



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:52 PM JST

PDB ID : 8IB4 / pdb_00008ib4
EMDB ID : EMD-35331
Title : Respiratory complex CI:CIII2, type IA, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

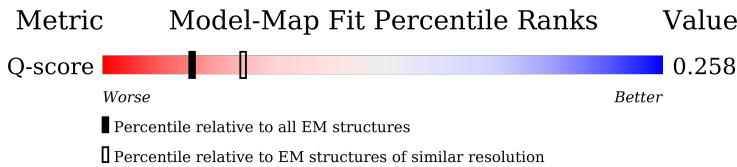
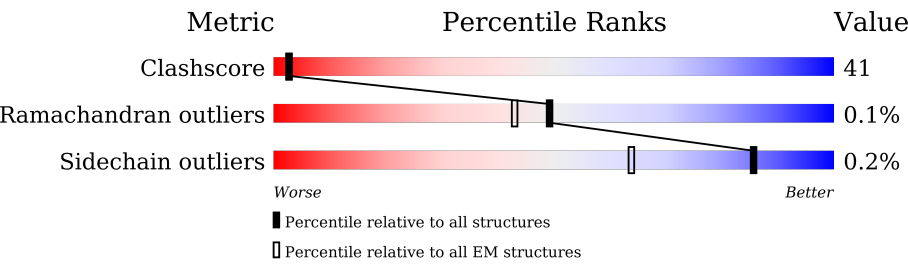
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	115	11% 17% 57% 7% 20%
2	B	224	6% 29% 34% 7% 30%
3	C	263	25% 36% 37% • 25%
4	D	463	13% 37% 50% 5% 8%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

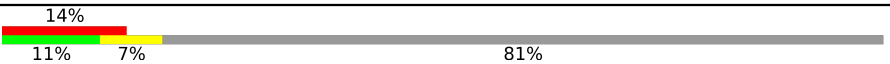
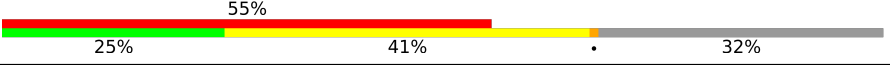
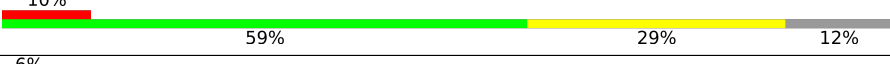
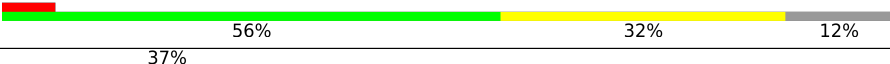
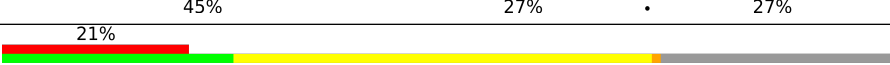
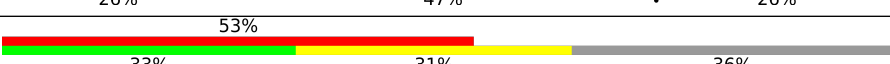
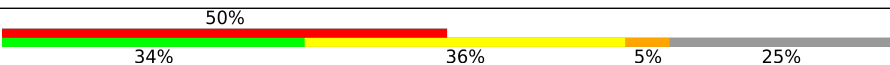
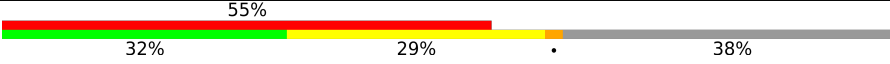
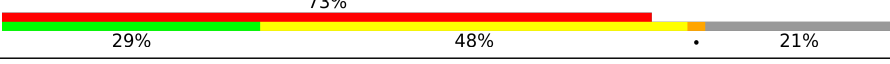
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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	

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Mol	Chain	Length	Quality of chain
49	AI	274	
49	Ae	274	
50	AF	111	
50	Af	111	
51	AG	82	
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

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
55	3PE	L	701	-	-	X	-
56	SF4	B	301	-	-	X	-
56	SF4	F	502	-	-	X	-
56	SF4	G	802	-	-	X	-
56	SF4	I	303	-	-	X	-
56	SF4	I	304	-	-	X	-
57	UQ1	B	302	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
62	CDL	a	101	-	-	X	-
70	HEC	AD	401	X	-	X	-
70	HEC	Ad	401	X	-	X	-

2 Entry composition

There are 71 unique types of molecules in this entry. The entry contains 97639 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1641	1060	279	299	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	424	Total	C	N	O	S	0	0
			3415	2182	587	622	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total	C	N	O	S	0	0
			3288	2073	588	605	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	314	Total	C	N	O	S	0	0
			2510	1687	380	421	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total	C	N	O	S	0	0
			1398	880	240	266	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	159	Total	C	N	O	S	0	0
			1205	814	171	205	15		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3622	2402	566	615	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	340	Total	C	N	O	S	0	0
			2730	1765	479	479	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	84	Total	C	N	O	S	0	0
			678	438	100	135	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			988	646	170	164	8		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			863	546	158	151	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	55	Total	C	N	O	S	0	0
			475	310	84	79	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	136	Total	C	N	O	S	0	0
			1146	754	191	198	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	94	Total	C	N	O	S	0	0
			796	520	139	134	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	71	Total	C	N	O	S	0	0
			569	375	99	93	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	158	Total	C	N	O	S	0	0
			1328	858	221	238	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	127	Total	C	N	O		0	0
			1054	678	190	186			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1027	647	192	179	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	904	258	268	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	14	Total	C	N	O	0	0
			115	75	17	23		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
46	Ab	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
47	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
48	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
49	AI	51	Total	C	N	O		0	0
			345	221	64	60			
49	Ae	185	Total	C	N	O	S	0	0
			1432	905	250	270	7		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	65	Total	C	N	O	S	0	0
			535	327	99	104	5		
52	Ah	66	Total	C	N	O	S	0	0
			544	333	101	105	5		

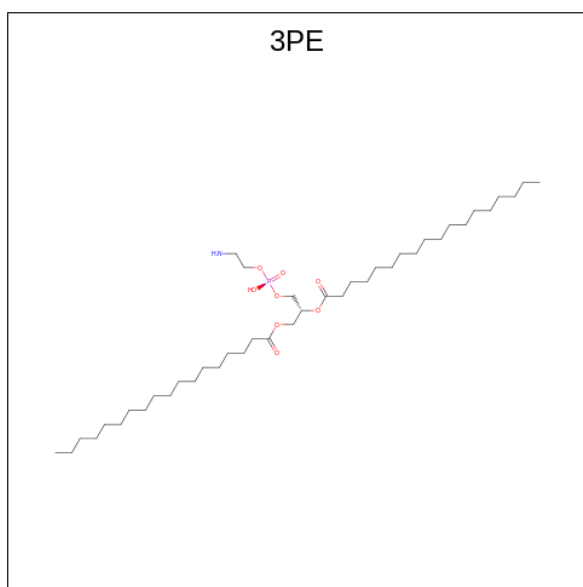
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
53	Aj	48	Total	C	N	O	0	0
			392	257	67	68		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	35	Total	C	N	O	S	0	0
			281	184	52	44	1		
54	Ak	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



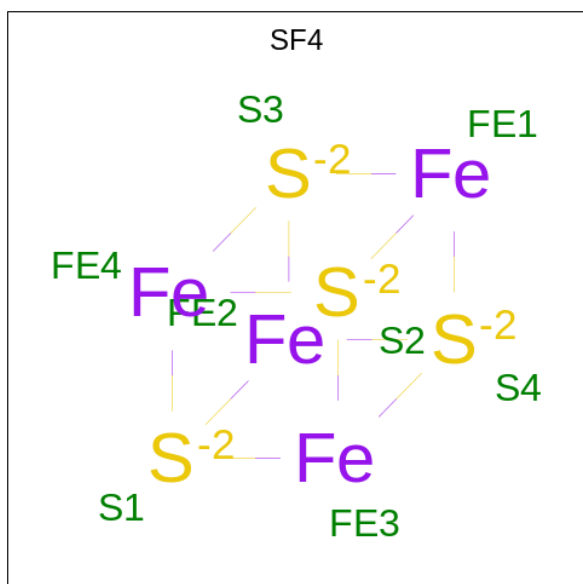
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
55	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



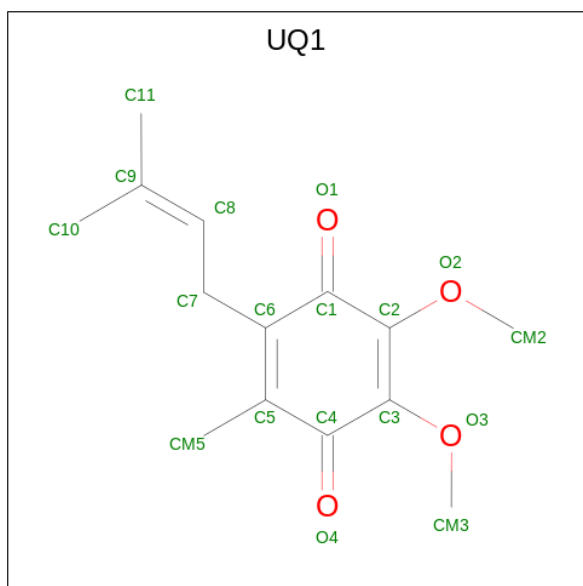
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	Fe	S	0
			8	4	4	
56	F	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	

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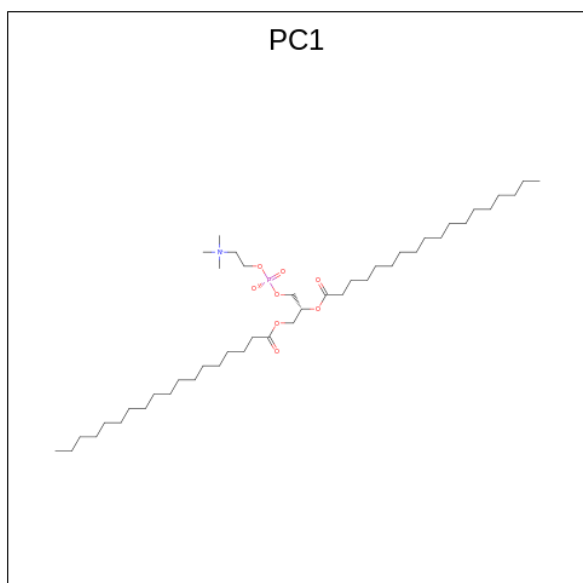
Mol	Chain	Residues	Atoms			AltConf
56	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 57 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



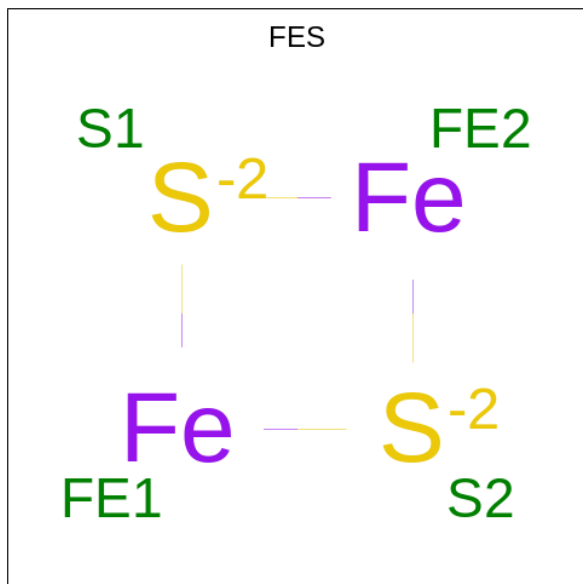
Mol	Chain	Residues	Atoms			AltConf
57	B	1	Total	C	O	0
			18	14	4	

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



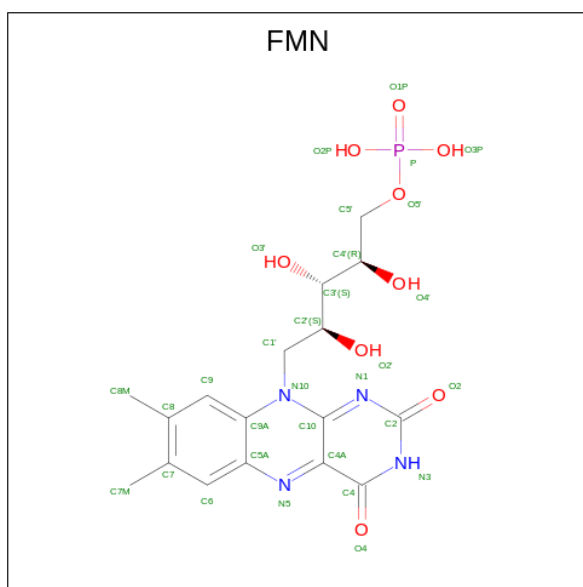
Mol	Chain	Residues	Atoms					AltConf
58	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	J	1	Total	C	N	O	P	0
			42	32	1	8	1	

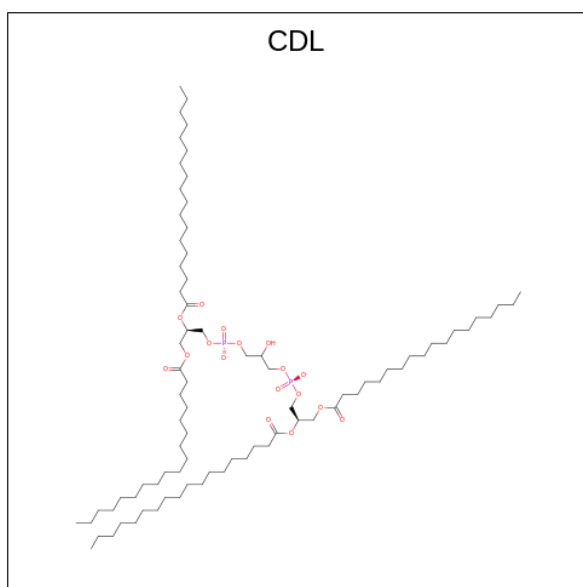
- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	

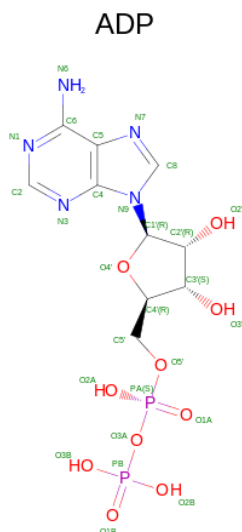
- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).





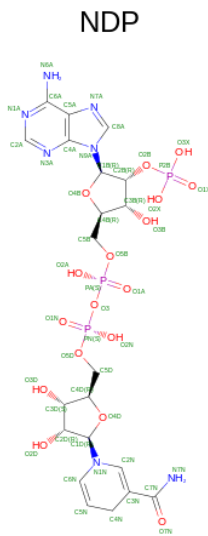
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			77	58	17	2	
62	L	1	Total	C	O	P	0
			86	67	17	2	
62	X	1	Total	C	O	P	0
			67	48	17	2	
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	AC	1	Total	C	O	P	0
			56	37	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ac	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
63	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 64 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

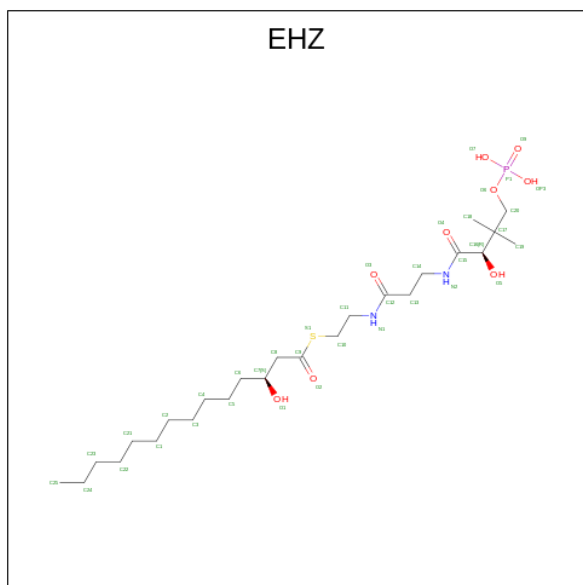


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

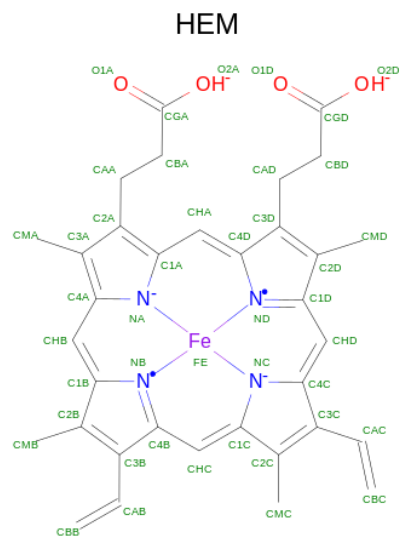
Mol	Chain	Residues	Atoms		AltConf
65	R	1	Total	Zn	0
			1	1	

- Molecule 66 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



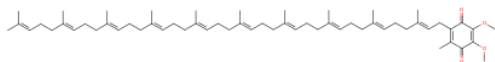
Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



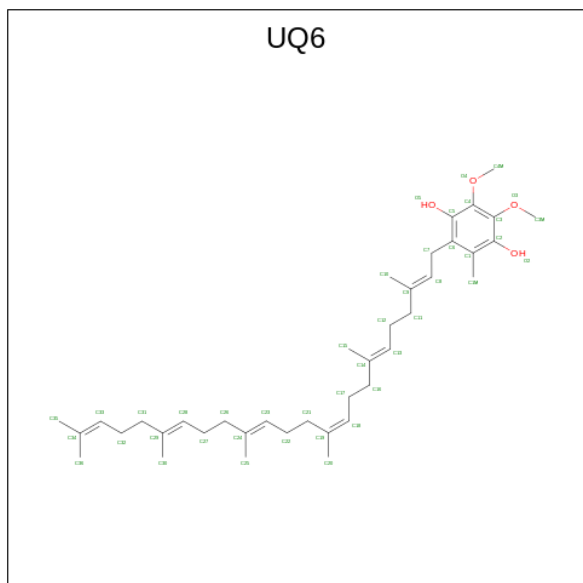
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
67	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
67	Ac	1	Total 43	C 34	Fe 1	N 4	O 4	0
67	Ac	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 68 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



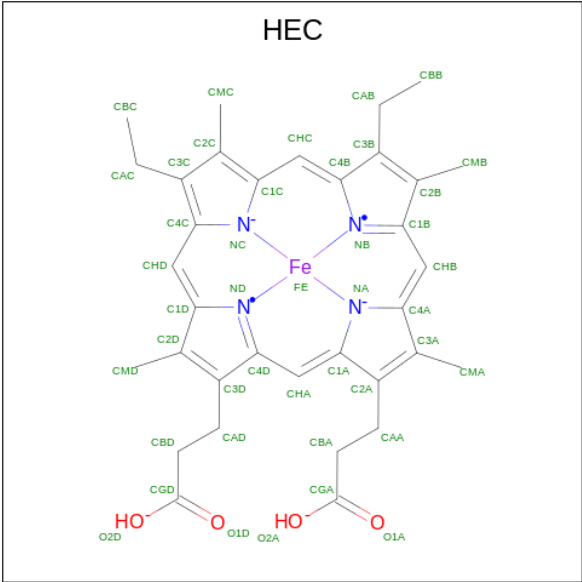
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			23	19	4	
68	Ac	1	Total	C	O	0
			38	34	4	

- Molecule 69 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



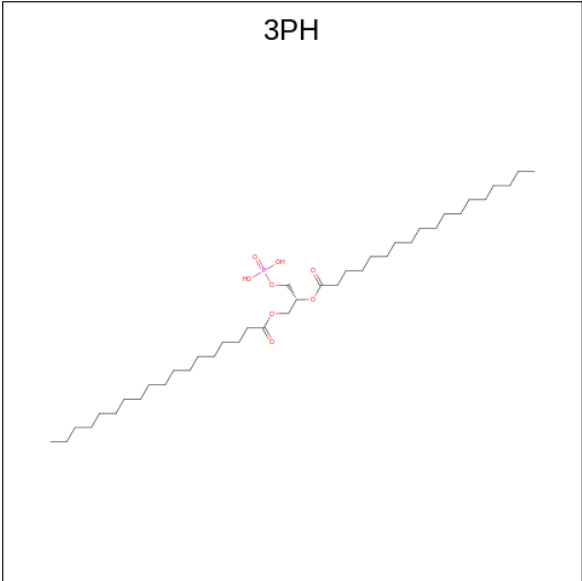
Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	
69	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total 43	C 34	Fe 1	N 4	O 4	0
70	Ad	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
71	AD	1	Total	C	O	P	0
			36	27	8	1	

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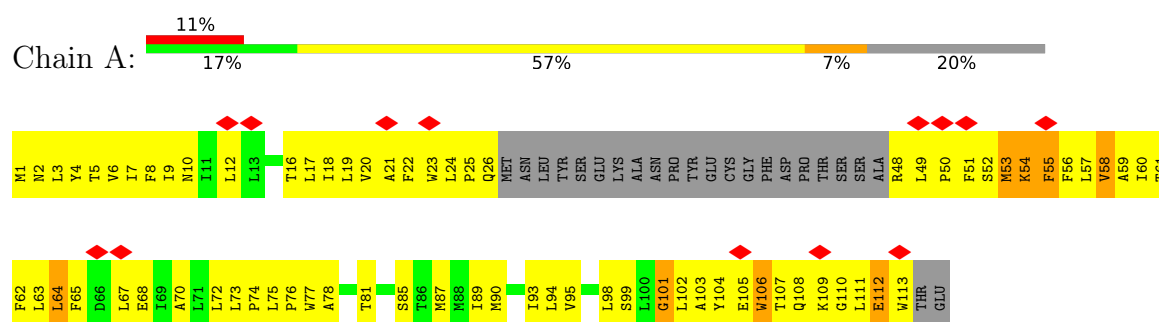
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
71	Ad	1	36	27	8	1	0

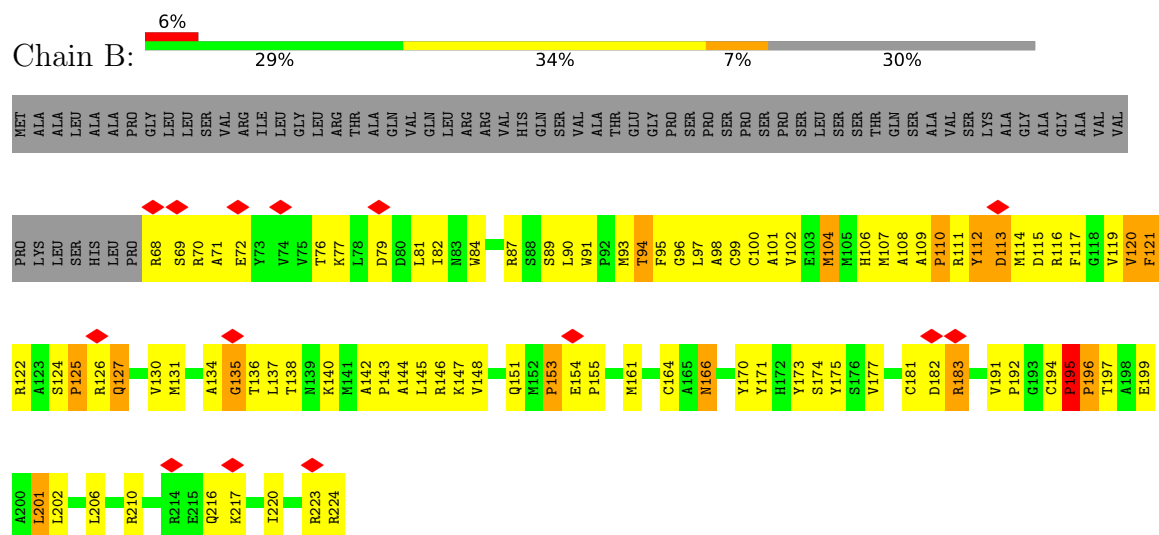
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

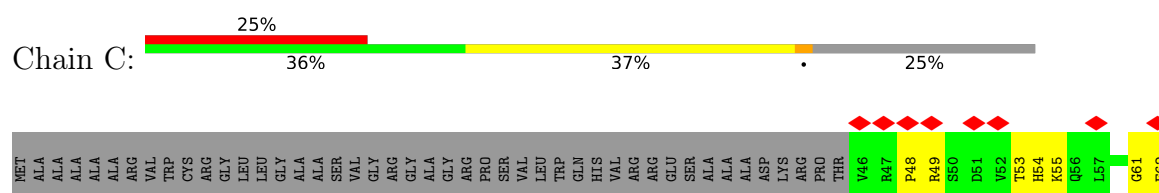
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

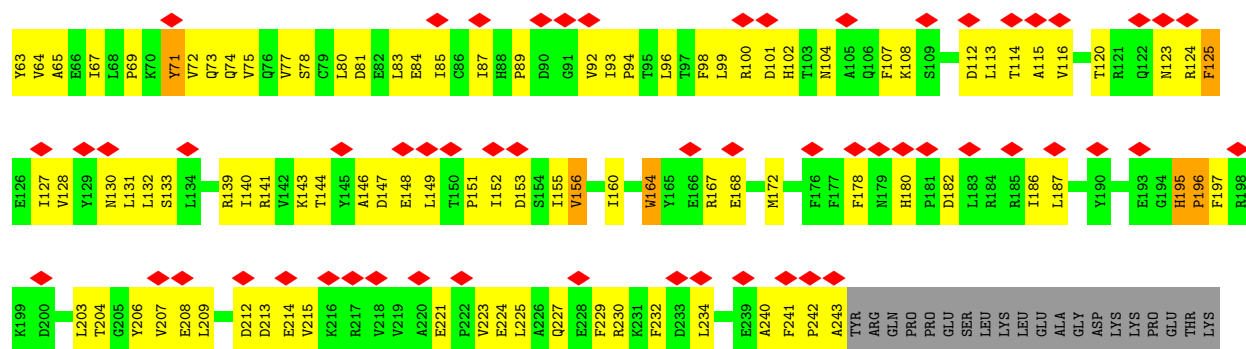


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

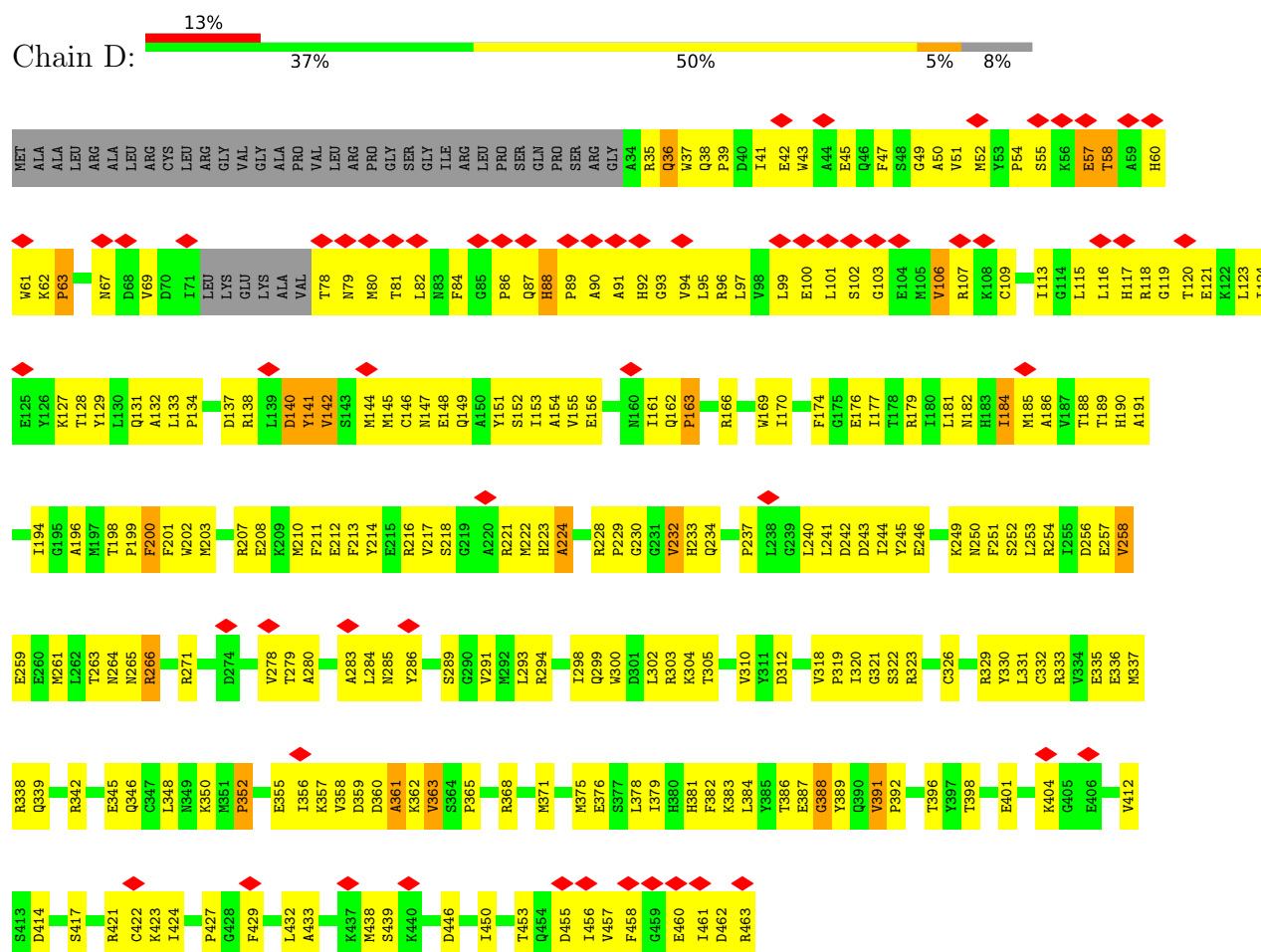


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

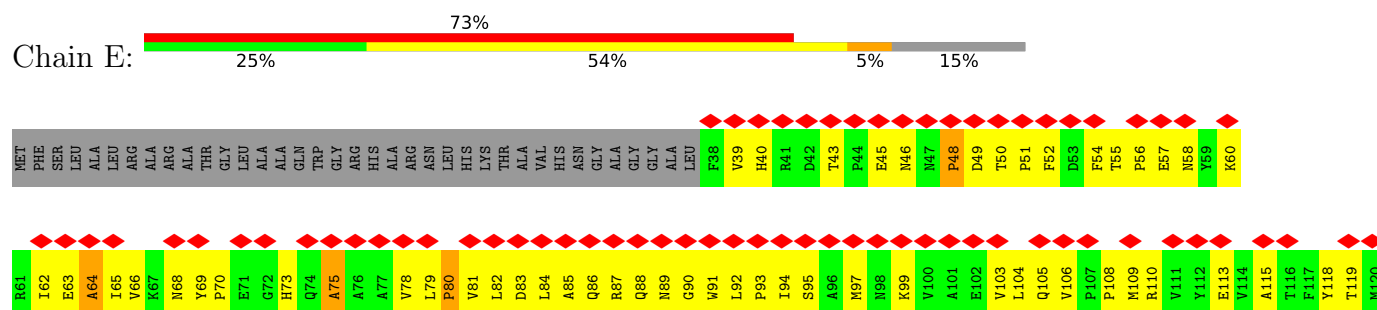


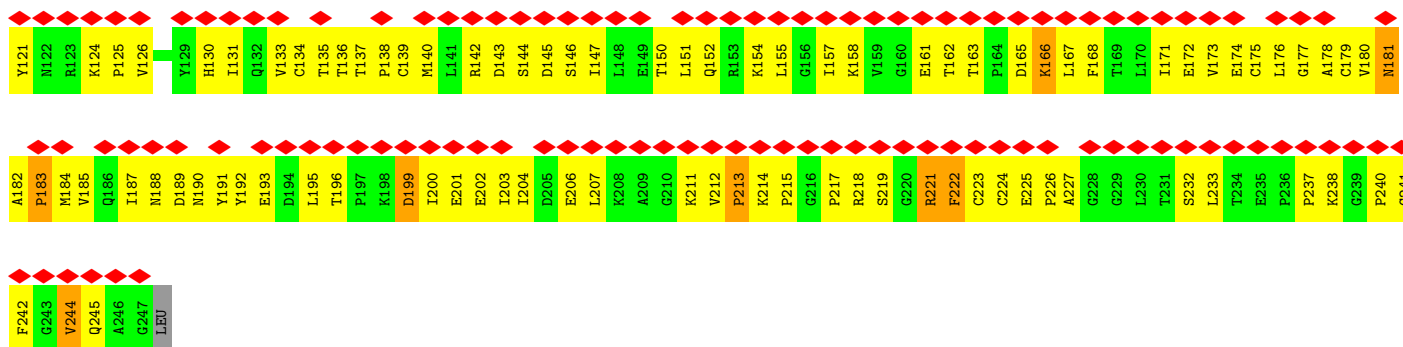


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

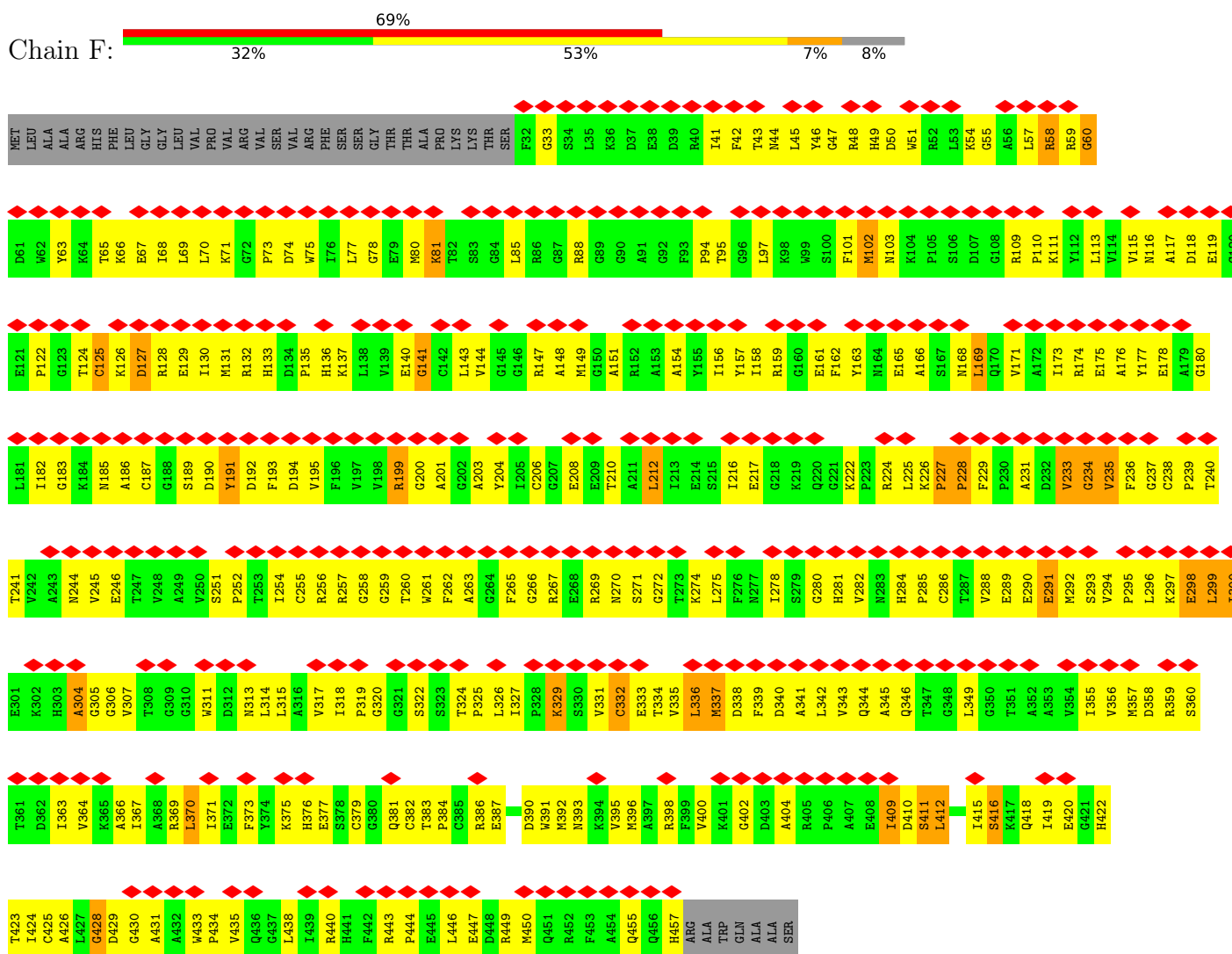


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

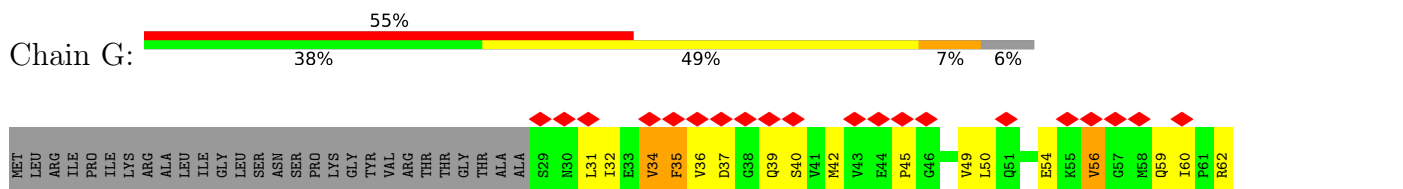


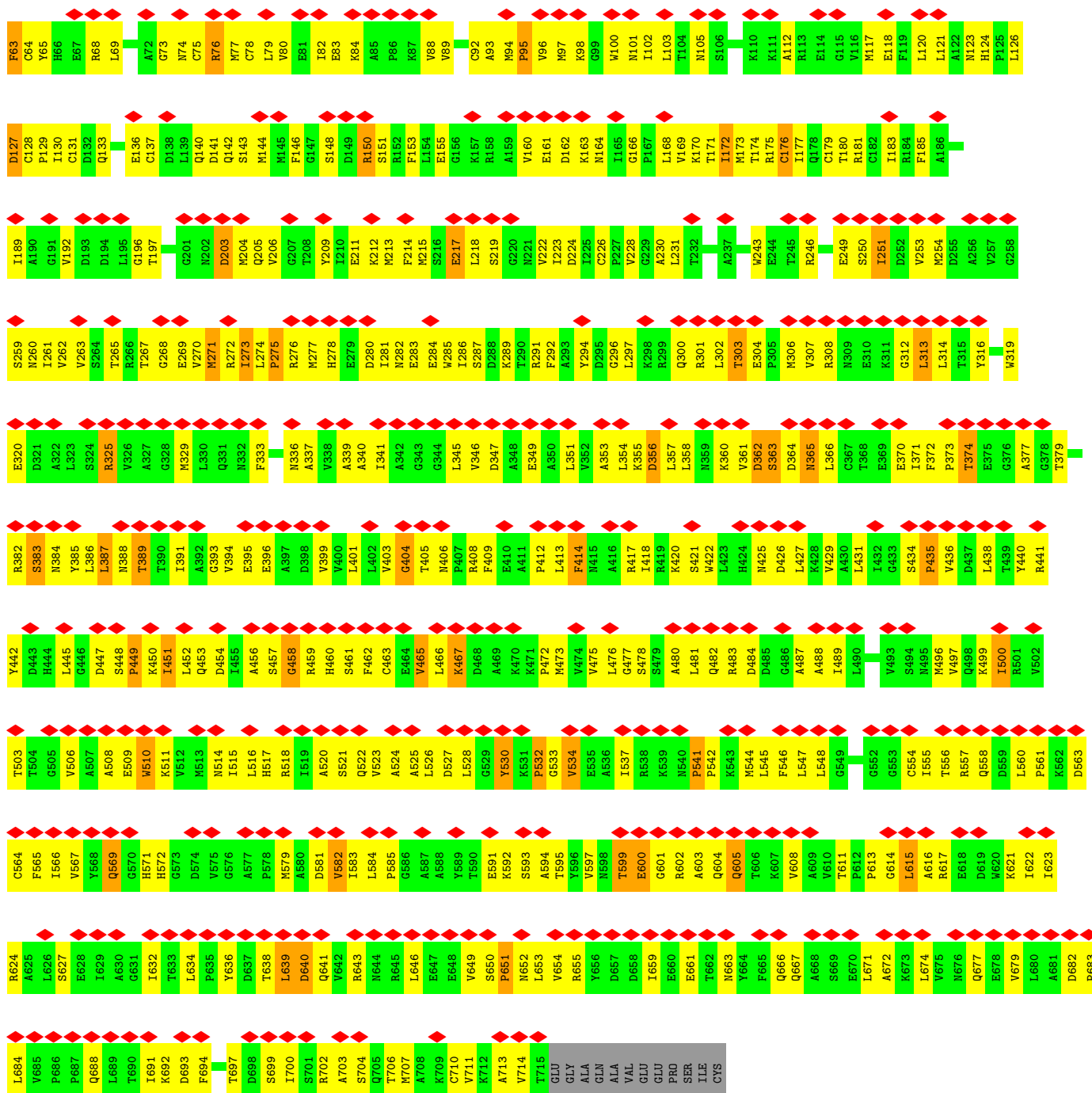


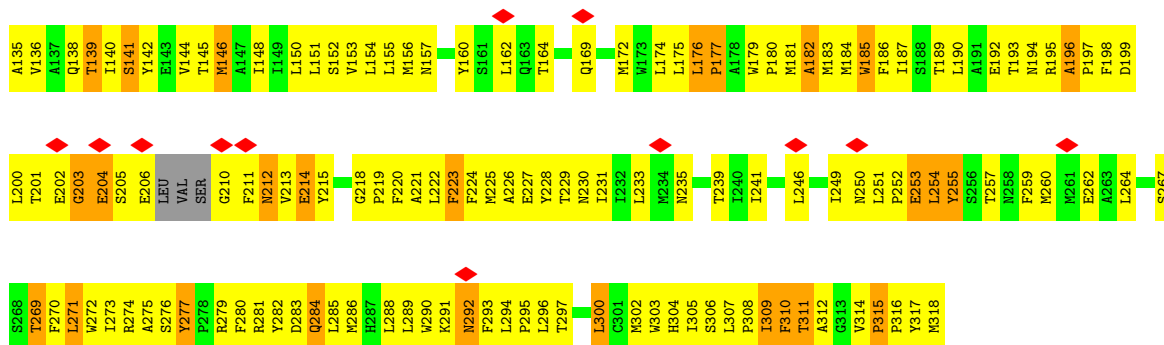
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



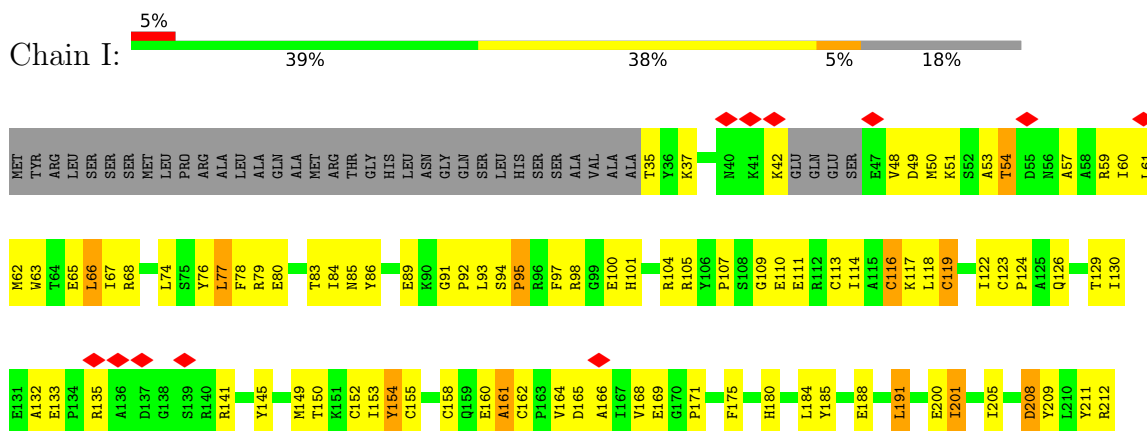
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



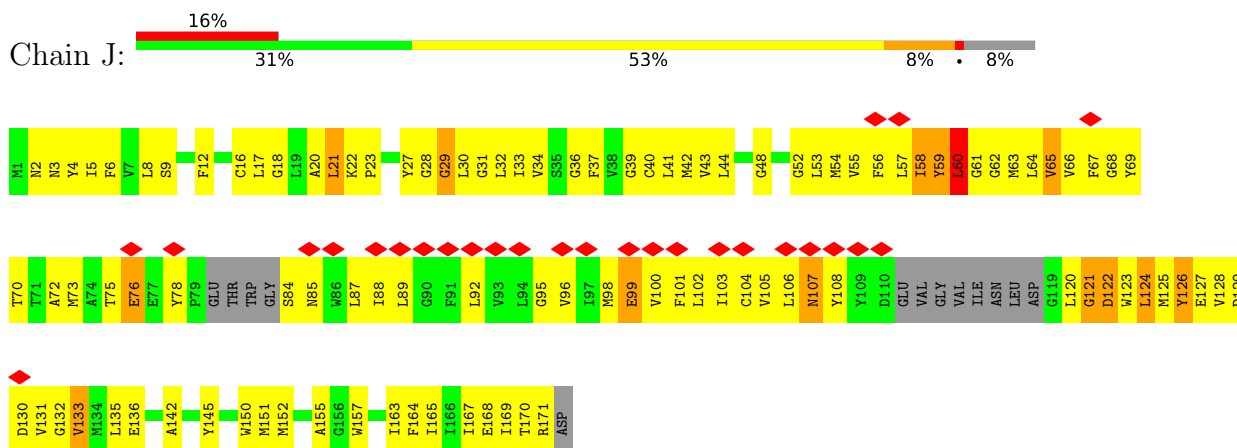




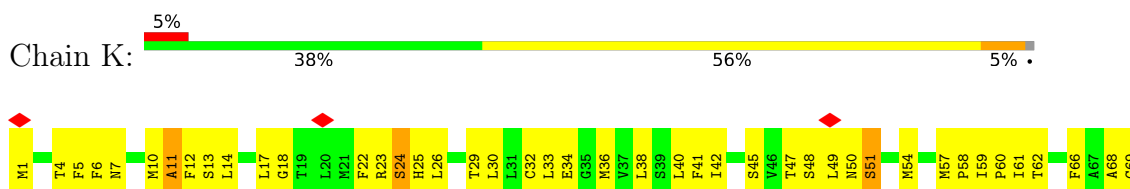
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

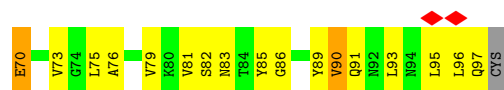


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



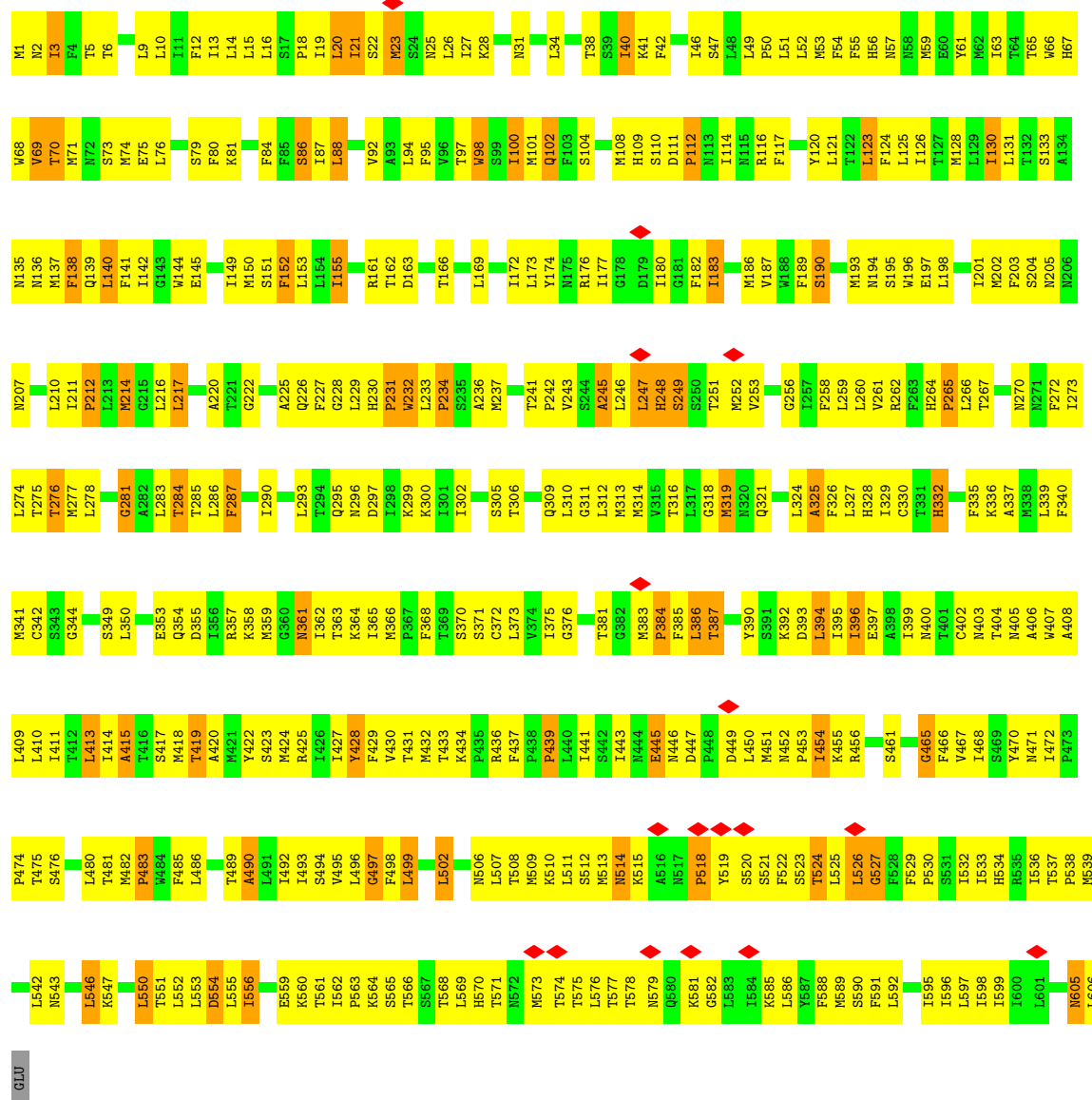
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L





• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

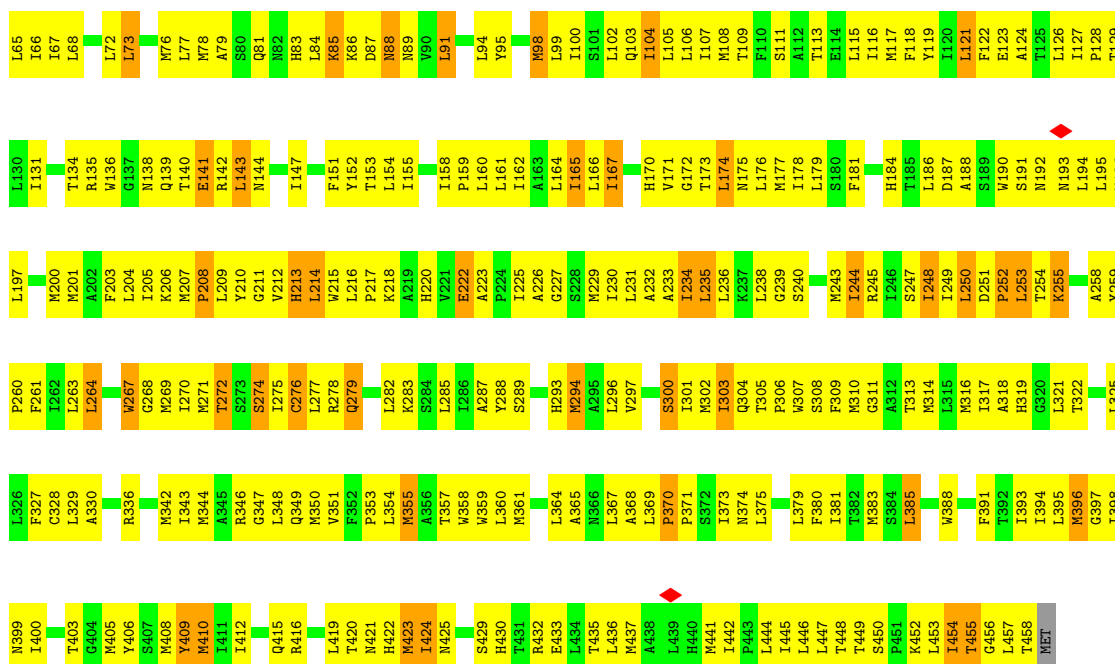
Chain L: 33% 56% 11%



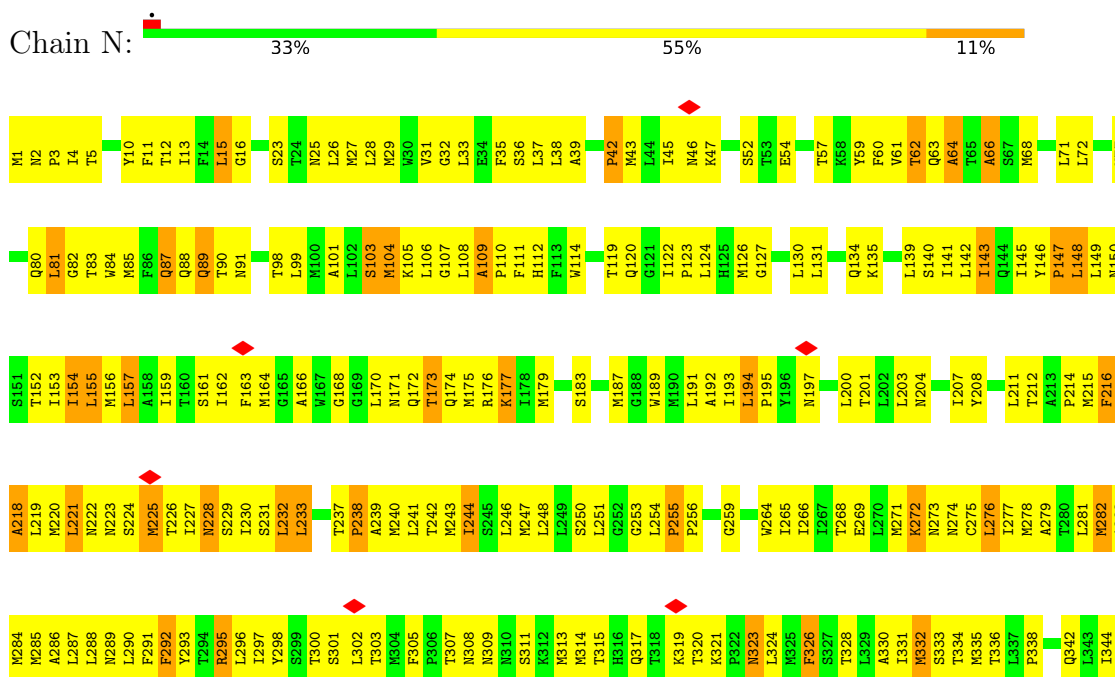
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 28% 60% 12%

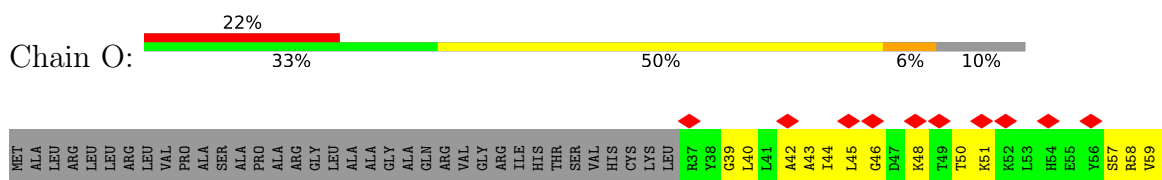


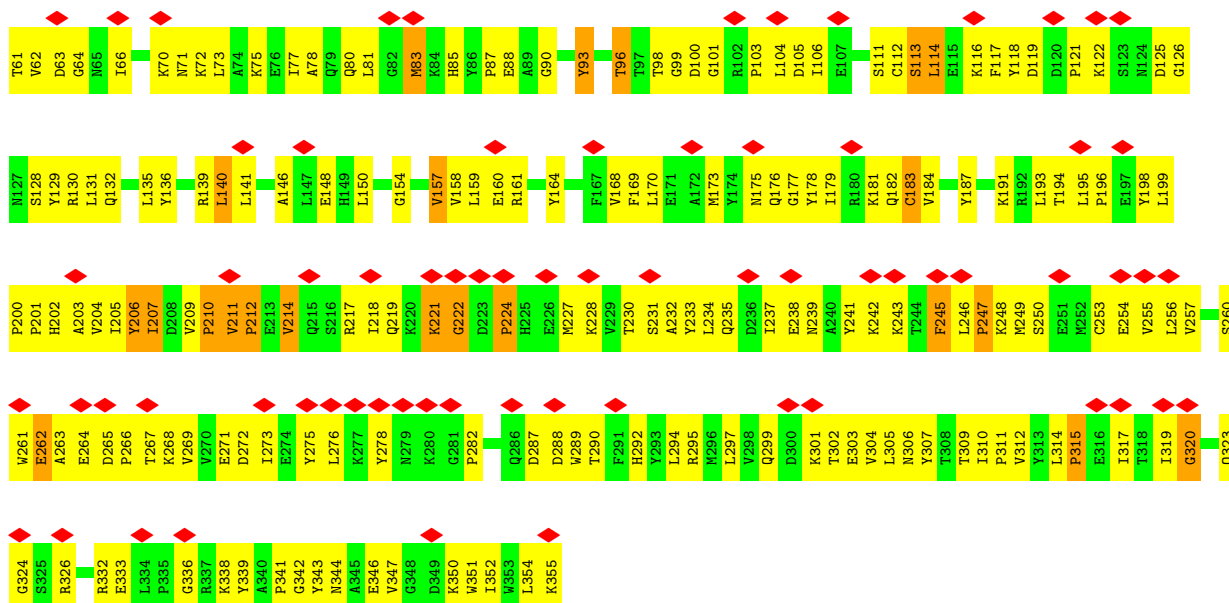


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

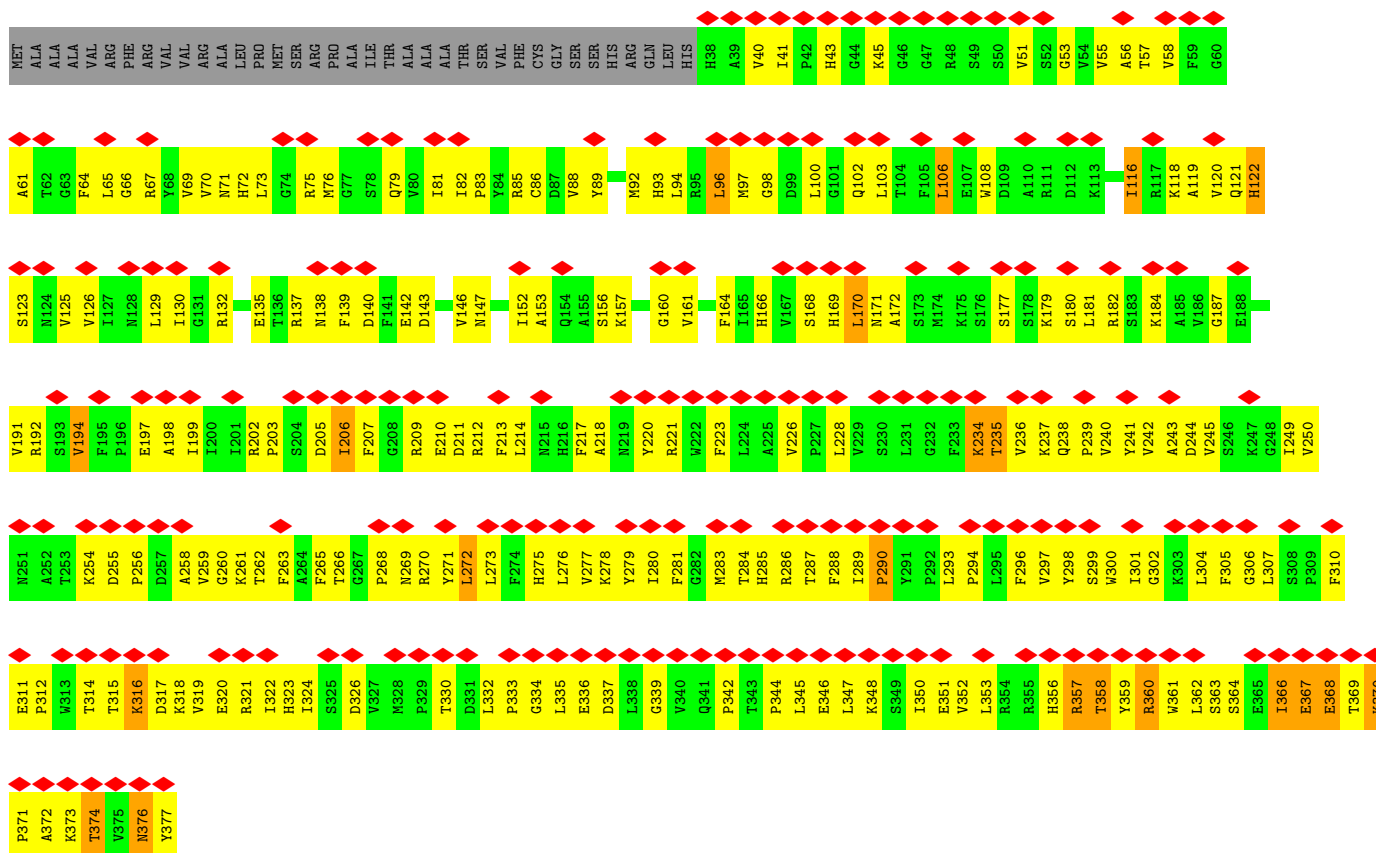


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

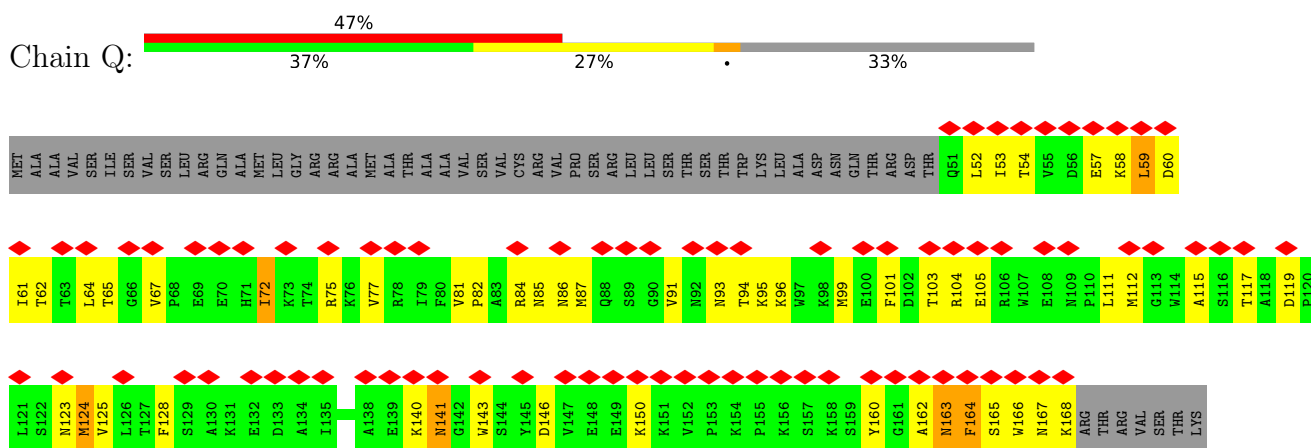




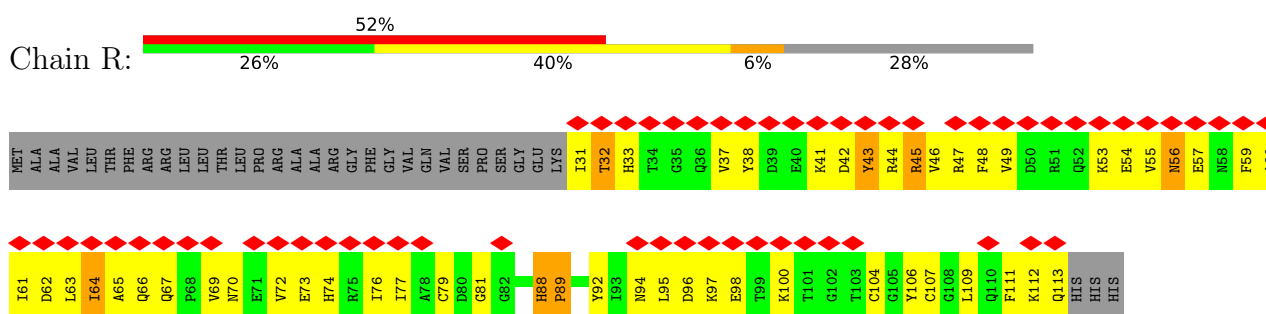
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



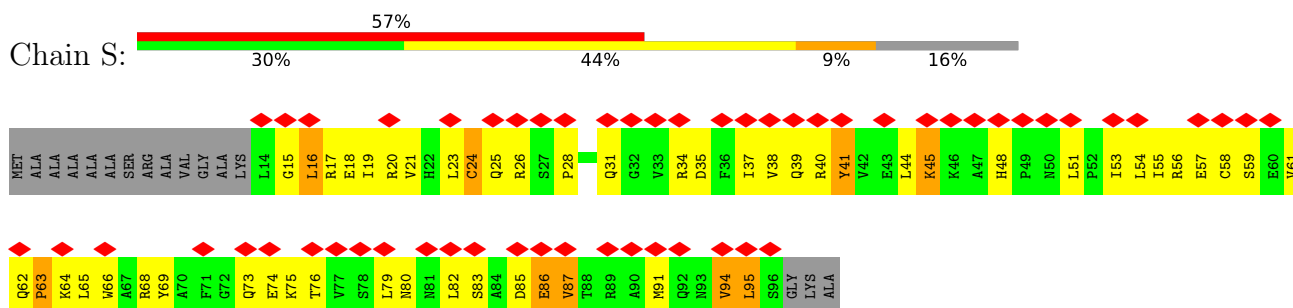
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



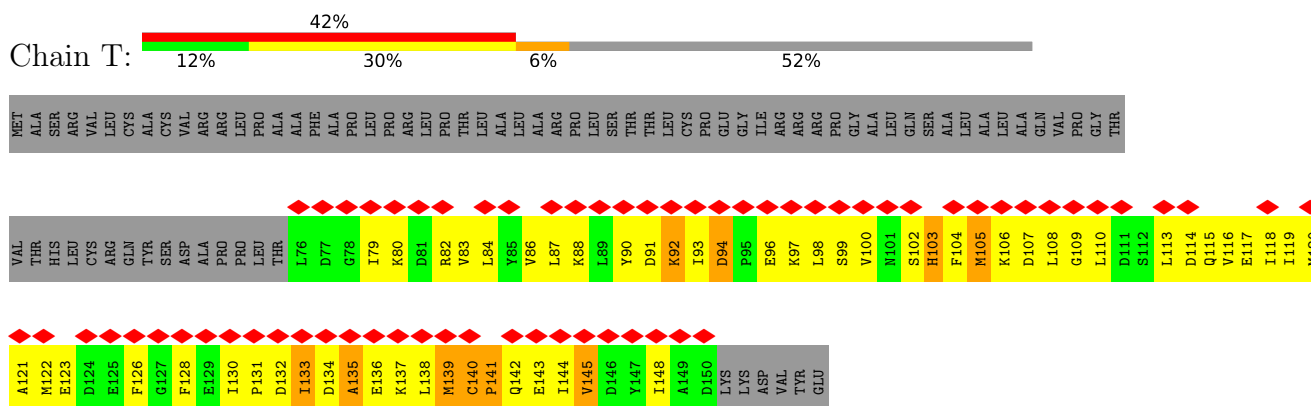
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



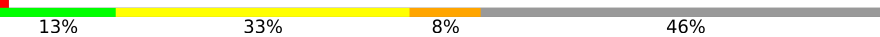
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

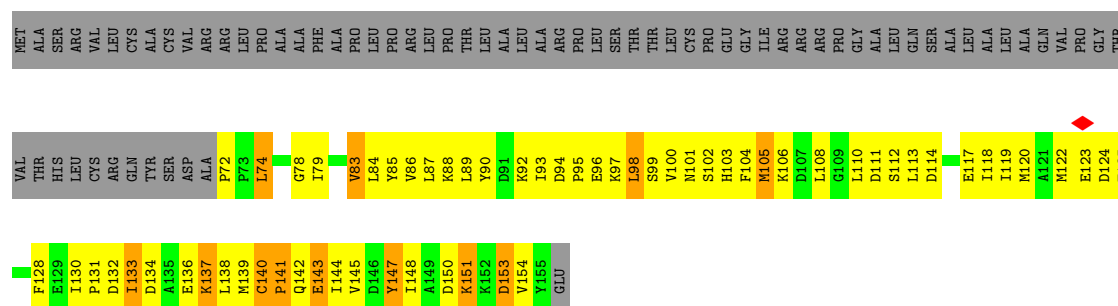


- Molecule 20: Acyl carrier protein, mitochondrial



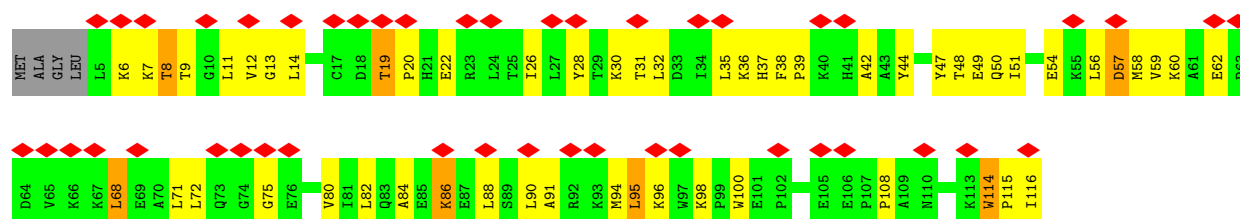
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U: 



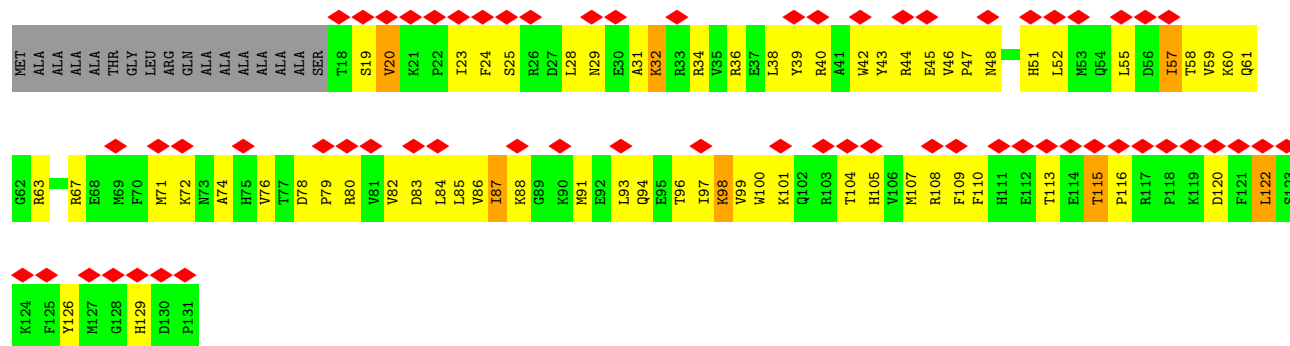
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V: 



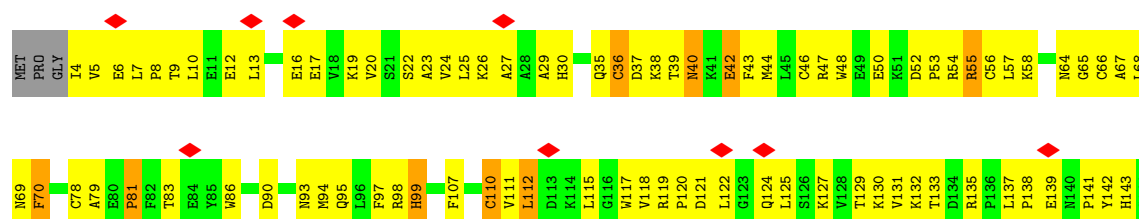
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

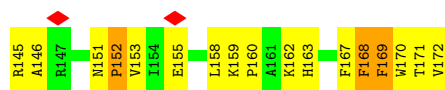
Chain W: 



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X: 

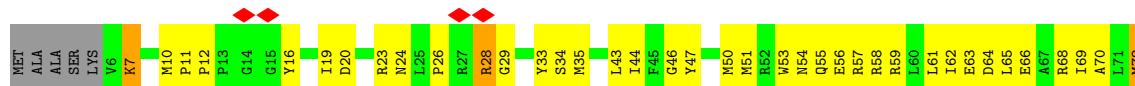




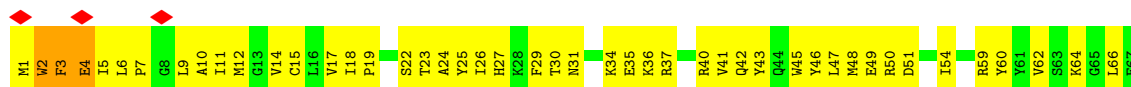
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



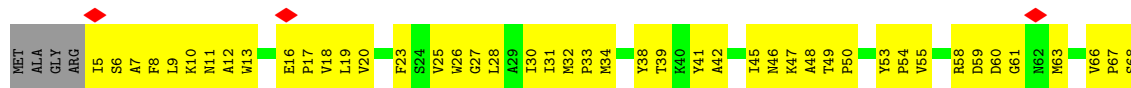
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



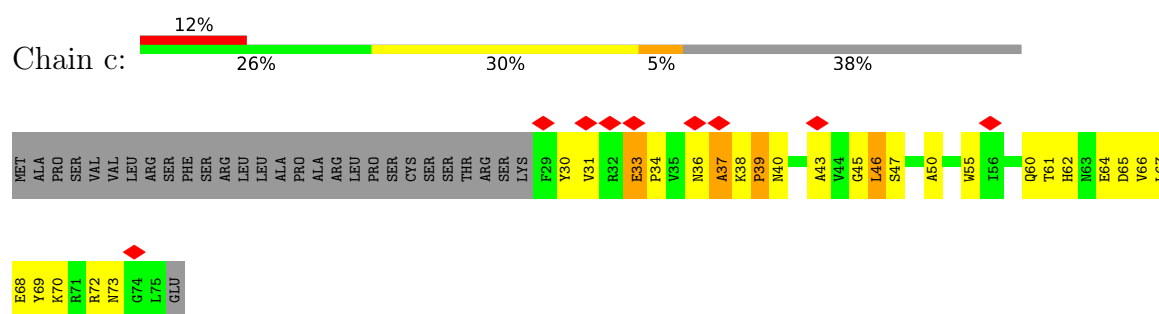
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



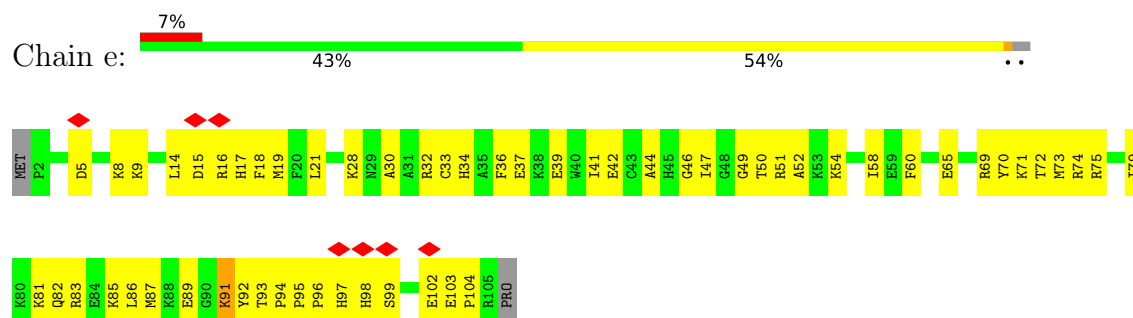
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



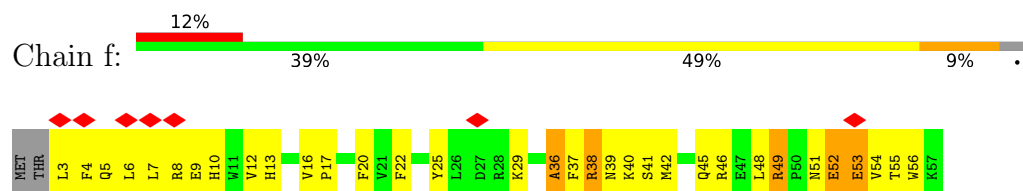
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



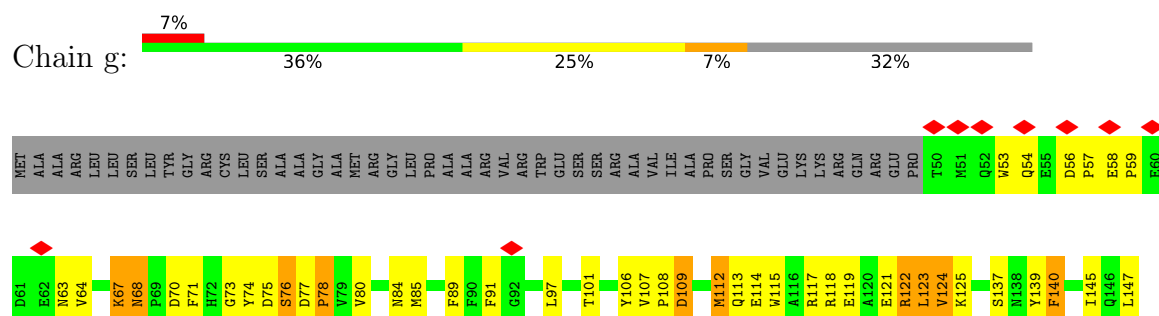
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

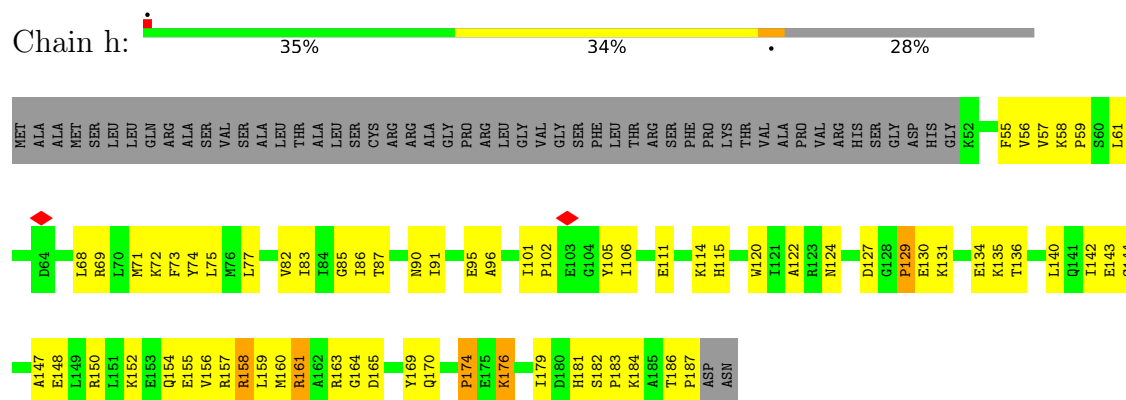


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

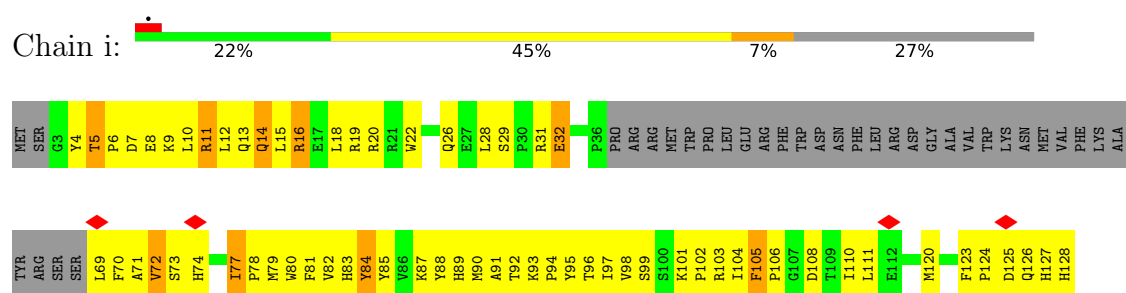




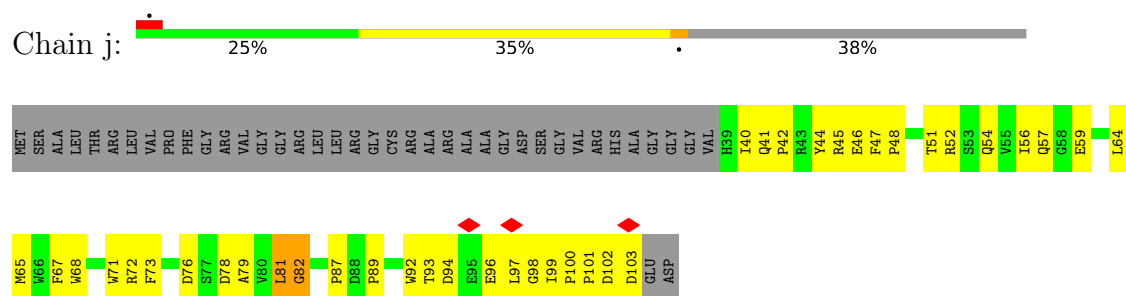
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



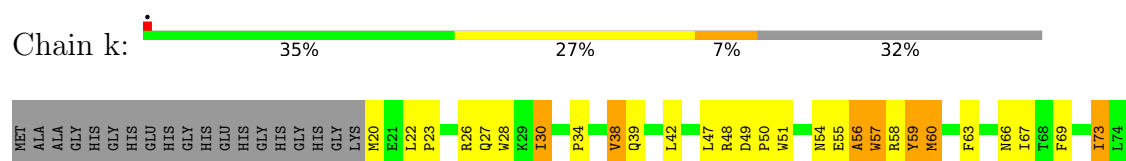
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

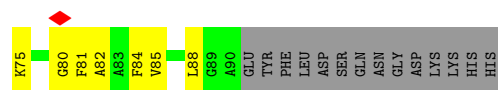


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

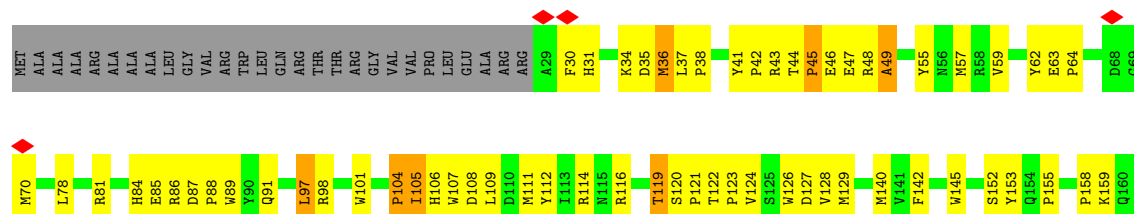


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

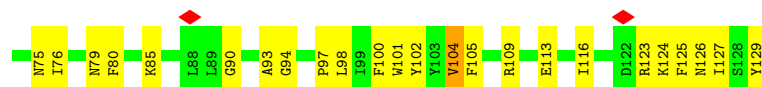
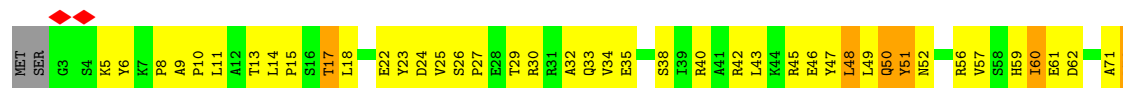




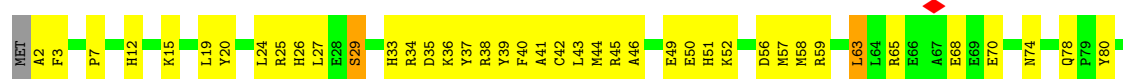
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

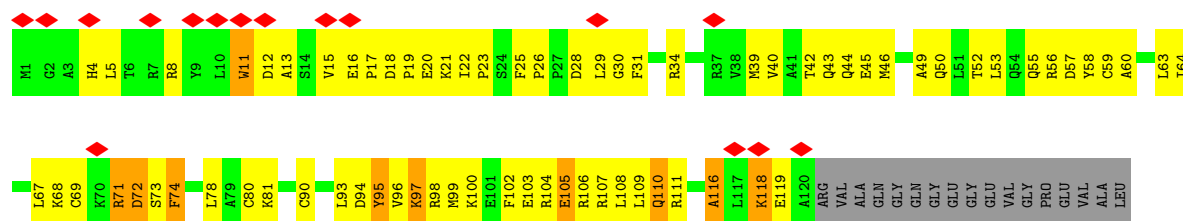


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

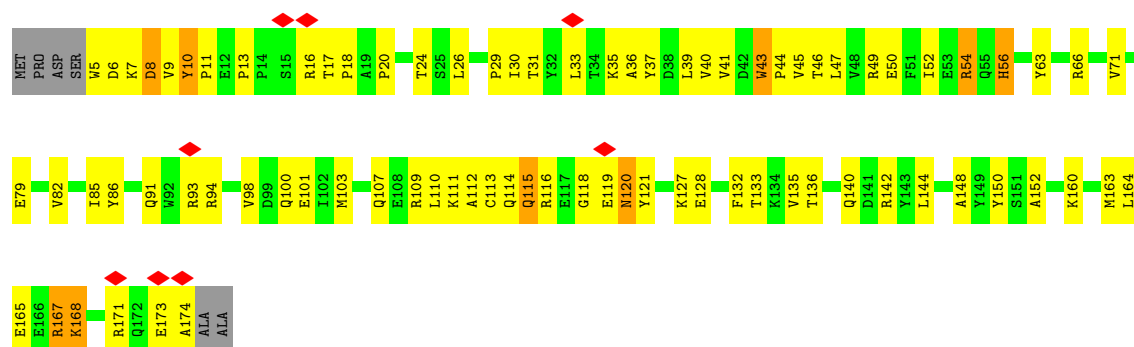


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

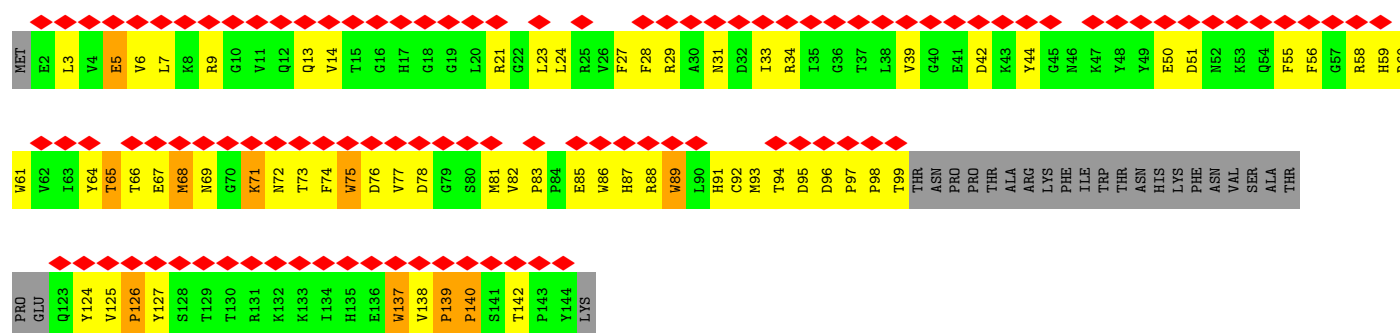
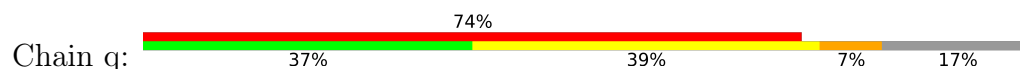




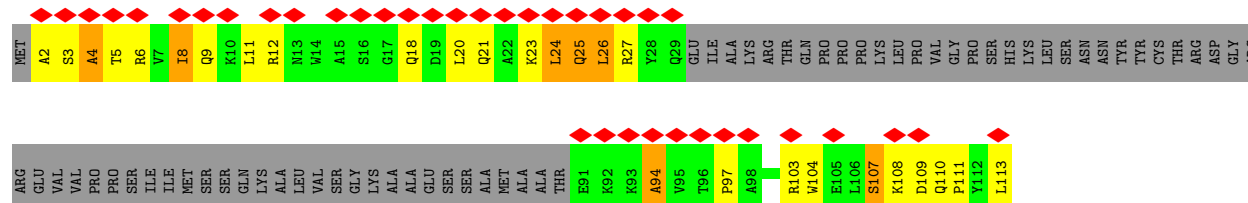
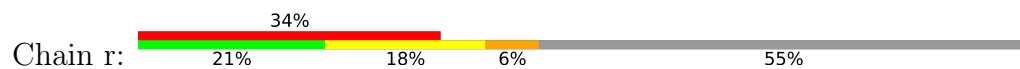
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET ALA VAL SER LEU LEU ARG GLY ARG GLN ILE ARG ALA LEU LYS VAL VAL LEU LEU LEU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL ARG LEU SER GLU THR GLU SER GLU LYS SER ALA LYS GLU LYS LEU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO

PRO THR ASP THR THR TYR LYS ASN LEU GLN HIS SER ASP TYR N76 T77 Y78 T79 F80 L81 D82 L83 N84 L85 D86 L87 S88 K89 PHE ARG LEU PRO PRO PRO SER SER SER ARG GLU PRO ARG HIS

• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



MET ALA ALA SER LEU LEU ARG GLY ARG ALA LEU LYS VAL VAL LEU LEU LEU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL ARG LEU SER GLU LYS SER ALA LYS GLU LYS LEU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO

S65 H66 A67 T68 C69 T70 N71 G72 L73 W74 W75 D76 A77 G78 S79 R80 Y81 E84 N87 F91 F92 L93 E94 H95 L96 A97 F98 F99 G100 T101 K102 N103 L109 E110 V113 E114 A118 H119 L120 N121 S124 E125 L132 L136 S137 K138 D139 L140 P141 K142 V143

L147 A148 V151 Q152 N153 S154 S155 L156 E157 D158 Q160 I161 E162 K163 E164 R165 I168 L169 M170 E171 M172 Q173 E174 N175 D176 A177 S178 M179 Q180 N181 V182 V183 Y186 L187 H188 F192 Q199 A200 V201 E202 G203 P204 S205 E206 N207 V208 R209 L210 L211 S212 R213 T214 D215

Y219 L220 H223 Y224 A226 N229 V230 L231 A232 G235 C236 V237 Q240 Q241 L242 L243 D244 L245 A246 Q247 K248 H249 L250 V253 S254 R255 V256 TYR GLU GLU ASP ALA VAL PRO GLY LEU THR C267 C268 R269 T270 T271 G272 G273 E274 L275 R276 D279 D280 A281 A285 H286

V287 A288 P294 G295 W296 A297 N298 P299 D300 N301 A307 I310 I311 G312 HIS TYR ASP CYS THR TYR GLY GLY VAL LEU SER SER PRO LEU ALA VAL VAL ALA ASN LYS LEU C338 Q339 S340 F341 Q342 S347 A356 H357 F358 V359 C360 D361 A362 M363 I365

D366 M368 V369 F370 F371 L372 Q373 Q374 Q375 Q376 L379 T384 E387 V388 T389 R390 G391 K392 R396 N397 A398 L399 V400 H401 H402 L403 D404 T407 P408 V409 C410 E411 D412 G414 R415 S416 L417 L418 T419 Y420 R423 L426 W429 I433 I444 P454 A455

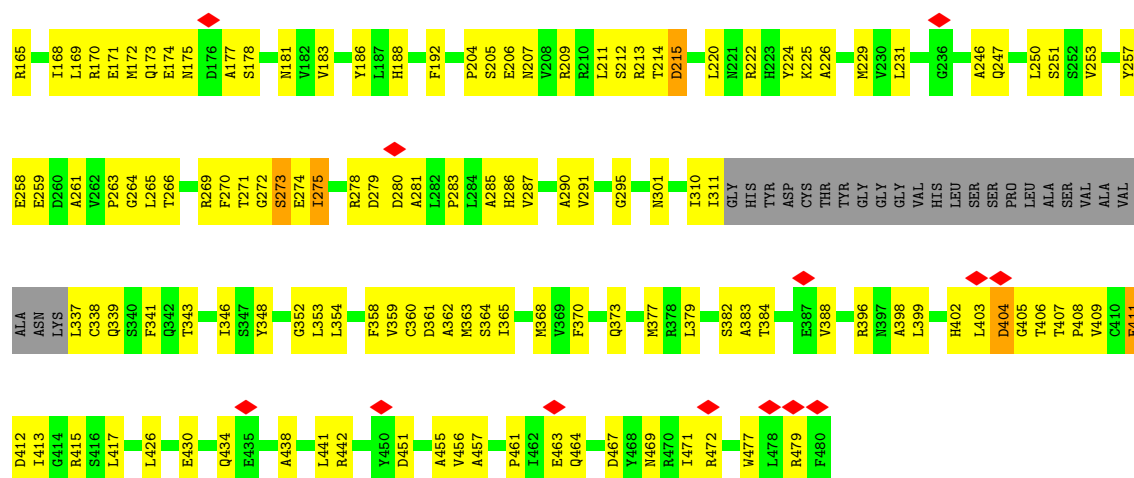
V456 P461 I462 E463 Q464 D467 Y468 N469 R470 G474 M475 F476 W477 L478 R479 PHE

• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

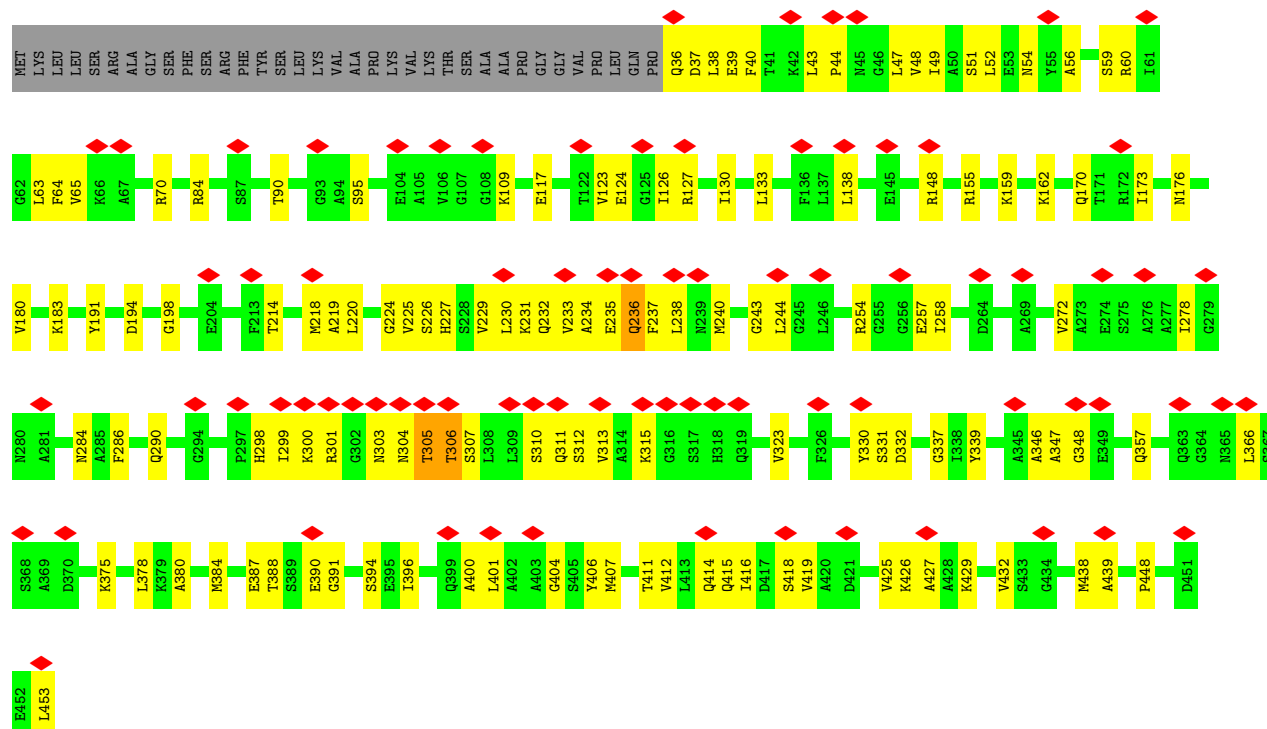


MET ALA ALA SER VAL CYS ARG ALA CYS GLY THR GLN VAL LEU LEU ARG THR ARG ARG SER PRO ALA LEU LEU LEU ARG LEU PRO ALA LEU ARG GLY THR PHE GLN ALA LEU GLN S44 V50 N55 S56 R58 V59 A60 S61 H66 A67 T68 V73

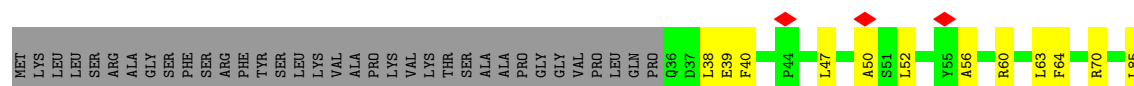
W74 G78 Y81 N86 N87 Y91 F92 L93 E94 H95 L96 A97 F98 K99 G100 T101 R104 N107 L108 E110 K111 E112 V113 E114 G117 L120 N121 A122 R126 A135 L136 L146 L147 A148 V151 Q152 M153 S154 S155 L156 E157 D158 S159 Q160 I161 E164

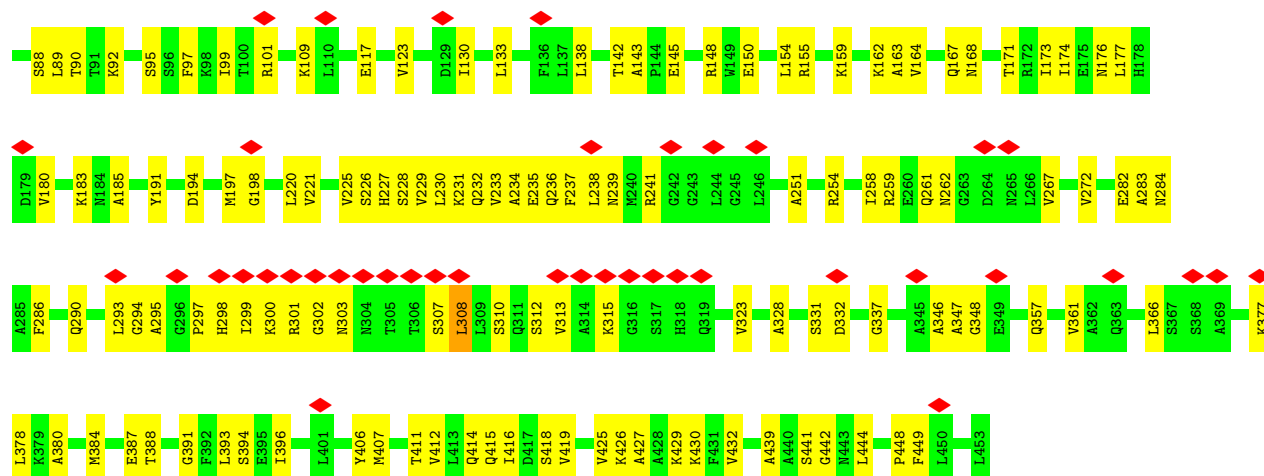


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



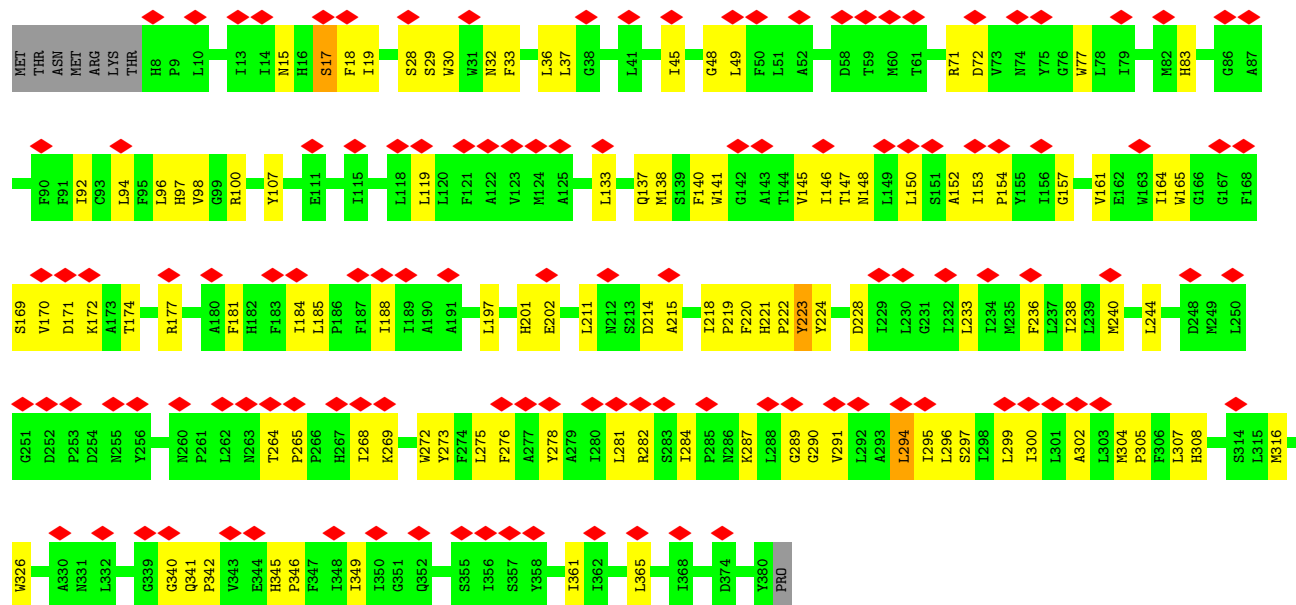
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial





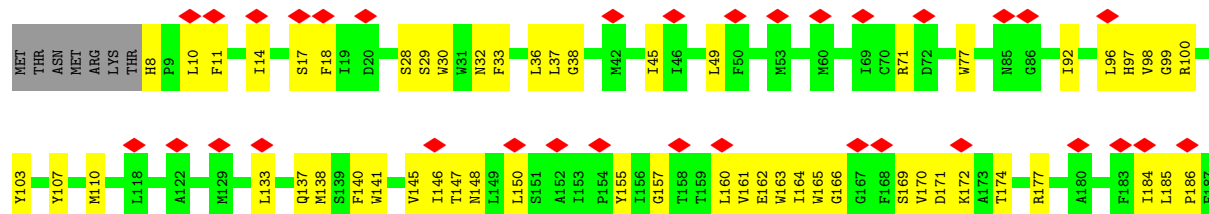
• Molecule 47: Cytochrome b

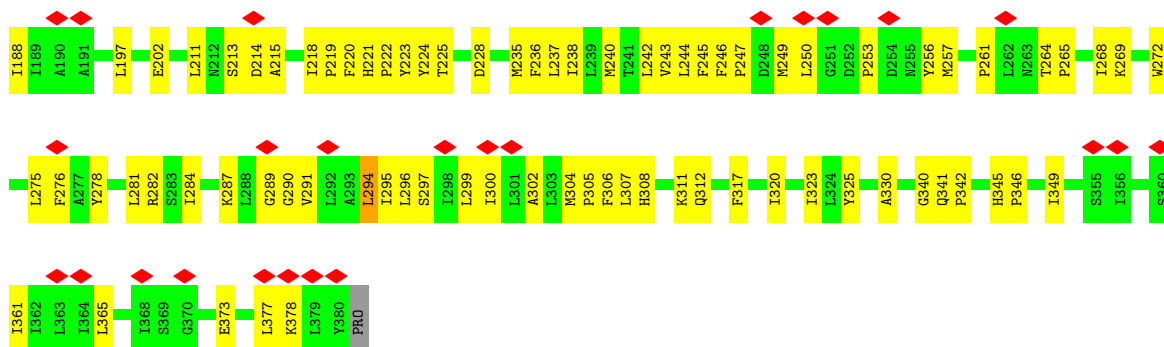
Chain AC: 32% 69% 28% ..



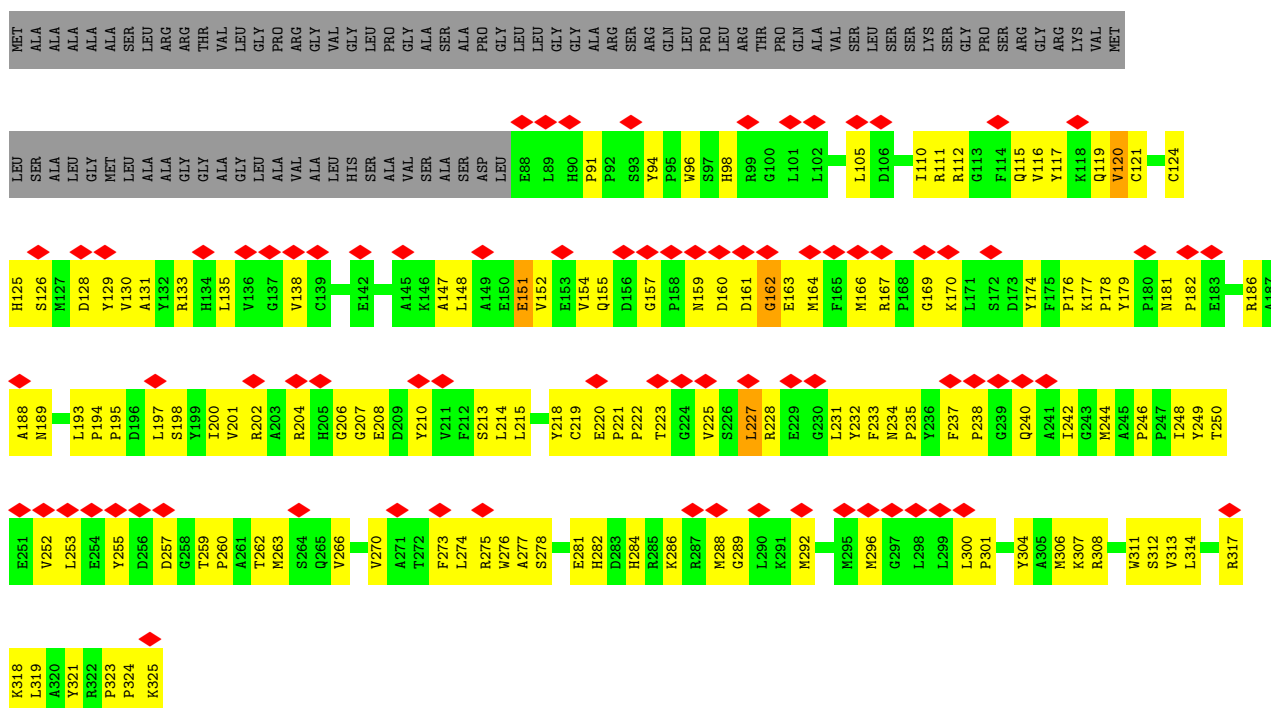
• Molecule 47: Cytochrome b

Chain AC: 15% 63% 35% .

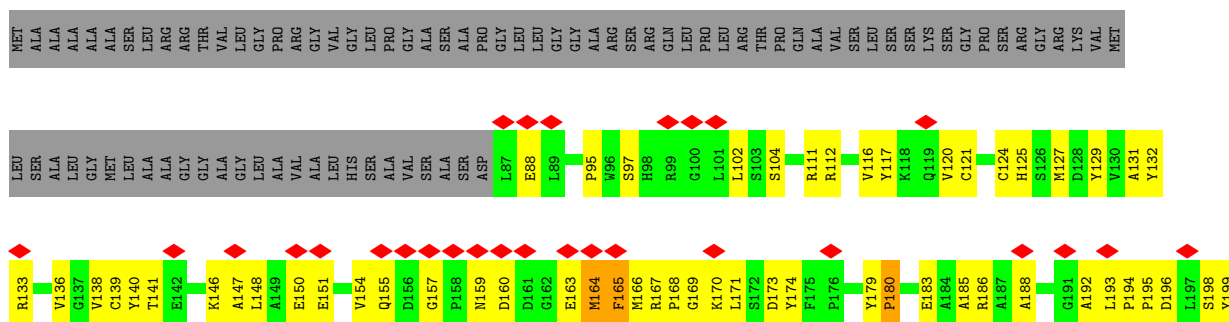


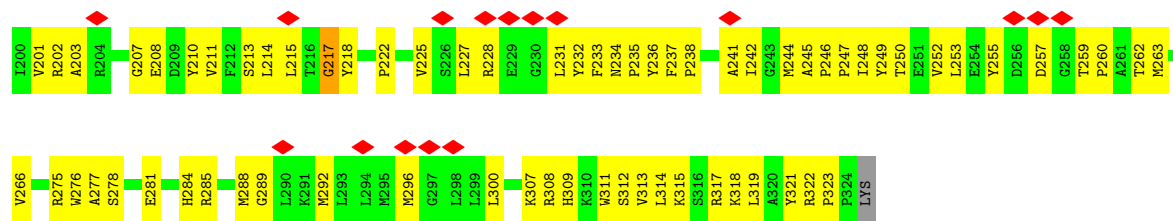


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

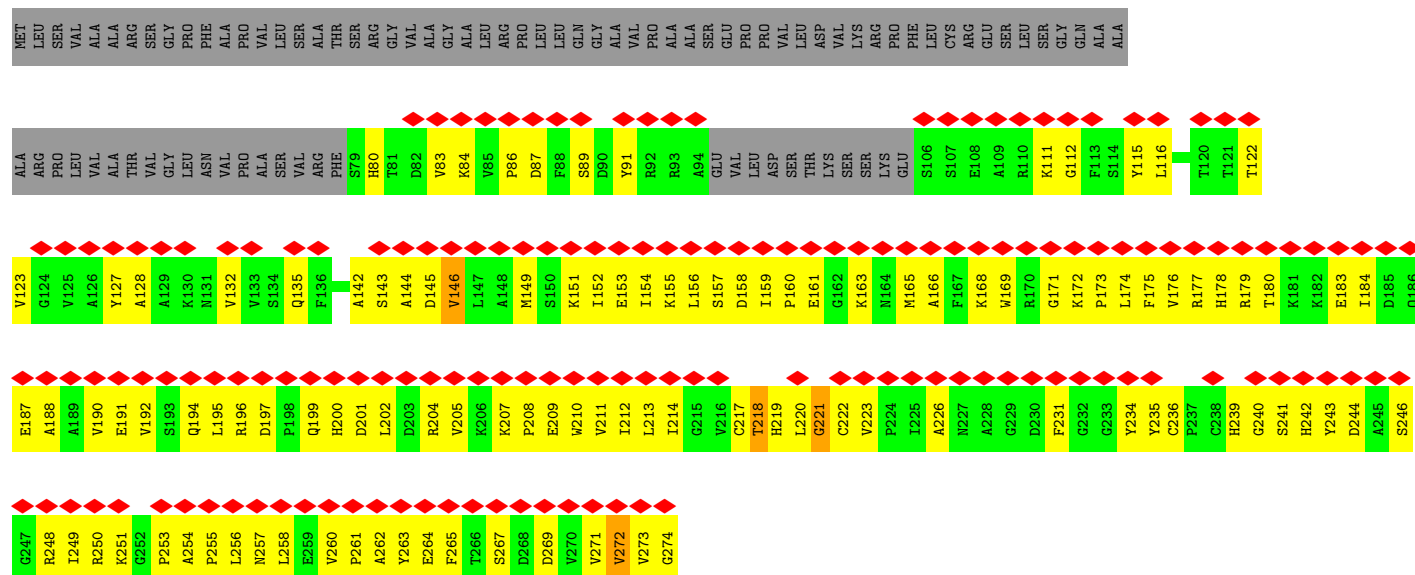


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

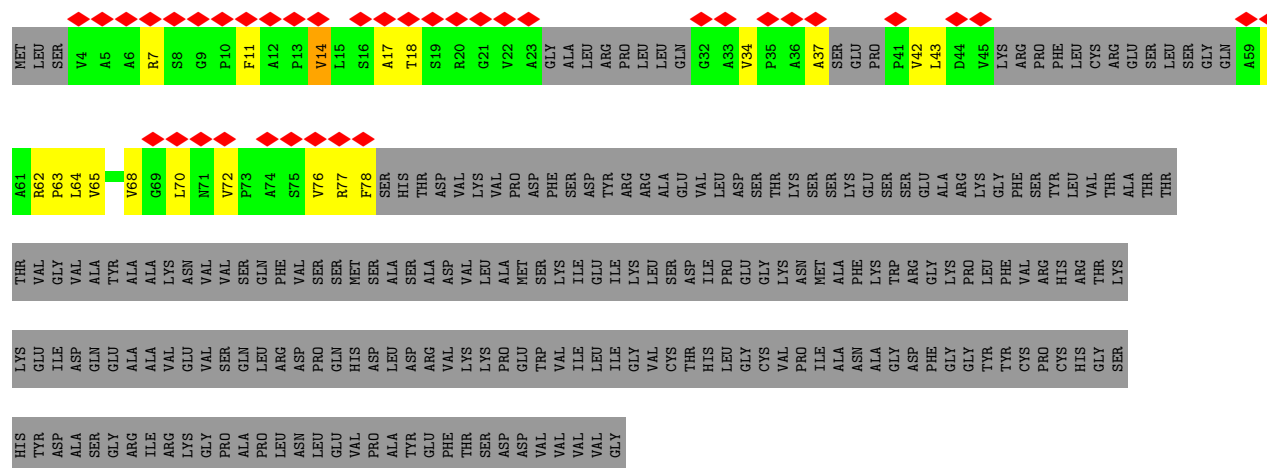




• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



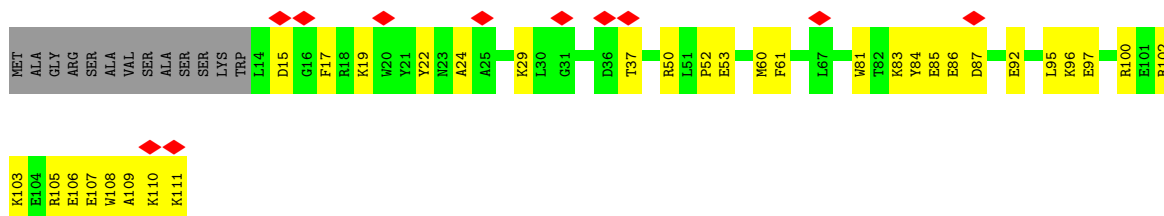
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



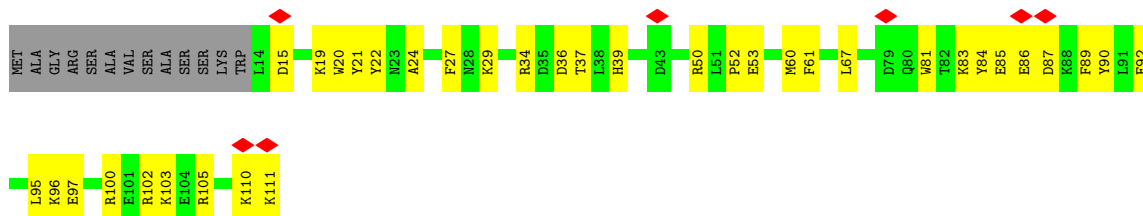
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



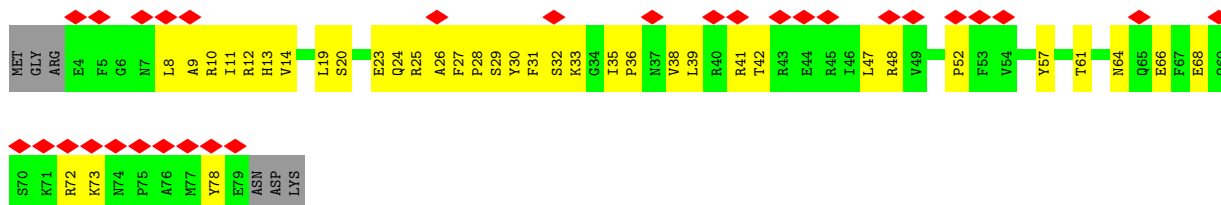
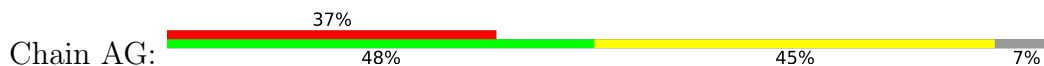
- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7

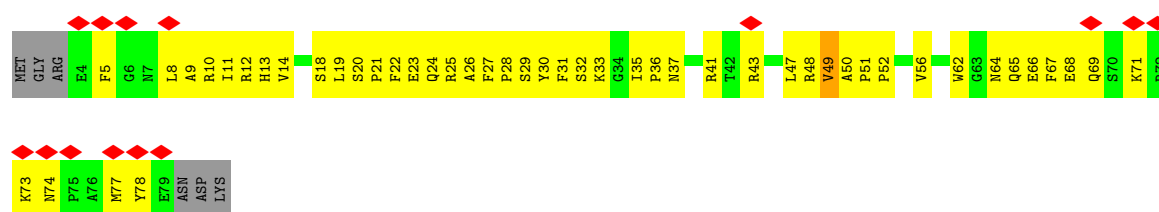


- Molecule 51: Cytochrome b-c1 complex subunit 8

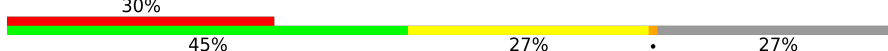


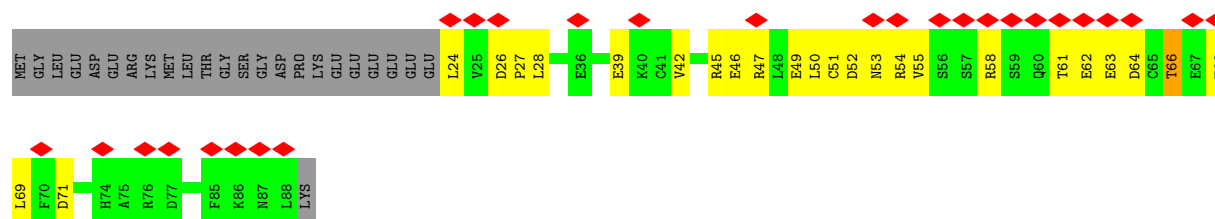
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain Ag: 

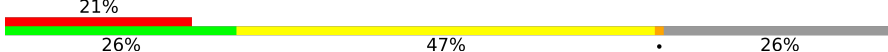


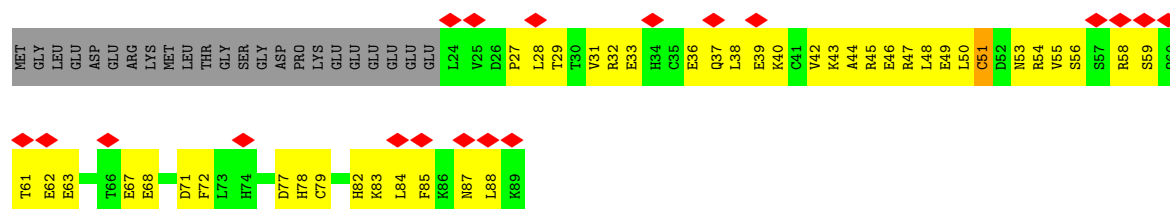
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH: 

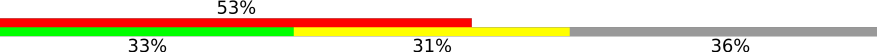


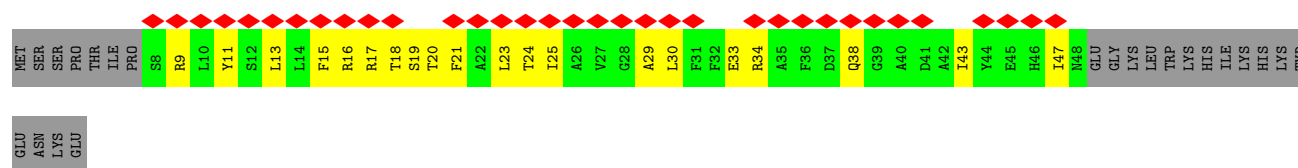
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah: 

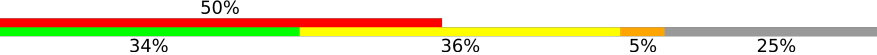


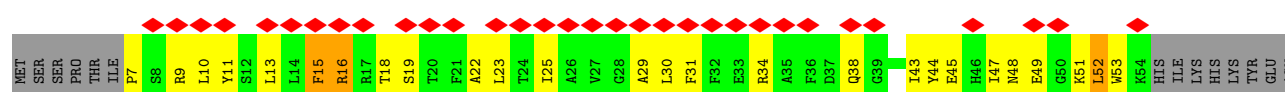
- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ: 



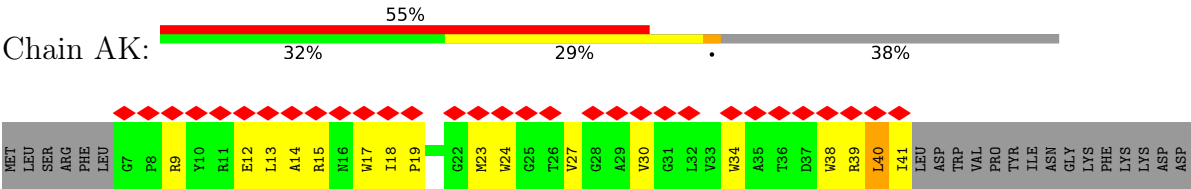
- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj: 

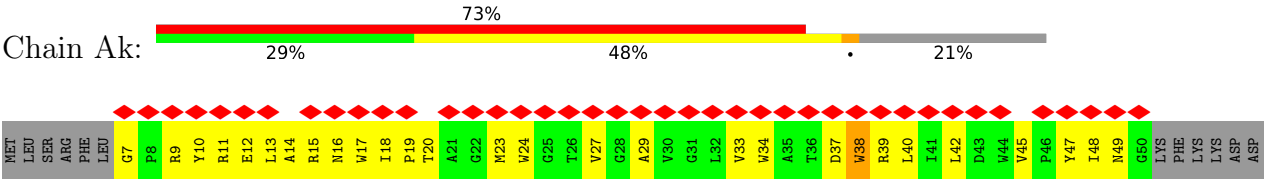


LYS
GLU

• Molecule 54: Cytochrome b-c1 complex subunit 10



• Molecule 54: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49613	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CDL, NDP, PC1, U10, HEC, UQ6, ZN, EHZ, 3PH, FMN, 3PE, ADP, FES, UQ1, UQ9, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/774	1.33	11/1056 (1.0%)
2	B	0.97	1/1289 (0.1%)	1.45	18/1744 (1.0%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.96	9/3504 (0.3%)	1.38	34/4747 (0.7%)
5	E	0.86	3/1675 (0.2%)	1.35	24/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	64/4543 (1.4%)
7	G	0.92	10/5374 (0.2%)	1.60	109/7281 (1.5%)
8	H	0.98	5/2585 (0.2%)	1.52	59/3529 (1.7%)
9	I	0.93	1/1427 (0.1%)	1.54	18/1927 (0.9%)
10	J	0.78	0/1233	1.35	16/1672 (1.0%)
11	K	0.90	0/740	1.54	13/1005 (1.3%)
12	L	0.99	8/4921 (0.2%)	1.59	114/6696 (1.7%)
13	M	1.01	7/3709 (0.2%)	1.56	85/5052 (1.7%)
14	N	1.01	4/2756 (0.1%)	1.56	62/3751 (1.7%)
15	O	1.02	9/2666 (0.3%)	1.44	43/3615 (1.2%)
16	P	0.88	4/2804 (0.1%)	1.35	43/3802 (1.1%)
17	Q	0.87	1/980 (0.1%)	1.29	12/1324 (0.9%)
18	R	0.87	1/671 (0.1%)	1.22	10/903 (1.1%)
19	S	1.09	3/678 (0.4%)	1.74	20/915 (2.2%)
20	T	1.03	1/613 (0.2%)	1.56	13/826 (1.6%)
20	U	0.96	1/690 (0.1%)	1.49	22/931 (2.4%)
21	V	0.86	0/937	1.47	14/1270 (1.1%)
22	W	0.80	0/993	1.32	15/1335 (1.1%)
23	X	0.87	2/1422 (0.1%)	1.42	26/1921 (1.4%)
24	Y	0.88	0/1054	0.97	2/1429 (0.1%)
25	Z	0.76	0/1183	1.10	7/1597 (0.4%)
26	a	0.83	0/561	1.47	7/755 (0.9%)
27	b	0.70	0/651	0.91	1/895 (0.1%)
28	c	0.92	1/400 (0.2%)	1.48	13/544 (2.4%)
29	d	1.02	2/1020 (0.2%)	1.15	11/1377 (0.8%)
30	e	0.63	0/885	0.91	1/1178 (0.1%)
31	f	0.92	1/488 (0.2%)	1.30	10/657 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.88	3/886 (0.3%)	1.35	20/1207 (1.7%)
33	h	0.76	1/1181 (0.1%)	1.27	8/1599 (0.5%)
34	i	0.79	0/823	1.31	13/1119 (1.2%)
35	j	0.82	0/588	1.32	8/805 (1.0%)
36	k	0.86	0/587	1.40	11/794 (1.4%)
37	l	0.97	3/1384 (0.2%)	1.24	11/1889 (0.6%)
38	m	0.79	1/1083 (0.1%)	1.17	14/1468 (1.0%)
39	n	0.89	1/1596 (0.1%)	1.27	17/2162 (0.8%)
40	o	0.83	0/1052	1.29	14/1411 (1.0%)
41	p	0.64	1/1471 (0.1%)	1.03	15/1988 (0.8%)
42	q	1.07	2/1037 (0.2%)	1.52	17/1408 (1.2%)
43	r	1.04	2/426 (0.5%)	1.57	11/573 (1.9%)
44	s	0.98	0/116	1.78	3/157 (1.9%)
45	AA	0.58	1/3187 (0.0%)	0.82	5/4320 (0.1%)
45	Aa	0.60	2/3288 (0.1%)	0.84	10/4462 (0.2%)
46	AB	0.44	1/3187 (0.0%)	0.67	5/4308 (0.1%)
46	Ab	0.45	0/3187	0.66	2/4308 (0.0%)
47	AC	0.43	1/3089 (0.0%)	0.69	3/4221 (0.1%)
47	Ac	0.45	0/3089	0.73	4/4221 (0.1%)
48	AD	0.53	0/1955	0.83	4/2655 (0.2%)
48	Ad	0.58	2/1954 (0.1%)	0.81	3/2655 (0.1%)
49	AE	0.66	0/1459	1.05	4/1976 (0.2%)
49	AI	0.75	0/349	1.15	2/476 (0.4%)
49	Ae	0.67	1/1464 (0.1%)	1.04	3/1983 (0.2%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.38	0/884	0.53	0/1184
51	AG	0.50	0/662	0.87	1/895 (0.1%)
51	Ag	0.65	0/662	1.00	2/895 (0.2%)
52	AH	0.38	0/542	0.80	2/728 (0.3%)
52	Ah	0.71	0/551	0.99	3/739 (0.4%)
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.65	0/402	1.01	3/541 (0.6%)
54	AK	0.48	0/291	0.83	1/399 (0.3%)
54	Ak	0.68	1/371 (0.3%)	0.92	1/511 (0.2%)
All	All	0.81	104/97759 (0.1%)	1.25	1131/132554 (0.9%)

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	247	PRO	N-CD	16.66	1.71	1.47
18	R	89	PRO	N-CD	-15.05	1.26	1.47
29	d	115	PRO	N-CD	-13.98	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	265	PRO	N-CD	13.84	1.67	1.47
14	N	255	PRO	N-CD	-13.54	1.28	1.47
42	q	139	PRO	N-CD	-13.44	1.28	1.47
28	c	39	PRO	N-CD	-13.32	1.29	1.47
16	P	371	PRO	N-CD	12.93	1.65	1.47
7	G	532	PRO	N-CD	-12.51	1.30	1.47
15	O	315	PRO	N-CD	-12.05	1.30	1.47
19	S	28	PRO	N-CD	-11.91	1.31	1.47
20	T	141	PRO	N-CD	11.75	1.64	1.47
12	L	234	PRO	N-CD	11.17	1.63	1.47
14	N	123	PRO	N-CD	-10.91	1.32	1.47
8	H	42	PRO	N-CD	10.87	1.62	1.47
13	M	370	PRO	N-CD	-10.55	1.32	1.47
15	O	210	PRO	N-CD	-10.49	1.33	1.47
6	F	234	GLY	CA-C	-10.22	1.41	1.52
15	O	224	PRO	N-CD	-10.22	1.33	1.47
23	X	152	PRO	N-CD	-10.14	1.33	1.47
6	F	227	PRO	N-CD	10.05	1.61	1.47
6	F	235	VAL	N-CA	-9.64	1.34	1.46
16	P	290	PRO	N-CD	9.62	1.61	1.47
32	g	78	PRO	N-CD	-9.52	1.34	1.47
7	G	275	PRO	N-CD	-9.48	1.34	1.47
29	d	15	PRO	N-CD	-9.41	1.34	1.47
8	H	75	PRO	N-CD	9.27	1.60	1.47
6	F	319	PRO	N-CD	9.11	1.60	1.47
15	O	212	PRO	N-CD	-8.89	1.35	1.47
46	AB	240	MET	C-N	8.63	1.45	1.33
13	M	20	PRO	N-CD	8.60	1.59	1.47
9	I	107	PRO	N-CD	8.56	1.59	1.47
4	D	163	PRO	N-CD	-8.44	1.35	1.47
12	L	212	PRO	N-CD	-8.28	1.36	1.47
48	Ad	180	PRO	N-CD	-8.17	1.36	1.47
39	n	155	PRO	N-CD	8.09	1.59	1.47
5	E	218	ARG	CA-C	7.96	1.62	1.53
4	D	352	PRO	N-CD	-7.90	1.36	1.47
12	L	513	MET	C-N	7.89	1.43	1.33
19	S	63	PRO	N-CD	-7.89	1.36	1.47
54	Ak	38	TRP	CA-C	-7.83	1.41	1.52
12	L	525	LEU	CA-C	7.81	1.62	1.53
17	Q	53	ILE	C-O	7.78	1.33	1.24
49	Ae	143	SER	C-N	7.66	1.44	1.33
43	r	111	PRO	N-CD	-7.44	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	138	ASN	CA-C	7.23	1.62	1.53
37	l	104	PRO	N-CD	-7.21	1.37	1.47
15	O	83	MET	C-N	7.20	1.43	1.33
13	M	208	PRO	N-CD	7.11	1.57	1.47
14	N	238	PRO	N-CD	-7.08	1.37	1.47
15	O	211	VAL	CA-C	6.95	1.60	1.52
7	G	449	PRO	N-CD	6.82	1.57	1.47
14	N	147	PRO	N-CD	-6.77	1.38	1.47
7	G	541	PRO	N-CD	-6.74	1.38	1.47
6	F	233	VAL	CA-C	-6.72	1.44	1.52
7	G	203	ASP	CA-C	6.71	1.62	1.52
32	g	113	GLN	CA-C	6.55	1.61	1.52
4	D	106	VAL	C-N	-6.55	1.24	1.33
7	G	600	GLU	CA-C	6.45	1.61	1.52
12	L	384	PRO	N-CD	6.41	1.56	1.47
2	B	110	PRO	C-O	-6.28	1.16	1.24
4	D	266	ARG	C-O	-6.25	1.16	1.24
7	G	127	ASP	CA-C	6.25	1.62	1.52
7	G	76	ARG	CA-C	6.14	1.61	1.53
6	F	384	PRO	N-CD	-6.12	1.39	1.47
32	g	137	SER	C-O	-6.09	1.16	1.24
12	L	514	ASN	C-N	-6.06	1.24	1.33
41	p	10	TYR	CA-C	-5.99	1.46	1.52
5	E	93	PRO	N-CD	-5.92	1.39	1.47
12	L	112	PRO	N-CD	5.90	1.56	1.47
7	G	361	VAL	CA-C	5.88	1.60	1.52
38	m	72	ARG	CA-C	5.85	1.60	1.52
23	X	54	ARG	CA-C	5.83	1.60	1.52
37	l	45	PRO	N-CD	-5.83	1.39	1.47
43	r	25	GLN	CA-C	5.82	1.60	1.52
4	D	88	HIS	CA-C	-5.79	1.45	1.52
8	H	60	PRO	N-CD	5.77	1.55	1.47
15	O	87	PRO	N-CD	-5.71	1.39	1.47
5	E	80	PRO	N-CD	5.70	1.55	1.47
13	M	454	ILE	CA-C	5.68	1.60	1.52
48	Ad	217	GLY	C-O	-5.66	1.16	1.23
13	M	252	PRO	N-CD	-5.61	1.40	1.47
37	l	119	THR	CA-C	-5.53	1.45	1.53
4	D	107	ARG	C-N	5.51	1.40	1.33
4	D	392	PRO	C-O	-5.50	1.20	1.24
19	S	95	LEU	CA-C	5.49	1.59	1.52
45	Aa	273	SER	CA-C	-5.43	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	683	PRO	N-CD	-5.42	1.40	1.47
42	q	126	PRO	N-CD	5.39	1.55	1.47
16	P	235	THR	CA-C	5.38	1.59	1.53
8	H	211	PHE	CA-C	5.33	1.59	1.52
15	O	103	PRO	N-CD	-5.32	1.40	1.47
4	D	266	ARG	CA-C	-5.23	1.45	1.52
45	AA	311	ILE	C-N	5.20	1.40	1.33
13	M	424	ILE	CA-C	-5.17	1.45	1.52
33	h	174	PRO	N-CD	-5.15	1.40	1.47
31	f	38	ARG	CA-C	-5.13	1.46	1.52
47	AC	223	TYR	C-O	-5.09	1.17	1.23
3	C	61	GLY	C-N	-5.08	1.27	1.33
20	U	140	CYS	C-O	-5.07	1.17	1.23
4	D	63	PRO	N-CD	-5.04	1.40	1.47
13	M	159	PRO	N-CD	5.04	1.54	1.47
45	Aa	59	VAL	CA-C	-5.01	1.48	1.53
8	H	310	PHE	CA-C	5.00	1.59	1.52

All (1131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.24	132.39	110.65
4	D	142	VAL	N-CA-C	-19.04	92.53	110.42
7	G	174	THR	N-CA-C	-16.81	89.08	114.64
6	F	125	CYS	N-CA-C	-15.64	93.46	113.17
6	F	332	CYS	N-CA-C	15.63	130.09	111.02
14	N	255	PRO	N-CA-C	14.59	128.50	110.70
13	M	370	PRO	N-CA-C	14.59	128.50	110.70
15	O	83	MET	O-C-N	14.43	140.50	122.89
15	O	118	TYR	N-CA-C	13.88	125.92	111.07
15	O	83	MET	CA-C-N	-13.70	100.06	120.75
15	O	83	MET	C-N-CA	-13.70	100.06	120.75
42	q	139	PRO	N-CA-CB	-13.60	95.57	103.19
39	n	165	PRO	N-CA-C	13.37	130.45	111.33
7	G	251	ILE	N-CA-C	13.33	126.83	108.17
7	G	77	MET	N-CA-C	-13.07	97.31	113.38
40	o	118	LYS	N-CA-C	-12.86	97.31	111.07
9	I	164	VAL	N-CA-C	-12.85	100.11	112.83
41	p	128	GLU	N-CA-C	12.55	125.04	111.36
7	G	500	ILE	N-CA-C	-12.52	98.77	110.53
26	a	3	PHE	CB-CA-C	-12.42	89.56	110.68
16	P	106	LEU	N-CA-C	12.25	128.79	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	171	VAL	N-CA-C	-11.82	99.42	110.53
15	O	157	VAL	N-CA-C	11.68	124.46	108.11
13	M	424	ILE	N-CA-C	-11.66	94.03	109.30
7	G	204	MET	N-CA-C	-11.65	91.43	109.25
6	F	449	ARG	N-CA-C	-11.61	98.70	111.36
34	i	14	GLN	N-CA-C	11.59	123.91	111.28
49	AI	60	ALA	N-CA-C	11.50	125.51	109.18
13	M	104	ILE	N-CA-C	-11.49	99.15	110.30
15	O	114	LEU	N-CA-C	-11.47	98.86	111.36
6	F	334	THR	N-CA-CB	11.47	127.25	109.82
12	L	194	ASN	N-CA-C	11.41	125.31	109.11
14	N	244	ILE	N-CA-C	-11.36	99.25	110.72
17	Q	60	ASP	N-CA-C	-11.34	90.30	109.24
7	G	599	THR	N-CA-C	11.32	126.19	112.38
12	L	278	LEU	N-CA-C	-11.26	98.98	111.14
19	S	39	GLN	N-CA-C	11.19	125.45	111.69
11	K	83	ASN	N-CA-C	-11.15	100.21	114.04
22	W	87	ILE	N-CA-C	-11.13	99.73	110.42
21	V	57	ASP	N-CA-C	-11.04	99.26	111.07
1	A	54	LYS	N-CA-C	-10.98	98.18	111.69
13	M	455	THR	N-CA-C	-10.96	95.44	110.35
8	H	259	PHE	N-CA-C	-10.96	99.41	111.36
44	s	86	ASP	N-CA-C	-10.95	99.32	111.14
12	L	582	GLY	N-CA-C	-10.83	99.47	114.64
12	L	556	ILE	N-CA-C	10.76	121.42	110.23
35	j	82	GLY	N-CA-C	-10.74	91.03	111.02
12	L	231	PRO	N-CA-C	10.71	127.76	113.84
23	X	70	PHE	N-CA-C	-10.60	99.73	111.07
33	h	101	ILE	N-CA-C	-10.53	98.63	108.95
9	I	77	LEU	N-CA-C	-10.46	99.68	111.71
5	E	68	ASN	N-CA-C	-10.41	99.93	111.07
53	Aj	16	ARG	N-CA-C	10.41	123.72	111.02
20	T	139	MET	N-CA-C	-10.40	97.46	113.89
15	O	96	THR	N-CA-C	-10.36	100.07	111.36
10	J	122	ASP	N-CA-C	-10.35	98.81	111.33
13	M	276	CYS	N-CA-C	-10.34	100.01	111.28
2	B	195	PRO	N-CA-C	-10.33	98.10	110.70
8	H	284	GLN	N-CA-C	-10.32	100.02	111.07
22	W	59	VAL	N-CA-C	-10.30	100.53	110.42
4	D	337	MET	N-CA-C	-10.30	100.05	111.07
45	Aa	261	ALA	N-CA-C	-10.29	95.20	109.71
7	G	280	ASP	N-CA-C	10.26	122.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	247	PRO	N-CA-CB	10.22	114.29	103.15
4	D	140	ASP	CB-CA-C	-10.20	98.06	111.42
16	P	366	ILE	N-CA-C	10.19	121.02	110.62
37	l	170	ARG	N-CA-C	-10.13	101.56	113.21
7	G	414	PHE	N-CA-C	-10.06	101.51	113.88
26	a	4	GLU	N-CA-C	10.05	124.81	112.54
9	I	161	ALA	N-CA-C	10.05	122.24	111.28
20	T	135	ALA	N-CA-C	-10.05	100.32	111.28
13	M	117	MET	N-CA-C	-9.99	100.39	111.28
46	AB	306	THR	N-CA-C	9.94	123.35	111.33
7	G	325	ARG	N-CA-C	-9.87	100.21	110.97
6	F	178	GLU	N-CA-C	-9.87	99.26	111.11
9	I	166	ALA	N-CA-C	-9.87	100.79	113.12
46	AB	303	ASN	N-CA-C	-9.86	100.16	112.88
53	Aj	15	PHE	N-CA-C	9.81	122.06	111.36
6	F	103	ASN	N-CA-C	-9.81	101.00	113.16
45	AA	187	LEU	N-CA-C	-9.80	100.42	112.38
13	M	423	MET	N-CA-C	-9.78	96.86	110.35
11	K	90	VAL	N-CA-C	-9.77	100.35	112.76
6	F	144	VAL	N-CA-C	-9.77	101.35	110.53
6	F	141	GLY	N-CA-C	-9.76	101.18	112.50
7	G	654	VAL	N-CA-C	9.76	123.28	111.09
14	N	255	PRO	CA-N-CD	9.70	125.58	112.00
7	G	35	PHE	N-CA-C	9.68	124.35	108.96
14	N	286	ALA	N-CA-C	-9.66	100.75	111.28
5	E	64	ALA	N-CA-C	-9.65	99.53	111.11
13	M	83	HIS	N-CA-C	-9.64	97.23	110.35
16	P	371	PRO	N-CA-CB	9.63	111.84	103.36
6	F	418	GLN	N-CA-C	-9.62	100.75	111.14
7	G	337	ALA	N-CA-C	-9.59	100.79	114.12
26	a	2	TRP	N-CA-C	-9.53	101.65	113.28
39	n	29	SER	N-CA-C	-9.52	101.56	113.55
12	L	375	ILE	N-CA-C	-9.52	101.28	110.42
8	H	52	ALA	N-CA-C	-9.50	100.90	111.07
29	d	115	PRO	N-CA-CB	-9.50	95.09	103.35
4	D	427	PRO	N-CA-C	-9.48	95.62	110.50
10	J	36	GLY	N-CA-C	-9.46	101.04	112.49
14	N	228	ASN	N-CA-C	-9.45	100.96	111.07
16	P	358	THR	N-CA-C	9.44	121.89	110.19
41	p	56	HIS	N-CA-C	9.44	121.56	111.28
31	f	51	ASN	CB-CA-C	-9.37	97.35	112.06
42	q	139	PRO	CA-N-CD	9.37	125.12	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	133	ILE	N-CA-C	9.35	119.89	110.82
13	M	104	ILE	N-CA-CB	9.35	120.81	110.62
7	G	694	PHE	N-CA-C	9.35	121.47	111.28
29	d	115	PRO	CA-N-CD	9.34	125.08	112.00
12	L	394	LEU	N-CA-C	-9.30	101.12	111.07
7	G	692	LYS	N-CA-C	-9.30	100.52	112.23
36	k	60	MET	N-CA-C	9.28	121.09	110.97
16	P	367	GLU	N-CA-C	9.26	122.56	111.82
16	P	369	THR	N-CA-CB	9.26	123.50	110.17
36	k	56	ALA	N-CA-C	9.26	121.45	111.36
12	L	40	ILE	N-CA-C	-9.23	101.40	110.72
7	G	640	ASP	N-CA-C	-9.22	101.31	111.36
12	L	467	VAL	N-CA-C	9.17	119.22	110.42
38	m	48	LEU	N-CA-C	9.16	124.01	113.01
12	L	483	PRO	N-CA-C	-9.16	96.81	111.38
14	N	326	PHE	N-CA-C	-9.15	101.28	111.07
16	P	157	LYS	N-CA-C	-9.14	101.39	111.36
7	G	389	THR	N-CA-C	-9.13	96.26	109.96
5	E	85	ALA	N-CA-C	-9.12	101.42	111.36
47	Ac	157	GLY	N-CA-C	9.12	123.08	112.50
14	N	87	GLN	N-CA-C	9.10	123.25	109.41
15	O	247	PRO	CA-N-CD	-9.09	99.27	112.00
13	M	442	ILE	N-CA-CB	9.09	117.54	110.45
28	c	64	GLU	N-CA-C	-9.07	101.36	111.07
28	c	39	PRO	N-CA-CB	-9.05	95.28	103.25
23	X	55	ARG	N-CA-C	9.04	130.06	110.80
12	L	524	THR	N-CA-C	8.99	122.25	111.82
40	o	97	LYS	N-CA-C	-8.97	101.47	111.07
41	p	115	GLN	N-CA-C	-8.95	102.88	113.88
11	K	70	GLU	N-CA-C	-8.93	100.39	111.11
2	B	121	PHE	CB-CA-C	8.91	124.69	110.96
12	L	406	ALA	N-CA-C	-8.90	101.65	111.36
6	F	411	SER	N-CA-C	-8.89	101.56	111.07
10	J	43	VAL	N-CA-C	-8.89	101.55	110.62
12	L	344	GLY	N-CA-C	-8.87	102.21	112.50
14	N	233	LEU	N-CA-C	-8.86	101.62	111.28
15	O	183	CYS	N-CA-C	-8.86	100.48	111.11
15	O	206	TYR	N-CA-CB	-8.83	92.81	110.64
39	n	70	GLU	N-CA-C	-8.79	101.67	111.07
13	M	255	LYS	N-CA-C	-8.77	101.68	111.07
14	N	255	PRO	N-CA-CB	-8.76	94.58	103.08
7	G	133	GLN	N-CA-CB	8.76	121.48	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	212	LYS	N-CA-C	-8.76	94.63	108.90
12	L	526	LEU	N-CA-CB	-8.75	99.00	112.30
7	G	365	ASN	N-CA-C	-8.74	102.17	112.92
40	o	72	ASP	N-CA-C	-8.73	99.01	110.53
14	N	81	LEU	N-CA-C	-8.71	94.44	108.55
8	H	60	PRO	N-CA-CB	8.69	108.56	102.65
9	I	154	TYR	N-CA-CB	-8.69	99.19	111.62
22	W	20	VAL	N-CA-C	8.68	120.78	108.36
52	Ah	83	LYS	N-CA-C	8.66	121.97	110.88
16	P	96	LEU	N-CA-C	8.65	121.66	111.71
8	H	212	ASN	N-CA-C	-8.63	101.88	114.39
34	i	12	LEU	N-CA-C	-8.60	101.11	111.69
13	M	248	ILE	N-CA-C	-8.60	102.17	110.42
10	J	29	GLY	N-CA-C	-8.59	102.25	112.64
12	L	212	PRO	N-CA-C	8.57	125.73	113.47
26	a	3	PHE	CA-CB-CG	8.55	122.35	113.80
19	S	86	GLU	N-CA-C	-8.53	102.07	111.36
15	O	315	PRO	CA-N-CD	8.52	123.93	112.00
18	R	57	GLU	N-CA-C	-8.51	98.25	110.59
19	S	18	GLU	N-CA-C	8.49	123.23	109.40
20	U	154	VAL	N-CA-C	8.47	119.75	106.88
16	P	373	LYS	N-CA-C	8.45	121.84	110.35
16	P	360	ARG	N-CA-C	8.44	121.67	110.53
22	W	100	TRP	N-CA-C	-8.43	99.90	112.04
14	N	221	LEU	N-CA-C	-8.43	101.13	111.33
12	L	281	GLY	N-CA-C	-8.42	102.73	112.50
23	X	99	HIS	N-CA-C	-8.40	102.20	111.36
15	O	212	PRO	N-CA-C	8.38	126.24	113.75
14	N	272	LYS	N-CA-C	-8.38	102.15	111.28
12	L	287	PHE	N-CA-C	-8.36	102.13	111.07
7	G	452	LEU	N-CA-C	-8.36	102.17	111.28
3	C	108	LYS	N-CA-C	8.35	120.00	111.07
22	W	57	ILE	N-CA-C	8.34	122.02	109.17
8	H	141	SER	N-CA-C	-8.34	102.15	111.07
17	Q	54	THR	N-CA-C	8.34	123.30	109.46
39	n	19	LEU	N-CA-C	-8.33	103.25	113.41
14	N	157	LEU	N-CA-C	-8.32	102.16	111.07
7	G	532	PRO	CA-N-CD	8.32	123.64	112.00
7	G	558	GLN	N-CA-C	-8.27	102.23	111.07
1	A	55	PHE	N-CA-C	-8.26	102.23	111.07
14	N	218	ALA	N-CA-C	-8.25	98.93	111.56
8	H	311	THR	N-CA-C	-8.23	102.55	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	218	ARG	CB-CA-C	-8.22	99.78	112.12
8	H	196	ALA	N-CA-C	8.22	127.99	109.81
12	L	88	LEU	N-CA-C	-8.19	102.29	111.14
3	C	196	PRO	N-CA-C	8.18	124.90	113.53
13	M	274	SER	N-CA-C	8.18	120.19	111.28
13	M	26	ASN	N-CA-C	-8.17	102.31	111.14
15	O	245	PHE	N-CA-C	8.15	120.17	111.28
12	L	169	LEU	N-CA-C	-8.15	102.48	111.36
7	G	691	ILE	N-CA-C	8.14	123.62	111.89
6	F	411	SER	N-CA-CB	8.14	121.81	110.01
7	G	484	ASP	N-CA-C	8.14	121.07	111.71
1	A	64	LEU	N-CA-C	-8.14	102.36	111.07
6	F	298	GLU	N-CA-C	8.13	120.14	111.28
14	N	32	GLY	N-CA-C	-8.13	103.07	112.50
22	W	96	THR	N-CA-C	-8.13	102.36	111.14
6	F	191	TYR	N-CA-C	8.12	121.69	110.24
12	L	151	SER	N-CA-C	-8.12	102.51	111.36
44	s	86	ASP	N-CA-CB	8.12	121.84	110.07
21	V	86	LYS	N-CA-C	-8.10	102.39	111.14
7	G	500	ILE	N-CA-CB	8.09	120.92	110.57
15	O	217	ARG	N-CA-C	-8.09	102.42	111.07
36	k	38	VAL	N-CA-C	-8.08	102.56	110.72
29	d	15	PRO	N-CA-CB	-8.08	96.32	103.35
45	AA	360	CYS	N-CA-C	8.08	121.44	109.24
2	B	110	PRO	N-CA-C	8.07	124.55	113.65
5	E	219	SER	N-CA-CB	8.07	124.07	111.56
39	n	170	ILE	N-CA-C	-8.07	103.03	111.58
13	M	205	ILE	N-CA-C	8.03	118.13	110.42
20	U	74	LEU	N-CA-C	8.03	122.04	108.23
12	L	276	THR	N-CA-CB	8.01	121.62	110.01
13	M	385	LEU	N-CA-C	-8.00	102.56	111.28
19	S	76	THR	N-CA-C	8.00	121.95	108.90
8	H	271	LEU	N-CA-C	-8.00	102.50	111.14
4	D	36	GLN	N-CA-C	-7.99	98.49	110.24
7	G	534	VAL	N-CA-C	-7.99	104.80	111.91
23	X	43	PHE	N-CA-C	-7.99	102.51	111.14
23	X	112	LEU	N-CA-C	-7.98	102.52	111.14
22	W	98	LYS	N-CA-C	-7.97	101.60	113.72
9	I	201	ILE	N-CA-C	-7.97	102.67	110.72
1	A	9	ILE	N-CA-C	-7.97	102.49	110.62
10	J	60	LEU	N-CA-C	7.95	120.72	111.02
42	q	67	GLU	CB-CA-C	-7.94	99.60	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	39	PRO	CA-N-CD	7.94	123.11	112.00
16	P	360	ARG	N-CA-CB	-7.93	99.02	110.36
7	G	651	PRO	CB-CA-C	-7.93	98.48	111.56
16	P	206	ILE	N-CA-C	7.93	120.92	108.87
2	B	121	PHE	CA-CB-CG	-7.92	105.88	113.80
23	X	46	CYS	N-CA-C	-7.90	102.75	111.36
19	S	28	PRO	CA-N-CD	7.90	123.06	112.00
13	M	141	GLU	N-CA-C	7.89	122.75	113.20
34	i	10	LEU	N-CA-C	-7.89	104.14	114.31
8	H	311	THR	N-CA-CB	7.86	123.50	110.92
21	V	6	LYS	N-CA-C	-7.86	100.15	110.53
28	c	45	GLY	N-CA-C	7.86	123.53	113.24
7	G	270	VAL	N-CA-CB	-7.85	100.66	110.31
41	p	128	GLU	N-CA-CB	-7.84	98.56	110.16
23	X	55	ARG	N-CA-CB	-7.84	97.24	110.49
9	I	160	GLU	N-CA-C	7.82	124.19	111.37
16	P	235	THR	CB-CA-C	-7.82	100.03	112.07
13	M	85	LYS	N-CA-C	-7.81	101.38	113.02
11	K	51	SER	N-CA-C	-7.81	102.84	113.30
12	L	265	PRO	N-CA-CB	7.81	111.66	103.15
38	m	50	GLN	N-CA-C	-7.80	102.78	114.64
7	G	389	THR	N-CA-CB	7.79	121.46	109.85
12	L	111	ASP	N-CA-C	-7.78	100.28	109.93
12	L	265	PRO	CA-N-CD	-7.77	101.13	112.00
13	M	330	ALA	N-CA-C	-7.76	102.75	111.14
23	X	58	LYS	N-CA-C	-7.76	102.77	111.07
1	A	53	MET	N-CA-C	-7.76	103.96	113.19
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
4	D	141	TYR	CA-C-N	7.73	130.16	120.72
4	D	141	TYR	C-N-CA	7.73	130.16	120.72
6	F	334	THR	N-CA-C	-7.70	101.62	111.02
12	L	265	PRO	N-CA-C	-7.70	101.31	113.78
12	L	415	ALA	N-CA-C	-7.68	102.91	111.28
42	q	44	TYR	N-CA-C	-7.68	98.91	110.28
52	AH	68	GLU	N-CA-C	-7.67	102.86	111.07
42	q	89	TRP	N-CA-C	-7.67	102.86	111.14
8	H	253	GLU	N-CA-C	7.67	121.90	112.54
6	F	58	ARG	N-CA-C	-7.65	103.02	111.36
10	J	124	LEU	N-CA-C	-7.64	103.81	113.43
31	f	48	LEU	N-CA-C	7.63	121.75	110.30
31	f	51	ASN	N-CA-C	7.63	121.94	111.17
7	G	56	VAL	N-CA-C	-7.63	103.02	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	171	VAL	N-CA-CB	7.62	120.33	110.57
2	B	153	PRO	CB-CA-C	-7.62	98.98	111.56
4	D	361	ALA	N-CA-C	-7.62	103.08	112.38
7	G	569	GLN	N-CA-C	7.60	122.00	108.24
32	g	124	VAL	N-CA-C	-7.59	103.05	110.72
5	E	68	ASN	N-CA-CB	7.59	121.02	110.01
19	S	35	ASP	N-CA-C	-7.59	103.09	111.36
18	R	32	THR	N-CA-C	7.58	119.60	110.19
5	E	166	LYS	N-CA-C	-7.57	102.22	113.72
18	R	74	HIS	N-CA-C	7.55	121.15	110.50
20	T	141	PRO	N-CA-C	-7.55	103.04	113.53
20	U	147	TYR	N-CA-C	-7.54	102.99	111.14
45	Aa	404	ASP	N-CA-C	-7.54	103.53	112.89
12	L	245	ALA	N-CA-C	7.54	119.14	111.07
8	H	223	PHE	CB-CA-C	-7.54	99.05	110.88
40	o	81	LYS	N-CA-C	-7.54	104.61	113.88
12	L	605	ASN	N-CA-CB	7.53	121.39	110.47
9	I	119	CYS	N-CA-C	-7.50	103.18	111.36
30	e	46	GLY	N-CA-C	-7.50	104.92	114.37
7	G	277	MET	N-CA-C	7.49	120.60	109.59
7	G	467	LYS	N-CA-C	-7.49	102.27	111.33
9	I	158	CYS	N-CA-C	-7.47	103.13	111.28
47	AC	202	GLU	N-CA-C	-7.45	103.18	111.82
11	K	14	LEU	N-CA-C	-7.44	103.25	111.36
7	G	510	TRP	N-CA-CB	7.43	120.93	109.85
12	L	392	LYS	N-CA-C	7.43	119.02	111.07
7	G	303	THR	N-CA-C	7.43	123.06	113.18
2	B	183	ARG	N-CA-C	-7.41	104.48	113.97
6	F	430	GLY	N-CA-C	7.41	121.62	112.73
48	Ad	164	MET	N-CA-C	7.41	120.50	107.61
12	L	138	PHE	N-CA-C	-7.40	103.21	111.28
12	L	123	LEU	N-CA-C	-7.39	103.30	111.36
29	d	113	LEU	N-CA-CB	-7.38	99.94	111.23
47	Ac	202	GLU	N-CA-C	-7.38	103.26	111.82
21	V	57	ASP	N-CA-CB	7.37	120.70	110.01
37	l	36	MET	N-CA-C	-7.37	103.42	113.30
12	L	21	ILE	N-CA-CB	7.37	121.63	110.58
4	D	350	LYS	CB-CA-C	-7.36	101.03	111.85
12	L	19	ILE	N-CA-C	7.36	117.49	110.42
37	l	97	LEU	N-CA-C	-7.36	103.89	113.17
12	L	526	LEU	N-CA-C	7.36	121.66	112.24
38	m	72	ARG	N-CA-C	7.36	122.55	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	250	LEU	N-CA-C	-7.35	103.61	112.58
12	L	28	LYS	N-CA-C	-7.34	103.28	111.28
42	q	24	LEU	N-CA-C	-7.34	103.28	111.28
19	S	94	VAL	N-CA-C	7.32	117.45	110.42
8	H	309	ILE	N-CA-C	7.32	117.40	110.30
23	X	152	PRO	N-CA-CB	-7.31	96.52	103.39
49	Ae	221	GLY	N-CA-C	7.28	126.87	113.76
20	T	105	MET	N-CA-C	7.28	119.29	111.36
28	c	37	ALA	N-CA-C	7.28	119.84	111.11
49	AE	221	GLY	N-CA-C	7.27	126.85	113.76
13	M	289	SER	N-CA-C	-7.27	103.29	111.07
40	o	118	LYS	N-CA-CB	7.27	120.55	110.01
39	n	165	PRO	CB-CA-C	-7.27	100.21	111.40
33	h	174	PRO	N-CA-C	7.26	122.66	111.11
12	L	527	GLY	N-CA-C	-7.25	105.71	115.36
3	C	195	HIS	CB-CA-C	7.25	117.35	110.17
7	G	374	THR	CB-CA-C	-7.24	99.85	111.28
7	G	384	ASN	N-CA-C	-7.23	103.43	111.82
7	G	497	VAL	N-CA-C	-7.23	103.25	110.62
8	H	212	ASN	N-CA-CB	7.22	120.50	110.98
15	O	224	PRO	N-CA-CB	-7.22	96.75	103.46
14	N	332	MET	N-CA-C	-7.21	103.36	111.07
8	H	50	ALA	N-CA-C	7.21	118.78	111.07
10	J	121	GLY	N-CA-C	-7.20	106.28	115.42
20	U	136	GLU	N-CA-C	-7.20	104.49	113.20
7	G	661	GLU	N-CA-C	7.19	118.81	110.97
8	H	139	THR	N-CA-CB	7.19	120.44	110.01
10	J	21	LEU	N-CA-C	-7.18	104.61	113.15
11	K	81	VAL	N-CA-C	7.18	117.94	110.62
6	F	73	PRO	N-CA-C	-7.17	103.79	113.40
11	K	24	SER	CB-CA-C	-7.17	107.48	117.23
21	V	68	LEU	N-CA-C	-7.17	103.47	111.28
36	k	73	ILE	N-CA-C	-7.17	103.31	110.62
6	F	81	LYS	N-CA-C	-7.16	103.55	111.36
7	G	465	VAL	N-CA-CB	7.15	118.45	110.51
15	O	210	PRO	CA-N-CD	7.15	122.01	112.00
7	G	217	GLU	N-CA-C	-7.13	101.63	110.41
8	H	254	LEU	N-CA-C	-7.13	103.55	111.82
8	H	214	GLU	N-CA-CB	-7.12	98.89	110.42
35	j	78	ASP	N-CA-C	-7.12	103.16	112.41
41	p	168	LYS	N-CA-C	-7.11	104.23	113.12
47	Ac	17	SER	N-CA-C	7.11	121.96	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	102	TRP	N-CA-C	-7.10	104.98	112.93
6	F	78	GLY	N-CA-C	-7.09	104.22	112.73
48	AD	120	VAL	N-CA-C	7.09	118.05	111.45
21	V	95	LEU	N-CA-C	-7.09	103.55	111.28
12	L	554	ASP	N-CA-CB	7.08	121.19	110.42
13	M	244	ILE	N-CA-C	7.08	117.84	110.62
13	M	325	LEU	N-CA-C	-7.08	103.50	111.07
11	K	48	SER	N-CA-C	-7.07	103.58	111.28
17	Q	162	ALA	N-CA-C	7.06	118.97	111.28
15	O	210	PRO	N-CA-C	7.05	122.27	111.34
7	G	461	SER	N-CA-C	7.05	119.86	111.33
14	N	103	SER	N-CA-C	-7.04	103.65	111.82
7	G	148	SER	N-CA-C	7.03	120.86	109.40
12	L	319	MET	N-CA-C	-7.03	104.70	112.72
8	H	176	LEU	CA-C-N	-7.03	113.56	120.52
8	H	176	LEU	C-N-CA	-7.03	113.56	120.52
13	M	365	ALA	N-CA-C	-7.02	103.70	111.36
35	j	65	MET	N-CA-C	-7.02	103.56	111.07
35	j	81	LEU	CA-C-O	7.02	126.02	119.00
13	M	34	ILE	N-CA-C	-7.01	103.47	110.62
6	F	169	LEU	N-CA-C	7.00	118.91	111.28
42	q	77	VAL	N-CA-C	-7.00	99.69	109.21
44	s	84	ASN	N-CA-C	7.00	118.55	111.07
49	Ae	218	THR	N-CA-C	-7.00	102.80	111.75
6	F	455	GLN	N-CA-C	6.99	118.55	111.07
7	G	150	ARG	N-CA-C	6.99	119.55	109.14
2	B	166	ASN	N-CA-C	-6.98	103.36	110.97
12	L	546	LEU	N-CA-C	6.98	119.53	111.02
13	M	264	LEU	N-CA-C	-6.97	103.61	111.07
6	F	418	GLN	N-CA-CB	6.97	120.18	110.07
6	F	428	GLY	N-CA-C	-6.97	103.85	112.77
13	M	213	HIS	CB-CA-C	-6.97	96.88	110.11
7	G	294	TYR	N-CA-C	-6.96	104.59	113.23
12	L	100	ILE	N-CA-C	6.96	119.75	111.05
8	H	292	ASN	N-CA-C	6.96	118.94	111.36
6	F	103	ASN	N-CA-CB	6.95	121.08	110.44
6	F	246	GLU	N-CA-C	-6.95	103.70	111.28
12	L	471	ASN	N-CA-C	6.95	118.93	111.36
7	G	582	VAL	N-CA-C	6.94	118.48	108.48
22	W	87	ILE	N-CA-CB	6.94	118.67	110.55
13	M	91	LEU	N-CA-C	-6.94	103.81	112.90
49	AE	218	THR	N-CA-C	-6.94	102.87	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	69	PRO	N-CA-C	-6.93	104.29	113.65
20	T	145	VAL	N-CA-C	-6.92	103.72	110.72
16	P	235	THR	CA-C-O	6.92	128.11	121.67
15	O	231	SER	N-CA-C	-6.92	103.82	111.36
8	H	204	GLU	N-CA-C	-6.92	104.96	113.19
12	L	86	SER	N-CA-C	6.91	118.46	111.07
5	E	152	GLN	N-CA-C	-6.90	103.69	111.07
7	G	300	GLN	N-CA-CB	6.90	122.50	112.08
6	F	148	ALA	N-CA-C	-6.89	103.85	111.36
13	M	235	LEU	N-CA-C	6.88	119.36	111.11
49	AE	272	VAL	N-CA-C	-6.88	99.85	109.21
12	L	26	LEU	N-CA-C	6.88	119.62	111.71
25	Z	34	SER	N-CA-C	-6.87	103.71	111.07
7	G	362	ASP	N-CA-C	6.87	125.44	110.80
39	n	117	ASP	N-CA-C	-6.87	103.85	111.82
32	g	78	PRO	CA-N-CD	6.87	121.61	112.00
54	Ak	38	TRP	CA-C-O	-6.86	113.39	120.80
13	M	276	CYS	N-CA-CB	6.86	120.20	110.12
13	M	442	ILE	N-CA-C	-6.86	104.12	112.35
6	F	233	VAL	O-C-N	6.85	131.12	123.10
11	K	83	ASN	N-CA-CB	6.85	120.95	110.81
13	M	165	ILE	N-CA-C	-6.85	102.53	111.09
36	k	59	TYR	N-CA-CB	-6.85	98.90	110.41
25	Z	28	ARG	N-CA-C	6.85	119.68	108.52
6	F	329	LYS	N-CA-C	6.83	119.59	111.33
8	H	300	LEU	N-CA-C	-6.82	104.22	112.54
1	A	112	GLU	N-CA-C	-6.82	102.25	111.87
8	H	305	ILE	N-CA-C	-6.82	103.37	113.39
7	G	133	GLN	N-CA-C	-6.81	101.21	110.68
14	N	194	LEU	CA-C-N	-6.80	112.69	120.04
14	N	194	LEU	C-N-CA	-6.80	112.69	120.04
18	R	56	ASN	N-CA-C	6.80	119.99	108.90
7	G	268	GLY	N-CA-C	6.80	124.75	115.30
11	K	70	GLU	N-CA-CB	6.80	120.07	109.94
12	L	547	LYS	N-CA-C	6.79	118.68	111.28
38	m	127	ILE	N-CA-C	-6.79	106.18	112.43
6	F	244	ASN	N-CA-C	-6.79	100.93	110.50
10	J	58	ILE	N-CA-C	6.79	117.40	111.56
15	O	93	TYR	N-CA-C	-6.79	103.96	111.36
14	N	162	ILE	N-CA-C	-6.79	103.91	110.42
35	j	79	ALA	N-CA-C	-6.78	103.98	111.36
34	i	5	THR	N-CA-C	-6.77	101.82	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	88	HIS	N-CA-C	-6.76	102.99	111.11
6	F	233	VAL	CA-C-O	-6.76	113.29	120.53
43	r	11	LEU	N-CA-C	-6.74	104.01	111.36
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
13	M	374	ASN	N-CA-C	-6.73	103.87	111.07
40	o	11	TRP	CB-CA-C	-6.73	108.80	116.54
32	g	76	SER	N-CA-C	6.72	118.26	111.07
20	U	140	CYS	N-CA-C	-6.72	100.81	110.08
13	M	248	ILE	N-CA-CB	6.71	118.40	110.55
20	U	150	ASP	CB-CA-C	6.71	121.93	110.79
8	H	8	THR	N-CA-C	-6.71	101.23	110.35
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
15	O	207	ILE	N-CA-C	-6.70	97.28	107.73
12	L	95	PHE	N-CA-C	-6.69	103.91	111.07
5	E	199	ASP	N-CA-C	-6.69	103.68	110.97
16	P	371	PRO	CA-N-CD	-6.68	102.64	112.00
20	U	151	LYS	N-CA-C	6.68	119.13	111.11
37	l	86	ARG	N-CA-C	-6.68	99.64	110.20
21	V	8	THR	N-CA-C	6.68	119.01	108.79
22	W	105	HIS	N-CA-C	-6.68	104.95	113.23
15	O	224	PRO	CA-N-CD	6.67	121.34	112.00
20	U	140	CYS	CA-C-N	-6.67	114.03	120.83
20	U	140	CYS	C-N-CA	-6.67	114.03	120.83
14	N	228	ASN	N-CA-CB	6.67	119.68	110.01
13	M	410	MET	N-CA-C	-6.66	103.94	111.07
20	T	141	PRO	N-CA-CB	6.66	110.66	103.33
21	V	114	TRP	N-CA-CB	6.66	120.22	110.30
7	G	601	GLY	N-CA-C	6.66	124.89	115.30
12	L	499	LEU	N-CA-C	-6.66	103.71	110.97
11	K	76	ALA	N-CA-C	-6.64	104.12	111.36
15	O	315	PRO	N-CA-CB	-6.64	96.02	103.33
23	X	129	THR	N-CA-C	6.64	120.86	110.17
3	C	125	PHE	N-CA-CB	-6.64	100.61	110.17
7	G	640	ASP	N-CA-CB	6.64	119.98	110.16
16	P	116	ILE	N-CA-C	-6.64	104.02	110.72
13	M	143	LEU	N-CA-C	-6.62	103.98	111.07
8	H	93	HIS	CB-CA-C	6.62	117.83	108.76
23	X	97	PHE	N-CA-C	6.62	118.58	111.36
6	F	344	GLN	N-CA-C	-6.62	103.99	111.07
14	N	323	ASN	N-CA-C	6.62	119.35	110.35
21	V	86	LYS	N-CA-CB	6.62	119.66	110.07
20	U	98	LEU	N-CA-C	-6.60	100.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
7	G	287	SER	N-CA-C	6.60	119.24	110.53
4	D	184	ILE	N-CA-C	-6.59	103.90	110.62
19	S	40	ARG	N-CA-C	6.59	122.83	113.02
13	M	303	ILE	N-CA-C	-6.58	104.07	110.72
48	Ad	165	PHE	N-CA-C	-6.58	99.26	108.54
5	E	166	LYS	CB-CA-C	6.58	123.47	110.65
8	H	182	ALA	N-CA-C	-6.57	104.04	111.07
36	k	57	TRP	N-CA-C	-6.57	104.52	112.54
6	F	336	LEU	N-CA-CB	-6.57	100.99	111.43
15	O	140	LEU	N-CA-C	-6.56	104.05	111.07
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
38	m	51	TYR	N-CA-C	-6.56	105.58	113.97
6	F	234	GLY	CA-C-N	-6.55	111.72	120.50
6	F	234	GLY	C-N-CA	-6.55	111.72	120.50
17	Q	141	ASN	N-CA-CB	6.55	120.74	110.46
12	L	130	ILE	N-CA-C	-6.54	103.94	110.62
14	N	173	THR	N-CA-C	-6.54	105.02	114.12
12	L	232	TRP	N-CA-C	6.54	120.52	112.54
46	AB	305	THR	N-CA-CB	-6.54	100.36	109.91
39	n	115	TYR	N-CA-CB	6.53	122.00	110.37
41	p	54	ARG	N-CA-C	-6.52	103.67	111.69
7	G	605	GLN	N-CA-C	6.52	119.15	108.52
8	H	223	PHE	N-CA-C	-6.51	104.10	111.07
13	M	161	LEU	N-CA-C	-6.50	104.12	111.07
19	S	16	LEU	N-CA-C	-6.50	98.31	108.90
23	X	152	PRO	CA-N-CD	6.50	121.10	112.00
8	H	267	SER	N-CA-C	-6.49	104.28	111.36
15	O	118	TYR	N-CA-CB	-6.49	100.59	110.01
7	G	275	PRO	CB-CA-C	-6.49	102.48	110.98
48	AD	162	GLY	N-CA-C	-6.49	102.08	113.76
23	X	81	PRO	N-CA-C	-6.49	104.19	113.47
20	T	141	PRO	CA-N-CD	-6.48	102.92	112.00
14	N	315	THR	N-CA-C	-6.47	104.22	111.28
23	X	98	ARG	N-CA-C	6.47	120.44	112.54
4	D	388	GLY	N-CA-C	6.47	119.57	110.38
12	L	423	SER	N-CA-C	-6.47	104.14	111.07
16	P	137	ARG	N-CA-C	6.46	122.04	111.37
42	q	75	TRP	N-CA-C	6.46	121.43	112.45
20	U	153	ASP	N-CA-CB	-6.46	101.54	111.74
12	L	329	ILE	N-CA-C	-6.46	104.22	110.42
18	R	81	GLY	N-CA-C	-6.46	106.82	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	49	GLU	N-CA-C	-6.45	104.25	111.28
7	G	250	SER	N-CA-C	6.45	116.78	108.34
24	Y	96	GLY	N-CA-C	-6.44	104.53	112.77
8	H	255	TYR	N-CA-CB	6.44	119.35	110.01
15	O	320	GLY	N-CA-C	-6.43	96.63	111.04
3	C	125	PHE	N-CA-C	6.43	119.57	110.50
45	AA	215	ASP	N-CA-C	-6.43	103.96	110.97
8	H	177	PRO	N-CA-C	-6.43	101.56	111.13
23	X	168	PHE	CB-CA-C	-6.42	101.91	109.80
43	r	24	LEU	N-CA-C	6.42	119.55	110.50
45	Aa	215	ASP	N-CA-C	-6.42	103.98	110.97
14	N	145	ILE	N-CA-C	-6.41	106.20	111.91
6	F	178	GLU	N-CA-CB	6.41	119.49	109.94
13	M	455	THR	N-CA-CB	6.41	119.46	110.04
4	D	140	ASP	N-CA-C	-6.40	96.54	107.23
7	G	273	ILE	N-CA-C	-6.40	98.29	107.77
7	G	275	PRO	CA-N-CD	6.40	120.97	112.00
18	R	43	TYR	N-CA-C	-6.40	99.80	109.79
9	I	66	LEU	N-CA-C	-6.40	104.39	111.36
12	L	325	ALA	N-CA-C	-6.40	104.31	111.28
6	F	370	LEU	N-CA-C	-6.39	104.39	111.36
11	K	11	ALA	N-CA-C	-6.38	104.24	111.07
8	H	271	LEU	N-CA-CB	6.38	119.32	110.07
12	L	234	PRO	CA-N-CD	-6.38	103.07	112.00
9	I	205	ILE	N-CA-C	-6.37	104.29	110.72
47	AC	17	SER	N-CA-C	6.37	122.00	113.72
7	G	95	PRO	N-CA-C	-6.37	101.19	110.80
32	g	112	MET	N-CA-C	6.36	120.82	113.38
12	L	70	THR	N-CA-C	-6.36	103.87	111.69
17	Q	59	LEU	N-CA-C	-6.35	100.77	110.30
12	L	387	THR	N-CA-C	6.35	119.01	111.71
29	d	15	PRO	CA-N-CD	6.34	120.88	112.00
13	M	32	PHE	N-CA-C	-6.34	104.29	111.07
6	F	144	VAL	N-CA-CB	6.33	118.68	110.57
12	L	439	PRO	N-CA-C	6.33	122.33	113.53
34	i	32	GLU	CA-C-N	-6.33	111.92	119.84
34	i	32	GLU	C-N-CA	-6.33	111.92	119.84
15	O	98	THR	N-CA-C	6.33	120.59	109.96
7	G	176	CYS	N-CA-C	6.32	119.64	110.42
13	M	26	ASN	N-CA-CB	6.31	119.22	110.07
12	L	490	ALA	N-CA-C	-6.30	104.32	111.07
43	r	8	ILE	N-CA-C	-6.29	104.36	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	337	ALA	N-CA-C	-6.29	104.42	111.28
21	V	71	LEU	N-CA-C	6.29	118.13	111.28
14	N	89	GLN	N-CA-C	6.29	120.51	112.34
26	a	26	ILE	N-CA-C	-6.29	104.52	113.07
42	q	28	PHE	N-CA-C	6.28	117.79	111.07
23	X	99	HIS	N-CA-CB	6.28	119.46	110.16
38	m	17	THR	N-CA-C	-6.28	102.24	110.53
5	E	64	ALA	N-CA-CB	6.28	119.29	109.94
37	l	105	ILE	CA-C-O	-6.27	115.13	121.59
28	c	47	SER	N-CA-CB	6.27	120.87	110.33
1	A	101	GLY	N-CA-C	-6.27	105.23	112.50
7	G	356	ASP	N-CA-CB	6.27	119.34	110.12
6	F	415	ILE	N-CA-C	-6.27	104.39	110.72
13	M	317	ILE	N-CA-C	-6.27	104.64	110.53
21	V	91	ALA	N-CA-C	-6.26	104.46	111.28
31	f	52	GLU	N-CA-CB	6.26	121.10	110.71
4	D	141	TYR	N-CA-C	6.25	120.91	113.16
52	Ah	53	ASN	N-CA-C	6.25	118.09	111.28
2	B	113	ASP	N-CA-CB	6.25	119.52	109.28
6	F	255	CYS	N-CA-C	-6.24	104.55	111.36
10	J	126	TYR	N-CA-C	6.24	119.02	111.40
42	q	69	ASN	N-CA-CB	6.24	121.39	111.66
14	N	46	ASN	N-CA-C	-6.23	105.70	113.55
45	Aa	398	ALA	N-CA-C	-6.23	104.84	112.88
6	F	101	PHE	N-CA-C	6.23	118.87	111.33
5	E	50	THR	N-CA-CB	6.22	121.45	110.37
32	g	123	LEU	N-CA-CB	6.22	119.09	110.07
7	G	383	SER	N-CA-C	-6.22	106.91	114.75
8	H	269	THR	N-CA-C	6.22	118.06	111.28
16	P	139	PHE	N-CA-CB	6.22	121.72	110.95
15	O	113	SER	N-CA-C	6.22	118.55	108.41
8	H	52	ALA	N-CA-CB	6.22	119.03	110.01
17	Q	141	ASN	N-CA-C	-6.21	105.71	113.28
20	U	137	LYS	CA-C-N	-6.21	113.66	122.41
20	U	137	LYS	C-N-CA	-6.21	113.66	122.41
12	L	502	LEU	N-CA-C	-6.20	104.52	111.28
6	F	192	ASP	N-CA-C	6.20	119.05	109.07
23	X	36	CYS	CB-CA-C	-6.20	97.25	110.76
20	U	105	MET	N-CA-C	6.20	119.31	111.69
8	H	76	THR	N-CA-C	-6.20	104.53	111.28
14	N	216	PHE	N-CA-C	6.19	118.11	111.36
14	N	276	LEU	N-CA-C	-6.19	105.37	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	451	ILE	N-CA-C	-6.18	104.96	113.00
19	S	28	PRO	N-CA-CB	-6.18	96.71	103.39
14	N	91	ASN	N-CA-CB	6.18	119.06	109.97
36	k	59	TYR	N-CA-C	6.18	120.66	113.18
43	r	26	LEU	N-CA-CB	-6.18	101.15	110.35
16	P	368	GLU	N-CA-CB	6.17	119.81	110.30
6	F	409	ILE	N-CA-C	6.17	116.34	110.42
16	P	118	LYS	N-CA-C	6.17	118.98	111.82
6	F	212	LEU	N-CA-C	-6.17	104.56	111.28
38	m	72	ARG	CA-C-O	6.17	125.92	119.14
40	o	110	GLN	N-CA-C	-6.17	104.64	111.36
7	G	418	ILE	N-CA-C	-6.16	103.42	112.04
12	L	98	TRP	N-CA-C	-6.14	104.67	111.36
33	h	101	ILE	N-CA-CB	6.14	115.79	110.08
25	Z	44	ILE	N-CA-C	-6.13	104.77	110.53
19	S	40	ARG	N-CA-CB	-6.13	101.09	111.27
4	D	291	VAL	N-CA-C	-6.13	103.43	111.09
31	f	49	ARG	N-CA-CB	6.13	119.06	110.11
39	n	63	LEU	N-CA-C	-6.13	104.15	111.69
48	AD	151	GLU	N-CA-C	-6.12	104.16	111.69
14	N	47	LYS	N-CA-C	-6.12	104.72	111.82
7	G	325	ARG	N-CA-CB	6.12	118.85	109.91
4	D	57	GLU	N-CA-CB	-6.12	102.84	112.08
36	k	30	ILE	N-CA-C	6.12	118.74	111.09
7	G	420	LYS	N-CA-C	6.12	118.73	111.33
12	L	361	ASN	CB-CA-C	-6.12	102.87	111.80
13	M	4	ILE	N-CA-C	-6.12	104.00	112.50
40	o	105	GLU	N-CA-C	-6.12	104.69	111.36
13	M	121	LEU	N-CA-C	-6.10	104.71	111.36
15	O	210	PRO	N-CA-CB	-6.10	97.66	103.39
7	G	508	ALA	N-CA-C	6.09	117.92	111.28
12	L	287	PHE	N-CA-CB	6.09	118.85	110.01
14	N	91	ASN	N-CA-C	-6.09	101.26	110.28
28	c	33	GLU	CA-C-N	-6.09	114.00	120.03
28	c	33	GLU	C-N-CA	-6.09	114.00	120.03
8	H	276	SER	N-CA-C	6.09	118.89	111.82
31	f	39	ASN	N-CA-C	-6.08	104.02	112.30
32	g	109	ASP	CA-CB-CG	6.07	118.67	112.60
13	M	57	SER	N-CA-C	6.06	119.08	109.50
40	o	116	ALA	N-CA-C	6.06	118.66	111.33
19	S	87	VAL	N-CA-C	-6.06	104.44	110.62
32	g	123	LEU	N-CA-C	-6.06	104.60	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	h	142	ILE	N-CA-C	-6.04	104.62	110.42
8	H	103	LEU	N-CA-C	-6.04	104.78	111.36
12	L	140	LEU	N-CA-C	-6.04	104.70	111.28
12	L	454	ILE	N-CA-C	-6.03	104.47	110.62
16	P	370	LYS	N-CA-C	6.03	119.26	108.47
8	H	185	TRP	N-CA-C	-6.03	104.07	112.45
13	M	3	LYS	N-CA-C	-6.03	106.06	113.41
13	M	213	HIS	N-CA-C	6.03	120.49	113.20
42	q	137	TRP	N-CA-C	-6.02	100.93	109.96
32	g	78	PRO	N-CA-C	6.02	121.90	113.53
13	M	396	MET	N-CA-C	-6.02	105.92	113.20
8	H	7	LEU	N-CA-C	-6.01	104.35	111.03
8	H	24	GLU	N-CA-C	-6.01	104.09	112.45
15	O	234	LEU	N-CA-C	-6.01	104.81	111.36
12	L	234	PRO	N-CA-CB	6.01	109.66	103.23
28	c	47	SER	N-CA-C	-6.01	104.69	112.68
43	r	108	LYS	N-CA-C	6.01	117.91	111.36
51	AG	31	PHE	N-CA-C	-6.01	105.99	113.38
12	L	102	GLN	N-CA-C	-6.00	104.81	111.36
14	N	295	ARG	N-CA-C	-6.00	104.73	111.28
19	S	61	VAL	N-CA-C	-6.00	99.60	107.88
7	G	353	ALA	N-CA-C	-6.00	104.67	112.23
7	G	532	PRO	N-CA-CB	-6.00	97.08	103.38
51	Ag	31	PHE	N-CA-C	-6.00	105.96	113.28
8	H	203	GLY	N-CA-C	-5.99	103.92	112.55
15	O	183	CYS	N-CA-CB	5.99	118.87	109.94
13	M	370	PRO	CA-N-CD	5.98	120.38	112.00
13	M	88	ASN	N-CA-C	5.98	120.20	113.02
13	M	222	GLU	N-CA-C	5.98	120.42	113.18
2	B	196	PRO	N-CA-C	-5.98	101.82	111.03
41	p	127	LYS	N-CA-C	-5.97	104.12	111.40
13	M	300	SER	N-CA-C	-5.96	106.99	114.56
7	G	638	THR	N-CA-C	-5.96	100.24	109.24
5	E	66	VAL	N-CA-C	5.96	116.62	110.36
6	F	291	GLU	N-CA-C	5.95	118.23	110.43
41	p	8	ASP	N-CA-C	5.95	120.61	113.23
9	I	116	CYS	N-CA-C	-5.94	105.52	112.89
46	AB	244	LEU	N-CA-C	-5.94	106.03	113.28
15	O	181	LYS	N-CA-C	5.94	117.43	111.07
14	N	98	THR	N-CA-C	-5.94	104.81	111.28
7	G	387	LEU	CB-CA-C	-5.93	101.72	111.68
23	X	40	ASN	N-CA-C	-5.93	104.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	234	ILE	N-CA-CB	-5.92	104.90	111.41
14	N	140	SER	N-CA-C	-5.91	104.92	111.36
31	f	53	GLU	N-CA-CB	-5.91	101.39	110.20
12	L	112	PRO	CB-CA-C	-5.91	103.05	111.68
12	L	278	LEU	N-CA-CB	5.91	118.64	110.07
42	q	5	GLU	N-CA-C	-5.91	104.92	111.36
13	M	253	LEU	N-CA-C	5.90	117.71	111.28
12	L	248	HIS	CB-CA-C	5.90	120.88	110.85
12	L	247	LEU	N-CA-CB	5.90	120.60	110.34
4	D	352	PRO	N-CA-CB	-5.89	97.36	103.08
12	L	88	LEU	N-CA-CB	5.89	118.61	110.07
10	J	155	ALA	N-CA-C	-5.89	104.94	111.36
36	k	80	GLY	N-CA-C	-5.89	105.67	112.50
14	N	66	ALA	N-CA-C	-5.88	104.95	111.36
15	O	130	ARG	N-CA-C	-5.88	104.87	111.28
20	U	143	GLU	N-CA-C	-5.88	104.23	111.75
14	N	16	GLY	CA-C-N	-5.87	112.45	118.85
14	N	16	GLY	C-N-CA	-5.87	112.45	118.85
1	A	58	VAL	CB-CA-C	-5.87	104.19	111.70
12	L	387	THR	CB-CA-C	-5.87	99.77	110.63
49	AI	60	ALA	N-CA-CB	-5.87	101.94	111.22
4	D	58	THR	N-CA-C	-5.87	105.88	114.39
20	T	94	ASP	N-CA-CB	-5.87	105.14	111.66
38	m	116	ILE	N-CA-C	-5.87	104.79	110.42
3	C	71	TYR	N-CA-C	5.86	120.23	113.38
15	O	221	LYS	N-CA-C	-5.85	101.75	110.23
6	F	127	ASP	N-CA-C	5.84	118.43	111.71
7	G	480	ALA	N-CA-C	-5.84	104.99	111.36
3	C	209	LEU	N-CA-CB	-5.84	100.66	110.83
15	O	222	GLY	N-CA-C	5.84	120.25	112.77
19	S	86	GLU	N-CA-CB	5.84	118.80	110.16
20	U	153	ASP	CB-CA-C	5.83	120.63	112.11
39	n	27	LEU	N-CA-C	-5.83	106.14	113.72
4	D	258	VAL	N-CA-C	-5.83	103.98	110.62
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
36	k	50	PRO	N-CA-C	5.83	121.63	113.53
45	Aa	59	VAL	CB-CA-C	-5.83	106.04	112.68
47	AC	17	SER	N-CA-CB	-5.82	102.09	110.65
7	G	289	LYS	N-CA-C	5.82	117.62	111.28
8	H	116	ILE	N-CA-C	-5.82	104.83	110.42
15	O	217	ARG	N-CA-CB	5.82	118.45	110.01
31	f	52	GLU	N-CA-C	-5.82	98.01	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	k	82	ALA	N-CA-C	-5.82	104.94	111.28
15	O	262	GLU	N-CA-C	-5.82	104.94	111.28
21	V	19	THR	N-CA-CB	5.82	120.72	110.37
42	q	65	THR	N-CA-C	5.82	119.15	110.14
8	H	315	PRO	O-C-N	5.81	123.88	121.15
16	P	367	GLU	CB-CA-C	-5.81	99.51	110.67
7	G	672	ALA	N-CA-C	-5.81	104.95	111.28
8	H	211	PHE	CA-C-O	5.80	126.97	119.95
16	P	157	LYS	N-CA-CB	5.80	118.75	110.16
13	M	272	THR	N-CA-C	-5.80	105.04	111.36
7	G	34	VAL	N-CA-C	5.79	116.22	108.11
12	L	428	TYR	N-CA-C	-5.79	104.88	111.14
29	d	62	LEU	N-CA-C	5.79	117.59	111.28
16	P	122	HIS	N-CA-C	5.79	120.03	112.92
39	n	52	LYS	N-CA-C	-5.78	105.89	113.12
17	Q	164	PHE	N-CA-CB	5.78	119.78	110.42
37	l	186	ILE	N-CA-CB	-5.78	101.68	111.50
26	a	3	PHE	N-CA-CB	5.77	118.72	110.06
18	R	45	ARG	N-CA-C	-5.77	104.96	113.61
6	F	102	MET	CB-CA-C	-5.77	101.43	110.94
4	D	414	ASP	N-CA-C	-5.76	101.42	110.36
6	F	299	LEU	N-CA-C	5.76	118.51	111.82
20	U	83	VAL	N-CA-C	-5.76	104.90	110.72
25	Z	72	MET	CA-C-N	-5.76	113.25	119.24
25	Z	72	MET	C-N-CA	-5.76	113.25	119.24
16	P	234	LYS	CB-CA-C	-5.76	103.39	111.80
12	L	23	MET	N-CA-CB	5.76	118.36	110.01
14	N	15	LEU	N-CA-C	-5.75	105.76	112.89
29	d	53	VAL	N-CA-C	5.75	116.40	110.36
35	j	73	PHE	N-CA-C	-5.75	104.92	111.07
10	J	76	GLU	N-CA-C	-5.74	105.61	113.30
12	L	467	VAL	N-CA-CB	-5.74	103.84	110.55
12	L	495	VAL	N-CA-C	5.74	115.93	110.42
40	o	71	ARG	N-CA-C	-5.73	104.41	111.40
7	G	275	PRO	N-CA-CB	-5.73	98.00	103.33
13	M	124	ALA	N-CA-C	-5.73	105.12	111.36
32	g	78	PRO	N-CA-CB	-5.73	97.03	103.33
6	F	393	ASN	N-CA-C	-5.73	104.94	111.07
12	L	177	ILE	N-CA-C	-5.72	104.78	110.62
13	M	19	SER	N-CA-C	5.72	117.80	109.84
19	S	73	GLN	N-CA-C	-5.72	100.38	109.59
46	Ab	308	LEU	N-CA-C	-5.72	104.41	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	126	LYS	N-CA-C	5.72	117.51	111.28
12	L	605	ASN	N-CA-C	-5.72	106.16	113.02
2	B	135	GLY	CA-C-O	-5.71	118.01	122.52
23	X	79	ALA	N-CA-C	5.71	117.18	111.07
5	E	119	THR	N-CA-C	-5.71	105.81	112.89
32	g	67	LYS	N-CA-C	-5.71	102.01	110.46
29	d	4	GLY	N-CA-C	-5.70	108.18	115.42
42	q	140	PRO	N-CA-C	-5.70	102.19	110.80
8	H	252	PRO	N-CA-CB	-5.70	98.04	103.51
13	M	424	ILE	O-C-N	5.69	128.31	122.79
1	A	55	PHE	N-CA-CB	5.69	118.26	110.01
13	M	279	GLN	N-CA-C	-5.69	98.62	108.69
31	f	36	ALA	N-CA-C	-5.69	103.41	110.41
16	P	272	LEU	N-CA-C	-5.68	101.87	110.28
6	F	41	ILE	N-CA-C	5.68	115.76	110.42
14	N	232	LEU	N-CA-C	-5.68	106.57	112.93
45	Aa	275	ILE	N-CA-C	-5.68	100.49	108.27
10	J	107	ASN	N-CA-C	-5.68	105.23	111.82
51	Ag	49	VAL	CB-CA-C	-5.68	106.05	111.44
12	L	371	SER	N-CA-C	-5.67	105.02	111.14
12	L	419	THR	N-CA-C	-5.67	105.10	111.28
45	Aa	265	LEU	N-CA-C	5.67	118.46	109.50
34	i	5	THR	N-CA-CB	5.66	118.07	109.75
34	i	14	GLN	N-CA-CB	-5.66	101.81	110.12
14	N	148	LEU	N-CA-C	5.65	117.52	111.36
38	m	104	VAL	N-CA-C	-5.65	105.59	111.58
34	i	84	TYR	N-CA-C	-5.65	105.12	111.28
7	G	59	GLN	N-CA-C	5.65	117.98	107.99
23	X	65	GLY	N-CA-C	-5.65	105.95	112.50
13	M	214	LEU	N-CA-C	-5.64	105.65	112.54
16	P	119	ALA	N-CA-C	-5.64	105.04	111.14
37	l	49	ALA	N-CA-C	-5.64	106.56	113.50
37	l	119	THR	N-CA-C	-5.64	95.76	107.67
6	F	457	HIS	N-CA-CB	-5.64	100.91	110.50
15	O	214	VAL	N-CA-CB	5.64	119.05	110.58
7	G	599	THR	CA-C-N	-5.63	114.16	122.83
7	G	599	THR	C-N-CA	-5.63	114.16	122.83
12	L	342	CYS	N-CA-CB	5.63	118.18	110.01
12	L	151	SER	N-CA-CB	5.63	118.49	110.16
6	F	416	SER	N-CA-C	5.62	117.86	111.11
38	m	60	ILE	N-CA-C	-5.62	101.94	109.30
6	F	304	ALA	CB-CA-C	-5.62	110.08	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	124	MET	CA-C-N	-5.61	115.01	122.98
17	Q	124	MET	C-N-CA	-5.61	115.01	122.98
2	B	112	TYR	N-CA-C	5.61	122.74	110.80
12	L	20	LEU	N-CA-C	5.61	119.84	112.89
32	g	122	ARG	N-CA-C	5.60	118.32	111.82
6	F	176	ALA	N-CA-C	5.60	118.11	111.33
5	E	222	PHE	CB-CA-C	-5.60	100.62	109.80
12	L	234	PRO	N-CA-C	-5.60	105.47	113.47
23	X	56	CYS	N-CA-C	5.60	119.80	112.92
32	g	107	VAL	N-CA-C	-5.59	102.86	108.96
4	D	352	PRO	N-CA-C	5.59	117.52	110.70
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
41	p	115	GLN	N-CA-CB	5.59	118.03	110.59
12	L	214	MET	N-CA-C	-5.59	105.27	111.36
19	S	63	PRO	CA-N-CD	5.59	119.82	112.00
7	G	530	TYR	N-CA-C	-5.58	102.02	110.28
14	N	192	ALA	N-CA-C	-5.58	105.20	111.28
32	g	113	GLN	CA-C-O	5.58	126.25	119.11
12	L	445	GLU	CB-CA-C	-5.58	101.98	111.02
7	G	615	LEU	N-CA-C	-5.58	106.25	113.16
18	R	89	PRO	N-CA-CB	-5.57	98.25	103.27
42	q	142	THR	N-CA-CB	5.57	119.87	109.68
2	B	71	ALA	N-CA-CB	-5.57	101.34	110.14
45	Aa	409	VAL	N-CA-C	-5.57	105.10	110.72
14	N	251	LEU	N-CA-C	-5.56	105.22	111.28
5	E	183	PRO	N-CA-C	-5.56	102.20	111.26
32	g	140	PHE	N-CA-CB	5.56	118.27	109.71
4	D	163	PRO	N-CA-CB	-5.55	97.69	103.08
20	U	154	VAL	CB-CA-C	-5.55	104.20	111.81
12	L	155	ILE	N-CA-C	-5.55	105.31	110.53
14	N	36	SER	N-CA-C	-5.55	105.23	111.28
23	X	54	ARG	CB-CA-C	5.55	119.50	110.96
2	B	201	LEU	N-CA-C	-5.54	105.14	111.07
41	p	120	ASN	N-CA-C	-5.54	105.14	113.89
38	m	46	GLU	N-CA-C	-5.53	106.53	113.72
7	G	127	ASP	CA-C-O	5.53	129.02	121.89
16	P	130	ILE	N-CA-C	5.53	115.22	107.37
2	B	120	VAL	CA-C-N	-5.53	113.36	120.65
2	B	120	VAL	C-N-CA	-5.53	113.36	120.65
6	F	294	VAL	CA-C-N	-5.53	114.07	119.76
6	F	294	VAL	C-N-CA	-5.53	114.07	119.76
42	q	68	MET	N-CA-C	5.52	119.28	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	q	71	LYS	N-CA-C	5.51	120.00	113.16
12	L	394	LEU	N-CA-CB	5.51	118.00	110.01
13	M	355	MET	N-CA-C	-5.51	104.66	111.33
12	L	465	GLY	N-CA-C	-5.51	105.72	112.77
14	N	123	PRO	CA-N-CD	5.50	119.71	112.00
20	T	135	ALA	N-CA-CB	5.50	118.21	110.12
41	p	94	ARG	N-CA-C	5.50	116.96	111.07
6	F	118	ASP	N-CA-C	-5.50	102.14	110.28
3	C	71	TYR	CB-CA-C	-5.50	102.27	111.23
12	L	370	SER	N-CA-C	-5.50	105.37	111.36
13	M	223	ALA	N-CA-CB	5.50	118.13	110.11
7	G	313	LEU	N-CA-C	5.49	118.51	109.72
12	L	152	PHE	N-CA-C	-5.49	105.19	111.07
13	M	370	PRO	N-CA-CB	-5.49	97.75	103.08
28	c	64	GLU	N-CA-CB	5.49	117.97	110.01
7	G	363	SER	N-CA-C	-5.49	100.23	109.07
13	M	234	ILE	N-CA-C	5.49	116.28	111.56
26	a	25	TYR	N-CA-C	-5.49	107.84	114.75
45	AA	255	ARG	N-CA-C	5.48	118.21	107.57
13	M	73	LEU	N-CA-C	-5.48	105.30	112.75
8	H	141	SER	N-CA-CB	5.47	117.94	110.01
43	r	94	ALA	N-CA-C	-5.47	101.75	109.96
4	D	200	PHE	CA-CB-CG	5.46	119.26	113.80
7	G	404	GLY	N-CA-C	5.46	121.45	113.48
14	N	62	THR	N-CA-C	-5.46	105.23	111.07
12	L	543	ASN	N-CA-C	-5.46	105.33	111.28
16	P	86	CYS	N-CA-C	-5.46	103.18	110.55
4	D	132	ALA	N-CA-C	-5.45	106.63	113.72
12	L	194	ASN	CB-CA-C	-5.45	103.38	111.72
39	n	136	GLU	CB-CA-C	5.45	121.26	110.42
7	G	682	ASP	CA-C-N	-5.45	114.15	119.76
7	G	682	ASP	C-N-CA	-5.45	114.15	119.76
43	r	111	PRO	N-CA-C	-5.45	106.44	113.57
32	g	137	SER	N-CA-CB	-5.44	101.27	110.41
7	G	150	ARG	N-CA-CB	-5.44	102.81	111.62
12	L	550	LEU	CA-C-O	-5.43	115.19	120.89
13	M	174	LEU	N-CA-C	-5.42	106.45	112.57
16	P	357	ARG	N-CA-C	5.42	117.53	110.43
14	N	177	LYS	N-CA-C	-5.42	105.38	111.28
7	G	420	LYS	N-CA-CB	-5.42	101.94	110.06
40	o	74	PHE	CA-C-N	-5.41	114.04	119.56
40	o	74	PHE	C-N-CA	-5.41	114.04	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	21	ILE	N-CA-C	-5.41	105.25	110.72
53	Aj	52	LEU	N-CA-C	-5.41	100.09	108.42
12	L	183	ILE	N-CA-C	-5.41	105.10	110.62
15	O	175	ASN	N-CA-C	-5.41	105.39	111.28
23	X	27	ALA	N-CA-C	-5.41	105.04	111.69
16	P	374	THR	N-CA-C	5.40	117.53	108.73
32	g	80	VAL	N-CA-C	-5.40	105.24	110.42
3	C	81	ASP	N-CA-C	-5.40	104.45	111.74
34	i	77	ILE	CB-CA-C	-5.40	108.63	114.35
14	N	89	GLN	N-CA-CB	-5.39	100.47	110.18
18	R	88	HIS	CB-CA-C	5.39	117.33	109.08
23	X	169	PHE	N-CA-C	5.39	119.44	112.86
20	T	92	LYS	N-CA-C	-5.39	106.29	112.92
38	m	52	ASN	N-CA-C	-5.39	105.15	112.26
5	E	48	PRO	N-CA-C	5.38	120.84	113.84
47	Ac	17	SER	N-CA-CB	-5.38	102.01	110.46
12	L	311	GLY	N-CA-C	-5.38	106.28	112.73
14	N	143	ILE	N-CA-C	-5.38	105.29	110.72
14	N	155	LEU	N-CA-CB	5.38	117.81	110.01
10	J	133	VAL	N-CA-C	-5.37	107.89	113.10
35	j	64	LEU	N-CA-C	-5.37	105.51	111.36
13	M	409	TYR	N-CA-C	-5.37	105.59	111.82
19	S	24	CYS	N-CA-C	-5.37	103.30	110.55
19	S	41	TYR	N-CA-C	-5.37	105.51	111.36
25	Z	50	MET	N-CA-C	-5.37	105.43	111.28
46	AB	236	GLN	N-CA-C	-5.36	106.00	112.54
39	n	104	LEU	N-CA-C	-5.36	106.77	113.15
6	F	199	ARG	N-CA-C	5.36	117.47	109.59
13	M	53	SER	N-CA-C	5.36	115.61	108.38
49	Ae	89	SER	N-CA-C	5.35	118.60	111.75
12	L	415	ALA	N-CA-CB	5.35	117.99	110.12
17	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
7	G	510	TRP	N-CA-C	-5.35	101.94	109.96
10	J	99	GLU	N-CA-C	-5.35	105.45	111.28
12	L	386	LEU	N-CA-C	-5.35	101.00	108.96
4	D	201	PHE	N-CA-C	-5.34	105.54	111.36
5	E	219	SER	N-CA-C	-5.34	100.61	108.79
12	L	413	LEU	N-CA-C	5.34	117.10	111.28
13	M	25	THR	CB-CA-C	-5.34	100.41	110.67
13	M	117	MET	N-CA-CB	5.34	117.97	110.12
25	Z	55	GLN	N-CA-C	-5.34	105.46	111.28
12	L	137	MET	N-CA-C	5.34	119.41	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	391	VAL	CA-C-N	-5.33	115.82	119.66
4	D	391	VAL	C-N-CA	-5.33	115.82	119.66
17	Q	164	PHE	N-CA-C	-5.33	106.75	113.20
7	G	356	ASP	N-CA-C	-5.33	105.47	111.28
8	H	94	PRO	N-CA-C	5.33	118.68	111.22
4	D	93	GLY	N-CA-C	5.33	121.84	114.92
20	U	141	PRO	N-CA-C	-5.32	109.14	114.68
45	Aa	411	GLU	N-CA-C	5.32	117.77	111.33
12	L	231	PRO	CB-CA-C	-5.32	104.30	111.85
13	M	343	ILE	N-CA-C	5.32	116.04	110.62
49	AE	89	SER	N-CA-C	5.31	118.55	111.75
13	M	167	ILE	N-CA-C	5.31	117.69	111.05
4	D	141	TYR	N-CA-CB	-5.31	102.32	110.44
8	H	252	PRO	CA-N-CD	5.30	119.43	112.00
16	P	339	GLY	N-CA-C	5.30	122.64	115.00
12	L	494	SER	N-CA-C	-5.30	105.42	111.14
14	N	218	ALA	N-CA-CB	5.30	118.41	110.14
22	W	32	LYS	N-CA-C	-5.30	104.92	111.33
15	O	219	GLN	N-CA-C	5.30	117.47	111.11
48	AD	227	LEU	N-CA-CB	-5.29	102.17	110.69
52	AH	66	THR	N-CA-C	5.29	116.73	110.97
17	Q	72	ILE	N-CA-C	-5.28	108.36	113.53
15	O	264	GLU	N-CA-C	-5.28	107.20	113.38
9	I	54	THR	N-CA-C	-5.27	104.95	111.33
16	P	330	THR	N-CA-C	-5.27	106.75	114.39
9	I	160	GLU	N-CA-CB	-5.27	100.77	109.72
12	L	190	SER	N-CA-C	-5.27	106.70	113.23
15	O	206	TYR	N-CA-C	5.27	118.87	107.49
4	D	363	VAL	N-CA-C	5.26	116.34	111.81
39	n	26	HIS	N-CA-C	-5.26	106.44	112.92
22	W	122	LEU	N-CA-C	-5.26	105.54	111.28
14	N	154	ILE	CB-CA-C	-5.26	103.73	112.26
7	G	435	PRO	CB-CA-C	-5.26	105.83	111.56
5	E	48	PRO	CB-CA-C	-5.26	104.39	111.85
45	AA	56	GLY	N-CA-C	-5.25	107.28	114.64
8	H	46	LEU	N-CA-C	-5.25	106.65	113.16
22	W	120	ASP	N-CA-C	-5.25	102.51	110.28
32	g	68	ASN	N-CA-CB	5.25	119.02	111.51
6	F	300	ILE	N-CA-CB	5.25	119.32	110.56
13	M	294	MET	N-CA-C	-5.25	106.90	113.72
6	F	412	LEU	N-CA-C	-5.24	105.74	111.82
8	H	146	MET	N-CA-C	-5.24	105.46	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	133	ILE	CB-CA-C	-5.24	104.03	112.16
39	n	12	HIS	N-CA-C	-5.24	105.00	111.40
7	G	362	ASP	CA-CB-CG	5.24	117.84	112.60
14	N	155	LEU	N-CA-C	-5.24	105.46	111.07
16	P	260	GLY	N-CA-C	-5.24	108.39	115.36
14	N	326	PHE	N-CA-CB	5.23	117.60	110.01
14	N	104	MET	N-CA-C	-5.23	105.47	111.07
12	L	375	ILE	N-CA-CB	5.23	116.67	110.55
33	h	129	PRO	N-CA-C	-5.23	106.72	113.57
5	E	221	ARG	N-CA-C	5.23	117.81	110.23
7	G	449	PRO	N-CA-CB	5.22	109.03	103.39
8	H	310	PHE	N-CA-C	5.22	119.28	113.01
7	G	277	MET	N-CA-CB	-5.22	101.67	109.71
34	i	105	PHE	N-CA-CB	-5.22	101.05	110.39
13	M	212	VAL	CB-CA-C	-5.22	105.21	112.36
13	M	20	PRO	N-CA-C	-5.21	106.28	113.53
16	P	192	ARG	N-CA-C	-5.21	105.60	111.28
12	L	497	GLY	N-CA-C	-5.21	106.46	112.50
33	h	158	ARG	N-CA-C	-5.21	105.52	111.14
41	p	167	ARG	CB-CA-C	5.21	117.25	109.13
43	r	111	PRO	CA-N-CD	5.21	119.29	112.00
43	r	107	SER	N-CA-C	-5.20	102.16	109.96
7	G	713	ALA	N-CA-C	-5.20	105.51	111.07
43	r	25	GLN	N-CA-C	5.20	118.88	112.54
16	P	194	VAL	N-CA-CB	5.20	118.38	110.58
12	L	396	ILE	O-C-N	5.20	127.00	121.91
7	G	556	THR	N-CA-C	-5.19	101.52	109.41
16	P	137	ARG	CA-C-N	-5.19	114.93	122.86
16	P	137	ARG	C-N-CA	-5.19	114.93	122.86
46	Ab	295	ALA	N-CA-C	-5.19	105.63	112.94
3	C	164	TRP	N-CA-C	5.18	117.01	111.36
7	G	600	GLU	CB-CA-C	-5.18	103.03	111.06
13	M	317	ILE	N-CA-CB	5.18	117.20	110.57
12	L	332	HIS	N-CA-C	-5.18	105.64	111.28
13	M	98	MET	N-CA-C	-5.18	105.53	111.07
20	U	133	ILE	N-CA-C	5.18	117.52	111.05
19	S	85	ASP	N-CA-C	5.17	117.82	111.82
12	L	284	THR	N-CA-C	-5.17	105.73	111.36
12	L	485	PHE	N-CA-CB	5.17	117.50	110.01
37	l	37	LEU	N-CA-C	-5.17	102.64	110.50
14	N	90	THR	N-CA-C	5.17	117.58	110.35
35	j	76	ASP	CB-CA-C	-5.16	104.71	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	172	ILE	N-CA-C	-5.16	98.62	109.34
8	H	277	TYR	N-CA-C	5.16	117.99	110.10
14	N	225	MET	N-CA-C	-5.16	106.58	112.92
29	d	37	LEU	N-CA-C	-5.15	105.66	111.28
2	B	125	PRO	CB-CA-C	-5.15	104.82	112.55
8	H	196	ALA	CA-C-N	-5.15	113.49	119.47
8	H	196	ALA	C-N-CA	-5.15	113.49	119.47
12	L	217	LEU	N-CA-C	-5.15	105.67	111.28
14	N	222	ASN	N-CA-C	-5.15	106.23	112.88
1	A	106	TRP	CB-CA-C	-5.15	102.44	110.94
6	F	337	MET	CB-CA-C	-5.15	103.03	111.68
7	G	63	PHE	CA-C-O	-5.15	115.09	121.06
7	G	569	GLN	CB-CA-C	-5.15	104.23	112.05
21	V	84	ALA	N-CA-C	5.15	116.58	111.07
7	G	387	LEU	N-CA-C	-5.14	98.32	107.98
16	P	198	ALA	N-CA-C	-5.14	100.14	108.52
41	p	13	PRO	O-C-N	5.14	123.56	121.15
38	m	61	GLU	N-CA-C	5.14	119.63	112.90
33	h	176	LYS	N-CA-C	-5.13	105.86	111.82
8	H	101	GLY	N-CA-C	5.13	118.45	112.50
12	L	386	LEU	CA-C-O	-5.13	115.96	121.45
16	P	360	ARG	CA-C-O	-5.13	115.92	121.87
8	H	90	PRO	CA-C-O	-5.13	117.43	121.38
27	b	82	LYS	N-CA-C	-5.13	103.76	110.53
7	G	458	GLY	N-CA-C	-5.13	108.25	115.32
4	D	391	VAL	N-CA-C	5.12	113.79	109.02
45	Aa	354	LEU	N-CA-C	-5.12	102.18	110.32
40	o	95	TYR	N-CA-C	-5.12	105.59	111.07
22	W	115	THR	CA-C-N	-5.12	113.44	119.84
22	W	115	THR	C-N-CA	-5.12	113.44	119.84
48	Ad	88	GLU	N-CA-C	5.12	117.76	109.06
12	L	249	SER	N-CA-C	5.12	116.66	111.14
28	c	60	GLN	N-CA-C	-5.11	105.60	111.07
2	B	94	THR	N-CA-CB	-5.11	102.25	110.69
40	o	11	TRP	N-CA-C	5.11	116.08	108.31
31	f	55	THR	N-CA-C	5.10	116.53	110.97
6	F	60	GLY	N-CA-C	-5.10	106.01	114.48
38	m	47	TYR	N-CA-C	-5.10	105.89	112.68
3	C	156	VAL	N-CA-C	-5.10	104.13	111.17
8	H	214	GLU	N-CA-C	5.09	119.36	113.20
22	W	91	MET	N-CA-C	-5.09	105.91	111.82
41	p	43	TRP	CA-C-N	-5.09	113.67	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	p	43	TRP	C-N-CA	-5.09	113.67	118.97
16	P	356	HIS	N-CA-C	-5.09	105.86	111.71
7	G	203	ASP	CA-C-O	5.08	127.22	121.32
14	N	292	PHE	CA-CB-CG	5.08	118.88	113.80
5	E	181	ASN	N-CA-C	-5.08	99.51	108.20
37	l	168	LEU	N-CA-C	-5.08	105.65	111.14
5	E	222	PHE	N-CA-C	5.08	117.89	109.46
4	D	63	PRO	N-CA-C	5.08	116.90	110.70
9	I	95	PRO	N-CA-C	5.08	121.17	113.81
24	Y	72	PHE	N-CA-C	-5.08	105.64	111.07
13	M	56	PHE	N-CA-C	5.08	116.80	108.52
13	M	86	LYS	N-CA-C	-5.08	106.33	112.88
13	M	30	TYR	N-CA-C	5.07	116.81	111.28
13	M	330	ALA	N-CA-CB	5.07	117.43	110.07
34	i	11	ARG	N-CA-C	-5.07	105.45	111.69
16	P	376	ASN	CB-CA-C	-5.07	102.23	110.85
32	g	137	SER	N-CA-C	5.07	119.31	113.18
14	N	42	PRO	CB-CA-C	-5.07	105.01	113.06
20	T	140	CYS	CB-CA-C	-5.06	104.08	109.85
34	i	16	ARG	N-CA-C	-5.06	105.76	111.28
13	M	32	PHE	N-CA-CB	5.06	117.35	110.01
16	P	170	LEU	N-CA-C	5.05	117.05	110.43
14	N	282	MET	N-CA-C	-5.05	105.66	111.07
39	n	169	HIS	CB-CA-C	5.05	118.71	110.17
8	H	254	LEU	N-CA-CB	5.05	118.11	110.28
7	G	280	ASP	N-CA-CB	-5.05	102.70	110.12
7	G	393	GLY	N-CA-C	-5.05	107.79	115.66
20	U	132	ASP	N-CA-C	5.05	117.18	111.02
23	X	42	GLU	N-CA-C	-5.05	105.86	111.36
28	c	39	PRO	N-CA-C	5.04	119.12	111.15
2	B	127	GLN	N-CA-CB	-5.04	103.16	110.47
12	L	384	PRO	N-CA-CB	5.04	107.73	103.35
28	c	46	LEU	CA-C-O	5.04	125.18	119.18
37	l	45	PRO	N-CA-C	5.04	120.45	113.65
43	r	4	ALA	N-CA-C	-5.04	105.88	112.23
1	A	54	LYS	N-CA-CB	5.04	117.70	110.20
3	C	208	GLU	CA-C-O	-5.04	115.71	121.40
32	g	109	ASP	CB-CA-C	5.04	119.04	111.89
13	M	234	ILE	CB-CA-C	5.03	116.22	111.44
19	S	45	LYS	N-CA-C	-5.03	105.87	111.36
4	D	224	ALA	CA-C-O	-5.03	115.52	120.90
15	O	212	PRO	CA-N-CD	5.03	119.04	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AK	40	LEU	N-CA-C	-5.03	105.24	111.33
3	C	221	GLU	N-CA-C	-5.03	102.42	108.25
5	E	213	PRO	CB-CA-C	-5.03	106.31	112.89
23	X	110	CYS	CB-CA-C	-5.03	103.22	110.96
29	d	60	ARG	N-CA-C	-5.03	105.71	111.14
52	Ah	51	CYS	N-CA-C	-5.02	105.72	111.14
13	M	229	MET	N-CA-C	-5.02	105.70	111.07
5	E	75	ALA	N-CA-C	5.01	117.39	111.33
14	N	64	ALA	N-CA-C	5.01	116.43	111.07
32	g	124	VAL	N-CA-CB	5.01	118.09	110.58
12	L	212	PRO	CA-N-CD	5.01	119.01	112.00
18	R	65	ALA	N-CA-C	-5.01	105.95	111.71
33	h	161	ARG	N-CA-C	-5.01	105.51	110.97
11	K	48	SER	N-CA-CB	5.00	117.48	110.12
20	T	140	CYS	N-CA-C	5.00	116.65	109.04
4	D	106	VAL	O-C-N	-5.00	116.84	122.94
10	J	59	TYR	N-CA-C	-5.00	105.30	111.40
13	M	267	TRP	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	187	0
2	B	1258	0	1270	160	0
3	C	1641	0	1596	134	0
4	D	3415	0	3353	341	0
5	E	1635	0	1626	185	0
6	F	3288	0	3243	357	0
7	G	5287	0	5323	551	0
8	H	2510	0	2593	430	0
9	I	1398	0	1359	151	0
10	J	1205	0	1229	260	0
11	K	729	0	764	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4798	0	4986	623	0
13	M	3622	0	3845	543	0
14	N	2694	0	2896	399	0
15	O	2599	0	2552	266	0
16	P	2730	0	2747	233	0
17	Q	957	0	949	74	0
18	R	660	0	639	78	0
19	S	667	0	685	72	0
20	T	604	0	596	92	0
20	U	678	0	677	90	0
21	V	915	0	954	82	0
22	W	970	0	991	78	0
23	X	1385	0	1366	111	0
24	Y	1030	0	1015	82	0
25	Z	1152	0	1148	145	0
26	a	548	0	562	83	0
27	b	628	0	628	93	0
28	c	389	0	385	27	0
29	d	988	0	989	90	0
30	e	863	0	850	105	0
31	f	475	0	472	42	0
32	g	858	0	787	70	0
33	h	1146	0	1153	124	0
34	i	796	0	797	122	0
35	j	563	0	510	67	0
36	k	569	0	568	53	0
37	l	1328	0	1218	89	0
38	m	1054	0	1064	97	0
39	n	1541	0	1470	139	0
40	o	1027	0	1018	101	0
41	p	1438	0	1404	124	0
42	q	1004	0	962	83	0
43	r	418	0	434	44	0
44	s	115	0	113	14	0
45	AA	3128	0	3052	191	0
45	Aa	3225	0	3141	196	0
46	AB	3137	0	3143	138	0
46	Ab	3137	0	3143	154	0
47	AC	2988	0	3045	145	0
47	Ac	2988	0	3045	162	0
48	AD	1896	0	1846	155	0
48	Ad	1895	0	1844	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	AE	1427	0	1409	180	0
49	AI	345	0	364	44	0
49	Ae	1432	0	1412	239	0
50	AF	864	0	854	31	0
50	Af	864	0	854	34	0
51	AG	643	0	643	57	0
51	Ag	643	0	643	73	0
52	AH	535	0	518	27	0
52	Ah	544	0	529	39	0
53	AJ	332	0	324	29	0
53	Aj	392	0	388	43	0
54	AK	281	0	277	19	0
54	Ak	357	0	347	38	0
55	A	46	0	69	12	0
55	AC	35	0	44	12	0
55	AF	42	0	61	7	0
55	Ac	58	0	64	6	0
55	Ag	39	0	52	9	0
55	I	51	0	82	14	0
55	J	46	0	66	5	0
55	L	225	0	332	54	0
55	M	153	0	246	26	0
55	N	37	0	48	14	0
55	O	31	0	36	5	0
55	Y	40	0	54	20	0
55	b	46	0	69	16	0
56	B	8	0	0	6	0
56	F	8	0	0	10	0
56	G	16	0	0	5	0
56	I	16	0	0	16	0
57	B	18	0	18	13	0
58	B	35	0	44	7	0
58	I	47	0	71	9	0
58	J	42	0	58	8	0
59	E	4	0	0	5	0
59	G	4	0	0	4	0
60	F	31	0	19	1	0
61	H	35	0	43	4	0
62	AC	56	0	56	4	0
62	Aa	46	0	36	8	0
62	Ac	42	0	28	3	0
62	Ag	56	0	56	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	L	163	0	217	38	0
62	X	67	0	81	9	0
62	a	57	0	58	22	0
62	h	70	0	87	15	0
63	O	27	0	12	6	0
64	P	48	0	26	7	0
65	R	1	0	0	0	0
66	W	32	0	0	7	0
66	n	32	0	0	0	0
67	AC	86	0	60	7	0
67	Ac	86	0	60	9	0
68	AC	23	0	23	4	0
68	Ac	38	0	47	5	0
69	AC	28	0	31	14	0
69	Ac	28	0	31	12	0
70	AD	43	0	32	24	0
70	Ad	43	0	32	25	0
71	AD	36	0	45	13	0
71	Ad	36	0	45	19	0
All	All	97639	0	97960	7968	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 41.

All (7968) 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)
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.39
48:Ad:170:LYS:CD	49:Ae:151:LYS:HD2	1.57	1.33
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
11:K:66:PHE:HZ	14:N:35:PHE:CZ	1.49	1.29
12:L:358:LYS:HG3	39:n:80:TYR:CZ	1.66	1.29
15:O:168:VAL:HG21	15:O:241:TYR:CZ	1.66	1.29
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
49:Ae:152:ILE:HG23	49:Ae:272:VAL:CG2	1.64	1.25
8:H:111:LEU:CD2	10:J:60:LEU:HD11	1.68	1.23
49:Ae:152:ILE:CG2	49:Ae:273:VAL:H	1.53	1.22
55:AC:403:3PE:H2C1	51:AG:41:ARG:NH2	1.52	1.22
16:P:93:HIS:CD2	16:P:94:LEU:HD12	1.75	1.22
11:K:66:PHE:CZ	14:N:35:PHE:CZ	2.26	1.21
1:A:63:LEU:HD21	10:J:62:GLY:O	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:170:LYS:CD	49:Ae:151:LYS:CD	2.20	1.20
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.20
12:L:13:ILE:HD11	55:L:701:3PE:C2C	1.70	1.20
7:G:126:LEU:HD12	7:G:126:LEU:O	1.37	1.19
12:L:437:PHE:CE1	12:L:441:ILE:HG12	1.77	1.19
20:U:90:TYR:CE2	20:U:92:LYS:HB2	1.76	1.19
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.38	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
10:J:5:ILE:CG1	11:K:4:THR:HG21	1.72	1.19
10:J:126:TYR:O	25:Z:120:LEU:HD12	1.40	1.18
21:V:44:TYR:CE1	21:V:48:THR:HG21	1.77	1.18
14:N:200:LEU:HD21	14:N:265:ILE:HG12	1.24	1.18
45:Aa:402:HIS:CD2	45:Aa:403:LEU:CD1	2.27	1.18
33:h:183:PRO:O	33:h:184:LYS:HG2	1.44	1.17
48:Ad:170:LYS:HD2	49:Ae:151:LYS:CD	1.74	1.17
1:A:63:LEU:HD21	10:J:62:GLY:C	1.67	1.17
14:N:29:MET:HE2	14:N:141:ILE:HG12	1.23	1.17
14:N:143:ILE:O	14:N:146:TYR:HD2	1.25	1.16
13:M:369:LEU:HD23	13:M:371:PRO:HD2	1.18	1.16
16:P:156:SER:HB2	16:P:161:VAL:CG2	1.75	1.16
10:J:5:ILE:HG12	11:K:4:THR:HG21	1.23	1.16
12:L:141:PHE:CE2	13:M:375:LEU:HD21	1.81	1.15
49:Ae:152:ILE:CG2	49:Ae:272:VAL:CG2	2.22	1.15
4:D:47:PHE:HB3	14:N:227:ILE:HD11	1.20	1.15
6:F:392:MET:CE	6:F:419:ILE:HD12	1.76	1.15
45:Aa:402:HIS:CD2	45:Aa:403:LEU:HD12	1.81	1.14
12:L:247:LEU:CD1	12:L:248:HIS:CD2	2.30	1.14
45:Aa:68:THR:HG21	46:Ab:384:MET:CG	1.76	1.13
13:M:162:ILE:HG23	14:N:271:MET:HE3	1.30	1.13
3:C:149:LEU:HD11	22:W:80:ARG:NH2	1.64	1.13
12:L:358:LYS:CG	39:n:80:TYR:CZ	2.30	1.13
19:S:51:LEU:HD13	19:S:95:LEU:HD21	1.23	1.12
45:Aa:68:THR:HG21	46:Ab:384:MET:HG2	1.15	1.12
6:F:382:CYS:SG	56:F:502:SF4:FE3	1.38	1.12
9:I:123:CYS:SG	56:I:303:SF4:FE1	1.40	1.12
10:J:3:ASN:ND2	10:J:120:LEU:HB2	1.63	1.12
62:L:706:CDL:H522	24:Y:107:THR:CG2	1.78	1.12
12:L:437:PHE:HE1	12:L:441:ILE:HG12	0.96	1.12
14:N:215:MET:CE	14:N:248:LEU:HD21	1.79	1.12
6:F:392:MET:HE3	6:F:419:ILE:CD1	1.78	1.12
29:d:14:LEU:O	29:d:14:LEU:HD12	1.49	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:16:LEU:HD11	55:L:701:3PE:H2H1	1.30	1.11
20:U:90:TYR:OH	20:U:92:LYS:HD2	1.48	1.11
12:L:229:LEU:HD12	12:L:229:LEU:O	1.51	1.10
12:L:365:ILE:HD12	12:L:366:MET:HG3	1.32	1.10
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.10
20:U:105:MET:SD	20:U:139:MET:HE3	1.92	1.10
12:L:141:PHE:CE2	13:M:375:LEU:CD2	2.35	1.10
16:P:40:VAL:HG22	18:R:43:TYR:CE2	1.86	1.10
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.10
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
49:AI:78:PHE:CZ	46:Ab:168:ASN:ND2	2.21	1.09
12:L:121:LEU:HD22	12:L:246:LEU:HD21	1.33	1.09
6:F:379:CYS:SG	56:F:502:SF4:FE4	1.43	1.09
10:J:126:TYR:O	25:Z:120:LEU:CD1	2.00	1.09
12:L:13:ILE:HD11	55:L:701:3PE:H2C2	1.33	1.09
45:AA:402:HIS:CE1	45:AA:403:LEU:CD1	2.36	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
49:Ae:152:ILE:HG21	49:Ae:273:VAL:H	0.96	1.08
34:i:11:ARG:HH22	39:n:154:LEU:HB2	0.99	1.08
49:AE:204:ARG:HB3	49:AE:260:VAL:HG21	1.35	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.08
36:k:34:PRO:HG2	36:k:59:TYR:CE1	1.88	1.08
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.10	1.07
8:H:111:LEU:HD21	10:J:60:LEU:CD1	1.84	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
12:L:141:PHE:CE2	13:M:370:PRO:HG3	1.87	1.07
12:L:141:PHE:HE2	13:M:375:LEU:CD2	1.67	1.07
49:Ae:152:ILE:CG2	49:Ae:272:VAL:HG22	1.82	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
12:L:569:LEU:HB2	24:Y:115:MET:HE1	1.36	1.06
62:L:705:CDL:HA62	33:h:68:LEU:HD13	1.37	1.06
16:P:299:SER:HB3	16:P:316:LYS:HE3	1.37	1.06
46:AB:48:VAL:CG2	46:AB:219:ALA:HB2	1.85	1.06
20:T:138:LEU:HD12	20:T:138:LEU:O	1.55	1.06
9:I:152:CYS:SG	56:I:303:SF4:FE2	1.46	1.06
45:AA:402:HIS:CE1	45:AA:403:LEU:HD11	1.91	1.06
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.33	1.06
13:M:143:LEU:HD21	14:N:303:THR:CG2	1.86	1.06
51:Ag:11:ILE:HG21	51:Ag:14:VAL:HG21	1.36	1.06
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.06
12:L:16:LEU:HD23	12:L:126:ILE:HD13	1.30	1.06
19:S:79:LEU:HA	19:S:82:LEU:HD12	1.37	1.06
49:Ae:93:ARG:HD2	49:Ae:110:ARG:HD2	1.38	1.06
8:H:111:LEU:HD21	10:J:60:LEU:HD11	1.36	1.05
35:j:97:LEU:HB3	40:o:104:ARG:HB2	1.36	1.05
2:B:100:CYS:SG	56:B:301:SF4:FE4	1.48	1.05
3:C:98:PHE:HA	21:V:90:LEU:HD11	1.37	1.05
12:L:141:PHE:HE2	13:M:375:LEU:HD22	1.22	1.05
12:L:141:PHE:HB2	12:L:182:PHE:CE2	1.92	1.05
21:V:44:TYR:CE1	21:V:48:THR:CG2	2.39	1.05
12:L:550:LEU:HD12	13:M:275:ILE:HB	1.32	1.05
3:C:102:HIS:HE1	21:V:48:THR:HG22	1.20	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
15:O:227:MET:O	15:O:228:LYS:HG2	1.57	1.05
37:l:30:PHE:CZ	37:l:31:HIS:HE1	1.75	1.05
43:r:2:ALA:N	43:r:26:LEU:HD12	1.69	1.05
55:L:701:3PE:H122	34:i:89:HIS:ND1	1.71	1.04
49:Ae:204:ARG:HB3	49:Ae:260:VAL:HG21	1.35	1.04
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
1:A:101:GLY:HA3	10:J:163:ILE:CD1	1.87	1.04
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.04
14:N:233:LEU:HD23	14:N:241:LEU:HD12	1.36	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
10:J:121:GLY:O	25:Z:133:MET:SD	2.14	1.04
13:M:249:ILE:O	13:M:250:LEU:HG	1.58	1.04
51:AG:11:ILE:HG21	51:AG:14:VAL:HG21	1.36	1.04
4:D:279:THR:HG23	21:V:13:GLY:HA3	1.36	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	1.03
12:L:553:LEU:HD11	38:m:93:ALA:HB3	1.41	1.03
16:P:156:SER:HB2	16:P:161:VAL:HG22	1.34	1.03
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
10:J:5:ILE:HG13	11:K:4:THR:CG2	1.88	1.03
13:M:127:ILE:CD1	14:N:256:PRO:HG3	1.89	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
12:L:173:LEU:HD23	55:L:703:3PE:H321	1.39	1.03
49:Ae:261:PRO:HB2	49:Ae:273:VAL:HG11	1.40	1.03
12:L:131:LEU:HD12	12:L:140:LEU:HD12	1.36	1.02
15:O:168:VAL:HG21	15:O:241:TYR:CE1	1.92	1.02
47:Ac:98:VAL:HG22	67:Ac:403:HEM:HBC2	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:69:CYS:O	40:o:80:CYS:SG	2.17	1.02
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.41	1.02
6:F:199:ARG:HD3	44:s:80:PHE:CE2	1.95	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
7:G:611:THR:HG21	17:Q:105:GLU:HA	1.42	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
47:AC:98:VAL:HG22	67:AC:402:HEM:HBC2	1.40	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.01
6:F:300:ILE:HG23	6:F:305:GLY:O	1.58	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
62:L:706:CDL:H522	24:Y:107:THR:HG23	1.40	1.01
13:M:179:LEU:HB3	13:M:249:ILE:HD11	1.42	1.01
8:H:111:LEU:CD2	10:J:60:LEU:CD1	2.39	1.01
16:P:358:THR:HG22	16:P:359:TYR:N	1.72	1.01
46:AB:48:VAL:CG2	46:AB:219:ALA:CB	2.39	1.01
12:L:228:GLY:O	12:L:229:LEU:HG	1.61	1.01
5:E:179:CYS:SG	59:E:301:FES:FE2	1.50	1.01
12:L:222:GLY:HA2	12:L:229:LEU:HD11	1.40	1.01
55:M:502:3PE:H3A2	14:N:246:LEU:HD11	1.39	1.01
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
8:H:121:TRP:CH2	10:J:27:TYR:CE1	2.48	1.00
10:J:60:LEU:HD13	10:J:60:LEU:C	1.86	1.00
15:O:256:LEU:HD11	15:O:276:LEU:HD23	1.43	1.00
12:L:358:LYS:HG3	39:n:80:TYR:OH	1.61	1.00
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.38	1.00
13:M:172:GLY:O	13:M:173:THR:HG23	1.61	1.00
53:Aj:52:LEU:HD13	53:Aj:53:TRP:H	1.22	1.00
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
9:I:155:CYS:SG	56:I:303:SF4:FE4	1.51	1.00
42:q:66:THR:HG22	42:q:74:PHE:HB2	1.39	1.00
1:A:90:MET:HE2	10:J:152:MET:HB3	1.42	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
10:J:126:TYR:HA	25:Z:120:LEU:HD11	1.42	1.00
21:V:44:TYR:CZ	21:V:48:THR:HG21	1.97	1.00
21:V:72:LEU:HD11	21:V:80:VAL:HG21	1.40	1.00
15:O:209:VAL:HG12	15:O:260:SER:HB2	1.43	0.99
34:i:11:ARG:NH2	39:n:154:LEU:HB2	1.76	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
46:Ab:142:THR:HG21	46:Ab:237:PHE:HB3	1.44	0.99
13:M:196:TRP:CD1	13:M:250:LEU:HD13	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:5:TRP:HZ3	41:p:10:TYR:O	1.45	0.99
15:O:168:VAL:HG11	15:O:241:TYR:CD1	1.97	0.99
34:i:105:PHE:CD2	40:o:68:LYS:HA	1.97	0.99
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.99
10:J:5:ILE:CG1	11:K:4:THR:CG2	2.41	0.99
49:Ae:93:ARG:HD2	49:Ae:110:ARG:CD	1.93	0.99
14:N:143:ILE:O	14:N:146:TYR:CD2	2.15	0.99
14:N:164:MET:CE	55:Y:201:3PE:H271	1.93	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
8:H:121:TRP:CH2	10:J:27:TYR:HE1	1.81	0.98
49:Ae:156:LEU:H	49:Ae:269:ASP:HA	1.27	0.98
4:D:36:GLN:HE22	13:M:135:ARG:NH1	1.60	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
10:J:3:ASN:HD22	10:J:120:LEU:HB2	1.20	0.98
55:AC:403:3PE:H2C1	51:AG:41:ARG:CZ	1.91	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
14:N:179:MET:CG	14:N:216:PHE:HE1	1.75	0.98
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.98
49:Ae:152:ILE:CG2	49:Ae:272:VAL:HG23	1.90	0.98
12:L:141:PHE:HB2	12:L:182:PHE:HE2	1.27	0.98
13:M:173:THR:CG2	33:h:147:ALA:HB2	1.94	0.98
13:M:275:ILE:HD11	13:M:288:TYR:CG	1.98	0.98
14:N:307:THR:HB	15:O:319:ILE:CD1	1.94	0.98
3:C:168:GLU:CB	3:C:186:ILE:HD11	1.92	0.98
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.46	0.97
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.45	0.97
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.43	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
45:Aa:222:ARG:CZ	45:Aa:263:PRO:HG3	1.95	0.97
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.97
45:AA:470:ARG:HD3	47:AC:222:PRO:HG3	1.47	0.97
49:AE:123:VAL:HG13	53:AJ:29:ALA:HA	1.42	0.97
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.97
8:H:114:TYR:CZ	10:J:65:VAL:HG23	1.99	0.97
26:a:64:LYS:HE2	26:a:66:LEU:HD12	1.43	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
49:AI:43:LEU:HD13	46:Ab:164:VAL:HG23	1.45	0.97
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
10:J:9:SER:CB	11:K:7:ASN:HD22	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:174:TYR:HD2	12:L:232:TRP:CD1	1.82	0.96
12:L:511:LEU:HD21	36:k:38:VAL:HG22	1.47	0.96
12:L:13:ILE:HD11	55:L:701:3PE:H2C1	1.45	0.96
1:A:101:GLY:HA3	10:J:163:ILE:HD13	1.43	0.96
13:M:250:LEU:HD12	13:M:250:LEU:O	1.65	0.96
8:H:121:TRP:HZ2	10:J:78:TYR:CZ	1.83	0.96
12:L:174:TYR:CD2	12:L:232:TRP:HD1	1.83	0.96
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.44	0.96
40:o:93:LEU:O	40:o:97:LYS:HG2	1.65	0.96
14:N:164:MET:HE1	55:Y:201:3PE:C26	1.96	0.96
49:Ae:152:ILE:C	49:Ae:272:VAL:HG23	1.91	0.96
16:P:376:ASN:OD1	16:P:377:TYR:N	1.98	0.96
48:Ad:170:LYS:HD3	49:Ae:151:LYS:CD	1.94	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
20:U:90:TYR:HE2	20:U:92:LYS:HB2	1.25	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
12:L:363:THR:HG23	12:L:431:THR:HB	1.48	0.96
45:AA:478:LEU:HD22	53:AJ:18:THR:HG21	1.45	0.96
49:Ae:152:ILE:HG21	49:Ae:273:VAL:N	1.81	0.95
6:F:379:CYS:HG	56:F:502:SF4:FE4	0.74	0.95
12:L:174:TYR:HD2	12:L:232:TRP:HD1	1.02	0.95
7:G:92:CYS:SG	59:G:803:FES:S1	2.63	0.95
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.95
12:L:247:LEU:HD12	12:L:248:HIS:CD2	1.98	0.95
12:L:302:ILE:CG2	12:L:340:PHE:CZ	2.48	0.95
12:L:319:MET:HE1	12:L:399:ILE:HA	1.47	0.95
14:N:31:VAL:O	14:N:35:PHE:CD2	2.19	0.95
16:P:40:VAL:HG22	18:R:43:TYR:CD2	1.99	0.95
48:Ad:249:TYR:CE1	48:Ad:252:VAL:HG23	2.02	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
19:S:16:LEU:HD11	19:S:51:LEU:HD11	1.46	0.95
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.94
13:M:216:LEU:HG	13:M:220:HIS:CE1	2.01	0.94
49:AI:78:PHE:HZ	46:Ab:168:ASN:ND2	1.60	0.94
51:Ag:19:LEU:HD23	51:Ag:24:GLN:HB3	1.49	0.94
13:M:4:ILE:HG22	13:M:107:ILE:HD13	1.47	0.94
19:S:19:ILE:HG13	19:S:95:LEU:HD11	1.49	0.94
30:e:96:PRO:HA	30:e:99:SER:HB2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:218:THR:HG21	49:Ae:256:LEU:O	1.68	0.94
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.47	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
49:AI:78:PHE:HE1	46:Ab:171:THR:HG1	1.11	0.94
9:I:152:CYS:HG	56:I:303:SF4:FE2	0.70	0.94
13:M:369:LEU:CD2	13:M:371:PRO:HD2	1.97	0.94
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.45	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
11:K:66:PHE:HZ	14:N:35:PHE:HZ	1.14	0.94
12:L:246:LEU:HD12	12:L:247:LEU:N	1.81	0.94
12:L:466:PHE:HB2	35:j:68:TRP:HZ2	1.33	0.94
20:U:140:CYS:HB2	20:U:143:GLU:HG2	1.49	0.94
55:AC:403:3PE:C2C	51:AG:41:ARG:NH2	2.30	0.94
49:Ae:152:ILE:CG2	49:Ae:273:VAL:N	2.30	0.94
13:M:1:MET:HG3	13:M:4:ILE:HD13	1.50	0.94
37:l:91:GLN:HE21	39:n:2:ALA:HB1	1.30	0.94
51:AG:19:LEU:HD23	51:AG:24:GLN:HB3	1.49	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.94
12:L:247:LEU:HD11	12:L:248:HIS:NE2	1.83	0.94
49:AI:43:LEU:HD13	46:Ab:164:VAL:CG2	1.97	0.94
9:I:113:CYS:SG	56:I:304:SF4:FE3	1.59	0.93
49:AE:218:THR:HG21	49:AE:256:LEU:O	1.68	0.93
12:L:274:LEU:HA	12:L:277:MET:HE3	1.49	0.93
10:J:12:PHE:CE2	11:K:42:ILE:CD1	2.51	0.93
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.49	0.93
47:Ac:197:LEU:HD12	69:Ac:406:UQ6:H1M2	1.48	0.93
10:J:12:PHE:CE2	11:K:42:ILE:HD13	2.03	0.93
13:M:453:LEU:CD1	13:M:454:ILE:HG23	1.99	0.93
48:AD:249:TYR:CE1	48:AD:252:VAL:HG23	2.02	0.93
49:Ae:152:ILE:HG22	49:Ae:272:VAL:HG22	1.51	0.93
55:L:702:3PE:H3C2	40:o:78:LEU:HD13	1.51	0.93
1:A:63:LEU:CD2	10:J:62:GLY:C	2.41	0.93
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.51	0.93
33:h:183:PRO:O	33:h:184:LYS:CG	2.17	0.93
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
16:P:93:HIS:CD2	16:P:94:LEU:CD1	2.52	0.92
47:Ac:137:GLN:HG3	47:Ac:265:PRO:HG3	1.48	0.92
48:Ad:121:CYS:SG	70:Ad:401:HEC:HBB3	2.09	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
12:L:41:LYS:HG3	12:L:98:TRP:CZ2	2.04	0.92
15:O:314:LEU:CD1	15:O:315:PRO:HD2	2.00	0.92
62:a:101:CDL:HB4	42:q:3:LEU:HD13	1.49	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
5:E:179:CYS:HG	59:E:301:FES:FE2	0.66	0.92
71:AD:402:3PH:H221	49:AE:135:GLN:HE22	1.35	0.92
24:Y:19:GLN:HE21	24:Y:22:ARG:HG2	1.32	0.92
45:Aa:402:HIS:NE2	45:Aa:403:LEU:HD11	1.85	0.92
34:i:14:GLN:HB3	39:n:164:PRO:HG3	1.52	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.92
12:L:136:ASN:HD21	62:h:201:CDL:H273	1.33	0.92
49:AI:78:PHE:HE1	46:Ab:171:THR:OG1	1.52	0.92
49:Ae:152:ILE:HG23	49:Ae:272:VAL:HG23	1.46	0.91
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.00	0.91
42:q:85:GLU:HG2	42:q:98:PRO:HB3	1.53	0.91
71:AD:402:3PH:H242	49:AE:132:VAL:HG22	1.50	0.91
49:AI:78:PHE:HZ	46:Ab:168:ASN:HD21	1.05	0.91
6:F:425:CYS:HG	56:F:502:SF4:FE1	0.63	0.91
12:L:466:PHE:HB2	35:j:68:TRP:CZ2	2.06	0.91
8:H:121:TRP:CZ2	10:J:78:TYR:OH	2.23	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.91
12:L:202:MET:HE3	12:L:265:PRO:HG3	1.53	0.91
12:L:245:ALA:O	12:L:249:SER:HB3	1.70	0.91
10:J:168:GLU:HA	10:J:171:ARG:HG2	1.52	0.91
12:L:362:ILE:HG23	12:L:366:MET:HE3	1.53	0.91
53:Aj:52:LEU:HD13	53:Aj:53:TRP:N	1.85	0.91
6:F:382:CYS:HG	56:F:502:SF4:FE3	0.72	0.91
15:O:106:ILE:HG12	15:O:111:SER:HA	1.50	0.91
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.01	0.90
47:AC:137:GLN:HG3	47:AC:265:PRO:HG3	1.50	0.90
48:Ad:170:LYS:HD3	49:Ae:151:LYS:HE2	1.53	0.90
37:l:30:PHE:CE2	37:l:31:HIS:CE1	2.60	0.90
10:J:9:SER:HB3	11:K:7:ASN:HD22	1.35	0.90
48:Ad:170:LYS:HD3	49:Ae:151:LYS:CE	2.01	0.90
2:B:120:VAL:HG21	61:H:400:UQ9:H1MA	1.52	0.90
8:H:200:LEU:HD12	8:H:201:THR:N	1.86	0.90
48:Ad:124:CYS:HA	48:Ad:179:TYR:HE2	1.37	0.90
49:Ae:155:LYS:HG3	49:Ae:269:ASP:HB3	1.53	0.90
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:38:PRO:HB2	38:m:75:ASN:HD22	1.36	0.90
55:L:702:3PE:H3B2	35:j:71:TRP:HH2	1.37	0.90
15:O:347:VAL:O	15:O:347:VAL:HG12	1.71	0.90
16:P:93:HIS:NE2	16:P:94:LEU:CD1	2.35	0.90
2:B:81:LEU:HG	58:B:303:PC1:H261	1.52	0.90
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.90
21:V:75:GLY:HA2	43:r:103:ARG:HD2	1.52	0.90
10:J:5:ILE:HG23	10:J:120:LEU:HD13	1.54	0.89
12:L:364:LYS:HE2	36:k:67:ILE:CD1	2.01	0.89
13:M:231:LEU:HD12	13:M:235:LEU:CD1	2.00	0.89
46:AB:305:THR:HG23	46:AB:306:THR:H	1.36	0.89
13:M:2:LEU:HA	13:M:5:ILE:HG12	1.53	0.89
13:M:453:LEU:HD12	13:M:454:ILE:N	1.87	0.89
4:D:36:GLN:HE22	13:M:135:ARG:HH12	1.19	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.89
10:J:5:ILE:HG13	11:K:4:THR:HG22	1.53	0.89
12:L:123:LEU:HD22	12:L:150:MET:SD	2.12	0.89
15:O:314:LEU:CG	15:O:315:PRO:HD2	2.02	0.89
32:g:145:ILE:HG23	41:p:160:LYS:HE2	1.53	0.89
42:q:76:ASP:OD1	42:q:76:ASP:O	1.90	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
62:L:706:CDL:H522	24:Y:107:THR:HG21	1.53	0.89
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.36	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
15:O:62:VAL:HG22	15:O:205:ILE:HB	1.52	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
12:L:9:LEU:HD11	55:L:701:3PE:H2B2	1.55	0.89
13:M:380:PHE:HA	13:M:383:MET:HE2	1.55	0.89
20:U:105:MET:SD	20:U:139:MET:CE	2.61	0.89
21:V:72:LEU:HD12	21:V:72:LEU:O	1.73	0.89
49:Ae:152:ILE:HD11	49:Ae:174:LEU:CD2	2.02	0.89
7:G:176:CYS:HG	56:G:802:SF4:FE4	0.62	0.89
26:a:37:ARG:HB2	26:a:48:MET:HE2	1.54	0.89
34:i:105:PHE:CE2	40:o:68:LYS:HA	2.08	0.89
45:Aa:403:LEU:HD21	46:Ab:56:ALA:HB1	1.53	0.89
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.35	0.89
7:G:226:CYS:HG	56:G:802:SF4:FE1	0.71	0.89
46:AB:48:VAL:HG21	46:AB:400:ALA:HB1	1.53	0.89
49:Ae:152:ILE:HG23	49:Ae:272:VAL:CA	2.03	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:96:LEU:HD12	16:P:97:MET:N	1.88	0.88
49:Ae:152:ILE:HD11	49:Ae:174:LEU:HD22	1.54	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.88
13:M:8:SER:HA	13:M:11:LEU:HD13	1.54	0.88
13:M:173:THR:HG21	33:h:147:ALA:HB2	1.55	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
9:I:61:LEU:HD21	27:b:17:PRO:O	1.74	0.88
47:Ac:236:PHE:HD2	71:Ad:402:3PH:H3B2	1.39	0.88
14:N:314:MET:HE2	14:N:319:LYS:HE2	1.54	0.88
45:Aa:68:THR:CG2	46:Ab:384:MET:HG2	2.03	0.88
45:AA:402:HIS:CE1	45:AA:403:LEU:HD12	2.07	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
45:Aa:87:ASN:H	45:Aa:207:ASN:HD22	1.17	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
12:L:428:TYR:HA	12:L:432:MET:HG2	1.56	0.87
19:S:16:LEU:HD22	19:S:19:ILE:HD11	1.53	0.87
27:b:60:ASP:OD1	27:b:61:GLY:N	2.07	0.87
13:M:368:ALA:HB1	13:M:375:LEU:HD13	1.56	0.87
13:M:447:LEU:HD11	13:M:454:ILE:HG21	1.54	0.87
14:N:307:THR:HB	15:O:319:ILE:HD11	1.56	0.87
30:e:17:HIS:CD2	30:e:18:PHE:HD1	1.92	0.87
12:L:496:LEU:HD12	12:L:497:GLY:N	1.90	0.87
16:P:344:PRO:HB2	16:P:347:LEU:HD13	1.55	0.87
43:r:2:ALA:N	43:r:26:LEU:CD1	2.37	0.87
1:A:90:MET:CE	10:J:152:MET:HB3	2.04	0.87
8:H:93:HIS:CE1	26:a:24:ALA:HA	2.10	0.87
12:L:41:LYS:HD3	55:L:702:3PE:H2A1	1.56	0.87
13:M:102:LEU:HD13	13:M:230:ILE:HG12	1.57	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.57	0.87
13:M:127:ILE:CD1	14:N:256:PRO:CG	2.53	0.87
12:L:358:LYS:HG2	39:n:80:TYR:CE1	2.10	0.87
13:M:142:ARG:HH21	14:N:303:THR:HG22	1.38	0.87
15:O:295:ARG:NH1	15:O:299:GLN:HB2	1.90	0.87
37:l:30:PHE:CZ	37:l:31:HIS:CE1	2.63	0.87
46:AB:48:VAL:HG23	46:AB:219:ALA:CB	2.03	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.87
51:AG:29:SER:HB2	51:AG:32:SER:HB2	1.57	0.87
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
45:Aa:402:HIS:NE2	45:Aa:403:LEU:CD1	2.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.86
13:M:1:MET:HE1	13:M:111:SER:HB2	1.58	0.86
20:T:79:ILE:HB	20:T:145:VAL:HG13	1.55	0.86
48:AD:292:MET:HA	71:AD:402:3PH:H331	1.57	0.86
51:AG:11:ILE:HG21	51:AG:14:VAL:CG2	2.05	0.86
12:L:79:SER:HB2	12:L:135:ASN:HB2	1.55	0.86
16:P:358:THR:CG2	16:P:359:TYR:N	2.37	0.86
19:S:16:LEU:HD12	19:S:16:LEU:O	1.76	0.86
20:T:138:LEU:HD13	20:T:144:ILE:HG12	1.56	0.86
25:Z:128:ARG:NH1	30:e:97:HIS:HB3	1.90	0.86
1:A:53:MET:HE1	10:J:170:THR:HG22	1.56	0.86
14:N:211:LEU:HD23	14:N:333:SER:HB2	1.58	0.86
8:H:199:ASP:O	8:H:279:ARG:HD2	1.74	0.86
46:AB:48:VAL:HG23	46:AB:219:ALA:HB1	1.55	0.86
1:A:53:MET:SD	11:K:79:VAL:CG1	2.64	0.86
3:C:168:GLU:HB2	3:C:186:ILE:CD1	2.04	0.86
10:J:37:PHE:CE2	10:J:41:LEU:HD11	2.10	0.86
7:G:78:CYS:SG	59:G:803:FES:FE2	1.68	0.86
48:AD:121:CYS:HB3	70:AD:401:HEC:HAB	1.58	0.86
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.76	0.86
48:AD:117:TYR:HA	48:AD:121:CYS:SG	2.14	0.86
47:Ac:138:MET:HE1	47:Ac:268:ILE:HG12	1.57	0.86
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
9:I:162:CYS:SG	56:I:304:SF4:FE4	1.68	0.85
15:O:314:LEU:HG	15:O:315:PRO:HD2	1.58	0.85
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
14:N:200:LEU:HD21	14:N:265:ILE:CG1	2.06	0.85
14:N:323:ASN:OD1	14:N:324:LEU:N	2.08	0.85
37:l:167:TYR:HD2	37:l:168:LEU:HD12	1.41	0.85
1:A:104:TYR:CE2	10:J:167:ILE:HD12	2.10	0.85
8:H:121:TRP:HZ2	10:J:78:TYR:CE1	1.94	0.85
16:P:156:SER:HB2	16:P:161:VAL:HG21	1.55	0.85
46:AB:48:VAL:HG22	46:AB:219:ALA:HB2	1.57	0.85
2:B:122:ARG:HH11	4:D:89:PRO:HB3	1.40	0.85
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.85
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.85
1:A:49:LEU:HD23	4:D:80:MET:HB2	1.57	0.85
1:A:101:GLY:CA	10:J:163:ILE:HD13	2.05	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:127:ILE:HD12	14:N:256:PRO:HG3	1.56	0.85
33:h:182:SER:HB3	33:h:183:PRO:HD2	1.58	0.85
51:Ag:29:SER:HB2	51:Ag:32:SER:HB2	1.56	0.85
12:L:417:SER:HB3	12:L:493:ILE:HG13	1.58	0.85
42:q:42:ASP:OD2	42:q:83:PRO:HG2	1.77	0.85
15:O:176:GLN:HG3	15:O:177:GLY:H	1.41	0.85
20:U:105:MET:HE2	20:U:112:SER:HA	1.59	0.85
12:L:437:PHE:HE1	12:L:441:ILE:CG1	1.85	0.85
13:M:29:SER:HB3	32:g:91:PHE:CD2	2.12	0.85
16:P:132:ARG:HG2	64:P:401:NDP:H8A	1.56	0.85
3:C:80:LEU:CD1	4:D:396:THR:HG22	2.07	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
8:H:114:TYR:CZ	10:J:65:VAL:CG2	2.60	0.85
20:T:110:LEU:HG	20:T:114:ASP:HB2	1.59	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
12:L:302:ILE:HG22	12:L:340:PHE:CE2	2.11	0.85
48:AD:121:CYS:HB3	70:AD:401:HEC:CAB	2.07	0.85
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
12:L:247:LEU:HD11	12:L:248:HIS:CD2	2.11	0.84
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.59	0.84
21:V:56:LEU:HD12	21:V:57:ASP:N	1.92	0.84
48:Ad:215:LEU:HD11	70:Ad:401:HEC:HMB1	1.57	0.84
49:Ae:152:ILE:O	49:Ae:272:VAL:HG23	1.76	0.84
4:D:89:PRO:HB2	8:H:204:GLU:HG3	1.58	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.84
12:L:128:MET:HG2	12:L:251:THR:HB	1.59	0.84
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.59	0.84
55:M:502:3PE:H261	55:O:401:3PE:H232	1.57	0.84
15:O:314:LEU:HD12	15:O:315:PRO:HD2	1.56	0.84
31:f:5:GLN:HB2	31:f:10:HIS:HD2	1.41	0.84
51:Ag:78:TYR:CE1	52:Ah:62:GLU:HB2	2.12	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
45:AA:255:ARG:O	45:AA:255:ARG:HG3	1.75	0.84
51:Ag:11:ILE:HG21	51:Ag:14:VAL:CG2	2.05	0.84
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.08	0.84
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.42	0.84
12:L:445:GLU:HB2	12:L:450:LEU:HD23	1.59	0.84
13:M:447:LEU:HD11	13:M:454:ILE:CG2	2.06	0.84
15:O:237:ILE:HG22	15:O:241:TYR:HE2	1.42	0.84
25:Z:128:ARG:HH12	30:e:97:HIS:HB3	1.42	0.84
49:Ae:156:LEU:N	49:Ae:269:ASP:HA	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
49:AE:263:TYR:HA	49:AE:273:VAL:O	1.77	0.84
46:AB:305:THR:HG23	46:AB:306:THR:N	1.92	0.84
54:Ak:12:GLU:HA	54:Ak:15:ARG:HD3	1.59	0.84
12:L:553:LEU:HD11	38:m:93:ALA:CB	2.06	0.84
14:N:215:MET:SD	14:N:248:LEU:HD21	2.18	0.84
37:l:167:TYR:CD2	37:l:168:LEU:HD12	2.13	0.84
47:AC:214:ASP:HB3	51:AG:9:ALA:HB2	1.58	0.84
2:B:93:MET:HE1	2:B:148:VAL:HG11	1.59	0.84
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.84
4:D:67:ASN:HB2	15:O:193:LEU:CD2	2.07	0.84
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.84
13:M:191:SER:HB2	55:N:401:3PE:O12	1.77	0.84
15:O:238:GLU:HA	15:O:241:TYR:HD2	1.43	0.84
16:P:275:HIS:HA	16:P:278:LYS:HE2	1.60	0.84
48:AD:204:ARG:HH21	70:AD:401:HEC:HBA2	1.40	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.84
5:E:178:ALA:HA	6:F:125:CYS:SG	2.18	0.84
12:L:20:LEU:HD12	12:L:21:ILE:N	1.92	0.84
13:M:196:TRP:NE1	13:M:250:LEU:HD13	1.92	0.84
14:N:276:LEU:HD13	55:N:401:3PE:H2	1.60	0.84
45:Aa:402:HIS:CD2	45:Aa:403:LEU:HD11	2.12	0.84
48:Ad:170:LYS:HD2	49:Ae:151:LYS:HD2	0.85	0.84
7:G:78:CYS:HG	59:G:803:FES:FE2	0.53	0.83
14:N:99:LEU:HD11	14:N:154:ILE:CG2	2.08	0.83
14:N:175:MET:HG2	14:N:219:LEU:HD22	1.60	0.83
30:e:14:LEU:HD12	30:e:15:ASP:HB2	1.57	0.83
8:H:114:TYR:CE1	10:J:33:ILE:CD1	2.60	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
13:M:373:ILE:HG12	13:M:454:ILE:HD11	1.60	0.83
14:N:164:MET:HE1	55:Y:201:3PE:H262	1.58	0.83
15:O:256:LEU:HD11	15:O:276:LEU:CD2	2.07	0.83
20:U:100:VAL:HA	20:U:141:PRO:HG2	1.59	0.83
13:M:361:MET:HB3	13:M:441:MET:HE3	1.60	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
12:L:16:LEU:HD23	12:L:126:ILE:CD1	2.08	0.83
47:AC:222:PRO:HG2	47:AC:223:TYR:HD1	1.43	0.83
51:AG:73:LYS:HZ3	52:AH:63:GLU:HG2	1.42	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.61	0.83
4:D:86:PRO:HG3	4:D:96:ARG:HG2	1.58	0.83
12:L:214:MET:HG3	55:L:704:3PE:H281	1.61	0.83
14:N:179:MET:HG3	14:N:216:PHE:CE1	2.14	0.83
27:b:23:PHE:HB3	55:b:201:3PE:H2D2	1.58	0.83
1:A:108:GLN:HG2	1:A:109:LYS:H	1.43	0.83
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.83
10:J:33:ILE:HG23	10:J:60:LEU:CD2	2.09	0.83
13:M:269:MET:HE1	13:M:396:MET:HA	1.61	0.83
16:P:358:THR:HG22	16:P:359:TYR:H	1.43	0.83
12:L:182:PHE:CE2	12:L:186:MET:HE3	2.14	0.82
13:M:162:ILE:HG23	14:N:271:MET:CE	2.08	0.82
48:AD:270:VAL:HG21	70:AD:401:HEC:HBB3	1.62	0.82
24:Y:34:CYS:HB3	55:Y:201:3PE:H381	1.61	0.82
12:L:432:MET:HG3	12:L:432:MET:O	1.78	0.82
49:AI:64:LEU:HA	49:AI:78:PHE:HA	1.59	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
12:L:131:LEU:CD1	12:L:140:LEU:HD12	2.09	0.82
14:N:170:LEU:HD12	14:N:292:PHE:CD2	2.15	0.82
37:l:30:PHE:CE2	37:l:31:HIS:HE1	1.97	0.82
3:C:186:ILE:CD1	4:D:429:PHE:HZ	1.93	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
8:H:1:MET:HG3	26:a:30:THR:HG22	1.58	0.82
12:L:222:GLY:HA2	12:L:229:LEU:CD1	2.08	0.82
12:L:542:LEU:HD11	55:L:703:3PE:H261	1.60	0.82
62:L:706:CDL:H351	24:Y:114:ALA:HB1	1.60	0.82
55:M:501:3PE:H2A1	62:h:201:CDL:H202	1.62	0.82
23:X:122:LEU:HD23	27:b:82:LYS:HG2	1.59	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.60	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
38:m:123:ARG:O	41:p:140:GLN:NE2	2.13	0.82
12:L:493:ILE:HD12	12:L:496:LEU:HD21	1.62	0.82
14:N:179:MET:CG	14:N:216:PHE:CE1	2.63	0.82
49:AI:43:LEU:HD11	46:Ab:163:ALA:HB3	1.60	0.82
49:Ae:152:ILE:CA	49:Ae:272:VAL:HG23	2.08	0.82
52:Ah:44:ALA:HA	52:Ah:47:ARG:HD3	1.62	0.82
1:A:67:LEU:CD1	11:K:68:ALA:HB3	2.10	0.82
12:L:552:LEU:HD12	37:l:70:MET:HE1	1.60	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:162:CYS:HG	56:I:304:SF4:FE4	0.52	0.81
55:L:703:3PE:H2G1	55:L:704:3PE:H3I1	1.61	0.81
16:P:358:THR:CG2	16:P:359:TYR:H	1.92	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
8:H:1:MET:HE3	26:a:29:PHE:CE2	2.15	0.81
11:K:22:PHE:HB2	12:L:585:LYS:HG2	1.59	0.81
32:g:139:TYR:HB2	41:p:142:ARG:CZ	2.10	0.81
36:k:34:PRO:HD2	36:k:59:TYR:CD1	2.16	0.81
47:Ac:37:LEU:HB3	67:Ac:403:HEM:HMB1	1.60	0.81
48:Ad:125:HIS:HE1	48:Ad:195:PRO:HD2	1.43	0.81
1:A:53:MET:CE	10:J:170:THR:HG22	2.09	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:1:MET:HG3	26:a:30:THR:CG2	2.08	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
12:L:16:LEU:CD2	12:L:126:ILE:HD13	2.10	0.81
49:AE:154:ILE:HD13	49:AE:273:VAL:HG23	1.61	0.81
45:Aa:117:GLY:HA2	46:Ab:377:LYS:HG2	1.59	0.81
46:Ab:259:ARG:HB3	46:Ab:444:LEU:HD13	1.60	0.81
8:H:121:TRP:HH2	10:J:27:TYR:HE1	1.27	0.81
20:U:105:MET:CG	20:U:139:MET:HE3	2.11	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
62:L:706:CDL:HB22	62:L:706:CDL:H512	1.62	0.81
36:k:30:ILE:HD11	36:k:39:GLN:HB2	1.61	0.81
42:q:71:LYS:O	42:q:72:ASN:OD1	1.99	0.81
43:r:4:ALA:HB1	43:r:9:GLN:HB2	1.60	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
13:M:336:ARG:NH2	13:M:429:SER:HA	1.95	0.81
17:Q:146:ASP:OD1	17:Q:146:ASP:O	1.97	0.81
36:k:38:VAL:HG13	39:n:39:TYR:HB2	1.62	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
3:C:102:HIS:CE1	21:V:48:THR:HG22	2.11	0.81
58:J:201:PC1:H342	58:J:201:PC1:H382	1.61	0.81
41:p:5:TRP:CZ3	41:p:10:TYR:O	2.34	0.81
1:A:104:TYR:HE2	10:J:167:ILE:HD12	1.44	0.81
14:N:277:ILE:HG23	14:N:278:MET:N	1.96	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
10:J:22:LYS:HD2	11:K:23:ARG:HG2	1.62	0.81
12:L:229:LEU:O	12:L:229:LEU:CD1	2.28	0.81
13:M:458:THR:CG2	41:p:148:ALA:HB1	2.10	0.81
14:N:277:ILE:CG2	14:N:278:MET:H	1.93	0.81
14:N:338:PRO:HB3	62:X:201:CDL:H712	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:110:GLU:HB2	46:AB:299:ILE:HD13	1.63	0.81
4:D:84:PHE:HZ	4:D:90:ALA:HB3	1.46	0.80
13:M:172:GLY:O	13:M:173:THR:CG2	2.28	0.80
45:Aa:87:ASN:HD22	45:Aa:204:PRO:HD3	1.46	0.80
4:D:47:PHE:CB	14:N:227:ILE:HD11	2.08	0.80
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.80
10:J:33:ILE:HG23	10:J:60:LEU:HD21	1.61	0.80
12:L:13:ILE:CD1	55:L:701:3PE:H2C2	2.11	0.80
12:L:424:MET:HE2	12:L:502:LEU:HB2	1.62	0.80
13:M:29:SER:HB3	32:g:91:PHE:HD2	1.46	0.80
55:AC:403:3PE:C29	51:AG:41:ARG:HH21	1.94	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.81	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
1:A:55:PHE:HB3	10:J:69:TYR:OH	1.82	0.80
12:L:364:LYS:HE2	36:k:67:ILE:HD11	1.64	0.80
13:M:453:LEU:HD12	13:M:454:ILE:HG23	1.63	0.80
15:O:227:MET:O	15:O:228:LYS:CG	2.30	0.80
47:AC:326:TRP:HZ2	55:AC:403:3PE:H11	1.44	0.80
52:Ah:39:GLU:HB3	52:Ah:43:LYS:HE2	1.61	0.80
7:G:73:GLY:HA2	59:G:803:FES:S1	2.21	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
13:M:173:THR:HG23	33:h:147:ALA:CB	2.11	0.80
1:A:53:MET:SD	11:K:79:VAL:HG12	2.20	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
9:I:80:GLU:HG3	26:a:1:MET:SD	2.22	0.80
12:L:358:LYS:HG2	39:n:80:TYR:CZ	2.16	0.80
13:M:216:LEU:HD12	13:M:236:LEU:HD21	1.60	0.80
49:AE:221:GLY:HA3	47:Ac:148:ASN:ND2	1.97	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
9:I:123:CYS:HG	56:I:303:SF4:FE1	0.51	0.80
12:L:466:PHE:CB	35:j:68:TRP:HZ2	1.94	0.80
20:T:87:LEU:HD21	20:T:104:PHE:HZ	1.47	0.80
45:AA:74:TRP:CZ2	45:AA:411:GLU:HA	2.16	0.80
15:O:117:PHE:CE1	15:O:173:MET:HE3	2.17	0.80
21:V:95:LEU:HA	21:V:100:TRP:HH2	1.46	0.80
40:o:29:LEU:HD23	40:o:108:LEU:HD13	1.64	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
9:I:171:PRO:HB3	42:q:93:MET:HE1	1.61	0.80
14:N:164:MET:CE	55:Y:201:3PE:C27	2.59	0.80
62:a:101:CDL:HB4	42:q:3:LEU:CD1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:HH12	57:B:302:UQ1:H71	1.45	0.79
14:N:29:MET:CE	14:N:141:ILE:HG12	2.09	0.79
15:O:199:LEU:HD11	15:O:294:LEU:HD22	1.64	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
52:AH:50:LEU:O	52:AH:54:ARG:HG2	1.82	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
12:L:552:LEU:HD21	38:m:90:GLY:HA2	1.63	0.79
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.62	0.79
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.79
4:D:47:PHE:HB3	14:N:227:ILE:CD1	2.10	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79
13:M:151:PHE:CZ	14:N:291:PHE:HB2	2.17	0.79
20:T:93:ILE:HG21	20:T:110:LEU:HD22	1.63	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:114:TYR:CZ	10:J:33:ILE:HD13	2.17	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
14:N:99:LEU:HD11	14:N:154:ILE:HG23	1.65	0.79
48:Ad:296:MET:HE2	71:Ad:402:3PH:H362	1.63	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
13:M:122:PHE:CZ	13:M:206:LYS:HD3	2.18	0.79
15:O:305:LEU:HD12	15:O:305:LEU:O	1.82	0.79
23:X:4:ILE:HG22	23:X:5:VAL:H	1.48	0.79
39:n:20:TYR:CE2	39:n:24:LEU:HD11	2.18	0.79
49:Ae:152:ILE:HG23	49:Ae:272:VAL:HG22	1.49	0.79
12:L:123:LEU:HD21	62:L:705:CDL:H741	1.63	0.79
12:L:130:ILE:HG23	12:L:139:GLN:HE21	1.46	0.79
23:X:120:PRO:CB	23:X:125:LEU:HD11	2.13	0.79
32:g:139:TYR:CD1	41:p:142:ARG:NH2	2.50	0.79
49:Ae:152:ILE:HD12	49:Ae:169:TRP:CG	2.17	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
13:M:367:LEU:HD21	13:M:408:MET:HE2	1.64	0.79
14:N:164:MET:CE	55:Y:201:3PE:C26	2.60	0.79
34:i:22:TRP:CD2	39:n:172:THR:HG22	2.17	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:114:TYR:CE1	10:J:33:ILE:HD11	2.18	0.79
12:L:131:LEU:HD12	12:L:140:LEU:CD1	2.12	0.79
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.63	0.79
15:O:206:TYR:CD1	15:O:246:LEU:HD21	2.17	0.79
49:Ae:152:ILE:HG22	49:Ae:272:VAL:CG2	2.07	0.79
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.24	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
13:M:173:THR:HG23	33:h:147:ALA:HB2	1.65	0.78
15:O:206:TYR:HB3	15:O:257:VAL:HA	1.63	0.78
19:S:51:LEU:HD13	19:S:95:LEU:CD2	2.11	0.78
49:AE:111:LYS:HE3	53:AJ:11:TYR:OH	1.83	0.78
49:Ae:155:LYS:HE2	49:Ae:157:SER:HB3	1.65	0.78
4:D:67:ASN:HB3	4:D:69:VAL:HG12	1.64	0.78
6:F:109:ARG:HD2	6:F:237:GLY:O	1.83	0.78
51:AG:19:LEU:HD11	51:AG:23:GLU:HG2	1.65	0.78
12:L:3:ILE:H	12:L:3:ILE:HD12	1.48	0.78
12:L:302:ILE:CG2	12:L:340:PHE:CE1	2.66	0.78
15:O:117:PHE:HE1	15:O:173:MET:CE	1.96	0.78
19:S:20:ARG:HG3	19:S:54:LEU:HB2	1.65	0.78
45:Aa:87:ASN:HB3	45:Aa:204:PRO:HD2	1.64	0.78
7:G:617:ARG:NH1	22:W:129:HIS:HA	1.97	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
8:H:30:TYR:OH	26:a:4:GLU:HB2	1.82	0.78
12:L:534:HIS:O	12:L:538:PRO:HG3	1.83	0.78
10:J:3:ASN:ND2	10:J:120:LEU:CB	2.46	0.78
13:M:9:LEU:HD23	13:M:104:ILE:HD13	1.65	0.78
13:M:248:ILE:HG13	13:M:249:ILE:HD12	1.64	0.78
15:O:314:LEU:HD12	15:O:315:PRO:CD	2.13	0.78
16:P:40:VAL:CG2	18:R:43:TYR:CE2	2.66	0.78
37:l:44:THR:OG1	37:l:45:PRO:HD2	1.83	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
12:L:136:ASN:HA	12:L:197:GLU:HA	1.66	0.78
13:M:388:TRP:CE2	38:m:109:ARG:HD2	2.19	0.78
9:I:113:CYS:HG	56:I:304:SF4:FE3	0.49	0.78
13:M:231:LEU:HD12	13:M:235:LEU:HD13	1.64	0.78
13:M:370:PRO:HA	13:M:375:LEU:CD2	2.13	0.78
20:T:87:LEU:HD22	20:T:104:PHE:CE1	2.19	0.78
48:AD:155:GLN:HA	48:AD:166:MET:HA	1.66	0.78
50:AF:52:PRO:HD3	46:Ab:148:ARG:NH2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.78
13:M:319:HIS:HA	13:M:322:THR:HG22	1.66	0.78
33:h:96:ALA:HB3	41:p:63:TYR:HD1	1.49	0.78
45:Aa:59:VAL:HG13	45:Aa:231:LEU:HD23	1.66	0.78
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.19	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
55:M:503:3PE:H2G2	38:m:97:PRO:HG3	1.65	0.78
14:N:120:GLN:HG3	14:N:177:LYS:CE	2.13	0.78
14:N:281:LEU:CD2	55:N:401:3PE:H281	2.13	0.78
16:P:142:GLU:O	16:P:146:VAL:HG12	1.83	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
14:N:215:MET:CE	14:N:248:LEU:CD2	2.62	0.78
20:T:83:VAL:CG2	20:T:126:PHE:HZ	1.97	0.78
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.99	0.77
10:J:67:PHE:CE2	11:K:75:LEU:HD21	2.19	0.77
22:W:47:PRO:HG3	22:W:63:ARG:HH21	1.48	0.77
45:AA:478:LEU:C	45:AA:478:LEU:HD13	2.08	0.77
48:Ad:167:ARG:HB2	48:Ad:168:PRO:HD2	1.64	0.77
51:Ag:19:LEU:HD11	51:Ag:23:GLU:HG2	1.65	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
10:J:3:ASN:HD22	10:J:120:LEU:CB	1.96	0.77
49:AE:115:TYR:HB3	53:AJ:21:PHE:HE1	1.47	0.77
48:Ad:155:GLN:HA	48:Ad:166:MET:HA	1.66	0.77
23:X:20:VAL:HG22	23:X:24:VAL:HG21	1.66	0.77
25:Z:90:ASN:OD1	30:e:98:HIS:NE2	2.17	0.77
30:e:17:HIS:CD2	30:e:18:PHE:CD1	2.72	0.77
45:AA:397:ASN:HD21	46:AB:126:ILE:HD11	1.50	0.77
51:AG:11:ILE:CG2	51:AG:14:VAL:CG2	2.62	0.77
51:Ag:11:ILE:CG2	51:Ag:14:VAL:CG2	2.63	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.77
13:M:274:SER:O	13:M:277:LEU:HB2	1.85	0.77
14:N:45:ILE:O	14:N:45:ILE:HG13	1.83	0.77
14:N:254:LEU:HD12	14:N:255:PRO:CD	2.14	0.77
37:l:169:GLU:C	37:l:171:GLY:H	1.92	0.77
48:Ad:120:VAL:HG12	70:Ad:401:HEC:HAB	1.67	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
45:AA:68:THR:HG21	46:AB:384:MET:HG3	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:204:LEU:HD22	13:M:209:LEU:HD12	1.65	0.77
15:O:168:VAL:HG21	15:O:241:TYR:OH	1.82	0.77
17:Q:81:VAL:HG21	17:Q:150:LYS:HG3	1.65	0.77
18:R:95:LEU:HD21	18:R:111:PHE:HB3	1.66	0.77
4:D:67:ASN:HB2	15:O:193:LEU:HD23	1.65	0.77
13:M:453:LEU:HD11	13:M:454:ILE:HG23	1.65	0.77
23:X:124:GLN:O	23:X:125:LEU:HD12	1.85	0.77
36:k:55:GLU:CD	39:n:34:ARG:HD2	2.09	0.77
1:A:61:THR:CG2	8:H:290:TRP:CH2	2.67	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
27:b:66:VAL:HG13	27:b:72:ASP:HB2	1.65	0.77
42:q:56:PHE:HA	42:q:59:HIS:HD2	1.50	0.77
45:Aa:360:CYS:SG	45:Aa:364:SER:HB2	2.24	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
10:J:126:TYR:HA	25:Z:120:LEU:CD1	2.13	0.77
13:M:208:PRO:HG2	13:M:216:LEU:HD13	1.67	0.77
3:C:80:LEU:CD1	4:D:396:THR:CG2	2.63	0.76
8:H:183:MET:HE2	58:I:302:PC1:H2A1	1.67	0.76
12:L:419:THR:HA	12:L:422:TYR:CE2	2.20	0.76
13:M:42:LEU:HG	13:M:67:ILE:HD11	1.67	0.76
13:M:98:MET:CE	13:M:128:PRO:HA	2.14	0.76
14:N:31:VAL:O	14:N:35:PHE:HD2	1.68	0.76
47:AC:18:PHE:CE1	69:AC:405:UQ6:H72	2.19	0.76
47:AC:137:GLN:HE21	47:AC:265:PRO:HD3	1.50	0.76
48:Ad:244:MET:HB2	70:Ad:401:HEC:C1D	2.15	0.76
1:A:112:GLU:O	1:A:112:GLU:CD	2.28	0.76
13:M:171:VAL:HG11	13:M:179:LEU:HD21	1.65	0.76
15:O:58:ARG:HG2	15:O:278:TYR:CE2	2.21	0.76
20:T:93:ILE:HG23	20:T:110:LEU:HD13	1.66	0.76
20:T:119:ILE:HD12	20:T:138:LEU:HD11	1.67	0.76
34:i:102:PRO:HB2	41:p:18:PRO:CD	2.15	0.76
46:AB:63:LEU:HD11	46:AB:238:LEU:HD21	1.65	0.76
47:AC:148:ASN:OD1	49:Ae:221:GLY:HA3	1.85	0.76
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.66	0.76
1:A:61:THR:HG21	8:H:290:TRP:CZ3	2.20	0.76
8:H:121:TRP:HH2	10:J:27:TYR:CE1	1.99	0.76
12:L:302:ILE:HG22	12:L:340:PHE:CE1	2.20	0.76
12:L:542:LEU:HB3	13:M:278:ARG:HD2	1.66	0.76
20:U:123:GLU:HG2	20:U:130:ILE:HG12	1.67	0.76
40:o:116:ALA:O	40:o:119:GLU:HB2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:99:LYS:HE2	46:Ab:302:GLY:HA3	1.67	0.76
49:Ae:152:ILE:O	49:Ae:272:VAL:CG2	2.32	0.76
11:K:95:LEU:HG	14:N:54:GLU:OE2	1.84	0.76
15:O:43:ALA:HA	15:O:46:GLY:O	1.86	0.76
47:Ac:214:ASP:HB3	51:Ag:9:ALA:HB2	1.66	0.76
49:Ae:270:VAL:O	49:Ae:271:VAL:HG23	1.86	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:M:60:PRO:O	13:M:64:PRO:HD3	1.85	0.76
14:N:314:MET:HB2	15:O:305:LEU:HD11	1.68	0.76
4:D:57:GLU:HA	4:D:60:HIS:CD2	2.21	0.76
12:L:496:LEU:HD12	12:L:496:LEU:C	2.09	0.76
14:N:179:MET:HG3	14:N:216:PHE:HE1	1.49	0.76
30:e:102:GLU:HG2	30:e:104:PRO:HD3	1.65	0.76
49:AE:111:LYS:HE3	53:AJ:11:TYR:CZ	2.20	0.76
49:AE:191:GLU:HB2	49:AE:194:GLN:HB2	1.66	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.67	0.76
17:Q:112:MET:SD	42:q:126:PRO:HB2	2.24	0.76
42:q:96:ASP:OD1	42:q:97:PRO:HD2	1.85	0.76
4:D:36:GLN:NE2	13:M:135:ARG:HH12	1.84	0.76
6:F:225:LEU:H	17:Q:160:TYR:HE2	1.32	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
12:L:232:TRP:CZ3	12:L:233:LEU:CD2	2.69	0.76
32:g:147:LEU:HD11	41:p:163:MET:HB3	1.65	0.76
34:i:102:PRO:HG2	41:p:18:PRO:HD3	1.66	0.76
46:AB:407:MET:HG2	46:AB:411:THR:OG1	1.85	0.76
48:AD:195:PRO:HG3	70:AD:401:HEC:HBA1	1.66	0.76
5:E:183:PRO:HB2	5:E:195:LEU:H	1.50	0.76
62:L:706:CDL:H801	62:L:706:CDL:H762	1.67	0.76
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.67	0.76
34:i:22:TRP:CE2	39:n:172:THR:HG22	2.21	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
12:L:605:ASN:OD1	12:L:605:ASN:O	2.03	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
12:L:126:ILE:HG21	62:L:705:CDL:H582	1.68	0.75
12:L:506:ASN:HA	12:L:509:MET:HE2	1.66	0.75
15:O:121:PRO:O	15:O:122:LYS:HG2	1.85	0.75
15:O:168:VAL:HG11	15:O:241:TYR:CE1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AG:11:ILE:HG22	51:AG:14:VAL:HG22	1.69	0.75
51:AG:73:LYS:NZ	52:AH:63:GLU:HG2	2.01	0.75
46:Ab:407:MET:HG2	46:Ab:411:THR:OG1	1.85	0.75
49:Ae:191:GLU:HB2	49:Ae:194:GLN:HB2	1.66	0.75
2:B:68:ARG:HD3	2:B:70:ARG:HG2	1.69	0.75
16:P:214:LEU:HG	16:P:353:LEU:HD21	1.68	0.75
39:n:20:TYR:CZ	39:n:24:LEU:HD11	2.21	0.75
45:AA:68:THR:HG22	45:AA:136:LEU:HD23	1.67	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
12:L:358:LYS:HG3	39:n:80:TYR:CE2	2.20	0.75
13:M:458:THR:HG22	41:p:148:ALA:HB1	1.68	0.75
15:O:48:LYS:O	15:O:51:LYS:HG2	1.86	0.75
16:P:348:LYS:O	16:P:351:GLU:HG2	1.86	0.75
49:Ae:169:TRP:CH2	49:Ae:273:VAL:HB	2.21	0.75
4:D:84:PHE:CZ	4:D:90:ALA:HB3	2.22	0.75
10:J:59:TYR:OH	11:K:34:GLU:HB3	1.86	0.75
10:J:60:LEU:CD1	10:J:60:LEU:C	2.59	0.75
12:L:387:THR:HG23	12:L:461:SER:O	1.85	0.75
14:N:170:LEU:HD12	14:N:292:PHE:HD2	1.49	0.75
33:h:57:VAL:HG22	39:n:104:LEU:HD11	1.69	0.75
45:AA:55:ASN:HB3	45:AA:226:ALA:CB	2.16	0.75
3:C:98:PHE:HA	21:V:90:LEU:CD1	2.16	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
17:Q:167:ASN:O	17:Q:168:LYS:CD	2.35	0.75
46:AB:429:LYS:HA	46:AB:432:VAL:HG12	1.67	0.75
49:AI:72:VAL:HG21	46:Ab:109:LYS:HD2	1.69	0.75
2:B:112:TYR:OH	9:I:91:GLY:CA	2.27	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
18:R:104:CYS:SG	18:R:107:CYS:HB2	2.27	0.75
49:Ae:173:PRO:HG2	49:Ae:223:VAL:HG22	1.67	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
14:N:227:ILE:HA	14:N:230:ILE:HG22	1.66	0.75
14:N:277:ILE:HG23	14:N:278:MET:H	1.50	0.75
1:A:90:MET:HE2	10:J:152:MET:CB	2.16	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
12:L:393:ASP:OD1	12:L:394:LEU:N	2.19	0.75
7:G:608:VAL:HG23	17:Q:103:THR:OG1	1.87	0.74
12:L:482:MET:HE2	12:L:486:LEU:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:336:GLU:HG3	16:P:342:PRO:HD3	1.67	0.74
42:q:55:PHE:CD1	43:r:26:LEU:HD22	2.21	0.74
45:AA:255:ARG:O	45:AA:256:VAL:C	2.29	0.74
48:AD:227:LEU:HD12	48:AD:227:LEU:O	1.87	0.74
49:AE:173:PRO:HG2	49:AE:223:VAL:HG22	1.67	0.74
53:AJ:23:LEU:HD22	54:AK:23:MET:SD	2.27	0.74
47:Ac:18:PHE:HE1	69:Ac:406:UQ6:C8	2.00	0.74
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.74
10:J:151:MET:HE2	14:N:28:LEU:HD13	1.69	0.74
12:L:475:THR:HA	40:o:55:GLN:NE2	2.01	0.74
25:Z:93:GLU:CD	30:e:95:PRO:HD2	2.12	0.74
34:i:11:ARG:HE	34:i:15:LEU:HD11	1.51	0.74
1:A:53:MET:SD	11:K:79:VAL:HG11	2.27	0.74
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.67	0.74
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.74
9:I:57:ALA:HB2	27:b:13:TRP:O	1.87	0.74
13:M:314:MET:HA	13:M:454:ILE:HD12	1.70	0.74
15:O:117:PHE:CE1	15:O:128:SER:HB2	2.22	0.74
15:O:333:GLU:O	15:O:333:GLU:CD	2.30	0.74
27:b:31:ILE:HA	27:b:34:MET:HE2	1.69	0.74
5:E:139:CYS:SG	59:E:301:FES:FE1	1.78	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
17:Q:61:ILE:O	17:Q:61:ILE:HD12	1.86	0.74
20:T:117:GLU:HA	20:T:120:MET:HE3	1.68	0.74
24:Y:71:MET:HG3	24:Y:102:THR:HG21	1.68	0.74
49:Ae:154:ILE:HD13	49:Ae:176:VAL:HG21	1.69	0.74
51:Ag:11:ILE:HG22	51:Ag:14:VAL:HG22	1.68	0.74
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.69	0.74
3:C:149:LEU:CD1	22:W:80:ARG:NH2	2.48	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
10:J:135:LEU:HD23	26:a:42:GLN:HG3	1.67	0.74
12:L:136:ASN:ND2	62:h:201:CDL:H273	2.01	0.74
14:N:43:MET:HB3	14:N:126:MET:SD	2.27	0.74
14:N:243:MET:HG2	29:d:44:MET:HE2	1.69	0.74
14:N:284:MET:HE2	55:N:401:3PE:H3B2	1.69	0.74
51:AG:78:TYR:CE1	52:AH:62:GLU:HB2	2.21	0.74
23:X:23:ALA:HB2	23:X:95:GLN:NE2	2.03	0.74
48:AD:200:ILE:HG21	48:AD:274:LEU:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD13	3:C:140:ILE:HD11	1.70	0.74
6:F:425:CYS:SG	56:F:502:SF4:FE1	1.78	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
8:H:316:PRO:HA	25:Z:58:ARG:HH11	1.52	0.74
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.70	0.74
15:O:59:VAL:HA	15:O:157:VAL:HG23	1.69	0.74
24:Y:76:THR:HG23	24:Y:95:GLY:HA3	1.70	0.74
33:h:57:VAL:HG12	39:n:99:VAL:HG21	1.69	0.74
37:l:91:GLN:NE2	39:n:2:ALA:HB1	2.03	0.74
45:AA:478:LEU:HD22	53:AJ:18:THR:CG2	2.18	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
8:H:195:ARG:O	8:H:199:ASP:HB2	1.87	0.74
8:H:272:TRP:HH2	58:I:302:PC1:H381	1.52	0.74
20:T:88:LYS:HG3	20:T:98:LEU:HD22	1.70	0.74
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.74
8:H:111:LEU:HD22	10:J:60:LEU:HD11	1.70	0.74
16:P:350:ILE:HB	16:P:366:ILE:HG23	1.70	0.74
1:A:61:THR:HG21	8:H:290:TRP:CH2	2.23	0.73
4:D:253:LEU:HB2	43:r:23:LYS:HD2	1.68	0.73
5:E:192:TYR:CE1	5:E:215:PRO:HA	2.23	0.73
9:I:110:GLU:OE2	18:R:64:ILE:HB	1.88	0.73
13:M:1:MET:HB2	13:M:52:PHE:CD2	2.23	0.73
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.23	0.73
20:T:103:HIS:CG	20:T:106:LYS:HD2	2.23	0.73
34:i:103:ARG:O	34:i:105:PHE:CE1	2.41	0.73
49:AI:42:VAL:HG11	45:Aa:283:PRO:HB2	1.69	0.73
49:Ae:112:GLY:HA2	53:Aj:15:PHE:HD2	1.52	0.73
2:B:122:ARG:NH1	57:B:302:UQ1:H71	2.02	0.73
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.73
55:L:702:3PE:H3B2	35:j:71:TRP:CH2	2.20	0.73
13:M:200:MET:HE1	13:M:247:SER:HB2	1.69	0.73
13:M:260:PRO:O	13:M:264:LEU:HG	1.88	0.73
45:AA:55:ASN:HB3	45:AA:226:ALA:HB1	1.68	0.73
48:Ad:217:GLY:O	48:Ad:235:PRO:HD2	1.88	0.73
49:Ae:93:ARG:CD	49:Ae:110:ARG:CD	2.66	0.73
8:H:111:LEU:HD11	10:J:56:PHE:CZ	2.22	0.73
12:L:232:TRP:CZ3	12:L:233:LEU:HD23	2.22	0.73
15:O:117:PHE:HE1	15:O:173:MET:HE3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:102:PRO:CG	41:p:18:PRO:HD3	2.17	0.73
46:AB:305:THR:CG2	46:AB:306:THR:H	2.01	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
20:T:94:ASP:HB3	20:T:98:LEU:HB2	1.69	0.73
21:V:54:GLU:HG2	21:V:58:MET:HE2	1.70	0.73
24:Y:143:VAL:HG23	33:h:157:ARG:HG2	1.69	0.73
1:A:90:MET:HG2	10:J:145:TYR:HD1	1.53	0.73
13:M:143:LEU:HD21	14:N:303:THR:HG23	1.68	0.73
13:M:167:ILE:HD11	13:M:195:LEU:HD21	1.70	0.73
15:O:99:GLY:HA2	28:c:30:TYR:HD1	1.53	0.73
35:j:102:ASP:OD1	40:o:111:ARG:HG3	1.89	0.73
71:Ad:402:3PH:H241	49:Ae:132:VAL:HG22	1.69	0.73
4:D:280:ALA:CB	21:V:11:LEU:HG	2.19	0.73
12:L:9:LEU:HD21	55:L:701:3PE:H2C1	1.69	0.73
12:L:20:LEU:HD12	12:L:20:LEU:C	2.13	0.73
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.12	0.73
13:M:216:LEU:HG	13:M:220:HIS:HE1	1.48	0.73
55:M:502:3PE:H3D1	55:M:502:3PE:H2B2	1.71	0.73
31:f:38:ARG:HH12	31:f:54:VAL:HG21	1.54	0.73
42:q:68:MET:SD	42:q:81:MET:HB3	2.28	0.73
47:Ac:220:PHE:HE2	69:Ac:406:UQ6:H4M2	1.53	0.73
12:L:579:ASN:OD1	12:L:579:ASN:O	2.06	0.73
16:P:40:VAL:CG2	18:R:43:TYR:CD2	2.71	0.73
27:b:69:HIS:HD2	27:b:70:PRO:HD2	1.54	0.73
45:AA:478:LEU:HD13	45:AA:478:LEU:O	1.88	0.73
49:Ae:263:TYR:HB2	49:Ae:271:VAL:CG1	2.18	0.73
16:P:203:PRO:HG2	64:P:401:NDP:H6N	1.69	0.73
23:X:151:ASN:HB2	23:X:152:PRO:HD2	1.70	0.73
47:AC:141:TRP:CD1	47:AC:265:PRO:HD3	2.23	0.73
47:AC:148:ASN:OD1	49:Ae:220:LEU:C	2.32	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
12:L:556:ILE:HG21	38:m:80:PHE:CE1	2.24	0.73
14:N:211:LEU:CD2	14:N:333:SER:HB2	2.19	0.73
15:O:59:VAL:HA	15:O:157:VAL:CG2	2.19	0.73
15:O:254:GLU:HG2	15:O:276:LEU:HD13	1.71	0.73
42:q:56:PHE:HA	42:q:59:HIS:CD2	2.24	0.73
42:q:56:PHE:HD1	42:q:59:HIS:HE2	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:269:LYS:HE3	47:AC:340:GLY:HA2	1.70	0.73
49:AE:132:VAL:O	49:AE:135:GLN:HG2	1.88	0.73
9:I:184:LEU:HD23	17:Q:112:MET:HG3	1.71	0.73
13:M:122:PHE:CD1	13:M:238:LEU:HG	2.23	0.73
13:M:441:MET:SD	13:M:444:LEU:HD23	2.29	0.73
22:W:110:PHE:HZ	66:W:201:EHZ:C2	2.00	0.73
46:AB:48:VAL:HG23	46:AB:48:VAL:O	1.88	0.73
48:AD:152:VAL:HG11	48:AD:176:PRO:HG3	1.71	0.73
49:AE:187:GLU:HB3	49:AE:201:ASP:HB3	1.71	0.73
9:I:68:ARG:NH2	25:Z:26:PRO:HD2	2.04	0.72
21:V:12:VAL:HG13	21:V:13:GLY:N	2.04	0.72
34:i:11:ARG:NE	34:i:15:LEU:HD11	2.04	0.72
49:Ae:187:GLU:HB3	49:Ae:201:ASP:HB3	1.71	0.72
10:J:121:GLY:HA3	25:Z:133:MET:HE1	1.71	0.72
10:J:165:ILE:HG23	14:N:42:PRO:HG3	1.69	0.72
14:N:155:LEU:HD12	24:Y:138:PHE:HA	1.71	0.72
32:g:106:TYR:CE2	33:h:86:ILE:HD12	2.24	0.72
41:p:7:LYS:O	41:p:11:PRO:HA	1.89	0.72
47:Ac:148:ASN:OD1	47:Ac:165:TRP:CH2	2.41	0.72
48:Ad:170:LYS:CD	49:Ae:151:LYS:CE	2.63	0.72
1:A:67:LEU:HD11	11:K:68:ALA:HB1	1.70	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
8:H:292:ASN:O	27:b:18:VAL:HG11	1.88	0.72
58:I:302:PC1:H112	25:Z:29:GLY:HA3	1.71	0.72
10:J:32:LEU:HG	10:J:64:LEU:HD21	1.71	0.72
12:L:9:LEU:HD22	34:i:82:VAL:HG13	1.71	0.72
12:L:141:PHE:HD2	13:M:370:PRO:HB3	1.54	0.72
12:L:316:THR:CG2	12:L:325:ALA:HB2	2.18	0.72
13:M:243:MET:HE1	13:M:302:MET:HE3	1.71	0.72
14:N:215:MET:SD	14:N:248:LEU:CD2	2.77	0.72
19:S:69:TYR:CE2	19:S:75:LYS:HG3	2.24	0.72
12:L:598:ILE:HD11	14:N:153:ILE:HG12	1.70	0.72
45:AA:74:TRP:HZ2	45:AA:411:GLU:HA	1.54	0.72
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.54	0.72
23:X:90:ASP:OD2	26:a:62:VAL:HG11	1.90	0.72
37:l:158:PRO:HD3	40:o:22:ILE:HB	1.71	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
7:G:126:LEU:CD1	18:R:89:PRO:CB	2.68	0.72
12:L:102:GLN:HE21	12:L:449:ASP:HA	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:576:LEU:HD12	12:L:577:THR:N	2.05	0.72
16:P:262:THR:H	16:P:332:LEU:HD12	1.54	0.72
19:S:51:LEU:CD1	19:S:95:LEU:HD21	2.12	0.72
25:Z:98:MET:HE3	25:Z:101:VAL:HG21	1.70	0.72
62:a:101:CDL:HA32	42:q:13:GLN:HE22	1.54	0.72
36:k:34:PRO:HG2	36:k:59:TYR:HE1	1.55	0.72
47:Ac:141:TRP:CD1	47:Ac:265:PRO:HD3	2.24	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.72
14:N:59:TYR:CE2	14:N:63:GLN:HG3	2.23	0.72
17:Q:167:ASN:O	17:Q:168:LYS:HD2	1.88	0.72
34:i:95:TYR:CD1	41:p:112:ALA:CB	2.72	0.72
47:AC:223:TYR:HE2	48:AD:314:LEU:HG	1.55	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
12:L:466:PHE:CZ	35:j:72:ARG:NH2	2.58	0.72
12:L:569:LEU:HB2	24:Y:115:MET:CE	2.17	0.72
13:M:127:ILE:HD11	14:N:256:PRO:CG	2.17	0.72
14:N:179:MET:SD	14:N:216:PHE:HE1	2.13	0.72
34:i:11:ARG:HH22	39:n:154:LEU:CB	1.92	0.72
49:AE:156:LEU:HG	49:AE:271:VAL:HG23	1.70	0.72
49:Ae:199:GLN:O	49:Ae:248:ARG:HD3	1.90	0.72
4:D:81:THR:HA	4:D:100:GLU:HA	1.71	0.72
7:G:617:ARG:HH11	22:W:129:HIS:HA	1.52	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
40:o:94:ASP:HA	40:o:97:LYS:HG2	1.71	0.72
45:AA:249:HIS:O	45:AA:250:LEU:HB2	1.89	0.72
49:AE:264:GLU:N	49:AE:272:VAL:O	2.21	0.72
1:A:4:TYR:CE2	55:A:401:3PE:H231	2.25	0.72
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.72
12:L:247:LEU:HD12	12:L:248:HIS:N	2.04	0.72
12:L:299:LYS:HB2	12:L:354:GLN:HE21	1.55	0.72
13:M:313:THR:HG21	13:M:456:GLY:HA3	1.72	0.72
13:M:373:ILE:CG1	13:M:454:ILE:HD11	2.19	0.72
47:AC:18:PHE:HE1	69:AC:405:UQ6:H72	1.54	0.72
48:Ad:292:MET:HA	71:Ad:402:3PH:H322	1.71	0.72
1:A:90:MET:HE3	10:J:152:MET:CG	2.20	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
14:N:232:LEU:HD23	14:N:307:THR:HG23	1.70	0.71
45:AA:171:GLU:O	45:AA:174:GLU:HG2	1.89	0.71
49:AE:123:VAL:CG1	53:AJ:29:ALA:HA	2.20	0.71
49:Ae:152:ILE:HG23	49:Ae:272:VAL:CB	2.20	0.71
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.72	0.71
3:C:102:HIS:HE1	21:V:48:THR:CG2	2.01	0.71
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
13:M:106:LEU:HD13	13:M:234:ILE:HG22	1.72	0.71
13:M:173:THR:HB	33:h:143:GLU:OE2	1.90	0.71
25:Z:111:PHE:HE1	30:e:65:GLU:C	1.98	0.71
45:AA:397:ASN:HD21	46:AB:126:ILE:CD1	2.03	0.71
6:F:236:PHE:HA	17:Q:166:TRP:CD1	2.25	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
12:L:141:PHE:CD2	13:M:370:PRO:HB3	2.25	0.71
13:M:173:THR:CG2	33:h:147:ALA:CB	2.68	0.71
15:O:100:ASP:OD1	15:O:101:GLY:N	2.24	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
12:L:466:PHE:CE1	35:j:72:ARG:NH2	2.58	0.71
1:A:90:MET:HG2	10:J:145:TYR:CD1	2.26	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
23:X:47:ARG:HH12	33:h:187:PRO:HB3	1.54	0.71
24:Y:34:CYS:HB3	55:Y:201:3PE:C38	2.20	0.71
37:l:106:HIS:CD2	37:l:107:TRP:H	2.08	0.71
49:AE:199:GLN:O	49:AE:248:ARG:HD3	1.90	0.71
1:A:50:PRO:HA	10:J:73:MET:HE3	1.70	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
58:I:302:PC1:H2D1	58:I:302:PC1:H291	1.73	0.71
15:O:336:GLY:H	15:O:344:ASN:ND2	1.89	0.71
23:X:93:ASN:OD1	23:X:94:MET:N	2.24	0.71
38:m:9:ALA:HB1	38:m:10:PRO:HD2	1.71	0.71
49:AE:220:LEU:HB3	47:Ac:145:VAL:HG13	1.71	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
13:M:220:HIS:CE1	13:M:231:LEU:HD23	2.26	0.71
13:M:370:PRO:HA	13:M:375:LEU:HD23	1.72	0.71
14:N:146:TYR:CG	14:N:147:PRO:HD3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AC:403:3PE:H2C1	51:AG:41:ARG:HH21	1.51	0.71
49:Ae:207:LYS:HB2	49:Ae:210:TRP:HB2	1.73	0.71
52:Ah:42:VAL:HG13	52:Ah:45:ARG:HH21	1.55	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:30:TYR:HE2	26:a:5:ILE:HG22	1.54	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
12:L:368:PHE:HB3	12:L:445:GLU:CD	2.15	0.71
16:P:170:LEU:O	16:P:171:ASN:OD1	2.09	0.71
19:S:48:HIS:ND1	19:S:95:LEU:HD23	2.05	0.71
20:U:144:ILE:O	20:U:148:ILE:HG12	1.91	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.73	0.71
15:O:237:ILE:HG22	15:O:241:TYR:CE2	2.24	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
8:H:121:TRP:CZ2	10:J:78:TYR:CZ	2.68	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:312:ALA:HB2	27:b:38:TYR:HB3	1.73	0.71
14:N:313:MET:CG	15:O:305:LEU:HD22	2.21	0.71
15:O:209:VAL:HG23	15:O:214:VAL:HG13	1.72	0.71
45:AA:310:ILE:HG21	45:AA:379:LEU:HD21	1.73	0.71
48:AD:159:ASN:O	48:AD:162:GLY:N	2.22	0.71
45:Aa:57:LEU:HD12	45:Aa:229:MET:HE2	1.73	0.71
49:Ae:178:HIS:HB2	49:Ae:210:TRP:CZ3	2.26	0.71
2:B:93:MET:HE1	2:B:148:VAL:CG1	2.21	0.70
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.72	0.70
8:H:187:ILE:HD12	55:I:301:3PE:H242	1.71	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
10:J:130:ASP:O	26:a:42:GLN:HB3	1.91	0.70
14:N:237:THR:HG23	14:N:237:THR:O	1.88	0.70
15:O:206:TYR:HD2	15:O:257:VAL:HG13	1.55	0.70
38:m:45:ARG:O	38:m:45:ARG:HG2	1.91	0.70
49:AE:152:ILE:HB	49:AE:169:TRP:NE1	2.06	0.70
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HG13	1.73	0.70
49:Ae:116:LEU:HA	53:Aj:15:PHE:CZ	2.26	0.70
49:Ae:264:GLU:H	49:Ae:271:VAL:HG13	1.56	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
8:H:318:MET:HG2	26:a:40:ARG:NH2	2.06	0.70
14:N:200:LEU:CD2	14:N:265:ILE:HG12	2.14	0.70
55:N:401:3PE:H3A2	55:N:401:3PE:H271	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:87:THR:HA	62:h:201:CDL:H512	1.73	0.70
49:AE:178:HIS:HB2	49:AE:210:TRP:CZ3	2.26	0.70
45:Aa:279:ASP:OD1	51:Ag:12:ARG:NE	2.24	0.70
48:Ad:248:ILE:HD11	70:Ad:401:HEC:HBB1	1.72	0.70
49:Ae:154:ILE:HD11	49:Ae:174:LEU:HD21	1.73	0.70
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
8:H:134:ARG:NH2	8:H:200:LEU:HD13	2.06	0.70
12:L:73:SER:HB3	41:p:100:GLN:NE2	2.06	0.70
12:L:455:LYS:NZ	35:j:57:GLN:OE1	2.23	0.70
13:M:373:ILE:HG12	13:M:454:ILE:CD1	2.20	0.70
14:N:23:SER:HB2	30:e:15:ASP:OD2	1.91	0.70
22:W:42:TRP:CD2	22:W:93:LEU:HD12	2.26	0.70
34:i:102:PRO:CB	41:p:18:PRO:HD2	2.21	0.70
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.70
15:O:135:LEU:HB3	15:O:139:ARG:HH12	1.57	0.70
49:AE:192:VAL:HA	49:AE:195:LEU:HD12	1.73	0.70
49:Ae:220:LEU:HD12	49:Ae:239:HIS:CE1	2.27	0.70
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.26	0.70
2:B:101:ALA:HB1	57:B:302:UQ1:HM53	1.73	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
12:L:9:LEU:CD2	55:L:701:3PE:H2C1	2.21	0.70
12:L:428:TYR:OH	39:n:33:HIS:CE1	2.44	0.70
45:AA:362:ALA:HB2	45:AA:461:PRO:HB2	1.72	0.70
13:M:446:LEU:HD13	32:g:101:THR:HG21	1.73	0.70
49:Ae:152:ILE:HG23	49:Ae:272:VAL:HA	1.73	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
8:H:30:TYR:CE2	26:a:5:ILE:CG2	2.75	0.70
8:H:67:SER:HA	58:J:201:PC1:H121	1.72	0.70
9:I:155:CYS:HG	56:I:303:SF4:FE4	1.08	0.70
12:L:428:TYR:HA	12:L:432:MET:CG	2.21	0.70
12:L:553:LEU:HD21	38:m:93:ALA:C	2.17	0.70
12:L:559:GLU:O	12:L:564:LYS:HB2	1.92	0.70
21:V:12:VAL:HG13	21:V:13:GLY:H	1.56	0.70
22:W:110:PHE:CZ	66:W:201:EHZ:C2	2.75	0.70
45:Aa:87:ASN:ND2	45:Aa:204:PRO:HD3	2.06	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
22:W:58:THR:HB	22:W:61:GLN:CB	2.22	0.70
25:Z:12:PRO:HD3	25:Z:16:TYR:CZ	2.25	0.70
47:Ac:269:LYS:HE3	47:Ac:340:GLY:HA2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:M:502:3PE:H3I3	62:X:201:CDL:H652	1.74	0.70
14:N:254:LEU:HD12	14:N:255:PRO:HD3	1.72	0.70
18:R:70:ASN:HB2	18:R:111:PHE:HD1	1.55	0.70
21:V:56:LEU:HD12	21:V:56:LEU:C	2.16	0.70
26:a:37:ARG:CB	26:a:48:MET:HE2	2.22	0.70
38:m:30:ARG:O	38:m:34:VAL:HG23	1.92	0.70
49:Ae:152:ILE:HG23	49:Ae:273:VAL:N	2.07	0.70
12:L:285:THR:HG22	12:L:415:ALA:CB	2.21	0.70
13:M:134:THR:O	13:M:142:ARG:HD2	1.92	0.70
15:O:206:TYR:CD2	15:O:257:VAL:HG13	2.27	0.70
18:R:67:GLN:HG2	18:R:109:LEU:CD2	2.21	0.70
47:Ac:147:THR:HG22	47:Ac:161:VAL:HG13	1.74	0.70
48:Ad:218:TYR:CD1	48:Ad:246:PRO:HG3	2.26	0.70
2:B:122:ARG:NH1	4:D:89:PRO:HB3	2.05	0.69
7:G:127:ASP:HA	18:R:106:TYR:OH	1.90	0.69
12:L:73:SER:HB3	41:p:100:GLN:HE21	1.57	0.69
14:N:308:ASN:HB3	15:O:317:ILE:HG22	1.72	0.69
21:V:35:LEU:HA	21:V:38:PHE:CD1	2.27	0.69
24:Y:19:GLN:HG3	24:Y:22:ARG:HB2	1.74	0.69
49:AE:220:LEU:HD12	49:AE:239:HIS:CE1	2.26	0.69
49:Ae:192:VAL:HA	49:Ae:195:LEU:HD12	1.73	0.69
12:L:480:LEU:HD23	12:L:480:LEU:O	1.93	0.69
13:M:447:LEU:HD21	13:M:454:ILE:HD13	1.73	0.69
30:e:42:GLU:HG2	33:h:176:LYS:HG3	1.74	0.69
32:g:106:TYR:OH	33:h:86:ILE:HG23	1.92	0.69
49:Ae:202:LEU:HA	49:Ae:205:VAL:HG22	1.74	0.69
14:N:342:GLN:HE21	29:d:30:ARG:HH11	1.36	0.69
20:T:100:VAL:HB	20:T:142:GLN:HB2	1.74	0.69
28:c:34:PRO:HG2	28:c:37:ALA:HB2	1.74	0.69
31:f:56:TRP:CE3	33:h:131:LYS:HG3	2.26	0.69
49:AE:159:ILE:HG23	49:AE:163:LYS:HE3	1.74	0.69
13:M:216:LEU:HD11	13:M:236:LEU:HD11	1.72	0.69
13:M:369:LEU:HD23	13:M:371:PRO:CD	2.12	0.69
34:i:94:PRO:HG3	41:p:10:TYR:CE2	2.28	0.69
12:L:305:SER:HB2	12:L:422:TYR:HE1	1.57	0.69
14:N:220:MET:C	14:N:223:ASN:H	2.00	0.69
14:N:248:LEU:HD13	14:N:296:LEU:HD23	1.75	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
10:J:3:ASN:HD21	10:J:120:LEU:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:220:LEU:O	47:Ac:145:VAL:HA	1.92	0.69
48:Ad:249:TYR:CZ	48:Ad:252:VAL:HA	2.28	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
9:I:93:LEU:O	42:q:93:MET:HG2	1.93	0.69
12:L:102:GLN:CD	12:L:453:PRO:HD3	2.18	0.69
15:O:40:LEU:HG	15:O:292:HIS:CE1	2.27	0.69
23:X:47:ARG:HH22	33:h:187:PRO:HG3	1.58	0.69
33:h:163:ARG:HG2	33:h:165:ASP:HB2	1.73	0.69
37:l:122:THR:HG21	37:l:129:MET:HE1	1.73	0.69
40:o:8:ARG:HB2	40:o:16:GLU:HG2	1.74	0.69
45:AA:186:TYR:CZ	49:AE:80:HIS:HB2	2.27	0.69
1:A:75:LEU:HD23	10:J:145:TYR:HE2	1.57	0.69
3:C:84:GLU:HG2	3:C:141:ARG:HH11	1.56	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
12:L:153:LEU:HD11	13:M:360:LEU:HD11	1.73	0.69
13:M:263:LEU:HD11	38:m:102:TYR:HD1	1.56	0.69
13:M:409:TYR:CD1	37:l:116:ARG:NH2	2.61	0.69
16:P:344:PRO:HD2	16:P:347:LEU:HD22	1.74	0.69
19:S:23:LEU:HD12	19:S:23:LEU:O	1.93	0.69
19:S:34:ARG:O	19:S:38:VAL:HG23	1.92	0.69
20:T:87:LEU:HD22	20:T:104:PHE:HE1	1.58	0.69
20:T:138:LEU:HD13	20:T:144:ILE:CG1	2.23	0.69
48:AD:244:MET:HB2	70:AD:401:HEC:C1D	2.23	0.69
49:AE:115:TYR:HB3	53:AJ:21:PHE:CE1	2.27	0.69
49:Ae:180:THR:H	49:Ae:183:GLU:HB2	1.58	0.69
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.22	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
9:I:200:GLU:OE2	42:q:93:MET:SD	2.51	0.69
49:AE:207:LYS:HB2	49:AE:210:TRP:HB2	1.73	0.69
49:AI:43:LEU:HD11	46:Ab:163:ALA:CB	2.23	0.69
53:AJ:17:ARG:HD2	53:AJ:20:THR:HG23	1.75	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
7:G:126:LEU:HD11	18:R:89:PRO:CB	2.23	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
10:J:4:TYR:CZ	10:J:8:LEU:HD11	2.28	0.69
11:K:66:PHE:CZ	14:N:35:PHE:CE1	2.80	0.69
12:L:332:HIS:NE2	12:L:336:LYS:HG3	2.07	0.69
14:N:215:MET:HE2	14:N:248:LEU:CD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:171:ASN:OD1	16:P:171:ASN:O	2.11	0.69
19:S:19:ILE:HG13	19:S:95:LEU:CD1	2.22	0.69
47:AC:146:ILE:HG13	68:AC:404:U10:H4M3	1.73	0.69
48:AD:244:MET:HB2	70:AD:401:HEC:ND	2.08	0.69
45:Aa:171:GLU:HA	45:Aa:174:GLU:HG2	1.74	0.69
45:Aa:403:LEU:HD12	45:Aa:403:LEU:N	2.08	0.69
46:Ab:412:VAL:HG13	46:Ab:415:GLN:HE21	1.58	0.69
48:Ad:214:LEU:HD11	48:Ad:237:PHE:HB2	1.75	0.69
5:E:190:ASN:HB3	5:E:192:TYR:CE2	2.28	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
20:U:74:LEU:HD23	20:U:79:ILE:HG12	1.75	0.68
49:AI:43:LEU:HB2	46:Ab:167:GLN:NE2	2.08	0.68
47:Ac:197:LEU:HD12	69:Ac:406:UQ6:C1M	2.22	0.68
48:Ad:186:ARG:HE	48:Ad:193:LEU:HB2	1.58	0.68
3:C:186:ILE:HB	4:D:113:ILE:HD11	1.76	0.68
12:L:18:PRO:O	12:L:21:ILE:HG22	1.92	0.68
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.75	0.68
16:P:191:VAL:HA	16:P:194:VAL:HG22	1.73	0.68
21:V:72:LEU:HD11	21:V:80:VAL:CG2	2.19	0.68
24:Y:77:CYS:SG	24:Y:78:VAL:N	2.66	0.68
40:o:20:GLU:O	40:o:21:LYS:HG2	1.93	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
12:L:312:LEU:HD21	12:L:395:ILE:HG21	1.76	0.68
15:O:140:LEU:HG	15:O:304:VAL:HG12	1.74	0.68
20:T:116:VAL:HG12	20:T:120:MET:HE2	1.75	0.68
36:k:34:PRO:CD	36:k:59:TYR:CD1	2.75	0.68
37:l:78:LEU:HD11	37:l:104:PRO:HB2	1.74	0.68
46:AB:233:VAL:HA	46:AB:236:GLN:HG2	1.76	0.68
48:AD:121:CYS:HA	70:AD:401:HEC:HMC2	1.74	0.68
48:AD:170:LYS:HD2	49:AE:151:LYS:HE2	1.74	0.68
8:H:33:LEU:HD23	43:r:25:GLN:HG2	1.76	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
13:M:311:GLY:HA2	13:M:314:MET:HE3	1.75	0.68
24:Y:143:VAL:CG2	33:h:157:ARG:HG2	2.23	0.68
30:e:8:LYS:HG2	30:e:16:ARG:HH12	1.58	0.68
48:AD:249:TYR:CZ	48:AD:252:VAL:HA	2.28	0.68
45:Aa:188:HIS:HE2	45:Aa:348:TYR:HE2	1.41	0.68
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HE3	1.74	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
19:S:19:ILE:HD12	19:S:94:VAL:HG11	1.76	0.68
24:Y:96:GLY:HA3	24:Y:121:GLY:HA2	1.75	0.68
34:i:102:PRO:HB2	41:p:18:PRO:HD2	1.74	0.68
49:AE:202:LEU:HA	49:AE:205:VAL:HG22	1.74	0.68
45:Aa:68:THR:HG21	46:Ab:384:MET:HG3	1.69	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
12:L:211:ILE:N	12:L:212:PRO:HD2	2.08	0.68
13:M:379:LEU:O	13:M:383:MET:HG3	1.93	0.68
14:N:313:MET:HG3	15:O:305:LEU:HD22	1.75	0.68
34:i:99:SER:O	41:p:116:ARG:HA	1.93	0.68
48:AD:117:TYR:HA	48:AD:121:CYS:HG	1.58	0.68
51:AG:19:LEU:HD11	51:AG:23:GLU:CG	2.24	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
13:M:39:LEU:HD23	13:M:67:ILE:HD13	1.74	0.68
13:M:344:MET:HE1	38:m:59:HIS:NE2	2.08	0.68
14:N:215:MET:HE1	14:N:248:LEU:HD21	1.71	0.68
62:a:101:CDL:H341	62:a:101:CDL:H171	1.74	0.68
38:m:48:LEU:HB3	39:n:166:LEU:HD23	1.74	0.68
45:Aa:68:THR:CG2	46:Ab:384:MET:CG	2.64	0.68
12:L:383:MET:SD	12:L:384:PRO:HD2	2.33	0.68
12:L:556:ILE:HD11	38:m:76:ILE:HG22	1.76	0.68
48:Ad:124:CYS:HA	48:Ad:179:TYR:CE2	2.24	0.68
49:Ae:197:ASP:HB3	49:Ae:257:ASN:CG	2.19	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
6:F:227:PRO:HG3	7:G:94:MET:SD	2.34	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
8:H:114:TYR:CE2	10:J:65:VAL:HG23	2.29	0.68
22:W:84:LEU:HD21	22:W:88:LYS:HE3	1.74	0.68
43:r:20:LEU:C	43:r:20:LEU:HD12	2.18	0.68
45:Aa:281:ALA:HB2	51:Ag:10:ARG:HH22	1.59	0.68
45:Aa:337:LEU:HB3	45:Aa:368:MET:SD	2.34	0.68
47:Ac:29:SER:OG	62:Ac:407:CDL:HA61	1.93	0.68
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.68
5:E:78:VAL:HG12	5:E:104:LEU:HD13	1.76	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
13:M:446:LEU:HD13	32:g:101:THR:CG2	2.23	0.68
20:U:119:ILE:HD11	20:U:138:LEU:HB2	1.76	0.68
21:V:116:ILE:HG23	21:V:116:ILE:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:64:ASN:O	23:X:68:LEU:HG	1.94	0.68
34:i:32:GLU:HG3	39:n:115:TYR:HA	1.76	0.68
46:AB:51:SER:HB2	46:AB:230:LEU:HD12	1.75	0.68
45:Aa:280:ASP:OD2	51:Ag:10:ARG:HA	1.94	0.68
1:A:61:THR:HG22	8:H:290:TRP:CH2	2.29	0.67
7:G:126:LEU:CD1	18:R:89:PRO:HB3	2.25	0.67
12:L:228:GLY:C	12:L:229:LEU:HG	2.19	0.67
15:O:224:PRO:HA	15:O:227:MET:HE3	1.74	0.67
23:X:78:CYS:SG	23:X:111:VAL:HG13	2.34	0.67
47:AC:147:THR:HG22	47:AC:161:VAL:HG13	1.74	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.67
10:J:12:PHE:HE2	11:K:42:ILE:CD1	2.06	0.67
11:K:95:LEU:HG	14:N:54:GLU:CD	2.20	0.67
15:O:347:VAL:O	15:O:347:VAL:CG1	2.42	0.67
46:AB:51:SER:HB2	46:AB:230:LEU:CD1	2.24	0.67
48:AD:218:TYR:CD1	48:AD:246:PRO:HG3	2.29	0.67
1:A:61:THR:HG22	8:H:290:TRP:HH2	1.59	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
14:N:26:LEU:HD23	14:N:29:MET:SD	2.34	0.67
14:N:66:ALA:HB2	14:N:104:MET:SD	2.34	0.67
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.24	0.67
24:Y:34:CYS:HB3	55:Y:201:3PE:C39	2.24	0.67
37:l:122:THR:HG23	37:l:123:PRO:HD2	1.75	0.67
45:AA:342:GLN:HE21	45:AA:357:HIS:HB3	1.59	0.67
46:AB:159:LYS:HE2	49:AI:37:ALA:O	1.94	0.67
46:AB:305:THR:HG23	46:AB:306:THR:HG23	1.77	0.67
2:B:93:MET:HE3	4:D:87:GLN:NE2	2.09	0.67
2:B:95:PHE:HZ	2:B:148:VAL:CB	2.05	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
12:L:456:ARG:HG2	55:L:702:3PE:H221	1.77	0.67
13:M:19:SER:HB2	31:f:8:ARG:HD2	1.77	0.67
13:M:275:ILE:HD11	13:M:288:TYR:CD1	2.29	0.67
13:M:310:MET:HG2	13:M:314:MET:HE2	1.75	0.67
14:N:175:MET:HG2	14:N:219:LEU:CD2	2.23	0.67
19:S:16:LEU:HB3	19:S:69:TYR:HD1	1.58	0.67
26:a:60:TYR:O	26:a:62:VAL:HG13	1.95	0.67
29:d:14:LEU:O	29:d:14:LEU:CD1	2.37	0.67
49:AE:180:THR:H	49:AE:183:GLU:HB2	1.58	0.67
47:Ac:197:LEU:CD1	69:Ac:406:UQ6:H1M2	2.23	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
12:L:80:PHE:C	12:L:135:ASN:ND2	2.53	0.67
13:M:11:LEU:HB3	13:M:100:ILE:HD13	1.76	0.67
13:M:142:ARG:NH2	14:N:303:THR:HG22	2.07	0.67
15:O:114:LEU:HA	15:O:131:LEU:CD2	2.25	0.67
25:Z:121:ILE:HD11	25:Z:136:ALA:CB	2.24	0.67
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.60	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
10:J:102:LEU:O	10:J:106:LEU:HG	1.95	0.67
12:L:9:LEU:HD21	55:L:701:3PE:C2B	2.25	0.67
13:M:30:TYR:O	13:M:34:ILE:HG12	1.95	0.67
16:P:180:SER:O	16:P:184:LYS:HG3	1.95	0.67
16:P:302:GLY:HA2	16:P:314:THR:HG23	1.77	0.67
25:Z:121:ILE:HD11	25:Z:136:ALA:HB1	1.77	0.67
32:g:109:ASP:CB	32:g:114:GLU:HB3	2.24	0.67
37:l:106:HIS:HD2	37:l:107:TRP:H	1.43	0.67
49:AE:154:ILE:CD1	49:AE:273:VAL:HG23	2.25	0.67
47:Ac:242:LEU:HD21	47:Ac:250:LEU:HD11	1.75	0.67
52:Ah:39:GLU:HA	52:Ah:42:VAL:HB	1.75	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
8:H:1:MET:HE3	26:a:29:PHE:HE2	1.58	0.67
9:I:188:GLU:CD	18:R:56:ASN:HB2	2.19	0.67
9:I:188:GLU:OE2	18:R:56:ASN:HB2	1.94	0.67
13:M:98:MET:HE2	13:M:131:ILE:HB	1.77	0.67
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.60	0.67
13:M:285:LEU:HD13	13:M:342:MET:HE1	1.75	0.67
14:N:320:THR:HG23	14:N:320:THR:O	1.93	0.67
29:d:60:ARG:O	29:d:61:GLN:C	2.37	0.67
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.25	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
15:O:305:LEU:HD12	15:O:305:LEU:C	2.20	0.67
19:S:26:ARG:H	19:S:34:ARG:NH1	1.92	0.67
33:h:129:PRO:HG3	41:p:66:ARG:NH2	2.10	0.67
40:o:105:GLU:O	40:o:109:LEU:HD23	1.94	0.67
1:A:112:GLU:O	1:A:112:GLU:OE1	2.12	0.67
4:D:36:GLN:HE21	4:D:38:GLN:NE2	1.93	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
8:H:1:MET:CE	26:a:29:PHE:HE2	2.08	0.67
10:J:121:GLY:C	25:Z:133:MET:SD	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:81:LYS:N	12:L:135:ASN:ND2	2.43	0.67
45:AA:470:ARG:CD	47:AC:222:PRO:HG3	2.24	0.67
48:Ad:120:VAL:CG1	70:Ad:401:HEC:HAB	2.24	0.67
49:Ae:270:VAL:O	49:Ae:271:VAL:CG2	2.42	0.67
4:D:92:HIS:HB2	4:D:458:PHE:CD2	2.30	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
12:L:552:LEU:CD2	12:L:553:LEU:HD12	2.25	0.67
12:L:577:THR:HA	55:Y:201:3PE:H222	1.76	0.67
55:L:701:3PE:C12	34:i:89:HIS:ND1	2.55	0.67
13:M:270:ILE:HG22	13:M:271:MET:HE2	1.76	0.67
13:M:395:LEU:HD21	38:m:101:TRP:CE2	2.29	0.67
15:O:60:ILE:HD12	15:O:203:ALA:HB3	1.77	0.67
16:P:320:GLU:O	16:P:324:ILE:HG12	1.95	0.67
30:e:14:LEU:CD1	30:e:15:ASP:HB2	2.25	0.67
42:q:138:VAL:CG2	42:q:139:PRO:HD2	2.25	0.67
46:AB:412:VAL:HG13	46:AB:415:GLN:HE21	1.58	0.67
45:Aa:66:HIS:CE1	45:Aa:402:HIS:HB2	2.31	0.67
49:Ae:261:PRO:CB	49:Ae:273:VAL:HG11	2.22	0.67
3:C:98:PHE:CA	21:V:90:LEU:HD11	2.21	0.66
12:L:201:ILE:HG22	12:L:266:LEU:HD11	1.75	0.66
16:P:197:GLU:HB3	16:P:259:VAL:CG2	2.24	0.66
24:Y:71:MET:HG3	24:Y:102:THR:CG2	2.26	0.66
44:s:78:TYR:HA	44:s:81:LEU:HD12	1.76	0.66
48:AD:186:ARG:NE	48:AD:193:LEU:HB2	2.09	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.78	0.66
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.76	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
8:H:310:PHE:HB3	27:b:33:PRO:HA	1.77	0.66
9:I:67:ILE:HG13	58:I:302:PC1:H251	1.77	0.66
11:K:1:MET:HG3	11:K:50:ASN:HD22	1.61	0.66
12:L:428:TYR:OH	39:n:33:HIS:HE1	1.76	0.66
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.78	0.66
13:M:123:GLU:HB3	14:N:255:PRO:HG2	1.77	0.66
13:M:361:MET:CB	13:M:441:MET:HE3	2.25	0.66
16:P:94:LEU:HA	16:P:97:MET:HE3	1.77	0.66
20:U:128:PHE:CZ	20:U:148:ILE:HD12	2.30	0.66
33:h:102:PRO:HD2	33:h:105:TYR:HB2	1.77	0.66
49:AE:153:GLU:C	49:AE:154:ILE:HD12	2.19	0.66
49:AE:197:ASP:HB3	49:AE:257:ASN:CG	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:248:ILE:HD11	70:Ad:401:HEC:CBB	2.25	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:240:PRO:HG3	6:F:57:LEU:O	1.94	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
12:L:407:TRP:CE3	12:L:410:LEU:HD11	2.29	0.66
15:O:343:TYR:HD1	15:O:352:ILE:HG23	1.59	0.66
24:Y:76:THR:HG22	24:Y:92:TYR:HA	1.77	0.66
32:g:147:LEU:HD21	41:p:163:MET:HB2	1.77	0.66
51:AG:11:ILE:CG2	51:AG:14:VAL:HG21	2.18	0.66
51:Ag:49:VAL:O	51:Ag:52:PRO:HD2	1.96	0.66
53:Aj:31:PHE:CD1	54:Ak:48:ILE:HG23	2.30	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:253:LEU:HB2	43:r:23:LYS:CD	2.26	0.66
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.77	0.66
10:J:55:VAL:HB	11:K:41:PHE:CE2	2.30	0.66
55:M:501:3PE:C2A	62:h:201:CDL:H202	2.25	0.66
14:N:273:ASN:ND2	24:Y:143:VAL:HA	2.11	0.66
16:P:288:PHE:CZ	16:P:290:PRO:HB3	2.30	0.66
37:l:38:PRO:HB2	38:m:75:ASN:ND2	2.10	0.66
45:AA:186:TYR:CE1	49:AE:80:HIS:HB2	2.30	0.66
46:AB:229:VAL:O	46:AB:232:GLN:HG2	1.95	0.66
51:AG:11:ILE:CG2	51:AG:14:VAL:HG22	2.25	0.66
49:Ae:112:GLY:HA2	53:Aj:15:PHE:CD2	2.30	0.66
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.49	0.66
8:H:114:TYR:CE1	10:J:33:ILE:HD13	2.29	0.66
9:I:35:THR:CG2	43:r:107:SER:HA	2.26	0.66
12:L:174:TYR:CD2	12:L:232:TRP:CD1	2.68	0.66
13:M:255:LYS:NZ	29:d:117:HIS:HB3	2.11	0.66
25:Z:93:GLU:OE2	30:e:95:PRO:HD2	1.96	0.66
51:Ag:19:LEU:HD11	51:Ag:23:GLU:CG	2.24	0.66
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.10	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.59	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
9:I:92:PRO:HA	42:q:91:HIS:O	1.96	0.66
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.31	0.66
12:L:518:PRO:HD2	12:L:520:SER:HB2	1.78	0.66
13:M:395:LEU:HD21	38:m:101:TRP:CZ2	2.30	0.66
14:N:197:ASN:CG	14:N:200:LEU:HD13	2.21	0.66
30:e:86:LEU:HB3	30:e:91:LYS:HB2	1.78	0.66
31:f:41:SER:O	31:f:45:GLN:HB2	1.96	0.66
33:h:57:VAL:HG12	39:n:99:VAL:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:25:PHE:HE2	40:o:109:LEU:HD22	1.60	0.66
49:Ae:169:TRP:CZ3	49:Ae:273:VAL:HB	2.31	0.66
55:A:401:3PE:H2C2	10:J:37:PHE:CZ	2.31	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.76	0.66
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.24	0.66
15:O:200:PRO:HG3	15:O:282:PRO:HD2	1.77	0.66
18:R:97:LYS:HE3	18:R:100:LYS:HD3	1.78	0.66
20:T:87:LEU:CD2	20:T:104:PHE:CZ	2.78	0.66
33:h:183:PRO:C	33:h:184:LYS:HG2	2.17	0.66
45:Aa:68:THR:HB	46:Ab:387:GLU:OE1	1.96	0.66
45:Aa:74:TRP:CZ2	45:Aa:411:GLU:HA	2.31	0.66
1:A:54:LYS:O	1:A:58:VAL:HG23	1.95	0.66
3:C:149:LEU:HD11	22:W:80:ARG:HH21	1.57	0.66
9:I:80:GLU:OE2	43:r:26:LEU:CD1	2.44	0.66
10:J:56:PHE:O	10:J:60:LEU:HB3	1.96	0.66
12:L:116:ARG:HG2	12:L:120:TYR:CE2	2.31	0.66
12:L:141:PHE:CD2	13:M:375:LEU:HD21	2.31	0.66
12:L:552:LEU:HD23	12:L:553:LEU:HD12	1.77	0.66
16:P:156:SER:CB	16:P:161:VAL:HG22	2.20	0.66
20:T:83:VAL:HG22	20:T:126:PHE:CZ	2.31	0.66
20:T:130:ILE:HG23	20:T:131:PRO:HD2	1.77	0.66
21:V:72:LEU:HD12	21:V:72:LEU:C	2.19	0.66
47:Ac:257:MET:HG3	48:Ad:203:ALA:HB1	1.78	0.66
49:Ae:152:ILE:HG23	49:Ae:273:VAL:H	1.56	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
10:J:9:SER:CB	11:K:7:ASN:ND2	2.54	0.66
12:L:25:ASN:OD1	12:L:25:ASN:O	2.14	0.66
13:M:318:ALA:HB2	13:M:373:ILE:HG23	1.76	0.66
14:N:25:ASN:ND2	30:e:18:PHE:CE2	2.64	0.66
15:O:249:MET:HB3	15:O:253:CYS:SG	2.36	0.66
16:P:199:ILE:HD11	16:P:258:ALA:O	1.96	0.66
16:P:268:PRO:HG2	16:P:344:PRO:HA	1.76	0.66
18:R:76:ILE:HD11	18:R:92:TYR:HB3	1.77	0.66
36:k:34:PRO:CG	36:k:59:TYR:CE1	2.72	0.66
47:Ac:240:MET:HE1	71:Ad:402:3PH:H231	1.76	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:303:TRP:CZ3	27:b:28:LEU:HG	2.31	0.66
21:V:44:TYR:CE1	21:V:48:THR:HG23	2.30	0.66
21:V:72:LEU:O	21:V:72:LEU:CD1	2.42	0.66
33:h:163:ARG:HG2	33:h:165:ASP:CB	2.26	0.66
51:Ag:11:ILE:CG2	51:Ag:14:VAL:HG22	2.25	0.66
16:P:263:PHE:HD2	16:P:333:PRO:O	1.79	0.65
20:U:134:ASP:OD2	39:n:2:ALA:N	2.29	0.65
25:Z:97:ILE:HG13	25:Z:98:MET:H	1.61	0.65
38:m:49:LEU:HD12	38:m:49:LEU:O	1.95	0.65
8:H:93:HIS:HE1	26:a:24:ALA:HA	1.61	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
8:H:311:THR:HB	25:Z:51:MET:SD	2.36	0.65
12:L:141:PHE:CE2	13:M:375:LEU:HD22	2.12	0.65
12:L:142:ILE:HA	13:M:370:PRO:HB2	1.78	0.65
12:L:293:LEU:HD11	12:L:418:MET:SD	2.36	0.65
12:L:481:THR:HB	40:o:95:TYR:CD2	2.31	0.65
13:M:373:ILE:CD1	13:M:454:ILE:HD11	2.25	0.65
47:AC:45:ILE:HA	67:AC:401:HEM:HAB	1.79	0.65
49:Ae:93:ARG:HH11	49:Ae:110:ARG:CG	2.09	0.65
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:671:LEU:HD21	19:S:45:LYS:HG2	1.77	0.65
12:L:186:MET:SD	13:M:379:LEU:HD21	2.36	0.65
13:M:175:ASN:HD22	33:h:143:GLU:HG2	1.61	0.65
19:S:24:CYS:HA	19:S:58:CYS:O	1.97	0.65
21:V:38:PHE:CD1	21:V:95:LEU:HD21	2.31	0.65
22:W:24:PHE:HB2	22:W:83:ASP:CG	2.20	0.65
23:X:158:LEU:HB3	29:d:21:LEU:HD21	1.77	0.65
25:Z:98:MET:CE	25:Z:101:VAL:HG21	2.27	0.65
48:Ad:121:CYS:SG	70:Ad:401:HEC:CBB	2.83	0.65
48:Ad:192:ALA:CB	70:Ad:401:HEC:HMD3	2.25	0.65
2:B:122:ARG:HH11	4:D:89:PRO:CB	2.08	0.65
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.65
10:J:22:LYS:HB2	11:K:23:ARG:HD3	1.78	0.65
12:L:141:PHE:CE2	13:M:370:PRO:CG	2.73	0.65
13:M:367:LEU:CD2	13:M:408:MET:HE2	2.25	0.65
18:R:70:ASN:HB2	18:R:111:PHE:CD1	2.31	0.65
49:AI:64:LEU:HD13	46:Ab:174:ILE:HG21	1.78	0.65
4:D:84:PHE:HZ	4:D:90:ALA:CB	2.09	0.65
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.25	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:TYR:CE2	26:a:5:ILE:HG22	2.31	0.65
12:L:190:SER:HB2	12:L:196:TRP:HE1	1.60	0.65
12:L:214:MET:CG	55:L:704:3PE:H281	2.26	0.65
14:N:120:GLN:HG3	14:N:177:LYS:HE3	1.78	0.65
14:N:156:MET:HA	14:N:159:ILE:HG22	1.77	0.65
15:O:73:LEU:HD21	15:O:269:VAL:HG11	1.76	0.65
19:S:16:LEU:HB3	19:S:69:TYR:CD1	2.32	0.65
20:T:118:ILE:HG23	20:T:122:MET:HE3	1.78	0.65
46:Ab:261:GLN:HA	46:Ab:442:GLY:O	1.97	0.65
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.65
10:J:105:VAL:O	10:J:108:TYR:HB3	1.96	0.65
14:N:332:MET:SD	14:N:336:THR:HG21	2.37	0.65
16:P:236:VAL:CG1	16:P:270:ARG:HH21	2.10	0.65
20:U:74:LEU:HD23	20:U:79:ILE:CG1	2.27	0.65
47:AC:137:GLN:CG	47:AC:265:PRO:HG3	2.27	0.65
48:AD:138:VAL:HG11	48:AD:276:TRP:NE1	2.11	0.65
1:A:75:LEU:HD23	10:J:145:TYR:CE2	2.32	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
10:J:12:PHE:CZ	11:K:42:ILE:CD1	2.80	0.65
12:L:88:LEU:HD23	12:L:326:PHE:CE2	2.32	0.65
16:P:226:VAL:HG21	16:P:281:PHE:CZ	2.32	0.65
25:Z:75:PHE:CD1	26:a:46:TYR:HE2	2.15	0.65
25:Z:111:PHE:CE1	30:e:65:GLU:HG3	2.31	0.65
49:AI:70:LEU:HD13	46:Ab:88:SER:HB3	1.78	0.65
47:Ac:240:MET:CE	71:Ad:402:3PH:H231	2.27	0.65
7:G:651:PRO:HG3	19:S:57:GLU:H	1.61	0.65
8:H:180:PRO:HD3	25:Z:43:LEU:HD21	1.79	0.65
10:J:33:ILE:CG2	10:J:60:LEU:HD21	2.26	0.65
10:J:39:GLY:HA2	10:J:42:MET:HE3	1.78	0.65
11:K:66:PHE:CE1	14:N:35:PHE:CZ	2.84	0.65
15:O:58:ARG:HA	15:O:202:HIS:ND1	2.11	0.65
16:P:156:SER:CB	16:P:161:VAL:CG2	2.66	0.65
32:g:106:TYR:OH	33:h:86:ILE:HD12	1.97	0.65
32:g:108:PRO:O	32:g:109:ASP:OD1	2.13	0.65
40:o:25:PHE:CE2	40:o:109:LEU:HD22	2.31	0.65
47:AC:197:LEU:O	47:AC:201:HIS:CD2	2.50	0.65
48:AD:181:ASN:HB2	48:AD:182:PRO:HD2	1.78	0.65
49:Ae:152:ILE:HD12	49:Ae:169:TRP:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.62	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.65
12:L:387:THR:HG22	12:L:465:GLY:H	1.61	0.65
62:L:705:CDL:HA62	33:h:68:LEU:CD1	2.21	0.65
13:M:388:TRP:NE1	38:m:109:ARG:HD2	2.12	0.65
16:P:363:SER:HB3	22:W:51:HIS:CD2	2.32	0.65
31:f:38:ARG:NH1	31:f:54:VAL:HG21	2.11	0.65
47:AC:287:LYS:HZ1	49:Ae:255:PRO:HG2	1.62	0.65
48:AD:202:ARG:HG3	48:AD:278:SER:HB3	1.78	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
8:H:118:TRP:CE2	10:J:30:LEU:HD22	2.32	0.65
11:K:96:LEU:O	11:K:97:GLN:C	2.40	0.65
13:M:122:PHE:HD1	13:M:238:LEU:HG	1.62	0.65
14:N:307:THR:O	15:O:319:ILE:N	2.30	0.65
15:O:168:VAL:CG2	15:O:241:TYR:CZ	2.62	0.65
15:O:343:TYR:CE1	15:O:355:LYS:HB2	2.32	0.65
16:P:169:HIS:H	16:P:184:LYS:HE3	1.61	0.65
33:h:127:ASP:OD1	33:h:127:ASP:O	2.15	0.65
34:i:123:PHE:CD2	40:o:40:VAL:HG11	2.32	0.65
49:AE:127:TYR:CE1	53:AJ:33:GLU:HG3	2.30	0.65
46:Ab:307:SER:HB2	46:Ab:310:SER:H	1.62	0.65
1:A:90:MET:CE	10:J:152:MET:CG	2.76	0.64
3:C:99:LEU:HD13	3:C:140:ILE:CD1	2.27	0.64
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
12:L:385:PHE:CD1	35:j:72:ARG:HG3	2.32	0.64
17:Q:163:ASN:OD1	17:Q:164:PHE:N	2.31	0.64
18:R:38:TYR:HB2	18:R:45:ARG:HD3	1.79	0.64
25:Z:110:VAL:HG11	30:e:72:THR:CG2	2.27	0.64
40:o:71:ARG:HB3	40:o:71:ARG:HH11	1.61	0.64
41:p:24:THR:HG22	41:p:26:LEU:H	1.63	0.64
45:AA:403:LEU:HD21	46:AB:56:ALA:HB1	1.79	0.64
47:Ac:141:TRP:HD1	47:Ac:265:PRO:HD3	1.62	0.64
4:D:52:MET:O	4:D:54:PRO:HD3	1.98	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
12:L:368:PHE:HB3	12:L:445:GLU:OE2	1.97	0.64
13:M:119:TYR:CD1	13:M:160:LEU:HD22	2.33	0.64
15:O:58:ARG:HG2	15:O:278:TYR:CD2	2.33	0.64
25:Z:69:ILE:HD12	27:b:53:TYR:HA	1.78	0.64
35:j:100:PRO:HG3	40:o:29:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:403:LEU:HD12	45:AA:403:LEU:N	2.12	0.64
45:Aa:50:VAL:HG11	45:Aa:417:LEU:HD11	1.80	0.64
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HA	1.80	0.64
48:Ad:248:ILE:HG22	48:Ad:263:MET:HG3	1.79	0.64
49:Ae:93:ARG:CD	49:Ae:110:ARG:HD3	2.26	0.64
49:Ae:152:ILE:HD11	49:Ae:174:LEU:HD21	1.78	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
13:M:167:ILE:O	13:M:171:VAL:HG12	1.98	0.64
55:M:503:3PE:H332	55:M:503:3PE:H372	1.78	0.64
15:O:117:PHE:CE1	15:O:173:MET:CE	2.77	0.64
15:O:194:THR:HG23	15:O:307:TYR:HB2	1.79	0.64
16:P:88:VAL:HG12	16:P:92:MET:HE2	1.79	0.64
22:W:115:THR:O	22:W:116:PRO:C	2.39	0.64
37:l:122:THR:CG2	37:l:123:PRO:HD2	2.27	0.64
47:AC:201:HIS:HE1	69:AC:405:UQ6:C1M	2.09	0.64
48:AD:214:LEU:HG	48:AD:234:ASN:ND2	2.12	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.13	0.64
10:J:99:GLU:O	10:J:103:ILE:HG12	1.98	0.64
12:L:81:LYS:N	12:L:135:ASN:HD21	1.96	0.64
12:L:366:MET:CG	12:L:443:ILE:HG21	2.28	0.64
12:L:385:PHE:CE1	35:j:72:ARG:HG3	2.33	0.64
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.78	0.64
24:Y:137:LEU:HD23	24:Y:138:PHE:CG	2.31	0.64
29:d:109:TYR:HA	29:d:112:ILE:CG2	2.28	0.64
37:l:158:PRO:HG3	40:o:23:PRO:HD3	1.79	0.64
45:Aa:87:ASN:H	45:Aa:207:ASN:ND2	1.94	0.64
49:Ae:153:GLU:HA	49:Ae:271:VAL:O	1.98	0.64
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.64
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
8:H:33:LEU:CD2	43:r:25:GLN:HG2	2.26	0.64
8:H:172:MET:HE1	25:Z:46:GLY:CA	2.28	0.64
12:L:40:ILE:HD13	12:L:97:THR:HG22	1.79	0.64
12:L:556:ILE:CG2	38:m:80:PHE:CZ	2.80	0.64
14:N:220:MET:HA	14:N:223:ASN:HA	1.78	0.64
14:N:275:CYS:SG	24:Y:139:PRO:HG2	2.37	0.64
20:T:83:VAL:HG23	20:T:126:PHE:HZ	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
12:L:556:ILE:HG23	38:m:80:PHE:CE2	2.33	0.64
13:M:300:SER:HB3	13:M:381:ILE:HG23	1.78	0.64
16:P:299:SER:CB	16:P:316:LYS:HE3	2.23	0.64
19:S:69:TYR:CD2	19:S:75:LYS:HG3	2.33	0.64
49:AE:218:THR:CG2	49:AE:256:LEU:O	2.45	0.64
49:AI:77:ARG:O	49:AI:78:PHE:C	2.40	0.64
47:Ac:220:PHE:CE2	69:Ac:406:UQ6:H4M2	2.33	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
11:K:66:PHE:CE1	14:N:35:PHE:CE1	2.86	0.64
12:L:41:LYS:HG3	12:L:98:TRP:CE2	2.33	0.64
12:L:246:LEU:HD12	12:L:246:LEU:C	2.22	0.64
14:N:37:LEU:HD12	14:N:63:GLN:HB3	1.79	0.64
49:Ae:93:ARG:HD2	49:Ae:110:ARG:HD3	1.76	0.64
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
13:M:160:LEU:HD11	13:M:203:PHE:CZ	2.33	0.64
16:P:106:LEU:HD21	18:R:49:VAL:HG11	1.79	0.64
20:T:138:LEU:O	20:T:138:LEU:CD1	2.40	0.64
39:n:97:TYR:HB2	39:n:178:PRO:HG2	1.77	0.64
45:AA:274:GLU:HG3	45:AA:456:VAL:HB	1.80	0.64
49:Ae:156:LEU:HB2	49:Ae:269:ASP:HA	1.80	0.64
49:Ae:234:TYR:HB2	49:Ae:243:TYR:HB2	1.79	0.64
10:J:39:GLY:HA2	10:J:42:MET:CE	2.27	0.64
18:R:112:LYS:O	18:R:113:GLN:C	2.40	0.64
34:i:102:PRO:CB	41:p:18:PRO:CD	2.76	0.64
48:AD:248:ILE:HG22	48:AD:263:MET:HG3	1.79	0.64
1:A:90:MET:CE	10:J:152:MET:CB	2.76	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.64
5:E:81:VAL:HB	5:E:104:LEU:HD11	1.79	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
12:L:550:LEU:HB2	13:M:275:ILE:HG22	1.80	0.64
62:L:706:CDL:C52	24:Y:107:THR:CG2	2.68	0.64
13:M:196:TRP:HZ3	13:M:261:PHE:HE2	1.44	0.64
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.32	0.64
16:P:333:PRO:HB2	16:P:337:ASP:HB2	1.80	0.64
20:T:87:LEU:HD21	20:T:104:PHE:CZ	2.32	0.64
24:Y:143:VAL:O	33:h:158:ARG:NH2	2.31	0.64
34:i:29:SER:HB2	34:i:32:GLU:OE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:106:HIS:CD2	37:l:107:TRP:N	2.66	0.64
45:Aa:171:GLU:O	45:Aa:175:ASN:N	2.28	0.64
46:Ab:426:LYS:O	46:Ab:429:LYS:HG2	1.97	0.64
47:Ac:137:GLN:HE21	47:Ac:265:PRO:HD3	1.62	0.64
49:Ae:152:ILE:CD1	49:Ae:174:LEU:HD22	2.28	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.63
8:H:172:MET:HE1	25:Z:46:GLY:HA2	1.80	0.63
12:L:305:SER:HB2	12:L:422:TYR:CE1	2.33	0.63
15:O:168:VAL:CG2	15:O:241:TYR:CE1	2.77	0.63
19:S:16:LEU:HD12	19:S:16:LEU:C	2.22	0.63
20:T:93:ILE:CG2	20:T:110:LEU:HD13	2.28	0.63
25:Z:62:ILE:HG12	27:b:49:THR:HG22	1.79	0.63
25:Z:97:ILE:HG22	30:e:92:TYR:CG	2.33	0.63
31:f:41:SER:OG	33:h:134:GLU:HG2	1.99	0.63
40:o:94:ASP:HA	40:o:97:LYS:CG	2.27	0.63
46:AB:48:VAL:CG2	46:AB:400:ALA:HB1	2.27	0.63
54:Ak:13:LEU:HB3	54:Ak:17:TRP:CH2	2.33	0.63
1:A:54:LYS:HD2	1:A:113:TRP:HB2	1.79	0.63
2:B:122:ARG:HG2	57:B:302:UQ1:H102	1.81	0.63
4:D:90:ALA:O	4:D:91:ALA:HB3	1.96	0.63
4:D:280:ALA:HB1	21:V:11:LEU:HG	1.78	0.63
4:D:348:LEU:O	25:Z:11:PRO:HB3	1.98	0.63
5:E:87:ARG:HD2	44:s:77:THR:HG22	1.80	0.63
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
8:H:118:TRP:CZ2	10:J:30:LEU:HD22	2.33	0.63
14:N:163:PHE:CD1	14:N:285:MET:HG3	2.33	0.63
23:X:167:PHE:HB3	23:X:170:TRP:CD1	2.33	0.63
40:o:17:PRO:HG3	40:o:106:ARG:HA	1.78	0.63
45:AA:92:PHE:CZ	45:AA:161:ILE:HG23	2.33	0.63
45:AA:182:VAL:HG12	45:AA:186:TYR:CE2	2.33	0.63
48:AD:323:PRO:HG2	48:AD:325:LYS:HD2	1.80	0.63
47:Ac:253:PRO:O	48:Ad:203:ALA:HA	1.98	0.63
49:Ae:188:ALA:HA	49:Ae:200:HIS:NE2	2.13	0.63
49:Ae:218:THR:CG2	49:Ae:256:LEU:O	2.45	0.63
1:A:50:PRO:HB3	10:J:73:MET:O	1.98	0.63
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.63
4:D:35:ARG:O	4:D:36:GLN:C	2.37	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:381:THR:HG21	12:L:498:PHE:CE2	2.33	0.63
13:M:250:LEU:O	13:M:250:LEU:CD1	2.44	0.63
14:N:193:ILE:HD13	14:N:200:LEU:CB	2.29	0.63
14:N:211:LEU:HD23	14:N:333:SER:CB	2.26	0.63
20:U:86:VAL:HB	20:U:122:MET:HE1	1.79	0.63
20:U:140:CYS:SG	20:U:143:GLU:OE2	2.52	0.63
21:V:38:PHE:CE1	21:V:95:LEU:HD21	2.33	0.63
23:X:145:ARG:NH1	30:e:58:ILE:HG13	2.13	0.63
34:i:102:PRO:CG	41:p:18:PRO:CD	2.77	0.63
39:n:94:TYR:CD2	39:n:177:ARG:HG3	2.34	0.63
49:AE:188:ALA:HA	49:AE:200:HIS:NE2	2.13	0.63
1:A:99:SER:HB3	55:b:201:3PE:H392	1.81	0.63
4:D:88:HIS:NE2	8:H:205:SER:HA	2.14	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
12:L:100:ILE:HD13	12:L:341:MET:SD	2.39	0.63
12:L:410:LEU:HD12	12:L:411:ILE:N	2.13	0.63
12:L:433:THR:HG22	12:L:434:LYS:N	2.13	0.63
62:L:706:CDL:C52	24:Y:107:THR:HG21	2.28	0.63
13:M:220:HIS:NE2	13:M:231:LEU:HB3	2.13	0.63
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.80	0.63
16:P:93:HIS:NE2	16:P:94:LEU:HD11	2.14	0.63
29:d:106:LYS:HB3	41:p:79:GLU:HB3	1.81	0.63
32:g:75:ASP:OD1	32:g:76:SER:N	2.32	0.63
48:AD:91:PRO:HB3	48:AD:213:SER:OG	1.99	0.63
48:AD:255:TYR:OH	48:AD:266:VAL:HA	1.98	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:375:MET:HE1	7:G:126:LEU:HA	1.80	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
11:K:70:GLU:HA	14:N:38:LEU:HD21	1.79	0.63
12:L:149:ILE:HG13	13:M:369:LEU:HD12	1.81	0.63
13:M:1:MET:HB2	13:M:52:PHE:HD2	1.60	0.63
13:M:105:LEU:O	13:M:109:THR:HG23	1.98	0.63
13:M:118:PHE:O	13:M:122:PHE:N	2.25	0.63
13:M:368:ALA:HB1	13:M:375:LEU:CD1	2.25	0.63
19:S:19:ILE:CG1	19:S:95:LEU:HD11	2.26	0.63
36:k:34:PRO:HG2	36:k:59:TYR:CD1	2.34	0.63
43:r:109:ASP:O	43:r:110:GLN:HG2	1.99	0.63
45:AA:204:PRO:HB2	45:AA:206:GLU:OE1	1.98	0.63
46:Ab:60:ARG:HD2	46:Ab:393:LEU:HD13	1.81	0.63
46:Ab:230:LEU:HA	46:Ab:233:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:37:LEU:HD13	67:Ac:403:HEM:C3B	2.34	0.63
1:A:75:LEU:CD2	10:J:145:TYR:CE2	2.82	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
11:K:1:MET:HG3	11:K:50:ASN:ND2	2.14	0.63
12:L:80:PHE:C	12:L:135:ASN:HD21	2.06	0.63
20:T:103:HIS:CD2	20:T:106:LYS:HD2	2.34	0.63
24:Y:19:GLN:NE2	24:Y:22:ARG:HG2	2.09	0.63
31:f:38:ARG:NH1	31:f:54:VAL:CG2	2.62	0.63
45:AA:96:LEU:HD11	45:AA:161:ILE:HG12	1.79	0.63
46:AB:40:PHE:CZ	46:AB:48:VAL:HB	2.34	0.63
46:AB:426:LYS:O	46:AB:429:LYS:HG2	1.97	0.63
47:AC:141:TRP:HD1	47:AC:265:PRO:HD3	1.61	0.63
47:AC:326:TRP:CZ2	55:AC:403:3PE:H11	2.31	0.63
48:AD:195:PRO:CG	70:AD:401:HEC:HBA1	2.29	0.63
45:Aa:266:THR:HG23	45:Aa:266:THR:O	1.99	0.63
45:Aa:403:LEU:HD21	46:Ab:56:ALA:CB	2.29	0.63
49:Ae:93:ARG:HH11	49:Ae:110:ARG:HG2	1.63	0.63
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.81	0.63
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.60	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
10:J:5:ILE:CG2	10:J:120:LEU:HD13	2.28	0.63
12:L:202:MET:HE3	12:L:265:PRO:CG	2.25	0.63
19:S:15:GLY:HA3	19:S:17:ARG:HH22	1.63	0.63
19:S:16:LEU:HA	19:S:69:TYR:HA	1.79	0.63
20:U:88:LYS:HG2	20:U:98:LEU:HD21	1.80	0.63
23:X:83:THR:HA	23:X:86:TRP:CD1	2.34	0.63
33:h:96:ALA:HB3	41:p:63:TYR:CD1	2.33	0.63
45:Aa:110:GLU:O	45:Aa:114:GLU:HG2	1.99	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
55:L:701:3PE:H122	34:i:89:HIS:CG	2.34	0.63
55:M:502:3PE:H2D2	55:M:502:3PE:H3E2	1.79	0.63
15:O:227:MET:C	15:O:228:LYS:HG2	2.23	0.63
16:P:132:ARG:HG2	64:P:401:NDP:C8A	2.29	0.63
33:h:155:GLU:O	33:h:159:LEU:HD13	1.99	0.63
34:i:28:LEU:HD22	34:i:32:GLU:HG2	1.79	0.63
45:AA:469:ASN:ND2	47:AC:223:TYR:CZ	2.67	0.63
46:AB:48:VAL:HG22	46:AB:219:ALA:CB	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:287:LYS:NZ	49:Ae:255:PRO:HG2	2.14	0.63
49:Ae:161:GLU:HA	49:Ae:178:HIS:CG	2.34	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
10:J:18:GLY:O	10:J:23:PRO:HD3	1.98	0.63
13:M:129:THR:HG21	13:M:235:LEU:HD13	1.80	0.63
14:N:172:GLN:OE1	14:N:177:LYS:HD3	1.98	0.63
14:N:193:ILE:HD11	14:N:200:LEU:HD22	1.81	0.63
55:AC:403:3PE:H291	51:AG:41:ARG:HE	1.62	0.63
52:AH:49:GLU:HA	52:AH:52:ASP:OD2	1.99	0.63
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.64	0.62
8:H:1:MET:HE3	26:a:29:PHE:CD2	2.33	0.62
9:I:188:GLU:HG3	18:R:55:VAL:HA	1.80	0.62
12:L:361:ASN:OD1	12:L:361:ASN:O	2.17	0.62
19:S:16:LEU:CD2	19:S:19:ILE:HD11	2.28	0.62
37:l:30:PHE:CD2	37:l:31:HIS:ND1	2.67	0.62
47:AC:218:ILE:HD11	47:AC:224:TYR:CE2	2.34	0.62
45:Aa:274:GLU:HG3	45:Aa:456:VAL:HB	1.80	0.62
46:Ab:92:LYS:HG2	46:Ab:145:GLU:HG3	1.81	0.62
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.62
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.62
12:L:437:PHE:CE1	12:L:441:ILE:CG1	2.69	0.62
12:L:445:GLU:HB2	12:L:450:LEU:CD2	2.29	0.62
13:M:73:LEU:CD2	13:M:103:GLN:NE2	2.61	0.62
55:M:503:3PE:H391	55:M:503:3PE:H232	1.80	0.62
22:W:83:ASP:O	22:W:86:VAL:HG22	1.99	0.62
23:X:53:PRO:O	23:X:57:LEU:HG	1.99	0.62
25:Z:65:LEU:HB3	27:b:50:PRO:O	1.99	0.62
47:Ac:223:TYR:O	48:Ad:311:TRP:NE1	2.27	0.62
48:Ad:186:ARG:NE	48:Ad:193:LEU:HB2	2.14	0.62
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.64	0.62
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.62
13:M:264:LEU:HD23	38:m:98:LEU:HD11	1.82	0.62
13:M:307:TRP:CE3	13:M:383:MET:HE3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:297:VAL:O	16:P:300:TRP:HB3	1.98	0.62
31:f:56:TRP:CZ3	33:h:131:LYS:HG3	2.35	0.62
43:r:20:LEU:HD12	43:r:21:GLN:N	2.14	0.62
48:AD:129:TYR:HD2	48:AD:198:SER:CB	2.12	0.62
49:AE:161:GLU:HA	49:AE:178:HIS:CG	2.34	0.62
49:AE:174:LEU:HD21	49:AE:273:VAL:HG21	1.81	0.62
47:Ac:138:MET:CE	47:Ac:268:ILE:HG23	2.28	0.62
48:Ad:255:TYR:OH	48:Ad:266:VAL:HA	1.98	0.62
49:Ae:179:ARG:HH12	49:Ae:201:ASP:HB2	1.64	0.62
49:Ae:213:LEU:HD23	49:Ae:260:VAL:HG22	1.81	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
10:J:169:ILE:HD13	14:N:45:ILE:HD11	1.81	0.62
13:M:318:ALA:CB	13:M:373:ILE:HG23	2.29	0.62
16:P:240:VAL:HB	16:P:266:THR:O	2.00	0.62
20:T:103:HIS:ND1	20:T:140:CYS:SG	2.73	0.62
45:AA:169:LEU:HD11	45:AA:209:ARG:HG2	1.82	0.62
55:AC:403:3PE:H292	51:AG:41:ARG:HH21	1.62	0.62
51:Ag:74:ASN:HB3	51:Ag:77:MET:HB2	1.81	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
62:L:705:CDL:H581	62:L:705:CDL:H792	1.80	0.62
13:M:16:TRP:CE3	55:O:401:3PE:H12	2.35	0.62
15:O:121:PRO:O	15:O:122:LYS:CG	2.46	0.62
20:U:72:PRO:HG3	35:j:42:PRO:HG2	1.81	0.62
23:X:115:LEU:HD13	23:X:117:TRP:CH2	2.34	0.62
25:Z:97:ILE:HG23	30:e:92:TYR:CE1	2.35	0.62
62:a:101:CDL:H1	43:r:3:SER:HB2	1.81	0.62
51:Ag:43:ARG:HD3	55:Ag:102:3PE:H3B2	1.81	0.62
1:A:94:LEU:HD22	10:J:152:MET:HE1	1.81	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
7:G:176:CYS:SG	56:G:802:SF4:FE4	1.78	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
12:L:9:LEU:HD21	55:L:701:3PE:C2C	2.29	0.62
12:L:365:ILE:HD11	12:L:366:MET:HE2	1.82	0.62
13:M:129:THR:HG21	13:M:235:LEU:CD1	2.30	0.62
14:N:124:LEU:CD2	14:N:176:ARG:HG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:113:SER:HB3	15:O:116:LYS:HB2	1.80	0.62
39:n:168:TRP:O	39:n:172:THR:OG1	2.18	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.30	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
14:N:207:ILE:O	14:N:211:LEU:HG	2.00	0.62
15:O:117:PHE:HE1	15:O:128:SER:HB2	1.63	0.62
15:O:132:GLN:HE22	15:O:169:PHE:HB2	1.64	0.62
20:T:87:LEU:CD2	20:T:104:PHE:HZ	2.12	0.62
23:X:167:PHE:HD2	23:X:170:TRP:NE1	1.96	0.62
49:AE:234:TYR:HB2	49:AE:243:TYR:HB2	1.79	0.62
1:A:3:LEU:HD23	55:A:401:3PE:H251	1.80	0.62
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.35	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
12:L:174:TYR:CE1	55:L:703:3PE:H331	2.34	0.62
12:L:187:VAL:HG22	13:M:383:MET:HG2	1.82	0.62
62:L:705:CDL:H321	33:h:71:MET:HE1	1.81	0.62
14:N:163:PHE:CE1	14:N:285:MET:HG3	2.34	0.62
15:O:323:GLN:HE22	32:g:54:GLN:HB3	1.64	0.62
20:U:104:PHE:HD1	20:U:108:LEU:HD12	1.65	0.62
45:AA:119:HIS:ND1	46:AB:298:HIS:HA	2.15	0.62
45:Aa:222:ARG:NH2	45:Aa:263:PRO:HB3	2.15	0.62
53:Aj:30:LEU:HD23	54:Ak:48:ILE:HG21	1.82	0.62
1:A:101:GLY:HA3	10:J:163:ILE:HD12	1.81	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:78:PHE:HD1	26:a:2:TRP:CD1	2.17	0.62
13:M:56:PHE:HE1	13:M:108:MET:HG2	1.64	0.62
45:AA:399:LEU:HB3	45:AA:426:LEU:CD2	2.30	0.62
46:Ab:117:GLU:OE2	46:Ab:331:SER:N	2.24	0.62
54:Ak:45:VAL:HB	54:Ak:48:ILE:HD11	1.82	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
12:L:10:LEU:HD23	12:L:46:ILE:HG21	1.82	0.62
12:L:358:LYS:CG	39:n:80:TYR:CE2	2.78	0.62
14:N:108:LEU:HD21	14:N:191:LEU:HD23	1.82	0.62
16:P:43:HIS:H	16:P:51:VAL:HG13	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:235:PRO:HA	48:AD:240:GLN:HG3	1.82	0.62
48:AD:244:MET:HB2	70:AD:401:HEC:C4D	2.30	0.62
70:AD:401:HEC:CGA	70:AD:401:HEC:HHA	2.30	0.62
49:AE:152:ILE:HB	49:AE:169:TRP:CD1	2.35	0.62
45:Aa:388:VAL:HG22	45:Aa:441:LEU:HD13	1.81	0.62
50:Af:110:LYS:O	50:Af:111:LYS:C	2.43	0.62
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
16:P:169:HIS:H	16:P:184:LYS:CE	2.13	0.61
16:P:179:LYS:HA	16:P:182:ARG:HG2	1.82	0.61
20:U:128:PHE:CZ	20:U:148:ILE:HG23	2.35	0.61
25:Z:28:ARG:HG3	25:Z:28:ARG:O	1.99	0.61
32:g:139:TYR:HB2	41:p:142:ARG:NH2	2.15	0.61
37:l:57:MET:HG2	37:l:104:PRO:HG2	1.82	0.61
46:AB:412:VAL:O	46:AB:415:GLN:HG2	2.00	0.61
45:Aa:92:PHE:CZ	45:Aa:161:ILE:HG23	2.35	0.61
46:Ab:412:VAL:O	46:Ab:415:GLN:HG2	2.00	0.61
49:Ae:261:PRO:HB2	49:Ae:273:VAL:CG1	2.25	0.61
4:D:89:PRO:HB2	8:H:204:GLU:CG	2.29	0.61
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.82	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.82	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
12:L:521:SER:O	12:L:522:PHE:C	2.41	0.61
13:M:73:LEU:CB	13:M:103:GLN:OE1	2.48	0.61
13:M:98:MET:HE3	13:M:128:PRO:HA	1.81	0.61
14:N:342:GLN:NE2	29:d:30:ARG:HH11	1.99	0.61
15:O:117:PHE:HD1	15:O:128:SER:HA	1.64	0.61
16:P:318:LYS:HA	16:P:321:ARG:NH1	2.15	0.61
34:i:95:TYR:CD1	41:p:112:ALA:HB2	2.36	0.61
45:AA:182:VAL:CG1	45:AA:186:TYR:CE2	2.83	0.61
50:Af:92:GLU:HG2	50:Af:96:LYS:HE2	1.82	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
12:L:559:GLU:HA	12:L:563:PRO:HG2	1.82	0.61
13:M:81:GLN:O	13:M:85:LYS:HB2	2.01	0.61
22:W:32:LYS:NZ	66:W:201:EHZ:C19	2.63	0.61
32:g:106:TYR:CZ	33:h:86:ILE:HD12	2.35	0.61
34:i:123:PHE:HD2	40:o:40:VAL:HG11	1.65	0.61
40:o:69:CYS:C	40:o:80:CYS:SG	2.82	0.61
45:AA:80:ARG:NH2	45:AA:268:CYS:SG	2.72	0.61
45:AA:384:THR:O	45:AA:387:GLU:HG2	2.00	0.61
49:AE:213:LEU:HD23	49:AE:260:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Ak:42:LEU:HD22	54:Ak:48:ILE:HD13	1.82	0.61
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.30	0.61
1:A:113:TRP:CE2	8:H:283:ASP:HB2	2.35	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
11:K:22:PHE:HZ	14:N:61:VAL:HG11	1.65	0.61
13:M:422:HIS:NE2	13:M:425:ASN:OD1	2.33	0.61
15:O:140:LEU:HD11	15:O:198:TYR:CZ	2.35	0.61
15:O:140:LEU:HD21	15:O:304:VAL:O	2.00	0.61
18:R:98:GLU:CD	18:R:98:GLU:H	2.07	0.61
23:X:151:ASN:HB3	30:e:51:ARG:HH11	1.65	0.61
62:a:101:CDL:H311	42:q:7:LEU:HD23	1.82	0.61
27:b:8:PHE:C	27:b:9:LEU:HD12	2.25	0.61
38:m:100:PHE:O	38:m:104:VAL:HG23	2.00	0.61
42:q:71:LYS:O	42:q:72:ASN:CG	2.43	0.61
50:AF:92:GLU:HG2	50:AF:96:LYS:HE2	1.82	0.61
46:Ab:183:LYS:HG3	46:Ab:254:ARG:HB3	1.82	0.61
1:A:51:PHE:CD1	4:D:102:SER:HB2	2.36	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
8:H:306:SER:HG	8:H:310:PHE:HE2	1.31	0.61
12:L:468:ILE:O	12:L:472:ILE:HG23	2.00	0.61
13:M:373:ILE:H	13:M:448:THR:HG22	1.65	0.61
14:N:218:ALA:HB1	14:N:240:MET:SD	2.40	0.61
20:U:138:LEU:HB3	20:U:144:ILE:HG12	1.83	0.61
22:W:24:PHE:HB2	22:W:83:ASP:HB3	1.82	0.61
22:W:25:SER:HB2	22:W:31:ALA:HB2	1.83	0.61
25:Z:58:ARG:NH2	27:b:49:THR:HG21	2.15	0.61
28:c:66:VAL:CG1	28:c:70:LYS:HE3	2.31	0.61
49:AE:221:GLY:HA3	47:Ac:148:ASN:HD22	1.63	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
13:M:98:MET:HE1	13:M:128:PRO:HA	1.83	0.61
13:M:109:THR:HG22	13:M:121:LEU:HB3	1.82	0.61
13:M:139:GLN:HB3	13:M:222:GLU:HG3	1.83	0.61
13:M:433:GLU:O	13:M:437:MET:HG2	2.01	0.61
14:N:240:MET:HE2	14:N:326:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:73:LEU:HD22	15:O:207:ILE:HD11	1.82	0.61
20:T:138:LEU:HD12	20:T:138:LEU:C	2.24	0.61
30:e:70:TYR:HA	30:e:73:MET:HG3	1.81	0.61
37:l:101:TRP:NE1	38:m:62:ASP:HA	2.14	0.61
46:AB:176:ASN:O	46:AB:258:ILE:HD11	2.00	0.61
50:AF:108:TRP:CZ2	46:Ab:101:ARG:HB3	2.35	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
6:F:426:ALA:HB3	60:F:501:FMN:HM81	1.81	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
10:J:169:ILE:CD1	14:N:45:ILE:HD11	2.31	0.61
13:M:318:ALA:HB2	13:M:373:ILE:CG2	2.30	0.61
14:N:179:MET:SD	14:N:216:PHE:CE1	2.94	0.61
15:O:72:LYS:O	15:O:75:LYS:HG2	2.01	0.61
17:Q:167:ASN:O	17:Q:168:LYS:CG	2.49	0.61
20:T:79:ILE:CB	20:T:145:VAL:HG13	2.28	0.61
37:l:62:TYR:CZ	37:l:64:PRO:HG3	2.36	0.61
41:p:6:ASP:HB3	41:p:9:VAL:HG22	1.83	0.61
42:q:34:ARG:NE	42:q:58:ARG:NH2	2.48	0.61
42:q:74:PHE:CD2	42:q:75:TRP:CD1	2.89	0.61
47:AC:138:MET:CE	47:AC:268:ILE:HG23	2.31	0.61
47:Ac:107:TYR:HB2	47:Ac:305:PRO:HG3	1.80	0.61
47:Ac:311:LYS:O	50:Af:39:HIS:N	2.27	0.61
1:A:104:TYR:CE2	10:J:167:ILE:CD1	2.83	0.61
3:C:100:ARG:HH12	21:V:86:LYS:NZ	1.99	0.61
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.61
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.83	0.61
5:E:233:LEU:HD22	6:F:43:THR:HA	1.83	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:246:ARG:NH2	17:Q:123:ASN:OD1	2.33	0.61
8:H:183:MET:HE2	58:I:302:PC1:H271	1.83	0.61
12:L:180:ILE:HD11	13:M:400:ILE:HB	1.83	0.61
12:L:424:MET:HE2	12:L:502:LEU:CB	2.31	0.61
14:N:275:CYS:SG	24:Y:139:PRO:CG	2.88	0.61
16:P:41:ILE:HB	16:P:43:HIS:CE1	2.35	0.61
31:f:38:ARG:HH12	31:f:54:VAL:CG2	2.14	0.61
35:j:97:LEU:HB3	40:o:104:ARG:CB	2.22	0.61
46:AB:307:SER:HB2	46:AB:310:SER:HB2	1.82	0.61
48:AD:262:THR:HG22	52:AH:24:LEU:HG	1.83	0.61
49:AE:244:ASP:HB3	49:AE:250:ARG:HH11	1.65	0.61
45:Aa:186:TYR:CE1	49:Ae:80:HIS:HB2	2.36	0.61
46:Ab:313:VAL:HG21	46:Ab:323:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.01	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:121:TRP:CZ2	10:J:78:TYR:CE1	2.84	0.61
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.61
12:L:100:ILE:HG21	12:L:246:LEU:HD23	1.83	0.61
12:L:302:ILE:HB	12:L:340:PHE:CE1	2.36	0.61
55:L:702:3PE:H3C1	35:j:72:ARG:HH22	1.65	0.61
25:Z:98:MET:SD	30:e:79:ILE:HA	2.40	0.61
28:c:66:VAL:HG12	28:c:70:LYS:HE3	1.83	0.61
48:AD:131:ALA:HB2	48:AD:174:TYR:CD2	2.36	0.61
48:AD:197:LEU:O	48:AD:198:SER:C	2.44	0.61
49:AE:179:ARG:HH12	49:AE:201:ASP:HB2	1.64	0.61
49:AE:263:TYR:HA	49:AE:273:VAL:C	2.26	0.61
46:Ab:300:LYS:HG2	46:Ab:301:ARG:HG3	1.83	0.61
48:Ad:244:MET:HB2	70:Ad:401:HEC:ND	2.15	0.61
49:Ae:244:ASP:HB3	49:Ae:250:ARG:HH11	1.65	0.61
4:D:86:PRO:HG3	4:D:96:ARG:CG	2.30	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
13:M:1:MET:CE	13:M:111:SER:HB2	2.29	0.61
13:M:423:MET:O	13:M:424:ILE:C	2.44	0.61
22:W:97:ILE:HG23	22:W:98:LYS:HG3	1.82	0.61
26:a:3:PHE:CE2	62:a:101:CDL:HA4	2.36	0.61
32:g:109:ASP:HB3	32:g:114:GLU:HB3	1.83	0.61
33:h:106:ILE:O	33:h:106:ILE:HG22	2.00	0.61
40:o:19:PRO:O	40:o:22:ILE:HG12	2.00	0.61
45:AA:341:PHE:HE1	45:AA:356:ALA:HB1	1.66	0.61
47:AC:265:PRO:HD2	47:AC:268:ILE:HD11	1.81	0.61
49:AI:62:ARG:CD	49:AI:63:PRO:HD2	2.31	0.61
3:C:186:ILE:HG13	3:C:187:LEU:HG	1.83	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.01	0.60
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.49	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:126:LEU:CD1	18:R:89:PRO:HB2	2.31	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
9:I:78:PHE:HB3	43:r:8:ILE:CG2	2.31	0.60
10:J:9:SER:HB2	11:K:7:ASN:HD22	1.63	0.60
10:J:61:GLY:O	10:J:65:VAL:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:209:LEU:HD23	13:M:210:TYR:N	2.16	0.60
14:N:179:MET:HB3	14:N:216:PHE:CE1	2.36	0.60
45:AA:168:ILE:O	45:AA:171:GLU:HG2	2.01	0.60
47:AC:222:PRO:HG2	47:AC:223:TYR:CD1	2.31	0.60
46:Ab:262:ASN:OD1	46:Ab:442:GLY:HA2	2.01	0.60
47:Ac:8:HIS:CE1	47:Ac:10:LEU:HB3	2.35	0.60
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.35	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
12:L:40:ILE:HD12	12:L:101:MET:HG3	1.82	0.60
13:M:151:PHE:CE2	14:N:291:PHE:HB2	2.35	0.60
16:P:146:VAL:HG23	16:P:187:GLY:HA2	1.83	0.60
16:P:169:HIS:HD2	16:P:181:LEU:HD11	1.65	0.60
20:T:103:HIS:HB2	20:T:106:LYS:HB2	1.83	0.60
23:X:159:LYS:O	23:X:160:PRO:C	2.43	0.60
29:d:2:MET:HE2	33:h:169:TYR:H	1.66	0.60
48:Ad:121:CYS:SG	70:Ad:401:HEC:CAB	2.89	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:93:HIS:CD2	26:a:27:HIS:ND1	2.70	0.60
8:H:118:TRP:CE2	10:J:30:LEU:CD2	2.84	0.60
12:L:466:PHE:CE1	35:j:72:ARG:CZ	2.84	0.60
12:L:482:MET:CE	12:L:486:LEU:HB3	2.31	0.60
13:M:178:ILE:HD12	33:h:143:GLU:HG3	1.83	0.60
14:N:59:TYR:CZ	14:N:63:GLN:HG3	2.36	0.60
14:N:108:LEU:HD21	14:N:191:LEU:CD2	2.31	0.60
23:X:53:PRO:HD3	25:Z:116:TRP:CD1	2.36	0.60
37:l:108:ASP:HB3	37:l:111:MET:HE2	1.83	0.60
40:o:31:PHE:HD2	40:o:104:ARG:HH12	1.47	0.60
47:AC:219:PRO:HG2	47:AC:223:TYR:CD1	2.37	0.60
45:Aa:403:LEU:CD1	45:Aa:403:LEU:N	2.65	0.60
46:Ab:97:PHE:CZ	46:Ab:101:ARG:HG3	2.36	0.60
52:Ah:39:GLU:O	52:Ah:40:LYS:C	2.41	0.60
1:A:54:LYS:HE3	1:A:55:PHE:CE1	2.37	0.60
1:A:94:LEU:HD22	10:J:152:MET:CE	2.31	0.60
1:A:113:TRP:O	1:A:113:TRP:CD1	2.54	0.60
2:B:100:CYS:SG	56:B:301:SF4:S2	2.99	0.60
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.60
12:L:16:LEU:CD1	55:L:701:3PE:H2H1	2.18	0.60
15:O:57:SER:C	15:O:58:ARG:HD2	2.25	0.60
22:W:58:THR:HB	22:W:61:GLN:HB2	1.83	0.60
23:X:168:PHE:O	23:X:170:TRP:CD1	2.54	0.60
25:Z:143:TYR:O	25:Z:144:THR:C	2.45	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
4:D:36:GLN:NE2	13:M:135:ARG:NH1	2.40	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
12:L:222:GLY:CA	12:L:229:LEU:HD11	2.26	0.60
14:N:281:LEU:HD23	55:N:401:3PE:C28	2.32	0.60
16:P:217:PHE:HA	16:P:220:TYR:CD2	2.37	0.60
21:V:35:LEU:HA	21:V:38:PHE:HD1	1.65	0.60
43:r:12:ARG:HB3	43:r:20:LEU:HD21	1.84	0.60
48:AD:195:PRO:HG3	70:AD:401:HEC:CBA	2.31	0.60
48:Ad:232:TYR:CZ	48:Ad:245:ALA:HB2	2.35	0.60
49:Ae:207:LYS:HD2	49:Ae:210:TRP:HD1	1.66	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
9:I:80:GLU:OE2	43:r:26:LEU:HD11	2.01	0.60
12:L:42:PHE:O	12:L:46:ILE:HG12	2.01	0.60
14:N:307:THR:HB	15:O:319:ILE:CG1	2.32	0.60
15:O:204:VAL:CG2	15:O:255:VAL:HG22	2.31	0.60
16:P:268:PRO:CG	16:P:344:PRO:HA	2.30	0.60
19:S:16:LEU:CB	19:S:69:TYR:HD1	2.15	0.60
20:U:153:ASP:OD2	39:n:176:GLU:HB2	2.02	0.60
29:d:16:ASP:O	29:d:19:ARG:HG3	2.00	0.60
45:AA:363:MET:HA	45:AA:464:GLN:OE1	2.01	0.60
51:AG:64:ASN:O	51:AG:68:GLU:HG2	2.01	0.60
49:AI:64:LEU:HD21	46:Ab:171:THR:HA	1.82	0.60
1:A:56:PHE:CD2	11:K:79:VAL:HG21	2.37	0.60
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
8:H:121:TRP:HZ3	10:J:27:TYR:HH	1.45	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
8:H:311:THR:O	25:Z:51:MET:HG3	2.01	0.60
10:J:98:MET:O	10:J:101:PHE:HB3	2.02	0.60
12:L:204:SER:HA	12:L:207:ASN:HD22	1.67	0.60
13:M:263:LEU:CD1	38:m:102:TYR:HD1	2.15	0.60
13:M:452:LYS:HA	13:M:455:THR:HG23	1.82	0.60
14:N:308:ASN:CB	15:O:317:ILE:HG22	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:209:VAL:HG23	15:O:214:VAL:CG1	2.31	0.60
42:q:85:GLU:HG2	42:q:98:PRO:CB	2.31	0.60
42:q:86:TRP:HA	42:q:98:PRO:HG2	1.84	0.60
45:AA:478:LEU:C	45:AA:478:LEU:CD1	2.74	0.60
47:AC:240:MET:SD	71:AD:402:3PH:H251	2.42	0.60
50:AF:108:TRP:HA	50:AF:111:LYS:NZ	2.17	0.60
54:Ak:48:ILE:HD12	54:Ak:49:ASN:N	2.17	0.60
2:B:121:PHE:HE1	57:B:302:UQ1:C11	2.14	0.60
4:D:88:HIS:ND1	4:D:90:ALA:HB3	2.16	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
12:L:141:PHE:CD2	13:M:370:PRO:HG3	2.35	0.60
13:M:269:MET:HE3	13:M:399:ASN:CB	2.32	0.60
14:N:224:SER:HB2	14:N:229:SER:CB	2.32	0.60
62:a:101:CDL:HA21	42:q:6:VAL:HG13	1.82	0.60
33:h:73:PHE:HD2	33:h:74:TYR:CD1	2.20	0.60
49:AE:207:LYS:HD2	49:AE:210:TRP:HD1	1.67	0.60
1:A:70:ALA:HB2	10:J:58:ILE:HG13	1.84	0.60
55:A:401:3PE:H2E1	55:A:401:3PE:H2I2	1.84	0.60
4:D:145:MET:HA	4:D:148:GLU:HG3	1.83	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
10:J:55:VAL:HB	11:K:41:PHE:HE2	1.65	0.60
12:L:295:GLN:HE22	12:L:526:LEU:HD12	1.65	0.60
12:L:598:ILE:HD11	14:N:153:ILE:CG1	2.32	0.60
62:L:705:CDL:H762	13:M:369:LEU:HD21	1.83	0.60
13:M:77:LEU:HD23	13:M:99:LEU:HD12	1.83	0.60
13:M:207:MET:HG3	13:M:239:GLY:HA3	1.84	0.60
26:a:2:TRP:HH2	62:a:101:CDL:H522	1.67	0.60
33:h:102:PRO:HD2	33:h:105:TYR:CB	2.32	0.60
39:n:143:GLU:OE1	39:n:155:PRO:HB3	2.02	0.60
39:n:176:GLU:O	39:n:178:PRO:HD3	2.02	0.60
45:AA:101:THR:HG22	45:AA:154:SER:HA	1.83	0.60
47:AC:302:ALA:O	47:AC:305:PRO:HD2	2.02	0.60
48:AD:121:CYS:HB3	70:AD:401:HEC:HHC	1.84	0.60
45:Aa:295:GLY:O	45:Aa:301:ASN:ND2	2.35	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
7:G:304:GLU:OE2	16:P:41:ILE:HG12	2.01	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
10:J:9:SER:HB2	11:K:7:ASN:ND2	2.16	0.60
12:L:65:THR:HA	34:i:90:MET:HE2	1.84	0.60
12:L:436:ARG:HA	36:k:58:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:276:LEU:C	14:N:276:LEU:HD12	2.27	0.60
21:V:82:LEU:O	21:V:86:LYS:HG3	2.00	0.60
22:W:43:TYR:CE1	22:W:63:ARG:HD3	2.37	0.60
22:W:122:LEU:HD11	22:W:126:TYR:CZ	2.37	0.60
23:X:16:GLU:CD	23:X:68:LEU:HD13	2.27	0.60
48:Ad:95:PRO:HG2	52:Ah:85:PHE:HB2	1.84	0.60
48:Ad:138:VAL:HG12	48:Ad:139:CYS:SG	2.42	0.60
48:Ad:146:LYS:O	48:Ad:150:GLU:HG2	2.00	0.60
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
13:M:126:LEU:HD21	13:M:153:THR:HB	1.83	0.59
13:M:144:ASN:HA	13:M:147:ILE:HD12	1.82	0.59
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.85	0.59
13:M:370:PRO:HA	13:M:375:LEU:HD22	1.83	0.59
14:N:307:THR:O	15:O:319:ILE:HG12	2.02	0.59
14:N:313:MET:O	14:N:317:GLN:OE1	2.19	0.59
20:U:90:TYR:CZ	20:U:92:LYS:HD2	2.35	0.59
20:U:97:LYS:O	20:U:98:LEU:C	2.43	0.59
23:X:20:VAL:HG12	23:X:25:LEU:HD21	1.84	0.59
33:h:73:PHE:CD2	33:h:74:TYR:CD1	2.90	0.59
46:AB:138:LEU:CD2	46:AB:238:LEU:HG	2.32	0.59
49:AE:111:LYS:CE	53:AJ:11:TYR:CZ	2.84	0.59
45:Aa:338:CYS:SG	45:Aa:368:MET:HB2	2.41	0.59
4:D:36:GLN:HA	13:M:138:ASN:HA	1.84	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:651:PRO:HD3	19:S:56:ARG:HB3	1.82	0.59
8:H:114:TYR:OH	10:J:65:VAL:HG23	2.01	0.59
12:L:247:LEU:HD12	12:L:248:HIS:CG	2.36	0.59
12:L:480:LEU:HD21	35:j:82:GLY:HA3	1.83	0.59
14:N:308:ASN:HB3	15:O:317:ILE:CG2	2.33	0.59
25:Z:61:LEU:HA	25:Z:64:ASP:OD2	2.02	0.59
28:c:34:PRO:CG	28:c:37:ALA:HB2	2.32	0.59
32:g:147:LEU:HD11	41:p:163:MET:HE2	1.84	0.59
45:AA:186:TYR:OH	49:AE:80:HIS:CB	2.50	0.59
45:AA:225:LYS:HE3	45:AA:256:VAL:HA	1.83	0.59
46:Ab:138:LEU:HB3	46:Ab:237:PHE:CD2	2.36	0.59
49:Ae:262:ALA:C	49:Ae:273:VAL:HG13	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ag:19:LEU:CD2	51:Ag:24:GLN:HB3	2.29	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
9:I:63:TRP:CZ2	55:I:301:3PE:H331	2.37	0.59
12:L:81:LYS:HB2	12:L:135:ASN:OD1	2.02	0.59
12:L:123:LEU:HD22	12:L:150:MET:CG	2.33	0.59
12:L:313:MET:HE2	12:L:328:HIS:CE1	2.38	0.59
13:M:115:LEU:O	13:M:118:PHE:HB3	2.02	0.59
13:M:294:MET:HE3	13:M:319:HIS:CD2	2.37	0.59
16:P:350:ILE:HB	16:P:366:ILE:CG2	2.32	0.59
24:Y:137:LEU:CD2	24:Y:138:PHE:CD2	2.84	0.59
25:Z:54:ASN:O	25:Z:58:ARG:HG2	2.02	0.59
49:AE:146:VAL:HA	49:AE:149:MET:HE3	1.84	0.59
54:AK:38:TRP:CD1	47:Ac:155:TYR:HH	2.21	0.59
47:Ac:28:SER:HB2	62:Ac:407:CDL:HA21	1.84	0.59
1:A:90:MET:HE3	10:J:152:MET:HG3	1.84	0.59
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.37	0.59
4:D:345:GLU:HB2	25:Z:19:ILE:HD12	1.83	0.59
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.38	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
8:H:114:TYR:CE2	10:J:65:VAL:CG2	2.84	0.59
12:L:12:PHE:HB3	55:L:701:3PE:H2G2	1.84	0.59
14:N:281:LEU:HD21	55:N:401:3PE:H281	1.83	0.59
14:N:314:MET:CB	15:O:305:LEU:HD11	2.32	0.59
15:O:164:TYR:CE2	15:O:195:LEU:HD21	2.36	0.59
26:a:36:LYS:HA	26:a:59:ARG:HH22	1.67	0.59
33:h:69:ARG:O	33:h:73:PHE:HB2	2.02	0.59
35:j:94:ASP:HB3	35:j:99:ILE:HB	1.83	0.59
45:AA:98:PHE:CE1	45:AA:120:LEU:HD21	2.37	0.59
45:AA:402:HIS:NE2	45:AA:403:LEU:HD12	2.17	0.59
45:AA:402:HIS:CD2	45:AA:403:LEU:HD12	2.38	0.59
46:AB:313:VAL:HG21	46:AB:323:VAL:HG21	1.83	0.59
47:Ac:138:MET:HE1	47:Ac:268:ILE:CG1	2.32	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
11:K:73:VAL:HG21	14:N:38:LEU:HD22	1.85	0.59
13:M:350:MET:HG2	39:n:99:VAL:HG12	1.84	0.59
16:P:318:LYS:HG2	16:P:322:ILE:HD11	1.84	0.59
45:AA:64:SER:OG	45:AA:235:GLY:HA2	2.02	0.59
47:Ac:302:ALA:O	47:Ac:305:PRO:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:320:ILE:HG23	55:Ag:102:3PE:H121	1.85	0.59
49:Ae:132:VAL:HA	49:Ae:135:GLN:NE2	2.17	0.59
4:D:35:ARG:NH2	32:g:57:PRO:C	2.60	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.59
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.83	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
12:L:227:PHE:CD2	12:L:283:LEU:CD2	2.86	0.59
20:U:105:MET:HB2	20:U:139:MET:CE	2.32	0.59
21:V:90:LEU:HD21	21:V:94:MET:CE	2.33	0.59
46:AB:286:PHE:CE1	46:AB:427:ALA:HB1	2.38	0.59
47:AC:345:HIS:CE1	47:AC:346:PRO:HB3	2.37	0.59
48:Ad:157:GLY:HA2	48:Ad:163:GLU:O	2.03	0.59
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.83	0.59
3:C:124:ARG:HD2	17:Q:140:LYS:NZ	2.17	0.59
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.59
4:D:35:ARG:HH22	32:g:56:ASP:C	2.11	0.59
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.99	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
12:L:149:ILE:HG21	13:M:364:LEU:HD21	1.84	0.59
12:L:214:MET:HG2	55:L:704:3PE:H261	1.84	0.59
12:L:302:ILE:CG2	12:L:340:PHE:CE2	2.80	0.59
12:L:562:ILE:HG23	55:L:707:3PE:H3B1	1.85	0.59
16:P:66:GLY:O	16:P:67:ARG:C	2.42	0.59
19:S:63:PRO:HB2	19:S:79:LEU:HB2	1.85	0.59
34:i:9:LYS:HG2	34:i:9:LYS:O	2.02	0.59
49:AE:123:VAL:HG13	53:AJ:29:ALA:CA	2.26	0.59
46:Ab:90:THR:HG23	46:Ab:95:SER:HA	1.83	0.59
49:Ae:163:LYS:O	49:Ae:177:ARG:HG3	2.02	0.59
52:Ah:28:LEU:HD13	52:Ah:84:LEU:HD22	1.84	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
1:A:108:GLN:HG2	1:A:109:LYS:N	2.16	0.59
3:C:224:GLU:OE2	16:P:45:LYS:HB3	2.01	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
7:G:267:THR:HB	17:Q:115:ALA:HB2	1.84	0.59
10:J:63:MET:SD	11:K:34:GLU:OE1	2.61	0.59
12:L:312:LEU:CD2	12:L:395:ILE:HG21	2.33	0.59
12:L:605:ASN:O	12:L:606:LEU:C	2.46	0.59
13:M:209:LEU:HD23	13:M:211:GLY:H	1.67	0.59
14:N:149:LEU:HD12	14:N:149:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:164:MET:HE1	55:Y:201:3PE:H271	1.85	0.59
15:O:343:TYR:HE1	15:O:355:LYS:HB2	1.67	0.59
16:P:96:LEU:HD12	16:P:96:LEU:C	2.28	0.59
42:q:51:ASP:O	42:q:59:HIS:HB2	2.03	0.59
42:q:96:ASP:OD1	42:q:97:PRO:CD	2.50	0.59
54:AK:18:ILE:N	54:AK:19:PRO:HD2	2.18	0.59
45:Aa:225:LYS:HG3	45:Aa:257:TYR:CZ	2.37	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
5:E:190:ASN:HB3	5:E:192:TYR:CD2	2.36	0.59
8:H:114:TYR:CZ	10:J:33:ILE:CD1	2.81	0.59
10:J:122:ASP:O	25:Z:122:GLY:HA3	2.01	0.59
12:L:570:HIS:O	12:L:571:THR:C	2.45	0.59
13:M:14:LEU:HD21	13:M:26:ASN:HB2	1.84	0.59
14:N:300:THR:HG23	14:N:301:SER:N	2.17	0.59
15:O:114:LEU:HA	15:O:131:LEU:HD21	1.84	0.59
21:V:31:THR:HG22	21:V:88:LEU:HD13	1.84	0.59
23:X:124:GLN:HA	23:X:127:LYS:HE3	1.83	0.59
25:Z:105:LYS:O	25:Z:106:VAL:C	2.46	0.59
30:e:69:ARG:HD2	30:e:72:THR:HG21	1.85	0.59
32:g:139:TYR:HD2	32:g:140:PHE:CD1	2.20	0.59
39:n:111:GLU:O	39:n:114:MET:HG2	2.03	0.59
45:AA:66:HIS:HE1	45:AA:402:HIS:HB2	1.68	0.59
45:AA:92:PHE:CE2	45:AA:161:ILE:HG23	2.38	0.59
45:AA:186:TYR:HB3	45:AA:275:ILE:HG21	1.84	0.59
46:AB:39:GLU:O	46:AB:227:HIS:CE1	2.56	0.59
48:AD:233:PHE:HA	48:AD:240:GLN:O	2.02	0.59
49:AE:163:LYS:O	49:AE:177:ARG:HG3	2.02	0.59
45:Aa:111:LYS:O	45:Aa:114:GLU:N	2.35	0.59
47:Ac:240:MET:CE	71:Ad:402:3PH:H251	2.33	0.59
51:Ag:47:LEU:HD12	55:Ag:102:3PE:H342	1.85	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.59
8:H:1:MET:CE	26:a:29:PHE:CE2	2.85	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.59
11:K:51:SER:HA	30:e:32:ARG:HH11	1.67	0.59
12:L:23:MET:HE1	62:L:705:CDL:H162	1.85	0.59
12:L:466:PHE:CE1	12:L:470:TYR:HE2	2.21	0.59
13:M:275:ILE:HD11	13:M:288:TYR:CB	2.33	0.59
13:M:396:MET:HG3	13:M:396:MET:O	2.03	0.59
14:N:170:LEU:CD1	14:N:292:PHE:HD2	2.16	0.59
45:AA:70:THR:HG21	45:AA:407:THR:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:236:PHE:CD2	71:Ad:402:3PH:H3B2	2.30	0.59
47:Ac:345:HIS:CE1	47:Ac:346:PRO:HB3	2.37	0.59
4:D:249:LYS:HA	25:Z:19:ILE:HG23	1.86	0.58
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.58
23:X:120:PRO:HB2	23:X:125:LEU:HD11	1.85	0.58
27:b:27:GLY:O	27:b:30:ILE:HG22	2.02	0.58
33:h:95:GLU:HB3	33:h:114:LYS:HG2	1.85	0.58
35:j:47:PHE:HA	36:k:63:PHE:CZ	2.38	0.58
46:AB:170:GLN:HG3	46:AB:339:TYR:OH	2.03	0.58
47:AC:197:LEU:HD12	69:AC:405:UQ6:H1M2	1.84	0.58
50:AF:24:ALA:O	51:AG:48:ARG:NH2	2.35	0.58
45:Aa:111:LYS:O	45:Aa:112:GLU:C	2.44	0.58
45:Aa:222:ARG:NH2	45:Aa:263:PRO:CB	2.66	0.58
46:Ab:60:ARG:CG	46:Ab:393:LEU:HD13	2.33	0.58
51:Ag:30:TYR:OH	62:Ag:101:CDL:H132	2.04	0.58
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.18	0.58
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
12:L:9:LEU:HD21	55:L:701:3PE:H2A1	1.83	0.58
12:L:385:PHE:CD1	35:j:72:ARG:CG	2.86	0.58
12:L:560:LYS:NZ	62:L:706:CDL:H321	2.18	0.58
13:M:449:THR:OG1	55:M:501:3PE:H281	2.03	0.58
55:M:502:3PE:H11	14:N:238:PRO:HB2	1.85	0.58
14:N:77:ASN:OD1	14:N:81:LEU:HD12	2.04	0.58
25:Z:82:ARG:O	25:Z:86:ILE:HG13	2.03	0.58
31:f:5:GLN:HB3	31:f:9:GLU:OE1	2.03	0.58
38:m:45:ARG:CZ	39:n:140:LEU:HD11	2.33	0.58
41:p:37:TYR:CZ	41:p:41:VAL:HG11	2.38	0.58
49:AE:122:THR:HG21	53:AJ:25:ILE:HG21	1.85	0.58
51:AG:11:ILE:HG22	51:AG:12:ARG:N	2.18	0.58
45:Aa:222:ARG:NH2	45:Aa:263:PRO:HG3	2.17	0.58
46:Ab:286:PHE:CE1	46:Ab:427:ALA:HB1	2.38	0.58
48:Ad:193:LEU:O	48:Ad:194:PRO:C	2.46	0.58
48:Ad:215:LEU:CD1	70:Ad:401:HEC:HMB1	2.29	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.32	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:382:CYS:SG	56:F:502:SF4:S1	3.02	0.58
8:H:175:LEU:HD21	58:I:302:PC1:H2C1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
12:L:52:LEU:HB2	41:p:30:ILE:HD11	1.85	0.58
12:L:161:ARG:HA	39:n:92:GLU:HB2	1.85	0.58
12:L:230:HIS:N	12:L:231:PRO:CD	2.66	0.58
12:L:417:SER:HB3	12:L:493:ILE:CG1	2.31	0.58
13:M:210:TYR:O	13:M:213:HIS:CD2	2.56	0.58
14:N:307:THR:CG2	14:N:311:SER:OG	2.51	0.58
47:AC:29:SER:HB3	62:AC:406:CDL:HB61	1.85	0.58
45:Aa:66:HIS:HE1	45:Aa:402:HIS:HB2	1.66	0.58
47:Ac:162:GLU:O	47:Ac:166:GLY:N	2.36	0.58
51:Ag:50:ALA:O	51:Ag:51:PRO:C	2.46	0.58
1:A:56:PHE:CZ	11:K:75:LEU:HB3	2.38	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
12:L:25:ASN:HB2	33:h:72:LYS:HZ1	1.68	0.58
12:L:407:TRP:CZ3	12:L:410:LEU:HD11	2.38	0.58
12:L:427:ILE:CD1	36:k:69:PHE:HE1	2.16	0.58
25:Z:128:ARG:HD3	30:e:98:HIS:CD2	2.39	0.58
51:AG:19:LEU:CD2	51:AG:24:GLN:HB3	2.29	0.58
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.84	0.58
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.51	0.58
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.02	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
12:L:404:THR:HG22	12:L:405:ASN:N	2.19	0.58
16:P:81:ILE:CD1	18:R:46:VAL:HG11	2.34	0.58
22:W:104:THR:O	22:W:108:ARG:HG3	2.02	0.58
23:X:124:GLN:O	27:b:70:PRO:HB2	2.04	0.58
23:X:171:THR:O	23:X:172:VAL:C	2.47	0.58
25:Z:93:GLU:OE1	30:e:92:TYR:OH	2.20	0.58
48:AD:197:LEU:HA	48:AD:200:ILE:HB	1.84	0.58
49:AE:156:LEU:HD13	49:AE:210:TRP:NE1	2.19	0.58
49:AI:18:THR:HG22	49:AI:18:THR:O	2.02	0.58
45:Aa:96:LEU:HG	45:Aa:164:GLU:HG3	1.84	0.58
47:Ac:163:TRP:O	47:Ac:177:ARG:NH1	2.36	0.58
49:Ae:159:ILE:O	49:Ae:210:TRP:HH2	1.86	0.58
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.85	0.58
4:D:37:TRP:CZ2	4:D:39:PRO:HA	2.38	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.01	0.58
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:217:GLU:CD	17:Q:166:TRP:HE1	2.10	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
13:M:196:TRP:HZ3	13:M:261:PHE:CE2	2.21	0.58
13:M:424:ILE:HG13	38:m:57:VAL:O	2.04	0.58
16:P:57:THR:HG23	16:P:123:SER:CB	2.33	0.58
22:W:67:ARG:HD3	22:W:71:MET:HG2	1.85	0.58
29:d:14:LEU:HD12	29:d:14:LEU:C	2.27	0.58
29:d:113:LEU:O	29:d:113:LEU:HG	2.02	0.58
38:m:75:ASN:O	38:m:75:ASN:OD1	2.20	0.58
47:AC:233:LEU:HD23	48:AD:300:LEU:HA	1.85	0.58
1:A:112:GLU:O	1:A:113:TRP:C	2.47	0.58
6:F:199:ARG:CD	44:s:80:PHE:CE2	2.79	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.86	0.58
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.58
8:H:111:LEU:HD21	10:J:60:LEU:HD12	1.84	0.58
12:L:15:LEU:O	12:L:18:PRO:HD2	2.03	0.58
14:N:26:LEU:O	14:N:27:MET:C	2.46	0.58
14:N:164:MET:HE3	55:Y:201:3PE:C27	2.33	0.58
14:N:179:MET:CB	14:N:216:PHE:HE1	2.16	0.58
14:N:193:ILE:HD13	14:N:200:LEU:HB3	1.86	0.58
15:O:326:ARG:HH21	32:g:56:ASP:CG	2.12	0.58
16:P:275:HIS:HB3	16:P:372:ALA:HB1	1.86	0.58
18:R:48:PHE:CD2	42:q:125:VAL:HG21	2.39	0.58
22:W:42:TRP:CZ2	66:W:201:EHZ:O1	2.56	0.58
25:Z:135:ASN:O	25:Z:139:GLY:HA3	2.04	0.58
45:AA:403:LEU:CD1	45:AA:403:LEU:H	2.16	0.58
49:AE:160:PRO:O	49:AE:178:HIS:HB3	2.03	0.58
48:Ad:284:HIS:NE2	48:Ad:288:MET:HE3	2.19	0.58
49:Ae:160:PRO:O	49:Ae:178:HIS:HB3	2.03	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
12:L:232:TRP:CZ3	12:L:233:LEU:HD21	2.37	0.58
12:L:514:ASN:HA	39:n:36:LYS:NZ	2.19	0.58
13:M:73:LEU:HB2	13:M:103:GLN:OE1	2.02	0.58
32:g:70:ASP:OD1	39:n:108:HIS:NE2	2.37	0.58
34:i:70:PHE:O	34:i:73:SER:HB3	2.04	0.58
34:i:103:ARG:CD	40:o:50:GLN:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:126:SER:HB3	48:AD:178:PRO:CD	2.34	0.58
45:Aa:104:ARG:HB3	45:Aa:108:ALA:HB3	1.85	0.58
45:Aa:220:LEU:O	45:Aa:224:TYR:HB2	2.04	0.58
51:Ag:11:ILE:HG22	51:Ag:12:ARG:N	2.18	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:62:LYS:HB2	4:D:63:PRO:HD2	1.86	0.58
8:H:85:LEU:CD2	8:H:108:THR:HB	2.33	0.58
8:H:114:TYR:CZ	10:J:65:VAL:HG22	2.39	0.58
12:L:592:LEU:O	12:L:596:ILE:HG12	2.03	0.58
14:N:142:LEU:HB3	14:N:194:LEU:HD21	1.85	0.58
15:O:88:GLU:HB2	15:O:160:GLU:OE1	2.04	0.58
15:O:117:PHE:CD1	15:O:128:SER:CB	2.87	0.58
16:P:57:THR:HG23	16:P:123:SER:HB2	1.86	0.58
23:X:160:PRO:HG3	29:d:22:PRO:HD3	1.86	0.58
28:c:72:ARG:HH11	29:d:19:ARG:HD3	1.68	0.58
32:g:121:GLU:HA	32:g:124:VAL:HG22	1.86	0.58
34:i:111:LEU:HD11	41:p:20:PRO:HD3	1.85	0.58
45:AA:220:LEU:O	45:AA:224:TYR:HB2	2.03	0.58
49:AE:159:ILE:O	49:AE:210:TRP:HH2	1.86	0.58
46:Ab:177:LEU:HD11	46:Ab:272:VAL:HG22	1.85	0.58
49:Ae:116:LEU:CA	53:Aj:15:PHE:CZ	2.86	0.58
52:Ah:33:GLU:O	52:Ah:37:GLN:HG3	2.04	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.58
12:L:425:ARG:HG3	12:L:429:PHE:CE2	2.39	0.58
62:L:706:CDL:H201	24:Y:119:TYR:HB3	1.86	0.58
16:P:245:VAL:O	16:P:249:ILE:HG13	2.04	0.58
19:S:16:LEU:HD11	19:S:51:LEU:CD1	2.29	0.58
22:W:25:SER:CB	22:W:31:ALA:HB2	2.34	0.58
30:e:14:LEU:HD12	30:e:15:ASP:CB	2.33	0.58
39:n:177:ARG:HG2	39:n:179:THR:OG1	2.04	0.58
46:AB:47:LEU:HA	46:AB:218:MET:O	2.03	0.58
49:Ae:156:LEU:H	49:Ae:269:ASP:CA	2.11	0.58
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.57
2:B:154:GLU:O	16:P:89:TYR:OH	2.20	0.57
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:164:PHE:HE2	14:N:4:ILE:HG12	1.68	0.57
12:L:598:ILE:HD11	14:N:153:ILE:CD1	2.34	0.57
13:M:109:THR:HG22	13:M:121:LEU:CB	2.34	0.57
17:Q:77:VAL:HG12	17:Q:101:PHE:HA	1.86	0.57
19:S:65:LEU:HB2	19:S:79:LEU:HD11	1.84	0.57
20:T:90:TYR:CE2	20:T:92:LYS:CB	2.87	0.57
21:V:28:TYR:HE2	21:V:59:VAL:HG21	1.69	0.57
38:m:125:PHE:CE1	41:p:133:THR:HG22	2.39	0.57
45:AA:57:LEU:HD13	45:AA:229:MET:HB3	1.85	0.57
47:AC:215:ALA:HA	51:AG:11:ILE:HD11	1.86	0.57
50:AF:106:GLU:O	50:AF:110:LYS:HG3	2.03	0.57
45:Aa:104:ARG:NH1	45:Aa:146:LEU:HD23	2.19	0.57
45:Aa:107:ASN:O	45:Aa:110:GLU:HG2	2.03	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:19:PHE:CE1	26:a:11:ILE:HD12	2.39	0.57
10:J:123:TRP:CZ2	30:e:73:MET:HG2	2.40	0.57
12:L:56:HIS:O	40:o:71:ARG:HG3	2.03	0.57
15:O:355:LYS:HE2	28:c:37:ALA:O	2.03	0.57
16:P:55:VAL:HA	16:P:79:GLN:HB3	1.86	0.57
20:U:84:LEU:O	20:U:88:LYS:HG3	2.05	0.57
20:U:100:VAL:O	20:U:101:ASN:HB2	2.04	0.57
23:X:122:LEU:HD21	27:b:81:LEU:HD23	1.86	0.57
29:d:113:LEU:HD22	32:g:148:PRO:HG3	1.86	0.57
45:AA:87:ASN:HD21	45:AA:199:GLN:HB2	1.69	0.57
48:AD:249:TYR:CE2	48:AD:252:VAL:HA	2.39	0.57
48:AD:284:HIS:NE2	48:AD:288:MET:HE3	2.18	0.57
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
20:T:90:TYR:CE2	20:T:92:LYS:HB3	2.39	0.57
34:i:103:ARG:O	34:i:105:PHE:CD1	2.57	0.57
51:AG:35:ILE:HB	51:AG:36:PRO:HD3	1.86	0.57
46:Ab:293:LEU:HD21	46:Ab:361:VAL:HG21	1.86	0.57
51:Ag:27:PHE:HB3	51:Ag:30:TYR:HB2	1.87	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
12:L:203:PHE:CZ	41:p:110:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:362:ILE:CG2	12:L:366:MET:HE3	2.32	0.57
13:M:73:LEU:HD22	13:M:103:GLN:NE2	2.18	0.57
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.85	0.57
13:M:297:VAL:O	13:M:301:ILE:HG12	2.03	0.57
16:P:214:LEU:HD23	16:P:352:VAL:CG1	2.34	0.57
16:P:220:TYR:HA	16:P:223:PHE:HD2	1.67	0.57
45:AA:158:ASP:HA	45:AA:161:ILE:HD12	1.86	0.57
54:AK:38:TRP:CZ2	54:AK:40:LEU:HD12	2.40	0.57
1:A:2:ASN:HB2	25:Z:143:TYR:HE1	1.69	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
8:H:318:MET:HG2	26:a:40:ARG:HH22	1.67	0.57
11:K:93:LEU:HA	14:N:54:GLU:OE2	2.03	0.57
12:L:145:GLU:HB3	13:M:370:PRO:CG	2.34	0.57
12:L:546:LEU:HD22	38:m:72:ARG:NH2	2.19	0.57
13:M:230:ILE:HG13	13:M:235:LEU:HG	1.87	0.57
14:N:273:ASN:O	14:N:274:ASN:HB2	2.05	0.57
14:N:284:MET:O	14:N:287:LEU:HB2	2.04	0.57
45:Aa:57:LEU:HA	45:Aa:226:ALA:O	2.05	0.57
47:Ac:45:ILE:HG12	67:Ac:402:HEM:HAB	1.85	0.57
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
12:L:227:PHE:CD2	12:L:283:LEU:HD21	2.38	0.57
13:M:444:LEU:O	13:M:448:THR:HG23	2.04	0.57
14:N:253:GLY:N	14:N:290:LEU:HD11	2.19	0.57
14:N:314:MET:HB2	15:O:305:LEU:CD1	2.33	0.57
20:U:130:ILE:HG23	20:U:147:TYR:CE2	2.40	0.57
26:a:36:LYS:HA	26:a:59:ARG:NH2	2.19	0.57
26:a:43:TYR:CZ	26:a:47:LEU:HD11	2.40	0.57
27:b:69:HIS:CD2	27:b:70:PRO:HD2	2.36	0.57
42:q:65:THR:HG22	42:q:66:THR:N	2.20	0.57
47:AC:141:TRP:NE1	47:AC:264:THR:HA	2.19	0.57
47:AC:150:LEU:HD13	47:AC:164:ILE:HD12	1.86	0.57
50:AF:107:GLU:OE2	50:AF:111:LYS:HD3	2.05	0.57
47:Ac:138:MET:HE1	47:Ac:268:ILE:HG23	1.86	0.57
47:Ac:185:LEU:HD11	68:Ac:405:U10:H221	1.86	0.57
48:Ad:195:PRO:HD2	70:Ad:401:HEC:CHA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.57
5:E:222:PHE:H	5:E:225:GLU:CD	2.13	0.57
12:L:306:THR:HA	12:L:336:LYS:HZ2	1.67	0.57
12:L:425:ARG:HG3	12:L:429:PHE:HE2	1.68	0.57
13:M:158:ILE:HG21	14:N:283:ALA:HB1	1.86	0.57
13:M:172:GLY:C	13:M:173:THR:HG23	2.28	0.57
16:P:315:THR:HG22	16:P:317:ASP:H	1.69	0.57
21:V:31:THR:O	21:V:35:LEU:HG	2.04	0.57
22:W:83:ASP:O	22:W:87:ILE:HG12	2.04	0.57
25:Z:89:GLU:OE1	30:e:97:HIS:CG	2.58	0.57
25:Z:110:VAL:HG11	30:e:72:THR:HA	1.87	0.57
32:g:121:GLU:OE2	41:p:10:TYR:CE2	2.58	0.57
45:AA:402:HIS:ND1	45:AA:403:LEU:CD1	2.67	0.57
47:AC:137:GLN:HG3	47:AC:265:PRO:CG	2.31	0.57
48:AD:223:THR:HG21	52:AH:55:VAL:HG21	1.86	0.57
49:AI:68:VAL:HG11	46:Ab:85:LEU:HD21	1.86	0.57
45:Aa:269:ARG:HD2	49:Ae:92:ARG:NH2	2.20	0.57
48:Ad:249:TYR:CE2	48:Ad:252:VAL:HA	2.40	0.57
52:Ah:84:LEU:O	52:Ah:88:LEU:HG	2.05	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.57
13:M:4:ILE:CG2	13:M:107:ILE:HD13	2.30	0.57
13:M:55:MET:HE1	62:X:201:CDL:CB5	2.34	0.57
13:M:447:LEU:HD21	13:M:454:ILE:CD1	2.33	0.57
14:N:109:ALA:HB2	14:N:161:SER:HB3	1.85	0.57
14:N:331:ILE:HG13	29:d:41:THR:HA	1.86	0.57
15:O:99:GLY:HA2	28:c:30:TYR:CD1	2.38	0.57
15:O:305:LEU:O	15:O:305:LEU:CD1	2.51	0.57
23:X:5:VAL:HG13	23:X:7:LEU:HG	1.87	0.57
23:X:130:LYS:HE3	27:b:67:PRO:HB3	1.86	0.57
26:a:50:ARG:NH1	26:a:54:ILE:HD11	2.20	0.57
34:i:87:LYS:HG2	34:i:87:LYS:O	2.05	0.57
37:l:166:LEU:HB2	37:l:170:ARG:NH2	2.19	0.57
42:q:55:PHE:CG	43:r:26:LEU:HD22	2.40	0.57
46:AB:162:LYS:NZ	46:AB:194:ASP:OD1	2.38	0.57
47:AC:147:THR:HG21	47:AC:165:TRP:CD1	2.40	0.57
47:AC:201:HIS:HE1	69:AC:405:UQ6:H1M1	1.68	0.57
49:AE:168:LYS:HE2	47:Ac:261:PRO:HG2	1.86	0.57
49:AE:207:LYS:HB3	49:AE:209:GLU:OE1	2.05	0.57
49:AE:272:VAL:HG12	49:AE:274:GLY:H	1.69	0.57
49:Ae:218:THR:HG21	49:Ae:256:LEU:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:MET:HG2	11:K:79:VAL:HG11	1.86	0.57
1:A:67:LEU:HD21	11:K:68:ALA:CB	2.35	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
10:J:44:LEU:HA	10:J:48:GLY:O	2.05	0.57
12:L:247:LEU:CD1	12:L:248:HIS:NE2	2.52	0.57
13:M:14:LEU:HD11	13:M:26:ASN:HB3	1.87	0.57
13:M:42:LEU:HD11	13:M:67:ILE:CD1	2.34	0.57
15:O:295:ARG:HH12	15:O:299:GLN:HB2	1.67	0.57
17:Q:125:VAL:HG23	17:Q:125:VAL:O	2.05	0.57
23:X:48:TRP:CD1	27:b:55:VAL:HG13	2.39	0.57
34:i:110:ILE:HD13	41:p:16:ARG:HD2	1.87	0.57
42:q:14:VAL:HG13	42:q:23:LEU:CD2	2.35	0.57
45:AA:158:ASP:O	45:AA:162:GLU:HG2	2.05	0.57
48:Ad:222:PRO:O	48:Ad:225:VAL:HG12	2.05	0.57
52:Ah:45:ARG:O	52:Ah:49:GLU:HG2	2.04	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
12:L:246:LEU:HD12	12:L:247:LEU:CA	2.34	0.57
12:L:253:VAL:CG2	12:L:310:LEU:HD11	2.35	0.57
62:L:705:CDL:H381	33:h:75:LEU:HB3	1.87	0.57
13:M:12:LEU:HB2	13:M:13:PRO:HD3	1.85	0.57
13:M:269:MET:HE3	13:M:399:ASN:HB2	1.86	0.57
14:N:43:MET:HE3	14:N:126:MET:SD	2.44	0.57
15:O:206:TYR:CD2	15:O:257:VAL:HG22	2.40	0.57
22:W:101:LYS:HZ1	22:W:109:PHE:HE2	1.53	0.57
33:h:57:VAL:CG1	39:n:99:VAL:CG2	2.83	0.57
35:j:101:PRO:O	35:j:102:ASP:C	2.46	0.57
48:AD:222:PRO:O	48:AD:225:VAL:HG12	2.05	0.57
48:AD:296:MET:CE	71:AD:402:3PH:H362	2.34	0.57
45:Aa:55:ASN:HB3	45:Aa:226:ALA:CB	2.35	0.57
45:Aa:92:PHE:HD1	45:Aa:168:ILE:HD12	1.68	0.57
46:Ab:142:THR:HG21	46:Ab:237:PHE:CB	2.28	0.57
48:Ad:136:VAL:HA	48:Ad:140:TYR:O	2.05	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:J:124:LEU:CB	25:Z:137:ASN:HD21	2.18	0.56
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:88:LEU:HD23	12:L:326:PHE:HE2	1.69	0.56
14:N:120:GLN:HG3	14:N:177:LYS:HE2	1.86	0.56
25:Z:131:GLU:O	25:Z:132:GLU:C	2.48	0.56
30:e:42:GLU:HG2	33:h:176:LYS:HE2	1.87	0.56
33:h:57:VAL:CG1	39:n:99:VAL:HG23	2.35	0.56
38:m:45:ARG:NE	39:n:140:LEU:HD11	2.20	0.56
45:AA:402:HIS:CG	45:AA:403:LEU:HD12	2.40	0.56
46:AB:40:PHE:CE1	46:AB:48:VAL:HB	2.40	0.56
46:AB:117:GLU:OE2	46:AB:330:TYR:HB3	2.05	0.56
48:Ad:185:ALA:O	48:Ad:186:ARG:C	2.46	0.56
49:Ae:156:LEU:HD13	49:Ae:210:TRP:NE1	2.19	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.56
2:B:115:ASP:HA	2:B:119:VAL:O	2.05	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.89	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
8:H:317:TYR:OH	10:J:136:GLU:OE2	2.22	0.56
11:K:89:TYR:C	11:K:91:GLN:N	2.59	0.56
12:L:518:PRO:C	12:L:520:SER:H	2.13	0.56
14:N:226:THR:HG22	14:N:228:ASN:H	1.70	0.56
15:O:176:GLN:HG3	15:O:177:GLY:N	2.16	0.56
20:T:134:ASP:OD1	20:T:134:ASP:O	2.23	0.56
24:Y:68:ILE:CG2	24:Y:120:MET:HE1	2.35	0.56
24:Y:92:TYR:CE1	24:Y:128:LYS:HD3	2.40	0.56
25:Z:7:LYS:HB2	25:Z:7:LYS:NZ	2.20	0.56
45:AA:74:TRP:CH2	45:AA:410:CYS:SG	2.97	0.56
47:AC:92:ILE:HG13	47:AC:272:TRP:HH2	1.69	0.56
47:AC:107:TYR:HB2	47:AC:305:PRO:HG3	1.87	0.56
51:AG:33:LYS:C	51:AG:36:PRO:HD2	2.30	0.56
46:Ab:425:VAL:HG12	46:Ab:429:LYS:HZ1	1.70	0.56
47:Ac:164:ILE:O	47:Ac:177:ARG:HD2	2.05	0.56
49:Ae:112:GLY:O	53:Aj:15:PHE:CE2	2.59	0.56
2:B:81:LEU:HD22	58:B:303:PC1:H352	1.87	0.56
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.27	0.56
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.86	0.56
7:G:136:GLU:CD	17:Q:87:MET:HG3	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:202:GLU:HA	8:H:206:GLU:OE2	2.05	0.56
10:J:12:PHE:CZ	11:K:42:ILE:HD12	2.40	0.56
10:J:33:ILE:HG23	10:J:60:LEU:HD22	1.85	0.56
12:L:229:LEU:HD12	12:L:229:LEU:C	2.28	0.56
12:L:264:HIS:O	12:L:265:PRO:C	2.49	0.56
12:L:466:PHE:CB	35:j:68:TRP:CZ2	2.79	0.56
13:M:118:PHE:O	13:M:122:PHE:CB	2.54	0.56
13:M:158:ILE:HG12	14:N:287:LEU:HD11	1.86	0.56
13:M:282:LEU:HD13	13:M:342:MET:HE2	1.87	0.56
14:N:164:MET:HE1	55:Y:201:3PE:C27	2.28	0.56
14:N:254:LEU:CD1	14:N:255:PRO:HD2	2.35	0.56
15:O:125:ASP:OD1	15:O:126:GLY:N	2.39	0.56
15:O:173:MET:HE2	15:O:179:ILE:HG23	1.87	0.56
16:P:156:SER:CB	16:P:161:VAL:HG21	2.30	0.56
18:R:62:ASP:O	18:R:66:GLN:HG3	2.06	0.56
23:X:160:PRO:HG3	29:d:22:PRO:CD	2.35	0.56
25:Z:70:ALA:O	25:Z:73:PRO:HD2	2.04	0.56
34:i:101:LYS:HB3	34:i:102:PRO:HD2	1.87	0.56
38:m:125:PHE:HE1	41:p:133:THR:HG22	1.70	0.56
41:p:39:LEU:O	41:p:44:PRO:HD3	2.05	0.56
45:AA:120:LEU:N	46:AB:298:HIS:O	2.38	0.56
49:AE:219:HIS:HB2	49:AE:254:ALA:HA	1.88	0.56
45:Aa:222:ARG:NH1	45:Aa:263:PRO:HG3	2.20	0.56
48:Ad:170:LYS:HZ3	49:Ae:151:LYS:HD3	1.70	0.56
51:Ag:51:PRO:HB2	51:Ag:52:PRO:HD3	1.87	0.56
1:A:62:PHE:CE2	10:J:62:GLY:HA2	2.40	0.56
3:C:124:ARG:HD2	17:Q:140:LYS:HZ2	1.71	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
11:K:89:TYR:C	11:K:91:GLN:H	2.13	0.56
13:M:78:MET:O	13:M:432:ARG:HD2	2.05	0.56
13:M:127:ILE:CG1	14:N:254:LEU:HD21	2.35	0.56
55:M:502:3PE:H3A2	14:N:246:LEU:CD1	2.27	0.56
14:N:193:ILE:HG21	14:N:266:ILE:HG12	1.88	0.56
15:O:77:ILE:HG23	15:O:81:LEU:HD12	1.86	0.56
19:S:23:LEU:HD12	19:S:23:LEU:C	2.29	0.56
33:h:165:ASP:OD1	33:h:165:ASP:O	2.22	0.56
34:i:80:TRP:HE1	41:p:44:PRO:HG2	1.68	0.56
35:j:99:ILE:HD12	40:o:107:ARG:HB2	1.88	0.56
39:n:50:GLU:HG2	39:n:51:HIS:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:171:ASP:CG	47:AC:172:LYS:H	2.12	0.56
48:AD:147:ALA:O	48:AD:151:GLU:HG3	2.05	0.56
49:AE:221:GLY:O	47:Ac:141:TRP:HZ3	1.88	0.56
49:AI:62:ARG:HB3	49:AI:78:PHE:O	2.06	0.56
45:Aa:363:MET:HA	45:Aa:464:GLN:OE1	2.04	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:161:GLU:OE1	18:R:97:LYS:HE2	2.06	0.56
7:G:655:ARG:HH12	19:S:59:SER:N	2.03	0.56
9:I:54:THR:HG21	25:Z:33:TYR:CZ	2.40	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
13:M:57:SER:HB3	13:M:113:THR:HG22	1.87	0.56
16:P:323:HIS:ND1	16:P:323:HIS:O	2.39	0.56
23:X:151:ASN:ND2	33:h:170:GLN:NE2	2.54	0.56
30:e:14:LEU:HD12	30:e:14:LEU:C	2.31	0.56
31:f:38:ARG:NH1	31:f:56:TRP:O	2.39	0.56
45:AA:402:HIS:ND1	45:AA:403:LEU:HD12	2.20	0.56
47:AC:138:MET:HE1	47:AC:268:ILE:HA	1.87	0.56
50:AF:22:TYR:CD2	50:AF:84:TYR:HB2	2.41	0.56
47:Ac:171:ASP:CG	47:Ac:172:LYS:H	2.13	0.56
49:Ae:270:VAL:C	49:Ae:271:VAL:HG23	2.31	0.56
50:Af:15:ASP:OD2	50:Af:19:LYS:NZ	2.39	0.56
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.56
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
11:K:36:MET:HE3	14:N:68:MET:HG3	1.87	0.56
11:K:45:SER:O	11:K:49:LEU:HG	2.06	0.56
14:N:108:LEU:CD2	14:N:191:LEU:CD2	2.83	0.56
15:O:114:LEU:O	15:O:117:PHE:HB3	2.06	0.56
17:Q:167:ASN:O	17:Q:168:LYS:HG2	2.05	0.56
20:T:130:ILE:HD11	20:T:148:ILE:HD11	1.86	0.56
20:U:87:LEU:HD21	20:U:118:ILE:HG23	1.86	0.56
25:Z:122:GLY:O	25:Z:126:GLY:N	2.36	0.56
34:i:95:TYR:HD1	41:p:112:ALA:CB	2.16	0.56
37:l:105:ILE:HG23	37:l:109:LEU:HD22	1.86	0.56
37:l:119:THR:HG22	38:m:13:THR:HG23	1.87	0.56
45:AA:74:TRP:HH2	45:AA:410:CYS:HG	1.51	0.56
49:AE:197:ASP:HB3	49:AE:257:ASN:OD1	2.06	0.56
49:Ae:207:LYS:HB3	49:Ae:209:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ag:35:ILE:HB	51:Ag:36:PRO:HD3	1.86	0.56
1:A:52:SER:C	1:A:54:LYS:H	2.11	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
2:B:173:TYR:O	3:C:203:LEU:HD22	2.05	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.56
10:J:22:LYS:HE2	11:K:18:GLY:O	2.06	0.56
12:L:397:GLU:HB2	12:L:482:MET:SD	2.46	0.56
13:M:196:TRP:HE1	13:M:250:LEU:HD13	1.69	0.56
18:R:38:TYR:OH	42:q:127:TYR:HB2	2.05	0.56
20:T:83:VAL:CG2	20:T:126:PHE:CZ	2.83	0.56
23:X:48:TRP:NE1	27:b:55:VAL:HG22	2.20	0.56
45:AA:403:LEU:CD1	45:AA:403:LEU:N	2.69	0.56
46:AB:236:GLN:HG3	46:AB:237:PHE:CD2	2.41	0.56
47:AC:119:LEU:HD22	67:AC:402:HEM:HBB2	1.86	0.56
48:AD:321:TYR:HB2	50:AF:61:PHE:CZ	2.41	0.56
50:AF:15:ASP:OD2	50:AF:19:LYS:NZ	2.39	0.56
48:Ad:116:VAL:HA	48:Ad:253:LEU:HD21	1.88	0.56
49:Ae:219:HIS:HB2	49:Ae:254:ALA:HA	1.88	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
55:J:202:3PE:H2C1	14:N:11:PHE:HZ	1.70	0.56
12:L:14:LEU:HD21	34:i:74:HIS:O	2.06	0.56
12:L:355:ASP:HB3	12:L:357:ARG:HG2	1.88	0.56
12:L:390:TYR:CE2	35:j:68:TRP:HH2	2.23	0.56
13:M:370:PRO:CA	13:M:375:LEU:CD2	2.84	0.56
14:N:307:THR:C	15:O:319:ILE:HG12	2.31	0.56
20:T:90:TYR:HE2	20:T:92:LYS:CB	2.19	0.56
26:a:14:VAL:O	26:a:18:ILE:HG13	2.06	0.56
27:b:11:ASN:OD1	27:b:12:ALA:N	2.39	0.56
32:g:123:LEU:HD12	41:p:98:VAL:CG1	2.36	0.56
35:j:97:LEU:O	40:o:104:ARG:NH1	2.38	0.56
39:n:57:MET:HE2	39:n:57:MET:HA	1.87	0.56
41:p:132:PHE:O	41:p:136:THR:OG1	2.17	0.56
45:AA:120:LEU:HD12	45:AA:121:ASN:H	1.71	0.56
46:AB:43:LEU:HB3	46:AB:44:PRO:HD2	1.88	0.56
47:Ac:97:HIS:CE1	47:Ac:100:ARG:HH21	2.24	0.56
71:Ad:402:3PH:H341	49:Ae:128:ALA:HB1	1.88	0.56
51:Ag:33:LYS:C	51:Ag:36:PRO:HD2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.87	0.56
1:A:73:LEU:HD11	10:J:57:LEU:HD23	1.87	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
8:H:42:PRO:HB3	42:q:27:PHE:CE2	2.41	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.56
12:L:353:GLU:OE1	39:n:80:TYR:OH	2.24	0.56
13:M:4:ILE:H	13:M:4:ILE:HD12	1.70	0.56
13:M:73:LEU:CD2	13:M:103:GLN:CD	2.79	0.56
13:M:422:HIS:HB3	38:m:51:TYR:CE2	2.41	0.56
14:N:253:GLY:H	14:N:290:LEU:HD11	1.71	0.56
18:R:77:ILE:HD11	18:R:111:PHE:CG	2.41	0.56
30:e:75:ARG:O	30:e:79:ILE:HG13	2.06	0.56
34:i:14:GLN:HE22	39:n:157:ALA:HB3	1.71	0.56
47:AC:201:HIS:CE1	69:AC:405:UQ6:H1M1	2.41	0.56
48:AD:124:CYS:SG	70:AD:401:HEC:CAC	2.94	0.56
48:AD:321:TYR:HB2	50:AF:61:PHE:CE1	2.40	0.56
49:AE:218:THR:HG21	49:AE:256:LEU:C	2.30	0.56
52:AH:47:ARG:HA	52:AH:50:LEU:HB2	1.86	0.56
53:AJ:30:LEU:HD12	54:AK:34:TRP:HB2	1.87	0.56
46:Ab:162:LYS:NZ	46:Ab:194:ASP:OD1	2.38	0.56
50:Af:22:TYR:CD2	50:Af:84:TYR:HB2	2.41	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
22:W:32:LYS:HZ3	66:W:201:EHZ:C19	2.19	0.56
23:X:124:GLN:C	23:X:125:LEU:HD12	2.31	0.56
46:AB:117:GLU:OE2	46:AB:331:SER:N	2.25	0.56
46:AB:300:LYS:HG2	46:AB:301:ARG:HG3	1.86	0.56
70:AD:401:HEC:HHA	70:AD:401:HEC:O2A	2.06	0.56
45:Aa:274:GLU:HG2	45:Aa:275:ILE:N	2.21	0.56
49:Ae:177:ARG:HB3	49:Ae:211:VAL:HG13	1.88	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.55
3:C:167:ARG:HB3	3:C:186:ILE:HG23	1.86	0.55
4:D:88:HIS:CE1	8:H:205:SER:HA	2.41	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
15:O:61:THR:HB	15:O:160:GLU:O	2.06	0.55
24:Y:76:THR:CG2	24:Y:95:GLY:HA3	2.34	0.55
34:i:105:PHE:CD2	40:o:68:LYS:CA	2.84	0.55
35:j:45:ARG:HD3	36:k:57:TRP:CD1	2.41	0.55
40:o:39:MET:HE1	40:o:58:TYR:HA	1.86	0.55
49:AE:156:LEU:HD22	49:AE:210:TRP:CE2	2.42	0.55
46:Ab:366:LEU:HD21	46:Ab:425:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:77:ASP:O	52:Ah:78:HIS:C	2.48	0.55
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.55
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.88	0.55
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.72	0.55
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.88	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
12:L:102:GLN:HE22	12:L:452:ASN:HB2	1.72	0.55
12:L:538:PRO:O	12:L:542:LEU:HD13	2.06	0.55
62:L:705:CDL:H161	13:M:361:MET:HE1	1.88	0.55
15:O:62:VAL:HG22	15:O:205:ILE:CB	2.33	0.55
16:P:64:PHE:HE1	16:P:209:ARG:O	1.88	0.55
17:Q:165:SER:HB3	17:Q:168:LYS:O	2.06	0.55
22:W:24:PHE:HB2	22:W:83:ASP:CB	2.37	0.55
32:g:106:TYR:CE2	33:h:86:ILE:CD1	2.89	0.55
47:AC:272:TRP:HA	47:AC:275:LEU:HG	1.87	0.55
71:AD:402:3PH:H261	71:AD:402:3PH:H371	1.88	0.55
49:AE:177:ARG:HB3	49:AE:211:VAL:HG13	1.88	0.55
51:AG:27:PHE:HB3	51:AG:30:TYR:HB2	1.87	0.55
53:Aj:30:LEU:HA	54:Ak:34:TRP:CD1	2.41	0.55
1:A:54:LYS:HG3	1:A:55:PHE:N	2.20	0.55
4:D:47:PHE:CE2	14:N:305:PHE:HZ	2.24	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.55
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.89	0.55
12:L:145:GLU:HG2	13:M:370:PRO:HD3	1.88	0.55
12:L:556:ILE:HG21	38:m:80:PHE:CZ	2.39	0.55
16:P:61:ALA:HB3	16:P:82:ILE:HG23	1.88	0.55
24:Y:71:MET:CG	24:Y:102:THR:HG21	2.37	0.55
29:d:106:LYS:CB	41:p:79:GLU:HB3	2.37	0.55
34:i:26:GLN:HA	39:n:118:TYR:HE1	1.71	0.55
34:i:127:HIS:O	34:i:128:HIS:C	2.47	0.55
40:o:69:CYS:O	40:o:69:CYS:SG	2.65	0.55
42:q:68:MET:HE1	42:q:81:MET:O	2.06	0.55
46:AB:366:LEU:HD21	46:AB:425:VAL:HG22	1.87	0.55
47:AC:153:ILE:HB	47:AC:157:GLY:CA	2.36	0.55
49:AE:248:ARG:HA	49:AE:257:ASN:CG	2.32	0.55
51:AG:78:TYR:HB3	52:AH:63:GLU:HB2	1.88	0.55
46:Ab:290:GLN:O	46:Ab:294:GLY:O	2.24	0.55
1:A:106:TRP:HZ3	27:b:19:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.55
12:L:71:MET:HE2	12:L:74:MET:O	2.05	0.55
14:N:237:THR:O	14:N:237:THR:CG2	2.55	0.55
24:Y:137:LEU:HD23	24:Y:138:PHE:CD2	2.41	0.55
25:Z:62:ILE:HD12	27:b:81:LEU:HD22	1.88	0.55
38:m:23:TYR:HB2	39:n:65:ARG:NH2	2.21	0.55
46:AB:36:GLN:O	46:AB:52:LEU:HD13	2.07	0.55
49:AI:11:PHE:O	49:AI:14:VAL:HG22	2.05	0.55
49:AI:65:VAL:HG11	49:AI:77:ARG:HH22	1.71	0.55
48:Ad:179:TYR:O	48:Ad:180:PRO:C	2.49	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
8:H:121:TRP:CH2	10:J:27:TYR:CZ	2.95	0.55
12:L:94:LEU:CD2	12:L:125:LEU:HD21	2.35	0.55
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.41	0.55
15:O:170:LEU:HG	15:O:179:ILE:HD13	1.87	0.55
15:O:224:PRO:HA	15:O:227:MET:CE	2.36	0.55
15:O:230:THR:HG22	15:O:233:TYR:H	1.72	0.55
20:U:88:LYS:HG3	20:U:98:LEU:HD11	1.87	0.55
22:W:58:THR:HG22	22:W:60:LYS:N	2.21	0.55
34:i:88:TYR:CE2	41:p:49:ARG:HB2	2.42	0.55
35:j:97:LEU:O	40:o:104:ARG:HG3	2.06	0.55
47:AC:148:ASN:OD1	49:Ae:221:GLY:CA	2.54	0.55
49:Ae:191:GLU:H	49:Ae:191:GLU:CD	2.14	0.55
3:C:120:THR:OG1	17:Q:128:PHE:HA	2.07	0.55
4:D:80:MET:HG2	8:H:126:LYS:HD3	1.89	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.36	0.55
6:F:382:CYS:SG	56:F:502:SF4:S4	3.05	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
12:L:162:THR:O	12:L:166:THR:HG23	2.06	0.55
13:M:62:SER:C	13:M:64:PRO:HD2	2.32	0.55
13:M:127:ILE:HG12	14:N:254:LEU:HD21	1.88	0.55
14:N:224:SER:HB2	14:N:229:SER:HB3	1.89	0.55
15:O:238:GLU:HA	15:O:241:TYR:CD2	2.33	0.55
16:P:273:LEU:O	16:P:277:VAL:HG23	2.06	0.55
17:Q:163:ASN:OD1	17:Q:163:ASN:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:41:LYS:H	18:R:41:LYS:HD2	1.71	0.55
35:j:92:TRP:CZ3	40:o:100:LYS:HA	2.41	0.55
42:q:64:TYR:CE2	42:q:82:VAL:HG13	2.42	0.55
47:AC:97:HIS:CE1	47:AC:100:ARG:HH21	2.23	0.55
47:AC:238:ILE:HD12	62:AC:406:CDL:H762	1.86	0.55
48:AD:253:LEU:HD12	48:AD:253:LEU:C	2.32	0.55
45:Aa:362:ALA:HB2	45:Aa:461:PRO:HB2	1.88	0.55
45:Aa:477:TRP:HA	62:Aa:501:CDL:OB4	2.07	0.55
48:Ad:253:LEU:C	48:Ad:253:LEU:HD12	2.32	0.55
49:Ae:156:LEU:HD22	49:Ae:210:TRP:CE2	2.42	0.55
55:A:401:3PE:H322	55:A:401:3PE:H262	1.88	0.55
8:H:134:ARG:NH2	8:H:200:LEU:CD1	2.70	0.55
10:J:75:THR:CG2	11:K:25:HIS:HB3	2.37	0.55
12:L:230:HIS:N	12:L:231:PRO:HD3	2.22	0.55
12:L:336:LYS:O	12:L:340:PHE:HD2	1.90	0.55
12:L:561:THR:O	12:L:565:SER:HB2	2.07	0.55
13:M:231:LEU:CA	13:M:235:LEU:HD12	2.36	0.55
14:N:230:ILE:O	14:N:233:LEU:HB2	2.07	0.55
14:N:321:LYS:HB2	29:d:49:ARG:HE	1.71	0.55
62:a:101:CDL:OB7	42:q:3:LEU:HD13	2.06	0.55
30:e:14:LEU:HD12	30:e:15:ASP:N	2.21	0.55
31:f:49:ARG:HG3	31:f:52:GLU:HG2	1.89	0.55
34:i:11:ARG:NH2	39:n:154:LEU:CB	2.60	0.55
35:j:100:PRO:HG3	40:o:30:GLY:HA3	1.89	0.55
36:k:30:ILE:CD1	36:k:39:GLN:HB2	2.33	0.55
45:AA:74:TRP:CD2	45:AA:414:GLY:HA3	2.42	0.55
47:AC:49:LEU:HD22	47:Ac:184:ILE:HD13	1.88	0.55
47:AC:233:LEU:CD2	48:AD:300:LEU:HA	2.37	0.55
47:AC:272:TRP:CE2	47:AC:273:TYR:HD2	2.25	0.55
48:AD:223:THR:CG2	52:AH:55:VAL:HG21	2.36	0.55
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.42	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
6:F:392:MET:CE	6:F:419:ILE:CD1	2.60	0.55
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.55
7:G:608:VAL:HG23	17:Q:103:THR:HG1	1.72	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.88	0.55
10:J:164:PHE:HD2	14:N:5:THR:HA	1.72	0.55
15:O:161:ARG:HH22	63:O:402:ADP:H5'1	1.72	0.55
16:P:217:PHE:HA	16:P:220:TYR:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:376:ASN:OD1	16:P:376:ASN:C	2.50	0.55
20:U:110:LEU:HD22	20:U:118:ILE:HD11	1.87	0.55
23:X:20:VAL:HG13	23:X:24:VAL:HB	1.87	0.55
23:X:55:ARG:HB3	23:X:135:ARG:HH22	1.72	0.55
25:Z:56:GLU:HA	25:Z:59:ARG:HH11	1.72	0.55
34:i:83:HIS:CD2	41:p:37:TYR:CE2	2.95	0.55
37:l:109:LEU:HG	37:l:109:LEU:O	2.06	0.55
48:AD:135:LEU:HD23	48:AD:276:TRP:CH2	2.41	0.55
48:AD:318:LYS:CD	49:AE:86:PRO:HB2	2.37	0.55
50:AF:102:ARG:HH21	50:AF:103:LYS:HE3	1.72	0.55
49:Ae:155:LYS:HA	49:Ae:269:ASP:O	2.07	0.55
49:Ae:192:VAL:HA	49:Ae:195:LEU:CD1	2.37	0.55
4:D:79:ASN:HB3	4:D:101:LEU:C	2.32	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.55
12:L:526:LEU:CD2	12:L:530:PRO:HG2	2.37	0.55
13:M:255:LYS:HZ3	29:d:117:HIS:HB3	1.72	0.55
16:P:237:LYS:HE3	16:P:322:ILE:O	2.07	0.55
20:T:128:PHE:CE2	20:T:130:ILE:HG13	2.42	0.55
31:f:46:ARG:HD2	33:h:106:ILE:HD13	1.87	0.55
33:h:73:PHE:CD2	33:h:74:TYR:CE1	2.94	0.55
45:AA:139:ASP:O	45:AA:143:VAL:HG23	2.07	0.55
45:AA:296:TRP:HH2	45:AA:415:ARG:HH11	1.55	0.55
55:AC:403:3PE:H291	51:AG:41:ARG:HH21	1.68	0.55
52:Ah:42:VAL:O	52:Ah:46:GLU:HG3	2.07	0.55
1:A:52:SER:C	1:A:54:LYS:N	2.62	0.55
1:A:56:PHE:HE1	10:J:70:THR:HG1	1.52	0.55
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.55
3:C:186:ILE:O	4:D:113:ILE:HG13	2.07	0.55
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:J:168:GLU:HA	10:J:171:ARG:CG	2.32	0.55
12:L:182:PHE:CE2	12:L:186:MET:CE	2.88	0.55
12:L:258:PHE:HE1	12:L:262:ARG:HH21	1.55	0.55
13:M:6:LEU:HB3	13:M:7:PRO:HD3	1.88	0.55
13:M:453:LEU:HD12	13:M:454:ILE:CG2	2.34	0.55
55:M:502:3PE:H261	55:O:401:3PE:C23	2.32	0.55
16:P:98:GLY:HA3	16:P:103:LEU:HG	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:236:VAL:HG13	16:P:270:ARG:HH21	1.71	0.55
17:Q:59:LEU:HD21	22:W:80:ARG:HH12	1.72	0.55
18:R:48:PHE:CD2	18:R:53:LYS:HB2	2.42	0.55
34:i:83:HIS:HE1	34:i:87:LYS:HD2	1.71	0.55
45:AA:74:TRP:HB3	45:AA:418:LEU:HD11	1.89	0.55
48:AD:124:CYS:SG	70:AD:401:HEC:CBC	2.95	0.55
49:Ae:132:VAL:O	49:Ae:135:GLN:HG2	2.06	0.55
49:Ae:248:ARG:HA	49:Ae:257:ASN:CG	2.32	0.55
53:Aj:11:TYR:HE2	53:Aj:16:ARG:HH21	1.55	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
7:G:655:ARG:HH12	19:S:59:SER:H	1.56	0.54
10:J:126:TYR:C	25:Z:120:LEU:CD1	2.78	0.54
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.43	0.54
16:P:357:ARG:HB2	16:P:362:LEU:HD23	1.89	0.54
20:T:87:LEU:HD22	20:T:104:PHE:CZ	2.41	0.54
20:U:103:HIS:NE2	20:U:140:CYS:SG	2.81	0.54
23:X:22:SER:HB2	26:a:47:LEU:HD23	1.89	0.54
30:e:32:ARG:O	30:e:33:CYS:HB2	2.06	0.54
30:e:42:GLU:CG	33:h:176:LYS:HE2	2.36	0.54
47:AC:138:MET:HE1	47:AC:268:ILE:HG23	1.89	0.54
47:AC:201:HIS:CE1	69:AC:405:UQ6:C1M	2.89	0.54
49:AE:127:TYR:HE1	53:AJ:33:GLU:HG3	1.71	0.54
45:Aa:101:THR:HA	45:Aa:155:SER:H	1.72	0.54
46:Ab:89:LEU:HD11	46:Ab:154:LEU:HD12	1.89	0.54
52:Ah:29:THR:O	52:Ah:33:GLU:HG3	2.07	0.54
52:Ah:46:GLU:O	52:Ah:50:LEU:HG	2.07	0.54
1:A:52:SER:HB3	1:A:54:LYS:HG2	1.88	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
12:L:190:SER:HB2	12:L:196:TRP:NE1	2.22	0.54
13:M:409:TYR:CE1	37:l:116:ARG:NH2	2.75	0.54
15:O:319:ILE:HG13	15:O:320:GLY:H	1.72	0.54
25:Z:53:TRP:O	25:Z:57:ARG:HG3	2.06	0.54
27:b:38:TYR:HA	27:b:41:TYR:CD2	2.42	0.54
34:i:16:ARG:O	34:i:20:ARG:HG2	2.08	0.54
37:l:152:SER:HA	40:o:5:LEU:HD21	1.88	0.54
45:AA:87:ASN:H	45:AA:207:ASN:HD22	1.53	0.54
49:AE:207:LYS:CD	49:AE:210:TRP:HD1	2.20	0.54
49:Ae:112:GLY:O	53:Aj:15:PHE:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:195:LEU:HD11	49:Ae:248:ARG:HH11	1.72	0.54
1:A:56:PHE:HZ	11:K:75:LEU:CB	2.20	0.54
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.90	0.54
4:D:61:TRP:HH2	12:L:579:ASN:HA	1.72	0.54
4:D:253:LEU:HD11	43:r:18:GLN:HG3	1.90	0.54
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:J:135:LEU:HA	11:K:54:MET:HE1	1.89	0.54
12:L:232:TRP:O	12:L:236:ALA:N	2.40	0.54
12:L:445:GLU:OE2	35:j:54:GLN:HG3	2.08	0.54
12:L:507:LEU:O	12:L:510:LYS:HG2	2.06	0.54
14:N:33:LEU:HD11	14:N:141:ILE:CD1	2.38	0.54
14:N:164:MET:HE2	55:Y:201:3PE:H271	1.86	0.54
14:N:179:MET:CB	14:N:216:PHE:CE1	2.89	0.54
14:N:314:MET:CE	14:N:319:LYS:HE2	2.34	0.54
20:U:85:TYR:HA	20:U:88:LYS:HD3	1.89	0.54
24:Y:68:ILE:HG12	24:Y:102:THR:OG1	2.07	0.54
25:Z:24:ASN:OD1	25:Z:24:ASN:O	2.24	0.54
32:g:106:TYR:HE2	33:h:86:ILE:CD1	2.20	0.54
40:o:103:GLU:OE2	40:o:106:ARG:HD2	2.07	0.54
45:AA:187:LEU:HD22	45:AA:288:ALA:HB1	1.89	0.54
46:AB:60:ARG:CZ	46:AB:390:GLU:HB3	2.37	0.54
47:AC:30:TRP:HB3	47:AC:100:ARG:HD3	1.90	0.54
49:AE:161:GLU:HA	49:AE:178:HIS:CD2	2.43	0.54
45:Aa:411:GLU:CD	45:Aa:415:ARG:HE	2.15	0.54
47:Ac:312:GLN:HE21	50:Af:37:THR:CB	2.21	0.54
48:Ad:155:GLN:HE21	48:Ad:164:MET:HB3	1.72	0.54
48:Ad:214:LEU:CD1	48:Ad:237:PHE:HB2	2.38	0.54
48:Ad:309:HIS:CE1	51:Ag:21:PRO:HB2	2.41	0.54
2:B:93:MET:HE2	2:B:95:PHE:CE1	2.42	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
8:H:133:LEU:HD13	10:J:73:MET:SD	2.47	0.54
12:L:66:TRP:HZ3	55:L:701:3PE:O14	1.90	0.54
12:L:174:TYR:HE1	55:L:703:3PE:H362	1.73	0.54
13:M:415:GLN:O	13:M:416:ARG:HG3	2.08	0.54
16:P:71:ASN:HA	16:P:97:MET:SD	2.47	0.54
18:R:32:THR:OG1	18:R:33:HIS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:131:PRO:HG2	20:U:134:ASP:HB2	1.90	0.54
44:s:85:LEU:O	44:s:85:LEU:HD23	2.07	0.54
69:AC:405:UQ6:C18	69:AC:405:UQ6:H151	2.37	0.54
48:AD:126:SER:HB2	48:AD:128:ASP:OD1	2.07	0.54
46:Ab:159:LYS:HB2	46:Ab:197:MET:SD	2.47	0.54
47:Ac:146:ILE:HG13	68:Ac:405:U10:O4	2.08	0.54
49:Ae:197:ASP:HB3	49:Ae:257:ASN:OD1	2.06	0.54
1:A:2:ASN:HB2	25:Z:143:TYR:CE1	2.41	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.07	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
9:I:123:CYS:SG	56:I:303:SF4:S3	3.06	0.54
12:L:232:TRP:CH2	12:L:233:LEU:HD21	2.42	0.54
12:L:510:LYS:HE3	12:L:512:SER:HB2	1.90	0.54
12:L:551:THR:HA	12:L:555:LEU:HD12	1.90	0.54
13:M:336:ARG:HH22	13:M:429:SER:HA	1.73	0.54
13:M:373:ILE:HD11	13:M:454:ILE:HD11	1.88	0.54
32:g:117:ARG:NE	41:p:10:TYR:OH	2.41	0.54
49:AE:272:VAL:HG12	49:AE:274:GLY:N	2.22	0.54
51:AG:39:LEU:O	51:AG:42:THR:HG22	2.08	0.54
49:Ae:263:TYR:HB2	49:Ae:271:VAL:HG13	1.89	0.54
1:A:54:LYS:CG	1:A:55:PHE:N	2.71	0.54
1:A:95:VAL:HG11	8:H:302:MET:CG	2.38	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
12:L:362:ILE:HA	12:L:365:ILE:HG13	1.90	0.54
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.38	0.54
13:M:313:THR:HG21	13:M:456:GLY:CA	2.38	0.54
13:M:421:ASN:HB2	38:m:51:TYR:OH	2.08	0.54
16:P:300:TRP:O	16:P:304:LEU:HG	2.08	0.54
17:Q:160:TYR:CZ	17:Q:164:PHE:HZ	2.26	0.54
19:S:44:LEU:HD13	19:S:91:MET:HG2	1.88	0.54
22:W:23:ILE:HG22	22:W:24:PHE:CD2	2.42	0.54
23:X:121:ASP:O	23:X:122:LEU:C	2.50	0.54
35:j:98:GLY:O	35:j:100:PRO:HD3	2.06	0.54
39:n:20:TYR:CE2	39:n:24:LEU:CD1	2.91	0.54
46:AB:60:ARG:HG3	46:AB:124:GLU:HB3	1.89	0.54
46:AB:290:GLN:NE2	49:AI:7:ARG:O	2.37	0.54
46:AB:300:LYS:HG2	46:AB:301:ARG:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:160:ASP:O	48:Ad:183:GLU:HB3	2.08	0.54
49:AE:195:LEU:HD11	49:AE:248:ARG:HH11	1.72	0.54
45:Aa:273:SER:O	45:Aa:455:ALA:HA	2.08	0.54
47:Ac:215:ALA:HA	51:Ag:11:ILE:HD11	1.90	0.54
48:Ad:155:GLN:HB3	48:Ad:166:MET:HG2	1.90	0.54
71:Ad:402:3PH:H222	49:Ae:135:GLN:HE22	1.73	0.54
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:J:9:SER:HB3	11:K:7:ASN:ND2	2.16	0.54
10:J:60:LEU:HD13	10:J:61:GLY:N	2.21	0.54
12:L:131:LEU:CD1	12:L:140:LEU:CD1	2.78	0.54
13:M:160:LEU:HD23	13:M:164:LEU:HD13	1.89	0.54
13:M:263:LEU:HD11	38:m:102:TYR:CD1	2.41	0.54
13:M:264:LEU:CD2	38:m:98:LEU:HD21	2.37	0.54
13:M:276:CYS:HB3	13:M:285:LEU:HG	1.89	0.54
14:N:33:LEU:HD11	14:N:141:ILE:HD12	1.90	0.54
15:O:170:LEU:HG	15:O:179:ILE:CD1	2.37	0.54
20:T:140:CYS:HB2	20:T:143:GLU:HG2	1.90	0.54
23:X:130:LYS:CE	27:b:67:PRO:HB3	2.38	0.54
34:i:22:TRP:CE3	39:n:172:THR:HG22	2.43	0.54
46:AB:148:ARG:NH2	50:Af:50:ARG:O	2.40	0.54
49:AE:190:VAL:HG11	49:AE:195:LEU:HD21	1.90	0.54
45:Aa:183:VAL:HG21	45:Aa:286:HIS:HB2	1.88	0.54
1:A:1:MET:O	1:A:2:ASN:C	2.49	0.54
1:A:55:PHE:CB	10:J:69:TYR:OH	2.54	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.54
4:D:35:ARG:HE	32:g:59:PRO:HD2	1.73	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.48	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:5:ASN:HD21	26:a:23:THR:HG23	1.73	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
12:L:247:LEU:HD11	12:L:248:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:31:SER:HA	13:M:34:ILE:HG12	1.90	0.54
13:M:79:ALA:HB1	13:M:225:ILE:HD13	1.90	0.54
15:O:48:LYS:H	15:O:51:LYS:HE3	1.71	0.54
19:S:25:GLN:HG2	19:S:57:GLU:HG2	1.89	0.54
19:S:41:TYR:HE1	19:S:53:ILE:HG23	1.73	0.54
20:T:97:LYS:HG3	20:T:97:LYS:O	2.08	0.54
33:h:96:ALA:O	41:p:63:TYR:HE1	1.90	0.54
33:h:129:PRO:HG3	41:p:66:ARG:CZ	2.37	0.54
38:m:109:ARG:O	38:m:113:GLU:HG2	2.08	0.54
47:AC:223:TYR:CE2	48:AD:314:LEU:HG	2.40	0.54
49:AE:143:SER:O	49:AE:146:VAL:HG22	2.08	0.54
51:AG:78:TYR:HE1	52:AH:62:GLU:HB2	1.70	0.54
49:AI:43:LEU:HD13	46:Ab:164:VAL:HG22	1.86	0.54
1:A:62:PHE:HE2	10:J:62:GLY:HA2	1.73	0.54
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.90	0.54
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.43	0.54
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.89	0.54
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.90	0.54
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
8:H:118:TRP:NE1	10:J:30:LEU:CD2	2.71	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
13:M:1:MET:HE2	13:M:52:PHE:CE2	2.42	0.54
13:M:283:LYS:HG3	13:M:327:PHE:CE1	2.43	0.54
14:N:108:LEU:HD22	14:N:191:LEU:HD22	1.90	0.54
14:N:164:MET:CE	55:Y:201:3PE:H261	2.37	0.54
16:P:207:PHE:CE1	16:P:214:LEU:HD22	2.43	0.54
16:P:239:PRO:HG2	16:P:345:LEU:HD12	1.90	0.54
17:Q:117:THR:HG22	17:Q:119:ASP:H	1.73	0.54
25:Z:53:TRP:NE1	25:Z:57:ARG:HD2	2.23	0.54
38:m:8:PRO:HB3	38:m:14:LEU:N	2.23	0.54
45:Aa:273:SER:HB3	51:Ag:18:SER:O	2.07	0.54
46:Ab:293:LEU:HD23	46:Ab:308:LEU:HD12	1.89	0.54
48:Ad:116:VAL:HG22	48:Ad:253:LEU:HD21	1.89	0.54
62:Ag:101:CDL:H532	62:Ag:101:CDL:H121	1.88	0.54
1:A:63:LEU:HG	10:J:66:VAL:HG21	1.90	0.54
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.90	0.54
5:E:187:ILE:O	5:E:188:ASN:C	2.48	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
9:I:109:GLY:O	18:R:63:LEU:HD12	2.08	0.54
10:J:124:LEU:HB2	25:Z:137:ASN:HD21	1.73	0.54
12:L:174:TYR:HE1	55:L:703:3PE:H331	1.71	0.54
12:L:481:THR:HG22	40:o:95:TYR:CE2	2.42	0.54
12:L:512:SER:HA	39:n:40:PHE:HZ	1.73	0.54
12:L:550:LEU:HD11	13:M:279:GLN:NE2	2.23	0.54
13:M:231:LEU:O	13:M:236:LEU:HG	2.06	0.54
13:M:423:MET:SD	38:m:59:HIS:NE2	2.81	0.54
14:N:179:MET:HB3	14:N:216:PHE:CZ	2.43	0.54
14:N:321:LYS:HB2	29:d:49:ARG:NE	2.23	0.54
22:W:58:THR:HG22	22:W:60:LYS:H	1.72	0.54
32:g:145:ILE:CG2	41:p:160:LYS:HE2	2.33	0.54
39:n:125:TRP:CE3	39:n:128:LEU:HD12	2.42	0.54
40:o:57:ASP:CG	40:o:59:CYS:H	2.16	0.54
41:p:31:THR:O	41:p:35:LYS:HG3	2.07	0.54
46:AB:237:PHE:O	46:AB:238:LEU:HB2	2.07	0.54
45:Aa:186:TYR:HB3	45:Aa:275:ILE:HG21	1.90	0.54
46:Ab:50:ALA:HB3	46:Ab:221:VAL:HG22	1.90	0.54
47:Ac:222:PRO:HG2	47:Ac:223:TYR:CD2	2.43	0.54
49:Ae:136:PHE:O	49:Ae:137:VAL:C	2.51	0.54
50:Af:102:ARG:HH21	50:Af:103:LYS:HE3	1.73	0.54
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
4:D:37:TRP:CE3	13:M:140:THR:HA	2.42	0.53
4:D:92:HIS:H	4:D:458:PHE:HE2	1.57	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.44	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.38	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
9:I:80:GLU:CB	43:r:26:LEU:HD11	2.38	0.53
12:L:102:GLN:NE2	12:L:452:ASN:HB2	2.23	0.53
12:L:427:ILE:HD11	36:k:69:PHE:CE1	2.43	0.53
12:L:554:ASP:OD2	13:M:213:HIS:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:79:LEU:HA	19:S:82:LEU:CD1	2.24	0.53
20:U:95:PRO:HG2	20:U:96:GLU:HG3	1.88	0.53
25:Z:62:ILE:HG23	27:b:50:PRO:HD3	1.89	0.53
27:b:59:ASP:HA	27:b:63:MET:HE2	1.89	0.53
32:g:140:PHE:HZ	41:p:152:ALA:HB1	1.72	0.53
46:AB:59:SER:OG	46:AB:130:ILE:HG21	2.08	0.53
47:AC:233:LEU:HD23	48:AD:300:LEU:HD23	1.90	0.53
49:AE:123:VAL:HG22	53:AJ:29:ALA:HB2	1.90	0.53
45:Aa:55:ASN:HB3	45:Aa:226:ALA:HB1	1.90	0.53
48:Ad:170:LYS:NZ	49:Ae:151:LYS:HD3	2.23	0.53
48:Ad:255:TYR:HB3	48:Ad:257:ASP:OD1	2.08	0.53
1:A:73:LEU:HD11	10:J:57:LEU:CD2	2.38	0.53
3:C:100:ARG:HH12	21:V:86:LYS:HZ1	1.56	0.53
4:D:92:HIS:HB2	4:D:458:PHE:CE2	2.44	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
12:L:141:PHE:CD2	13:M:370:PRO:CG	2.91	0.53
12:L:407:TRP:HE1	37:l:140:MET:CE	2.21	0.53
12:L:559:GLU:HG2	12:L:564:LYS:HD3	1.90	0.53
12:L:578:THR:HG21	14:N:168:GLY:HA2	1.89	0.53
16:P:58:VAL:O	16:P:83:PRO:HD2	2.09	0.53
20:U:99:SER:O	20:U:100:VAL:C	2.51	0.53
55:Y:201:3PE:H251	55:Y:201:3PE:H331	1.89	0.53
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.53
45:AA:170:ARG:HG3	45:AA:171:GLU:N	2.22	0.53
47:AC:164:ILE:O	47:AC:177:ARG:HD2	2.08	0.53
68:AC:404:U10:H111	68:AC:404:U10:C1M	2.39	0.53
52:AH:45:ARG:O	52:AH:49:GLU:HG2	2.09	0.53
62:Aa:501:CDL:HB31	62:Aa:501:CDL:H111	1.90	0.53
47:Ac:18:PHE:CE1	69:Ac:406:UQ6:C8	2.89	0.53
48:Ad:125:HIS:CE1	48:Ad:194:PRO:HB3	2.43	0.53
49:Ae:161:GLU:HA	49:Ae:178:HIS:CD2	2.43	0.53
51:Ag:74:ASN:O	51:Ag:77:MET:HB3	2.08	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.08	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:121:TRP:CZ3	10:J:27:TYR:CZ	2.96	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
12:L:79:SER:CB	12:L:135:ASN:HB2	2.36	0.53
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.90	0.53
14:N:193:ILE:CD1	14:N:200:LEU:HD22	2.38	0.53
15:O:40:LEU:O	15:O:44:ILE:HG13	2.09	0.53
15:O:114:LEU:HA	15:O:131:LEU:HD22	1.91	0.53
16:P:122:HIS:CB	18:R:46:VAL:HG22	2.39	0.53
16:P:262:THR:N	16:P:332:LEU:HD12	2.23	0.53
16:P:370:LYS:HG3	16:P:370:LYS:O	2.08	0.53
40:o:93:LEU:C	40:o:96:VAL:HG12	2.33	0.53
41:p:103:MET:CE	41:p:135:VAL:HG12	2.38	0.53
45:AA:119:HIS:HA	46:AB:298:HIS:O	2.09	0.53
48:AD:121:CYS:HA	70:AD:401:HEC:CMC	2.38	0.53
49:AE:191:GLU:CD	49:AE:191:GLU:H	2.14	0.53
49:AE:192:VAL:HA	49:AE:195:LEU:CD1	2.37	0.53
55:AF:201:3PE:H392	55:AF:201:3PE:H241	1.89	0.53
45:Aa:99:LYS:HE2	46:Ab:302:GLY:CA	2.39	0.53
45:Aa:403:LEU:CD1	45:Aa:403:LEU:H	2.22	0.53
48:Ad:165:PHE:O	48:Ad:166:MET:C	2.52	0.53
49:Ae:207:LYS:CD	49:Ae:210:TRP:HD1	2.20	0.53
53:Aj:31:PHE:HA	54:Ak:48:ILE:CG2	2.39	0.53
5:E:131:ILE:HG13	5:E:187:ILE:HG12	1.89	0.53
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
12:L:9:LEU:HD21	55:L:701:3PE:C2A	2.38	0.53
12:L:226:GLN:OE1	12:L:284:THR:HG21	2.07	0.53
12:L:387:THR:HG22	12:L:465:GLY:N	2.24	0.53
12:L:400:ASN:HD21	12:L:413:LEU:HD11	1.73	0.53
15:O:140:LEU:HD11	15:O:198:TYR:OH	2.08	0.53
18:R:94:ASN:OD1	18:R:96:ASP:HB2	2.08	0.53
20:T:87:LEU:HD23	20:T:122:MET:HE1	1.91	0.53
34:i:83:HIS:HD2	41:p:37:TYR:CE2	2.27	0.53
42:q:95:ASP:OD1	42:q:96:ASP:N	2.41	0.53
48:AD:255:TYR:HB3	48:AD:257:ASP:OD1	2.08	0.53
49:AE:264:GLU:HB3	49:AE:272:VAL:HB	1.89	0.53
45:Aa:338:CYS:HB2	45:Aa:368:MET:SD	2.48	0.53
47:Ac:294:LEU:HD21	68:Ac:405:U10:H1M2	1.90	0.53
48:Ad:139:CYS:C	53:Aj:53:TRP:CZ3	2.87	0.53
1:A:61:THR:CG2	8:H:290:TRP:CZ3	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:ASN:ND2	21:V:108:PRO:HG2	2.24	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
10:J:40:CYS:SG	10:J:56:PHE:HB2	2.49	0.53
11:K:22:PHE:CB	12:L:585:LYS:HG2	2.35	0.53
12:L:509:MET:HG2	39:n:33:HIS:CE1	2.43	0.53
12:L:518:PRO:C	12:L:520:SER:N	2.62	0.53
12:L:563:PRO:HG3	13:M:152:TYR:OH	2.08	0.53
15:O:80:GLN:HE22	15:O:267:THR:HG22	1.73	0.53
15:O:319:ILE:HG13	15:O:320:GLY:N	2.23	0.53
15:O:352:ILE:HG21	29:d:52:PRO:HG2	1.91	0.53
17:Q:82:PRO:O	17:Q:94:THR:HG23	2.08	0.53
21:V:114:TRP:O	21:V:115:PRO:C	2.52	0.53
27:b:28:LEU:HA	27:b:31:ILE:HG22	1.90	0.53
42:q:88:ARG:HD2	42:q:94:THR:OG1	2.08	0.53
45:AA:478:LEU:HA	53:AJ:18:THR:HG21	1.90	0.53
46:AB:47:LEU:HD11	46:AB:238:LEU:HD13	1.91	0.53
48:AD:222:PRO:HD2	48:AD:225:VAL:HG11	1.89	0.53
46:Ab:229:VAL:HA	46:Ab:232:GLN:HG2	1.89	0.53
49:Ae:180:THR:N	49:Ae:183:GLU:HB2	2.23	0.53
53:Aj:7:PRO:HB2	53:Aj:10:LEU:HG	1.91	0.53
53:Aj:45:GLU:O	53:Aj:49:GLU:N	2.42	0.53
4:D:35:ARG:HE	32:g:59:PRO:CD	2.21	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:199:ARG:HD3	44:s:80:PHE:CD2	2.41	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.53
14:N:99:LEU:HD11	14:N:154:ILE:HG22	1.90	0.53
14:N:328:THR:HG23	29:d:68:PHE:CZ	2.43	0.53
16:P:164:PHE:CE2	16:P:166:HIS:HB2	2.44	0.53
20:T:118:ILE:HG23	20:T:122:MET:CE	2.37	0.53
25:Z:12:PRO:HD3	25:Z:16:TYR:CE1	2.43	0.53
36:k:49:ASP:OD1	39:n:38:ARG:HG3	2.09	0.53
39:n:56:ASP:O	39:n:57:MET:C	2.50	0.53
48:Ad:170:LYS:CD	49:Ae:151:LYS:HD3	2.32	0.53
49:Ae:263:TYR:HA	49:Ae:273:VAL:HG22	1.89	0.53
1:A:53:MET:CG	11:K:79:VAL:HG11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.53
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.53
4:D:166:ARG:HH22	25:Z:10:MET:HG2	1.74	0.53
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
9:I:54:THR:HA	27:b:13:TRP:HE1	1.73	0.53
9:I:62:MET:SD	25:Z:35:MET:HG2	2.49	0.53
9:I:80:GLU:HB3	43:r:26:LEU:HD11	1.90	0.53
12:L:358:LYS:CG	39:n:80:TYR:CE1	2.74	0.53
12:L:361:ASN:HA	12:L:431:THR:O	2.09	0.53
55:L:701:3PE:H2I1	62:L:705:CDL:C59	2.39	0.53
62:L:706:CDL:H822	55:Y:201:3PE:C39	2.38	0.53
13:M:55:MET:HG3	13:M:56:PHE:CD2	2.44	0.53
13:M:269:MET:CE	13:M:396:MET:HA	2.36	0.53
13:M:453:LEU:HD12	13:M:453:LEU:C	2.33	0.53
14:N:99:LEU:HD21	14:N:157:LEU:HD12	1.90	0.53
14:N:328:THR:HG23	29:d:68:PHE:HZ	1.74	0.53
19:S:16:LEU:HD13	19:S:19:ILE:CD1	2.38	0.53
21:V:48:THR:HA	21:V:51:ILE:HD12	1.90	0.53
23:X:158:LEU:HD13	29:d:17:GLU:HG3	1.91	0.53
29:d:109:TYR:O	29:d:110:ALA:C	2.50	0.53
39:n:39:TYR:CZ	39:n:43:LEU:HD11	2.44	0.53
42:q:125:VAL:HG23	42:q:125:VAL:O	2.08	0.53
45:AA:136:LEU:HD21	46:AB:380:ALA:HA	1.91	0.53
47:AC:77:TRP:CD2	48:AD:281:GLU:HG3	2.44	0.53
49:AE:132:VAL:HA	49:AE:135:GLN:NE2	2.23	0.53
49:AE:204:ARG:HB3	49:AE:260:VAL:CG2	2.25	0.53
45:Aa:136:LEU:HD21	46:Ab:380:ALA:HA	1.90	0.53
45:Aa:270:PHE:HE1	45:Aa:353:LEU:HD22	1.72	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
10:J:12:PHE:HE2	11:K:42:ILE:HD11	1.74	0.53
12:L:124:PHE:HZ	12:L:252:MET:HB2	1.74	0.53
13:M:57:SER:CB	13:M:113:THR:HG22	2.39	0.53
13:M:59:ASP:O	13:M:60:PRO:C	2.49	0.53
13:M:73:LEU:HD23	13:M:103:GLN:NE2	2.23	0.53
14:N:203:LEU:HD13	14:N:344:ILE:HG22	1.90	0.53
15:O:73:LEU:CD2	15:O:207:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:170:LEU:HD13	15:O:187:TYR:CD2	2.44	0.53
16:P:265:PHE:HD1	16:P:334:GLY:HA3	1.74	0.53
24:Y:50:SER:HB3	24:Y:53:GLU:HG2	1.91	0.53
26:a:51:ASP:HA	26:a:54:ILE:HD12	1.91	0.53
33:h:156:VAL:CG1	33:h:160:MET:HE3	2.39	0.53
36:k:38:VAL:CG1	39:n:39:TYR:HB2	2.34	0.53
48:AD:111:ARG:O	48:AD:115:GLN:HG3	2.09	0.53
53:AJ:43:ILE:O	53:AJ:47:ILE:HG13	2.09	0.53
1:A:54:LYS:HD2	1:A:113:TRP:CB	2.38	0.53
4:D:36:GLN:OE1	13:M:136:TRP:HA	2.09	0.53
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.21	0.53
5:E:81:VAL:CB	5:E:104:LEU:HD11	2.38	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
12:L:20:LEU:C	12:L:20:LEU:CD1	2.81	0.53
13:M:15:THR:HG21	13:M:100:ILE:HD12	1.90	0.53
13:M:188:ALA:H	13:M:253:LEU:HD11	1.74	0.53
13:M:348:LEU:HD12	13:M:415:GLN:NE2	2.24	0.53
14:N:193:ILE:HD12	14:N:266:ILE:HA	1.91	0.53
18:R:69:VAL:HG12	18:R:112:LYS:N	2.24	0.53
18:R:98:GLU:HA	18:R:113:GLN:CD	2.33	0.53
19:S:82:LEU:HD13	19:S:86:GLU:OE1	2.08	0.53
32:g:139:TYR:CD2	32:g:140:PHE:CD1	2.96	0.53
35:j:99:ILE:HA	40:o:108:LEU:HD21	1.90	0.53
37:l:55:TYR:O	37:l:104:PRO:HG3	2.09	0.53
39:n:136:GLU:OE2	39:n:167:TRP:NE1	2.42	0.53
45:AA:255:ARG:O	45:AA:255:ARG:CG	2.51	0.53
46:AB:257:GLU:HA	46:AB:438:MET:O	2.09	0.53
49:AE:262:ALA:O	49:AE:273:VAL:O	2.27	0.53
49:AI:76:VAL:HG22	49:AI:78:PHE:H	1.73	0.53
47:Ac:30:TRP:HB3	47:Ac:100:ARG:HD3	1.90	0.53
47:Ac:275:LEU:O	47:Ac:276:PHE:C	2.51	0.53
48:Ad:213:SER:O	48:Ad:217:GLY:N	2.42	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.53
11:K:5:PHE:HE1	11:K:47:THR:HG23	1.74	0.53
11:K:24:SER:O	11:K:90:VAL:HG13	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:450:LEU:HG	12:L:454:ILE:HD12	1.91	0.53
12:L:598:ILE:CD1	14:N:153:ILE:HG12	2.38	0.53
13:M:314:MET:HE1	13:M:380:PHE:CD2	2.44	0.53
14:N:81:LEU:HD23	30:e:60:PHE:HE1	1.74	0.53
14:N:155:LEU:HD13	14:N:278:MET:HG3	1.91	0.53
14:N:331:ILE:O	14:N:335:MET:HB2	2.09	0.53
15:O:77:ILE:HD13	15:O:273:ILE:HD11	1.90	0.53
16:P:275:HIS:HA	16:P:278:LYS:HG2	1.91	0.53
33:h:184:LYS:HE3	33:h:186:THR:O	2.08	0.53
34:i:106:PRO:HD2	40:o:64:ILE:CG2	2.38	0.53
36:k:47:LEU:CD1	39:n:43:LEU:HD23	2.39	0.53
38:m:85:LYS:O	38:m:85:LYS:HG2	2.09	0.53
45:AA:74:TRP:HH2	45:AA:410:CYS:SG	2.31	0.53
46:AB:348:GLY:HA2	46:AB:448:PRO:HD3	1.91	0.53
47:AC:141:TRP:CD1	47:AC:265:PRO:CD	2.90	0.53
47:AC:148:ASN:OD1	49:Ae:220:LEU:O	2.26	0.53
47:AC:170:VAL:HG23	47:AC:174:THR:CB	2.39	0.53
48:AD:206:GLY:HA3	48:AD:210:TYR:HB2	1.91	0.53
48:AD:227:LEU:HD12	48:AD:227:LEU:C	2.34	0.53
45:Aa:311:ILE:HB	45:Aa:343:THR:HG21	1.91	0.53
46:Ab:226:SER:O	46:Ab:229:VAL:HG22	2.09	0.53
47:Ac:170:VAL:HG23	47:Ac:174:THR:CB	2.39	0.53
51:Ag:43:ARG:HD3	55:Ag:102:3PE:C3B	2.39	0.53
51:Ag:48:ARG:HE	55:Ag:102:3PE:H332	1.74	0.53
4:D:145:MET:O	4:D:148:GLU:N	2.41	0.52
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.91	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
10:J:120:LEU:C	10:J:122:ASP:H	2.16	0.52
12:L:128:MET:CG	12:L:251:THR:HB	2.36	0.52
12:L:247:LEU:O	12:L:252:MET:HB3	2.09	0.52
13:M:73:LEU:HD21	13:M:100:ILE:HG12	1.90	0.52
14:N:313:MET:HG2	15:O:305:LEU:HD22	1.91	0.52
16:P:179:LYS:O	16:P:182:ARG:HG2	2.10	0.52
16:P:203:PRO:HG2	64:P:401:NDP:C6N	2.37	0.52
16:P:206:ILE:HG13	64:P:401:NDP:H42N	1.89	0.52
20:U:78:GLY:O	20:U:79:ILE:C	2.51	0.52
25:Z:68:ARG:O	25:Z:69:ILE:C	2.49	0.52
31:f:49:ARG:CG	31:f:52:GLU:HG3	2.39	0.52
42:q:56:PHE:HD1	42:q:59:HIS:NE2	2.06	0.52
49:AE:207:LYS:HD2	49:AE:210:TRP:CD1	2.44	0.52
49:AI:43:LEU:HB2	46:Ab:167:GLN:HE21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:60:ARG:HG2	46:Ab:393:LEU:HD13	1.90	0.52
47:Ac:312:GLN:HE21	50:Af:37:THR:HB	1.74	0.52
49:Ae:116:LEU:HB2	53:Aj:15:PHE:CE2	2.44	0.52
4:D:51:VAL:HG21	4:D:58:THR:HG22	1.90	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:300:ILE:CG2	6:F:305:GLY:O	2.45	0.52
6:F:392:MET:HE1	6:F:419:ILE:HD12	1.79	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
12:L:108:MET:HB2	12:L:114:ILE:HD13	1.90	0.52
12:L:228:GLY:O	12:L:229:LEU:CG	2.47	0.52
12:L:332:HIS:CD2	12:L:336:LYS:HG3	2.44	0.52
13:M:160:LEU:CD2	13:M:164:LEU:HD13	2.39	0.52
13:M:354:LEU:O	13:M:357:THR:N	2.41	0.52
13:M:447:LEU:HD11	13:M:454:ILE:HG23	1.90	0.52
14:N:227:ILE:HA	14:N:230:ILE:CG2	2.39	0.52
15:O:350:LYS:O	15:O:351:TRP:HB2	2.09	0.52
16:P:85:ARG:HE	64:P:401:NDP:C2A	2.22	0.52
16:P:283:MET:HE2	16:P:366:ILE:HG22	1.92	0.52
17:Q:72:ILE:HD13	17:Q:143:TRP:NE1	2.24	0.52
18:R:95:LEU:HD21	18:R:111:PHE:CB	2.37	0.52
18:R:113:GLN:CD	18:R:113:GLN:N	2.66	0.52
30:e:41:ILE:HD13	33:h:174:PRO:HD2	1.92	0.52
36:k:20:MET:HE3	36:k:22:LEU:HD21	1.91	0.52
39:n:163:LEU:O	39:n:164:PRO:C	2.51	0.52
71:AD:402:3PH:H371	71:AD:402:3PH:C26	2.40	0.52
49:AE:180:THR:N	49:AE:183:GLU:HB2	2.23	0.52
47:Ac:223:TYR:C	48:Ad:311:TRP:HE1	2.14	0.52
71:Ad:402:3PH:H12	49:Ae:131:ASN:HD21	1.73	0.52
52:Ah:27:PRO:HB3	52:Ah:87:ASN:CG	2.34	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.92	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:133:VAL:HA	26:a:41:VAL:HB	1.91	0.52
13:M:196:TRP:HE1	13:M:254:THR:HB	1.75	0.52
13:M:213:HIS:O	13:M:217:PRO:HD3	2.09	0.52
13:M:313:THR:HA	13:M:316:MET:HE3	1.89	0.52
13:M:388:TRP:CD1	38:m:109:ARG:HD2	2.44	0.52
15:O:121:PRO:C	15:O:122:LYS:HG2	2.33	0.52
16:P:153:ALA:CB	16:P:191:VAL:HG23	2.39	0.52
16:P:305:PHE:CG	16:P:314:THR:HG22	2.45	0.52
26:a:64:LYS:HG3	26:a:66:LEU:H	1.75	0.52
48:AD:284:HIS:CE1	48:AD:288:MET:HE3	2.43	0.52
50:AF:108:TRP:HA	50:AF:111:LYS:HZ2	1.74	0.52
45:Aa:57:LEU:CA	45:Aa:226:ALA:O	2.57	0.52
48:Ad:192:ALA:HB3	70:Ad:401:HEC:HMD3	1.92	0.52
48:Ad:214:LEU:HA	48:Ad:234:ASN:HD21	1.73	0.52
48:Ad:321:TYR:CD2	48:Ad:323:PRO:HD3	2.44	0.52
49:Ae:190:VAL:HG11	49:Ae:195:LEU:HD21	1.90	0.52
49:Ae:207:LYS:HD2	49:Ae:210:TRP:CD1	2.43	0.52
49:Ae:241:SER:OG	49:Ae:253:PRO:HD2	2.10	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.91	0.52
7:G:126:LEU:HD13	18:R:89:PRO:HB3	1.90	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
8:H:307:LEU:HD11	25:Z:47:TYR:CG	2.45	0.52
9:I:80:GLU:OE2	43:r:26:LEU:HD13	2.08	0.52
12:L:536:ILE:HG23	12:L:537:THR:N	2.25	0.52
13:M:403:THR:HA	13:M:406:TYR:CE2	2.44	0.52
14:N:10:TYR:O	14:N:13:ILE:HG22	2.09	0.52
14:N:220:MET:O	14:N:221:LEU:C	2.51	0.52
15:O:310:ILE:HG13	15:O:311:PRO:HD2	1.91	0.52
20:T:130:ILE:CG2	20:T:131:PRO:HD2	2.40	0.52
20:U:74:LEU:HD23	20:U:79:ILE:HD11	1.91	0.52
23:X:35:GLN:HB2	23:X:70:PHE:CE1	2.44	0.52
25:Z:65:LEU:O	25:Z:69:ILE:HG12	2.09	0.52
26:a:1:MET:HG3	62:a:101:CDL:HB21	1.92	0.52
27:b:66:VAL:HG11	27:b:70:PRO:HA	1.92	0.52
34:i:19:ARG:HH11	39:n:173:ARG:HH21	1.56	0.52
37:l:119:THR:HG23	38:m:11:LEU:HA	1.91	0.52
42:q:68:MET:SD	42:q:81:MET:CB	2.95	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:85:LEU:HA	44:s:88:SER:HB2	1.92	0.52
45:AA:339:GLN:HB2	45:AA:359:VAL:O	2.10	0.52
47:AC:28:SER:HB2	62:AC:406:CDL:OA3	2.09	0.52
49:AI:62:ARG:HD2	49:AI:63:PRO:HD2	1.90	0.52
47:Ac:37:LEU:CB	67:Ac:403:HEM:HMB1	2.35	0.52
49:Ae:204:ARG:HB3	49:Ae:260:VAL:CG2	2.25	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.51	0.52
2:B:170:TYR:OH	4:D:131:GLN:O	2.28	0.52
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.52
3:C:104:ASN:O	43:r:97:PRO:HD3	2.09	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:135:ALA:HB2	8:H:201:THR:OG1	2.09	0.52
11:K:38:LEU:HG	11:K:42:ILE:CD1	2.39	0.52
12:L:297:ASP:HB3	12:L:300:LYS:CG	2.39	0.52
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.90	0.52
55:L:707:3PE:H3C1	13:M:155:ILE:HD11	1.91	0.52
13:M:171:VAL:HG11	13:M:179:LEU:CD2	2.35	0.52
13:M:278:ARG:HH22	37:l:108:ASP:CG	2.18	0.52
14:N:320:THR:O	14:N:320:THR:CG2	2.58	0.52
15:O:336:GLY:N	15:O:344:ASN:ND2	2.57	0.52
17:Q:58:LYS:O	17:Q:59:LEU:C	2.49	0.52
18:R:45:ARG:HD2	18:R:48:PHE:CD1	2.44	0.52
20:T:103:HIS:HD1	20:T:140:CYS:HG	1.51	0.52
26:a:7:PRO:HD3	62:a:101:CDL:H181	1.91	0.52
34:i:31:ARG:O	34:i:32:GLU:C	2.51	0.52
38:m:49:LEU:HA	39:n:133:TRP:HH2	1.74	0.52
47:AC:346:PRO:O	47:AC:349:ILE:HG22	2.10	0.52
48:AD:228:ARG:HG2	48:AD:231:LEU:HD12	1.91	0.52
48:AD:248:ILE:CG2	48:AD:263:MET:HG3	2.40	0.52
48:Ad:147:ALA:O	48:Ad:151:GLU:HG3	2.09	0.52
51:Ag:77:MET:HG3	51:Ag:78:TYR:CD2	2.45	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:99:LEU:HD12	4:D:99:LEU:O	2.10	0.52
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
11:K:57:MET:N	11:K:58:PRO:HD2	2.24	0.52
15:O:168:VAL:CG2	15:O:241:TYR:OH	2.56	0.52
16:P:336:GLU:CG	16:P:342:PRO:HD3	2.38	0.52
19:S:16:LEU:O	19:S:16:LEU:CD1	2.51	0.52
22:W:94:GLN:HA	22:W:97:ILE:HG22	1.92	0.52
24:Y:68:ILE:CD1	24:Y:103:LEU:HB2	2.39	0.52
26:a:6:LEU:O	26:a:7:PRO:C	2.52	0.52
29:d:62:LEU:O	29:d:66:THR:OG1	2.22	0.52
33:h:87:THR:HG22	62:h:201:CDL:H512	1.90	0.52
33:h:111:GLU:O	41:p:63:TYR:HA	2.08	0.52
62:h:201:CDL:H721	34:i:84:TYR:CD2	2.44	0.52
47:AC:145:VAL:HG13	49:Ae:220:LEU:HD13	1.92	0.52
48:AD:112:ARG:HD3	48:AD:257:ASP:OD2	2.10	0.52
48:AD:296:MET:HE2	71:AD:402:3PH:H362	1.90	0.52
51:Ag:68:GLU:HA	51:Ag:71:LYS:HE2	1.92	0.52
2:B:194:CYS:O	56:B:301:SF4:S2	2.67	0.52
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.34	0.52
5:E:87:ARG:HD2	44:s:77:THR:CG2	2.40	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.92	0.52
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.52
8:H:134:ARG:CZ	8:H:200:LEU:HD13	2.39	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
10:J:121:GLY:C	10:J:123:TRP:N	2.64	0.52
12:L:123:LEU:HD22	12:L:150:MET:HG3	1.91	0.52
12:L:481:THR:CG2	40:o:95:TYR:CD2	2.93	0.52
12:L:496:LEU:C	12:L:496:LEU:CD1	2.79	0.52
15:O:170:LEU:HD13	15:O:187:TYR:CG	2.44	0.52
25:Z:94:GLU:HA	25:Z:97:ILE:CG1	2.39	0.52
41:p:50:GLU:HG3	41:p:54:ARG:HH21	1.75	0.52
42:q:29:ARG:HD3	42:q:74:PHE:CE1	2.44	0.52
46:AB:226:SER:O	46:AB:229:VAL:HG22	2.09	0.52
47:AC:146:ILE:CG1	68:AC:404:U10:H4M3	2.39	0.52
47:AC:169:SER:HB3	49:Ae:172:LYS:HD2	1.91	0.52
45:Aa:169:LEU:HA	45:Aa:172:MET:HE2	1.92	0.52
46:Ab:60:ARG:CD	46:Ab:393:LEU:HD13	2.40	0.52
1:A:54:LYS:CD	1:A:113:TRP:HB2	2.39	0.52
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.90	0.52
4:D:67:ASN:HB2	15:O:193:LEU:HD22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:196:THR:O	5:E:200:ILE:HD12	2.10	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
12:L:108:MET:HB2	12:L:114:ILE:CD1	2.39	0.52
12:L:145:GLU:HB3	13:M:370:PRO:HG2	1.90	0.52
12:L:427:ILE:HD11	36:k:69:PHE:HE1	1.73	0.52
55:L:707:3PE:H121	14:N:295:ARG:HG3	1.92	0.52
13:M:68:LEU:HG	13:M:234:ILE:HD11	1.92	0.52
13:M:84:LEU:HD21	13:M:95:TYR:HB3	1.90	0.52
13:M:346:ARG:O	13:M:419:LEU:HA	2.09	0.52
16:P:236:VAL:HG11	16:P:270:ARG:HH21	1.75	0.52
20:T:79:ILE:CG2	20:T:145:VAL:HG13	2.40	0.52
21:V:12:VAL:CG1	21:V:13:GLY:N	2.72	0.52
27:b:82:LYS:O	27:b:83:ASN:C	2.52	0.52
32:g:121:GLU:OE2	41:p:10:TYR:CZ	2.63	0.52
35:j:81:LEU:O	35:j:82:GLY:C	2.51	0.52
42:q:138:VAL:HG23	42:q:139:PRO:HD2	1.92	0.52
46:AB:432:VAL:HG22	46:AB:432:VAL:O	2.09	0.52
48:AD:125:HIS:HB3	48:AD:197:LEU:HG	1.91	0.52
45:Aa:479:ARG:NH1	62:Aa:501:CDL:OB2	2.42	0.52
47:Ac:148:ASN:OD1	47:Ac:165:TRP:HH2	1.90	0.52
48:Ad:125:HIS:CE1	48:Ad:195:PRO:HD2	2.34	0.52
54:Ak:14:ALA:O	54:Ak:18:ILE:HG12	2.10	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
9:I:89:GLU:HG3	42:q:61:TRP:HB3	1.92	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
12:L:49:LEU:HD12	41:p:33:LEU:HD23	1.92	0.52
12:L:533:ILE:HG23	12:L:534:HIS:HD2	1.74	0.52
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.91	0.52
20:U:128:PHE:CE1	20:U:148:ILE:HG23	2.45	0.52
21:V:95:LEU:HA	21:V:100:TRP:CH2	2.35	0.52
45:AA:170:ARG:HA	45:AA:173:GLN:CD	2.34	0.52
47:AC:141:TRP:CD1	47:AC:264:THR:HA	2.45	0.52
49:AI:43:LEU:CD1	46:Ab:164:VAL:HG23	2.29	0.52
45:Aa:212:SER:O	45:Aa:213:ARG:C	2.50	0.52
46:Ab:70:ARG:NH2	46:Ab:332:ASP:OD2	2.43	0.52
49:Ae:90:ASP:O	51:Ag:25:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
9:I:155:CYS:SG	56:I:303:SF4:S2	3.08	0.52
12:L:483:PRO:HG2	12:L:486:LEU:HD13	1.91	0.52
14:N:200:LEU:HD22	14:N:269:GLU:HG3	1.92	0.52
27:b:7:ALA:C	27:b:9:LEU:N	2.68	0.52
37:l:169:GLU:C	37:l:171:GLY:N	2.55	0.52
39:n:168:TRP:HD1	39:n:169:HIS:CE1	2.27	0.52
45:AA:118:ALA:O	46:AB:298:HIS:HB3	2.09	0.52
49:AE:241:SER:OG	49:AE:253:PRO:HD2	2.10	0.52
49:AE:242:HIS:CD2	49:AE:251:LYS:HB3	2.45	0.52
45:Aa:107:ASN:HB2	45:Aa:110:GLU:CD	2.35	0.52
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
8:H:23:VAL:HG11	26:a:9:LEU:HD21	1.91	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
10:J:60:LEU:CD1	10:J:61:GLY:N	2.72	0.51
12:L:286:LEU:HG	12:L:290:ILE:CD1	2.40	0.51
13:M:103:GLN:O	13:M:107:ILE:HB	2.10	0.51
13:M:139:GLN:HB3	13:M:222:GLU:CG	2.40	0.51
15:O:121:PRO:HB3	15:O:178:TYR:CE1	2.45	0.51
20:U:133:ILE:HG23	20:U:134:ASP:N	2.26	0.51
30:e:44:ALA:HA	30:e:47:ILE:HG12	1.92	0.51
36:k:47:LEU:HD12	39:n:43:LEU:HD23	1.91	0.51
39:n:143:GLU:O	39:n:143:GLU:HG2	2.10	0.51
41:p:164:LEU:O	41:p:168:LYS:N	2.42	0.51
42:q:29:ARG:HD3	42:q:74:PHE:CD1	2.44	0.51
45:AA:207:ASN:O	45:AA:211:LEU:HG	2.09	0.51
45:AA:407:THR:O	45:AA:408:PRO:C	2.49	0.51
47:AC:140:PHE:CE1	47:AC:170:VAL:HG13	2.45	0.51
48:AD:304:TYR:CZ	48:AD:308:ARG:HD2	2.45	0.51
45:Aa:186:TYR:HE1	49:Ae:80:HIS:HB2	1.75	0.51
2:B:126:ARG:NH1	8:H:61:MET:SD	2.83	0.51
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
7:G:611:THR:HG21	17:Q:105:GLU:CA	2.27	0.51
10:J:63:MET:O	10:J:64:LEU:C	2.53	0.51
10:J:150:TRP:CD1	14:N:28:LEU:HD21	2.44	0.51
12:L:556:ILE:HD11	38:m:76:ILE:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:115:LEU:HD21	13:M:176:LEU:CD2	2.37	0.51
25:Z:99:LYS:HG3	25:Z:100:ASP:N	2.25	0.51
30:e:50:THR:O	30:e:54:LYS:NZ	2.44	0.51
31:f:37:PHE:HA	31:f:40:LYS:HB2	1.92	0.51
45:AA:338:CYS:SG	45:AA:339:GLN:N	2.84	0.51
48:AD:321:TYR:CD2	48:AD:323:PRO:HD3	2.44	0.51
50:AF:97:GLU:HA	50:AF:100:ARG:HH11	1.75	0.51
45:Aa:399:LEU:HD22	45:Aa:426:LEU:CD2	2.40	0.51
46:Ab:95:SER:O	46:Ab:99:ILE:HG13	2.10	0.51
48:Ad:167:ARG:HB2	48:Ad:168:PRO:CD	2.39	0.51
51:Ag:62:TRP:O	51:Ag:65:GLN:HG3	2.11	0.51
1:A:106:TRP:CZ3	27:b:19:LEU:HD21	2.45	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
7:G:31:LEU:HB3	7:G:42:MET:HE2	1.93	0.51
7:G:136:GLU:HB3	17:Q:87:MET:HB3	1.92	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
12:L:49:LEU:HB3	12:L:50:PRO:HD3	1.91	0.51
12:L:202:MET:CE	12:L:265:PRO:HG3	2.33	0.51
12:L:539:MET:SD	38:m:11:LEU:HD21	2.50	0.51
12:L:569:LEU:O	12:L:573:MET:HG2	2.11	0.51
20:T:140:CYS:HB2	20:T:143:GLU:CG	2.40	0.51
30:e:8:LYS:HG2	30:e:16:ARG:NH1	2.23	0.51
34:i:85:TYR:CE2	34:i:90:MET:HE3	2.46	0.51
45:AA:225:LYS:HD2	45:AA:256:VAL:H	1.74	0.51
49:AE:155:LYS:O	49:AE:158:ASP:HB2	2.09	0.51
49:AE:248:ARG:HG2	49:AE:257:ASN:ND2	2.25	0.51
54:AK:14:ALA:O	54:AK:18:ILE:HG12	2.09	0.51
46:Ab:142:THR:HG21	46:Ab:238:LEU:H	1.74	0.51
48:Ad:112:ARG:HD3	48:Ad:257:ASP:OD2	2.09	0.51
53:Aj:19:SER:HB2	54:Ak:23:MET:CB	2.41	0.51
54:Ak:18:ILE:N	54:Ak:19:PRO:HD2	2.25	0.51
1:A:75:LEU:CD2	10:J:145:TYR:HE2	2.21	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
11:K:59:ILE:O	11:K:60:PRO:C	2.49	0.51
16:P:69:VAL:HG21	16:P:129:LEU:HD11	1.91	0.51
25:Z:62:ILE:HG23	27:b:50:PRO:CD	2.41	0.51
34:i:77:ILE:HD13	34:i:80:TRP:CZ3	2.46	0.51
41:p:5:TRP:CE3	41:p:10:TYR:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:65:THR:CG2	42:q:66:THR:N	2.72	0.51
46:AB:56:ALA:O	46:AB:127:ARG:HD2	2.10	0.51
50:AF:50:ARG:O	46:Ab:148:ARG:NH2	2.44	0.51
47:Ac:110:MET:HE1	47:Ac:306:PHE:CE1	2.45	0.51
48:Ad:228:ARG:HG2	48:Ad:231:LEU:CD1	2.40	0.51
48:Ad:248:ILE:CG2	48:Ad:263:MET:HG3	2.40	0.51
2:B:87:ARG:HH11	58:B:303:PC1:P	2.34	0.51
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.43	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:126:LEU:HD11	18:R:89:PRO:HB3	1.91	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:121:TRP:CZ3	10:J:27:TYR:CE1	2.99	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
12:L:261:VAL:O	12:L:264:HIS:HD2	1.93	0.51
13:M:20:PRO:HB3	13:M:89:ASN:ND2	2.25	0.51
13:M:275:ILE:CD1	13:M:288:TYR:CG	2.84	0.51
14:N:174:GLN:HB2	14:N:177:LYS:HD2	1.92	0.51
14:N:307:THR:HB	15:O:319:ILE:HG12	1.91	0.51
15:O:332:ARG:NH1	29:d:50:MET:HE1	2.26	0.51
22:W:71:MET:O	22:W:72:LYS:C	2.51	0.51
27:b:23:PHE:CB	55:b:201:3PE:H2D2	2.37	0.51
29:d:28:ASP:O	29:d:29:PRO:C	2.53	0.51
29:d:87:ASP:O	29:d:88:HIS:C	2.51	0.51
34:i:101:LYS:HB3	34:i:102:PRO:CD	2.41	0.51
34:i:106:PRO:HD2	40:o:64:ILE:HG21	1.93	0.51
47:AC:150:LEU:HB2	47:AC:161:VAL:HG22	1.93	0.51
47:Ac:346:PRO:O	47:Ac:349:ILE:HG22	2.10	0.51
48:Ad:218:TYR:CG	48:Ad:246:PRO:HG3	2.45	0.51
49:Ae:242:HIS:CD2	49:Ae:251:LYS:HB3	2.45	0.51
49:Ae:248:ARG:HG2	49:Ae:257:ASN:ND2	2.25	0.51
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.91	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.29	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:530:PRO:O	12:L:534:HIS:HB2	2.11	0.51
13:M:11:LEU:O	13:M:15:THR:HG23	2.09	0.51
13:M:31:SER:HA	13:M:34:ILE:CG1	2.41	0.51
13:M:129:THR:CG2	13:M:235:LEU:HD11	2.40	0.51
13:M:251:ASP:N	13:M:252:PRO:HD2	2.26	0.51
14:N:149:LEU:HD12	14:N:149:LEU:C	2.34	0.51
17:Q:77:VAL:HG12	17:Q:101:PHE:CG	2.46	0.51
21:V:62:GLU:HB3	21:V:68:LEU:HD13	1.93	0.51
31:f:49:ARG:CG	31:f:52:GLU:CG	2.88	0.51
34:i:83:HIS:CD2	41:p:37:TYR:HE2	2.28	0.51
34:i:83:HIS:CE1	34:i:87:LYS:HD2	2.46	0.51
36:k:34:PRO:HD2	36:k:59:TYR:CG	2.46	0.51
36:k:39:GLN:HE22	36:k:49:ASP:HB3	1.75	0.51
42:q:88:ARG:HG3	42:q:89:TRP:N	2.26	0.51
45:AA:169:LEU:O	45:AA:173:GLN:HG3	2.11	0.51
53:AJ:30:LEU:CD1	54:AK:30:VAL:HG13	2.40	0.51
46:Ab:185:ALA:HB3	46:Ab:251:ALA:HB2	1.93	0.51
47:Ac:140:PHE:CE1	47:Ac:170:VAL:HG13	2.45	0.51
47:Ac:373:GLU:HG2	50:Af:21:TYR:OH	2.11	0.51
1:A:59:ALA:HB1	10:J:66:VAL:HG13	1.92	0.51
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.51
3:C:84:GLU:CG	3:C:141:ARG:HH11	2.23	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
9:I:48:VAL:O	27:b:10:LYS:NZ	2.42	0.51
15:O:60:ILE:HG12	15:O:83:MET:HE1	1.93	0.51
16:P:197:GLU:HB3	16:P:259:VAL:HG23	1.93	0.51
20:T:87:LEU:HD23	20:T:122:MET:CE	2.40	0.51
25:Z:81:ARG:HG3	25:Z:82:ARG:N	2.25	0.51
33:h:159:LEU:HD23	33:h:163:ARG:HH12	1.75	0.51
45:AA:73:VAL:HG23	45:AA:147:LEU:HD13	1.93	0.51
45:AA:148:ALA:HA	45:AA:250:LEU:HD21	1.92	0.51
48:AD:94:TYR:HB2	48:AD:96:TRP:NE1	2.26	0.51
48:AD:237:PHE:CG	48:AD:242:ILE:HB	2.46	0.51
49:AE:196:ARG:HD2	49:AE:249:ILE:CG2	2.41	0.51
49:Ae:184:ILE:HG21	49:Ae:208:PRO:HB3	1.93	0.51
50:Af:97:GLU:HA	50:Af:100:ARG:HH11	1.75	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:111:LEU:HD23	10:J:60:LEU:CD1	2.35	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
8:H:200:LEU:HD12	8:H:200:LEU:C	2.36	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.51
10:J:84:SER:OG	10:J:87:LEU:HB3	2.10	0.51
12:L:161:ARG:NE	12:L:163:ASP:HB2	2.26	0.51
12:L:595:ILE:O	12:L:599:ILE:HG13	2.11	0.51
13:M:304:GLN:HA	13:M:309:PHE:CE1	2.45	0.51
14:N:239:ALA:HB1	29:d:47:MET:HG2	1.93	0.51
14:N:333:SER:O	14:N:334:THR:OG1	2.26	0.51
16:P:172:ALA:H	16:P:202:ARG:NH2	2.08	0.51
17:Q:91:VAL:HG13	17:Q:95:LYS:NZ	2.26	0.51
19:S:16:LEU:HD21	19:S:95:LEU:CD1	2.41	0.51
20:U:74:LEU:HD23	20:U:79:ILE:CD1	2.40	0.51
23:X:25:LEU:O	23:X:29:ALA:N	2.44	0.51
23:X:78:CYS:C	23:X:81:PRO:HD2	2.36	0.51
25:Z:80:ASP:O	25:Z:84:LEU:HG	2.11	0.51
25:Z:93:GLU:O	25:Z:97:ILE:HG12	2.11	0.51
35:j:67:PHE:CE1	36:k:84:PHE:HA	2.46	0.51
38:m:23:TYR:HB2	39:n:65:ARG:HH21	1.76	0.51
45:AA:392:LYS:HE3	45:AA:433:ILE:O	2.11	0.51
54:AK:12:GLU:HA	54:AK:15:ARG:HH11	1.74	0.51
47:Ac:221:HIS:O	47:Ac:225:THR:HB	2.10	0.51
47:Ac:291:VAL:O	47:Ac:295:ILE:HG12	2.11	0.51
48:Ad:124:CYS:SG	70:Ad:401:HEC:CAC	2.99	0.51
48:Ad:237:PHE:CG	48:Ad:242:ILE:HB	2.46	0.51
1:A:67:LEU:CD1	11:K:68:ALA:CB	2.75	0.51
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.51
4:D:279:THR:HA	21:V:12:VAL:HG13	1.93	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.41	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
12:L:404:THR:HG22	12:L:405:ASN:H	1.75	0.51
12:L:414:ILE:O	12:L:418:MET:HG2	2.10	0.51
13:M:166:LEU:HD11	55:N:401:3PE:O14	2.11	0.51
13:M:249:ILE:HG22	13:M:250:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:75:ARG:HH12	17:Q:104:ARG:HG2	1.76	0.51
21:V:7:LYS:O	21:V:8:THR:OG1	2.29	0.51
30:e:70:TYR:OH	30:e:74:ARG:HD3	2.11	0.51
37:l:155:PRO:HG3	40:o:4:HIS:CG	2.46	0.51
42:q:88:ARG:HB2	42:q:93:MET:HB2	1.91	0.51
47:AC:77:TRP:HZ2	48:AD:284:HIS:CD2	2.28	0.51
47:AC:147:THR:HG21	47:AC:165:TRP:NE1	2.26	0.51
49:AI:64:LEU:HD12	49:AI:78:PHE:HB3	1.93	0.51
45:Aa:96:LEU:HD11	45:Aa:161:ILE:HA	1.92	0.51
45:Aa:104:ARG:HH12	45:Aa:146:LEU:HD23	1.75	0.51
46:Ab:89:LEU:HD22	46:Ab:150:GLU:HB3	1.93	0.51
47:Ac:92:ILE:HG13	47:Ac:272:TRP:CH2	2.45	0.51
48:Ad:201:VAL:HG22	48:Ad:278:SER:CB	2.41	0.51
71:Ad:402:3PH:C23	49:Ae:135:GLN:HE22	2.23	0.51
49:Ae:242:HIS:HD2	49:Ae:251:LYS:HB3	1.76	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.46	0.51
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
12:L:451:MET:O	12:L:452:ASN:C	2.53	0.51
13:M:4:ILE:HD11	13:M:41:LEU:HD21	1.92	0.51
14:N:45:ILE:HA	14:N:52:SER:OG	2.11	0.51
14:N:183:SER:O	14:N:187:MET:HE2	2.11	0.51
15:O:289:TRP:HA	15:O:289:TRP:CE3	2.46	0.51
20:U:122:MET:HA	20:U:122:MET:HE2	1.91	0.51
20:U:134:ASP:OD2	39:n:3:PHE:N	2.41	0.51
22:W:28:LEU:HG	22:W:32:LYS:HE2	1.93	0.51
23:X:44:MET:SD	25:Z:73:PRO:HA	2.51	0.51
23:X:145:ARG:HG2	23:X:146:ALA:N	2.25	0.51
45:AA:226:ALA:HB2	45:AA:253:VAL:HB	1.93	0.51
46:AB:425:VAL:HG12	46:AB:429:LYS:HZ1	1.75	0.51
49:AI:62:ARG:NH1	46:Ab:290:GLN:HE22	2.09	0.51
71:Ad:402:3PH:H371	49:Ae:128:ALA:HB1	1.93	0.51
51:Ag:77:MET:HE3	51:Ag:78:TYR:CZ	2.46	0.51
52:Ah:79:CYS:O	52:Ah:82:HIS:HB3	2.10	0.51
1:A:57:LEU:O	1:A:58:VAL:C	2.54	0.50
2:B:224:ARG:HG3	16:P:85:ARG:HH22	1.76	0.50
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LYS:CE	11:K:18:GLY:O	2.59	0.50
55:J:202:3PE:H2C1	14:N:11:PHE:CZ	2.46	0.50
12:L:21:ILE:HG12	12:L:27:ILE:HG23	1.93	0.50
13:M:123:GLU:CG	14:N:255:PRO:HG2	2.41	0.50
14:N:159:ILE:HG12	14:N:163:PHE:CE2	2.46	0.50
15:O:182:GLN:O	15:O:183:CYS:C	2.54	0.50
16:P:65:LEU:HD23	16:P:129:LEU:HD22	1.93	0.50
16:P:209:ARG:N	16:P:352:VAL:HG22	2.26	0.50
18:R:72:VAL:HG12	18:R:73:GLU:N	2.26	0.50
20:T:105:MET:HB2	20:T:139:MET:SD	2.51	0.50
20:U:119:ILE:CD1	20:U:138:LEU:HB2	2.40	0.50
21:V:31:THR:HA	21:V:88:LEU:HD13	1.92	0.50
23:X:141:PRO:HG2	23:X:142:TYR:HD1	1.75	0.50
25:Z:121:ILE:HG23	25:Z:122:GLY:N	2.26	0.50
25:Z:130:LYS:O	25:Z:131:GLU:C	2.52	0.50
28:c:46:LEU:O	28:c:50:ALA:HB2	2.12	0.50
33:h:73:PHE:CE2	33:h:74:TYR:CE1	2.98	0.50
41:p:49:ARG:O	41:p:52:ILE:HB	2.10	0.50
41:p:113:CYS:O	41:p:113:CYS:SG	2.69	0.50
47:AC:269:LYS:CE	47:AC:340:GLY:HA2	2.39	0.50
48:AD:201:VAL:HG21	48:AD:275:ARG:HA	1.92	0.50
48:AD:215:LEU:HD21	70:AD:401:HEC:CMB	2.41	0.50
46:Ab:348:GLY:HA2	46:Ab:448:PRO:HD3	1.91	0.50
47:Ac:140:PHE:HE1	47:Ac:170:VAL:HG13	1.76	0.50
48:Ad:146:LYS:CD	48:Ad:171:LEU:HG	2.41	0.50
49:Ae:155:LYS:O	49:Ae:158:ASP:HB2	2.09	0.50
49:Ae:196:ARG:HD2	49:Ae:249:ILE:CG2	2.40	0.50
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.93	0.50
5:E:75:ALA:O	5:E:78:VAL:HG22	2.11	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
10:J:96:VAL:O	10:J:99:GLU:HG2	2.11	0.50
58:J:201:PC1:H3B1	58:J:201:PC1:H261	1.92	0.50
12:L:395:ILE:O	12:L:399:ILE:HG13	2.11	0.50
55:L:704:3PE:H2	55:L:704:3PE:H112	1.93	0.50
14:N:104:MET:HE3	14:N:111:PHE:CE1	2.47	0.50
14:N:189:TRP:HB2	14:N:204:ASN:HD21	1.76	0.50
14:N:313:MET:HG3	15:O:305:LEU:CD2	2.40	0.50
16:P:234:LYS:HG2	16:P:234:LYS:O	2.10	0.50
16:P:305:PHE:HB2	16:P:314:THR:HG22	1.92	0.50
16:P:348:LYS:HB3	16:P:351:GLU:OE2	2.11	0.50
16:P:374:THR:HG23	16:P:374:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:167:ASN:C	17:Q:168:LYS:HG2	2.36	0.50
19:S:54:LEU:HD22	19:S:56:ARG:NH1	2.25	0.50
23:X:9:THR:HG23	23:X:12:GLU:H	1.77	0.50
27:b:20:VAL:HG22	55:b:201:3PE:H282	1.92	0.50
32:g:115:TRP:HA	32:g:118:ARG:HH11	1.75	0.50
34:i:19:ARG:HA	39:n:171:VAL:HG13	1.94	0.50
37:l:87:ASP:OD1	37:l:88:PRO:HD2	2.11	0.50
38:m:22:GLU:OE2	39:n:15:LYS:HD3	2.11	0.50
44:s:85:LEU:HD23	44:s:85:LEU:C	2.36	0.50
45:AA:109:LEU:O	45:AA:113:VAL:HG12	2.11	0.50
48:AD:242:ILE:CD1	48:AD:244:MET:HE2	2.41	0.50
49:AE:242:HIS:HD2	49:AE:251:LYS:HB3	1.76	0.50
45:Aa:57:LEU:C	45:Aa:57:LEU:HD23	2.35	0.50
53:Aj:9:ARG:NH2	53:Aj:13:LEU:HD21	2.26	0.50
4:D:90:ALA:O	4:D:91:ALA:CB	2.59	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.50
12:L:117:PHE:HE1	12:L:243:VAL:CG2	2.23	0.50
12:L:264:HIS:O	12:L:267:THR:N	2.43	0.50
12:L:349:SER:HB2	12:L:443:ILE:HG23	1.93	0.50
12:L:365:ILE:CD1	12:L:366:MET:HE2	2.42	0.50
13:M:154:LEU:HD13	14:N:287:LEU:CD2	2.41	0.50
13:M:294:MET:HE3	13:M:319:HIS:HD2	1.76	0.50
13:M:354:LEU:O	13:M:355:MET:C	2.52	0.50
14:N:248:LEU:CD1	14:N:296:LEU:HD23	2.41	0.50
15:O:40:LEU:H	15:O:40:LEU:HD12	1.76	0.50
15:O:326:ARG:NH2	32:g:56:ASP:OD1	2.45	0.50
16:P:212:ARG:O	16:P:213:PHE:C	2.55	0.50
18:R:55:VAL:HG22	18:R:56:ASN:H	1.77	0.50
20:T:130:ILE:HG23	20:T:131:PRO:CD	2.40	0.50
21:V:44:TYR:CD1	21:V:48:THR:HG23	2.46	0.50
26:a:31:ASN:ND2	26:a:36:LYS:HB2	2.26	0.50
37:l:38:PRO:HG2	38:m:71:ALA:HB2	1.93	0.50
43:r:6:ARG:HG2	43:r:6:ARG:O	2.11	0.50
45:AA:274:GLU:OE2	45:AA:276:ARG:NH1	2.44	0.50
46:AB:38:LEU:H	46:AB:38:LEU:HD22	1.76	0.50
46:Ab:229:VAL:O	46:Ab:232:GLN:HG2	2.10	0.50
46:Ab:429:LYS:HA	46:Ab:432:VAL:HG12	1.93	0.50
49:Ae:152:ILE:HG23	49:Ae:272:VAL:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
12:L:70:THR:HG21	41:p:101:GLU:OE2	2.12	0.50
12:L:109:HIS:O	12:L:110:SER:HB2	2.11	0.50
12:L:383:MET:CB	12:L:386:LEU:HD12	2.30	0.50
13:M:63:THR:N	13:M:64:PRO:HD2	2.26	0.50
15:O:211:VAL:HB	15:O:212:PRO:HD3	1.91	0.50
55:O:401:3PE:O22	55:O:401:3PE:H322	2.12	0.50
19:S:21:VAL:CG2	19:S:91:MET:HE1	2.41	0.50
20:U:93:ILE:HD11	20:U:118:ILE:HD11	1.92	0.50
22:W:97:ILE:C	22:W:99:VAL:H	2.18	0.50
23:X:48:TRP:CD1	27:b:55:VAL:HG22	2.46	0.50
24:Y:90:LEU:O	24:Y:94:ILE:HG12	2.11	0.50
26:a:37:ARG:CB	26:a:48:MET:CE	2.90	0.50
32:g:63:ASN:OD1	39:n:106:TYR:HE1	1.95	0.50
32:g:74:TYR:CE2	32:g:85:MET:HB3	2.47	0.50
62:h:201:CDL:H132	62:h:201:CDL:H172	1.92	0.50
34:i:108:ASP:OD2	41:p:18:PRO:HB2	2.11	0.50
39:n:114:MET:O	39:n:115:TYR:C	2.52	0.50
47:AC:291:VAL:O	47:AC:295:ILE:HG12	2.11	0.50
52:AH:52:ASP:O	52:AH:55:VAL:HB	2.11	0.50
45:Aa:109:LEU:HD23	45:Aa:113:VAL:HG23	1.94	0.50
48:Ad:192:ALA:HB1	70:Ad:401:HEC:HMD3	1.92	0.50
54:Ak:38:TRP:HE1	54:Ak:40:LEU:HD12	1.76	0.50
1:A:108:GLN:CG	1:A:109:LYS:H	2.18	0.50
1:A:109:LYS:O	1:A:109:LYS:HG2	2.12	0.50
3:C:186:ILE:HG13	3:C:187:LEU:N	2.27	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
12:L:424:MET:HE2	12:L:502:LEU:HA	1.93	0.50
13:M:118:PHE:O	13:M:122:PHE:HB2	2.11	0.50
21:V:90:LEU:HD21	21:V:94:MET:HE3	1.93	0.50
36:k:34:PRO:CG	36:k:59:TYR:CD1	2.94	0.50
45:AA:158:ASP:OD1	45:AA:213:ARG:HD2	2.11	0.50
46:AB:148:ARG:NH2	50:Af:52:PRO:HD3	2.26	0.50
46:AB:384:MET:O	46:AB:387:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:126:SER:HB3	48:AD:178:PRO:HD2	1.94	0.50
48:AD:232:TYR:HD1	48:AD:242:ILE:O	1.93	0.50
49:AE:195:LEU:HD11	49:AE:248:ARG:NH1	2.26	0.50
45:Aa:188:HIS:HE2	45:Aa:348:TYR:HH	1.57	0.50
62:Aa:501:CDL:H312	47:Ac:221:HIS:CE1	2.46	0.50
49:Ae:123:VAL:HG13	53:Aj:29:ALA:HA	1.94	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
13:M:248:ILE:HG13	13:M:249:ILE:N	2.25	0.50
14:N:326:PHE:CE2	29:d:48:LEU:HD13	2.46	0.50
16:P:205:ASP:OD1	16:P:205:ASP:O	2.30	0.50
16:P:315:THR:HB	16:P:318:LYS:HB2	1.92	0.50
16:P:367:GLU:HG2	16:P:368:GLU:N	2.26	0.50
23:X:151:ASN:HB3	30:e:51:ARG:NH1	2.26	0.50
26:a:1:MET:HG3	62:a:101:CDL:CB2	2.41	0.50
32:g:139:TYR:HD1	41:p:142:ARG:HH22	1.52	0.50
37:l:49:ALA:HA	37:l:59:VAL:HG13	1.93	0.50
45:AA:180:GLN:HG3	45:AA:181:ASN:N	2.25	0.50
48:Ad:242:ILE:HG12	48:Ad:244:MET:H	1.77	0.50
49:Ae:165:MET:O	49:Ae:176:VAL:N	2.44	0.50
52:Ah:51:CYS:O	52:Ah:55:VAL:HG23	2.11	0.50
1:A:1:MET:O	1:A:4:TYR:N	2.45	0.50
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.79	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.77	0.50
5:E:199:ASP:O	5:E:202:GLU:HB3	2.11	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.50
6:F:225:LEU:N	17:Q:160:TYR:HE2	2.07	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
10:J:52:GLY:O	10:J:55:VAL:HG12	2.12	0.50
10:J:68:GLY:O	10:J:69:TYR:C	2.54	0.50
12:L:515:LYS:HD2	39:n:74:ASN:HB3	1.94	0.50
13:M:19:SER:HB2	31:f:8:ARG:CD	2.42	0.50
13:M:122:PHE:CE1	13:M:238:LEU:HG	2.46	0.50
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.51	0.50
13:M:370:PRO:CA	13:M:375:LEU:HD22	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:32:THR:HA	18:R:59:PHE:CZ	2.46	0.50
18:R:70:ASN:HD22	18:R:111:PHE:HE1	1.60	0.50
20:T:90:TYR:CE2	20:T:92:LYS:HB2	2.46	0.50
37:l:34:LYS:HG3	37:l:35:ASP:OD1	2.12	0.50
38:m:124:LYS:HE2	38:m:125:PHE:CE2	2.47	0.50
45:AA:285:ALA:O	45:AA:359:VAL:HA	2.11	0.50
46:AB:176:ASN:CA	46:AB:258:ILE:HD11	2.42	0.50
46:AB:227:HIS:HD2	46:AB:231:LYS:HE2	1.76	0.50
48:AD:148:LEU:HA	48:AD:151:GLU:CD	2.36	0.50
45:Aa:73:VAL:HG23	45:Aa:147:LEU:HD13	1.93	0.50
45:Aa:399:LEU:HD22	45:Aa:426:LEU:HD22	1.93	0.50
46:Ab:180:VAL:O	46:Ab:254:ARG:HG3	2.12	0.50
1:A:67:LEU:HD13	11:K:68:ALA:HB3	1.91	0.50
1:A:75:LEU:HD21	10:J:145:TYR:CE2	2.47	0.50
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.27	0.50
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.50
4:D:304:LYS:HE2	9:I:35:THR:N	2.26	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.93	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
7:G:401:LEU:HD23	7:G:496:MET:HE1	1.92	0.50
8:H:93:HIS:CE1	26:a:24:ALA:CA	2.89	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
10:J:121:GLY:CA	25:Z:133:MET:HE1	2.41	0.50
12:L:149:ILE:HG21	13:M:364:LEU:CD2	2.42	0.50
12:L:306:THR:HA	12:L:336:LYS:NZ	2.27	0.50
12:L:336:LYS:O	12:L:340:PHE:CD2	2.65	0.50
12:L:354:GLN:O	12:L:354:GLN:HG2	2.12	0.50
12:L:514:ASN:HA	39:n:36:LYS:HZ1	1.77	0.50
13:M:432:ARG:HA	13:M:435:THR:HG22	1.94	0.50
20:T:140:CYS:O	20:T:144:ILE:HG13	2.12	0.50
20:U:86:VAL:HG13	36:k:54:ASN:ND2	2.27	0.50
20:U:90:TYR:HD2	20:U:93:ILE:H	1.60	0.50
23:X:119:ARG:HD2	23:X:120:PRO:HD2	1.94	0.50
24:Y:12:HIS:NE2	24:Y:127:PHE:HZ	2.09	0.50
27:b:28:LEU:HA	27:b:31:ILE:CG2	2.42	0.50
27:b:38:TYR:HA	27:b:41:TYR:HD2	1.76	0.50
45:AA:397:ASN:ND2	46:AB:126:ILE:HD11	2.24	0.50
46:AB:48:VAL:HG21	46:AB:219:ALA:HB2	1.87	0.50
46:AB:173:ILE:HD11	46:AB:439:ALA:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:232:GLN:O	46:AB:235:GLU:HG3	2.11	0.50
49:AE:184:ILE:HG21	49:AE:208:PRO:HB3	1.93	0.50
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:66:THR:O	58:J:201:PC1:H153	2.12	0.50
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.50
10:J:122:ASP:O	25:Z:122:GLY:CA	2.60	0.50
12:L:302:ILE:CB	12:L:340:PHE:CE1	2.95	0.50
12:L:560:LYS:HZ2	62:L:706:CDL:H321	1.75	0.50
15:O:136:TYR:OH	15:O:191:LYS:HA	2.11	0.50
20:U:142:GLN:O	20:U:145:VAL:N	2.43	0.50
25:Z:102:PRO:O	25:Z:103:ASN:C	2.53	0.50
38:m:35:GLU:O	38:m:38:SER:N	2.43	0.50
47:AC:211:LEU:HD21	50:AF:37:THR:HA	1.94	0.50
49:AE:154:ILE:HG22	49:AE:155:LYS:N	2.27	0.50
53:AJ:30:LEU:HD13	54:AK:30:VAL:HG13	1.94	0.50
45:Aa:404:ASP:O	45:Aa:408:PRO:HG2	2.12	0.50
48:Ad:154:VAL:HG21	48:Ad:173:ASP:OD2	2.12	0.50
48:Ad:249:TYR:O	48:Ad:250:THR:C	2.55	0.50
1:A:63:LEU:HD21	10:J:63:MET:HA	1.94	0.49
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.77	0.49
2:B:126:ARG:NH2	2:B:151:GLN:HG2	2.27	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
6:F:225:LEU:HB2	17:Q:160:TYR:CE2	2.47	0.49
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.49
8:H:30:TYR:CE2	26:a:5:ILE:HG23	2.46	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
12:L:123:LEU:CD2	12:L:150:MET:HG3	2.43	0.49
12:L:141:PHE:CD2	13:M:370:PRO:CB	2.94	0.49
13:M:388:TRP:NE1	38:m:109:ARG:CD	2.74	0.49
13:M:441:MET:HG3	13:M:445:ILE:HD12	1.94	0.49
14:N:336:THR:CG2	29:d:37:LEU:HD11	2.42	0.49
15:O:60:ILE:O	15:O:158:VAL:HA	2.12	0.49
15:O:237:ILE:CG2	15:O:241:TYR:CE2	2.95	0.49
15:O:276:LEU:HD11	15:O:278:TYR:CE2	2.47	0.49
15:O:319:ILE:HD12	15:O:324:GLY:HA3	1.94	0.49
16:P:70:VAL:HG12	16:P:97:MET:SD	2.52	0.49
47:AC:218:ILE:HB	47:AC:219:PRO:HD2	1.94	0.49
48:AD:249:TYR:O	48:AD:250:THR:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:91:TYR:CZ	45:Aa:95:HIS:HE1	2.30	0.49
48:Ad:116:VAL:HA	48:Ad:253:LEU:CD2	2.41	0.49
48:Ad:133:ARG:HB3	48:Ad:171:LEU:O	2.12	0.49
49:Ae:179:ARG:HA	49:Ae:183:GLU:OE1	2.12	0.49
2:B:94:THR:CG2	2:B:104:MET:SD	3.00	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
3:C:241:PHE:H	7:G:146:PHE:HE1	1.59	0.49
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.27	0.49
5:E:78:VAL:CG1	5:E:104:LEU:HD13	2.42	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
12:L:203:PHE:CE1	41:p:114:GLN:HG3	2.47	0.49
15:O:170:LEU:HD21	15:O:184:VAL:HG22	1.95	0.49
16:P:122:HIS:HB2	18:R:46:VAL:HG22	1.94	0.49
16:P:207:PHE:HE1	16:P:214:LEU:HD22	1.76	0.49
16:P:359:TYR:CD1	16:P:360:ARG:N	2.80	0.49
25:Z:140:PHE:O	25:Z:141:THR:C	2.56	0.49
32:g:139:TYR:CG	41:p:142:ARG:NH2	2.80	0.49
34:i:95:TYR:HE2	41:p:10:TYR:HB3	1.77	0.49
37:l:159:LYS:HA	40:o:98:ARG:HE	1.76	0.49
46:AB:48:VAL:CG2	46:AB:48:VAL:O	2.60	0.49
48:AD:323:PRO:HG2	48:AD:325:LYS:CD	2.41	0.49
47:Ac:346:PRO:HG3	51:Ag:66:GLU:HG2	1.94	0.49
48:Ad:255:TYR:HH	48:Ad:266:VAL:HA	1.76	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
2:B:68:ARG:HD3	2:B:70:ARG:CG	2.41	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.94	0.49
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.49
11:K:38:LEU:HG	11:K:42:ILE:HD11	1.94	0.49
12:L:434:LYS:NZ	36:k:66:ASN:HA	2.27	0.49
12:L:445:GLU:CB	12:L:450:LEU:HD23	2.37	0.49
62:L:706:CDL:H362	24:Y:118:VAL:HG21	1.95	0.49
13:M:88:ASN:O	13:M:89:ASN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:184:HIS:CD2	13:M:249:ILE:HG23	2.47	0.49
13:M:207:MET:SD	13:M:240:SER:HA	2.52	0.49
14:N:317:GLN:HE21	15:O:141:LEU:HD13	1.76	0.49
16:P:40:VAL:HB	16:P:53:GLY:HA2	1.93	0.49
23:X:48:TRP:HD1	27:b:55:VAL:HG13	1.77	0.49
26:a:51:ASP:O	26:a:54:ILE:HB	2.11	0.49
34:i:95:TYR:CE2	41:p:10:TYR:HB3	2.47	0.49
38:m:124:LYS:C	38:m:126:ASN:N	2.70	0.49
45:AA:296:TRP:NE1	45:AA:347:SER:O	2.45	0.49
45:AA:341:PHE:HE1	45:AA:356:ALA:CB	2.26	0.49
47:Ac:37:LEU:HB3	67:Ac:403:HEM:CMB	2.38	0.49
48:Ad:213:SER:HB3	48:Ad:236:TYR:CE1	2.47	0.49
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CE2	2.47	0.49
49:Ae:195:LEU:HD11	49:Ae:248:ARG:NH1	2.26	0.49
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.49
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:273:ILE:HD11	55:I:301:3PE:H2A1	1.93	0.49
12:L:217:LEU:HD13	12:L:273:ILE:HG23	1.94	0.49
12:L:296:ASN:HB3	12:L:357:ARG:HH11	1.77	0.49
12:L:393:ASP:OD1	12:L:393:ASP:C	2.56	0.49
12:L:399:ILE:HG22	12:L:409:LEU:HD13	1.93	0.49
13:M:311:GLY:HA2	13:M:314:MET:CE	2.40	0.49
15:O:114:LEU:CD2	63:O:402:ADP:H1'	2.43	0.49
16:P:64:PHE:CZ	16:P:211:ASP:HB3	2.48	0.49
20:T:138:LEU:HD13	20:T:144:ILE:CD1	2.42	0.49
21:V:39:PRO:HB2	21:V:42:ALA:HB2	1.94	0.49
25:Z:127:LEU:O	30:e:98:HIS:ND1	2.45	0.49
34:i:90:MET:O	34:i:91:ALA:C	2.53	0.49
37:l:81:ARG:HD3	37:l:85:GLU:OE2	2.13	0.49
46:AB:70:ARG:NH2	46:AB:332:ASP:OD2	2.45	0.49
47:AC:140:PHE:HE1	47:AC:170:VAL:HG13	1.77	0.49
48:AD:318:LYS:HD2	49:AE:86:PRO:HB2	1.95	0.49
52:AH:66:THR:O	52:AH:69:LEU:HB3	2.13	0.49
48:Ad:242:ILE:CD1	48:Ad:244:MET:HE2	2.42	0.49
49:Ae:184:ILE:CG2	49:Ae:208:PRO:HB3	2.42	0.49
4:D:79:ASN:O	4:D:80:MET:C	2.53	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ASP:OD1	4:D:148:GLU:HG2	2.11	0.49
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.49
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.49
10:J:127:GLU:CD	30:e:32:ARG:HG2	2.36	0.49
10:J:131:VAL:HG23	10:J:131:VAL:O	2.12	0.49
12:L:316:THR:CG2	12:L:325:ALA:CB	2.89	0.49
12:L:390:TYR:HE2	35:j:68:TRP:CH2	2.31	0.49
13:M:391:PHE:HE2	55:M:503:3PE:H232	1.77	0.49
13:M:420:THR:HG21	13:M:423:MET:HG2	1.93	0.49
14:N:164:MET:HE3	55:Y:201:3PE:H271	1.85	0.49
14:N:243:MET:CG	29:d:44:MET:HE2	2.40	0.49
16:P:346:GLU:H	16:P:346:GLU:CD	2.20	0.49
18:R:67:GLN:HG2	18:R:109:LEU:HD21	1.95	0.49
20:T:88:LYS:NZ	20:T:96:GLU:H	2.11	0.49
21:V:56:LEU:HA	21:V:59:VAL:HB	1.94	0.49
26:a:4:GLU:O	26:a:7:PRO:HD2	2.11	0.49
35:j:92:TRP:O	40:o:107:ARG:NH2	2.46	0.49
37:l:167:TYR:OH	37:l:176:LYS:O	2.14	0.49
45:AA:186:TYR:OH	49:AE:80:HIS:HB3	2.12	0.49
46:AB:375:LYS:NZ	46:AB:419:VAL:O	2.36	0.49
48:AD:128:ASP:OD1	48:AD:177:LYS:HD2	2.11	0.49
47:Ac:107:TYR:HE1	47:Ac:308:HIS:HB2	1.77	0.49
49:Ae:152:ILE:CB	49:Ae:272:VAL:HG23	2.40	0.49
49:Ae:197:ASP:HB3	49:Ae:257:ASN:ND2	2.27	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.12	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
10:J:16:CYS:SG	11:K:11:ALA:HB1	2.53	0.49
10:J:66:VAL:O	10:J:69:TYR:HB3	2.12	0.49
12:L:67:HIS:HE2	12:L:69:VAL:C	2.21	0.49
13:M:5:ILE:HG13	13:M:6:LEU:N	2.28	0.49
15:O:146:ALA:HB2	15:O:159:LEU:HD21	1.95	0.49
17:Q:64:LEU:HG	22:W:84:LEU:HD22	1.94	0.49
21:V:12:VAL:CG1	21:V:13:GLY:H	2.22	0.49
23:X:115:LEU:HD13	23:X:117:TRP:CZ3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:68:GLU:HG3	29:d:19:ARG:HH21	1.76	0.49
32:g:53:TRP:CD1	32:g:53:TRP:H	2.30	0.49
45:AA:171:GLU:O	45:AA:175:ASN:N	2.45	0.49
45:AA:373:GLN:O	45:AA:374:GLY:C	2.53	0.49
46:AB:304:ASN:ND2	46:AB:307:SER:OG	2.45	0.49
46:AB:305:THR:CG2	46:AB:306:THR:N	2.60	0.49
46:Ab:261:GLN:NE2	46:Ab:444:LEU:HB2	2.28	0.49
47:Ac:221:HIS:CE1	55:Ac:401:3PE:H31	2.48	0.49
47:Ac:278:TYR:CZ	47:Ac:282:ARG:HD2	2.48	0.49
67:Ac:402:HEM:O1A	67:Ac:402:HEM:HHA	2.12	0.49
49:Ae:204:ARG:O	49:Ae:260:VAL:HG11	2.12	0.49
1:A:51:PHE:CD2	4:D:103:GLY:HA3	2.47	0.49
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.49
2:B:164:CYS:SG	56:B:301:SF4:S4	3.10	0.49
4:D:96:ARG:HG3	4:D:115:LEU:HD21	1.95	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
6:F:163:TYR:CE1	44:s:80:PHE:HB3	2.48	0.49
6:F:379:CYS:SG	56:F:502:SF4:S1	3.11	0.49
8:H:203:GLY:C	8:H:205:SER:H	2.19	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
9:I:114:ILE:HD13	18:R:106:TYR:CD1	2.48	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
10:J:54:MET:HE1	10:J:58:ILE:HG13	1.94	0.49
55:J:202:3PE:H242	55:J:202:3PE:H3A2	1.93	0.49
13:M:285:LEU:HD22	13:M:410:MET:SD	2.53	0.49
14:N:149:LEU:HD11	14:N:195:PRO:HG3	1.95	0.49
14:N:230:ILE:HG21	14:N:296:LEU:HD11	1.94	0.49
14:N:240:MET:HE2	14:N:326:PHE:CE2	2.47	0.49
15:O:260:SER:O	15:O:263:ALA:HB3	2.13	0.49
15:O:351:TRP:HB3	28:c:39:PRO:HG3	1.95	0.49
16:P:315:THR:HB	16:P:318:LYS:H	1.78	0.49
17:Q:72:ILE:HD13	17:Q:143:TRP:HE1	1.76	0.49
20:U:88:LYS:CG	20:U:98:LEU:HD11	2.43	0.49
28:c:62:HIS:O	28:c:66:VAL:HG23	2.12	0.49
31:f:25:TYR:OH	31:f:29:LYS:HE3	2.13	0.49
39:n:20:TYR:OH	39:n:45:ARG:HB2	2.11	0.49
45:AA:279:ASP:OD1	51:AG:12:ARG:NE	2.45	0.49
48:AD:105:LEU:HB3	48:AD:110:ILE:HD11	1.95	0.49
46:Ab:298:HIS:C	46:Ab:299:ILE:HD12	2.38	0.49
54:Ak:15:ARG:NH1	54:Ak:15:ARG:HB2	2.28	0.49
1:A:56:PHE:HZ	11:K:75:LEU:HB3	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.47	0.49
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.94	0.49
57:B:302:UQ1:CM2	4:D:189:THR:HG21	2.43	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.49
7:G:179:CYS:HG	56:G:802:SF4:FE3	1.28	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:187:ILE:CD1	55:I:301:3PE:H242	2.41	0.49
12:L:227:PHE:CD2	12:L:283:LEU:HD23	2.48	0.49
12:L:566:THR:HG21	55:L:707:3PE:H381	1.95	0.49
13:M:139:GLN:HG3	13:M:140:THR:N	2.27	0.49
13:M:248:ILE:CG1	13:M:249:ILE:HD12	2.39	0.49
13:M:348:LEU:HD12	13:M:415:GLN:HE22	1.78	0.49
14:N:231:SER:HA	14:N:300:THR:HA	1.93	0.49
16:P:238:GLN:HB2	16:P:270:ARG:HG2	1.94	0.49
20:U:94:ASP:OD1	20:U:95:PRO:HD2	2.12	0.49
30:e:36:PHE:O	30:e:39:GLU:N	2.45	0.49
30:e:102:GLU:CG	30:e:104:PRO:HD3	2.41	0.49
34:i:92:THR:O	41:p:5:TRP:HD1	1.95	0.49
38:m:75:ASN:OD1	38:m:79:ASN:ND2	2.46	0.49
45:AA:186:TYR:C	45:AA:188:HIS:N	2.68	0.49
45:AA:280:ASP:OD2	51:AG:10:ARG:HA	2.13	0.49
47:AC:48:GLY:HA3	67:AC:401:HEM:C2B	2.47	0.49
49:AE:179:ARG:HA	49:AE:183:GLU:OE1	2.12	0.49
49:AE:192:VAL:O	49:AE:195:LEU:HB2	2.13	0.49
45:Aa:92:PHE:HZ	45:Aa:161:ILE:HG23	1.76	0.49
46:Ab:307:SER:O	46:Ab:308:LEU:C	2.54	0.49
47:Ac:361:ILE:HA	47:Ac:365:LEU:HB2	1.95	0.49
48:Ad:222:PRO:HD3	48:Ad:233:PHE:CZ	2.48	0.49
51:Ag:77:MET:HE3	51:Ag:78:TYR:CE2	2.48	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
10:J:89:LEU:HB2	58:J:201:PC1:O31	2.12	0.49
12:L:68:TRP:CE3	12:L:76:LEU:HD21	2.47	0.49
12:L:403:ASN:OD1	37:l:153:TYR:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:496:LEU:HA	12:L:499:LEU:HB2	1.94	0.49
13:M:1:MET:HB2	13:M:52:PHE:CE2	2.47	0.49
13:M:123:GLU:CD	14:N:255:PRO:HG2	2.37	0.49
15:O:306:ASN:O	15:O:309:THR:HG22	2.13	0.49
21:V:90:LEU:HD23	21:V:94:MET:HG2	1.94	0.49
34:i:69:LEU:HG	34:i:71:ALA:HB3	1.94	0.49
45:AA:387:GLU:HB2	45:AA:390:ARG:HH22	1.78	0.49
45:AA:467:ASP:OD2	47:AC:223:TYR:CE1	2.66	0.49
48:AD:115:GLN:O	48:AD:119:GLN:HG3	2.13	0.49
47:Ac:281:LEU:HD12	47:Ac:290:GLY:HA3	1.95	0.49
51:Ag:78:TYR:CZ	52:Ah:62:GLU:HB2	2.48	0.49
53:Aj:43:ILE:O	53:Aj:47:ILE:HG12	2.13	0.49
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.13	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:55:SER:HB3	12:L:575:THR:HG21	1.95	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
5:E:137:THR:HG22	6:F:370:LEU:HD21	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
13:M:134:THR:O	13:M:142:ARG:CD	2.59	0.49
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.43	0.49
13:M:348:LEU:HB2	13:M:415:GLN:OE1	2.13	0.49
14:N:124:LEU:CD2	14:N:176:ARG:CG	2.91	0.49
14:N:220:MET:O	14:N:223:ASN:N	2.45	0.49
34:i:103:ARG:NE	40:o:49:ALA:O	2.45	0.49
37:l:153:TYR:CD2	40:o:19:PRO:HB3	2.48	0.49
39:n:114:MET:HG3	39:n:115:TYR:HD2	1.78	0.49
45:Aa:207:ASN:O	45:Aa:211:LEU:HG	2.13	0.49
45:Aa:346:ILE:O	45:Aa:353:LEU:N	2.40	0.49
47:Ac:242:LEU:HD21	47:Ac:250:LEU:CD1	2.40	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
55:A:401:3PE:H2C2	10:J:37:PHE:HZ	1.76	0.48
2:B:96:GLY:HA3	57:B:302:UQ1:O4	2.13	0.48
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.48	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
4:D:36:GLN:HG3	4:D:38:GLN:HE21	1.78	0.48
4:D:92:HIS:HB2	4:D:458:PHE:HD2	1.78	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
10:J:126:TYR:CA	25:Z:120:LEU:CD1	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:126:TYR:HD1	25:Z:120:LEU:HD11	1.78	0.48
12:L:390:TYR:HE2	35:j:68:TRP:HH2	1.61	0.48
13:M:193:ASN:HA	13:M:253:LEU:HD23	1.94	0.48
13:M:227:GLY:HA2	13:M:230:ILE:HG22	1.95	0.48
14:N:200:LEU:HD23	14:N:265:ILE:HG23	1.95	0.48
14:N:317:GLN:HG2	15:O:301:LYS:HB3	1.95	0.48
14:N:321:LYS:HB2	29:d:49:ARG:HD3	1.94	0.48
16:P:235:THR:O	16:P:236:VAL:C	2.56	0.48
16:P:318:LYS:O	16:P:322:ILE:HG13	2.13	0.48
20:T:90:TYR:HE2	20:T:92:LYS:HB3	1.78	0.48
23:X:158:LEU:HD13	29:d:17:GLU:CG	2.43	0.48
24:Y:60:ARG:CZ	24:Y:60:ARG:HB2	2.41	0.48
24:Y:143:VAL:HG23	33:h:157:ARG:O	2.13	0.48
25:Z:72:MET:O	25:Z:73:PRO:C	2.56	0.48
34:i:7:ASP:OD1	34:i:8:GLU:N	2.46	0.48
45:AA:96:LEU:HD23	45:AA:164:GLU:HG3	1.94	0.48
47:AC:244:LEU:HD13	48:AD:289:GLY:HA2	1.94	0.48
47:AC:278:TYR:CZ	47:AC:282:ARG:HD2	2.48	0.48
49:AE:155:LYS:HZ3	49:AE:157:SER:HB3	1.77	0.48
49:AE:156:LEU:HB2	49:AE:269:ASP:CA	2.43	0.48
49:AI:64:LEU:HA	49:AI:78:PHE:CA	2.38	0.48
45:Aa:226:ALA:HB2	45:Aa:253:VAL:HB	1.94	0.48
46:Ab:38:LEU:HD11	46:Ab:396:ILE:HD13	1.95	0.48
48:Ad:179:TYR:CD2	48:Ad:185:ALA:HB2	2.48	0.48
49:Ae:192:VAL:O	49:Ae:195:LEU:HB2	2.13	0.48
53:Aj:19:SER:HB2	54:Ak:23:MET:HB2	1.94	0.48
2:B:68:ARG:HG2	2:B:69:SER:N	2.28	0.48
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.48
4:D:88:HIS:HE2	8:H:205:SER:HA	1.77	0.48
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.94	0.48
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.48
8:H:16:ALA:HB2	26:a:15:CYS:HB2	1.94	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
10:J:121:GLY:O	10:J:122:ASP:C	2.52	0.48
12:L:390:TYR:CE2	35:j:68:TRP:CH2	3.01	0.48
12:L:521:SER:O	12:L:524:THR:N	2.46	0.48
13:M:4:ILE:HG22	13:M:107:ILE:CD1	2.32	0.48
13:M:190:TRP:CE2	24:Y:89:PRO:HG2	2.48	0.48
13:M:216:LEU:HD12	13:M:236:LEU:CD2	2.39	0.48
13:M:309:PHE:HB2	13:M:458:THR:HG21	1.95	0.48
13:M:351:VAL:HA	33:h:59:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:221:ARG:CD	16:P:286:ARG:HD3	2.43	0.48
16:P:298:TYR:HA	16:P:301:ILE:HG12	1.95	0.48
18:R:32:THR:HA	18:R:59:PHE:HZ	1.78	0.48
19:S:79:LEU:CA	19:S:82:LEU:HD12	2.26	0.48
20:U:133:ILE:HD13	39:n:7:PRO:HD3	1.95	0.48
32:g:109:ASP:HB2	32:g:114:GLU:HB3	1.94	0.48
45:AA:409:VAL:O	45:AA:410:CYS:C	2.55	0.48
47:AC:185:LEU:HD23	47:AC:188:ILE:HD12	1.95	0.48
71:AD:402:3PH:H221	49:AE:135:GLN:NE2	2.16	0.48
49:AE:142:ALA:HB1	49:AE:146:VAL:CG2	2.43	0.48
49:AE:184:ILE:CG2	49:AE:208:PRO:HB3	2.42	0.48
46:Ab:388:THR:HG23	46:Ab:391:GLY:H	1.78	0.48
49:Ae:217:CYS:O	49:Ae:218:THR:C	2.56	0.48
51:Ag:78:TYR:CB	52:Ah:63:GLU:HB2	2.43	0.48
53:Aj:43:ILE:O	53:Aj:44:TYR:C	2.54	0.48
53:Aj:52:LEU:CD1	53:Aj:53:TRP:N	2.68	0.48
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.38	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.48
10:J:22:LYS:CD	11:K:23:ARG:HG2	2.39	0.48
12:L:144:TRP:HH2	12:L:256:GLY:HA2	1.78	0.48
12:L:350:LEU:HD23	12:L:443:ILE:HD11	1.96	0.48
12:L:357:ARG:HD3	39:n:80:TYR:HB2	1.95	0.48
12:L:402:CYS:SG	12:L:403:ASN:N	2.87	0.48
13:M:16:TRP:HE3	55:O:401:3PE:H12	1.78	0.48
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.47	0.48
13:M:313:THR:HA	13:M:316:MET:CE	2.43	0.48
14:N:321:LYS:HB2	29:d:49:ARG:CD	2.43	0.48
16:P:228:LEU:HD11	16:P:288:PHE:HZ	1.78	0.48
18:R:31:ILE:HD11	18:R:37:VAL:HG23	1.95	0.48
22:W:122:LEU:HD11	22:W:126:TYR:CE2	2.47	0.48
23:X:5:VAL:O	23:X:6:GLU:C	2.54	0.48
25:Z:111:PHE:CE1	30:e:65:GLU:CG	2.95	0.48
27:b:48:ALA:O	27:b:49:THR:C	2.53	0.48
46:AB:388:THR:HG23	46:AB:391:GLY:H	1.78	0.48
46:AB:429:LYS:HA	46:AB:432:VAL:CG1	2.39	0.48
48:Ad:195:PRO:HG3	70:Ad:401:HEC:HAA1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:38:LEU:O	52:Ah:42:VAL:HG23	2.13	0.48
4:D:42:GLU:HA	4:D:45:GLU:HG2	1.96	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
6:F:46:TYR:O	6:F:48:ARG:HG2	2.13	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48
12:L:41:LYS:HG3	12:L:98:TRP:CH2	2.45	0.48
12:L:101:MET:HE1	12:L:121:LEU:CB	2.43	0.48
12:L:152:PHE:HE1	13:M:412:ILE:HD11	1.79	0.48
12:L:316:THR:HG21	12:L:325:ALA:HA	1.95	0.48
12:L:361:ASN:O	12:L:361:ASN:CG	2.54	0.48
12:L:424:MET:HE2	12:L:502:LEU:CA	2.43	0.48
14:N:31:VAL:HB	14:N:35:PHE:CE2	2.48	0.48
14:N:243:MET:HE2	14:N:330:ALA:HB1	1.95	0.48
20:T:119:ILE:HG13	20:T:135:ALA:HB1	1.95	0.48
22:W:32:LYS:HG2	66:W:201:EHZ:C19	2.44	0.48
22:W:42:TRP:O	22:W:43:TYR:C	2.55	0.48
25:Z:89:GLU:HG2	25:Z:128:ARG:NH1	2.27	0.48
27:b:23:PHE:HD1	55:b:201:3PE:H3B2	1.77	0.48
27:b:26:TRP:CZ3	55:b:201:3PE:H2G2	2.48	0.48
27:b:78:LEU:HA	27:b:80:TRP:CD1	2.49	0.48
33:h:73:PHE:O	33:h:77:LEU:N	2.46	0.48
34:i:14:GLN:CB	39:n:164:PRO:HG3	2.35	0.48
34:i:69:LEU:O	34:i:72:VAL:HG22	2.12	0.48
39:n:51:HIS:HB3	39:n:63:LEU:HD13	1.95	0.48
40:o:4:HIS:ND1	40:o:102:PHE:HE2	2.11	0.48
47:AC:148:ASN:CB	49:Ae:220:LEU:HA	2.43	0.48
47:AC:316:MET:HG3	55:AC:403:3PE:H232	1.95	0.48
48:AD:116:VAL:HA	48:AD:253:LEU:CD2	2.43	0.48
49:AE:197:ASP:HB3	49:AE:257:ASN:ND2	2.27	0.48
50:AF:110:LYS:HA	54:Ak:10:TYR:HE2	1.77	0.48
45:Aa:469:ASN:ND2	47:Ac:223:TYR:CZ	2.80	0.48
46:Ab:109:LYS:O	46:Ab:123:VAL:HA	2.13	0.48
47:Ac:218:ILE:HB	47:Ac:219:PRO:HD2	1.94	0.48
3:C:107:PHE:CE2	3:C:140:ILE:HD13	2.48	0.48
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
12:L:372:CYS:SG	12:L:454:ILE:HG22	2.54	0.48
14:N:4:ILE:HG23	14:N:5:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:172:GLN:OE1	14:N:177:LYS:CD	2.59	0.48
19:S:31:GLN:CD	19:S:34:ARG:NH2	2.71	0.48
23:X:170:TRP:CZ3	62:X:201:CDL:H521	2.48	0.48
25:Z:110:VAL:HG11	30:e:72:THR:HG23	1.95	0.48
25:Z:111:PHE:CE1	30:e:65:GLU:C	2.85	0.48
26:a:18:ILE:N	26:a:19:PRO:CD	2.76	0.48
27:b:19:LEU:HD21	55:b:201:3PE:H332	1.95	0.48
31:f:4:PHE:O	31:f:5:GLN:C	2.57	0.48
31:f:5:GLN:HB2	31:f:10:HIS:CD2	2.33	0.48
32:g:106:TYR:HE2	33:h:86:ILE:HD12	1.78	0.48
32:g:117:ARG:NH2	41:p:10:TYR:OH	2.45	0.48
43:r:12:ARG:HE	43:r:20:LEU:HD21	1.78	0.48
46:AB:286:PHE:CZ	46:AB:427:ALA:HB1	2.49	0.48
47:AC:32:ASN:ND2	47:AC:228:ASP:OD1	2.46	0.48
47:AC:361:ILE:HA	47:AC:365:LEU:HB2	1.95	0.48
48:AD:98:HIS:HB3	48:AD:105:LEU:HD23	1.95	0.48
48:AD:307:LYS:O	48:AD:311:TRP:HB2	2.13	0.48
49:AE:218:THR:OG1	49:AE:254:ALA:HB1	2.13	0.48
45:Aa:338:CYS:HB3	45:Aa:359:VAL:O	2.13	0.48
47:Ac:185:LEU:HD23	47:Ac:188:ILE:HD12	1.95	0.48
47:Ac:304:MET:HA	47:Ac:307:LEU:HD12	1.95	0.48
48:Ad:296:MET:CE	71:Ad:402:3PH:H362	2.41	0.48
49:Ae:218:THR:OG1	49:Ae:254:ALA:HB1	2.13	0.48
53:Aj:10:LEU:O	53:Aj:11:TYR:C	2.56	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:93:HIS:HE1	26:a:24:ALA:CA	2.25	0.48
8:H:300:LEU:HD23	27:b:25:VAL:HG11	1.96	0.48
10:J:28:GLY:O	10:J:31:GLY:N	2.46	0.48
12:L:141:PHE:HD1	12:L:182:PHE:CD2	2.31	0.48
12:L:433:THR:HG21	12:L:436:ARG:NH2	2.29	0.48
13:M:154:LEU:HD13	14:N:287:LEU:HD22	1.95	0.48
13:M:166:LEU:HD21	13:M:170:HIS:CE1	2.48	0.48
13:M:307:TRP:CE3	13:M:383:MET:CE	2.97	0.48
16:P:318:LYS:HA	16:P:321:ARG:HH12	1.78	0.48
18:R:43:TYR:CD1	18:R:44:ARG:HB2	2.49	0.48
29:d:109:TYR:HE2	41:p:85:ILE:HD12	1.79	0.48
30:e:47:ILE:HG13	30:e:47:ILE:O	2.12	0.48
33:h:73:PHE:HE2	33:h:74:TYR:HE1	1.62	0.48
34:i:69:LEU:HD23	34:i:72:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:69:PHE:CE1	36:k:73:ILE:HD11	2.48	0.48
37:l:167:TYR:HD2	37:l:168:LEU:CD1	2.19	0.48
48:AD:282:HIS:O	48:AD:286:LYS:HG2	2.13	0.48
49:AE:204:ARG:O	49:AE:260:VAL:HG11	2.13	0.48
45:Aa:405:GLY:C	45:Aa:408:PRO:HD2	2.38	0.48
62:Aa:501:CDL:OB5	55:Ac:401:3PE:N	2.47	0.48
46:Ab:63:LEU:HD11	46:Ab:238:LEU:HD21	1.95	0.48
49:Ae:231:PHE:HD2	49:Ae:250:ARG:NH1	2.12	0.48
1:A:49:LEU:HD23	4:D:80:MET:CB	2.35	0.48
1:A:106:TRP:CE3	55:b:201:3PE:H331	2.48	0.48
2:B:96:GLY:HA3	57:B:302:UQ1:HM52	1.96	0.48
3:C:131:LEU:O	3:C:139:ARG:HG3	2.12	0.48
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.48
4:D:375:MET:HE1	7:G:126:LEU:CA	2.43	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
8:H:111:LEU:CD2	10:J:60:LEU:HD12	2.35	0.48
8:H:121:TRP:CZ3	10:J:27:TYR:OH	2.60	0.48
8:H:296:LEU:HD21	55:I:301:3PE:H351	1.95	0.48
11:K:6:PHE:CZ	11:K:10:MET:HE3	2.49	0.48
12:L:496:LEU:HD12	12:L:497:GLY:CA	2.44	0.48
14:N:281:LEU:HD23	55:N:401:3PE:C29	2.44	0.48
15:O:314:LEU:HD12	15:O:315:PRO:HD3	1.93	0.48
17:Q:82:PRO:HG2	17:Q:93:ASN:O	2.14	0.48
20:T:104:PHE:CZ	20:T:118:ILE:HG21	2.48	0.48
21:V:11:LEU:HD23	21:V:14:LEU:HD13	1.96	0.48
23:X:17:GLU:HB3	23:X:19:LYS:HG3	1.96	0.48
26:a:3:PHE:CZ	62:a:101:CDL:HA4	2.49	0.48
34:i:103:ARG:HD2	40:o:50:GLN:HB2	1.94	0.48
46:AB:109:LYS:O	46:AB:123:VAL:HA	2.14	0.48
47:AC:304:MET:HA	47:AC:307:LEU:HD12	1.96	0.48
46:Ab:286:PHE:CZ	46:Ab:427:ALA:HB1	2.49	0.48
47:Ac:197:LEU:HD21	69:Ac:406:UQ6:H13	1.95	0.48
47:Ac:378:LYS:HE3	50:Af:89:PHE:HE2	1.78	0.48
49:Ae:178:HIS:HD2	49:Ae:179:ARG:N	2.11	0.48
1:A:48:ARG:HD3	10:J:76:GLU:CD	2.39	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:L:274:LEU:O	12:L:277:MET:HG2	2.14	0.48
13:M:42:LEU:HG	13:M:67:ILE:CD1	2.42	0.48
14:N:227:ILE:CA	14:N:230:ILE:HG22	2.38	0.48
15:O:114:LEU:HD21	63:O:402:ADP:H1'	1.94	0.48
16:P:79:GLN:NE2	16:P:102:GLN:O	2.47	0.48
23:X:132:LYS:HB3	27:b:59:ASP:HB3	1.96	0.48
23:X:153:VAL:O	23:X:155:GLU:HG3	2.14	0.48
62:X:201:CDL:HB32	29:d:29:PRO:HB2	1.95	0.48
34:i:102:PRO:HG3	41:p:16:ARG:O	2.14	0.48
37:l:162:PRO:HG3	40:o:39:MET:HE3	1.94	0.48
42:q:14:VAL:HG13	42:q:23:LEU:HD22	1.95	0.48
42:q:60:ARG:HH12	42:q:95:ASP:HA	1.78	0.48
46:AB:49:ILE:CD1	46:AB:220:LEU:HB3	2.43	0.48
46:AB:90:THR:HG23	46:AB:95:SER:HA	1.95	0.48
46:AB:176:ASN:C	46:AB:258:ILE:HD11	2.39	0.48
47:AC:220:PHE:HE2	69:AC:405:UQ6:H4M3	1.77	0.48
48:AD:242:ILE:HD11	48:AD:244:MET:HE2	1.95	0.48
49:AE:217:CYS:O	49:AE:218:THR:C	2.56	0.48
45:Aa:373:GLN:NE2	45:Aa:471:ILE:HG23	2.29	0.48
45:Aa:479:ARG:O	54:Ak:20:THR:HG21	2.13	0.48
46:Ab:92:LYS:HE2	46:Ab:143:ALA:HB1	1.96	0.48
46:Ab:142:THR:CG2	46:Ab:237:PHE:HB3	2.30	0.48
47:Ac:32:ASN:ND2	47:Ac:228:ASP:OD1	2.47	0.48
48:Ad:121:CYS:HG	70:Ad:401:HEC:HBB3	1.77	0.48
49:Ae:176:VAL:HG13	49:Ae:212:ILE:HG12	1.95	0.48
51:Ag:65:GLN:O	51:Ag:69:GLN:HG2	2.13	0.48
53:Aj:22:ALA:O	53:Aj:23:LEU:C	2.57	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:149:LEU:CD1	22:W:80:ARG:HH21	2.19	0.48
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.48
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.49	0.48
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
10:J:20:ALA:C	10:J:22:LYS:H	2.21	0.48
12:L:57:ASN:OD1	12:L:59:MET:HG3	2.14	0.48
12:L:319:MET:O	12:L:319:MET:HG2	2.13	0.48
13:M:269:MET:HE3	13:M:399:ASN:HB3	1.96	0.48
13:M:422:HIS:CE1	13:M:425:ASN:OD1	2.66	0.48
15:O:63:ASP:OD1	15:O:64:GLY:N	2.43	0.48
16:P:294:PRO:HB3	16:P:296:PHE:HD1	1.79	0.48
28:c:72:ARG:HD2	29:d:20:SER:HA	1.96	0.48
29:d:119:VAL:O	29:d:120:ARG:C	2.55	0.48
32:g:58:GLU:HB2	37:l:30:PHE:HE1	1.79	0.48
49:AE:231:PHE:HD2	49:AE:250:ARG:NH1	2.12	0.48
52:AH:47:ARG:O	52:AH:51:CYS:N	2.41	0.48
45:Aa:104:ARG:N	45:Aa:104:ARG:HD2	2.29	0.48
48:Ad:146:LYS:HD3	48:Ad:171:LEU:HG	1.95	0.48
48:Ad:154:VAL:HG21	48:Ad:173:ASP:CG	2.39	0.48
51:Ag:78:TYR:HB3	52:Ah:63:GLU:HB2	1.95	0.48
1:A:67:LEU:HD21	11:K:68:ALA:HB2	1.96	0.48
2:B:121:PHE:CD1	2:B:121:PHE:C	2.89	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.76	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
10:J:124:LEU:HB3	25:Z:137:ASN:OD1	2.14	0.48
11:K:73:VAL:HG21	14:N:38:LEU:CD2	2.44	0.48
13:M:176:LEU:HD13	13:M:245:ARG:HH11	1.79	0.48
16:P:335:LEU:O	16:P:336:GLU:HB2	2.14	0.48
18:R:79:CYS:O	18:R:88:HIS:CE1	2.67	0.48
20:T:82:ARG:NH1	20:T:126:PHE:HA	2.29	0.48
20:U:90:TYR:CD1	36:k:51:TRP:CE2	3.02	0.48
20:U:128:PHE:HZ	20:U:148:ILE:HD12	1.76	0.48
24:Y:83:ARG:HH11	24:Y:91:ASN:HD21	1.61	0.48
29:d:8:HIS:O	29:d:10:PRO:HD3	2.14	0.48
36:k:84:PHE:CZ	36:k:88:LEU:HD22	2.49	0.48
37:l:111:MET:HE3	37:l:112:TYR:CZ	2.49	0.48
38:m:25:VAL:HB	38:m:29:THR:HB	1.96	0.48
42:q:23:LEU:HD11	42:q:33:ILE:HG12	1.96	0.48
45:AA:338:CYS:N	45:AA:368:MET:SD	2.87	0.48
49:AE:178:HIS:HD2	49:AE:179:ARG:N	2.11	0.48
45:Aa:287:VAL:HB	45:Aa:358:PHE:CE1	2.49	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
11:K:29:THR:O	11:K:32:CYS:N	2.47	0.47
11:K:66:PHE:HE1	14:N:35:PHE:CE1	2.31	0.47
12:L:3:ILE:HG22	12:L:49:LEU:HD21	1.96	0.47
12:L:588:PHE:CZ	14:N:61:VAL:HG12	2.48	0.47
13:M:7:PRO:HG3	31:f:20:PHE:HA	1.94	0.47
13:M:127:ILE:CD1	14:N:256:PRO:HG2	2.43	0.47
13:M:336:ARG:HH21	13:M:429:SER:HA	1.78	0.47
15:O:60:ILE:CG1	15:O:83:MET:HE1	2.43	0.47
17:Q:99:MET:SD	17:Q:128:PHE:HE2	2.36	0.47
37:l:89:TRP:CZ2	39:n:86:PRO:HD3	2.49	0.47
38:m:125:PHE:CD1	41:p:132:PHE:CE2	3.03	0.47
45:AA:113:VAL:HG13	46:AB:299:ILE:HD11	1.95	0.47
49:AE:156:LEU:HB2	49:AE:269:ASP:HA	1.96	0.47
49:AE:172:LYS:HD2	47:Ac:169:SER:HB3	1.96	0.47
45:Aa:463:GLU:OE1	51:Ag:8:LEU:HB2	2.14	0.47
46:Ab:227:HIS:CD2	46:Ab:231:LYS:HG3	2.49	0.47
47:Ac:10:LEU:O	47:Ac:14:ILE:HG12	2.14	0.47
47:Ac:297:SER:O	47:Ac:300:ILE:HG22	2.13	0.47
49:Ae:273:VAL:O	49:Ae:273:VAL:HG12	2.14	0.47
3:C:73:GLN:O	3:C:74:GLN:C	2.57	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.28	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:233:VAL:HG11	17:Q:164:PHE:HB2	1.95	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
12:L:542:LEU:HD21	37:l:116:ARG:HD3	1.96	0.47
13:M:192:ASN:C	13:M:194:LEU:N	2.72	0.47
16:P:55:VAL:HG12	16:P:123:SER:HA	1.96	0.47
20:T:117:GLU:HG2	22:W:43:TYR:CZ	2.48	0.47
23:X:20:VAL:CG2	23:X:24:VAL:HG21	2.40	0.47
23:X:168:PHE:O	23:X:169:PHE:CG	2.67	0.47
27:b:68:SER:O	27:b:69:HIS:C	2.56	0.47
34:i:90:MET:SD	34:i:97:ILE:HD11	2.54	0.47
38:m:124:LYS:C	38:m:126:ASN:H	2.21	0.47
42:q:68:MET:SD	42:q:81:MET:HG2	2.55	0.47
45:AA:172:MET:HA	45:AA:175:ASN:ND2	2.30	0.47
45:AA:407:THR:HB	45:AA:408:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:176:VAL:HG13	49:AE:212:ILE:HG12	1.95	0.47
47:Ac:243:VAL:O	47:Ac:247:PRO:HB3	2.13	0.47
47:Ac:265:PRO:HD2	47:Ac:268:ILE:HD11	1.95	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
10:J:3:ASN:HD22	10:J:120:LEU:CG	2.27	0.47
12:L:31:ASN:HD22	12:L:34:LEU:HB2	1.79	0.47
62:L:706:CDL:H551	62:L:706:CDL:H582	1.66	0.47
13:M:94:LEU:O	13:M:98:MET:HG2	2.14	0.47
13:M:309:PHE:O	13:M:313:THR:HG23	2.14	0.47
14:N:173:THR:O	14:N:227:ILE:HG23	2.14	0.47
16:P:304:LEU:O	16:P:307:LEU:HB3	2.14	0.47
18:R:32:THR:O	18:R:33:HIS:C	2.57	0.47
62:X:201:CDL:H522	62:X:201:CDL:HB62	1.96	0.47
37:l:48:ARG:HH22	37:l:64:PRO:HD2	1.80	0.47
43:r:12:ARG:HB3	43:r:20:LEU:CD2	2.44	0.47
45:AA:341:PHE:CZ	45:AA:372:LEU:HD13	2.49	0.47
47:AC:94:LEU:HD13	67:AC:402:HEM:HAB	1.96	0.47
47:AC:281:LEU:HD12	47:AC:290:GLY:HA3	1.95	0.47
47:AC:297:SER:O	47:AC:300:ILE:HG22	2.13	0.47
47:Ac:71:ARG:NH2	48:Ad:277:ALA:O	2.47	0.47
47:Ac:96:LEU:HD23	55:Ac:404:3PE:H292	1.95	0.47
48:Ad:170:LYS:HD3	49:Ae:151:LYS:HD3	1.92	0.47
48:Ad:183:GLU:CD	48:Ad:183:GLU:H	2.21	0.47
1:A:90:MET:CG	10:J:145:TYR:CD1	2.97	0.47
4:D:43:TRP:CZ2	13:M:143:LEU:CD1	2.97	0.47
4:D:55:SER:HB3	12:L:575:THR:CG2	2.44	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:118:TRP:CZ2	10:J:30:LEU:CD2	2.97	0.47
10:J:95:GLY:HA2	10:J:98:MET:HB2	1.95	0.47
12:L:54:PHE:CZ	12:L:84:PHE:HB2	2.49	0.47
12:L:296:ASN:ND2	12:L:357:ARG:HE	2.12	0.47
12:L:362:ILE:HG12	12:L:430:VAL:O	2.13	0.47
12:L:433:THR:CG2	12:L:434:LYS:N	2.78	0.47
62:L:705:CDL:H152	13:M:358:TRP:CH2	2.49	0.47
13:M:458:THR:HG21	41:p:148:ALA:HB1	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:70:LYS:HG3	15:O:71:ASN:N	2.30	0.47
16:P:108:TRP:CZ2	64:P:401:NDP:H2A	2.49	0.47
16:P:311:GLU:O	16:P:312:PRO:C	2.57	0.47
23:X:69:ASN:OD1	23:X:70:PHE:N	2.47	0.47
25:Z:110:VAL:HG11	30:e:72:THR:CA	2.44	0.47
26:a:3:PHE:HE2	62:a:101:CDL:HA4	1.77	0.47
27:b:46:ASN:OD1	27:b:47:LYS:N	2.47	0.47
29:d:73:TYR:O	29:d:77:LYS:HB2	2.14	0.47
30:e:42:GLU:CD	33:h:176:LYS:HE2	2.39	0.47
31:f:37:PHE:O	31:f:38:ARG:C	2.57	0.47
34:i:95:TYR:CE1	41:p:112:ALA:CB	2.97	0.47
34:i:102:PRO:HG3	41:p:17:THR:HA	1.96	0.47
39:n:44:MET:HE2	39:n:44:MET:HB2	1.74	0.47
39:n:156:PRO:HD2	39:n:158:ARG:NH1	2.29	0.47
45:AA:137:SER:HB3	45:AA:236:GLY:O	2.15	0.47
45:Aa:274:GLU:HA	45:Aa:456:VAL:O	2.14	0.47
47:Ac:296:LEU:O	47:Ac:300:ILE:N	2.45	0.47
2:B:127:GLN:NE2	8:H:215:TYR:O	2.47	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
4:D:43:TRP:CZ2	13:M:143:LEU:HD12	2.50	0.47
4:D:299:GLN:HB3	43:r:104:TRP:CE3	2.49	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
8:H:172:MET:HE1	25:Z:46:GLY:HA3	1.95	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
12:L:63:ILE:HG23	34:i:97:ILE:CD1	2.45	0.47
12:L:277:MET:SD	12:L:318:GLY:HA2	2.54	0.47
13:M:78:MET:HG2	13:M:432:ARG:HG3	1.97	0.47
13:M:177:MET:HE1	41:p:86:TYR:CE1	2.49	0.47
13:M:370:PRO:CA	13:M:375:LEU:HD23	2.42	0.47
14:N:1:MET:HE1	14:N:43:MET:SD	2.54	0.47
14:N:89:GLN:H	14:N:89:GLN:CD	2.22	0.47
15:O:343:TYR:CE1	15:O:355:LYS:CB	2.96	0.47
62:a:101:CDL:HA21	42:q:6:VAL:CG1	2.44	0.47
34:i:79:MET:O	34:i:80:TRP:C	2.57	0.47
45:AA:101:THR:O	45:AA:102:LYS:C	2.55	0.47
45:AA:160:GLN:HA	45:AA:163:LYS:NZ	2.29	0.47
45:AA:478:LEU:O	54:AK:24:TRP:HZ2	1.98	0.47
47:AC:148:ASN:OD1	49:Ae:221:GLY:N	2.47	0.47
47:Ac:275:LEU:O	47:Ac:278:TYR:N	2.48	0.47
49:Ae:152:ILE:N	49:Ae:272:VAL:HG23	2.29	0.47
51:Ag:11:ILE:CG2	51:Ag:12:ARG:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:PHE:CE1	2:B:131:MET:HE2	2.40	0.47
3:C:195:HIS:HE1	22:W:88:LYS:NZ	2.12	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
5:E:70:PRO:HG2	6:F:236:PHE:CE2	2.50	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:401:LEU:HD23	7:G:496:MET:CE	2.43	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:1:MET:CB	26:a:30:THR:HG21	2.45	0.47
11:K:69:CYS:O	11:K:70:GLU:C	2.57	0.47
13:M:430:HIS:HB3	32:g:73:GLY:HA3	1.97	0.47
14:N:1:MET:O	14:N:2:ASN:C	2.54	0.47
14:N:26:LEU:O	14:N:29:MET:N	2.47	0.47
15:O:99:GLY:O	28:c:30:TYR:HA	2.14	0.47
16:P:76:MET:HE1	16:P:254:LYS:CE	2.45	0.47
20:T:132:ASP:HB3	22:W:40:ARG:HH12	1.78	0.47
20:U:90:TYR:CE2	20:U:110:LEU:HD21	2.50	0.47
30:e:41:ILE:CD1	33:h:174:PRO:HD2	2.45	0.47
34:i:108:ASP:OD2	41:p:18:PRO:CB	2.62	0.47
37:l:42:PRO:HB2	37:l:48:ARG:HG2	1.97	0.47
45:AA:152:GLN:O	45:AA:153:ASN:HB2	2.15	0.47
46:AB:306:THR:O	46:AB:307:SER:C	2.58	0.47
48:AD:242:ILE:HG12	48:AD:244:MET:H	1.80	0.47
49:AI:68:VAL:HG11	46:Ab:85:LEU:CD2	2.45	0.47
45:Aa:266:THR:O	45:Aa:266:THR:CG2	2.62	0.47
48:Ad:207:GLY:O	48:Ad:208:GLU:C	2.58	0.47
49:Ae:166:ALA:HA	49:Ae:174:LEU:O	2.15	0.47
52:Ah:44:ALA:HA	52:Ah:47:ARG:HH11	1.79	0.47
1:A:53:MET:CG	11:K:79:VAL:CG1	2.92	0.47
4:D:58:THR:HG23	4:D:61:TRP:CZ3	2.49	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.98	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
6:F:166:ALA:HB1	44:s:80:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:425:CYS:SG	56:F:502:SF4:S4	3.13	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
9:I:188:GLU:OE1	18:R:56:ASN:CB	2.63	0.47
11:K:57:MET:C	11:K:60:PRO:HD2	2.39	0.47
12:L:102:GLN:NE2	12:L:449:ASP:HA	2.27	0.47
12:L:264:HIS:HA	12:L:267:THR:OG1	2.14	0.47
12:L:439:PRO:HA	36:k:57:TRP:CZ2	2.49	0.47
12:L:552:LEU:HD22	12:L:553:LEU:HD12	1.97	0.47
12:L:576:LEU:HA	12:L:579:ASN:ND2	2.29	0.47
13:M:51:ASN:O	33:h:135:LYS:HD2	2.13	0.47
13:M:57:SER:OG	13:M:113:THR:HG22	2.15	0.47
13:M:122:PHE:HZ	13:M:206:LYS:HD3	1.75	0.47
13:M:196:TRP:HD1	13:M:250:LEU:HB2	1.80	0.47
13:M:231:LEU:CD1	13:M:235:LEU:HD12	2.42	0.47
13:M:263:LEU:HD21	38:m:105:PHE:HD2	1.80	0.47
14:N:89:GLN:HG2	30:e:60:PHE:CD2	2.50	0.47
15:O:62:VAL:CG1	15:O:207:ILE:HG12	2.44	0.47
15:O:116:LYS:HA	15:O:119:ASP:OD1	2.14	0.47
15:O:135:LEU:HB3	15:O:139:ARG:NH1	2.26	0.47
16:P:170:LEU:HG	16:P:171:ASN:N	2.28	0.47
17:Q:85:ASN:N	17:Q:85:ASN:OD1	2.48	0.47
19:S:16:LEU:HD21	19:S:95:LEU:HD12	1.97	0.47
20:U:128:PHE:CE2	20:U:151:LYS:HG2	2.50	0.47
21:V:116:ILE:O	21:V:116:ILE:CG2	2.61	0.47
22:W:29:ASN:O	22:W:29:ASN:OD1	2.33	0.47
22:W:113:THR:O	22:W:113:THR:HG22	2.15	0.47
23:X:36:CYS:O	23:X:39:THR:HG22	2.15	0.47
23:X:139:GLU:CD	23:X:139:GLU:H	2.22	0.47
24:Y:64:THR:O	24:Y:68:ILE:HG13	2.15	0.47
24:Y:142:LYS:O	24:Y:143:VAL:C	2.57	0.47
26:a:43:TYR:CE1	26:a:47:LEU:HD11	2.50	0.47
27:b:23:PHE:CD1	55:b:201:3PE:H3B2	2.50	0.47
28:c:46:LEU:O	28:c:50:ALA:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:51:ARG:O	29:d:52:PRO:C	2.55	0.47
30:e:28:LYS:HB3	33:h:184:LYS:HA	1.96	0.47
31:f:38:ARG:HD3	31:f:56:TRP:NE1	2.30	0.47
34:i:26:GLN:CD	39:n:118:TYR:HH	2.16	0.47
37:l:48:ARG:NH2	37:l:64:PRO:HD2	2.30	0.47
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.50	0.47
44:s:76:ASN:HB3	44:s:79:THR:HB	1.96	0.47
45:AA:74:TRP:C	45:AA:75:ILE:HG13	2.40	0.47
45:AA:138:LYS:O	45:AA:141:PRO:HD2	2.14	0.47
47:AC:153:ILE:HG23	47:AC:154:PRO:HD2	1.96	0.47
48:AD:318:LYS:HE3	49:AE:87:ASP:O	2.15	0.47
52:AH:26:ASP:O	52:AH:27:PRO:C	2.58	0.47
45:Aa:107:ASN:HB2	45:Aa:110:GLU:OE2	2.15	0.47
45:Aa:152:GLN:O	45:Aa:153:ASN:HB2	2.15	0.47
45:Aa:396:ARG:NH2	45:Aa:434:GLN:HB3	2.30	0.47
46:Ab:142:THR:HA	46:Ab:241:ARG:HH22	1.80	0.47
47:Ac:162:GLU:HA	47:Ac:165:TRP:HB2	1.97	0.47
48:Ad:124:CYS:HB3	48:Ad:194:PRO:HG2	1.96	0.47
48:Ad:227:LEU:HD13	48:Ad:231:LEU:HB2	1.97	0.47
52:Ah:28:LEU:HA	52:Ah:84:LEU:HD13	1.95	0.47
1:A:58:VAL:CG2	8:H:286:MET:HE1	2.45	0.47
2:B:135:GLY:HA2	56:B:301:SF4:S3	2.54	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
9:I:68:ARG:HH22	25:Z:26:PRO:HD2	1.78	0.47
10:J:6:PHE:HB2	10:J:120:LEU:HD11	1.96	0.47
11:K:29:THR:O	11:K:30:LEU:C	2.56	0.47
11:K:75:LEU:O	11:K:79:VAL:HG23	2.15	0.47
12:L:121:LEU:HD22	12:L:246:LEU:CD2	2.24	0.47
12:L:296:ASN:HD22	12:L:357:ARG:NH1	2.13	0.47
12:L:420:ALA:HB1	12:L:498:PHE:CD2	2.50	0.47
13:M:305:THR:O	13:M:306:PRO:C	2.58	0.47
14:N:146:TYR:CD1	14:N:147:PRO:HD3	2.49	0.47
15:O:48:LYS:HE2	15:O:289:TRP:CH2	2.50	0.47
15:O:341:PRO:HB2	28:c:34:PRO:HB3	1.96	0.47
16:P:221:ARG:HD3	16:P:286:ARG:HD3	1.97	0.47
26:a:22:SER:O	26:a:23:THR:C	2.57	0.47
27:b:16:GLU:CD	55:b:201:3PE:H12	2.39	0.47
35:j:44:TYR:HD2	36:k:23:PRO:HD2	1.80	0.47
37:l:44:THR:CG2	37:l:47:GLU:HG3	2.45	0.47
39:n:50:GLU:O	39:n:51:HIS:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:29:PRO:O	41:p:33:LEU:HD13	2.14	0.47
42:q:76:ASP:OD1	42:q:76:ASP:C	2.57	0.47
43:r:109:ASP:O	43:r:110:GLN:OE1	2.32	0.47
49:AE:143:SER:HB2	49:AE:145:ASP:OD1	2.15	0.47
51:AG:11:ILE:CG2	51:AG:12:ARG:N	2.77	0.47
46:Ab:228:SER:HA	46:Ab:231:LYS:HE2	1.97	0.47
47:Ac:140:PHE:CE1	47:Ac:170:VAL:CG1	2.98	0.47
1:A:63:LEU:O	1:A:67:LEU:HG	2.14	0.47
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.47
4:D:254:ARG:HH11	43:r:25:GLN:HB2	1.80	0.47
5:E:191:TYR:O	5:E:192:TYR:C	2.58	0.47
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
8:H:306:SER:OG	27:b:33:PRO:HG3	2.15	0.47
58:J:201:PC1:O14	58:J:201:PC1:H122	2.15	0.47
12:L:183:ILE:HD13	13:M:400:ILE:HD13	1.96	0.47
12:L:237:MET:HE1	12:L:248:HIS:HB2	1.97	0.47
14:N:307:THR:HG22	14:N:308:ASN:N	2.29	0.47
16:P:207:PHE:CD2	16:P:241:TYR:HD1	2.33	0.47
16:P:237:LYS:HZ2	16:P:322:ILE:HG23	1.79	0.47
17:Q:99:MET:SD	17:Q:128:PHE:CE2	3.08	0.47
24:Y:116:GLY:O	24:Y:120:MET:HB2	2.15	0.47
27:b:69:HIS:CD2	27:b:71:GLN:H	2.33	0.47
41:p:93:ARG:NH2	41:p:150:TYR:CE1	2.83	0.47
45:AA:375:GLN:O	45:AA:376:TRP:C	2.58	0.47
46:AB:284:ASN:HB3	46:AB:419:VAL:CG2	2.45	0.47
46:AB:312:SER:OG	46:AB:357:GLN:NE2	2.40	0.47
48:AD:242:ILE:HG13	70:AD:401:HEC:HBD1	1.97	0.47
50:AF:29:LYS:HA	50:AF:81:TRP:CD1	2.49	0.47
50:Af:29:LYS:HA	50:Af:81:TRP:CD1	2.50	0.47
1:A:54:LYS:O	1:A:55:PHE:C	2.58	0.47
55:A:401:3PE:C2C	10:J:37:PHE:CZ	2.97	0.47
3:C:67:ILE:HD11	21:V:47:TYR:CD2	2.50	0.47
8:H:310:PHE:O	27:b:38:TYR:HB2	2.15	0.47
10:J:157:TRP:HE1	14:N:11:PHE:HD2	1.62	0.47
12:L:474:PRO:HD2	40:o:67:LEU:HD21	1.96	0.47
15:O:129:TYR:CE2	15:O:183:CYS:HB3	2.50	0.47
16:P:245:VAL:HA	16:P:265:PHE:CD2	2.49	0.47
18:R:47:ARG:HG3	18:R:48:PHE:CD1	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:54:GLU:HB2	42:q:124:TYR:CD1	2.51	0.47
23:X:120:PRO:CB	23:X:125:LEU:CD1	2.91	0.47
23:X:120:PRO:HB3	23:X:125:LEU:HD11	1.94	0.47
32:g:151:ASP:C	41:p:171:ARG:HH22	2.23	0.47
33:h:55:PHE:HB2	34:i:28:LEU:HD21	1.95	0.47
37:l:127:ASP:O	37:l:128:VAL:C	2.58	0.47
39:n:57:MET:O	39:n:58:MET:C	2.58	0.47
41:p:43:TRP:O	41:p:44:PRO:C	2.58	0.47
47:AC:140:PHE:CE1	47:AC:170:VAL:CG1	2.98	0.47
47:AC:218:ILE:HG21	48:AD:314:LEU:HD11	1.97	0.47
48:AD:130:VAL:HG21	48:AD:277:ALA:HB1	1.97	0.47
48:AD:215:LEU:HD21	70:AD:401:HEC:HMB1	1.96	0.47
49:AE:231:PHE:CD2	49:AE:250:ARG:HG3	2.50	0.47
49:AE:246:SER:HB3	49:AE:248:ARG:HE	1.79	0.47
45:Aa:222:ARG:HH22	45:Aa:263:PRO:HA	1.80	0.47
45:Aa:310:ILE:HG21	45:Aa:379:LEU:HD21	1.96	0.47
45:Aa:352:GLY:O	45:Aa:353:LEU:HD23	2.15	0.47
47:Ac:294:LEU:O	47:Ac:297:SER:HB3	2.15	0.47
47:Ac:323:ILE:HD11	55:Ag:102:3PE:H12	1.97	0.47
68:Ac:405:U10:H272	68:Ac:405:U10:H251	1.56	0.47
48:Ad:167:ARG:CB	48:Ad:168:PRO:HD2	2.38	0.47
50:Af:85:GLU:CD	50:Af:85:GLU:H	2.23	0.47
51:Ag:29:SER:CB	51:Ag:32:SER:HB2	2.38	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.46
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.46
8:H:249:ILE:HD13	23:X:99:HIS:CG	2.50	0.46
10:J:75:THR:HG21	11:K:25:HIS:HB3	1.96	0.46
13:M:232:ALA:HA	13:M:236:LEU:HD12	1.98	0.46
14:N:3:PRO:HG2	15:O:289:TRP:CH2	2.51	0.46
14:N:101:ALA:O	14:N:104:MET:HB3	2.14	0.46
14:N:217:MET:HA	14:N:220:MET:HG2	1.97	0.46
19:S:19:ILE:HD12	19:S:94:VAL:CG1	2.44	0.46
21:V:56:LEU:HD12	21:V:57:ASP:CA	2.44	0.46
22:W:58:THR:HB	22:W:61:GLN:HB3	1.94	0.46
25:Z:98:MET:SD	30:e:79:ILE:HG12	2.55	0.46
31:f:38:ARG:O	31:f:56:TRP:NE1	2.48	0.46
35:j:51:THR:O	35:j:52:ARG:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:14:LEU:HD12	38:m:15:PRO:HD2	1.96	0.46
42:q:137:TRP:CH2	42:q:140:PRO:HD3	2.50	0.46
45:AA:160:GLN:HA	45:AA:163:LYS:HZ3	1.80	0.46
49:Ae:156:LEU:HD11	49:Ae:265:PHE:CE2	2.50	0.46
55:A:401:3PE:H262	55:A:401:3PE:C32	2.45	0.46
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.46
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.46
10:J:132:GLY:O	26:a:42:GLN:HB2	2.15	0.46
11:K:13:SER:O	11:K:17:LEU:HG	2.15	0.46
12:L:86:SER:OG	12:L:133:SER:HB3	2.15	0.46
12:L:172:ILE:O	12:L:176:ARG:HG2	2.16	0.46
12:L:305:SER:C	12:L:336:LYS:HZ3	2.24	0.46
14:N:159:ILE:HB	14:N:278:MET:HE1	1.98	0.46
16:P:287:THR:HG23	16:P:289:ILE:HD11	1.97	0.46
16:P:318:LYS:O	16:P:319:VAL:C	2.58	0.46
21:V:50:GLN:HE22	43:r:94:ALA:H	1.63	0.46
23:X:8:PRO:HB3	23:X:12:GLU:CD	2.39	0.46
23:X:115:LEU:HD13	23:X:117:TRP:CZ2	2.51	0.46
25:Z:97:ILE:CG2	30:e:92:TYR:CD1	2.99	0.46
29:d:59:HIS:CE1	29:d:60:ARG:HG3	2.50	0.46
31:f:37:PHE:O	33:h:134:GLU:HB3	2.15	0.46
35:j:99:ILE:CD1	40:o:107:ARG:HB2	2.45	0.46
37:l:153:TYR:CZ	40:o:19:PRO:HD3	2.50	0.46
46:AB:38:LEU:HD13	46:AB:52:LEU:HB2	1.96	0.46
47:AC:220:PHE:HE2	69:AC:405:UQ6:C4M	2.29	0.46
47:AC:294:LEU:O	47:AC:297:SER:HB3	2.15	0.46
49:AE:156:LEU:HD11	49:AE:265:PHE:CE1	2.50	0.46
49:AE:205:VAL:HG12	49:AE:211:VAL:HG23	1.98	0.46
49:AE:265:PHE:CD1	49:AE:271:VAL:HG22	2.50	0.46
49:Ae:226:ALA:HB2	49:Ae:234:TYR:HE1	1.80	0.46
2:B:93:MET:HE3	4:D:87:GLN:HE21	1.79	0.46
5:E:78:VAL:HG12	5:E:104:LEU:CD1	2.44	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:249:ILE:HG21	23:X:99:HIS:CE1	2.50	0.46
12:L:277:MET:CG	12:L:318:GLY:HA2	2.45	0.46
12:L:373:LEU:CD2	12:L:427:ILE:HG22	2.45	0.46
12:L:427:ILE:CD1	36:k:69:PHE:CE1	2.99	0.46
13:M:4:ILE:HD12	13:M:4:ILE:N	2.30	0.46
13:M:300:SER:HB2	13:M:308:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:380:PHE:HD1	13:M:380:PHE:N	2.13	0.46
55:M:501:3PE:O22	62:h:201:CDL:H122	2.15	0.46
14:N:250:SER:HB2	14:N:334:THR:HG22	1.98	0.46
14:N:336:THR:HG23	29:d:37:LEU:HD11	1.97	0.46
16:P:209:ARG:O	16:P:210:GLU:HB2	2.15	0.46
18:R:72:VAL:HG21	18:R:77:ILE:HG21	1.97	0.46
20:U:130:ILE:HG21	20:U:138:LEU:HD11	1.97	0.46
21:V:22:GLU:O	21:V:26:ILE:HG12	2.16	0.46
23:X:167:PHE:HD2	23:X:170:TRP:HE1	1.62	0.46
25:Z:99:LYS:HB2	25:Z:99:LYS:HE3	1.77	0.46
29:d:78:ARG:O	29:d:81:TYR:N	2.49	0.46
31:f:16:VAL:O	31:f:17:PRO:C	2.57	0.46
35:j:40:ILE:HG13	35:j:41:GLN:H	1.80	0.46
39:n:35:ASP:OD1	39:n:36:LYS:N	2.47	0.46
40:o:31:PHE:CG	40:o:34:ARG:HD2	2.51	0.46
47:AC:296:LEU:O	47:AC:300:ILE:N	2.45	0.46
49:AE:223:VAL:HG23	47:Ac:141:TRP:CH2	2.51	0.46
49:AE:267:SER:C	49:AE:269:ASP:H	2.23	0.46
45:Aa:192:PHE:CZ	45:Aa:353:LEU:HD21	2.50	0.46
46:Ab:225:VAL:HG22	46:Ab:229:VAL:CG2	2.46	0.46
48:Ad:192:ALA:HB1	70:Ad:401:HEC:HBD2	1.97	0.46
48:Ad:309:HIS:NE2	51:Ag:21:PRO:HB2	2.30	0.46
71:Ad:402:3PH:C24	49:Ae:132:VAL:HG22	2.41	0.46
49:Ae:231:PHE:CD2	49:Ae:250:ARG:HG3	2.50	0.46
51:Ag:47:LEU:O	51:Ag:51:PRO:HG2	2.14	0.46
54:Ak:37:ASP:O	54:Ak:38:TRP:C	2.58	0.46
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.96	0.46
2:B:174:SER:HA	3:C:203:LEU:CD2	2.46	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.97	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46
8:H:201:THR:O	8:H:202:GLU:C	2.58	0.46
8:H:307:LEU:HD11	25:Z:47:TYR:CD1	2.50	0.46
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:ILE:O	11:K:62:THR:C	2.58	0.46
12:L:21:ILE:HG12	12:L:27:ILE:CG2	2.45	0.46
12:L:74:MET:HE3	13:M:307:TRP:HH2	1.80	0.46
13:M:213:HIS:O	13:M:217:PRO:CD	2.63	0.46
13:M:380:PHE:N	13:M:380:PHE:CD1	2.82	0.46
55:M:503:3PE:H2G2	38:m:97:PRO:CG	2.41	0.46
14:N:120:GLN:HG3	14:N:177:LYS:CG	2.45	0.46
14:N:175:MET:HE1	14:N:227:ILE:HG22	1.97	0.46
15:O:204:VAL:HG22	15:O:255:VAL:HG22	1.97	0.46
15:O:232:ALA:O	15:O:235:GLN:HB3	2.14	0.46
16:P:55:VAL:HG22	16:P:79:GLN:HB3	1.97	0.46
16:P:153:ALA:HB3	16:P:194:VAL:CG2	2.46	0.46
20:U:114:ASP:O	20:U:117:GLU:N	2.48	0.46
23:X:35:GLN:O	23:X:36:CYS:CB	2.64	0.46
23:X:94:MET:O	23:X:95:GLN:C	2.59	0.46
62:a:101:CDL:H141	62:a:101:CDL:H321	1.97	0.46
46:AB:183:LYS:HG3	46:AB:254:ARG:HB3	1.96	0.46
47:AC:201:HIS:CE1	69:AC:405:UQ6:O2	2.68	0.46
49:AE:166:ALA:HA	49:AE:174:LEU:O	2.15	0.46
62:Ag:101:CDL:H121	62:Ag:101:CDL:H512	1.97	0.46
52:Ah:68:GLU:HA	52:Ah:71:ASP:OD2	2.15	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.80	0.46
5:E:62:ILE:HD12	5:E:81:VAL:HG13	1.97	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
12:L:225:ALA:CB	12:L:233:LEU:HD12	2.45	0.46
13:M:348:LEU:O	13:M:351:VAL:N	2.38	0.46
21:V:72:LEU:C	21:V:72:LEU:CD1	2.89	0.46
23:X:4:ILE:HG22	23:X:5:VAL:N	2.25	0.46
38:m:17:THR:HB	39:n:68:GLU:OE1	2.15	0.46
39:n:133:TRP:O	39:n:137:VAL:HG22	2.15	0.46
49:AE:165:MET:O	49:AE:176:VAL:N	2.44	0.46
49:AE:214:ILE:HG12	49:AE:261:PRO:HD3	1.98	0.46
50:AF:17:PHE:HA	55:AF:201:3PE:H111	1.98	0.46
49:AI:63:PRO:HB3	46:Ab:328:ALA:HB1	1.97	0.46
53:AJ:19:SER:HA	54:AK:24:TRP:CH2	2.51	0.46
45:Aa:279:ASP:HA	51:Ag:12:ARG:HA	1.97	0.46
45:Aa:384:THR:HA	54:Ak:12:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:47:LEU:CD2	46:Ab:234:ALA:HB1	2.45	0.46
47:Ac:37:LEU:CB	67:Ac:403:HEM:CMB	2.93	0.46
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.50	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
6:F:224:ARG:HD3	17:Q:164:PHE:CE1	2.51	0.46
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.28	0.46
8:H:312:ALA:CB	27:b:38:TYR:HB3	2.44	0.46
10:J:164:PHE:HB3	14:N:5:THR:HG23	1.97	0.46
13:M:10:MET:C	13:M:13:PRO:HD2	2.41	0.46
13:M:139:GLN:HG3	13:M:141:GLU:H	1.80	0.46
15:O:50:THR:OG1	15:O:288:ASP:HB3	2.16	0.46
20:T:87:LEU:CD2	20:T:122:MET:HE1	2.46	0.46
23:X:120:PRO:HB2	23:X:125:LEU:CD1	2.44	0.46
23:X:133:THR:HG23	27:b:58:ARG:HH12	1.81	0.46
25:Z:28:ARG:O	25:Z:28:ARG:CG	2.64	0.46
35:j:71:TRP:HA	36:k:84:PHE:CE1	2.50	0.46
39:n:136:GLU:O	39:n:139:GLN:N	2.49	0.46
41:p:50:GLU:CG	41:p:54:ARG:HH21	2.28	0.46
45:AA:174:GLU:C	45:AA:176:ASP:N	2.73	0.46
47:AC:92:ILE:HG13	47:AC:272:TRP:CH2	2.48	0.46
49:AE:220:LEU:HD13	47:Ac:145:VAL:HG13	1.97	0.46
50:AF:53:GLU:OE2	51:AG:12:ARG:NH1	2.47	0.46
50:AF:83:LYS:HB3	50:AF:85:GLU:OE2	2.15	0.46
45:Aa:114:GLU:OE2	46:Ab:298:HIS:HB2	2.16	0.46
45:Aa:285:ALA:HB3	45:Aa:365:ILE:HD11	1.97	0.46
45:Aa:338:CYS:O	45:Aa:339:GLN:C	2.57	0.46
45:Aa:407:THR:HB	45:Aa:408:PRO:HD3	1.96	0.46
46:Ab:228:SER:HA	46:Ab:231:LYS:CE	2.45	0.46
50:Af:83:LYS:HB3	50:Af:85:GLU:OE2	2.15	0.46
51:Ag:37:ASN:ND2	62:Ag:101:CDL:OA3	2.49	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.46
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
7:G:655:ARG:NH1	19:S:59:SER:H	2.14	0.46
12:L:52:LEU:CB	41:p:30:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:407:TRP:HE1	37:l:140:MET:HE1	1.81	0.46
12:L:434:LYS:HZ2	36:k:66:ASN:HA	1.80	0.46
12:L:581:LYS:HB2	12:L:586:LEU:HD22	1.97	0.46
13:M:116:ILE:HD12	13:M:119:TYR:HB3	1.97	0.46
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.98	0.46
14:N:321:LYS:HG3	14:N:321:LYS:O	2.15	0.46
15:O:246:LEU:O	15:O:247:PRO:C	2.57	0.46
15:O:343:TYR:HB3	29:d:52:PRO:HD3	1.98	0.46
16:P:276:LEU:O	16:P:280:ILE:HG13	2.15	0.46
19:S:25:GLN:NE2	19:S:34:ARG:HH11	2.13	0.46
21:V:56:LEU:HD13	21:V:60:LYS:HE2	1.98	0.46
22:W:99:VAL:HG13	22:W:99:VAL:O	2.15	0.46
23:X:107:PHE:O	23:X:110:CYS:SG	2.73	0.46
26:a:45:TRP:O	26:a:46:TYR:C	2.58	0.46
27:b:28:LEU:O	27:b:32:MET:HG2	2.15	0.46
28:c:67:LEU:O	28:c:68:GLU:C	2.59	0.46
33:h:69:ARG:O	33:h:73:PHE:CB	2.63	0.46
38:m:9:ALA:O	38:m:10:PRO:C	2.56	0.46
45:AA:339:GLN:O	45:AA:340:SER:C	2.56	0.46
45:Aa:383:ALA:O	45:Aa:442:ARG:NH1	2.48	0.46
47:Ac:160:LEU:O	47:Ac:163:TRP:HB3	2.15	0.46
48:Ad:146:LYS:N	48:Ad:171:LEU:HD21	2.31	0.46
49:Ae:246:SER:HB3	49:Ae:248:ARG:HE	1.79	0.46
54:Ak:23:MET:O	54:Ak:27:VAL:HG23	2.15	0.46
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.97	0.46
5:E:136:THR:HB	59:E:301:FES:S2	2.56	0.46
7:G:275:PRO:HB2	17:Q:86:ASN:ND2	2.30	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
12:L:31:ASN:ND2	12:L:34:LEU:HB2	2.31	0.46
12:L:529:PHE:CZ	12:L:533:ILE:HG21	2.50	0.46
12:L:560:LYS:HZ3	62:L:706:CDL:C32	2.28	0.46
62:L:706:CDL:H732	62:L:706:CDL:OB8	2.16	0.46
13:M:15:THR:HG21	13:M:100:ILE:CD1	2.46	0.46
13:M:173:THR:HG22	33:h:150:ARG:NH1	2.31	0.46
13:M:319:HIS:CA	13:M:322:THR:HG22	2.41	0.46
13:M:435:THR:O	13:M:436:LEU:C	2.59	0.46
13:M:453:LEU:CD1	13:M:454:ILE:CG2	2.84	0.46
14:N:37:LEU:HD21	14:N:60:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:104:MET:CE	14:N:111:PHE:CE1	2.99	0.46
14:N:197:ASN:ND2	14:N:200:LEU:HD13	2.30	0.46
14:N:277:ILE:HG22	14:N:278:MET:H	1.79	0.46
14:N:319:LYS:HA	15:O:302:THR:HG21	1.98	0.46
19:S:37:ILE:HD12	19:S:55:ILE:HD12	1.98	0.46
23:X:5:VAL:CG1	23:X:7:LEU:HG	2.46	0.46
24:Y:74:LEU:HD23	24:Y:74:LEU:C	2.41	0.46
27:b:19:LEU:CD2	55:b:201:3PE:H332	2.46	0.46
40:o:71:ARG:HB3	40:o:71:ARG:NH1	2.27	0.46
40:o:93:LEU:O	40:o:96:VAL:CG1	2.64	0.46
42:q:14:VAL:HA	42:q:23:LEU:HD22	1.98	0.46
46:AB:278:ILE:HB	46:AB:331:SER:HA	1.98	0.46
55:AF:201:3PE:H3B2	51:AG:47:LEU:O	2.16	0.46
53:AJ:11:TYR:HA	53:AJ:15:PHE:HB2	1.97	0.46
54:AK:41:ILE:HD12	54:AK:41:ILE:N	2.31	0.46
45:Aa:109:LEU:HG	45:Aa:146:LEU:HD22	1.97	0.46
45:Aa:157:GLU:HB2	45:Aa:160:GLN:HB2	1.97	0.46
46:Ab:177:LEU:HD21	46:Ab:272:VAL:CG1	2.46	0.46
47:Ac:245:PHE:CE1	48:Ad:102:LEU:HD23	2.51	0.46
4:D:338:ARG:NH1	25:Z:23:ARG:HA	2.31	0.46
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.51	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
55:I:301:3PE:H241	55:I:301:3PE:H272	1.60	0.46
10:J:29:GLY:O	10:J:30:LEU:C	2.58	0.46
10:J:103:ILE:HG22	10:J:107:ASN:HD21	1.81	0.46
12:L:12:PHE:O	12:L:16:LEU:HG	2.15	0.46
12:L:101:MET:HE1	12:L:121:LEU:HB2	1.98	0.46
13:M:6:LEU:HD21	31:f:22:PHE:HD2	1.81	0.46
13:M:186:LEU:HD22	13:M:250:LEU:HA	1.97	0.46
14:N:243:MET:CE	14:N:330:ALA:HB1	2.46	0.46
14:N:276:LEU:HD13	55:N:401:3PE:C2	2.38	0.46
16:P:261:LYS:HB2	16:P:263:PHE:CE1	2.51	0.46
23:X:7:LEU:CD1	25:Z:87:LEU:HB3	2.46	0.46
27:b:45:ILE:N	27:b:80:TRP:HH2	2.14	0.46
28:c:38:LYS:HA	28:c:39:PRO:HD3	1.58	0.46
32:g:77:ASP:HA	32:g:78:PRO:HD3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:82:VAL:O	33:h:85:GLY:N	2.49	0.46
45:AA:183:VAL:HG21	45:AA:286:HIS:HB2	1.96	0.46
47:AC:150:LEU:CD1	47:AC:164:ILE:HD12	2.46	0.46
49:AI:62:ARG:CG	49:AI:63:PRO:HD2	2.46	0.46
45:Aa:59:VAL:HG21	45:Aa:246:ALA:HB1	1.97	0.46
45:Aa:117:GLY:HA3	46:Ab:377:LYS:HA	1.98	0.46
45:Aa:222:ARG:NH2	45:Aa:263:PRO:CG	2.79	0.46
45:Aa:250:LEU:O	45:Aa:253:VAL:HG23	2.16	0.46
45:Aa:338:CYS:HB3	45:Aa:360:CYS:HB2	1.55	0.46
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CD2	2.51	0.46
48:Ad:214:LEU:O	48:Ad:234:ASN:ND2	2.49	0.46
51:Ag:64:ASN:O	51:Ag:68:GLU:HG2	2.16	0.46
1:A:63:LEU:HD11	10:J:63:MET:HA	1.98	0.46
1:A:90:MET:CE	10:J:152:MET:HG2	2.46	0.46
1:A:106:TRP:CH2	8:H:291:LYS:HA	2.51	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.46
5:E:73:HIS:ND1	17:Q:166:TRP:CE3	2.84	0.46
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.46
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.46
8:H:114:TYR:CE1	10:J:65:VAL:HG22	2.50	0.46
8:H:316:PRO:HG3	25:Z:57:ARG:HB3	1.98	0.46
9:I:60:ILE:CG2	55:I:301:3PE:H111	2.46	0.46
11:K:26:LEU:O	11:K:29:THR:N	2.48	0.46
12:L:324:LEU:HA	12:L:327:LEU:HD12	1.97	0.46
12:L:339:LEU:HD11	12:L:376:GLY:HA3	1.98	0.46
12:L:475:THR:O	12:L:476:SER:HB2	2.16	0.46
12:L:590:SER:HB2	24:Y:45:LEU:HD11	1.98	0.46
14:N:119:THR:O	14:N:122:ILE:HG13	2.16	0.46
14:N:241:LEU:O	14:N:244:ILE:HG22	2.15	0.46
15:O:59:VAL:HA	15:O:157:VAL:HG22	1.97	0.46
15:O:71:ASN:C	15:O:75:LYS:HE3	2.40	0.46
15:O:344:ASN:OD1	15:O:346:GLU:HG2	2.15	0.46
16:P:66:GLY:O	16:P:69:VAL:N	2.48	0.46
16:P:170:LEU:HD12	16:P:171:ASN:H	1.81	0.46
18:R:54:GLU:HB2	42:q:124:TYR:HD1	1.81	0.46
20:U:118:ILE:O	20:U:122:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:19:GLN:HE21	24:Y:22:ARG:CG	2.15	0.46
25:Z:93:GLU:OE1	30:e:95:PRO:HD2	2.14	0.46
27:b:38:TYR:O	27:b:39:THR:C	2.59	0.46
27:b:45:ILE:CA	27:b:80:TRP:HH2	2.28	0.46
29:d:13:PHE:O	29:d:78:ARG:NE	2.43	0.46
29:d:107:LYS:HB3	29:d:111:GLU:HB3	1.98	0.46
33:h:95:GLU:OE1	33:h:114:LYS:HD3	2.15	0.46
33:h:96:ALA:CB	41:p:63:TYR:HD1	2.25	0.46
35:j:92:TRP:O	35:j:93:THR:C	2.59	0.46
36:k:39:GLN:NE2	36:k:49:ASP:HB3	2.31	0.46
36:k:69:PHE:CZ	36:k:73:ILE:HG13	2.51	0.46
37:l:166:LEU:HD12	37:l:170:ARG:HH22	1.81	0.46
39:n:58:MET:HE1	45:Aa:264:GLY:HA2	1.98	0.46
48:AD:237:PHE:CD1	48:AD:238:PRO:HD2	2.51	0.46
48:AD:321:TYR:HB2	50:AF:61:PHE:CD1	2.51	0.46
52:AH:46:GLU:O	52:AH:50:LEU:HG	2.16	0.46
45:Aa:412:ASP:O	45:Aa:413:ILE:C	2.58	0.46
47:Ac:246:PHE:HB3	47:Ac:249:MET:HE3	1.98	0.46
48:Ad:236:TYR:O	48:Ad:237:PHE:C	2.59	0.46
48:Ad:237:PHE:CD1	48:Ad:238:PRO:HD2	2.51	0.46
48:Ad:242:ILE:HD13	48:Ad:244:MET:HE2	1.98	0.46
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.51	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
5:E:245:GLN:HB3	6:F:256:ARG:O	2.16	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.30	0.45
7:G:32:ILE:HD11	7:G:45:PRO:HG3	1.98	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
11:K:57:MET:O	11:K:58:PRO:C	2.58	0.45
12:L:161:ARG:HA	39:n:92:GLU:CB	2.45	0.45
12:L:277:MET:HG3	12:L:318:GLY:CA	2.46	0.45
12:L:550:LEU:O	12:L:554:ASP:HB3	2.16	0.45
13:M:122:PHE:CZ	13:M:206:LYS:CD	2.95	0.45
13:M:158:ILE:CG2	14:N:283:ALA:HB1	2.45	0.45
13:M:282:LEU:HD11	13:M:410:MET:HE3	1.96	0.45
14:N:300:THR:CG2	14:N:301:SER:N	2.79	0.45
14:N:326:PHE:HE2	29:d:48:LEU:HD13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:140:LEU:HD11	15:O:198:TYR:CE2	2.51	0.45
15:O:271:GLU:OE1	21:V:30:LYS:NZ	2.48	0.45
23:X:37:ASP:OD2	27:b:70:PRO:HD3	2.16	0.45
31:f:49:ARG:HG2	31:f:52:GLU:HG3	1.98	0.45
34:i:15:LEU:HD21	39:n:167:TRP:HB3	1.97	0.45
34:i:18:LEU:CD2	39:n:125:TRP:HH2	2.29	0.45
39:n:37:TYR:O	39:n:38:ARG:C	2.58	0.45
49:AE:143:SER:O	49:AE:144:ALA:C	2.59	0.45
53:AJ:9:ARG:O	53:AJ:13:LEU:HD23	2.16	0.45
45:Aa:270:PHE:CE1	45:Aa:353:LEU:HD22	2.51	0.45
49:Ae:188:ALA:HA	49:Ae:200:HIS:HE2	1.79	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.45
4:D:79:ASN:O	4:D:101:LEU:N	2.49	0.45
5:E:69:TYR:HE2	5:E:80:PRO:HG2	1.81	0.45
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.45
7:G:163:LYS:HE2	18:R:97:LYS:NZ	2.31	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
8:H:30:TYR:HE2	26:a:5:ILE:CG2	2.16	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.45
8:H:292:ASN:HD21	55:I:301:3PE:HN2	1.63	0.45
8:H:302:MET:SD	27:b:26:TRP:CD1	3.09	0.45
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.45
9:I:123:CYS:SG	56:I:303:SF4:S4	3.13	0.45
12:L:55:PHE:CB	40:o:74:PHE:HE1	2.29	0.45
12:L:142:ILE:HA	13:M:370:PRO:CB	2.45	0.45
12:L:204:SER:HA	12:L:207:ASN:ND2	2.31	0.45
12:L:357:ARG:NH2	39:n:29:SER:HA	2.31	0.45
62:L:705:CDL:H341	33:h:71:MET:SD	2.57	0.45
13:M:22:LYS:HG2	13:M:22:LYS:O	2.17	0.45
13:M:56:PHE:CE1	13:M:108:MET:HG2	2.47	0.45
13:M:61:LEU:C	13:M:64:PRO:HD2	2.42	0.45
13:M:207:MET:O	13:M:208:PRO:C	2.59	0.45
14:N:148:LEU:H	14:N:148:LEU:HD12	1.82	0.45
14:N:154:ILE:HB	14:N:191:LEU:HG	1.98	0.45
14:N:281:LEU:HD23	55:N:401:3PE:H292	1.98	0.45
15:O:63:ASP:O	15:O:161:ARG:HG2	2.16	0.45
22:W:42:TRP:CZ2	22:W:93:LEU:HB2	2.51	0.45
31:f:12:VAL:HG23	31:f:13:HIS:N	2.31	0.45
36:k:47:LEU:HD13	39:n:42:CYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:44:MET:O	39:n:45:ARG:C	2.54	0.45
46:AB:225:VAL:HG22	46:AB:229:VAL:CG2	2.46	0.45
47:AC:30:TRP:HZ3	47:AC:96:LEU:HD22	1.81	0.45
47:AC:223:TYR:O	48:AD:311:TRP:NE1	2.49	0.45
48:AD:116:VAL:HA	48:AD:253:LEU:HD21	1.99	0.45
48:AD:121:CYS:CB	70:AD:401:HEC:CAB	2.89	0.45
49:AE:156:LEU:HD23	49:AE:156:LEU:HA	1.62	0.45
50:AF:85:GLU:H	50:AF:85:GLU:CD	2.24	0.45
45:Aa:269:ARG:HG3	45:Aa:271:THR:HG23	1.98	0.45
47:Ac:30:TRP:HZ3	47:Ac:96:LEU:HD22	1.81	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.45
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.45
3:C:100:ARG:NH1	21:V:86:LYS:NZ	2.64	0.45
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.05	0.45
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.45
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.47	0.45
7:G:176:CYS:SG	56:G:802:SF4:S1	3.14	0.45
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
9:I:188:GLU:OE1	18:R:56:ASN:HB2	2.16	0.45
11:K:59:ILE:HD12	14:N:27:MET:HG2	1.98	0.45
12:L:135:ASN:O	12:L:198:LEU:HD13	2.16	0.45
12:L:210:LEU:HD23	12:L:210:LEU:C	2.41	0.45
13:M:19:SER:H	31:f:8:ARG:HD2	1.82	0.45
13:M:42:LEU:HD21	13:M:67:ILE:HD12	1.97	0.45
13:M:393:ILE:O	13:M:397:GLY:N	2.49	0.45
14:N:130:LEU:O	14:N:134:GLN:HB2	2.16	0.45
15:O:265:ASP:O	15:O:266:PRO:C	2.58	0.45
24:Y:75:THR:HB	24:Y:95:GLY:HA2	1.98	0.45
30:e:18:PHE:O	30:e:18:PHE:CD2	2.69	0.45
36:k:48:ARG:HG3	36:k:48:ARG:O	2.15	0.45
37:l:101:TRP:HE1	38:m:62:ASP:HA	1.80	0.45
39:n:45:ARG:O	39:n:49:GLU:N	2.37	0.45
40:o:63:LEU:O	40:o:64:ILE:C	2.59	0.45
40:o:73:SER:HA	41:p:24:THR:OG1	2.17	0.45
41:p:173:GLU:O	41:p:174:ALA:C	2.59	0.45
42:q:98:PRO:O	42:q:99:THR:C	2.59	0.45
45:AA:341:PHE:CE1	45:AA:356:ALA:HB1	2.48	0.45
49:AE:226:ALA:HB2	49:AE:234:TYR:HE1	1.80	0.45
49:AE:231:PHE:CE2	49:AE:250:ARG:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:98:PHE:CZ	45:Aa:122:ALA:HB2	2.51	0.45
45:Aa:169:LEU:HD23	45:Aa:172:MET:CE	2.46	0.45
71:Ad:402:3PH:C22	49:Ae:135:GLN:HE22	2.29	0.45
49:Ae:205:VAL:HG12	49:Ae:211:VAL:HG23	1.98	0.45
49:Ae:231:PHE:CE2	49:Ae:250:ARG:HB3	2.51	0.45
2:B:126:ARG:HG3	8:H:213:VAL:O	2.17	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
12:L:23:MET:O	62:L:705:CDL:HA61	2.16	0.45
14:N:26:LEU:HG	14:N:85:MET:SD	2.56	0.45
14:N:124:LEU:HD21	14:N:176:ARG:CG	2.46	0.45
14:N:215:MET:SD	14:N:244:ILE:HD11	2.56	0.45
15:O:112:CYS:HB3	15:O:131:LEU:HA	1.97	0.45
15:O:246:LEU:O	15:O:250:SER:N	2.48	0.45
15:O:342:GLY:O	15:O:355:LYS:NZ	2.50	0.45
16:P:218:ALA:HB2	16:P:280:ILE:CG2	2.47	0.45
18:R:97:LYS:CE	18:R:100:LYS:HD3	2.45	0.45
19:S:31:GLN:OE1	19:S:34:ARG:NH2	2.49	0.45
19:S:65:LEU:HD23	19:S:65:LEU:O	2.16	0.45
20:T:119:ILE:CD1	20:T:138:LEU:HD11	2.43	0.45
24:Y:39:SER:HB2	24:Y:58:VAL:HA	1.98	0.45
26:a:45:TRP:O	26:a:48:MET:N	2.50	0.45
30:e:19:MET:HE2	30:e:19:MET:HB3	1.85	0.45
34:i:5:THR:HG22	34:i:6:PRO:HD2	1.98	0.45
37:l:57:MET:HE2	37:l:57:MET:HB3	1.75	0.45
40:o:118:LYS:HD2	40:o:118:LYS:HA	1.85	0.45
41:p:24:THR:HG22	41:p:26:LEU:N	2.31	0.45
46:Ab:267:VAL:HA	46:Ab:441:SER:O	2.17	0.45
48:Ad:311:TRP:O	48:Ad:315:LYS:HG3	2.16	0.45
49:Ae:156:LEU:HD11	49:Ae:265:PHE:HE2	1.81	0.45
49:Ae:214:ILE:HG12	49:Ae:261:PRO:HD3	1.98	0.45
49:Ae:241:SER:OG	49:Ae:254:ALA:HB2	2.17	0.45
1:A:78:ALA:HB2	10:J:142:ALA:HB1	1.99	0.45
2:B:91:TRP:HA	2:B:120:VAL:HG12	1.99	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.45
10:J:28:GLY:O	10:J:29:GLY:C	2.59	0.45
12:L:74:MET:HE3	12:L:74:MET:HB2	1.76	0.45
12:L:145:GLU:CG	13:M:370:PRO:HD3	2.47	0.45
12:L:195:SER:O	12:L:201:ILE:HD11	2.16	0.45
12:L:310:LEU:HA	12:L:313:MET:HB2	1.99	0.45
12:L:366:MET:SD	12:L:443:ILE:HG21	2.57	0.45
12:L:403:ASN:HA	37:l:152:SER:O	2.17	0.45
13:M:42:LEU:HD11	13:M:67:ILE:HD12	1.99	0.45
13:M:42:LEU:CG	13:M:67:ILE:HD11	2.43	0.45
13:M:208:PRO:CD	13:M:236:LEU:HD22	2.38	0.45
13:M:283:LYS:HG3	13:M:327:PHE:HE1	1.78	0.45
15:O:249:MET:HE3	15:O:253:CYS:SG	2.56	0.45
20:U:133:ILE:CD1	39:n:7:PRO:HD3	2.46	0.45
21:V:32:LEU:O	21:V:36:LYS:HG2	2.16	0.45
22:W:32:LYS:HZ2	66:W:201:EHZ:C19	2.28	0.45
23:X:48:TRP:HZ3	33:h:186:THR:C	2.24	0.45
62:X:201:CDL:OA4	31:f:29:LYS:HD2	2.16	0.45
62:a:101:CDL:H321	62:a:101:CDL:C14	2.46	0.45
32:g:67:LYS:O	32:g:68:ASN:C	2.60	0.45
33:h:73:PHE:HD2	33:h:74:TYR:CE1	2.33	0.45
36:k:26:ARG:O	36:k:27:GLN:C	2.57	0.45
36:k:42:LEU:HG	39:n:39:TYR:HD1	1.82	0.45
40:o:13:ALA:C	40:o:15:VAL:N	2.74	0.45
41:p:107:GLN:O	41:p:111:LYS:HG3	2.15	0.45
42:q:71:LYS:HB2	42:q:73:THR:HG23	1.98	0.45
42:q:85:GLU:CG	42:q:98:PRO:HB3	2.36	0.45
45:AA:74:TRP:HB3	45:AA:418:LEU:CD1	2.46	0.45
45:AA:287:VAL:HB	45:AA:358:PHE:CZ	2.50	0.45
45:AA:387:GLU:HB2	45:AA:390:ARG:NH2	2.30	0.45
46:AB:49:ILE:HD13	46:AB:220:LEU:HB3	1.98	0.45
49:AE:155:LYS:HB3	49:AE:158:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Aj:34:ARG:NH1	53:Aj:38:GLN:HB2	2.31	0.45
45:Aa:278:ARG:NH2	51:Ag:9:ALA:O	2.50	0.45
48:Ad:139:CYS:HA	53:Aj:53:TRP:CZ3	2.51	0.45
48:Ad:159:ASN:O	48:Ad:160:ASP:C	2.59	0.45
49:Ae:126:ALA:C	54:Ak:34:TRP:HH2	2.24	0.45
51:Ag:67:PHE:CE2	51:Ag:71:LYS:HD3	2.52	0.45
1:A:63:LEU:CD2	10:J:63:MET:HA	2.46	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
9:I:61:LEU:O	55:I:301:3PE:H332	2.15	0.45
11:K:85:TYR:OH	11:K:95:LEU:HD11	2.17	0.45
12:L:246:LEU:C	12:L:246:LEU:CD1	2.90	0.45
12:L:247:LEU:HD12	12:L:247:LEU:C	2.41	0.45
12:L:446:ASN:HD21	35:j:51:THR:HG21	1.82	0.45
12:L:446:ASN:ND2	35:j:51:THR:HG21	2.32	0.45
12:L:508:THR:HG22	39:n:33:HIS:CD2	2.51	0.45
12:L:589:MET:O	12:L:592:LEU:HB3	2.16	0.45
13:M:65:LEU:O	13:M:66:ILE:C	2.59	0.45
15:O:351:TRP:HB2	15:O:355:LYS:HE3	1.98	0.45
16:P:259:VAL:H	16:P:261:LYS:HG2	1.82	0.45
17:Q:77:VAL:HG21	17:Q:99:MET:HE3	1.97	0.45
19:S:44:LEU:CD1	19:S:91:MET:HG2	2.45	0.45
19:S:74:GLU:OE1	19:S:74:GLU:N	2.49	0.45
20:U:102:SER:O	20:U:141:PRO:HD3	2.16	0.45
25:Z:110:VAL:HG21	30:e:72:THR:HG23	1.98	0.45
34:i:7:ASP:HB2	39:n:156:PRO:HD3	1.99	0.45
40:o:93:LEU:O	40:o:96:VAL:HG12	2.16	0.45
45:AA:114:GLU:HG2	46:AB:299:ILE:CD1	2.47	0.45
47:AC:37:LEU:HB3	67:AC:402:HEM:HMB1	1.98	0.45
49:AE:168:LYS:HZ3	49:AE:171:GLY:HA2	1.82	0.45
49:AE:188:ALA:HA	49:AE:200:HIS:HE2	1.80	0.45
45:Aa:285:ALA:CB	45:Aa:365:ILE:HD11	2.47	0.45
45:Aa:467:ASP:OD2	47:Ac:223:TYR:CE2	2.69	0.45
46:Ab:267:VAL:HG13	46:Ab:444:LEU:CD2	2.46	0.45
48:Ad:167:ARG:NH1	48:Ad:169:GLY:HA2	2.31	0.45
53:Aj:34:ARG:NH1	53:Aj:38:GLN:HB2	2.31	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.97	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
12:L:47:SER:O	12:L:50:PRO:HD2	2.17	0.45
12:L:241:THR:N	12:L:242:PRO:HD2	2.31	0.45
12:L:560:LYS:NZ	62:L:706:CDL:C32	2.80	0.45
55:L:704:3PE:C3B	55:L:704:3PE:H271	2.47	0.45
13:M:25:THR:HG22	32:g:84:ASN:CG	2.42	0.45
14:N:293:TYR:O	14:N:297:ILE:HG12	2.16	0.45
15:O:60:ILE:CD1	15:O:203:ALA:HB3	2.45	0.45
20:T:87:LEU:CD2	20:T:104:PHE:CE1	2.94	0.45
20:T:130:ILE:CG2	20:T:131:PRO:CD	2.95	0.45
21:V:56:LEU:HD11	21:V:57:ASP:OD1	2.17	0.45
28:c:65:ASP:O	28:c:66:VAL:C	2.56	0.45
34:i:95:TYR:HD1	41:p:112:ALA:HB2	1.77	0.45
35:j:59:GLU:HG2	36:k:75:LYS:HZ1	1.82	0.45
36:k:57:TRP:O	36:k:58:ARG:C	2.59	0.45
40:o:44:GLN:O	40:o:45:GLU:C	2.59	0.45
45:AA:92:PHE:HZ	45:AA:161:ILE:HG23	1.81	0.45
45:AA:294:PRO:HB2	45:AA:298:ASN:HB3	1.98	0.45
45:AA:463:GLU:OE1	51:AG:8:LEU:HB2	2.17	0.45
46:AB:37:ASP:O	46:AB:38:LEU:C	2.60	0.45
48:AD:121:CYS:HB3	70:AD:401:HEC:CHC	2.46	0.45
49:AE:178:HIS:CD2	49:AE:209:GLU:O	2.70	0.45
49:AE:255:PRO:HG2	47:Ac:287:LYS:HZ1	1.82	0.45
51:AG:38:VAL:HA	51:AG:41:ARG:HD3	1.98	0.45
45:Aa:399:LEU:HB3	45:Aa:426:LEU:HD22	1.98	0.45
46:Ab:429:LYS:O	46:Ab:432:VAL:HG12	2.16	0.45
48:Ad:218:TYR:CE2	48:Ad:246:PRO:HA	2.51	0.45
49:Ae:116:LEU:CB	53:Aj:15:PHE:CZ	3.00	0.45
49:Ae:178:HIS:CD2	49:Ae:209:GLU:O	2.70	0.45
49:Ae:261:PRO:HB2	49:Ae:273:VAL:HG21	1.98	0.45
50:Af:20:TRP:CH2	55:Ag:102:3PE:H32	2.52	0.45
51:Ag:12:ARG:HB3	51:Ag:13:HIS:CD2	2.52	0.45
2:B:94:THR:HG21	2:B:104:MET:SD	2.57	0.45
4:D:266:ARG:NH2	9:I:59:ARG:O	2.50	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:107:ALA:HB1	10:J:56:PHE:HD2	1.81	0.45
8:H:224:PHE:CE2	61:H:400:UQ9:C14	3.00	0.45
10:J:17:LEU:O	10:J:21:LEU:HG	2.16	0.45
12:L:387:THR:HA	12:L:465:GLY:HA3	1.98	0.45
12:L:532:ILE:HG23	12:L:533:ILE:N	2.31	0.45
12:L:591:PHE:N	12:L:591:PHE:CD1	2.83	0.45
12:L:591:PHE:N	12:L:591:PHE:HD1	2.15	0.45
55:L:701:3PE:H221	34:i:89:HIS:NE2	2.32	0.45
13:M:3:LYS:HA	13:M:7:PRO:HD2	1.99	0.45
13:M:42:LEU:CG	13:M:67:ILE:CD1	2.94	0.45
13:M:129:THR:CG2	13:M:235:LEU:CD1	2.95	0.45
13:M:272:THR:O	13:M:275:ILE:HG13	2.17	0.45
14:N:82:GLY:HA3	30:e:21:LEU:HG	1.98	0.45
14:N:176:ARG:CZ	14:N:225:MET:SD	3.05	0.45
17:Q:65:THR:HG23	17:Q:67:VAL:HG23	1.99	0.45
20:T:83:VAL:HG21	20:T:145:VAL:HG22	1.99	0.45
20:T:90:TYR:O	20:T:91:ASP:HB2	2.17	0.45
20:T:117:GLU:HA	20:T:120:MET:CE	2.41	0.45
20:U:103:HIS:CD2	20:U:140:CYS:SG	3.10	0.45
23:X:7:LEU:HD13	25:Z:87:LEU:HB3	1.99	0.45
29:d:2:MET:HE3	29:d:2:MET:HB3	1.88	0.45
29:d:13:PHE:CE2	29:d:14:LEU:HD23	2.52	0.45
35:j:87:PRO:HG3	40:o:96:VAL:HG23	1.99	0.45
37:l:30:PHE:CE1	37:l:31:HIS:CE1	3.05	0.45
40:o:4:HIS:HD1	40:o:102:PHE:HE2	1.64	0.45
41:p:110:LEU:O	41:p:111:LYS:C	2.58	0.45
47:AC:138:MET:HE1	47:AC:268:ILE:CD1	2.47	0.45
49:AE:155:LYS:HZ3	49:AE:157:SER:CB	2.28	0.45
49:AE:156:LEU:HG	49:AE:271:VAL:CG2	2.43	0.45
49:AE:241:SER:OG	49:AE:254:ALA:HB2	2.17	0.45
45:Aa:170:ARG:HG3	45:Aa:171:GLU:N	2.32	0.45
49:Ae:201:ASP:OD1	49:Ae:202:LEU:N	2.50	0.45
54:Ak:29:ALA:O	54:Ak:33:VAL:HG23	2.17	0.45
2:B:94:THR:OG1	57:B:302:UQ1:H72	2.17	0.45
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:179:TRP:CD1	25:Z:43:LEU:HD21	2.52	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
10:J:126:TYR:CD2	11:K:50:ASN:HB2	2.52	0.45
12:L:81:LYS:CA	12:L:135:ASN:HD21	2.29	0.45
12:L:100:ILE:O	12:L:104:SER:N	2.42	0.45
12:L:226:GLN:HG3	12:L:314:MET:HE2	1.98	0.45
12:L:231:PRO:CG	12:L:529:PHE:HD2	2.30	0.45
12:L:287:PHE:CZ	12:L:527:GLY:HA3	2.52	0.45
12:L:508:THR:HG22	39:n:33:HIS:HD2	1.82	0.45
12:L:578:THR:CG2	14:N:168:GLY:HA2	2.47	0.45
13:M:73:LEU:HB3	13:M:103:GLN:OE1	2.15	0.45
13:M:87:ASP:HB3	13:M:91:LEU:HB2	1.99	0.45
13:M:151:PHE:HZ	14:N:291:PHE:CA	2.30	0.45
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.81	0.45
16:P:209:ARG:CA	16:P:352:VAL:HG22	2.47	0.45
20:T:133:ILE:HG23	20:T:134:ASP:N	2.32	0.45
20:U:110:LEU:CD2	20:U:118:ILE:HD11	2.46	0.45
22:W:71:MET:O	22:W:74:ALA:N	2.43	0.45
29:d:3:ASN:C	29:d:5:ARG:H	2.25	0.45
62:h:201:CDL:H162	62:h:201:CDL:H191	1.75	0.45
38:m:40:ARG:NH1	39:n:152:GLU:OE1	2.49	0.45
41:p:49:ARG:O	41:p:50:GLU:C	2.57	0.45
42:q:55:PHE:CD1	43:r:26:LEU:CD2	2.96	0.45
47:AC:138:MET:HE1	47:AC:268:ILE:HD13	1.98	0.45
49:AE:207:LYS:HE3	49:AE:265:PHE:CG	2.51	0.45
49:AE:263:TYR:HA	49:AE:273:VAL:HA	1.98	0.45
51:AG:12:ARG:HB3	51:AG:13:HIS:CD2	2.52	0.45
49:AI:34:VAL:O	49:AI:34:VAL:HG13	2.17	0.45
46:Ab:229:VAL:O	46:Ab:233:VAL:HG13	2.16	0.45
46:Ab:300:LYS:C	46:Ab:302:GLY:H	2.24	0.45
3:C:98:PHE:HE1	21:V:44:TYR:CE1	2.35	0.45
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.52	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.45
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
12:L:149:ILE:CG2	13:M:364:LEU:HD21	2.47	0.45
13:M:249:ILE:O	13:M:250:LEU:CG	2.47	0.45
14:N:214:PRO:HB2	14:N:247:MET:SD	2.56	0.45
15:O:60:ILE:HB	15:O:83:MET:HE1	1.99	0.45
15:O:129:TYR:CD2	15:O:183:CYS:HB3	2.52	0.45
16:P:220:TYR:HA	16:P:223:PHE:CD2	2.51	0.45
16:P:238:GLN:HB3	16:P:326:ASP:OD2	2.17	0.45
20:T:133:ILE:O	20:T:136:GLU:N	2.46	0.45
20:U:118:ILE:HA	36:k:51:TRP:CH2	2.52	0.45
21:V:8:THR:CG2	21:V:9:THR:N	2.79	0.45
22:W:97:ILE:C	22:W:99:VAL:N	2.73	0.45
23:X:9:THR:O	23:X:12:GLU:HB3	2.17	0.45
27:b:20:VAL:HA	55:b:201:3PE:H282	1.99	0.45
30:e:70:TYR:O	30:e:71:LYS:C	2.60	0.45
32:g:64:VAL:HG11	32:g:71:PHE:CE1	2.52	0.45
43:r:109:ASP:O	43:r:110:GLN:CG	2.64	0.45
47:AC:170:VAL:HG13	47:AC:170:VAL:O	2.16	0.45
47:AC:346:PRO:HG3	51:AG:66:GLU:HG2	1.99	0.45
48:AD:234:ASN:O	48:AD:235:PRO:C	2.59	0.45
52:AH:58:ARG:HD3	52:AH:61:THR:HB	1.99	0.45
46:Ab:259:ARG:HB3	46:Ab:444:LEU:CD1	2.41	0.45
47:Ac:245:PHE:CZ	48:Ad:289:GLY:C	2.95	0.45
48:Ad:141:THR:CG2	53:Aj:53:TRP:CZ2	3.00	0.45
50:Af:86:GLU:O	50:Af:87:ASP:C	2.60	0.45
52:Ah:47:ARG:NH1	52:Ah:47:ARG:HB2	2.32	0.45
1:A:4:TYR:HE2	55:A:401:3PE:H231	1.80	0.44
3:C:78:SER:C	3:C:80:LEU:H	2.24	0.44
4:D:78:THR:O	4:D:100:GLU:HB3	2.17	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.31	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
7:G:136:GLU:OE1	17:Q:87:MET:HG3	2.17	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.34	0.44
13:M:187:ASP:H	13:M:192:ASN:ND2	2.15	0.44
14:N:109:ALA:HB3	14:N:110:PRO:HD3	1.99	0.44
15:O:39:GLY:O	15:O:40:LEU:C	2.60	0.44
15:O:230:THR:HG22	15:O:232:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:245:PHE:CE1	15:O:249:MET:HG3	2.52	0.44
15:O:336:GLY:HA2	15:O:344:ASN:HB3	1.99	0.44
16:P:55:VAL:HA	16:P:79:GLN:O	2.18	0.44
16:P:116:ILE:HG21	16:P:152:ILE:HA	1.98	0.44
16:P:245:VAL:HA	16:P:265:PHE:HD2	1.82	0.44
16:P:357:ARG:NH2	16:P:364:SER:O	2.47	0.44
17:Q:77:VAL:CG1	17:Q:101:PHE:CD2	3.00	0.44
23:X:115:LEU:HB3	23:X:117:TRP:CE2	2.52	0.44
24:Y:68:ILE:HD13	24:Y:103:LEU:HB2	1.98	0.44
25:Z:62:ILE:O	25:Z:66:GLU:HG3	2.16	0.44
29:d:11:LEU:HD12	29:d:11:LEU:HA	1.69	0.44
29:d:78:ARG:O	29:d:79:GLN:C	2.59	0.44
33:h:56:VAL:O	33:h:58:LYS:HG3	2.16	0.44
33:h:73:PHE:CE2	33:h:74:TYR:HE1	2.35	0.44
33:h:120:TRP:NE1	33:h:124:ASN:ND2	2.64	0.44
34:i:92:THR:O	41:p:5:TRP:CD1	2.69	0.44
45:AA:139:ASP:O	45:AA:140:LEU:C	2.59	0.44
45:AA:162:GLU:HA	45:AA:165:ARG:NH1	2.32	0.44
45:AA:246:ALA:O	45:AA:249:HIS:O	2.34	0.44
46:AB:39:GLU:O	46:AB:227:HIS:HE1	2.00	0.44
46:AB:418:SER:O	46:AB:419:VAL:C	2.59	0.44
47:AC:107:TYR:HE1	47:AC:308:HIS:HB2	1.82	0.44
47:AC:141:TRP:CH2	49:Ae:223:VAL:HG23	2.52	0.44
48:AD:259:THR:O	48:AD:260:PRO:C	2.60	0.44
71:AD:402:3PH:H352	49:AE:128:ALA:HB1	1.99	0.44
55:AF:201:3PE:H371	51:AG:47:LEU:HD13	2.00	0.44
49:AI:43:LEU:CD1	46:Ab:164:VAL:N	2.80	0.44
45:Aa:68:THR:CG2	46:Ab:384:MET:HG3	2.42	0.44
46:Ab:39:GLU:HG3	46:Ab:227:HIS:ND1	2.32	0.44
46:Ab:173:ILE:HD11	46:Ab:439:ALA:C	2.43	0.44
46:Ab:312:SER:HA	46:Ab:315:LYS:HE3	1.99	0.44
46:Ab:418:SER:O	46:Ab:419:VAL:C	2.59	0.44
47:Ac:211:LEU:HD21	50:Af:37:THR:HA	1.97	0.44
47:Ac:218:ILE:HD11	47:Ac:224:TYR:CE2	2.52	0.44
47:Ac:256:TYR:OH	48:Ad:202:ARG:NH1	2.50	0.44
48:Ad:104:SER:H	53:Aj:48:ASN:ND2	2.15	0.44
48:Ad:167:ARG:HH11	48:Ad:169:GLY:HA2	1.82	0.44
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:94:VAL:HB	4:D:115:LEU:CB	2.48	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:186:PHE:CE2	55:I:301:3PE:H2B1	2.52	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
8:H:293:PHE:CE1	55:I:301:3PE:H32	2.52	0.44
9:I:48:VAL:HG12	27:b:10:LYS:HZ2	1.82	0.44
10:J:54:MET:HE3	10:J:54:MET:HB3	1.70	0.44
12:L:117:PHE:CE1	12:L:243:VAL:CG2	3.00	0.44
12:L:155:ILE:HG12	12:L:248:HIS:CE1	2.53	0.44
12:L:231:PRO:C	12:L:234:PRO:HD2	2.41	0.44
12:L:437:PHE:CZ	12:L:441:ILE:HG12	2.43	0.44
55:L:707:3PE:H261	55:L:707:3PE:H322	1.98	0.44
13:M:43:TRP:HZ2	33:h:122:ALA:HB2	1.82	0.44
14:N:164:MET:HE3	55:Y:201:3PE:C26	2.44	0.44
14:N:239:ALA:CB	29:d:47:MET:HG2	2.48	0.44
15:O:70:LYS:HE3	63:O:402:ADP:O2A	2.17	0.44
15:O:350:LYS:HD3	15:O:351:TRP:N	2.32	0.44
16:P:298:TYR:O	16:P:299:SER:C	2.60	0.44
17:Q:99:MET:HG2	17:Q:128:PHE:HE2	1.82	0.44
19:S:62:GLN:HB2	19:S:80:ASN:CG	2.42	0.44
20:T:79:ILE:O	20:T:83:VAL:HG23	2.17	0.44
20:U:137:LYS:O	34:i:4:TYR:CE2	2.70	0.44
25:Z:94:GLU:HA	25:Z:97:ILE:HG12	1.99	0.44
25:Z:110:VAL:HG11	30:e:72:THR:HG22	1.98	0.44
29:d:108:THR:O	29:d:109:TYR:C	2.60	0.44
33:h:182:SER:HB3	33:h:183:PRO:CD	2.39	0.44
40:o:49:ALA:O	40:o:50:GLN:C	2.60	0.44
45:AA:92:PHE:HE1	45:AA:165:ARG:N	2.14	0.44
45:AA:140:LEU:O	45:AA:141:PRO:C	2.59	0.44
46:AB:84:ARG:NE	49:AI:17:ALA:CB	2.81	0.44
46:AB:305:THR:O	46:AB:311:GLN:HG3	2.17	0.44
47:AC:341:GLN:HE21	47:AC:342:PRO:HD2	1.82	0.44
45:Aa:121:ASN:OD1	46:Ab:300:LYS:HD2	2.17	0.44
45:Aa:275:ILE:HG23	45:Aa:457:ALA:HA	1.99	0.44
47:Ac:213:SER:HA	50:Af:67:LEU:HD11	1.99	0.44
47:Ac:341:GLN:HE21	47:Ac:342:PRO:HD2	1.82	0.44
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CG	2.52	0.44
48:Ad:138:VAL:HG11	48:Ad:276:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:259:THR:O	48:Ad:260:PRO:C	2.61	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.17	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44
3:C:133:SER:O	3:C:133:SER:OG	2.32	0.44
3:C:149:LEU:O	22:W:23:ILE:HD11	2.17	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.51	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.44
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.44
9:I:60:ILE:HG23	55:I:301:3PE:H111	1.99	0.44
12:L:2:ASN:O	12:L:3:ILE:C	2.59	0.44
12:L:54:PHE:CB	12:L:87:ILE:HD11	2.47	0.44
12:L:366:MET:SD	12:L:443:ILE:CG2	3.06	0.44
12:L:526:LEU:CB	12:L:530:PRO:HG2	2.47	0.44
13:M:98:MET:SD	55:M:502:3PE:H3C1	2.57	0.44
13:M:321:LEU:HD23	13:M:321:LEU:HA	1.81	0.44
13:M:415:GLN:O	13:M:416:ARG:CG	2.64	0.44
14:N:208:TYR:O	14:N:212:THR:HG22	2.18	0.44
14:N:250:SER:O	14:N:259:GLY:HA3	2.17	0.44
15:O:342:GLY:HA3	28:c:36:ASN:OD1	2.18	0.44
15:O:351:TRP:O	15:O:355:LYS:HG2	2.16	0.44
16:P:168:SER:O	16:P:202:ARG:HA	2.17	0.44
17:Q:62:THR:HG22	17:Q:141:ASN:O	2.18	0.44
19:S:20:ARG:HG3	19:S:54:LEU:CB	2.43	0.44
19:S:83:SER:O	19:S:87:VAL:HG23	2.17	0.44
20:U:106:LYS:HE2	20:U:106:LYS:HB3	1.79	0.44
24:Y:88:ASP:H	24:Y:128:LYS:HZ3	1.64	0.44
31:f:3:LEU:O	31:f:4:PHE:C	2.60	0.44
33:h:55:PHE:C	33:h:55:PHE:CD1	2.94	0.44
33:h:87:THR:HG22	62:h:201:CDL:C51	2.46	0.44
40:o:110:GLN:O	40:o:111:ARG:C	2.59	0.44
45:AA:286:HIS:CG	45:AA:359:VAL:HG22	2.51	0.44
45:AA:311:ILE:CG2	45:AA:341:PHE:CZ	3.01	0.44
46:AB:426:LYS:HA	46:AB:429:LYS:HZ3	1.82	0.44
49:AE:178:HIS:NE2	49:AE:209:GLU:HB2	2.33	0.44
49:AE:217:CYS:C	49:AE:219:HIS:N	2.72	0.44
45:Aa:442:ARG:NH1	54:Ak:16:ASN:HD21	2.15	0.44
47:Ac:165:TRP:CE3	47:Ac:169:SER:HA	2.52	0.44
47:Ac:312:GLN:HG2	50:Af:37:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:195:PRO:O	48:Ad:196:ASP:C	2.58	0.44
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD1	2.53	0.44
54:Ak:42:LEU:HD22	54:Ak:48:ILE:CD1	2.47	0.44
54:Ak:45:VAL:HB	54:Ak:48:ILE:CD1	2.48	0.44
1:A:48:ARG:C	1:A:49:LEU:HD22	2.43	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:284:GLU:OE2	17:Q:84:ARG:NH2	2.51	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
10:J:3:ASN:HD22	10:J:120:LEU:HD12	1.83	0.44
10:J:121:GLY:O	25:Z:133:MET:CE	2.65	0.44
10:J:150:TRP:CZ3	55:J:202:3PE:H251	2.52	0.44
12:L:537:THR:N	12:L:538:PRO:HD2	2.32	0.44
13:M:154:LEU:HD22	14:N:287:LEU:HD21	2.00	0.44
13:M:177:MET:HB3	33:h:140:LEU:HD21	2.00	0.44
13:M:200:MET:HE2	13:M:250:LEU:HD21	2.00	0.44
55:M:502:3PE:H242	29:d:47:MET:HE1	1.99	0.44
14:N:193:ILE:HD13	14:N:200:LEU:HB2	1.99	0.44
15:O:211:VAL:N	15:O:212:PRO:CD	2.80	0.44
16:P:305:PHE:CB	16:P:314:THR:HG22	2.47	0.44
23:X:137:LEU:HA	23:X:138:PRO:HD3	1.85	0.44
24:Y:120:MET:HE2	24:Y:120:MET:HB3	1.90	0.44
25:Z:131:GLU:O	25:Z:134:SER:N	2.51	0.44
62:a:101:CDL:CA2	42:q:6:VAL:HG13	2.47	0.44
34:i:19:ARG:HH11	39:n:173:ARG:NH2	2.16	0.44
37:l:30:PHE:CD2	37:l:31:HIS:CE1	3.00	0.44
38:m:32:ALA:O	38:m:35:GLU:N	2.48	0.44
43:r:109:ASP:OD1	43:r:110:GLN:N	2.51	0.44
45:AA:410:CYS:O	45:AA:411:GLU:C	2.59	0.44
46:AB:64:PHE:HZ	46:AB:394:SER:HA	1.83	0.44
47:AC:19:ILE:HG23	47:AC:221:HIS:CB	2.48	0.44
48:AD:219:CYS:SG	48:AD:220:GLU:N	2.90	0.44
49:AE:161:GLU:HA	49:AE:178:HIS:CB	2.48	0.44
49:AE:243:TYR:CD2	49:AE:258:LEU:HG	2.52	0.44
51:AG:72:ARG:NH1	52:AH:71:ASP:OD2	2.50	0.44
45:Aa:377:MET:HG3	45:Aa:477:TRP:NE1	2.32	0.44
45:Aa:406:THR:O	45:Aa:407:THR:C	2.58	0.44
48:Ad:201:VAL:HG22	48:Ad:278:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:248:ILE:HD12	48:Ad:266:VAL:HG11	2.00	0.44
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.53	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.31	0.44
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.32	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
7:G:32:ILE:CG2	7:G:98:LYS:HD2	2.47	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:93:HIS:NE2	26:a:27:HIS:ND1	2.66	0.44
11:K:33:LEU:HA	11:K:36:MET:HE2	2.00	0.44
11:K:73:VAL:CG2	14:N:38:LEU:HD22	2.47	0.44
12:L:152:PHE:HD2	12:L:153:LEU:HD12	1.83	0.44
12:L:482:MET:HE2	12:L:486:LEU:CB	2.45	0.44
62:L:705:CDL:H531	62:L:705:CDL:H212	2.00	0.44
13:M:22:LYS:HG2	13:M:26:ASN:ND2	2.33	0.44
13:M:24:TRP:CE3	13:M:81:GLN:HG2	2.52	0.44
13:M:424:ILE:O	13:M:424:ILE:CG2	2.65	0.44
14:N:87:GLN:O	14:N:88:GLN:C	2.59	0.44
14:N:175:MET:HE1	14:N:296:LEU:HD13	1.98	0.44
14:N:309:ASN:N	15:O:317:ILE:O	2.48	0.44
15:O:200:PRO:HG3	15:O:282:PRO:CD	2.47	0.44
15:O:262:GLU:HB3	15:O:268:LYS:NZ	2.33	0.44
26:a:43:TYR:O	26:a:47:LEU:HD13	2.18	0.44
26:a:62:VAL:HG23	26:a:62:VAL:O	2.18	0.44
30:e:96:PRO:C	30:e:99:SER:H	2.25	0.44
38:m:24:ASP:OD2	45:Aa:264:GLY:N	2.51	0.44
40:o:13:ALA:C	40:o:15:VAL:H	2.25	0.44
42:q:74:PHE:HD2	42:q:75:TRP:CD1	2.33	0.44
43:r:5:THR:HG22	43:r:5:THR:O	2.18	0.44
45:AA:389:THR:O	45:AA:390:ARG:C	2.59	0.44
48:AD:161:ASP:HB3	48:AD:163:GLU:HB2	2.00	0.44
50:AF:86:GLU:O	50:AF:87:ASP:C	2.60	0.44
49:AI:63:PRO:HB3	46:Ab:328:ALA:CB	2.48	0.44
45:Aa:247:GLN:O	45:Aa:251:SER:HB2	2.18	0.44
48:Ad:322:ARG:O	51:Ag:13:HIS:HB3	2.17	0.44
49:Ae:243:TYR:CD2	49:Ae:258:LEU:HG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:32:ARG:O	52:Ah:33:GLU:C	2.61	0.44
3:C:101:ASP:OD1	21:V:86:LYS:HE3	2.16	0.44
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.44
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.98	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:177:GLY:O	59:E:301:FES:S1	2.75	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
8:H:121:TRP:HZ3	10:J:27:TYR:OH	1.96	0.44
8:H:203:GLY:C	8:H:205:SER:N	2.76	0.44
8:H:277:TYR:CE2	55:I:301:3PE:H271	2.53	0.44
10:J:104:CYS:O	10:J:108:TYR:N	2.46	0.44
12:L:526:LEU:HD12	12:L:526:LEU:N	2.32	0.44
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.44
13:M:18:SER:OG	13:M:26:ASN:ND2	2.51	0.44
13:M:42:LEU:CD1	13:M:67:ILE:CD1	2.96	0.44
13:M:123:GLU:CB	14:N:255:PRO:HG2	2.44	0.44
13:M:263:LEU:CD2	38:m:105:PHE:HD2	2.31	0.44
14:N:122:ILE:HD11	14:N:127:GLY:HA2	1.99	0.44
14:N:239:ALA:HA	29:d:47:MET:HE2	1.99	0.44
15:O:238:GLU:HG3	15:O:242:LYS:HD3	1.99	0.44
15:O:272:ASP:O	15:O:275:TYR:HB2	2.18	0.44
16:P:345:LEU:C	16:P:345:LEU:HD23	2.43	0.44
20:U:104:PHE:O	20:U:108:LEU:HB2	2.18	0.44
22:W:20:VAL:HG21	22:W:80:ARG:CZ	2.48	0.44
23:X:30:HIS:CE1	25:Z:63:GLU:HG3	2.51	0.44
24:Y:7:PHE:CZ	24:Y:26:ILE:HG12	2.52	0.44
24:Y:141:PRO:HB2	33:h:161:ARG:NH1	2.33	0.44
55:Y:201:3PE:H31	55:Y:201:3PE:H112	1.98	0.44
29:d:27:ASN:O	29:d:28:ASP:C	2.61	0.44
29:d:93:TYR:CD2	33:h:156:VAL:HG13	2.53	0.44
30:e:91:LYS:NZ	30:e:91:LYS:HB3	2.32	0.44
33:h:179:ILE:HB	33:h:181:HIS:CE1	2.52	0.44
46:AB:214:THR:OG1	46:AB:243:GLY:O	2.35	0.44
48:AD:312:SER:O	48:AD:313:VAL:C	2.59	0.44
71:AD:402:3PH:H252	71:AD:402:3PH:H281	1.52	0.44
49:AE:161:GLU:HA	49:AE:178:HIS:HB3	1.99	0.44
49:AE:178:HIS:HA	49:AE:209:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:169:LEU:O	45:Aa:173:GLN:HG3	2.18	0.44
47:Ac:33:PHE:HE1	62:Ag:101:CDL:H782	1.82	0.44
47:Ac:317:PHE:HB3	50:Af:27:PHE:HD2	1.83	0.44
49:Ae:161:GLU:HA	49:Ae:178:HIS:HB3	2.00	0.44
54:Ak:15:ARG:HB2	54:Ak:15:ARG:CZ	2.48	0.44
1:A:48:ARG:HD3	10:J:76:GLU:OE1	2.18	0.44
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.48	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.47	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
12:L:231:PRO:CG	12:L:529:PHE:CD2	3.00	0.44
12:L:231:PRO:HG2	12:L:529:PHE:CD2	2.52	0.44
13:M:29:SER:HB3	32:g:91:PHE:CE2	2.50	0.44
13:M:446:LEU:CD1	32:g:97:LEU:HD12	2.47	0.44
13:M:450:SER:HB3	55:M:501:3PE:H32	2.00	0.44
14:N:227:ILE:HG13	14:N:228:ASN:N	2.32	0.44
14:N:281:LEU:HD23	55:N:401:3PE:H281	1.84	0.44
16:P:310:PHE:O	16:P:311:GLU:C	2.59	0.44
22:W:58:THR:HB	22:W:61:GLN:H	1.82	0.44
24:Y:12:HIS:CD2	24:Y:131:LYS:HE2	2.53	0.44
28:c:33:GLU:CD	28:c:33:GLU:H	2.26	0.44
28:c:61:THR:HG22	28:c:65:ASP:OD2	2.18	0.44
29:d:57:GLY:O	29:d:60:ARG:N	2.51	0.44
41:p:140:GLN:HG2	41:p:144:LEU:CD1	2.47	0.44
46:AB:312:SER:HA	46:AB:315:LYS:HE3	1.99	0.44
47:AC:72:ASP:OD1	48:AD:133:ARG:NH1	2.51	0.44
47:AC:152:ALA:O	47:AC:153:ILE:C	2.58	0.44
49:AE:91:TYR:CD1	51:AG:28:PRO:HG2	2.52	0.44
45:Aa:78:GLY:H	45:Aa:81:TYR:HD2	1.65	0.44
45:Aa:212:SER:O	45:Aa:215:ASP:N	2.50	0.44
69:Ac:406:UQ6:H172	69:Ac:406:UQ6:H151	1.54	0.44
48:Ad:170:LYS:NZ	49:Ae:151:LYS:CD	2.80	0.44
49:Ae:178:HIS:HA	49:Ae:209:GLU:O	2.18	0.44
3:C:130:ASN:ND2	3:C:141:ARG:HE	2.13	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.47	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.44
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.44
8:H:196:ALA:C	8:H:198:PHE:N	2.75	0.44
58:I:302:PC1:H112	25:Z:29:GLY:CA	2.45	0.44
12:L:529:PHE:O	12:L:533:ILE:HG22	2.17	0.44
55:L:703:3PE:H331	55:L:703:3PE:H362	1.64	0.44
13:M:8:SER:O	13:M:11:LEU:HB2	2.18	0.44
13:M:186:LEU:HD13	13:M:250:LEU:HA	2.00	0.44
13:M:264:LEU:HD23	38:m:98:LEU:CD1	2.47	0.44
13:M:344:MET:HE3	13:M:423:MET:CE	2.48	0.44
14:N:31:VAL:C	14:N:35:PHE:CD2	2.91	0.44
15:O:132:GLN:HE22	63:O:402:ADP:HN62	1.66	0.44
16:P:64:PHE:CE1	16:P:209:ARG:O	2.69	0.44
17:Q:77:VAL:HG21	17:Q:99:MET:CE	2.48	0.44
24:Y:7:PHE:O	24:Y:8:PHE:C	2.61	0.44
25:Z:97:ILE:HG13	25:Z:98:MET:N	2.30	0.44
29:d:101:PHE:CZ	33:h:156:VAL:HG22	2.53	0.44
29:d:101:PHE:CZ	33:h:159:LEU:HD22	2.52	0.44
30:e:50:THR:HB	33:h:164:GLY:HA3	1.99	0.44
39:n:150:MET:HE2	39:n:150:MET:HB3	1.87	0.44
45:AA:93:LEU:HD21	45:AA:156:LEU:HD11	1.99	0.44
46:AB:138:LEU:CD1	46:AB:233:VAL:HB	2.47	0.44
46:AB:180:VAL:O	46:AB:254:ARG:HG3	2.18	0.44
46:AB:233:VAL:HA	46:AB:236:GLN:CG	2.47	0.44
47:AC:15:ASN:OD1	47:AC:19:ILE:HB	2.18	0.44
48:AD:321:TYR:HB2	50:AF:61:PHE:CE2	2.53	0.44
49:AE:122:THR:O	49:AE:123:VAL:C	2.61	0.44
49:Ae:161:GLU:HA	49:Ae:178:HIS:CB	2.48	0.44
49:Ae:263:TYR:HB2	49:Ae:271:VAL:HG11	1.97	0.44
1:A:105:GLU:OE2	1:A:110:GLY:HA3	2.18	0.44
2:B:114:MET:SD	2:B:121:PHE:HA	2.58	0.44
58:B:303:PC1:H133	58:B:303:PC1:H111	1.72	0.44
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.44
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
10:J:84:SER:HG	10:J:87:LEU:HB3	1.83	0.44
11:K:57:MET:O	11:K:60:PRO:HD2	2.18	0.44
12:L:55:PHE:HB2	40:o:74:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:68:TRP:HE3	12:L:76:LEU:HD21	1.83	0.44
12:L:556:ILE:CG2	38:m:80:PHE:CE2	3.00	0.44
13:M:126:LEU:HD11	13:M:153:THR:HG21	2.00	0.44
13:M:165:ILE:HD11	14:N:264:TRP:HE1	1.83	0.44
15:O:148:GLU:HG3	15:O:295:ARG:NH1	2.33	0.44
16:P:72:HIS:HB2	16:P:250:VAL:HG21	2.00	0.44
16:P:169:HIS:CD2	16:P:181:LEU:HD11	2.49	0.44
24:Y:89:PRO:HG3	24:Y:129:ILE:HG12	1.99	0.44
25:Z:89:GLU:OE1	30:e:97:HIS:ND1	2.51	0.44
33:h:83:ILE:HG12	62:h:201:CDL:H561	2.00	0.44
34:i:5:THR:O	34:i:6:PRO:C	2.57	0.44
34:i:95:TYR:HE1	41:p:116:ARG:HH22	1.66	0.44
37:l:41:TYR:HD2	37:l:43:ARG:HD3	1.82	0.44
37:l:142:PHE:O	37:l:145:TRP:N	2.51	0.44
40:o:39:MET:HE1	40:o:57:ASP:O	2.17	0.44
42:q:21:ARG:HD2	42:q:21:ARG:HA	1.80	0.44
45:AA:172:MET:HE1	45:AA:205:SER:HA	2.00	0.44
48:AD:112:ARG:HB3	48:AD:255:TYR:CE1	2.53	0.44
48:AD:167:ARG:NH1	48:AD:169:GLY:HA2	2.32	0.44
48:AD:189:ASN:ND2	48:AD:194:PRO:HG3	2.33	0.44
51:AG:25:ARG:NH2	51:AG:29:SER:H	2.16	0.44
46:Ab:63:LEU:HD12	46:Ab:220:LEU:HD13	2.00	0.44
46:Ab:297:PRO:HB3	46:Ab:303:ASN:HD22	1.83	0.44
49:Ae:217:CYS:C	49:Ae:219:HIS:N	2.72	0.44
50:Af:97:GLU:HA	50:Af:100:ARG:NH1	2.33	0.44
5:E:140:MET:HE1	6:F:366:ALA:HA	2.00	0.43
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.43
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.43
10:J:30:LEU:O	10:J:34:VAL:HG23	2.17	0.43
12:L:305:SER:OG	12:L:336:LYS:HE2	2.18	0.43
12:L:537:THR:HG21	55:L:703:3PE:H352	2.00	0.43
13:M:46:ASP:OD1	13:M:47:GLU:N	2.50	0.43
14:N:164:MET:HE3	55:Y:201:3PE:H261	2.00	0.43
14:N:193:ILE:CD1	14:N:200:LEU:CD2	2.96	0.43
55:N:401:3PE:H231	55:N:401:3PE:H262	1.87	0.43
16:P:126:VAL:HG23	16:P:161:VAL:HG11	2.00	0.43
16:P:197:GLU:HB3	16:P:259:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:91:VAL:HG22	17:Q:91:VAL:O	2.18	0.43
20:T:92:LYS:O	20:T:92:LYS:HG2	2.16	0.43
22:W:47:PRO:HG3	22:W:63:ARG:NH2	2.26	0.43
24:Y:26:ILE:O	24:Y:30:LEU:HG	2.17	0.43
24:Y:83:ARG:O	24:Y:84:GLU:HB3	2.18	0.43
25:Z:68:ARG:HG3	25:Z:69:ILE:N	2.33	0.43
41:p:165:GLU:C	41:p:167:ARG:H	2.26	0.43
45:AA:71:VAL:HG21	45:AA:140:LEU:CD1	2.48	0.43
45:AA:78:GLY:H	45:AA:81:TYR:HD2	1.65	0.43
45:AA:225:LYS:HG3	45:AA:256:VAL:HG12	2.00	0.43
46:AB:54:ASN:OD1	46:AB:224:GLY:HA2	2.18	0.43
46:AB:411:THR:O	46:AB:414:GLN:HG2	2.18	0.43
48:AD:186:ARG:HE	48:AD:193:LEU:HB2	1.80	0.43
48:AD:262:THR:O	48:AD:263:MET:C	2.61	0.43
48:AD:288:MET:HE2	71:AD:402:3PH:H11	2.00	0.43
49:AE:173:PRO:HG2	49:AE:223:VAL:CG2	2.45	0.43
46:Ab:282:GLU:OE2	46:Ab:430:LYS:HD2	2.18	0.43
47:Ac:170:VAL:HG13	47:Ac:170:VAL:O	2.16	0.43
49:Ae:145:ASP:O	49:Ae:149:MET:HG3	2.17	0.43
49:Ae:195:LEU:HD13	49:Ae:248:ARG:HD2	1.99	0.43
1:A:4:TYR:O	1:A:5:THR:C	2.61	0.43
2:B:121:PHE:HZ	2:B:122:ARG:HH21	1.65	0.43
2:B:122:ARG:HH11	4:D:89:PRO:CA	2.30	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
4:D:41:ILE:HD11	32:g:53:TRP:HB3	2.00	0.43
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.43
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.83	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:128:SER:HA	8:H:210:GLY:O	2.18	0.43
11:K:26:LEU:HG	11:K:30:LEU:HD13	1.98	0.43
11:K:66:PHE:CZ	14:N:35:PHE:CE2	2.97	0.43
12:L:226:GLN:OE1	12:L:284:THR:CG2	2.66	0.43
55:L:703:3PE:C2G	55:L:704:3PE:H3I1	2.40	0.43
13:M:1:MET:HB3	13:M:1:MET:HE3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:TYR:CZ	13:M:457:LEU:HD11	2.52	0.43
14:N:12:THR:CG2	14:N:39:ALA:HB2	2.48	0.43
14:N:166:ALA:HB1	14:N:288:LEU:HB3	1.99	0.43
14:N:265:ILE:HD12	14:N:344:ILE:HG21	2.00	0.43
17:Q:59:LEU:O	17:Q:140:LYS:HA	2.18	0.43
23:X:35:GLN:HB2	23:X:70:PHE:CD1	2.53	0.43
28:c:40:ASN:O	28:c:43:ALA:N	2.50	0.43
30:e:87:MET:HE3	30:e:94:PRO:HD3	2.00	0.43
47:AC:71:ARG:NH2	48:AD:277:ALA:O	2.51	0.43
47:AC:287:LYS:NZ	49:Ae:255:PRO:CG	2.81	0.43
49:AE:235:TYR:CE1	49:AE:240:GLY:HA2	2.53	0.43
45:Aa:157:GLU:O	45:Aa:160:GLN:N	2.51	0.43
47:Ac:77:TRP:CD2	48:Ad:281:GLU:HG3	2.52	0.43
48:Ad:112:ARG:HB3	48:Ad:255:TYR:CE1	2.53	0.43
51:Ag:19:LEU:HG	51:Ag:20:SER:N	2.33	0.43
53:Aj:18:THR:HG22	54:Ak:24:TRP:HH2	1.83	0.43
1:A:106:TRP:CH2	8:H:295:PRO:HG2	2.53	0.43
4:D:97:LEU:HD21	4:D:109:CYS:HB3	1.99	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
12:L:22:SER:HA	12:L:27:ILE:HG21	2.00	0.43
12:L:136:ASN:HD21	62:h:201:CDL:C27	2.18	0.43
12:L:309:GLN:HB2	12:L:336:LYS:HZ1	1.83	0.43
13:M:307:TRP:HB2	38:m:129:TYR:O	2.19	0.43
13:M:423:MET:C	13:M:424:ILE:O	2.56	0.43
13:M:452:LYS:HA	13:M:455:THR:CG2	2.48	0.43
20:T:113:LEU:O	20:T:116:VAL:HB	2.17	0.43
21:V:19:THR:N	21:V:20:PRO:CD	2.81	0.43
23:X:66:CYS:O	23:X:67:ALA:C	2.61	0.43
24:Y:19:GLN:OE1	24:Y:19:GLN:HA	2.17	0.43
27:b:82:LYS:HB3	27:b:82:LYS:HE2	1.81	0.43
29:d:72:GLY:O	29:d:73:TYR:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:95:TYR:OH	41:p:11:PRO:O	2.34	0.43
45:AA:178:SER:O	45:AA:179:MET:C	2.60	0.43
45:AA:371:PHE:CZ	45:AA:375:GLN:NE2	2.74	0.43
45:AA:392:LYS:O	45:AA:396:ARG:HG3	2.18	0.43
45:AA:401:SER:O	45:AA:404:ASP:N	2.51	0.43
47:AC:171:ASP:CG	47:AC:172:LYS:N	2.76	0.43
47:AC:181:PHE:HA	47:AC:184:ILE:HG22	2.00	0.43
48:AD:270:VAL:HG21	70:AD:401:HEC:CBB	2.39	0.43
50:AF:97:GLU:HA	50:AF:100:ARG:NH1	2.33	0.43
46:Ab:97:PHE:CE2	46:Ab:101:ARG:HG3	2.53	0.43
46:Ab:297:PRO:CB	46:Ab:303:ASN:HD22	2.30	0.43
48:Ad:307:LYS:O	48:Ad:311:TRP:HB2	2.19	0.43
2:B:96:GLY:CA	57:B:302:UQ1:HM52	2.49	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
9:I:35:THR:HG22	43:r:107:SER:HA	1.97	0.43
10:J:85:ASN:OD1	58:J:201:PC1:C31	2.67	0.43
11:K:32:CYS:O	11:K:33:LEU:C	2.59	0.43
12:L:53:MET:HE2	12:L:53:MET:HB3	1.78	0.43
12:L:92:VAL:HG21	12:L:330:CYS:HB3	2.00	0.43
12:L:283:LEU:CD1	37:l:140:MET:HE2	2.48	0.43
12:L:296:ASN:ND2	12:L:357:ARG:NE	2.67	0.43
13:M:348:LEU:O	13:M:349:GLN:C	2.60	0.43
13:M:353:PRO:HG3	33:h:61:LEU:CD2	2.48	0.43
14:N:29:MET:HE1	14:N:141:ILE:HA	2.01	0.43
15:O:214:VAL:O	15:O:218:ILE:HG13	2.18	0.43
16:P:164:PHE:HE2	16:P:166:HIS:HB2	1.82	0.43
16:P:170:LEU:O	16:P:171:ASN:CG	2.61	0.43
17:Q:101:PHE:CE1	17:Q:124:MET:HE3	2.53	0.43
19:S:16:LEU:HD21	19:S:95:LEU:HG	2.00	0.43
22:W:23:ILE:HG22	22:W:24:PHE:HD2	1.81	0.43
23:X:39:THR:HG23	23:X:40:ASN:N	2.33	0.43
23:X:145:ARG:HG2	23:X:146:ALA:O	2.18	0.43
24:Y:19:GLN:O	24:Y:23:LYS:HG2	2.19	0.43
32:g:58:GLU:CD	32:g:59:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:89:PHE:HB3	33:h:74:TYR:HD2	1.84	0.43
39:n:131:GLU:O	39:n:131:GLU:HG2	2.17	0.43
39:n:163:LEU:HA	39:n:164:PRO:HD2	1.75	0.43
41:p:103:MET:HE1	41:p:135:VAL:HG12	1.98	0.43
46:AB:63:LEU:HD12	46:AB:220:LEU:HD13	2.00	0.43
46:AB:155:ARG:HD2	46:AB:198:GLY:H	1.82	0.43
46:AB:378:LEU:HD23	46:AB:416:ILE:CG2	2.49	0.43
69:AC:405:UQ6:H72	69:AC:405:UQ6:H1M3	1.83	0.43
49:AI:62:ARG:HH12	46:Ab:290:GLN:HE22	1.66	0.43
45:Aa:151:VAL:HG21	45:Aa:250:LEU:HD21	2.00	0.43
46:Ab:130:ILE:HA	46:Ab:133:LEU:HB2	2.00	0.43
48:Ad:321:TYR:HB2	50:Af:61:PHE:CG	2.53	0.43
49:Ae:155:LYS:HB3	49:Ae:158:ASP:OD2	2.19	0.43
49:Ae:178:HIS:NE2	49:Ae:209:GLU:HB2	2.33	0.43
51:Ag:25:ARG:NH2	51:Ag:29:SER:H	2.16	0.43
52:Ah:54:ARG:O	52:Ah:58:ARG:N	2.46	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
1:A:63:LEU:HD21	10:J:63:MET:CA	2.47	0.43
3:C:167:ARG:CZ	3:C:186:ILE:HG22	2.49	0.43
4:D:279:THR:CG2	21:V:13:GLY:HA3	2.26	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.01	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.00	0.43
6:F:44:ASN:HB2	6:F:59:ARG:HD3	1.99	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.43
8:H:303:TRP:HB2	27:b:25:VAL:CG1	2.49	0.43
11:K:93:LEU:CD2	14:N:57:THR:HG21	2.47	0.43
12:L:70:THR:O	12:L:75:GLU:HA	2.17	0.43
12:L:81:LYS:HD3	12:L:262:ARG:NH1	2.34	0.43
13:M:63:THR:N	13:M:64:PRO:CD	2.81	0.43
13:M:304:GLN:HA	13:M:309:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:120:GLN:CG	14:N:177:LYS:HE3	2.47	0.43
14:N:240:MET:O	14:N:240:MET:HG2	2.18	0.43
14:N:254:LEU:HA	14:N:255:PRO:HD3	1.60	0.43
14:N:279:ALA:HA	14:N:282:MET:HE2	2.00	0.43
15:O:239:ASN:HA	15:O:242:LYS:HE2	2.01	0.43
15:O:332:ARG:O	15:O:338:LYS:HA	2.19	0.43
16:P:81:ILE:HD13	18:R:46:VAL:HG11	2.00	0.43
16:P:135:GLU:HG3	16:P:140:ASP:HA	2.00	0.43
20:U:105:MET:HG3	20:U:139:MET:HE3	1.98	0.43
21:V:56:LEU:CD1	21:V:57:ASP:OD1	2.67	0.43
23:X:151:ASN:CB	23:X:152:PRO:HD2	2.39	0.43
62:a:101:CDL:H311	42:q:7:LEU:CD2	2.49	0.43
27:b:42:ALA:HA	27:b:45:ILE:HG22	2.01	0.43
29:d:93:TYR:OH	33:h:163:ARG:HD2	2.18	0.43
40:o:59:CYS:SG	40:o:90:CYS:C	3.01	0.43
48:AD:157:GLY:O	48:AD:164:MET:HA	2.18	0.43
49:AE:195:LEU:HD13	49:AE:248:ARG:HD2	1.99	0.43
46:Ab:236:GLN:HG3	46:Ab:237:PHE:CD2	2.53	0.43
46:Ab:411:THR:O	46:Ab:414:GLN:HG2	2.18	0.43
48:Ad:247:PRO:HB3	70:Ad:401:HEC:CHC	2.48	0.43
49:Ae:222:CYS:HB2	49:Ae:236:CYS:SG	2.59	0.43
49:Ae:263:TYR:CA	49:Ae:273:VAL:HG22	2.47	0.43
54:Ak:7:GLY:O	54:Ak:11:ARG:HD3	2.18	0.43
1:A:56:PHE:HD1	10:J:70:THR:HG1	1.60	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
4:D:36:GLN:NE2	4:D:38:GLN:NE2	2.62	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:279:THR:HG23	21:V:13:GLY:CA	2.26	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.43
8:H:134:ARG:HH21	8:H:200:LEU:CD1	2.32	0.43
9:I:78:PHE:HB3	43:r:8:ILE:HG22	1.99	0.43
12:L:246:LEU:HD12	12:L:247:LEU:CB	2.49	0.43
12:L:327:LEU:HD21	12:L:472:ILE:HD13	2.00	0.43
12:L:427:ILE:HG13	12:L:428:TYR:N	2.33	0.43
55:L:707:3PE:H251	14:N:288:LEU:CD1	2.48	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.19	0.43
13:M:207:MET:SD	13:M:240:SER:CA	3.06	0.43
14:N:120:GLN:CG	14:N:177:LYS:HG3	2.48	0.43
14:N:150:ASN:ND2	14:N:152:THR:OG1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:203:ALA:CB	15:O:254:GLU:HB3	2.48	0.43
16:P:76:MET:HE1	16:P:254:LYS:HE2	2.01	0.43
16:P:269:ASN:ND2	16:P:271:TYR:OH	2.51	0.43
20:U:72:PRO:HD3	35:j:42:PRO:HG3	1.99	0.43
20:U:113:LEU:HD11	39:n:20:TYR:CD1	2.53	0.43
21:V:36:LYS:HA	21:V:36:LYS:HD3	1.89	0.43
23:X:50:GLU:OE1	23:X:55:ARG:HB3	2.18	0.43
25:Z:53:TRP:CE2	25:Z:57:ARG:HD2	2.53	0.43
25:Z:62:ILE:CG1	27:b:49:THR:HG22	2.48	0.43
27:b:53:TYR:HA	27:b:54:PRO:HD3	1.92	0.43
29:d:78:ARG:HG2	29:d:82:LEU:HD23	2.00	0.43
29:d:94:ILE:HD13	33:h:152:LYS:HE3	2.01	0.43
30:e:72:THR:O	30:e:73:MET:C	2.60	0.43
33:h:127:ASP:OD1	33:h:127:ASP:C	2.60	0.43
34:i:18:LEU:HD22	39:n:125:TRP:CH2	2.54	0.43
39:n:94:TYR:HB3	39:n:178:PRO:HD2	2.01	0.43
40:o:17:PRO:HG3	40:o:106:ARG:CA	2.45	0.43
45:AA:183:VAL:HG21	45:AA:286:HIS:CB	2.48	0.43
55:AF:201:3PE:H381	55:AF:201:3PE:H351	1.70	0.43
45:Aa:57:LEU:N	45:Aa:226:ALA:O	2.52	0.43
45:Aa:339:GLN:OE1	45:Aa:339:GLN:N	2.51	0.43
62:Aa:501:CDL:H121	55:Ac:401:3PE:H221	2.00	0.43
46:Ab:378:LEU:HD23	46:Ab:416:ILE:CG2	2.49	0.43
47:Ac:377:LEU:HB3	50:Af:34:ARG:HD2	1.99	0.43
49:Ae:93:ARG:CD	49:Ae:110:ARG:HD2	2.28	0.43
49:Ae:143:SER:HB2	49:Ae:145:ASP:OD1	2.19	0.43
1:A:52:SER:O	1:A:55:PHE:N	2.51	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.43
10:J:67:PHE:O	10:J:68:GLY:C	2.59	0.43
10:J:128:VAL:O	10:J:129:ASP:C	2.60	0.43
10:J:135:LEU:HG	10:J:135:LEU:O	2.18	0.43
11:K:5:PHE:CE1	11:K:47:THR:HG23	2.53	0.43
12:L:193:MET:HE1	38:m:125:PHE:CD2	2.54	0.43
12:L:446:ASN:O	12:L:447:ASP:C	2.57	0.43
12:L:532:ILE:HG13	37:l:126:TRP:CH2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:569:LEU:CD1	62:L:706:CDL:H131	2.49	0.43
55:L:703:3PE:H2G1	55:L:704:3PE:C3I	2.41	0.43
13:M:73:LEU:HD23	13:M:103:GLN:HE22	1.84	0.43
13:M:119:TYR:HD1	13:M:160:LEU:HD22	1.80	0.43
14:N:11:PHE:O	14:N:15:LEU:N	2.49	0.43
15:O:303:GLU:O	15:O:304:VAL:C	2.59	0.43
16:P:280:ILE:HG23	16:P:353:LEU:HD22	2.00	0.43
17:Q:99:MET:O	17:Q:99:MET:HG3	2.18	0.43
20:U:87:LEU:HB2	20:U:98:LEU:CD1	2.49	0.43
22:W:36:ARG:O	22:W:39:TYR:N	2.51	0.43
26:a:37:ARG:H	26:a:59:ARG:NH2	2.17	0.43
37:l:97:LEU:O	37:l:98:ARG:C	2.60	0.43
38:m:17:THR:O	38:m:18:LEU:HB3	2.17	0.43
38:m:45:ARG:O	38:m:45:ARG:CG	2.61	0.43
44:s:87:LEU:HD23	44:s:87:LEU:HA	1.84	0.43
45:AA:271:THR:HG22	45:AA:273:SER:OG	2.18	0.43
49:AE:155:LYS:HE2	49:AE:157:SER:HB3	1.99	0.43
49:AE:220:LEU:C	47:Ac:148:ASN:HD22	2.26	0.43
49:AE:222:CYS:HB2	49:AE:236:CYS:SG	2.59	0.43
50:AF:109:ALA:HB1	54:Ak:9:ARG:HH21	1.84	0.43
45:Aa:175:ASN:C	45:Aa:177:ALA:N	2.76	0.43
46:Ab:92:LYS:HA	46:Ab:145:GLU:OE1	2.18	0.43
52:Ah:27:PRO:HB3	52:Ah:87:ASN:ND2	2.34	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
3:C:78:SER:C	3:C:80:LEU:N	2.76	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:148:GLU:O	4:D:149:GLN:C	2.62	0.43
4:D:279:THR:HA	21:V:12:VAL:CG1	2.49	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.43
7:G:651:PRO:HB3	19:S:58:CYS:HA	2.01	0.43
9:I:162:CYS:SG	56:I:304:SF4:S2	3.17	0.43
10:J:124:LEU:CD2	25:Z:138:PHE:CE1	3.02	0.43
12:L:496:LEU:CD1	12:L:497:GLY:N	2.73	0.43
12:L:569:LEU:CB	24:Y:115:MET:HE1	2.27	0.43
13:M:231:LEU:CD1	13:M:235:LEU:CD1	2.85	0.43
13:M:263:LEU:CD1	38:m:102:TYR:CD1	2.99	0.43
14:N:12:THR:HG22	14:N:39:ALA:HB2	2.00	0.43
14:N:39:ALA:O	14:N:42:PRO:HD2	2.18	0.43
14:N:219:LEU:CD2	14:N:230:ILE:HD12	2.49	0.43
16:P:81:ILE:HD11	18:R:46:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:315:THR:O	16:P:316:LYS:C	2.57	0.43
17:Q:59:LEU:HD23	17:Q:59:LEU:HA	1.84	0.43
20:T:93:ILE:HD11	20:T:118:ILE:HD11	2.00	0.43
20:U:142:GLN:O	20:U:143:GLU:C	2.60	0.43
21:V:8:THR:HG22	21:V:9:THR:N	2.34	0.43
22:W:25:SER:OG	22:W:34:ARG:NH2	2.52	0.43
29:d:120:ARG:O	38:m:109:ARG:NH2	2.52	0.43
30:e:49:GLY:O	30:e:50:THR:C	2.61	0.43
33:h:90:ASN:OD1	33:h:115:HIS:NE2	2.52	0.43
46:AB:47:LEU:HD12	46:AB:218:MET:O	2.18	0.43
49:AE:166:ALA:HB2	49:AE:175:PHE:HD1	1.84	0.43
50:AF:95:LEU:O	50:AF:96:LYS:C	2.62	0.43
45:Aa:98:PHE:CE1	45:Aa:120:LEU:HD11	2.53	0.43
47:Ac:33:PHE:CE1	62:Ag:101:CDL:H782	2.52	0.43
48:Ad:179:TYR:CG	48:Ad:185:ALA:HB2	2.54	0.43
53:Aj:34:ARG:HG3	54:Ak:47:TYR:CZ	2.54	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:180:HIS:CD2	3:C:182:ASP:H	2.37	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
5:E:70:PRO:HG2	6:F:236:PHE:CD2	2.54	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
8:H:21:THR:HG21	61:H:400:UQ9:H16	2.01	0.43
10:J:72:ALA:O	10:J:76:GLU:HG2	2.18	0.43
11:K:22:PHE:O	12:L:585:LYS:HE3	2.19	0.43
11:K:33:LEU:HD11	14:N:64:ALA:HB1	2.01	0.43
12:L:172:ILE:HD13	12:L:172:ILE:HA	1.89	0.43
12:L:493:ILE:O	12:L:496:LEU:HG	2.19	0.43
13:M:51:ASN:ND2	33:h:136:THR:HG23	2.34	0.43
13:M:100:ILE:O	13:M:103:GLN:HG2	2.19	0.43
13:M:154:LEU:HA	13:M:154:LEU:HD23	1.84	0.43
13:M:367:LEU:C	13:M:367:LEU:HD12	2.44	0.43
13:M:369:LEU:CD2	13:M:371:PRO:CD	2.84	0.43
14:N:43:MET:CE	14:N:126:MET:SD	3.07	0.43
14:N:109:ALA:O	14:N:112:HIS:HB3	2.19	0.43
14:N:189:TRP:CB	14:N:204:ASN:HD21	2.32	0.43
15:O:96:THR:O	28:c:31:VAL:HG21	2.18	0.43
16:P:142:GLU:O	16:P:146:VAL:CG1	2.61	0.43
16:P:153:ALA:HB2	16:P:191:VAL:HG23	2.01	0.43
16:P:376:ASN:O	16:P:377:TYR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:72:VAL:HG11	18:R:77:ILE:CG2	2.49	0.43
18:R:72:VAL:HG11	18:R:77:ILE:HG22	2.01	0.43
20:T:109:GLY:O	20:T:110:LEU:C	2.61	0.43
23:X:52:ASP:HA	25:Z:116:TRP:CD1	2.54	0.43
24:Y:115:MET:O	24:Y:119:TYR:HD2	2.02	0.43
25:Z:121:ILE:HD11	25:Z:136:ALA:HB3	1.98	0.43
26:a:4:GLU:C	26:a:7:PRO:HD2	2.44	0.43
27:b:6:SER:OG	27:b:10:LYS:HD2	2.18	0.43
30:e:102:GLU:HG2	30:e:103:GLU:N	2.33	0.43
39:n:45:ARG:O	39:n:46:ALA:C	2.61	0.43
41:p:118:GLY:O	41:p:119:GLU:HB2	2.19	0.43
45:AA:402:HIS:NE2	45:AA:403:LEU:CD1	2.75	0.43
46:AB:230:LEU:O	46:AB:233:VAL:HG22	2.18	0.43
48:AD:167:ARG:NH1	48:AD:170:LYS:HE2	2.34	0.43
49:AE:83:VAL:HG22	49:AE:84:LYS:N	2.34	0.43
49:AE:143:SER:HB2	49:AE:146:VAL:HG13	2.00	0.43
49:AE:221:GLY:CA	47:Ac:148:ASN:HD22	2.32	0.43
55:AF:201:3PE:H3H1	51:AG:52:PRO:HG3	2.00	0.43
46:Ab:283:ALA:O	46:Ab:284:ASN:C	2.60	0.43
49:Ae:153:GLU:C	49:Ae:154:ILE:HG13	2.44	0.43
49:Ae:156:LEU:HD23	49:Ae:156:LEU:HA	1.62	0.43
49:Ae:235:TYR:CE1	49:Ae:240:GLY:HA2	2.53	0.43
50:Af:53:GLU:OE2	51:Ag:12:ARG:NH1	2.52	0.43
53:Aj:9:ARG:O	53:Aj:13:LEU:HD23	2.19	0.43
1:A:87:MET:HA	10:J:145:TYR:HB3	2.01	0.43
2:B:81:LEU:CD2	58:B:303:PC1:H352	2.48	0.43
2:B:116:ARG:NH2	9:I:86:TYR:H	2.17	0.43
3:C:102:HIS:CE1	21:V:44:TYR:HE1	2.37	0.43
4:D:51:VAL:HB	14:N:171:ASN:OD1	2.19	0.43
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
9:I:152:CYS:SG	56:I:303:SF4:S3	3.17	0.43
10:J:55:VAL:HG13	10:J:56:PHE:N	2.33	0.43
11:K:50:ASN:C	11:K:50:ASN:OD1	2.62	0.43
12:L:38:THR:O	12:L:41:LYS:HB3	2.19	0.43
12:L:141:PHE:CB	12:L:182:PHE:CE2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:217:LEU:CD1	12:L:273:ILE:HG23	2.49	0.43
12:L:253:VAL:HG21	12:L:310:LEU:HD11	1.99	0.43
12:L:296:ASN:CB	12:L:357:ARG:HH11	2.32	0.43
12:L:357:ARG:HG3	39:n:80:TYR:CD1	2.54	0.43
12:L:441:ILE:HD12	35:j:46:GLU:O	2.19	0.43
13:M:208:PRO:HG2	13:M:216:LEU:CD1	2.44	0.43
14:N:106:LEU:HD21	14:N:139:LEU:HG	2.00	0.43
14:N:108:LEU:HD12	14:N:187:MET:HB3	2.01	0.43
14:N:308:ASN:C	15:O:319:ILE:HG23	2.43	0.43
15:O:121:PRO:HB3	15:O:178:TYR:HE1	1.83	0.43
16:P:259:VAL:N	16:P:261:LYS:HG2	2.33	0.43
17:Q:104:ARG:HA	17:Q:104:ARG:HD3	1.88	0.43
19:S:58:CYS:SG	19:S:59:SER:N	2.92	0.43
19:S:75:LYS:HE2	19:S:75:LYS:HA	2.01	0.43
20:T:113:LEU:HD22	22:W:71:MET:HE2	2.01	0.43
22:W:57:ILE:HG23	22:W:107:MET:HE1	2.00	0.43
26:a:50:ARG:O	26:a:54:ILE:HG13	2.18	0.43
30:e:30:ALA:HB3	33:h:186:THR:HG21	2.00	0.43
34:i:22:TRP:CZ2	39:n:172:THR:HG22	2.53	0.43
40:o:57:ASP:OD2	40:o:59:CYS:HB2	2.19	0.43
47:AC:148:ASN:HB3	49:Ae:220:LEU:HA	1.99	0.43
49:AI:78:PHE:CE1	46:Ab:171:THR:OG1	2.42	0.43
53:AJ:23:LEU:HA	54:AK:27:VAL:HG22	2.00	0.43
45:Aa:157:GLU:O	45:Aa:158:ASP:C	2.62	0.43
47:Ac:215:ALA:HB2	50:Af:60:MET:HE3	2.01	0.43
48:Ad:318:LYS:CD	49:Ae:86:PRO:HB2	2.49	0.43
52:Ah:32:ARG:O	52:Ah:36:GLU:HG3	2.19	0.43
1:A:73:LEU:N	1:A:74:PRO:HD2	2.34	0.42
1:A:99:SER:HB3	55:b:201:3PE:C38	2.49	0.42
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
8:H:33:LEU:HD21	43:r:25:GLN:HG2	2.01	0.42
8:H:200:LEU:CD1	8:H:201:THR:N	2.70	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.42
12:L:138:PHE:CD1	62:h:201:CDL:H271	2.54	0.42
12:L:246:LEU:CD1	12:L:247:LEU:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:275:THR:HG23	12:L:276:THR:N	2.34	0.42
13:M:131:ILE:HD13	14:N:302:LEU:HD21	2.01	0.42
14:N:28:LEU:HD22	30:e:15:ASP:CG	2.44	0.42
14:N:219:LEU:HD23	14:N:230:ILE:HD12	2.01	0.42
15:O:117:PHE:HD1	15:O:128:SER:CA	2.31	0.42
15:O:224:PRO:O	15:O:228:LYS:NZ	2.52	0.42
16:P:306:GLY:HA2	16:P:312:PRO:HB3	2.01	0.42
16:P:361:TRP:HE3	16:P:364:SER:HB2	1.84	0.42
20:T:87:LEU:HD11	20:T:141:PRO:HB3	2.01	0.42
21:V:37:HIS:O	21:V:38:PHE:C	2.62	0.42
22:W:83:ASP:O	22:W:86:VAL:CG2	2.66	0.42
25:Z:108:GLU:O	25:Z:109:SER:C	2.61	0.42
26:a:12:MET:HE2	26:a:12:MET:HB3	1.90	0.42
33:h:59:PRO:O	33:h:61:LEU:HG	2.19	0.42
38:m:5:LYS:HB2	38:m:5:LYS:HE3	1.73	0.42
40:o:46:MET:HE2	40:o:60:ALA:HB3	2.00	0.42
46:AB:64:PHE:HB3	46:AB:401:LEU:HD11	2.01	0.42
46:AB:300:LYS:HE2	46:AB:301:ARG:HH11	1.83	0.42
49:AE:205:VAL:CG1	49:AE:211:VAL:HG23	2.49	0.42
49:AE:221:GLY:HA3	47:Ac:148:ASN:HD21	1.82	0.42
54:AK:9:ARG:O	54:AK:13:LEU:HG	2.18	0.42
45:Aa:291:VAL:O	45:Aa:353:LEU:HA	2.19	0.42
46:Ab:307:SER:HB2	46:Ab:310:SER:HB2	2.01	0.42
47:Ac:256:TYR:CD2	48:Ad:202:ARG:HB3	2.54	0.42
48:Ad:97:SER:O	53:Aj:51:LYS:NZ	2.52	0.42
52:Ah:55:VAL:O	52:Ah:59:SER:HA	2.19	0.42
52:Ah:56:SER:O	52:Ah:59:SER:HB3	2.19	0.42
2:B:69:SER:O	2:B:70:ARG:C	2.61	0.42
2:B:122:ARG:HH22	57:B:302:UQ1:C8	2.32	0.42
2:B:194:CYS:SG	4:D:138:ARG:NE	2.90	0.42
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.44	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.55	0.42
10:J:100:VAL:HG12	10:J:104:CYS:SG	2.59	0.42
12:L:34:LEU:HD12	12:L:34:LEU:HA	1.88	0.42
12:L:521:SER:C	12:L:523:SER:N	2.75	0.42
62:L:706:CDL:H512	62:L:706:CDL:HB4	1.71	0.42
15:O:77:ILE:CG2	15:O:81:LEU:HD12	2.49	0.42
15:O:310:ILE:HG23	15:O:312:VAL:HG23	2.01	0.42
15:O:323:GLN:HB2	32:g:56:ASP:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:298:TYR:C	16:P:300:TRP:N	2.71	0.42
19:S:16:LEU:HD13	19:S:19:ILE:HD11	2.01	0.42
21:V:56:LEU:C	21:V:56:LEU:CD1	2.85	0.42
24:Y:8:PHE:CD1	24:Y:30:LEU:HD21	2.53	0.42
27:b:45:ILE:HG23	27:b:46:ASN:N	2.34	0.42
34:i:93:LYS:HE3	34:i:96:THR:HG21	2.01	0.42
36:k:28:TRP:CE3	36:k:60:MET:HG2	2.54	0.42
37:l:36:MET:O	37:l:36:MET:HG2	2.19	0.42
41:p:36:ALA:O	41:p:37:TYR:C	2.60	0.42
45:AA:71:VAL:HG21	45:AA:140:LEU:HD12	2.01	0.42
45:AA:410:CYS:O	45:AA:413:ILE:N	2.52	0.42
46:AB:286:PHE:CD1	46:AB:427:ALA:HB1	2.54	0.42
48:AD:120:VAL:HG23	48:AD:253:LEU:HD23	2.00	0.42
49:AE:196:ARG:HD2	49:AE:249:ILE:HG23	2.01	0.42
49:AE:201:ASP:OD1	49:AE:202:LEU:N	2.50	0.42
49:AE:249:ILE:HG12	49:AE:254:ALA:HB3	2.01	0.42
49:AE:263:TYR:CB	49:AE:273:VAL:HA	2.49	0.42
46:Ab:40:PHE:CZ	46:Ab:406:TYR:HB2	2.54	0.42
46:Ab:176:ASN:HB3	46:Ab:258:ILE:HD11	2.00	0.42
47:Ac:169:SER:O	47:Ac:170:VAL:C	2.62	0.42
48:Ad:312:SER:O	48:Ad:313:VAL:C	2.59	0.42
1:A:50:PRO:HA	10:J:73:MET:CE	2.43	0.42
1:A:81:THR:O	27:b:46:ASN:ND2	2.52	0.42
55:A:401:3PE:H261	10:J:41:LEU:CD2	2.50	0.42
3:C:149:LEU:HD21	17:Q:59:LEU:HD22	2.00	0.42
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:78:VAL:O	5:E:82:LEU:HB2	2.20	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.42
12:L:5:THR:O	12:L:6:THR:C	2.62	0.42
12:L:272:PHE:O	12:L:275:THR:HG22	2.19	0.42
12:L:489:THR:HG23	12:L:490:ALA:N	2.33	0.42
13:M:14:LEU:HD21	13:M:26:ASN:CB	2.50	0.42
13:M:68:LEU:HD23	13:M:234:ILE:CD1	2.50	0.42
13:M:72:LEU:HD12	13:M:234:ILE:HG12	2.01	0.42
13:M:214:LEU:C	13:M:217:PRO:HD2	2.45	0.42
13:M:306:PRO:HA	13:M:458:THR:HG21	2.01	0.42
55:M:502:3PE:O22	14:N:242:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:80:GLN:O	14:N:80:GLN:HG2	2.19	0.42
14:N:89:GLN:HB3	30:e:60:PHE:CZ	2.53	0.42
16:P:235:THR:HG21	16:P:323:HIS:CD2	2.55	0.42
17:Q:64:LEU:HD12	22:W:85:LEU:HD21	2.00	0.42
23:X:10:LEU:HD12	23:X:13:LEU:HD12	2.01	0.42
24:Y:68:ILE:HG21	24:Y:120:MET:HE1	2.01	0.42
25:Z:10:MET:HE2	25:Z:10:MET:HB3	1.72	0.42
30:e:82:GLN:O	30:e:86:LEU:HG	2.19	0.42
30:e:89:GLU:HB2	30:e:91:LYS:HG2	2.00	0.42
33:h:129:PRO:HD2	33:h:130:GLU:OE1	2.19	0.42
34:i:4:TYR:O	34:i:5:THR:C	2.62	0.42
34:i:22:TRP:O	34:i:26:GLN:HG2	2.19	0.42
34:i:81:PHE:O	34:i:82:VAL:C	2.60	0.42
35:j:44:TYR:CE2	35:j:45:ARG:HG3	2.54	0.42
45:AA:157:GLU:O	45:AA:161:ILE:HG13	2.19	0.42
46:AB:162:LYS:HG3	46:AB:191:TYR:HB3	2.00	0.42
47:AC:29:SER:CB	62:AC:406:CDL:HB61	2.49	0.42
47:AC:153:ILE:HB	47:AC:157:GLY:HA2	2.01	0.42
48:AD:284:HIS:HE2	48:AD:288:MET:HE3	1.83	0.42
46:Ab:39:GLU:OE2	46:Ab:227:HIS:HB2	2.19	0.42
49:Ae:83:VAL:HG22	49:Ae:84:LYS:N	2.34	0.42
49:Ae:93:ARG:CZ	51:Ag:22:PHE:O	2.67	0.42
53:Aj:30:LEU:HD12	54:Ak:34:TRP:HB2	2.00	0.42
1:A:50:PRO:CA	10:J:73:MET:HE3	2.45	0.42
4:D:101:LEU:HD11	4:D:106:VAL:CG2	2.39	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.42
5:E:233:LEU:CD2	6:F:43:THR:HA	2.48	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.84	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:39:ILE:HG13	42:q:31:ASN:ND2	2.35	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:J:125:MET:HG2	25:Z:137:ASN:OD1	2.19	0.42
12:L:9:LEU:HG	55:L:701:3PE:H2D2	2.01	0.42
12:L:309:GLN:CG	12:L:336:LYS:HZ1	2.32	0.42
12:L:335:PHE:O	12:L:339:LEU:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:357:ARG:HG2	12:L:357:ARG:H	1.59	0.42
12:L:358:LYS:CG	39:n:80:TYR:OH	2.47	0.42
13:M:47:GLU:O	13:M:48:ASN:C	2.62	0.42
14:N:80:GLN:O	14:N:81:LEU:HG	2.19	0.42
14:N:241:LEU:HG	14:N:301:SER:OG	2.19	0.42
14:N:272:LYS:HE3	33:h:154:GLN:HG2	2.00	0.42
15:O:170:LEU:HD21	15:O:184:VAL:HG13	2.00	0.42
15:O:242:LYS:HE2	15:O:242:LYS:HB2	1.92	0.42
15:O:297:LEU:C	15:O:297:LEU:HD23	2.44	0.42
15:O:339:TYR:CE1	29:d:52:PRO:HA	2.54	0.42
16:P:207:PHE:O	16:P:241:TYR:HA	2.20	0.42
16:P:279:TYR:O	16:P:280:ILE:C	2.62	0.42
16:P:300:TRP:NE1	16:P:304:LEU:HD21	2.35	0.42
19:S:26:ARG:N	19:S:34:ARG:NH1	2.63	0.42
20:U:125:GLU:OE2	35:j:44:TYR:CE1	2.73	0.42
21:V:35:LEU:HA	21:V:38:PHE:CE1	2.55	0.42
23:X:130:LYS:HG2	27:b:67:PRO:HA	2.01	0.42
25:Z:97:ILE:HG23	30:e:92:TYR:CD1	2.54	0.42
25:Z:129:THR:O	25:Z:130:LYS:C	2.61	0.42
34:i:103:ARG:NH2	40:o:67:LEU:HD13	2.33	0.42
36:k:58:ARG:HH12	39:n:34:ARG:HH11	1.68	0.42
39:n:110:SER:O	39:n:113:ALA:HB3	2.20	0.42
39:n:139:GLN:HA	39:n:142:GLU:HG2	2.01	0.42
41:p:6:ASP:OD1	41:p:8:ASP:HB2	2.20	0.42
41:p:43:TRP:NE1	41:p:47:LEU:HD11	2.33	0.42
47:AC:278:TYR:CE2	47:AC:282:ARG:HD2	2.54	0.42
48:AD:252:VAL:HG13	48:AD:253:LEU:N	2.34	0.42
49:AE:152:ILE:HD12	49:AE:153:GLU:H	1.84	0.42
52:AH:39:GLU:HA	52:AH:42:VAL:HG12	2.02	0.42
45:Aa:451:ASP:HA	45:Aa:472:ARG:HH12	1.84	0.42
47:Ac:99:GLY:HA3	55:Ac:404:3PE:H2A1	2.01	0.42
48:Ad:252:VAL:HG13	48:Ad:253:LEU:N	2.33	0.42
48:Ad:262:THR:O	48:Ad:263:MET:C	2.61	0.42
49:Ae:112:GLY:O	49:Ae:116:LEU:HB2	2.19	0.42
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG23	2.01	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.01	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.34	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
8:H:202:GLU:HA	8:H:206:GLU:CD	2.45	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
58:J:201:PC1:H342	58:J:201:PC1:C38	2.42	0.42
12:L:591:PHE:O	12:L:595:ILE:HG13	2.20	0.42
55:L:707:3PE:H3B2	55:L:707:3PE:H3E1	1.72	0.42
13:M:29:SER:CB	32:g:91:PHE:HD2	2.24	0.42
13:M:44:GLN:HG2	13:M:46:ASP:O	2.18	0.42
13:M:77:LEU:O	13:M:81:GLN:HG3	2.19	0.42
13:M:118:PHE:HE2	13:M:203:PHE:CE1	2.37	0.42
13:M:131:ILE:HD12	14:N:302:LEU:HD21	2.01	0.42
13:M:206:LYS:HA	13:M:215:TRP:CZ2	2.54	0.42
13:M:293:HIS:O	13:M:294:MET:HE2	2.20	0.42
13:M:347:GLY:O	13:M:348:LEU:C	2.63	0.42
15:O:209:VAL:HA	15:O:210:PRO:HD3	1.80	0.42
15:O:350:LYS:HD3	15:O:351:TRP:CD1	2.54	0.42
19:S:16:LEU:CB	19:S:69:TYR:CD1	2.97	0.42
20:U:124:ASP:CG	39:n:25:ARG:HH12	2.27	0.42
22:W:38:LEU:O	22:W:39:TYR:C	2.62	0.42
23:X:130:LYS:HG2	27:b:67:PRO:CA	2.50	0.42
26:a:17:VAL:O	26:a:18:ILE:C	2.62	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CE2	2.54	0.42
29:d:114:GLU:O	29:d:114:GLU:HG2	2.18	0.42
37:l:57:MET:HG2	37:l:104:PRO:CG	2.49	0.42
45:AA:74:TRP:CZ3	45:AA:232:ALA:HB3	2.54	0.42
45:AA:174:GLU:C	45:AA:176:ASP:H	2.27	0.42
45:AA:372:LEU:HD21	45:AA:376:TRP:CH2	2.55	0.42
46:AB:130:ILE:HA	46:AB:133:LEU:HB2	2.01	0.42
48:AD:248:ILE:HD12	48:AD:266:VAL:HG11	2.00	0.42
49:AE:263:TYR:HA	49:AE:273:VAL:CA	2.50	0.42
52:AH:58:ARG:HB3	52:AH:61:THR:HB	2.01	0.42
45:Aa:95:HIS:CE1	46:Ab:301:ARG:HD3	2.54	0.42
45:Aa:170:ARG:O	45:Aa:173:GLN:HB2	2.20	0.42
46:Ab:225:VAL:HG22	46:Ab:229:VAL:HG21	2.01	0.42
47:Ac:141:TRP:CD1	47:Ac:265:PRO:CD	2.97	0.42
48:Ad:318:LYS:HD2	49:Ae:86:PRO:HB2	2.01	0.42
49:Ae:122:THR:HG21	53:Aj:25:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:31:VAL:HG21	52:Ah:84:LEU:HA	2.01	0.42
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.02	0.42
5:E:196:THR:O	5:E:199:ASP:HB2	2.19	0.42
6:F:300:ILE:CG2	6:F:306:GLY:HA2	2.35	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
12:L:220:ALA:HB2	12:L:260:LEU:CD1	2.49	0.42
12:L:396:ILE:HD13	12:L:396:ILE:HA	1.89	0.42
13:M:181:PHE:CZ	41:p:86:TYR:HD1	2.37	0.42
13:M:200:MET:CE	13:M:247:SER:HB2	2.46	0.42
13:M:207:MET:HE3	13:M:240:SER:HB2	2.02	0.42
13:M:210:TYR:O	13:M:213:HIS:HD2	2.01	0.42
13:M:230:ILE:HG23	13:M:235:LEU:HD11	2.01	0.42
14:N:226:THR:HG22	14:N:228:ASN:N	2.34	0.42
16:P:324:ILE:HD13	16:P:324:ILE:HA	1.81	0.42
17:Q:58:LYS:O	17:Q:58:LYS:HG3	2.20	0.42
18:R:64:ILE:HD12	18:R:64:ILE:HA	1.95	0.42
23:X:127:LYS:HB2	27:b:76:PRO:HD2	2.02	0.42
24:Y:45:LEU:O	24:Y:46:ASN:C	2.62	0.42
24:Y:76:THR:CG2	24:Y:92:TYR:HA	2.48	0.42
24:Y:141:PRO:HB2	33:h:161:ARG:NE	2.35	0.42
25:Z:64:ASP:OD1	25:Z:65:LEU:N	2.52	0.42
32:g:119:GLU:OE1	32:g:122:ARG:NH1	2.53	0.42
32:g:147:LEU:O	32:g:148:PRO:C	2.62	0.42
36:k:42:LEU:HD11	39:n:39:TYR:HA	2.02	0.42
37:l:62:TYR:CE2	37:l:64:PRO:HG3	2.55	0.42
38:m:26:SER:HB2	38:m:27:PRO:HD2	2.00	0.42
45:AA:172:MET:HA	45:AA:175:ASN:CG	2.44	0.42
45:AA:230:VAL:HG21	45:AA:417:LEU:HB3	2.00	0.42
47:AC:17:SER:O	69:AC:405:UQ6:H1M1	2.19	0.42
45:Aa:156:LEU:O	45:Aa:213:ARG:NE	2.52	0.42
45:Aa:212:SER:C	45:Aa:214:THR:N	2.74	0.42
45:Aa:272:GLY:O	51:Ag:19:LEU:HD12	2.19	0.42
45:Aa:370:PHE:HE1	62:Aa:501:CDL:H1O1	1.66	0.42
45:Aa:396:ARG:HE	45:Aa:430:GLU:HG2	1.85	0.42
46:Ab:284:ASN:HB3	46:Ab:419:VAL:CG2	2.48	0.42
46:Ab:332:ASP:OD1	46:Ab:332:ASP:N	2.52	0.42
46:Ab:396:ILE:HG12	46:Ab:406:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:231:LEU:HD13	48:Ad:241:ALA:HB1	2.01	0.42
49:Ae:155:LYS:HD3	49:Ae:158:ASP:OD1	2.20	0.42
49:Ae:177:ARG:HB3	49:Ae:211:VAL:CG1	2.49	0.42
51:Ag:47:LEU:HD12	55:Ag:102:3PE:C34	2.48	0.42
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
9:I:80:GLU:N	26:a:1:MET:HE1	2.34	0.42
12:L:21:ILE:HG23	12:L:27:ILE:CG2	2.50	0.42
12:L:81:LYS:HD3	12:L:262:ARG:HH11	1.83	0.42
12:L:189:PHE:CZ	12:L:212:PRO:HB2	2.55	0.42
12:L:277:MET:CG	12:L:318:GLY:CA	2.98	0.42
12:L:365:ILE:CD1	12:L:366:MET:HG3	2.24	0.42
12:L:405:ASN:HB2	12:L:408:ALA:HB3	2.01	0.42
13:M:16:TRP:HZ2	55:M:502:3PE:H282	1.84	0.42
13:M:123:GLU:OE2	13:M:154:LEU:HD21	2.20	0.42
13:M:191:SER:O	13:M:194:LEU:HB2	2.20	0.42
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.42
15:O:272:ASP:HA	15:O:275:TYR:HD2	1.85	0.42
16:P:172:ALA:H	16:P:202:ARG:HH21	1.66	0.42
16:P:220:TYR:CG	16:P:226:VAL:HG13	2.55	0.42
16:P:242:VAL:HG13	16:P:243:ALA:N	2.35	0.42
19:S:19:ILE:O	19:S:53:ILE:HD12	2.20	0.42
20:U:84:LEU:HD11	20:U:98:LEU:HG	2.02	0.42
23:X:38:LYS:O	23:X:42:GLU:HG3	2.20	0.42
25:Z:120:LEU:HD12	25:Z:121:ILE:H	1.85	0.42
27:b:5:ILE:HD12	27:b:6:SER:N	2.34	0.42
27:b:69:HIS:HD2	27:b:70:PRO:CD	2.26	0.42
28:c:55:TRP:CZ2	29:d:66:THR:HG22	2.55	0.42
35:j:96:GLU:HG2	35:j:97:LEU:HD23	2.01	0.42
37:l:120:SER:O	37:l:121:PRO:C	2.60	0.42
45:AA:120:LEU:HD23	46:AB:299:ILE:HG23	2.00	0.42
46:AB:407:MET:HE1	46:AB:415:GLN:CD	2.45	0.42
48:AD:155:GLN:HA	48:AD:166:MET:CA	2.44	0.42
48:AD:189:ASN:HB3	70:AD:401:HEC:HMD2	2.01	0.42
48:AD:221:PRO:HB2	48:AD:225:VAL:HG13	2.01	0.42
49:AE:178:HIS:CD2	49:AE:179:ARG:N	2.88	0.42
52:AH:42:VAL:HG23	52:AH:45:ARG:HH21	1.84	0.42
54:AK:38:TRP:HB3	54:AK:41:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:359:VAL:O	45:Aa:360:CYS:HB2	2.19	0.42
45:Aa:463:GLU:CD	51:Ag:8:LEU:HB2	2.44	0.42
47:Ac:278:TYR:CE2	47:Ac:282:ARG:HD2	2.54	0.42
69:Ac:406:UQ6:H111	69:Ac:406:UQ6:H72	1.80	0.42
48:Ad:201:VAL:HG22	48:Ad:278:SER:HB2	2.00	0.42
49:Ae:173:PRO:HG2	49:Ae:223:VAL:CG2	2.45	0.42
49:Ae:266:THR:HB	49:Ae:270:VAL:HG11	2.01	0.42
50:Af:95:LEU:O	50:Af:96:LYS:C	2.61	0.42
52:Ah:54:ARG:HH21	52:Ah:55:VAL:CG2	2.32	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:99:SER:HB3	55:b:201:3PE:C39	2.48	0.42
4:D:37:TRP:CE3	4:D:37:TRP:O	2.73	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:264:ASN:O	9:I:65:GLU:OE1	2.38	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:92:PRO:HB3	42:q:92:CYS:HB2	2.01	0.42
12:L:112:PRO:HD2	39:n:97:TYR:CE2	2.55	0.42
12:L:264:HIS:HA	12:L:267:THR:HG23	2.02	0.42
12:L:552:LEU:HD12	37:l:70:MET:CE	2.42	0.42
13:M:445:ILE:HG23	55:M:501:3PE:H292	2.02	0.42
14:N:154:ILE:CG2	14:N:191:LEU:HD11	2.49	0.42
14:N:281:LEU:CD2	55:N:401:3PE:C28	2.88	0.42
16:P:316:LYS:O	16:P:320:GLU:HG2	2.19	0.42
19:S:64:LYS:HE2	19:S:66:TRP:CZ2	2.55	0.42
20:U:125:GLU:OE2	35:j:44:TYR:HE1	2.02	0.42
22:W:42:TRP:CE2	22:W:93:LEU:HB2	2.54	0.42
22:W:55:LEU:HB3	22:W:57:ILE:HG12	2.01	0.42
23:X:26:LYS:HD3	23:X:95:GLN:OE1	2.19	0.42
27:b:31:ILE:HG23	27:b:32:MET:N	2.34	0.42
27:b:32:MET:N	27:b:33:PRO:CD	2.82	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CD2	2.55	0.42
32:g:123:LEU:CD1	41:p:98:VAL:HG11	2.49	0.42
33:h:144:SER:HB2	41:p:82:VAL:HG21	2.02	0.42
37:l:167:TYR:CG	37:l:178:PRO:HG3	2.55	0.42
40:o:104:ARG:O	40:o:108:LEU:HG	2.20	0.42
43:r:18:GLN:OE1	43:r:18:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:397:ASN:N	45:AA:397:ASN:HD22	2.18	0.42
47:AC:33:PHE:O	47:AC:36:LEU:HB2	2.19	0.42
52:AH:49:GLU:O	52:AH:53:ASN:N	2.50	0.42
46:Ab:162:LYS:HG3	46:Ab:191:TYR:HB3	2.00	0.42
47:Ac:150:LEU:HD23	47:Ac:150:LEU:HA	1.92	0.42
49:Ae:153:GLU:CA	49:Ae:271:VAL:O	2.66	0.42
49:Ae:160:PRO:C	49:Ae:178:HIS:HB3	2.45	0.42
49:Ae:249:ILE:HG12	49:Ae:254:ALA:HB3	2.01	0.42
4:D:94:VAL:HB	4:D:115:LEU:HB3	2.02	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:39:VAL:HG21	7:G:163:LYS:HZ1	1.85	0.42
5:E:181:ASN:HB3	5:E:193:GLU:HB2	2.01	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.42
10:J:120:LEU:C	10:J:122:ASP:N	2.78	0.42
12:L:23:MET:SD	62:L:705:CDL:H112	2.60	0.42
12:L:226:GLN:OE1	12:L:281:GLY:HA2	2.20	0.42
12:L:534:HIS:O	12:L:538:PRO:CG	2.60	0.42
14:N:215:MET:SD	14:N:244:ILE:CD1	3.08	0.42
15:O:66:ILE:HG23	63:O:402:ADP:O3'	2.19	0.42
15:O:195:LEU:N	15:O:196:PRO:HD2	2.34	0.42
16:P:179:LYS:O	16:P:180:SER:C	2.63	0.42
17:Q:75:ARG:NH1	17:Q:104:ARG:HG2	2.34	0.42
19:S:26:ARG:HA	19:S:34:ARG:HH12	1.84	0.42
20:T:132:ASP:O	22:W:40:ARG:NH2	2.53	0.42
22:W:76:VAL:HG13	22:W:82:VAL:HG22	2.02	0.42
26:a:34:LYS:O	26:a:35:GLU:C	2.63	0.42
29:d:100:ASP:HB3	33:h:159:LEU:HD21	2.01	0.42
31:f:6:LEU:O	31:f:7:LEU:HB2	2.19	0.42
33:h:55:PHE:HE1	33:h:57:VAL:HA	1.84	0.42
37:l:84:HIS:NE2	37:l:114:ARG:HA	2.34	0.42
39:n:100:PRO:HB2	39:n:102:TRP:NE1	2.35	0.42
40:o:22:ILE:N	40:o:23:PRO:HD2	2.35	0.42
40:o:31:PHE:CD1	40:o:34:ARG:HD2	2.55	0.42
45:AA:342:GLN:HE21	45:AA:357:HIS:CB	2.31	0.42
49:AE:112:GLY:O	49:AE:116:LEU:HB2	2.19	0.42
49:AE:177:ARG:HB3	49:AE:211:VAL:CG1	2.49	0.42
51:AG:19:LEU:HG	51:AG:20:SER:N	2.33	0.42
45:Aa:178:SER:OG	45:Aa:181:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:247:PRO:CB	70:Ad:401:HEC:CHC	2.98	0.42
49:Ae:111:LYS:HE3	53:Aj:11:TYR:CZ	2.55	0.42
49:Ae:122:THR:O	49:Ae:123:VAL:C	2.61	0.42
49:Ae:195:LEU:CD1	49:Ae:248:ARG:HD2	2.50	0.42
52:Ah:58:ARG:CZ	52:Ah:61:THR:HB	2.50	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.35	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
9:I:152:CYS:SG	56:I:303:SF4:S1	3.17	0.42
10:J:20:ALA:C	10:J:22:LYS:N	2.77	0.42
11:K:59:ILE:HB	11:K:60:PRO:HD3	2.01	0.42
12:L:51:LEU:HA	12:L:87:ILE:HD12	2.02	0.42
12:L:193:MET:CE	38:m:125:PHE:CD2	3.03	0.42
12:L:293:LEU:O	12:L:425:ARG:HD2	2.20	0.42
12:L:568:THR:O	12:L:569:LEU:C	2.61	0.42
12:L:597:LEU:HD21	24:Y:37:ILE:HD12	2.02	0.42
13:M:263:LEU:HD13	38:m:102:TYR:HB2	2.01	0.42
14:N:25:ASN:HB3	30:e:15:ASP:CG	2.45	0.42
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.85	0.42
15:O:209:VAL:CG1	15:O:260:SER:HB2	2.31	0.42
16:P:283:MET:HE3	16:P:357:ARG:HH11	1.85	0.42
19:S:31:GLN:CD	19:S:34:ARG:HH21	2.28	0.42
20:T:118:ILE:HD13	20:T:118:ILE:HA	1.83	0.42
20:U:103:HIS:HB2	20:U:106:LYS:HG2	2.02	0.42
25:Z:94:GLU:HA	25:Z:97:ILE:HD11	2.01	0.42
29:d:24:PRO:HD2	29:d:73:TYR:CE2	2.55	0.42
30:e:44:ALA:HA	30:e:47:ILE:CG1	2.49	0.42
30:e:81:LYS:O	30:e:85:LYS:HG3	2.19	0.42
30:e:83:ARG:HG2	30:e:87:MET:SD	2.60	0.42
34:i:9:LYS:O	34:i:13:GLN:HB2	2.20	0.42
37:l:159:LYS:HE3	37:l:161:TYR:HE1	1.85	0.42
38:m:8:PRO:HD3	38:m:14:LEU:HD13	2.02	0.42
46:AB:272:VAL:HA	46:AB:337:GLY:HA3	2.02	0.42
47:AC:83:HIS:CD2	67:AC:401:HEM:ND	2.88	0.42
55:AC:403:3PE:C2B	51:AG:41:ARG:NH2	2.82	0.42
49:AE:195:LEU:CD1	49:AE:248:ARG:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:164:GLU:O	45:Aa:165:ARG:C	2.60	0.42
47:Ac:330:ALA:HB1	51:Ag:56:VAL:CG2	2.50	0.42
71:Ad:402:3PH:H371	49:Ae:128:ALA:CB	2.50	0.42
49:Ae:166:ALA:HB2	49:Ae:175:PHE:HD1	1.84	0.42
1:A:3:LEU:O	1:A:4:TYR:C	2.60	0.41
1:A:60:ILE:O	1:A:61:THR:C	2.62	0.41
1:A:102:LEU:HD23	55:b:201:3PE:H371	2.02	0.41
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:102:HIS:CE1	21:V:48:THR:CG2	2.89	0.41
4:D:280:ALA:CB	21:V:11:LEU:CG	2.95	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
8:H:16:ALA:HB2	26:a:15:CYS:CB	2.50	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:J:84:SER:O	10:J:88:ILE:HG12	2.19	0.41
12:L:117:PHE:HZ	12:L:242:PRO:HG2	1.85	0.41
12:L:407:TRP:CE3	12:L:410:LEU:HD21	2.54	0.41
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.02	0.41
13:M:158:ILE:HG21	14:N:283:ALA:CB	2.48	0.41
13:M:258:ALA:O	13:M:259:TYR:C	2.62	0.41
15:O:58:ARG:HB3	15:O:202:HIS:HB2	2.01	0.41
16:P:255:ASP:OD1	16:P:256:PRO:HD2	2.20	0.41
16:P:265:PHE:N	16:P:265:PHE:CD1	2.87	0.41
20:T:80:LYS:O	20:T:84:LEU:HG	2.20	0.41
22:W:45:GLU:O	22:W:46:VAL:C	2.62	0.41
22:W:93:LEU:HD23	22:W:93:LEU:C	2.45	0.41
62:X:201:CDL:OB7	62:X:201:CDL:HB61	2.20	0.41
24:Y:10:SER:O	24:Y:11:TYR:C	2.62	0.41
25:Z:93:GLU:OE2	30:e:95:PRO:CD	2.65	0.41
27:b:59:ASP:HA	27:b:63:MET:CE	2.50	0.41
30:e:36:PHE:O	30:e:37:GLU:C	2.62	0.41
30:e:96:PRO:HA	30:e:99:SER:CB	2.33	0.41
33:h:90:ASN:HD21	62:h:201:CDL:PA1	2.43	0.41
37:l:59:VAL:O	37:l:59:VAL:HG12	2.20	0.41
39:n:132:SER:O	39:n:133:TRP:C	2.62	0.41
39:n:164:PRO:HA	39:n:165:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:42:THR:O	40:o:43:GLN:C	2.62	0.41
41:p:9:VAL:O	41:p:109:ARG:NH2	2.51	0.41
42:q:74:PHE:HE2	42:q:75:TRP:HE1	1.68	0.41
45:AA:53:LEU:HD21	45:AA:243:LEU:CD1	2.50	0.41
45:AA:361:ASP:OD1	45:AA:361:ASP:N	2.52	0.41
45:AA:479:ARG:HG3	54:AK:17:TRP:HZ2	1.85	0.41
47:AC:18:PHE:CE1	69:AC:405:UQ6:H103	2.54	0.41
47:AC:184:ILE:HD13	47:Ac:49:LEU:HD22	2.02	0.41
48:AD:167:ARG:NH1	48:AD:170:LYS:HG3	2.35	0.41
48:AD:300:LEU:O	48:AD:301:PRO:C	2.61	0.41
48:AD:323:PRO:HB2	48:AD:325:LYS:HG3	2.02	0.41
49:AE:172:LYS:HE2	49:AE:172:LYS:HA	2.02	0.41
49:AE:231:PHE:CD2	49:AE:250:ARG:NH1	2.88	0.41
52:AH:26:ASP:C	52:AH:28:LEU:N	2.77	0.41
45:Aa:117:GLY:HA2	46:Ab:377:LYS:CG	2.41	0.41
45:Aa:382:SER:HA	54:Ak:16:ASN:HD22	1.85	0.41
46:Ab:155:ARG:HD2	46:Ab:198:GLY:H	1.84	0.41
46:Ab:307:SER:HB2	46:Ab:310:SER:CB	2.50	0.41
47:Ac:33:PHE:O	47:Ac:36:LEU:HB2	2.19	0.41
48:Ad:199:TYR:HA	48:Ad:278:SER:OG	2.20	0.41
48:Ad:317:ARG:HD2	48:Ad:319:LEU:HD21	2.02	0.41
4:D:35:ARG:HH21	32:g:59:PRO:HD3	1.84	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.35	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
8:H:12:PRO:O	26:a:15:CYS:HB3	2.20	0.41
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
10:J:39:GLY:HA2	10:J:42:MET:HE2	1.99	0.41
10:J:124:LEU:HB3	25:Z:137:ASN:HD21	1.85	0.41
12:L:16:LEU:HD11	55:L:701:3PE:C2H	2.23	0.41
12:L:355:ASP:O	12:L:359:MET:HG3	2.20	0.41
12:L:489:THR:O	12:L:492:ILE:HG13	2.20	0.41
12:L:553:LEU:HD21	38:m:94:GLY:N	2.34	0.41
14:N:154:ILE:HD11	14:N:195:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:218:ALA:CB	14:N:240:MET:SD	3.08	0.41
15:O:267:THR:O	15:O:271:GLU:HG3	2.19	0.41
16:P:214:LEU:HD23	16:P:352:VAL:HG12	2.01	0.41
16:P:284:THR:HG22	16:P:286:ARG:HG3	2.02	0.41
20:T:90:TYR:CD2	20:T:92:LYS:HB3	2.54	0.41
20:U:128:PHE:HZ	20:U:148:ILE:CD1	2.33	0.41
24:Y:91:ASN:HD22	24:Y:91:ASN:HA	1.71	0.41
25:Z:91:LEU:HD13	25:Z:91:LEU:C	2.45	0.41
27:b:7:ALA:C	27:b:9:LEU:H	2.27	0.41
27:b:61:GLY:O	27:b:63:MET:HG3	2.20	0.41
29:d:108:THR:HG23	29:d:110:ALA:HB3	2.02	0.41
30:e:33:CYS:O	30:e:34:HIS:C	2.62	0.41
34:i:20:ARG:HH11	34:i:20:ARG:HG3	1.84	0.41
39:n:56:ASP:O	39:n:59:ARG:N	2.54	0.41
39:n:114:MET:HG3	39:n:115:TYR:CD2	2.55	0.41
45:AA:120:LEU:HD12	45:AA:132:LEU:O	2.20	0.41
45:AA:148:ALA:O	45:AA:152:GLN:HG2	2.20	0.41
45:AA:152:GLN:NE2	45:AA:250:LEU:HA	2.36	0.41
45:AA:271:THR:HG23	51:AG:23:GLU:HG2	2.02	0.41
45:AA:467:ASP:OD2	47:AC:223:TYR:CZ	2.73	0.41
68:AC:404:U10:H1M3	68:AC:404:U10:H72	1.93	0.41
48:AD:201:VAL:HG23	48:AD:202:ARG:N	2.35	0.41
50:AF:102:ARG:HA	50:AF:105:ARG:CZ	2.49	0.41
45:Aa:205:SER:O	45:Aa:209:ARG:HG3	2.19	0.41
45:Aa:359:VAL:HG12	45:Aa:360:CYS:N	2.33	0.41
46:Ab:38:LEU:HD13	46:Ab:52:LEU:HB2	2.02	0.41
46:Ab:346:ALA:O	46:Ab:347:ALA:C	2.62	0.41
47:Ac:237:LEU:HD22	48:Ad:300:LEU:HD11	2.02	0.41
47:Ac:284:ILE:HG21	47:Ac:289:GLY:HA3	2.02	0.41
47:Ac:317:PHE:CD1	50:Af:27:PHE:HB3	2.55	0.41
48:Ad:248:ILE:HD11	70:Ad:401:HEC:HBB2	2.01	0.41
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
1:A:56:PHE:CZ	1:A:60:ILE:HD11	2.55	0.41
1:A:101:GLY:CA	10:J:163:ILE:CD1	2.70	0.41
2:B:100:CYS:SG	56:B:301:SF4:S3	3.19	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
57:B:302:UQ1:HM22	4:D:189:THR:HG21	2.03	0.41
4:D:81:THR:HB	4:D:100:GLU:HG2	2.03	0.41
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	1.99	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
12:L:142:ILE:HG12	13:M:370:PRO:HB2	2.01	0.41
12:L:598:ILE:HD11	14:N:153:ILE:HD13	2.02	0.41
13:M:151:PHE:CZ	14:N:291:PHE:CB	2.97	0.41
13:M:177:MET:HB3	13:M:177:MET:HE3	1.70	0.41
13:M:270:ILE:HD11	13:M:395:LEU:HA	2.03	0.41
13:M:319:HIS:HA	13:M:322:THR:CG2	2.44	0.41
14:N:285:MET:HE1	14:N:288:LEU:HD22	2.03	0.41
15:O:146:ALA:CB	15:O:159:LEU:HD21	2.50	0.41
15:O:179:ILE:CD1	15:O:184:VAL:HG22	2.50	0.41
15:O:179:ILE:HD12	15:O:184:VAL:HG22	2.02	0.41
15:O:243:LYS:HB2	15:O:243:LYS:HE2	1.64	0.41
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.89	0.41
16:P:156:SER:O	16:P:160:GLY:N	2.45	0.41
18:R:60:ALA:O	18:R:61:ILE:C	2.63	0.41
19:S:21:VAL:HG23	19:S:91:MET:HE1	2.02	0.41
19:S:31:GLN:NE2	19:S:34:ARG:NH2	2.68	0.41
20:T:87:LEU:CD2	20:T:122:MET:CE	2.97	0.41
20:T:115:GLN:O	20:T:116:VAL:C	2.63	0.41
23:X:70:PHE:CE1	23:X:117:TRP:CZ3	3.08	0.41
25:Z:96:ILE:H	25:Z:96:ILE:HG13	1.72	0.41
30:e:85:LYS:HG3	30:e:85:LYS:H	1.58	0.41
31:f:42:MET:HB3	41:p:71:VAL:HG23	2.02	0.41
38:m:42:ARG:O	38:m:43:LEU:C	2.62	0.41
40:o:15:VAL:HG13	40:o:110:GLN:HG2	2.01	0.41
45:AA:373:GLN:OE1	45:AA:474:GLY:HA3	2.20	0.41
45:AA:454:PRO:O	45:AA:468:TYR:OH	2.34	0.41
47:AC:233:LEU:HD21	48:AD:300:LEU:N	2.35	0.41
48:AD:98:HIS:CE1	48:AD:208:GLU:OE1	2.73	0.41
48:AD:119:GLN:OE1	48:AD:253:LEU:HB2	2.20	0.41
53:AJ:19:SER:HA	54:AK:24:TRP:CZ2	2.55	0.41
45:Aa:278:ARG:CZ	45:Aa:463:GLU:HB2	2.50	0.41
46:Ab:239:ASN:OD1	46:Ab:239:ASN:N	2.53	0.41
47:Ac:171:ASP:CG	47:Ac:172:LYS:N	2.76	0.41
47:Ac:240:MET:SD	71:Ad:402:3PH:H272	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:210:TYR:O	48:Ad:211:VAL:C	2.63	0.41
48:Ad:244:MET:HB2	70:Ad:401:HEC:C4D	2.50	0.41
49:Ae:205:VAL:CG1	49:Ae:211:VAL:HG23	2.49	0.41
52:Ah:67:GLU:HG3	52:Ah:68:GLU:N	2.35	0.41
52:Ah:71:ASP:OD1	52:Ah:72:PHE:N	2.53	0.41
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.20	0.41
2:B:224:ARG:HG3	16:P:85:ARG:HH12	1.84	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:49:GLY:O	14:N:173:THR:HG21	2.21	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
5:E:136:THR:HG21	6:F:122:PRO:HG3	2.01	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:J:100:VAL:O	10:J:101:PHE:C	2.63	0.41
12:L:23:MET:HE1	62:L:705:CDL:H132	2.02	0.41
12:L:202:MET:HE3	12:L:265:PRO:CB	2.50	0.41
12:L:231:PRO:O	12:L:234:PRO:HD2	2.20	0.41
12:L:286:LEU:HG	12:L:290:ILE:HD11	2.01	0.41
55:L:707:3PE:H3C1	13:M:155:ILE:CD1	2.51	0.41
13:M:142:ARG:HG3	13:M:143:LEU:N	2.35	0.41
13:M:270:ILE:HD12	13:M:395:LEU:HD22	2.02	0.41
15:O:261:TRP:H	15:O:261:TRP:HE3	1.68	0.41
15:O:295:ARG:HH12	15:O:299:GLN:CB	2.33	0.41
16:P:177:SER:O	16:P:182:ARG:NH2	2.53	0.41
16:P:228:LEU:HD11	16:P:288:PHE:CZ	2.54	0.41
20:T:123:GLU:HG2	20:T:130:ILE:HD12	2.02	0.41
20:U:87:LEU:C	20:U:89:LEU:N	2.78	0.41
20:U:105:MET:SD	20:U:139:MET:HE1	2.58	0.41
23:X:23:ALA:HB2	23:X:95:GLN:HE22	1.82	0.41
23:X:112:LEU:HD13	23:X:118:VAL:HG22	2.03	0.41
24:Y:20:CYS:O	24:Y:21:HIS:C	2.63	0.41
27:b:78:LEU:O	27:b:81:LEU:N	2.53	0.41
34:i:102:PRO:HB2	41:p:18:PRO:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:124:LYS:O	38:m:126:ASN:N	2.54	0.41
40:o:4:HIS:HB3	40:o:16:GLU:OE1	2.21	0.41
40:o:26:PRO:C	40:o:28:ASP:N	2.75	0.41
40:o:53:LEU:HD23	40:o:56:ARG:NE	2.34	0.41
42:q:5:GLU:HG2	42:q:9:ARG:HE	1.85	0.41
42:q:39:VAL:HG21	42:q:89:TRP:CZ2	2.55	0.41
42:q:87:HIS:O	42:q:91:HIS:HD2	2.04	0.41
46:AB:138:LEU:HD22	46:AB:238:LEU:HG	2.01	0.41
46:AB:346:ALA:O	46:AB:347:ALA:C	2.62	0.41
46:AB:396:ILE:HG12	46:AB:406:TYR:HE1	1.85	0.41
49:AE:160:PRO:C	49:AE:178:HIS:HB3	2.45	0.41
47:Ac:186:PRO:HG2	67:Ac:402:HEM:CHC	2.50	0.41
49:Ae:244:ASP:OD2	49:Ae:248:ARG:NE	2.54	0.41
52:Ah:45:ARG:O	52:Ah:48:LEU:HB3	2.20	0.41
4:D:87:GLN:O	4:D:88:HIS:C	2.61	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
6:F:131:MET:HE3	6:F:131:MET:HB2	1.91	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.41
10:J:22:LYS:HE3	11:K:22:PHE:HA	2.02	0.41
10:J:29:GLY:O	10:J:33:ILE:HG13	2.21	0.41
10:J:168:GLU:OE2	10:J:171:ARG:HG3	2.21	0.41
13:M:85:LYS:O	13:M:85:LYS:HG2	2.21	0.41
13:M:247:SER:OG	13:M:304:GLN:NE2	2.53	0.41
15:O:117:PHE:CZ	15:O:173:MET:HE3	2.54	0.41
15:O:263:ALA:C	15:O:265:ASP:N	2.77	0.41
16:P:358:THR:HG23	16:P:359:TYR:H	1.81	0.41
17:Q:85:ASN:C	17:Q:87:MET:N	2.76	0.41
18:R:55:VAL:HG22	18:R:56:ASN:N	2.35	0.41
20:T:134:ASP:HA	20:T:137:LYS:NZ	2.35	0.41
20:U:74:LEU:CD2	20:U:79:ILE:HD11	2.49	0.41
20:U:120:MET:HE1	39:n:24:LEU:HD12	2.03	0.41
22:W:44:ARG:O	22:W:47:PRO:HG2	2.20	0.41
27:b:25:VAL:O	27:b:26:TRP:C	2.64	0.41
35:j:40:ILE:HD12	35:j:40:ILE:HA	1.93	0.41
35:j:44:TYR:CD2	35:j:45:ARG:HG3	2.56	0.41
35:j:52:ARG:HG2	35:j:56:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:50:GLU:HA	42:q:59:HIS:O	2.20	0.41
43:r:12:ARG:HH21	43:r:20:LEU:CD1	2.33	0.41
43:r:24:LEU:HD23	43:r:24:LEU:HA	1.85	0.41
45:AA:356:ALA:HB3	45:AA:372:LEU:HD21	2.03	0.41
46:AB:37:ASP:N	46:AB:37:ASP:OD1	2.52	0.41
48:AD:167:ARG:HH12	48:AD:170:LYS:HG3	1.86	0.41
48:AD:317:ARG:HD2	48:AD:319:LEU:HD21	2.02	0.41
51:AG:28:PRO:O	51:AG:29:SER:C	2.63	0.41
51:AG:35:ILE:O	51:AG:36:PRO:C	2.63	0.41
47:Ac:197:LEU:HD11	69:Ac:406:UQ6:C7	2.51	0.41
48:Ad:185:ALA:O	48:Ad:188:ALA:N	2.54	0.41
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG21	2.03	0.41
49:Ae:231:PHE:CD2	49:Ae:250:ARG:NH1	2.88	0.41
54:Ak:48:ILE:O	54:Ak:49:ASN:C	2.62	0.41
1:A:108:GLN:HE22	10:J:171:ARG:HD3	1.84	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:210:ARG:NE	42:q:78:ASP:OD1	2.53	0.41
3:C:229:PHE:O	17:Q:123:ASN:ND2	2.54	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.55	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
10:J:60:LEU:O	10:J:64:LEU:HB2	2.20	0.41
10:J:98:MET:HE2	10:J:98:MET:HB3	1.82	0.41
12:L:112:PRO:CD	39:n:97:TYR:CE2	3.03	0.41
12:L:182:PHE:HE2	12:L:186:MET:CE	2.32	0.41
12:L:258:PHE:O	12:L:261:VAL:HG22	2.20	0.41
12:L:296:ASN:CG	12:L:357:ARG:HE	2.28	0.41
12:L:466:PHE:HB2	35:j:68:TRP:CH2	2.50	0.41
13:M:4:ILE:CD1	13:M:41:LEU:HD21	2.51	0.41
13:M:178:ILE:O	13:M:179:LEU:C	2.60	0.41
13:M:250:LEU:HD12	13:M:250:LEU:C	2.39	0.41
13:M:301:ILE:HG22	13:M:301:ILE:O	2.19	0.41
14:N:152:THR:HG22	24:Y:138:PHE:HB3	2.02	0.41
14:N:233:LEU:CD2	14:N:241:LEU:HD12	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:164:TYR:CE1	15:O:201:PRO:HD3	2.56	0.41
17:Q:52:LEU:HD23	22:W:19:SER:O	2.20	0.41
17:Q:111:LEU:HD11	42:q:126:PRO:HG2	2.03	0.41
18:R:38:TYR:HE2	18:R:44:ARG:NE	2.19	0.41
20:T:87:LEU:HD11	20:T:141:PRO:HG3	2.03	0.41
20:T:100:VAL:O	20:T:141:PRO:HD2	2.20	0.41
22:W:78:ASP:HA	22:W:79:PRO:HD3	1.94	0.41
23:X:162:LYS:HE3	23:X:163:HIS:CD2	2.55	0.41
62:a:101:CDL:CA3	42:q:13:GLN:HE22	2.29	0.41
28:c:69:TYR:O	28:c:73:ASN:ND2	2.54	0.41
30:e:49:GLY:O	30:e:52:ALA:N	2.53	0.41
31:f:5:GLN:O	31:f:9:GLU:HB2	2.20	0.41
32:g:71:PHE:CE2	32:g:73:GLY:HA2	2.55	0.41
34:i:74:HIS:O	34:i:78:PRO:HG2	2.20	0.41
34:i:106:PRO:HG3	34:i:120:MET:HG2	2.02	0.41
35:j:99:ILE:HA	40:o:108:LEU:CD2	2.51	0.41
42:q:56:PHE:HD2	43:r:27:ARG:HH22	1.68	0.41
45:AA:92:PHE:HD1	45:AA:168:ILE:HD12	1.85	0.41
46:AB:64:PHE:CZ	46:AB:394:SER:HA	2.56	0.41
46:AB:225:VAL:HG22	46:AB:229:VAL:HG21	2.01	0.41
47:AC:133:LEU:HD23	47:AC:133:LEU:HA	1.85	0.41
47:AC:215:ALA:HB2	50:AF:60:MET:HE3	2.02	0.41
47:AC:264:THR:O	47:AC:265:PRO:C	2.59	0.41
48:AD:306:MET:C	48:AD:308:ARG:N	2.78	0.41
49:AI:42:VAL:CG1	45:Aa:283:PRO:HB2	2.42	0.41
46:Ab:284:ASN:HB3	46:Ab:419:VAL:HG21	2.01	0.41
46:Ab:286:PHE:CD1	46:Ab:427:ALA:HB1	2.54	0.41
46:Ab:407:MET:HE1	46:Ab:415:GLN:CD	2.45	0.41
55:Ac:404:3PE:H12	62:Ac:407:CDL:OB3	2.21	0.41
48:Ad:117:TYR:CE1	48:Ad:127:MET:HG2	2.55	0.41
48:Ad:202:ARG:HG3	48:Ad:278:SER:HB3	2.02	0.41
51:Ag:41:ARG:NH1	62:Ag:101:CDL:OA3	2.51	0.41
53:Aj:52:LEU:HD22	53:Aj:52:LEU:HA	1.86	0.41
1:A:61:THR:O	1:A:62:PHE:C	2.64	0.41
1:A:63:LEU:CD1	10:J:63:MET:HA	2.50	0.41
1:A:108:GLN:CG	1:A:109:LYS:N	2.80	0.41
3:C:77:VAL:HG22	3:C:83:LEU:HD13	2.03	0.41
4:D:50:ALA:C	4:D:51:VAL:HG13	2.45	0.41
5:E:78:VAL:CA	5:E:104:LEU:HD13	2.46	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.01	0.41
7:G:163:LYS:HD3	7:G:163:LYS:HA	1.84	0.41
8:H:23:VAL:HG11	26:a:9:LEU:CD2	2.50	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
58:I:302:PC1:H122	25:Z:35:MET:HE1	2.01	0.41
10:J:87:LEU:HD23	10:J:87:LEU:C	2.46	0.41
12:L:253:VAL:HB	12:L:310:LEU:CD1	2.50	0.41
12:L:296:ASN:ND2	39:n:78:GLN:HB3	2.36	0.41
62:L:705:CDL:H361	33:h:72:LYS:HG3	2.03	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.03	0.41
13:M:329:LEU:HD23	13:M:437:MET:CE	2.49	0.41
14:N:83:THR:HG22	14:N:84:TRP:N	2.35	0.41
14:N:317:GLN:HB3	15:O:301:LYS:HB2	2.01	0.41
15:O:262:GLU:O	15:O:265:ASP:HB3	2.21	0.41
16:P:75:ARG:HH21	22:W:113:THR:HG23	1.86	0.41
16:P:285:HIS:ND1	16:P:361:TRP:HB3	2.36	0.41
16:P:293:LEU:HD12	16:P:294:PRO:HD2	2.01	0.41
18:R:72:VAL:HG12	18:R:73:GLU:H	1.85	0.41
28:c:72:ARG:HD2	29:d:20:SER:CA	2.50	0.41
30:e:32:ARG:O	30:e:33:CYS:CB	2.69	0.41
30:e:93:THR:HA	30:e:94:PRO:HD3	1.92	0.41
35:j:47:PHE:O	35:j:48:PRO:C	2.62	0.41
35:j:102:ASP:O	35:j:103:ASP:HB2	2.21	0.41
37:l:122:THR:HG22	37:l:124:VAL:H	1.85	0.41
40:o:39:MET:CE	40:o:58:TYR:HA	2.51	0.41
41:p:91:GLN:O	41:p:91:GLN:HG2	2.21	0.41
43:r:113:LEU:HD12	43:r:113:LEU:HA	1.77	0.41
45:AA:192:PHE:HD1	45:AA:269:ARG:O	2.04	0.41
47:AC:236:PHE:CE1	71:AD:402:3PH:H291	2.56	0.41
47:AC:284:ILE:HG21	47:AC:289:GLY:HA3	2.02	0.41
48:AD:221:PRO:HB3	48:AD:233:PHE:HB2	2.03	0.41
51:AG:26:ALA:C	51:AG:28:PRO:HD3	2.46	0.41
52:AH:49:GLU:HA	52:AH:52:ASP:CG	2.45	0.41
45:Aa:464:GLN:HA	51:Ag:5:PHE:HB3	2.03	0.41
46:Ab:426:LYS:HA	46:Ab:429:LYS:NZ	2.36	0.41
47:Ac:235:MET:HB2	62:Ag:101:CDL:H762	2.02	0.41
48:Ad:141:THR:HG23	53:Aj:53:TRP:CZ2	2.56	0.41
48:Ad:195:PRO:CG	70:Ad:401:HEC:HAA1	2.50	0.41
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.41
55:A:401:3PE:H291	10:J:37:PHE:HZ	1.84	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:193:GLU:HG3	5:E:217:PRO:HG3	2.02	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
5:E:241:GLY:HA3	6:F:63:TYR:CZ	2.56	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.41
10:J:92:LEU:HD23	10:J:92:LEU:C	2.46	0.41
12:L:368:PHE:HB3	12:L:445:GLU:OE1	2.20	0.41
12:L:519:TYR:O	12:L:520:SER:C	2.62	0.41
12:L:571:THR:O	12:L:574:THR:HG22	2.20	0.41
12:L:586:LEU:HD21	24:Y:47:PRO:HD3	2.03	0.41
55:L:707:3PE:H2A1	14:N:288:LEU:HD13	2.02	0.41
55:L:707:3PE:H341	55:L:707:3PE:H371	1.91	0.41
13:M:16:TRP:HZ2	55:M:502:3PE:C28	2.34	0.41
13:M:22:LYS:HE3	13:M:26:ASN:HD21	1.86	0.41
13:M:216:LEU:CG	13:M:220:HIS:CE1	2.88	0.41
13:M:264:LEU:HD23	38:m:98:LEU:HD21	2.01	0.41
13:M:350:MET:HE3	13:M:350:MET:HB2	1.80	0.41
14:N:81:LEU:CD2	30:e:60:PHE:HE1	2.33	0.41
14:N:103:SER:O	14:N:107:GLY:N	2.54	0.41
14:N:200:LEU:CD2	14:N:265:ILE:HG23	2.51	0.41
15:O:117:PHE:CE1	15:O:128:SER:CB	2.96	0.41
15:O:150:LEU:O	15:O:154:GLY:HA2	2.20	0.41
15:O:287:ASP:HB3	15:O:290:THR:HG23	2.02	0.41
25:Z:19:ILE:HG22	25:Z:20:ASP:N	2.36	0.41
25:Z:89:GLU:CD	30:e:97:HIS:CG	2.98	0.41
27:b:49:THR:HA	27:b:50:PRO:HD3	1.89	0.41
30:e:65:GLU:OE2	30:e:71:LYS:N	2.54	0.41
31:f:36:ALA:O	31:f:37:PHE:C	2.61	0.41
32:g:148:PRO:O	41:p:167:ARG:NH2	2.53	0.41
34:i:102:PRO:CG	41:p:18:PRO:HD2	2.49	0.41
35:j:81:LEU:O	35:j:81:LEU:HD23	2.20	0.41
37:l:44:THR:HG23	37:l:46:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:63:GLU:O	37:l:64:PRO:C	2.63	0.41
49:AE:152:ILE:HD13	49:AE:169:TRP:CD1	2.56	0.41
49:AE:159:ILE:HG23	49:AE:163:LYS:HB3	2.03	0.41
49:AE:255:PRO:HG2	47:Ac:287:LYS:NZ	2.35	0.41
45:Aa:171:GLU:O	45:Aa:174:GLU:HG2	2.21	0.41
45:Aa:206:GLU:H	45:Aa:206:GLU:CD	2.27	0.41
45:Aa:361:ASP:OD1	45:Aa:361:ASP:N	2.54	0.41
47:Ac:8:HIS:HB3	47:Ac:11:PHE:HD2	1.85	0.41
47:Ac:133:LEU:HD23	47:Ac:133:LEU:HA	1.85	0.41
47:Ac:264:THR:O	47:Ac:265:PRO:C	2.63	0.41
48:Ad:124:CYS:HB3	48:Ad:194:PRO:CG	2.51	0.41
48:Ad:131:ALA:O	48:Ad:132:TYR:C	2.64	0.41
48:Ad:148:LEU:HA	48:Ad:151:GLU:CD	2.46	0.41
48:Ad:154:VAL:HG11	48:Ad:173:ASP:OD1	2.21	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.41
1:A:52:SER:O	1:A:55:PHE:HB2	2.21	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.51	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.84	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:99:ASN:OD1	26:a:40:ARG:HG3	2.21	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
8:H:303:TRP:HZ3	27:b:28:LEU:HG	1.84	0.41
8:H:317:TYR:CZ	26:a:40:ARG:NH1	2.78	0.41
10:J:33:ILE:HG12	10:J:64:LEU:HD23	2.02	0.41
10:J:107:ASN:O	10:J:108:TYR:C	2.63	0.41
10:J:126:TYR:O	25:Z:120:LEU:HD13	2.08	0.41
12:L:3:ILE:HG22	12:L:49:LEU:CD2	2.51	0.41
12:L:61:TYR:HA	34:i:98:VAL:O	2.21	0.41
12:L:321:GLN:NE2	12:L:324:LEU:HD13	2.36	0.41
12:L:441:ILE:HD13	35:j:48:PRO:HD3	2.02	0.41
12:L:466:PHE:HE1	35:j:72:ARG:CZ	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:481:THR:CG2	40:o:95:TYR:CE2	3.03	0.41
12:L:570:HIS:O	12:L:573:MET:N	2.54	0.41
55:L:701:3PE:H122	34:i:89:HIS:CB	2.51	0.41
13:M:6:LEU:O	13:M:7:PRO:C	2.60	0.41
13:M:7:PRO:HG3	31:f:20:PHE:CA	2.51	0.41
13:M:72:LEU:O	13:M:76:MET:N	2.45	0.41
13:M:160:LEU:O	13:M:164:LEU:HD13	2.21	0.41
13:M:164:LEU:HB3	13:M:174:LEU:HD11	2.03	0.41
13:M:175:ASN:ND2	33:h:143:GLU:HG2	2.31	0.41
13:M:303:ILE:HG13	13:M:385:LEU:HD23	2.03	0.41
13:M:391:PHE:HE2	55:M:503:3PE:C23	2.34	0.41
14:N:89:GLN:HG2	30:e:60:PHE:CE2	2.56	0.41
14:N:124:LEU:CD2	14:N:176:ARG:HD3	2.51	0.41
14:N:131:LEU:O	14:N:135:LYS:HG3	2.21	0.41
14:N:194:LEU:HD13	14:N:201:THR:HG21	2.03	0.41
14:N:215:MET:HE3	14:N:215:MET:HB3	1.96	0.41
15:O:42:ALA:O	15:O:45:LEU:C	2.64	0.41
15:O:63:ASP:HB3	15:O:245:PHE:HE2	1.84	0.41
15:O:90:GLY:H	15:O:93:TYR:HB2	1.85	0.41
15:O:105:ASP:OD1	15:O:106:ILE:N	2.54	0.41
15:O:354:LEU:HD12	15:O:354:LEU:HA	1.95	0.41
16:P:243:ALA:O	16:P:244:ASP:C	2.63	0.41
18:R:42:ASP:C	18:R:43:TYR:O	2.61	0.41
18:R:48:PHE:CE2	18:R:53:LYS:HB2	2.56	0.41
20:T:99:SER:HB2	20:T:102:SER:HB2	2.02	0.41
20:U:83:VAL:HG13	20:U:122:MET:SD	2.61	0.41
20:U:128:PHE:CZ	20:U:148:ILE:CD1	3.04	0.41
21:V:98:LYS:HG2	21:V:100:TRP:CZ2	2.55	0.41
22:W:24:PHE:HB2	22:W:83:ASP:OD2	2.20	0.41
24:Y:5:LYS:C	24:Y:7:PHE:N	2.77	0.41
24:Y:51:THR:HG23	24:Y:52:LEU:N	2.35	0.41
62:a:101:CDL:HA62	42:q:6:VAL:O	2.21	0.41
29:d:11:LEU:HD22	30:e:5:ASP:O	2.20	0.41
29:d:25:LYS:HE3	29:d:27:ASN:OD1	2.21	0.41
29:d:45:ASP:O	29:d:46:ASN:C	2.62	0.41
30:e:83:ARG:O	30:e:87:MET:HG3	2.20	0.41
34:i:29:SER:O	34:i:32:GLU:HB2	2.21	0.41
34:i:125:ASP:O	34:i:126:GLN:C	2.63	0.41
35:j:89:PRO:O	40:o:103:GLU:HG2	2.21	0.41
37:l:129:MET:HE3	37:l:129:MET:HB2	1.89	0.41
38:m:50:GLN:O	38:m:50:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:59:HIS:O	38:m:60:ILE:C	2.64	0.41
39:n:41:ALA:C	39:n:43:LEU:N	2.78	0.41
39:n:165:PRO:O	39:n:166:LEU:C	2.64	0.41
40:o:50:GLN:OE1	41:p:120:ASN:ND2	2.54	0.41
40:o:71:ARG:NH1	40:o:72:ASP:OD1	2.54	0.41
41:p:40:VAL:O	41:p:44:PRO:HG2	2.20	0.41
45:AA:365:ILE:O	45:AA:369:VAL:HG23	2.21	0.41
45:AA:412:ASP:O	45:AA:416:SER:OG	2.32	0.41
46:AB:176:ASN:CB	46:AB:258:ILE:HD11	2.51	0.41
47:AC:49:LEU:HD13	47:Ac:184:ILE:HD12	2.03	0.41
47:AC:295:ILE:HG22	47:AC:299:LEU:HD12	2.03	0.41
48:AD:235:PRO:HA	48:AD:240:GLN:CG	2.50	0.41
48:AD:281:GLU:O	48:AD:282:HIS:C	2.64	0.41
49:AE:244:ASP:OD2	49:AE:248:ARG:NE	2.54	0.41
55:AF:201:3PE:H381	55:AF:201:3PE:H222	2.03	0.41
51:AG:29:SER:CB	51:AG:32:SER:HB2	2.38	0.41
51:AG:57:TYR:O	51:AG:61:THR:HG23	2.21	0.41
45:Aa:92:PHE:CE2	45:Aa:161:ILE:HG23	2.56	0.41
45:Aa:93:LEU:O	45:Aa:97:ALA:N	2.53	0.41
45:Aa:341:PHE:O	45:Aa:341:PHE:CG	2.70	0.41
62:Aa:501:CDL:HB32	62:Aa:501:CDL:H1	2.02	0.41
46:Ab:64:PHE:HZ	46:Ab:394:SER:HA	1.86	0.41
46:Ab:272:VAL:HA	46:Ab:337:GLY:HA3	2.02	0.41
47:Ac:8:HIS:CG	47:Ac:11:PHE:HD2	2.38	0.41
49:Ae:162:GLY:N	49:Ae:178:HIS:O	2.53	0.41
49:Ae:172:LYS:HA	49:Ae:172:LYS:HE2	2.02	0.41
49:Ae:178:HIS:CD2	49:Ae:179:ARG:N	2.88	0.41
51:Ag:26:ALA:C	51:Ag:28:PRO:HD3	2.46	0.41
53:Aj:48:ASN:HB3	53:Aj:51:LYS:HG3	2.03	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.85	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
5:E:190:ASN:O	5:E:191:TYR:C	2.63	0.41
5:E:223:CYS:CB	6:F:133:HIS:CE1	3.04	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
6:F:45:LEU:O	6:F:46:TYR:HB2	2.21	0.41
6:F:199:ARG:HD3	44:s:80:PHE:CZ	2.48	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:357:LEU:HD13	7:G:627:SER:HG	1.84	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:THR:HG21	25:Z:33:TYR:CE2	2.56	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
10:J:2:ASN:O	10:J:3:ASN:HB2	2.20	0.41
10:J:59:TYR:HH	11:K:34:GLU:C	2.28	0.41
12:L:52:LEU:O	12:L:53:MET:C	2.62	0.41
13:M:165:ILE:HG21	14:N:268:THR:HA	2.02	0.41
13:M:248:ILE:HG13	13:M:249:ILE:H	1.85	0.41
13:M:422:HIS:CE1	38:m:56:ARG:HH22	2.38	0.41
15:O:104:LEU:HD23	15:O:104:LEU:HA	1.90	0.41
15:O:263:ALA:C	15:O:265:ASP:H	2.29	0.41
15:O:268:LYS:HA	15:O:271:GLU:OE1	2.21	0.41
16:P:96:LEU:HD12	16:P:97:MET:CA	2.51	0.41
16:P:143:ASP:OD1	16:P:147:ASN:ND2	2.54	0.41
23:X:38:LYS:HD2	23:X:131:VAL:HG12	2.02	0.41
62:X:201:CDL:H521	62:X:201:CDL:H552	1.90	0.41
30:e:49:GLY:HA2	30:e:52:ALA:HB3	2.02	0.41
31:f:7:LEU:O	31:f:8:ARG:HB2	2.21	0.41
33:h:91:ILE:O	41:p:56:HIS:CD2	2.74	0.41
36:k:81:PHE:O	36:k:85:VAL:HG23	2.21	0.41
37:l:159:LYS:HE3	37:l:161:TYR:CE1	2.56	0.41
39:n:139:GLN:O	39:n:140:LEU:C	2.64	0.41
40:o:52:THR:O	40:o:53:LEU:C	2.62	0.41
45:AA:95:HIS:HB3	45:AA:164:GLU:OE1	2.21	0.41
46:AB:40:PHE:CE1	46:AB:404:GLY:O	2.73	0.41
46:AB:258:ILE:HD13	46:AB:258:ILE:HG21	1.79	0.41
47:AC:275:LEU:O	47:AC:276:PHE:C	2.64	0.41
47:AC:294:LEU:C	47:AC:294:LEU:HD23	2.46	0.41
48:AD:306:MET:HE2	48:AD:306:MET:HB3	1.92	0.41
53:AJ:21:PHE:O	53:AJ:24:THR:HG22	2.20	0.41
45:Aa:290:ALA:HB1	45:Aa:353:LEU:HB3	2.03	0.41
45:Aa:388:VAL:HG21	45:Aa:438:ALA:HA	2.02	0.41
47:Ac:38:GLY:HA3	69:Ac:406:UQ6:H161	2.01	0.41
47:Ac:103:TYR:HD1	47:Ac:325:TYR:CD2	2.38	0.41
47:Ac:295:ILE:HG22	47:Ac:299:LEU:HD12	2.03	0.41
48:Ad:250:THR:HG23	48:Ad:262:THR:HA	2.03	0.41
49:Ae:116:LEU:HB2	53:Aj:15:PHE:CZ	2.56	0.41
49:Ae:154:ILE:N	49:Ae:271:VAL:O	2.54	0.41
51:Ag:28:PRO:O	51:Ag:29:SER:C	2.64	0.41
51:Ag:73:LYS:HD3	52:Ah:63:GLU:OE2	2.21	0.41
54:Ak:10:TYR:HA	54:Ak:13:LEU:HD12	2.03	0.41
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NE	1:A:48:ARG:HA	2.36	0.40
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.83	0.40
1:A:62:PHE:HD1	8:H:144:VAL:CG2	2.34	0.40
1:A:87:MET:HB3	1:A:87:MET:HE3	1.84	0.40
1:A:111:LEU:HD13	8:H:290:TRP:HB3	2.02	0.40
55:A:401:3PE:H332	10:J:53:LEU:HD21	2.03	0.40
2:B:84:TRP:CZ3	58:B:303:PC1:H351	2.56	0.40
2:B:117:PHE:CD2	2:B:206:LEU:HD21	2.55	0.40
2:B:120:VAL:HG21	61:H:400:UQ9:C1M	2.36	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.40
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.40
6:F:300:ILE:CG2	6:F:306:GLY:CA	2.95	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.03	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
9:I:180:HIS:CE1	16:P:100:LEU:HD21	2.55	0.40
10:J:135:LEU:CD2	26:a:42:GLN:HG3	2.44	0.40
11:K:51:SER:HA	30:e:32:ARG:NH1	2.34	0.40
12:L:68:TRP:CE3	12:L:76:LEU:CD2	3.04	0.40
12:L:283:LEU:HD12	37:l:140:MET:HE2	2.03	0.40
12:L:324:LEU:HB3	12:L:395:ILE:CD1	2.51	0.40
62:L:705:CDL:H162	62:L:705:CDL:H132	1.81	0.40
13:M:197:LEU:O	13:M:201:MET:HB2	2.21	0.40
14:N:189:TRP:CZ3	14:N:282:MET:HE3	2.57	0.40
14:N:224:SER:HB2	14:N:229:SER:HB2	2.01	0.40
14:N:323:ASN:OD1	14:N:323:ASN:C	2.61	0.40
16:P:56:ALA:HA	16:P:125:VAL:O	2.21	0.40
20:T:107:ASP:OD1	20:T:108:LEU:N	2.54	0.40
23:X:169:PHE:HD1	23:X:169:PHE:O	2.04	0.40
26:a:64:LYS:CE	26:a:66:LEU:HD12	2.31	0.40
31:f:56:TRP:CD1	33:h:134:GLU:OE1	2.73	0.40
32:g:112:MET:HE3	32:g:115:TRP:CE3	2.56	0.40
34:i:22:TRP:CE3	39:n:172:THR:CG2	3.04	0.40
34:i:32:GLU:OE2	39:n:117:ASP:N	2.53	0.40
34:i:69:LEU:HD23	34:i:69:LEU:N	2.36	0.40
39:n:157:ALA:O	39:n:158:ARG:HB2	2.21	0.40
40:o:95:TYR:O	40:o:99:MET:HG3	2.21	0.40
45:AA:298:ASN:OD1	45:AA:299:PRO:HD2	2.20	0.40
48:AD:207:GLY:O	48:AD:208:GLU:C	2.63	0.40
49:AI:64:LEU:HD12	49:AI:78:PHE:HA	2.03	0.40
45:Aa:258:GLU:C	45:Aa:259:GLU:HG2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:341:PHE:HB2	45:Aa:368:MET:HE2	2.03	0.40
46:Ab:312:SER:OG	46:Ab:357:GLN:NE2	2.40	0.40
48:Ad:129:TYR:HD2	48:Ad:198:SER:CB	2.34	0.40
49:Ae:152:ILE:O	49:Ae:272:VAL:CB	2.68	0.40
50:Af:36:ASP:OD1	50:Af:90:TYR:OH	2.38	0.40
54:Ak:39:ARG:HA	54:Ak:42:LEU:HB2	2.02	0.40
54:Ak:45:VAL:O	54:Ak:49:ASN:HB2	2.21	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
2:B:82:ILE:CG1	8:H:57:MET:CE	2.83	0.40
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.75	0.40
57:B:302:UQ1:HM21	4:D:189:THR:HG21	2.04	0.40
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.56	0.40
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.36	0.40
3:C:243:ALA:C	7:G:105:ASN:ND2	2.79	0.40
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
4:D:299:GLN:OE1	43:r:104:TRP:HB2	2.20	0.40
6:F:47:GLY:O	6:F:48:ARG:HB2	2.22	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
10:J:32:LEU:O	10:J:33:ILE:C	2.64	0.40
12:L:14:LEU:CD2	34:i:74:HIS:O	2.69	0.40
12:L:22:SER:HA	12:L:27:ILE:CG2	2.52	0.40
12:L:203:PHE:CE2	41:p:110:LEU:HD11	2.56	0.40
12:L:205:ASN:ND2	41:p:121:TYR:OH	2.52	0.40
12:L:210:LEU:O	12:L:211:ILE:C	2.62	0.40
12:L:400:ASN:HD22	12:L:409:LEU:HD11	1.85	0.40
13:M:162:ILE:CG2	14:N:271:MET:HE3	2.22	0.40
13:M:435:THR:HG23	13:M:436:LEU:N	2.36	0.40
16:P:180:SER:HB2	16:P:321:ARG:HH21	1.87	0.40
16:P:272:LEU:HD23	16:P:272:LEU:HA	1.92	0.40
17:Q:57:GLU:O	17:Q:58:LYS:C	2.65	0.40
20:U:111:ASP:OD1	20:U:112:SER:N	2.55	0.40
25:Z:59:ARG:HH21	27:b:84:LEU:H	1.68	0.40
26:a:41:VAL:O	26:a:42:GLN:C	2.64	0.40
30:e:69:ARG:CD	30:e:72:THR:HG21	2.50	0.40
32:g:125:LYS:HD3	41:p:6:ASP:OD2	2.21	0.40
33:h:87:THR:O	33:h:91:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:148:GLU:O	33:h:152:LYS:HG3	2.21	0.40
36:k:57:TRP:HA	36:k:60:MET:HB3	2.02	0.40
37:l:122:THR:CG2	37:l:129:MET:HE1	2.45	0.40
38:m:6:TYR:HB3	38:m:18:LEU:HD21	2.01	0.40
41:p:43:TRP:HB3	41:p:44:PRO:HD3	2.03	0.40
45:AA:341:PHE:O	45:AA:341:PHE:CG	2.74	0.40
46:AB:65:VAL:HG22	46:AB:218:MET:HG2	2.03	0.40
46:AB:183:LYS:HE2	46:Ab:449:PHE:CG	2.57	0.40
48:AD:218:TYR:CE1	48:AD:246:PRO:HG3	2.57	0.40
48:AD:324:PRO:O	48:AD:325:LYS:C	2.63	0.40
49:AE:196:ARG:HD2	49:AE:249:ILE:HG21	2.03	0.40
51:AG:10:ARG:NH2	51:AG:12:ARG:HD2	2.36	0.40
45:Aa:68:THR:HG23	45:Aa:135:ALA:O	2.21	0.40
45:Aa:148:ALA:O	45:Aa:152:GLN:HG2	2.20	0.40
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD2	2.57	0.40
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HB3	2.03	0.40
49:Ae:249:ILE:HG23	49:Ae:249:ILE:O	2.22	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.40
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.40
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.52	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
8:H:296:LEU:CD2	55:I:301:3PE:H351	2.51	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.40
10:J:63:MET:O	10:J:66:VAL:N	2.54	0.40
11:K:82:SER:HA	11:K:86:GLY:H	1.85	0.40
12:L:172:ILE:HG22	13:M:405:MET:HE1	2.04	0.40
12:L:553:LEU:HD21	38:m:93:ALA:O	2.22	0.40
13:M:53:SER:O	13:M:54:ASN:C	2.63	0.40
13:M:394:ILE:O	13:M:398:ILE:HG13	2.22	0.40
55:M:502:3PE:H2H2	55:M:502:3PE:H3I1	2.03	0.40
14:N:59:TYR:O	14:N:63:GLN:HG2	2.21	0.40
16:P:96:LEU:C	16:P:96:LEU:CD1	2.94	0.40
16:P:120:VAL:O	16:P:121:GLN:C	2.64	0.40
20:T:82:ARG:O	20:T:86:VAL:HG23	2.20	0.40
20:T:120:MET:O	20:T:121:ALA:C	2.63	0.40
20:U:86:VAL:CB	20:U:122:MET:HE1	2.49	0.40
20:U:113:LEU:HD23	39:n:45:ARG:NH1	2.36	0.40
20:U:133:ILE:CG2	20:U:134:ASP:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:132:LYS:HB3	23:X:132:LYS:HE2	1.84	0.40
26:a:45:TRP:NE1	26:a:49:GLU:HG3	2.36	0.40
34:i:98:VAL:HG13	41:p:115:GLN:HG2	2.03	0.40
34:i:102:PRO:HG2	34:i:104:ILE:HG23	2.03	0.40
38:m:32:ALA:O	38:m:33:GLN:C	2.63	0.40
45:AA:404:ASP:O	45:AA:408:PRO:HG2	2.21	0.40
47:AC:30:TRP:CB	47:AC:100:ARG:HD3	2.52	0.40
48:AD:179:TYR:CE1	48:AD:188:ALA:HB3	2.56	0.40
54:AK:23:MET:O	54:AK:27:VAL:HG23	2.21	0.40
45:Aa:60:ALA:O	45:Aa:61:SER:HB3	2.21	0.40
45:Aa:278:ARG:NH1	51:Ag:11:ILE:HD13	2.36	0.40
46:Ab:227:HIS:HD2	46:Ab:231:LYS:HE2	1.85	0.40
46:Ab:232:GLN:O	46:Ab:235:GLU:HG3	2.20	0.40
47:Ac:238:ILE:HD12	62:Ag:101:CDL:H772	2.03	0.40
48:Ad:192:ALA:HB3	70:Ad:401:HEC:CMD	2.51	0.40
50:Af:24:ALA:O	51:Ag:48:ARG:NH2	2.53	0.40
53:Aj:48:ASN:O	53:Aj:49:GLU:C	2.64	0.40
54:Ak:11:ARG:HD3	54:Ak:11:ARG:N	2.37	0.40
1:A:48:ARG:HB3	10:J:76:GLU:OE2	2.21	0.40
3:C:71:TYR:O	3:C:87:ILE:HA	2.21	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.65	0.40
4:D:271:ARG:HG2	8:H:281:ARG:CG	2.44	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40
8:H:264:LEU:HD21	26:a:12:MET:HE2	2.03	0.40
9:I:93:LEU:O	42:q:93:MET:CG	2.65	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.40
55:J:202:3PE:H332	55:J:202:3PE:O11	2.22	0.40
12:L:1:MET:HE1	12:L:59:MET:HE1	2.03	0.40
12:L:67:HIS:HD2	12:L:76:LEU:O	2.05	0.40
12:L:586:LEU:CD2	24:Y:47:PRO:HD3	2.50	0.40
13:M:259:TYR:HB2	13:M:260:PRO:HD3	2.03	0.40
15:O:78:ALA:CB	15:O:85:HIS:HB2	2.51	0.40
15:O:170:LEU:CD2	15:O:184:VAL:HG13	2.51	0.40
15:O:221:LYS:HD3	15:O:222:GLY:H	1.86	0.40
15:O:235:GLN:HE21	15:O:239:ASN:ND2	2.19	0.40
16:P:40:VAL:HG13	18:R:43:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:300:TRP:CE2	16:P:304:LEU:HD21	2.57	0.40
16:P:315:THR:H	16:P:318:LYS:HB3	1.86	0.40
17:Q:166:TRP:O	17:Q:167:ASN:C	2.64	0.40
18:R:38:TYR:HE2	18:R:44:ARG:HE	1.69	0.40
20:U:87:LEU:C	20:U:89:LEU:H	2.29	0.40
21:V:96:LYS:HE2	21:V:96:LYS:HB2	1.95	0.40
22:W:48:ASN:O	22:W:52:LEU:HG	2.22	0.40
23:X:143:HIS:CG	23:X:143:HIS:O	2.73	0.40
26:a:9:LEU:O	26:a:10:ALA:C	2.64	0.40
29:d:104:LYS:HB3	29:d:104:LYS:HE2	1.85	0.40
31:f:49:ARG:HG3	31:f:52:GLU:CG	2.51	0.40
31:f:53:GLU:C	31:f:54:VAL:HG13	2.46	0.40
34:i:101:LYS:HB2	40:o:50:GLN:HE21	1.87	0.40
35:j:71:TRP:HZ3	35:j:72:ARG:NH2	2.19	0.40
38:m:49:LEU:O	38:m:49:LEU:CD1	2.65	0.40
40:o:11:TRP:CD1	40:o:12:ASP:N	2.89	0.40
42:q:89:TRP:HB2	42:q:98:PRO:HD3	2.03	0.40
45:AA:73:VAL:HG11	45:AA:151:VAL:HG11	2.03	0.40
48:AD:110:ILE:HG23	48:AD:273:PHE:HA	2.04	0.40
48:AD:154:VAL:N	48:AD:167:ARG:O	2.52	0.40
48:AD:262:THR:HG22	52:AH:24:LEU:CG	2.49	0.40
50:AF:109:ALA:HB1	54:Ak:9:ARG:NH2	2.36	0.40
45:Aa:86:ASN:OD1	45:Aa:86:ASN:N	2.54	0.40
47:Ac:296:LEU:O	47:Ac:297:SER:C	2.64	0.40
71:Ad:402:3PH:H232	49:Ae:135:GLN:NE2	2.36	0.40
49:Ae:156:LEU:HB2	49:Ae:269:ASP:CA	2.50	0.40
49:Ae:216:VAL:HG13	49:Ae:221:GLY:HA2	2.03	0.40
49:Ae:254:ALA:HA	49:Ae:255:PRO:HD3	1.96	0.40
50:Af:102:ARG:HA	50:Af:105:ARG:NH2	2.37	0.40
51:Ag:10:ARG:NH2	51:Ag:12:ARG:HD2	2.37	0.40
51:Ag:43:ARG:HD3	55:Ag:102:3PE:C39	2.51	0.40
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
3:C:128:VAL:HG22	3:C:143:LYS:HB3	2.04	0.40
5:E:109:MET:HE2	7:G:196:GLY:HA3	2.04	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.37	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:145:THR:HG22	8:H:289:LEU:HD11	2.03	0.40
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:123:TRP:HB2	10:J:126:TYR:CE1	2.57	0.40
12:L:210:LEU:HD12	12:L:270:ASN:HD21	1.86	0.40
12:L:399:ILE:HG22	12:L:409:LEU:CD1	2.52	0.40
13:M:5:ILE:CG1	13:M:6:LEU:N	2.85	0.40
13:M:186:LEU:CB	13:M:253:LEU:HD13	2.52	0.40
13:M:285:LEU:CD2	13:M:410:MET:SD	3.09	0.40
14:N:220:MET:HG3	14:N:221:LEU:N	2.36	0.40
14:N:273:ASN:HD21	24:Y:143:VAL:HA	1.84	0.40
14:N:297:ILE:O	14:N:298:TYR:C	2.63	0.40
15:O:117:PHE:HE1	15:O:173:MET:HE1	1.80	0.40
15:O:247:PRO:O	15:O:248:LYS:C	2.65	0.40
15:O:276:LEU:C	15:O:276:LEU:HD12	2.46	0.40
16:P:40:VAL:HG13	18:R:43:TYR:OH	2.22	0.40
18:R:45:ARG:HD2	18:R:48:PHE:CE1	2.57	0.40
20:T:140:CYS:HB2	20:T:143:GLU:HB2	2.02	0.40
55:b:201:3PE:H361	55:b:201:3PE:H391	1.89	0.40
29:d:11:LEU:HB2	30:e:9:LYS:HB2	2.04	0.40
30:e:65:GLU:OE2	30:e:71:LYS:HB2	2.21	0.40
36:k:56:ALA:O	36:k:60:MET:N	2.53	0.40
38:m:49:LEU:HD12	38:m:49:LEU:C	2.47	0.40
38:m:124:LYS:HG2	38:m:125:PHE:CD2	2.57	0.40
40:o:18:ASP:HB3	40:o:21:LYS:HE2	2.04	0.40
40:o:25:PHE:O	40:o:26:PRO:C	2.64	0.40
41:p:45:VAL:O	41:p:46:THR:C	2.64	0.40
45:AA:57:LEU:HD12	45:AA:229:MET:O	2.22	0.40
45:AA:98:PHE:CD1	45:AA:120:LEU:HD21	2.57	0.40
46:AB:234:ALA:C	46:AB:237:PHE:O	2.65	0.40
46:AB:426:LYS:HA	46:AB:429:LYS:NZ	2.36	0.40
46:AB:453:LEU:O	46:AB:453:LEU:HD23	2.21	0.40
49:AE:168:LYS:NZ	49:AE:171:GLY:HA2	2.36	0.40
49:AE:172:LYS:HD2	47:Ac:169:SER:CB	2.51	0.40
51:AG:73:LYS:NZ	52:AH:64:ASP:O	2.55	0.40
53:AJ:11:TYR:CZ	53:AJ:16:ARG:HB2	2.56	0.40
54:AK:39:ARG:O	54:AK:40:LEU:C	2.62	0.40
45:Aa:126:ARG:HD2	45:Aa:348:TYR:OH	2.21	0.40
47:Ac:218:ILE:HG21	48:Ad:314:LEU:HD11	2.03	0.40
47:Ac:244:LEU:HA	48:Ad:285:ARG:HD2	2.02	0.40
47:Ac:294:LEU:C	47:Ac:294:LEU:HD23	2.46	0.40
68:Ac:405:U10:H121	68:Ac:405:U10:H8	1.48	0.40
48:Ad:111:ARG:HG3	48:Ad:140:TYR:CZ	2.57	0.40
48:Ad:155:GLN:HB3	48:Ad:166:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	21	58
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	420/463 (91%)	391 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	36	71
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	153/172 (89%)	144 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	573 (95%)	30 (5%)	1 (0%)	43	77
13	M	456/459 (99%)	438 (96%)	18 (4%)	0	100	100
14	N	342/345 (99%)	330 (96%)	11 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
16	P	338/377 (90%)	317 (94%)	21 (6%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	77 (95%)	4 (5%)	0	100	100
19	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	82/156 (53%)	76 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
26	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
27	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
30	e	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
31	f	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	134/189 (71%)	127 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	76 (84%)	13 (14%)	1 (1%)	11	45
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	69/104 (66%)	67 (97%)	2 (3%)	0	100	100
37	l	156/186 (84%)	143 (92%)	13 (8%)	0	100	100
38	m	125/129 (97%)	117 (94%)	8 (6%)	0	100	100
39	n	176/179 (98%)	162 (92%)	13 (7%)	1 (1%)	21	58
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
41	p	168/176 (96%)	153 (91%)	15 (9%)	0	100	100
42	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	12/104 (12%)	12 (100%)	0	0	100	100
45	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
45	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
46	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
46	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
49	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
49	Ae	181/274 (66%)	166 (92%)	15 (8%)	0	100	100
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
52	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
52	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
54	AK	33/56 (59%)	33 (100%)	0	0	100	100
54	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	11769/14118 (83%)	11186 (95%)	577 (5%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
14	N	109	ALA
34	i	124	PRO
2	B	195	PRO
39	n	156	PRO
12	L	518	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	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	365 (100%)	1 (0%)	86	84
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	81
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	127/138 (92%)	125 (98%)	2 (2%)	55	69
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	414/415 (100%)	413 (100%)	1 (0%)	87	85
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	84
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	297/325 (91%)	296 (100%)	1 (0%)	86	84
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	91/94 (97%)	90 (99%)	1 (1%)	65	74
31	f	51/53 (96%)	51 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	121/162 (75%)	121 (100%)	0	100	100
34	i	89/120 (74%)	88 (99%)	1 (1%)	65	74
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	110/121 (91%)	110 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	108/131 (82%)	108 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	14/95 (15%)	14 (100%)	0	100	100
45	AA	338/398 (85%)	337 (100%)	1 (0%)	86	84
45	Aa	349/398 (88%)	349 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	328 (100%)	0	100	100
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	203 (100%)	0	100	100
49	AE	155/224 (69%)	154 (99%)	1 (1%)	78	80
49	AI	34/224 (15%)	33 (97%)	1 (3%)	37	58
49	Ae	156/224 (70%)	155 (99%)	1 (1%)	78	80
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	62/83 (75%)	62 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	AK	26/46 (56%)	26 (100%)	0	100	100
54	AK	34/46 (74%)	34 (100%)	0	100	100
All	All	10334/12037 (86%)	10310 (100%)	24 (0%)	85	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104	MET
4	D	232	VAL
5	E	244	VAL
7	G	271	MET
10	J	60	LEU
10	J	65	VAL
12	L	3	ILE
12	L	69	VAL
13	M	218	LYS
14	N	105	LYS
16	P	316	LYS
17	Q	96	LYS
18	R	64	ILE
19	S	68	ARG
20	T	103	HIS
25	Z	7	LYS
30	e	91	LYS
34	i	72	VAL
45	AA	478	LEU
47	AC	294	LEU
49	AE	146	VAL
49	AI	14	VAL
47	Ac	294	LEU
49	Ae	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (250) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS

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Mol	Chain	Res	Type
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	36	GLN
4	D	38	GLN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	101	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	569	GLN

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Mol	Chain	Res	Type
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	32	GLN
8	H	47	GLN
8	H	97	ASN
8	H	169	GLN
8	H	171	HIS
8	H	258	ASN
8	H	284	GLN
8	H	292	ASN
9	I	126	GLN
10	J	3	ASN
10	J	107	ASN
11	K	7	ASN
12	L	2	ASN
12	L	25	ASN
12	L	102	GLN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	170	GLN
12	L	192	ASN
12	L	194	ASN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	269	ASN
12	L	296	ASN
12	L	321	GLN
12	L	354	GLN
12	L	400	ASN
12	L	452	ASN
12	L	572	ASN
12	L	579	ASN
13	M	26	ASN
13	M	44	GLN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN

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Mol	Chain	Res	Type
13	M	170	HIS
13	M	175	ASN
13	M	213	HIS
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	415	GLN
14	N	112	HIS
14	N	120	GLN
14	N	150	ASN
14	N	204	ASN
14	N	273	ASN
14	N	289	ASN
14	N	317	GLN
14	N	342	GLN
15	O	54	HIS
15	O	85	HIS
15	O	132	GLN
15	O	175	ASN
15	O	225	HIS
15	O	239	ASN
15	O	286	GLN
15	O	292	HIS
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	43	HIS
16	P	71	ASN
16	P	79	GLN
16	P	169	HIS
16	P	216	HIS
16	P	251	ASN
16	P	269	ASN
16	P	275	HIS
16	P	323	HIS
16	P	341	GLN
17	Q	51	GLN
17	Q	88	GLN
19	S	25	GLN
20	U	101	ASN
21	V	41	HIS
21	V	50	GLN

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Mol	Chain	Res	Type
22	W	29	ASN
22	W	54	GLN
23	X	30	HIS
23	X	77	HIS
23	X	151	ASN
24	Y	19	GLN
24	Y	21	HIS
24	Y	91	ASN
25	Z	112	HIS
26	a	58	ASN
27	b	69	HIS
27	b	83	ASN
29	d	59	HIS
29	d	61	GLN
29	d	79	GLN
30	e	34	HIS
31	f	10	HIS
31	f	13	HIS
32	g	52	GLN
33	h	109	HIS
33	h	154	GLN
33	h	170	GLN
33	h	181	HIS
34	i	83	HIS
35	j	83	HIS
36	k	39	GLN
36	k	66	ASN
37	l	31	HIS
37	l	83	GLN
37	l	91	GLN
37	l	106	HIS
37	l	154	GLN
38	m	75	ASN
38	m	79	ASN
39	n	13	GLN
39	n	14	GLN
39	n	26	HIS
39	n	33	HIS
39	n	53	ASN
39	n	62	GLN
39	n	74	ASN
39	n	139	GLN

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Mol	Chain	Res	Type
40	o	85	HIS
41	p	91	GLN
41	p	104	ASN
41	p	124	ASN
42	q	13	GLN
42	q	31	ASN
42	q	52	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS
43	r	21	GLN
43	r	110	GLN
44	s	84	ASN
45	AA	87	ASN
45	AA	103	ASN
45	AA	173	GLN
45	AA	207	ASN
45	AA	240	GLN
45	AA	277	HIS
45	AA	301	ASN
45	AA	305	GLN
45	AA	342	GLN
45	AA	345	ASN
45	AA	397	ASN
45	AA	402	HIS
46	AB	284	ASN
46	AB	304	ASN
46	AB	357	GLN
46	AB	365	ASN
46	AB	415	GLN
47	AC	32	ASN
47	AC	201	HIS
47	AC	260	ASN
47	AC	312	GLN
48	AD	98	HIS
48	AD	115	GLN
48	AD	189	ASN
48	AD	190	ASN
49	AE	131	ASN
49	AE	135	GLN
49	AE	227	ASN
49	AE	242	HIS

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Mol	Chain	Res	Type
50	AF	80	GLN
54	AK	16	ASN
45	Aa	49	GLN
45	Aa	87	ASN
45	Aa	103	ASN
45	Aa	119	HIS
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	207	ASN
45	Aa	240	GLN
46	Ab	227	HIS
46	Ab	284	ASN
46	Ab	290	GLN
46	Ab	291	HIS
46	Ab	303	ASN
46	Ab	304	ASN
46	Ab	357	GLN
46	Ab	415	GLN
46	Ab	443	ASN
47	Ac	32	ASN
47	Ac	148	ASN
47	Ac	260	ASN
47	Ac	312	GLN
48	Ad	115	GLN
48	Ad	155	GLN
48	Ad	190	ASN
49	Ae	131	ASN
49	Ae	135	GLN
49	Ae	227	ASN
49	Ae	242	HIS
50	Af	80	GLN
51	Ag	69	GLN
52	Ah	60	GLN
52	Ah	82	HIS
53	Aj	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 1 is monoatomic - leaving 59 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$
66	EHZ	n	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.85	11 (29%)
55	3PE	M	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
55	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
56	SF4	G	802	7	0,12,12	-	-	-	-	-
71	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
55	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
59	FES	G	803	7	0,4,4	-	-	-	-	-
62	CDL	X	201	-	66,66,99	1.09	4 (6%)	72,78,111	1.26	6 (8%)
56	SF4	I	303	9	0,12,12	-	-	-	-	-
55	3PE	L	703	-	50,50,50	0.90	2 (4%)	53,55,55	1.12	3 (5%)
58	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
68	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
69	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
55	3PE	L	707	-	44,44,50	0.96	2 (4%)	47,49,55	1.08	3 (6%)
55	3PE	M	502	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	4 (7%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
55	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
62	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.68	11 (16%)
55	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
62	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
56	SF4	I	304	9	0,12,12	-	-	-		
56	SF4	G	801	7	0,12,12	-	-	-		
69	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
55	3PE	M	501	-	50,50,50	0.91	2 (4%)	53,55,55	1.11	4 (7%)
56	SF4	B	301	2	0,12,12	-	-	-		
66	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
70	HEC	AD	401	48	50,50,50	2.80	26 (52%)	68,82,82	2.48	30 (44%)
63	ADP	O	402	-	27,29,29	1.37	4 (14%)	42,45,45	1.98	11 (26%)
55	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
55	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0
55	3PE	O	401	-	30,30,50	1.16	2 (6%)	33,35,55	1.27	3 (9%)
55	3PE	L	701	-	41,41,50	0.99	2 (4%)	44,46,55	1.03	2 (4%)
55	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
61	UQ9	H	400	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
67	HEM	AC	402	47	50,50,50	1.69	11 (22%)	66,82,82	2.17	23 (34%)
67	HEM	Ac	402	47	50,50,50	1.63	9 (18%)	66,82,82	1.98	16 (24%)
56	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	L	702	-	39,39,50	1.03	2 (5%)	42,44,55	1.10	4 (9%)
62	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
55	3PE	J	202	-	45,45,50	0.96	2 (4%)	48,50,55	1.06	3 (6%)
55	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
58	PC1	J	201	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)
59	FES	E	301	5	0,4,4	-	-	-		
60	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
62	CDL	L	706	-	85,85,99	0.99	4 (4%)	91,97,111	1.13	5 (5%)
67	HEM	AC	401	47	50,50,50	1.58	8 (16%)	66,82,82	1.76	14 (21%)
67	HEM	Ac	403	47	50,50,50	1.65	10 (20%)	66,82,82	1.70	13 (19%)
58	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
62	CDL	L	705	-	76,76,99	1.02	4 (5%)	82,88,111	1.17	5 (6%)
62	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
55	3PE	L	704	-	46,46,50	0.95	2 (4%)	49,51,55	1.08	3 (6%)
70	HEC	Ad	401	48	50,50,50	2.80	25 (50%)	68,82,82	2.44	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
55	3PE	Y	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.14	3 (7%)
57	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
55	3PE	N	401	-	36,36,50	1.06	2 (5%)	39,41,55	1.18	4 (10%)

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
66	EHZ	n	201	-	-	21/39/39/45	-
55	3PE	M	503	-	-	17/54/54/54	-
55	3PE	Ag	102	-	-	5/42/42/54	-
56	SF4	G	802	7	-	-	0/6/5/5
71	3PH	AD	402	-	-	8/37/37/49	-
55	3PE	AC	403	-	-	12/38/38/54	-
59	FES	G	803	7	-	-	0/1/1/1
62	CDL	X	201	-	-	27/77/77/110	-
56	SF4	I	303	9	-	-	0/6/5/5
55	3PE	L	703	-	-	13/54/54/54	-
58	PC1	I	302	-	-	13/50/50/57	-
68	U10	AC	404	-	-	0/15/39/87	0/1/1/1
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
71	3PH	Ad	402	-	-	8/37/37/49	-
55	3PE	L	707	-	-	13/48/48/54	-
55	3PE	M	502	-	-	14/54/54/54	-
62	CDL	h	201	-	-	23/80/80/110	-
55	3PE	I	301	-	-	17/54/54/54	-
62	CDL	Ag	101	-	-	12/66/66/110	-
64	NDP	P	401	-	-	6/34/77/77	0/5/5/5
55	3PE	AF	201	-	-	9/45/45/54	-
62	CDL	Aa	501	-	-	16/56/56/110	-
56	SF4	I	304	9	-	-	0/6/5/5
56	SF4	G	801	7	-	-	0/6/5/5
69	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
55	3PE	M	501	-	-	15/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	EHZ	W	201	-	-	22/39/39/45	-
70	HEC	AD	401	48	1/1/3/7	7/14/54/54	-
56	SF4	B	301	2	-	-	0/6/5/5
63	ADP	O	402	-	-	5/16/32/32	0/3/3/3
55	3PE	A	401	-	-	14/49/49/54	-
55	3PE	O	401	-	-	10/34/34/54	-
55	3PE	Ac	401	-	-	10/26/26/54	-
55	3PE	L	701	-	-	13/45/45/54	-
55	3PE	b	201	-	-	8/49/49/54	-
61	UQ9	H	400	-	-	13/30/54/81	0/1/1/1
67	HEM	AC	402	47	-	6/14/54/54	-
67	HEM	Ac	402	47	-	5/14/54/54	-
56	SF4	F	502	6	-	-	0/6/5/5
55	3PE	L	702	-	-	8/43/43/54	-
62	CDL	Ac	407	-	-	11/52/52/110	-
55	3PE	J	202	-	-	12/49/49/54	-
55	3PE	Ac	404	-	-	8/38/38/54	-
58	PC1	J	201	-	-	14/45/45/57	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
62	CDL	a	101	-	-	14/67/67/110	-
59	FES	E	301	5	-	-	0/1/1/1
62	CDL	L	706	-	-	27/96/96/110	-
67	HEM	AC	401	47	-	8/14/54/54	-
67	HEM	Ac	403	47	-	10/14/54/54	-
58	PC1	B	303	-	-	11/38/38/57	-
62	CDL	L	705	-	-	24/87/87/110	-
62	CDL	AC	406	-	-	18/66/66/110	-
55	3PE	L	704	-	-	13/50/50/54	-
70	HEC	Ad	401	48	1/1/3/7	7/14/54/54	-
68	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
55	3PE	Y	201	-	-	5/43/43/54	-
57	UQ1	B	302	-	-	3/9/33/33	0/1/1/1
55	3PE	N	401	-	-	8/40/40/54	-

All (217) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	404	U10	C6-C1	7.59	1.49	1.35
68	Ac	405	U10	C6-C1	7.42	1.48	1.35
69	AC	405	UQ6	C2-C3	5.95	1.49	1.39
69	Ac	406	UQ6	C2-C3	5.90	1.49	1.39
69	Ac	406	UQ6	C5-C4	5.87	1.48	1.39
69	Ac	406	UQ6	C5-C6	5.87	1.49	1.40
69	AC	405	UQ6	C5-C4	5.67	1.48	1.39
67	Ac	402	HEM	FE-NB	5.66	2.12	1.94
69	AC	405	UQ6	C5-C6	5.60	1.48	1.40
69	AC	405	UQ6	C6-C1	5.57	1.49	1.40
69	Ac	406	UQ6	C6-C1	5.46	1.49	1.40
66	W	201	EHZ	C15-N2	5.38	1.45	1.33
66	n	201	EHZ	C15-N2	5.37	1.45	1.33
70	AD	401	HEC	FE-NB	5.28	2.11	1.94
66	n	201	EHZ	C12-N1	5.19	1.45	1.33
67	AC	401	HEM	FE-NB	5.17	2.10	1.94
66	W	201	EHZ	C12-N1	5.11	1.45	1.33
67	Ac	403	HEM	FE-NB	5.08	2.10	1.94
70	AD	401	HEC	C2A-C3A	4.99	1.47	1.36
70	Ad	401	HEC	C2A-C3A	4.94	1.47	1.36
70	AD	401	HEC	C3D-C2D	4.94	1.47	1.36
70	Ad	401	HEC	FE-NB	4.93	2.10	1.94
70	AD	401	HEC	FE-ND	4.93	2.10	1.94
70	Ad	401	HEC	CHB-C4A	4.89	1.47	1.38
70	AD	401	HEC	CHB-C4A	4.87	1.47	1.38
70	Ad	401	HEC	FE-ND	4.86	2.09	1.94
70	AD	401	HEC	CHA-C1A	4.84	1.47	1.38
70	Ad	401	HEC	C3D-C2D	4.83	1.47	1.36
60	F	501	FMN	C9A-C5A	4.79	1.49	1.41
70	Ad	401	HEC	CHA-C1A	4.79	1.47	1.38
70	AD	401	HEC	C3B-C2B	4.72	1.46	1.36
69	Ac	406	UQ6	C4-C3	4.68	1.49	1.39
70	AD	401	HEC	CHD-C1D	4.68	1.48	1.38
70	Ad	401	HEC	C3B-C2B	4.67	1.46	1.36
70	Ad	401	HEC	FE-NC	4.63	2.10	1.95
67	AC	402	HEM	FE-NB	4.58	2.09	1.94
69	AC	405	UQ6	C4-C3	4.53	1.48	1.39
63	O	402	ADP	C5-C4	4.53	1.47	1.39
70	Ad	401	HEC	FE-NA	4.47	2.10	1.95
70	AD	401	HEC	FE-NA	4.42	2.10	1.95
69	AC	405	UQ6	C2-C1	4.40	1.49	1.40
62	AC	406	CDL	OB8-CB7	4.34	1.46	1.33
55	M	503	3PE	O31-C31	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	Ag	101	CDL	OB8-CB7	4.27	1.45	1.33
64	P	401	NDP	C5A-C4A	4.27	1.47	1.39
55	J	202	3PE	O31-C31	4.26	1.45	1.33
62	L	706	CDL	OB8-CB7	4.26	1.45	1.33
62	Ac	407	CDL	OA8-CA7	4.26	1.45	1.33
62	Ac	407	CDL	OB8-CB7	4.26	1.45	1.33
70	Ad	401	HEC	CHC-C4B	4.25	1.47	1.38
69	Ac	406	UQ6	C2-C1	4.25	1.48	1.40
71	AD	402	3PH	O31-C31	4.24	1.45	1.33
62	L	705	CDL	OB8-CB7	4.24	1.45	1.33
55	L	702	3PE	O31-C31	4.24	1.45	1.33
58	J	201	PC1	O31-C31	4.24	1.45	1.33
71	Ad	402	3PH	O31-C31	4.23	1.45	1.33
55	Y	201	3PE	O31-C31	4.22	1.45	1.33
55	Ag	102	3PE	O31-C31	4.22	1.45	1.33
62	a	101	CDL	OB8-CB7	4.20	1.45	1.33
55	Ac	404	3PE	O31-C31	4.20	1.45	1.33
55	M	501	3PE	O31-C31	4.19	1.45	1.33
55	L	704	3PE	O31-C31	4.18	1.45	1.33
62	L	706	CDL	OA8-CA7	4.18	1.45	1.33
55	AF	201	3PE	O31-C31	4.18	1.45	1.33
58	B	303	PC1	O31-C31	4.17	1.45	1.33
58	I	302	PC1	O31-C31	4.17	1.45	1.33
62	X	201	CDL	OB6-CB5	4.17	1.46	1.34
55	L	707	3PE	O31-C31	4.16	1.45	1.33
55	AC	403	3PE	O31-C31	4.15	1.45	1.33
55	O	401	3PE	O31-C31	4.15	1.45	1.33
55	M	502	3PE	O31-C31	4.14	1.45	1.33
62	a	101	CDL	OB6-CB5	4.14	1.46	1.34
55	b	201	3PE	O31-C31	4.14	1.45	1.33
55	L	701	3PE	O31-C31	4.13	1.45	1.33
62	L	706	CDL	OB6-CB5	4.11	1.45	1.34
62	a	101	CDL	OA8-CA7	4.11	1.45	1.33
62	h	201	CDL	OA8-CA7	4.11	1.45	1.33
62	h	201	CDL	OB8-CB7	4.11	1.45	1.33
62	L	705	CDL	OA8-CA7	4.11	1.45	1.33
55	A	401	3PE	O31-C31	4.10	1.45	1.33
55	L	701	3PE	O21-C21	4.10	1.45	1.34
58	J	201	PC1	O21-C21	4.10	1.45	1.34
58	I	302	PC1	O21-C21	4.09	1.45	1.34
62	AC	406	CDL	OA8-CA7	4.09	1.45	1.33
62	L	706	CDL	OA6-CA5	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	N	401	3PE	O21-C21	4.08	1.45	1.34
67	AC	401	HEM	FE-NC	4.08	2.09	1.95
62	X	201	CDL	OB8-CB7	4.08	1.45	1.33
62	h	201	CDL	OB6-CB5	4.08	1.45	1.34
55	I	301	3PE	O31-C31	4.08	1.45	1.33
55	N	401	3PE	O31-C31	4.07	1.45	1.33
55	M	503	3PE	O21-C21	4.06	1.45	1.34
55	AF	201	3PE	O21-C21	4.05	1.45	1.34
62	X	201	CDL	OA8-CA7	4.05	1.45	1.33
70	AD	401	HEC	FE-NC	4.05	2.08	1.95
62	a	101	CDL	OA6-CA5	4.05	1.45	1.34
55	L	702	3PE	O21-C21	4.05	1.45	1.34
62	AC	406	CDL	OB6-CB5	4.04	1.45	1.34
62	Ag	101	CDL	OA8-CA7	4.04	1.45	1.33
62	Ag	101	CDL	OB6-CB5	4.04	1.45	1.34
58	B	303	PC1	O21-C21	4.04	1.45	1.34
55	L	703	3PE	O21-C21	4.03	1.45	1.34
62	Ac	407	CDL	OA6-CA5	4.03	1.45	1.34
55	L	704	3PE	O21-C21	4.02	1.45	1.34
62	h	201	CDL	OA6-CA5	4.02	1.45	1.34
55	b	201	3PE	O21-C21	4.01	1.45	1.34
55	AC	403	3PE	O21-C21	4.01	1.45	1.34
55	Ag	102	3PE	O21-C21	4.00	1.45	1.34
55	L	703	3PE	O31-C31	4.00	1.45	1.33
55	J	202	3PE	O21-C21	3.99	1.45	1.34
55	O	401	3PE	O21-C21	3.99	1.45	1.34
62	L	705	CDL	OB6-CB5	3.98	1.45	1.34
55	I	301	3PE	O21-C21	3.97	1.45	1.34
55	A	401	3PE	O21-C21	3.96	1.45	1.34
67	Ac	403	HEM	C1B-NB	-3.95	1.33	1.40
55	M	501	3PE	O21-C21	3.95	1.45	1.34
62	Ag	101	CDL	OA6-CA5	3.95	1.45	1.34
55	L	707	3PE	O21-C21	3.94	1.45	1.34
62	Ac	407	CDL	OB6-CB5	3.93	1.45	1.34
55	Y	201	3PE	O21-C21	3.93	1.45	1.34
67	AC	402	HEM	FE-NC	3.91	2.08	1.95
71	AD	402	3PH	O21-C21	3.91	1.45	1.34
67	Ac	403	HEM	FE-NC	3.91	2.08	1.95
67	AC	402	HEM	C1B-NB	-3.91	1.33	1.40
71	Ad	402	3PH	O21-C21	3.91	1.45	1.34
62	X	201	CDL	OA6-CA5	3.90	1.45	1.34
55	Ac	404	3PE	O21-C21	3.89	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	AC	406	CDL	OA6-CA5	3.89	1.45	1.34
70	Ad	401	HEC	CHD-C1D	3.88	1.46	1.38
55	M	502	3PE	O21-C21	3.86	1.45	1.34
67	Ac	402	HEM	FE-NC	3.80	2.08	1.95
67	Ac	402	HEM	C1B-NB	-3.80	1.33	1.40
70	Ad	401	HEC	CHB-C1B	3.76	1.47	1.39
70	AD	401	HEC	CHC-C4B	3.75	1.46	1.38
62	L	705	CDL	OA6-CA5	3.73	1.44	1.34
67	Ac	403	HEM	C4D-ND	-3.66	1.34	1.40
70	AD	401	HEC	CHD-C4C	3.65	1.47	1.39
70	AD	401	HEC	CHA-C4D	3.64	1.47	1.39
70	Ad	401	HEC	CHD-C4C	3.57	1.47	1.39
67	AC	402	HEM	C4D-ND	-3.55	1.34	1.40
70	Ad	401	HEC	CHA-C4D	3.53	1.47	1.39
70	Ad	401	HEC	C1D-ND	-3.51	1.34	1.40
67	AC	401	HEM	C4D-ND	-3.44	1.34	1.40
67	AC	401	HEM	C1B-NB	-3.43	1.34	1.40
67	Ac	402	HEM	C4D-ND	-3.39	1.34	1.40
70	AD	401	HEC	C4B-NB	-3.35	1.34	1.40
70	Ad	401	HEC	C4B-NB	-3.34	1.34	1.40
70	Ad	401	HEC	CHC-C1C	3.29	1.46	1.39
64	P	401	NDP	C6N-C5N	3.26	1.39	1.33
70	AD	401	HEC	CHC-C1C	3.18	1.46	1.39
60	F	501	FMN	C8-C7	3.15	1.48	1.40
70	Ad	401	HEC	C3C-C2C	3.15	1.47	1.38
70	AD	401	HEC	CHB-C1B	3.10	1.46	1.39
68	AC	404	U10	C4-C3	3.08	1.48	1.36
67	Ac	402	HEM	C1C-C2C	-3.08	1.39	1.45
68	Ac	405	U10	C4-C3	3.04	1.48	1.36
67	AC	402	HEM	C4B-NB	-2.98	1.32	1.38
70	AD	401	HEC	C1C-NC	-2.96	1.34	1.39
57	B	302	UQ1	C3-C4	-2.96	1.40	1.48
67	AC	402	HEM	C1B-C2B	-2.94	1.38	1.44
70	AD	401	HEC	C3C-C2C	2.83	1.46	1.38
60	F	501	FMN	C4-N3	-2.75	1.33	1.38
67	AC	402	HEM	FE-ND	-2.74	1.86	1.94
70	AD	401	HEC	C1D-ND	-2.74	1.35	1.40
63	O	402	ADP	C5-C6	2.71	1.48	1.41
67	Ac	403	HEM	C1C-C2C	-2.68	1.40	1.45
61	H	400	UQ9	C4-C5	-2.68	1.41	1.48
61	H	400	UQ9	C3-C2	-2.61	1.41	1.48
67	AC	401	HEM	C1C-C2C	-2.60	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Ac	403	HEM	FE-ND	-2.58	1.86	1.94
67	AC	402	HEM	C1C-C2C	-2.57	1.40	1.45
66	n	201	EHZ	P1-O7	2.55	1.64	1.54
66	W	201	EHZ	P1-O7	2.55	1.64	1.54
64	P	401	NDP	C5A-C6A	2.52	1.48	1.41
67	Ac	402	HEM	C3C-C4C	-2.48	1.41	1.46
66	W	201	EHZ	O4-C15	-2.48	1.18	1.23
67	AC	401	HEM	FE-ND	-2.45	1.87	1.94
66	n	201	EHZ	O4-C15	-2.44	1.18	1.23
70	Ad	401	HEC	C4A-NA	-2.44	1.35	1.39
70	AD	401	HEC	C1A-NA	-2.42	1.35	1.39
70	AD	401	HEC	C4A-NA	-2.41	1.35	1.39
70	Ad	401	HEC	C1A-NA	-2.41	1.35	1.39
70	Ad	401	HEC	C4C-NC	-2.41	1.35	1.39
60	F	501	FMN	C5A-N5	-2.41	1.34	1.39
66	W	201	EHZ	C9-S1	2.40	1.81	1.76
57	B	302	UQ1	C2-C1	-2.40	1.42	1.48
70	Ad	401	HEC	C1B-C2B	2.39	1.49	1.44
66	n	201	EHZ	C9-S1	2.38	1.81	1.76
70	AD	401	HEC	C1B-C2B	2.38	1.49	1.44
66	n	201	EHZ	O3-C12	-2.38	1.18	1.23
70	Ad	401	HEC	C1C-NC	-2.37	1.35	1.39
67	Ac	403	HEM	C4B-NB	-2.36	1.33	1.38
70	AD	401	HEC	C4C-NC	-2.36	1.35	1.39
70	Ad	401	HEC	C1C-C2C	2.35	1.48	1.43
64	P	401	NDP	C8A-N7A	2.34	1.36	1.31
64	P	401	NDP	C5A-N7A	-2.34	1.34	1.39
70	AD	401	HEC	C1A-C2A	2.34	1.49	1.45
66	W	201	EHZ	O3-C12	-2.33	1.18	1.23
67	AC	402	HEM	C3C-C4C	-2.33	1.41	1.46
67	AC	402	HEM	C1D-ND	-2.29	1.34	1.38
63	O	402	ADP	C8-N7	2.27	1.35	1.31
66	n	201	EHZ	P1-OP3	-2.27	1.46	1.54
67	Ac	403	HEM	C3C-C4C	-2.26	1.42	1.46
70	Ad	401	HEC	C4D-C3D	2.23	1.48	1.45
66	W	201	EHZ	P1-OP3	-2.22	1.46	1.54
67	Ac	402	HEM	C1D-ND	-2.22	1.34	1.38
67	Ac	403	HEM	C1D-ND	-2.20	1.34	1.38
67	Ac	402	HEM	FE-ND	-2.19	1.88	1.94
63	O	402	ADP	C5-N7	-2.18	1.34	1.39
70	AD	401	HEC	C1D-C2D	2.16	1.48	1.44
67	Ac	402	HEM	C3B-C4B	2.14	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AC	401	HEM	C4B-NB	-2.13	1.34	1.38
67	AC	402	HEM	C3B-C2B	-2.11	1.33	1.37
70	AD	401	HEC	C4D-C3D	2.08	1.48	1.45
67	AC	401	HEM	C1D-ND	-2.06	1.34	1.38
60	F	501	FMN	C4A-N5	2.05	1.34	1.30
67	Ac	403	HEM	C1A-C2A	-2.02	1.40	1.44

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
63	O	402	ADP	C5-C4-N3	-6.41	118.39	126.75
66	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
66	n	201	EHZ	C8-C9-S1	6.30	121.43	113.63
67	AC	402	HEM	CHC-C4B-NB	6.28	131.24	124.42
70	AD	401	HEC	C1B-C2B-C3B	-6.23	100.41	106.96
70	AD	401	HEC	C2B-C1B-NB	6.06	117.14	109.88
64	P	401	NDP	C5A-C4A-N3A	-6.05	118.85	126.75
70	Ad	401	HEC	C1B-C2B-C3B	-5.58	101.09	106.96
69	AC	405	UQ6	C7-C8-C9	-5.55	118.63	127.24
67	AC	401	HEM	CHC-C4B-NB	5.48	130.37	124.42
70	Ad	401	HEC	C2D-C1D-ND	5.42	116.26	109.84
70	Ad	401	HEC	C1C-C2C-C3C	-5.24	100.70	106.83
70	Ad	401	HEC	C2A-C1A-NA	5.03	115.22	110.32
62	X	201	CDL	OA6-CA5-C11	5.01	122.30	111.50
63	O	402	ADP	N3-C4-N9	4.93	135.21	127.08
70	AD	401	HEC	C2A-C1A-NA	4.92	115.11	110.32
70	AD	401	HEC	C3D-C4D-ND	4.92	115.12	110.36
67	Ac	402	HEM	C3B-C2B-C1B	4.83	110.07	106.49
67	AC	402	HEM	CHD-C1D-ND	4.80	129.63	124.42
64	P	401	NDP	N3A-C4A-N9A	4.76	134.92	127.08
67	AC	402	HEM	C3B-C2B-C1B	-4.70	103.00	106.49
67	AC	402	HEM	CHB-C1B-NB	4.67	130.13	124.37
70	Ad	401	HEC	C3D-C4D-ND	4.60	114.81	110.36
67	AC	401	HEM	CHD-C1D-ND	4.55	129.36	124.42
70	Ad	401	HEC	C2B-C1B-NB	4.54	115.32	109.88
55	M	503	3PE	O21-C21-C22	4.50	121.20	111.50
62	h	201	CDL	OB6-CB5-C51	4.46	121.11	111.50
67	Ac	403	HEM	CHC-C4B-NB	4.43	129.23	124.42
67	Ac	402	HEM	CHD-C1D-ND	4.43	129.23	124.42
55	N	401	3PE	O21-C21-C22	4.37	120.92	111.50
55	M	502	3PE	O21-C21-C22	4.37	120.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	L	703	3PE	O21-C21-C22	4.35	120.89	111.50
67	AC	402	HEM	C4B-C3B-C2B	4.35	110.57	107.11
70	AD	401	HEC	C3B-C4B-NB	4.34	115.00	110.17
62	a	101	CDL	OA6-CA5-C11	4.33	120.84	111.50
67	Ac	403	HEM	CHD-C1D-ND	4.32	129.11	124.42
55	O	401	3PE	O21-C21-C22	4.32	120.80	111.50
70	AD	401	HEC	C2D-C1D-ND	4.27	114.90	109.84
70	Ad	401	HEC	C2C-C1C-NC	4.25	116.55	110.08
58	I	302	PC1	O21-C21-C22	4.23	120.61	111.50
62	X	201	CDL	OB6-CB5-C51	4.23	120.61	111.50
55	Ac	404	3PE	O21-C21-C22	4.22	120.61	111.50
62	L	706	CDL	OA6-CA5-C11	4.20	120.56	111.50
62	L	706	CDL	OB6-CB5-C51	4.20	120.55	111.50
70	Ad	401	HEC	C1D-C2D-C3D	-4.20	102.54	106.96
55	Ag	102	3PE	O21-C21-C22	4.11	120.36	111.50
62	a	101	CDL	OB6-CB5-C51	4.07	120.28	111.50
67	Ac	403	HEM	CHA-C4D-ND	4.07	129.39	124.37
67	Ac	402	HEM	CHC-C4B-NB	4.06	128.83	124.42
70	AD	401	HEC	C1C-C2C-C3C	-4.05	102.09	106.83
68	AC	404	U10	C7-C8-C9	-4.04	120.07	126.79
62	Ag	101	CDL	OA6-CA5-C11	4.02	120.17	111.50
70	AD	401	HEC	CMC-C2C-C3C	4.02	134.30	125.61
55	J	202	3PE	O21-C21-C22	4.01	120.14	111.50
58	J	201	PC1	O21-C21-C22	4.01	120.13	111.50
62	Ac	407	CDL	OB6-CB5-C51	4.00	120.12	111.50
62	h	201	CDL	OA6-CA5-C11	3.96	120.03	111.50
70	AD	401	HEC	C1D-C2D-C3D	-3.95	102.80	106.96
62	Ag	101	CDL	OB6-CB5-C51	3.95	120.01	111.50
67	AC	402	HEM	CHA-C4D-ND	3.93	129.23	124.37
63	O	402	ADP	C2-N3-C4	3.92	121.01	111.75
70	Ad	401	HEC	CBB-CAB-C3B	3.89	123.16	112.43
70	AD	401	HEC	C2C-C1C-NC	3.86	115.96	110.08
55	M	501	3PE	O21-C21-C22	3.86	119.82	111.50
67	AC	401	HEM	CHA-C4D-ND	3.85	129.12	124.37
55	AC	403	3PE	O21-C21-C22	3.84	119.77	111.50
70	AD	401	HEC	CBB-CAB-C3B	3.82	122.95	112.43
58	B	303	PC1	O21-C21-C22	3.81	119.71	111.50
64	P	401	NDP	C2A-N3A-C4A	3.81	120.74	111.75
55	A	401	3PE	O21-C21-C22	3.76	119.61	111.50
62	AC	406	CDL	OA6-CA5-C11	3.76	119.61	111.50
55	L	704	3PE	O21-C21-C22	3.75	119.58	111.50
55	Y	201	3PE	O21-C21-C22	3.75	119.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Ac	405	U10	C22-C23-C24	-3.74	118.65	127.66
67	AC	401	HEM	C1B-NB-C4B	3.72	108.92	105.07
62	AC	406	CDL	OB6-CB5-C51	3.72	119.52	111.50
68	Ac	405	U10	C12-C13-C14	-3.71	118.72	127.66
62	X	201	CDL	CA4-OA6-CA5	-3.71	108.67	117.79
67	AC	401	HEM	CHB-C1B-NB	3.68	128.91	124.37
55	I	301	3PE	O21-C21-C22	3.68	119.43	111.50
67	AC	402	HEM	CHB-C1B-C2B	-3.64	116.61	126.73
55	L	707	3PE	O21-C21-C22	3.64	119.34	111.50
55	L	701	3PE	O21-C21-C22	3.62	119.30	111.50
69	AC	405	UQ6	C15-C14-C16	3.60	121.33	115.27
55	L	702	3PE	O21-C21-C22	3.58	119.22	111.50
62	L	705	CDL	OA6-CA5-C11	3.58	119.22	111.50
67	Ac	403	HEM	CHB-C1B-NB	3.57	128.77	124.37
64	P	401	NDP	PN-O3-PA	-3.56	120.62	132.83
67	Ac	402	HEM	CHA-C4D-ND	3.55	128.76	124.37
71	AD	402	3PH	O21-C21-C22	3.54	119.13	111.50
70	AD	401	HEC	C1A-C2A-C3A	-3.52	102.54	107.13
55	b	201	3PE	O21-C21-C22	3.51	119.07	111.50
70	Ad	401	HEC	C3C-C4C-NC	3.49	114.05	110.15
70	Ad	401	HEC	CBC-CAC-C3C	3.48	122.04	112.43
55	b	201	3PE	C2-O21-C21	-3.48	109.22	117.79
71	Ad	402	3PH	O21-C21-C22	3.44	118.91	111.50
62	L	705	CDL	CA4-OA6-CA5	-3.41	109.40	117.79
62	Ac	407	CDL	OA6-CA5-C11	3.41	120.31	110.80
69	Ac	406	UQ6	C7-C8-C9	-3.40	121.97	127.24
63	O	402	ADP	C4-C5-N7	-3.40	106.48	110.62
62	L	705	CDL	OB6-CB5-C51	3.38	118.79	111.50
62	Ac	407	CDL	OB8-CB7-C71	3.38	120.24	111.38
70	Ad	401	HEC	C1A-C2A-C3A	-3.36	102.74	107.13
67	Ac	403	HEM	C1B-NB-C4B	3.34	108.53	105.07
55	AF	201	3PE	O21-C21-C22	3.33	118.67	111.50
55	M	502	3PE	C2-O21-C21	-3.33	109.60	117.79
70	Ad	401	HEC	C3B-C4B-NB	3.32	113.86	110.17
64	P	401	NDP	C4A-C5A-N7A	-3.31	106.59	110.62
67	AC	401	HEM	C4C-NC-C1C	3.25	108.53	105.35
67	Ac	402	HEM	CHD-C4C-NC	3.22	127.92	124.44
70	AD	401	HEC	CHC-C1C-C2C	-3.20	118.20	127.24
67	AC	402	HEM	C4C-NC-C1C	3.19	108.47	105.35
67	AC	402	HEM	C1B-NB-C4B	3.17	108.35	105.07
70	Ad	401	HEC	CBD-CAD-C3D	-3.13	103.93	112.63
63	O	402	ADP	N3-C2-N1	-3.13	123.71	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Ac	405	U10	C15-C14-C16	3.11	120.51	115.27
68	AC	404	U10	C10-C9-C11	3.11	120.50	115.27
66	W	201	EHZ	C13-C12-N1	3.10	121.64	116.42
66	n	201	EHZ	C13-C12-N1	3.09	121.62	116.42
64	P	401	NDP	N3A-C2A-N1A	-3.09	123.78	128.60
55	M	501	3PE	O31-C31-C32	3.08	121.58	111.91
62	L	705	CDL	OB8-CB7-C71	3.07	121.55	111.91
63	O	402	ADP	PA-O3A-PB	-3.07	122.31	132.83
67	Ac	403	HEM	C4C-NC-C1C	3.05	108.33	105.35
67	Ac	402	HEM	C1B-NB-C4B	3.05	108.22	105.07
68	Ac	405	U10	C10-C9-C11	3.04	120.39	115.27
67	Ac	402	HEM	CHD-C1D-C2D	-3.04	120.23	124.98
66	n	201	EHZ	C14-C13-C12	-3.03	107.31	112.36
67	AC	402	HEM	C4D-ND-C1D	3.03	108.20	105.07
66	W	201	EHZ	C14-C13-C12	-3.02	107.33	112.36
55	M	503	3PE	O31-C31-C32	3.02	121.38	111.91
55	L	702	3PE	O31-C31-C32	3.02	121.37	111.91
62	Ag	101	CDL	CA4-OA6-CA5	-3.02	110.37	117.79
55	Ac	404	3PE	C2-O21-C21	-3.00	110.40	117.79
70	Ad	401	HEC	CAD-C3D-C4D	2.97	129.85	124.66
70	AD	401	HEC	C3A-C4A-NA	2.96	115.16	109.69
68	Ac	405	U10	C20-C19-C21	2.96	120.25	115.27
70	Ad	401	HEC	C3A-C4A-NA	2.96	115.14	109.69
68	Ac	405	U10	C1M-C1-C6	-2.92	119.63	124.40
67	Ac	402	HEM	C4C-NC-C1C	2.92	108.21	105.35
70	Ad	401	HEC	C4D-C3D-C2D	-2.91	102.66	106.90
55	O	401	3PE	O31-C31-C32	2.91	121.04	111.91
66	W	201	EHZ	OP3-P1-O9	-2.90	99.33	110.68
67	AC	402	HEM	CHD-C4C-NC	2.89	127.57	124.44
66	n	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
66	W	201	EHZ	C7-C8-C9	-2.89	107.30	113.89
67	AC	402	HEM	C2B-C1B-NB	2.89	113.26	109.84
66	n	201	EHZ	C7-C8-C9	-2.88	107.33	113.89
55	Ag	102	3PE	O31-C31-C32	2.86	120.89	111.91
64	P	401	NDP	C4A-N9A-C8A	2.86	108.83	105.73
55	M	501	3PE	C2-O21-C21	-2.86	110.76	117.79
68	Ac	405	U10	C17-C18-C19	-2.85	120.80	127.66
70	Ad	401	HEC	C4A-C3A-C2A	-2.85	102.78	106.94
69	AC	405	UQ6	C10-C9-C11	2.85	120.06	115.27
55	N	401	3PE	O31-C31-C32	2.84	120.82	111.91
58	I	302	PC1	C2-O21-C21	-2.83	110.83	117.79
70	AD	401	HEC	CAA-C2A-C1A	2.82	130.21	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AC	403	3PE	C2-O21-C21	-2.82	110.85	117.79
71	AD	402	3PH	O31-C31-C32	2.81	120.74	111.91
62	L	706	CDL	OB8-CB7-C71	2.81	120.73	111.91
70	Ad	401	HEC	CMB-C2B-C1B	2.81	129.32	125.04
62	h	201	CDL	OB8-CB7-C71	2.81	120.72	111.91
67	AC	402	HEM	C4A-CHB-C1B	-2.80	119.69	126.34
62	L	706	CDL	OA8-CA7-C31	2.80	120.69	111.91
64	P	401	NDP	C5A-N7A-C8A	2.79	107.47	103.51
58	B	303	PC1	O31-C31-C32	2.78	120.62	111.91
62	Ac	407	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
70	Ad	401	HEC	CHD-C1D-C2D	-2.77	119.04	126.73
69	Ac	406	UQ6	C10-C9-C11	2.77	119.92	115.27
69	Ac	406	UQ6	C4M-O4-C4	2.76	122.35	114.78
62	Ac	407	CDL	CB4-OB6-CB5	-2.75	111.01	117.79
69	AC	405	UQ6	C12-C13-C14	-2.75	121.03	127.66
55	J	202	3PE	C2-O21-C21	-2.75	111.03	117.79
67	AC	402	HEM	CHD-C1D-C2D	-2.74	120.69	124.98
63	O	402	ADP	C5-N7-C8	2.74	107.40	103.51
62	a	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
62	a	101	CDL	CA4-OA6-CA5	-2.74	111.06	117.79
55	Y	201	3PE	O31-C31-C32	2.73	120.49	111.91
55	L	703	3PE	O31-C31-C32	2.73	120.47	111.91
70	AD	401	HEC	C4D-C3D-C2D	-2.73	102.92	106.90
70	Ad	401	HEC	CAA-CBA-CGA	-2.72	107.76	113.60
70	AD	401	HEC	C4A-C3A-C2A	-2.72	102.97	106.94
67	AC	401	HEM	CHD-C4C-NC	2.70	127.36	124.44
58	B	303	PC1	C2-O21-C21	-2.69	111.16	117.79
67	AC	402	HEM	CBD-CAD-C3D	-2.69	105.15	112.63
55	L	701	3PE	O31-C31-C32	2.69	120.34	111.91
71	Ad	402	3PH	C2-O21-C21	-2.68	111.19	117.79
55	I	301	3PE	O31-C31-C32	2.67	120.28	111.91
70	AD	401	HEC	CAC-C3C-C4C	2.67	128.62	124.92
55	L	704	3PE	O31-C31-C32	2.66	120.26	111.91
69	Ac	406	UQ6	C6-C7-C8	-2.65	107.97	112.17
60	F	501	FMN	C4A-C10-N1	-2.63	118.62	124.73
70	AD	401	HEC	CHB-C1B-C2B	-2.63	120.87	124.98
55	Y	201	3PE	C2-O21-C21	-2.63	111.32	117.79
62	AC	406	CDL	OB8-CB7-C71	2.62	120.13	111.91
62	h	201	CDL	CA4-OA6-CA5	-2.61	111.38	117.79
62	L	705	CDL	OA8-CA7-C31	2.60	120.07	111.91
62	X	201	CDL	OA8-CA7-C31	2.60	120.06	111.91
67	Ac	403	HEM	CBD-CAD-C3D	-2.60	105.41	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	403	HEM	CHD-C4C-NC	2.59	127.24	124.44
58	I	302	PC1	O31-C31-C32	2.59	120.04	111.91
55	L	707	3PE	C2-O21-C21	-2.58	111.43	117.79
55	AC	403	3PE	O31-C31-C32	2.58	119.99	111.91
67	AC	401	HEM	C4D-ND-C1D	2.57	107.73	105.07
67	AC	401	HEM	CAA-CBA-CGA	-2.57	108.07	113.60
70	AD	401	HEC	CAD-C3D-C4D	2.57	129.15	124.66
55	A	401	3PE	O31-C31-C32	2.56	119.95	111.91
67	Ac	403	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
70	AD	401	HEC	CBC-CAC-C3C	2.56	119.48	112.43
67	Ac	403	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
69	Ac	406	UQ6	C17-C18-C19	-2.55	119.05	127.75
67	Ac	402	HEM	C4A-NA-C1A	2.55	107.84	105.35
55	Ac	404	3PE	O31-C31-C32	2.54	119.88	111.91
55	L	704	3PE	C2-O21-C21	-2.54	111.53	117.79
69	Ac	406	UQ6	C21-C19-C20	2.54	120.22	114.60
62	Ag	101	CDL	OA8-CA7-C31	2.54	119.87	111.91
70	AD	401	HEC	CMD-C2D-C1D	2.53	128.89	125.04
70	Ad	401	HEC	CMC-C2C-C3C	2.53	131.08	125.61
60	F	501	FMN	O4-C4-C4A	-2.53	119.90	126.60
70	AD	401	HEC	CMB-C2B-C1B	2.53	128.89	125.04
62	Ag	101	CDL	CB4-OB6-CB5	-2.52	111.59	117.79
71	Ad	402	3PH	O31-C31-C32	2.52	119.81	111.91
62	h	201	CDL	CB4-OB6-CB5	-2.51	111.62	117.79
55	b	201	3PE	O31-C31-C32	2.49	119.74	111.91
62	h	201	CDL	OA8-CA7-C31	2.49	119.73	111.91
55	AF	201	3PE	O31-C31-C32	2.49	119.73	111.91
63	O	402	ADP	C3'-C2'-C1'	2.49	106.15	101.43
67	Ac	402	HEM	C1A-CHA-C4D	-2.49	120.44	126.34
68	Ac	405	U10	C27-C28-C29	-2.48	119.27	127.75
67	AC	402	HEM	CHB-C4A-NA	2.47	128.40	123.85
69	AC	405	UQ6	C21-C19-C20	2.47	120.06	114.60
67	AC	401	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
64	P	401	NDP	C3D-C2D-C1D	2.47	106.11	101.43
68	AC	404	U10	C16-C14-C15	2.45	120.02	114.60
67	AC	402	HEM	C4A-NA-C1A	2.45	107.75	105.35
62	Ag	101	CDL	OB8-CB7-C71	2.45	119.59	111.91
62	Ac	407	CDL	OA8-CA7-C31	2.45	119.59	111.91
55	M	502	3PE	O31-C31-C32	2.43	119.54	111.91
66	W	201	EHZ	C5-C6-C7	-2.39	107.98	114.85
62	a	101	CDL	OB8-CB7-C71	2.39	119.40	111.91
68	AC	404	U10	C1M-C1-C6	-2.38	120.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	402	HEM	CHC-C1C-NC	2.38	127.01	124.44
71	AD	402	3PH	C2-O21-C21	-2.37	111.94	117.79
66	n	201	EHZ	C5-C6-C7	-2.37	108.02	114.85
62	AC	406	CDL	OA8-CA7-C31	2.37	119.34	111.91
67	AC	401	HEM	CHA-C4D-C3D	-2.37	120.88	125.33
69	AC	405	UQ6	C4M-O4-C4	2.36	121.25	114.78
67	Ac	402	HEM	CHC-C4B-C3B	-2.35	120.07	125.13
62	L	706	CDL	CB4-OB6-CB5	-2.35	112.01	117.79
62	X	201	CDL	OA6-CA5-OA7	-2.34	118.05	123.70
58	J	201	PC1	C2-O21-C21	-2.33	112.04	117.79
58	J	201	PC1	O31-C31-C32	2.33	119.23	111.91
63	O	402	ADP	C4-N9-C8	2.32	108.25	105.73
62	AC	406	CDL	CB4-OB6-CB5	-2.32	112.07	117.79
67	Ac	402	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
67	Ac	403	HEM	CHB-C1B-C2B	-2.32	120.29	126.73
67	Ac	402	HEM	CHB-C1B-NB	2.31	127.23	124.37
70	Ad	401	HEC	CMA-C3A-C4A	2.31	128.78	124.71
55	J	202	3PE	O31-C31-C32	2.30	119.13	111.91
63	O	402	ADP	O4'-C1'-N9	2.30	112.59	108.06
69	AC	405	UQ6	C7-C6-C5	-2.30	117.80	120.82
68	Ac	405	U10	C31-C29-C30	2.30	119.68	114.60
67	Ac	403	HEM	C4D-ND-C1D	2.28	107.43	105.07
70	AD	401	HEC	C3C-C4C-NC	2.27	112.68	110.15
66	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
67	Ac	402	HEM	CHA-C1A-NA	2.27	128.02	123.85
55	L	703	3PE	O21-C21-O22	-2.26	118.24	123.70
66	n	201	EHZ	C10-S1-C9	2.26	108.91	101.87
67	Ac	403	HEM	C1A-CHA-C4D	-2.25	120.99	126.34
55	M	502	3PE	O21-C21-O22	-2.25	118.26	123.70
55	N	401	3PE	C2-O21-C21	-2.25	112.26	117.79
55	L	707	3PE	O31-C31-C32	2.25	118.95	111.91
70	AD	401	HEC	CHB-C1B-NB	-2.24	121.98	124.42
68	AC	404	U10	C12-C13-C14	-2.23	120.11	127.75
69	AC	405	UQ6	C17-C18-C19	-2.23	120.11	127.75
62	a	101	CDL	CB4-OB6-CB5	-2.23	112.30	117.79
62	X	201	CDL	OB8-CB7-C71	2.22	118.87	111.91
64	P	401	NDP	C6A-C5A-N7A	2.21	136.15	132.02
64	P	401	NDP	N9A-C8A-N7A	-2.21	110.89	113.91
60	F	501	FMN	C4-C4A-N5	2.19	121.35	118.23
70	AD	401	HEC	CMA-C3A-C4A	2.19	128.57	124.71
66	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
67	AC	402	HEM	C4C-CHD-C1D	-2.17	121.38	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Ad	401	HEC	CHC-C1C-C2C	-2.17	121.11	127.24
67	AC	401	HEM	CHB-C1B-C2B	-2.17	120.71	126.73
70	Ad	401	HEC	CMD-C2D-C3D	2.16	131.99	126.12
55	O	401	3PE	C2-O21-C21	-2.16	112.47	117.79
70	AD	401	HEC	CBD-CAD-C3D	-2.15	106.65	112.63
62	AC	406	CDL	CA4-OA6-CA5	-2.14	112.52	117.79
66	n	201	EHZ	C11-N1-C12	-2.14	118.86	122.84
63	O	402	ADP	C6-C5-N7	2.13	135.99	132.02
55	M	503	3PE	O21-C21-O22	-2.13	118.56	123.70
60	F	501	FMN	C4A-C10-N10	2.12	119.58	116.48
66	W	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
66	n	201	EHZ	O3-C12-N1	-2.11	119.02	123.01
69	AC	405	UQ6	C1M-C1-C6	-2.11	117.37	120.42
62	Ac	407	CDL	OB6-CB5-OB7	-2.10	118.62	123.70
66	W	201	EHZ	O6-P1-O9	2.10	112.36	106.47
66	n	201	EHZ	O6-P1-O9	2.10	112.36	106.47
55	N	401	3PE	O31-C31-O32	-2.10	118.30	123.59
55	Ag	102	3PE	C2-O21-C21	-2.09	112.63	117.79
67	AC	402	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
68	Ac	405	U10	C7-C6-C5	2.09	121.00	118.48
68	Ac	405	U10	C25-C24-C26	2.09	118.78	115.27
70	Ad	401	HEC	CHA-C1A-C2A	-2.09	121.56	124.94
66	n	201	EHZ	O2-C9-S1	-2.09	119.91	122.61
55	L	702	3PE	O21-C21-O22	-2.08	118.66	123.70
69	AC	405	UQ6	C1M-C1-C2	2.08	124.03	120.50
67	AC	402	HEM	C1A-CHA-C4D	-2.08	121.41	126.34
69	Ac	406	UQ6	C7-C6-C5	-2.08	118.09	120.82
67	AC	402	HEM	CMB-C2B-C1B	2.08	128.20	125.04
66	W	201	EHZ	O3-C12-N1	-2.07	119.11	123.01
67	AC	402	HEM	CAA-CBA-CGA	-2.07	109.15	113.60
70	AD	401	HEC	C4B-NB-C1B	-2.07	102.94	105.07
60	F	501	FMN	O2-C2-N1	-2.06	118.41	121.83
55	L	702	3PE	C2-O21-C21	-2.06	112.72	117.79
60	F	501	FMN	C10-N1-C2	2.06	121.02	116.90
70	AD	401	HEC	CHA-C1A-NA	-2.06	122.21	124.44
55	Ac	404	3PE	O21-C21-O22	-2.06	118.73	123.70
67	AC	401	HEM	C4C-CHD-C1D	-2.05	121.63	126.06
55	M	501	3PE	O21-C21-O22	-2.05	118.76	123.70
69	Ac	406	UQ6	C3M-O3-C3	2.04	120.38	114.78
69	Ac	406	UQ6	C17-C16-C14	-2.04	106.26	112.98
68	Ac	405	U10	C7-C8-C9	-2.04	123.40	126.79
67	AC	402	HEM	C2A-C1A-NA	-2.03	107.87	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	AD	401	HEC	CHA-C4D-C3D	-2.03	121.85	124.84
55	I	301	3PE	O31-C31-O32	-2.03	118.47	123.59
58	J	201	PC1	C11-C12-N	-2.01	109.05	115.78
55	Ag	102	3PE	O31-C31-O32	-2.01	118.52	123.59
55	I	301	3PE	C2-O21-C21	-2.01	112.85	117.79
67	AC	401	HEM	C4A-CHB-C1B	-2.01	121.58	126.34
60	F	501	FMN	C4A-C4-N3	2.00	118.28	113.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
70	AD	401	HEC	NA
70	Ad	401	HEC	NA

All (586) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C12-C11-O13-P
55	A	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C32-C31-O31-C3
55	I	301	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O12
55	L	701	3PE	C1-O11-P-O13
55	L	701	3PE	C1-O11-P-O14
55	L	702	3PE	C11-O13-P-O14
55	L	703	3PE	C1-O11-P-O14
55	L	703	3PE	O22-C21-O21-C2
55	L	703	3PE	C22-C21-O21-C2
55	L	704	3PE	C1-O11-P-O12
55	L	707	3PE	C11-O13-P-O11
55	L	707	3PE	C11-O13-P-O12
55	M	501	3PE	C1-O11-P-O12
55	M	501	3PE	C1-O11-P-O13
55	M	501	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O11
55	M	501	3PE	C11-O13-P-O12
55	M	501	3PE	C11-O13-P-O14
55	M	502	3PE	C11-O13-P-O12
55	M	502	3PE	C11-O13-P-O14
55	M	503	3PE	C1-O11-P-O12
55	M	503	3PE	C1-O11-P-O13
55	M	503	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
55	M	503	3PE	C11-O13-P-O12
55	M	503	3PE	C11-O13-P-O14
55	M	503	3PE	C22-C21-O21-C2
55	N	401	3PE	C11-O13-P-O11
55	N	401	3PE	C11-O13-P-O12
55	N	401	3PE	C11-O13-P-O14
55	O	401	3PE	C11-O13-P-O12
55	O	401	3PE	C11-O13-P-O14
55	O	401	3PE	C22-C21-O21-C2
55	b	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C22-C21-O21-C2
55	AC	403	3PE	C1-O11-P-O12
55	AC	403	3PE	C1-O11-P-O13
55	AC	403	3PE	C1-O11-P-O14
55	AC	403	3PE	C11-O13-P-O12
55	AC	403	3PE	C11-O13-P-O14
55	Ac	401	3PE	C1-O11-P-O12
55	Ac	401	3PE	C22-C21-O21-C2
55	Ag	102	3PE	C11-O13-P-O11
55	Ag	102	3PE	C11-O13-P-O12
55	Ag	102	3PE	C11-O13-P-O14
57	B	302	UQ1	C7-C8-C9-C11
58	B	303	PC1	C1-O11-P-O12
58	B	303	PC1	C1-O11-P-O14
58	B	303	PC1	C1-O11-P-O13
58	B	303	PC1	C22-C21-O21-C2
58	I	302	PC1	C11-O13-P-O12
58	I	302	PC1	C11-O13-P-O14
58	I	302	PC1	C11-O13-P-O11
58	I	302	PC1	C1-O11-P-O12
58	J	201	PC1	C11-O13-P-O12
58	J	201	PC1	C11-O13-P-O14
58	J	201	PC1	C1-O11-P-O12
58	J	201	PC1	C1-O11-P-O13
58	J	201	PC1	C12-C11-O13-P
60	F	501	FMN	N10-C1'-C2'-O2'
60	F	501	FMN	C5'-O5'-P-O1P
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C22-C23-C24-C26
61	H	400	UQ9	C22-C23-C24-C25
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
61	H	400	UQ9	C7-C8-C9-C10
62	L	705	CDL	CA2-OA2-PA1-OA4
62	L	705	CDL	CA3-OA5-PA1-OA3
62	L	705	CDL	C11-CA5-OA6-CA4
62	L	705	CDL	C51-CB5-OB6-CB4
62	L	706	CDL	C11-CA5-OA6-CA4
62	L	706	CDL	CB2-OB2-PB2-OB4
62	L	706	CDL	OB7-CB5-OB6-CB4
62	L	706	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CB3-OB5-PB2-OB3
62	X	201	CDL	CB3-OB5-PB2-OB4
62	X	201	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	C71-CB7-OB8-CB6
62	a	101	CDL	CA3-OA5-PA1-OA2
62	a	101	CDL	CA3-OA5-PA1-OA3
62	a	101	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB2-OB2-PB2-OB3
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	AC	406	CDL	CA2-OA2-PA1-OA4
62	AC	406	CDL	CA3-OA5-PA1-OA3
62	AC	406	CDL	CA3-OA5-PA1-OA4
62	AC	406	CDL	C31-CA7-OA8-CA6
62	Aa	501	CDL	CA3-OA5-PA1-OA2
62	Aa	501	CDL	CB4-CB3-OB5-PB2
62	Ac	407	CDL	CB2-OB2-PB2-OB3
62	Ac	407	CDL	CB2-OB2-PB2-OB4
62	Ac	407	CDL	CB2-OB2-PB2-OB5
62	Ac	407	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
63	O	402	ADP	C5'-O5'-PA-O2A
63	O	402	ADP	C5'-O5'-PA-O3A
64	P	401	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C7-C8-C9-S1
66	W	201	EHZ	S1-C10-C11-N1
66	W	201	EHZ	C11-C10-S1-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	C20-O6-P1-O7
66	W	201	EHZ	C20-O6-P1-O9
66	W	201	EHZ	C20-O6-P1-OP3
66	n	201	EHZ	O1-C7-C8-C9
66	n	201	EHZ	C6-C7-C8-C9
66	n	201	EHZ	C7-C8-C9-S1
66	n	201	EHZ	S1-C10-C11-N1
66	n	201	EHZ	C11-C10-S1-C9
66	n	201	EHZ	C16-C17-C20-O6
66	n	201	EHZ	C20-O6-P1-O7
66	n	201	EHZ	C20-O6-P1-O9
66	n	201	EHZ	C20-O6-P1-OP3
67	AC	401	HEM	C2C-C3C-CAC-CBC
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C2C-C3C-CAC-CBC
67	Ac	403	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C4B-C3B-CAB-CBB
68	Ac	405	U10	C5-C6-C7-C8
69	AC	405	UQ6	C13-C14-C16-C17
69	AC	405	UQ6	C15-C14-C16-C17
69	Ac	406	UQ6	C1-C6-C7-C8
69	Ac	406	UQ6	C13-C14-C16-C17
69	Ac	406	UQ6	C15-C14-C16-C17
71	Ad	402	3PH	C22-C21-O21-C2
55	O	401	3PE	O32-C31-O31-C3
58	I	302	PC1	O32-C31-O31-C3
62	AC	406	CDL	OA9-CA7-OA8-CA6
55	O	401	3PE	C32-C31-O31-C3
58	I	302	PC1	C32-C31-O31-C3
70	AD	401	HEC	C2B-C3B-CAB-CBB
70	AD	401	HEC	C4B-C3B-CAB-CBB
70	Ad	401	HEC	C2B-C3B-CAB-CBB
70	Ad	401	HEC	C4B-C3B-CAB-CBB
55	AF	201	3PE	O32-C31-O31-C3
58	J	201	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
62	L	705	CDL	OA9-CA7-OA8-CA6
70	AD	401	HEC	C4C-C3C-CAC-CBC
70	Ad	401	HEC	C4C-C3C-CAC-CBC
70	AD	401	HEC	C2C-C3C-CAC-CBC
70	Ad	401	HEC	C2C-C3C-CAC-CBC
55	M	503	3PE	O22-C21-O21-C2
55	O	401	3PE	O22-C21-O21-C2
55	Ac	401	3PE	O22-C21-O21-C2
58	B	303	PC1	O22-C21-O21-C2
62	L	705	CDL	OA7-CA5-OA6-CA4
62	L	705	CDL	OB7-CB5-OB6-CB4
62	L	706	CDL	OA7-CA5-OA6-CA4
62	X	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
62	AC	406	CDL	OA7-CA5-OA6-CA4
71	Ad	402	3PH	O22-C21-O21-C2
55	M	502	3PE	C32-C31-O31-C3
58	J	201	PC1	C32-C31-O31-C3
55	J	202	3PE	C22-C21-O21-C2
68	Ac	405	U10	C25-C24-C26-C27
61	H	400	UQ9	C18-C19-C21-C22
55	AF	201	3PE	C32-C31-O31-C3
62	L	705	CDL	C31-CA7-OA8-CA6
62	X	201	CDL	C31-CA7-OA8-CA6
55	Y	201	3PE	O32-C31-O31-C3
55	AC	403	3PE	O32-C31-O31-C3
55	Y	201	3PE	C32-C31-O31-C3
55	AC	403	3PE	C32-C31-O31-C3
55	M	502	3PE	O32-C31-O31-C3
62	X	201	CDL	OA9-CA7-OA8-CA6
62	AC	406	CDL	C11-CA5-OA6-CA4
57	B	302	UQ1	C7-C8-C9-C10
55	J	202	3PE	O22-C21-O21-C2
62	h	201	CDL	CA4-CA3-OA5-PA1
62	Ag	101	CDL	CB4-CB3-OB5-PB2
61	H	400	UQ9	C25-C24-C26-C27
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C23-C24-C26-C27
61	H	400	UQ9	C13-C14-C16-C17
62	AC	406	CDL	OB9-CB7-OB8-CB6
62	AC	406	CDL	C71-CB7-OB8-CB6
55	A	401	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
62	Aa	501	CDL	CA2-C1-CB2-OB2
58	J	201	PC1	C11-C12-N-C13
55	I	301	3PE	C32-C31-O31-C3
55	b	201	3PE	C32-C31-O31-C3
62	Aa	501	CDL	O1-C1-CB2-OB2
71	AD	402	3PH	O21-C2-C3-O31
55	Y	201	3PE	C23-C24-C25-C26
62	a	101	CDL	C12-C13-C14-C15
62	L	705	CDL	C13-C14-C15-C16
62	h	201	CDL	C71-CB7-OB8-CB6
62	Ag	101	CDL	C31-CA7-OA8-CA6
58	I	302	PC1	C11-C12-N-C15
67	Ac	403	HEM	C3D-CAD-CBD-CGD
55	I	301	3PE	O32-C31-O31-C3
55	b	201	3PE	O32-C31-O31-C3
61	H	400	UQ9	C19-C21-C22-C23
69	Ac	406	UQ6	C9-C11-C12-C13
55	A	401	3PE	O22-C21-O21-C2
62	Ag	101	CDL	OA9-CA7-OA8-CA6
55	M	501	3PE	C22-C21-O21-C2
55	A	401	3PE	C11-O13-P-O11
55	I	301	3PE	C1-O11-P-O13
55	I	301	3PE	C11-O13-P-O11
55	J	202	3PE	C11-O13-P-O11
55	L	702	3PE	C11-O13-P-O11
55	L	703	3PE	C1-O11-P-O13
55	L	704	3PE	C1-O11-P-O13
55	M	502	3PE	C11-O13-P-O11
55	M	503	3PE	C11-O13-P-O11
55	O	401	3PE	C11-O13-P-O11
55	AC	403	3PE	C11-O13-P-O11
55	AF	201	3PE	C1-O11-P-O13
55	AF	201	3PE	C11-O13-P-O11
58	I	302	PC1	C1-O11-P-O13
58	J	201	PC1	C11-O13-P-O11
62	L	705	CDL	CA2-OA2-PA1-OA5
62	L	706	CDL	CA2-OA2-PA1-OA5
62	L	706	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CB3-OB5-PB2-OB2
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
62	AC	406	CDL	CA2-OA2-PA1-OA5
62	AC	406	CDL	CA3-OA5-PA1-OA2
62	AC	406	CDL	CB2-OB2-PB2-OB5
62	Ac	407	CDL	CB3-OB5-PB2-OB2
55	L	703	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
68	Ac	405	U10	C23-C24-C26-C27
58	J	201	PC1	C11-C12-N-C15
55	L	703	3PE	C24-C25-C26-C27
62	Aa	501	CDL	C11-CA5-OA6-CA4
55	AF	201	3PE	C34-C35-C36-C37
62	h	201	CDL	C18-C19-C20-C21
62	h	201	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	CB6-CB4-OB6-CB5
55	M	501	3PE	O22-C21-O21-C2
62	Aa	501	CDL	OA7-CA5-OA6-CA4
68	Ac	405	U10	C12-C11-C9-C10
68	Ac	405	U10	C20-C19-C21-C22
62	X	201	CDL	C61-C62-C63-C64
55	M	502	3PE	O13-C11-C12-N
55	L	703	3PE	O32-C31-O31-C3
62	a	101	CDL	OA9-CA7-OA8-CA6
68	Ac	405	U10	C12-C11-C9-C8
55	M	501	3PE	C23-C24-C25-C26
58	I	302	PC1	C11-C12-N-C13
58	J	201	PC1	C11-C12-N-C14
62	Ag	101	CDL	C74-C75-C76-C77
67	Ac	402	HEM	C2A-CAA-CBA-CGA
67	Ac	403	HEM	C2A-CAA-CBA-CGA
55	L	702	3PE	C22-C21-O21-C2
68	Ac	405	U10	C18-C19-C21-C22
55	Ac	401	3PE	O21-C21-C22-C23
62	Aa	501	CDL	C72-C71-CB7-OB8
55	Ac	404	3PE	C32-C31-O31-C3
62	L	706	CDL	CB5-C51-C52-C53
55	M	503	3PE	C39-C3A-C3B-C3C
67	AC	402	HEM	C2C-C3C-CAC-CBC
55	A	401	3PE	C31-C32-C33-C34
62	X	201	CDL	C11-CA5-OA6-CA4
62	a	101	CDL	C51-CB5-OB6-CB4
67	AC	401	HEM	C4C-C3C-CAC-CBC
67	Ac	402	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
62	X	201	CDL	OA7-CA5-OA6-CA4
62	a	101	CDL	OB7-CB5-OB6-CB4
62	AC	406	CDL	OB6-CB4-CB6-OB8
58	I	302	PC1	C11-C12-N-C14
71	Ad	402	3PH	C25-C26-C27-C28
55	L	704	3PE	C27-C28-C29-C2A
55	M	501	3PE	C3C-C3D-C3E-C3F
55	L	702	3PE	O22-C21-O21-C2
55	I	301	3PE	C22-C21-O21-C2
55	AC	403	3PE	C22-C21-O21-C2
55	Ac	404	3PE	C22-C21-O21-C2
55	AC	403	3PE	C22-C23-C24-C25
62	L	705	CDL	CA3-OA5-PA1-OA2
62	L	706	CDL	CB2-OB2-PB2-OB5
62	h	201	CDL	CB3-OB5-PB2-OB2
70	AD	401	HEC	C2A-CAA-CBA-CGA
71	AD	402	3PH	C1-C2-C3-O31
71	Ad	402	3PH	C1-C2-C3-O31
70	AD	401	HEC	C1A-C2A-CAA-CBA
68	Ac	405	U10	C1-C6-C7-C8
62	L	706	CDL	C72-C73-C74-C75
55	L	704	3PE	C31-C32-C33-C34
55	Ac	404	3PE	O32-C31-O31-C3
55	L	704	3PE	C38-C39-C3A-C3B
55	Y	201	3PE	C2A-C2B-C2C-C2D
55	N	401	3PE	C37-C38-C39-C3A
55	L	707	3PE	C32-C31-O31-C3
62	L	705	CDL	CB6-CB4-OB6-CB5
62	AC	406	CDL	CA6-CA4-OA6-CA5
55	M	503	3PE	C2C-C2D-C2E-C2F
62	L	706	CDL	C31-CA7-OA8-CA6
62	L	705	CDL	C56-C57-C58-C59
55	I	301	3PE	C24-C25-C26-C27
55	b	201	3PE	C2A-C2B-C2C-C2D
55	M	503	3PE	C2D-C2E-C2F-C2G
55	I	301	3PE	O22-C21-O21-C2
55	AC	403	3PE	O22-C21-O21-C2
55	N	401	3PE	C32-C33-C34-C35
55	J	202	3PE	C32-C31-O31-C3
58	B	303	PC1	C2-C1-O11-P
58	B	303	PC1	C32-C33-C34-C35
71	AD	402	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
62	AC	406	CDL	CB3-CB4-CB6-OB8
66	W	201	EHZ	N2-C15-C16-C17
66	n	201	EHZ	N2-C15-C16-C17
62	h	201	CDL	CB2-OB2-PB2-OB5
66	W	201	EHZ	C3-C4-C5-C6
55	Ag	102	3PE	C32-C31-O31-C3
55	L	707	3PE	O32-C31-O31-C3
66	n	201	EHZ	C3-C4-C5-C6
62	L	706	CDL	OA9-CA7-OA8-CA6
66	W	201	EHZ	C5-C6-C7-O1
66	n	201	EHZ	C5-C6-C7-O1
55	J	202	3PE	O21-C2-C3-O31
71	Ad	402	3PH	O21-C2-C3-O31
58	B	303	PC1	C32-C31-O31-C3
55	Ac	404	3PE	O22-C21-O21-C2
62	L	705	CDL	C1-CA2-OA2-PA1
62	Aa	501	CDL	C1-CB2-OB2-PB2
62	h	201	CDL	C14-C15-C16-C17
66	W	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	O2-C9-S1-C10
70	AD	401	HEC	C3A-C2A-CAA-CBA
63	O	402	ADP	PB-O3A-PA-O5'
55	L	703	3PE	C28-C29-C2A-C2B
55	J	202	3PE	C22-C23-C24-C25
55	L	704	3PE	C22-C21-O21-C2
62	Ac	407	CDL	C51-CB5-OB6-CB4
69	Ac	406	UQ6	C5-C6-C7-C8
55	N	401	3PE	C32-C31-O31-C3
55	A	401	3PE	C3-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C2C-C3C-CAC-CBC
55	L	704	3PE	C22-C23-C24-C25
62	L	705	CDL	C16-C17-C18-C19
55	J	202	3PE	C25-C26-C27-C28
55	L	701	3PE	C2-C1-O11-P
62	L	705	CDL	CA4-CA3-OA5-PA1
62	h	201	CDL	CB4-CB3-OB5-PB2
67	AC	402	HEM	C4C-C3C-CAC-CBC
55	L	704	3PE	O22-C21-O21-C2
71	AD	402	3PH	O32-C31-O31-C3
55	L	701	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
55	J	202	3PE	O32-C31-O31-C3
64	P	401	NDP	C2B-O2B-P2B-O2X
55	Ag	102	3PE	O32-C31-O31-C3
58	B	303	PC1	O32-C31-O31-C3
62	Ac	407	CDL	OB7-CB5-OB6-CB4
55	Ac	404	3PE	C23-C24-C25-C26
71	Ad	402	3PH	C2-C3-O31-C31
55	O	401	3PE	C1-O11-P-O13
55	Ac	401	3PE	C1-O11-P-O13
62	L	705	CDL	CB2-OB2-PB2-OB5
55	A	401	3PE	C2E-C2F-C2G-C2H
55	L	701	3PE	C24-C25-C26-C27
55	A	401	3PE	C2-C1-O11-P
62	L	706	CDL	C1-CA2-OA2-PA1
62	a	101	CDL	CA4-CA3-OA5-PA1
62	AC	406	CDL	CA4-CA3-OA5-PA1
55	N	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C11-O13-P-O14
55	I	301	3PE	C1-O11-P-O12
55	I	301	3PE	C1-O11-P-O14
55	I	301	3PE	C11-O13-P-O14
55	J	202	3PE	C11-O13-P-O14
55	L	702	3PE	C11-O13-P-O12
55	L	703	3PE	C1-O11-P-O12
55	L	704	3PE	C1-O11-P-O14
55	L	707	3PE	C11-O13-P-O14
55	AF	201	3PE	C1-O11-P-O14
55	AF	201	3PE	C11-O13-P-O12
55	AF	201	3PE	C11-O13-P-O14
55	Ac	401	3PE	C1-O11-P-O14
58	J	201	PC1	C1-O11-P-O14
62	L	705	CDL	CA2-OA2-PA1-OA3
62	L	705	CDL	CA3-OA5-PA1-OA4
62	L	706	CDL	CA2-OA2-PA1-OA3
62	L	706	CDL	CA2-OA2-PA1-OA4
62	L	706	CDL	CA3-OA5-PA1-OA4
62	L	706	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CA2-OA2-PA1-OA4
62	X	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	AC	406	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
62	Aa	501	CDL	CA3-OA5-PA1-OA4
62	Ac	407	CDL	CB3-OB5-PB2-OB4
62	Ag	101	CDL	CB2-OB2-PB2-OB4
55	A	401	3PE	O11-C1-C2-C3
55	L	703	3PE	C34-C35-C36-C37
55	J	202	3PE	C12-C11-O13-P
55	M	502	3PE	C12-C11-O13-P
62	X	201	CDL	C59-C60-C61-C62
62	L	705	CDL	C77-C78-C79-C80
55	A	401	3PE	O11-C1-C2-O21
55	L	701	3PE	C1-C2-C3-O31
58	B	303	PC1	O13-C11-C12-N
58	J	201	PC1	O13-C11-C12-N
62	Ag	101	CDL	C54-C55-C56-C57
55	I	301	3PE	O21-C2-C3-O31
62	L	706	CDL	C56-C57-C58-C59
55	AF	201	3PE	C35-C36-C37-C38
55	O	401	3PE	C2-C1-O11-P
55	Ac	401	3PE	C2-C1-O11-P
69	Ac	406	UQ6	C3-C4-O4-C4M
66	W	201	EHZ	O4-C15-C16-O5
66	n	201	EHZ	O4-C15-C16-O5
55	M	503	3PE	C21-C22-C23-C24
55	L	703	3PE	C3C-C3D-C3E-C3F
66	W	201	EHZ	C19-C17-C20-O6
66	n	201	EHZ	C19-C17-C20-O6
62	L	706	CDL	C71-CB7-OB8-CB6
55	M	503	3PE	C32-C31-O31-C3
55	L	707	3PE	C36-C37-C38-C39
55	O	401	3PE	C32-C33-C34-C35
55	L	707	3PE	C22-C21-O21-C2
55	b	201	3PE	C2B-C2C-C2D-C2E
55	M	503	3PE	O32-C31-O31-C3
55	L	707	3PE	C1-O11-P-O13
55	M	502	3PE	C1-O11-P-O13
62	X	201	CDL	CB2-OB2-PB2-OB5
62	a	101	CDL	CB2-OB2-PB2-OB5
55	M	503	3PE	C26-C27-C28-C29
62	L	705	CDL	C33-C34-C35-C36
71	AD	402	3PH	C2-C3-O31-C31
55	J	202	3PE	C1-C2-C3-O31
66	W	201	EHZ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
66	n	201	EHZ	C2-C3-C4-C5
64	P	401	NDP	O4D-C1D-N1N-C6N
62	L	706	CDL	OB9-CB7-OB8-CB6
57	B	302	UQ1	C1-C2-O2-CM2
55	L	704	3PE	C29-C2A-C2B-C2C
55	L	704	3PE	C32-C33-C34-C35
62	X	201	CDL	CB4-CB3-OB5-PB2
62	a	101	CDL	C1-CB2-OB2-PB2
62	AC	406	CDL	CB4-CB3-OB5-PB2
62	Ac	407	CDL	C1-CA2-OA2-PA1
58	B	303	PC1	C34-C35-C36-C37
70	Ad	401	HEC	C3D-CAD-CBD-CGD
67	Ac	403	HEM	CAD-CBD-CGD-O1D
71	AD	402	3PH	C25-C26-C27-C28
55	M	501	3PE	C2B-C2C-C2D-C2E
55	M	501	3PE	O11-C1-C2-O21
67	Ac	403	HEM	C4C-C3C-CAC-CBC
62	L	705	CDL	OB9-CB7-OB8-CB6
62	Aa	501	CDL	CA4-CA6-OA8-CA7
62	L	706	CDL	C74-C75-C76-C77
55	M	502	3PE	C34-C35-C36-C37
55	J	202	3PE	C28-C29-C2A-C2B
55	L	707	3PE	O21-C2-C3-O31
62	L	706	CDL	CB4-CB3-OB5-PB2
55	M	503	3PE	C38-C39-C3A-C3B
55	L	707	3PE	O22-C21-O21-C2
64	P	401	NDP	C2D-C1D-N1N-C6N
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	AC	401	HEM	CAD-CBD-CGD-O1D
62	Aa	501	CDL	C33-C34-C35-C36
55	AC	403	3PE	C24-C25-C26-C27
55	L	707	3PE	C1-C2-C3-O31
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O1D
55	I	301	3PE	C37-C38-C39-C3A
55	L	702	3PE	C38-C39-C3A-C3B
55	L	701	3PE	C3-C2-O21-C21
62	Aa	501	CDL	CA6-CA4-OA6-CA5
62	L	705	CDL	C71-CB7-OB8-CB6
58	J	201	PC1	C34-C35-C36-C37
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	AC	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
62	h	201	CDL	C31-CA7-OA8-CA6
55	M	502	3PE	C25-C26-C27-C28
55	Y	201	3PE	C27-C28-C29-C2A
55	b	201	3PE	C24-C25-C26-C27
55	M	501	3PE	C26-C27-C28-C29
58	I	302	PC1	C2E-C2F-C2G-C2H
67	AC	401	HEM	CAA-CBA-CGA-O2A
67	Ac	403	HEM	CAD-CBD-CGD-O2D
64	P	401	NDP	PN-O3-PA-O2A
62	h	201	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C12-C11-C9-C10
71	Ad	402	3PH	C37-C38-C39-C3A
67	Ac	402	HEM	CAD-CBD-CGD-O2D
55	I	301	3PE	C35-C36-C37-C38
55	I	301	3PE	C33-C34-C35-C36
55	M	501	3PE	O11-C1-C2-C3
55	L	701	3PE	C36-C37-C38-C39
62	Ag	101	CDL	C11-C12-C13-C14
63	O	402	ADP	O4'-C4'-C5'-O5'
60	F	501	FMN	C5'-O5'-P-O2P
66	W	201	EHZ	N2-C15-C16-O5
66	n	201	EHZ	N2-C15-C16-O5
71	AD	402	3PH	C1-O11-P-O13
55	M	503	3PE	C33-C34-C35-C36
66	W	201	EHZ	C18-C17-C20-O6
66	n	201	EHZ	C18-C17-C20-O6
55	L	701	3PE	C32-C31-O31-C3
55	L	703	3PE	C3D-C3E-C3F-C3G
62	X	201	CDL	C12-C11-CA5-OA6
55	Ac	401	3PE	C1-C2-O21-C21
66	W	201	EHZ	C8-C9-S1-C10
55	N	401	3PE	C33-C34-C35-C36
62	L	706	CDL	C34-C35-C36-C37
55	M	502	3PE	O21-C21-C22-C23
62	L	706	CDL	C52-C51-CB5-OB6
68	Ac	405	U10	C5-C4-O4-C4M
69	AC	405	UQ6	C14-C16-C17-C18
62	L	706	CDL	C19-C20-C21-C22
55	L	704	3PE	C2-C1-O11-P
62	L	706	CDL	C55-C56-C57-C58
71	AD	402	3PH	O22-C21-O21-C2
55	Ac	404	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	403	HEM	CAA-CBA-CGA-O1A
66	W	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C18
62	X	201	CDL	OA6-CA4-CA6-OA8
62	Aa	501	CDL	C72-C71-CB7-OB9
67	Ac	403	HEM	CAA-CBA-CGA-O2A
64	P	401	NDP	C2B-O2B-P2B-O3X
66	W	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C18
55	L	701	3PE	O32-C31-O31-C3
62	X	201	CDL	C52-C51-CB5-OB6
69	Ac	406	UQ6	C5-C4-O4-C4M
55	L	707	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C39-C3A-C3B-C3C
62	a	101	CDL	C32-C31-CA7-OA8
55	M	502	3PE	C22-C21-O21-C2
62	X	201	CDL	C12-C11-CA5-OA7
55	L	703	3PE	C39-C3A-C3B-C3C
61	H	400	UQ9	C12-C11-C9-C8
63	O	402	ADP	C2'-C1'-N9-C8
55	M	502	3PE	O22-C21-C22-C23
55	Ac	404	3PE	O22-C21-C22-C23
55	M	501	3PE	C39-C3A-C3B-C3C
62	L	706	CDL	C52-C51-CB5-OB7
55	Ac	401	3PE	O22-C21-C22-C23
62	Ac	407	CDL	C71-CB7-OB8-CB6
55	I	301	3PE	C1-C2-C3-O31
55	L	702	3PE	C1-O11-P-O13
62	Aa	501	CDL	O1-C1-CA2-OA2
55	Ac	404	3PE	C2-C3-O31-C31
55	L	702	3PE	C1-O11-P-O14
62	X	201	CDL	CA2-OA2-PA1-OA3
62	Aa	501	CDL	CB3-OB5-PB2-OB3
55	A	401	3PE	O13-C11-C12-N
55	L	701	3PE	O13-C11-C12-N
55	Ac	401	3PE	C3-C2-O21-C21
58	I	302	PC1	C12-C11-O13-P
66	W	201	EHZ	O4-C15-C16-C17
66	n	201	EHZ	O4-C15-C16-C17
62	X	201	CDL	CA5-C11-C12-C13
62	L	705	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
55	L	704	3PE	C2B-C2C-C2D-C2E
71	Ad	402	3PH	C23-C24-C25-C26
70	Ad	401	HEC	C2D-C3D-CAD-CBD
62	X	201	CDL	C52-C51-CB5-OB7
62	a	101	CDL	OA7-CA5-OA6-CA4
55	I	301	3PE	C2-C1-O11-P
55	L	701	3PE	O21-C21-C22-C23
62	h	201	CDL	C72-C71-CB7-OB8
62	Ac	407	CDL	OB9-CB7-OB8-CB6
55	L	707	3PE	C2B-C2C-C2D-C2E
62	a	101	CDL	C32-C31-CA7-OA9
70	Ad	401	HEC	CAA-CBA-CGA-O2A
55	b	201	3PE	C39-C3A-C3B-C3C
58	I	302	PC1	C2C-C2D-C2E-C2F
62	Aa	501	CDL	C12-C11-CA5-OA6

There are no ring outliers.

57 monomers are involved in 537 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	M	503	3PE	6	0
55	Ag	102	3PE	9	0
56	G	802	SF4	5	0
71	AD	402	3PH	13	0
55	AC	403	3PE	12	0
59	G	803	FES	4	0
62	X	201	CDL	9	0
56	I	303	SF4	11	0
55	L	703	3PE	10	0
58	I	302	PC1	9	0
68	AC	404	U10	4	0
69	AC	405	UQ6	14	0
71	Ad	402	3PH	19	0
55	L	707	3PE	10	0
55	M	502	3PE	14	0
62	h	201	CDL	15	0
55	I	301	3PE	14	0
62	Ag	101	CDL	9	0
64	P	401	NDP	7	0
55	AF	201	3PE	7	0
62	Aa	501	CDL	8	0
56	I	304	SF4	5	0

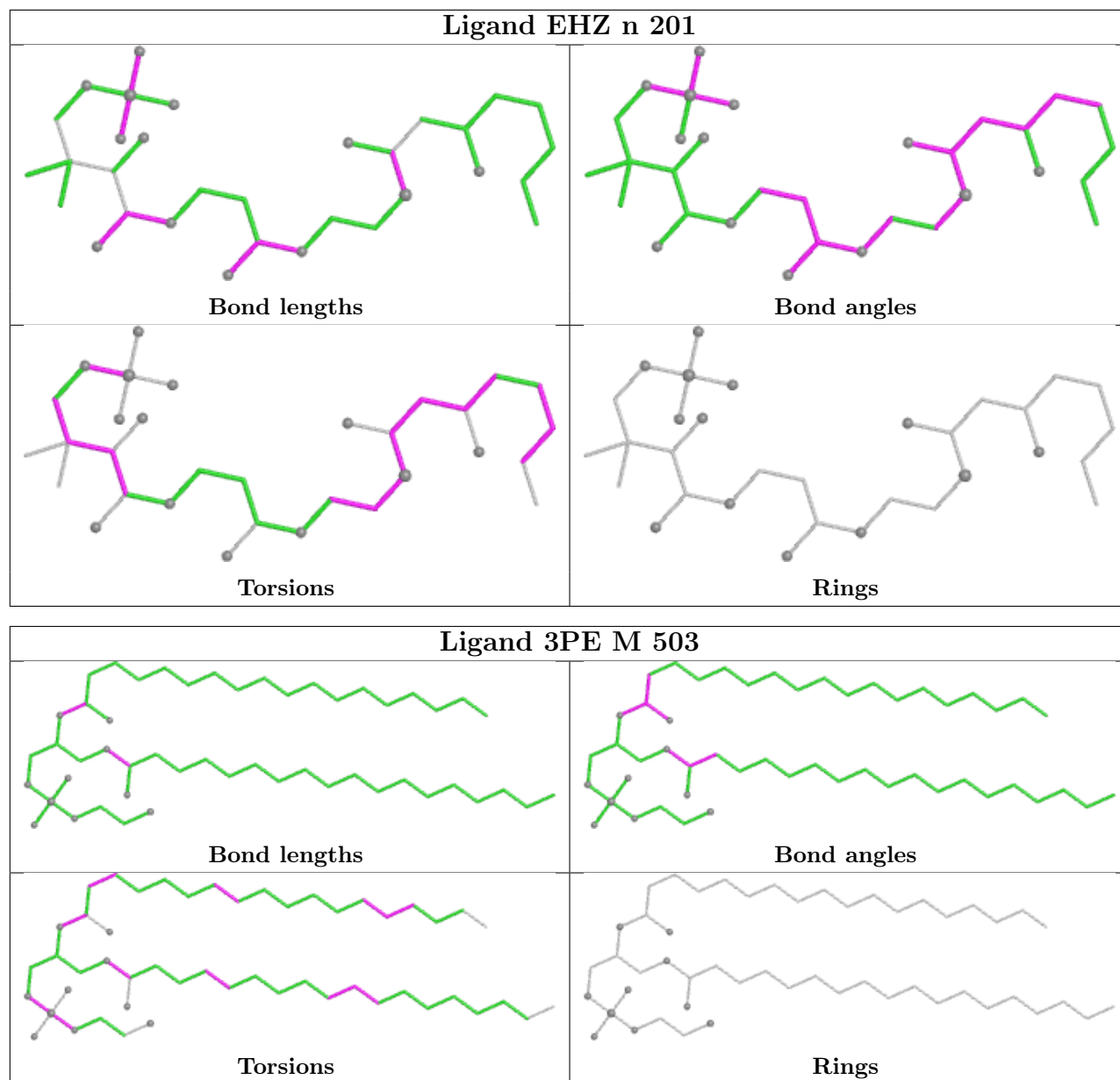
Continued on next page...

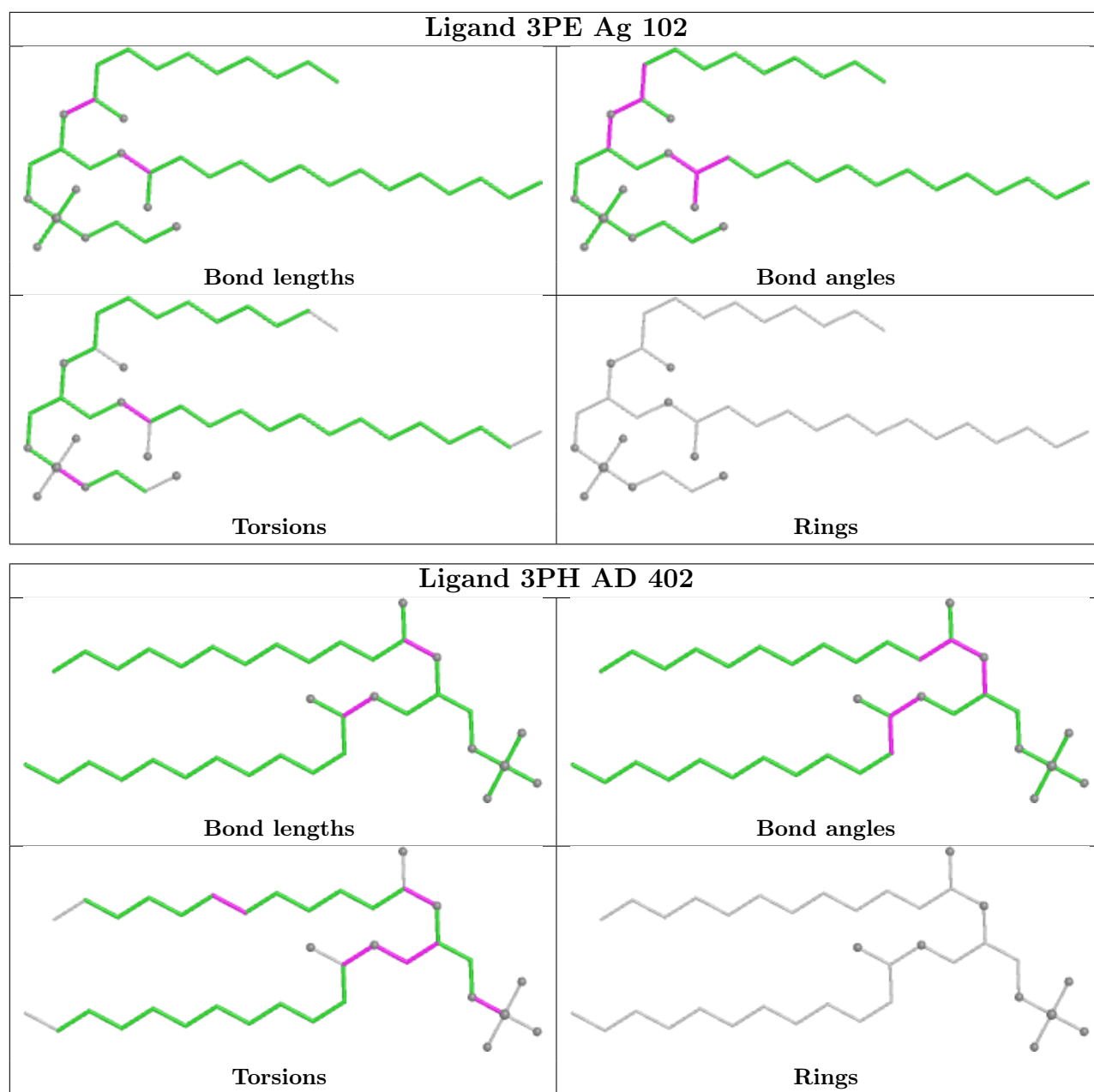
Continued from previous page...

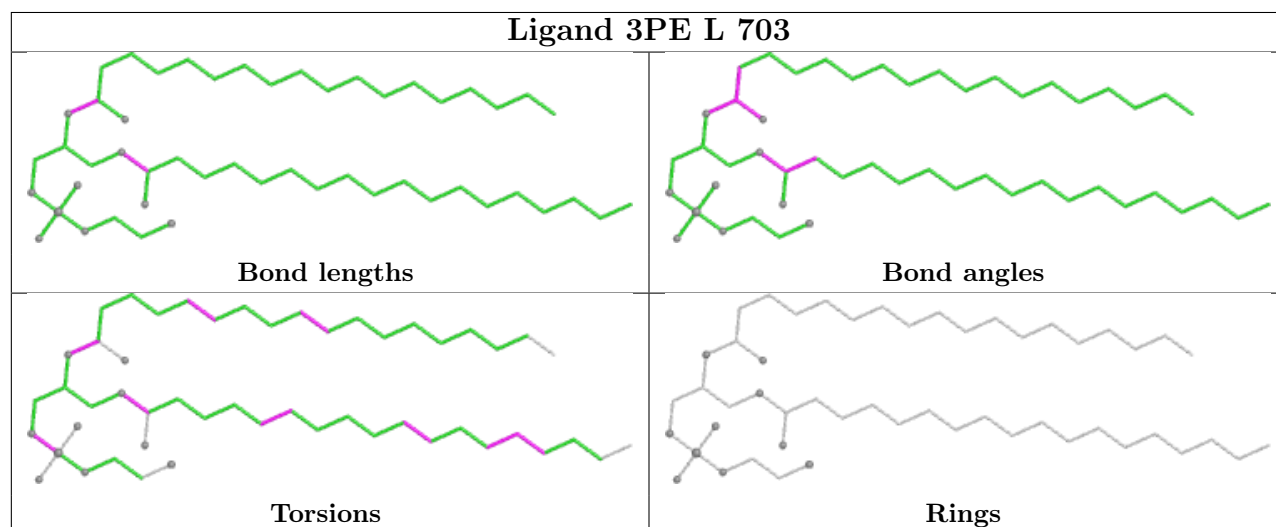
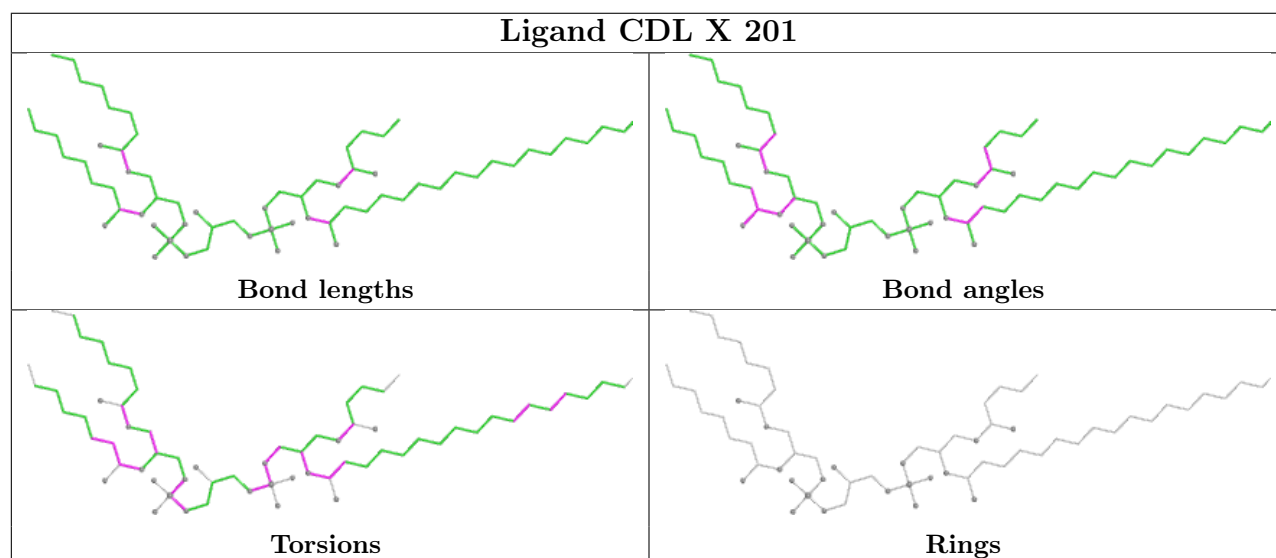
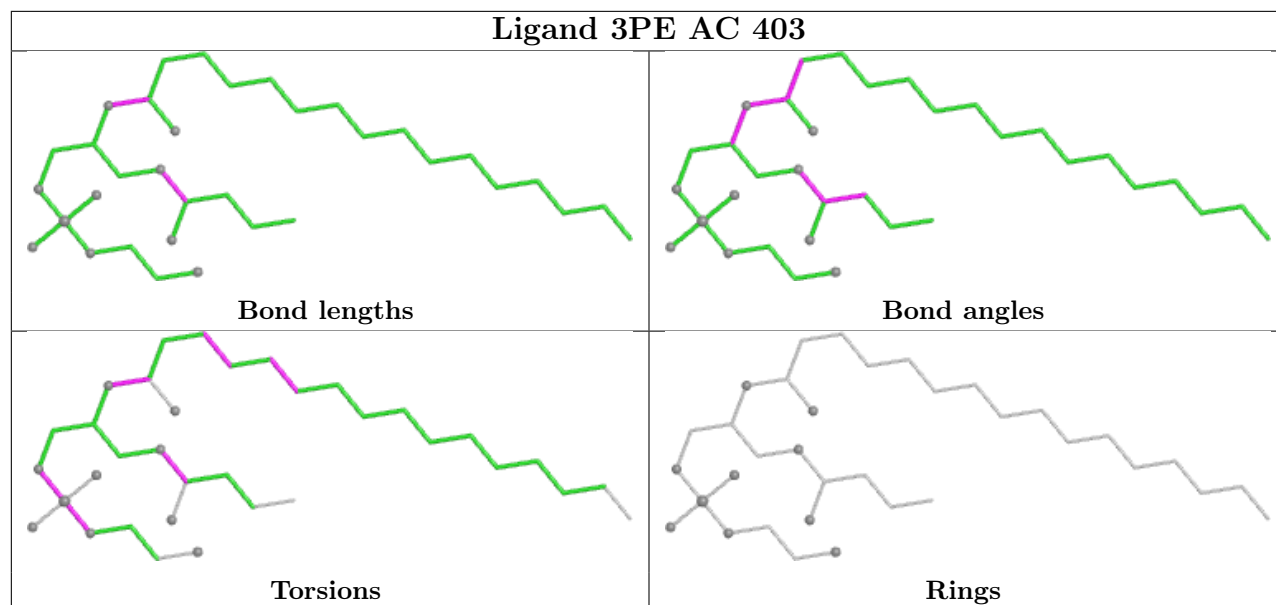
Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	Ac	406	UQ6	12	0
55	M	501	3PE	6	0
56	B	301	SF4	6	0
66	W	201	EHZ	7	0
70	AD	401	HEC	24	0
63	O	402	ADP	6	0
55	A	401	3PE	12	0
55	Ac	401	3PE	3	0
55	O	401	3PE	5	0
55	L	701	3PE	23	0
55	b	201	3PE	16	0
61	H	400	UQ9	4	0
67	AC	402	HEM	4	0
67	Ac	402	HEM	3	0
56	F	502	SF4	10	0
55	L	702	3PE	6	0
62	Ac	407	CDL	3	0
55	J	202	3PE	5	0
55	Ac	404	3PE	3	0
58	J	201	PC1	8	0
59	E	301	FES	5	0
60	F	501	FMN	1	0
62	a	101	CDL	22	0
62	L	706	CDL	19	0
67	AC	401	HEM	3	0
67	Ac	403	HEM	6	0
58	B	303	PC1	7	0
62	L	705	CDL	19	0
62	AC	406	CDL	4	0
55	L	704	3PE	8	0
70	Ad	401	HEC	25	0
68	Ac	405	U10	5	0
55	Y	201	3PE	20	0
57	B	302	UQ1	13	0
55	N	401	3PE	14	0

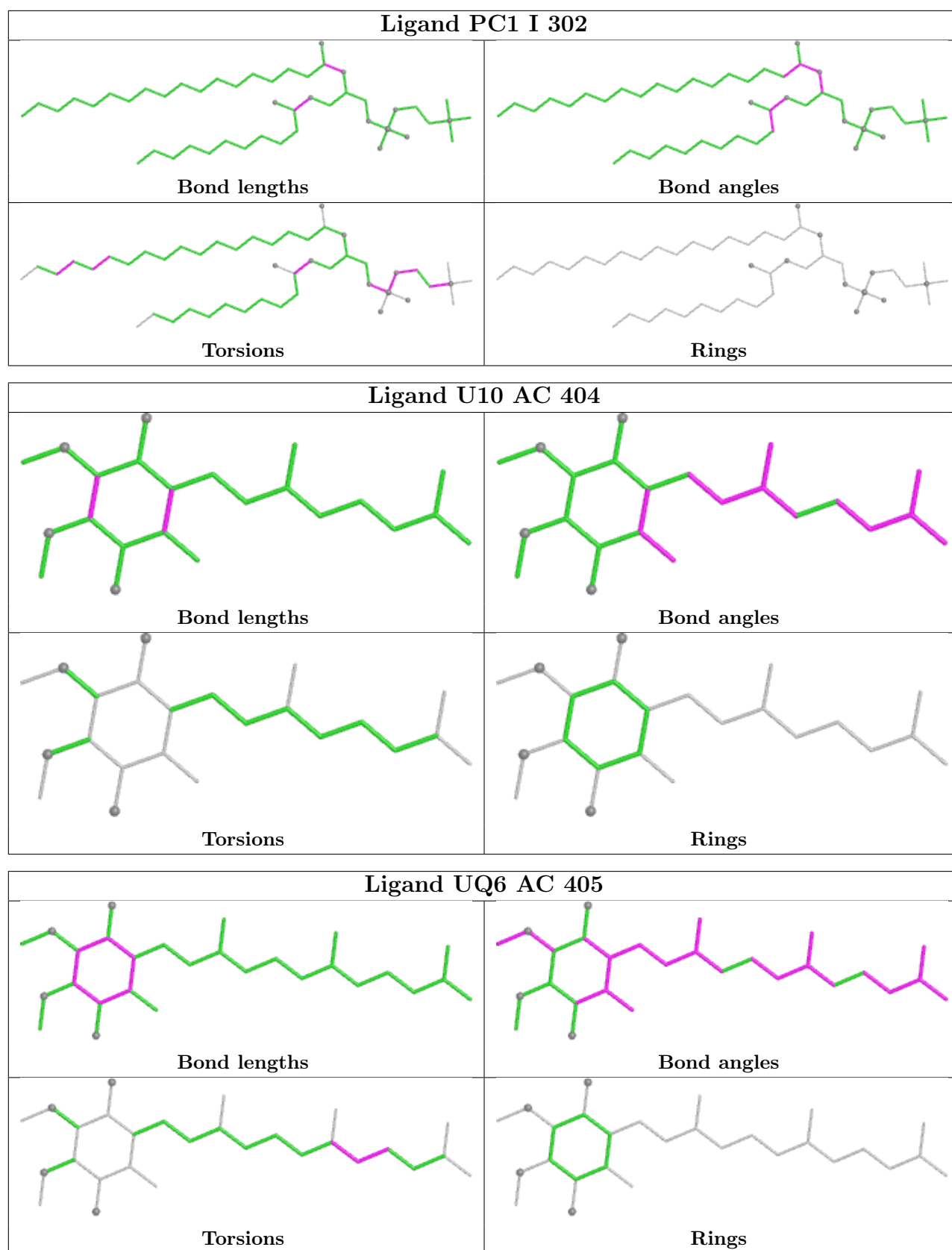
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

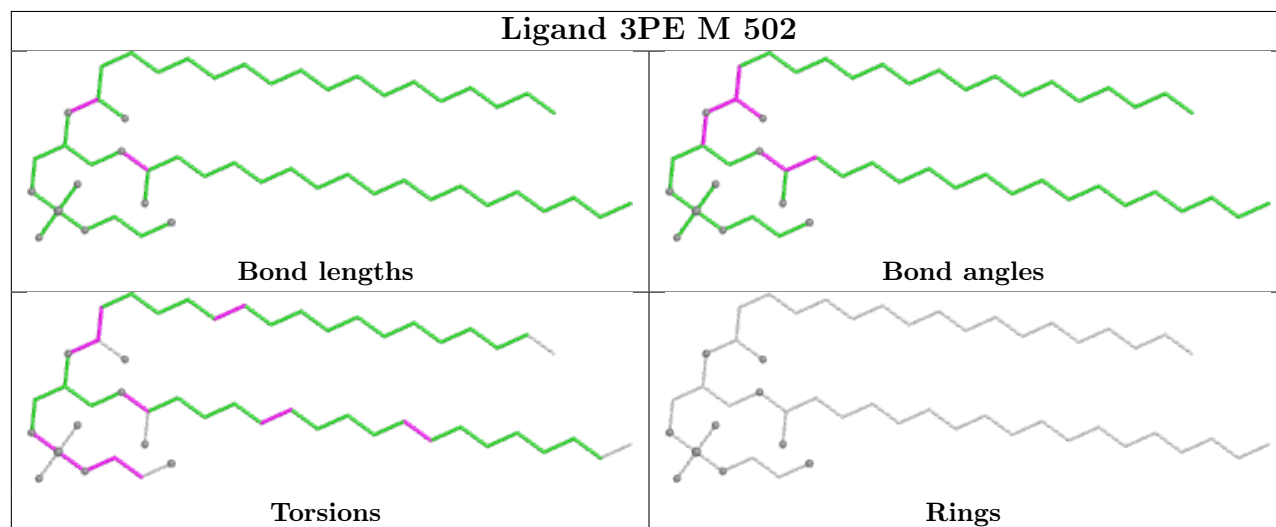
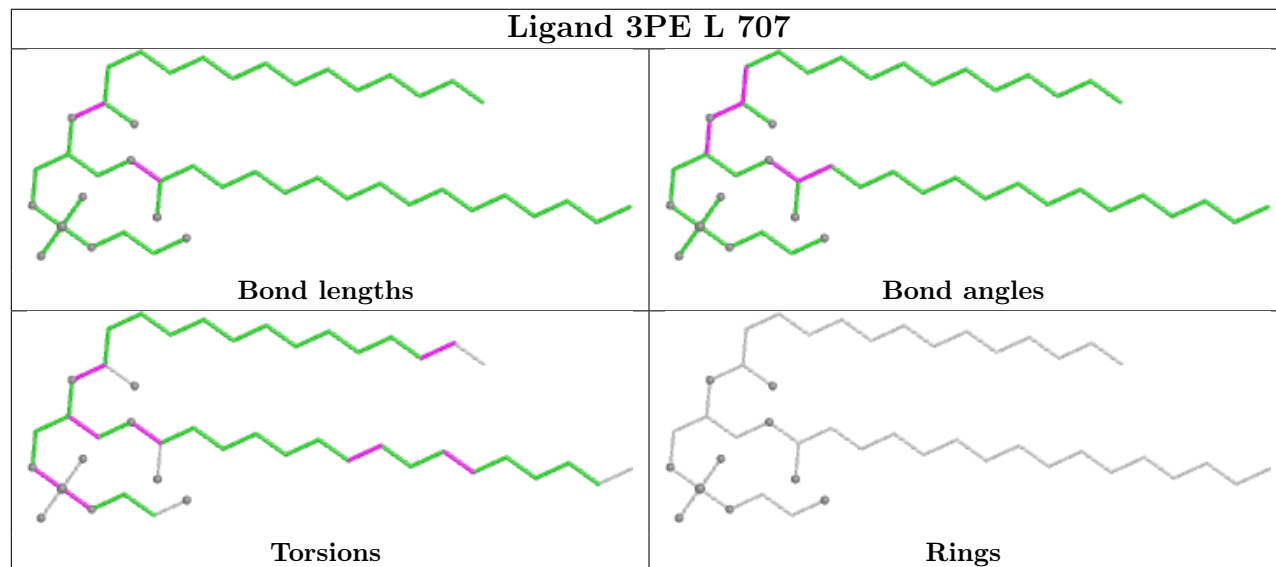
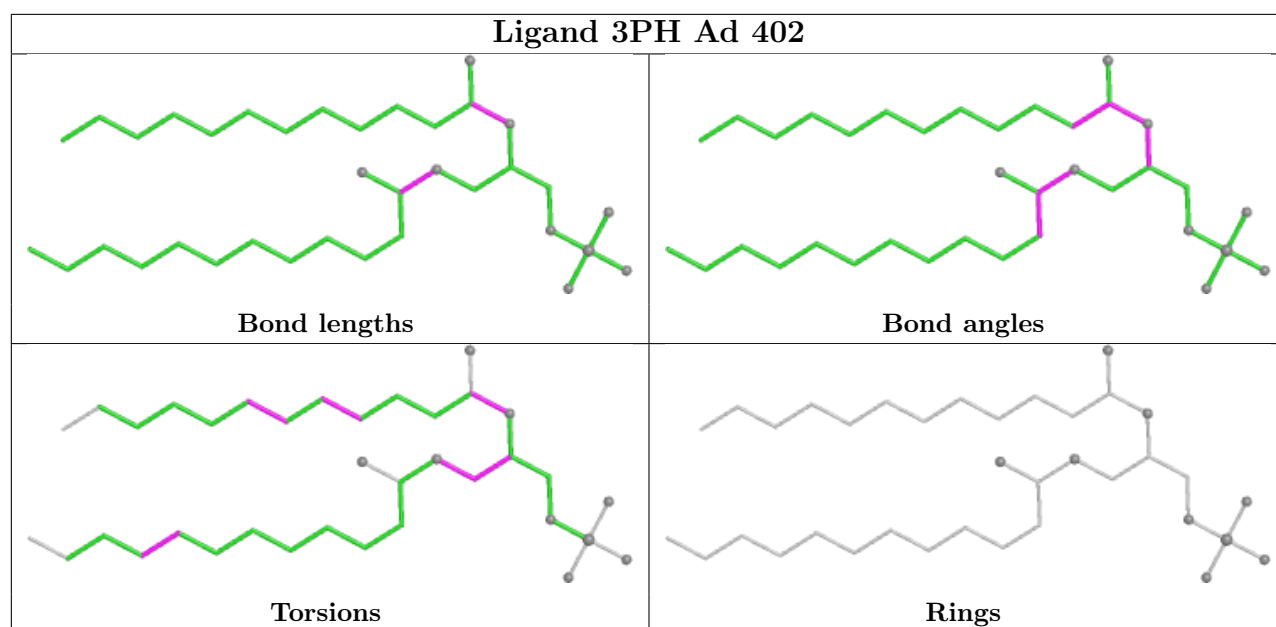
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

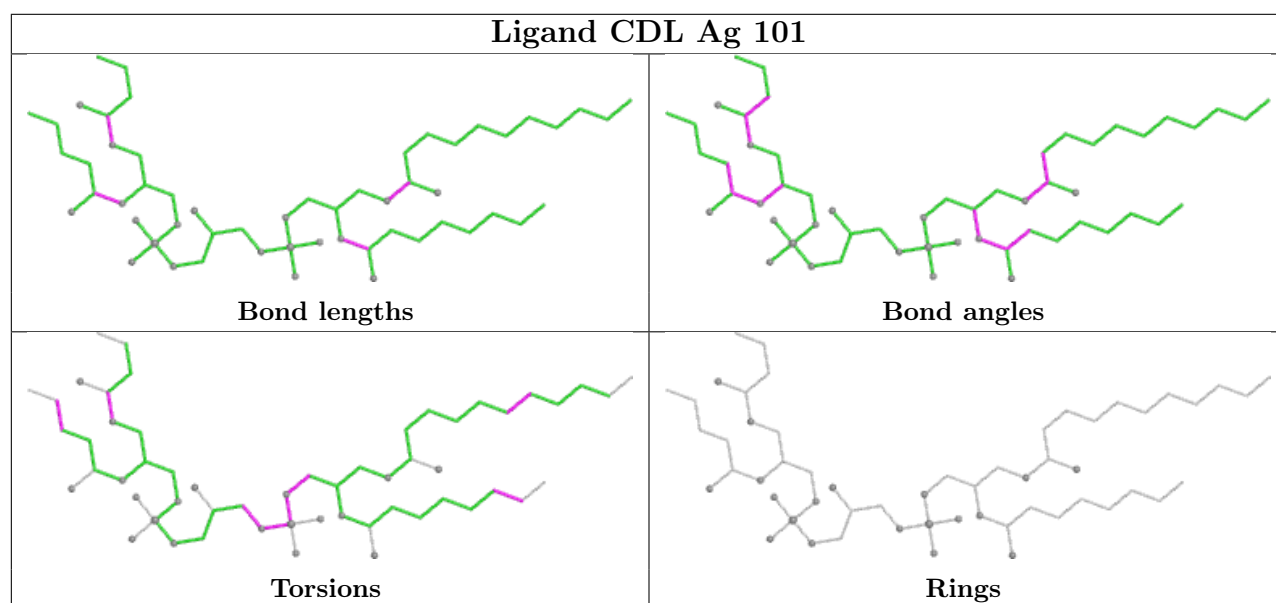
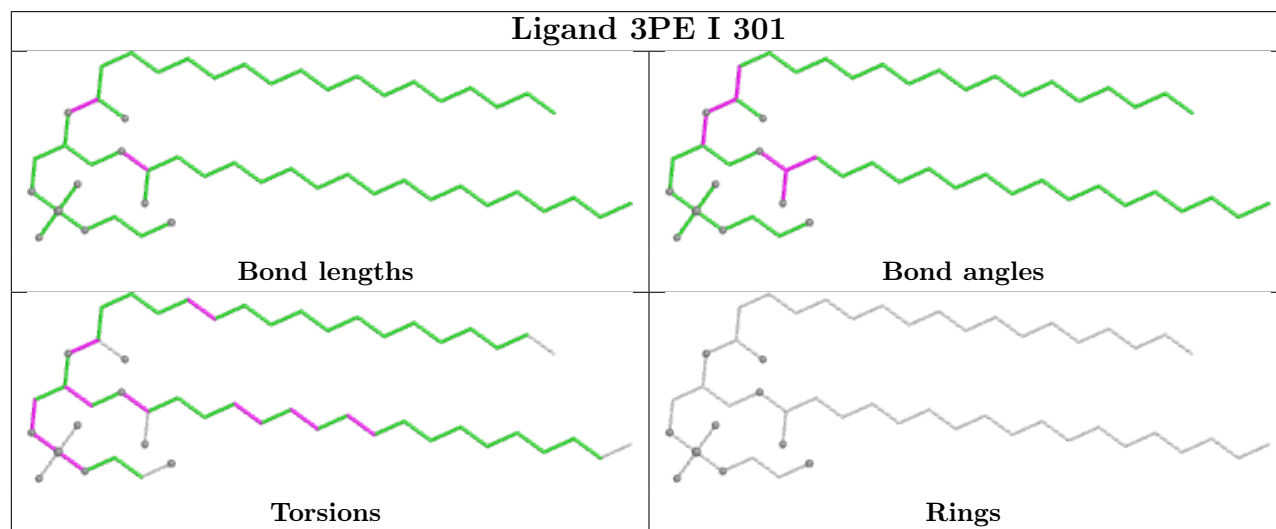
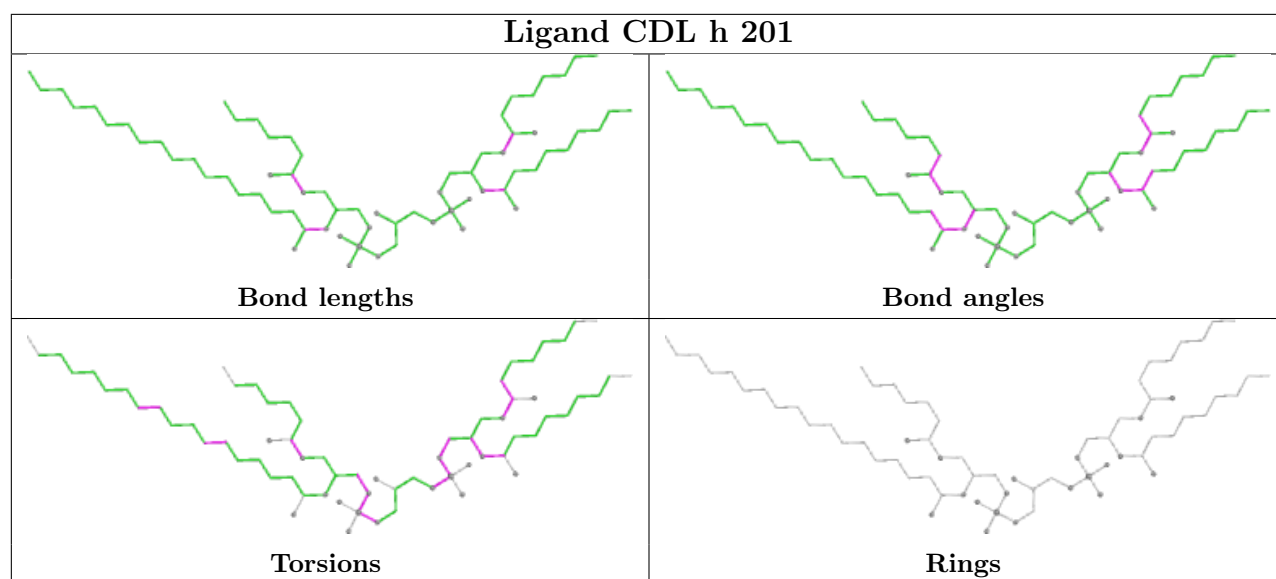


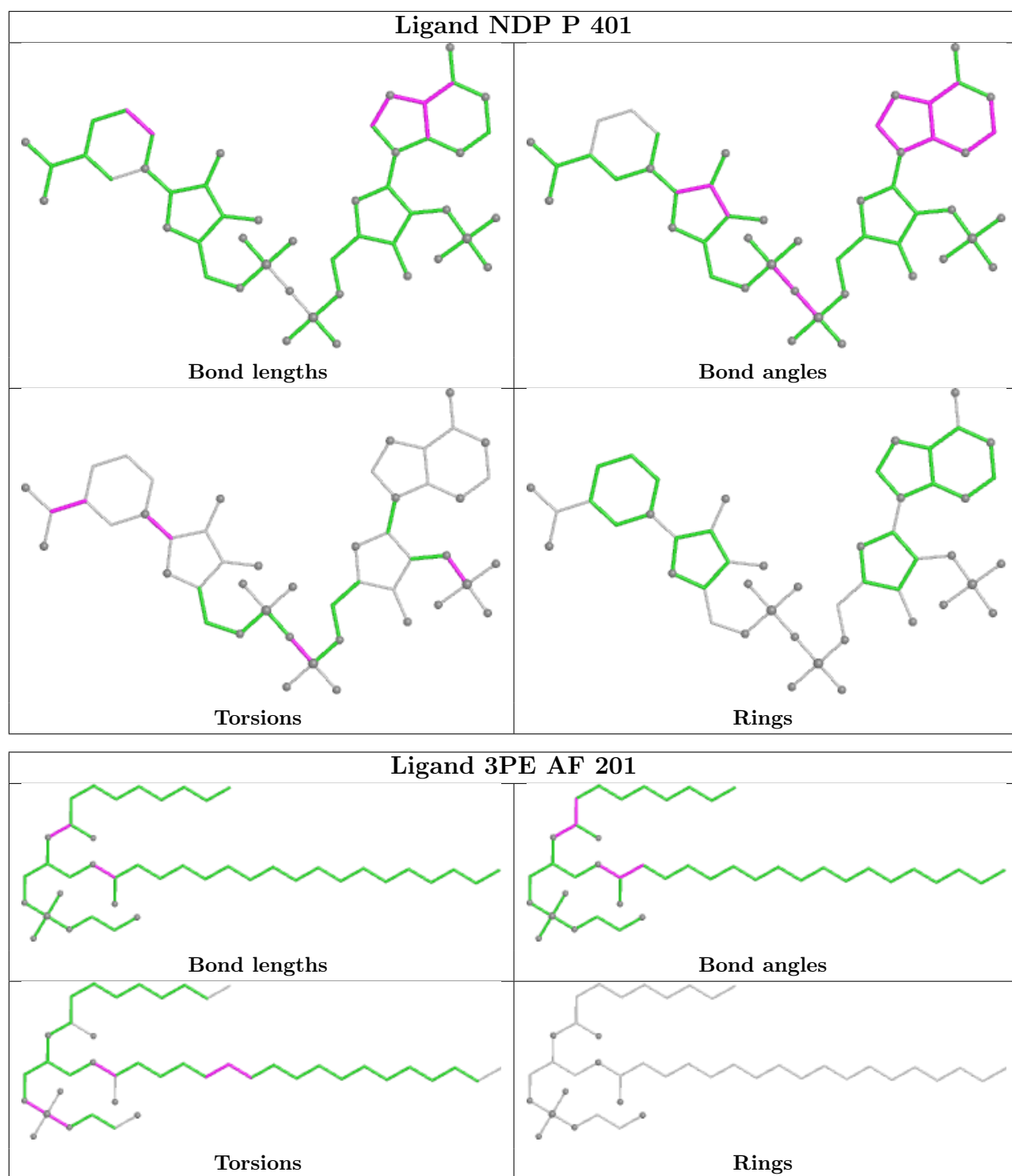


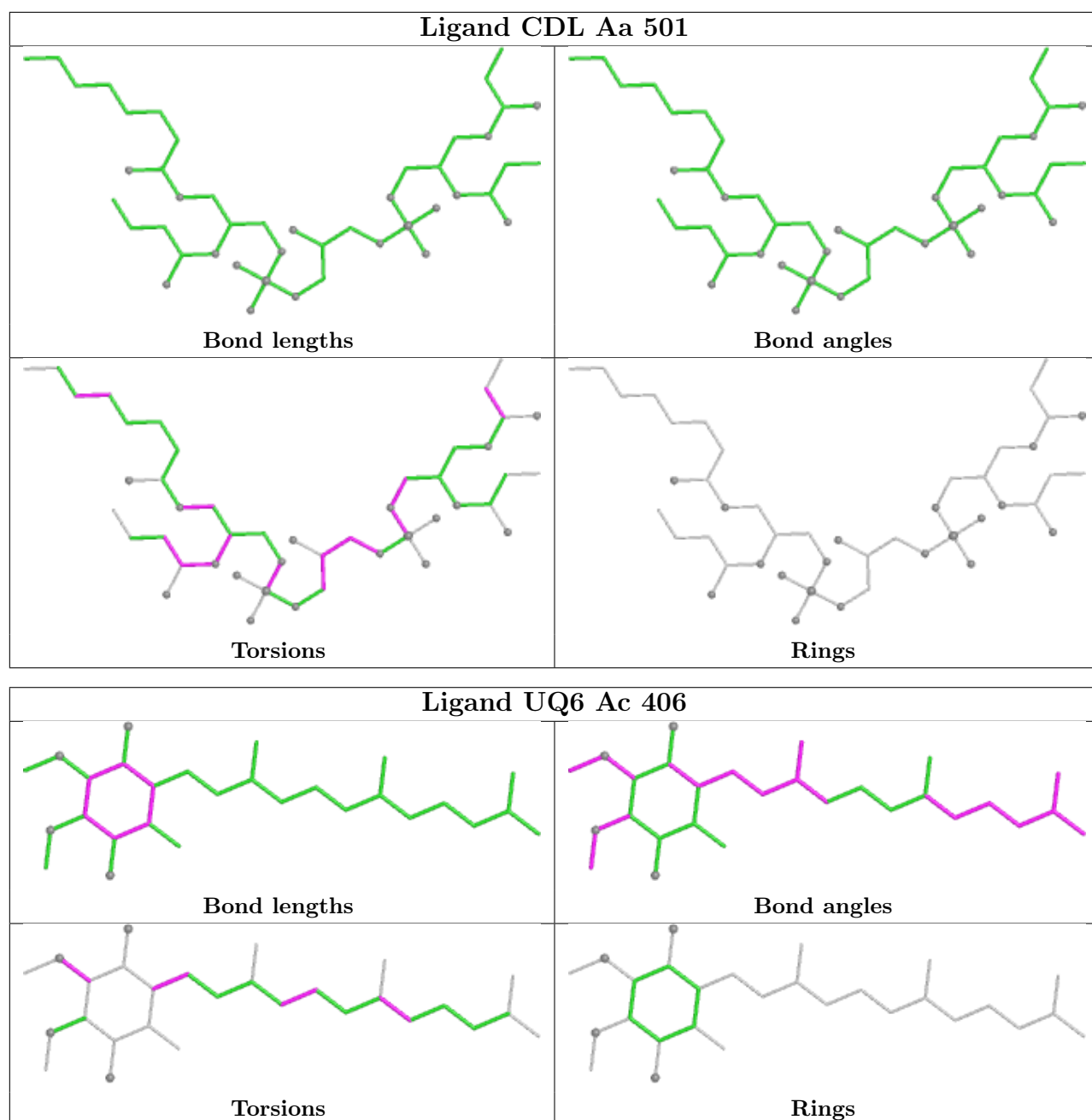


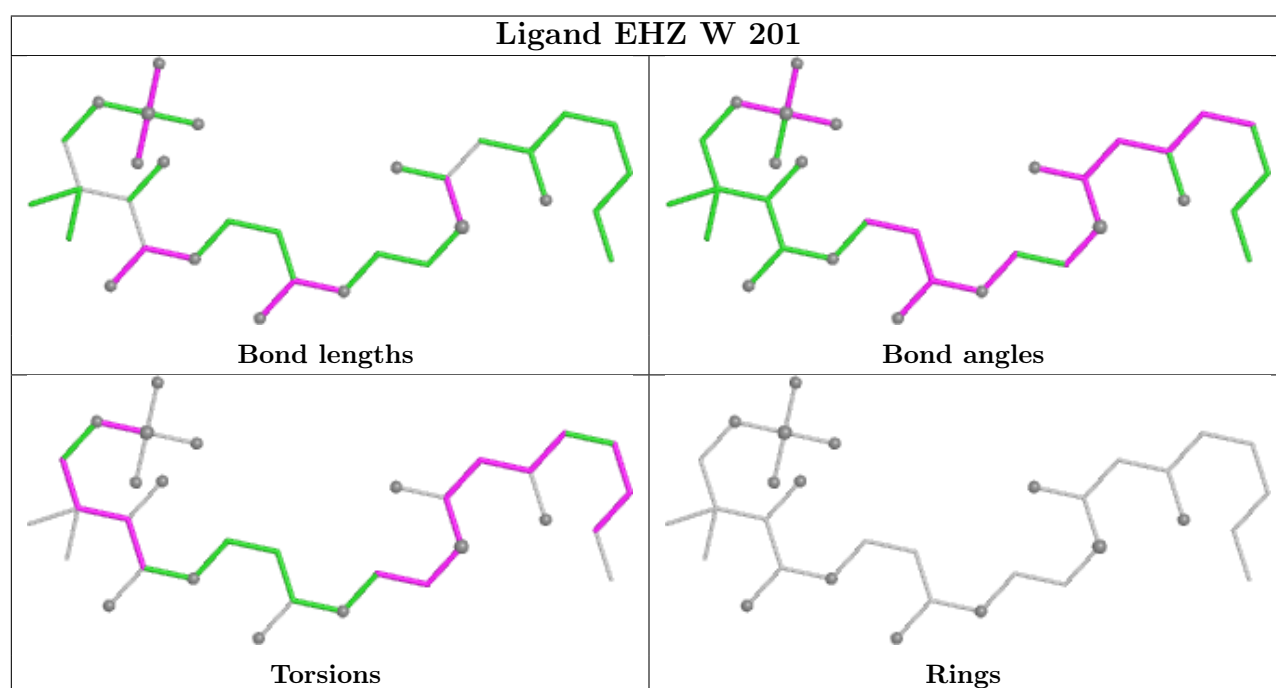
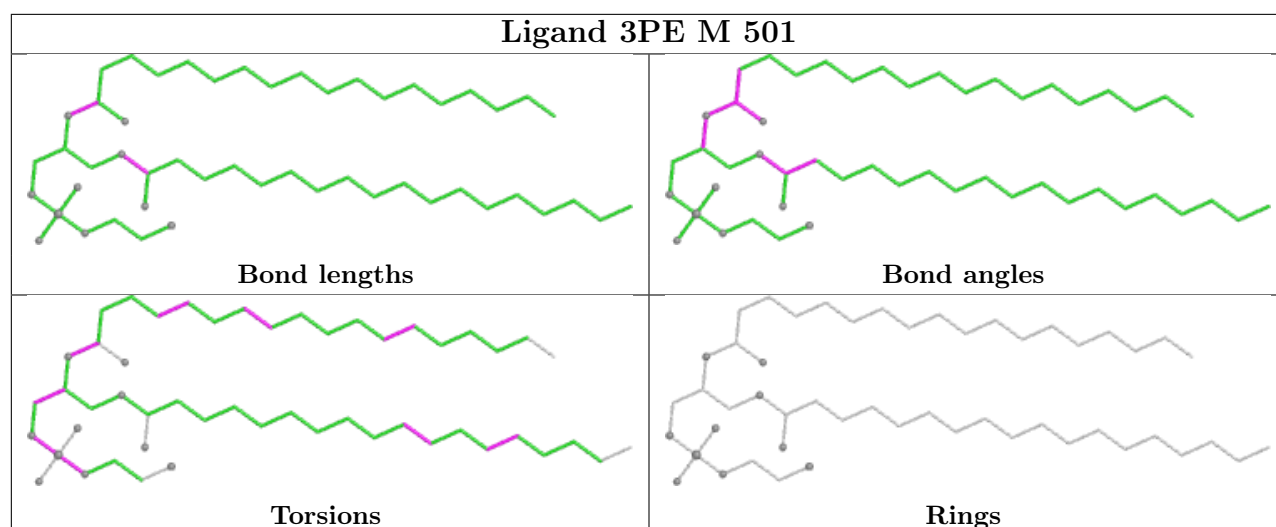




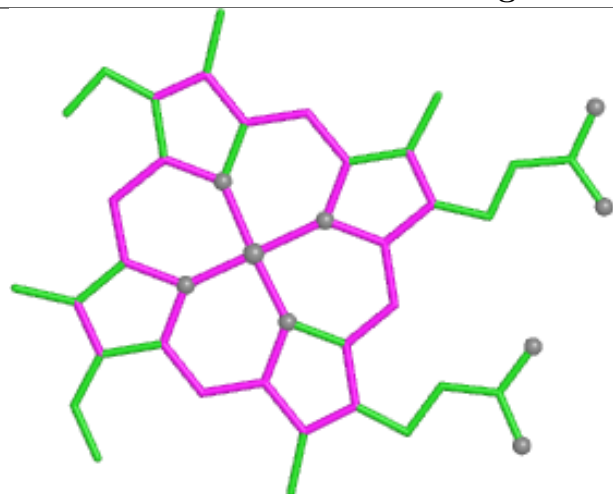




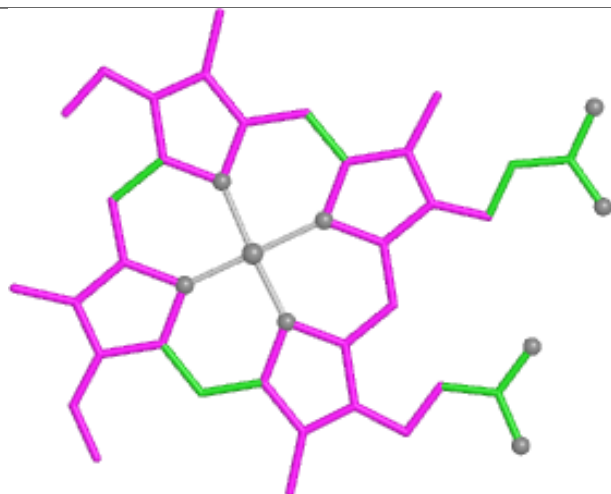




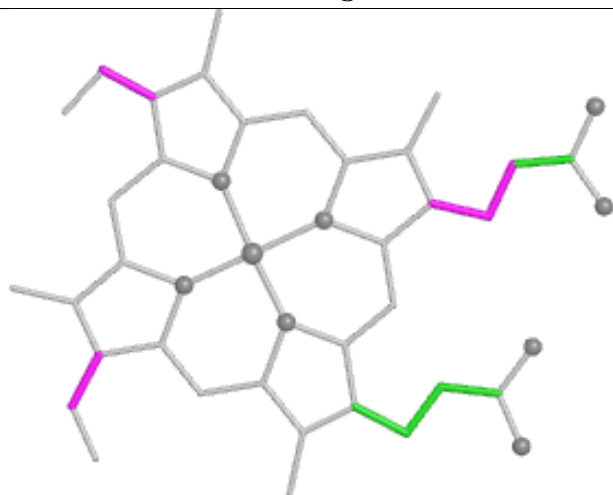
Ligand HEC AD 401



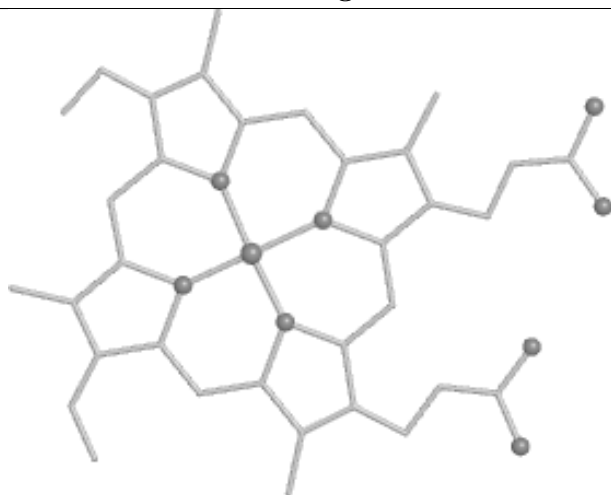
Bond lengths



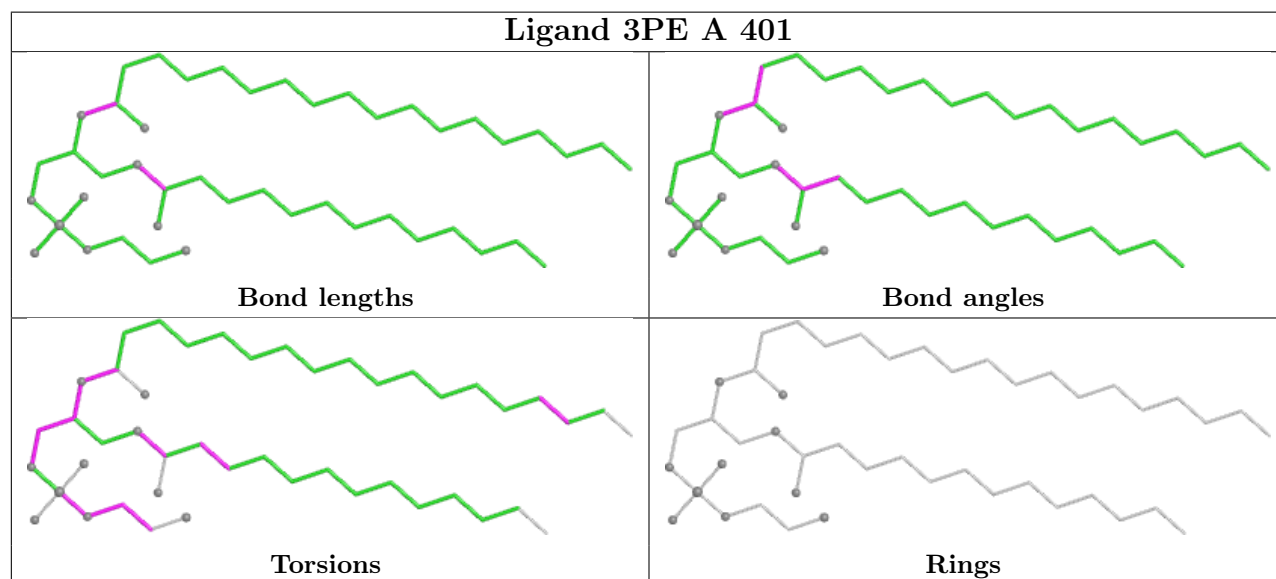
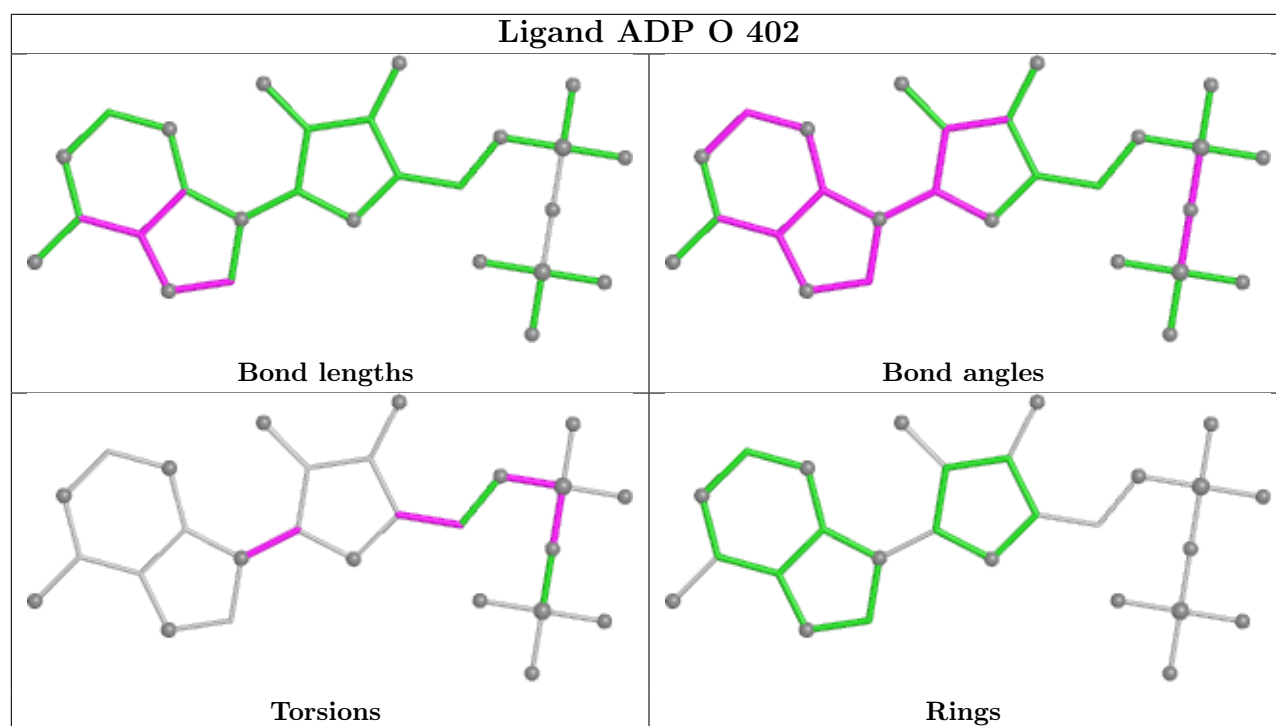
Bond angles

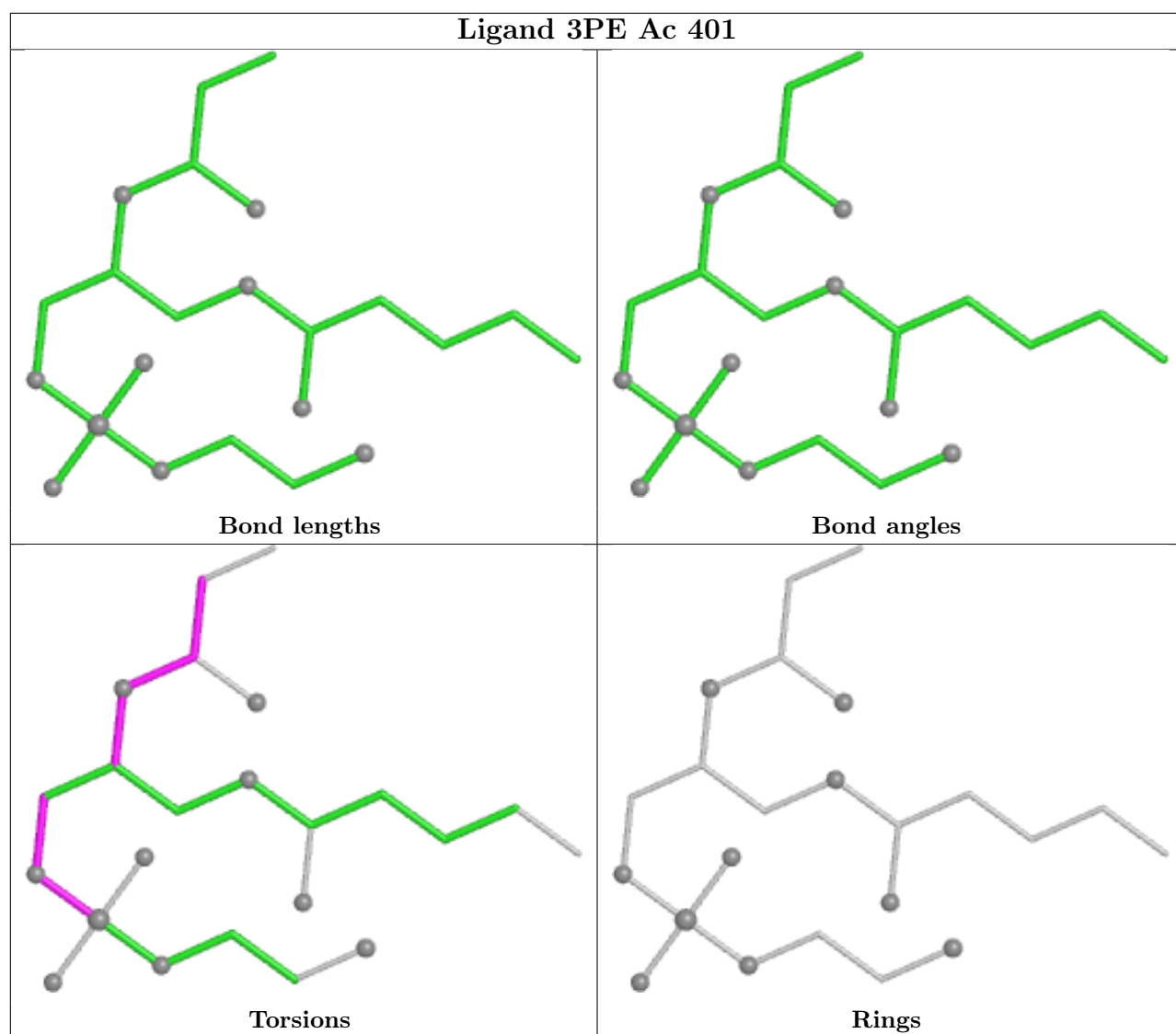


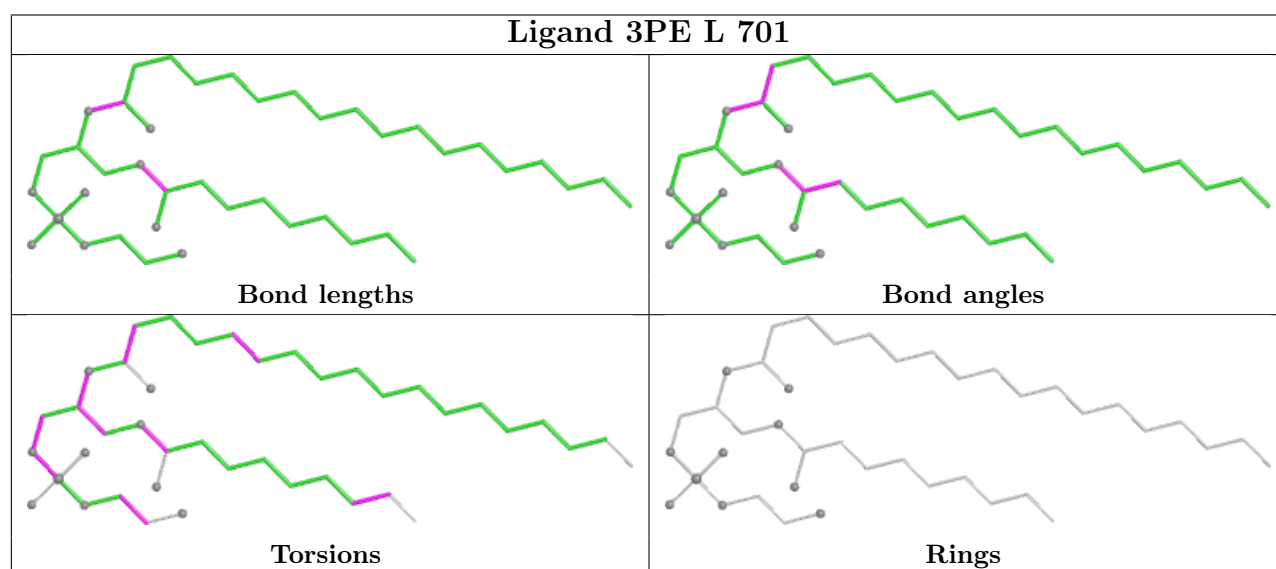
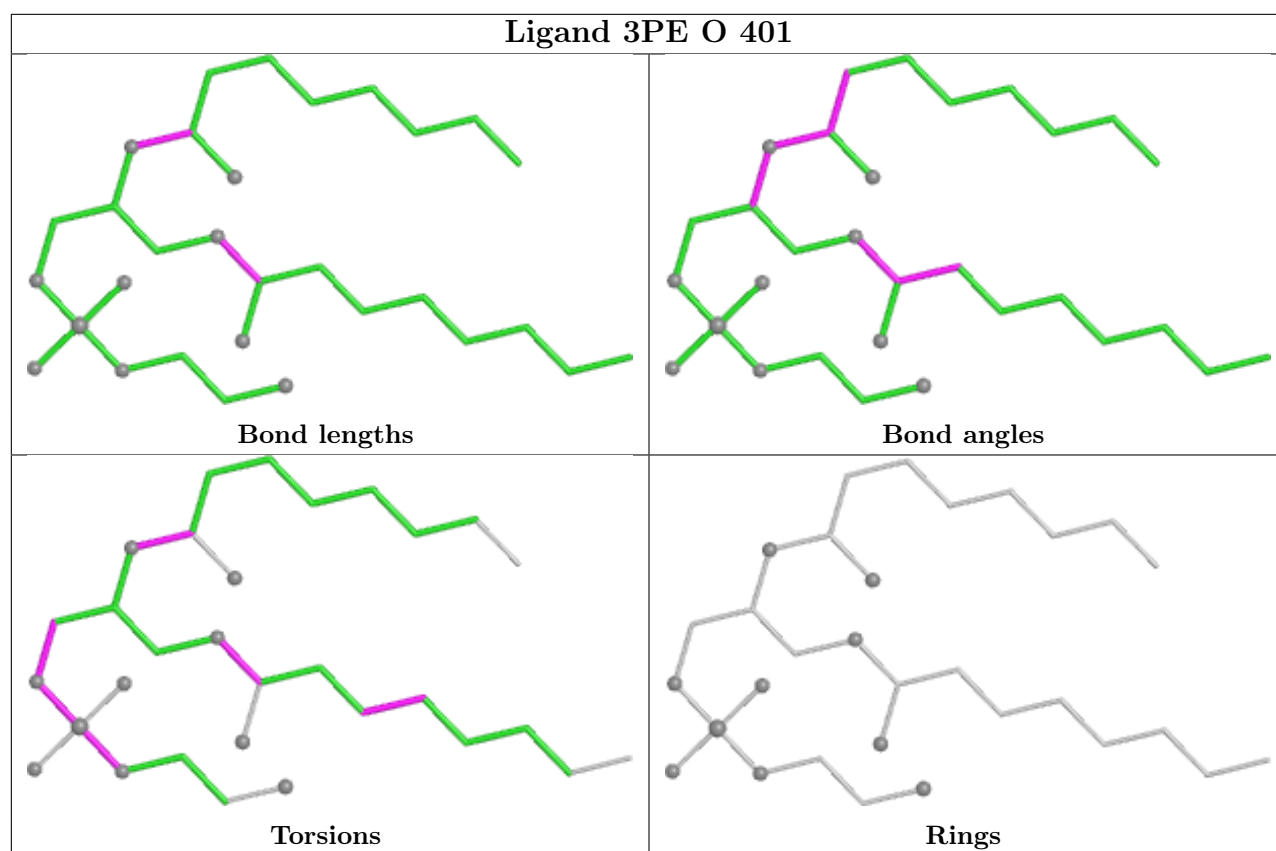
Torsions

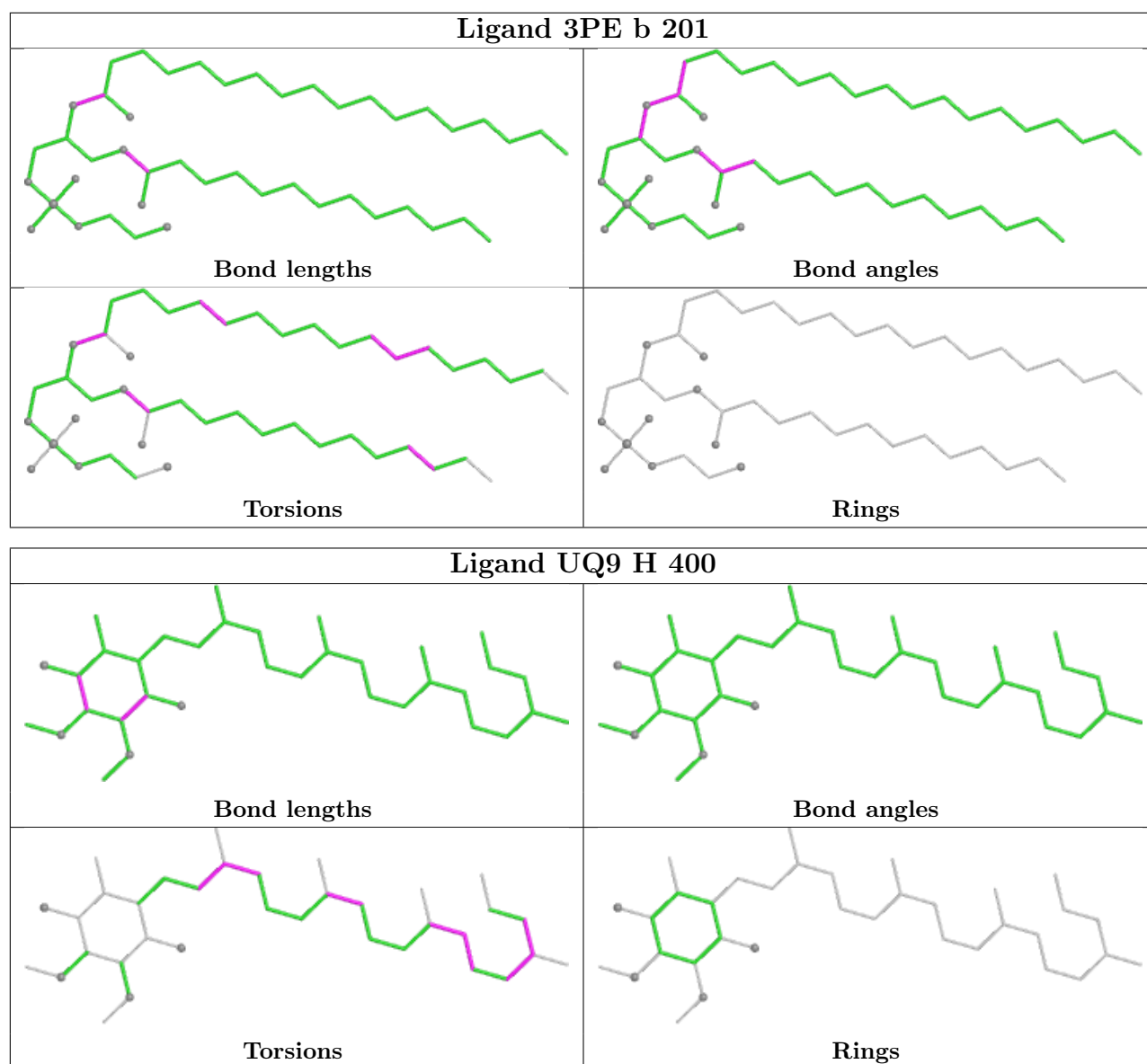


Rings

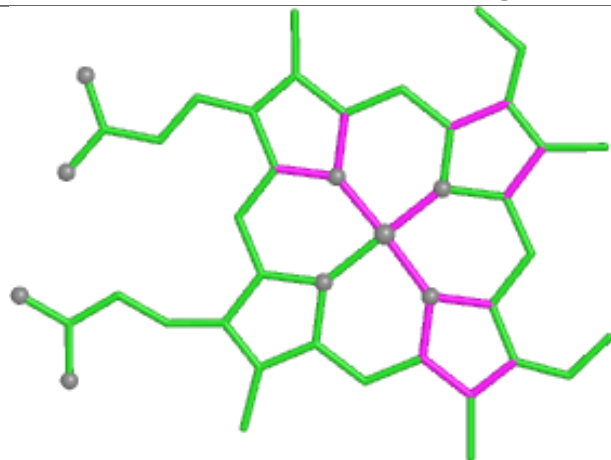




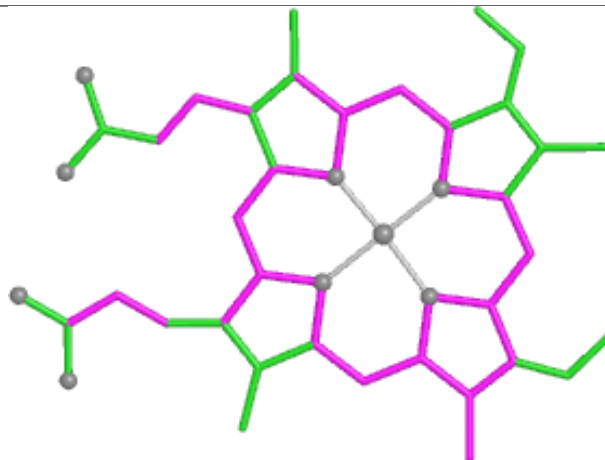




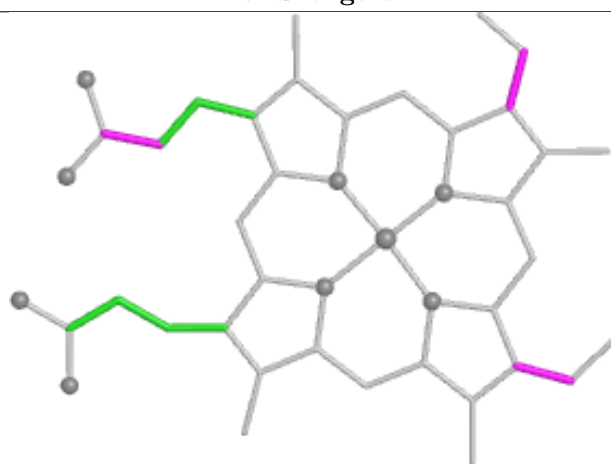
Ligand HEM AC 402



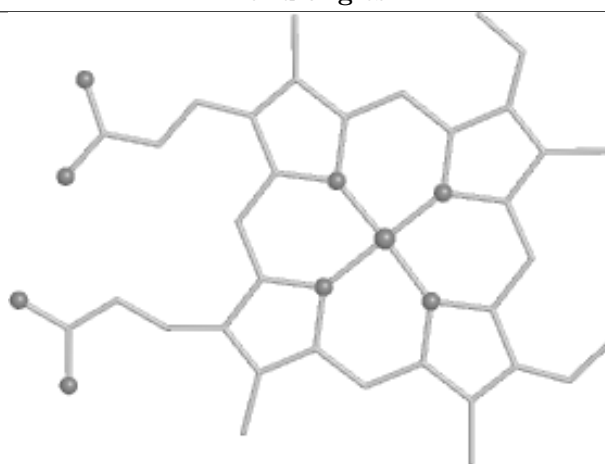
Bond lengths



Bond angles

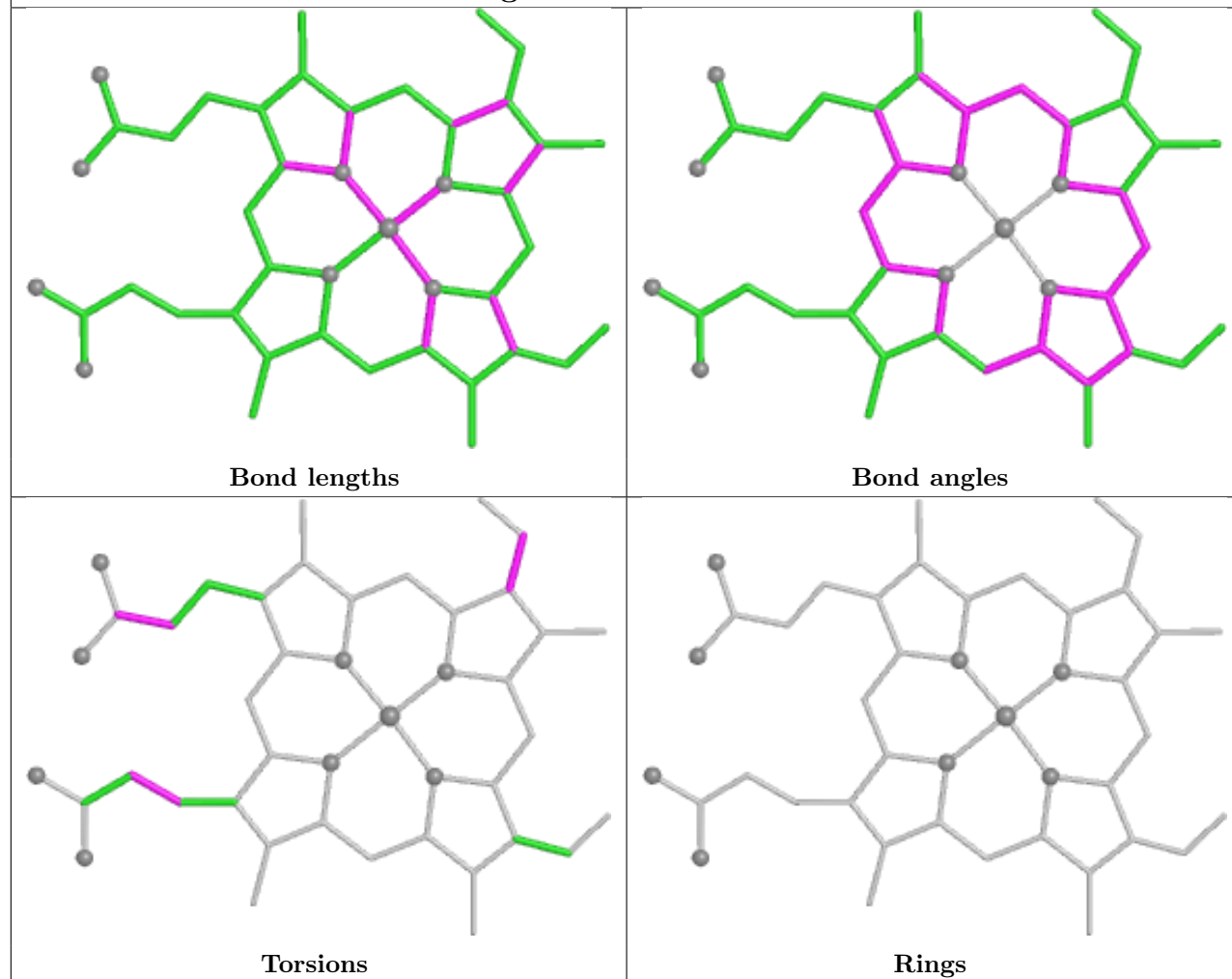


Torsions

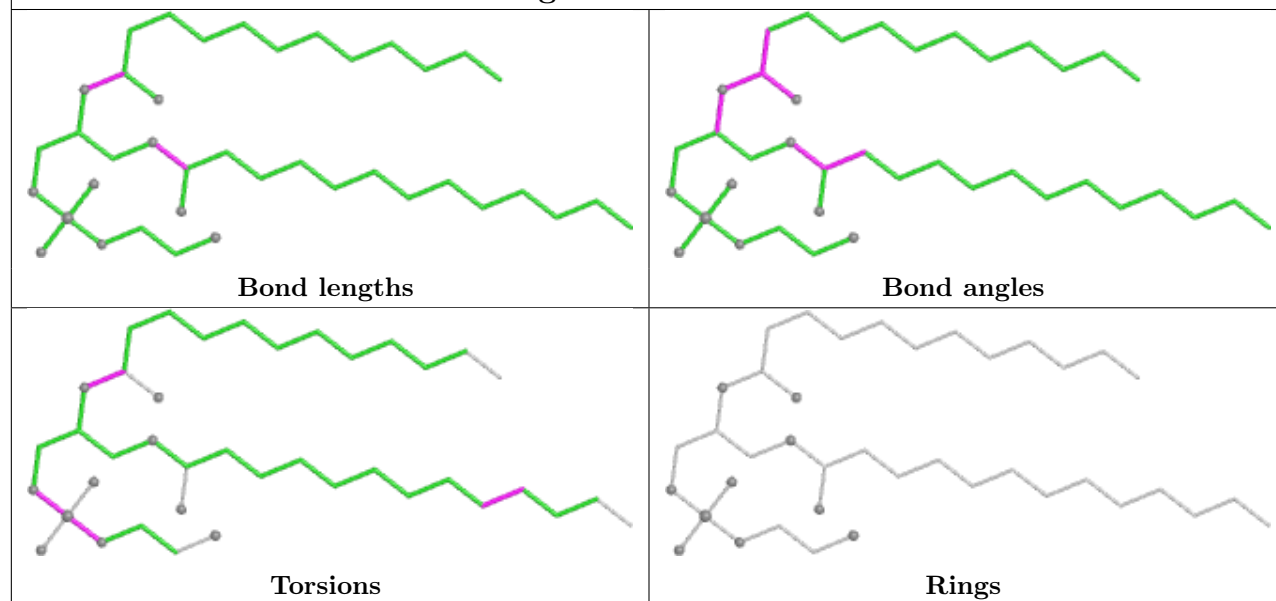


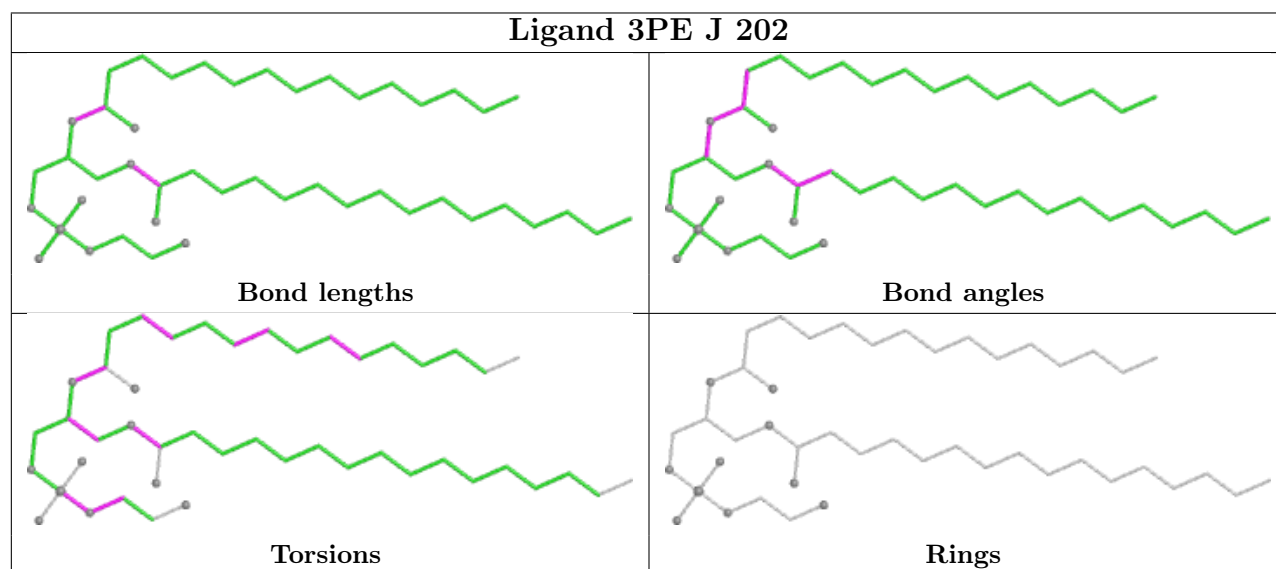
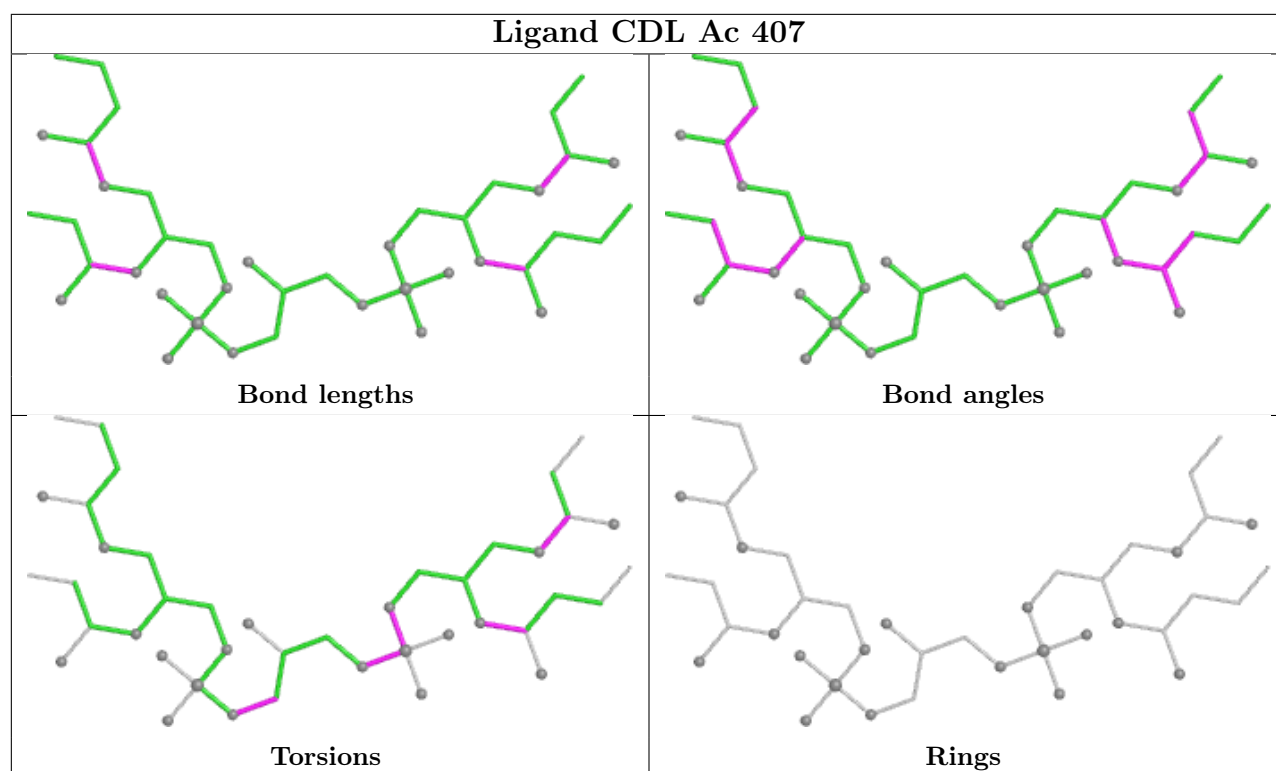
Rings

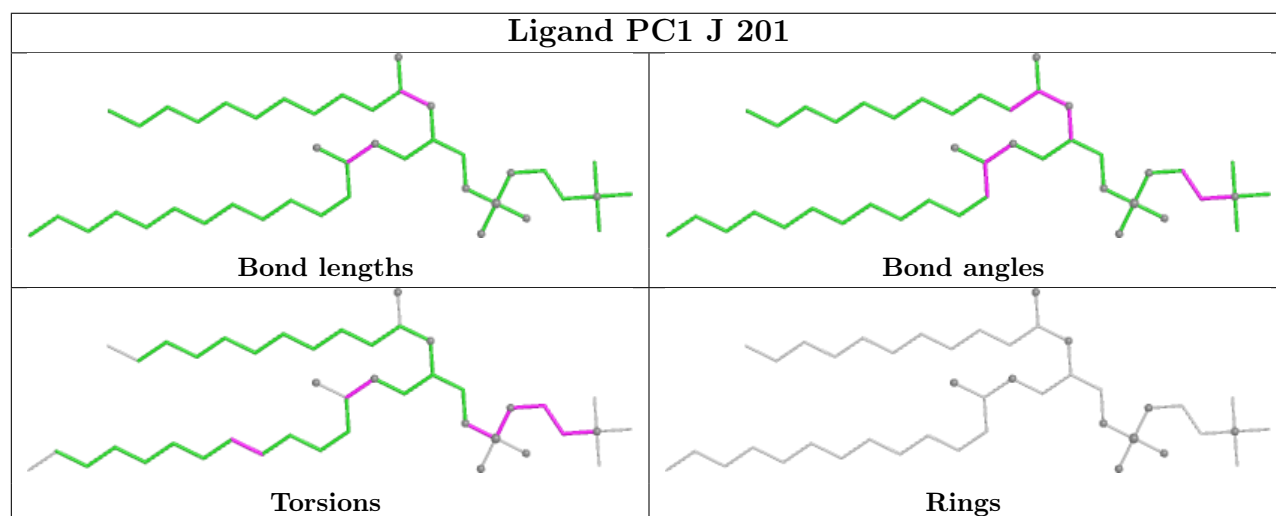
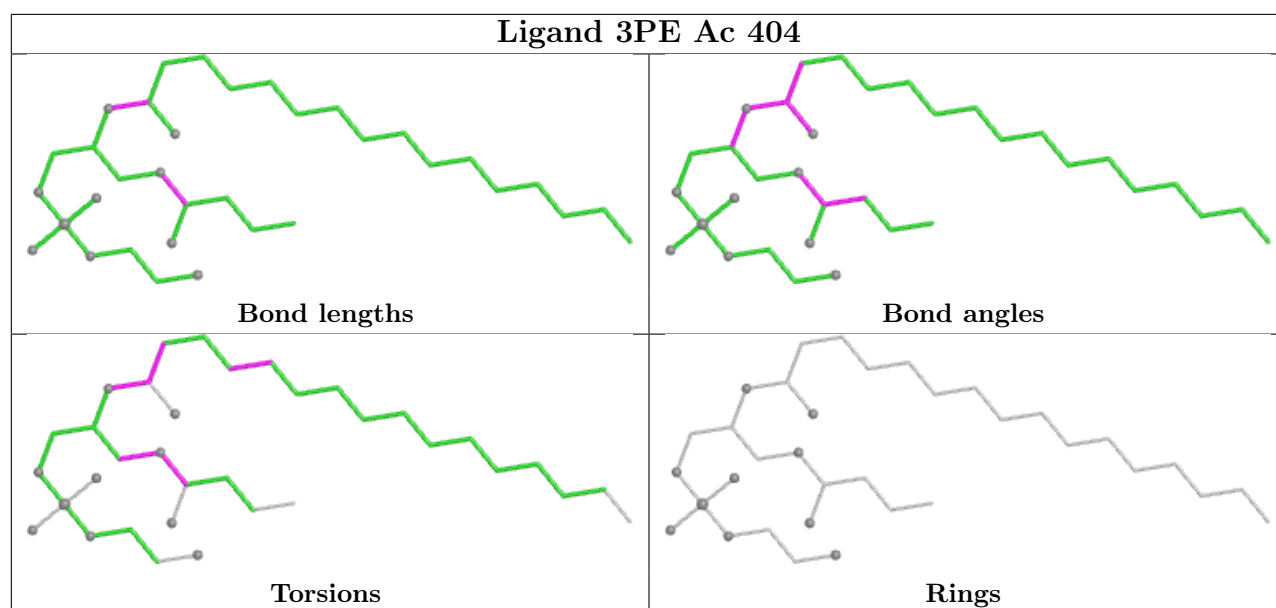
Ligand HEM Ac 402

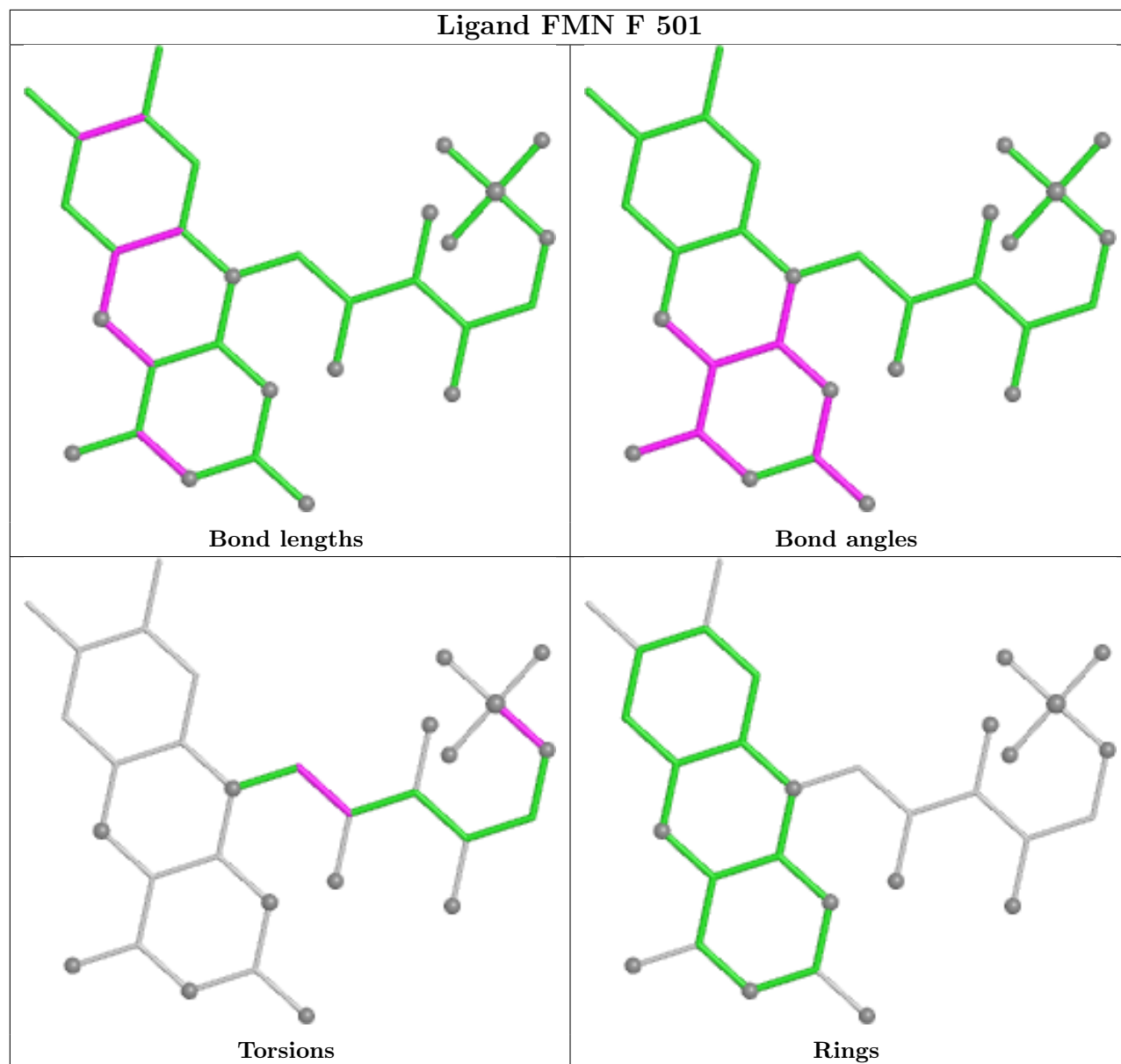


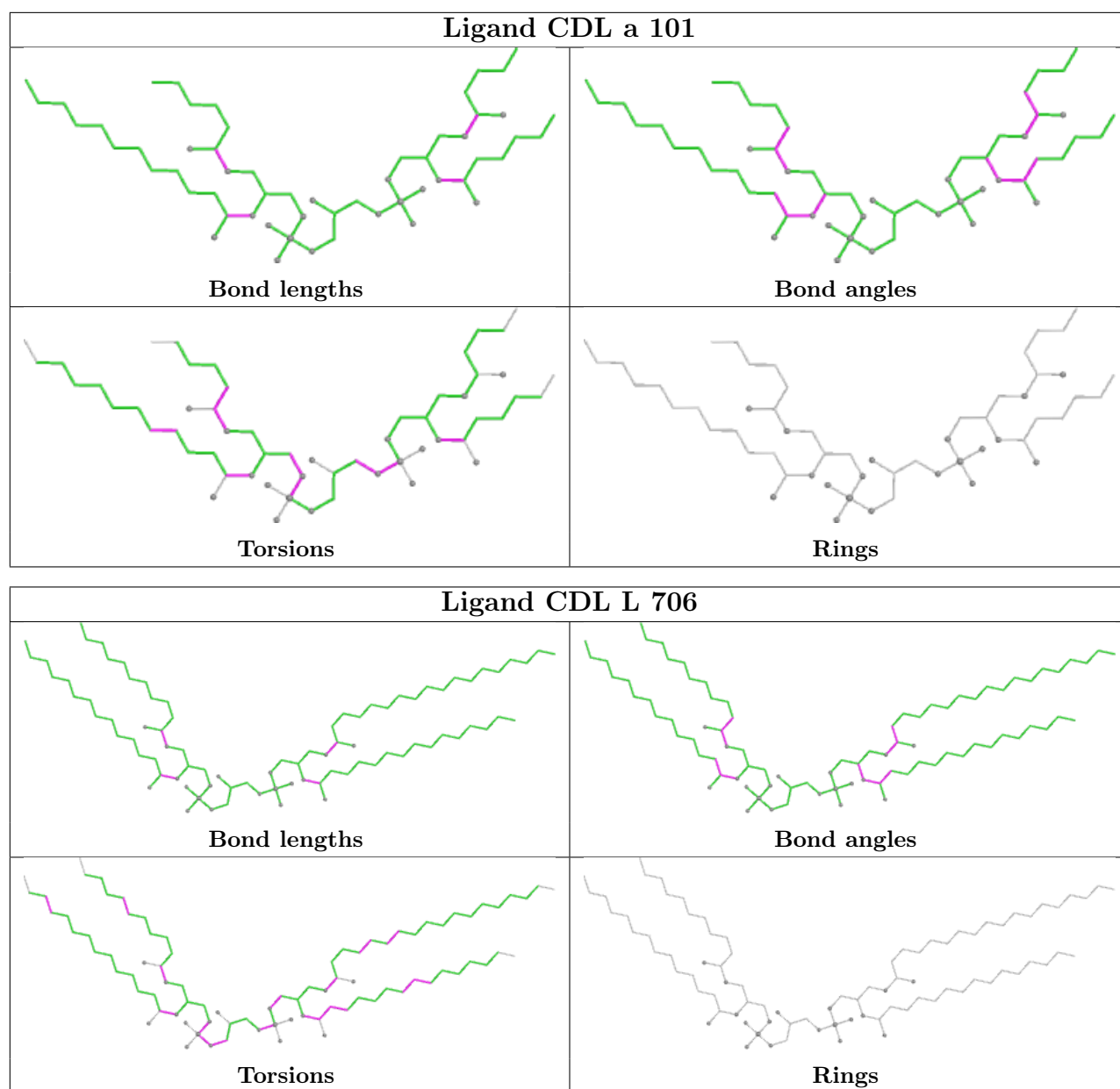
Ligand 3PE L 702



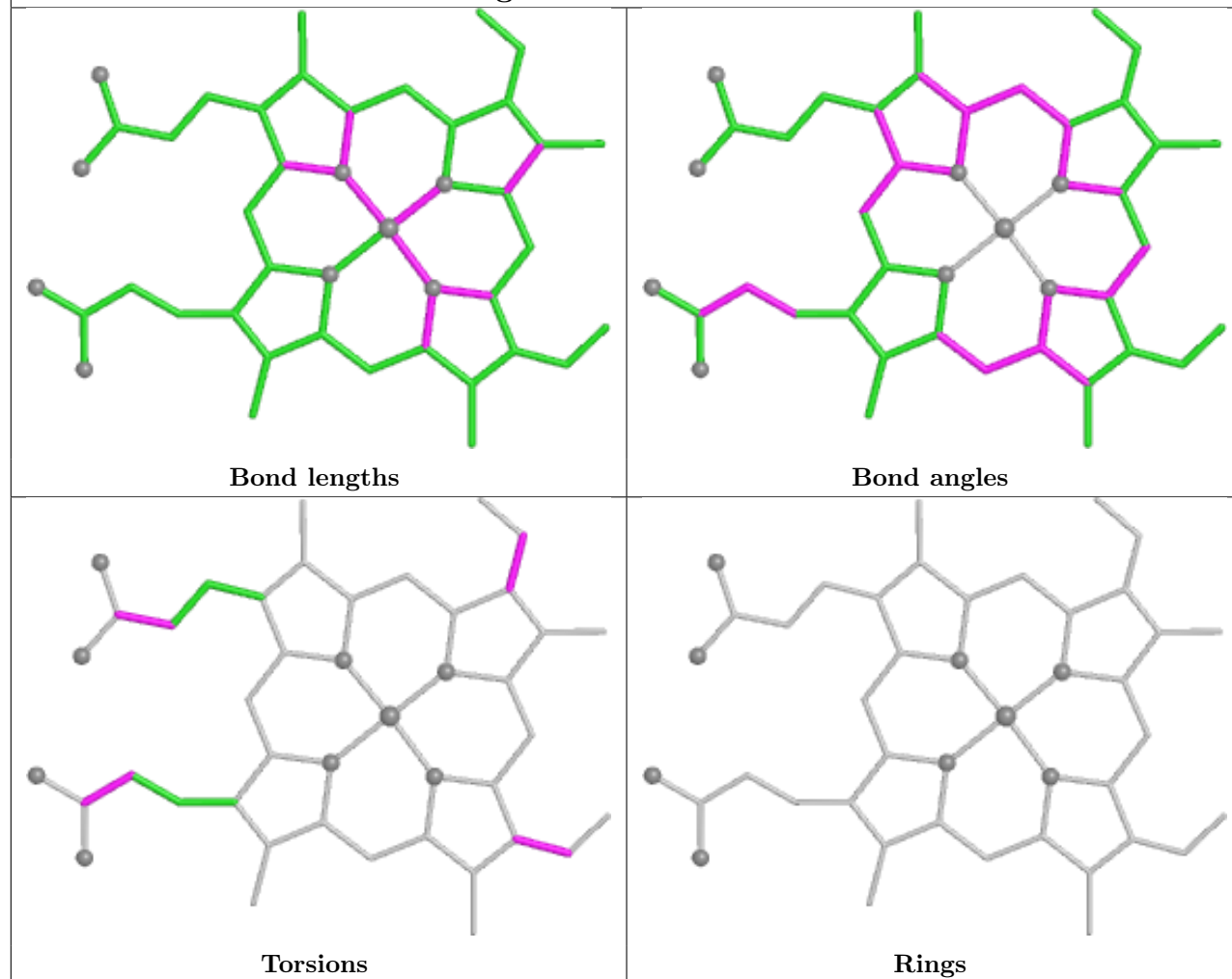




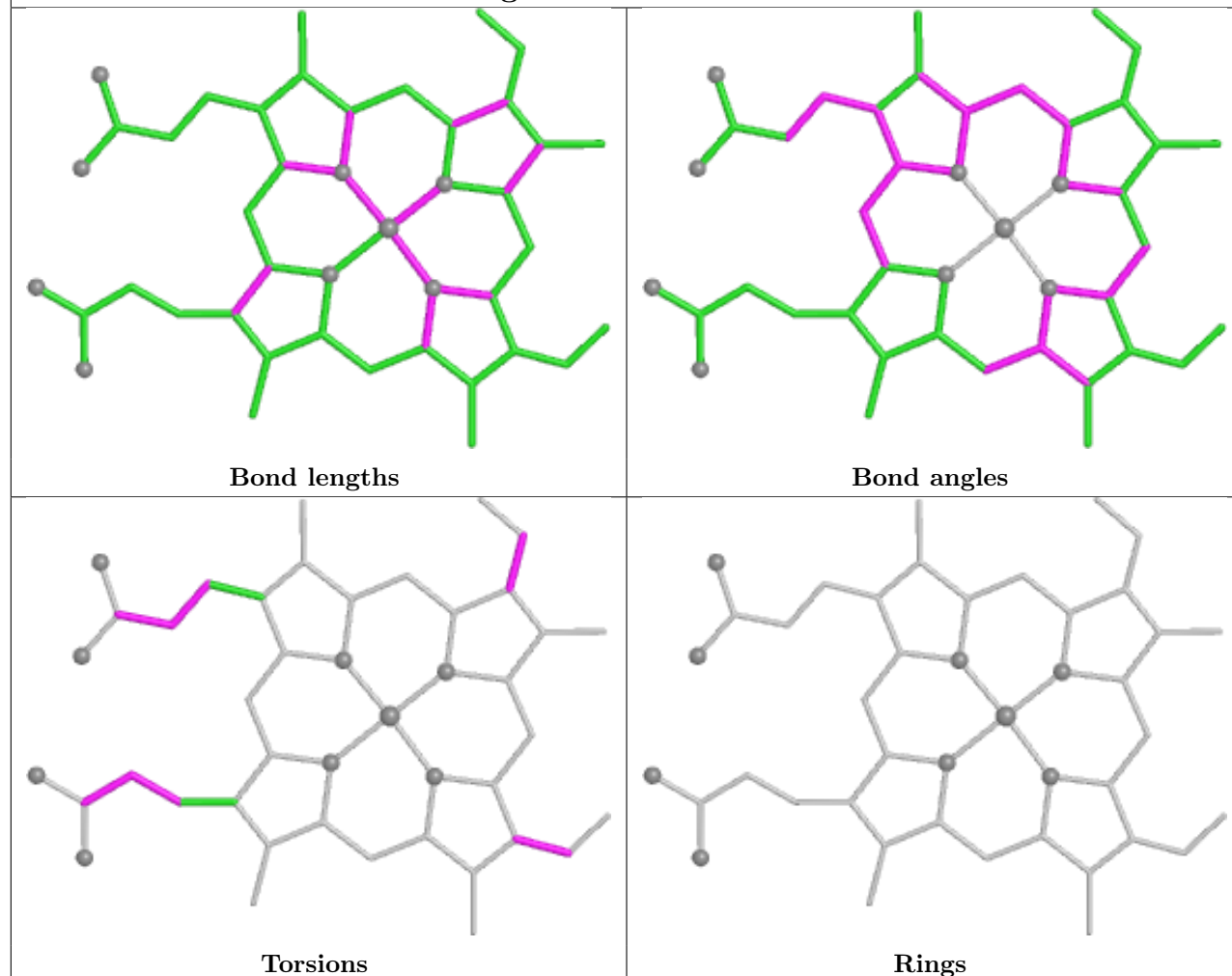




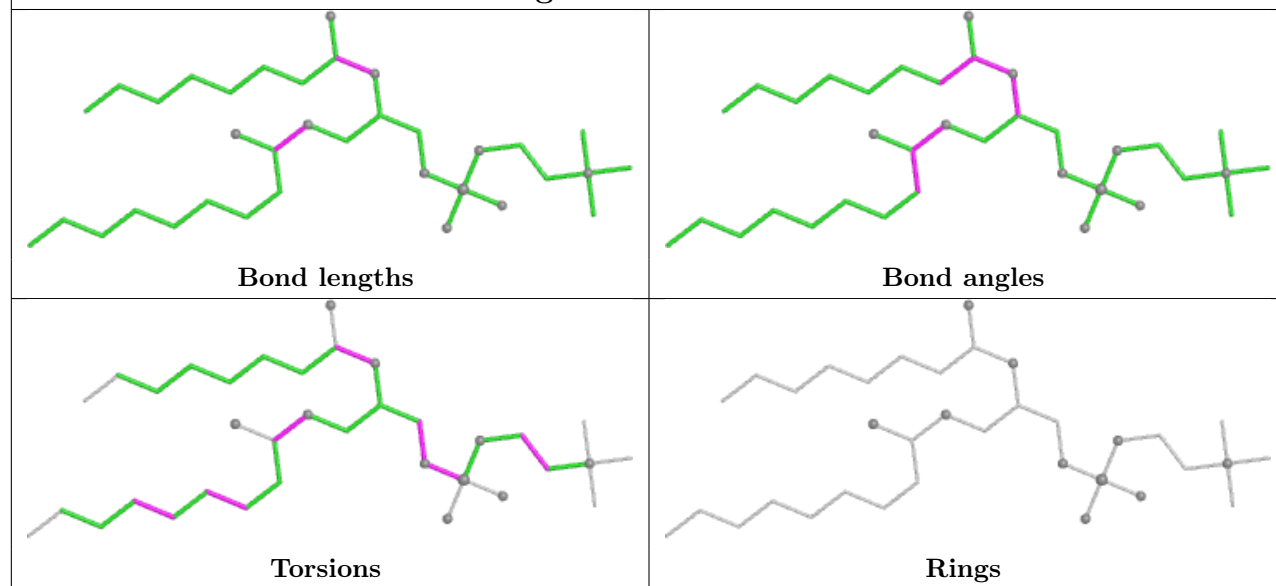
Ligand HEM AC 401

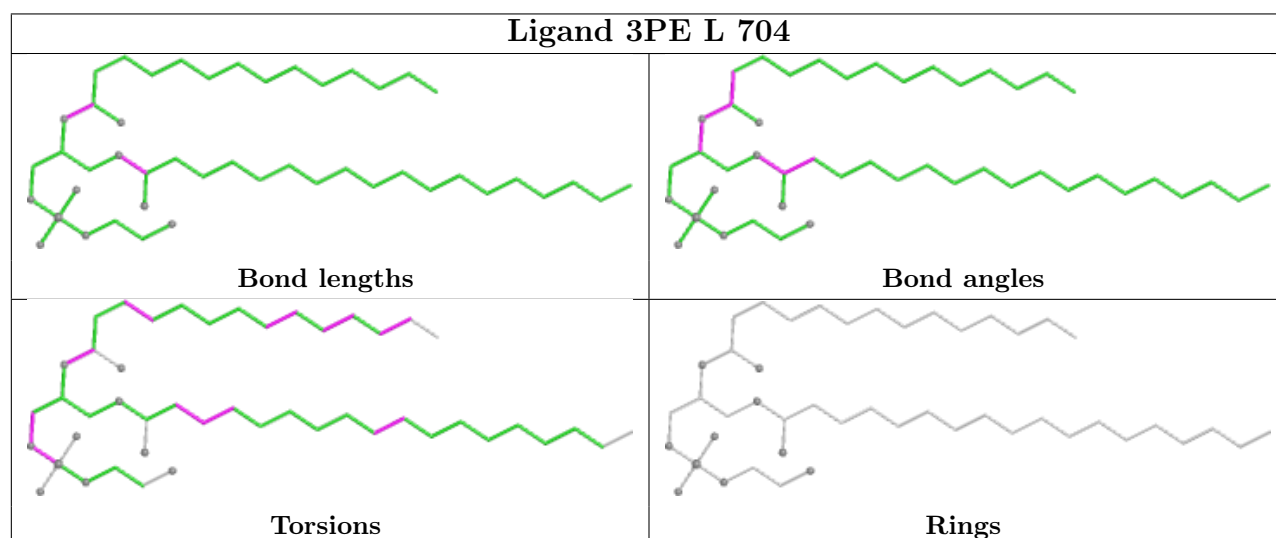
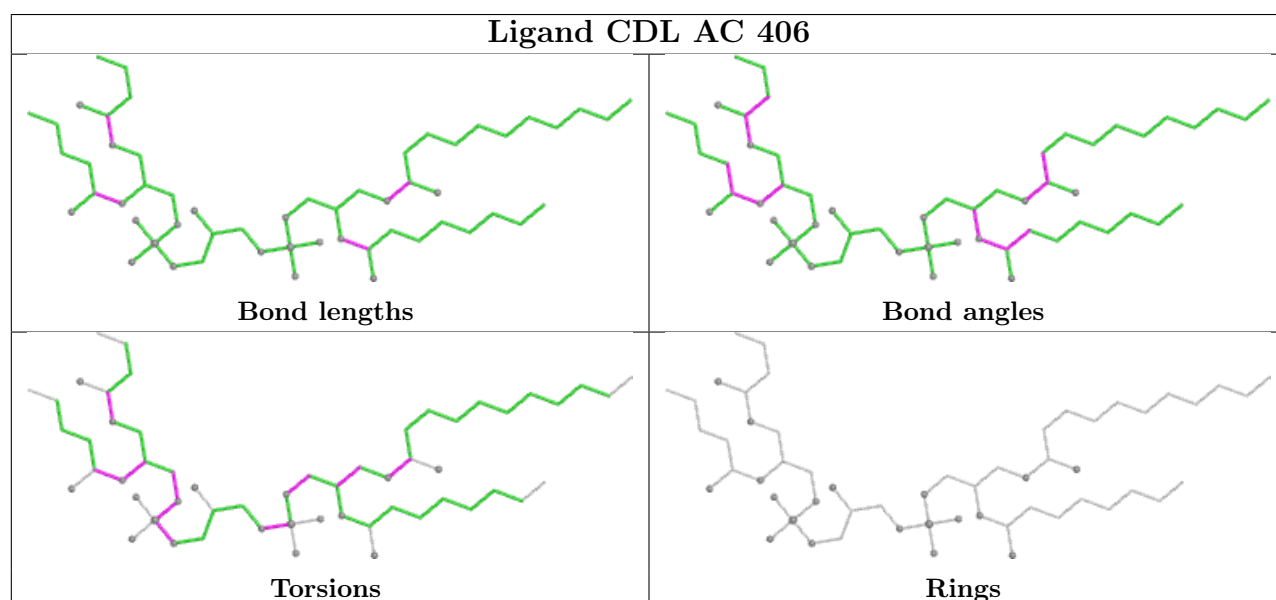
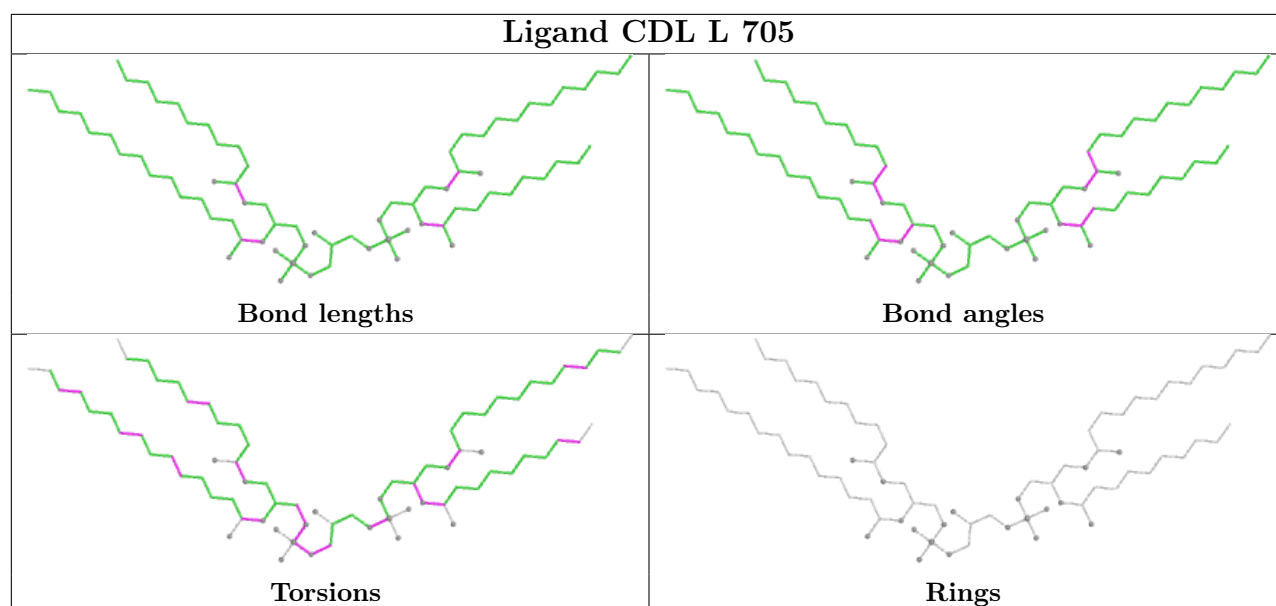


Ligand HEM Ac 403

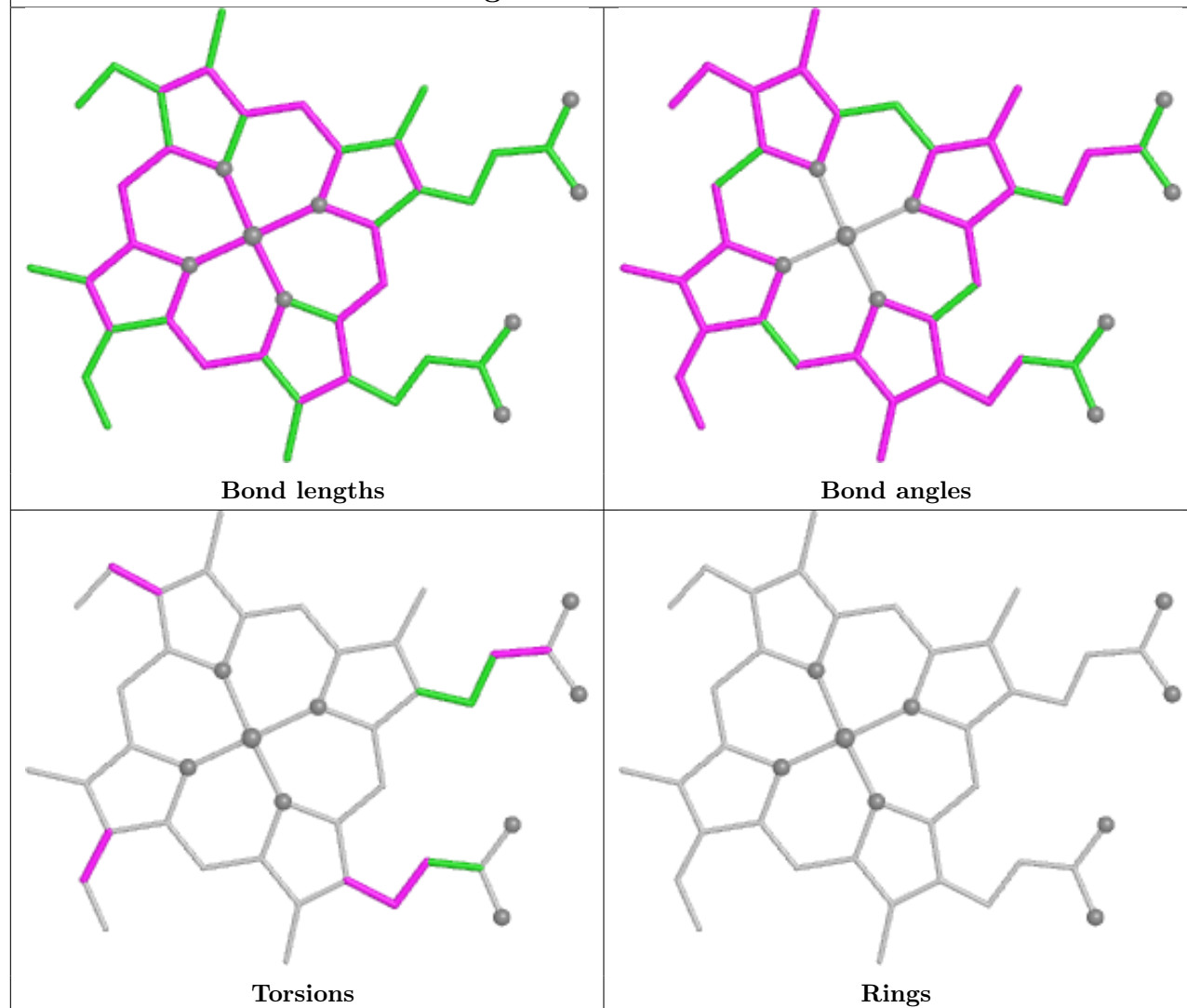


Ligand PC1 B 303

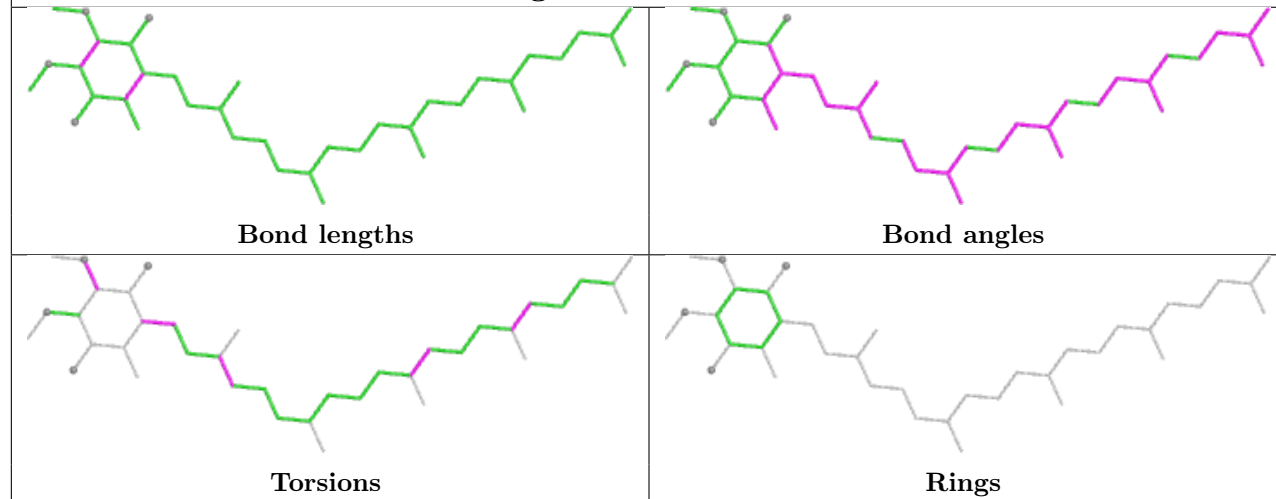




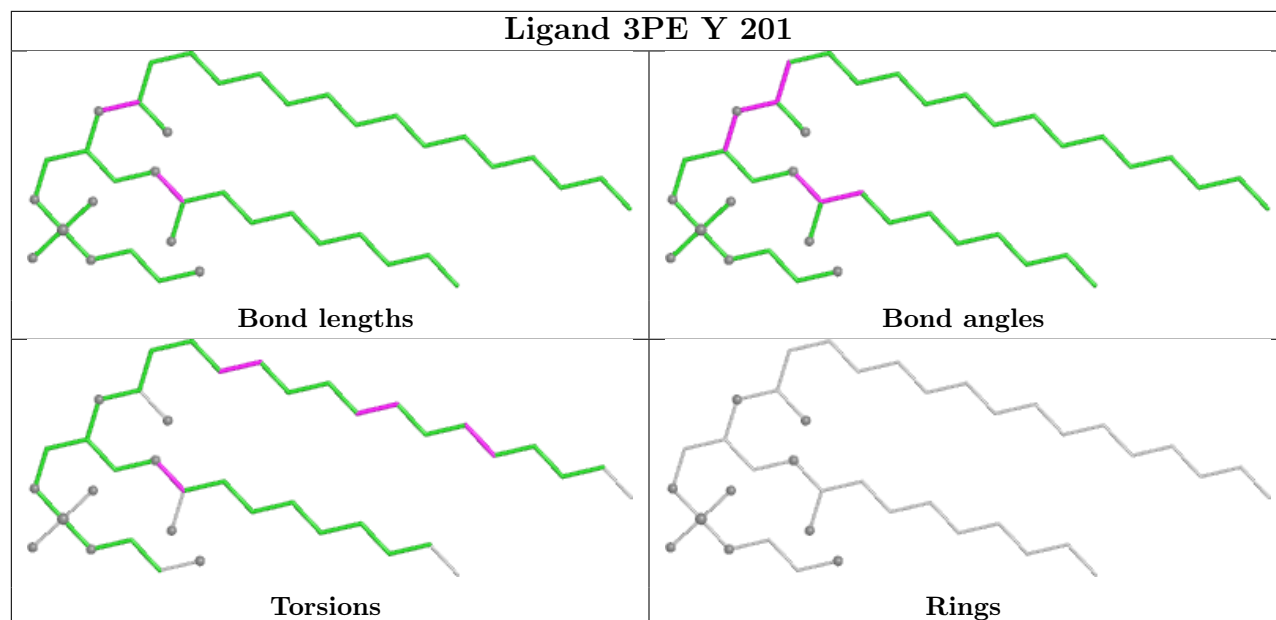
Ligand HEC Ad 401



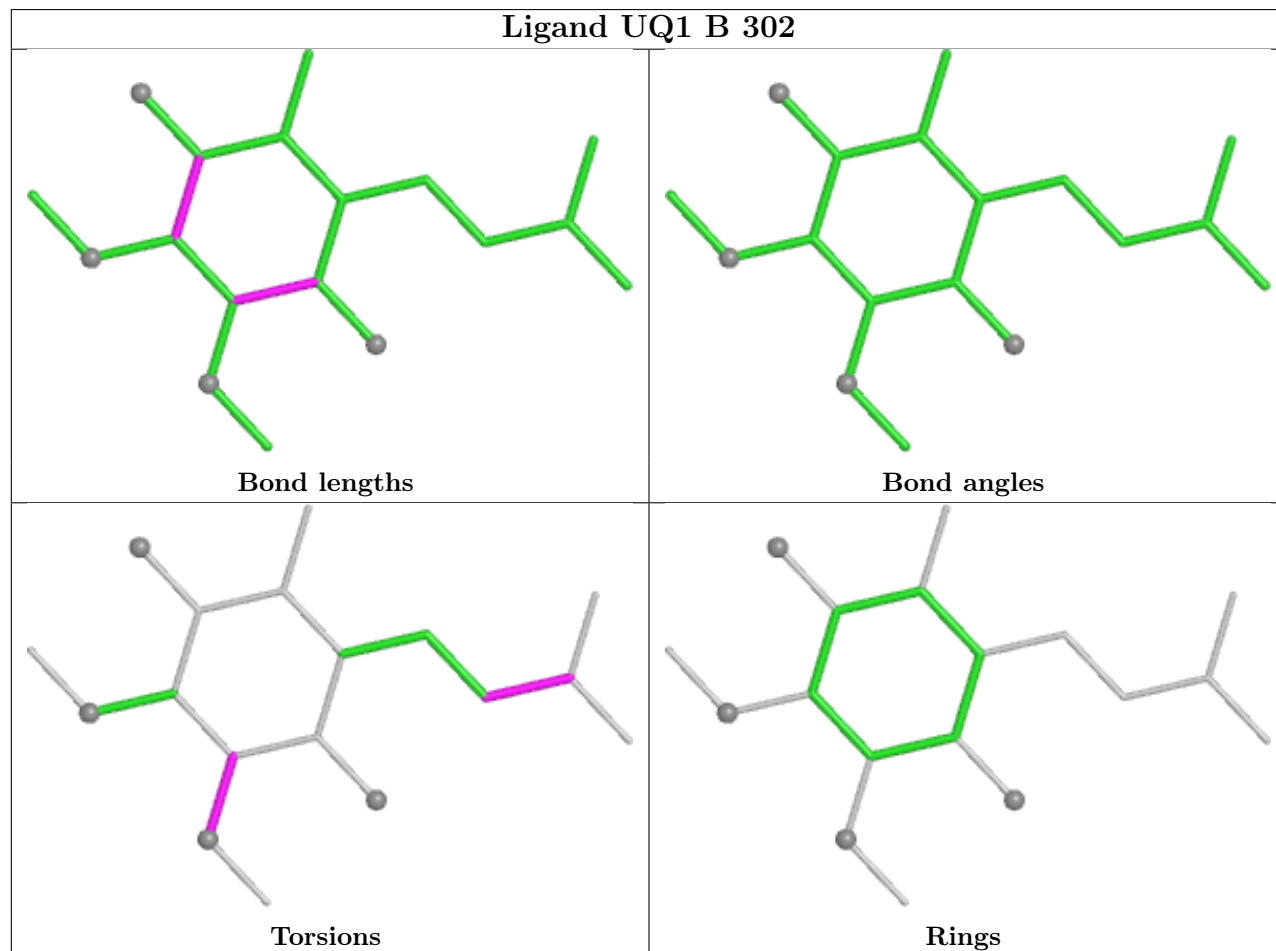
Ligand U10 Ac 405

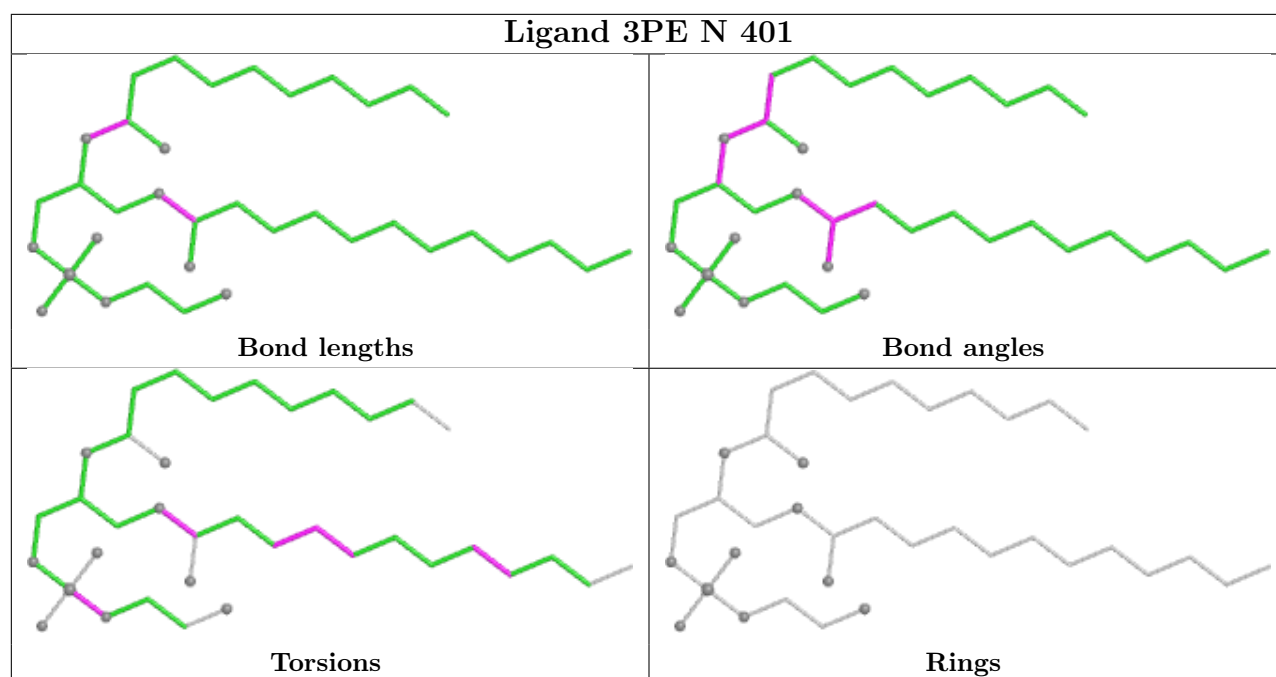


Ligand 3PE Y 201



Ligand UQ1 B 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

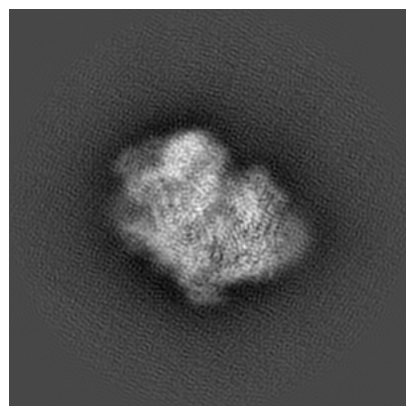
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35331. These allow visual inspection of the internal detail of the map and identification of artifacts.

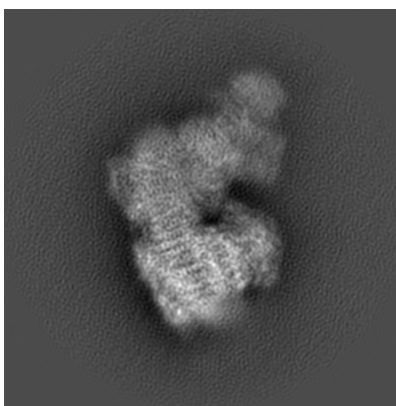
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

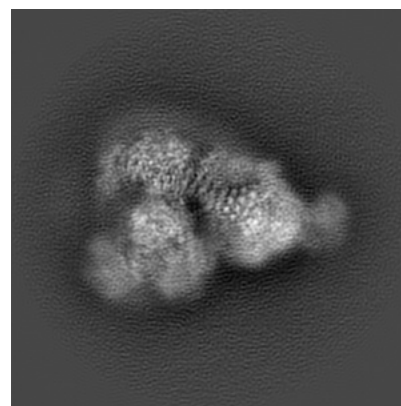
6.1.1 Primary map



X

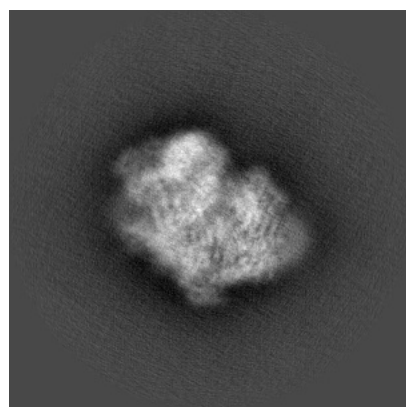


Y

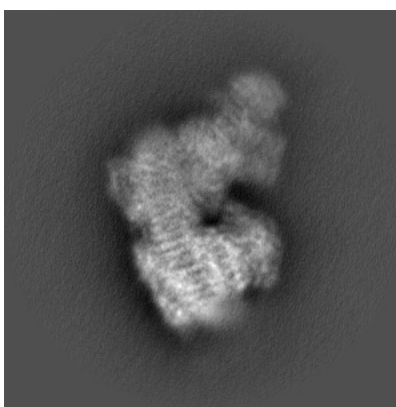


Z

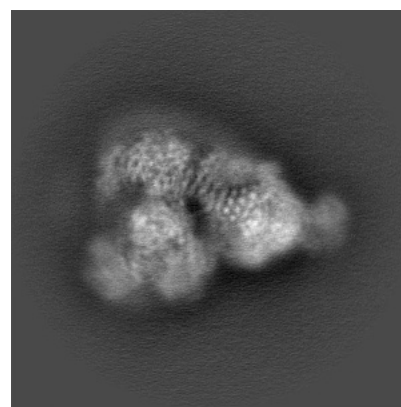
6.1.2 Raw map



X



Y

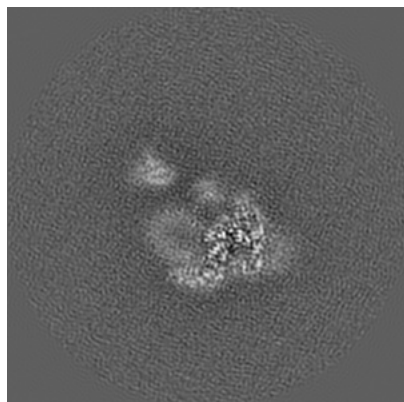


Z

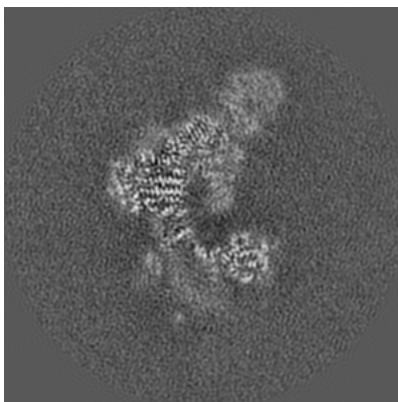
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

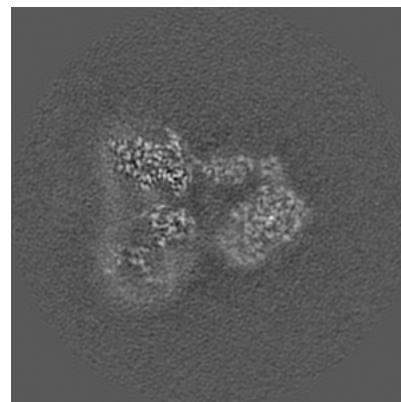
6.2.1 Primary map



X Index: 192

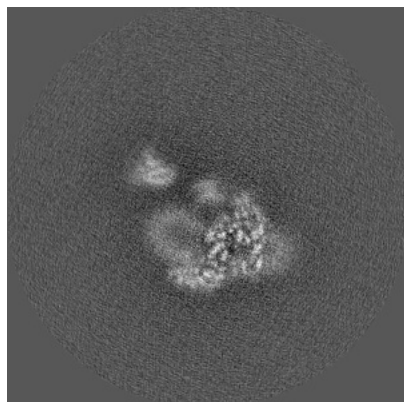


Y Index: 192

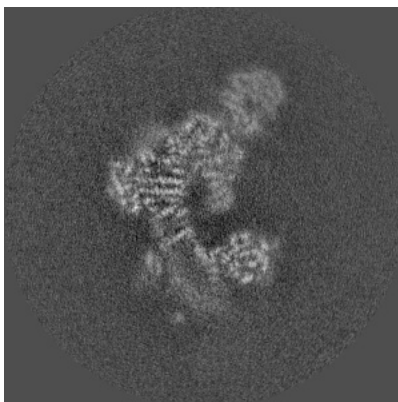


Z Index: 192

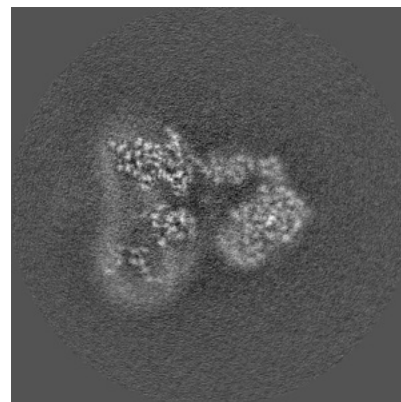
6.2.2 Raw map



X Index: 192



Y Index: 192

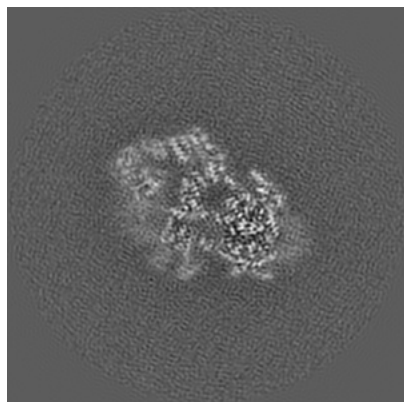


Z Index: 192

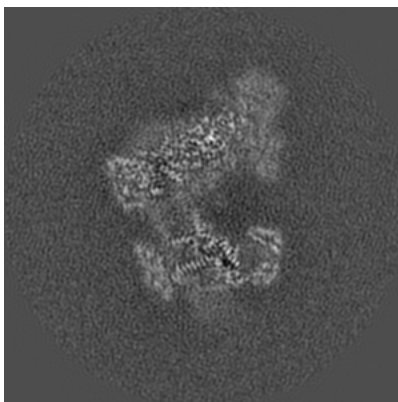
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

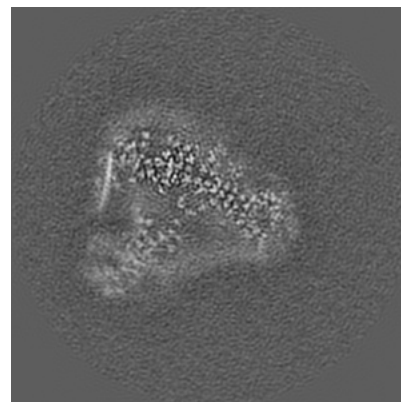
6.3.1 Primary map



X Index: 154

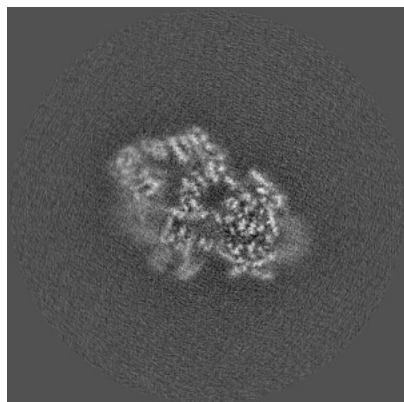


Y Index: 177

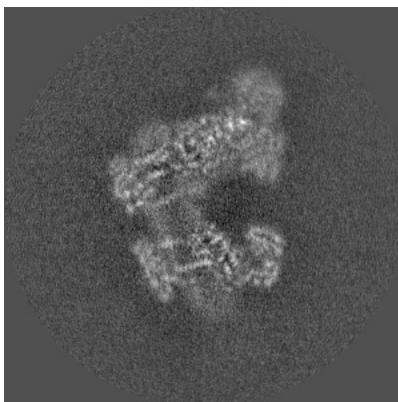


Z Index: 167

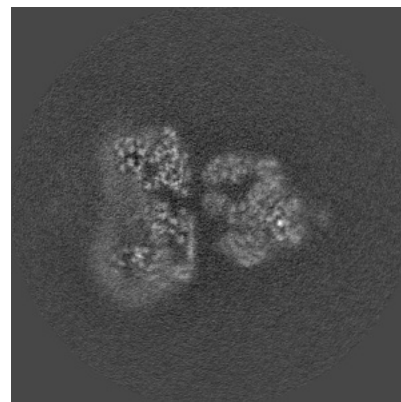
6.3.2 Raw map



X Index: 154



Y Index: 174

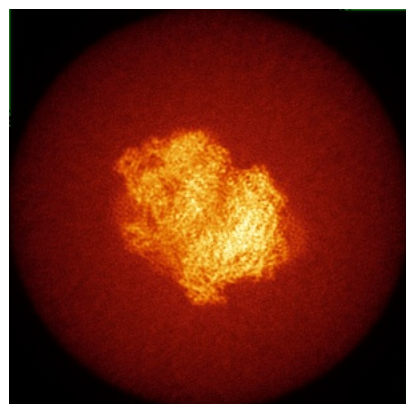


Z Index: 198

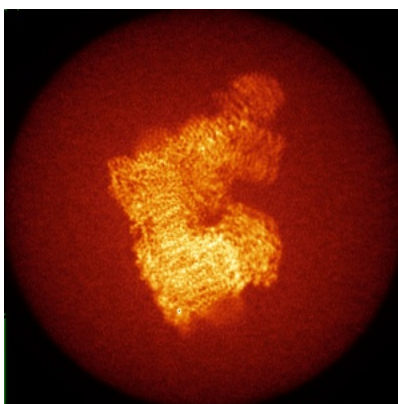
The images above show the largest variance slices of the map in three orthogonal directions.

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

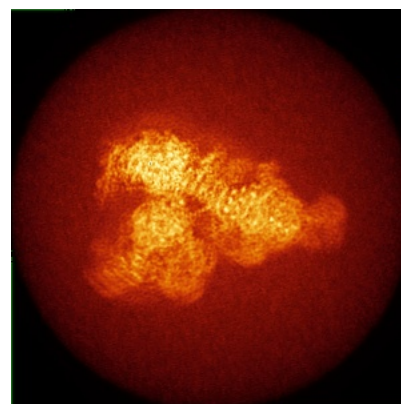
6.4.1 Primary map



X

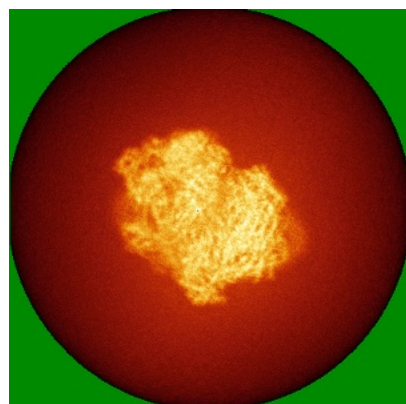


Y

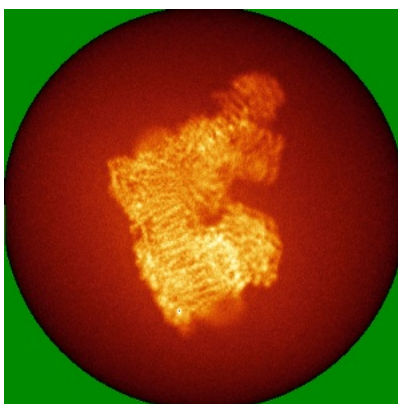


Z

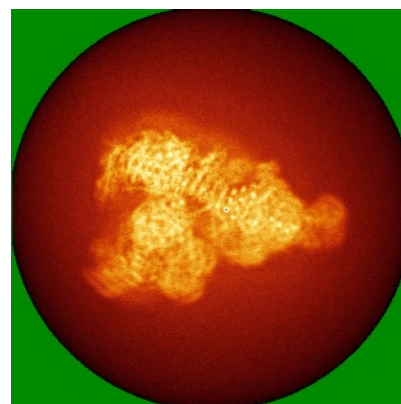
6.4.2 Raw map



X



Y

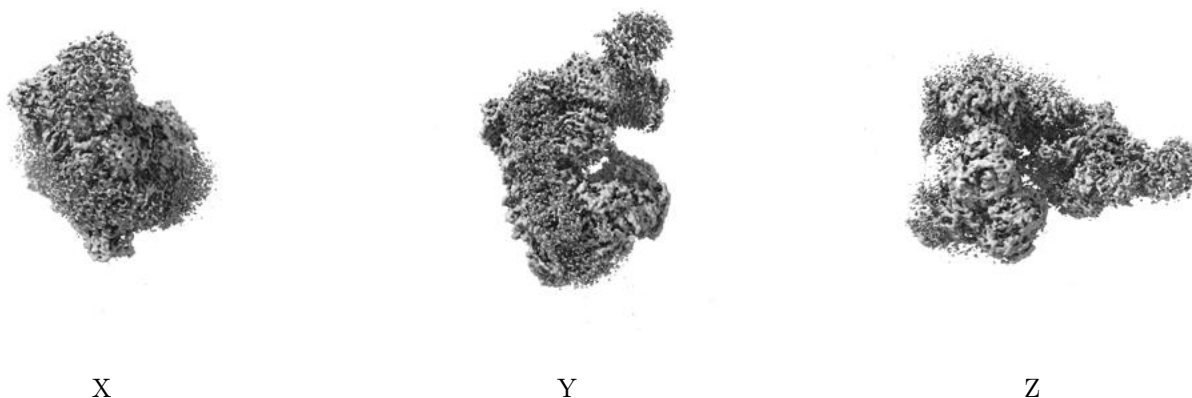


Z

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

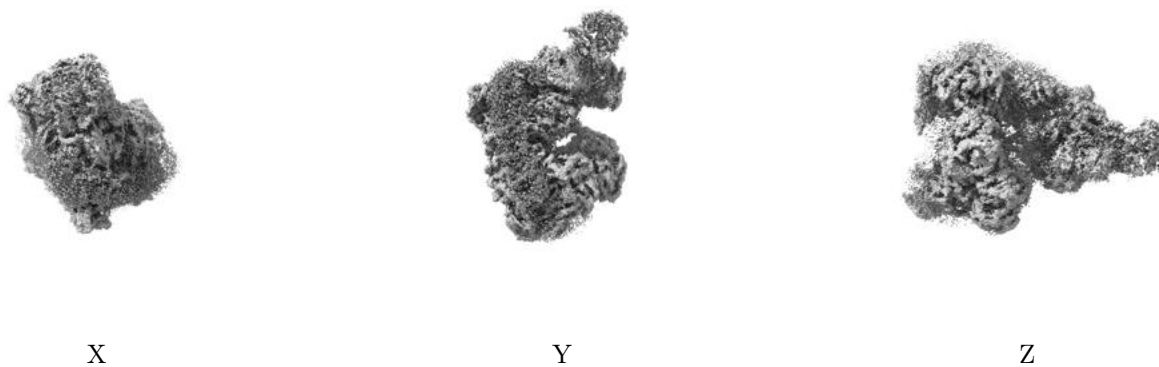
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

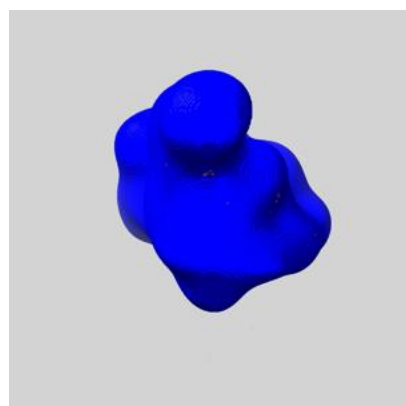
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

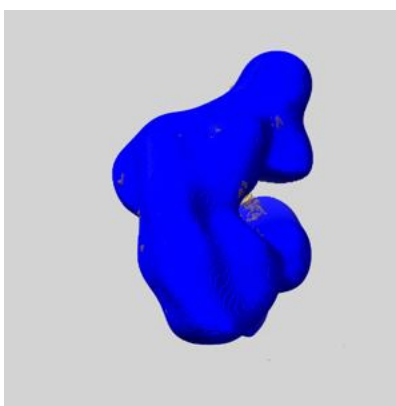
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

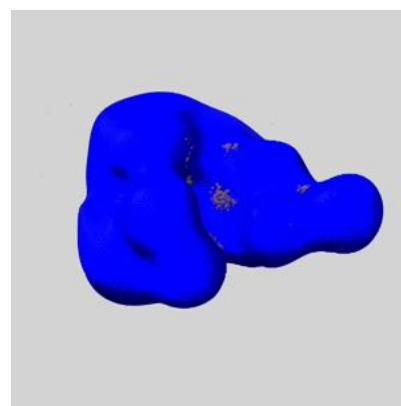
6.6.1 emd_35331_msk_1.map [i](#)



X



Y

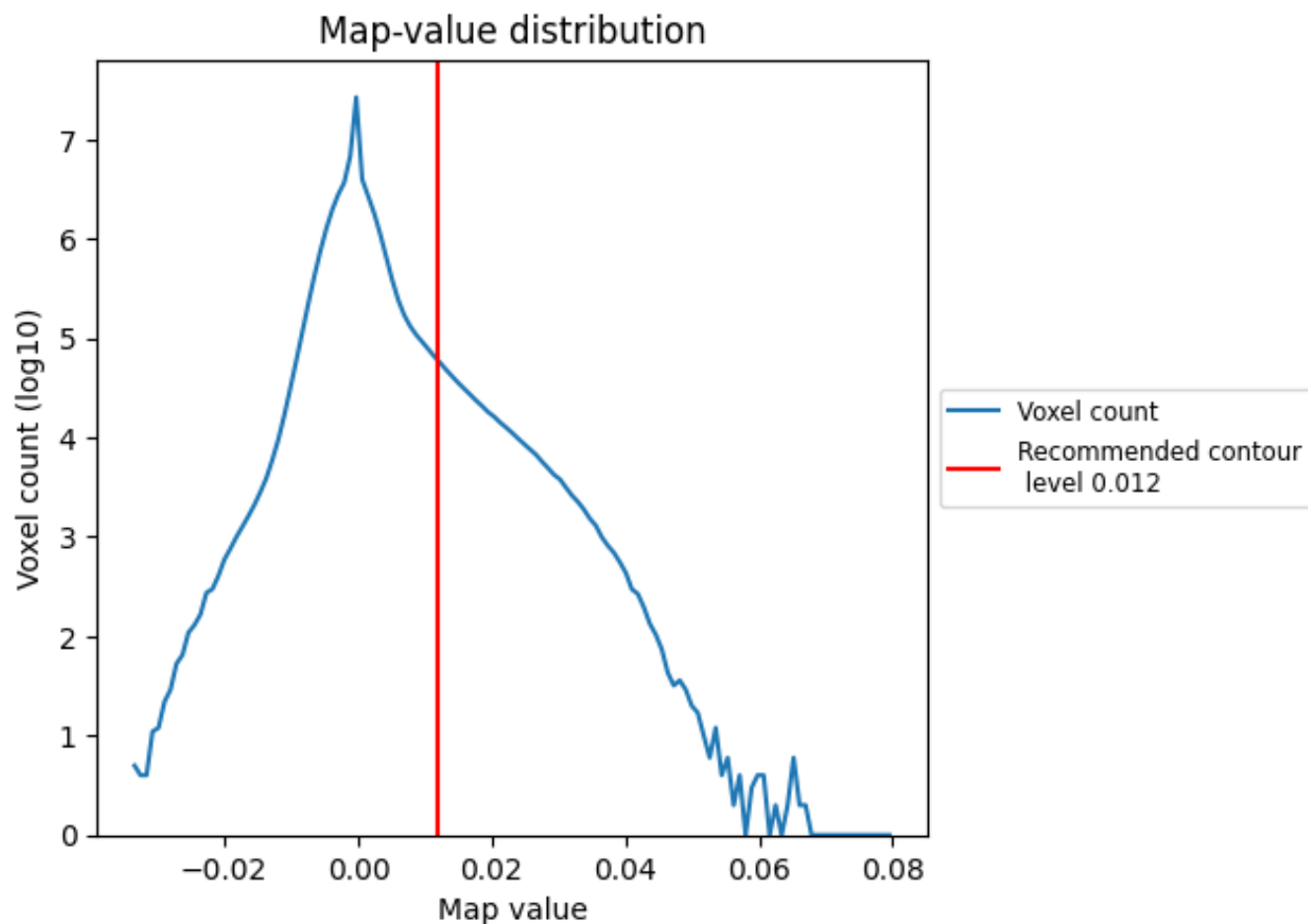


Z

7 Map analysis [i](#)

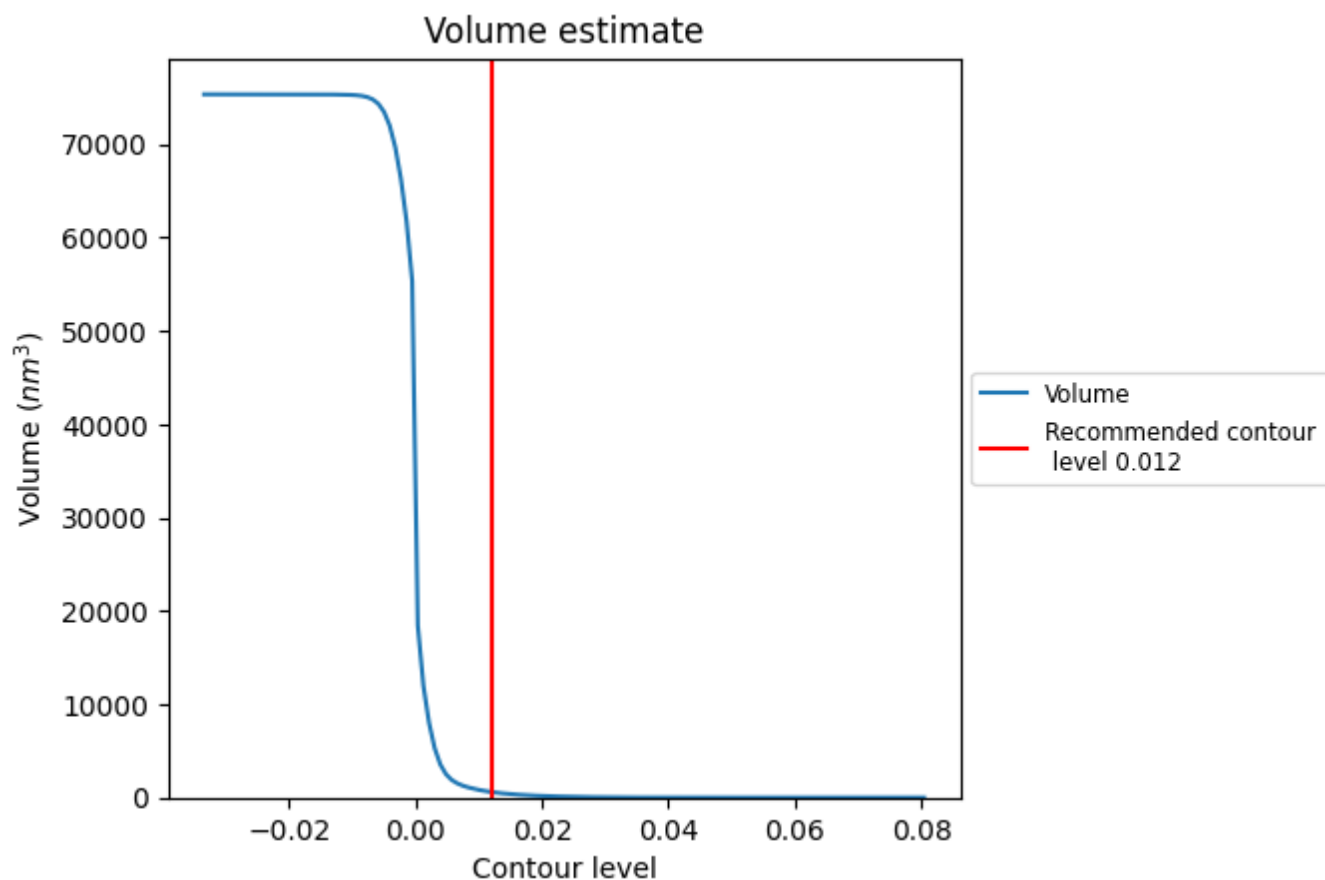
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

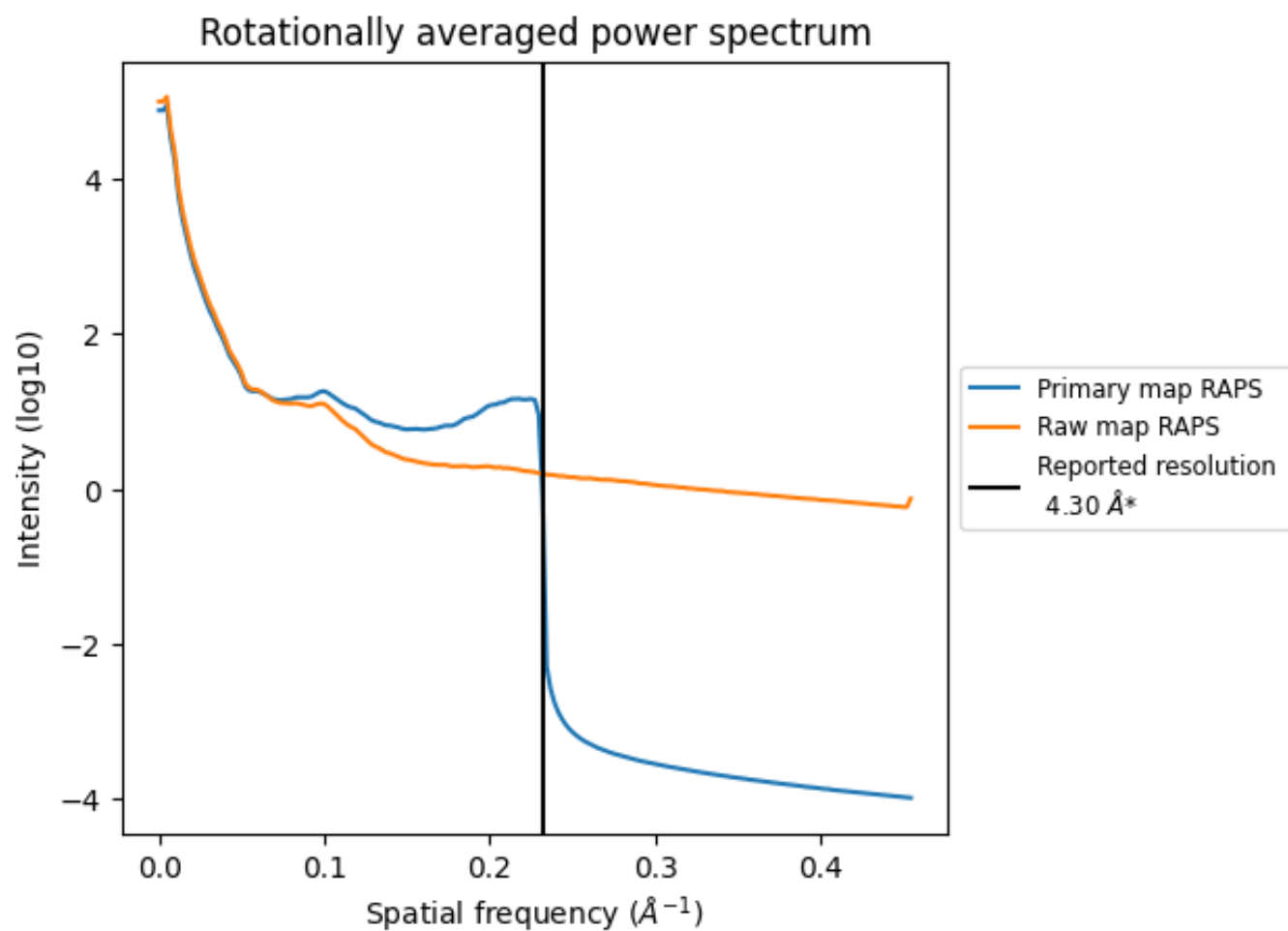
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 593 nm³; this corresponds to an approximate mass of 536 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

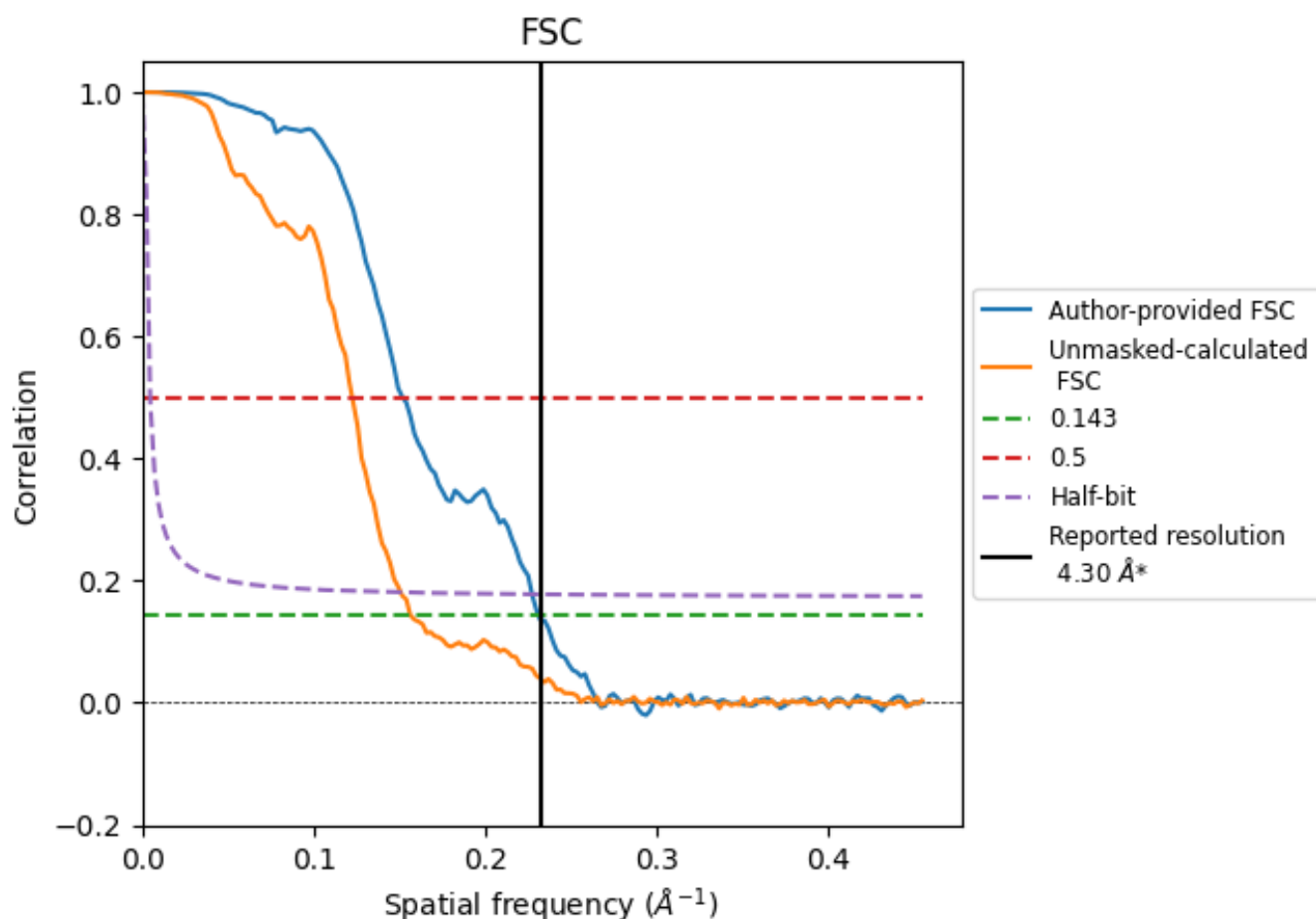


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates

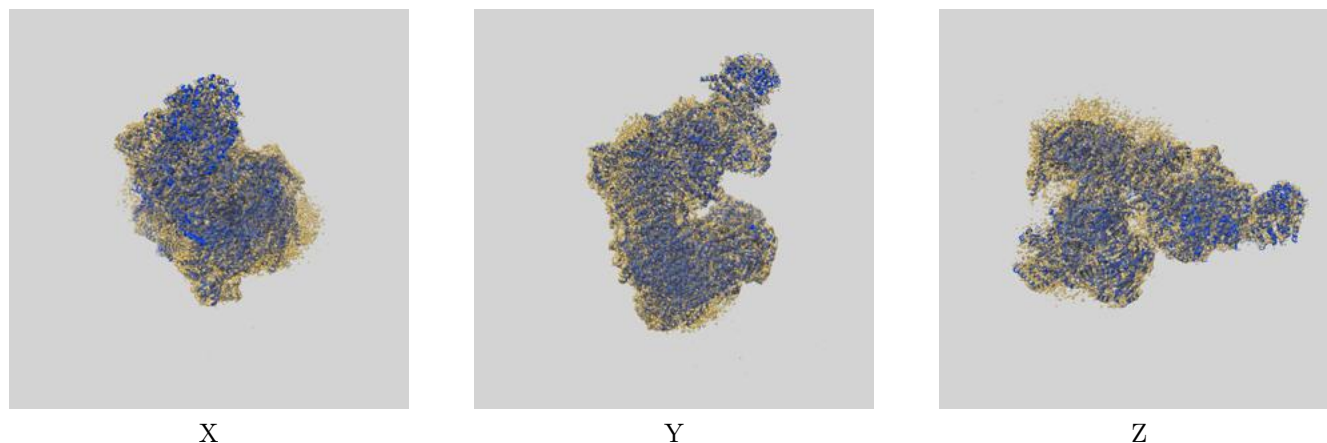
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.59	4.40
Unmasked-calculated*	6.39	8.17	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

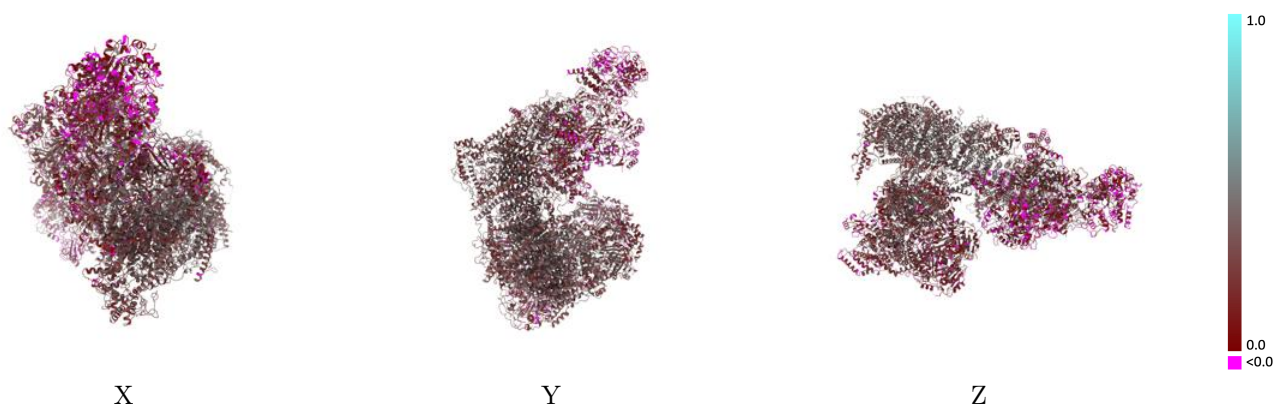
This section contains information regarding the fit between EMDB map EMD-35331 and PDB model 8IB4. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



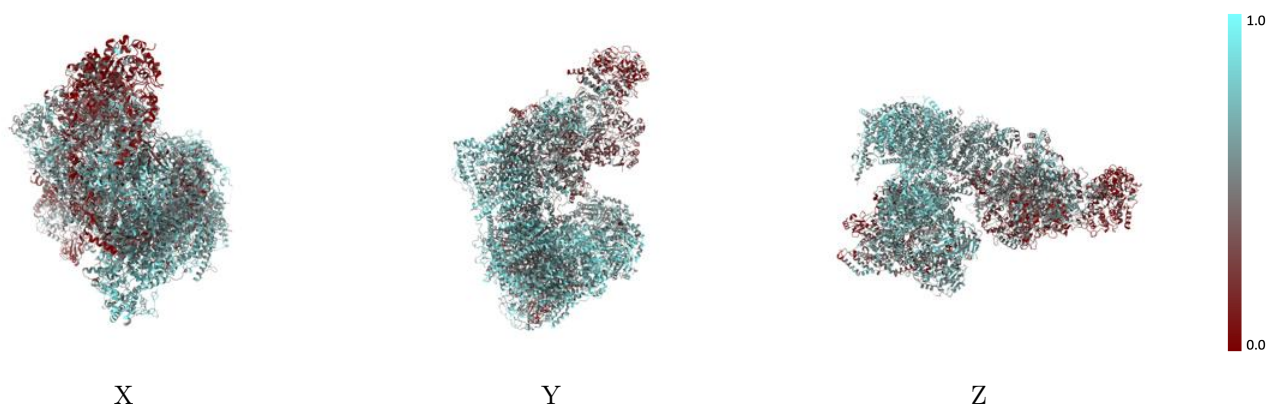
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



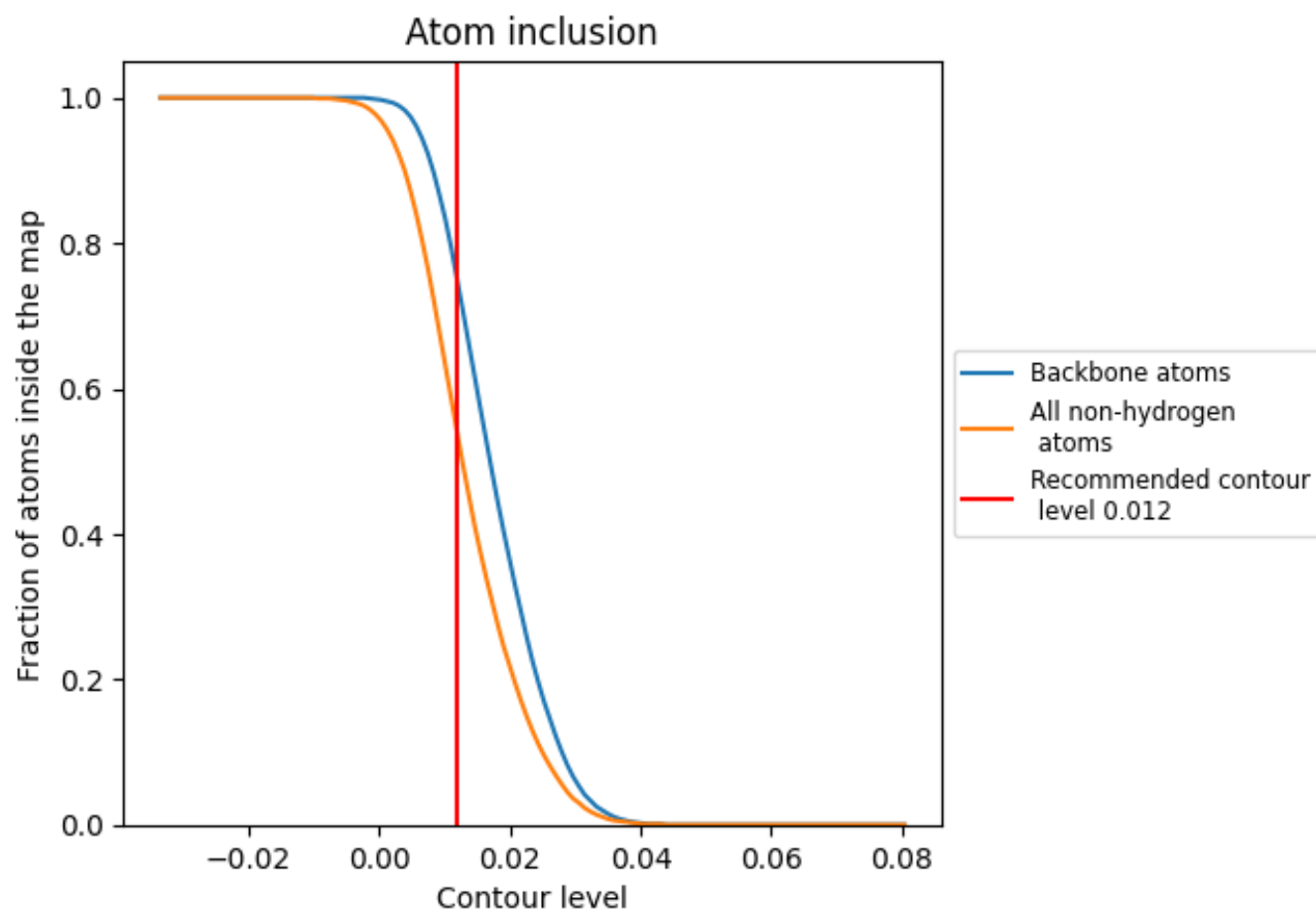
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5370	 0.2580
A	 0.5630	 0.3210
AA	 0.5930	 0.2210
AB	 0.5900	 0.2290
AC	 0.4970	 0.2570
AD	 0.5020	 0.1900
AE	 0.1630	 0.1300
AF	 0.6180	 0.2580
AG	 0.4350	 0.1990
AH	 0.4400	 0.1220
AI	 0.2820	 0.2100
AJ	 0.1830	 0.1680
AK	 0.1720	 0.1620
Aa	 0.6900	 0.3210
Ab	 0.6560	 0.2690
Ac	 0.5620	 0.2860
Ad	 0.5900	 0.2170
Ae	 0.1790	 0.1480
Af	 0.6290	 0.2990
Ag	 0.5350	 0.2910
Ah	 0.5510	 0.1690
Aj	 0.3540	 0.2340
Ak	 0.1580	 0.1740
B	 0.6170	 0.3110
C	 0.5140	 0.2050
D	 0.6100	 0.3010
E	 0.1830	 0.0850
F	 0.2410	 0.1140
G	 0.3630	 0.1480
H	 0.6240	 0.3380
I	 0.6400	 0.2880
J	 0.5270	 0.2930
K	 0.6230	 0.3560
L	 0.6340	 0.3490
M	 0.6740	 0.3770



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Chain	Atom inclusion	Q-score
N	 0.6600	 0.3700
O	 0.5300	 0.2840
P	 0.3430	 0.1390
Q	 0.3060	 0.1770
R	 0.2130	 0.1200
S	 0.2980	 0.1030
T	 0.2020	 0.0800
U	 0.7410	 0.3560
V	 0.4580	 0.1640
W	 0.3570	 0.1420
X	 0.6760	 0.2990
Y	 0.6030	 0.3310
Z	 0.6950	 0.3090
a	 0.6500	 0.3120
b	 0.6520	 0.2950
c	 0.5930	 0.2730
d	 0.7040	 0.3470
e	 0.6680	 0.3140
f	 0.6080	 0.2920
g	 0.6530	 0.3140
h	 0.6790	 0.3300
i	 0.7090	 0.3220
j	 0.6840	 0.3020
k	 0.7380	 0.3450
l	 0.7390	 0.3840
m	 0.7130	 0.3500
n	 0.7500	 0.3470
o	 0.6400	 0.2640
p	 0.7140	 0.3320
q	 0.1600	 0.1780
r	 0.2320	 0.1530
s	 0.1050	 0.0160