	12:M:414:PHE:HE1	1.73	0.53
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	0.53
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.53
1:A:317:VAL:HG13	1:A:356:VAL:HA	1.91	0.53
63:AF:36:ASP:OD1	63:AF:62:ARG:NH1	2.42	0.53
75:AL:502:CDL:C76	76:AL:503:PEE:H74	2.38	0.53
68:AY:473:SER:HB3	76:AY:502:PEE:H10	1.91	0.53
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.91	0.53
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.53
18:T:52:ARG:HB3	18:T:55:ARG:HH12	1.74	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
66:AJ:173:PRO:O	66:AJ:177:ARG:HG2	2.09	0.53
67:AK:57:PRO:HG2	68:AL:400:VAL:HG11	1.91	0.53
2:B:90:PRO:HD2	3:C:100:ARG:HH11	1.74	0.53
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.53
7:H:97:TRP:HB3	7:H:100:TRP:CH2	2.43	0.53
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.53
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.53
19:U:69:HIS:ND1	19:U:70:PRO:HA	2.24	0.53
48:O:67:SER:OG	48:O:70:GLU:HG3	2.08	0.52
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.91	0.52
62:AE:34:ARG:HD3	62:AE:78:ARG:CZ	2.36	0.52
60:AP:131:ASN:ND2	76:AU:401:PEE:H7	2.24	0.52
11:L:120:PRO:HB2	15:P:203:PRO:HG3	1.91	0.52
15:P:115:THR:HG22	16:Q:423:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:0:40:LEU:HD13	48:0:59:LEU:HD13	1.91	0.52
1:A:116:ASN:HD22	70:A:502:FMN:C9	2.22	0.52
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	0.52
58:AN:20:SER:HB3	58:AN:23:GLU:HG2	1.91	0.52
64:AT:19:PRO:HA	64:AT:22:TYR:HD2	1.74	0.52
9:J:223:PHE:O	9:J:225:PRO:HD2	2.09	0.52
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.52
60:AC:80:HIS:CE1	68:AL:185:ASN:HD22	2.27	0.52
75:AG:101:CDL:H741	66:AV:156:ILE:HG23	1.91	0.52
67:AK:299:VAL:HG21	68:AL:110:GLU:HG3	1.91	0.52
68:AY:70:THR:HG1	68:AY:410:CYS:HG	1.57	0.52
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	0.52
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.52
12:M:519:ILE:HD13	12:M:522:GLN:HB2	1.90	0.52
12:M:613:PRO:HB3	13:N:134:ILE:HG21	1.91	0.52
51:3:42:ARG:HH11	51:3:42:ARG:HG3	1.74	0.52
66:AJ:281:LEU:HD11	66:AJ:294:LEU:HD22	1.90	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
9:J:64:PHE:CD1	9:J:210:GLU:HB3	2.44	0.52
11:L:61:ILE:HG22	11:L:64:LEU:HD12	1.91	0.52
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.52
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.52
48:0:23:PRO:HD2	49:1:34:ASN:HD22	1.74	0.52
50:2:8:THR:OG1	50:2:11:GLU:HG2	2.09	0.52
76:AH:401:PEE:C40	76:AH:401:PEE:C18	2.86	0.52
68:AL:361:ASP:OD1	68:AL:362:ARG:N	2.42	0.52
60:AP:128:ALA:HB1	76:AU:401:PEE:H55	1.90	0.52
6:G:123:GLU:HB2	6:G:128:PHE:O	2.09	0.52
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	0.52
15:P:113:ASP:HB3	15:P:115:THR:HG23	1.91	0.52
16:Q:338:ARG:NH2	21:W:23:ARG:HB3	2.24	0.52
48:0:40:LEU:HD22	48:0:59:LEU:HD13	1.91	0.52
1:A:181:LEU:HA	1:A:187:CYS:HB3	1.91	0.52
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.52
1:A:68:ILE:HD11	1:A:256:ARG:HG2	1.91	0.52
68:AL:285:ALA:HB3	68:AL:360:CYS:SG	2.50	0.52
62:AR:37:CYS:SG	62:AR:85:LYS:CE	2.97	0.52
66:AV:333:LEU:HD21	76:AV:403:PEE:C38	2.39	0.52
75:AJ:405:CDL:H111	76:AY:502:PEE:C45	2.30	0.52
6:G:137:LYS:O	6:G:139:MET:N	2.42	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)
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
15:P:186:ARG:NH2	15:P:193:PHE:O	2.40	0.52
21:W:35:MET:HA	21:W:38:ILE:HD12	1.91	0.52
8:I:41:LEU:C	21:W:8:GLN:HE22	2.13	0.52
75:AJ:405:CDL:H312	75:AJ:405:CDL:OB4	2.10	0.52
60:AP:239:HIS:HB2	74:AP:301:FES:S1	2.50	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.92	0.52
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.91	0.52
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.52
20:V:58:GLN:O	20:V:62:THR:HG23	2.10	0.52
21:W:33:TYR:CG	21:W:34:SER:N	2.77	0.52
51:3:8:HIS:O	51:3:10:GLY:N	2.42	0.52
67:AK:116:ARG:NH2	67:AK:175:GLU:HG3	2.24	0.52
68:AY:134:LYS:NZ	68:AY:407:THR:OG1	2.42	0.52
68:AY:96:LEU:CD2	68:AY:161:ILE:HD13	2.40	0.52
12:M:645:ARG:O	12:M:648:GLU:HG2	2.10	0.52
17:S:37:ARG:O	21:W:143:TYR:OH	2.27	0.52
18:T:56:PHE:CD1	18:T:61:LYS:HB2	2.45	0.52
1:A:423:THR:OG1	69:A:501:SF4:S4	2.68	0.52
58:AA:41:ARG:NE	75:AA:101:CDL:OA4	2.35	0.52
66:AJ:191:ALA:O	66:AJ:194:THR:OG1	2.20	0.52
67:AK:146:PHE:HD2	67:AK:206:HIS:CE1	2.28	0.52
67:AK:352:LYS:HE2	67:AK:453:LEU:CB	2.40	0.52
72:E:201:8Q1:C30	72:E:201:8Q1:N36	2.73	0.52
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.52
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.92	0.52
16:Q:39:PRO:HB3	16:Q:43:TRP:CE3	2.45	0.52
1:A:86:ARG:NE	1:A:92:GLY:O	2.40	0.52
68:AL:334:ALA:H	68:AL:336:LYS:H	1.58	0.52
68:AL:470:ARG:NH1	75:AL:502:CDL:HA31	2.25	0.52
65:AU:125:HIS:HB3	65:AU:197:LEU:HD13	1.91	0.52
66:AV:173:PRO:HB2	66:AV:177:ARG:HH12	1.74	0.52
68:AY:437:ASP:OD1	68:AY:438:ALA:N	2.43	0.52
68:AY:462:ILE:HG23	68:AY:465:LEU:HB3	1.91	0.52
6:G:143:GLU:HA	6:G:146:ASP:HB3	1.92	0.52
7:H:24:LEU:HD21	7:H:81:ILE:HG22	1.92	0.52
12:M:319:TRP:HZ2	12:M:615:LEU:O	1.92	0.52
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.52
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.91	0.52
58:AA:78:TYR:HE1	62:AE:64:GLU:C	1.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:135:LEU:HA	65:AH:138:VAL:HG12	1.91	0.51
12:M:61:PRO:HG2	12:M:113:ARG:HE	1.74	0.51
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.51
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.25	0.51
19:U:84:LEU:O	21:W:59:ARG:NH1	2.41	0.51
48:O:128:VAL:O	48:O:134:PHE:HB3	2.09	0.51
60:AC:244:ASP:OD1	60:AC:248:ARG:N	2.44	0.51
61:AD:43:ILE:O	61:AD:47:ILE:HD12	2.10	0.51
75:AJ:405:CDL:OA9	75:AJ:405:CDL:H332	2.10	0.51
60:AP:153:GLU:HB3	60:AP:273:VAL:HB	1.91	0.51
76:AU:401:PEE:H57	66:AV:236:LEU:HD13	1.92	0.51
68:AY:160:GLN:O	68:AY:164:GLU:HG2	2.09	0.51
3:C:209:ILE:HG21	9:J:86:CYS:O	2.11	0.51
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.51
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.51
67:AK:438:MET:HB2	67:AK:450:VAL:HG11	1.89	0.51
68:AL:460:GLY:HA2	68:AL:462:ILE:HG13	1.92	0.51
60:AP:194:GLN:O	60:AP:250:ARG:NH1	2.41	0.51
64:AG:9:ARG:HD3	63:AS:109:ALA:O	2.10	0.51
65:AU:270:VAL:HG11	81:AU:402:HEC:HMB1	1.93	0.51
66:AV:97:HIS:CE1	66:AV:100:ARG:HH21	2.27	0.51
67:AW:57:PRO:O	67:AW:127:ARG:HG3	2.11	0.51
67:AW:309:LEU:HD23	67:AW:323:VAL:HG12	1.93	0.51
68:AY:230:VAL:HG21	68:AY:418:LEU:HD11	1.92	0.51
9:J:168:SER:N	9:J:201:VAL:O	2.40	0.51
12:M:464:GLN:HE22	12:M:467:LYS:HE2	1.75	0.51
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.51
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	0.51
16:Q:304:LYS:HE3	16:Q:316:PHE:CE1	2.46	0.51
49:1:63:SER:O	49:1:67:ILE:HG13	2.10	0.51
1:A:300:ILE:HA	1:A:304:ALA:HB3	1.93	0.51
75:AG:101:CDL:C54	75:AG:101:CDL:C73	2.85	0.51
75:AL:502:CDL:H772	76:AL:503:PEE:C43	2.41	0.51
61:AQ:51:LYS:O	65:AU:107:HIS:ND1	2.32	0.51
63:AF:109:ALA:O	64:AT:9:ARG:HD3	2.11	0.51
67:AW:101:ARG:NH1	68:AY:325:SER:O	2.44	0.51
4:E:50:PHE:HB2	4:E:52:LEU:CD1	2.41	0.51
6:G:147:TYR:O	6:G:151:LYS:N	2.43	0.51
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:278:HIS:CD2	12:M:280:ASP:HB2	2.44	0.51
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.51
16:Q:228:ARG:CZ	16:Q:233:HIS:HB2	2.40	0.51
20:V:12:ILE:HG22	20:V:13:PRO:O	2.11	0.51
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.45	0.51
60:AC:183:GLU:HA	60:AC:186:GLN:HG2	1.93	0.51
67:AK:159:LYS:HG3	67:AK:197:ILE:HG21	1.92	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
62:AE:21:GLU:O	62:AE:24:GLU:CB	2.59	0.51
66:AV:263:ASN:OD1	66:AV:264:THR:N	2.44	0.51
68:AY:304:LEU:HD13	68:AY:354:LEU:HD11	1.93	0.51
2:B:127:THR:HB	2:B:144:ASP:OD1	2.10	0.51
2:B:79:PRO:HD2	17:S:1:MET:SD	2.50	0.51
3:C:162:TYR:O	16:Q:123:LEU:HD21	2.10	0.51
16:Q:203:LEU:HD11	16:Q:258:LEU:HD11	1.93	0.51
6:X:77:GLU:HB2	23:Z:13:LYS:HE2	1.93	0.51
63:AF:43:ASP:OD2	63:AF:102:ARG:NH1	2.44	0.51
66:AJ:103:TYR:O	66:AJ:315:MET:HB2	2.10	0.51
67:AK:65:ILE:HG13	67:AK:218:MET:HG2	1.92	0.51
67:AW:107:GLY:O	68:AY:397:ASN:ND2	2.41	0.51
67:AW:214:THR:HG22	67:AW:216:ALA:H	1.75	0.51
68:AY:230:VAL:HG21	68:AY:418:LEU:HD13	1.92	0.51
3:C:112:ALA:O	3:C:113:SER:OG	2.29	0.51
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.51
11:L:107:TRP:HZ3	11:L:118:ALA:HB2	1.76	0.51
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	0.51
62:AE:75:LEU:HD23	62:AE:78:ARG:HD3	1.92	0.51
63:AF:63:ILE:HD13	66:AJ:211:ILE:HG21	1.93	0.51
66:AV:141:TRP:HZ2	66:AV:260:ASN:O	1.93	0.51
66:AV:326:TRP:CH2	76:AV:403:PEE:H13	2.46	0.51
66:AV:47:THR:HG23	66:AV:79:ILE:HG23	1.93	0.51
67:AW:180:ALA:HA	67:AW:254:ARG:NH1	2.26	0.51
67:AW:95:SER:O	67:AW:99:ILE:HD12	2.11	0.51
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	0.51
12:M:76:ARG:HE	12:M:79:LEU:HD21	1.74	0.51
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
13:N:18:GLY:O	13:N:20:LEU:N	2.44	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
16:Q:381:HIS:O	16:Q:385:TYR:HD2	1.93	0.51
18:T:83:ARG:NH1	18:T:103:LEU:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AC:219:HIS:ND1	74:AC:301:FES:S1	2.74	0.51
64:AG:16:ASN:ND2	68:AL:442:ARG:HH12	2.09	0.51
67:AK:92:LYS:HD2	67:AK:143:ALA:HB1	1.93	0.51
66:AV:151:SER:HB2	66:AV:161:VAL:HG21	1.92	0.51
66:AV:96:LEU:CD2	76:AV:403:PEE:H26	2.40	0.51
68:AY:182:VAL:HG12	68:AY:186:TYR:CE2	2.46	0.51
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.10	0.51
9:J:84:TYR:HB2	9:J:91:ILE:HD11	1.92	0.51
12:M:372:PHE:CD1	12:M:481:LEU:HD13	2.46	0.51
64:AG:39:ARG:HB2	75:AG:101:CDL:HB31	1.93	0.51
67:AW:288:VAL:O	67:AW:292:VAL:HG23	2.11	0.51
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.34	0.51
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.51
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.51
11:L:61:ILE:HG12	11:L:140:LYS:O	2.10	0.51
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.51
13:N:40:GLY:HA3	13:N:48:TYR:HB2	1.92	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
18:T:80:VAL:HG12	18:T:82:THR:H	1.76	0.51
6:X:85:TYR:HE2	22:Y:45:ARG:NH1	2.09	0.51
81:AH:402:HEC:HHC	81:AH:402:HEC:HBB3	1.92	0.50
58:AN:29:HIS:ND1	58:AN:33:LYS:HB2	2.27	0.50
60:AP:242:HIS:HB2	60:AP:251:LEU:HB2	1.92	0.50
66:AV:282:ARG:NH1	66:AV:343:VAL:HG22	2.27	0.50
68:AY:412:ASP:O	68:AY:416:SER:CB	2.56	0.50
2:B:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.50
2:B:37:LYS:O	16:Q:320:VAL:N	2.38	0.50
9:J:142:GLU:OE2	9:J:146:VAL:HG21	2.11	0.50
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.50
12:M:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.50
12:M:506:VAL:HG12	12:M:508:GLY:N	2.24	0.50
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.50
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:HB3	1.93	0.50
60:AC:197:ASP:O	60:AC:257:ASN:ND2	2.45	0.50
67:AK:183:ARG:CG	67:AK:183:ARG:NH2	2.73	0.50
68:AL:285:ALA:HB2	68:AL:461:PRO:O	2.11	0.50
58:AN:42:ILE:HG22	58:AN:46:PHE:CE2	2.47	0.50
66:AV:173:PRO:HB2	66:AV:177:ARG:NH1	2.27	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.50
15:P:74:GLN:HB2	15:P:87:CYS:HB2	1.93	0.50
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.47	0.50
1:A:87:GLY:N	1:A:93:PHE:O	2.44	0.50
60:AC:132:ALA:CB	76:AH:401:PEE:H24	2.41	0.50
63:AF:39:TYR:HD1	63:AF:40:GLU:H	1.59	0.50
67:AK:309:LEU:HD23	67:AK:323:VAL:HG12	1.92	0.50
64:AT:40:LEU:CD1	64:AT:41:ILE:N	2.56	0.50
65:AU:193:LEU:HD12	65:AU:194:PRO:HD2	1.93	0.50
63:AS:71:LEU:HD21	66:AV:25:SER:HB2	1.92	0.50
66:AV:87:ALA:HB2	82:AV:401:HEM:HBB	1.92	0.50
5:F:30:SER:OG	5:F:63:PRO:HG3	2.11	0.50
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.50
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	0.50
9:J:62:THR:HB	73:J:401:NDP:HO3A	1.76	0.50
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.50
51:3:44:ARG:HD2	51:3:74:ARG:O	2.11	0.50
51:3:5:LYS:NZ	51:3:5:LYS:HB3	2.27	0.50
58:AA:74:ASN:N	58:AA:75:PRO:HD2	2.27	0.50
66:AJ:326:TRP:CH2	76:AJ:403:PEE:H50	2.46	0.50
68:AL:161:ILE:O	68:AL:165:ARG:HG3	2.12	0.50
65:AU:104:SER:OG	65:AU:283:ASP:OD1	2.27	0.50
68:AY:168:ILE:O	68:AY:172:MET:HG2	2.11	0.50
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
12:M:213:MET:HG3	12:M:215:MET:HG3	1.93	0.50
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.50
16:Q:82:LEU:N	16:Q:99:MET:O	2.41	0.50
2:B:108:GLU:OE1	18:T:68:ALA:HB1	2.12	0.50
60:AC:123:VAL:HG13	61:AD:29:VAL:HG22	1.94	0.50
82:AJ:402:HEM:HBB2	82:AJ:402:HEM:HMB1	1.92	0.50
9:J:159:ALA:HB3	9:J:161:VAL:HG23	1.93	0.50
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.50
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	0.50
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	0.50
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	0.50
12:M:92:CYS:SG	74:M:803:FES:S2	3.10	0.50
15:P:202:PHE:HB2	15:P:203:PRO:HD2	1.92	0.50
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.50
16:Q:69:VAL:HG12	16:Q:72:PRO:CD	2.41	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:CB	2.40	0.50
63:AF:71:LEU:N	63:AF:71:LEU:HD23	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AL:502:CDL:H572	76:AL:503:PEE:C39	2.38	0.50
60:AP:160:PRO:HD2	60:AP:163:LYS:HD3	1.94	0.50
4:E:25:MET:CB	4:E:29:LYS:CE	2.59	0.50
12:M:569:GLN:NE2	12:M:622:ILE:HD12	2.26	0.50
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.50
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.50
48:O:64:PHE:CE1	49:1:66:ARG:HD2	2.46	0.50
1:A:118:ASP:O	1:A:159:ARG:CD	2.60	0.50
62:AE:29:PRO:HD2	65:AH:262:THR:HG21	1.91	0.50
59:AO:28:PRO:HG3	67:AW:324:SER:OG	2.10	0.50
67:AW:254:ARG:HG2	67:AW:256:GLY:H	1.77	0.50
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.50
22:Y:74:TRP:CE3	22:Y:74:TRP:C	2.85	0.50
50:2:37:LYS:HD3	50:2:37:LYS:N	2.27	0.50
51:3:5:LYS:HD2	51:3:5:LYS:C	2.32	0.50
1:A:112:TYR:CD1	1:A:155:TYR:HE2	2.29	0.50
1:A:443:ARG:HB3	1:A:444:PRO:HD3	1.94	0.50
58:AA:28:PRO:HB2	58:AA:29:HIS:CE1	2.47	0.50
65:AH:125:HIS:HB3	65:AH:197:LEU:HD13	1.94	0.50
65:AH:323:PRO:HB2	65:AH:325:LYS:HG2	1.93	0.50
67:AK:185:ALA:HB2	67:AK:249:ALA:HB1	1.92	0.50
67:AK:299:VAL:HG13	68:AL:120:LEU:HD11	1.94	0.50
68:AL:308:ASN:HD21	68:AL:345:SER:HB3	1.77	0.50
64:AT:38:TRP:CD2	64:AT:41:ILE:HD13	2.47	0.50
4:E:50:PHE:HE1	4:E:96:VAL:HG13	1.76	0.50
2:B:36:TYR:HD2	8:I:104:TRP:HB2	1.76	0.50
9:J:268:PRO:HG3	9:J:344:PRO:HA	1.94	0.50
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.50
12:M:381:LEU:HB2	12:M:384:ASN:OD1	2.12	0.50
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.50
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
16:Q:65:PRO:HG2	16:Q:69:VAL:HG22	1.94	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
58:AA:20:SER:HB3	58:AA:23:GLU:HG2	1.94	0.50
6:G:112:SER:O	6:G:115:GLN:HB3	2.11	0.50
9:J:206:ILE:HB	9:J:242:VAL:HG23	1.90	0.50
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.50
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.50
16:Q:291:VAL:N	16:Q:294:ARG:HH21	2.09	0.50
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:87:GLN:O	16:Q:88:HIS:O	2.30	0.50
20:V:14:ASP:O	20:V:21:LYS:NZ	2.45	0.50
1:A:63:TYR:HD2	1:A:256:ARG:HD2	1.76	0.49
68:AL:257:TYR:CD2	68:AL:262:VAL:HG22	2.45	0.49
61:AQ:34:ARG:NH1	61:AQ:38:GLN:HB3	2.26	0.49
65:AU:155:GLN:HA	65:AU:166:MET:HA	1.94	0.49
66:AV:140:PHE:CD1	66:AV:140:PHE:C	2.85	0.49
68:AY:164:GLU:O	68:AY:168:ILE:HG12	2.12	0.49
60:AP:126:ALA:HA	76:AY:502:PEE:H61	1.95	0.49
12:M:168:LEU:HD23	12:M:292:PHE:CD2	2.46	0.49
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.49
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.44	0.49
18:T:89:GLY:HA2	18:T:115:CYS:SG	2.52	0.49
51:3:42:ARG:HD2	51:3:42:ARG:O	2.13	0.49
67:AK:299:VAL:HG22	68:AL:120:LEU:HG	1.94	0.49
62:AR:66:ASP:OD1	62:AR:67:CYS:N	2.44	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:186:PRO:HA	66:AV:189:ILE:HD12	1.94	0.49
68:AY:119:HIS:HB2	68:AY:134:LYS:HB3	1.93	0.49
68:AY:96:LEU:HD12	68:AY:96:LEU:C	2.32	0.49
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.49
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.49
10:K:104:GLU:OE1	10:K:104:GLU:N	2.46	0.49
13:N:87:HIS:O	13:N:91:HIS:HD2	1.96	0.49
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
65:AH:289:GLY:HA2	65:AH:292:MET:HG2	1.93	0.49
67:AK:239:ASN:OD1	67:AK:240:MET:N	2.45	0.49
68:AL:168:ILE:O	68:AL:172:MET:HG2	2.13	0.49
67:AW:105:ALA:HA	68:AY:390:ARG:HG3	1.94	0.49
7:H:115:PRO:HG3	16:Q:393:PRO:HB2	1.94	0.49
9:J:85:ARG:NH1	9:J:85:ARG:CG	2.72	0.49
12:M:209:TYR:O	12:M:210:ILE:HG22	2.12	0.49
12:M:385:TYR:O	12:M:517:HIS:NE2	2.43	0.49
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.75	0.49
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
76:V:202:PEE:C35	76:V:202:PEE:H40	2.42	0.49
59:AB:30:VAL:O	59:AB:33:THR:OG1	2.22	0.49
67:AK:49:ILE:HG12	67:AK:50:ALA:N	2.26	0.49
61:AD:16:ARG:NH1	68:AL:446:SER:OG	2.42	0.49
62:AR:80:HIS:CD2	62:AR:80:HIS:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AW:230:LEU:HA	67:AW:233:VAL:HG22	1.94	0.49
68:AY:296:TRP:CD1	68:AY:419:THR:CB	2.67	0.49
3:C:79:LEU:HB2	3:C:108:VAL:HG12	1.95	0.49
3:C:73:TRP:HD1	3:C:76:ARG:NH2	2.10	0.49
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	0.49
9:J:201:VAL:HG13	9:J:265:PHE:CE2	2.47	0.49
12:M:61:PRO:HG2	12:M:113:ARG:NE	2.26	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
65:AH:93:SER:HB2	65:AH:99:ARG:HH12	1.77	0.49
68:AL:75:ILE:HG21	68:AL:224:TYR:CD1	2.48	0.49
66:AV:150:LEU:HD23	66:AV:164:ILE:CD1	2.43	0.49
68:AY:75:ILE:HG12	68:AY:229:MET:SD	2.52	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
9:J:179:ARG:HB3	9:J:179:ARG:NH1	2.27	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	0.49
12:M:348:ALA:O	12:M:352:VAL:HG23	2.12	0.49
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	0.49
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.49
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	0.49
16:Q:424:ILE:O	16:Q:463:ARG:NE	2.45	0.49
20:V:62:THR:HG22	20:V:104:ARG:NE	2.27	0.49
51:3:42:ARG:NH1	51:3:74:ARG:HH21	2.10	0.49
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.49
1:A:202:GLY:O	12:M:200:ARG:NH2	2.42	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
65:AH:291:LYS:HD2	76:AH:401:PEE:C3	2.37	0.49
66:AJ:131:TYR:O	66:AJ:134:PRO:HD2	2.11	0.49
66:AJ:186:PRO:HA	66:AJ:189:ILE:HD12	1.94	0.49
67:AK:173:VAL:HG11	67:AK:339:TYR:HE1	1.77	0.49
61:AQ:53:TRP:NE1	65:AU:139:CYS:O	2.45	0.49
65:AU:288:MET:CG	76:AU:401:PEE:O4	2.61	0.49
75:AG:101:CDL:H741	66:AV:156:ILE:CG2	2.43	0.49
66:AV:281:LEU:HD11	66:AV:294:LEU:HD22	1.94	0.49
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.49
9:J:217:PHE:CZ	9:J:322:MET:CE	2.86	0.49
9:J:350:ILE:HG21	9:J:366:ILE:HG12	1.95	0.49
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.49
14:O:193:TYR:HB3	14:O:196:LEU:HD11	1.94	0.49
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.49
16:Q:323:ARG:N	16:Q:328:ASP:OD2	2.46	0.49
66:AJ:126:THR:O	66:AJ:182:HIS:ND1	2.46	0.49
67:AK:305:THR:HA	67:AK:311:GLN:HE21	1.78	0.49
67:AK:64:PHE:CE2	67:AK:397:GLY:HA3	2.48	0.49
67:AK:378:LEU:HD13	67:AK:416:ILE:HD11	1.94	0.49
68:AL:75:ILE:HG21	68:AL:224:TYR:HD1	1.77	0.49
61:AQ:43:ILE:O	61:AQ:47:ILE:HD12	2.13	0.49
65:AU:296:MET:HE2	76:AU:401:PEE:C33	2.40	0.49
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.49
9:J:62:THR:HB	73:J:401:NDP:O2X	2.12	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.49
12:M:711:VAL:HA	12:M:714:VAL:HG12	1.94	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.49
20:V:39:TYR:HD2	75:V:201:CDL:H721	1.76	0.49
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.27	0.49
68:AL:426:LEU:HA	68:AL:429:TRP:HD1	1.78	0.49
66:AV:286:ASN:OD1	66:AV:287:LYS:N	2.46	0.49
68:AY:294:PRO:HG3	68:AY:448:TYR:CE1	2.48	0.49
66:AV:10:LEU:CD2	76:AY:502:PEE:C26	2.91	0.49
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.49
11:L:75:ARG:HH11	11:L:104:ARG:NE	2.09	0.49
16:Q:175:GLY:O	16:Q:178:THR:OG1	2.29	0.49
16:Q:358:VAL:HG12	16:Q:360:ASP:H	1.78	0.49
1:A:274:LYS:HB2	1:A:292:MET:SD	2.53	0.49
75:AJ:405:CDL:H762	75:AJ:405:CDL:H132	1.95	0.49
67:AK:116:ARG:NH1	67:AK:188:ASN:O	2.46	0.49
66:AV:254:ASP:OD2	66:AV:267:HIS:NE2	2.46	0.49
68:AY:101:THR:OG1	68:AY:149:ASP:OD1	2.31	0.49
2:B:51:VAL:HG22	2:B:54:ARG:NH1	2.26	0.49
6:G:123:GLU:OE1	6:G:130:ILE:N	2.39	0.49
9:J:212:ARG:CG	9:J:212:ARG:NH1	2.73	0.49
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.37	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
12:M:610:VAL:O	12:M:611:THR:OG1	2.25	0.49
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.49
76:V:202:PEE:H41	76:V:202:PEE:C37	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
50:2:49:VAL:HG21	50:2:74:LEU:HD12	1.95	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
66:AJ:97:HIS:HE1	66:AJ:100:ARG:HH21	1.58	0.49
68:AL:192:PHE:HB2	68:AL:198:ALA:HB2	1.95	0.49
63:AS:34:ARG:NH2	63:AS:92:GLU:OE2	2.45	0.49
66:AV:366:MET:HB3	66:AV:367:PRO:HD3	1.95	0.49
9:J:238:GLN:NE2	9:J:267:GLY:O	2.43	0.49
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.49
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.49
48:O:68:PHE:HA	48:O:71:MET:HG2	1.95	0.48
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.77	0.48
67:AK:259:ARG:HH12	67:AK:438:MET:CE	2.26	0.48
67:AK:438:MET:HB2	67:AK:450:VAL:HG12	1.94	0.48
68:AL:304:LEU:HD13	68:AL:354:LEU:HD11	1.95	0.48
64:AT:39:ARG:CG	64:AT:39:ARG:NH2	2.73	0.48
66:AV:195:LEU:HD22	66:AV:199:PHE:CE2	2.48	0.48
75:AN:101:CDL:C58	76:AV:403:PEE:H52	2.42	0.48
7:H:46:LYS:HE3	8:I:90:THR:OG1	2.13	0.48
12:M:136:GLU:N	12:M:136:GLU:OE1	2.46	0.48
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.48
13:N:11:LEU:HA	13:N:14:ILE:HD12	1.94	0.48
20:V:62:THR:HG22	20:V:104:ARG:HD3	1.95	0.48
23:Z:28:PRO:O	23:Z:31:THR:OG1	2.22	0.48
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	0.48
63:AF:29:LYS:NZ	63:AF:29:LYS:CB	2.73	0.48
61:AQ:27:VAL:O	61:AQ:30:MET:HB2	2.13	0.48
68:AY:187:LEU:HD11	68:AY:290:ALA:HB3	1.94	0.48
68:AY:424:ILE:HG13	68:AY:429:TRP:NE1	2.27	0.48
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.48
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.48
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.96	0.48
14:O:155:LYS:HZ3	14:O:205:ILE:HB	1.77	0.48
17:S:50:ARG:CZ	17:S:54:ILE:HD11	2.43	0.48
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.48
60:AC:136:PHE:CE2	76:AH:401:PEE:H34	2.48	0.48
76:AH:401:PEE:H17	66:AJ:240:MET:HE2	1.95	0.48
65:AU:307:LYS:HE2	75:AU:403:CDL:CA3	2.43	0.48
66:AV:131:TYR:O	66:AV:134:PRO:HD2	2.13	0.48
68:AY:98:PHE:N	68:AY:98:PHE:CD1	2.79	0.48
9:J:93:HIS:O	9:J:96:PRO:HD2	2.14	0.48
12:M:37:ASP:OD1	12:M:38:GLY:N	2.41	0.48
12:M:392:ALA:HA	12:M:417:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:115:VAL:O	14:O:119:TYR:HD2	1.96	0.48
12:M:200:ARG:HH21	14:O:120:THR:HG23	1.78	0.48
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.48
1:A:318:ILE:HD11	1:A:355:ILE:HD13	1.94	0.48
63:AF:83:LYS:HB2	63:AF:86:GLU:HB2	1.95	0.48
66:AJ:22:PRO:HB3	66:AJ:217:LYS:HB3	1.94	0.48
67:AK:82:LEU:HD21	67:AK:151:VAL:HG13	1.94	0.48
67:AK:207:TYR:HA	67:AK:210:GLN:NE2	2.28	0.48
62:AR:34:ARG:CG	62:AR:78:ARG:NH1	2.61	0.48
66:AV:246:SER:HB3	66:AV:249:LEU:HD23	1.95	0.48
68:AY:119:HIS:HB2	68:AY:134:LYS:HD2	1.93	0.48
9:J:197:GLU:N	9:J:197:GLU:OE1	2.45	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	0.48
12:M:365:THR:HG22	12:M:537:ILE:HD11	1.95	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
20:V:29:ALA:O	20:V:63:ALA:HB1	2.14	0.48
21:W:47:HIS:O	21:W:51:MET:HG3	2.13	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48
66:AJ:223:TYR:OH	68:AL:469:ASN:ND2	2.44	0.48
65:AU:284:HIS:O	65:AU:288:MET:HG3	2.13	0.48
67:AW:384:MET:SD	68:AY:68:THR:HG21	2.54	0.48
67:AW:413:LEU:HA	67:AW:416:ILE:HG22	1.94	0.48
64:AT:17:TRP:NE1	68:AY:382:SER:OG	2.41	0.48
9:J:152:ILE:HG22	9:J:164:PHE:HE1	1.77	0.48
12:M:636:TYR:HB2	12:M:641:GLN:HB3	1.95	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
17:S:28:ARG:O	17:S:33:GLY:N	2.47	0.48
13:N:129:THR:HA	18:T:44:GLN:NE2	2.28	0.48
52:4:24:ASN:ND2	52:4:26:THR:H	2.11	0.48
1:A:132:ARG:HG2	1:A:165:GLU:OE1	2.13	0.48
63:AF:51:LEU:HD22	63:AF:55:LEU:HB3	1.96	0.48
68:AL:179:MET:O	68:AL:181:ASP:N	2.45	0.48
66:AV:96:LEU:HD23	76:AV:403:PEE:C17	2.39	0.48
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
4:E:128:PRO:HG3	11:L:74:THR:OG1	2.14	0.48
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.48
11:L:75:ARG:NH2	11:L:101:PHE:HB3	2.29	0.48
11:L:98:LYS:HA	11:L:126:LEU:O	2.13	0.48
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.48	0.48
12:M:564:CYS:O	12:M:566:ILE:HG12	2.14	0.48
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:233:SER:OG	14:O:234:LEU:N	2.47	0.48
16:Q:149:GLN:HG3	16:Q:171:ARG:HD3	1.94	0.48
53:5:39:VAL:O	53:5:42:LYS:HE2	2.14	0.48
66:AJ:177:ARG:NH2	60:AP:140:MET:O	2.47	0.48
65:AU:115:GLN:HA	65:AU:118:LYS:HE2	1.96	0.48
66:AV:45:ILE:HA	82:AV:401:HEM:CMC	2.44	0.48
4:E:20:ILE:H	4:E:77:ARG:HG2	1.78	0.48
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.48
68:AL:186:TYR:CD1	68:AL:275:ILE:HG21	2.48	0.48
68:AL:183:VAL:HG21	68:AL:286:HIS:HD2	1.79	0.48
61:AQ:56:ILE:O	61:AQ:59:LYS:HG2	2.14	0.48
4:E:52:LEU:HB3	4:E:54:ILE:HG13	1.96	0.48
7:H:35:LEU:O	7:H:45:ARG:NE	2.43	0.48
9:J:250:VAL:O	9:J:254:LYS:HG2	2.13	0.48
16:Q:301:ASP:OD1	16:Q:302:LEU:N	2.47	0.48
16:Q:124:ILE:HG22	16:Q:419:PRO:HG3	1.96	0.48
22:Y:71:TRP:C	22:Y:71:TRP:CE3	2.87	0.48
54:6:8:LYS:NZ	54:6:8:LYS:HB3	2.28	0.48
1:A:370:LEU:O	1:A:373:PHE:HB3	2.14	0.48
63:AF:36:ASP:CG	63:AF:62:ARG:NH1	2.67	0.48
58:AA:66:GLU:HG2	66:AJ:346:PRO:HB3	1.96	0.48
68:AL:101:THR:HA	68:AL:154:CYS:HA	1.95	0.48
68:AL:326:SER:O	68:AL:330:SER:N	2.43	0.48
60:AP:88:PHE:O	60:AP:92:ARG:HG3	2.14	0.48
64:AT:40:LEU:HD12	64:AT:41:ILE:CA	2.36	0.48
66:AJ:13:LEU:HD11	66:AV:198:LEU:HD11	1.95	0.48
68:AY:286:HIS:ND1	68:AY:359:VAL:HG22	2.29	0.48
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.94	0.48
9:J:357:ARG:HG3	9:J:362:LEU:HA	1.94	0.48
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.95	0.48
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.48
20:V:47:GLY:O	20:V:48:THR:OG1	2.25	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
54:6:16:ASN:ND2	54:6:16:ASN:H	2.12	0.48
1:A:208:GLU:OE1	1:A:211:ALA:N	2.38	0.48
65:AH:96:TRP:CZ3	65:AH:208:GLU:HG3	2.49	0.48
67:AK:267:VAL:HG21	67:AK:447:THR:HG21	1.95	0.48
67:AK:38:LEU:HB3	67:AK:52:LEU:HB2	1.94	0.48
76:AL:503:PEE:C33	76:AL:503:PEE:H26	2.44	0.48
59:AO:26:LEU:HA	59:AO:27:ARG:O	2.14	0.48
62:AR:34:ARG:NH1	62:AR:78:ARG:CZ	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AV:278:TYR:CE2	66:AV:282:ARG:HD2	2.48	0.48
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.48
8:I:96:THR:OG1	8:I:98:ALA:O	2.19	0.48
9:J:203:PRO:O	73:J:401:NDP:H5N	2.14	0.48
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.48
20:V:37:ALA:HB1	20:V:56:VAL:HG22	1.95	0.48
51:3:5:LYS:HZ3	51:3:5:LYS:HB3	1.79	0.47
65:AH:249:TYR:O	65:AH:252:VAL:HG23	2.14	0.47
67:AK:425:ILE:HG22	67:AK:429:LYS:HE2	1.95	0.47
58:AN:28:PRO:HB2	58:AN:29:HIS:CD2	2.50	0.47
60:AP:138:SER:O	66:AV:74:ASN:ND2	2.44	0.47
66:AV:65:SER:O	66:AV:68:HIS:HB3	2.14	0.47
67:AW:443:ASN:OD1	67:AW:445:GLY:N	2.43	0.47
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.47
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.47
1:A:51:TRP:HE1	10:K:76:HIS:HD1	1.62	0.47
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	0.47
12:M:383:SER:HA	12:M:386:LEU:HD12	1.96	0.47
9:J:52:SER:HB3	16:Q:103:GLY:HA3	59.47	0.47
75:V:201:CDL:H522	75:V:201:CDL:H552	1.70	0.47
20:V:40:ARG:HG3	75:V:201:CDL:HB22	1.96	0.47
76:W:201:PEE:P	76:W:201:PEE:N	2.87	0.47
2:B:52:THR:CG2	21:W:33:TYR:CE1	2.98	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
75:AJ:405:CDL:OB9	75:AJ:405:CDL:HA4	2.13	0.47
66:AJ:62:ALA:O	66:AJ:65:SER:OG	2.22	0.47
68:AL:113:VAL:HG11	68:AL:120:LEU:HD23	1.95	0.47
68:AL:133:ILE:HG22	68:AL:134:LYS:H	1.79	0.47
68:AL:437:ASP:OD1	68:AL:438:ALA:N	2.44	0.47
60:AP:124:GLY:HA3	65:AU:299:LEU:HD21	1.94	0.47
67:AW:136:PHE:O	67:AW:140:VAL:HG23	2.13	0.47
2:B:40:ASN:O	2:B:42:GLN:N	2.43	0.47
5:F:35:ASP:O	5:F:39:LYS:HG2	2.14	0.47
9:J:176:SER:CA	9:J:182:ARG:NH2	2.67	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
12:M:704:SER:OG	12:M:706:THR:HG22	2.14	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
52:4:60:TYR:CD1	52:4:60:TYR:C	2.88	0.47
1:A:114:VAL:O	1:A:242:VAL:HA	2.13	0.47
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.47
66:AJ:82:LEU:HD23	66:AJ:243:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AJ:47:THR:HG23	66:AJ:79:ILE:HG23	1.96	0.47
67:AK:115:THR:HG23	67:AK:118:ASN:H	1.80	0.47
60:AP:236:CYS:HA	60:AP:237:PRO:HD2	1.75	0.47
61:AQ:56:ILE:HG23	61:AQ:59:LYS:HE3	1.96	0.47
63:AS:14:LEU:HA	63:AS:17:ILE:HG12	1.96	0.47
65:AU:128:ASP:OD1	65:AU:177:LYS:NZ	2.47	0.47
66:AV:129:MET:HE1	66:AV:185:LEU:CD1	2.44	0.47
68:AY:294:PRO:HG3	68:AY:448:TYR:CZ	2.50	0.47
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.47
12:M:287:SER:HB3	12:M:290:THR:HG23	1.96	0.47
13:N:38:LEU:HD22	13:N:50:GLU:HB2	1.96	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.47
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.47
16:Q:136:PHE:CE2	16:Q:151:TYR:HB2	2.49	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47
64:AG:14:VAL:O	64:AG:18:VAL:HG23	2.14	0.47
76:AL:503:PEE:H16	76:AL:503:PEE:C30	2.44	0.47
62:AR:71:LEU:HD22	65:AU:222:PRO:HG3	1.97	0.47
65:AU:214:LEU:O	65:AU:234:ASN:ND2	2.44	0.47
60:AP:136:PHE:HB3	66:AV:50:PHE:CE2	2.49	0.47
67:AW:138:LEU:O	67:AW:142:THR:OG1	2.25	0.47
67:AW:157:GLN:NE2	68:AY:317:THR:O	2.45	0.47
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	0.47
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	0.47
10:K:91:LEU:HA	10:K:94:PHE:HD2	1.79	0.47
12:M:360:ARG:NH1	12:M:635:PRO:HD3	2.29	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
20:V:96:ALA:HA	20:V:99:LEU:HD12	1.95	0.47
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.88	0.47
59:AB:26:LEU:HA	59:AB:27:ARG:C	2.35	0.47
67:AK:84:ARG:HH11	67:AK:114:ALA:HB3	1.79	0.47
68:AL:376:TRP:HB3	68:AL:449:ILE:HG21	1.95	0.47
68:AY:296:TRP:HB3	68:AY:349:ALA:HA	1.96	0.47
67:AW:301:ARG:HD2	68:AY:95:HIS:CD2	2.49	0.47
2:B:151:ILE:HD13	3:C:159:TYR:CD2	2.50	0.47
11:L:115:ALA:O	15:P:228:GLN:N	2.44	0.47
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.47
11:L:162:ALA:HA	11:L:168:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:92:ASN:O	11:L:95:LYS:HG2	2.15	0.47
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.47
18:T:109:THR:HB	18:T:118:GLN:HB3	1.95	0.47
22:Y:50:LEU:O	22:Y:51:THR:OG1	2.27	0.47
51:3:67:HIS:CD2	51:3:78:LEU:HD11	2.50	0.47
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.79	0.47
59:AB:34:VAL:HB	59:AB:35:PRO:HD3	1.95	0.47
63:AF:28:ASN:O	63:AF:31:GLY:N	2.42	0.47
61:AD:38:GLN:NE2	64:AG:47:TYR:OH	2.48	0.47
76:AH:401:PEE:C30	76:AH:401:PEE:C11	2.92	0.47
75:AJ:405:CDL:H371	75:AJ:405:CDL:H341	1.67	0.47
67:AK:183:ARG:NH2	67:AK:254:ARG:CB	2.78	0.47
66:AV:141:TRP:CZ2	66:AV:260:ASN:O	2.67	0.47
68:AY:322:VAL:HG12	68:AY:323:HIS:N	2.27	0.47
2:B:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.97	0.47
10:K:89:LEU:HD13	14:O:65:ALA:HB2	1.95	0.47
12:M:236:TYR:CZ	12:M:272:ARG:HD3	2.50	0.47
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.47
63:AF:70:ASN:HD22	66:AJ:209:LEU:HG	1.80	0.47
67:AK:64:PHE:CE1	67:AK:120:ALA:HB1	2.49	0.47
67:AK:277:VAL:HG22	67:AK:278:ALA:HA	1.96	0.47
68:AL:96:LEU:HA	68:AL:99:LYS:HG2	1.96	0.47
66:AV:14:ILE:HD11	76:AY:502:PEE:H41	1.80	0.47
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.47
2:B:78:GLU:HA	17:S:1:MET:SD	2.53	0.47
8:I:69:ILE:O	8:I:71:SER:N	2.48	0.47
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.47
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.47
12:M:546:PHE:CE2	12:M:566:ILE:HD12	2.50	0.47
12:M:303:THR:O	12:M:615:LEU:HB2	2.15	0.47
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
21:W:101:VAL:HG13	21:W:102:PRO:HD2	1.96	0.47
48:O:33:LEU:HD22	48:O:37:GLN:HB3	1.97	0.47
50:2:31:TYR:HE1	50:2:98:HIS:HE1	1.62	0.47
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.47
59:AB:35:PRO:HB3	67:AK:320:PRO:HA	1.96	0.47
68:AL:373:GLN:HE22	68:AL:471:ILE:HG23	1.80	0.47
62:AR:30:LEU:HD13	62:AR:86:LEU:CD1	2.44	0.47
67:AW:444:LEU:HD23	67:AW:447:THR:CG2	2.42	0.47
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
16:Q:205:GLU:HG3	16:Q:209:LYS:NZ	2.29	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.14	0.47
48:O:23:PRO:HB3	49:1:70:VAL:CG2	2.45	0.47
60:AC:207:LYS:HD3	60:AC:265:PHE:CE2	2.50	0.47
58:AA:27:TYR:HE2	65:AH:305:THR:HG22	1.80	0.47
66:AV:111:GLU:O	66:AV:115:ILE:HG12	2.15	0.47
5:F:48:ASN:HD21	5:F:53:ILE:HD11	1.77	0.47
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.79	0.47
12:M:535:GLU:O	12:M:538:ARG:HG2	2.15	0.47
17:S:35:GLU:HG2	17:S:35:GLU:O	2.14	0.47
76:W:201:PEE:H28	76:W:201:PEE:H22	1.50	0.47
21:W:48:TRP:O	21:W:51:MET:HB2	2.15	0.47
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
58:AA:78:TYR:CE1	62:AE:65:GLU:CA	2.87	0.47
63:AF:45:LYS:HB3	63:AF:45:LYS:HZ2	1.80	0.47
59:AO:11:PHE:H	59:AO:27:ARG:CZ	2.27	0.47
75:AU:403:CDL:H732	75:AU:403:CDL:HB62	1.96	0.47
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.49	0.47
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	0.47
12:M:69:LEU:HD22	12:M:181:ARG:HG3	1.95	0.47
1:A:123:GLY:N	14:O:180:CYS:SG	2.72	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.30	0.47
16:Q:338:ARG:NH1	21:W:23:ARG:HB3	2.29	0.47
22:Y:88:ASP:N	22:Y:89:PRO:CD	2.78	0.47
62:AE:30:LEU:C	62:AE:30:LEU:HD12	2.35	0.47
76:AH:401:PEE:C11	76:AH:401:PEE:C31	2.93	0.47
66:AJ:221:HIS:HB3	66:AJ:222:PRO:HD3	1.97	0.47
68:AL:164:GLU:O	68:AL:168:ILE:HG12	2.14	0.47
60:AP:177:ARG:HB3	60:AP:211:VAL:HG13	1.97	0.47
63:AS:44:VAL:O	63:AS:48:ILE:HG12	2.14	0.47
65:AU:262:THR:HG22	65:AU:264:SER:H	1.78	0.47
67:AW:450:VAL:HA	67:AW:453:LEU:HD13	1.94	0.47
64:AT:24:TRP:CH2	75:AY:501:CDL:H551	2.50	0.47
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.47
9:J:238:GLN:HG3	9:J:269:SER:O	2.15	0.47
9:J:281:PHE:HA	9:J:284:ALA:HB3	1.97	0.47
9:J:365:GLU:N	9:J:365:GLU:OE1	2.45	0.47
11:L:77:VAL:HG22	11:L:78:ARG:H	1.80	0.47
14:O:54:ASP:OD1	14:O:55:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.47
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	0.47
17:S:4:GLU:O	17:S:7:PRO:HD2	2.15	0.47
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.47
60:AC:164:ASN:HD21	60:AC:175:PHE:HB3	1.80	0.46
66:AJ:97:HIS:CE1	66:AJ:100:ARG:HH21	2.32	0.46
60:AP:199:GLN:NE2	60:AP:204:ARG:HG2	2.29	0.46
64:AT:9:ARG:HH22	71:AT:101:PLX:H1A1	1.79	0.46
65:AU:131:ALA:HA	65:AU:174:TYR:HA	1.97	0.46
65:AU:215:LEU:HD11	81:AU:402:HEC:HMB1	1.97	0.46
59:AO:43:LEU:HD11	68:AY:179:MET:HG3	1.97	0.46
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.46
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.46
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.97	0.46
16:Q:71:PRO:N	16:Q:72:PRO:CD	2.78	0.46
22:Y:74:TRP:CE3	22:Y:75:HIS:CA	2.91	0.46
65:AH:133:ARG:O	65:AH:135:LEU:N	2.37	0.46
62:AR:62:HIS:O	62:AR:62:HIS:ND1	2.48	0.46
66:AV:343:VAL:CG1	66:AV:348:THR:HG22	2.46	0.46
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.46
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.46
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.46
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.46
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.46
16:Q:156:GLU:OE2	16:Q:163:PRO:HG3	2.15	0.46
21:W:77:ALA:O	21:W:80:ASP:HB3	2.16	0.46
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.46
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.46
58:AA:16:SER:HA	65:AH:319:LEU:HA	1.98	0.46
65:AH:321:TYR:CD2	65:AH:323:PRO:HD3	2.51	0.46
67:AK:214:THR:HG22	67:AK:216:ALA:H	1.80	0.46
67:AK:305:THR:HA	67:AK:311:GLN:NE2	2.30	0.46
76:AL:503:PEE:C17	76:AL:503:PEE:H49	2.44	0.46
63:AS:55:LEU:HD11	63:AS:90:TYR:HB2	1.97	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.51	0.46
6:G:84:LEU:HD23	6:G:87:LEU:HD12	1.97	0.46
12:M:620:TRP:NE1	12:M:639:LEU:HD13	2.30	0.46
12:M:645:ARG:HG3	12:M:648:GLU:OE2	2.16	0.46
14:O:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:159:LEU:O	16:Q:161:ILE:HG13	2.16	0.46
17:S:47:LEU:HA	17:S:50:ARG:HB3	1.98	0.46
54:6:11:LEU:HD23	54:6:11:LEU:O	2.15	0.46
48:0:102:TYR:CD2	57:9:35:TYR:HE1	2.33	0.46
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.46
3:C:59:ARG:HH22	3:C:61:GLU:CB	2.25	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.46
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.96	0.46
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.49	0.46
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.46
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.16	0.46
16:Q:97:LEU:O	16:Q:97:LEU:HD12	2.15	0.46
20:V:121:ALA:O	20:V:125:VAL:HG23	2.16	0.46
48:0:33:LEU:HD13	48:0:41:LYS:HG3	1.97	0.46
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.46
76:AJ:403:PEE:H61	76:AJ:403:PEE:C17	2.42	0.46
68:AL:101:THR:HA	68:AL:155:SER:H	1.81	0.46
68:AL:166:ASP:OD1	68:AL:167:VAL:N	2.49	0.46
59:AO:50:LEU:O	59:AO:51:SER:OG	2.33	0.46
63:AS:35:ASP:O	63:AS:38:ILE:HG22	2.15	0.46
6:G:77:GLU:N	6:G:77:GLU:OE1	2.38	0.46
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.62	0.46
11:L:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
12:M:68:ARG:NH2	12:M:284:GLU:OE1	2.33	0.46
12:M:299:ARG:O	12:M:301:ARG:HG2	2.15	0.46
16:Q:412:VAL:O	16:Q:420:TYR:N	2.43	0.46
21:W:31:SER:C	21:W:32:GLY:O	2.51	0.46
48:0:41:LYS:HD3	48:0:62:LEU:HD23	1.97	0.46
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	0.46
59:AB:11:PHE:CD1	59:AB:24:GLY:HA3	2.50	0.46
67:AK:370:ASP:OD1	67:AK:371:VAL:N	2.49	0.46
68:AL:332:ALA:O	68:AL:337:LEU:N	2.43	0.46
59:AO:11:PHE:CD1	59:AO:27:ARG:HD2	2.51	0.46
60:AP:136:PHE:HD1	66:AV:50:PHE:HD2	1.62	0.46
62:AR:75:LEU:HA	62:AR:75:LEU:HD23	1.80	0.46
67:AW:152:ALA:HA	67:AW:155:GLN:HG2	1.98	0.46
67:AW:298:HIS:HE1	67:AW:377:LYS:HG2	1.81	0.46
67:AW:306:THR:OG1	68:AY:111:LYS:NZ	2.45	0.46
2:B:192:GLY:O	2:B:196:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.46
2:B:151:ILE:HD13	3:C:159:TYR:CE2	2.51	0.46
5:F:14:LEU:N	5:F:17:ARG:HH22	2.13	0.46
7:H:36:GLU:HA	7:H:45:ARG:NH2	2.19	0.46
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.46
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
16:Q:216:ARG:HE	16:Q:240:LEU:HD23	1.80	0.46
50:2:40:SER:OG	50:2:45:ASP:HB3	2.16	0.46
58:AA:74:ASN:OD1	58:AA:78:TYR:HE2	1.99	0.46
76:AL:503:PEE:H16	76:AL:503:PEE:H49	1.95	0.46
60:AP:181:GLN:HA	60:AP:184:ILE:HD12	1.98	0.46
8:I:33:LYS:NZ	8:I:36:GLN:HA	2.30	0.46
9:J:207:PHE:CE2	9:J:348:LYS:HB2	2.49	0.46
11:L:107:TRP:O	11:L:116:SER:HB2	2.16	0.46
13:N:49:TYR:HD2	13:N:61:TRP:CZ3	2.33	0.46
13:N:83:PRO:HG2	13:N:86:TRP:HB2	1.98	0.46
14:O:84:ASP:O	14:O:88:ARG:N	2.47	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
16:Q:205:GLU:O	16:Q:209:LYS:HG3	2.16	0.46
16:Q:255:LEU:HD11	16:Q:337:MET:HG2	1.98	0.46
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	0.46
17:S:43:TYR:CZ	21:W:68:ARG:HD2	2.51	0.46
48:O:108:PRO:HG2	48:O:111:PHE:CD2	2.50	0.46
62:AE:74:PHE:CZ	62:AE:78:ARG:HD2	2.51	0.46
66:AJ:246:SER:HB3	66:AJ:249:LEU:HD23	1.98	0.46
68:AL:125:THR:HG22	68:AL:126:ARG:H	1.81	0.46
63:AS:93:PRO:O	63:AS:97:GLU:HG2	2.15	0.46
58:AN:67:PHE:CB	66:AV:346:PRO:HG3	2.42	0.46
3:C:81:PRO:HA	3:C:119:VAL:O	2.15	0.46
5:F:36:PHE:CE1	5:F:40:ARG:HB2	2.51	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.46
12:M:457:SER:O	12:M:499:LYS:NZ	2.49	0.46
23:Z:31:THR:O	23:Z:34:LYS:HB3	2.16	0.46
76:AH:401:PEE:C30	76:AH:401:PEE:C10	2.93	0.46
67:AK:178:HIS:HE1	67:AK:330:TYR:CE2	2.34	0.46
67:AK:277:VAL:HG11	67:AK:329:SER:HA	1.97	0.46
58:AA:12:ARG:NH1	68:AL:279:ASP:OD1	2.49	0.46
60:AP:136:PHE:HB3	66:AV:50:PHE:HE2	1.81	0.46
60:AP:167:PHE:HB2	60:AP:174:LEU:HB3	1.97	0.46
67:AW:259:ARG:NH1	67:AW:449:PHE:CZ	2.83	0.46
68:AY:148:GLY:O	68:AY:152:GLN:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46
9:J:220:MET:O	9:J:223:PHE:HB2	2.16	0.46
9:J:311:GLU:HA	9:J:312:PRO:HD3	1.79	0.46
1:A:174:ARG:HB2	10:K:91:LEU:HD11	1.96	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	0.46
12:M:589:TYR:CE2	12:M:590:THR:HG23	2.50	0.46
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.46
16:Q:446:ASP:O	16:Q:450:ILE:HG13	2.16	0.46
48:O:66:GLU:O	49:1:66:ARG:NH2	2.49	0.46
57:9:1:ILE:HG23	57:9:1:ILE:O	2.15	0.46
1:A:392:MET:O	1:A:396:MET:HG2	2.16	0.46
66:AJ:300:ILE:H	66:AJ:300:ILE:HG13	1.57	0.46
66:AV:24:PRO:HD2	66:AV:27:ILE:HD11	1.97	0.46
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.96	0.46
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.46
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.46
12:M:692:LYS:HG3	12:M:714:VAL:HG13	1.98	0.46
14:O:58:GLU:O	14:O:62:ARG:HG3	2.15	0.46
1:A:128:ARG:O	1:A:132:ARG:HG3	2.15	0.45
60:AC:164:ASN:HB3	60:AC:226:ALA:HB1	1.98	0.45
65:AH:291:LYS:CD	76:AH:401:PEE:H8	2.42	0.45
67:AK:57:PRO:HG2	68:AL:400:VAL:CG1	2.47	0.45
58:AN:41:ARG:HH21	75:AN:101:CDL:H1	1.81	0.45
67:AW:38:LEU:HD21	67:AW:406:TYR:CD1	2.51	0.45
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.45
6:G:133:ILE:O	6:G:136:GLU:HB2	2.15	0.45
9:J:220:MET:SD	9:J:223:PHE:HD2	2.39	0.45
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	0.45
18:T:68:ALA:O	18:T:72:ILE:HG13	2.16	0.45
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.97	0.45
22:Y:42:PRO:HD2	23:Z:14:MET:HG3	1.98	0.45
1:A:321:GLY:HA2	1:A:353:ALA:HB3	1.97	0.45
1:A:116:ASN:HD21	70:A:502:FMN:C8	2.22	0.45
66:AJ:362:ILE:HG13	66:AJ:363:LEU:HD12	1.98	0.45
63:AF:34:ARG:HH11	66:AJ:379:TRP:HE1	1.60	0.45
60:AC:135:GLN:HG3	66:AJ:75:TYR:CD2	2.51	0.45
60:AP:159:ILE:HA	60:AP:160:PRO:HD3	1.76	0.45
65:AU:204:ARG:HE	81:AU:402:HEC:CGA	2.29	0.45
58:AN:67:PHE:HD1	66:AV:344:SER:HG	1.61	0.45
68:AY:192:PHE:HB2	68:AY:198:ALA:HB2	1.98	0.45
68:AY:424:ILE:HD12	68:AY:424:ILE:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.45
12:M:64:CYS:SG	12:M:75:CYS:HB3	2.55	0.45
16:Q:94:VAL:HG21	16:Q:458:PHE:HB2	1.99	0.45
17:S:16:LEU:O	17:S:19:PRO:HD2	2.16	0.45
49:1:70:VAL:HG12	49:1:71:VAL:N	2.31	0.45
60:AC:178:HIS:HD2	60:AC:209:GLU:O	1.99	0.45
64:AG:39:ARG:HE	64:AG:51:LYS:HD2	1.80	0.45
66:AJ:366:MET:HB3	66:AJ:367:PRO:HD3	1.98	0.45
68:AL:286:HIS:ND1	68:AL:359:VAL:HG22	2.31	0.45
68:AL:294:PRO:HB2	68:AL:301:ASN:HD21	1.82	0.45
65:AU:313:VAL:HG13	65:AU:314:LEU:HD12	1.97	0.45
67:AW:49:ILE:HD11	67:AW:230:LEU:HB3	1.98	0.45
68:AY:66:GLN:OE1	68:AY:67:PRO:HD2	2.16	0.45
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	0.45
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.45
7:H:31:ILE:HG12	7:H:88:LEU:HA	1.99	0.45
12:M:221:ASN:OD1	12:M:291:ARG:NH2	2.35	0.45
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	0.45
20:V:17:ASP:OD1	58:AA:69:ARG:NH2	2.48	0.45
52:4:57:ARG:NH1	52:4:57:ARG:HB3	2.31	0.45
53:5:21:ILE:HA	53:5:21:ILE:HD12	1.81	0.45
1:A:371:ILE:HD11	1:A:435:VAL:HB	1.97	0.45
68:AL:140:LEU:HD21	68:AL:237:VAL:HG13	1.99	0.45
63:AS:83:LYS:HB2	63:AS:86:GLU:HB2	1.98	0.45
14:O:196:LEU:HD21	14:O:204:ILE:HG13	1.98	0.45
15:P:170:ILE:HG23	15:P:174:PHE:CD2	2.52	0.45
16:Q:136:PHE:CD2	16:Q:151:TYR:HB2	2.52	0.45
18:T:52:ARG:HB3	18:T:55:ARG:NH1	2.31	0.45
21:W:111:PHE:CD2	21:W:117:VAL:HG21	2.51	0.45
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.45
62:AE:53:CYS:O	62:AE:57:VAL:HG23	2.17	0.45
67:AK:259:ARG:HH21	67:AK:259:ARG:CB	2.10	0.45
59:AO:36:ALA:HB3	67:AW:320:PRO:HB3	1.97	0.45
66:AV:25:SER:HB3	66:AV:218:ILE:HD12	1.98	0.45
67:AW:312:ALA:HA	67:AW:315:LYS:HE3	1.98	0.45
68:AY:465:LEU:HD12	68:AY:466:PRO:HD2	1.97	0.45
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	0.45
4:E:120:SER:O	4:E:124:VAL:HG23	2.17	0.45
4:E:43:VAL:HB	4:E:44:PRO:HD3	1.98	0.45
8:I:30:GLU:HG2	8:I:31:ILE:N	2.32	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:688:GLN:O	12:M:690:THR:N	2.50	0.45
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.45
14:O:80:LEU:HB2	14:O:81:PRO:HD3	1.99	0.45
16:Q:145:MET:HG3	16:Q:174:PHE:HB3	1.99	0.45
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.98	0.45
16:Q:70:ASP:N	16:Q:71:PRO:CD	2.80	0.45
1:A:44:ASN:HD22	1:A:59:ARG:NH2	2.14	0.45
63:AF:38:ILE:HG12	63:AF:39:TYR:N	2.30	0.45
75:AG:101:CDL:H371	75:AG:101:CDL:H341	1.78	0.45
65:AH:158:PRO:HG3	65:AU:181:ASN:HD22	1.82	0.45
68:AL:126:ARG:NH1	68:AL:199:GLN:O	2.50	0.45
65:AU:88:GLU:HB3	65:AU:238:PRO:HA	1.97	0.45
66:AV:18:PHE:O	66:AV:220:PHE:HB3	2.17	0.45
66:AV:333:LEU:CD2	76:AV:403:PEE:C40	2.94	0.45
3:C:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.45
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	0.45
12:M:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.45
12:M:446:GLY:N	12:M:451:ILE:HD11	2.32	0.45
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.81	0.45
15:P:164:ASN:HA	15:P:181:HIS:HE2	1.82	0.45
16:Q:304:LYS:HE3	16:Q:316:PHE:CZ	2.52	0.45
16:Q:316:PHE:HD1	16:Q:339:GLN:NE2	2.14	0.45
75:V:201:CDL:H541	75:V:201:CDL:H572	1.46	0.45
50:2:31:TYR:HE1	50:2:98:HIS:CE1	2.34	0.45
51:3:3:ALA:O	51:3:4:ALA:HB2	2.17	0.45
51:3:42:ARG:NH1	51:3:42:ARG:HG3	2.32	0.45
56:8:35:ALA:HB3	56:8:36:PRO:HD3	1.99	0.45
59:AB:46:LYS:HD2	59:AB:49:PHE:CZ	2.52	0.45
65:AH:288:MET:SD	76:AH:401:PEE:O4	2.75	0.45
66:AJ:372:ILE:O	66:AJ:376:MET:HG2	2.17	0.45
68:AL:332:ALA:HA	68:AL:337:LEU:HB2	1.98	0.45
65:AU:201:VAL:O	65:AU:207:GLY:HA2	2.17	0.45
66:AV:10:LEU:HD21	76:AY:502:PEE:H45	1.77	0.45
68:AY:166:ASP:OD1	68:AY:167:VAL:N	2.49	0.45
6:G:123:GLU:O	6:G:127:GLY:N	2.50	0.45
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.45
11:L:102:ASP:N	11:L:102:ASP:OD1	2.50	0.45
12:M:421:SER:O	12:M:425:ASN:N	2.49	0.45
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:602:ARG:NE	12:M:659:ILE:HD11	2.30	0.45
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.45
50:2:33:ILE:HG22	50:2:34:LEU:HD12	1.98	0.45
50:2:98:HIS:ND1	50:2:98:HIS:N	2.64	0.45
1:A:440:ARG:HE	1:A:441:HIS:CE1	2.35	0.45
75:AJ:404:CDL:OB9	75:AJ:404:CDL:O1	2.33	0.45
68:AL:42:LEU:HD11	68:AL:430:GLU:OE1	2.17	0.45
61:AQ:53:TRP:HA	61:AQ:56:ILE:HB	1.99	0.45
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.45
9:J:108:TRP:HZ3	9:J:110:ALA:HA	1.82	0.45
9:J:178:SER:OG	9:J:181:LEU:HB2	2.17	0.45
9:J:273:LEU:O	9:J:276:LEU:HB3	2.17	0.45
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	0.45
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	0.45
16:Q:235:ASP:OD1	16:Q:356:ILE:HD12	2.17	0.45
16:Q:369:ALA:HA	18:T:93:ALA:HB2	1.99	0.45
22:Y:74:TRP:HE3	22:Y:75:HIS:N	2.15	0.45
1:A:319:PRO:HB2	1:A:347:THR:HG21	1.98	0.45
66:AJ:278:TYR:O	66:AJ:281:LEU:HB2	2.17	0.45
67:AK:148:ARG:NH1	63:AS:50:ARG:O	2.50	0.45
68:AL:113:VAL:HG21	68:AL:120:LEU:HD23	1.99	0.45
68:AL:75:ILE:HD13	68:AL:224:TYR:CD1	2.51	0.45
61:AQ:14:LEU:O	61:AQ:20:THR:OG1	2.33	0.45
61:AQ:26:ILE:HD12	64:AT:27:VAL:HG13	1.98	0.45
66:AV:191:ALA:O	66:AV:194:THR:OG1	2.24	0.45
66:AV:276:PHE:O	66:AV:279:THR:OG1	2.24	0.45
67:AW:444:LEU:HA	67:AW:447:THR:HG23	1.99	0.45
68:AY:101:THR:HA	68:AY:155:SER:N	2.30	0.45
68:AY:479:ARG:HH11	75:AY:501:CDL:HB62	1.82	0.45
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	0.45
5:F:22:HIS:HB2	5:F:64:LYS:HB3	1.97	0.45
7:H:28:TYR:CD2	7:H:56:LEU:HD13	2.52	0.45
9:J:217:PHE:HZ	9:J:322:MET:HE1	1.80	0.45
9:J:163:LYS:HE2	9:J:253:VAL:HA	1.98	0.45
14:O:207:GLU:HG2	14:O:213:ILE:HG13	1.99	0.45
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	0.45
16:Q:259:GLU:O	16:Q:263:THR:OG1	2.34	0.45
20:V:2:ALA:O	20:V:6:PHE:N	2.45	0.45
48:O:79:LYS:NZ	55:7:15:ASN:HD21	2.15	0.45
59:AB:26:LEU:HG	59:AB:28:PRO:HA	1.99	0.45
65:AH:304:TYR:CE1	75:AH:403:CDL:OA3	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AJ:16:HIS:O	66:AJ:21:LEU:HB3	2.16	0.45
68:AL:63:GLN:HE22	68:AL:238:GLU:HA	1.81	0.45
67:AW:328:ALA:HB3	67:AW:335:LEU:HB2	1.99	0.45
68:AY:96:LEU:CD1	68:AY:96:LEU:C	2.86	0.45
68:AY:96:LEU:HD23	68:AY:161:ILE:CD1	2.47	0.45
3:C:88:CYS:SG	16:Q:223:HIS:CE1	3.10	0.45
12:M:382:ARG:O	12:M:386:LEU:HG	2.16	0.45
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	0.45
14:O:198:ALA:HA	14:O:201:ILE:HD12	1.99	0.45
48:O:40:LEU:HD22	48:O:59:LEU:CD1	2.47	0.44
60:AC:195:LEU:HD13	60:AC:248:ARG:HD2	1.99	0.44
60:AC:81:THR:O	60:AC:83:ILE:N	2.48	0.44
61:AD:34:ARG:NH1	61:AD:38:GLN:HB3	2.32	0.44
63:AF:34:ARG:NH1	66:AJ:379:TRP:NE1	2.60	0.44
65:AH:221:PRO:HA	65:AH:222:PRO:HD3	1.77	0.44
66:AJ:265:PRO:HA	66:AJ:266:PRO:HD3	1.82	0.44
60:AC:80:HIS:CE1	68:AL:182:VAL:HG22	2.52	0.44
60:AC:140:MET:HA	66:AV:177:ARG:HH21	1.81	0.44
66:AV:7:THR:O	66:AV:12:LYS:HE3	2.17	0.44
68:AY:421:GLY:O	68:AY:422:ARG:HG3	2.16	0.44
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.44
12:M:307:VAL:HG22	12:M:582:VAL:HG13	1.99	0.44
12:M:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.18	0.44
18:T:96:HIS:NE2	18:T:115:CYS:SG	2.90	0.44
76:V:202:PEE:H60	76:V:202:PEE:H40	1.99	0.44
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.44
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.44
59:AB:41:PRO:HB2	67:AK:167:GLN:NE2	2.31	0.44
61:AD:27:VAL:O	61:AD:30:MET:HB2	2.17	0.44
68:AL:373:GLN:NE2	68:AL:471:ILE:HG23	2.31	0.44
63:AS:51:LEU:HD22	63:AS:55:LEU:HD22	1.99	0.44
63:AS:71:LEU:HD21	66:AV:25:SER:CB	2.48	0.44
66:AV:160:LEU:O	66:AV:164:ILE:HD12	2.17	0.44
67:AW:277:VAL:HA	67:AW:278:ALA:HA	1.73	0.44
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44
7:H:32:LEU:HA	7:H:35:LEU:HG	1.97	0.44
8:I:38:PRO:HA	8:I:39:PRO:HD3	1.58	0.44
73:J:401:NDP:O2X	73:J:401:NDP:O3B	2.33	0.44
11:L:136:SER:O	11:L:140:LYS:HG3	2.16	0.44
12:M:157:LYS:HB2	18:T:100:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.44
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.98	0.44
20:V:69:VAL:HG21	20:V:100:THR:HG21	1.98	0.44
21:W:111:PHE:CE2	21:W:117:VAL:HG11	2.49	0.44
1:A:317:VAL:HG22	1:A:356:VAL:HA	1.99	0.44
59:AB:50:LEU:O	59:AB:51:SER:OG	2.32	0.44
65:AH:301:PRO:O	65:AH:305:THR:HG23	2.17	0.44
66:AJ:8:ASN:HB3	66:AJ:11:MET:HB2	2.00	0.44
67:AK:155:GLN:NE2	67:AK:200:VAL:O	2.50	0.44
64:AT:40:LEU:CD1	64:AT:40:LEU:C	2.85	0.44
65:AU:249:TYR:O	65:AU:252:VAL:HG23	2.17	0.44
65:AU:253:LEU:HD23	65:AU:254:GLU:N	2.32	0.44
66:AV:155:TYR:O	66:AV:155:TYR:CD1	2.70	0.44
68:AY:333:VAL:HG13	68:AY:336:LYS:HD2	1.99	0.44
67:AW:108:GLY:HA2	68:AY:397:ASN:ND2	2.33	0.44
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.44
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.81	0.44
9:J:329:LEU:HD12	9:J:329:LEU:O	2.17	0.44
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
17:S:31:ASN:HD21	17:S:36:LYS:HD3	1.83	0.44
20:V:40:ARG:HE	75:V:201:CDL:CA2	2.30	0.44
61:AD:25:ILE:O	61:AD:29:VAL:HG23	2.18	0.44
63:AF:44:VAL:O	63:AF:48:ILE:HG12	2.17	0.44
66:AJ:198:LEU:CD1	75:AJ:404:CDL:H332	2.48	0.44
68:AL:225:LYS:HD2	68:AL:257:TYR:CE1	2.52	0.44
66:AV:315:MET:SD	66:AV:318:ARG:NH2	2.90	0.44
58:AN:17:TYR:HD1	68:AY:275:ILE:HG12	1.83	0.44
67:AW:104:GLU:OE1	68:AY:325:SER:HA	2.17	0.44
68:AY:64:SER:HB3	68:AY:235:GLY:HA2	1.99	0.44
68:AY:92:PHE:O	68:AY:92:PHE:HD1	2.00	0.44
2:B:69:GLY:O	2:B:72:LEU:HB3	2.17	0.44
2:B:91:LEU:HD23	2:B:95:PHE:CD2	2.52	0.44
9:J:169:HIS:CD2	73:J:401:NDP:C5N	2.79	0.44
12:M:221:ASN:HB3	12:M:285:TRP:HE3	1.82	0.44
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.99	0.44
12:M:306:MET:HA	12:M:315:THR:O	2.18	0.44
12:M:371:VAL:HG12	12:M:533:GLY:O	2.17	0.44
12:M:541:PRO:HA	12:M:542:PRO:HD2	1.77	0.44
12:M:612:PRO:HB3	12:M:616:ALA:HB3	1.99	0.44
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:195:ASP:HB2	14:O:219:ARG:H	1.83	0.44
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.44
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
18:T:67:PHE:O	18:T:71:LEU:HD13	2.17	0.44
18:T:81:GLU:HA	18:T:122:HIS:O	2.17	0.44
22:Y:85:PRO:O	22:Y:86:TYR:CD1	2.71	0.44
1:A:194:ASP:OD2	10:K:96:MET:N	2.41	0.44
66:AJ:156:ILE:HG21	66:AJ:160:LEU:HD13	2.00	0.44
67:AK:126:LEU:HB3	68:AL:38:PHE:CZ	2.52	0.44
68:AL:125:THR:HG22	68:AL:126:ARG:N	2.31	0.44
68:AL:286:HIS:CE1	68:AL:359:VAL:HG22	2.52	0.44
63:AS:99:ILE:O	63:AS:103:LYS:HG2	2.17	0.44
65:AU:114:PHE:CE2	65:AU:148:LEU:HD21	2.52	0.44
65:AU:197:LEU:HD23	65:AU:274:LEU:HD21	1.99	0.44
67:AW:323:VAL:HG13	67:AW:340:THR:HG22	1.99	0.44
67:AW:452:GLU:HG2	67:AW:453:LEU:N	2.31	0.44
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.44
7:H:23:ARG:O	7:H:26:ILE:HB	2.18	0.44
9:J:141:PHE:CD2	9:J:183:ASN:ND2	2.86	0.44
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.44
11:L:72:ILE:HA	11:L:143:TRP:NE1	2.33	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.44
12:M:229:GLY:O	12:M:232:THR:HG23	2.18	0.44
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.65	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
49:I:78:HIS:CE1	53:5:12:LEU:HD22	2.52	0.44
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	0.44
1:A:225:LEU:HB2	1:A:424:ILE:HD11	1.99	0.44
75:AL:502:CDL:H511	76:AL:503:PEE:H67	1.98	0.44
66:AV:129:MET:CE	66:AV:185:LEU:CD1	2.95	0.44
75:AN:101:CDL:C58	76:AV:403:PEE:C33	2.96	0.44
68:AY:225:LYS:NZ	68:AY:258:ALA:H	2.15	0.44
68:AY:324:LEU:O	68:AY:325:SER:OG	2.33	0.44
7:H:12:VAL:HG13	7:H:13:GLY:N	2.33	0.44
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.44
12:M:385:TYR:HB2	12:M:517:HIS:CE1	2.53	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	0.44
16:Q:190:HIS:HD2	16:Q:452:GLY:CA	2.26	0.44
53:5:61:GLU:OE1	53:5:64:ARG:NH1	2.51	0.44
53:5:68:ILE:HG13	53:5:69:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:6:3:ASN:ND2	54:6:5:VAL:HG13	2.33	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
66:AJ:105:GLY:HA2	66:AJ:107:PHE:CE2	2.53	0.44
63:AF:34:ARG:HD2	66:AJ:377:LEU:HB3	2.00	0.44
68:AL:279:ASP:OD2	68:AL:282:LEU:HG	2.17	0.44
75:AU:403:CDL:H112	66:AV:234:LEU:HD12	2.00	0.44
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.44
4:E:35:LEU:HD11	4:E:39:TRP:HE1	1.81	0.44
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.44
9:J:130:ILE:HG21	73:J:401:NDP:N7A	2.23	0.44
12:M:510:TRP:HD1	12:M:512:VAL:HG22	1.82	0.44
16:Q:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.44
55:7:9:PHE:HD1	55:7:10:HIS:HD2	1.64	0.44
58:AA:12:ARG:HG2	58:AA:13:HIS:HD1	1.78	0.44
58:AA:27:TYR:CE2	65:AH:305:THR:HG22	2.53	0.44
76:AJ:403:PEE:H61	76:AJ:403:PEE:C18	2.45	0.44
68:AL:231:LEU:HD22	68:AL:250:LEU:HD12	2.00	0.44
62:AR:43:CYS:SG	62:AR:78:ARG:HA	2.57	0.44
67:AW:81:HIS:CD2	67:AW:158:LEU:HD22	2.53	0.44
2:B:131:GLU:OE1	2:B:141:THR:HG21	2.18	0.44
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.44
8:I:37:PRO:HA	8:I:38:PRO:HD3	1.81	0.44
12:M:37:ASP:HA	12:M:103:LEU:HD23	1.98	0.44
14:O:132:ILE:O	14:O:172:ILE:HG22	2.18	0.44
16:Q:55:SER:N	16:Q:58:THR:OG1	2.50	0.44
76:W:201:PEE:H51	76:W:201:PEE:H56	1.33	0.44
51:3:78:LEU:HA	51:3:78:LEU:HD12	1.75	0.44
60:AC:145:ASP:OD1	60:AC:146:VAL:N	2.51	0.44
60:AC:179:ARG:NE	60:AC:208:PRO:O	2.43	0.44
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.44
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	0.44
12:M:278:HIS:NE2	12:M:280:ASP:HB2	2.33	0.44
12:M:358:LEU:HD22	12:M:363:SER:HB2	1.99	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.18	0.44
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	0.44
16:Q:265:ASN:OD1	16:Q:267:ILE:HD12	2.17	0.44
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.49	0.44
53:5:26:MET:N	53:5:26:MET:SD	2.91	0.43
54:6:2:GLU:CG	54:6:3:ASN:H	2.30	0.43
54:6:30:ILE:HG13	54:6:31:LEU:N	2.33	0.43
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AE:34:ARG:HE	62:AE:34:ARG:HB2	1.62	0.43
67:AK:158:LEU:HB2	67:AK:197:ILE:HG23	1.99	0.43
68:AL:152:GLN:NE2	68:AL:249:HIS:O	2.51	0.43
68:AL:414:GLY:O	68:AL:418:LEU:HD13	2.18	0.43
67:AW:228:PRO:O	67:AW:231:LYS:HB2	2.18	0.43
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.43
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.43
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
14:O:236:GLU:HB3	14:O:238:PRO:HD2	2.00	0.43
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.43
52:4:84:LYS:HD2	52:4:84:LYS:HA	1.83	0.43
75:AJ:404:CDL:H152	75:AJ:404:CDL:H121	1.70	0.43
67:AK:155:GLN:N	67:AK:156:PRO:HD2	2.33	0.43
67:AK:257:GLU:HG3	67:AK:450:VAL:HG21	1.98	0.43
59:AB:1:MET:SD	67:AK:412:VAL:HG13	2.58	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
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	0.43
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.43
9:J:83:PRO:HA	9:J:106:LEU:O	2.18	0.43
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	0.43
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.43
12:M:646:LEU:HD13	12:M:653:LEU:HB3	2.00	0.43
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	0.43
15:P:55:HIS:NE2	15:P:78:VAL:HG12	2.33	0.43
16:Q:391:VAL:O	16:Q:415:GLY:HA2	2.18	0.43
20:V:51:GLU:HB3	20:V:55:LYS:NZ	2.34	0.43
67:AK:60:ARG:HB3	67:AK:223:LEU:HD12	2.00	0.43
66:AJ:155:TYR:HE2	64:AT:38:TRP:CZ2	2.35	0.43
67:AW:379:LYS:HG2	67:AW:413:LEU:HG	2.00	0.43
67:AW:444:LEU:HA	67:AW:444:LEU:HD23	1.78	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43
12:M:455:ILE:HG12	12:M:463:SER:HB3	1.99	0.43
12:M:566:ILE:HD11	12:M:579:ILE:HG22	1.99	0.43
17:S:43:TYR:CE2	21:W:68:ARG:HD2	2.53	0.43
48:0:37:GLN:O	48:0:41:LYS:HG2	2.18	0.43
49:1:27:TRP:CH2	50:2:86:GLY:HA2	2.54	0.43
51:3:5:LYS:CD	51:3:6:GLY:N	2.82	0.43
1:A:73:PRO:HB2	1:A:74:ASP:H	1.58	0.43
65:AH:131:ALA:HB3	65:AH:133:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AH:131:ALA:HA	65:AH:174:TYR:HA	2.00	0.43
60:AP:214:ILE:HG22	60:AP:216:VAL:H	1.83	0.43
60:AP:127:TYR:HE1	61:AQ:33:GLU:HG2	1.83	0.43
63:AS:36:ASP:OD1	63:AS:90:TYR:OH	2.37	0.43
65:AU:291:LYS:HE3	76:AU:401:PEE:O1P	2.18	0.43
65:AU:288:MET:HE2	66:AV:77:TRP:HH2	1.82	0.43
59:AO:37:THR:N	68:AY:174:GLU:OE2	2.41	0.43
68:AY:57:LEU:HD13	68:AY:250:LEU:HB3	1.99	0.43
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.43
5:F:65:LEU:O	5:F:76:ASN:HA	2.18	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.43
11:L:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	0.43
13:N:5:GLN:O	13:N:9:ARG:HG2	2.17	0.43
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.43
16:Q:147:ASN:O	16:Q:150:ALA:HB3	2.17	0.43
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.43
62:AE:40:LEU:O	62:AE:44:VAL:HG23	2.19	0.43
67:AK:227:HIS:N	67:AK:228:PRO:HD2	2.33	0.43
60:AP:125:VAL:CG2	71:AQ:101:PLX:H141	2.49	0.43
62:AR:86:LEU:CD2	62:AR:86:LEU:C	2.86	0.43
65:AU:91:PRO:HA	65:AU:92:PRO:HD3	1.84	0.43
67:AW:346:ALA:O	67:AW:350:VAL:HG23	2.19	0.43
67:AW:79:THR:HG23	67:AW:205:LEU:HD23	2.00	0.43
2:B:166:VAL:HG11	2:B:199:ILE:HG23	2.00	0.43
6:G:138:LEU:O	6:G:143:GLU:HB2	2.18	0.43
10:K:78:ASP:HA	14:O:215:LYS:HD3	2.00	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:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.43
15:P:55:HIS:HD2	15:P:79:SER:O	2.01	0.43
15:P:188:LEU:HA	16:Q:114:GLY:HA3	2.00	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
23:Z:65:ASP:O	23:Z:69:LYS:HB2	2.19	0.43
48:O:126:MET:HG3	48:O:128:VAL:HG23	2.00	0.43
54:6:36:MET:O	54:6:40:LEU:HG	2.18	0.43
63:AF:99:ILE:O	63:AF:103:LYS:HG2	2.19	0.43
66:AJ:331:ASP:HA	66:AJ:334:ILE:HD12	2.01	0.43
66:AJ:8:ASN:OD1	66:AJ:9:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AK:127:ARG:NH1	67:AK:224:GLY:O	2.49	0.43
68:AL:133:ILE:HG22	68:AL:134:LYS:N	2.33	0.43
68:AL:58:ARG:HB2	68:AL:230:VAL:HG22	2.01	0.43
65:AU:156:ASP:OD1	65:AU:157:GLY:N	2.43	0.43
65:AU:290:LEU:C	65:AU:290:LEU:CD2	2.86	0.43
65:AU:292:MET:HE1	66:AV:241:THR:CG2	2.48	0.43
65:AU:296:MET:HE2	76:AU:401:PEE:C32	2.49	0.43
68:AY:287:VAL:HG12	68:AY:458:GLY:HA2	2.01	0.43
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.43
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	0.43
14:O:104:VAL:HG12	14:O:105:LEU:HD12	2.00	0.43
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.43
57:9:37:LEU:HA	57:9:37:LEU:HD23	1.84	0.43
63:AF:70:ASN:ND2	66:AJ:209:LEU:HG	2.33	0.43
64:AG:45:VAL:HA	64:AG:46:PRO:HD3	1.80	0.43
75:AH:403:CDL:O1	75:AH:403:CDL:OB8	2.35	0.43
67:AK:326:PHE:HB3	67:AK:337:GLY:O	2.19	0.43
67:AK:293:LEU:HD21	67:AK:358:VAL:HG22	2.00	0.43
68:AL:322:VAL:HG12	68:AL:323:HIS:N	2.31	0.43
60:AP:80:HIS:CD2	60:AP:81:THR:HG23	2.54	0.43
60:AP:82:ASP:OD1	60:AP:83:ILE:N	2.51	0.43
66:AV:171:ASP:OD1	66:AV:172:SER:N	2.50	0.43
66:AV:206:ASN:H	82:AV:402:HEM:CGD	2.31	0.43
67:AW:262:ASN:O	67:AW:443:ASN:HA	2.18	0.43
67:AW:323:VAL:HG22	67:AW:340:THR:HG22	1.99	0.43
68:AY:295:GLY:HA2	68:AY:351:THR:O	2.19	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.43
9:J:56:ALA:HA	9:J:125:VAL:HG23	2.01	0.43
9:J:167:VAL:HG22	9:J:201:VAL:HB	2.00	0.43
11:L:77:VAL:HG22	11:L:78:ARG:N	2.33	0.43
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.43
71:V:203:PLX:H141	71:V:203:PLX:H332	2.01	0.43
50:2:53:THR:HG22	50:2:54:ASN:OD1	2.19	0.43
55:7:44:PRO:HA	55:7:47:ARG:NH1	2.34	0.43
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	0.43
58:AA:74:ASN:OD1	58:AA:78:TYR:CE2	2.72	0.43
60:AC:200:HIS:O	60:AC:204:ARG:HG3	2.18	0.43
58:AA:78:TYR:CD1	62:AE:64:GLU:C	2.91	0.43
68:AL:121:ASN:HB3	68:AL:132:TYR:CZ	2.54	0.43
68:AL:350:GLU:HG2	68:AL:351:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AQ:44:TYR:HB2	65:AU:290:LEU:HD13	2.01	0.43
65:AU:292:MET:CE	66:AV:241:THR:CG2	2.96	0.43
75:AU:403:CDL:H742	75:AU:403:CDL:H711	1.77	0.43
66:AV:333:LEU:HD21	76:AV:403:PEE:C40	2.48	0.43
3:C:156:GLY:O	3:C:161:HIS:ND1	2.52	0.43
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.43
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	0.43
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
15:P:163:ALA:O	15:P:167:GLU:HB2	2.17	0.43
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.43
16:Q:82:LEU:HD23	16:Q:82:LEU:HA	1.78	0.43
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.54	0.43
63:AF:27:PHE:HD1	63:AF:28:ASN:N	2.17	0.43
67:AK:105:ALA:HA	68:AL:390:ARG:HG3	2.00	0.43
75:AU:403:CDL:OA6	66:AV:230:LEU:HD23	2.19	0.43
67:AW:61:ILE:HG22	67:AW:222:GLY:HA2	1.99	0.43
2:B:175:THR:HB	2:B:180:GLU:OE1	2.19	0.43
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	0.43
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.43
9:J:283:VAL:O	9:J:357:ARG:NH2	2.51	0.43
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.00	0.43
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.43
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.43
15:P:171:TRP:CZ3	15:P:177:PHE:HA	2.54	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	0.43
53:5:21:ILE:O	53:5:25:PHE:HD2	2.02	0.43
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.43
62:AE:21:GLU:HA	62:AE:24:GLU:CB	2.49	0.43
63:AF:51:LEU:CD2	63:AF:55:LEU:HD13	2.49	0.43
59:AO:28:PRO:O	67:AW:170:GLN:NE2	2.52	0.43
65:AU:114:PHE:HE2	65:AU:148:LEU:HD21	1.83	0.43
68:AY:74:TRP:CG	68:AY:414:GLY:HA3	2.54	0.43
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.43
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.43
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.43
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.43
9:J:131:GLY:HA3	73:J:401:NDP:O3D	2.19	0.43
12:M:342:ALA:O	12:M:369:GLU:HG2	2.19	0.43
13:N:73:THR:HG22	13:N:74:PHE:N	2.34	0.43
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	2.01	0.43
16:Q:99:MET:HE2	16:Q:447:VAL:HG21	2.01	0.43
21:W:33:TYR:O	21:W:34:SER:OG	2.27	0.43
21:W:72:LEU:HD23	21:W:72:LEU:HA	1.84	0.43
1:A:403:ASP:HA	1:A:453:PHE:CE2	2.54	0.42
63:AF:110:LYS:HG3	63:AF:111:LYS:HG3	2.02	0.42
75:AH:403:CDL:H122	66:AJ:234:LEU:HD12	2.01	0.42
66:AJ:197:LEU:HD22	75:AJ:404:CDL:H162	2.01	0.42
67:AK:178:HIS:HE1	67:AK:330:TYR:HE2	1.66	0.42
67:AK:355:TYR:CE2	67:AK:359:LYS:HD2	2.54	0.42
67:AK:82:LEU:O	67:AK:86:THR:HG23	2.20	0.42
76:AL:503:PEE:H13	76:AL:503:PEE:H1	1.74	0.42
59:AO:46:LYS:HG2	59:AO:47:ARG:O	2.18	0.42
2:B:78:GLU:HG3	17:S:1:MET:SD	2.59	0.42
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.42
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.42
9:J:124:ASN:OD1	9:J:125:VAL:N	2.51	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.19	0.42
9:J:221:HIS:C	9:J:221:HIS:ND1	2.73	0.42
9:J:221:HIS:ND1	9:J:222:ARG:HG3	2.31	0.42
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.42
16:Q:372:LYS:HD2	18:T:93:ALA:HA	2.00	0.42
20:V:62:THR:HG22	20:V:104:ARG:CD	2.49	0.42
20:V:95:CYS:O	20:V:99:LEU:HG	2.19	0.42
1:A:274:LYS:NZ	1:A:351:THR:O	2.51	0.42
58:AA:78:TYR:HB3	62:AE:65:GLU:CD	2.30	0.42
76:AH:401:PEE:H61	66:AJ:236:LEU:HD13	2.01	0.42
66:AJ:312:GLN:HG3	66:AJ:379:TRP:HH2	1.84	0.42
67:AK:138:LEU:O	67:AK:142:THR:N	2.52	0.42
67:AK:195:TYR:CE2	67:AK:196:ARG:HG2	2.54	0.42
68:AL:156:LEU:HB3	68:AL:161:ILE:HD11	2.01	0.42
68:AL:267:PRO:HA	68:AL:350:GLU:OE1	2.18	0.42
63:AS:8:SER:OG	63:AS:9:ALA:N	2.51	0.42
66:AV:326:TRP:CZ2	76:AV:403:PEE:O5	2.72	0.42
67:AW:82:LEU:O	67:AW:86:THR:HG23	2.19	0.42
68:AY:64:SER:N	68:AY:235:GLY:O	2.49	0.42
2:B:158:GLU:O	16:Q:368:ARG:NH2	2.52	0.42
2:B:117:CYS:HB2	69:B:301:SF4:S1	2.59	0.42
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.42
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.42
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:133:GLN:HA	12:M:136:GLU:OE2	2.17	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.20	0.42
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.42
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.54	0.42
18:T:102:ASN:HD21	18:T:104:ASP:HB2	1.84	0.42
20:V:133:TRP:CG	76:V:202:PEE:H7	2.54	0.42
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.42
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.42
70:A:502:FMN:H4'	70:A:502:FMN:H1'2	1.63	0.42
58:AA:3:ARG:HH12	66:AJ:217:LYS:CE	2.32	0.42
59:AB:50:LEU:HD23	59:AB:51:SER:O	2.20	0.42
62:AE:78:ARG:O	62:AE:82:VAL:HG23	2.19	0.42
60:AP:244:ASP:OD2	60:AP:248:ARG:HB2	2.18	0.42
65:AU:292:MET:CE	66:AV:241:THR:HG22	2.49	0.42
66:AV:123:THR:HG22	66:AV:189:ILE:HD13	2.00	0.42
67:AW:90:THR:HG22	67:AW:150:GLU:OE1	2.19	0.42
67:AK:449:PHE:CE2	67:AW:183:ARG:HB3	2.54	0.42
15:P:109:LYS:O	15:P:110:SER:OG	2.31	0.42
15:P:97:LEU:HD11	15:P:130:TYR:CE2	2.54	0.42
15:P:90:PRO:O	15:P:93:VAL:HG23	2.18	0.42
16:Q:116:LEU:O	16:Q:118:ARG:HG3	2.19	0.42
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.42
16:Q:338:ARG:O	16:Q:341:LEU:HB2	2.19	0.42
18:T:79:GLU:OE1	18:T:122:HIS:HB3	2.19	0.42
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.52	0.42
53:5:35:TYR:O	53:5:39:VAL:HB	2.19	0.42
54:6:31:LEU:HD23	54:6:31:LEU:HA	1.83	0.42
1:A:129:GLU:OE1	1:A:132:ARG:NH1	2.49	0.42
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.00	0.42
1:A:282:VAL:HA	1:A:307:VAL:HA	2.00	0.42
1:A:314:LEU:O	1:A:315:LEU:HD12	2.19	0.42
60:AC:239:HIS:HB2	74:AC:301:FES:S1	2.59	0.42
60:AC:132:ALA:HB1	76:AH:401:PEE:H27	2.00	0.42
68:AL:294:PRO:HB2	68:AL:301:ASN:ND2	2.34	0.42
76:AL:503:PEE:C33	76:AL:503:PEE:C17	2.97	0.42
68:AL:51:SER:HB2	68:AL:59:VAL:HB	2.01	0.42
68:AL:87:ASN:HD21	68:AL:199:GLN:HB2	1.85	0.42
60:AP:207:LYS:HA	60:AP:208:PRO:HD3	1.84	0.42
65:AU:290:LEU:HD23	65:AU:290:LEU:O	2.19	0.42
67:AW:373:ALA:O	67:AW:377:LYS:HG3	2.19	0.42
68:AY:88:GLY:O	68:AY:92:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	0.42
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.42
11:L:79:ILE:HD12	11:L:145:TYR:CD2	2.54	0.42
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	0.42
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.42
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.42
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	0.42
14:O:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
17:S:7:PRO:O	17:S:10:SER:OG	2.23	0.42
18:T:52:ARG:O	18:T:55:ARG:HG2	2.20	0.42
19:U:40:LYS:O	19:U:44:MET:HG2	2.18	0.42
8:I:40:LYS:HG2	21:W:8:GLN:HA	2.00	0.42
50:2:86:GLY:O	50:2:87:THR:O	2.37	0.42
51:3:54:ARG:CD	51:3:54:ARG:N	2.80	0.42
56:8:41:ARG:HD2	57:9:40:TYR:CZ	2.54	0.42
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.42
65:AH:214:LEU:O	65:AH:234:ASN:ND2	2.41	0.42
66:AJ:214:HIS:ND1	66:AJ:217:LYS:NZ	2.68	0.42
67:AK:330:TYR:HB2	67:AK:333:SER:O	2.20	0.42
58:AN:82:LYS:HE2	62:AR:65:GLU:HB2	2.02	0.42
66:AV:346:PRO:O	66:AV:349:ILE:HG22	2.19	0.42
59:AO:14:VAL:HA	67:AW:113:THR:HA	2.01	0.42
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.42
9:J:128:ASN:O	9:J:129:LEU:HD12	2.19	0.42
11:L:170:THR:HG22	12:M:423:LEU:O	2.18	0.42
12:M:542:PRO:HB2	12:M:543:LYS:HD3	2.01	0.42
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.42
1:A:32:PHE:HB3	1:A:294:VAL:HA	2.02	0.42
68:AL:233:ALA:HB3	68:AL:242:LEU:HD22	2.01	0.42
68:AL:324:LEU:O	68:AL:325:SER:OG	2.32	0.42
65:AU:221:PRO:HA	65:AU:222:PRO:HD3	1.85	0.42
75:AU:403:CDL:HB61	75:AU:403:CDL:O1	2.20	0.42
58:AN:49:VAL:HG21	76:AV:403:PEE:H7	2.02	0.42
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42
16:Q:281:GLU:CD	16:Q:281:GLU:N	2.73	0.42
61:AD:39:GLY:O	61:AD:43:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AN:48:ARG:HE	66:AV:319:PRO:HB3	1.84	0.42
3:C:150:MET:SD	3:C:190:LEU:HD13	2.60	0.42
4:E:102:HIS:HA	4:E:105:ARG:HG3	2.02	0.42
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	0.42
12:M:254:MET:CB	12:M:290:THR:HG22	2.46	0.42
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	0.42
16:Q:275:ILE:HD13	16:Q:446:ASP:OD1	2.20	0.42
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	0.42
16:Q:70:ASP:HB2	16:Q:71:PRO:HD3	2.02	0.42
19:U:69:HIS:CE1	19:U:70:PRO:HA	2.54	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
1:A:159:ARG:HD3	1:A:162:PHE:CE2	2.55	0.42
64:AG:16:ASN:CG	68:AL:442:ARG:HH12	2.23	0.42
66:AJ:163:TRP:CG	75:AJ:405:CDL:H331	2.55	0.42
67:AK:347:ALA:O	67:AK:351:ILE:HG12	2.20	0.42
58:AN:11:MET:SD	63:AS:64:LYS:HD2	2.60	0.42
58:AN:19:LEU:HD11	60:AP:88:PHE:CB	2.50	0.42
71:AT:101:PLX:H21	71:AT:101:PLX:H1A2	1.78	0.42
64:AT:17:TRP:HE1	68:AY:382:SER:HG	1.61	0.42
67:AW:271:PHE:CZ	67:AW:338:ILE:HB	2.55	0.42
61:AQ:18:THR:HG22	68:AY:480:PHE:OXT	2.19	0.42
68:AY:58:ARG:HH11	68:AY:230:VAL:HG22	1.85	0.42
4:E:25:MET:O	4:E:29:LYS:N	2.44	0.42
4:E:78:VAL:O	4:E:82:LEU:HD13	2.20	0.42
5:F:62:GLN:HE21	5:F:64:LYS:NZ	2.17	0.42
6:G:87:LEU:HA	6:G:90:TYR:HB3	2.00	0.42
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.42
9:J:171:ASN:O	9:J:181:LEU:HG	2.18	0.42
9:J:283:VAL:HG13	9:J:369:VAL:HG11	2.02	0.42
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.42
12:M:49:VAL:HG23	12:M:94:MET:O	2.20	0.42
12:M:33:GLU:O	12:M:98:LYS:HA	2.20	0.42
13:N:10:GLY:O	13:N:14:ILE:HG13	2.20	0.42
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.42
16:Q:371:MET:HA	16:Q:377:SER:OG	2.20	0.42
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.42
2:B:133:ARG:NH2	18:T:69:ILE:HG13	2.34	0.42
18:T:83:ARG:HH12	18:T:103:LEU:H	1.68	0.42
51:3:42:ARG:NH1	51:3:74:ARG:NH2	2.68	0.42
52:4:24:ASN:HD22	52:4:25:GLN:N	2.18	0.42
48:0:102:TYR:HD2	57:9:35:TYR:HE1	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:O	1:A:456:GLN:HG2	2.20	0.42
66:AJ:316:MET:HB3	76:AJ:403:PEE:O2P	2.20	0.42
75:AJ:405:CDL:H741	75:AJ:405:CDL:H711	1.59	0.42
67:AK:65:ILE:HG21	67:AK:213:PHE:HD1	1.83	0.42
76:AL:503:PEE:C30	76:AL:503:PEE:H19	2.47	0.42
60:AP:145:ASP:OD1	60:AP:146:VAL:N	2.53	0.42
81:AU:402:HEC:HHD	81:AU:402:HEC:HBC3	2.01	0.42
2:B:166:VAL:HG11	2:B:199:ILE:CG2	2.49	0.42
9:J:263:PHE:CE1	9:J:333:PRO:HG2	2.55	0.42
11:L:130:THR:O	11:L:133:ASP:HB3	2.19	0.42
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.42
12:M:560:LEU:HD12	12:M:561:PRO:HD2	2.02	0.42
12:M:598:ASN:N	12:M:602:ARG:O	2.48	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
14:O:176:CYS:HA	74:O:301:FES:S1	2.60	0.42
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	0.42
15:P:210:LEU:HA	15:P:221:ALA:HA	2.01	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
16:Q:190:HIS:CE1	16:Q:268:TRP:CH2	3.08	0.42
16:Q:233:HIS:CD2	16:Q:234:GLN:HB2	2.55	0.42
16:Q:235:ASP:HA	16:Q:356:ILE:HD12	2.01	0.42
1:A:122:PRO:HB2	1:A:322:SER:HB2	2.01	0.42
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.42
60:AC:200:HIS:CE1	60:AC:202:LEU:HB3	2.55	0.42
63:AF:39:TYR:CE2	66:AJ:108:LEU:HD13	2.55	0.42
66:AJ:171:ASP:CG	66:AJ:172:SER:H	2.23	0.42
66:AJ:320:LEU:HB2	66:AJ:373:GLU:OE2	2.20	0.42
67:AK:79:THR:HG23	67:AK:205:LEU:HD23	2.02	0.42
68:AL:233:ALA:HB1	68:AL:237:VAL:HG21	2.01	0.42
68:AL:424:ILE:HA	68:AL:425:PRO:HD2	1.91	0.42
66:AV:271:GLU:HG3	66:AV:273:TYR:CZ	2.55	0.42
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.42
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
12:M:357:LEU:O	12:M:361:VAL:HG22	2.20	0.42
12:M:543:LYS:HD2	12:M:543:LYS:N	2.35	0.42
12:M:711:VAL:O	12:M:715:THR:HG23	2.19	0.42
14:O:144:ASN:O	14:O:147:SER:OG	2.35	0.42
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.42
15:P:202:PHE:HB2	15:P:207:TYR:CE2	2.55	0.42
15:P:240:GLU:OE1	15:P:246:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:40:THR:OG1	18:T:44:GLN:HG2	2.20	0.42
20:V:23:TYR:O	20:V:24:SER:HB2	2.20	0.42
60:AC:136:PHE:O	60:AC:139:SER:OG	2.28	0.41
60:AC:200:HIS:HE1	60:AC:202:LEU:HB3	1.84	0.41
60:AC:246:SER:OG	60:AC:248:ARG:NE	2.47	0.41
61:AD:30:MET:SD	64:AG:34:TRP:HB2	2.60	0.41
63:AF:63:ILE:HD13	66:AJ:211:ILE:CG2	2.50	0.41
64:AG:17:TRP:HE1	68:AL:382:SER:HG	1.67	0.41
68:AL:240:GLN:HE22	68:AL:243:LEU:HD23	1.84	0.41
68:AL:407:THR:HB	68:AL:408:PRO:HD3	2.02	0.41
66:AV:149:LEU:O	66:AV:152:ALA:HB3	2.19	0.41
67:AW:43:LEU:HD13	67:AW:238:LEU:HD11	2.01	0.41
67:AW:257:GLU:HG2	67:AW:450:VAL:HB	2.02	0.41
68:AY:407:THR:HB	68:AY:408:PRO:HD3	2.01	0.41
68:AY:40:GLN:HB3	68:AY:44:PHE:HE2	1.84	0.41
64:AT:24:TRP:HZ3	75:AY:501:CDL:H551	1.79	0.41
2:B:96:ARG:HB3	2:B:167:GLU:HG2	2.01	0.41
6:G:103:HIS:N	6:G:107:ASP:HB2	2.35	0.41
9:J:179:ARG:HB3	9:J:179:ARG:HH11	1.84	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.41
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.41
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.41
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.41
16:Q:199:PRO:HB3	16:Q:258:LEU:HD21	2.01	0.41
16:Q:368:ARG:HA	16:Q:371:MET:HG2	2.01	0.41
16:Q:83:ASN:CA	16:Q:98:VAL:HG22	2.44	0.41
18:T:80:VAL:O	18:T:121:GLN:HA	2.20	0.41
51:3:77:PRO:HA	51:3:82:TYR:HA	2.01	0.41
1:A:27:PRO:HB2	1:A:28:LYS:H	1.65	0.41
60:AC:181:GLN:HA	60:AC:184:ILE:HD12	2.01	0.41
62:AE:29:PRO:HD3	65:AH:262:THR:CG2	2.37	0.41
63:AF:76:LEU:HD12	63:AF:77:PRO:HD2	2.02	0.41
66:AJ:160:LEU:O	66:AJ:164:ILE:HD12	2.20	0.41
66:AJ:9:PRO:HB3	66:AV:202:GLU:OE1	2.20	0.41
67:AK:80:THR:HA	67:AK:83:LEU:HB3	2.03	0.41
68:AL:35:THR:OG1	68:AL:36:ALA:N	2.52	0.41
58:AN:13:HIS:H	68:AY:279:ASP:H	1.67	0.41
68:AY:373:GLN:NE2	68:AY:471:ILE:HG23	2.35	0.41
68:AY:392:LYS:O	68:AY:396:ARG:HG3	2.20	0.41
66:AV:10:LEU:HD22	76:AY:502:PEE:C27	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.55	0.41
7:H:18:ASN:O	7:H:19:THR:OG1	2.31	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.85	0.41
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.41
16:Q:341:LEU:HD23	16:Q:341:LEU:HA	1.88	0.41
19:U:19:LEU:O	19:U:22:SER:OG	2.29	0.41
20:V:126:LYS:HE3	20:V:130:LEU:HD11	2.02	0.41
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.41
59:AB:53:GLU:O	68:AL:402:HIS:ND1	2.47	0.41
75:AG:101:CDL:C52	75:AG:101:CDL:C71	2.86	0.41
65:AH:266:ILE:O	65:AH:270:VAL:HG23	2.20	0.41
66:AJ:147:THR:HG22	66:AJ:161:VAL:HG13	2.02	0.41
68:AL:360:CYS:SG	68:AL:365:ILE:HG12	2.60	0.41
60:AP:207:LYS:HE3	60:AP:209:GLU:OE2	2.20	0.41
62:AR:34:ARG:NH1	62:AR:78:ARG:NH2	2.63	0.41
66:AJ:9:PRO:HG2	66:AV:199:PHE:CE1	2.55	0.41
66:AV:33:PHE:HA	66:AV:36:LEU:HD12	2.01	0.41
67:AW:125:CYS:SG	67:AW:130:VAL:HG22	2.60	0.41
67:AW:195:TYR:CE2	67:AW:196:ARG:HG2	2.55	0.41
2:B:140:THR:HG1	2:B:185:LYS:HZ2	1.60	0.41
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	0.41
7:H:50:GLN:HE22	8:I:93:LYS:HD2	1.85	0.41
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.84	0.41
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.41
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.41
18:T:32:VAL:HG22	18:T:38:LYS:HE3	2.02	0.41
48:O:130:PRO:O	48:O:136:ALA:HB2	2.21	0.41
52:4:57:ARG:HA	52:4:60:TYR:CD2	2.55	0.41
1:A:223:PRO:HB2	1:A:425:CYS:SG	2.60	0.41
64:AG:45:VAL:HG21	64:AG:48:ILE:HB	2.02	0.41
67:AK:261:GLN:H	67:AK:444:LEU:HD12	1.86	0.41
75:AN:101:CDL:OB4	63:AS:73:HIS:CE1	2.73	0.41
63:AS:42:GLU:HA	63:AS:45:LYS:HD3	2.03	0.41
68:AY:314:TYR:HB3	68:AY:341:PHE:CE1	2.56	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
10:K:101:SER:OG	10:K:102:GLY:N	2.53	0.41
11:L:131:LYS:HD2	11:L:147:ILE:HG23	2.03	0.41
12:M:234:LYS:N	12:M:235:PRO:HD2	2.36	0.41
12:M:598:ASN:HD22	12:M:602:ARG:NH1	2.19	0.41
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:157:VAL:HG21	15:P:181:HIS:CD2	2.46	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
50:2:49:VAL:O	50:2:91:LEU:HD12	2.21	0.41
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.41
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.41
1:A:116:ASN:HB3	70:A:502:FMN:HM83	2.01	0.41
63:AF:76:LEU:O	63:AF:81:TRP:NE1	2.37	0.41
66:AJ:146:ILE:HA	66:AJ:149:LEU:HD13	2.02	0.41
67:AK:81:HIS:CD2	67:AK:158:LEU:HD22	2.55	0.41
67:AK:452:GLU:HG3	67:AK:452:GLU:O	2.20	0.41
60:AP:155:LYS:NZ	60:AP:273:VAL:HG21	2.36	0.41
61:AQ:4:ALA:HB3	61:AQ:9:LYS:HE3	2.02	0.41
65:AU:177:LYS:HA	65:AU:178:PRO:HD3	1.87	0.41
66:AV:105:GLY:HA2	66:AV:107:PHE:CE2	2.56	0.41
67:AW:64:PHE:HZ	67:AW:393:LEU:HD23	1.86	0.41
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	0.41
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.41
12:M:557:ARG:HE	12:M:579:ILE:HG23	1.86	0.41
1:A:382:CYS:HA	12:M:75:CYS:H	1.86	0.41
54:6:5:VAL:O	54:6:9:GLN:HG3	2.21	0.41
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
60:AC:248:ARG:HG2	60:AC:257:ASN:ND2	2.36	0.41
60:AC:88:PHE:O	60:AC:92:ARG:HG3	2.20	0.41
65:AH:197:LEU:HA	65:AH:200:ILE:HB	2.03	0.41
68:AL:156:LEU:HB2	68:AL:213:ARG:HE	1.85	0.41
76:AL:503:PEE:H53	76:AL:503:PEE:H25	2.01	0.41
58:AN:17:TYR:CD1	68:AY:275:ILE:HG12	2.55	0.41
66:AV:171:ASP:CG	66:AV:172:SER:H	2.23	0.41
67:AW:290:GLN:HB3	67:AW:336:PHE:HE1	1.86	0.41
67:AW:450:VAL:CA	67:AW:453:LEU:CD1	2.89	0.41
68:AY:225:LYS:O	68:AY:228:ARG:HB3	2.20	0.41
68:AY:274:GLU:OE2	68:AY:468:TYR:HB2	2.20	0.41
3:C:187:ALA:O	3:C:190:LEU:HB3	2.20	0.41
9:J:201:VAL:HG13	9:J:265:PHE:CD2	2.55	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
14:O:156:LEU:HD13	14:O:158:ILE:HD12	2.03	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
48:O:86:MET:O	55:7:25:CYS:HB2	2.20	0.41
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	0.41
66:AJ:132:VAL:HG22	66:AJ:143:ALA:HB2	2.03	0.41
59:AO:13:PRO:HB2	67:AW:84:ARG:HH12	1.86	0.41
59:AO:20:ARG:NH2	59:AO:48:PRO:HG2	2.36	0.41
60:AP:218:THR:HG21	60:AP:256:LEU:HD12	2.02	0.41
65:AU:201:VAL:HG13	65:AU:208:GLU:N	2.36	0.41
76:AU:401:PEE:H49	76:AU:401:PEE:H55	1.81	0.41
66:AV:249:LEU:CD1	66:AV:250:LEU:HD12	2.50	0.41
66:AV:87:ALA:HB2	82:AV:401:HEM:CHB	2.50	0.41
67:AW:214:THR:HG21	67:AW:244:LEU:N	2.34	0.41
67:AW:88:SER:O	67:AW:96:SER:OG	2.33	0.41
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.41
51:3:44:ARG:HA	51:3:45:PRO:HD2	1.76	0.41
52:4:65:PRO:HG2	52:4:68:TRP:CG	2.56	0.41
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.41
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.92	0.41
60:AC:127:TYR:HE1	61:AD:33:GLU:HG2	1.85	0.41
65:AH:112:ARG:O	65:AH:116:VAL:HG23	2.21	0.41
66:AJ:111:GLU:O	66:AJ:115:ILE:HG12	2.20	0.41
66:AJ:2:THR:HG21	68:AL:335:ASN:HD22	1.86	0.41
58:AA:64:THR:HG23	66:AJ:337:TRP:HZ2	1.86	0.41
67:AK:227:HIS:HD1	67:AK:231:LYS:HE2	1.86	0.41
67:AK:67:ALA:HB2	67:AK:212:HIS:HB3	2.03	0.41
64:AT:9:ARG:HH22	71:AT:101:PLX:C1A	2.33	0.41
65:AU:266:ILE:O	65:AU:270:VAL:HG23	2.20	0.41
66:AV:156:ILE:HG22	66:AV:160:LEU:HB2	2.01	0.41
67:AW:51:SER:HB2	67:AW:230:LEU:HD12	2.02	0.41
67:AW:299:VAL:HG22	68:AY:120:LEU:HG	2.03	0.41
68:AY:282:LEU:HB2	68:AY:461:PRO:HD3	2.03	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
4:E:41:ARG:HE	6:G:120:MET:HE3	1.85	0.41
5:F:23:LEU:HD21	5:F:34:ARG:HG2	2.03	0.41
9:J:62:THR:HG21	73:J:401:NDP:O1X	2.21	0.41
11:L:117:THR:OG1	15:P:229:GLU:OE1	2.39	0.41
12:M:646:LEU:O	12:M:651:PRO:HA	2.20	0.41
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.41
15:P:77:GLN:HB2	15:P:85:GLU:HB2	2.03	0.41
48:O:137:LYS:O	48:O:145:TRP:HE3	2.03	0.41
53:5:42:LYS:HB3	53:5:42:LYS:HE2	1.83	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AC:196:ARG:HB3	60:AC:249:ILE:HG23	2.01	0.41
58:AA:78:TYR:CD1	62:AE:65:GLU:CG	3.04	0.41
65:AH:128:ASP:OD1	65:AH:177:LYS:HE2	2.20	0.41
66:AJ:221:HIS:HA	66:AJ:225:THR:HG23	2.02	0.41
67:AK:449:PHE:HE2	67:AW:183:ARG:HB3	1.86	0.41
68:AL:170:ARG:O	68:AL:174:GLU:HG3	2.20	0.41
68:AL:91:TYR:O	68:AL:94:GLU:HB3	2.21	0.41
60:AP:186:GLN:O	60:AP:190:VAL:HG23	2.20	0.41
62:AR:34:ARG:NH1	62:AR:78:ARG:HH22	2.10	0.41
65:AU:156:ASP:HB2	65:AU:167:ARG:HB2	2.03	0.41
67:AW:155:GLN:N	67:AW:156:PRO:HD2	2.35	0.41
67:AW:209:VAL:HG13	67:AW:213:PHE:CD2	2.55	0.41
67:AW:352:LYS:O	67:AW:356:ASN:ND2	2.54	0.41
60:AP:111:LYS:NZ	68:AY:451:ASP:O	2.32	0.41
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.41
3:C:213:ARG:HG2	3:C:213:ARG:O	2.19	0.41
7:H:45:ARG:O	7:H:49:GLU:HG3	2.21	0.41
9:J:130:ILE:HA	73:J:401:NDP:H8A	2.03	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:246:ARG:NH2	15:P:229:GLU:OE2	2.54	0.41
12:M:522:GLN:HE21	12:M:526:LEU:HG	1.85	0.41
12:M:568:TYR:HB2	12:M:580:ALA:CB	2.51	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
15:P:227:ALA:O	15:P:229:GLU:N	2.47	0.41
16:Q:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
16:Q:80:ILE:HG22	16:Q:81:THR:N	2.35	0.41
18:T:110:GLY:N	18:T:119:PHE:O	2.28	0.41
20:V:114:ALA:HB1	20:V:118:PHE:CE2	2.56	0.41
21:W:86:MET:HG2	21:W:128:ARG:HH22	1.86	0.41
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.41
48:O:24:LEU:HB3	49:1:30:ARG:HG2	2.03	0.41
49:1:21:LYS:O	49:1:57:ARG:NH1	2.53	0.41
50:2:10:GLU:HG2	50:2:25:ARG:HH22	1.86	0.41
51:3:25:LEU:HA	51:3:25:LEU:HD23	1.91	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.41
1:A:339:PHE:HA	1:A:342:LEU:HD12	2.03	0.41
60:AC:209:GLU:HG2	60:AC:210:TRP:CD1	2.56	0.41
65:AH:85:SER:OG	65:AH:86:ASP:N	2.52	0.41
67:AK:239:ASN:OD1	67:AK:240:MET:HG2	2.21	0.41
68:AL:141:PRO:HA	68:AL:245:LEU:HD13	2.03	0.41
68:AL:462:ILE:HG23	68:AL:465:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:150:ALA:C	60:AP:152:ILE:H	2.24	0.41
61:AQ:21:PHE:CE2	61:AQ:25:ILE:HD11	2.56	0.41
65:AU:199:TYR:OH	66:AV:71:ARG:NH1	2.53	0.41
66:AV:146:ILE:O	66:AV:149:LEU:HB2	2.21	0.41
67:AW:205:LEU:O	67:AW:209:VAL:HG23	2.21	0.41
67:AW:305:THR:HA	67:AW:311:GLN:NE2	2.36	0.41
2:B:143:TYR:HB3	2:B:185:LYS:HB2	2.03	0.41
2:B:146:ASP:OD2	2:B:149:LYS:HE2	2.21	0.41
2:B:160:CYS:HA	2:B:161:PRO:HD2	1.83	0.41
71:B:303:PLX:H332	71:B:303:PLX:H301	1.80	0.41
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
9:J:271:TYR:HE1	9:J:374:THR:HB	1.85	0.41
9:J:329:LEU:HD22	9:J:332:LEU:HD12	2.01	0.41
16:Q:316:PHE:HD1	16:Q:339:GLN:HE21	1.67	0.41
17:S:47:LEU:O	17:S:50:ARG:HB3	2.20	0.41
22:Y:62:SER:O	22:Y:65:MET:HB3	2.21	0.41
50:2:30:PRO:HG2	50:2:31:TYR:CD1	2.56	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:176:VAL:HG22	60:AC:212:ILE:HG12	2.02	0.41
76:AH:401:PEE:C30	76:AH:401:PEE:H13	2.50	0.41
65:AH:91:PRO:HA	65:AH:92:PRO:HD3	1.91	0.41
66:AJ:103:TYR:OH	66:AJ:322:GLN:NE2	2.54	0.41
66:AJ:3:PRO:HB2	66:AJ:5:ARG:HG2	2.03	0.41
66:AJ:198:LEU:HD12	75:AJ:404:CDL:H311	2.02	0.41
67:AK:58:VAL:HG23	68:AL:400:VAL:HG11	2.03	0.41
68:AL:234:ALA:HB2	68:AL:413:ILE:HD12	2.03	0.41
60:AP:141:SER:OG	60:AP:142:ALA:N	2.51	0.41
71:AQ:101:PLX:H21	71:AQ:101:PLX:H1C3	1.84	0.41
67:AW:449:PHE:N	67:AW:452:GLU:CD	2.73	0.41
67:AW:67:ALA:HA	67:AW:71:TYR:CD2	2.56	0.41
68:AY:113:VAL:HG13	68:AY:118:ALA:HB3	2.03	0.41
68:AY:98:PHE:HE2	68:AY:120:LEU:CD1	2.19	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	0.41
9:J:168:SER:CA	9:J:184:LYS:CE	2.99	0.41
9:J:202:LYS:N	9:J:263:PHE:O	2.54	0.41
11:L:123:ASN:HB3	15:P:232:LYS:HD2	2.02	0.41
12:M:128:CYS:CB	12:M:129:PRO:CD	2.86	0.41
14:O:148:ILE:O	14:O:152:ILE:HG13	2.21	0.41
14:O:198:ALA:O	14:O:202:GLU:HG2	2.21	0.41
15:P:148:ASP:HB2	15:P:151:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:153:LEU:O	16:Q:157:LYS:HG3	2.21	0.41
18:T:33:SER:HB3	18:T:45:VAL:HG21	2.03	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
50:2:74:LEU:HA	50:2:74:LEU:HD23	1.86	0.40
65:AH:89:LEU:HD23	65:AH:236:TYR:CZ	2.56	0.40
75:AL:502:CDL:HB62	75:AL:502:CDL:H712	1.75	0.40
60:AP:173:PRO:HD2	60:AP:216:VAL:HG23	2.03	0.40
60:AP:248:ARG:HG2	60:AP:257:ASN:ND2	2.36	0.40
61:AQ:15:PHE:O	71:AQ:101:PLX:H1A1	2.21	0.40
61:AQ:25:ILE:O	61:AQ:29:VAL:HG23	2.21	0.40
67:AW:177:LEU:HD21	67:AW:272:VAL:HG21	2.02	0.40
67:AW:261:GLN:H	67:AW:444:LEU:HD12	1.85	0.40
68:AY:334:ALA:H	68:AY:336:LYS:H	1.68	0.40
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.40
2:B:155:PHE:HB2	69:B:302:SF4:S2	2.61	0.40
2:B:90:PRO:O	2:B:91:LEU:HD12	2.21	0.40
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.40
4:E:42:GLU:OE2	4:E:46:THR:OG1	2.40	0.40
5:F:89:ARG:HD2	5:F:92:GLU:OE2	2.21	0.40
73:J:401:NDP:P2B	73:J:401:NDP:O3B	2.79	0.40
12:M:401:LEU:HD13	12:M:462:PHE:CE2	2.56	0.40
12:M:483:ARG:O	12:M:483:ARG:HG3	2.21	0.40
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.40
16:Q:65:PRO:CG	16:Q:69:VAL:HG22	2.51	0.40
16:Q:71:PRO:HB2	16:Q:72:PRO:HD3	2.03	0.40
75:V:201:CDL:H722	75:V:201:CDL:H752	1.75	0.40
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.86	0.40
54:6:12:PHE:O	54:6:23:LYS:HE2	2.21	0.40
54:6:21:HIS:CD2	54:6:22:LEU:HG	2.57	0.40
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.40
75:AG:101:CDL:C55	75:AG:101:CDL:H512	2.43	0.40
75:AH:403:CDL:H311	75:AH:403:CDL:H341	1.79	0.40
67:AK:288:VAL:O	67:AK:292:VAL:HG23	2.21	0.40
58:AA:17:TYR:CD1	68:AL:275:ILE:HG12	2.56	0.40
68:AL:314:TYR:HB3	68:AL:341:PHE:CZ	2.55	0.40
60:AP:155:LYS:HB2	60:AP:271:VAL:HG13	2.04	0.40
63:AS:76:LEU:O	63:AS:81:TRP:NE1	2.37	0.40
66:AV:128:PHE:O	66:AV:132:VAL:HG23	2.22	0.40
66:AV:3:PRO:HG2	66:AV:6:LYS:HG2	2.03	0.40
67:AW:317:THR:HB	67:AW:318:GLN:H	1.69	0.40
6:G:154:VAL:O	6:G:156:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:75:GLY:CA	8:I:103:ARG:HH11	2.34	0.40
12:M:128:CYS:HA	69:M:801:SF4:S4	2.61	0.40
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.96	0.40
12:M:436:VAL:HG21	12:M:686:PRO:HG2	2.02	0.40
14:O:99:ASN:O	14:O:103:GLU:HG3	2.21	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
15:P:61:PHE:O	15:P:64:TYR:HB3	2.20	0.40
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	0.40
71:U:101:PLX:H1B3	71:U:101:PLX:H22	1.86	0.40
71:V:203:PLX:H342	71:V:203:PLX:H371	1.76	0.40
22:Y:74:TRP:CZ3	22:Y:75:HIS:HA	2.53	0.40
50:2:16:LEU:O	50:2:20:VAL:HG13	2.21	0.40
57:9:35:TYR:HD2	57:9:36:HIS:CE1	2.39	0.40
1:A:55:GLY:O	1:A:58:SER:OG	2.32	0.40
65:AH:175:PHE:HA	65:AH:176:PRO:HD3	1.84	0.40
66:AJ:150:LEU:HA	66:AJ:150:LEU:HD12	1.87	0.40
66:AJ:345:TYR:N	66:AJ:346:PRO:HD2	2.36	0.40
68:AL:294:PRO:HG3	68:AL:448:TYR:CE1	2.56	0.40
68:AL:301:ASN:O	68:AL:305:GLN:HG2	2.21	0.40
60:AP:125:VAL:HG21	71:AQ:101:PLX:H141	2.03	0.40
66:AV:21:LEU:O	66:AV:21:LEU:HD12	2.22	0.40
59:AO:35:PRO:CB	67:AW:320:PRO:HA	2.48	0.40
68:AY:331:GLY:O	68:AY:337:LEU:HD12	2.21	0.40
67:AW:126:LEU:HB3	68:AY:38:PHE:HZ	1.85	0.40
68:AY:61:SER:HA	68:AY:233:ALA:O	2.21	0.40
68:AY:61:SER:HB2	68:AY:242:LEU:HD23	2.03	0.40
2:B:84:TYR:CD1	2:B:85:PRO:HA	2.56	0.40
2:B:96:ARG:HD2	2:B:154:GLY:HA3	2.03	0.40
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.40
9:J:329:LEU:HD13	9:J:332:LEU:HD12	2.03	0.40
11:L:163:ASN:O	11:L:171:ARG:N	2.55	0.40
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40
14:O:110:MET:HA	14:O:113:TYR:CD2	2.57	0.40
14:O:197:THR:N	14:O:200:ASP:HB3	2.36	0.40
16:Q:120:THR:O	16:Q:124:ILE:HG13	2.22	0.40
16:Q:310:VAL:O	16:Q:314:VAL:HG23	2.21	0.40
21:W:111:PHE:CE2	21:W:117:VAL:HG21	2.56	0.40
22:Y:45:ARG:O	22:Y:45:ARG:HG2	2.22	0.40
60:AC:207:LYS:HA	60:AC:208:PRO:HD3	1.86	0.40
65:AH:228:ARG:NH1	65:AH:229:GLU:HB3	2.36	0.40
59:AO:37:THR:O	67:AW:266:LEU:HD21	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AP:184:ILE:HD13	60:AP:208:PRO:HB2	2.04	0.40
65:AU:304:TYR:OH	75:AU:403:CDL:H732	2.22	0.40
68:AY:296:TRP:HB2	68:AY:348:TYR:C	2.42	0.40
68:AY:53:LEU:HD12	68:AY:57:LEU:HB3	2.04	0.40
68:AY:71:VAL:HG22	68:AY:233:ALA:HB2	2.02	0.40
2:B:104:TYR:N	2:B:108:GLU:O	2.33	0.40
5:F:14:LEU:N	5:F:17:ARG:HH12	2.20	0.40
9:J:319:VAL:C	9:J:323:HIS:HD1	2.22	0.40
12:M:645:ARG:O	12:M:649:VAL:HG12	2.21	0.40
5:F:66:TRP:CZ2	12:M:648:GLU:HB2	2.57	0.40
13:N:39:VAL:HG12	13:N:40:GLY:O	2.21	0.40
16:Q:331:LEU:O	16:Q:335:GLU:HG3	2.20	0.40
16:Q:316:PHE:HB2	16:Q:339:GLN:CG	2.51	0.40
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.03	0.40
48:O:127:LYS:O	48:O:130:PRO:HD3	2.20	0.40
52:4:33:TYR:O	52:4:37:HIS:HD2	2.05	0.40
1:A:53:LEU:O	1:A:56:SER:OG	2.24	0.40
66:AJ:171:ASP:OD1	66:AJ:172:SER:N	2.51	0.40
67:AK:104:GLU:OE1	68:AL:325:SER:HA	2.21	0.40
67:AK:159:LYS:HG2	67:AK:197:ILE:HD13	2.03	0.40
60:AP:151:LYS:O	60:AP:153:GLU:N	2.51	0.40
64:AT:38:TRP:CD1	64:AT:40:LEU:HG	2.56	0.40
65:AU:281:GLU:HG3	66:AV:77:TRP:CD2	2.56	0.40
66:AV:132:VAL:HG11	66:AV:178:PHE:HD2	1.87	0.40
66:AV:186:PRO:O	66:AV:189:ILE:HB	2.21	0.40
66:AV:222:PRO:HG3	68:AY:470:ARG:HD3	2.04	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
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	0.40
4:E:37:ARG:HH21	4:E:41:ARG:HH22	1.68	0.40
6:G:123:GLU:HB3	6:G:130:ILE:HG12	2.04	0.40
11:L:121:LEU:HA	11:L:121:LEU:HD23	4.50	0.40
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.40
14:O:186:VAL:HG12	14:O:188:ILE:HG13	2.03	0.40
16:Q:314:VAL:HG12	16:Q:316:PHE:HD2	1.87	0.40
16:Q:50:ALA:HB2	16:Q:63:PRO:HB3	2.03	0.40
17:S:37:ARG:NH1	17:S:51:ASP:OD2	2.51	0.40
18:T:105:LYS:HB3	18:T:107:THR:HG22	2.04	0.40
19:U:8:PHE:O	19:U:11:ASN:HB3	2.21	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%)	8	48
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	28	70
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	5	40
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	10	51
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	7	45
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	30
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	3	31
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	23
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	48
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	1	13
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	4	39
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	4	39
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	29
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	39
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	28
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	11	53
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	5	42
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	3	32
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	15	58
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	8	47
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	4	36
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	11
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	8	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	33
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	3	30
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	28	70
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	5	40
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	8	47
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	28
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	2	25
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	11	52
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	6	43
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	5	40
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	11	52
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	2	26
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	4	36
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	5	40
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	10	51
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	9	49
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	6	43
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	5	41
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	6	43
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	6	43
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	22	65
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	14	57
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	32
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	2	25
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	13	55
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	4	36
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	6	44
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	14	57
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	27
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	10
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	6	44
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	12	54
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%)	6	43
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	13	55
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	18	61
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%)	22	65
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	22	65
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	22	65
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	22	65
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	15	58
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	15	58
68	AL	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	13	55
68	AY	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	11	53
All	All	14029/14219 (99%)	12872 (92%)	849 (6%)	308 (2%)	12	47

All (308) 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

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Mol	Chain	Res	Type
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
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

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Mol	Chain	Res	Type
54	6	2	GLU
66	AJ	268	ILE
67	AK	241	ARG
59	AO	23	ALA
60	AP	141	SER
68	AY	424	ILE
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
31	h	24	GLU

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Mol	Chain	Res	Type
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
1	A	74	ASP
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
1	A	94	PRO
12	M	575	VAL
36	m	23	PRO
50	2	15	GLY

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Mol	Chain	Res	Type
59	AO	30	VAL
3	C	144	PRO
16	Q	307	PRO
21	W	32	GLY
16	Q	69	VAL
67	AK	320	PRO
10	K	102	GLY
32	i	338	PRO
28	e	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
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	82	92
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	71	87
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	94	97
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	369 (100%)	2 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	49 (86%)	8 (14%)	4	27
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	68	86
25	b	118/118 (100%)	114 (97%)	4 (3%)	42	73
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	25	62
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	41	72
35	l	531/532 (100%)	510 (96%)	21 (4%)	36	69
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	156 (99%)	1 (1%)	89	95
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	x	427/427 (100%)	389 (91%)	38 (9%)	11	44
46	y	211/211 (100%)	191 (90%)	20 (10%)	10	41
47	z	226/226 (100%)	199 (88%)	27 (12%)	6	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	0	128/128 (100%)	120 (94%)	8 (6%)	21	57
49	1	95/95 (100%)	89 (94%)	6 (6%)	21	57
50	2	81/81 (100%)	76 (94%)	5 (6%)	21	58
51	3	68/68 (100%)	50 (74%)	18 (26%)	0	5
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	28
53	5	58/58 (100%)	53 (91%)	5 (9%)	12	46
54	6	47/47 (100%)	40 (85%)	7 (15%)	3	24
55	7	39/39 (100%)	37 (95%)	2 (5%)	28	63
56	8	40/40 (100%)	38 (95%)	2 (5%)	28	64
57	9	37/37 (100%)	34 (92%)	3 (8%)	14	49
58	AA	74/74 (100%)	68 (92%)	6 (8%)	14	49
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%)	52 (100%)	0	100	100
62	AE	61/71 (86%)	59 (97%)	2 (3%)	43	73
62	AR	61/71 (86%)	59 (97%)	2 (3%)	43	73
63	AF	95/95 (100%)	84 (88%)	11 (12%)	6	33
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%)	30	65
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	91	96
66	AJ	330/330 (100%)	327 (99%)	3 (1%)	82	92
66	AV	330/330 (100%)	322 (98%)	8 (2%)	54	79
67	AK	334/335 (100%)	331 (99%)	3 (1%)	82	92
67	AW	335/335 (100%)	332 (99%)	3 (1%)	82	92
68	AL	367/367 (100%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	AY	367/367 (100%)	361 (98%)	6 (2%)	68	86
All	All	12164/12289 (99%)	11911 (98%)	253 (2%)	62	82

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
22	Y	73	PHE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	83	HIS
22	Y	87	PRO
22	Y	97	LEU
24	a	53	ARG
24	a	55	PHE
25	b	21	ARG
25	b	38	GLN
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	115	TYR
27	d	117	GLN
34	k	1	MET
34	k	3	LEU
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN

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Mol	Chain	Res	Type
35	l	87	MET
35	l	88	MET
35	l	94	LEU
35	l	95	PHE
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER
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	447	ASN
35	l	450	LEU
35	l	452	ASN
35	l	513	MET
39	p	124	GLN
45	x	18	LEU
45	x	35	LEU
45	x	92	MET
45	x	96	ARG
45	x	105	LEU
45	x	109	PHE
45	x	115	SER
45	x	138	HIS
45	x	150	LEU
45	x	159	LEU
45	x	187	SER
45	x	188	VAL
45	x	199	LEU
45	x	213	ARG
45	x	238	PHE
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

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Mol	Chain	Res	Type
45	x	347	LEU
45	x	353	LEU
45	x	354	THR
45	x	365	ILE
45	x	369	ASP
45	x	373	VAL
45	x	383	MET
45	x	417	MET
45	x	465	VAL
45	x	467	LEU
45	x	474	GLU
45	x	486	ASP
45	x	492	LEU
45	x	508	PRO
45	x	509	THR
45	x	512	ASN
46	y	7	LEU
46	y	31	VAL
46	y	52	HIS
46	y	60	GLU
46	y	63	THR
46	y	65	TRP
46	y	88	ASP
46	y	92	ASN
46	y	113	TYR
46	y	125	THR
46	y	130	PRO
46	y	134	ARG
46	y	142	VAL
46	y	147	GLU
46	y	148	MET
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

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Mol	Chain	Res	Type
47	z	22	LEU
47	z	38	ASN
47	z	39	SER
47	z	85	LEU
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	159	MET
47	z	160	LEU
47	z	163	LEU
47	z	188	ILE
47	z	196	THR
47	z	199	VAL
47	z	214	PHE
47	z	222	GLN
47	z	258	TRP
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	37	LYS
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	38	HIS
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	69	PHE
51	3	78	LEU
52	4	19	ARG
52	4	24	ASN
52	4	28	ASN
52	4	29	CYS
52	4	51	SER
52	4	53	CYS
52	4	57	ARG
52	4	60	TYR
52	4	75	ARG
53	5	2	THR
53	5	8	GLN
53	5	26	MET
53	5	44	LYS
53	5	64	ARG
54	6	1	PHE
54	6	2	GLU
54	6	3	ASN
54	6	8	LYS
54	6	16	ASN
54	6	23	LYS
54	6	27	THR
55	7	48	VAL
55	7	49	THR
56	8	15	VAL
56	8	22	LEU
57	9	13	LYS

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Mol	Chain	Res	Type
57	9	42	LYS
57	9	43	SER
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	40	GLU
63	AF	41	ASP
63	AF	49	ARG
63	AF	60	MET
63	AF	71	LEU
63	AF	74	GLN
66	AJ	124	MET
66	AJ	150	LEU
66	AJ	300	ILE
67	AK	49	ILE
67	AK	365	ASN
67	AK	451	ASP
62	AR	78	ARG
62	AR	81	CYS
64	AT	39	ARG
64	AT	40	LEU
65	AU	292	MET
66	AV	147	THR
66	AV	149	LEU
66	AV	183	PHE
66	AV	185	LEU
66	AV	192	LEU
66	AV	195	LEU
66	AV	299	LEU
66	AV	345	TYR
67	AW	254	ARG
67	AW	451	ASP

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Mol	Chain	Res	Type
67	AW	453	LEU
68	AY	92	PHE
68	AY	96	LEU
68	AY	416	SER
68	AY	418	LEU
68	AY	422	ARG
68	AY	423	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	101	ASN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
12	M	425	ASN

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Mol	Chain	Res	Type
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	688	GLN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	59	ASN
14	O	69	ASN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	38	GLN
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
17	S	68	ASN
18	T	64	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
22	Y	75	HIS
24	a	90	ASN
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS

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Mol	Chain	Res	Type
25	b	126	GLN
26	c	56	ASN
26	c	84	HIS
26	c	154	GLN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	113	GLN
27	d	117	GLN
27	d	138	GLN
30	g	60	GLN
30	g	96	HIS
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	139	GLN
35	l	192	HIS
35	l	199	GLN
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	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	45	ASN
36	m	117	ASN

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Mol	Chain	Res	Type
37	n	40	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	48	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	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	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	85	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	GLN
45	x	11	ASN
45	x	12	HIS
45	x	43	GLN
45	x	99	ASN
45	x	170	ASN
45	x	256	HIS
45	x	360	ASN
45	x	413	HIS
45	x	512	ASN
46	y	103	GLN
46	y	203	ASN
47	z	6	HIS
47	z	12	ASN
47	z	133	ASN

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Mol	Chain	Res	Type
47	z	148	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	52	HIS
52	4	23	GLN
52	4	24	ASN
52	4	25	GLN
52	4	28	ASN
52	4	37	HIS
54	6	3	ASN
54	6	16	ASN
55	7	10	HIS
55	7	15	ASN
55	7	41	ASN
57	9	39	ASN
58	AA	29	HIS
59	AB	31	GLN
60	AC	80	HIS
60	AC	135	GLN
60	AC	178	HIS
63	AF	23	ASN
63	AF	70	ASN
63	AF	73	HIS
64	AG	16	ASN
65	AH	107	HIS
65	AH	205	HIS
66	AJ	8	ASN
66	AJ	97	HIS
66	AJ	322	GLN
67	AK	167	GLN
67	AK	178	HIS
67	AK	184	ASN
67	AK	206	HIS
67	AK	212	HIS
67	AK	310	HIS
67	AK	311	GLN
67	AK	343	GLN
67	AK	399	GLN

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Mol	Chain	Res	Type
68	AL	87	ASN
68	AL	188	HIS
68	AL	239	HIS
68	AL	240	GLN
68	AL	301	ASN
68	AL	308	ASN
60	AP	135	GLN
60	AP	178	HIS
61	AQ	38	GLN
62	AR	80	HIS
62	AR	84	HIS
63	AS	70	ASN
63	AS	73	HIS
65	AU	284	HIS
66	AV	97	HIS
66	AV	137	GLN
66	AV	255	ASN
66	AV	260	ASN
67	AW	81	HIS
67	AW	139	ASN
67	AW	155	GLN
67	AW	206	HIS
67	AW	212	HIS
67	AW	227	HIS
67	AW	291	HIS
67	AW	298	HIS
67	AW	310	HIS
67	AW	421	ASN
67	AW	446	HIS
68	AY	87	ASN
68	AY	121	ASN
68	AY	152	GLN
68	AY	223	HIS
68	AY	301	ASN
68	AY	342	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 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$
69	SF4	A	501	1	0,12,12	0.00	-	0,24,24	0.00	-
70	FMN	A	502	-	31,33,33	1.47	5 (16%)	38,50,50	1.95	8 (21%)
75	CDL	AA	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.13	5 (7%)
74	FES	AC	301	60	0,4,4	0.00	-	0,4,4	0.00	-
75	CDL	AG	101	-	63,63,99	1.13	4 (6%)	65,75,111	1.23	5 (7%)
76	PEE	AH	401	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
81	HEC	AH	402	65	28,50,50	2.31	3 (10%)	16,82,82	1.56	2 (12%)
75	CDL	AH	403	-	63,63,99	1.23	5 (7%)	65,75,111	1.09	5 (7%)
82	HEM	AJ	401	66	28,50,50	2.15	6 (21%)	17,82,82	1.52	3 (17%)
82	HEM	AJ	402	66	28,50,50	2.14	6 (21%)	17,82,82	1.42	4 (23%)
76	PEE	AJ	403	-	48,48,50	0.99	2 (4%)	50,53,55	0.93	2 (4%)
75	CDL	AJ	404	-	63,63,99	1.22	5 (7%)	65,75,111	1.08	4 (6%)
75	CDL	AJ	405	-	63,63,99	1.11	4 (6%)	65,75,111	1.29	5 (7%)
71	PLX	AL	501	-	51,51,51	0.76	1 (1%)	54,59,59	0.64	1 (1%)
75	CDL	AL	502	-	63,63,99	1.23	5 (7%)	65,75,111	1.11	4 (6%)
76	PEE	AL	503	-	48,48,50	1.05	2 (4%)	50,53,55	0.84	2 (4%)
75	CDL	AN	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.08	4 (6%)
74	FES	AP	301	60	0,4,4	0.00	-	0,4,4	0.00	-
71	PLX	AQ	101	-	51,51,51	0.76	1 (1%)	54,59,59	0.62	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
71	PLX	AT	101	-	51,51,51	0.74	1 (1%)	54,59,59	0.61	1 (1%)
76	PEE	AU	401	-	40,40,50	1.10	2 (5%)	42,45,55	0.86	2 (4%)
81	HEC	AU	402	65	28,50,50	2.39	3 (10%)	16,82,82	1.61	3 (18%)
75	CDL	AU	403	-	63,63,99	1.22	6 (9%)	65,75,111	1.10	4 (6%)
82	HEM	AV	401	66	28,50,50	2.23	6 (21%)	17,82,82	1.59	3 (17%)
82	HEM	AV	402	66	28,50,50	2.15	6 (21%)	17,82,82	1.52	4 (23%)
76	PEE	AV	403	-	48,48,50	1.02	2 (4%)	50,53,55	0.98	2 (4%)
75	CDL	AY	501	-	63,63,99	1.22	5 (7%)	65,75,111	1.06	4 (6%)
76	PEE	AY	502	-	48,48,50	1.06	2 (4%)	50,53,55	0.90	2 (4%)
69	SF4	B	301	2	0,12,12	0.00	-	0,24,24	0.00	-
69	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
71	PLX	B	303	-	51,51,51	0.76	1 (1%)	54,59,59	0.69	1 (1%)
69	SF4	C	301	3	0,12,12	0.00	-	0,24,24	0.00	-
72	8Q1	E	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.54	8 (20%)
73	NDP	J	401	-	43,52,52	0.99	2 (4%)	49,80,80	1.41	3 (6%)
69	SF4	M	801	12	0,12,12	0.00	-	0,24,24	0.00	-
69	SF4	M	802	12	0,12,12	0.00	-	0,24,24	0.00	-
74	FES	M	803	-	0,4,4	0.00	-	0,4,4	0.00	-
74	FES	O	301	14	0,4,4	0.00	-	0,4,4	0.00	-
71	PLX	U	101	-	51,51,51	0.73	1 (1%)	54,59,59	0.74	2 (3%)
75	CDL	V	201	-	61,61,99	1.24	5 (8%)	60,71,111	0.99	3 (5%)
76	PEE	V	202	-	50,50,50	0.87	4 (8%)	52,55,55	0.85	2 (3%)
71	PLX	V	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.61	1 (1%)
76	PEE	W	201	-	50,50,50	0.86	4 (8%)	52,55,55	0.92	2 (3%)
71	PLX	b	201	-	51,51,51	0.60	0	54,59,59	0.64	0
71	PLX	g	201	-	51,51,51	0.81	1 (1%)	54,59,59	0.69	1 (1%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	54,59,59	0.62	1 (1%)
71	PLX	g	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.59	1 (1%)
75	CDL	i	401	-	63,63,99	1.19	5 (7%)	65,75,111	1.10	5 (7%)
76	PEE	l	701	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
76	PEE	l	702	-	50,50,50	0.88	4 (8%)	52,55,55	0.93	2 (3%)
75	CDL	l	703	-	63,63,99	1.19	5 (7%)	65,75,111	1.12	4 (6%)
75	CDL	l	704	-	63,63,99	1.25	5 (7%)	65,75,111	1.06	4 (6%)
75	CDL	n	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.12	4 (6%)
72	8Q1	p	201	-	32,34,34	1.67	5 (15%)	39,43,43	1.80	5 (12%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	54,59,59	0.66	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
71	PLX	r	502	-	51,51,51	0.67	0	54,59,59	0.67	1 (1%)
79	HEA	x	603	45	44,67,67	1.63	8 (18%)	37,103,103	1.87	9 (24%)
79	HEA	x	604	45	44,67,67	1.54	4 (9%)	37,103,103	1.37	8 (21%)

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
69	SF4	A	501	1	-	0/0/48/48	0/6/5/5
70	FMN	A	502	-	-	0/16/18/18	0/3/3/3
75	CDL	AA	101	-	-	0/74/74/110	0/0/0/0
74	FES	AC	301	60	-	0/0/4/4	0/1/1/1
75	CDL	AG	101	-	-	0/74/74/110	0/0/0/0
76	PEE	AH	401	-	-	0/52/52/54	0/0/0/0
81	HEC	AH	402	65	-	0/6/54/54	0/0/8/8
75	CDL	AH	403	-	-	1/74/74/110	0/0/0/0
82	HEM	AJ	401	66	-	0/6/54/54	0/0/8/8
82	HEM	AJ	402	66	-	0/6/54/54	0/0/8/8
76	PEE	AJ	403	-	-	0/52/52/54	0/0/0/0
75	CDL	AJ	404	-	-	0/74/74/110	0/0/0/0
75	CDL	AJ	405	-	-	0/74/74/110	0/0/0/0
71	PLX	AL	501	-	-	0/54/55/55	0/0/0/0
75	CDL	AL	502	-	-	0/74/74/110	0/0/0/0
76	PEE	AL	503	-	-	2/52/52/54	0/0/0/0
75	CDL	AN	101	-	-	0/74/74/110	0/0/0/0
74	FES	AP	301	60	-	0/0/4/4	0/1/1/1
71	PLX	AQ	101	-	-	0/54/55/55	0/0/0/0
71	PLX	AT	101	-	-	0/54/55/55	0/0/0/0
76	PEE	AU	401	-	-	0/44/44/54	0/0/0/0
81	HEC	AU	402	65	-	0/6/54/54	0/0/8/8
75	CDL	AU	403	-	-	0/74/74/110	0/0/0/0
82	HEM	AV	401	66	-	0/6/54/54	0/0/8/8
82	HEM	AV	402	66	-	0/6/54/54	0/0/8/8
76	PEE	AV	403	-	-	0/52/52/54	0/0/0/0
75	CDL	AY	501	-	-	0/74/74/110	0/0/0/0
76	PEE	AY	502	-	-	0/52/52/54	0/0/0/0
69	SF4	B	301	2	-	0/0/48/48	0/6/5/5
69	SF4	B	302	2	-	0/0/48/48	0/6/5/5
71	PLX	B	303	-	-	0/54/55/55	0/0/0/0
69	SF4	C	301	3	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	8Q1	E	201	-	-	2/41/41/41	0/0/0/0
73	NDP	J	401	-	-	0/30/77/77	0/5/5/5
69	SF4	M	801	12	-	0/0/48/48	0/6/5/5
69	SF4	M	802	12	-	0/0/48/48	0/6/5/5
74	FES	M	803	-	-	0/0/4/4	0/1/1/1
74	FES	O	301	14	-	0/0/4/4	0/1/1/1
71	PLX	U	101	-	-	0/54/55/55	0/0/0/0
75	CDL	V	201	-	-	0/69/69/110	0/0/0/0
76	PEE	V	202	-	-	0/54/54/54	0/0/0/0
71	PLX	V	203	-	-	0/54/55/55	0/0/0/0
76	PEE	W	201	-	-	0/54/54/54	0/0/0/0
71	PLX	b	201	-	-	0/54/55/55	0/0/0/0
71	PLX	g	201	-	-	0/54/55/55	0/0/0/0
71	PLX	g	202	-	-	0/54/55/55	0/0/0/0
71	PLX	g	203	-	-	0/54/55/55	0/0/0/0
75	CDL	i	401	-	-	0/74/74/110	0/0/0/0
76	PEE	l	701	-	-	0/52/52/54	0/0/0/0
76	PEE	l	702	-	-	0/54/54/54	0/0/0/0
75	CDL	l	703	-	-	0/74/74/110	0/0/0/0
75	CDL	l	704	-	-	0/74/74/110	0/0/0/0
75	CDL	n	101	-	-	2/74/74/110	0/0/0/0
72	8Q1	p	201	-	-	2/41/41/41	0/0/0/0
71	PLX	r	501	-	-	0/54/55/55	0/0/0/0
71	PLX	r	502	-	-	0/54/55/55	0/0/0/0
79	HEA	x	603	45	3/3/7/16	0/24/76/76	0/0/8/8
79	HEA	x	604	45	3/3/7/16	0/24/76/76	0/0/8/8

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AU	402	HEC	C3C-C2C	-6.89	1.33	1.40
79	x	604	HEA	C3A-C2A	-6.82	1.31	1.40
81	AU	402	HEC	C3B-C2B	-6.62	1.33	1.40
81	AH	402	HEC	C3B-C2B	-6.48	1.33	1.40
81	AH	402	HEC	C3C-C2C	-6.47	1.33	1.40
82	AV	401	HEM	C3C-C2C	-5.73	1.32	1.40
82	AV	402	HEM	C3B-C2B	-4.36	1.34	1.40
82	AJ	401	HEM	C3C-C2C	-4.35	1.34	1.40
82	AJ	401	HEM	C3B-C2B	-4.29	1.34	1.40
82	AV	402	HEM	C3C-C2C	-4.18	1.34	1.40
82	AJ	402	HEM	C3C-C2C	-4.16	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AJ	402	HEM	C3B-C2B	-4.15	1.34	1.40
82	AV	401	HEM	C3B-C2B	-4.03	1.35	1.40
79	x	604	HEA	C3A-CMA	-3.89	1.37	1.46
79	x	603	HEA	C3C-C2C	-3.33	1.35	1.40
71	B	303	PLX	O6-C4	-2.89	1.40	1.44
79	x	604	HEA	C3C-C2C	-2.87	1.36	1.40
79	x	603	HEA	C3A-CMA	-2.87	1.39	1.46
71	g	203	PLX	O6-C4	-2.83	1.40	1.44
71	g	201	PLX	O6-C4	-2.69	1.40	1.44
71	V	203	PLX	O6-C4	-2.68	1.40	1.44
75	n	101	CDL	OB6-CB4	-2.65	1.39	1.46
71	AL	501	PLX	O6-C4	-2.61	1.41	1.44
72	E	201	8Q1	O35-C34	-2.53	1.18	1.23
72	p	201	8Q1	O35-C34	-2.53	1.18	1.23
75	AL	502	CDL	OB6-CB4	-2.52	1.40	1.46
71	AQ	101	PLX	O6-C4	-2.52	1.41	1.44
75	V	201	CDL	OB6-CB4	-2.51	1.40	1.46
71	U	101	PLX	O6-C4	-2.50	1.41	1.44
75	AH	403	CDL	OB6-CB4	-2.50	1.40	1.46
75	AA	101	CDL	OB6-CB4	-2.48	1.40	1.46
75	AJ	404	CDL	OB6-CB4	-2.45	1.40	1.46
75	AN	101	CDL	OB6-CB4	-2.44	1.40	1.46
75	AU	403	CDL	OB6-CB4	-2.41	1.40	1.46
71	AT	101	PLX	O6-C4	-2.41	1.41	1.44
75	i	401	CDL	OB6-CB4	-2.39	1.40	1.46
71	g	202	PLX	O6-C4	-2.37	1.41	1.44
75	AY	501	CDL	OB6-CB4	-2.36	1.40	1.46
79	x	603	HEA	C3A-C2A	-2.34	1.37	1.40
71	r	501	PLX	O6-C4	-2.32	1.41	1.44
76	V	202	PEE	O3-C3	-2.27	1.40	1.45
72	E	201	8Q1	O40-C39	-2.27	1.18	1.23
72	p	201	8Q1	O40-C39	-2.27	1.18	1.23
75	l	704	CDL	OB6-CB4	-2.26	1.40	1.46
76	l	702	PEE	O3-C3	-2.25	1.40	1.45
75	l	703	CDL	OB6-CB4	-2.25	1.40	1.46
76	W	201	PEE	O3-C3	-2.19	1.40	1.45
76	l	702	PEE	O2-C2	-2.16	1.41	1.46
76	V	202	PEE	O2-C2	-2.15	1.41	1.46
76	W	201	PEE	O2-C2	-2.09	1.41	1.46
70	A	502	FMN	C6-C5A	-2.01	1.38	1.41
72	E	201	8Q1	C6-C1	2.03	1.53	1.50
75	AU	403	CDL	C11-CA5	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	x	603	HEA	C1C-NC	2.15	1.40	1.36
76	W	201	PEE	O2-C10	2.16	1.40	1.34
79	x	604	HEA	C1A-NA	2.18	1.39	1.36
76	W	201	PEE	O3-C30	2.23	1.39	1.33
76	V	202	PEE	O3-C30	2.24	1.39	1.33
76	l	702	PEE	O2-C10	2.32	1.41	1.34
76	l	702	PEE	O3-C30	2.32	1.40	1.33
76	V	202	PEE	O2-C10	2.33	1.41	1.34
82	AV	401	HEM	C4D-ND	2.37	1.39	1.36
82	AV	402	HEM	C4D-ND	2.38	1.39	1.36
82	AJ	401	HEM	C4D-ND	2.39	1.39	1.36
82	AJ	402	HEM	C4D-ND	2.39	1.39	1.36
72	p	201	8Q1	C1-S44	2.46	1.81	1.76
73	J	401	NDP	C5A-C4A	2.58	1.46	1.40
79	x	603	HEA	C4C-NC	2.61	1.41	1.36
72	E	201	8Q1	C1-S44	2.63	1.81	1.76
70	A	502	FMN	C9A-C5A	2.91	1.48	1.42
75	i	401	CDL	OB6-CB5	2.99	1.43	1.34
70	A	502	FMN	C8-C7	3.00	1.48	1.41
79	x	603	HEA	C4D-ND	3.01	1.42	1.36
75	AL	502	CDL	OB6-CB5	3.02	1.43	1.34
75	V	201	CDL	OB6-CB5	3.03	1.43	1.34
76	AH	401	PEE	O2-C10	3.03	1.43	1.34
73	J	401	NDP	C6N-C5N	3.06	1.38	1.33
75	AU	403	CDL	OB6-CB5	3.06	1.43	1.34
76	AV	403	PEE	O2-C10	3.07	1.43	1.34
75	AA	101	CDL	OB6-CB5	3.07	1.43	1.34
76	AU	401	PEE	O2-C10	3.10	1.43	1.34
75	AH	403	CDL	OB6-CB5	3.12	1.43	1.34
75	l	703	CDL	OB6-CB5	3.14	1.43	1.34
75	AN	101	CDL	OB6-CB5	3.14	1.43	1.34
76	AJ	403	PEE	O2-C10	3.15	1.43	1.34
75	AJ	404	CDL	OB6-CB5	3.15	1.43	1.34
75	n	101	CDL	OB6-CB5	3.19	1.43	1.34
75	AY	501	CDL	OB6-CB5	3.20	1.43	1.34
76	l	701	PEE	O2-C10	3.24	1.43	1.34
75	l	704	CDL	OB6-CB5	3.26	1.43	1.34
76	AL	503	PEE	O2-C10	3.36	1.44	1.34
76	AY	502	PEE	O2-C10	3.37	1.44	1.34
82	AV	401	HEM	C3C-CAC	3.56	1.54	1.47
75	i	401	CDL	OA8-CA7	3.69	1.44	1.33
82	AJ	402	HEM	C3C-CAC	3.75	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	C3B-CAB	3.77	1.55	1.47
70	A	502	FMN	C4A-C10	3.78	1.47	1.41
70	A	502	FMN	C4-C4A	3.79	1.48	1.41
82	AJ	401	HEM	C3B-CAB	3.79	1.55	1.47
75	l	703	CDL	OA8-CA7	3.80	1.44	1.33
82	AV	401	HEM	C3B-CAB	3.84	1.55	1.47
82	AJ	402	HEM	C3B-CAB	3.85	1.55	1.47
82	AJ	401	HEM	C3C-CAC	3.86	1.55	1.47
75	AJ	405	CDL	OA6-CA5	3.87	1.45	1.34
75	AA	101	CDL	OA8-CA7	3.88	1.44	1.33
75	AN	101	CDL	OA8-CA7	3.88	1.44	1.33
75	i	401	CDL	OA6-CA5	3.89	1.45	1.34
75	AL	502	CDL	OA8-CA7	3.89	1.44	1.33
75	n	101	CDL	OA8-CA7	3.89	1.44	1.33
75	AU	403	CDL	OA8-CA7	3.91	1.44	1.33
75	AH	403	CDL	OA8-CA7	3.91	1.44	1.33
75	AG	101	CDL	OB6-CB5	3.92	1.45	1.34
82	AV	402	HEM	C3C-CAC	3.93	1.55	1.47
75	AY	501	CDL	OA8-CA7	3.93	1.44	1.33
75	AJ	404	CDL	OA8-CA7	3.95	1.44	1.33
76	AJ	403	PEE	O3-C30	3.96	1.45	1.33
75	AJ	405	CDL	OB6-CB5	3.98	1.45	1.34
75	l	704	CDL	OA6-CA5	4.04	1.46	1.34
75	i	401	CDL	OB8-CB7	4.04	1.45	1.33
75	AN	101	CDL	OA6-CA5	4.04	1.46	1.34
75	AA	101	CDL	OA6-CA5	4.06	1.46	1.34
75	n	101	CDL	OB8-CB7	4.09	1.45	1.33
75	V	201	CDL	OA8-CA7	4.09	1.45	1.32
76	AU	401	PEE	O3-C30	4.09	1.45	1.33
76	AV	403	PEE	O3-C30	4.10	1.45	1.33
75	AN	101	CDL	OB8-CB7	4.10	1.45	1.33
76	l	701	PEE	O3-C30	4.11	1.45	1.33
75	AG	101	CDL	OA6-CA5	4.12	1.46	1.34
75	l	704	CDL	OA8-CA7	4.12	1.45	1.33
75	AJ	405	CDL	OB8-CB7	4.14	1.45	1.33
75	l	703	CDL	OA6-CA5	4.14	1.46	1.34
75	AJ	404	CDL	OA6-CA5	4.15	1.46	1.34
75	V	201	CDL	OA6-CA5	4.16	1.46	1.34
75	AJ	404	CDL	OB8-CB7	4.16	1.45	1.33
75	AA	101	CDL	OB8-CB7	4.16	1.45	1.33
75	AU	403	CDL	OA6-CA5	4.17	1.46	1.34
76	AH	401	PEE	O3-C30	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	V	201	CDL	OB8-CB7	4.17	1.45	1.33
75	AY	501	CDL	OA6-CA5	4.18	1.46	1.34
75	n	101	CDL	OA6-CA5	4.19	1.46	1.34
76	AY	502	PEE	O3-C30	4.19	1.45	1.33
75	AG	101	CDL	OA8-CA7	4.19	1.45	1.33
75	AY	501	CDL	OB8-CB7	4.19	1.45	1.33
75	AL	502	CDL	OB8-CB7	4.20	1.45	1.33
75	l	703	CDL	OB8-CB7	4.20	1.45	1.33
75	AL	502	CDL	OA6-CA5	4.21	1.46	1.34
75	AU	403	CDL	OB8-CB7	4.21	1.45	1.33
76	AL	503	PEE	O3-C30	4.22	1.45	1.33
75	AH	403	CDL	OA6-CA5	4.22	1.46	1.34
75	AJ	405	CDL	OA8-CA7	4.25	1.45	1.33
75	AG	101	CDL	OB8-CB7	4.27	1.45	1.33
75	AH	403	CDL	OB8-CB7	4.28	1.45	1.33
75	l	704	CDL	OB8-CB7	4.32	1.46	1.33
72	E	201	8Q1	C39-N41	4.74	1.44	1.33
79	x	603	HEA	C1A-NA	4.81	1.42	1.36
79	x	603	HEA	C4B-NB	4.94	1.42	1.36
72	p	201	8Q1	C39-N41	5.05	1.45	1.33
82	AV	401	HEM	C3D-C2D	5.25	1.53	1.37
82	AJ	402	HEM	C3D-C2D	5.29	1.53	1.37
82	AV	402	HEM	C3D-C2D	5.32	1.53	1.37
82	AJ	401	HEM	C3D-C2D	5.32	1.53	1.37
81	AH	402	HEC	C3D-C2D	5.38	1.53	1.37
81	AU	402	HEC	C3D-C2D	5.43	1.53	1.37
72	E	201	8Q1	C34-N36	5.63	1.45	1.33
72	p	201	8Q1	C34-N36	5.71	1.45	1.33

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	J	401	NDP	N3A-C2A-N1A	-6.94	122.81	128.86
72	p	201	8Q1	O4-C1-C6	-4.87	119.68	123.95
79	x	603	HEA	C4B-C3B-C2B	-4.60	103.66	106.87
70	A	502	FMN	C4-C4A-C10	-3.93	116.78	119.96
79	x	603	HEA	CMB-C2B-C1B	-3.91	122.45	128.46
79	x	603	HEA	C17-C18-C19	-3.82	118.09	127.68
70	A	502	FMN	C4A-C4-N3	-3.40	118.65	123.48
72	E	201	8Q1	O4-C1-C6	-3.35	121.01	123.95
82	AV	401	HEM	CAD-CBD-CGD	-3.20	107.20	112.66
75	AG	101	CDL	CB4-OB6-CB5	-3.06	110.64	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	x	603	HEA	C13-C14-C15	-3.01	120.13	127.68
72	p	201	8Q1	O4-C1-S44	-2.85	119.85	122.84
82	AV	401	HEM	C1D-C2D-C3D	-2.66	105.15	107.00
73	J	401	NDP	C4A-C5A-N7A	-2.64	106.86	109.41
72	E	201	8Q1	O4-C1-S44	-2.51	120.21	122.84
81	AH	402	HEC	CMC-C2C-C1C	-2.51	124.61	128.46
72	E	201	8Q1	O35-C34-N36	-2.43	118.40	123.07
81	AU	402	HEC	CAA-CBA-CGA	-2.38	108.59	112.66
79	x	604	HEA	C4B-C3B-C2B	-2.35	105.23	106.87
72	E	201	8Q1	C42-N41-C39	-2.33	118.36	122.84
79	x	603	HEA	C17-C16-C15	-2.33	105.04	112.93
79	x	603	HEA	C16-C17-C18	-2.29	104.10	111.97
72	E	201	8Q1	C37-N36-C34	-2.27	118.36	122.59
81	AH	402	HEC	CAA-CBA-CGA	-2.24	108.84	112.66
79	x	603	HEA	C12-C13-C14	-2.23	106.47	112.33
82	AV	402	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
75	AJ	405	CDL	OB8-CB7-OB9	-2.23	118.02	123.55
82	AJ	401	HEM	CAD-CBD-CGD	-2.22	108.86	112.66
71	U	101	PLX	C5-C4-C3	-2.21	106.88	111.86
81	AU	402	HEC	CMB-C2B-C1B	-2.20	125.08	128.46
82	AV	402	HEM	CAD-CBD-CGD	-2.19	108.92	112.66
79	x	604	HEA	C13-C14-C15	-2.16	122.25	127.68
81	AU	402	HEC	C1D-C2D-C3D	-2.14	105.50	107.00
71	r	502	PLX	C2-C1-N1	-2.08	108.79	115.86
75	AA	101	CDL	CB4-OB6-CB5	-2.08	112.97	117.88
71	AQ	101	PLX	C2-C1-N1	-2.04	108.95	115.86
79	x	604	HEA	CMC-C2C-C1C	-2.03	125.35	128.46
75	i	401	CDL	CA4-OA6-CA5	-2.03	113.09	117.88
82	AJ	402	HEM	C1D-C2D-C3D	-2.02	105.59	107.00
75	AH	403	CDL	CB4-OB6-CB5	-2.01	113.12	117.88
70	A	502	FMN	C1'-N10-C9A	2.02	120.20	118.35
82	AJ	402	HEM	CMB-C2B-C3B	2.05	128.69	124.89
82	AJ	402	HEM	CMC-C2C-C3C	2.08	128.76	124.89
82	AV	402	HEM	CMB-C2B-C3B	2.13	128.84	124.89
82	AJ	402	HEM	C4A-C3A-C2A	2.13	108.48	107.00
79	x	604	HEA	C26-C15-C16	2.14	119.00	115.29
71	AQ	101	PLX	C1C-N1-C1	2.16	118.22	109.93
82	AV	402	HEM	C4A-C3A-C2A	2.16	108.50	107.00
73	J	401	NDP	C3D-C2D-C1D	2.17	105.59	101.43
71	r	501	PLX	C1C-N1-C1	2.20	118.36	109.93
82	AV	401	HEM	CMB-C2B-C3B	2.24	129.04	124.89
79	x	604	HEA	C25-C23-C24	2.24	119.82	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AJ	401	HEM	CMC-C2C-C3C	2.27	129.11	124.89
79	x	603	HEA	C20-C19-C18	2.33	125.87	121.10
71	g	202	PLX	C1C-N1-C1	2.33	118.89	109.93
71	g	201	PLX	C1C-N1-C1	2.34	118.91	109.93
79	x	604	HEA	CMC-C2C-C3C	2.36	129.27	124.89
82	AJ	401	HEM	CMB-C2B-C3B	2.40	129.35	124.89
71	g	203	PLX	C1C-N1-C1	2.42	119.20	109.93
71	U	101	PLX	C1C-N1-C1	2.44	119.30	109.93
72	p	201	8Q1	C38-C39-N41	2.45	120.71	116.49
71	V	203	PLX	C1C-N1-C1	2.47	119.40	109.93
76	l	701	PEE	O3-C30-C31	2.47	119.09	111.90
76	AY	502	PEE	O3-C30-C31	2.48	119.11	111.90
76	AU	401	PEE	O3-C30-C31	2.49	119.16	111.90
71	AL	501	PLX	C1C-N1-C1	2.50	119.53	109.93
71	B	303	PLX	C1C-N1-C1	2.52	119.58	109.93
72	p	201	8Q1	C43-S44-C1	2.55	110.34	101.90
76	AJ	403	PEE	O3-C30-C31	2.57	119.39	111.90
79	x	604	HEA	CBA-CAA-C2A	2.59	117.41	112.47
71	AT	101	PLX	C1C-N1-C1	2.59	119.87	109.93
75	i	401	CDL	OA8-CA7-C31	2.61	119.49	111.90
72	E	201	8Q1	C32-C34-N36	2.62	122.03	116.58
72	E	201	8Q1	C43-S44-C1	2.62	110.57	101.90
76	AL	503	PEE	O3-C30-C31	2.67	119.66	111.90
75	AH	403	CDL	OA8-CA7-C31	2.70	119.76	111.90
75	AN	101	CDL	OB8-CB7-C71	2.72	119.81	111.90
75	AY	501	CDL	OB8-CB7-C71	2.72	119.81	111.90
75	AY	501	CDL	OA8-CA7-C31	2.72	119.82	111.90
75	V	201	CDL	OB8-CB7-C71	2.74	119.86	111.90
75	AJ	404	CDL	OB8-CB7-C71	2.74	119.87	111.90
75	AG	101	CDL	OA8-CA7-C31	2.77	119.96	111.90
75	AU	403	CDL	OB8-CB7-C71	2.80	120.05	111.90
75	AA	101	CDL	OB8-CB7-C71	2.82	120.11	111.90
76	AH	401	PEE	O3-C30-C31	2.86	120.23	111.90
75	AJ	404	CDL	OA8-CA7-C31	2.87	120.25	111.90
75	AU	403	CDL	OA8-CA7-C31	2.87	120.25	111.90
75	l	704	CDL	OB8-CB7-C71	2.88	120.28	111.90
75	AH	403	CDL	OB8-CB7-C71	2.89	120.30	111.90
76	W	201	PEE	O3-C30-C31	2.90	120.33	111.90
75	AN	101	CDL	OA8-CA7-C31	2.90	120.33	111.90
70	A	502	FMN	C5A-C9A-N10	2.90	119.81	117.66
75	n	101	CDL	OB8-CB7-C71	2.90	120.34	111.90
75	AL	502	CDL	OB8-CB7-C71	2.91	120.36	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	l	703	CDL	OB8-CB7-C71	2.91	120.36	111.90
75	AJ	405	CDL	OA8-CA7-C31	2.92	120.40	111.90
75	l	704	CDL	OA8-CA7-C31	2.94	120.45	111.90
75	AL	502	CDL	OA8-CA7-C31	2.94	120.46	111.90
75	AG	101	CDL	OB8-CB7-C71	2.96	120.51	111.90
75	n	101	CDL	OA8-CA7-C31	2.97	120.54	111.90
75	i	401	CDL	OB8-CB7-C71	2.98	120.57	111.90
79	x	604	HEA	CBD-CAD-C3D	3.03	118.28	112.48
76	l	702	PEE	O3-C30-C31	3.07	120.82	111.90
76	V	202	PEE	O3-C30-C31	3.08	120.85	111.90
75	AA	101	CDL	OA8-CA7-C31	3.20	121.22	111.90
75	l	703	CDL	OA8-CA7-C31	3.23	121.29	111.90
70	A	502	FMN	C4-C4A-N5	3.23	122.22	118.68
70	A	502	FMN	C1'-N10-C10	3.23	121.82	118.50
76	AV	403	PEE	O3-C30-C31	3.30	121.52	111.90
76	AU	401	PEE	O2-C10-C11	3.33	118.46	111.55
70	A	502	FMN	C4A-N5-C5A	3.39	120.34	116.76
75	AJ	405	CDL	OB8-CB7-C71	3.51	122.11	111.90
75	V	201	CDL	OA6-CA5-C11	3.55	118.93	111.55
75	i	401	CDL	OB6-CB5-C51	3.60	119.03	111.55
76	AL	503	PEE	O2-C10-C11	3.62	119.06	111.55
75	AJ	405	CDL	OA6-CA5-C11	3.66	119.15	111.55
76	AH	401	PEE	O2-C10-C11	3.67	119.16	111.55
75	AG	101	CDL	OA6-CA5-C11	3.69	119.21	111.55
76	V	202	PEE	O2-C10-C11	3.72	119.28	111.55
76	W	201	PEE	O2-C10-C11	3.81	119.45	111.55
75	AL	502	CDL	OB6-CB5-C51	3.97	119.79	111.55
75	AN	101	CDL	OB6-CB5-C51	3.99	119.83	111.55
75	AY	501	CDL	OB6-CB5-C51	4.01	119.87	111.55
76	AV	403	PEE	O2-C10-C11	4.04	119.93	111.55
75	l	704	CDL	OB6-CB5-C51	4.04	119.95	111.55
75	AH	403	CDL	OB6-CB5-C51	4.05	119.95	111.55
75	n	101	CDL	OA6-CA5-C11	4.06	119.97	111.55
75	AN	101	CDL	OA6-CA5-C11	4.08	120.01	111.55
75	l	703	CDL	OB6-CB5-C51	4.08	120.02	111.55
75	AA	101	CDL	OB6-CB5-C51	4.11	120.10	111.55
76	l	701	PEE	O2-C10-C11	4.13	120.13	111.55
76	AJ	403	PEE	O2-C10-C11	4.16	120.19	111.55
75	AJ	404	CDL	OB6-CB5-C51	4.16	120.19	111.55
75	AU	403	CDL	OB6-CB5-C51	4.17	120.20	111.55
75	n	101	CDL	OB6-CB5-C51	4.21	120.30	111.55
75	AA	101	CDL	OA6-CA5-C11	4.21	120.30	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	l	704	CDL	OA6-CA5-C11	4.22	120.31	111.55
75	V	201	CDL	OB6-CB5-C51	4.22	120.31	111.55
75	AJ	404	CDL	OA6-CA5-C11	4.26	120.39	111.55
75	i	401	CDL	OA6-CA5-C11	4.27	120.41	111.55
75	AU	403	CDL	OA6-CA5-C11	4.28	120.45	111.55
75	AH	403	CDL	OA6-CA5-C11	4.29	120.47	111.55
75	AG	101	CDL	OB6-CB5-C51	4.33	120.53	111.55
75	l	703	CDL	OA6-CA5-C11	4.33	120.54	111.55
75	AY	501	CDL	OA6-CA5-C11	4.33	120.55	111.55
75	AL	502	CDL	OA6-CA5-C11	4.40	120.69	111.55
75	AJ	405	CDL	OB6-CB5-C51	4.43	120.74	111.55
76	AY	502	PEE	O2-C10-C11	4.45	120.78	111.55
76	l	702	PEE	O2-C10-C11	4.52	120.95	111.55
79	x	603	HEA	C1B-C2B-C3B	4.75	110.30	107.00
72	E	201	8Q1	C6-C1-S44	5.46	118.77	113.28
72	p	201	8Q1	C6-C1-S44	7.13	120.47	113.28
70	A	502	FMN	C4-N3-C2	7.26	121.51	115.16

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	x	603	HEA	ND
79	x	603	HEA	NA
79	x	603	HEA	NB
79	x	604	HEA	ND
79	x	604	HEA	NA
79	x	604	HEA	NB

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	O35-C34-C32-C29
75	AH	403	CDL	CB4-OB6-CB5-C51
75	n	101	CDL	CA4-OA6-CA5-OA7
75	n	101	CDL	CA4-OA6-CA5-C11
72	p	201	8Q1	C6-C1-S44-C43
76	AL	503	PEE	C2-O2-C10-O4
72	p	201	8Q1	O4-C1-S44-C43
76	AL	503	PEE	C2-O2-C10-C11

There are no ring outliers.



41 monomers are involved in 365 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	A	501	SF4	6	0
70	A	502	FMN	17	0
75	AA	101	CDL	1	0
74	AC	301	FES	3	0
75	AG	101	CDL	29	0
76	AH	401	PEE	30	0
81	AH	402	HEC	5	0
75	AH	403	CDL	6	0
82	AJ	401	HEM	3	0
82	AJ	402	HEM	4	0
76	AJ	403	PEE	8	0
75	AJ	404	CDL	6	0
75	AJ	405	CDL	17	0
71	AL	501	PLX	3	0
75	AL	502	CDL	23	0
76	AL	503	PEE	38	0
75	AN	101	CDL	8	0
74	AP	301	FES	2	0
71	AQ	101	PLX	7	0
71	AT	101	PLX	3	0
76	AU	401	PEE	25	0
81	AU	402	HEC	7	0
75	AU	403	CDL	12	0
82	AV	401	HEM	7	0
82	AV	402	HEM	6	0
76	AV	403	PEE	21	0
75	AY	501	CDL	4	0
76	AY	502	PEE	22	0
69	B	301	SF4	1	0
69	B	302	SF4	2	0
71	B	303	PLX	1	0
72	E	201	8Q1	4	0
73	J	401	NDP	27	0
69	M	801	SF4	3	0
74	M	803	FES	1	0
74	O	301	FES	2	0
71	U	101	PLX	1	0
75	V	201	CDL	8	0
76	V	202	PEE	12	0
71	V	203	PLX	2	0
76	W	201	PEE	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.