



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:45 PM JST

PDB ID : 8IAO / pdb_00008iao
EMDB ID : EMD-35313
Title : Respiratory complex CI:CIII2, type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 4.20 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:

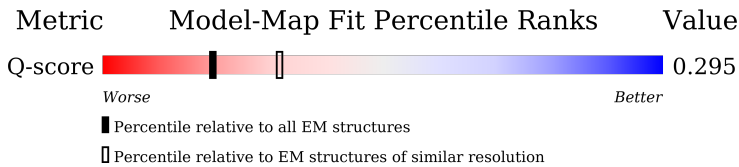
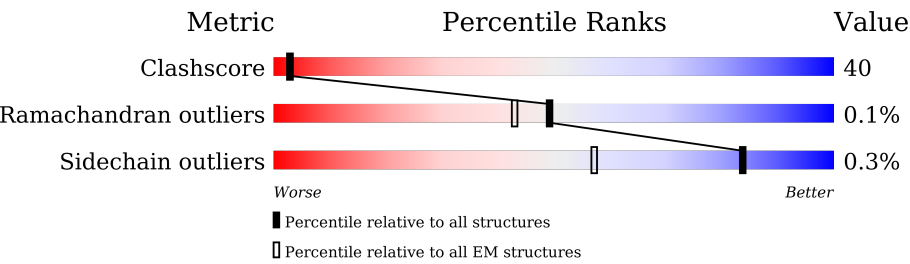
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 4.20 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	5410 (3.70 - 4.70)

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	13% 24% 54% 20%
2	B	224	6% 33% 31% 5% 30%
3	C	263	8% 36% 37% 25%
4	D	463	9% 36% 50% 5% 8%

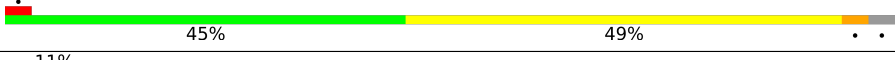
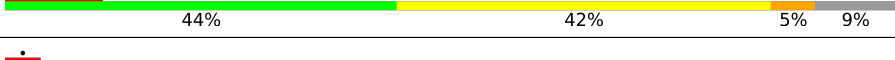
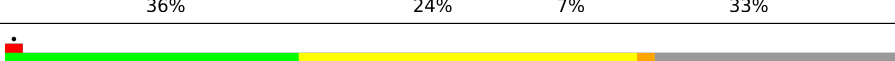
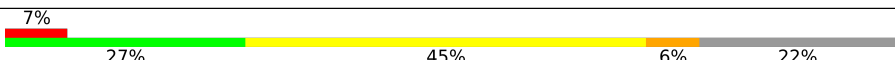
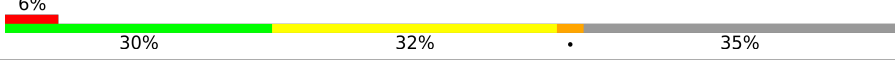
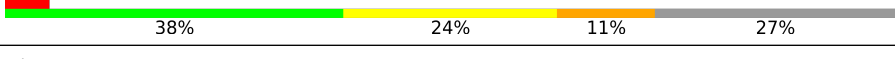
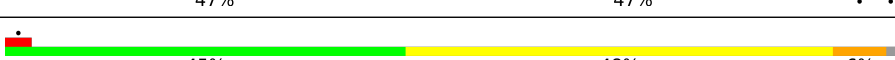
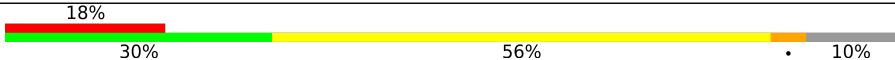
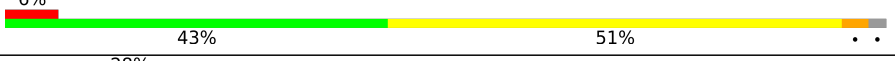
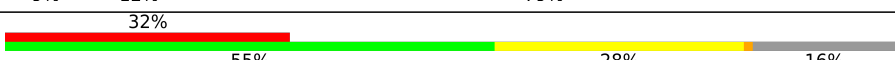
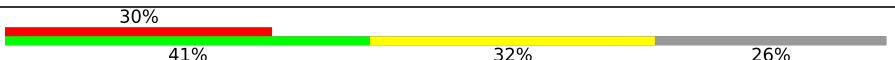
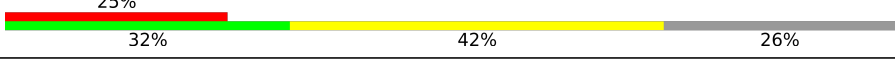
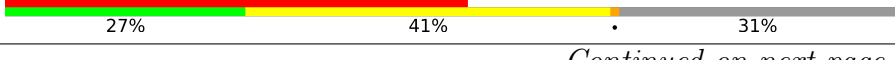
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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	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	
49	Ai	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
56	CDL	A	402	-	-	X	-
57	SF4	B	301	-	-	X	-
57	SF4	F	502	-	-	X	-
57	SF4	G	802	-	-	X	-
57	SF4	I	302	-	-	X	-
57	SF4	I	303	-	-	X	-
58	UQ1	D	501	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
68	U10	Ac	404	-	-	X	-
69	UQ6	AC	406	-	-	X	-
70	HEC	AD	401	X	-	-	-
70	HEC	Ad	401	X	-	-	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 98999 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
			3416	2184	587	621	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	317	Total	C	N	O	S	0	0
			2532	1702	383	425	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1287	866	183	223	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	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- 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	339	Total	C	N	O	S	0	0
			2720	1759	476	478	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	87	Total	C	N	O	S	0	0
			700	450	103	142	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	140	Total	C	N	O	S	0	0
			1037	662	175	192	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	79	Total	C	N	O	S	0	0
			620	408	98	110	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	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			447	290	80	75	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	100	Total	C	N	O	S	0	0
			839	546	146	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	68	Total	C	N	O	S	0	0
			578	378	96	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	76	Total	C	N	O	S	0	0
			618	410	105	101	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	125	Total	C	N	O		0	0
			1044	673	188	183			

- 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	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	22	Total	C	N	O	0	0
			189	124	29	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	403	Total	C	N	O	S	0	0
			3153	1970	560	607	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	412	Total	C	N	O	S	0	0
			3094	1945	542	598	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	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		
48	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	AI	30	Total	C	N	O		0	0
			217	138	42	37			
49	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	Ai	28	Total	C	N	O		0	0
			207	133	40	34			

- 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		
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	68	Total	C	N	O	S	0	0
			562	343	103	111	5		
52	Ah	68	Total	C	N	O	S	0	0
			562	343	103	111	5		

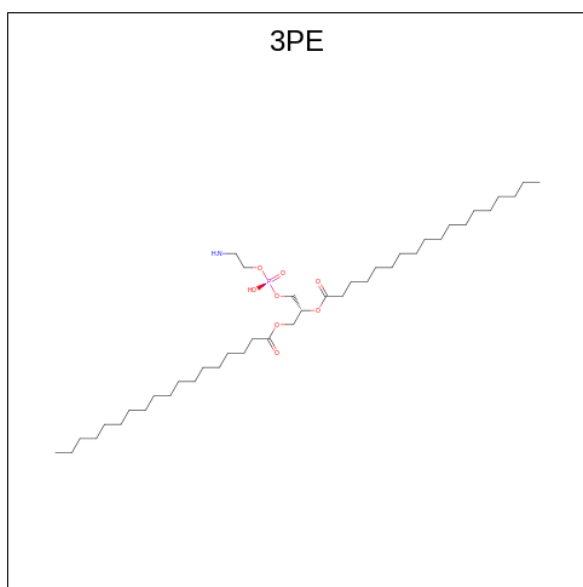
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

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
			391	257	66	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		
54	Ak	49	Total	C	N	O	S	0	0
			401	266	71	63	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



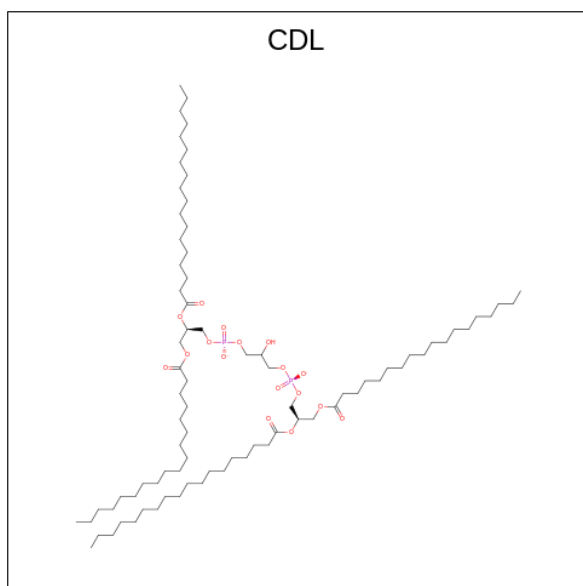
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
55	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	i	1	Total	C	N	O	P	0
			40	30	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
			41	31	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	

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Mol	Chain	Residues	Atoms					AltConf
55	AG	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Aa	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
			51	41	1	8	1	

- Molecule 56 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



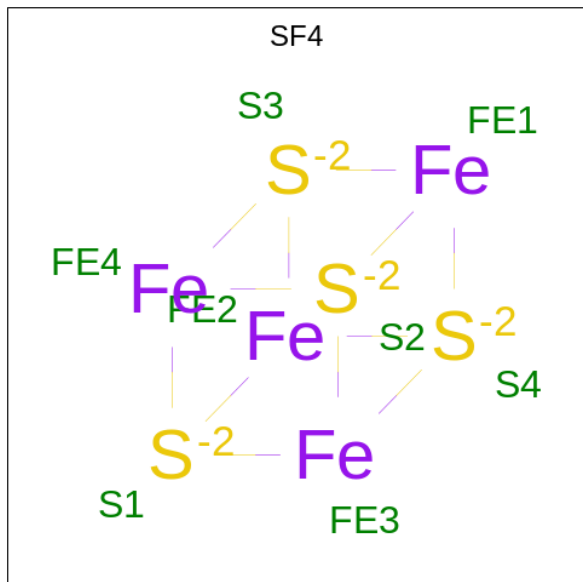
Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	O	P	0
			92	73	17	2	
56	L	1	Total	C	O	P	0
			74	55	17	2	
56	M	1	Total	C	O	P	0
			79	60	17	2	
56	Y	1	Total	C	O	P	0
			81	62	17	2	
56	d	1	Total	C	O	P	0
			84	65	17	2	
56	h	1	Total	C	O	P	0
			93	74	17	2	
56	q	1	Total	C	O	P	0
			57	38	17	2	

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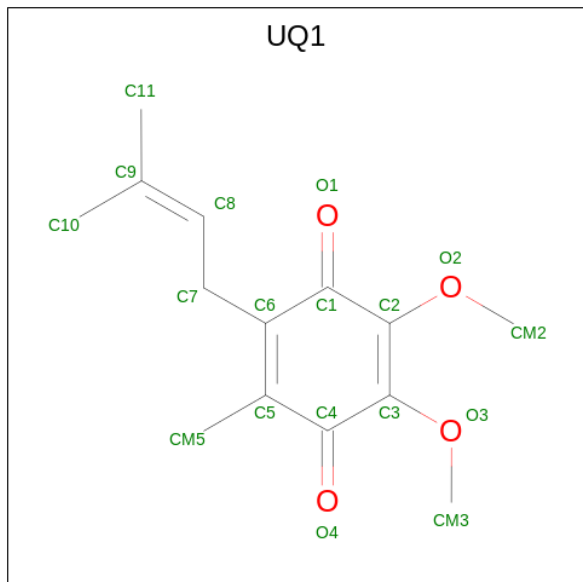
Mol	Chain	Residues	Atoms				AltConf
56	AG	1	Total	C	O	P	0
			42	23	17	2	
56	AG	1	Total	C	O	P	0
			56	37	17	2	
56	Aa	1	Total	C	O	P	0
			46	27	17	2	
56	Ag	1	Total	C	O	P	0
			42	23	17	2	
56	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



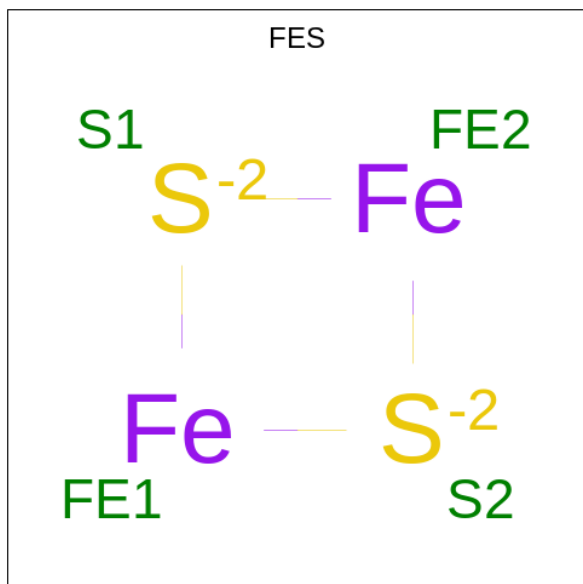
Mol	Chain	Residues	Atoms			AltConf
57	B	1	Total	Fe	S	0
			8	4	4	
57	F	1	Total	Fe	S	0
			8	4	4	
57	G	1	Total	Fe	S	0
			8	4	4	
57	G	1	Total	Fe	S	0
			8	4	4	
57	I	1	Total	Fe	S	0
			8	4	4	
57	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 58 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
58	D	1	Total	C	O	0
			18	14	4	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



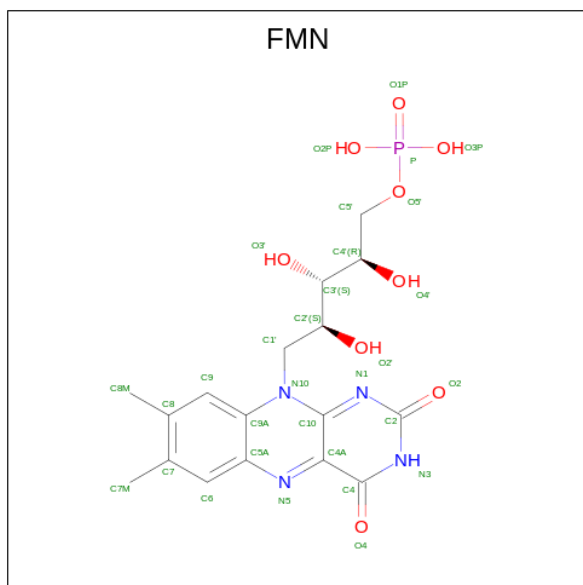
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	

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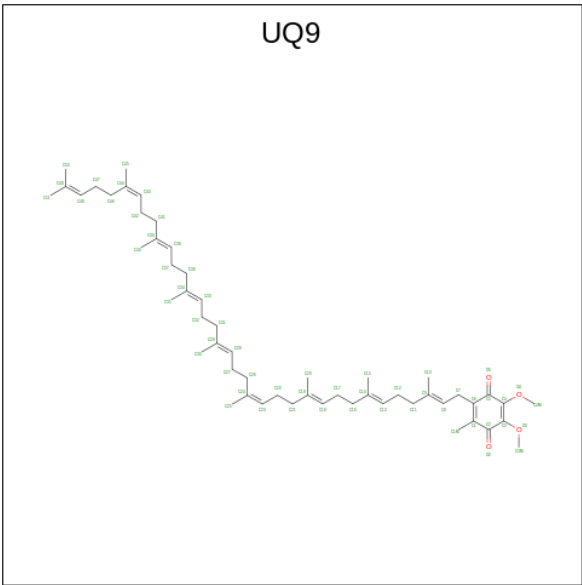
Mol	Chain	Residues	Atoms			AltConf
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



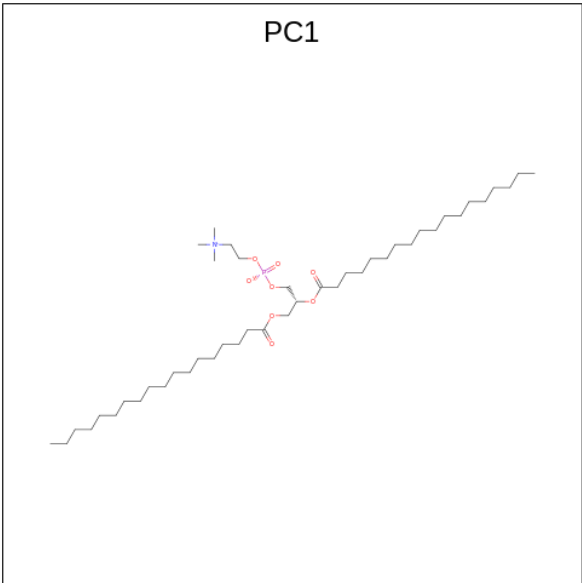
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 61 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



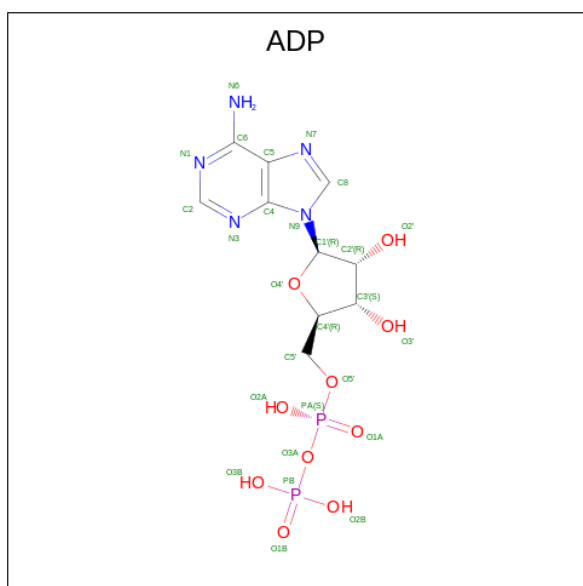
Mol	Chain	Residues	Atoms					AltConf
62	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
62	L	1	Total	C	N	O	P	0
			48	38	1	8	1	

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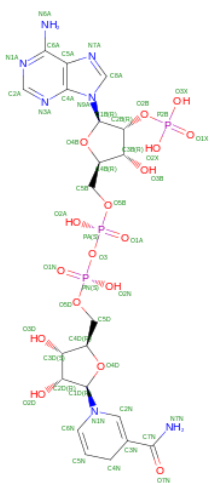
Mol	Chain	Residues	Atoms					AltConf
62	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
62	q	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	Ae	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

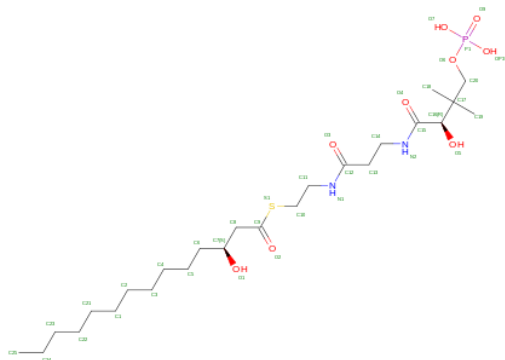


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

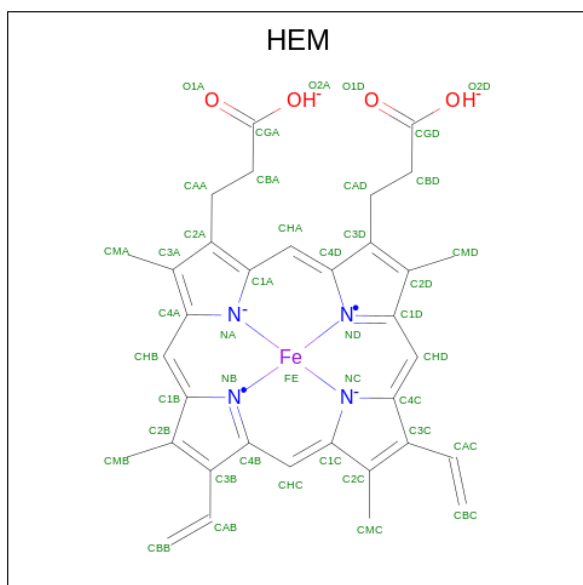
Mol	Chain	Residues	Atoms	AltConf
65	R	1	Total Zn 1 1	0

- 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: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



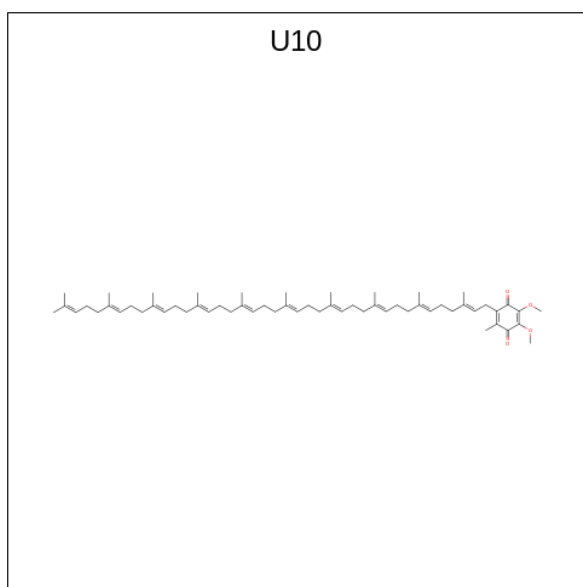
Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



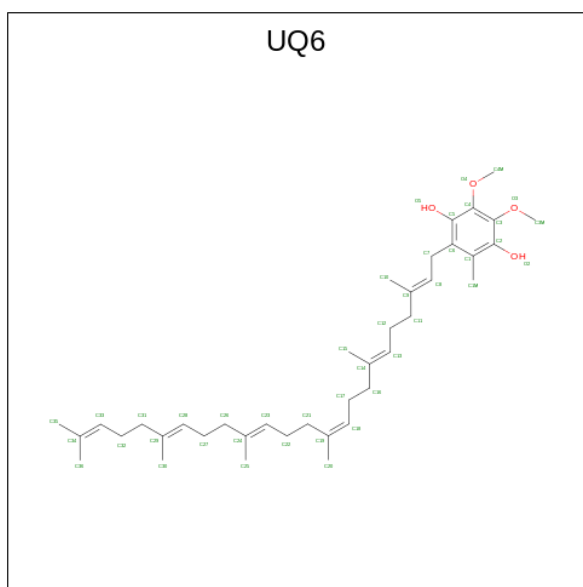
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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
			23	19	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).



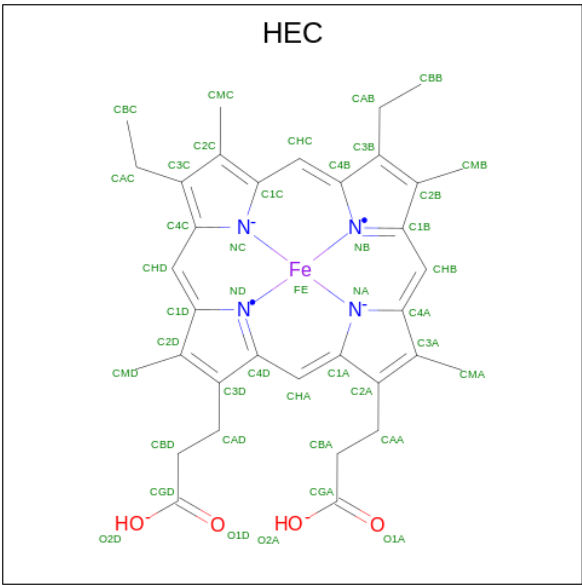
Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	

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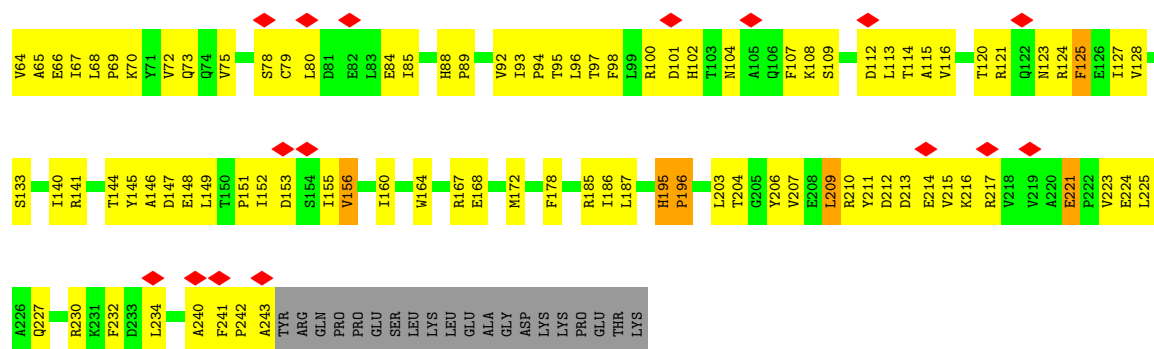
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Mol	Chain	Residues	Atoms			AltConf
69	Ac	1	Total	C	O	0
			28	24	4	

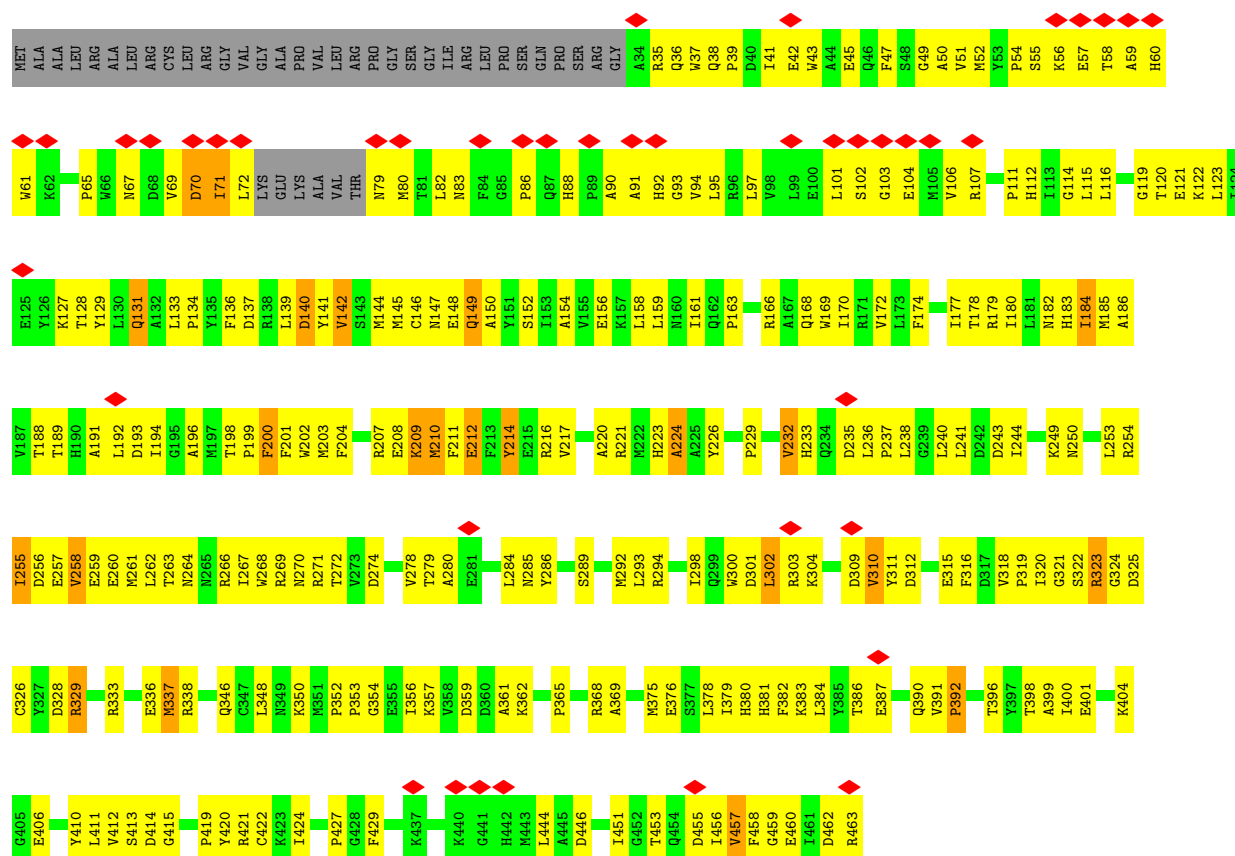
- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



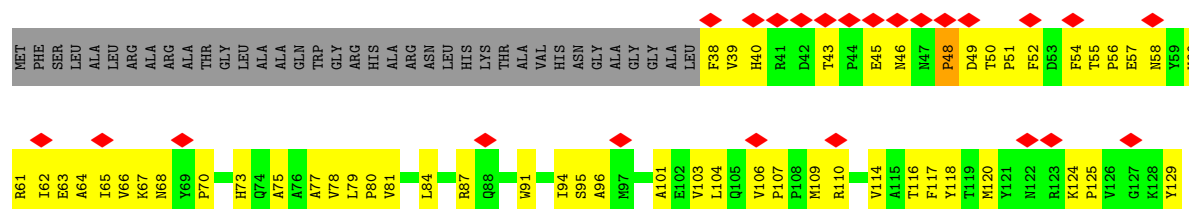
Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

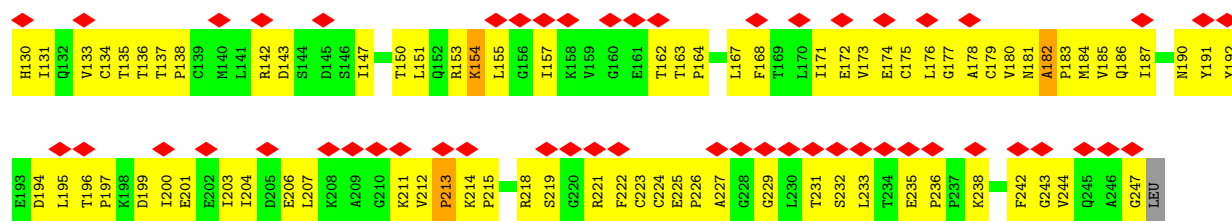


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

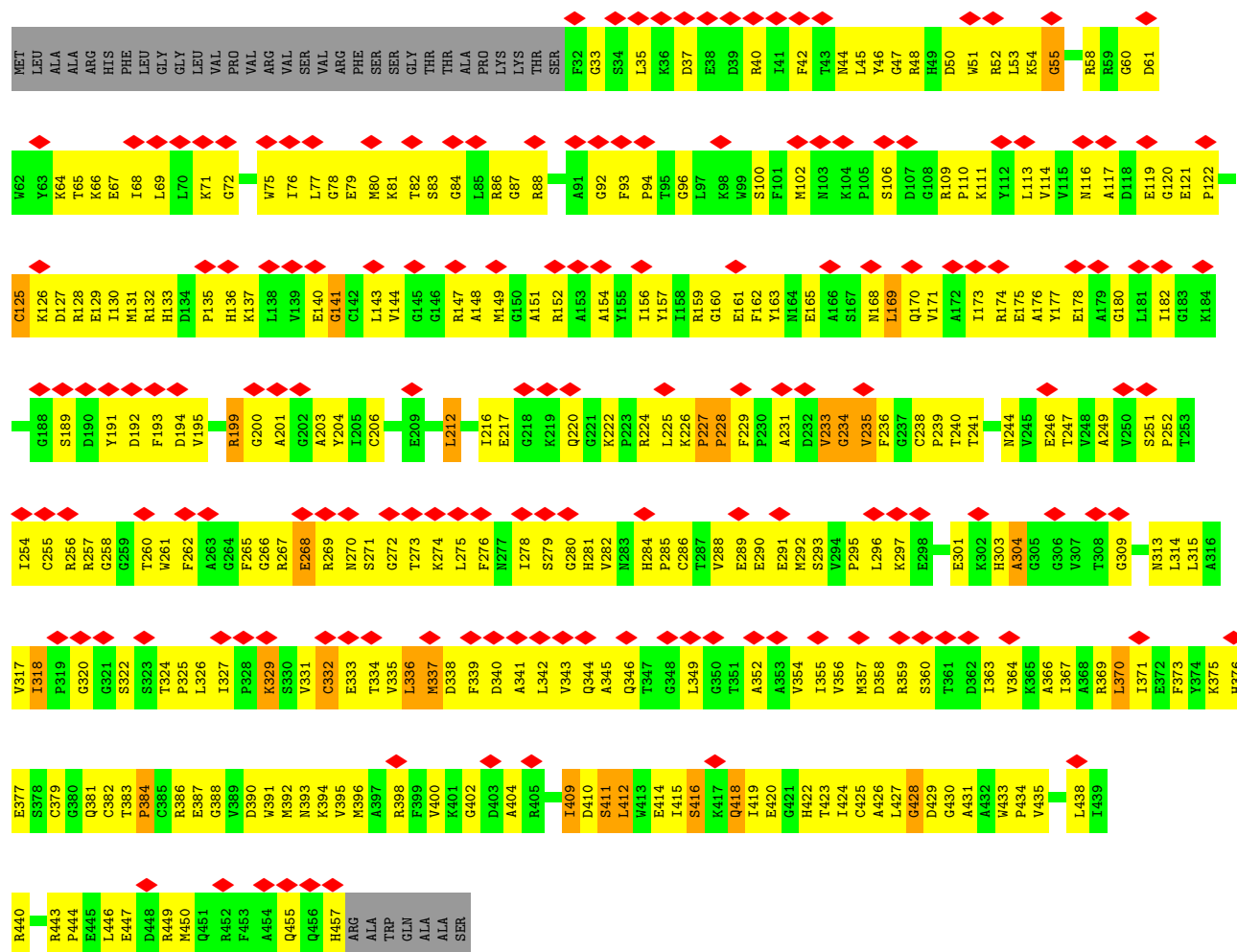


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

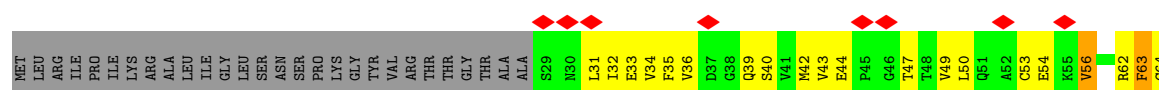


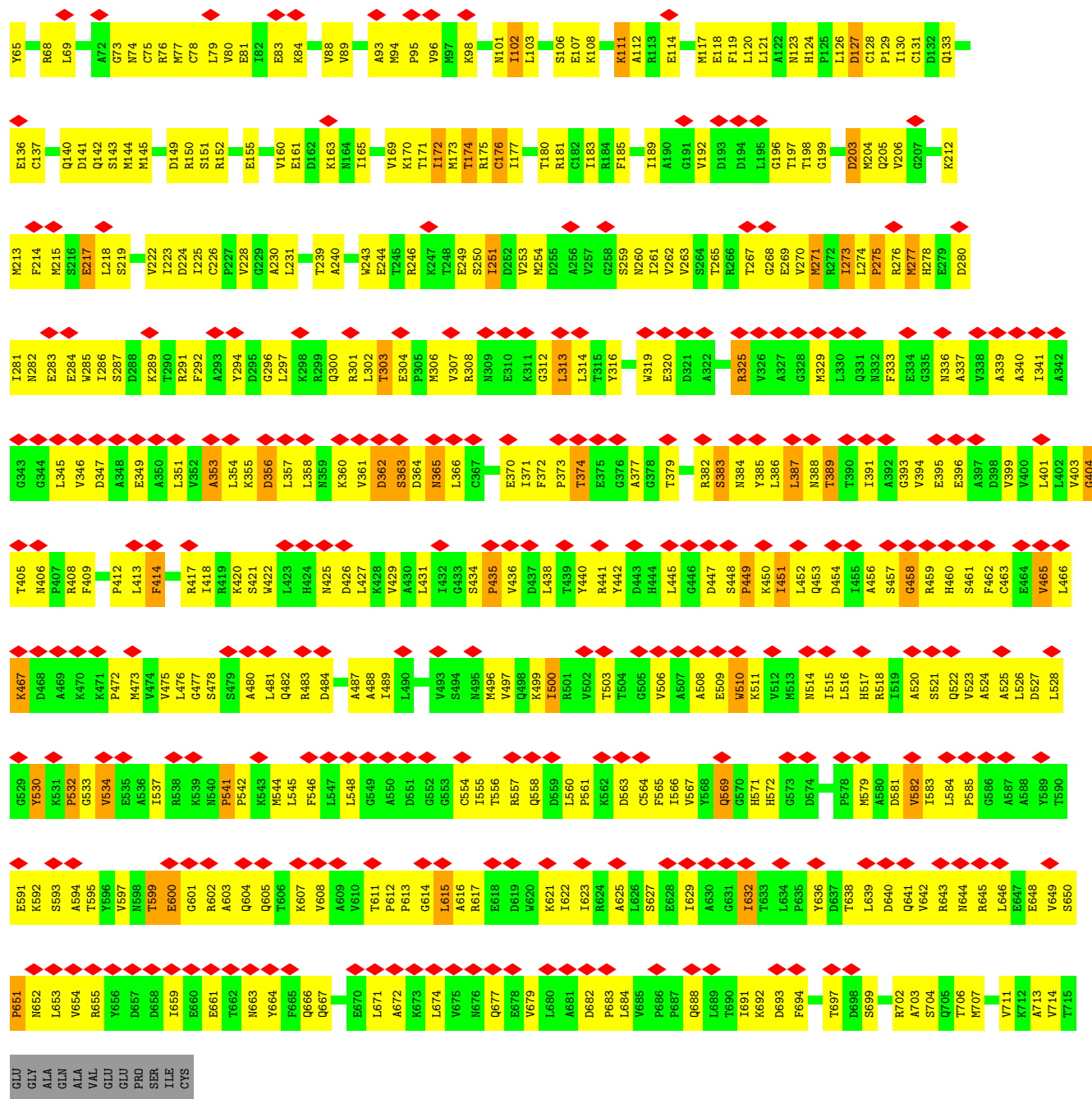


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

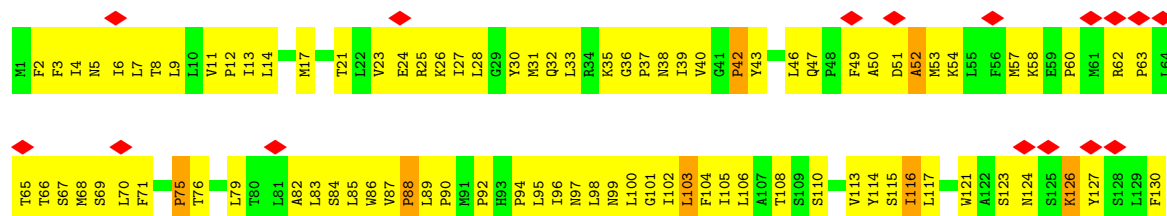


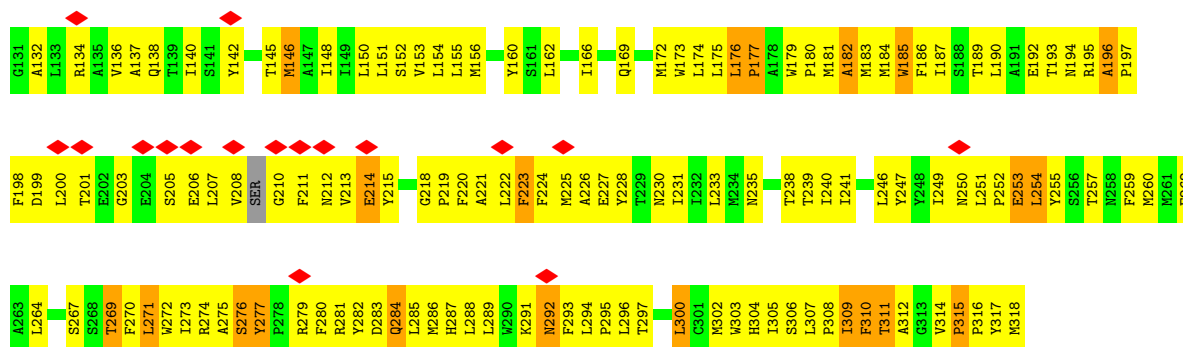
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



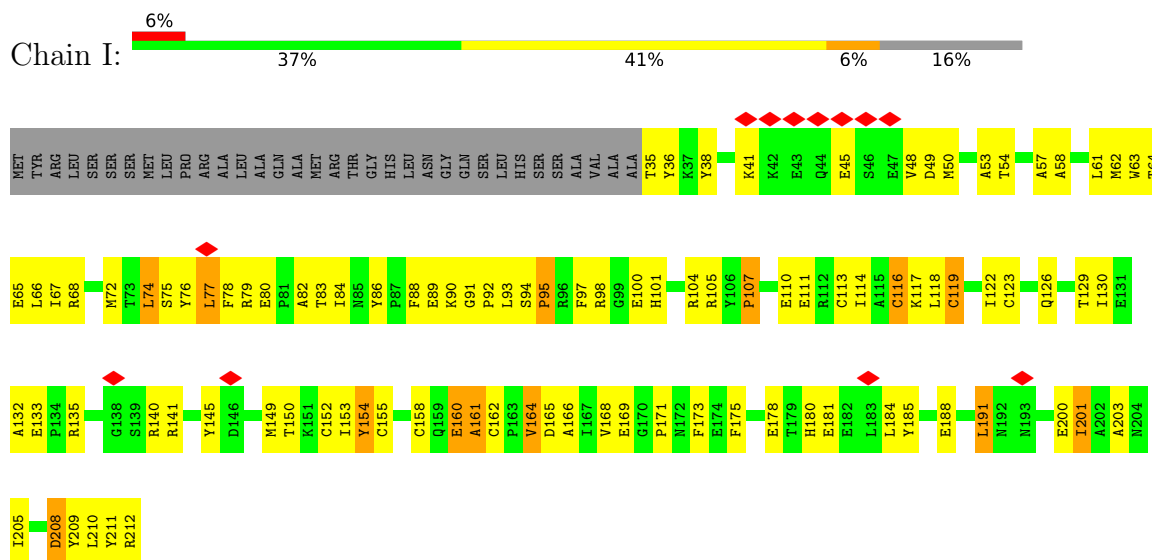


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

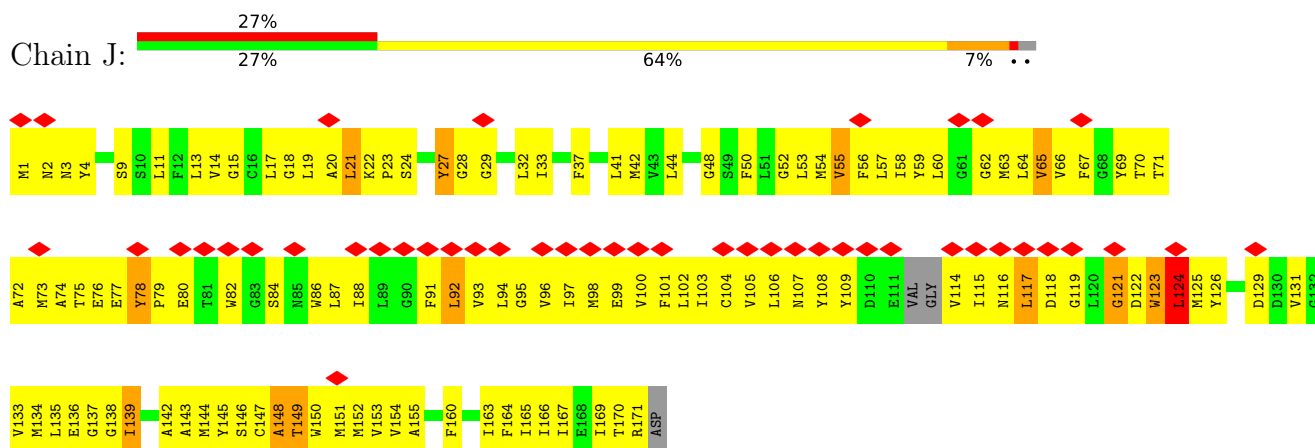




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

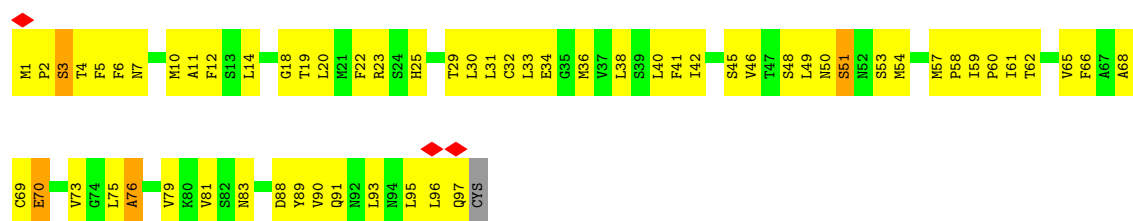


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

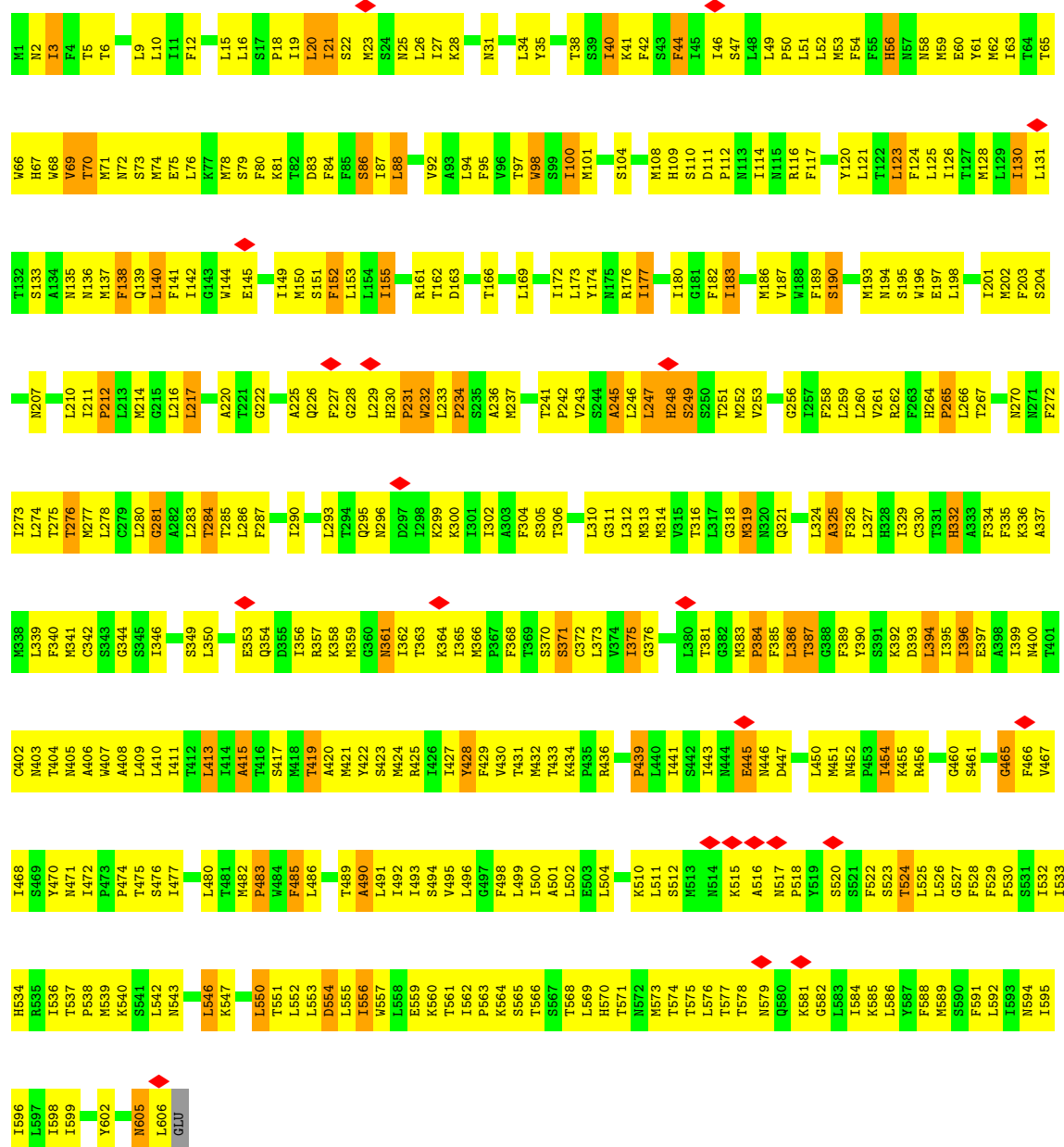


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



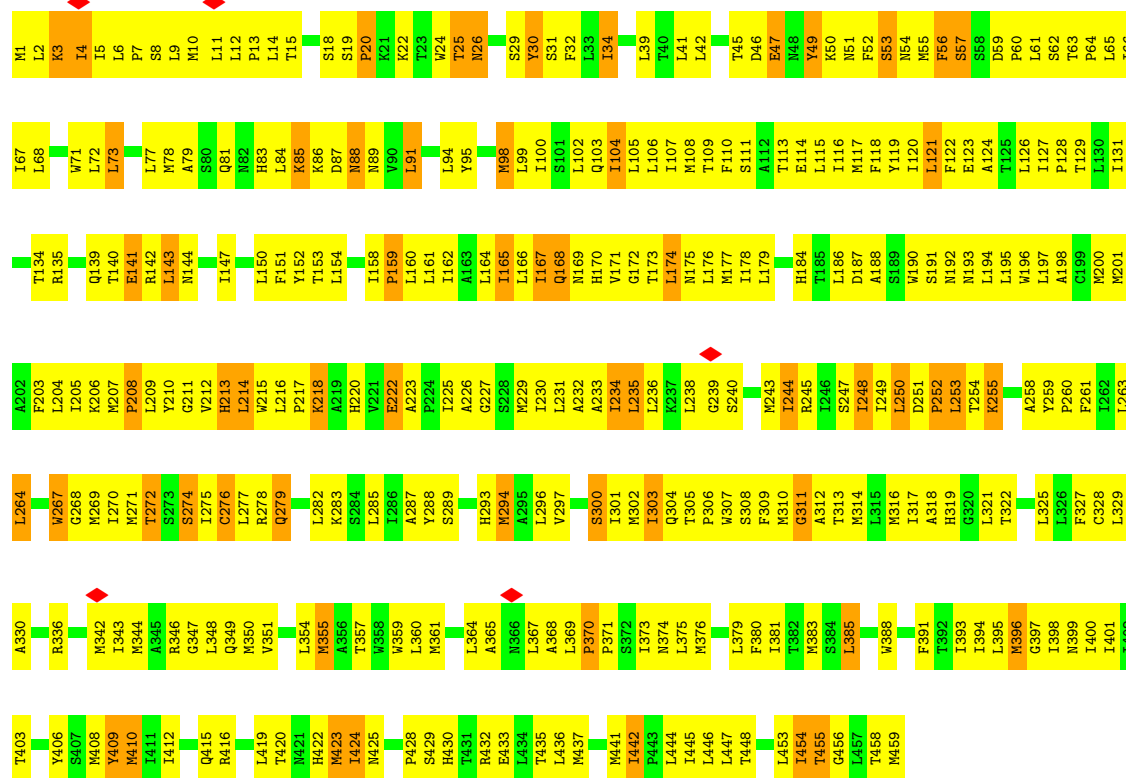


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



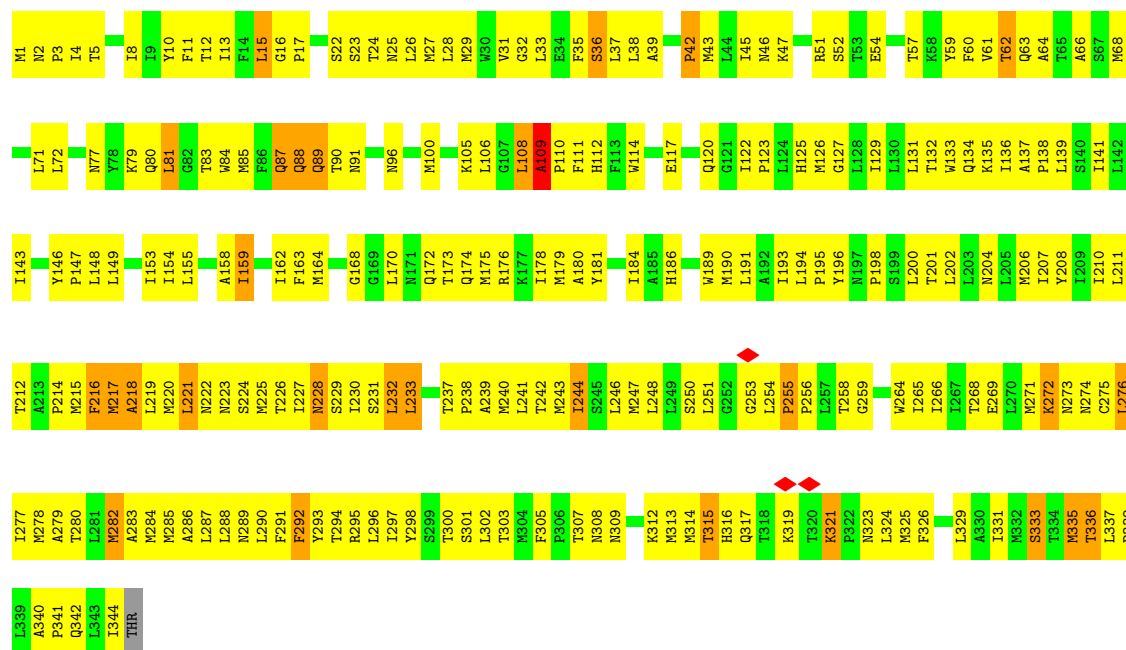
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

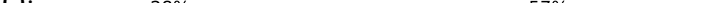
Chain M: 

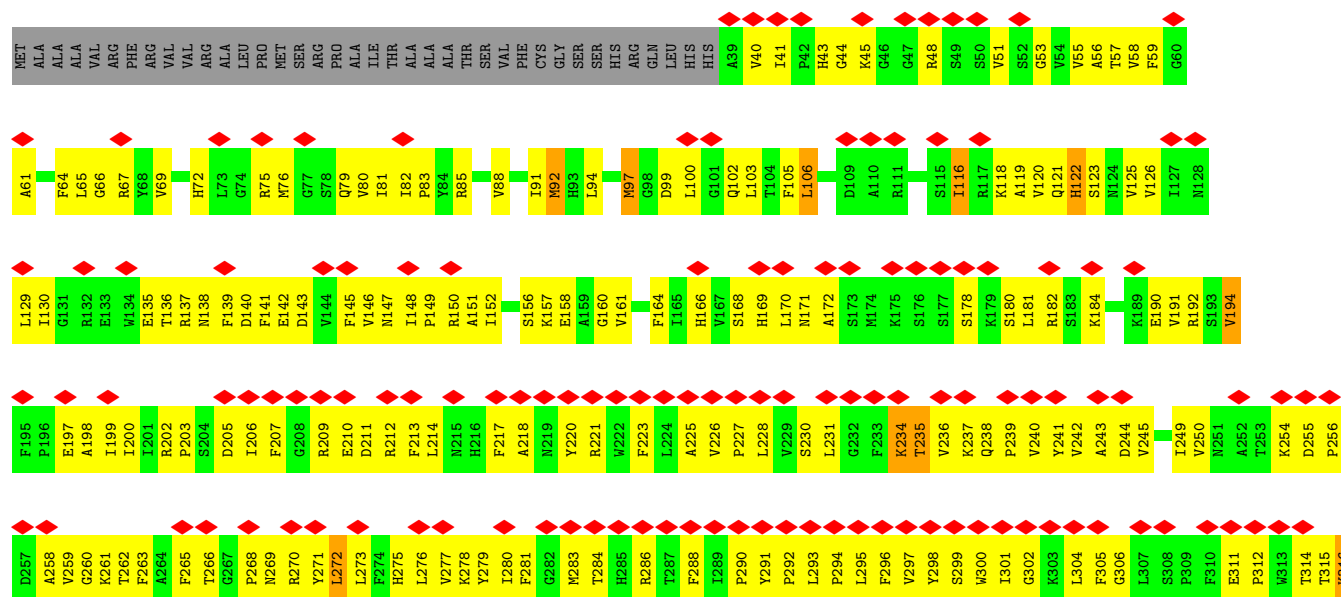
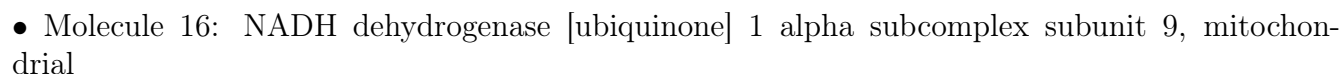


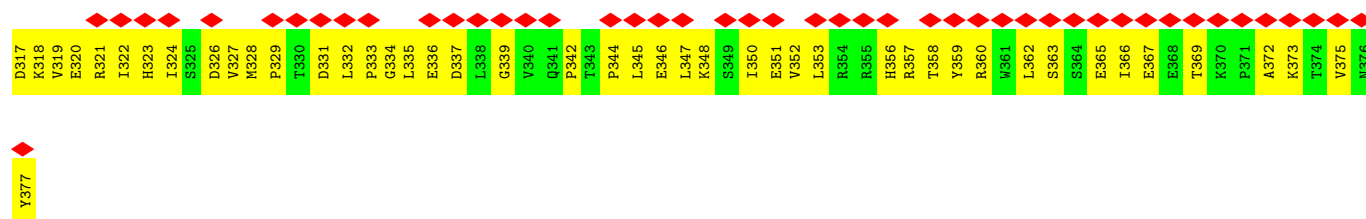
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 

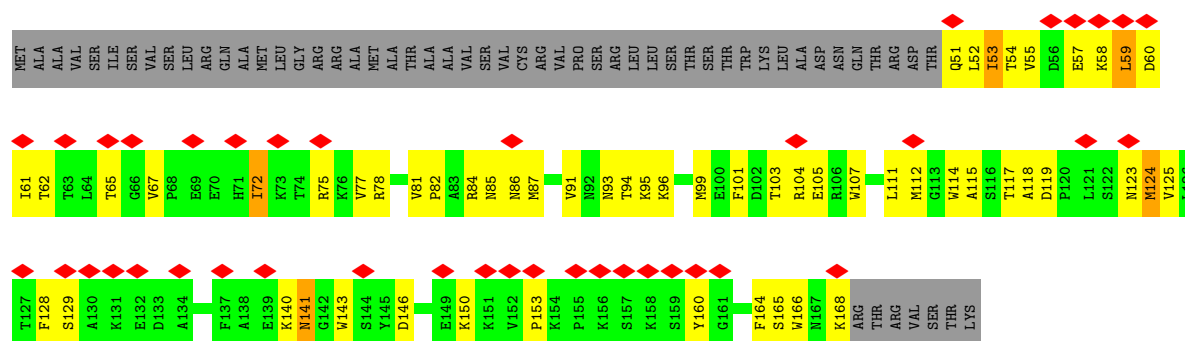


- Chain O:  11% 28% 57% 5% 10%

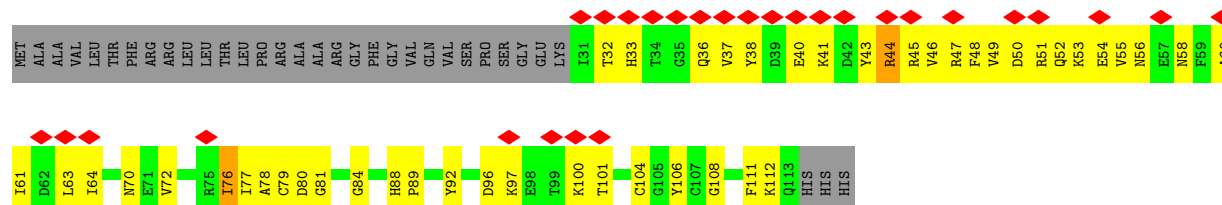




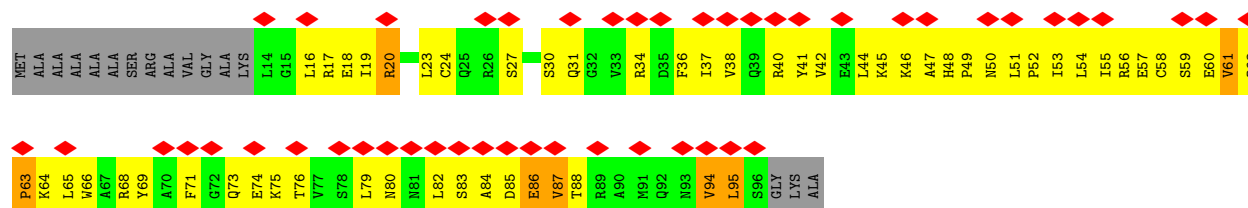
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

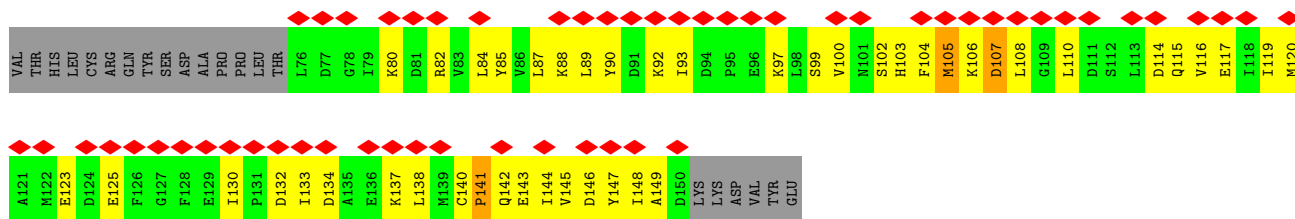


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



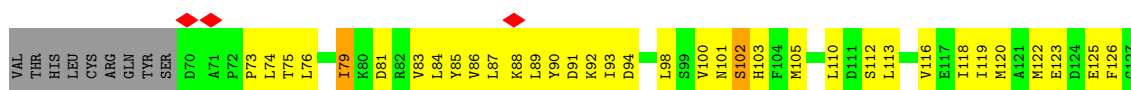
- Molecule 20: Acyl carrier protein, mitochondrial





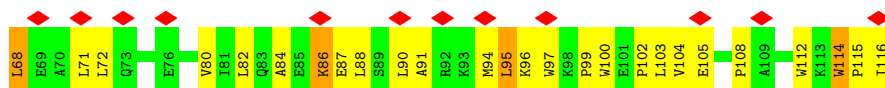
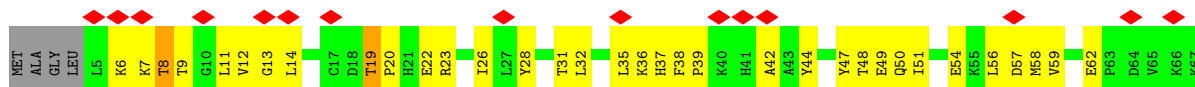
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U: 20% 31% 44%



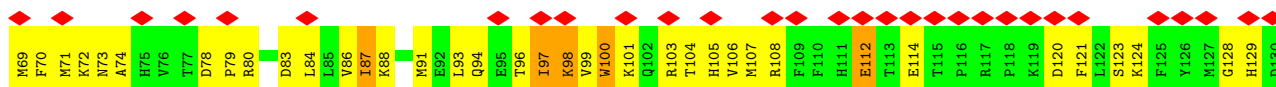
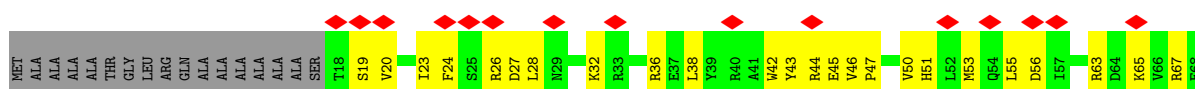
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V: 23% 45% 47% 5%



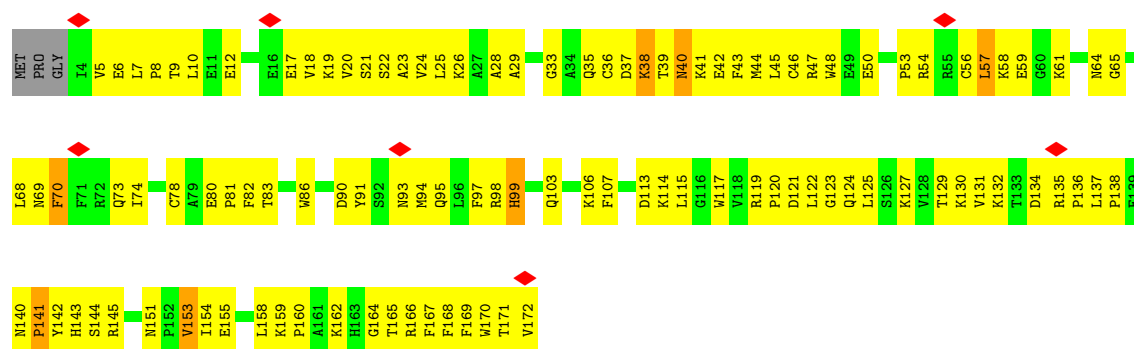
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W: 35% 40% 44% 13%

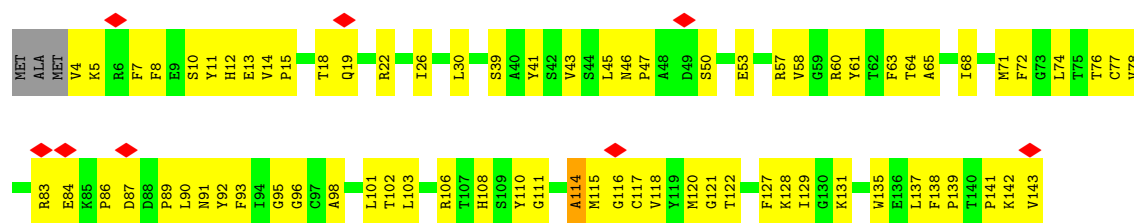


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

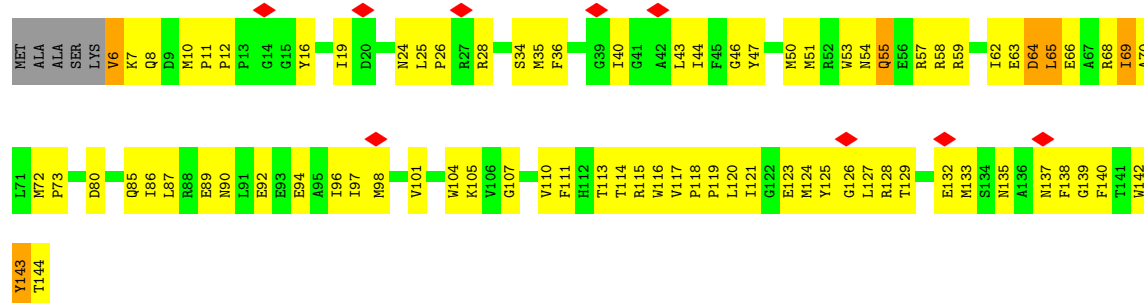
Chain X: 34% 60% 6%



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



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

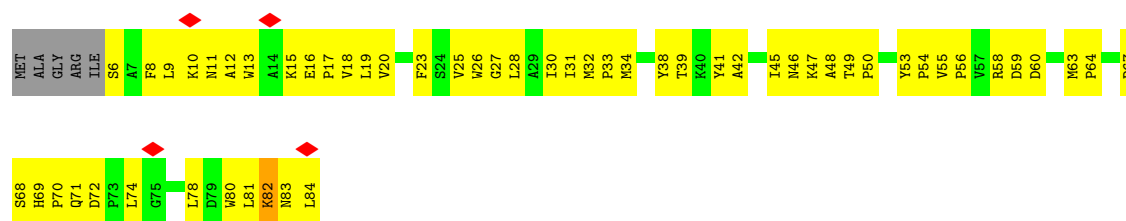


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

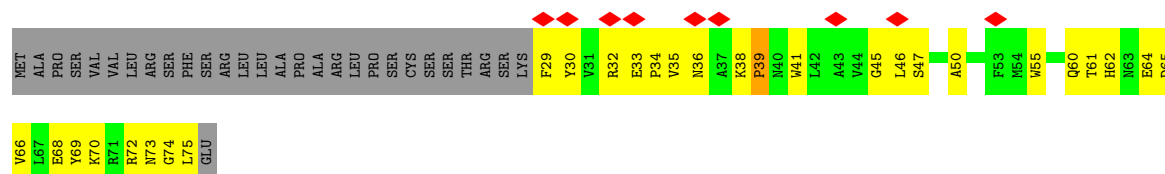
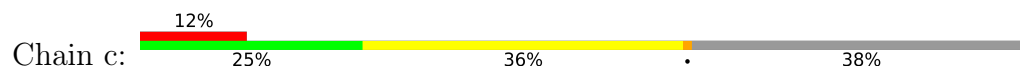


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

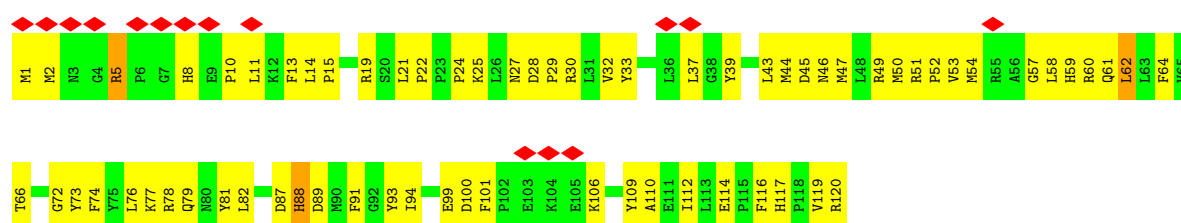
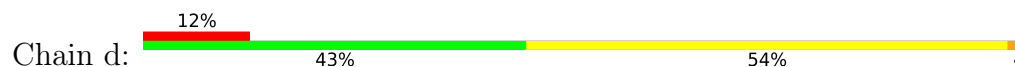




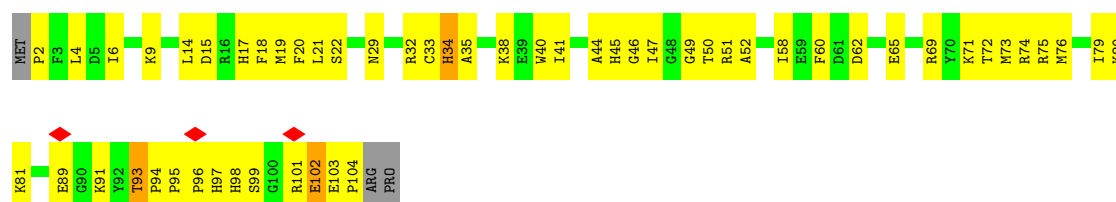
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



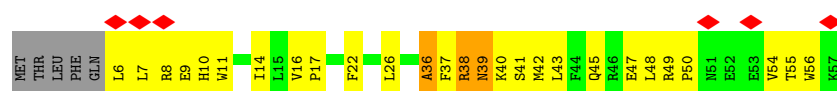
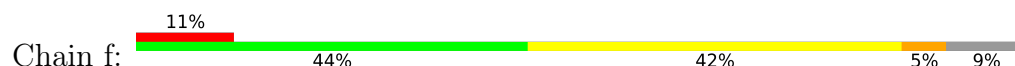
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



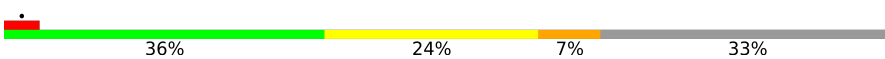
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

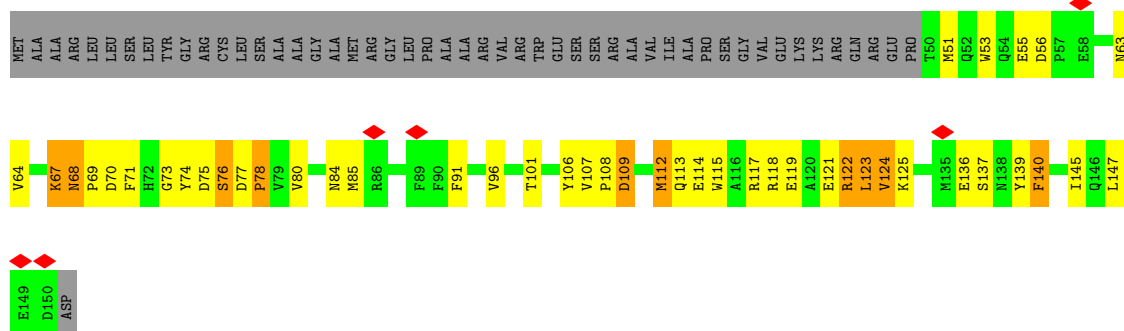


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

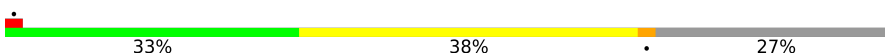


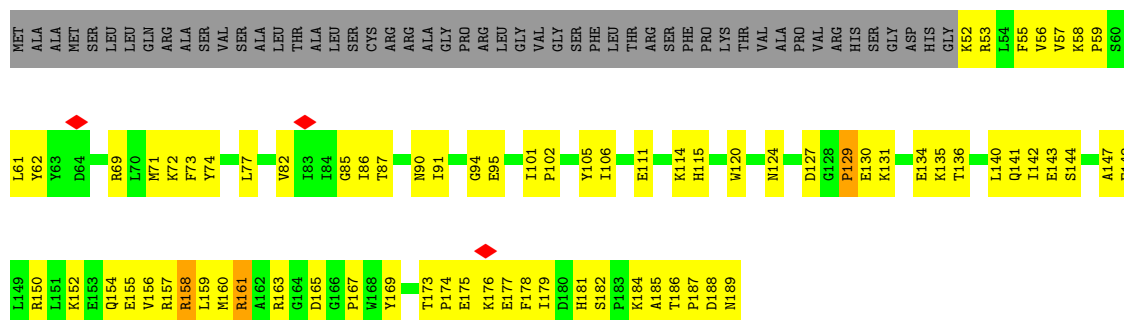
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 

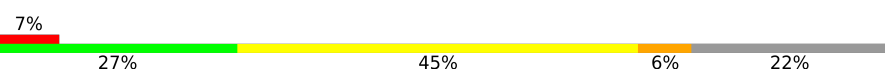


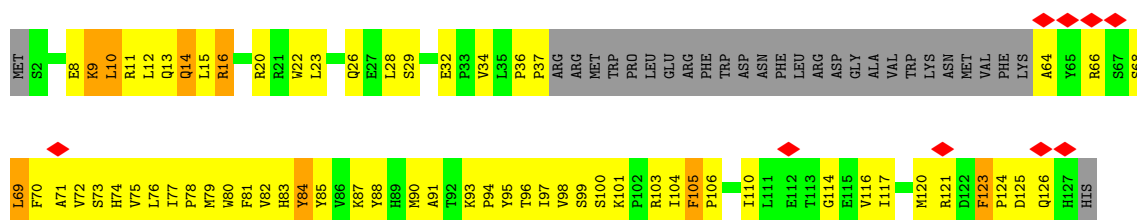
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 

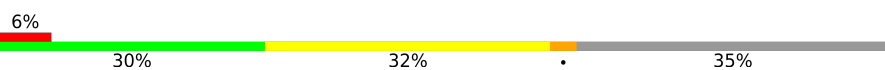


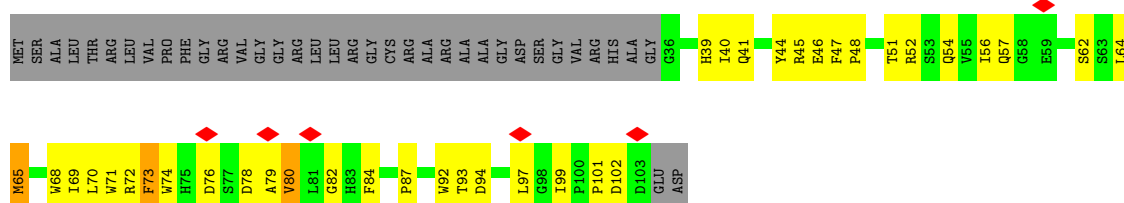
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 

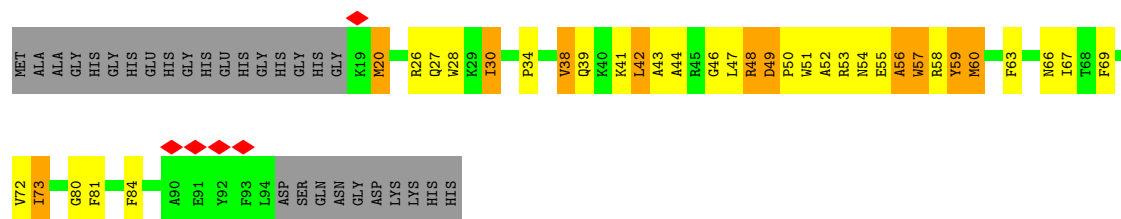


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

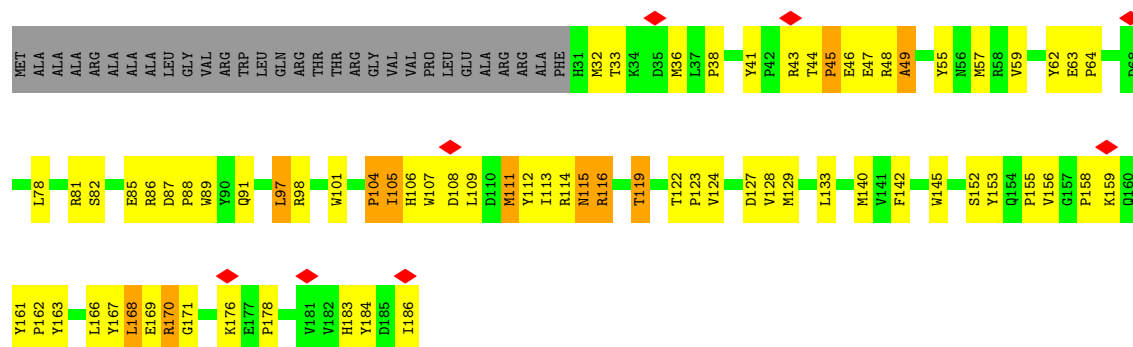
Chain j: 



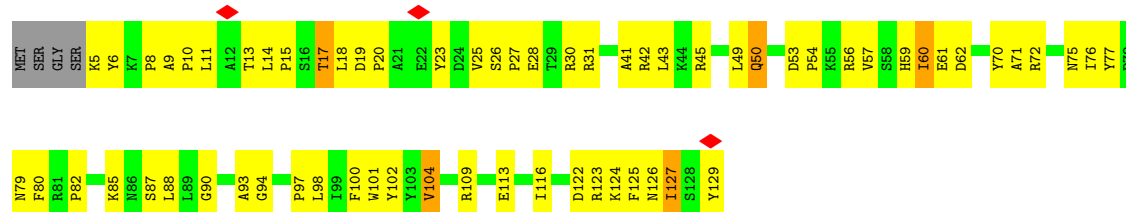
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



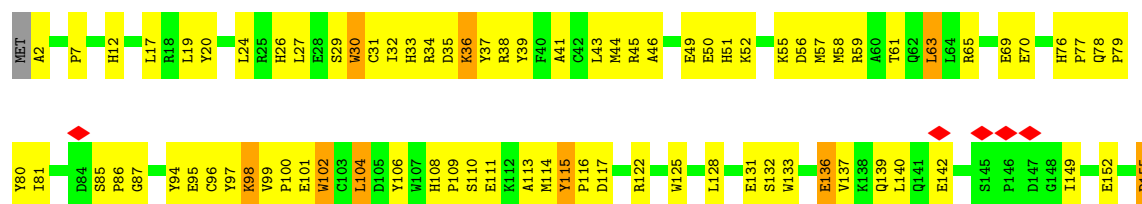
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

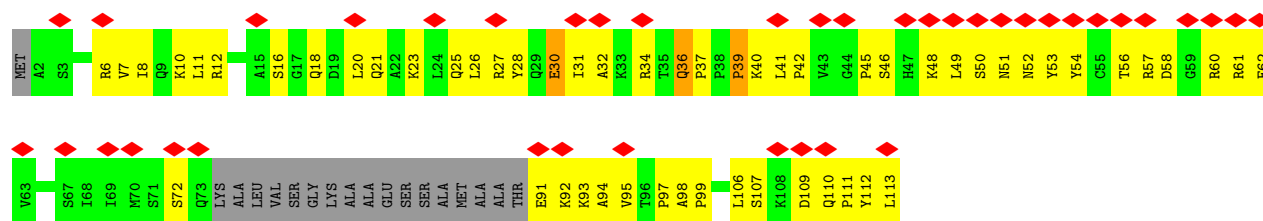


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

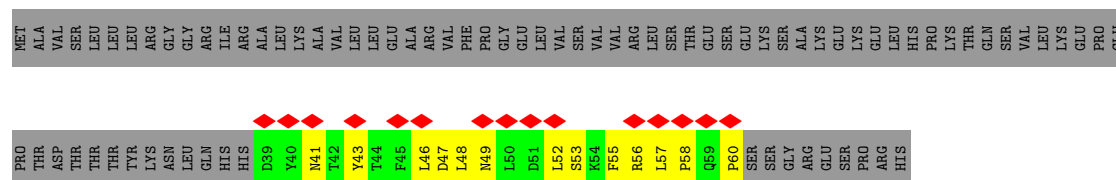


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

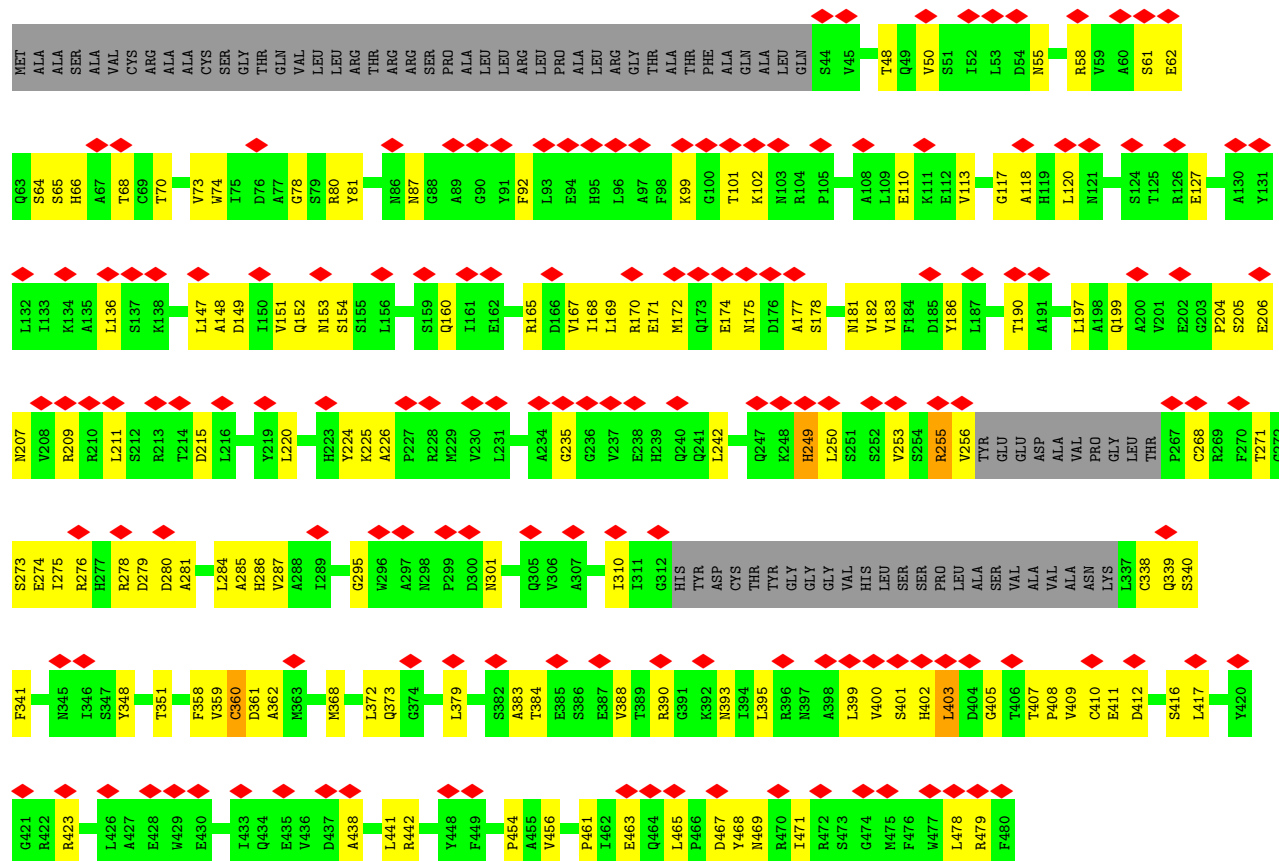




- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

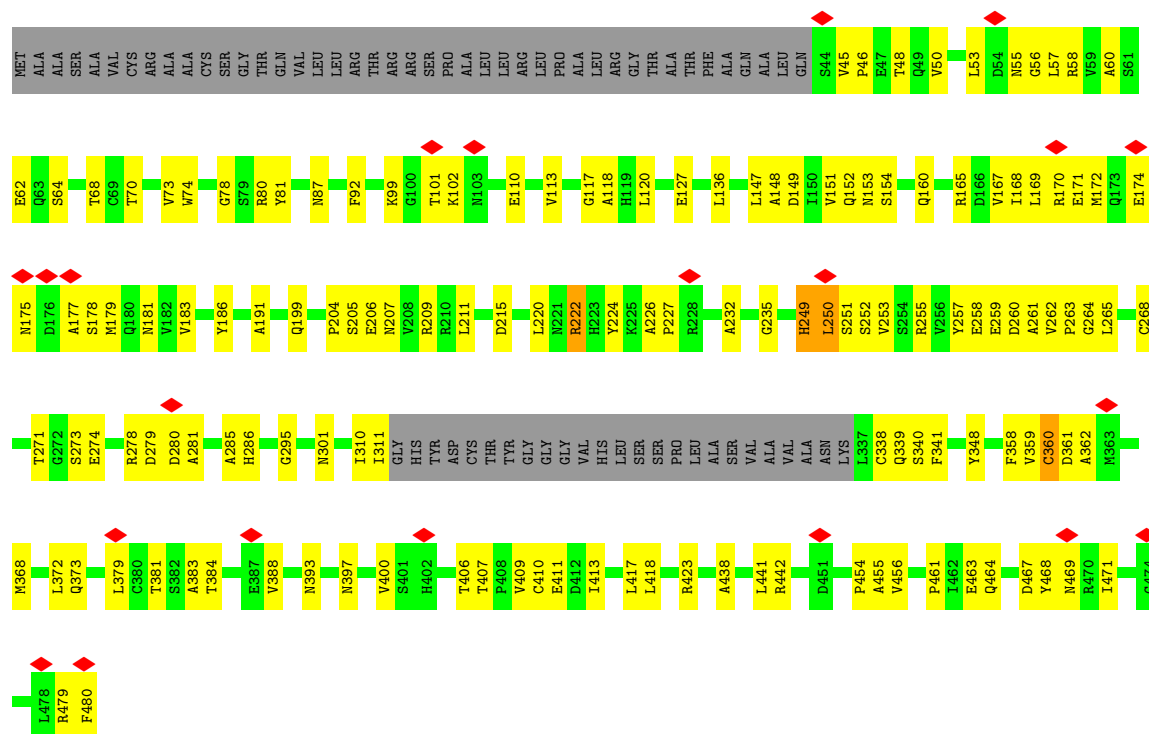


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

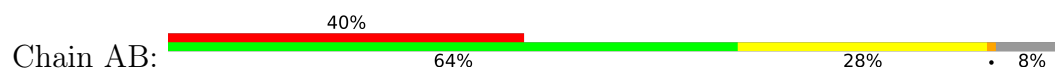


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



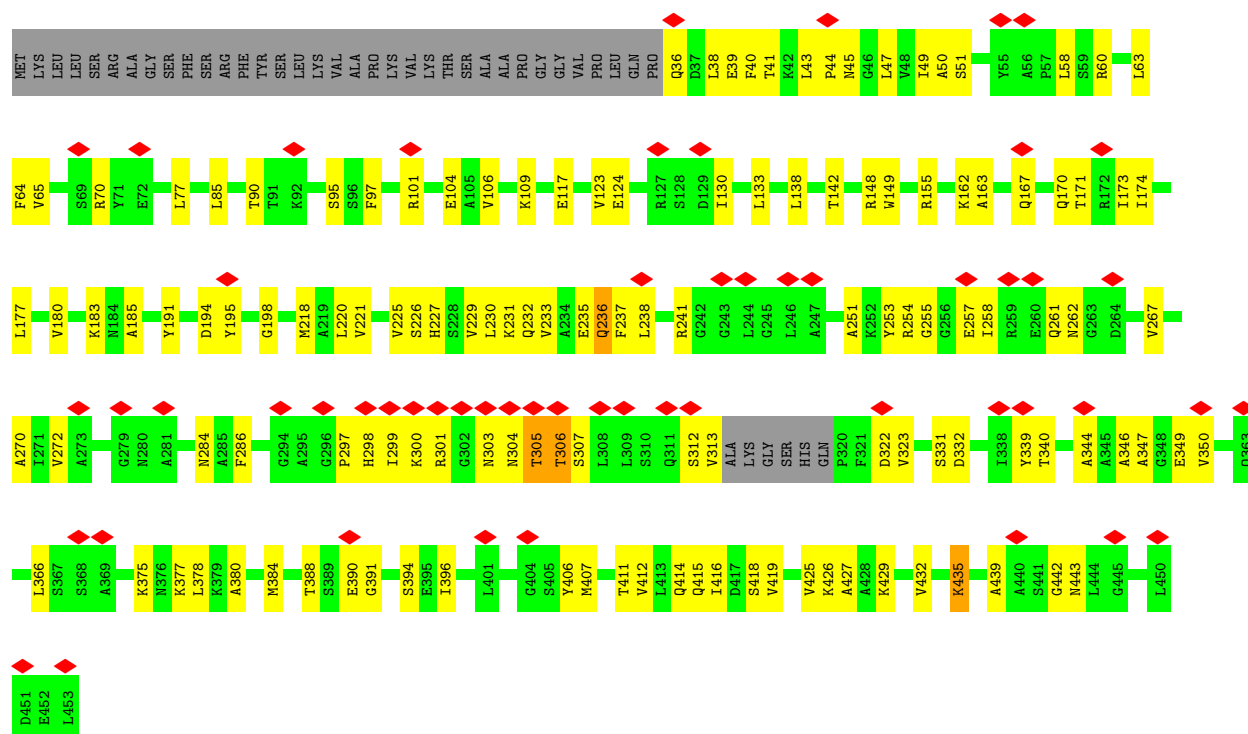


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



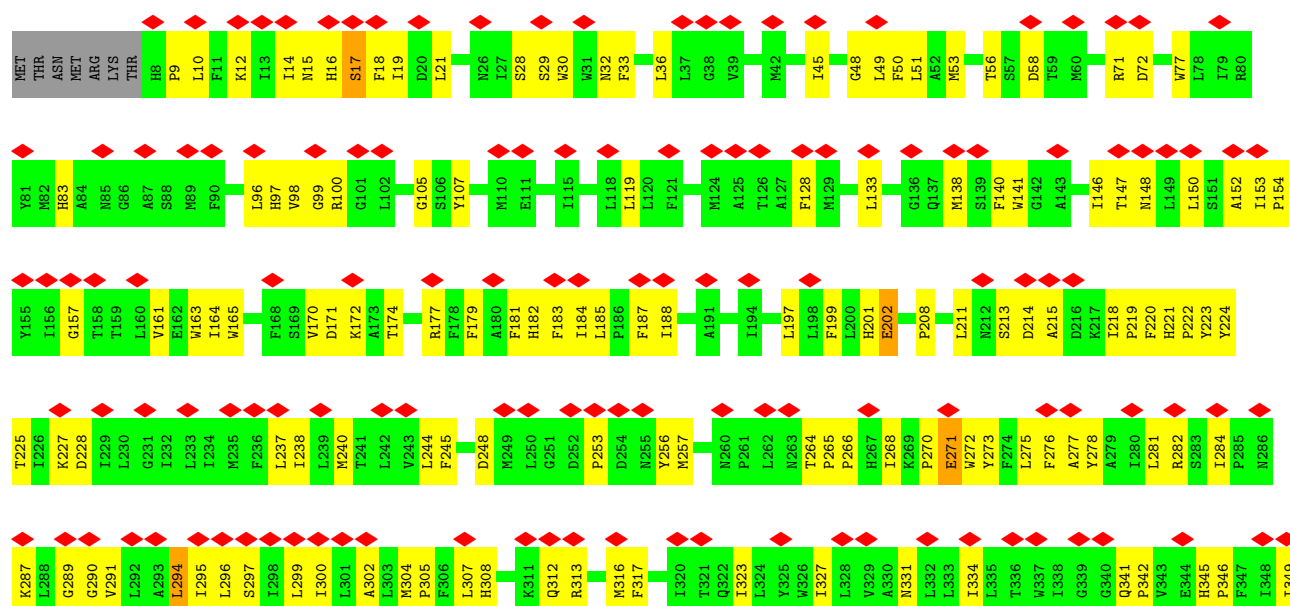
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

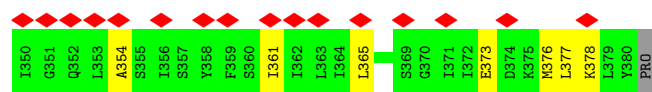
Chain Ab: 



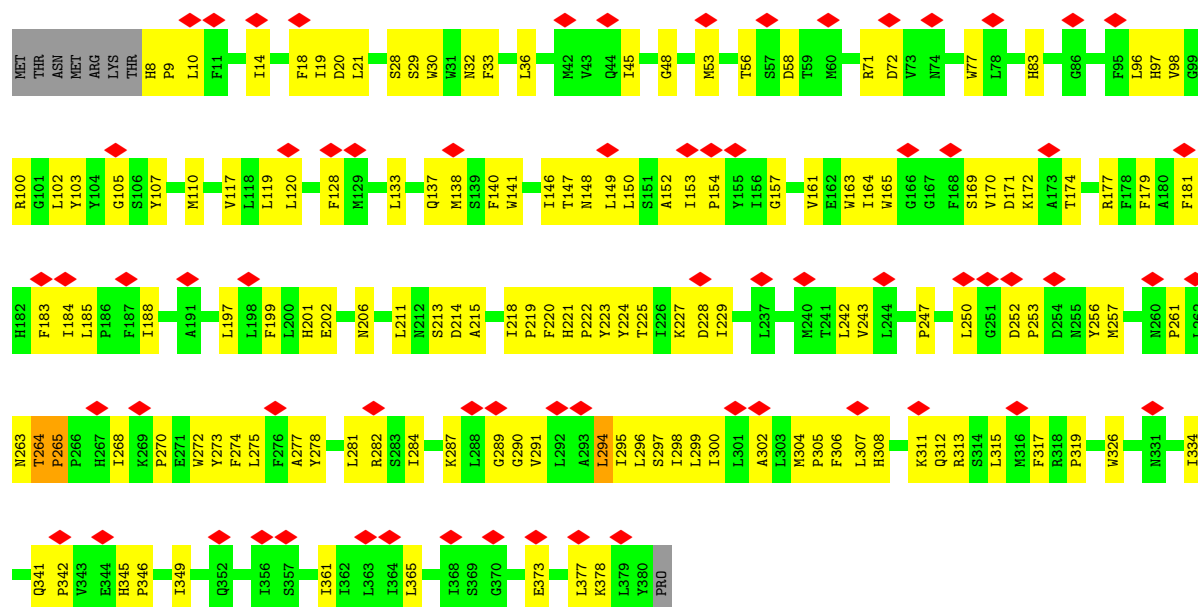
• Molecule 47: Cytochrome b

Chain AC: 

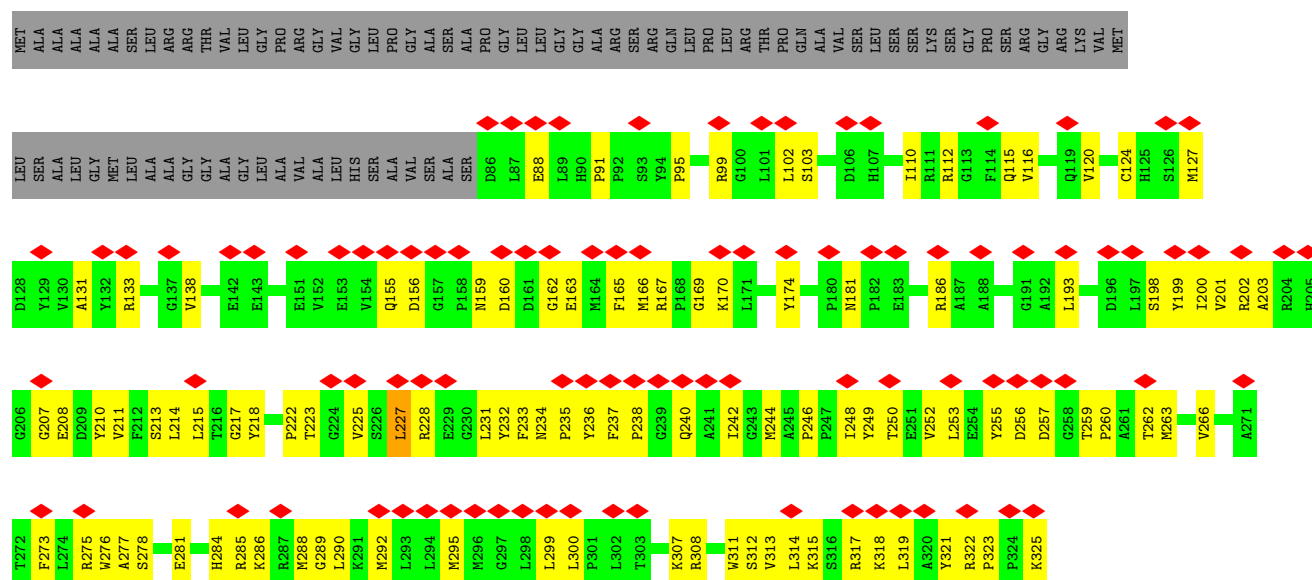
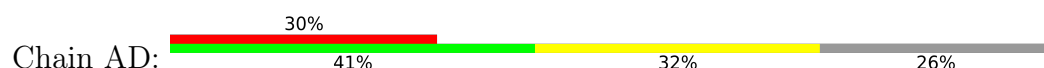




• Molecule 47: Cytochrome b

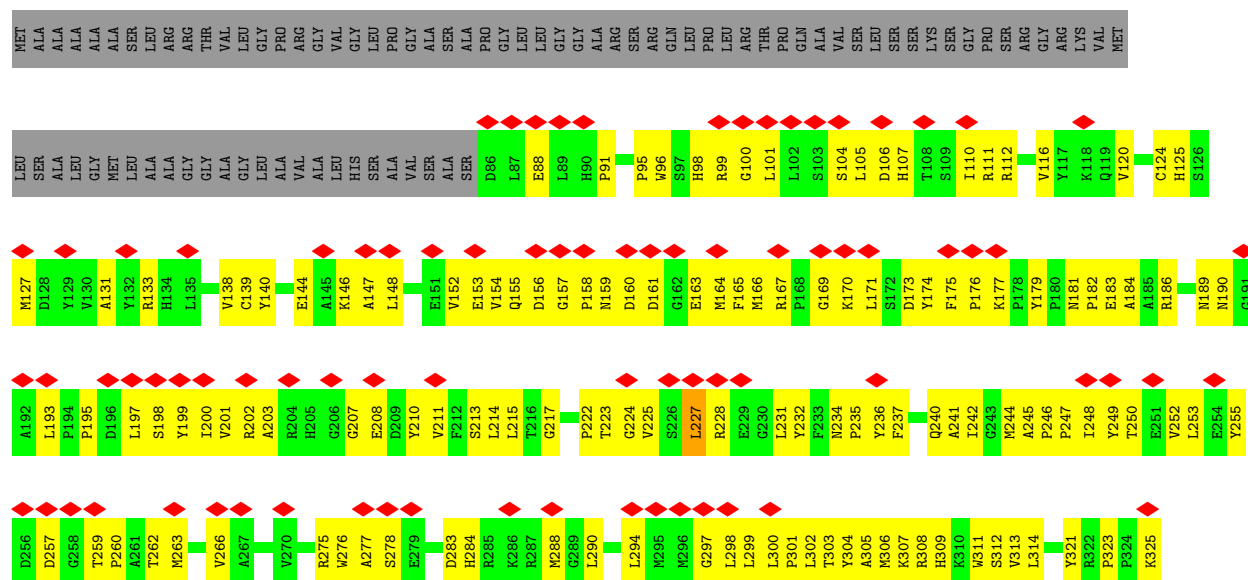


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

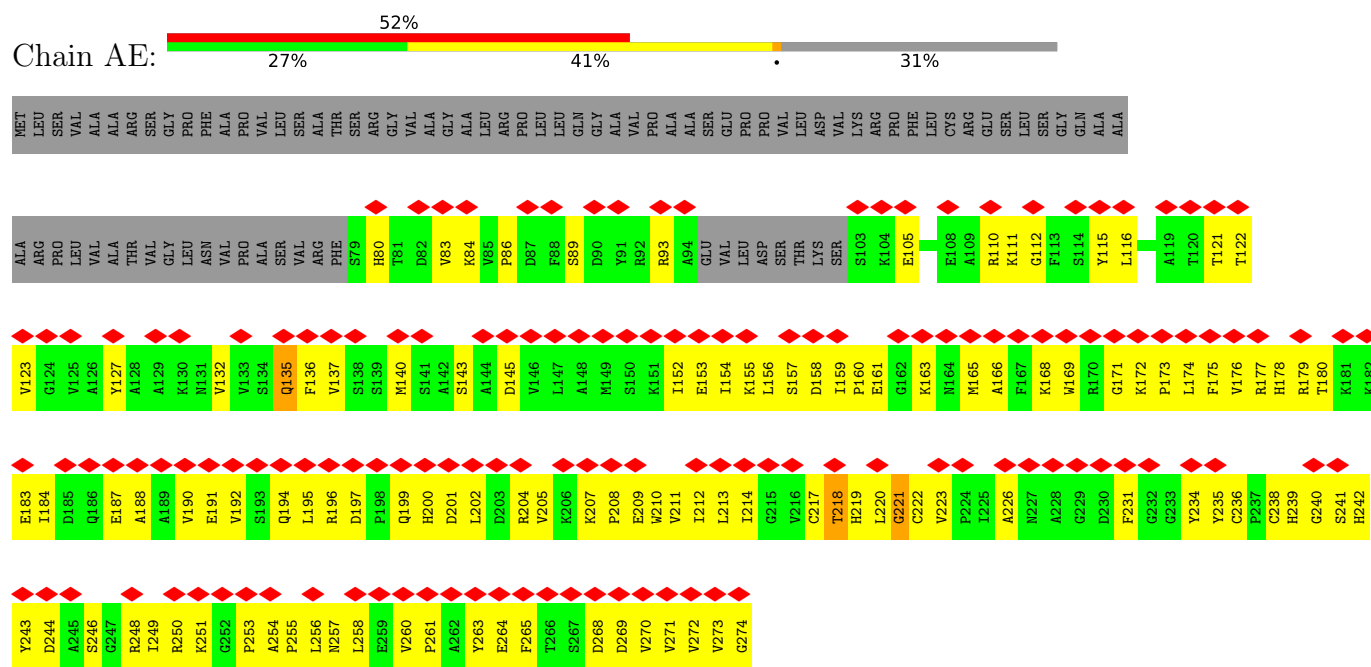


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

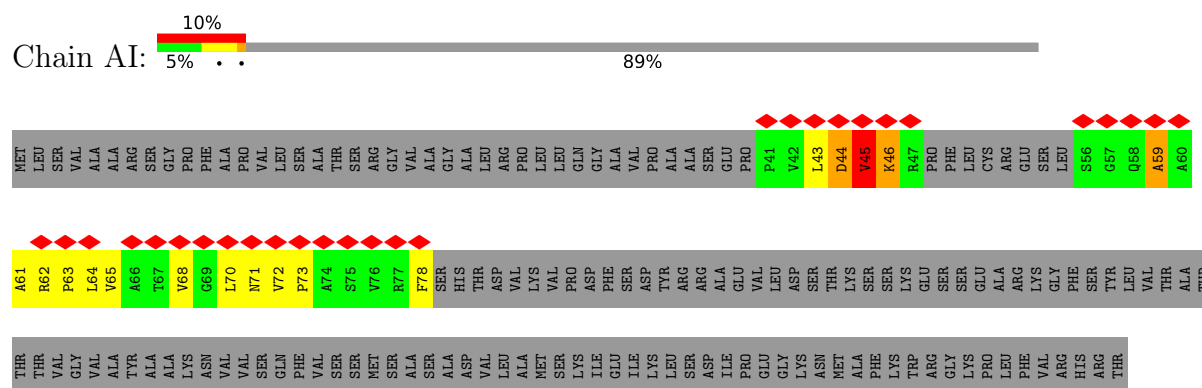


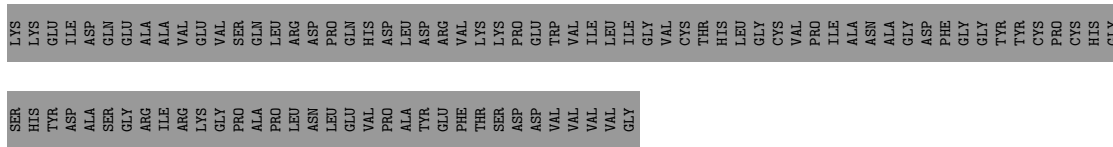


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

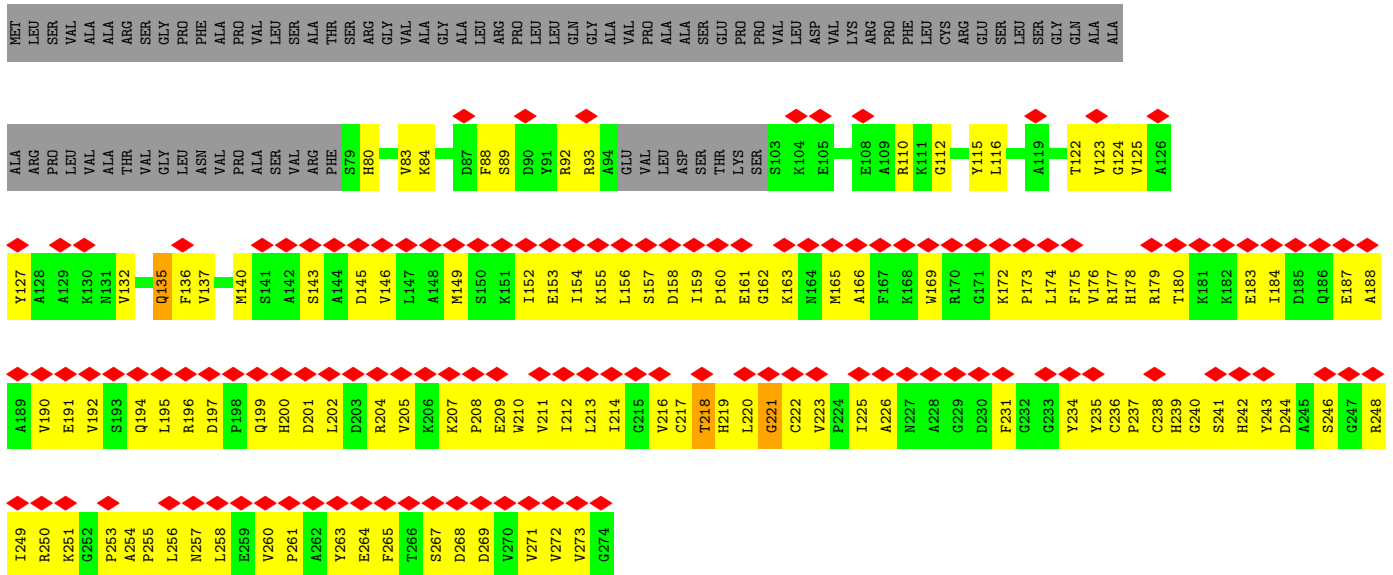


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

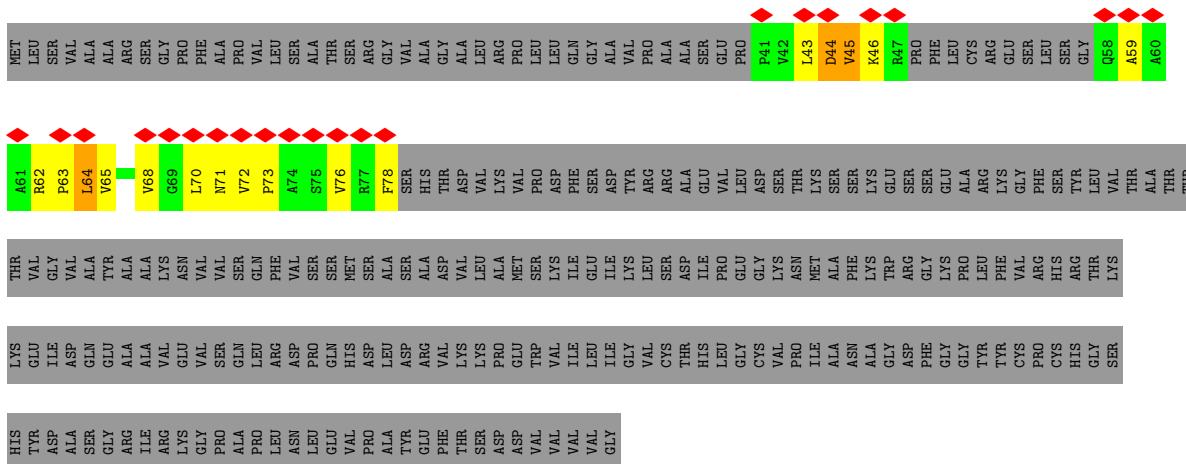




- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

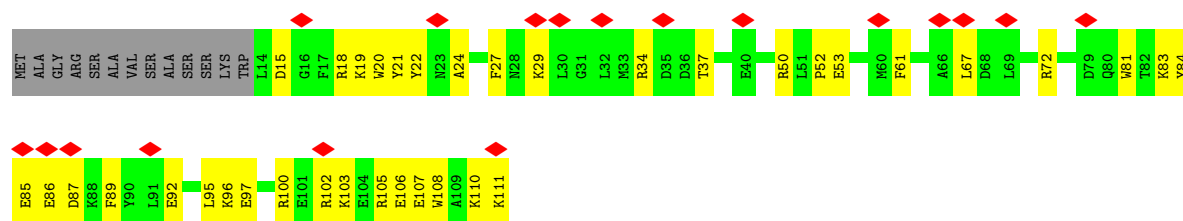


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

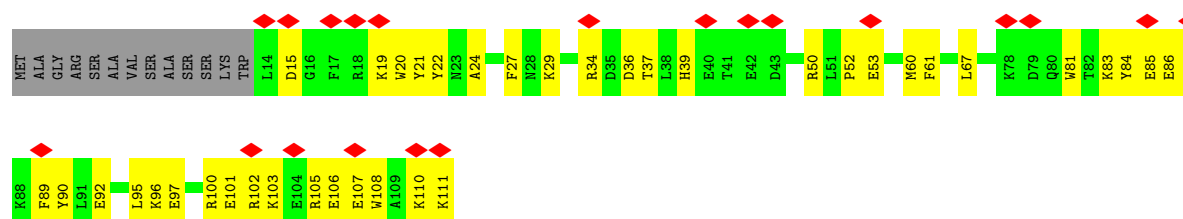


- Molecule 50: Cytochrome b-c1 complex subunit 7

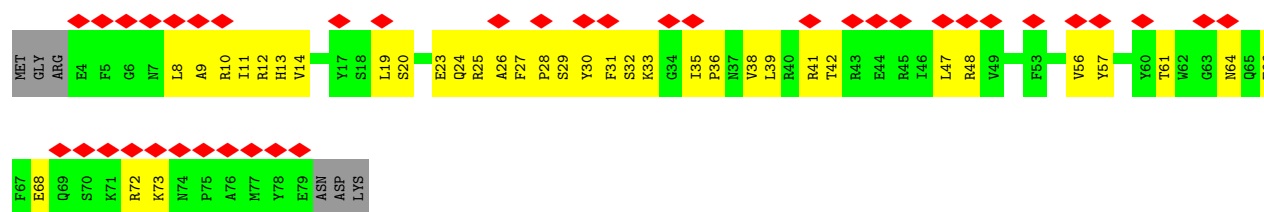




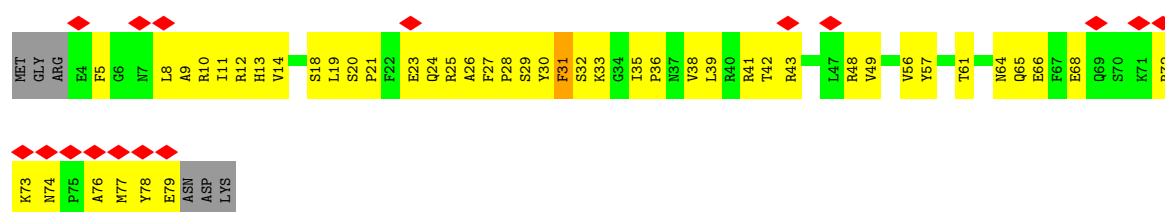
• Molecule 50: Cytochrome b-c1 complex subunit 7



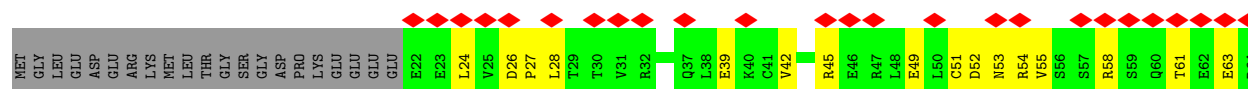
• Molecule 51: Cytochrome b-c1 complex subunit 8



• Molecule 51: Cytochrome b-c1 complex subunit 8

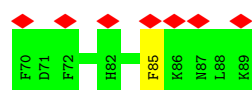
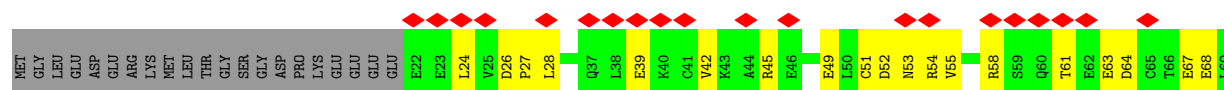


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

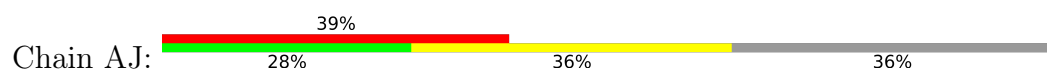




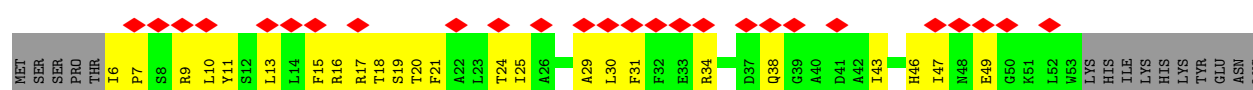
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



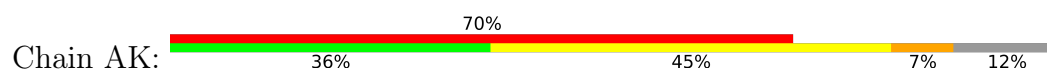
- Molecule 53: Cytochrome b-c1 complex subunit 9



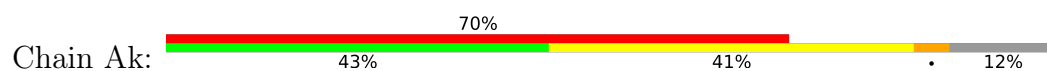
- Molecule 53: Cytochrome b-c1 complex subunit 9



- 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	28091	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	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: 3PE, HEM, U10, NDP, CDL, FMN, ADP, UQ1, FES, ZN, UQ6, EHZ, SF4, UQ9, PC1, HEC

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	0.79	0/774	1.12	7/1056 (0.7%)
2	B	0.93	1/1289 (0.1%)	1.46	20/1744 (1.1%)
3	C	0.87	0/1687	1.26	11/2297 (0.5%)
4	D	0.93	5/3505 (0.1%)	1.46	40/4748 (0.8%)
5	E	0.72	1/1675 (0.1%)	1.11	13/2282 (0.6%)
6	F	0.90	5/3363 (0.1%)	1.43	54/4543 (1.2%)
7	G	0.93	10/5374 (0.2%)	1.56	101/7281 (1.4%)
8	H	1.00	3/2608 (0.1%)	1.42	48/3563 (1.3%)
9	I	0.92	1/1461 (0.1%)	1.51	20/1974 (1.0%)
10	J	0.90	6/1318 (0.5%)	1.16	13/1791 (0.7%)
11	K	0.90	0/740	1.49	13/1005 (1.3%)
12	L	1.00	9/4921 (0.2%)	1.57	107/6696 (1.6%)
13	M	1.02	7/3717 (0.2%)	1.58	87/5062 (1.7%)
14	N	1.00	4/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.94	8/2666 (0.3%)	1.24	29/3615 (0.8%)
16	P	0.74	1/2793 (0.0%)	1.12	17/3787 (0.4%)
17	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
18	R	0.66	0/671	0.92	2/903 (0.2%)
19	S	0.92	2/678 (0.3%)	1.39	10/915 (1.1%)
20	T	0.68	1/613 (0.2%)	0.95	3/826 (0.4%)
20	U	1.01	1/712 (0.1%)	1.46	21/962 (2.2%)
21	V	0.81	0/937	1.38	12/1270 (0.9%)
22	W	0.80	1/993 (0.1%)	1.06	7/1335 (0.5%)
23	X	0.72	0/1422	1.20	14/1921 (0.7%)
24	Y	0.86	0/1061	1.03	4/1439 (0.3%)
25	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
26	a	0.84	0/561	1.11	3/755 (0.4%)
27	b	0.78	1/643 (0.2%)	1.01	3/884 (0.3%)
28	c	0.96	1/400 (0.2%)	1.34	10/544 (1.8%)
29	d	0.89	1/1028 (0.1%)	1.02	8/1387 (0.6%)
30	e	0.88	3/881 (0.3%)	1.07	6/1173 (0.5%)
31	f	0.82	1/459 (0.2%)	0.96	2/618 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.88	3/878 (0.3%)	1.35	18/1196 (1.5%)
33	h	0.75	0/1197	1.21	7/1621 (0.4%)
34	i	0.94	3/867 (0.3%)	1.35	17/1179 (1.4%)
35	j	0.74	0/603	1.21	8/825 (1.0%)
36	k	1.10	2/638 (0.3%)	1.49	19/862 (2.2%)
37	l	1.00	4/1367 (0.3%)	1.26	11/1866 (0.6%)
38	m	0.78	1/1073 (0.1%)	1.10	9/1455 (0.6%)
39	n	0.96	2/1596 (0.1%)	1.28	20/2162 (0.9%)
40	o	0.84	2/1075 (0.2%)	1.12	10/1442 (0.7%)
41	p	0.68	0/1485	0.96	11/2007 (0.5%)
42	q	0.91	4/1234 (0.3%)	1.27	19/1681 (1.1%)
43	r	0.60	0/782	1.04	6/1058 (0.6%)
44	s	0.43	0/194	0.69	0/264
45	AA	0.38	0/3213	0.69	5/4355 (0.1%)
45	Aa	0.50	1/3288 (0.0%)	0.69	3/4462 (0.1%)
46	AB	0.36	0/3187	0.64	5/4308 (0.1%)
46	Ab	0.43	0/3142	0.68	4/4246 (0.1%)
47	AC	0.48	1/3089 (0.0%)	0.68	3/4221 (0.1%)
47	Ac	0.46	1/3089 (0.0%)	0.73	7/4221 (0.2%)
48	AD	0.41	0/1971	0.70	3/2677 (0.1%)
48	Ad	0.54	0/1971	0.81	5/2677 (0.2%)
49	AE	0.63	0/1483	1.03	3/2007 (0.1%)
49	AI	1.83	2/219 (0.9%)	1.48	5/296 (1.7%)
49	Ae	0.63	0/1483	1.03	3/2007 (0.1%)
49	Ai	1.51	1/209 (0.5%)	1.16	1/283 (0.4%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.38	0/884	0.52	0/1184
51	AG	0.49	0/662	0.87	1/895 (0.1%)
51	Ag	0.50	0/662	0.89	1/895 (0.1%)
52	AH	0.38	0/569	0.68	0/763
52	Ah	0.38	0/569	0.68	0/763
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.55	0/401	0.71	0/542
54	AK	0.53	0/416	0.97	5/571 (0.9%)
54	Ak	0.53	0/416	0.81	2/571 (0.4%)
All	All	0.79	102/99004 (0.1%)	1.18	967/134251 (0.7%)

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Ai	44	ASP	C-N	20.05	1.52	1.33
49	AI	44	ASP	C-N	20.05	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Aa	250	LEU	C-N	19.52	1.58	1.33
15	O	247	PRO	N-CD	16.57	1.71	1.47
49	AI	45	VAL	C-N	15.63	1.53	1.33
8	H	214	GLU	C-N	15.51	1.56	1.33
12	L	265	PRO	N-CD	13.85	1.67	1.47
36	k	50	PRO	N-CD	-13.68	1.28	1.47
47	AC	271	GLU	C-N	13.65	1.52	1.34
14	N	255	PRO	N-CD	-13.54	1.28	1.47
42	q	139	PRO	N-CD	-13.37	1.29	1.47
28	c	39	PRO	N-CD	-13.30	1.29	1.47
7	G	532	PRO	N-CD	-12.53	1.30	1.47
15	O	315	PRO	N-CD	-12.07	1.30	1.47
42	q	102	PRO	N-CD	-11.23	1.32	1.47
34	i	124	PRO	C-N	11.15	1.48	1.33
12	L	234	PRO	N-CD	11.14	1.63	1.47
8	H	42	PRO	N-CD	10.89	1.62	1.47
13	M	370	PRO	N-CD	-10.67	1.32	1.47
6	F	234	GLY	CA-C	-10.42	1.40	1.52
36	k	20	MET	C-N	10.36	1.47	1.33
15	O	210	PRO	N-CD	-10.27	1.33	1.47
6	F	227	PRO	N-CD	10.13	1.61	1.47
30	e	101	ARG	CA-C	-9.94	1.39	1.53
15	O	318	THR	C-N	-9.82	1.21	1.33
6	F	235	VAL	N-CA	-9.65	1.34	1.46
7	G	275	PRO	N-CD	-9.55	1.34	1.47
32	g	78	PRO	N-CD	-9.49	1.34	1.47
10	J	117	LEU	C-N	-9.45	1.21	1.33
29	d	15	PRO	N-CD	-9.43	1.34	1.47
15	O	319	ILE	C-N	9.35	1.43	1.32
8	H	75	PRO	N-CD	9.26	1.60	1.47
30	e	102	GLU	N-CA	-9.25	1.35	1.46
34	i	125	ASP	C-N	8.80	1.44	1.33
10	J	123	TRP	C-N	-8.71	1.23	1.33
9	I	107	PRO	N-CD	8.66	1.59	1.47
13	M	20	PRO	N-CD	8.62	1.59	1.47
27	b	64	PRO	N-CD	8.54	1.59	1.47
42	q	121	PRO	N-CD	-8.40	1.35	1.47
47	Ac	265	PRO	N-CD	8.19	1.59	1.47
12	L	212	PRO	N-CD	-8.19	1.36	1.47
39	n	155	PRO	N-CD	8.15	1.59	1.47
4	D	140	ASP	C-O	-8.05	1.14	1.24
12	L	522	PHE	CA-C	-8.00	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S	63	PRO	N-CD	-7.94	1.36	1.47
5	E	218	ARG	CA-C	7.93	1.62	1.53
17	Q	53	ILE	C-O	7.84	1.33	1.24
10	J	118	ASP	C-N	7.71	1.44	1.33
20	T	141	PRO	N-CD	-7.68	1.36	1.47
40	o	120	ALA	C-N	-7.49	1.22	1.33
34	i	126	GLN	C-N	-7.44	1.23	1.33
4	D	365	PRO	N-CD	-7.41	1.37	1.47
37	l	115	ASN	C-N	-7.38	1.24	1.33
37	l	104	PRO	N-CD	-7.31	1.37	1.47
13	M	208	PRO	N-CD	7.24	1.57	1.47
42	q	126	PRO	N-CD	-7.10	1.37	1.47
14	N	238	PRO	N-CD	-7.08	1.37	1.47
15	O	206	TYR	C-N	6.80	1.42	1.33
7	G	449	PRO	N-CD	6.71	1.57	1.47
7	G	541	PRO	N-CD	-6.71	1.38	1.47
6	F	233	VAL	CA-C	-6.68	1.44	1.52
7	G	203	ASP	CA-C	6.65	1.62	1.52
32	g	113	GLN	CA-C	6.65	1.61	1.52
39	n	116	PRO	N-CD	6.52	1.56	1.47
4	D	140	ASP	CA-C	-6.45	1.44	1.52
7	G	600	GLU	CA-C	6.43	1.61	1.52
7	G	632	ILE	CA-C	-6.41	1.44	1.52
15	O	205	ILE	C-N	6.40	1.42	1.33
25	Z	63	GLU	C-N	-6.25	1.24	1.33
10	J	148	ALA	C-O	6.24	1.31	1.24
12	L	384	PRO	N-CD	6.21	1.56	1.47
7	G	127	ASP	CA-C	6.20	1.62	1.52
6	F	384	PRO	N-CD	-6.13	1.39	1.47
12	L	112	PRO	N-CD	6.10	1.56	1.47
2	B	110	PRO	C-O	-6.09	1.16	1.24
4	D	392	PRO	C-O	-5.96	1.20	1.25
32	g	137	SER	C-O	-5.94	1.16	1.24
38	m	72	ARG	CA-C	5.92	1.60	1.52
7	G	361	VAL	CA-C	5.85	1.60	1.52
30	e	34	HIS	C-O	-5.83	1.16	1.24
37	l	45	PRO	N-CD	-5.82	1.39	1.47
15	O	87	PRO	N-CD	-5.79	1.39	1.47
10	J	124	LEU	C-N	5.76	1.41	1.33
12	L	523	SER	CA-C	-5.76	1.45	1.52
13	M	252	PRO	N-CD	-5.63	1.39	1.47
13	M	454	ILE	CA-C	5.63	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	333	SER	C-O	-5.61	1.17	1.23
10	J	78	TYR	CA-C	-5.48	1.50	1.53
22	W	98	LYS	CA-C	-5.48	1.46	1.52
7	G	683	PRO	N-CD	-5.47	1.40	1.47
19	S	95	LEU	CA-C	5.47	1.59	1.52
16	P	235	THR	CA-C	5.38	1.59	1.53
20	U	140	CYS	C-O	-5.35	1.17	1.24
12	L	523	SER	N-CA	-5.27	1.39	1.46
13	M	424	ILE	CA-C	-5.24	1.45	1.52
37	l	111	MET	C-O	-5.14	1.17	1.24
31	f	38	ARG	CA-C	-5.14	1.46	1.52
13	M	159	PRO	N-CD	5.10	1.54	1.47
4	D	310	VAL	C-O	-5.06	1.16	1.23
12	L	56	HIS	CA-C	-5.02	1.46	1.52
14	N	88	GLN	CA-C	5.01	1.59	1.52
40	o	121	ARG	C-N	5.00	1.40	1.33

All (967) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.60	130.05	111.02
13	M	370	PRO	N-CA-C	14.64	128.56	110.70
14	N	255	PRO	N-CA-C	14.43	128.31	110.70
15	O	118	TYR	N-CA-C	13.77	125.80	111.07
7	G	632	ILE	N-CA-C	-13.65	88.01	107.80
42	q	139	PRO	N-CA-CB	-13.45	95.66	103.19
7	G	251	ILE	N-CA-C	13.29	126.78	108.17
6	F	125	CYS	N-CA-C	-12.93	93.46	113.89
7	G	500	ILE	N-CA-C	-12.51	98.77	110.53
12	L	522	PHE	N-CA-C	-12.30	97.86	111.14
2	B	199	GLU	N-CA-C	-12.20	98.06	111.36
16	P	106	LEU	N-CA-C	12.19	128.70	109.07
22	W	98	LYS	N-CA-C	-12.06	88.99	108.41
10	J	65	VAL	N-CA-C	-12.04	98.34	110.62
6	F	171	VAL	N-CA-C	-11.88	99.36	110.53
2	B	80	ASP	N-CA-C	-11.68	98.58	111.07
6	F	449	ARG	N-CA-C	-11.62	98.69	111.36
7	G	204	MET	N-CA-C	-11.61	91.49	109.25
34	i	14	GLN	N-CA-C	11.60	123.92	111.28
13	M	424	ILE	N-CA-C	-11.59	94.11	109.30
13	M	104	ILE	N-CA-C	-11.56	99.09	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	334	THR	N-CA-CB	11.50	127.31	109.82
15	O	114	LEU	N-CA-C	-11.48	98.84	111.36
12	L	194	ASN	N-CA-C	11.44	125.35	109.11
13	M	311	GLY	N-CA-C	-11.35	99.33	112.50
7	G	599	THR	N-CA-C	11.35	126.22	112.38
14	N	244	ILE	N-CA-C	-11.32	99.28	110.72
17	Q	60	ASP	N-CA-C	-11.32	90.34	109.24
12	L	278	LEU	N-CA-C	-11.26	98.98	111.14
37	l	116	ARG	N-CA-C	11.22	123.20	110.97
11	K	83	ASN	N-CA-C	-11.20	100.15	114.04
8	H	259	PHE	N-CA-C	-11.02	99.35	111.36
20	U	79	ILE	N-CA-C	-11.00	102.34	112.90
7	G	77	MET	N-CA-C	-10.84	97.35	113.61
12	L	582	GLY	N-CA-C	-10.81	99.50	114.64
2	B	105	MET	N-CA-C	-10.72	99.38	111.71
12	L	556	ILE	N-CA-C	10.70	121.36	110.23
9	I	164	VAL	N-CA-C	-10.67	100.09	113.22
12	L	231	PRO	N-CA-C	10.65	127.69	113.84
33	h	101	ILE	N-CA-C	-10.65	98.52	108.95
39	n	117	ASP	N-CA-C	-10.52	99.62	111.82
9	I	77	LEU	N-CA-C	-10.47	99.67	111.71
13	M	276	CYS	N-CA-C	-10.35	100.00	111.28
7	G	280	ASP	N-CA-C	10.32	122.53	111.28
15	O	247	PRO	N-CA-CB	10.31	114.26	103.23
37	l	170	ARG	N-CA-C	-10.19	101.49	113.21
7	G	414	PHE	N-CA-C	-10.11	101.44	113.88
9	I	161	ALA	N-CA-C	10.07	122.26	111.28
13	M	117	MET	N-CA-C	-10.04	100.33	111.28
4	D	114	GLY	N-CA-C	-9.99	100.87	114.95
46	AB	306	THR	N-CA-C	9.96	123.38	111.33
46	Ab	306	THR	N-CA-C	9.92	123.33	111.33
9	I	166	ALA	N-CA-C	-9.89	100.75	113.12
46	AB	303	ASN	N-CA-C	-9.88	100.14	112.88
2	B	195	PRO	N-CA-C	-9.87	98.66	110.70
46	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
6	F	178	GLU	N-CA-C	-9.84	99.30	111.11
7	G	325	ARG	N-CA-C	-9.84	100.25	110.97
4	D	311	TYR	N-CA-C	-9.84	98.37	113.02
6	F	141	GLY	N-CA-C	-9.83	101.09	112.50
45	Aa	250	LEU	O-C-N	-9.83	112.22	121.56
7	G	654	VAL	N-CA-C	9.81	123.36	111.09
36	k	50	PRO	CA-N-CD	9.75	125.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	423	MET	N-CA-C	-9.73	96.92	110.35
6	F	144	VAL	N-CA-C	-9.71	101.40	110.53
14	N	255	PRO	CA-N-CD	9.65	125.51	112.00
6	F	418	GLN	N-CA-C	-9.64	100.73	111.14
14	N	286	ALA	N-CA-C	-9.64	100.78	111.28
13	M	83	HIS	N-CA-C	-9.63	97.25	110.35
20	U	74	LEU	N-CA-C	9.61	122.23	110.41
39	n	29	SER	N-CA-C	-9.60	101.46	113.55
34	i	12	LEU	N-CA-C	-9.57	101.16	113.12
7	G	337	ALA	N-CA-C	-9.55	100.84	114.12
22	W	87	ILE	N-CA-C	-9.55	101.26	110.42
8	H	52	ALA	N-CA-C	-9.54	100.86	111.07
4	D	427	PRO	N-CA-C	-9.53	95.55	110.50
23	X	70	PHE	N-CA-C	-9.49	99.72	111.11
12	L	375	ILE	N-CA-C	-9.47	101.33	110.42
14	N	228	ASN	N-CA-C	-9.39	101.02	111.07
42	q	123	GLN	N-CA-C	9.38	123.83	110.23
42	q	139	PRO	CA-N-CD	9.36	125.11	112.00
12	L	40	ILE	N-CA-C	-9.31	101.32	110.72
7	G	692	LYS	N-CA-C	-9.30	100.51	112.23
36	k	56	ALA	N-CA-C	9.27	121.46	111.36
13	M	104	ILE	N-CA-CB	9.26	120.71	110.62
36	k	60	MET	N-CA-C	9.25	121.05	110.97
7	G	694	PHE	N-CA-C	9.24	121.36	111.28
25	Z	69	ILE	N-CA-C	-9.24	100.66	110.36
12	L	394	LEU	N-CA-C	-9.23	101.19	111.07
12	L	483	PRO	N-CA-C	-9.19	96.77	111.38
7	G	389	THR	N-CA-C	-9.17	96.20	109.96
15	O	247	PRO	CA-N-CD	-9.12	99.23	112.00
28	c	64	GLU	N-CA-C	-9.10	101.33	111.07
4	D	212	GLU	N-CA-C	-9.10	100.32	111.33
14	N	87	GLN	N-CA-C	9.08	123.21	109.41
4	D	323	ARG	N-CA-C	9.08	124.79	112.90
12	L	467	VAL	N-CA-C	9.06	119.12	110.42
26	a	57	VAL	N-CA-C	-9.02	105.14	113.71
28	c	39	PRO	N-CA-CB	-9.01	95.32	103.25
13	M	442	ILE	N-CA-CB	8.98	117.46	110.45
41	p	115	GLN	N-CA-C	-8.98	102.83	113.88
25	Z	143	TYR	N-CA-C	8.98	121.96	108.31
11	K	70	GLU	N-CA-C	-8.95	100.37	111.11
6	F	411	SER	N-CA-C	-8.92	101.53	111.07
12	L	406	ALA	N-CA-C	-8.88	101.68	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	344	GLY	N-CA-C	-8.88	102.20	112.50
14	N	233	LEU	N-CA-C	-8.85	101.63	111.28
2	B	170	TYR	N-CA-C	-8.85	97.76	110.24
15	O	183	CYS	N-CA-C	-8.85	100.49	111.11
7	G	133	GLN	N-CA-CB	8.83	121.58	110.45
49	AI	46	LYS	N-CA-C	8.81	121.70	110.33
39	n	70	GLU	N-CA-C	-8.81	101.65	111.07
13	M	255	LYS	N-CA-C	-8.78	101.67	111.07
7	G	365	ASN	N-CA-C	-8.78	102.12	112.92
7	G	212	LYS	N-CA-C	-8.78	94.59	108.90
14	N	81	LEU	N-CA-C	-8.75	94.37	108.55
14	N	255	PRO	N-CA-CB	-8.70	94.64	103.08
40	o	72	ASP	N-CA-C	-8.69	99.06	110.53
9	I	154	TYR	N-CA-CB	-8.67	99.23	111.62
43	r	62	GLU	N-CA-C	-8.61	102.76	113.18
13	M	248	ILE	N-CA-C	-8.59	102.17	110.42
4	D	209	LYS	N-CA-C	-8.58	101.89	111.07
12	L	212	PRO	N-CA-C	8.58	125.74	113.47
19	S	86	GLU	N-CA-C	-8.55	102.04	111.36
15	O	315	PRO	CA-N-CD	8.52	123.93	112.00
15	O	245	PHE	N-CA-C	8.47	120.14	111.07
12	L	265	PRO	N-CA-C	-8.46	101.37	113.47
4	D	140	ASP	N-CA-C	-8.45	94.75	108.52
14	N	221	LEU	N-CA-C	-8.44	101.11	111.33
4	D	214	TYR	CB-CA-C	-8.43	97.64	110.88
12	L	287	PHE	N-CA-C	-8.43	102.05	111.07
14	N	272	LYS	N-CA-C	-8.42	102.10	111.28
23	X	99	HIS	N-CA-C	-8.41	102.19	111.36
5	E	154	LYS	N-CA-C	-8.39	101.82	110.97
3	C	108	LYS	N-CA-C	8.39	120.05	111.07
14	N	109	ALA	CA-C-N	-8.38	110.82	120.12
14	N	109	ALA	C-N-CA	-8.38	110.82	120.12
12	L	281	GLY	N-CA-C	-8.38	102.78	112.50
17	Q	54	THR	N-CA-C	8.34	123.31	109.46
7	G	532	PRO	CA-N-CD	8.33	123.66	112.00
7	G	452	LEU	N-CA-C	-8.32	102.21	111.28
7	G	558	GLN	N-CA-C	-8.30	102.19	111.07
39	n	19	LEU	N-CA-C	-8.27	103.33	113.41
14	N	218	ALA	N-CA-C	-8.26	98.93	111.56
36	k	50	PRO	N-CA-CB	-8.26	93.51	102.76
13	M	274	SER	N-CA-C	8.25	120.27	111.28
5	E	218	ARG	CB-CA-C	-8.23	99.78	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	88	LEU	N-CA-C	-8.21	102.28	111.14
8	H	196	ALA	N-CA-C	8.21	127.94	109.81
8	H	311	THR	N-CA-C	-8.20	102.59	112.59
12	L	169	LEU	N-CA-C	-8.19	102.44	111.36
12	L	151	SER	N-CA-C	-8.18	102.44	111.36
1	A	64	LEU	N-CA-C	-8.18	102.32	111.07
7	G	691	ILE	N-CA-C	8.18	123.66	111.89
36	k	38	VAL	N-CA-C	-8.17	102.47	110.72
7	G	500	ILE	N-CA-CB	8.15	121.00	110.57
14	N	32	GLY	N-CA-C	-8.15	103.05	112.50
7	G	484	ASP	N-CA-C	8.14	121.08	111.71
3	C	196	PRO	N-CA-C	8.14	124.84	113.53
13	M	26	ASN	N-CA-C	-8.13	102.36	111.14
6	F	411	SER	N-CA-CB	8.12	121.78	110.01
29	d	15	PRO	N-CA-CB	-8.09	96.31	103.35
42	q	118	SER	N-CA-C	8.09	120.82	111.11
21	V	86	LYS	N-CA-C	-8.06	102.43	111.14
7	G	534	VAL	N-CA-C	-8.06	104.74	111.91
19	S	76	THR	N-CA-C	8.05	122.02	108.90
5	E	219	SER	N-CA-CB	8.03	124.01	111.56
13	M	385	LEU	N-CA-C	-8.03	102.53	111.28
9	I	201	ILE	N-CA-C	-8.03	102.61	110.72
12	L	276	THR	N-CA-CB	8.01	121.62	110.01
23	X	43	PHE	N-CA-C	-7.99	102.52	111.07
13	M	205	ILE	N-CA-C	7.98	118.08	110.42
8	H	271	LEU	N-CA-C	-7.97	102.53	111.14
12	L	524	THR	N-CA-C	7.97	122.27	112.23
1	A	9	ILE	N-CA-C	-7.95	102.52	110.62
7	G	651	PRO	CB-CA-C	-7.94	98.45	111.56
28	c	45	GLY	N-CA-C	7.94	123.64	113.24
28	c	39	PRO	CA-N-CD	7.94	123.11	112.00
16	P	206	ILE	N-CA-C	7.93	120.93	108.87
39	n	170	ILE	N-CA-C	-7.92	103.18	111.58
45	AA	360	CYS	N-CA-C	7.91	120.92	109.14
12	L	265	PRO	N-CA-CB	7.91	111.69	103.23
21	V	6	LYS	N-CA-C	-7.90	100.11	110.53
45	Aa	360	CYS	N-CA-C	7.87	120.87	109.14
30	e	101	ARG	CA-C-N	-7.87	111.90	123.00
30	e	101	ARG	C-N-CA	-7.87	111.90	123.00
8	H	311	THR	N-CA-CB	7.86	123.50	110.92
9	I	160	GLU	N-CA-C	7.85	124.25	111.37
13	M	141	GLU	N-CA-C	7.85	122.70	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	270	VAL	N-CA-CB	-7.84	100.66	110.31
42	q	28	PHE	N-CA-C	7.83	122.60	112.89
16	P	235	THR	CB-CA-C	-7.82	100.03	112.07
11	K	51	SER	N-CA-C	-7.82	102.83	113.30
13	M	330	ALA	N-CA-C	-7.81	102.71	111.14
12	L	111	ASP	N-CA-C	-7.79	100.27	109.93
14	N	336	THR	N-CA-C	-7.78	103.31	114.12
7	G	389	THR	N-CA-CB	7.76	121.42	109.85
25	Z	143	TYR	CB-CA-C	-7.76	107.61	116.54
12	L	265	PRO	CA-N-CD	-7.76	101.14	112.00
13	M	85	LYS	N-CA-C	-7.76	101.46	113.02
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
15	O	318	THR	O-C-N	-7.73	112.31	122.59
4	D	233	HIS	N-CA-C	7.72	119.48	111.14
6	F	58	ARG	N-CA-C	-7.71	102.95	111.36
8	H	253	GLU	N-CA-C	7.71	121.94	112.54
12	L	415	ALA	N-CA-C	-7.70	102.88	111.28
42	q	89	TRP	N-CA-C	-7.69	102.83	111.14
6	F	334	THR	N-CA-C	-7.67	101.66	111.02
4	D	184	ILE	N-CA-C	-7.67	102.80	110.62
7	G	56	VAL	N-CA-C	-7.66	102.99	110.72
4	D	257	GLU	N-CA-C	7.61	119.57	111.28
7	G	569	GLN	N-CA-C	7.61	122.01	108.24
10	J	104	CYS	N-CA-C	-7.60	103.00	111.28
9	I	119	CYS	N-CA-C	-7.56	103.11	111.36
6	F	171	VAL	N-CA-CB	7.56	120.25	110.57
43	r	30	GLU	N-CA-C	-7.54	104.98	114.56
8	H	214	GLU	N-CA-CB	-7.53	98.86	110.46
12	L	245	ALA	N-CA-C	7.52	119.12	111.07
40	o	81	LYS	N-CA-C	-7.52	104.63	113.88
9	I	158	CYS	N-CA-C	-7.51	103.09	111.28
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
7	G	277	MET	N-CA-C	7.50	120.61	109.59
20	U	147	TYR	N-CA-C	-7.50	103.04	111.14
32	g	124	VAL	N-CA-C	-7.48	103.16	110.72
4	D	180	ILE	N-CA-C	-7.48	103.24	110.42
11	K	14	LEU	N-CA-C	-7.48	103.21	111.36
6	F	430	GLY	N-CA-C	7.45	121.67	112.73
7	G	467	LYS	N-CA-C	-7.44	102.33	111.33
30	e	46	GLY	N-CA-C	-7.44	105.00	114.37
12	L	605	ASN	N-CA-CB	7.44	121.25	110.47
12	L	392	LYS	N-CA-C	7.43	119.03	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	123	LEU	N-CA-C	-7.43	103.27	111.36
42	q	102	PRO	CA-N-CD	7.43	122.40	112.00
22	W	100	TRP	N-CA-C	-7.42	103.80	114.12
19	S	94	VAL	N-CA-C	7.42	117.54	110.42
13	M	250	LEU	N-CA-C	-7.42	103.53	112.58
2	B	80	ASP	N-CA-CB	7.41	120.76	110.01
12	L	138	PHE	N-CA-C	-7.41	103.20	111.28
7	G	510	TRP	N-CA-CB	7.41	120.89	109.85
12	L	21	ILE	N-CA-CB	7.39	121.67	110.58
35	j	82	GLY	N-CA-C	-7.37	103.56	112.48
8	H	309	ILE	N-CA-C	7.37	117.45	110.30
47	AC	202	GLU	N-CA-C	-7.36	103.28	111.82
13	M	47	GLU	N-CA-C	7.35	121.50	112.54
7	G	303	THR	N-CA-C	7.33	122.92	113.18
38	m	72	ARG	N-CA-C	7.31	122.49	113.50
12	L	28	LYS	N-CA-C	-7.30	103.32	111.28
13	M	455	THR	N-CA-C	-7.30	100.42	110.35
37	l	97	LEU	N-CA-C	-7.29	103.98	113.17
47	Ac	8	HIS	CA-C-N	7.29	127.00	119.56
47	Ac	8	HIS	C-N-CA	7.29	127.00	119.56
34	i	123	PHE	N-CA-C	-7.29	100.89	110.07
49	AE	221	GLY	N-CA-C	7.29	126.88	113.76
7	G	661	GLU	N-CA-C	7.29	118.91	110.97
7	G	384	ASN	N-CA-C	-7.28	103.38	111.82
3	C	195	HIS	CB-CA-C	7.27	117.37	110.17
49	Ae	221	GLY	N-CA-C	7.26	126.83	113.76
13	M	289	SER	N-CA-C	-7.24	103.32	111.07
21	V	68	LEU	N-CA-C	-7.24	103.39	111.28
7	G	374	THR	CB-CA-C	-7.22	99.88	111.28
4	D	210	MET	N-CA-C	7.20	119.12	111.28
36	k	73	ILE	N-CA-C	-7.19	103.29	110.62
11	K	81	VAL	N-CA-C	7.18	117.94	110.62
12	L	19	ILE	N-CA-C	7.17	117.31	110.42
19	S	20	ARG	N-CA-C	7.16	120.66	107.99
4	D	177	ILE	N-CA-C	-7.15	103.33	110.62
7	G	461	SER	N-CA-C	7.15	119.98	111.33
54	AK	47	TYR	N-CA-C	7.15	122.19	112.68
20	U	136	GLU	N-CA-C	-7.14	104.56	113.20
8	H	50	ALA	N-CA-C	7.14	118.71	111.07
7	G	465	VAL	N-CA-CB	7.14	118.43	110.51
12	L	554	ASP	N-CA-CB	7.14	121.27	110.42
7	G	497	VAL	N-CA-C	-7.13	103.34	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	244	ILE	N-CA-C	7.13	117.89	110.62
6	F	455	GLN	N-CA-C	7.12	118.69	111.07
41	p	168	LYS	N-CA-C	-7.10	104.24	113.12
8	H	254	LEU	N-CA-C	-7.10	103.58	111.82
4	D	457	VAL	N-CA-C	-7.09	98.18	108.11
15	O	70	LYS	N-CA-C	7.08	119.85	111.71
4	D	119	GLY	N-CA-C	-7.08	103.47	115.08
9	I	45	GLU	N-CA-C	7.08	120.87	108.56
21	V	95	LEU	N-CA-C	-7.08	103.57	111.28
11	K	48	SER	N-CA-C	-7.07	103.58	111.28
13	M	34	ILE	N-CA-C	-7.07	103.41	110.62
12	L	319	MET	N-CA-C	-7.06	104.67	112.72
39	n	102	TRP	N-CA-C	-7.05	105.03	112.93
47	AC	17	SER	N-CA-C	7.05	122.05	113.38
13	M	325	LEU	N-CA-C	-7.04	103.54	111.07
7	G	217	GLU	N-CA-C	-7.03	101.76	110.41
8	H	176	LEU	CA-C-N	-7.02	113.57	120.52
8	H	176	LEU	C-N-CA	-7.02	113.57	120.52
35	j	65	MET	N-CA-C	-7.02	103.56	111.07
23	X	153	VAL	N-CA-C	7.02	117.97	107.80
13	M	264	LEU	N-CA-C	-7.00	103.58	111.07
13	M	213	HIS	CB-CA-C	-7.00	96.81	110.11
42	q	102	PRO	N-CA-CB	-7.00	96.29	103.08
6	F	428	GLY	N-CA-C	-6.99	103.82	112.77
12	L	546	LEU	N-CA-C	6.99	119.55	111.02
16	P	235	THR	CA-C-O	6.99	128.17	121.67
34	i	9	LYS	N-CA-C	-6.99	104.75	112.72
7	G	294	TYR	N-CA-C	-6.99	104.57	113.23
24	Y	118	VAL	N-CA-C	6.98	117.12	110.42
20	U	75	THR	N-CA-CB	6.98	123.83	111.69
6	F	246	GLU	N-CA-C	-6.97	103.69	111.28
12	L	86	SER	N-CA-C	6.97	118.52	111.07
49	Ae	218	THR	N-CA-C	-6.96	102.84	111.75
6	F	418	GLN	N-CA-CB	6.96	120.16	110.07
6	F	169	LEU	N-CA-C	6.96	118.86	111.28
13	M	365	ALA	N-CA-C	-6.96	103.77	111.36
6	F	148	ALA	N-CA-C	-6.95	103.78	111.36
34	i	124	PRO	O-C-N	6.95	130.56	122.98
14	N	132	THR	N-CA-C	6.95	122.86	113.97
25	Z	34	SER	N-CA-C	-6.94	103.72	111.28
13	M	91	LEU	N-CA-C	-6.94	103.81	112.90
49	AE	218	THR	N-CA-C	-6.93	102.88	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	300	GLN	N-CA-CB	6.93	122.54	112.08
49	AI	45	VAL	CA-C-N	-6.92	108.62	120.95
49	AI	45	VAL	C-N-CA	-6.92	108.62	120.95
12	L	100	ILE	N-CA-C	6.91	119.69	111.05
12	L	26	LEU	N-CA-C	6.91	119.66	111.71
7	G	582	VAL	N-CA-C	6.91	118.42	108.48
13	M	442	ILE	N-CA-C	-6.91	104.06	112.35
8	H	98	LEU	N-CA-CB	-6.90	98.82	110.83
6	F	233	VAL	O-C-N	6.90	131.18	123.10
36	k	59	TYR	N-CA-CB	-6.90	98.81	110.41
2	B	78	LEU	N-CA-C	6.90	119.83	111.82
12	L	471	ASN	N-CA-C	6.90	118.88	111.36
22	W	99	VAL	N-CA-C	6.89	117.16	107.37
13	M	276	CYS	N-CA-CB	6.89	120.25	110.12
8	H	203	GLY	N-CA-C	-6.89	102.72	112.37
10	J	65	VAL	N-CA-CB	6.89	119.91	110.54
7	G	102	ILE	N-CA-C	6.88	119.69	111.09
8	H	292	ASN	N-CA-C	6.88	118.86	111.36
18	R	108	GLY	N-CA-C	-6.88	105.98	114.92
13	M	235	LEU	N-CA-C	6.87	119.35	111.11
34	i	11	ARG	N-CA-C	-6.87	104.90	113.28
7	G	362	ASP	N-CA-C	6.86	125.40	110.80
7	G	133	GLN	N-CA-C	-6.84	101.18	110.68
11	K	83	ASN	N-CA-CB	6.83	120.92	110.81
8	H	305	ILE	N-CA-C	-6.83	103.36	113.39
6	F	244	ASN	N-CA-C	-6.82	100.88	110.50
6	F	329	LYS	N-CA-C	6.82	119.58	111.33
6	F	233	VAL	CA-C-O	-6.82	113.24	120.53
8	H	300	LEU	N-CA-C	-6.81	104.23	112.54
13	M	165	ILE	N-CA-C	-6.79	102.60	111.09
15	O	175	ASN	N-CA-C	-6.78	103.95	111.82
11	K	70	GLU	N-CA-CB	6.78	120.04	109.94
32	g	78	PRO	CA-N-CD	6.78	121.49	112.00
25	Z	63	GLU	O-C-N	-6.78	114.94	122.12
2	B	196	PRO	N-CA-C	-6.77	100.60	111.03
12	L	547	LYS	N-CA-C	6.77	118.66	111.28
7	G	268	GLY	N-CA-C	6.77	124.71	115.30
15	O	210	PRO	CA-N-CD	6.77	121.47	112.00
16	P	91	ILE	CB-CA-C	-6.76	102.62	111.88
5	E	154	LYS	N-CA-CB	6.75	119.77	109.91
38	m	127	ILE	N-CA-C	-6.75	106.22	112.43
20	U	140	CYS	CA-C-N	-6.74	113.95	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	140	CYS	C-N-CA	-6.74	113.95	120.83
4	D	329	ARG	CB-CA-C	6.73	121.97	110.79
7	G	434	SER	N-CA-C	-6.73	101.00	110.29
2	B	110	PRO	N-CA-C	6.73	122.73	113.65
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
37	l	86	ARG	N-CA-C	-6.69	99.62	110.20
11	K	76	ALA	N-CA-C	-6.69	104.06	111.36
21	V	114	TRP	N-CA-CB	6.68	120.26	110.30
36	k	49	ASP	CA-C-N	-6.68	113.32	120.47
36	k	49	ASP	C-N-CA	-6.68	113.32	120.47
13	M	374	ASN	N-CA-C	-6.68	103.92	111.07
21	V	8	THR	N-CA-C	6.68	119.01	108.79
12	L	95	PHE	N-CA-C	-6.68	103.93	111.07
14	N	228	ASN	N-CA-CB	6.67	119.69	110.01
32	g	76	SER	N-CA-C	6.67	118.21	111.07
13	M	248	ILE	N-CA-CB	6.67	118.35	110.55
15	O	315	PRO	N-CA-CB	-6.67	95.99	103.33
20	U	150	ASP	CB-CA-C	6.67	121.86	110.79
13	M	49	TYR	N-CA-CB	-6.66	100.25	110.04
13	M	410	MET	N-CA-C	-6.66	103.94	111.07
6	F	344	GLN	N-CA-C	-6.65	104.03	111.28
10	J	117	LEU	O-C-N	-6.65	114.46	122.11
29	d	88	HIS	N-CA-C	-6.64	103.14	111.11
16	P	116	ILE	N-CA-C	-6.64	104.01	110.72
34	i	8	GLU	N-CA-C	-6.64	104.77	114.39
13	M	161	LEU	N-CA-C	-6.63	103.97	111.07
21	V	86	LYS	N-CA-CB	6.63	119.68	110.07
13	M	143	LEU	N-CA-C	-6.62	103.98	111.07
23	X	129	THR	N-CA-C	6.62	120.84	110.17
3	C	125	PHE	N-CA-CB	-6.62	100.64	110.17
8	H	267	SER	N-CA-C	-6.61	104.15	111.36
4	D	70	ASP	N-CA-C	6.61	120.66	110.42
7	G	601	GLY	N-CA-C	6.60	124.81	115.30
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
17	Q	141	ASN	N-CA-CB	6.59	120.81	110.46
20	U	102	SER	N-CA-C	6.59	119.58	107.99
39	n	115	TYR	N-CA-CB	6.58	122.08	110.37
2	B	79	ASP	N-CA-C	-6.57	103.61	111.69
41	p	30	ILE	CB-CA-C	-6.57	103.27	112.14
2	B	154	GLU	CA-C-N	-6.56	112.37	119.98
2	B	154	GLU	C-N-CA	-6.56	112.37	119.98
7	G	287	SER	N-CA-C	6.55	119.18	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	435	PRO	N-CA-C	-6.55	100.21	110.50
23	X	97	PHE	N-CA-C	6.55	118.50	111.36
13	M	303	ILE	N-CA-C	-6.55	104.10	110.72
6	F	234	GLY	CA-C-N	-6.55	111.73	120.50
6	F	234	GLY	C-N-CA	-6.55	111.73	120.50
8	H	223	PHE	N-CA-C	-6.54	104.07	111.07
47	Ac	265	PRO	N-CA-C	-6.54	102.72	110.70
12	L	232	TRP	N-CA-C	6.53	120.51	112.54
8	H	182	ALA	N-CA-C	-6.53	104.08	111.07
36	k	57	TRP	N-CA-C	-6.53	104.58	112.54
12	L	423	SER	N-CA-C	-6.53	104.09	111.07
7	G	250	SER	N-CA-C	6.52	116.89	108.34
25	Z	65	LEU	N-CA-C	-6.52	104.25	111.36
15	O	118	TYR	N-CA-CB	-6.52	100.56	110.01
36	k	46	GLY	N-CA-C	-6.51	106.94	114.69
46	AB	305	THR	N-CA-CB	-6.51	100.41	109.91
4	D	237	PRO	N-CA-C	-6.50	101.65	111.41
16	P	92	MET	N-CA-C	-6.50	104.23	111.71
6	F	336	LEU	N-CA-CB	-6.50	101.10	111.43
12	L	130	ILE	N-CA-C	-6.50	103.99	110.62
7	G	275	PRO	CB-CA-C	-6.49	102.48	110.98
46	Ab	305	THR	N-CA-CB	-6.49	100.43	109.91
12	L	329	ILE	N-CA-C	-6.48	104.20	110.42
15	O	140	LEU	N-CA-C	-6.47	104.14	111.07
15	O	320	GLY	N-CA-C	-6.46	96.56	111.04
14	N	315	THR	N-CA-C	-6.46	104.16	111.07
7	G	605	GLN	N-CA-C	6.46	119.05	108.52
45	Aa	215	ASP	N-CA-C	-6.45	103.94	110.97
4	D	149	GLN	N-CA-C	-6.45	105.57	113.50
8	H	255	TYR	N-CA-CB	6.45	119.36	110.01
9	I	66	LEU	N-CA-C	-6.44	104.34	111.36
8	H	177	PRO	N-CA-C	-6.44	101.54	111.13
45	AA	215	ASP	N-CA-C	-6.43	103.96	110.97
23	X	98	ARG	N-CA-C	6.43	120.39	112.54
11	K	11	ALA	N-CA-C	-6.43	104.19	111.07
6	F	178	GLU	N-CA-CB	6.43	119.52	109.94
9	I	205	ILE	N-CA-C	-6.42	104.23	110.72
21	V	49	GLU	N-CA-C	-6.42	104.28	111.28
3	C	125	PHE	N-CA-C	6.42	119.56	110.50
6	F	370	LEU	N-CA-C	-6.41	104.37	111.36
7	G	275	PRO	CA-N-CD	6.41	120.98	112.00
13	M	32	PHE	N-CA-C	-6.41	104.21	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	LEU	N-CA-C	-6.41	105.32	113.01
45	AA	402	HIS	N-CA-C	-6.41	102.27	110.53
10	J	149	THR	N-CA-C	-6.40	106.05	114.31
12	L	325	ALA	N-CA-C	-6.40	104.31	111.28
29	d	15	PRO	CA-N-CD	6.39	120.95	112.00
37	l	119	THR	N-CA-C	-6.38	98.14	108.41
7	G	273	ILE	N-CA-C	-6.37	98.34	107.77
49	AI	44	ASP	O-C-N	6.37	131.23	121.23
36	k	42	LEU	N-CA-C	-6.37	103.60	111.75
49	Ai	44	ASP	O-C-N	6.36	131.22	121.23
21	V	91	ALA	N-CA-C	-6.36	104.35	111.28
12	L	70	THR	N-CA-C	-6.35	103.88	111.69
12	L	439	PRO	N-CA-C	6.35	122.35	113.53
17	Q	59	LEU	N-CA-C	-6.34	100.80	110.30
20	T	107	ASP	N-CA-C	6.33	122.85	110.56
8	H	271	LEU	N-CA-CB	6.33	119.25	110.07
6	F	144	VAL	N-CA-CB	6.33	118.67	110.57
12	L	234	PRO	CA-N-CD	-6.32	103.15	112.00
28	c	47	SER	N-CA-CB	6.32	120.95	110.33
34	i	105	PHE	CA-C-N	-6.32	113.27	119.90
34	i	105	PHE	C-N-CA	-6.32	113.27	119.90
12	L	387	THR	N-CA-C	6.31	118.97	111.71
38	m	50	GLN	N-CA-C	-6.30	106.18	114.31
12	L	337	ALA	N-CA-C	-6.29	104.42	111.28
32	g	112	MET	N-CA-C	6.29	120.74	113.38
23	X	99	HIS	N-CA-CB	6.29	119.47	110.16
21	V	71	LEU	N-CA-C	6.29	118.13	111.28
2	B	135	GLY	CA-C-O	-6.29	117.92	122.45
28	c	72	ARG	N-CA-C	-6.29	104.34	111.07
7	G	176	CYS	N-CA-C	6.28	119.59	110.42
13	M	317	ILE	N-CA-C	-6.28	104.62	110.53
5	E	50	THR	N-CA-CB	6.28	121.54	110.37
17	Q	141	ASN	N-CA-C	-6.27	105.63	113.28
14	N	91	ASN	N-CA-CB	6.27	119.18	109.97
42	q	65	THR	N-CA-C	6.26	118.11	110.41
13	M	26	ASN	N-CA-CB	6.25	119.14	110.07
26	a	26	ILE	N-CA-C	-6.25	104.57	113.07
6	F	415	ILE	N-CA-C	-6.25	104.41	110.72
14	N	337	LEU	CA-C-N	-6.25	113.69	119.82
14	N	337	LEU	C-N-CA	-6.25	113.69	119.82
22	W	97	ILE	CB-CA-C	-6.25	104.36	111.55
7	G	356	ASP	N-CA-CB	6.25	119.31	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	255	CYS	N-CA-C	-6.25	104.55	111.36
12	L	490	ALA	N-CA-C	-6.25	104.39	111.07
5	E	182	ALA	CA-C-N	-6.24	112.74	119.98
5	E	182	ALA	C-N-CA	-6.24	112.74	119.98
15	O	113	SER	N-CA-C	6.23	118.56	108.41
8	H	269	THR	N-CA-C	6.22	118.06	111.28
16	P	118	LYS	N-CA-C	6.22	119.03	111.82
7	G	383	SER	N-CA-C	-6.21	106.92	114.75
8	H	52	ALA	N-CA-CB	6.21	119.02	110.01
14	N	89	GLN	N-CA-C	6.21	120.42	112.34
35	j	78	ASP	N-CA-C	-6.21	102.85	110.61
25	Z	69	ILE	N-CA-CB	6.21	117.40	110.51
7	G	451	ILE	N-CA-C	-6.20	104.94	113.00
32	g	123	LEU	N-CA-CB	6.20	119.06	110.07
8	H	76	THR	N-CA-C	-6.20	104.53	111.28
39	n	63	LEU	N-CA-C	-6.20	104.07	111.69
37	l	105	ILE	CA-C-O	-6.20	115.21	121.59
14	N	276	LEU	N-CA-C	-6.19	105.37	113.17
14	N	216	PHE	N-CA-C	6.19	118.10	111.36
1	A	101	GLY	N-CA-C	-6.17	105.34	112.50
6	F	409	ILE	N-CA-C	6.17	116.34	110.42
14	N	47	LYS	N-CA-C	-6.17	104.66	111.82
13	M	121	LEU	N-CA-C	-6.16	104.64	111.36
38	m	72	ARG	CA-C-O	6.16	125.92	119.14
2	B	98	ALA	N-CA-C	6.16	117.67	108.31
6	F	212	LEU	N-CA-C	-6.16	104.57	111.28
7	G	420	LYS	N-CA-C	6.16	118.78	111.33
36	k	59	TYR	N-CA-C	6.16	120.63	113.18
14	N	46	ASN	N-CA-C	-6.13	105.82	113.55
7	G	325	ARG	N-CA-CB	6.13	118.86	109.91
13	M	4	ILE	N-CA-C	-6.13	103.98	112.50
19	S	61	VAL	N-CA-C	-6.13	99.65	108.42
4	D	122	LYS	N-CA-C	-6.13	105.96	113.50
12	L	361	ASN	CB-CA-C	-6.12	102.86	111.80
7	G	418	ILE	N-CA-C	-6.12	103.47	112.04
24	Y	114	ALA	N-CA-C	-6.12	104.24	111.03
33	h	101	ILE	N-CA-CB	6.12	115.77	110.08
36	k	30	ILE	N-CA-C	6.11	118.73	111.09
31	f	39	ASN	N-CA-C	-6.11	103.99	112.30
6	F	304	ALA	CB-CA-C	-6.10	109.52	116.54
12	L	454	ILE	N-CA-C	-6.10	104.40	110.62
19	S	87	VAL	N-CA-C	-6.09	104.41	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	p	127	LYS	N-CA-C	-6.09	104.19	111.69
15	O	72	LYS	N-CA-CB	6.09	119.08	109.82
39	n	30	TRP	N-CA-C	-6.08	104.21	111.69
13	M	57	SER	N-CA-C	6.08	119.11	109.50
8	H	276	SER	N-CA-C	6.08	118.87	111.82
6	F	268	GLU	CB-CA-C	-6.08	109.55	116.54
13	M	396	MET	N-CA-C	-6.08	105.85	113.20
12	L	287	PHE	N-CA-CB	6.07	118.82	110.01
4	D	258	VAL	N-CA-C	-6.07	103.31	111.44
15	O	160	GLU	CB-CA-C	-6.07	109.56	116.54
14	N	91	ASN	N-CA-C	-6.06	101.31	110.28
8	H	185	TRP	N-CA-C	-6.06	104.03	112.45
7	G	353	ALA	N-CA-C	-6.06	104.60	112.23
13	M	168	GLN	N-CA-C	-6.05	104.76	111.36
25	Z	65	LEU	N-CA-CB	6.05	119.12	110.16
28	c	47	SER	N-CA-C	-6.05	104.63	112.68
10	J	55	VAL	N-CA-C	-6.05	104.61	110.42
32	g	109	ASP	CA-CB-CG	6.05	118.65	112.60
7	G	508	ALA	N-CA-C	6.04	117.87	111.28
51	AG	31	PHE	N-CA-C	-6.04	105.95	113.38
33	h	142	ILE	N-CA-C	-6.04	104.62	110.42
32	g	123	LEU	N-CA-C	-6.03	104.62	111.14
13	M	3	LYS	N-CA-C	-6.03	106.05	113.41
12	L	44	PHE	N-CA-C	-6.03	104.79	111.36
8	H	103	LEU	N-CA-C	-6.02	104.80	111.36
13	M	370	PRO	CA-N-CD	6.02	120.42	112.00
45	AA	401	SER	N-CA-C	-6.02	104.64	111.14
20	T	141	PRO	N-CA-CB	-6.01	96.89	103.39
35	j	39	HIS	N-CA-C	-6.01	106.07	113.41
4	D	444	LEU	N-CA-C	-6.01	104.72	111.28
12	L	248	HIS	CB-CA-C	6.01	121.07	110.85
13	M	213	HIS	N-CA-C	6.01	120.47	113.20
12	L	140	LEU	N-CA-C	-6.00	104.74	111.28
15	O	181	LYS	N-CA-C	6.00	117.49	111.07
4	D	414	ASP	N-CA-C	-5.99	101.07	110.36
12	L	98	TRP	N-CA-C	-5.97	104.77	111.28
51	Ag	31	PHE	N-CA-C	-5.97	106.03	113.38
15	O	183	CYS	N-CA-CB	5.97	118.84	109.94
42	q	104	THR	N-CA-C	5.97	118.45	108.96
7	G	532	PRO	N-CA-CB	-5.96	97.12	103.38
13	M	300	SER	N-CA-C	-5.96	106.99	114.56
7	G	387	LEU	CB-CA-C	-5.95	101.69	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	88	LEU	N-CA-CB	5.95	118.69	110.07
14	N	295	ARG	N-CA-C	-5.95	104.80	111.28
46	AB	244	LEU	N-CA-C	-5.95	106.02	113.28
54	AK	16	ASN	N-CA-C	-5.95	104.92	111.82
27	b	60	ASP	N-CA-C	-5.95	105.29	112.54
54	AK	38	TRP	N-CA-C	-5.95	101.38	110.30
15	O	205	ILE	O-C-N	5.94	129.11	122.75
12	L	112	PRO	CB-CA-C	-5.94	103.01	111.68
23	X	38	LYS	N-CA-C	-5.94	104.72	111.07
32	g	78	PRO	N-CA-C	5.94	121.78	113.53
12	L	247	LEU	N-CA-CB	5.93	120.67	110.34
7	G	480	ALA	N-CA-C	-5.92	104.90	111.36
13	M	88	ASN	N-CA-C	5.92	120.12	113.02
14	N	15	LEU	N-CA-C	-5.92	105.56	112.89
13	M	253	LEU	N-CA-C	5.91	117.73	111.28
23	X	141	PRO	N-CA-C	-5.91	102.55	111.41
22	W	98	LYS	N-CA-CB	5.91	119.60	110.21
12	L	234	PRO	N-CA-CB	5.90	109.55	103.23
40	o	120	ALA	O-C-N	-5.90	115.00	122.26
14	N	16	GLY	CA-C-N	-5.89	112.42	118.85
14	N	16	GLY	C-N-CA	-5.89	112.42	118.85
12	L	387	THR	CB-CA-C	-5.89	99.74	110.63
13	M	222	GLU	N-CA-C	5.88	120.30	113.18
34	i	10	LEU	N-CA-C	-5.88	107.09	114.56
40	o	11	TRP	CB-CA-C	-5.88	109.81	116.63
15	O	67	CYS	N-CA-CB	-5.88	100.06	111.11
39	n	27	LEU	N-CA-C	-5.88	106.08	113.72
54	Ak	16	ASN	N-CA-C	-5.87	105.01	111.82
9	I	116	CYS	N-CA-C	-5.87	105.62	112.89
36	k	80	GLY	N-CA-C	-5.87	105.70	112.50
12	L	428	TYR	N-CA-C	-5.86	104.81	111.14
6	F	127	ASP	N-CA-C	5.86	118.45	111.71
13	M	272	THR	N-CA-C	-5.86	104.97	111.36
12	L	278	LEU	N-CA-CB	5.85	118.55	110.07
43	r	11	LEU	N-CA-C	-5.85	104.82	111.14
8	H	116	ILE	N-CA-C	-5.85	104.81	110.42
39	n	116	PRO	CB-CA-C	-5.84	103.79	112.55
15	O	130	ARG	N-CA-C	-5.83	104.92	111.28
31	f	36	ALA	N-CA-C	-5.82	103.25	110.41
3	C	209	LEU	N-CA-CB	-5.82	100.70	110.83
8	H	315	PRO	O-C-N	5.82	123.89	121.15
2	B	98	ALA	CB-CA-C	-5.82	109.85	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	122	HIS	N-CA-C	5.82	120.08	112.92
19	S	86	GLU	N-CA-CB	5.81	118.75	110.16
7	G	672	ALA	N-CA-C	-5.80	104.95	111.28
13	M	424	ILE	O-C-N	5.80	128.42	122.79
21	V	19	THR	N-CA-CB	5.79	120.68	110.37
16	P	97	MET	N-CA-C	-5.78	102.35	110.50
42	q	100	THR	N-CA-C	5.78	117.26	111.07
20	U	137	LYS	CA-C-N	-5.78	113.50	122.05
20	U	137	LYS	C-N-CA	-5.78	113.50	122.05
4	D	212	GLU	N-CA-CB	5.77	118.72	110.06
32	g	67	LYS	N-CA-C	-5.77	101.92	110.46
7	G	289	LYS	N-CA-C	5.77	117.57	111.28
29	d	53	VAL	N-CA-C	5.77	116.42	110.36
43	r	72	SER	N-CA-C	-5.77	106.08	113.23
14	N	321	LYS	N-CA-C	5.76	118.50	110.20
37	l	186	ILE	N-CA-CB	-5.76	101.71	111.50
20	U	101	ASN	N-CA-C	-5.76	106.11	113.02
48	AD	163	GLU	N-CA-C	5.75	118.16	109.41
35	j	73	PHE	N-CA-C	-5.75	104.92	111.07
42	q	121	PRO	N-CA-CB	-5.75	98.06	103.52
23	X	36	CYS	CB-CA-C	-5.74	102.61	111.74
12	L	177	ILE	N-CA-C	-5.74	104.77	110.62
13	M	124	ALA	N-CA-C	-5.74	105.11	111.36
13	M	279	GLN	N-CA-C	-5.74	98.53	108.69
7	G	275	PRO	N-CA-CB	-5.73	98.00	103.33
12	L	419	THR	N-CA-C	-5.73	105.03	111.28
39	n	52	LYS	N-CA-C	-5.73	105.95	113.12
8	H	126	LYS	N-CA-C	5.73	117.53	111.28
14	N	66	ALA	N-CA-C	-5.73	105.11	111.36
16	P	272	LEU	N-CA-C	-5.73	101.80	110.28
12	L	467	VAL	N-CA-CB	-5.73	103.85	110.55
16	P	234	LYS	CB-CA-C	-5.72	103.44	111.80
38	m	104	VAL	N-CA-C	-5.72	105.52	111.58
4	D	337	MET	N-CA-C	-5.72	105.05	111.28
29	d	62	LEU	N-CA-C	5.72	117.52	111.28
34	i	84	TYR	N-CA-C	-5.71	105.05	111.28
11	K	6	PHE	N-CA-C	-5.71	106.44	113.41
6	F	393	ASN	N-CA-C	-5.71	104.96	111.07
8	H	252	PRO	N-CA-CB	-5.70	98.04	103.51
32	g	78	PRO	N-CA-CB	-5.70	97.06	103.33
10	J	74	ALA	N-CA-C	5.68	121.24	113.97
47	AC	17	SER	N-CA-CB	-5.68	102.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	e	34	HIS	N-CA-C	-5.68	106.19	113.01
6	F	176	ALA	N-CA-C	5.68	118.20	111.33
19	S	73	GLN	N-CA-C	-5.68	100.45	109.59
14	N	232	LEU	N-CA-C	-5.68	106.57	112.93
12	L	214	MET	N-CA-C	-5.67	105.17	111.36
12	L	342	CYS	N-CA-CB	5.67	118.24	110.01
10	J	123	TRP	O-C-N	-5.67	116.05	122.23
12	L	523	SER	CA-C-N	-5.67	111.04	120.68
12	L	523	SER	C-N-CA	-5.67	111.04	120.68
38	m	116	ILE	N-CA-C	-5.67	104.98	110.42
16	P	119	ALA	N-CA-C	-5.67	105.02	111.14
40	o	71	ARG	N-CA-C	-5.67	104.49	111.40
12	L	605	ASN	N-CA-C	-5.67	106.22	113.02
10	J	21	LEU	N-CA-C	-5.66	106.46	113.19
18	R	44	ARG	N-CA-C	-5.66	106.08	112.87
12	L	155	ILE	N-CA-C	-5.66	105.21	110.53
47	Ac	252	ASP	CA-C-N	-5.65	112.91	119.47
47	Ac	252	ASP	C-N-CA	-5.65	112.91	119.47
34	i	14	GLN	N-CA-CB	-5.65	101.81	110.12
10	J	121	GLY	N-CA-C	-5.65	107.87	115.21
37	l	49	ALA	N-CA-C	-5.64	106.56	113.50
4	D	186	ALA	N-CA-C	5.64	117.10	111.07
6	F	416	SER	N-CA-C	5.63	117.87	111.11
12	L	151	SER	N-CA-CB	5.63	118.50	110.16
4	D	192	LEU	N-CA-C	-5.62	105.16	111.28
42	q	140	PRO	N-CA-C	-5.62	102.32	110.80
13	M	19	SER	N-CA-C	5.61	117.64	109.84
13	M	214	LEU	N-CA-C	-5.61	105.70	112.54
4	D	455	ASP	CB-CA-C	-5.61	103.93	111.89
12	L	371	SER	N-CA-C	-5.61	105.07	111.07
6	F	457	HIS	N-CA-CB	-5.61	100.97	110.50
7	G	599	THR	CA-C-N	-5.61	114.20	122.83
7	G	599	THR	C-N-CA	-5.61	114.20	122.83
10	J	27	TYR	N-CA-C	-5.61	105.25	111.36
29	d	5	ARG	CA-C-N	-5.59	114.20	119.90
29	d	5	ARG	C-N-CA	-5.59	114.20	119.90
32	g	140	PHE	N-CA-CB	5.59	118.32	109.71
38	m	60	ILE	N-CA-C	-5.59	101.98	109.30
41	p	115	GLN	N-CA-CB	5.59	118.02	110.59
9	I	191	LEU	N-CA-C	-5.58	105.28	111.36
12	L	20	LEU	N-CA-C	5.58	119.81	112.89
23	X	40	ASN	N-CA-C	-5.58	104.89	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	o	22	ILE	CB-CA-C	-5.58	108.43	114.35
12	L	445	GLU	CB-CA-C	-5.58	101.98	111.02
7	G	530	TYR	N-CA-C	-5.58	102.03	110.28
32	g	122	ARG	N-CA-C	5.57	118.28	111.82
14	N	36	SER	N-CA-C	-5.57	105.21	111.28
17	Q	124	MET	CA-C-N	-5.57	115.08	122.98
17	Q	124	MET	C-N-CA	-5.57	115.08	122.98
32	g	107	VAL	N-CA-C	-5.57	102.89	108.96
47	Ac	265	PRO	N-CA-CB	5.56	108.47	103.08
19	S	63	PRO	CA-N-CD	5.56	119.78	112.00
10	J	92	LEU	N-CA-C	-5.56	105.12	111.07
32	g	113	GLN	CA-C-O	5.56	126.22	119.11
5	E	223	CYS	CB-CA-C	-5.56	110.15	116.54
26	a	25	TYR	N-CA-C	-5.55	107.75	114.75
11	K	3	SER	N-CA-C	-5.55	106.41	114.12
7	G	127	ASP	CA-C-O	5.55	129.05	121.89
41	p	120	ASN	N-CA-C	-5.54	105.13	113.89
24	Y	13	GLU	N-CA-C	5.54	117.76	111.11
14	N	251	LEU	N-CA-C	-5.53	105.25	111.28
12	L	370	SER	N-CA-C	-5.52	105.34	111.36
12	L	234	PRO	N-CA-C	-5.52	105.57	113.47
39	n	136	GLU	CB-CA-C	5.52	121.41	110.42
49	AI	59	ALA	N-CA-CB	-5.51	101.40	109.95
7	G	615	LEU	N-CA-C	-5.51	106.33	113.16
15	O	269	VAL	N-CA-C	5.51	116.24	110.62
4	D	350	LYS	CB-CA-C	-5.50	103.77	111.85
13	M	73	LEU	N-CA-C	-5.50	105.27	112.75
35	j	64	LEU	N-CA-C	-5.50	105.44	111.82
48	AD	88	GLU	N-CA-C	5.50	117.75	109.23
48	Ad	177	LYS	CA-C-N	-5.50	114.59	120.47
48	Ad	177	LYS	C-N-CA	-5.50	114.59	120.47
45	AA	255	ARG	N-CA-C	5.49	118.23	107.57
12	L	465	GLY	N-CA-C	-5.49	105.74	112.77
12	L	394	LEU	N-CA-CB	5.48	117.96	110.01
28	c	64	GLU	N-CA-CB	5.48	117.96	110.01
13	M	370	PRO	N-CA-CB	-5.47	97.78	103.08
12	L	152	PHE	N-CA-C	-5.46	105.22	111.07
7	G	313	LEU	N-CA-C	5.46	118.46	109.72
40	o	74	PHE	CA-C-N	-5.46	113.99	119.56
40	o	74	PHE	C-N-CA	-5.46	113.99	119.56
13	M	234	ILE	N-CA-C	5.46	116.32	111.90
36	k	20	MET	CA-C-N	-5.46	111.18	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	k	20	MET	C-N-CA	-5.46	111.18	121.66
7	G	363	SER	N-CA-C	-5.45	100.29	109.07
7	G	404	GLY	N-CA-C	5.45	121.44	113.48
39	n	178	PRO	N-CA-C	-5.45	106.95	113.98
42	q	126	PRO	N-CA-CB	-5.45	98.46	103.31
23	X	113	ASP	N-CA-C	-5.45	106.57	113.43
2	B	155	PRO	N-CA-C	-5.44	102.13	110.95
7	G	682	ASP	CA-C-N	-5.44	114.16	119.76
7	G	682	ASP	C-N-CA	-5.44	114.16	119.76
10	J	139	ILE	N-CA-C	-5.44	104.42	110.62
14	N	108	LEU	N-CA-C	5.44	118.11	109.24
25	Z	55	GLN	N-CA-C	-5.44	105.35	111.28
4	D	200	PHE	CA-CB-CG	5.44	119.24	113.80
14	N	62	THR	N-CA-C	-5.44	105.25	111.07
13	M	355	MET	N-CA-C	-5.43	104.75	111.33
12	L	194	ASN	CB-CA-C	-5.43	103.41	111.72
7	G	420	LYS	N-CA-CB	-5.43	101.92	110.06
34	i	69	LEU	N-CA-C	-5.43	106.43	113.16
46	AB	236	GLN	N-CA-C	-5.43	105.92	112.54
15	O	154	GLY	N-CA-C	-5.43	107.53	114.37
2	B	104	MET	N-CA-C	-5.42	107.21	113.88
32	g	137	SER	N-CA-CB	-5.42	101.30	110.41
4	D	255	ILE	N-CA-C	-5.41	105.25	110.72
7	G	510	TRP	N-CA-C	-5.41	101.84	109.96
13	M	223	ALA	N-CA-CB	5.41	118.01	110.11
2	B	146	ARG	N-CA-C	-5.40	105.39	111.28
54	Ak	18	ILE	N-CA-C	5.40	120.55	108.88
14	N	89	GLN	N-CA-CB	-5.40	100.46	110.18
35	j	80	VAL	CB-CA-C	-5.40	106.31	111.44
42	q	121	PRO	CA-N-CD	5.39	119.55	112.00
20	U	143	GLU	N-CA-C	-5.38	104.81	111.33
13	M	409	TYR	N-CA-C	-5.38	105.58	111.82
33	h	173	THR	O-C-N	5.38	125.75	121.55
5	E	219	SER	N-CA-C	-5.38	100.56	108.79
13	M	174	LEU	N-CA-C	-5.38	106.49	112.57
2	B	105	MET	N-CA-CB	5.38	118.50	110.22
41	p	94	ARG	N-CA-C	5.38	116.83	111.07
4	D	131	GLN	CB-CA-C	5.38	120.32	110.11
20	U	73	PRO	N-CA-C	5.38	119.93	111.38
12	L	21	ILE	N-CA-C	-5.37	105.29	110.72
12	L	494	SER	N-CA-C	-5.37	105.34	111.14
25	Z	50	MET	N-CA-C	-5.37	105.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	AE	89	SER	N-CA-C	5.37	118.62	111.75
54	AK	18	ILE	N-CA-C	5.37	120.48	108.88
13	M	117	MET	N-CA-CB	5.37	118.01	110.12
46	Ab	236	GLN	N-CA-C	-5.36	106.00	112.54
34	i	125	ASP	O-C-N	5.36	129.19	122.65
12	L	550	LEU	CA-C-O	-5.36	115.27	120.89
39	n	116	PRO	N-CA-C	5.36	120.58	113.40
5	E	48	PRO	N-CA-C	5.35	120.79	113.84
42	q	30	ALA	N-CA-CB	5.35	118.50	110.53
6	F	199	ARG	N-CA-C	5.34	117.45	109.59
38	m	17	THR	N-CA-C	-5.34	103.09	110.35
5	E	143	ASP	N-CA-C	5.33	118.47	111.28
13	M	169	ASN	N-CA-C	-5.33	105.55	111.36
12	L	183	ILE	N-CA-C	-5.32	105.19	110.62
48	Ad	227	LEU	N-CA-CB	-5.32	102.12	110.69
39	n	104	LEU	N-CA-C	-5.32	106.82	113.15
49	Ae	89	SER	N-CA-C	5.32	118.56	111.75
12	L	543	ASN	N-CA-C	-5.32	105.48	111.28
12	L	386	LEU	N-CA-C	-5.32	101.04	108.96
13	M	343	ILE	N-CA-C	5.32	116.04	110.62
8	H	98	LEU	N-CA-C	-5.31	100.74	109.40
13	M	25	THR	CB-CA-C	-5.31	100.47	110.67
20	U	141	PRO	N-CA-C	-5.31	109.16	114.68
14	N	218	ALA	N-CA-CB	5.31	118.43	110.14
8	H	252	PRO	CA-N-CD	5.31	119.43	112.00
12	L	311	GLY	N-CA-C	-5.30	106.36	112.73
48	AD	227	LEU	N-CA-CB	-5.30	102.15	110.69
36	k	48	ARG	N-CA-C	-5.30	98.93	108.48
13	M	294	MET	N-CA-C	-5.30	106.83	113.72
25	Z	64	ASP	N-CA-C	5.30	119.80	113.23
6	F	84	GLY	N-CA-C	-5.30	107.93	115.30
17	Q	72	ILE	N-CA-C	-5.30	108.34	113.53
42	q	102	PRO	N-CA-C	-5.30	104.24	110.70
13	M	167	ILE	N-CA-C	5.29	117.66	111.05
32	g	80	VAL	N-CA-C	-5.29	105.34	110.42
33	h	129	PRO	N-CA-C	-5.29	106.64	113.57
8	H	146	MET	N-CA-C	-5.29	105.41	111.07
7	G	449	PRO	N-CA-CB	5.29	109.10	103.39
8	H	284	GLN	N-CA-C	-5.29	105.60	111.36
39	n	36	LYS	N-CA-C	-5.29	105.52	111.28
12	L	415	ALA	N-CA-CB	5.28	117.89	110.12
8	H	214	GLU	N-CA-C	5.28	119.43	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Ad	160	ASP	N-CA-C	-5.28	105.53	111.28
16	P	260	GLY	N-CA-C	-5.28	108.34	115.36
42	q	67	GLU	N-CA-CB	-5.28	102.17	110.77
13	M	53	SER	N-CA-C	5.27	115.50	108.38
12	L	190	SER	N-CA-C	-5.27	106.69	113.23
7	G	356	ASP	N-CA-C	-5.27	105.54	111.28
7	G	111	LYS	N-CA-C	-5.27	105.59	112.23
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
12	L	386	LEU	CA-C-O	-5.26	115.82	121.45
12	L	231	PRO	CB-CA-C	-5.26	104.38	111.85
13	M	212	VAL	CB-CA-C	-5.26	105.15	112.36
15	O	54	HIS	N-CA-C	5.26	115.48	108.38
12	L	137	MET	N-CA-C	5.26	119.32	113.01
6	F	55	GLY	N-CA-C	-5.25	106.42	112.83
5	E	48	PRO	CB-CA-C	-5.25	104.39	111.85
7	G	362	ASP	CA-CB-CG	5.24	117.84	112.60
12	L	413	LEU	N-CA-C	5.24	117.00	111.28
6	F	412	LEU	N-CA-C	-5.24	105.74	111.82
16	P	339	GLY	N-CA-C	5.24	122.55	115.00
25	Z	118	PRO	CA-C-N	-5.24	113.91	120.51
25	Z	118	PRO	C-N-CA	-5.24	113.91	120.51
4	D	369	ALA	N-CA-C	5.24	116.99	111.28
8	H	46	LEU	N-CA-C	-5.24	106.67	113.16
13	M	20	PRO	N-CA-C	-5.23	106.26	113.53
20	U	94	ASP	CA-C-N	-5.23	115.50	120.83
20	U	94	ASP	C-N-CA	-5.23	115.50	120.83
12	L	217	LEU	N-CA-C	-5.22	105.58	111.28
12	L	485	PHE	N-CA-CB	5.22	117.58	110.01
20	U	133	ILE	N-CA-C	5.22	117.58	111.05
6	F	318	ILE	CA-C-N	5.22	124.85	119.05
6	F	318	ILE	C-N-CA	5.22	124.85	119.05
32	g	68	ASN	N-CA-CB	5.22	118.98	111.51
7	G	458	GLY	N-CA-C	-5.22	108.12	115.32
21	V	84	ALA	N-CA-C	5.22	116.66	111.07
20	U	133	ILE	CB-CA-C	-5.21	104.08	112.16
7	G	277	MET	N-CA-CB	-5.21	101.68	109.71
47	Ac	264	THR	N-CA-C	5.21	116.96	109.04
2	B	167	GLY	N-CA-C	-5.21	106.11	112.68
4	D	312	ASP	N-CA-C	-5.21	107.09	113.50
8	H	310	PHE	N-CA-C	5.21	119.26	113.01
15	O	206	TYR	CA-C-N	-5.21	114.95	122.45
15	O	206	TYR	C-N-CA	-5.21	114.95	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	76	ASP	CB-CA-C	-5.21	104.64	112.09
13	M	98	MET	N-CA-C	-5.20	105.51	111.07
14	N	335	MET	CB-CA-C	-5.20	104.41	111.95
39	n	26	HIS	N-CA-C	-5.20	106.53	112.92
7	G	600	GLU	CB-CA-C	-5.20	103.01	111.06
16	P	194	VAL	N-CA-CB	5.20	118.37	110.58
39	n	12	HIS	N-CA-C	-5.20	105.06	111.40
54	AK	49	ASN	N-CA-C	-5.20	103.28	110.35
7	G	713	ALA	N-CA-C	-5.19	105.51	111.07
41	p	43	TRP	CA-C-N	-5.19	113.57	118.97
41	p	43	TRP	C-N-CA	-5.19	113.57	118.97
7	G	435	PRO	CB-CA-C	-5.19	105.91	111.56
12	L	332	HIS	N-CA-C	-5.19	105.63	111.28
13	M	330	ALA	N-CA-CB	5.19	117.59	110.07
7	G	556	THR	N-CA-C	-5.18	101.53	109.41
4	D	103	GLY	N-CA-C	-5.18	100.90	113.18
41	p	167	ARG	CB-CA-C	5.18	117.21	109.13
13	M	317	ILE	N-CA-CB	5.18	117.19	110.57
14	N	222	ASN	N-CA-C	-5.18	106.20	112.88
12	L	375	ILE	N-CA-CB	5.17	116.60	110.55
36	k	44	ALA	N-CA-C	-5.17	105.64	111.28
43	r	18	GLN	N-CA-C	5.17	117.25	109.23
19	S	85	ASP	N-CA-C	5.17	117.82	111.82
43	r	36	GLN	N-CA-C	-5.17	102.51	110.01
3	C	79	CYS	N-CA-C	-5.17	107.04	113.19
33	h	158	ARG	N-CA-C	-5.17	105.56	111.14
14	N	90	THR	N-CA-C	5.17	117.58	110.35
6	F	337	MET	CB-CA-C	-5.17	103.00	111.68
23	X	33	GLY	N-CA-C	-5.16	107.92	114.16
7	G	63	PHE	CA-C-O	-5.16	115.08	121.06
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
12	L	284	THR	N-CA-C	-5.16	105.74	111.36
34	i	66	ARG	CB-CA-C	-5.15	110.23	117.23
40	o	121	ARG	CA-C-N	-5.15	116.10	123.10
40	o	121	ARG	C-N-CA	-5.15	116.10	123.10
6	F	60	GLY	N-CA-C	-5.14	105.94	114.48
24	Y	72	PHE	N-CA-C	-5.14	105.57	111.07
27	b	82	LYS	N-CA-C	-5.14	103.74	110.53
3	C	164	TRP	N-CA-C	5.14	116.96	111.36
3	C	156	VAL	N-CA-C	-5.14	104.08	111.17
37	l	168	LEU	N-CA-C	-5.14	105.59	111.14
16	P	198	ALA	N-CA-C	-5.13	100.15	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	101	GLY	N-CA-C	5.13	118.45	112.50
14	N	225	MET	N-CA-C	-5.13	106.61	112.92
38	m	61	GLU	N-CA-C	5.13	119.62	112.90
8	H	277	TYR	N-CA-C	5.12	117.94	110.10
8	H	196	ALA	CA-C-N	-5.12	113.53	119.47
8	H	196	ALA	C-N-CA	-5.12	113.53	119.47
12	L	396	ILE	O-C-N	5.12	126.93	121.91
48	Ad	88	GLU	N-CA-C	5.12	117.77	109.06
1	A	2	ASN	CA-C-N	-5.12	113.02	120.29
1	A	2	ASN	C-N-CA	-5.12	113.02	120.29
28	c	39	PRO	N-CA-C	5.12	119.24	111.15
28	c	60	GLN	N-CA-C	-5.12	105.60	111.07
13	M	86	LYS	N-CA-C	-5.11	106.28	112.88
27	b	63	MET	N-CA-C	5.11	118.87	109.10
29	d	37	LEU	N-CA-C	-5.11	105.71	111.28
11	K	48	SER	N-CA-CB	5.11	117.62	110.12
7	G	569	GLN	CB-CA-C	-5.10	104.30	112.05
7	G	387	LEU	N-CA-C	-5.10	98.40	107.98
9	I	95	PRO	N-CA-C	5.09	121.20	113.81
4	D	71	ILE	N-CA-C	5.09	118.26	111.44
12	L	249	SER	N-CA-C	5.09	116.64	111.14
3	C	221	GLU	N-CA-C	-5.08	102.35	108.25
13	M	32	PHE	N-CA-CB	5.08	117.38	110.01
41	p	31	THR	N-CA-C	-5.08	105.63	111.07
1	A	73	LEU	CA-C-N	-5.08	114.48	120.12
1	A	73	LEU	C-N-CA	-5.08	114.48	120.12
14	N	42	PRO	CB-CA-C	-5.07	104.99	113.06
8	H	254	LEU	N-CA-CB	5.07	118.14	110.28
20	U	132	ASP	N-CA-C	5.06	117.20	111.02
6	F	366	ALA	N-CA-C	-5.06	105.45	110.97
7	G	280	ASP	N-CA-CB	-5.06	102.68	110.12
14	N	64	ALA	N-CA-C	5.06	116.49	111.07
34	i	114	GLY	N-CA-C	-5.06	108.33	115.32
14	N	292	PHE	CA-CB-CG	5.06	118.86	113.80
20	T	105	MET	N-CA-C	-5.06	105.77	111.28
3	C	109	SER	N-CA-C	5.05	118.05	109.76
9	I	61	LEU	N-CA-C	5.05	116.59	111.14
7	G	203	ASP	CA-C-O	5.05	127.17	121.32
34	i	16	ARG	N-CA-C	-5.05	105.78	111.28
8	H	67	SER	N-CA-C	-5.04	103.87	110.53
7	G	393	GLY	N-CA-C	-5.04	107.80	115.66
13	M	30	TYR	N-CA-C	5.04	116.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	137	SER	N-CA-C	5.04	119.27	113.18
13	M	267	TRP	N-CA-C	-5.03	105.87	111.36
14	N	282	MET	N-CA-C	-5.03	105.69	111.07
37	l	45	PRO	N-CA-C	5.03	120.44	113.65
22	W	112	GLU	N-CA-C	5.03	116.84	111.36
30	e	93	THR	CA-C-N	-5.03	115.20	120.38
30	e	93	THR	C-N-CA	-5.03	115.20	120.38
39	n	169	HIS	CB-CA-C	5.03	118.66	110.17
4	D	232	VAL	CA-C-O	-5.02	116.35	121.67
33	h	161	ARG	N-CA-C	-5.02	105.49	110.97
15	O	250	SER	N-CA-CB	5.02	117.50	110.12
20	U	81	ASP	N-CA-C	-5.02	106.33	112.90
9	I	90	LYS	N-CA-C	5.02	117.58	109.40
5	E	213	PRO	CB-CA-C	-5.01	106.32	112.89
6	F	249	ALA	N-CA-C	5.01	116.74	111.28
37	l	163	TYR	CB-CA-C	5.01	120.39	110.42
13	M	229	MET	N-CA-C	-5.01	105.71	111.07
4	D	224	ALA	CA-C-O	-5.01	115.54	120.90
42	q	89	TRP	N-CA-CB	5.01	117.33	110.07
13	M	56	PHE	N-CA-C	5.00	116.68	108.52
14	N	217	MET	N-CA-C	-5.00	107.01	113.01

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	132	0
2	B	1258	0	1269	148	0
3	C	1641	0	1596	159	0
4	D	3416	0	3357	342	0
5	E	1635	0	1624	146	0
6	F	3288	0	3243	383	0
7	G	5287	0	5323	561	0
8	H	2532	0	2621	412	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1431	0	1385	176	0
10	J	1287	0	1303	280	0
11	K	729	0	764	128	0
12	L	4798	0	4986	620	0
13	M	3630	0	3854	560	0
14	N	2694	0	2896	376	0
15	O	2599	0	2552	272	0
16	P	2720	0	2740	251	0
17	Q	957	0	949	75	0
18	R	660	0	639	64	0
19	S	667	0	683	70	0
20	T	604	0	596	65	0
20	U	700	0	691	72	0
21	V	915	0	954	97	0
22	W	970	0	991	86	0
23	X	1385	0	1370	149	0
24	Y	1037	0	1022	89	0
25	Z	1152	0	1148	157	0
26	a	548	0	562	46	0
27	b	620	0	617	96	0
28	c	389	0	385	27	0
29	d	996	0	1001	89	0
30	e	859	0	849	107	0
31	f	447	0	444	34	0
32	g	850	0	783	71	0
33	h	1162	0	1163	129	0
34	i	839	0	839	73	0
35	j	578	0	525	66	0
36	k	618	0	616	55	0
37	l	1312	0	1204	100	0
38	m	1044	0	1056	137	0
39	n	1541	0	1470	142	0
40	o	1050	0	1045	110	0
41	p	1452	0	1413	133	0
42	q	1192	0	1145	92	0
43	r	764	0	789	84	0
44	s	189	0	181	18	0
45	AA	3153	0	3077	144	0
45	Aa	3225	0	3141	173	0
46	AB	3137	0	3143	170	0
46	Ab	3094	0	3102	176	0
47	AC	2988	0	3045	214	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	Ac	2988	0	3045	188	0
48	AD	1912	0	1860	141	0
48	Ad	1912	0	1860	150	0
49	AE	1451	0	1433	160	0
49	AI	217	0	234	41	0
49	Ae	1451	0	1433	162	0
49	Ai	207	0	226	37	0
50	AF	864	0	854	54	0
50	Af	864	0	854	47	0
51	AG	643	0	643	50	0
51	Ag	643	0	643	66	0
52	AH	562	0	543	24	0
52	Ah	562	0	543	26	0
53	AJ	332	0	324	31	0
53	Aj	391	0	385	25	0
54	AK	401	0	396	46	0
54	Ak	401	0	396	46	0
55	A	46	0	69	10	0
55	AC	58	0	64	8	0
55	AG	51	0	82	16	0
55	Aa	23	0	20	7	0
55	Ac	35	0	44	4	0
55	Ag	51	0	82	5	0
55	H	46	0	69	16	0
55	J	46	0	66	6	0
55	L	87	0	125	8	0
55	M	88	0	130	11	0
55	Y	39	0	52	4	0
55	b	46	0	69	13	0
55	i	40	0	54	9	0
55	m	92	0	138	25	0
56	A	92	0	134	21	0
56	AG	98	0	84	16	0
56	Aa	46	0	36	4	0
56	Ag	98	0	84	9	0
56	L	74	0	92	11	0
56	M	79	0	105	12	0
56	Y	81	0	106	18	0
56	d	84	0	118	11	0
56	h	93	0	136	11	0
56	q	57	0	58	8	0
57	B	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	F	8	0	0	9	0
57	G	16	0	0	3	0
57	I	16	0	0	16	0
58	D	18	0	18	14	0
59	E	4	0	0	3	0
59	G	4	0	0	6	0
60	F	31	0	19	2	0
61	H	35	0	43	10	0
62	Ae	35	0	44	6	0
62	I	47	0	71	9	0
62	L	48	0	70	12	0
62	l	50	0	74	5	0
62	q	35	0	44	6	0
63	O	27	0	12	8	0
64	P	48	0	26	2	0
65	R	1	0	0	0	0
66	W	32	0	0	0	0
66	n	32	0	0	0	0
67	AC	86	0	60	15	0
67	Ac	86	0	60	12	0
68	AC	23	0	23	19	0
68	Ac	23	0	23	21	0
69	AC	28	0	31	27	0
69	Ac	28	0	31	12	0
70	AD	43	0	31	12	0
70	Ad	43	0	31	11	0
All	All	98999	0	99365	7839	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 40.

All (7839) 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)
48:AD:124:CYS:SG	70:AD:401:HEC:HAC	1.40	1.60
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.44
12:L:485:PHE:CE1	12:L:486:LEU:CD1	2.13	1.31
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
46:AB:297:PRO:CG	46:AB:304:ASN:HD21	1.43	1.29
46:Ab:297:PRO:CG	46:Ab:304:ASN:HD21	1.43	1.28
47:AC:21:LEU:HD22	69:AC:406:UQ6:C3M	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:140:LEU:CD1	39:n:165:PRO:HB3	1.68	1.23
12:L:358:LYS:HG3	39:n:80:TYR:CZ	1.73	1.22
48:AD:124:CYS:SG	70:AD:401:HEC:CAC	2.28	1.21
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.21
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.28	1.20
46:AB:297:PRO:HG3	46:AB:304:ASN:ND2	1.57	1.20
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.20
20:U:90:TYR:CE2	20:U:92:LYS:HB2	1.76	1.20
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
4:D:189:THR:HB	58:D:501:UQ1:CM2	1.73	1.18
1:A:104:TYR:HE2	10:J:167:ILE:CD1	1.54	1.17
11:K:22:PHE:HB2	12:L:585:LYS:HG2	1.18	1.17
46:Ab:297:PRO:HG3	46:Ab:304:ASN:ND2	1.57	1.17
10:J:150:TRP:NE1	14:N:28:LEU:HD21	1.58	1.16
12:L:485:PHE:CD1	12:L:486:LEU:HD12	1.80	1.16
13:M:369:LEU:HD23	13:M:371:PRO:HD2	1.18	1.16
39:n:140:LEU:HD11	39:n:165:PRO:CB	1.75	1.15
4:D:47:PHE:HB3	14:N:227:ILE:HD11	1.22	1.15
8:H:317:TYR:CE2	10:J:136:GLU:OE2	1.99	1.14
54:AK:4:ARG:HA	50:Af:110:LYS:HE2	1.24	1.14
6:F:379:CYS:SG	57:F:502:SF4:FE4	1.38	1.14
12:L:141:PHE:CE2	13:M:375:LEU:HD11	1.82	1.14
12:L:247:LEU:CD1	12:L:248:HIS:CD2	2.31	1.14
49:AE:263:TYR:HA	49:AE:273:VAL:HA	1.14	1.13
12:L:261:VAL:O	12:L:264:HIS:CD2	2.02	1.12
4:D:189:THR:HB	58:D:501:UQ1:HM23	1.16	1.12
14:N:215:MET:CE	14:N:248:LEU:HD21	1.79	1.12
24:Y:19:GLN:HG2	51:Ag:65:GLN:OE1	1.46	1.12
20:T:104:PHE:HZ	20:T:115:GLN:HG2	1.08	1.11
24:Y:108:HIS:HE1	55:Ag:103:3PE:H392	1.13	1.11
25:Z:144:THR:CG2	26:a:48:MET:SD	2.38	1.11
25:Z:144:THR:HG21	26:a:48:MET:SD	1.90	1.11
20:U:90:TYR:OH	20:U:92:LYS:HD2	1.48	1.11
29:d:14:LEU:O	29:d:14:LEU:HD12	1.49	1.11
42:q:59:HIS:ND1	42:q:60:ARG:HG3	1.64	1.11
46:Ab:167:GLN:HE21	49:Ai:43:LEU:CB	1.63	1.11
12:L:229:LEU:HD12	12:L:229:LEU:O	1.51	1.11
12:L:365:ILE:HD12	12:L:366:MET:HG3	1.32	1.11
12:L:553:LEU:HD11	38:m:93:ALA:HB3	1.33	1.10
46:Ab:167:GLN:HG2	49:Ai:43:LEU:HD13	1.32	1.10
18:R:80:ASP:OD2	18:R:84:GLY:HA2	1.49	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:8:ARG:HB2	40:o:16:GLU:HG2	1.32	1.10
10:J:80:GLU:HA	16:P:360:ARG:HD2	1.33	1.10
7:G:611:THR:HG21	17:Q:105:GLU:HA	1.32	1.10
47:AC:264:THR:CG2	49:Ae:225:ILE:HD11	1.80	1.10
3:C:98:PHE:HA	21:V:90:LEU:HD11	1.22	1.09
9:I:123:CYS:SG	57:I:302:SF4:FE1	1.42	1.09
47:AC:21:LEU:HD22	69:AC:406:UQ6:H3M1	1.10	1.09
50:AF:110:LYS:HE2	54:Ak:4:ARG:HA	1.27	1.09
12:L:121:LEU:HD22	12:L:246:LEU:HD21	1.33	1.09
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.35	1.09
8:H:65:THR:HG21	16:P:359:TYR:HD1	1.15	1.09
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
49:AE:204:ARG:HB3	49:AE:260:VAL:HG21	1.35	1.08
48:Ad:124:CYS:SG	70:Ad:401:HEC:HAC	1.93	1.08
3:C:203:LEU:HD11	4:D:123:LEU:HD23	1.30	1.08
46:Ab:167:GLN:HE21	49:Ai:43:LEU:HB3	1.11	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.34	1.08
9:I:152:CYS:SG	57:I:302:SF4:FE2	1.43	1.08
46:Ab:297:PRO:CB	46:Ab:304:ASN:HD21	1.66	1.08
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.08
8:H:65:THR:CG2	16:P:359:TYR:HD1	1.66	1.08
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
36:k:34:PRO:HG2	36:k:59:TYR:CE1	1.88	1.08
47:AC:146:ILE:HG13	68:AC:405:U10:C4M	1.83	1.08
46:AB:297:PRO:CB	46:AB:304:ASN:HD21	1.66	1.08
46:Ab:297:PRO:HG3	46:Ab:304:ASN:HD21	1.07	1.07
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.64	1.07
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.07
16:P:299:SER:HB3	16:P:316:LYS:HE3	1.37	1.07
12:L:511:LEU:HD21	36:k:38:VAL:HG22	1.29	1.06
12:L:550:LEU:HD12	13:M:275:ILE:HB	1.34	1.06
12:L:16:LEU:HD23	12:L:126:ILE:HD13	1.30	1.06
2:B:82:ILE:HG23	8:H:57:MET:SD	1.95	1.06
3:C:241:PHE:CD2	43:r:61:ARG:HB2	1.91	1.06
10:J:154:VAL:CG2	14:N:35:PHE:HZ	1.69	1.06
22:W:101:LYS:HG3	22:W:105:HIS:HB2	1.34	1.05
46:Ab:167:GLN:CG	49:Ai:43:LEU:HD13	1.85	1.05
51:Ag:11:ILE:HG21	51:Ag:14:VAL:HG21	1.36	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
48:AD:215:LEU:HD11	70:AD:401:HEC:HMB1	1.35	1.05
47:AC:21:LEU:HD13	69:AC:406:UQ6:O2	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:HD11	8:H:233:LEU:CD1	1.87	1.05
23:X:19:LYS:HG2	30:e:104:PRO:HG3	1.36	1.05
30:e:20:PHE:CZ	33:h:178:PHE:HB2	1.92	1.05
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.22	1.05
7:G:353:ALA:HA	7:G:636:TYR:OH	1.54	1.05
10:J:165:ILE:HG23	14:N:42:PRO:HG3	1.38	1.05
12:L:141:PHE:HE2	13:M:375:LEU:HD11	1.05	1.05
12:L:485:PHE:CE1	12:L:486:LEU:HD11	1.92	1.05
19:S:79:LEU:HA	19:S:82:LEU:HD12	1.37	1.05
13:M:142:ARG:HH21	14:N:303:THR:HG22	1.14	1.04
47:AC:21:LEU:CD2	69:AC:406:UQ6:H3M1	1.87	1.04
47:Ac:146:ILE:HG13	68:Ac:404:U10:C4M	1.86	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.04
14:N:233:LEU:HD23	14:N:241:LEU:HD12	1.36	1.04
48:Ad:215:LEU:HD11	70:Ad:401:HEC:CMB	1.87	1.04
4:D:238:LEU:HD13	9:I:211:TYR:OH	1.55	1.04
12:L:358:LYS:CG	39:n:80:TYR:CZ	2.40	1.04
37:l:91:GLN:HE21	39:n:2:ALA:HB1	1.15	1.04
47:AC:146:ILE:HG13	68:AC:405:U10:H4M2	1.38	1.04
48:AD:215:LEU:HD11	70:AD:401:HEC:CMB	1.87	1.04
51:AG:11:ILE:HG21	51:AG:14:VAL:HG21	1.36	1.04
2:B:89:SER:O	8:H:54:LYS:CD	2.06	1.04
48:Ad:215:LEU:HD11	70:Ad:401:HEC:HMB1	1.34	1.04
13:M:249:ILE:O	13:M:250:LEU:HG	1.58	1.03
41:p:40:VAL:O	41:p:44:PRO:HG2	1.59	1.03
49:Ae:204:ARG:HB3	49:Ae:260:VAL:HG21	1.35	1.03
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.03
46:AB:167:GLN:CG	49:AI:43:LEU:HD13	1.87	1.03
46:Ab:167:GLN:NE2	49:AI:43:LEU:HB3	1.73	1.03
5:E:247:GLY:HA2	6:F:64:LYS:HE2	1.36	1.02
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.39	1.02
12:L:131:LEU:HD12	12:L:140:LEU:HD12	1.36	1.02
20:T:104:PHE:CZ	20:T:115:GLN:HG2	1.94	1.02
40:o:69:CYS:O	40:o:80:CYS:SG	2.17	1.02
3:C:149:LEU:HD11	22:W:80:ARG:NH2	1.75	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.42	1.02
13:M:179:LEU:HB3	13:M:249:ILE:HD11	1.42	1.02
8:H:317:TYR:HH	10:J:136:GLU:CD	1.68	1.01
10:J:124:LEU:HB2	25:Z:137:ASN:HD21	1.25	1.01
16:P:272:LEU:HG	16:P:375:VAL:HG21	1.36	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:228:GLY:O	12:L:229:LEU:HG	1.61	1.01
12:L:222:GLY:HA2	12:L:229:LEU:HD11	1.40	1.01
23:X:48:TRP:CE2	27:b:55:VAL:HG22	1.94	1.01
45:AA:341:PHE:HD2	45:AA:368:MET:CE	1.74	1.01
5:E:247:GLY:CA	6:F:64:LYS:HE2	1.89	1.01
21:V:72:LEU:HD11	21:V:80:VAL:HG21	1.40	1.01
3:C:241:PHE:HD2	43:r:61:ARG:HB2	1.24	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
10:J:166:ILE:HD11	11:K:76:ALA:HB2	1.42	1.00
13:M:172:GLY:O	13:M:173:THR:HG23	1.61	1.00
46:AB:297:PRO:HG3	46:AB:304:ASN:HD21	1.07	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
40:o:117:LEU:CD2	40:o:118:LYS:HG3	1.92	1.00
25:Z:86:ILE:HG23	25:Z:128:ARG:HE	1.24	1.00
33:h:163:ARG:HG2	33:h:165:ASP:HB2	1.44	1.00
45:Aa:341:PHE:HD2	45:Aa:368:MET:CE	1.74	0.99
13:M:127:ILE:CD1	14:N:256:PRO:HG3	1.92	0.99
37:l:38:PRO:HB2	38:m:75:ASN:HD22	1.23	0.99
13:M:196:TRP:CD1	13:M:250:LEU:HD13	1.96	0.99
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
14:N:232:LEU:HD23	14:N:307:THR:HG23	1.39	0.99
4:D:259:GLU:HG3	25:Z:25:LEU:HD11	1.43	0.99
7:G:401:LEU:HD11	7:G:462:PHE:CE2	1.98	0.99
32:g:147:LEU:HD11	41:p:163:MET:HB3	1.44	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
13:M:173:THR:CG2	33:h:147:ALA:HB2	1.92	0.99
10:J:154:VAL:HG22	14:N:35:PHE:HZ	1.25	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
11:K:22:PHE:CB	12:L:585:LYS:HG2	1.93	0.98
9:I:113:CYS:SG	57:I:303:SF4:FE3	1.55	0.98
10:J:67:PHE:CE2	11:K:34:GLU:HG3	1.99	0.98
10:J:154:VAL:CG2	14:N:35:PHE:CZ	2.45	0.98
46:AB:167:GLN:HG2	49:AI:43:LEU:HD13	1.45	0.98
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
13:M:275:ILE:HD11	13:M:288:TYR:CG	1.98	0.98
22:W:55:LEU:HB3	22:W:107:MET:CE	1.94	0.98
62:l:201:PC1:H2A1	62:l:201:PC1:H3A2	1.45	0.98
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.44	0.98
42:q:78:ASP:OD1	42:q:81:MET:HG3	1.61	0.98
9:I:155:CYS:SG	57:I:302:SF4:FE4	1.55	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:339:GLN:HB3	49:AI:45:VAL:HG22	1.45	0.97
16:P:363:SER:HB3	22:W:51:HIS:CE1	1.98	0.97
48:AD:223:THR:HG21	52:AH:52:ASP:HA	1.43	0.97
12:L:485:PHE:CE1	12:L:486:LEU:HD12	1.91	0.97
3:C:203:LEU:HD21	4:D:123:LEU:HD21	1.47	0.97
7:G:75:CYS:HG	59:G:803:FES:FE1	0.80	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.45	0.97
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.47	0.97
1:A:104:TYR:CE2	10:J:167:ILE:CD1	2.47	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.79	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.44	0.96
12:L:174:TYR:HD2	12:L:232:TRP:CD1	1.82	0.96
26:a:64:LYS:HE2	26:a:66:LEU:HD12	1.43	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
4:D:189:THR:CB	58:D:501:UQ1:HM23	1.94	0.96
12:L:174:TYR:CD2	12:L:232:TRP:HD1	1.83	0.96
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.96
13:M:250:LEU:HD12	13:M:250:LEU:O	1.65	0.96
12:L:364:LYS:HE2	36:k:67:ILE:CD1	1.94	0.96
42:q:59:HIS:CE1	42:q:60:ARG:HG3	2.00	0.96
12:L:363:THR:HG23	12:L:431:THR:HB	1.48	0.96
25:Z:110:VAL:HG23	30:e:65:GLU:HG2	1.48	0.96
6:F:318:ILE:HD11	6:F:355:ILE:HD12	1.47	0.95
8:H:127:TYR:CD1	8:H:207:LEU:HD22	2.00	0.95
12:L:174:TYR:HD2	12:L:232:TRP:HD1	1.02	0.95
12:L:466:PHE:CZ	35:j:72:ARG:NH2	2.34	0.95
20:T:102:SER:O	20:T:141:PRO:HD3	1.66	0.95
30:e:20:PHE:HZ	33:h:178:PHE:HB2	1.25	0.95
40:o:75:PRO:HD3	41:p:28:ASN:OD1	1.65	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
23:X:132:LYS:HB3	27:b:59:ASP:HB2	1.48	0.95
12:L:247:LEU:HD12	12:L:248:HIS:CD2	1.98	0.95
12:L:466:PHE:HB2	35:j:68:TRP:HZ2	1.31	0.95
12:L:141:PHE:HE2	13:M:375:LEU:CD1	1.79	0.95
12:L:319:MET:HE1	12:L:399:ILE:HA	1.47	0.95
20:U:90:TYR:HE2	20:U:92:LYS:HB2	1.25	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:466:PHE:HB2	35:j:68:TRP:CZ2	2.02	0.95
48:Ad:249:TYR:CE1	48:Ad:252:VAL:HG23	2.02	0.95
46:Ab:297:PRO:CG	46:Ab:304:ASN:ND2	2.22	0.95
51:Ag:19:LEU:HD23	51:Ag:24:GLN:HB3	1.49	0.95
14:N:31:VAL:O	14:N:35:PHE:CD2	2.19	0.95
12:L:302:ILE:CG2	12:L:340:PHE:CZ	2.49	0.95
45:Aa:120:LEU:N	46:Ab:298:HIS:O	2.00	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
30:e:41:ILE:HG23	33:h:179:ILE:HD11	1.48	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
8:H:318:MET:HE1	10:J:133:VAL:HG12	1.49	0.94
13:M:216:LEU:HG	13:M:220:HIS:CE1	2.01	0.94
12:L:9:LEU:HD21	55:i:201:3PE:H2A2	1.50	0.94
4:D:128:THR:HG22	4:D:131:GLN:HG2	1.45	0.94
49:Ae:218:THR:HG21	49:Ae:256:LEU:O	1.68	0.94
13:M:369:LEU:CD2	13:M:371:PRO:HD2	1.97	0.94
2:B:89:SER:O	8:H:54:LYS:HD3	1.67	0.94
4:D:128:THR:CG2	4:D:131:GLN:HG2	1.98	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
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
12:L:246:LEU:HD12	12:L:247:LEU:N	1.81	0.94
13:M:4:ILE:HG22	13:M:107:ILE:HD13	1.47	0.94
20:T:104:PHE:HE1	20:T:115:GLN:HB2	1.32	0.94
51:AG:19:LEU:HD23	51:AG:24:GLN:HB3	1.49	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
12:L:247:LEU:HD11	12:L:248:HIS:NE2	1.83	0.94
49:AE:218:THR:HG21	49:AE:256:LEU:O	1.68	0.94
38:m:25:VAL:HG23	45:Aa:261:ALA:HA	1.47	0.94
12:L:362:ILE:HD12	12:L:430:VAL:HG12	1.51	0.93
13:M:1:MET:HG3	13:M:4:ILE:HD13	1.50	0.93
8:H:65:THR:HG21	16:P:359:TYR:CD1	2.04	0.93
45:AA:190:THR:HG21	45:AA:275:ILE:HB	1.49	0.93
12:L:274:LEU:HA	12:L:277:MET:HE3	1.50	0.93
13:M:127:ILE:HD12	14:N:256:PRO:HG3	1.48	0.93
45:AA:58:ARG:HE	45:AA:417:LEU:HD12	1.33	0.93
48:AD:249:TYR:CE1	48:AD:252:VAL:HG23	2.02	0.93
13:M:453:LEU:CD1	13:M:454:ILE:HG23	1.99	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
47:Ac:146:ILE:HG13	68:Ac:404:U10:H4M2	1.44	0.93
12:L:41:LYS:HG3	12:L:98:TRP:CZ2	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:12:ARG:HB3	43:r:20:LEU:HD21	1.48	0.93
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.51	0.92
45:Aa:117:GLY:HA2	46:Ab:377:LYS:HG2	1.52	0.92
11:K:22:PHE:O	12:L:585:LYS:HE3	1.69	0.92
15:O:314:LEU:CD1	15:O:315:PRO:HD2	2.00	0.92
48:Ad:223:THR:HG21	52:Ah:52:ASP:HA	1.52	0.92
6:F:318:ILE:HG22	6:F:326:LEU:HB3	1.50	0.92
45:Aa:58:ARG:NH2	45:Aa:417:LEU:O	2.03	0.92
6:F:147:ARG:HD3	6:F:191:TYR:CD2	2.03	0.92
13:M:173:THR:HG21	33:h:147:ALA:HB2	1.50	0.92
10:J:154:VAL:HG23	14:N:35:PHE:CZ	2.05	0.92
15:O:205:ILE:HD13	15:O:256:LEU:HB2	1.52	0.92
53:Aj:6:ILE:HB	53:Aj:7:PRO:HD2	1.52	0.92
24:Y:108:HIS:CE1	55:Ag:103:3PE:H392	2.03	0.92
32:g:145:ILE:HG23	41:p:160:LYS:HE2	1.50	0.92
3:C:203:LEU:HD11	4:D:123:LEU:CD2	2.00	0.92
4:D:238:LEU:HD11	43:r:39:PRO:HB3	1.49	0.92
6:F:382:CYS:SG	57:F:502:SF4:FE3	1.60	0.92
9:I:152:CYS:HG	57:I:302:SF4:FE2	0.77	0.92
10:J:166:ILE:CD1	11:K:76:ALA:HB2	2.00	0.91
13:M:127:ILE:CD1	14:N:256:PRO:CG	2.47	0.91
55:Aa:501:3PE:H332	62:Ae:301:PC1:H321	1.51	0.91
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.91
10:J:151:MET:HE1	14:N:28:LEU:HD13	1.51	0.91
3:C:98:PHE:HA	21:V:90:LEU:CD1	2.01	0.91
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.36	0.91
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.00	0.91
54:AK:10:TYR:CE1	50:Af:110:LYS:HA	2.06	0.91
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.52	0.91
4:D:361:ALA:O	4:D:384:LEU:HD11	1.71	0.91
22:W:55:LEU:HB3	22:W:107:MET:HE1	1.52	0.91
42:q:25:ARG:O	42:q:29:ARG:HG2	1.69	0.91
12:L:245:ALA:O	12:L:249:SER:HB3	1.70	0.91
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.36	0.91
16:P:363:SER:HB3	22:W:51:HIS:NE2	1.86	0.91
8:H:317:TYR:HE2	10:J:136:GLU:OE2	1.45	0.91
12:L:202:MET:HE3	12:L:265:PRO:HG3	1.53	0.91
15:O:106:ILE:HG12	15:O:111:SER:HA	1.50	0.91
25:Z:87:LEU:HD21	25:Z:119:PRO:HG3	1.53	0.91
1:A:93:ILE:HD11	56:A:402:CDL:H591	1.51	0.90
2:B:111:ARG:HB3	4:D:208:GLU:OE1	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:CYS:SG	59:G:803:FES:FE2	1.63	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
1:A:104:TYR:HE2	10:J:167:ILE:HD11	1.33	0.90
10:J:150:TRP:CD1	14:N:28:LEU:HD11	2.06	0.90
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.52	0.90
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.06	0.90
13:M:151:PHE:CZ	14:N:291:PHE:HB2	2.05	0.90
47:Ac:214:ASP:HB3	51:Ag:9:ALA:HB2	1.52	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.53	0.90
15:O:63:ASP:OD2	15:O:241:TYR:CE1	2.23	0.90
49:AE:263:TYR:CA	49:AE:273:VAL:HA	2.01	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
37:l:91:GLN:NE2	39:n:2:ALA:HB1	1.87	0.90
7:G:176:CYS:HG	57:G:802:SF4:FE4	0.66	0.90
13:M:231:LEU:HD12	13:M:235:LEU:CD1	2.00	0.90
16:P:333:PRO:HB2	16:P:337:ASP:HB2	1.53	0.90
47:AC:223:TYR:O	48:AD:311:TRP:NE1	2.04	0.90
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.53	0.90
15:O:347:VAL:O	15:O:347:VAL:HG12	1.71	0.90
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.53	0.90
12:L:466:PHE:CB	35:j:68:TRP:HZ2	1.84	0.90
40:o:117:LEU:HD23	40:o:118:LYS:HG3	1.51	0.90
1:A:89:ILE:HD11	56:A:402:CDL:H541	1.54	0.90
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.02	0.90
12:L:123:LEU:HD22	12:L:150:MET:SD	2.12	0.90
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
10:J:55:VAL:HG22	11:K:41:PHE:CE2	2.07	0.89
15:O:314:LEU:CG	15:O:315:PRO:HD2	2.02	0.89
46:AB:305:THR:HG23	46:AB:306:THR:H	1.36	0.89
12:L:556:ILE:HG21	38:m:80:PHE:CE1	2.07	0.89
13:M:453:LEU:HD12	13:M:454:ILE:N	1.87	0.89
9:I:67:ILE:HG13	62:I:301:PC1:H251	1.53	0.89
6:F:314:LEU:HD11	6:F:317:VAL:HG23	1.55	0.89
13:M:2:LEU:HA	13:M:5:ILE:HG12	1.53	0.89
13:M:380:PHE:HA	13:M:383:MET:HE2	1.55	0.89
25:Z:111:PHE:CZ	25:Z:117:VAL:HG21	2.06	0.89
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.53	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
13:M:29:SER:HB3	32:g:91:PHE:CD2	2.08	0.89
1:A:70:ALA:HB1	10:J:54:MET:HE1	1.54	0.89
12:L:261:VAL:O	12:L:264:HIS:HD2	1.50	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:168:GLN:OE1	23:X:168:PHE:CE1	2.25	0.89
24:Y:143:VAL:HG23	33:h:157:ARG:HG2	1.53	0.89
37:l:158:PRO:HD3	40:o:22:ILE:HB	1.55	0.89
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.08	0.89
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.89
21:V:72:LEU:HD12	21:V:72:LEU:O	1.73	0.89
6:F:424:ILE:HD11	7:G:73:GLY:O	1.72	0.89
12:L:552:LEU:HD21	38:m:90:GLY:HA2	1.54	0.89
6:F:225:LEU:H	17:Q:160:TYR:HE2	1.21	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
13:M:50:LYS:HE2	13:M:52:PHE:HE1	1.36	0.89
2:B:82:ILE:HG12	8:H:57:MET:CE	2.03	0.88
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.55	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.55	0.88
8:H:318:MET:HE1	10:J:133:VAL:CG1	2.02	0.88
13:M:8:SER:HA	13:M:11:LEU:HD13	1.54	0.88
16:P:344:PRO:HB2	16:P:347:LEU:HD13	1.55	0.88
54:AK:4:ARG:HA	50:Af:110:LYS:CE	2.02	0.88
3:C:240:ALA:HB1	43:r:61:ARG:HD2	1.56	0.88
39:n:101:GLU:O	39:n:122:ARG:NH2	2.06	0.88
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.38	0.88
10:J:150:TRP:NE1	14:N:28:LEU:HD11	1.89	0.88
8:H:65:THR:CG2	16:P:359:TYR:CD1	2.56	0.88
46:Ab:305:THR:HG23	46:Ab:306:THR:H	1.36	0.88
5:E:134:CYS:HG	59:E:301:FES:FE1	0.68	0.88
6:F:379:CYS:HG	57:F:502:SF4:FE4	0.62	0.88
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.88
8:H:183:MET:HE2	62:I:301:PC1:H2A1	1.56	0.88
15:O:209:VAL:HG12	15:O:260:SER:HB2	1.56	0.88
46:AB:297:PRO:CG	46:AB:304:ASN:ND2	2.23	0.88
6:F:266:GLY:HA3	6:F:271:SER:HA	1.54	0.88
13:M:310:MET:SD	13:M:455:THR:HB	2.13	0.88
7:G:608:VAL:HG23	17:Q:103:THR:OG1	1.74	0.87
13:M:447:LEU:HD11	13:M:454:ILE:HG21	1.54	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
12:L:428:TYR:HA	12:L:432:MET:HG2	1.56	0.87
12:L:485:PHE:HE1	12:L:486:LEU:HD11	1.38	0.87
30:e:17:HIS:CD2	30:e:18:PHE:HD1	1.92	0.87
45:AA:341:PHE:CD2	45:AA:368:MET:CE	2.56	0.87
45:Aa:341:PHE:CD2	45:Aa:368:MET:CE	2.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD23	55:A:401:3PE:H251	1.56	0.87
2:B:89:SER:O	8:H:54:LYS:HE2	1.72	0.87
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.08	0.87
12:L:362:ILE:HD12	12:L:430:VAL:CG1	2.04	0.87
34:i:110:ILE:HD13	41:p:16:ARG:HD2	1.56	0.87
2:B:89:SER:O	8:H:54:LYS:CE	2.22	0.87
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.88	0.87
47:Ac:138:MET:HE1	47:Ac:268:ILE:HA	1.56	0.87
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.57	0.87
13:M:102:LEU:HD13	13:M:230:ILE:HG12	1.57	0.87
13:M:142:ARG:NH2	14:N:303:THR:HG22	1.90	0.87
51:AG:29:SER:HB2	51:AG:32:SER:HB2	1.57	0.87
3:C:98:PHE:CA	21:V:90:LEU:HD11	2.04	0.87
12:L:553:LEU:HD11	38:m:93:ALA:CB	2.04	0.87
25:Z:97:ILE:CD1	30:e:79:ILE:HG23	2.04	0.87
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.57	0.87
16:P:296:PHE:CE1	16:P:297:VAL:HG23	2.10	0.87
45:AA:120:LEU:N	46:AB:298:HIS:O	2.08	0.87
45:AA:190:THR:HG21	45:AA:275:ILE:CB	2.04	0.87
4:D:146:CYS:SG	4:D:178:THR:OG1	2.32	0.86
12:L:79:SER:HB2	12:L:135:ASN:HB2	1.55	0.86
13:M:143:LEU:HD21	14:N:303:THR:CG2	2.05	0.86
58:D:501:UQ1:O1	58:D:501:UQ1:H8	1.74	0.86
25:Z:110:VAL:CG2	30:e:65:GLU:HG2	2.05	0.86
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.40	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
45:Aa:102:LYS:HZ1	45:Aa:153:ASN:HA	1.38	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
15:O:211:VAL:HG21	15:O:235:GLN:HA	1.57	0.86
51:AG:11:ILE:HG21	51:AG:14:VAL:CG2	2.05	0.86
45:Aa:384:THR:HG21	54:Ak:9:ARG:CG	2.05	0.86
10:J:80:GLU:HA	16:P:360:ARG:CD	2.05	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
13:M:1:MET:HE1	13:M:111:SER:HB2	1.58	0.86
22:W:55:LEU:HD22	22:W:107:MET:HE2	1.58	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
47:AC:98:VAL:HG22	67:AC:403:HEM:HBC2	1.56	0.86
7:G:607:LYS:HG3	17:Q:78:ARG:HH12	1.41	0.85
8:H:127:TYR:CD1	8:H:207:LEU:CD2	2.59	0.85
37:l:167:TYR:HD2	37:l:168:LEU:HD12	1.41	0.85
45:AA:190:THR:O	45:AA:273:SER:OG	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:294:LEU:HD11	68:AC:405:U10:H1M3	1.58	0.85
49:Ae:174:LEU:HD11	49:Ae:273:VAL:HG11	1.57	0.85
4:D:101:LEU:HD23	4:D:106:VAL:HG22	1.57	0.85
6:F:288:VAL:HG21	6:F:303:HIS:HD2	1.41	0.85
12:L:417:SER:HB3	12:L:493:ILE:HG13	1.58	0.85
12:L:466:PHE:CE1	35:j:72:ARG:NH2	2.44	0.85
46:AB:45:ASN:ND2	46:AB:239:ASN:HA	1.90	0.85
47:AC:18:PHE:CE1	69:AC:406:UQ6:H1M2	2.10	0.85
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.40	0.85
56:h:201:CDL:H572	55:i:201:3PE:H372	1.57	0.85
45:AA:255:ARG:O	45:AA:255:ARG:HG3	1.75	0.85
47:Ac:294:LEU:HD11	68:Ac:404:U10:H1M3	1.56	0.85
3:C:203:LEU:HD21	4:D:123:LEU:CD2	2.06	0.85
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.91	0.85
18:R:72:VAL:HG11	18:R:77:ILE:HD12	1.59	0.85
51:Ag:29:SER:HB2	51:Ag:32:SER:HB2	1.56	0.85
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.59	0.85
12:L:475:THR:HA	40:o:55:GLN:NE2	1.90	0.85
12:L:54:PHE:O	12:L:58:ASN:N	2.10	0.85
34:i:15:LEU:HD21	39:n:164:PRO:HB2	1.59	0.85
49:Ae:155:LYS:HE2	49:Ae:157:SER:HB3	1.57	0.85
6:F:425:CYS:SG	57:F:502:SF4:FE1	1.68	0.85
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.59	0.85
2:B:141:MET:HE1	4:D:86:PRO:HB2	1.59	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.59	0.84
37:l:89:TRP:CZ2	39:n:86:PRO:HD2	2.12	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
12:L:128:MET:HG2	12:L:251:THR:HB	1.59	0.84
10:J:150:TRP:NE1	14:N:28:LEU:CD2	2.40	0.84
12:L:247:LEU:HD11	12:L:248:HIS:CD2	2.11	0.84
12:L:445:GLU:HB2	12:L:450:LEU:HD23	1.59	0.84
12:L:466:PHE:CE1	35:j:72:ARG:CZ	2.59	0.84
20:T:104:PHE:CZ	20:T:115:GLN:CG	2.61	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
13:M:447:LEU:HD11	13:M:454:ILE:CG2	2.06	0.84
47:AC:146:ILE:CG1	68:AC:405:U10:H4M3	2.07	0.84
4:D:185:MET:HE3	58:D:501:UQ1:HM33	1.58	0.84
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.12	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
12:L:302:ILE:HG22	12:L:340:PHE:CE2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:29:SER:HB3	32:g:91:PHE:HD2	1.42	0.84
20:T:104:PHE:HD1	20:T:110:LEU:HB3	1.41	0.84
30:e:14:LEU:HD12	30:e:15:ASP:HB2	1.57	0.84
46:AB:305:THR:HG23	46:AB:306:THR:N	1.92	0.84
9:I:123:CYS:HG	57:I:302:SF4:FE1	0.58	0.84
14:N:215:MET:SD	14:N:248:LEU:HD21	2.18	0.84
15:O:258:TYR:HB3	15:O:262:GLU:HB2	1.56	0.84
15:O:314:LEU:HD12	15:O:315:PRO:HD2	1.56	0.84
17:Q:112:MET:SD	42:q:126:PRO:HB2	2.17	0.84
20:T:93:ILE:HD11	20:T:110:LEU:HD22	1.58	0.84
26:a:53:ARG:HB3	30:e:102:GLU:HB3	1.59	0.84
37:l:167:TYR:CD2	37:l:168:LEU:HD12	2.13	0.84
51:Ag:11:ILE:HG21	51:Ag:14:VAL:CG2	2.05	0.84
20:T:104:PHE:HZ	20:T:115:GLN:CG	1.87	0.84
48:AD:103:SER:O	48:AD:286:LYS:NZ	2.09	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
16:P:275:HIS:HA	16:P:278:LYS:HE2	1.60	0.84
45:AA:58:ARG:NH2	45:AA:417:LEU:O	2.10	0.84
12:L:20:LEU:HD12	12:L:21:ILE:N	1.92	0.84
12:L:364:LYS:HE2	36:k:67:ILE:HD11	1.59	0.84
13:M:196:TRP:NE1	13:M:250:LEU:HD13	1.92	0.84
20:T:117:GLU:HA	20:T:120:MET:HE3	1.60	0.84
47:Ac:223:TYR:O	48:Ad:311:TRP:NE1	2.09	0.84
45:AA:117:GLY:HA2	46:AB:377:LYS:HG2	1.59	0.84
45:Aa:179:MET:SD	49:AI:46:LYS:NZ	2.51	0.84
46:Ab:305:THR:HG23	46:Ab:306:THR:N	1.92	0.84
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.60	0.83
15:O:314:LEU:HG	15:O:315:PRO:HD2	1.58	0.83
49:AE:123:VAL:HG13	53:AJ:29:ALA:HA	1.59	0.83
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.61	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
25:Z:97:ILE:HD11	30:e:79:ILE:HG23	1.60	0.83
46:AB:167:GLN:HE21	49:AI:43:LEU:CB	1.91	0.83
47:Ac:146:ILE:CG1	68:Ac:404:U10:H4M3	2.08	0.83
4:D:67:ASN:HB3	4:D:69:VAL:HG12	1.58	0.83
8:H:136:VAL:HG13	10:J:69:TYR:HE1	1.40	0.83
9:I:162:CYS:SG	57:I:303:SF4:FE4	1.71	0.83
13:M:123:GLU:HB3	14:N:255:PRO:HG2	1.60	0.83
12:L:16:LEU:HD23	12:L:126:ILE:CD1	2.08	0.83
13:M:373:ILE:HG12	13:M:454:ILE:HD11	1.60	0.83
46:AB:51:SER:HB2	46:AB:230:LEU:HD12	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Aj:31:PHE:HA	54:Ak:48:ILE:HD11	1.60	0.83
54:Ak:42:LEU:HD22	54:Ak:48:ILE:HG21	1.58	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
10:J:150:TRP:CD1	14:N:28:LEU:HD21	2.12	0.83
13:M:446:LEU:HD21	56:h:201:CDL:H822	1.61	0.83
13:M:361:MET:HB3	13:M:441:MET:HE3	1.60	0.83
19:S:48:HIS:CE1	19:S:95:LEU:HD22	2.13	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.41	0.83
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.58	0.83
8:H:317:TYR:CZ	10:J:136:GLU:OE2	2.31	0.83
10:J:135:LEU:HA	11:K:54:MET:HE1	1.61	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
10:J:131:VAL:O	25:Z:68:ARG:NH1	2.12	0.83
4:D:271:ARG:HD2	8:H:281:ARG:CG	2.09	0.83
10:J:24:SER:HB3	10:J:27:TYR:HD2	1.44	0.83
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.09	0.82
13:M:173:THR:HG23	33:h:147:ALA:CB	2.08	0.82
13:M:269:MET:HE1	13:M:396:MET:HA	1.61	0.82
56:d:201:CDL:H742	56:d:201:CDL:H151	1.61	0.82
54:AK:10:TYR:HE1	50:Af:110:LYS:HA	1.43	0.82
8:H:293:PHE:HE1	55:H:402:3PE:H321	1.42	0.82
12:L:131:LEU:CD1	12:L:140:LEU:HD12	2.09	0.82
30:e:41:ILE:CG2	33:h:179:ILE:HD11	2.09	0.82
7:G:651:PRO:HG3	19:S:57:GLU:H	1.44	0.82
14:N:335:MET:HG3	14:N:335:MET:O	1.79	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
47:AC:146:ILE:CG1	68:AC:405:U10:C4M	2.57	0.82
46:Ab:51:SER:HB2	46:Ab:230:LEU:HD12	1.61	0.82
4:D:280:ALA:CB	21:V:11:LEU:HG	2.09	0.82
12:L:222:GLY:HA2	12:L:229:LEU:CD1	2.08	0.82
12:L:432:MET:HG3	12:L:432:MET:O	1.78	0.82
12:L:456:ARG:HG2	62:L:701:PC1:H31	1.62	0.82
17:Q:146:ASP:OD1	17:Q:146:ASP:O	1.97	0.82
47:AC:264:THR:HG23	49:Ae:225:ILE:HD11	1.61	0.82
7:G:114:GLU:OE2	43:r:53:TYR:HA	1.79	0.82
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.82
45:Aa:102:LYS:NZ	45:Aa:153:ASN:HA	1.94	0.82
12:L:73:SER:HB3	41:p:100:GLN:NE2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.62	0.81
5:E:84:LEU:HD12	44:s:46:LEU:HD13	1.61	0.81
8:H:94:PRO:HG2	8:H:97:ASN:HB3	1.61	0.81
9:I:162:CYS:HG	57:I:303:SF4:FE4	0.54	0.81
10:J:22:LYS:NZ	11:K:18:GLY:O	2.11	0.81
29:d:47:MET:HE1	56:d:201:CDL:H122	1.62	0.81
45:AA:341:PHE:CE2	45:AA:372:LEU:HD13	2.15	0.81
45:Aa:341:PHE:CE2	45:Aa:372:LEU:HD13	2.15	0.81
4:D:101:LEU:CD2	4:D:106:VAL:HG22	2.09	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
7:G:614:GLY:HA2	16:P:41:ILE:CD1	2.10	0.81
8:H:89:LEU:HD11	8:H:233:LEU:HD11	1.62	0.81
9:I:135:ARG:HD2	18:R:61:ILE:HG12	1.61	0.81
20:U:140:CYS:HB2	20:U:143:GLU:HG2	1.62	0.81
25:Z:86:ILE:HG23	25:Z:128:ARG:NE	1.95	0.81
36:k:34:PRO:HD2	36:k:59:TYR:CD1	2.15	0.81
39:n:140:LEU:HD11	39:n:165:PRO:HB3	0.84	0.81
45:AA:102:LYS:NZ	45:AA:153:ASN:HA	1.94	0.81
46:Ab:297:PRO:CB	46:Ab:304:ASN:ND2	2.41	0.81
7:G:225:ILE:HD11	7:G:285:TRP:CZ3	2.16	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
10:J:55:VAL:CG2	11:K:41:PHE:HE2	1.93	0.81
10:J:87:LEU:HD21	10:J:91:PHE:CE2	2.16	0.81
12:L:16:LEU:CD2	12:L:126:ILE:HD13	2.10	0.81
14:N:164:MET:HE2	56:Y:202:CDL:H592	1.62	0.81
24:Y:143:VAL:CG2	33:h:157:ARG:HG2	2.09	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
4:D:102:SER:HB2	4:D:107:ARG:HG3	1.61	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
10:J:144:MET:HA	10:J:148:ALA:O	1.80	0.81
22:W:55:LEU:CD2	22:W:107:MET:HE2	2.09	0.81
35:j:92:TRP:CZ3	40:o:100:LYS:HA	2.16	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.69	0.81
12:L:556:ILE:CG2	38:m:80:PHE:CZ	2.63	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
14:N:277:ILE:HG23	14:N:278:MET:N	1.95	0.81
14:N:307:THR:HG22	14:N:308:ASN:H	1.46	0.81
25:Z:126:GLY:HA3	30:e:76:MET:HE1	1.63	0.81
40:o:117:LEU:HD23	40:o:118:LYS:CG	2.10	0.81
4:D:304:LYS:HE2	9:I:35:THR:N	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:296:LEU:HB2	6:F:337:MET:HE3	1.61	0.81
12:L:358:LYS:HG3	39:n:80:TYR:CE2	2.15	0.81
20:T:110:LEU:HG	20:T:114:ASP:HB2	1.61	0.81
36:k:30:ILE:HD11	36:k:39:GLN:HB2	1.61	0.81
12:L:229:LEU:O	12:L:229:LEU:CD1	2.28	0.81
9:I:171:PRO:HB3	42:q:93:MET:HE1	1.60	0.80
14:N:200:LEU:HD21	14:N:265:ILE:HG12	1.62	0.80
14:N:277:ILE:CG2	14:N:278:MET:H	1.93	0.80
20:T:104:PHE:CD1	20:T:110:LEU:HB3	2.16	0.80
45:AA:190:THR:CG2	45:AA:275:ILE:HB	2.10	0.80
47:Ac:270:PRO:HG2	47:Ac:275:LEU:HD23	1.63	0.80
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.44	0.80
13:M:172:GLY:O	13:M:173:THR:CG2	2.28	0.80
13:M:453:LEU:HD12	13:M:454:ILE:HG23	1.63	0.80
25:Z:97:ILE:HD11	30:e:79:ILE:CG2	2.10	0.80
7:G:607:LYS:HG3	17:Q:78:ARG:NH1	1.94	0.80
25:Z:120:LEU:HG	30:e:69:ARG:HH21	1.44	0.80
53:Aj:46:HIS:HA	53:Aj:49:GLU:HG3	1.62	0.80
13:M:216:LEU:HD12	13:M:236:LEU:HD21	1.60	0.80
25:Z:110:VAL:CG1	30:e:71:LYS:HB3	2.10	0.80
4:D:47:PHE:CB	14:N:227:ILE:HD11	2.07	0.80
10:J:165:ILE:HG23	14:N:42:PRO:CG	2.11	0.80
13:M:55:MET:HE1	56:M:503:CDL:HA61	1.62	0.80
18:R:80:ASP:OD2	18:R:84:GLY:CA	2.27	0.80
27:b:20:VAL:HG13	55:b:201:3PE:H2A1	1.64	0.80
40:o:117:LEU:HD22	40:o:118:LYS:HG3	1.64	0.80
5:E:247:GLY:HA2	6:F:64:LYS:CE	2.12	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.80
11:K:22:PHE:HB2	12:L:585:LYS:CG	2.07	0.80
4:D:88:HIS:CE1	8:H:205:SER:O	2.34	0.80
8:H:311:THR:HB	25:Z:51:MET:SD	2.21	0.80
45:AA:102:LYS:HZ1	45:AA:153:ASN:HA	1.46	0.80
45:Aa:341:PHE:CZ	45:Aa:372:LEU:HD13	2.17	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
12:L:556:ILE:HG23	38:m:80:PHE:CE2	2.17	0.80
7:G:226:CYS:HG	57:G:802:SF4:FE1	0.99	0.80
7:G:614:GLY:HA2	16:P:41:ILE:HD13	1.63	0.80
56:Y:202:CDL:H511	56:Y:202:CDL:H731	1.64	0.80
49:AE:263:TYR:HA	49:AE:273:VAL:CA	2.04	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:PHE:CZ	11:K:34:GLU:HG3	2.17	0.80
15:O:117:PHE:CE1	15:O:173:MET:HE3	2.17	0.80
45:AA:190:THR:HG21	45:AA:275:ILE:CG2	2.10	0.80
45:AA:339:GLN:CB	49:AI:45:VAL:HG22	2.12	0.80
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
15:O:199:LEU:HD11	15:O:294:LEU:HD22	1.64	0.79
20:T:108:LEU:O	20:T:108:LEU:HD23	1.82	0.79
22:W:96:THR:HG22	22:W:101:LYS:HD2	1.64	0.79
47:AC:21:LEU:CD1	69:AC:406:UQ6:O2	2.30	0.79
50:AF:110:LYS:CE	54:AK:4:ARG:HA	2.11	0.79
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.13	0.79
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.17	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
62:I:301:PC1:H2D1	62:I:301:PC1:H291	1.64	0.79
12:L:358:LYS:HG3	39:n:80:TYR:OH	1.80	0.79
22:W:101:LYS:HG3	22:W:105:HIS:CB	2.12	0.79
24:Y:83:ARG:HH12	24:Y:90:LEU:HB3	1.45	0.79
47:AC:214:ASP:HB3	51:AG:9:ALA:HB2	1.65	0.79
13:M:122:PHE:CZ	13:M:206:LYS:HD3	2.18	0.79
20:U:76:LEU:HD12	20:U:156:GLU:HB2	1.62	0.79
32:g:70:ASP:OD1	39:n:108:HIS:NE2	2.15	0.79
41:p:24:THR:HG22	41:p:26:LEU:H	1.46	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.62	0.79
45:AA:341:PHE:CZ	45:AA:372:LEU:HD13	2.17	0.79
47:AC:45:ILE:HA	67:AC:402:HEM:HAB	1.63	0.79
13:M:127:ILE:CG1	14:N:254:LEU:HD21	2.12	0.79
24:Y:96:GLY:HA3	24:Y:121:GLY:HA2	1.64	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
12:L:130:ILE:HG23	12:L:139:GLN:HE21	1.46	0.79
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.63	0.79
39:n:20:TYR:CE2	39:n:24:LEU:HD11	2.18	0.79
50:AF:52:PRO:HD3	46:Ab:148:ARG:NH2	1.98	0.79
47:Ac:146:ILE:CG1	68:Ac:404:U10:C4M	2.61	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:127:TYR:CE1	8:H:207:LEU:HD23	2.17	0.79
12:L:131:LEU:HD12	12:L:140:LEU:CD1	2.12	0.79
13:M:175:ASN:HD22	33:h:143:GLU:HG2	1.47	0.79
13:M:367:LEU:HD21	13:M:408:MET:HE2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:120:PRO:CB	23:X:125:LEU:HD11	2.13	0.79
46:AB:163:ALA:HB1	49:AI:43:LEU:HD23	1.62	0.79
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
10:J:150:TRP:HE1	14:N:28:LEU:HD21	1.45	0.79
25:Z:126:GLY:HA3	30:e:76:MET:CE	2.12	0.79
9:I:211:TYR:CE2	43:r:39:PRO:HG3	2.17	0.79
14:N:123:PRO:HG2	14:N:126:MET:HG2	1.63	0.79
16:P:44:GLY:HA2	17:Q:107:TRP:CZ3	2.18	0.79
6:F:174:ARG:HA	44:s:52:LEU:HD21	1.65	0.78
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.13	0.78
4:D:170:ILE:HD13	4:D:236:LEU:CD1	2.13	0.78
13:M:248:ILE:HG13	13:M:249:ILE:HD12	1.64	0.78
21:V:48:THR:OG1	21:V:87:GLU:OE2	2.01	0.78
25:Z:120:LEU:HG	30:e:69:ARG:NH2	1.97	0.78
28:c:55:TRP:CZ2	29:d:66:THR:HG22	2.18	0.78
10:J:78:TYR:HA	11:K:25:HIS:HE1	1.46	0.78
13:M:231:LEU:HD12	13:M:235:LEU:HD13	1.64	0.78
15:O:207:ILE:HD12	15:O:263:ALA:HB2	1.64	0.78
54:AK:4:ARG:CA	50:Af:110:LYS:HE2	2.10	0.78
6:F:66:LYS:HZ3	6:F:189:SER:HA	1.48	0.78
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.13	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
13:M:151:PHE:CE2	14:N:291:PHE:HB2	2.17	0.78
15:O:117:PHE:HE1	15:O:173:MET:CE	1.96	0.78
51:AG:19:LEU:HD11	51:AG:23:GLU:HG2	1.66	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	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	2.67	0.78
12:L:534:HIS:O	12:L:538:PRO:HG3	1.83	0.78
15:O:314:LEU:HD12	15:O:315:PRO:CD	2.13	0.78
37:l:44:THR:OG1	37:l:45:PRO:HD2	1.83	0.78
42:q:85:GLU:OE2	42:q:103:PRO:HD3	1.83	0.78
8:H:17:MET:HE1	8:H:225:MET:HE3	1.66	0.78
8:H:39:ILE:HD11	62:q:202:PC1:H131	1.65	0.78
13:M:319:HIS:HA	13:M:322:THR:HG22	1.66	0.78
20:T:90:TYR:HD2	20:T:93:ILE:HG12	1.48	0.78
46:Ab:297:PRO:HA	46:Ab:304:ASN:OD1	1.84	0.78
2:B:82:ILE:HA	8:H:57:MET:HE1	1.65	0.78
10:J:55:VAL:CG2	11:K:41:PHE:CE2	2.66	0.78
12:L:136:ASN:HA	12:L:197:GLU:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:168:GLN:OE1	23:X:168:PHE:HE1	1.65	0.78
50:AF:110:LYS:HA	54:Ak:10:TYR:CE1	2.19	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
11:K:42:ILE:O	11:K:46:VAL:HG23	1.84	0.78
46:AB:167:GLN:HG3	49:AI:43:LEU:HD13	1.64	0.78
50:AF:108:TRP:CZ2	46:Ab:101:ARG:HB3	2.19	0.78
45:Aa:62:GLU:OE1	45:Aa:409:VAL:HG13	1.83	0.78
51:Ag:19:LEU:HD11	51:Ag:23:GLU:HG2	1.66	0.78
1:A:63:LEU:HD21	10:J:62:GLY:O	1.83	0.78
8:H:316:PRO:HA	25:Z:58:ARG:HH11	1.48	0.78
14:N:215:MET:CE	14:N:248:LEU:CD2	2.62	0.78
23:X:168:PHE:O	23:X:170:TRP:CD1	2.37	0.78
45:Aa:384:THR:CB	54:Ak:9:ARG:HG3	2.14	0.78
4:D:271:ARG:NH2	8:H:206:GLU:OE2	2.17	0.78
5:E:136:THR:HB	59:E:301:FES:S2	2.24	0.78
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.78
8:H:317:TYR:OH	10:J:136:GLU:CD	2.27	0.78
15:O:91:ILE:HD11	15:O:131:LEU:HD11	1.65	0.78
15:O:211:VAL:HG13	15:O:234:LEU:HB2	1.66	0.78
23:X:48:TRP:CD1	27:b:55:VAL:HG13	2.19	0.78
1:A:89:ILE:CD1	56:A:402:CDL:H541	2.14	0.77
13:M:9:LEU:HD23	13:M:104:ILE:HD13	1.65	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
14:N:170:LEU:HD11	14:N:288:LEU:HG	1.65	0.77
46:AB:297:PRO:CB	46:AB:304:ASN:ND2	2.41	0.77
12:L:525:LEU:HD21	39:n:77:PRO:HB3	1.66	0.77
15:O:305:LEU:HD12	15:O:305:LEU:O	1.83	0.77
25:Z:111:PHE:CZ	25:Z:117:VAL:CG2	2.66	0.77
46:AB:167:GLN:HE21	49:AI:43:LEU:HB3	1.49	0.77
47:AC:327:ILE:HG12	55:AG:103:3PE:H2A2	1.67	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
17:Q:81:VAL:HG21	17:Q:150:LYS:HG3	1.65	0.77
24:Y:18:THR:HG22	24:Y:19:GLN:HG3	1.66	0.77
4:D:128:THR:HG22	4:D:131:GLN:CG	2.13	0.77
30:e:17:HIS:CD2	30:e:18:PHE:CD1	2.72	0.77
51:AG:11:ILE:CG2	51:AG:14:VAL:CG2	2.62	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
13:M:204:LEU:HD22	13:M:209:LEU:HD12	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:254:LEU:HD12	14:N:255:PRO:CD	2.14	0.77
19:S:19:ILE:HB	19:S:53:ILE:CD1	2.15	0.77
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.15	0.77
12:L:141:PHE:HB2	12:L:182:PHE:CE2	2.20	0.77
25:Z:97:ILE:CD1	30:e:79:ILE:CG2	2.62	0.77
37:l:169:GLU:C	37:l:171:GLY:H	1.92	0.77
47:AC:21:LEU:HD22	69:AC:406:UQ6:H3M2	1.63	0.77
45:Aa:62:GLU:HB2	45:Aa:413:ILE:HD11	1.65	0.77
4:D:280:ALA:HB1	21:V:11:LEU:HG	1.65	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
13:M:98:MET:CE	13:M:128:PRO:HA	2.14	0.77
51:Ag:11:ILE:CG2	51:Ag:14:VAL:CG2	2.62	0.77
4:D:271:ARG:HD2	8:H:281:ARG:HG3	1.66	0.77
13:M:453:LEU:HD11	13:M:454:ILE:HG23	1.66	0.77
16:P:231:LEU:HD13	16:P:292:PRO:HD3	1.66	0.77
37:l:113:ILE:HG23	37:l:115:ASN:H	1.50	0.77
4:D:198:THR:CG2	8:H:32:GLN:HE21	1.98	0.77
14:N:31:VAL:O	14:N:35:PHE:HD2	1.68	0.77
14:N:232:LEU:CD2	14:N:307:THR:HG23	2.15	0.77
23:X:124:GLN:O	23:X:125:LEU:HD12	1.85	0.77
27:b:20:VAL:HA	55:b:201:3PE:H282	1.67	0.77
35:j:94:ASP:HB2	35:j:99:ILE:HB	1.67	0.77
46:AB:63:LEU:HD11	46:AB:238:LEU:HD21	1.65	0.77
46:AB:297:PRO:HA	46:AB:304:ASN:OD1	1.84	0.77
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.20	0.76
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.76
12:L:419:THR:HA	12:L:422:TYR:CE2	2.20	0.76
13:M:171:VAL:HG11	13:M:179:LEU:HD21	1.65	0.76
13:M:208:PRO:HG2	13:M:216:LEU:HD13	1.67	0.76
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.65	0.76
42:q:24:LEU:HD22	42:q:28:PHE:HE2	1.50	0.76
54:Ak:6:LEU:HA	54:Ak:11:ARG:HH12	1.49	0.76
6:F:234:GLY:HA3	6:F:238:CYS:O	1.85	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
7:G:225:ILE:HD11	7:G:285:TRP:HZ3	1.48	0.76
15:O:217:ARG:O	15:O:220:LYS:HG2	1.85	0.76
20:U:86:VAL:HB	20:U:122:MET:HE1	1.67	0.76
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.67	0.76
12:L:353:GLU:OE1	39:n:80:TYR:OH	2.03	0.76
13:M:42:LEU:HG	13:M:67:ILE:HD11	1.68	0.76
20:U:123:GLU:HG2	20:U:130:ILE:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:245:PHE:HE1	48:AD:102:LEU:HD23	1.51	0.76
46:Ab:63:LEU:HD11	46:Ab:238:LEU:HD21	1.66	0.76
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.99	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.67	0.76
49:Ae:191:GLU:HB2	49:Ae:194:GLN:HB2	1.66	0.76
3:C:88:HIS:CE1	21:V:105:GLU:HB3	2.20	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
8:H:200:LEU:HD22	8:H:282:TYR:HA	1.64	0.76
13:M:60:PRO:O	13:M:64:PRO:HD3	1.85	0.76
16:P:143:ASP:HA	16:P:147:ASN:HB2	1.67	0.76
34:i:101:LYS:HG2	41:p:116:ARG:O	1.85	0.76
49:AE:191:GLU:HB2	49:AE:194:GLN:HB2	1.66	0.76
54:AK:6:LEU:HA	54:AK:11:ARG:HH12	1.49	0.76
1:A:93:ILE:HD13	56:A:402:CDL:H592	1.67	0.76
12:L:9:LEU:HD22	34:i:82:VAL:HG13	1.68	0.76
12:L:302:ILE:HG22	12:L:340:PHE:CE1	2.20	0.76
56:L:703:CDL:H782	13:M:371:PRO:HG3	1.68	0.76
13:M:446:LEU:HD13	32:g:101:THR:HG21	1.67	0.76
14:N:211:LEU:HD23	14:N:333:SER:HB2	1.68	0.76
47:Ac:146:ILE:HD11	68:Ac:404:U10:C3	2.15	0.76
7:G:126:LEU:CD1	18:R:89:PRO:HB3	2.16	0.76
12:L:142:ILE:HA	13:M:370:PRO:HB2	1.68	0.76
12:L:232:TRP:CZ3	12:L:233:LEU:CD2	2.69	0.76
20:T:104:PHE:CE1	20:T:115:GLN:HB2	2.21	0.76
40:o:117:LEU:CD2	40:o:118:LYS:CG	2.64	0.76
3:C:241:PHE:HD2	43:r:61:ARG:CB	1.97	0.76
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.20	0.76
5:E:75:ALA:O	5:E:78:VAL:HG23	1.85	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
4:D:321:GLY:HA3	4:D:328:ASP:OD1	1.86	0.76
5:E:120:MET:HE1	6:F:160:GLY:HA3	1.66	0.76
6:F:192:ASP:HB3	44:s:57:LEU:HD11	1.67	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
9:I:113:CYS:HG	57:I:303:SF4:FE3	0.45	0.76
12:L:605:ASN:OD1	12:L:605:ASN:O	2.04	0.76
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.67	0.76
16:P:348:LYS:O	16:P:351:GLU:HG2	1.86	0.76
46:Ab:407:MET:HG2	46:Ab:411:THR:OG1	1.85	0.76
47:Ac:146:ILE:HG13	68:Ac:404:U10:H4M3	1.67	0.76
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:173:MET:HE2	7:G:231:LEU:HD23	1.68	0.75
46:AB:407:MET:HG2	46:AB:411:THR:OG1	1.85	0.75
47:AC:146:ILE:HD11	68:AC:405:U10:C3	2.16	0.75
51:AG:11:ILE:HG22	51:AG:14:VAL:HG22	1.68	0.75
9:I:68:ARG:NH2	25:Z:26:PRO:O	2.19	0.75
39:n:20:TYR:CZ	39:n:24:LEU:HD11	2.21	0.75
12:L:387:THR:HG23	12:L:461:SER:O	1.85	0.75
15:O:121:PRO:O	15:O:122:LYS:HG2	1.85	0.75
22:W:97:ILE:HG13	22:W:98:LYS:N	2.02	0.75
37:l:38:PRO:HB2	38:m:75:ASN:ND2	2.00	0.75
42:q:14:VAL:HG13	42:q:23:LEU:HD22	1.67	0.75
2:B:173:TYR:O	3:C:203:LEU:HD22	1.86	0.75
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.21	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
10:J:169:ILE:HG23	14:N:45:ILE:HD11	1.68	0.75
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.21	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
4:D:259:GLU:CG	25:Z:25:LEU:HD11	2.16	0.75
8:H:292:ASN:HD21	55:H:402:3PE:H122	1.50	0.75
12:L:153:LEU:HD11	13:M:360:LEU:HD11	1.68	0.75
12:L:553:LEU:HD21	38:m:93:ALA:C	2.12	0.75
14:N:227:ILE:HA	14:N:230:ILE:HG22	1.66	0.75
17:Q:61:ILE:O	17:Q:61:ILE:HD12	1.86	0.75
1:A:104:TYR:CE2	10:J:167:ILE:HD11	2.17	0.75
4:D:362:LYS:HE2	43:r:54:TYR:CE2	2.22	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
15:O:333:GLU:O	15:O:333:GLU:CD	2.30	0.75
48:Ad:227:LEU:HD12	48:Ad:227:LEU:O	1.87	0.75
12:L:393:ASP:OD1	12:L:394:LEU:N	2.19	0.75
12:L:482:MET:HE2	12:L:486:LEU:HB3	1.68	0.75
14:N:277:ILE:HG23	14:N:278:MET:H	1.50	0.75
22:W:55:LEU:HB3	22:W:107:MET:HE2	1.66	0.75
45:AA:255:ARG:O	45:AA:256:VAL:C	2.29	0.75
48:Ad:186:ARG:HE	48:Ad:193:LEU:HB2	1.51	0.75
1:A:51:PHE:HD2	10:J:73:MET:HB2	1.51	0.74
6:F:297:LYS:HD3	6:F:333:GLU:CB	2.17	0.74
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.74
10:J:124:LEU:HB2	25:Z:137:ASN:ND2	2.01	0.74
12:L:362:ILE:HG23	12:L:366:MET:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:210:PRO:HD2	15:O:213:GLU:HG3	1.69	0.74
19:S:19:ILE:HB	19:S:53:ILE:HD12	1.68	0.74
48:AD:227:LEU:HD12	48:AD:227:LEU:O	1.87	0.74
1:A:63:LEU:HD21	10:J:63:MET:HA	1.69	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
13:M:263:LEU:HD11	38:m:102:TYR:HD1	1.51	0.74
20:T:110:LEU:HG	20:T:114:ASP:CB	2.17	0.74
40:o:117:LEU:HD22	40:o:118:LYS:HE3	1.67	0.74
51:Ag:11:ILE:HG22	51:Ag:14:VAL:HG22	1.68	0.74
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
7:G:651:PRO:HD3	19:S:56:ARG:HB3	1.67	0.74
8:H:97:ASN:ND2	26:a:38:VAL:HG13	2.02	0.74
10:J:82:TRP:CE3	16:P:360:ARG:HB2	2.22	0.74
16:P:214:LEU:HG	16:P:353:LEU:HD21	1.68	0.74
28:c:30:TYR:HB2	28:c:34:PRO:HD3	1.70	0.74
47:AC:148:ASN:OD1	49:Ae:221:GLY:HA3	1.87	0.74
49:AE:173:PRO:HG2	49:AE:223:VAL:HG22	1.67	0.74
49:Ae:173:PRO:HG2	49:Ae:223:VAL:HG22	1.67	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:239:ASN:HB3	15:O:243:LYS:HD3	1.69	0.74
16:P:336:GLU:HG3	16:P:342:PRO:HD3	1.67	0.74
27:b:31:ILE:HA	27:b:34:MET:HE2	1.69	0.74
3:C:203:LEU:CD1	4:D:123:LEU:HD23	2.15	0.74
7:G:75:CYS:SG	59:G:803:FES:FE1	1.79	0.74
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.22	0.74
8:H:295:PRO:HB3	55:b:201:3PE:H3A1	1.69	0.74
20:T:103:HIS:ND1	20:T:140:CYS:HB3	2.01	0.74
3:C:100:ARG:HH12	21:V:86:LYS:HZ1	1.32	0.74
6:F:288:VAL:HG21	6:F:303:HIS:CD2	2.22	0.74
13:M:1:MET:HB2	13:M:52:PHE:CD2	2.22	0.74
20:T:103:HIS:HB2	20:T:106:LYS:HG2	1.67	0.74
56:A:402:CDL:H852	56:A:402:CDL:H532	1.69	0.74
7:G:88:VAL:HG13	7:G:108:LYS:HE2	1.67	0.74
13:M:310:MET:HG3	13:M:455:THR:HA	1.70	0.74
46:AB:85:LEU:HD23	49:AI:68:VAL:HG21	1.70	0.74
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.74
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.70	0.74
16:P:351:GLU:HB3	22:W:56:ASP:OD2	1.87	0.74
35:j:47:PHE:HA	36:k:63:PHE:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:127:ILE:HG12	14:N:254:LEU:HD21	1.69	0.74
13:M:395:LEU:HD21	38:m:101:TRP:CE2	2.23	0.74
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.23	0.74
47:AC:17:SER:O	69:AC:406:UQ6:O2	2.06	0.74
46:Ab:323:VAL:HG13	46:Ab:340:THR:HG22	1.68	0.74
1:A:24:LEU:N	1:A:25:PRO:HD2	2.03	0.74
4:D:238:LEU:CD1	43:r:39:PRO:HB3	2.17	0.74
6:F:318:ILE:CG2	6:F:326:LEU:HB3	2.17	0.74
7:G:611:THR:HG21	17:Q:105:GLU:CA	2.15	0.74
49:Ae:123:VAL:HG13	53:Aj:29:ALA:HA	1.70	0.74
2:B:163:SER:HB2	9:I:150:THR:O	1.88	0.73
4:D:375:MET:HE1	7:G:126:LEU:HA	1.70	0.73
9:I:211:TYR:CZ	43:r:39:PRO:HG3	2.23	0.73
13:M:200:MET:HE1	13:M:247:SER:HB2	1.69	0.73
14:N:202:LEU:O	14:N:206:MET:HG2	1.87	0.73
16:P:293:LEU:HD12	16:P:294:PRO:HD2	1.69	0.73
47:Ac:137:GLN:HE21	47:Ac:265:PRO:HD3	1.51	0.73
48:Ad:232:TYR:HD1	48:Ad:242:ILE:O	1.71	0.73
12:L:174:TYR:CD2	12:L:232:TRP:CD1	2.68	0.73
50:AF:24:ALA:O	51:AG:48:ARG:NH2	2.21	0.73
12:L:232:TRP:CZ3	12:L:233:LEU:HD23	2.22	0.73
5:E:68:ASN:HD21	44:s:49:ASN:HD21	1.35	0.73
6:F:66:LYS:NZ	6:F:189:SER:HA	2.03	0.73
7:G:382:ARG:HD2	19:S:56:ARG:CD	2.18	0.73
12:L:358:LYS:HG2	39:n:80:TYR:CE1	2.22	0.73
13:M:260:PRO:O	13:M:264:LEU:HG	1.88	0.73
45:Aa:80:ARG:HE	45:Aa:265:LEU:HD11	1.53	0.73
1:A:106:TRP:CE3	55:b:201:3PE:H342	2.24	0.73
4:D:279:THR:HA	21:V:12:VAL:HG13	1.68	0.73
13:M:391:PHE:HE2	55:m:201:3PE:H242	1.52	0.73
15:O:117:PHE:HE1	15:O:173:MET:HE3	1.53	0.73
16:P:94:LEU:HA	16:P:97:MET:HE2	1.68	0.73
26:a:7:PRO:HG3	56:q:201:CDL:H181	1.68	0.73
46:AB:305:THR:CG2	46:AB:306:THR:H	2.01	0.73
1:A:93:ILE:CD1	56:A:402:CDL:H591	2.18	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
12:L:20:LEU:HD12	12:L:20:LEU:C	2.13	0.73
13:M:167:ILE:HD11	13:M:195:LEU:HD21	1.70	0.73
16:P:44:GLY:HA2	17:Q:107:TRP:CE3	2.23	0.73
21:V:54:GLU:HG2	21:V:58:MET:HE2	1.70	0.73
34:i:104:ILE:HG13	40:o:48:ASP:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:305:THR:CG2	46:Ab:306:THR:H	2.02	0.73
48:Ad:96:TRP:HD1	48:Ad:99:ARG:HH21	1.34	0.73
4:D:326:CYS:HB3	4:D:453:THR:HG21	1.69	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.12	0.73
49:AE:187:GLU:HB3	49:AE:201:ASP:HB3	1.71	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.19	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
10:J:129:ASP:HB2	10:J:135:LEU:HD13	1.70	0.73
12:L:579:ASN:OD1	12:L:579:ASN:O	2.06	0.73
13:M:122:PHE:CD1	13:M:238:LEU:HG	2.23	0.73
13:M:216:LEU:HG	13:M:220:HIS:HE1	1.48	0.73
21:V:12:VAL:HG13	21:V:13:GLY:N	2.04	0.73
23:X:48:TRP:CZ2	27:b:55:VAL:HG22	2.23	0.73
42:q:42:ASP:OD2	42:q:83:PRO:HG2	1.87	0.73
47:Ac:21:LEU:HD22	69:Ac:405:UQ6:H3M1	1.71	0.73
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.70	0.73
10:J:76:GLU:HG3	10:J:77:GLU:H	1.53	0.73
12:L:424:MET:HE2	12:L:502:LEU:HA	1.70	0.73
20:U:79:ILE:HD11	20:U:148:ILE:HG22	1.71	0.73
46:Ab:163:ALA:HB1	49:Ai:43:LEU:HD23	1.69	0.73
47:Ac:146:ILE:HD11	68:Ac:404:U10:H3M2	1.69	0.73
49:Ae:187:GLU:HB3	49:Ae:201:ASP:HB3	1.71	0.73
2:B:166:ASN:O	9:I:150:THR:HB	1.89	0.73
4:D:323:ARG:O	21:V:12:VAL:HG21	1.88	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
14:N:215:MET:SD	14:N:248:LEU:CD2	2.76	0.73
47:AC:21:LEU:CD2	69:AC:406:UQ6:C3M	2.53	0.73
47:AC:29:SER:HB2	56:AG:102:CDL:H712	1.71	0.73
13:M:388:TRP:CE2	38:m:109:ARG:HD2	2.23	0.72
13:M:441:MET:SD	13:M:444:LEU:HD23	2.29	0.72
16:P:169:HIS:H	16:P:184:LYS:HE3	1.54	0.72
19:S:69:TYR:CE2	19:S:75:LYS:HG3	2.24	0.72
33:h:57:VAL:HG22	39:n:104:LEU:HD11	1.71	0.72
46:AB:297:PRO:CA	46:AB:304:ASN:HD21	2.01	0.72
8:H:181:MET:CE	8:H:304:HIS:CE1	2.72	0.72
10:J:63:MET:CE	11:K:68:ALA:HB2	2.19	0.72
12:L:73:SER:HB3	41:p:100:GLN:HE21	1.51	0.72
13:M:173:THR:CG2	33:h:147:ALA:CB	2.63	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:243:MET:HE1	13:M:302:MET:HE3	1.71	0.72
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.72	0.72
40:o:39:MET:HE1	40:o:58:TYR:HA	1.70	0.72
50:AF:110:LYS:HE2	54:AK:4:ARG:CA	2.15	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.72
6:F:273:THR:HG22	6:F:291:GLU:HA	1.70	0.72
20:T:120:MET:HG2	22:W:44:ARG:HH11	1.53	0.72
20:T:140:CYS:SG	20:T:143:GLU:HB2	2.29	0.72
25:Z:65:LEU:O	25:Z:69:ILE:HG12	1.89	0.72
34:i:22:TRP:CE2	39:n:172:THR:HG22	2.24	0.72
53:AJ:34:ARG:HB2	54:AK:48:ILE:HG13	1.69	0.72
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HA	1.71	0.72
9:I:184:LEU:HD23	17:Q:112:MET:HG3	1.72	0.72
14:N:242:THR:HG21	56:d:201:CDL:H132	1.70	0.72
15:O:176:GLN:HB2	15:O:178:TYR:HD2	1.55	0.72
49:AE:221:GLY:HA3	47:Ac:148:ASN:OD1	1.88	0.72
46:Ab:85:LEU:HD21	49:AI:68:VAL:HG11	1.72	0.72
9:I:57:ALA:HB2	27:b:13:TRP:O	1.88	0.72
12:L:123:LEU:HD21	56:L:703:CDL:H741	1.70	0.72
56:M:503:CDL:H731	56:M:503:CDL:H771	1.71	0.72
20:U:112:SER:HB2	39:n:17:LEU:HD11	1.72	0.72
25:Z:6:VAL:CG1	43:r:40:LYS:HB3	2.19	0.72
46:Ab:297:PRO:CA	46:Ab:304:ASN:HD21	2.01	0.72
4:D:392:PRO:HG3	43:r:60:ARG:O	1.89	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
10:J:63:MET:CE	11:K:68:ALA:CB	2.68	0.72
10:J:150:TRP:CD1	14:N:28:LEU:CD1	2.72	0.72
12:L:141:PHE:HB2	12:L:182:PHE:HE2	1.54	0.72
12:L:566:THR:HG21	55:L:704:3PE:H361	1.70	0.72
27:b:23:PHE:HD2	55:b:201:3PE:H281	1.54	0.72
46:AB:163:ALA:HB1	49:AI:43:LEU:CD2	2.20	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.20	0.72
55:H:402:3PE:H322	9:I:63:TRP:HE1	1.55	0.72
9:I:68:ARG:NH2	25:Z:26:PRO:HD2	2.05	0.72
14:N:59:TYR:CE2	14:N:63:GLN:HG3	2.23	0.72
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.13	0.72
8:H:17:MET:SD	8:H:225:MET:HB3	2.30	0.72
12:L:316:THR:CG2	12:L:325:ALA:HB2	2.19	0.72
12:L:576:LEU:HD12	12:L:577:THR:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:163:ARG:HG2	33:h:165:ASP:CB	2.19	0.72
49:Ae:199:GLN:O	49:Ae:248:ARG:HD3	1.90	0.72
1:A:73:LEU:O	1:A:76:PRO:HD2	1.90	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
15:O:81:LEU:HD11	15:O:270:VAL:HG13	1.70	0.72
6:F:35:LEU:HD22	6:F:273:THR:HG21	1.72	0.72
6:F:318:ILE:O	6:F:318:ILE:HG13	1.90	0.72
13:M:127:ILE:HD11	14:N:256:PRO:CG	2.20	0.72
22:W:42:TRP:CH2	22:W:93:LEU:HA	2.24	0.72
53:AJ:30:LEU:HA	54:AK:34:TRP:CD1	2.25	0.72
5:E:155:LEU:HB3	5:E:157:ILE:HG22	1.72	0.71
7:G:544:MET:HE3	7:G:565:PHE:HE2	1.54	0.71
8:H:17:MET:HE1	8:H:225:MET:HB3	1.72	0.71
8:H:96:ILE:HG23	25:Z:143:TYR:OH	1.90	0.71
9:I:64:THR:HG22	62:I:301:PC1:H222	1.72	0.71
9:I:107:PRO:HG3	42:q:106:ARG:NH1	2.05	0.71
12:L:247:LEU:HD12	12:L:248:HIS:N	2.03	0.71
12:L:299:LYS:HB2	12:L:354:GLN:HE21	1.55	0.71
13:M:373:ILE:CG1	13:M:454:ILE:HD11	2.19	0.71
14:N:243:MET:HG2	29:d:44:MET:HE2	1.72	0.71
25:Z:6:VAL:HG13	25:Z:7:LYS:H	1.53	0.71
48:Ad:306:MET:HE1	62:Ae:301:PC1:H331	1.70	0.71
6:F:110:PRO:HD2	6:F:238:CYS:SG	2.30	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
8:H:310:PHE:HA	27:b:39:THR:HA	1.72	0.71
13:M:106:LEU:HD13	13:M:234:ILE:HG22	1.72	0.71
13:M:154:LEU:HD13	14:N:287:LEU:CD2	2.20	0.71
3:C:217:ARG:NH1	22:W:112:GLU:HB2	2.04	0.71
9:I:135:ARG:HH11	18:R:61:ILE:HG23	1.55	0.71
12:L:180:ILE:HD11	13:M:400:ILE:HB	1.72	0.71
13:M:45:THR:O	13:M:46:ASP:OD1	2.09	0.71
15:O:336:GLY:H	15:O:344:ASN:ND2	1.88	0.71
2:B:210:ARG:NH1	42:q:78:ASP:HB3	2.05	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.20	0.71
10:J:116:ASN:ND2	10:J:123:TRP:HE1	1.87	0.71
12:L:310:LEU:HD23	12:L:313:MET:SD	2.31	0.71
13:M:313:THR:HG21	13:M:456:GLY:HA3	1.71	0.71
14:N:146:TYR:CD1	14:N:147:PRO:HD3	2.26	0.71
45:AA:58:ARG:NE	45:AA:417:LEU:HD12	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:384:THR:HB	54:Ak:9:ARG:HG3	1.73	0.71
3:C:67:ILE:HD11	21:V:47:TYR:HD2	1.55	0.71
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.71
8:H:5:ASN:HD21	26:a:23:THR:HG23	1.54	0.71
12:L:149:ILE:HG13	13:M:369:LEU:HD12	1.72	0.71
49:AE:199:GLN:O	49:AE:248:ARG:HD3	1.90	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:21:THR:HG21	61:H:401:UQ9:H16A	1.72	0.71
10:J:67:PHE:HE2	11:K:34:GLU:HG3	1.56	0.71
15:O:54:HIS:HE1	15:O:56:TYR:HB2	1.53	0.71
23:X:93:ASN:OD1	23:X:94:MET:N	2.24	0.71
37:l:106:HIS:CD2	37:l:107:TRP:H	2.08	0.71
38:m:9:ALA:HB1	38:m:10:PRO:HD2	1.71	0.71
6:F:318:ILE:HG22	6:F:326:LEU:CB	2.20	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
12:L:187:VAL:HG22	13:M:383:MET:HG2	1.73	0.71
20:U:144:ILE:O	20:U:148:ILE:HG12	1.91	0.71
25:Z:120:LEU:HD21	30:e:32:ARG:HH21	1.55	0.71
35:j:99:ILE:HA	40:o:108:LEU:HD21	1.73	0.71
45:AA:190:THR:HG21	45:AA:275:ILE:HG22	1.72	0.71
47:AC:294:LEU:CD1	68:AC:405:U10:H1M3	2.20	0.71
6:F:44:ASN:ND2	6:F:133:HIS:O	2.24	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
13:M:370:PRO:HA	13:M:375:LEU:HD13	1.72	0.71
13:M:446:LEU:HD13	32:g:101:THR:CG2	2.20	0.71
15:O:96:THR:HA	15:O:101:GLY:HA2	1.73	0.71
47:AC:245:PHE:CE1	48:AD:102:LEU:HD23	2.26	0.71
47:Ac:294:LEU:CD1	68:Ac:404:U10:H1M3	2.20	0.71
49:Ae:207:LYS:HB2	49:Ae:210:TRP:HB2	1.73	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.79	0.71
8:H:306:SER:OG	27:b:33:PRO:HG3	1.90	0.71
13:M:220:HIS:CE1	13:M:231:LEU:HD23	2.26	0.71
13:M:424:ILE:HG13	38:m:57:VAL:O	1.90	0.71
46:AB:297:PRO:HA	46:AB:304:ASN:CG	2.16	0.71
49:AE:154:ILE:HB	49:AE:271:VAL:O	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:102:SER:O	20:U:141:PRO:HD3	1.91	0.71
24:Y:77:CYS:SG	24:Y:78:VAL:N	2.64	0.71
25:Z:144:THR:HG22	26:a:48:MET:SD	2.30	0.71
48:Ad:222:PRO:HD2	48:Ad:225:VAL:HG11	1.72	0.71
4:D:238:LEU:CD1	9:I:211:TYR:OH	2.35	0.70
13:M:373:ILE:HG12	13:M:454:ILE:CD1	2.20	0.70
14:N:109:ALA:CB	14:N:110:PRO:HD3	2.21	0.70
38:m:30:ARG:NH1	45:Aa:260:ASP:HB2	2.05	0.70
49:Ae:178:HIS:HB2	49:Ae:210:TRP:CZ3	2.26	0.70
1:A:63:LEU:HG	10:J:66:VAL:HG21	1.74	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
9:I:188:GLU:OE1	18:R:56:ASN:N	2.24	0.70
15:O:54:HIS:CE1	15:O:56:TYR:HB2	2.26	0.70
39:n:61:THR:HG21	45:Aa:262:VAL:HG21	1.73	0.70
39:n:149:ILE:H	39:n:149:ILE:HD12	1.56	0.70
43:r:46:SER:C	43:r:52:ASN:HD21	1.99	0.70
45:Aa:113:VAL:CG1	46:Ab:299:ILE:HD11	2.21	0.70
49:Ae:220:LEU:HD12	49:Ae:239:HIS:CE1	2.27	0.70
2:B:116:ARG:HG2	8:H:36:GLY:O	1.91	0.70
4:D:198:THR:HG22	8:H:32:GLN:NE2	2.07	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.56	0.70
48:AD:222:PRO:HD2	48:AD:225:VAL:HG11	1.72	0.70
49:Ae:192:VAL:HA	49:Ae:195:LEU:HD12	1.73	0.70
3:C:67:ILE:HD11	21:V:47:TYR:CD2	2.25	0.70
4:D:82:LEU:HD12	8:H:126:LYS:HD2	1.73	0.70
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.55	0.70
6:F:110:PRO:O	6:F:238:CYS:HB3	1.91	0.70
10:J:150:TRP:HE1	14:N:28:LEU:CD2	2.03	0.70
10:J:154:VAL:HG22	14:N:35:PHE:CZ	2.16	0.70
14:N:237:THR:HG23	14:N:237:THR:O	1.88	0.70
15:O:135:LEU:HB3	15:O:139:ARG:HH12	1.57	0.70
46:AB:183:LYS:HG3	46:AB:254:ARG:HB3	1.73	0.70
49:AE:93:ARG:HD2	49:AE:110:ARG:HD2	1.72	0.70
47:Ac:45:ILE:HA	67:Ac:401:HEM:HAB	1.71	0.70
2:B:166:ASN:HB2	2:B:190:TYR:HD2	1.55	0.70
7:G:81:GLU:OE2	7:G:108:LYS:HD3	1.92	0.70
8:H:127:TYR:HD1	8:H:207:LEU:HD22	1.50	0.70
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.73	0.70
9:I:155:CYS:HG	57:I:302:SF4:FE4	1.08	0.70
12:L:428:TYR:HA	12:L:432:MET:CG	2.20	0.70
12:L:556:ILE:HG21	38:m:80:PHE:CZ	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:140:PHE:CE2	41:p:74:ILE:CG2	2.75	0.70
49:AE:178:HIS:HB2	49:AE:210:TRP:CZ3	2.26	0.70
49:AE:192:VAL:HA	49:AE:195:LEU:HD12	1.73	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
12:L:559:GLU:O	12:L:564:LYS:HB2	1.92	0.70
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.74	0.70
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.44	0.70
13:M:158:ILE:HG21	14:N:283:ALA:HB1	1.74	0.70
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.57	0.70
48:AD:215:LEU:HD11	70:AD:401:HEC:HMB3	1.72	0.70
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE1	2.27	0.70
46:Ab:297:PRO:HA	46:Ab:304:ASN:CG	2.16	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.21	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
13:M:134:THR:O	13:M:142:ARG:HD2	1.91	0.70
13:M:447:LEU:HD21	13:M:454:ILE:HD13	1.73	0.70
19:S:16:LEU:HD21	19:S:19:ILE:HD11	1.74	0.70
45:AA:341:PHE:CD2	45:AA:368:MET:HE1	2.27	0.70
48:Ad:152:VAL:HG21	48:Ad:176:PRO:HG2	1.74	0.70
49:Ae:202:LEU:HA	49:Ae:205:VAL:HG22	1.74	0.70
12:L:56:HIS:HA	40:o:74:PHE:CD1	2.27	0.70
20:U:125:GLU:OE2	35:j:44:TYR:CE1	2.45	0.70
41:p:28:ASN:O	41:p:31:THR:HG22	1.91	0.70
45:AA:68:THR:HG22	45:AA:136:LEU:HD23	1.73	0.70
49:AE:159:ILE:HG23	49:AE:163:LYS:HE3	1.74	0.70
53:Aj:6:ILE:HB	53:Aj:7:PRO:CD	2.21	0.70
12:L:285:THR:HG22	12:L:415:ALA:CB	2.22	0.69
21:V:35:LEU:HA	21:V:38:PHE:CD1	2.27	0.69
37:l:152:SER:HA	40:o:5:LEU:HD21	1.73	0.69
47:AC:265:PRO:HD2	47:AC:268:ILE:HD11	1.74	0.69
2:B:120:VAL:HG21	61:H:401:UQ9:C1M	2.22	0.69
3:C:100:ARG:HH12	21:V:86:LYS:NZ	1.88	0.69
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.72	0.69
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.57	0.69
7:G:614:GLY:CA	16:P:41:ILE:HD13	2.22	0.69
12:L:480:LEU:HD23	12:L:480:LEU:O	1.93	0.69
14:N:254:LEU:HD12	14:N:255:PRO:HD3	1.72	0.69
25:Z:12:PRO:HD3	25:Z:16:TYR:CZ	2.25	0.69
41:p:30:ILE:HG13	41:p:31:THR:N	2.06	0.69
43:r:98:ALA:HB1	43:r:99:PRO:HD2	1.74	0.69
3:C:123:ASN:ND2	21:V:108:PRO:HG2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:THR:HG21	4:D:139:LEU:HD21	1.74	0.69
21:V:12:VAL:HG13	21:V:13:GLY:H	1.56	0.69
45:Aa:62:GLU:OE1	45:Aa:409:VAL:CG1	2.40	0.69
47:Ac:147:THR:HG22	47:Ac:161:VAL:HG13	1.75	0.69
49:Ae:263:TYR:HA	49:Ae:273:VAL:HA	1.74	0.69
8:H:97:ASN:HD21	26:a:38:VAL:HG13	1.58	0.69
14:N:248:LEU:HD13	14:N:296:LEU:HD23	1.75	0.69
16:P:365:GLU:HB2	16:P:367:GLU:OE2	1.92	0.69
25:Z:6:VAL:HG13	43:r:40:LYS:HB3	1.75	0.69
25:Z:110:VAL:HG11	30:e:71:LYS:HB3	1.72	0.69
4:D:88:HIS:HE1	8:H:205:SER:O	1.74	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
15:O:201:PRO:CG	15:O:249:MET:HE2	2.23	0.69
47:AC:264:THR:HG22	49:Ae:225:ILE:HD11	1.75	0.69
49:Ae:180:THR:H	49:Ae:183:GLU:HB2	1.58	0.69
1:A:77:TRP:CZ3	10:J:50:PHE:CD2	2.80	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
8:H:317:TYR:OH	10:J:136:GLU:OE1	2.11	0.69
12:L:141:PHE:CD1	12:L:182:PHE:CD2	2.80	0.69
12:L:305:SER:HB2	12:L:422:TYR:HE1	1.57	0.69
12:L:306:THR:HA	12:L:336:LYS:HZ2	1.58	0.69
13:M:369:LEU:HD23	13:M:371:PRO:CD	2.12	0.69
16:P:171:ASN:OD1	16:P:171:ASN:O	2.11	0.69
37:l:156:VAL:HG11	40:o:95:TYR:CZ	2.27	0.69
48:Ad:249:TYR:CZ	48:Ad:252:VAL:HA	2.28	0.69
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.08	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.74	0.69
13:M:216:LEU:HD11	13:M:236:LEU:HD11	1.72	0.69
37:l:122:THR:HG21	37:l:129:MET:HE1	1.73	0.69
49:AE:220:LEU:HD12	49:AE:239:HIS:CE1	2.27	0.69
55:A:401:3PE:H241	10:J:41:LEU:HD22	1.74	0.69
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.75	0.69
5:E:61:ARG:NE	44:s:47:ASP:OD1	2.22	0.69
6:F:278:ILE:HG12	6:F:304:ALA:HB2	1.73	0.69
8:H:17:MET:CE	8:H:225:MET:HB3	2.23	0.69
8:H:293:PHE:CE1	55:H:402:3PE:H321	2.25	0.69
10:J:150:TRP:CD1	14:N:28:LEU:CD2	2.76	0.69
13:M:50:LYS:HE2	13:M:52:PHE:CE1	2.25	0.69
14:N:109:ALA:CB	14:N:110:PRO:CD	2.70	0.69
14:N:109:ALA:HB1	14:N:110:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:51:LEU:HD13	19:S:95:LEU:HD12	1.75	0.69
23:X:122:LEU:HD21	27:b:81:LEU:HD23	1.73	0.69
24:Y:4:VAL:O	24:Y:4:VAL:HG12	1.92	0.69
38:m:97:PRO:HB3	55:m:201:3PE:H2G2	1.75	0.69
47:AC:18:PHE:CE1	69:AC:406:UQ6:C1M	2.75	0.69
49:AE:207:LYS:HB2	49:AE:210:TRP:HB2	1.73	0.69
1:A:94:LEU:HD22	10:J:152:MET:HE3	1.75	0.69
7:G:117:MET:HE3	7:G:143:SER:HA	1.74	0.69
7:G:171:THR:HB	7:G:173:MET:HG3	1.74	0.69
12:L:455:LYS:NZ	35:j:57:GLN:OE1	2.25	0.69
38:m:97:PRO:HG3	55:m:201:3PE:H2I3	1.73	0.69
48:AD:214:LEU:HD11	48:AD:237:PHE:HB2	1.75	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:236:PHE:O	17:Q:166:TRP:HE3	1.76	0.69
10:J:150:TRP:HE1	14:N:28:LEU:CG	2.04	0.69
12:L:203:PHE:CZ	41:p:110:LEU:HD11	2.28	0.69
12:L:312:LEU:HD21	12:L:395:ILE:HG21	1.75	0.69
12:L:332:HIS:NE2	12:L:336:LYS:HG3	2.07	0.69
12:L:357:ARG:HG2	39:n:32:ILE:HG12	1.75	0.69
14:N:324:LEU:HD11	29:d:64:PHE:CZ	2.28	0.69
34:i:123:PHE:CZ	40:o:65:ARG:HD2	2.28	0.69
53:AJ:17:ARG:HD2	53:AJ:20:THR:HG23	1.75	0.69
46:Ab:412:VAL:HG13	46:Ab:415:GLN:HE21	1.58	0.69
1:A:93:ILE:CD1	56:A:402:CDL:C59	2.72	0.68
4:D:88:HIS:CD2	8:H:208:VAL:HG13	2.27	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
7:G:401:LEU:HD11	7:G:462:PHE:CZ	2.28	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
12:L:542:LEU:HB3	13:M:278:ARG:HD2	1.74	0.68
14:N:215:MET:HE2	14:N:248:LEU:CD2	2.23	0.68
16:P:148:ILE:HB	16:P:149:PRO:HD3	1.74	0.68
46:AB:101:ARG:HB3	50:Af:108:TRP:CZ2	2.28	0.68
48:Ad:125:HIS:HE1	48:Ad:195:PRO:HD2	1.56	0.68
48:Ad:214:LEU:HD11	48:Ad:237:PHE:HB2	1.75	0.68
3:C:217:ARG:HH12	22:W:112:GLU:HB2	1.58	0.68
4:D:156:GLU:HG2	4:D:161:ILE:HD11	1.74	0.68
10:J:63:MET:CE	11:K:68:ALA:HA	2.23	0.68
10:J:107:ASN:HD21	10:J:117:LEU:HB2	1.59	0.68
12:L:18:PRO:O	12:L:21:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.75	0.68
20:T:90:TYR:HE2	20:T:110:LEU:HD11	1.58	0.68
36:k:34:PRO:CD	36:k:59:TYR:CD1	2.75	0.68
41:p:73:ASP:OD1	41:p:91:GLN:OE1	2.10	0.68
46:AB:233:VAL:HA	46:AB:236:GLN:HG2	1.76	0.68
46:AB:297:PRO:CA	46:AB:304:ASN:ND2	2.57	0.68
49:AE:202:LEU:HA	49:AE:205:VAL:HG22	1.74	0.68
45:Aa:384:THR:CG2	54:Ak:9:ARG:HG3	2.22	0.68
55:Aa:501:3PE:H331	47:Ac:229:ILE:HD11	1.76	0.68
46:Ab:297:PRO:CA	46:Ab:304:ASN:ND2	2.57	0.68
2:B:111:ARG:CB	4:D:208:GLU:OE1	2.40	0.68
5:E:233:LEU:H	6:F:37:ASP:CG	2.02	0.68
6:F:382:CYS:HG	57:F:502:SF4:FE3	1.10	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
12:L:358:LYS:HG2	39:n:80:TYR:CZ	2.26	0.68
16:P:191:VAL:HA	16:P:194:VAL:HG22	1.72	0.68
21:V:72:LEU:HD11	21:V:80:VAL:CG2	2.19	0.68
38:m:125:PHE:HE1	41:p:133:THR:HG22	1.59	0.68
4:D:95:LEU:HG	4:D:97:LEU:HG	1.76	0.68
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.68
16:P:344:PRO:HD2	16:P:347:LEU:HD22	1.74	0.68
26:a:31:ASN:ND2	26:a:36:LYS:HB2	2.08	0.68
37:l:78:LEU:HD11	37:l:104:PRO:HB2	1.74	0.68
38:m:125:PHE:CE1	41:p:133:THR:HG22	2.28	0.68
43:r:112:TYR:O	43:r:113:LEU:HB2	1.93	0.68
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HE3	1.74	0.68
4:D:67:ASN:HB2	15:O:193:LEU:CD2	2.22	0.68
11:K:66:PHE:HE1	14:N:35:PHE:CZ	2.12	0.68
12:L:211:ILE:N	12:L:212:PRO:HD2	2.08	0.68
19:S:42:VAL:HB	19:S:46:LYS:HE3	1.75	0.68
54:AK:33:VAL:HG12	54:AK:42:LEU:HG	1.75	0.68
46:Ab:233:VAL:HA	46:Ab:236:GLN:HG2	1.76	0.68
48:Ad:186:ARG:NE	48:Ad:193:LEU:HB2	2.09	0.68
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.29	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
9:I:93:LEU:O	42:q:93:MET:HG2	1.94	0.68
15:O:140:LEU:HG	15:O:304:VAL:HG12	1.74	0.68
28:c:55:TRP:HE1	29:d:66:THR:HG21	1.57	0.68
32:g:145:ILE:CG2	41:p:160:LYS:HE2	2.24	0.68
51:AG:19:LEU:HD11	51:AG:23:GLU:CG	2.24	0.68
49:Ae:197:ASP:HB3	49:Ae:257:ASN:CG	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:GLU:HG3	4:D:229:PRO:O	1.93	0.68
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.76	0.68
13:M:395:LEU:HD21	38:m:101:TRP:CZ2	2.28	0.68
14:N:215:MET:HE1	14:N:248:LEU:HD21	1.71	0.68
16:P:263:PHE:HD2	16:P:333:PRO:O	1.77	0.68
20:U:100:VAL:O	20:U:141:PRO:HG2	1.94	0.68
41:p:51:PHE:HA	41:p:54:ARG:NE	2.09	0.68
47:AC:16:HIS:CE1	47:AC:201:HIS:NE2	2.62	0.68
48:AD:249:TYR:CZ	48:AD:252:VAL:HA	2.28	0.68
45:Aa:68:THR:HG22	45:Aa:136:LEU:HD23	1.74	0.68
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.76	0.68
7:G:78:CYS:HG	59:G:803:FES:FE2	0.46	0.68
7:G:617:ARG:HH11	22:W:129:HIS:HA	1.59	0.68
12:L:383:MET:SD	12:L:384:PRO:HD2	2.33	0.68
13:M:379:LEU:O	13:M:383:MET:HG3	1.93	0.68
46:AB:148:ARG:NH2	50:Af:52:PRO:HD3	2.09	0.68
45:Aa:80:ARG:NE	45:Aa:265:LEU:HD11	2.09	0.68
45:Aa:101:THR:HG22	45:Aa:154:SER:HA	1.76	0.68
45:Aa:384:THR:HG21	54:Ak:9:ARG:HG3	1.73	0.68
48:Ad:124:CYS:HA	48:Ad:179:TYR:HE2	1.59	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
12:L:145:GLU:HB3	13:M:370:PRO:CG	2.24	0.68
13:M:311:GLY:HA2	13:M:314:MET:HE3	1.76	0.68
20:T:104:PHE:HB2	20:T:110:LEU:HB2	1.74	0.68
25:Z:65:LEU:HB3	27:b:50:PRO:O	1.93	0.68
55:i:201:3PE:H2B2	55:i:201:3PE:H342	1.74	0.68
52:AH:45:ARG:O	52:AH:49:GLU:HG2	1.94	0.68
45:Aa:118:ALA:O	46:Ab:298:HIS:HB3	1.94	0.68
48:Ad:215:LEU:HD11	70:Ad:401:HEC:HMB3	1.73	0.68
2:B:155:PRO:HG2	8:H:58:LYS:HA	1.75	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
6:F:147:ARG:HD3	6:F:191:TYR:CE2	2.29	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
9:I:110:GLU:OE1	18:R:64:ILE:HB	1.94	0.68
12:L:228:GLY:C	12:L:229:LEU:HG	2.19	0.68
40:o:31:PHE:CD1	40:o:34:ARG:HB3	2.29	0.68
47:Ac:146:ILE:HD11	68:Ac:404:U10:C3M	2.23	0.68
4:D:142:VAL:HG11	4:D:185:MET:HG2	1.76	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
13:M:39:LEU:HD23	13:M:67:ILE:HD13	1.74	0.67
22:W:45:GLU:CD	22:W:97:ILE:HG22	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:110:VAL:CG2	30:e:65:GLU:CG	2.72	0.67
29:d:5:ARG:HD2	29:d:89:ASP:OD2	1.93	0.67
37:l:122:THR:HG23	37:l:123:PRO:HD2	1.75	0.67
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.60	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
14:N:149:LEU:HD13	14:N:154:ILE:HG21	1.75	0.67
16:P:197:GLU:HB3	16:P:259:VAL:CG2	2.24	0.67
19:S:20:ARG:HB2	19:S:66:TRP:HB2	1.75	0.67
49:AE:180:THR:H	49:AE:183:GLU:HB2	1.58	0.67
2:B:202:LEU:CD2	9:I:86:TYR:CB	2.73	0.67
7:G:651:PRO:CD	19:S:56:ARG:HB3	2.23	0.67
10:J:80:GLU:CA	16:P:360:ARG:HD2	2.20	0.67
13:M:30:TYR:O	13:M:34:ILE:HG12	1.95	0.67
13:M:275:ILE:HD11	13:M:288:TYR:CD1	2.29	0.67
15:O:206:TYR:HD2	15:O:257:VAL:HG13	1.59	0.67
15:O:347:VAL:O	15:O:347:VAL:CG1	2.42	0.67
16:P:296:PHE:CZ	16:P:297:VAL:HG23	2.29	0.67
32:g:109:ASP:CB	32:g:114:GLU:HB3	2.24	0.67
38:m:18:LEU:HD21	39:n:69:GLU:HA	1.76	0.67
43:r:12:ARG:HH21	43:r:20:LEU:CD1	2.07	0.67
45:AA:101:THR:HG22	45:AA:154:SER:HA	1.76	0.67
45:AA:274:GLU:HG3	45:AA:456:VAL:HB	1.77	0.67
47:AC:146:ILE:HD11	68:AC:405:U10:H3M2	1.76	0.67
50:AF:110:LYS:HA	54:Ak:10:TYR:HE1	1.56	0.67
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.24	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.77	0.67
10:J:9:SER:HB3	11:K:7:ASN:HD22	1.60	0.67
12:L:80:PHE:C	12:L:135:ASN:ND2	2.53	0.67
14:N:26:LEU:HD23	14:N:29:MET:SD	2.35	0.67
37:l:158:PRO:HD3	40:o:22:ILE:CB	2.24	0.67
45:AA:190:THR:CG2	45:AA:275:ILE:CG2	2.72	0.67
47:AC:147:THR:HG22	47:AC:161:VAL:HG13	1.75	0.67
49:Ae:156:LEU:HB2	49:Ae:269:ASP:HA	1.76	0.67
4:D:47:PHE:HB3	14:N:227:ILE:CD1	2.14	0.67
7:G:73:GLY:HA2	59:G:803:FES:S1	2.35	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.77	0.67
12:L:25:ASN:HB2	33:h:72:LYS:HZ1	1.57	0.67
15:O:114:LEU:HA	15:O:131:LEU:CD2	2.24	0.67
32:g:63:ASN:OD1	39:n:106:TYR:HE1	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:45:ARG:HD3	36:k:57:TRP:CD1	2.30	0.67
12:L:427:ILE:CD1	36:k:69:PHE:HE1	2.08	0.67
13:M:98:MET:HE2	13:M:131:ILE:HB	1.77	0.67
16:P:302:GLY:HA2	16:P:314:THR:HG23	1.77	0.67
25:Z:62:ILE:HD12	27:b:81:LEU:HD22	1.76	0.67
42:q:138:VAL:CG2	42:q:139:PRO:HD2	2.25	0.67
46:AB:305:THR:HG23	46:AB:306:THR:HG23	1.77	0.67
53:AJ:30:LEU:HD12	54:AK:34:TRP:HB2	1.77	0.67
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.25	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
11:K:62:THR:O	11:K:66:PHE:HD2	1.78	0.67
12:L:552:LEU:CD2	12:L:553:LEU:HD12	2.25	0.67
37:l:106:HIS:HD2	37:l:107:TRP:H	1.43	0.67
51:Ag:19:LEU:HD11	51:Ag:23:GLU:CG	2.24	0.67
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.24	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
8:H:207:LEU:O	8:H:208:VAL:C	2.38	0.67
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.60	0.67
53:AJ:17:ARG:HD2	53:AJ:20:THR:HG23	1.75	0.67
6:F:233:VAL:HG11	17:Q:164:PHE:HB2	1.76	0.67
13:M:278:ARG:HH22	37:l:108:ASP:CG	2.03	0.67
13:M:285:LEU:HD13	13:M:342:MET:HE1	1.75	0.67
23:X:7:LEU:HD13	25:Z:87:LEU:HB3	1.77	0.67
29:d:14:LEU:O	29:d:14:LEU:CD1	2.37	0.67
34:i:28:LEU:HD22	34:i:32:GLU:HG2	1.75	0.67
52:Ah:45:ARG:O	52:Ah:49:GLU:HG2	1.94	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
8:H:185:TRP:CD1	8:H:238:THR:HG1	2.13	0.67
12:L:81:LYS:N	12:L:135:ASN:ND2	2.43	0.67
20:T:97:LYS:HZ3	20:T:108:LEU:N	1.93	0.67
47:Ac:20:ASP:O	51:Ag:5:PHE:HE2	1.78	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
8:H:317:TYR:OH	10:J:136:GLU:OE2	2.13	0.66
9:I:62:MET:HE1	25:Z:36:PHE:HA	1.77	0.66
9:I:200:GLU:OE2	42:q:93:MET:SD	2.53	0.66
13:M:154:LEU:HD13	14:N:287:LEU:HD22	1.77	0.66
13:M:270:ILE:HG22	13:M:271:MET:HE2	1.76	0.66
14:N:307:THR:HB	15:O:319:ILE:HD11	1.76	0.66
17:Q:111:LEU:HD11	42:q:126:PRO:HG2	1.77	0.66
24:Y:76:THR:HG22	24:Y:92:TYR:HA	1.77	0.66
38:m:23:TYR:CG	39:n:65:ARG:HG2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:156:ASP:HB2	48:AD:167:ARG:HE	1.58	0.66
49:AE:197:ASP:HB3	49:AE:257:ASN:CG	2.19	0.66
51:AG:11:ILE:CG2	51:AG:14:VAL:HG22	2.25	0.66
45:Aa:400:VAL:HB	46:Ab:58:LEU:HG	1.77	0.66
1:A:51:PHE:CZ	11:K:79:VAL:HG13	2.30	0.66
2:B:81:LEU:CG	8:H:53:MET:HE1	2.25	0.66
2:B:95:PHE:HB3	2:B:97:LEU:CD1	2.25	0.66
3:C:98:PHE:HE1	21:V:44:TYR:CE1	2.13	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
12:L:149:ILE:HG21	13:M:364:LEU:HD21	1.78	0.66
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.78	0.66
16:P:122:HIS:HB2	18:R:46:VAL:HG12	1.77	0.66
23:X:130:LYS:HG2	27:b:68:SER:HA	1.77	0.66
30:e:14:LEU:CD1	30:e:15:ASP:HB2	2.25	0.66
33:h:102:PRO:HD2	33:h:105:TYR:HB2	1.78	0.66
51:AG:11:ILE:CG2	51:AG:14:VAL:HG21	2.18	0.66
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.26	0.66
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.24	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
12:L:407:TRP:CE3	12:L:410:LEU:HD11	2.29	0.66
13:M:173:THR:HG23	33:h:147:ALA:HB2	1.68	0.66
13:M:361:MET:CB	13:M:441:MET:HE3	2.25	0.66
15:O:343:TYR:HD1	15:O:352:ILE:HG23	1.59	0.66
16:P:268:PRO:HG2	16:P:344:PRO:HA	1.76	0.66
20:U:125:GLU:OE2	35:j:44:TYR:HE1	1.77	0.66
20:U:128:PHE:CZ	20:U:148:ILE:HD12	2.31	0.66
40:o:89:TYR:CE2	40:o:93:LEU:HD11	2.30	0.66
46:AB:412:VAL:HG13	46:AB:415:GLN:HE21	1.58	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.66
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.60	0.66
8:H:136:VAL:HG13	10:J:69:TYR:CE1	2.27	0.66
12:L:201:ILE:HG22	12:L:266:LEU:HD11	1.76	0.66
13:M:173:THR:HB	33:h:143:GLU:OE2	1.95	0.66
16:P:262:THR:H	16:P:332:LEU:HD12	1.61	0.66
46:Ab:270:ALA:HB2	46:Ab:339:TYR:HD1	1.61	0.66
3:C:47:ARG:HG3	3:C:48:PRO:HD2	1.77	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:279:THR:HA	21:V:12:VAL:CG1	2.25	0.66
6:F:275:LEU:HA	6:F:289:GLU:HA	1.77	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
8:H:300:LEU:HD23	27:b:25:VAL:HG11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:424:MET:HE2	12:L:502:LEU:CA	2.25	0.66
13:M:11:LEU:HB3	13:M:100:ILE:HD13	1.77	0.66
46:AB:229:VAL:O	46:AB:232:GLN:HG2	1.95	0.66
7:G:246:ARG:NH2	17:Q:123:ASN:OD1	2.28	0.66
14:N:242:THR:HG23	56:d:201:CDL:H382	1.77	0.66
20:U:89:LEU:HA	36:k:53:ARG:HH22	1.60	0.66
22:W:121:PHE:HA	22:W:124:LYS:HE2	1.76	0.66
23:X:48:TRP:CE2	27:b:55:VAL:CG2	2.75	0.66
23:X:57:LEU:HG	23:X:61:LYS:NZ	2.10	0.66
24:Y:108:HIS:HE1	55:Ag:103:3PE:C39	2.00	0.66
32:g:53:TRP:CD1	32:g:53:TRP:H	2.14	0.66
47:Ac:215:ALA:HA	51:Ag:11:ILE:HD11	1.76	0.66
51:Ag:35:ILE:HD11	56:Ag:102:CDL:H322	1.78	0.66
4:D:83:ASN:OD1	4:D:83:ASN:O	2.14	0.66
8:H:187:ILE:HD12	55:H:402:3PE:H242	1.77	0.66
10:J:70:THR:HG21	11:K:75:LEU:HD22	1.78	0.66
12:L:552:LEU:HD23	12:L:553:LEU:HD12	1.77	0.66
13:M:318:ALA:HB2	13:M:373:ILE:HG23	1.76	0.66
15:O:201:PRO:HG2	15:O:249:MET:HE2	1.77	0.66
16:P:320:GLU:O	16:P:324:ILE:HG12	1.96	0.66
21:V:72:LEU:HD12	21:V:72:LEU:C	2.19	0.66
21:V:72:LEU:O	21:V:72:LEU:CD1	2.42	0.66
38:m:97:PRO:HG3	55:m:201:3PE:C2I	2.26	0.66
41:p:70:ARG:CZ	41:p:91:GLN:HE21	2.09	0.66
46:Ab:229:VAL:O	46:Ab:232:GLN:HG2	1.95	0.66
47:Ac:257:MET:HG3	48:Ad:203:ALA:HB1	1.78	0.66
4:D:359:ASP:HB3	7:G:150:ARG:NH2	2.11	0.66
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.61	0.66
6:F:297:LYS:HD3	6:F:333:GLU:HB3	1.77	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
15:O:62:VAL:HA	15:O:205:ILE:O	1.96	0.66
16:P:169:HIS:H	16:P:184:LYS:CE	2.09	0.66
46:AB:339:TYR:HD2	49:AI:59:ALA:HB1	1.61	0.66
47:Ac:18:PHE:CZ	69:Ac:405:UQ6:H1M3	2.31	0.66
2:B:81:LEU:HG	8:H:53:MET:HE1	1.77	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.29	0.66
11:K:70:GLU:HA	14:N:38:LEU:HD21	1.77	0.66
12:L:116:ARG:HG2	12:L:120:TYR:CE2	2.31	0.66
23:X:160:PRO:HG3	29:d:22:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:148:PRO:O	41:p:167:ARG:NH2	2.29	0.66
36:k:34:PRO:CG	36:k:59:TYR:CE1	2.72	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.26	0.66
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.66
8:H:317:TYR:CD2	10:J:134:MET:HE1	2.31	0.66
12:L:173:LEU:HD23	55:L:702:3PE:H322	1.77	0.66
15:O:38:TYR:HB3	15:O:299:GLN:NE2	2.11	0.66
4:D:102:SER:CB	4:D:107:ARG:HG3	2.26	0.65
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.22	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
7:G:667:GLN:NE2	19:S:38:VAL:HA	2.11	0.65
10:J:9:SER:CB	11:K:7:ASN:HD22	2.08	0.65
12:L:25:ASN:OD1	12:L:25:ASN:O	2.14	0.65
13:M:373:ILE:CD1	13:M:454:ILE:HD11	2.25	0.65
15:O:200:PRO:HG3	15:O:282:PRO:HD2	1.78	0.65
25:Z:114:THR:O	25:Z:114:THR:HG22	1.94	0.65
47:AC:28:SER:HB2	56:AG:101:CDL:HA21	1.78	0.65
49:AE:122:THR:HG21	53:AJ:25:ILE:HD13	1.79	0.65
51:Ag:11:ILE:CG2	51:Ag:14:VAL:HG22	2.25	0.65
4:D:178:THR:HG22	4:D:214:TYR:OH	1.96	0.65
4:D:384:LEU:CD2	7:G:144:MET:HE1	2.26	0.65
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.94	0.65
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.30	0.65
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.32	0.65
12:L:66:TRP:HZ3	12:L:68:TRP:CD1	2.14	0.65
16:P:59:PHE:HB2	16:P:130:ILE:HD11	1.79	0.65
48:AD:223:THR:CG2	52:AH:52:ASP:HA	2.23	0.65
6:F:293:SER:HA	6:F:338:ASP:HB3	1.78	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
8:H:17:MET:HE1	8:H:225:MET:CE	2.25	0.65
14:N:275:CYS:SG	24:Y:139:PRO:HG2	2.36	0.65
19:S:58:CYS:HB2	19:S:61:VAL:HG12	1.78	0.65
25:Z:143:TYR:CD1	25:Z:144:THR:N	2.65	0.65
34:i:22:TRP:CD2	39:n:172:THR:HG22	2.31	0.65
46:AB:339:TYR:CD2	49:AI:59:ALA:HB1	2.31	0.65
45:Aa:136:LEU:HD21	46:Ab:380:ALA:HA	1.78	0.65
4:D:198:THR:HG22	8:H:32:GLN:CG	2.26	0.65
4:D:211:PHE:O	4:D:214:TYR:HB2	1.96	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
13:M:367:LEU:CD2	13:M:408:MET:HE2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:220:MET:C	14:N:223:ASN:H	2.04	0.65
16:P:199:ILE:HD11	16:P:258:ALA:O	1.96	0.65
19:S:16:LEU:HD11	19:S:19:ILE:HD11	1.78	0.65
32:g:140:PHE:CE2	41:p:74:ILE:HG22	2.32	0.65
45:AA:341:PHE:CD2	45:AA:368:MET:HE3	2.32	0.65
1:A:64:LEU:HD13	10:J:163:ILE:HG12	1.78	0.65
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.65
2:B:95:PHE:CZ	2:B:145:LEU:HA	2.31	0.65
11:K:93:LEU:CD2	14:N:54:GLU:HG2	2.26	0.65
12:L:485:PHE:CD1	12:L:486:LEU:CD1	2.55	0.65
14:N:258:THR:HB	14:N:333:SER:O	1.96	0.65
21:V:38:PHE:CD1	21:V:95:LEU:HD21	2.31	0.65
47:AC:257:MET:HG3	48:AD:203:ALA:HB1	1.78	0.65
45:Aa:381:THR:O	54:Ak:16:ASN:ND2	2.30	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.97	0.65
8:H:310:PHE:O	27:b:38:TYR:HB2	1.96	0.65
12:L:190:SER:HB2	12:L:196:TRP:HE1	1.61	0.65
37:l:82:SER:HA	37:l:112:TYR:HB3	1.79	0.65
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.31	0.65
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.61	0.65
8:H:292:ASN:HD21	55:H:402:3PE:C12	2.10	0.65
10:J:150:TRP:HE1	14:N:28:LEU:HD11	1.59	0.65
12:L:88:LEU:HD23	12:L:326:PHE:CE2	2.32	0.65
24:Y:110:TYR:OH	51:Ag:43:ARG:NH2	2.30	0.65
32:g:108:PRO:O	32:g:109:ASP:OD1	2.13	0.65
38:m:28:GLU:HG2	38:m:31:ARG:HH22	1.61	0.65
40:o:25:PHE:CE2	40:o:109:LEU:HD22	2.32	0.65
47:AC:96:LEU:HD23	55:AC:404:3PE:H292	1.78	0.65
45:Aa:110:GLU:HB2	46:Ab:299:ILE:HD13	1.78	0.65
47:Ac:110:MET:HE1	47:Ac:306:PHE:CE1	2.32	0.65
12:L:387:THR:HG22	12:L:465:GLY:H	1.61	0.65
16:P:236:VAL:CG1	16:P:270:ARG:HH21	2.10	0.65
18:R:40:GLU:HA	18:R:45:ARG:NH1	2.12	0.65
23:X:53:PRO:HB3	25:Z:80:ASP:OD2	1.97	0.65
37:l:38:PRO:CB	38:m:75:ASN:HD22	2.05	0.65
39:n:30:TRP:CD2	39:n:76:HIS:HD2	2.15	0.65
45:AA:339:GLN:HB3	49:AI:45:VAL:CG2	2.22	0.65
47:AC:58:ASP:HB2	47:Ac:56:THR:HG21	1.77	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65
10:J:144:MET:CA	10:J:148:ALA:O	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:PHE:HD1	13:M:238:LEU:HG	1.62	0.65
14:N:275:CYS:SG	24:Y:139:PRO:CG	2.85	0.65
15:O:168:VAL:HG21	15:O:241:TYR:CZ	2.32	0.65
15:O:194:THR:HG23	15:O:307:TYR:HB2	1.79	0.65
15:O:343:TYR:CE1	15:O:355:LYS:HB2	2.31	0.65
20:U:91:ASP:OD2	36:k:48:ARG:NH2	2.30	0.65
23:X:141:PRO:O	23:X:142:TYR:HB2	1.96	0.65
31:f:38:ARG:NH1	31:f:54:VAL:HB	2.11	0.65
40:o:71:ARG:HB3	40:o:71:ARG:HH11	1.61	0.65
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.77	0.65
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.61	0.65
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.96	0.65
8:H:287:HIS:HE1	55:H:402:3PE:N	1.94	0.65
12:L:466:PHE:CB	35:j:68:TRP:CZ2	2.70	0.65
20:U:134:ASP:OD2	39:n:2:ALA:N	2.30	0.65
23:X:162:LYS:HB3	23:X:166:ARG:HH21	1.61	0.65
67:AC:403:HEM:HBA1	69:AC:406:UQ6:C4M	2.27	0.65
46:Ab:167:GLN:NE2	49:Ai:43:LEU:CB	2.40	0.65
46:Ab:305:THR:HG23	46:Ab:306:THR:HG23	1.77	0.65
55:A:401:3PE:H341	10:J:56:PHE:HE2	1.62	0.64
7:G:89:VAL:HB	7:G:94:MET:HG3	1.78	0.64
9:I:181:GLU:HB2	42:q:126:PRO:HG3	1.79	0.64
11:K:20:LEU:HA	12:L:588:PHE:HD2	1.62	0.64
12:L:368:PHE:HB3	12:L:445:GLU:OE2	1.97	0.64
33:h:127:ASP:OD1	33:h:127:ASP:O	2.15	0.64
41:p:51:PHE:O	41:p:55:GLN:HG2	1.97	0.64
67:Ac:402:HEM:HBA1	69:Ac:405:UQ6:C4M	2.27	0.64
48:Ad:161:ASP:HB2	48:Ad:163:GLU:HG2	1.79	0.64
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HA	1.79	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
7:G:614:GLY:C	16:P:41:ILE:HG21	2.22	0.64
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.64
55:H:402:3PE:H322	9:I:63:TRP:NE1	2.12	0.64
10:J:78:TYR:HE2	10:J:82:TRP:HA	1.62	0.64
13:M:119:TYR:CD1	13:M:160:LEU:HD22	2.32	0.64
13:M:167:ILE:O	13:M:171:VAL:HG12	1.98	0.64
14:N:307:THR:HG22	14:N:308:ASN:N	2.12	0.64
45:Aa:249:HIS:O	45:Aa:250:LEU:HB2	1.97	0.64
4:D:198:THR:HG22	8:H:32:GLN:HG3	1.79	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
8:H:249:ILE:HD13	23:X:99:HIS:CG	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LYS:CD	11:K:23:ARG:HG2	2.27	0.64
55:J:201:3PE:H391	24:Y:43:VAL:HG12	1.80	0.64
11:K:22:PHE:CD2	12:L:584:ILE:HG23	2.32	0.64
13:M:154:LEU:HD22	14:N:287:LEU:HD21	1.80	0.64
13:M:307:TRP:CD1	13:M:459:MET:SD	2.91	0.64
15:O:117:PHE:CE1	15:O:173:MET:CE	2.77	0.64
16:P:226:VAL:HG21	16:P:281:PHE:CZ	2.32	0.64
19:S:48:HIS:CE1	19:S:95:LEU:CD2	2.80	0.64
24:Y:137:LEU:HD23	24:Y:138:PHE:CG	2.31	0.64
37:l:122:THR:CG2	37:l:123:PRO:HD2	2.27	0.64
42:q:3:LEU:O	42:q:6:VAL:HG22	1.97	0.64
47:AC:146:ILE:HG12	68:AC:405:U10:H4M3	1.79	0.64
45:Aa:274:GLU:HG3	45:Aa:456:VAL:HB	1.80	0.64
3:C:68:LEU:HD13	3:C:95:THR:HG23	1.80	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.78	0.64
23:X:65:GLY:HA2	23:X:68:LEU:HD12	1.78	0.64
23:X:167:PHE:HD2	23:X:170:TRP:NE1	1.94	0.64
41:p:74:ILE:HD13	41:p:85:ILE:HG13	1.80	0.64
48:Ad:248:ILE:HG22	48:Ad:263:MET:HG3	1.79	0.64
1:A:7:ILE:HG21	55:A:401:3PE:H292	1.80	0.64
3:C:241:PHE:CD2	43:r:61:ARG:CB	2.75	0.64
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
13:M:458:THR:CG2	41:p:148:ALA:HB1	2.27	0.64
15:O:63:ASP:OD2	15:O:241:TYR:HE1	1.79	0.64
15:O:124:ASN:O	32:g:51:MET:HE3	1.98	0.64
19:S:69:TYR:CD2	19:S:75:LYS:HG3	2.33	0.64
20:T:80:LYS:HD3	20:T:100:VAL:HG11	1.79	0.64
46:Ab:191:TYR:OH	49:Ai:76:VAL:HB	1.98	0.64
47:Ac:311:LYS:O	50:Af:39:HIS:N	2.25	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
4:D:67:ASN:HB2	15:O:193:LEU:HD23	1.78	0.64
4:D:104:GLU:HG3	8:H:130:PHE:HZ	1.63	0.64
5:E:58:ASN:HB3	5:E:84:LEU:HD21	1.80	0.64
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.61	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
12:L:193:MET:HE1	38:m:125:PHE:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:366:MET:CG	12:L:443:ILE:HG21	2.28	0.64
12:L:480:LEU:HD22	35:j:84:PHE:CD2	2.33	0.64
13:M:300:SER:HB3	13:M:381:ILE:HG23	1.78	0.64
25:Z:120:LEU:HD21	30:e:32:ARG:NH2	2.13	0.64
31:f:37:PHE:CZ	41:p:83:LEU:HD13	2.33	0.64
42:q:60:ARG:HH12	42:q:95:ASP:HA	1.60	0.64
49:AE:218:THR:CG2	49:AE:256:LEU:O	2.45	0.64
46:Ab:183:LYS:HG3	46:Ab:254:ARG:HB3	1.78	0.64
48:Ad:96:TRP:CD1	48:Ad:99:ARG:HH21	2.16	0.64
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.78	0.64
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.28	0.64
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.28	0.64
6:F:379:CYS:SG	57:F:502:SF4:S1	2.96	0.64
7:G:557:ARG:HD3	42:q:144:TYR:CE1	2.32	0.64
12:L:40:ILE:HD13	12:L:97:THR:HG22	1.79	0.64
12:L:41:LYS:HG3	12:L:98:TRP:CE2	2.33	0.64
12:L:81:LYS:N	12:L:135:ASN:HD21	1.96	0.64
12:L:246:LEU:HD12	12:L:246:LEU:C	2.23	0.64
12:L:280:LEU:HD21	62:l:201:PC1:H3G1	1.80	0.64
14:N:37:LEU:HD12	14:N:63:GLN:HB3	1.79	0.64
29:d:60:ARG:O	29:d:61:GLN:C	2.40	0.64
46:AB:115:THR:HG22	49:AI:65:VAL:HG22	1.79	0.64
4:D:102:SER:HB2	4:D:107:ARG:CG	2.26	0.64
4:D:217:VAL:HG22	4:D:226:TYR:CZ	2.33	0.64
7:G:152:ARG:HD2	43:r:49:LEU:HA	1.80	0.64
8:H:249:ILE:HG21	23:X:99:HIS:CE1	2.33	0.64
12:L:141:PHE:HD1	12:L:182:PHE:CD2	2.14	0.64
13:M:160:LEU:HD11	13:M:203:PHE:CZ	2.33	0.64
14:N:143:ILE:HA	14:N:194:LEU:HD11	1.79	0.64
16:P:296:PHE:CZ	16:P:297:VAL:CG2	2.81	0.64
23:X:50:GLU:HG2	23:X:138:PRO:HG3	1.79	0.64
48:AD:248:ILE:HG22	48:AD:263:MET:HG3	1.79	0.64
48:AD:323:PRO:HG2	48:AD:325:LYS:HD2	1.80	0.64
49:Ae:234:TYR:HB2	49:Ae:243:TYR:HB2	1.79	0.64
4:D:156:GLU:HG2	4:D:161:ILE:CD1	2.28	0.64
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.80	0.64
6:F:227:PRO:HG3	7:G:94:MET:SD	2.38	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
10:J:59:TYR:OH	11:K:34:GLU:HB3	1.98	0.64
14:N:179:MET:HG3	14:N:216:PHE:HE1	1.63	0.64
36:k:38:VAL:HG13	39:n:39:TYR:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:31:CYS:SG	39:n:36:LYS:NZ	2.71	0.64
42:q:29:ARG:O	62:q:202:PC1:C14	2.46	0.64
45:AA:403:LEU:HD23	45:AA:409:VAL:HG22	1.78	0.64
47:Ac:253:PRO:O	48:Ad:203:ALA:HA	1.98	0.64
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.80	0.64
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.64
12:L:247:LEU:CD1	12:L:248:HIS:NE2	2.52	0.64
13:M:196:TRP:HZ3	13:M:261:PHE:HE2	1.44	0.64
14:N:220:MET:HA	14:N:223:ASN:HA	1.79	0.64
16:P:150:ARG:HE	16:P:190:GLU:HG2	1.62	0.64
16:P:299:SER:CB	16:P:316:LYS:HE3	2.22	0.64
19:S:20:ARG:HG2	19:S:54:LEU:HD12	1.79	0.64
23:X:37:ASP:OD1	23:X:38:LYS:N	2.31	0.64
32:g:123:LEU:HD12	41:p:98:VAL:CG1	2.28	0.64
37:l:101:TRP:NE1	38:m:62:ASP:HA	2.13	0.64
37:l:106:HIS:CD2	37:l:107:TRP:N	2.66	0.64
47:Ac:107:TYR:HB2	47:Ac:305:PRO:HG3	1.79	0.64
5:E:48:PRO:HA	5:E:95:SER:HB2	1.80	0.63
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.33	0.63
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.61	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
12:L:385:PHE:CD1	35:j:72:ARG:HG3	2.33	0.63
13:M:191:SER:OG	55:M:501:3PE:H12	1.98	0.63
14:N:314:MET:HB2	15:O:305:LEU:HD11	1.79	0.63
16:P:180:SER:O	16:P:184:LYS:HG3	1.98	0.63
23:X:17:GLU:HB2	30:e:104:PRO:HG2	1.79	0.63
48:AD:255:TYR:OH	48:AD:266:VAL:HA	1.98	0.63
54:AK:45:VAL:CG1	54:AK:48:ILE:HG22	2.29	0.63
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE3	2.32	0.63
46:Ab:426:LYS:O	46:Ab:429:LYS:HG2	1.97	0.63
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.78	0.63
2:B:202:LEU:CD2	9:I:86:TYR:HB2	2.29	0.63
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.63	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
8:H:90:PRO:HB2	8:H:166:ILE:HD11	1.80	0.63
8:H:181:MET:CE	8:H:304:HIS:ND1	2.62	0.63
8:H:310:PHE:HB3	27:b:33:PRO:HA	1.80	0.63
13:M:1:MET:HB2	13:M:52:PHE:HD2	1.60	0.63
13:M:250:LEU:O	13:M:250:LEU:CD1	2.44	0.63
15:O:275:TYR:OH	21:V:23:ARG:NH2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:74:TRP:CZ2	45:AA:411:GLU:HA	2.33	0.63
46:AB:109:LYS:HD2	49:AI:71:ASN:HD22	1.62	0.63
47:AC:100:ARG:HH12	67:AC:403:HEM:CBD	2.11	0.63
48:AD:186:ARG:HE	48:AD:193:LEU:HB2	1.62	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
8:H:85:LEU:HD21	8:H:108:THR:HB	1.80	0.63
8:H:316:PRO:HG3	25:Z:57:ARG:HB3	1.80	0.63
10:J:151:MET:CE	14:N:28:LEU:HD13	2.25	0.63
12:L:100:ILE:HD13	12:L:341:MET:SD	2.38	0.63
12:L:305:SER:HB2	12:L:422:TYR:CE1	2.34	0.63
13:M:220:HIS:NE2	13:M:231:LEU:HB3	2.13	0.63
15:O:176:GLN:HB2	15:O:178:TYR:CD2	2.32	0.63
30:e:89:GLU:HB3	30:e:91:LYS:HE2	1.80	0.63
45:Aa:467:ASP:OD2	47:Ac:223:TYR:CE2	2.51	0.63
2:B:116:ARG:HA	8:H:37:PRO:HA	1.80	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
12:L:433:THR:HG22	12:L:434:LYS:N	2.13	0.63
13:M:105:LEU:O	13:M:109:THR:HG23	1.98	0.63
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.80	0.63
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.33	0.63
14:N:273:ASN:ND2	24:Y:143:VAL:HA	2.13	0.63
20:T:104:PHE:CE1	20:T:115:GLN:CB	2.80	0.63
21:V:38:PHE:CE1	21:V:95:LEU:HD21	2.33	0.63
39:n:95:GLU:HA	39:n:98:LYS:HG3	1.81	0.63
45:AA:204:PRO:HB2	45:AA:206:GLU:OE1	1.98	0.63
46:AB:307:SER:HB2	46:AB:310:SER:HB2	1.78	0.63
49:Ae:188:ALA:HA	49:Ae:200:HIS:NE2	2.13	0.63
2:B:194:CYS:O	57:B:301:SF4:S4	2.56	0.63
10:J:150:TRP:NE1	14:N:28:LEU:CD1	2.61	0.63
12:L:410:LEU:HD12	12:L:411:ILE:N	2.13	0.63
12:L:439:PRO:HA	36:k:57:TRP:CZ2	2.32	0.63
13:M:388:TRP:NE1	38:m:109:ARG:HD2	2.13	0.63
14:N:319:LYS:HA	15:O:302:THR:HG21	1.80	0.63
15:O:215:GLN:HE22	15:O:231:SER:HB3	1.63	0.63
15:O:347:VAL:HG11	28:c:29:PHE:HA	1.79	0.63
16:P:284:THR:HG23	16:P:356:HIS:HB2	1.79	0.63
16:P:365:GLU:CB	16:P:367:GLU:OE2	2.46	0.63
30:e:69:ARG:HD2	30:e:72:THR:HG21	1.80	0.63
32:g:75:ASP:OD1	32:g:76:SER:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:34:PRO:HG2	36:k:59:TYR:CD1	2.34	0.63
49:AE:188:ALA:HA	49:AE:200:HIS:NE2	2.13	0.63
47:Ac:107:TYR:HE1	47:Ac:308:HIS:HB2	1.63	0.63
8:H:172:MET:HE1	25:Z:46:GLY:HA2	1.79	0.63
12:L:202:MET:HE3	12:L:265:PRO:CG	2.25	0.63
13:M:118:PHE:O	13:M:122:PHE:N	2.25	0.63
14:N:149:LEU:HD13	14:N:154:ILE:CG2	2.28	0.63
16:P:66:GLY:O	16:P:67:ARG:C	2.42	0.63
23:X:83:THR:HA	23:X:86:TRP:CD1	2.34	0.63
25:Z:97:ILE:HD12	30:e:79:ILE:HG23	1.79	0.63
45:AA:388:VAL:HG22	45:AA:441:LEU:HD13	1.81	0.63
53:AJ:30:LEU:O	54:AK:48:ILE:HD12	1.98	0.63
48:Ad:255:TYR:OH	48:Ad:266:VAL:HA	1.98	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
7:G:126:LEU:HD11	18:R:89:PRO:HB3	1.80	0.63
10:J:63:MET:HE2	11:K:68:ALA:HA	1.80	0.63
12:L:80:PHE:C	12:L:135:ASN:HD21	2.06	0.63
12:L:361:ASN:OD1	12:L:361:ASN:O	2.17	0.63
12:L:493:ILE:HD12	12:L:496:LEU:HD21	1.81	0.63
14:N:131:LEU:O	14:N:135:LYS:HG2	1.98	0.63
15:O:76:GLU:O	15:O:80:GLN:HG2	1.99	0.63
15:O:81:LEU:HD12	15:O:81:LEU:N	2.13	0.63
18:R:44:ARG:HG2	18:R:47:ARG:NH1	2.14	0.63
18:R:76:ILE:HD11	18:R:92:TYR:HB3	1.79	0.63
20:T:104:PHE:HE1	20:T:115:GLN:CB	2.07	0.63
25:Z:65:LEU:O	25:Z:68:ARG:HG2	1.98	0.63
42:q:29:ARG:O	62:q:202:PC1:H141	1.97	0.63
46:AB:426:LYS:O	46:AB:429:LYS:HG2	1.97	0.63
47:AC:253:PRO:O	48:AD:203:ALA:HA	1.98	0.63
2:B:91:TRP:CE3	61:H:401:UQ9:H1MA	2.33	0.63
6:F:275:LEU:HG	6:F:289:GLU:HB3	1.80	0.63
6:F:425:CYS:SG	57:F:502:SF4:S4	2.96	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.79	0.63
32:g:125:LYS:HE3	41:p:8:ASP:CB	2.28	0.63
33:h:155:GLU:O	33:h:159:LEU:HD13	1.99	0.63
41:p:66:ARG:HD2	41:p:68:TYR:CZ	2.34	0.63
49:AE:234:TYR:HB2	49:AE:243:TYR:HB2	1.79	0.63
45:Aa:55:ASN:HB3	45:Aa:226:ALA:CB	2.29	0.63
48:Ad:217:GLY:O	48:Ad:235:PRO:HD2	1.99	0.63
49:Ae:161:GLU:HA	49:Ae:178:HIS:CG	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:218:THR:CG2	49:Ae:256:LEU:O	2.45	0.63
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.79	0.63
1:A:90:MET:CE	10:J:152:MET:HB3	2.28	0.63
2:B:98:ALA:O	4:D:141:TYR:CZ	2.52	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
4:D:198:THR:HA	8:H:32:GLN:HG2	1.80	0.63
46:AB:38:LEU:HD11	46:AB:396:ILE:HD13	1.80	0.63
48:AD:217:GLY:O	48:AD:235:PRO:HD2	1.99	0.63
45:Aa:204:PRO:HB2	45:Aa:206:GLU:OE1	1.98	0.63
49:Ae:179:ARG:HH12	49:Ae:201:ASP:HB2	1.64	0.63
1:A:7:ILE:HG13	55:A:401:3PE:H271	1.81	0.62
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.32	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	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
13:M:129:THR:HG21	13:M:235:LEU:HD13	1.80	0.62
13:M:263:LEU:CD1	38:m:102:TYR:HD1	2.12	0.62
13:M:264:LEU:CD2	38:m:98:LEU:HD21	2.27	0.62
14:N:158:ALA:O	14:N:162:ILE:HG12	1.99	0.62
15:O:305:LEU:HD12	15:O:305:LEU:C	2.24	0.62
22:W:55:LEU:CB	22:W:107:MET:CE	2.75	0.62
25:Z:6:VAL:HG11	43:r:40:LYS:HD3	1.80	0.62
35:j:84:PHE:HE2	40:o:88:ASP:HB3	1.63	0.62
46:AB:45:ASN:HD21	46:AB:239:ASN:HA	1.63	0.62
47:Ac:146:ILE:HG12	68:Ac:404:U10:H4M3	1.81	0.62
51:Ag:31:PHE:CE1	56:Ag:102:CDL:H312	2.34	0.62
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.59	0.62
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.79	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.35	0.62
7:G:360:LYS:CE	7:G:632:ILE:HB	2.27	0.62
10:J:2:ASN:HB3	10:J:121:GLY:HA3	1.81	0.62
48:AD:201:VAL:HG21	48:AD:275:ARG:HA	1.79	0.62
48:Ad:167:ARG:HH12	48:Ad:173:ASP:HB2	1.64	0.62
49:Ae:213:LEU:HD23	49:Ae:260:VAL:HG22	1.81	0.62
56:A:402:CDL:H391	10:J:150:TRP:HZ3	1.64	0.62
5:E:238:LYS:HE2	5:E:242:PHE:CE2	2.34	0.62
6:F:87:GLY:H	6:F:92:GLY:HA2	1.64	0.62
7:G:382:ARG:HD2	19:S:56:ARG:HD3	1.82	0.62
13:M:178:ILE:HD12	33:h:143:GLU:HG3	1.80	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)
14:N:100:MET:HE3	14:N:111:PHE:CZ	2.34	0.62
15:O:113:SER:HB3	15:O:116:LYS:HB2	1.80	0.62
23:X:158:LEU:HB3	29:d:21:LEU:HD21	1.80	0.62
28:c:55:TRP:HE1	29:d:66:THR:CG2	2.12	0.62
45:Aa:53:LEU:CD1	45:Aa:57:LEU:HD23	2.28	0.62
1:A:60:ILE:HG21	10:J:166:ILE:HG12	1.81	0.62
4:D:102:SER:HB2	4:D:107:ARG:CD	2.29	0.62
4:D:139:LEU:O	4:D:460:GLU:N	2.32	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
9:I:92:PRO:HG2	42:q:56:PHE:CE2	2.35	0.62
15:O:217:ARG:HG2	15:O:220:LYS:HE3	1.81	0.62
16:P:297:VAL:O	16:P:300:TRP:HB3	1.98	0.62
22:W:55:LEU:CB	22:W:107:MET:HE2	2.30	0.62
25:Z:69:ILE:HG23	27:b:54:PRO:HD3	1.81	0.62
38:m:23:TYR:CD1	39:n:65:ARG:HG2	2.34	0.62
48:AD:290:LEU:HD23	53:AJ:44:TYR:HB2	1.80	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.40	0.62
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.80	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
10:J:78:TYR:HA	11:K:25:HIS:CE1	2.32	0.62
10:J:124:LEU:HG	25:Z:138:PHE:HZ	1.63	0.62
12:L:365:ILE:HD11	12:L:366:MET:HE2	1.82	0.62
12:L:485:PHE:CE1	12:L:486:LEU:HD13	2.26	0.62
20:U:113:LEU:HD23	39:n:17:LEU:CD2	2.29	0.62
25:Z:110:VAL:HG21	30:e:65:GLU:OE2	2.00	0.62
45:AA:478:LEU:HD11	55:AC:401:3PE:H11	1.80	0.62
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.82	0.62
12:L:66:TRP:CZ3	56:h:201:CDL:H591	2.34	0.62
13:M:129:THR:HG21	13:M:235:LEU:CD1	2.30	0.62
13:M:307:TRP:HD1	13:M:459:MET:SD	2.23	0.62
13:M:318:ALA:CB	13:M:373:ILE:HG23	2.29	0.62
15:O:117:PHE:HE1	15:O:128:SER:HB2	1.63	0.62
15:O:121:PRO:O	15:O:122:LYS:CG	2.46	0.62
24:Y:64:THR:OG1	24:Y:106:ARG:HG2	2.00	0.62
39:n:168:TRP:O	39:n:172:THR:OG1	2.18	0.62
45:AA:249:HIS:O	45:AA:250:LEU:HB2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:262:THR:HG22	52:AH:24:LEU:HG	1.81	0.62
49:AE:161:GLU:HA	49:AE:178:HIS:CG	2.34	0.62
46:Ab:412:VAL:O	46:Ab:415:GLN:HG2	2.00	0.62
47:Ac:220:PHE:HE2	69:Ac:405:UQ6:H4M2	1.65	0.62
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.80	0.62
6:F:87:GLY:O	6:F:88:ARG:HB2	1.99	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
55:J:201:3PE:H382	12:L:589:MET:SD	2.39	0.62
14:N:207:ILE:O	14:N:211:LEU:HG	2.00	0.62
14:N:335:MET:O	14:N:335:MET:CG	2.41	0.62
15:O:132:GLN:HE22	15:O:169:PHE:HB2	1.64	0.62
16:P:43:HIS:H	16:P:51:VAL:HG13	1.64	0.62
16:P:318:LYS:HA	16:P:321:ARG:NH1	2.15	0.62
46:AB:412:VAL:O	46:AB:415:GLN:HG2	2.00	0.62
49:AE:152:ILE:HG21	49:AE:274:GLY:H	1.64	0.62
45:Aa:280:ASP:OD2	51:Ag:10:ARG:HA	1.99	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
3:C:212:ASP:OD2	16:P:75:ARG:NH2	2.32	0.62
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.34	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
13:M:56:PHE:HE1	13:M:108:MET:HG2	1.64	0.62
13:M:158:ILE:HG21	14:N:283:ALA:CB	2.30	0.62
16:P:240:VAL:HB	16:P:266:THR:O	2.00	0.62
23:X:7:LEU:CD1	25:Z:87:LEU:HB3	2.30	0.62
25:Z:107:GLY:HA2	30:e:75:ARG:NH2	2.15	0.62
40:o:5:LEU:HB3	40:o:9:TYR:CE2	2.34	0.62
47:AC:202:GLU:OE1	47:Ac:9:PRO:HG3	2.00	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
8:H:17:MET:HE3	8:H:225:MET:HG2	1.82	0.62
8:H:186:PHE:CD1	8:H:270:PHE:HE1	2.14	0.62
11:K:1:MET:N	11:K:2:PRO:HD2	2.15	0.62
15:O:211:VAL:HG21	15:O:235:GLN:CA	2.28	0.62
37:l:38:PRO:HG2	38:m:71:ALA:HB2	1.82	0.62
47:Ac:138:MET:HE1	47:Ac:268:ILE:HG12	1.81	0.62
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.64	0.62
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.24	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.62
15:O:117:PHE:HD1	15:O:128:SER:HA	1.64	0.62
25:Z:143:TYR:HD1	25:Z:144:THR:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:106:ARG:HG2	40:o:110:GLN:HE21	1.64	0.62
45:AA:120:LEU:HB3	46:AB:299:ILE:HA	1.81	0.62
50:AF:20:TRP:HE1	55:AG:103:3PE:H3B2	1.64	0.62
45:Aa:259:GLU:O	45:Aa:260:ASP:C	2.43	0.62
4:D:368:ARG:NH1	9:I:160:GLU:O	2.33	0.61
5:E:180:VAL:HG13	5:E:181:ASN:N	2.15	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.61
7:G:636:TYR:CD1	7:G:642:VAL:HG22	2.34	0.61
9:I:92:PRO:HA	42:q:91:HIS:O	2.00	0.61
13:M:98:MET:HE3	13:M:128:PRO:HA	1.81	0.61
13:M:350:MET:HG2	39:n:99:VAL:HG12	1.82	0.61
15:O:211:VAL:CG2	15:O:235:GLN:HA	2.30	0.61
16:P:156:SER:HB2	16:P:161:VAL:HG21	1.81	0.61
36:k:34:PRO:HG2	36:k:59:TYR:HE1	1.55	0.61
37:l:57:MET:HG2	37:l:104:PRO:HG2	1.82	0.61
56:q:201:CDL:H331	56:q:201:CDL:H722	1.82	0.61
49:AE:213:LEU:HD23	49:AE:260:VAL:HG22	1.81	0.61
48:Ad:223:THR:CG2	52:Ah:52:ASP:HA	2.28	0.61
50:Af:92:GLU:HG2	50:Af:96:LYS:HE2	1.82	0.61
2:B:97:LEU:HD11	2:B:141:MET:HE2	1.82	0.61
4:D:145:MET:HA	4:D:148:GLU:HG2	1.82	0.61
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.80	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
12:L:10:LEU:HD23	12:L:46:ILE:HG21	1.82	0.61
14:N:175:MET:HE1	14:N:227:ILE:HA	1.80	0.61
15:O:140:LEU:HD11	15:O:198:TYR:CZ	2.35	0.61
15:O:326:ARG:HH21	32:g:56:ASP:CG	2.08	0.61
19:S:48:HIS:HE1	19:S:95:LEU:HD22	1.63	0.61
23:X:164:GLY:O	23:X:165:THR:C	2.41	0.61
40:o:69:CYS:C	40:o:80:CYS:SG	2.82	0.61
48:AD:235:PRO:HA	48:AD:240:GLN:HG3	1.82	0.61
12:L:550:LEU:HB2	13:M:275:ILE:HG22	1.83	0.61
13:M:73:LEU:CB	13:M:103:GLN:OE1	2.48	0.61
13:M:81:GLN:O	13:M:85:LYS:HB2	2.01	0.61
16:P:41:ILE:HB	16:P:43:HIS:CE1	2.35	0.61
16:P:106:LEU:HD21	18:R:49:VAL:HG11	1.81	0.61
18:R:72:VAL:HG21	18:R:77:ILE:HD13	1.82	0.61
23:X:18:VAL:HG11	23:X:25:LEU:HD21	1.80	0.61
24:Y:46:ASN:HD22	56:Y:202:CDL:HB22	1.64	0.61
33:h:55:PHE:HB2	34:i:28:LEU:HD21	1.81	0.61
38:m:100:PHE:O	38:m:104:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AF:50:ARG:O	46:Ab:148:ARG:NH2	2.34	0.61
46:Ab:262:ASN:OD1	46:Ab:442:GLY:HA2	2.00	0.61
1:A:93:ILE:HD13	56:A:402:CDL:C59	2.30	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.28	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:317:TYR:HH	26:a:40:ARG:HH22	1.47	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
13:M:105:LEU:HD21	56:M:503:CDL:H411	1.82	0.61
13:M:123:GLU:CB	14:N:255:PRO:HG2	2.28	0.61
13:M:373:ILE:H	13:M:448:THR:HG22	1.65	0.61
13:M:422:HIS:NE2	13:M:425:ASN:OD1	2.33	0.61
14:N:17:PRO:HG2	14:N:133:TRP:CE2	2.35	0.61
14:N:218:ALA:HB1	14:N:240:MET:SD	2.40	0.61
15:O:140:LEU:HD21	15:O:304:VAL:O	2.00	0.61
20:U:128:PHE:CZ	20:U:148:ILE:HG23	2.36	0.61
27:b:11:ASN:O	27:b:15:LYS:N	2.31	0.61
40:o:5:LEU:HB3	40:o:9:TYR:CD2	2.36	0.61
42:q:84:PRO:HD2	42:q:113:HIS:CD2	2.36	0.61
45:AA:268:CYS:SG	45:AA:351:THR:HG21	2.40	0.61
47:AC:29:SER:OG	56:AG:101:CDL:HA61	2.00	0.61
45:Aa:113:VAL:HG13	46:Ab:299:ILE:HD11	1.81	0.61
5:E:65:ILE:HD11	44:s:46:LEU:HD22	1.83	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
12:L:559:GLU:HA	12:L:563:PRO:HG2	1.82	0.61
13:M:391:PHE:CE2	55:m:201:3PE:H242	2.36	0.61
50:AF:92:GLU:HG2	50:AF:96:LYS:HE2	1.82	0.61
51:AG:47:LEU:HB3	55:AG:103:3PE:O22	2.00	0.61
4:D:271:ARG:HD2	8:H:281:ARG:HG2	1.82	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.81	0.61
10:J:150:TRP:HE1	14:N:28:LEU:CD1	2.14	0.61
12:L:427:ILE:HD11	36:k:69:PHE:CE1	2.36	0.61
13:M:98:MET:HE1	13:M:128:PRO:HA	1.83	0.61
13:M:139:GLN:HB3	13:M:222:GLU:HG3	1.83	0.61
13:M:318:ALA:HB2	13:M:373:ILE:CG2	2.30	0.61
13:M:433:GLU:O	13:M:437:MET:HG2	2.01	0.61
15:O:209:VAL:CG1	15:O:260:SER:HB2	2.31	0.61
16:P:363:SER:CB	22:W:51:HIS:NE2	2.60	0.61
32:g:125:LYS:HE3	41:p:8:ASP:HB2	1.82	0.61
33:h:106:ILE:O	33:h:106:ILE:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:62:TYR:CZ	37:l:64:PRO:HG3	2.36	0.61
49:AE:179:ARG:HH12	49:AE:201:ASP:HB2	1.64	0.61
49:AE:244:ASP:HB3	49:AE:250:ARG:HH11	1.66	0.61
45:Aa:388:VAL:HG22	45:Aa:441:LEU:HD13	1.81	0.61
46:Ab:174:ILE:HG21	49:Ai:64:LEU:HD13	1.83	0.61
49:Ae:154:ILE:HB	49:Ae:271:VAL:HG13	1.82	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.81	0.61
12:L:100:ILE:HG21	12:L:246:LEU:HD23	1.82	0.61
12:L:594:ASN:ND2	14:N:110:PRO:HB2	2.15	0.61
20:U:89:LEU:HA	36:k:53:ARG:NH2	2.14	0.61
23:X:46:CYS:SG	23:X:59:GLU:HG3	2.41	0.61
24:Y:111:GLY:HA3	55:Y:201:3PE:H12	1.81	0.61
32:g:109:ASP:HB3	32:g:114:GLU:HB3	1.82	0.61
45:AA:110:GLU:HB2	46:AB:299:ILE:HD13	1.81	0.61
46:AB:167:GLN:NE2	49:AI:43:LEU:HB3	2.16	0.61
48:Ad:124:CYS:HA	48:Ad:179:TYR:CE2	2.35	0.61
51:Ag:64:ASN:O	51:Ag:68:GLU:HG2	2.01	0.61
2:B:120:VAL:HG11	61:H:401:UQ9:H1MB	1.83	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.61
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.30	0.61
12:L:65:THR:HA	34:i:90:MET:HE2	1.82	0.61
12:L:302:ILE:HB	12:L:340:PHE:CE1	2.36	0.61
12:L:468:ILE:O	12:L:472:ILE:HG23	2.00	0.61
13:M:175:ASN:ND2	33:h:143:GLU:HG2	2.16	0.61
20:U:138:LEU:HB3	20:U:144:ILE:HG12	1.83	0.61
29:d:119:VAL:HG21	41:p:147:GLY:CA	2.30	0.61
30:e:32:ARG:O	30:e:33:CYS:HB2	1.99	0.61
46:AB:167:GLN:HG2	49:AI:43:LEU:CD1	2.25	0.61
45:Aa:281:ALA:HB2	51:Ag:10:ARG:HH22	1.66	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:667:GLN:HE21	19:S:38:VAL:HA	1.66	0.61
8:H:89:LEU:HD11	8:H:233:LEU:HD13	1.80	0.61
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.30	0.61
10:J:22:LYS:HD2	11:K:23:ARG:HG2	1.83	0.61
13:M:109:THR:HG22	13:M:121:LEU:HB3	1.82	0.61
13:M:209:LEU:HD23	13:M:210:TYR:N	2.16	0.61
13:M:370:PRO:CA	13:M:375:LEU:HD13	2.29	0.61
16:P:169:HIS:HD2	16:P:181:LEU:HD11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:268:PRO:CG	16:P:344:PRO:HA	2.30	0.61
21:V:95:LEU:HA	21:V:100:TRP:HH2	1.66	0.61
34:i:71:ALA:O	34:i:75:VAL:HB	2.00	0.61
45:AA:92:PHE:HD1	45:AA:168:ILE:HD12	1.66	0.61
67:AC:403:HEM:HMA1	69:AC:406:UQ6:O5	2.01	0.61
53:Aj:30:LEU:HA	54:Ak:34:TRP:CD1	2.36	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
8:H:39:ILE:HG13	42:q:31:ASN:ND2	2.15	0.61
12:L:70:THR:HG21	41:p:101:GLU:OE2	2.00	0.61
12:L:182:PHE:CE2	12:L:186:MET:SD	2.94	0.61
13:M:263:LEU:HD11	38:m:102:TYR:CD1	2.35	0.61
13:M:423:MET:O	13:M:424:ILE:C	2.43	0.61
15:O:201:PRO:HD2	15:O:249:MET:CE	2.30	0.61
23:X:160:PRO:HG3	29:d:22:PRO:CD	2.30	0.61
35:j:84:PHE:CE2	40:o:88:ASP:HB3	2.35	0.61
48:Ad:248:ILE:HD11	70:Ad:401:HEC:HBB1	1.83	0.61
1:A:77:TRP:HZ3	10:J:50:PHE:CE2	2.19	0.60
4:D:128:THR:HG23	4:D:131:GLN:HG2	1.81	0.60
4:D:256:ASP:O	4:D:259:GLU:HB3	2.02	0.60
4:D:323:ARG:O	21:V:12:VAL:CG2	2.49	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
13:M:446:LEU:HB3	55:M:502:3PE:H322	1.82	0.60
31:f:38:ARG:NH1	31:f:56:TRP:O	2.34	0.60
48:AD:156:ASP:CB	48:AD:167:ARG:HE	2.14	0.60
51:AG:64:ASN:O	51:AG:68:GLU:HG2	2.01	0.60
46:Ab:305:THR:CG2	46:Ab:306:THR:N	2.60	0.60
4:D:55:SER:HB2	12:L:575:THR:HG23	1.83	0.60
6:F:69:LEU:HD11	6:F:143:LEU:CD2	2.31	0.60
11:K:22:PHE:CD2	12:L:584:ILE:CG2	2.84	0.60
12:L:40:ILE:HD12	12:L:101:MET:HG3	1.82	0.60
12:L:445:GLU:OE2	35:j:54:GLN:HG3	2.01	0.60
14:N:59:TYR:CZ	14:N:63:GLN:HG3	2.36	0.60
25:Z:110:VAL:HG21	30:e:65:GLU:CG	2.31	0.60
40:o:17:PRO:HB3	40:o:105:GLU:CD	2.26	0.60
48:AD:162:GLY:HA2	48:Ad:183:GLU:HB2	1.82	0.60
47:Ac:128:PHE:CE1	68:Ac:404:U10:H4M2	2.36	0.60
1:A:104:TYR:HE2	10:J:167:ILE:HD13	1.58	0.60
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.14	0.60
4:D:170:ILE:CD1	4:D:236:LEU:CD1	2.79	0.60
4:D:261:MET:HE1	8:H:276:SER:HA	1.83	0.60
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.83	0.60
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.84	0.60
10:J:22:LYS:HB2	11:K:23:ARG:HD3	1.81	0.60
10:J:71:THR:CG2	10:J:75:THR:HG21	2.31	0.60
12:L:145:GLU:HG2	13:M:370:PRO:HD3	1.84	0.60
12:L:482:MET:CE	12:L:486:LEU:HB3	2.31	0.60
40:o:15:VAL:HB	40:o:110:GLN:HG2	1.83	0.60
43:r:12:ARG:HH21	43:r:20:LEU:HD11	1.65	0.60
45:AA:407:THR:HB	45:AA:408:PRO:HD3	1.83	0.60
46:AB:45:ASN:HD22	46:AB:239:ASN:HA	1.67	0.60
47:AC:16:HIS:NE2	47:AC:201:HIS:NE2	2.49	0.60
47:AC:119:LEU:HD22	67:AC:403:HEM:HBB2	1.83	0.60
5:E:134:CYS:SG	5:E:175:CYS:HA	2.41	0.60
6:F:318:ILE:HD11	6:F:355:ILE:CD1	2.28	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
13:M:1:MET:CE	13:M:111:SER:HB2	2.30	0.60
14:N:100:MET:HE3	14:N:111:PHE:HZ	1.66	0.60
21:V:82:LEU:O	21:V:86:LYS:HG3	2.00	0.60
23:X:159:LYS:O	23:X:160:PRO:C	2.43	0.60
24:Y:76:THR:HG23	24:Y:95:GLY:HA3	1.83	0.60
38:m:30:ARG:NE	45:Aa:259:GLU:O	2.33	0.60
49:AE:152:ILE:CG2	49:AE:274:GLY:H	2.13	0.60
45:Aa:55:ASN:HB3	45:Aa:226:ALA:HB1	1.83	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
9:I:188:GLU:HG3	18:R:55:VAL:HA	1.81	0.60
12:L:42:PHE:O	12:L:46:ILE:HG12	2.01	0.60
25:Z:144:THR:O	26:a:36:LYS:HD2	2.02	0.60
49:Ae:207:LYS:HD2	49:Ae:210:TRP:HD1	1.67	0.60
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.84	0.60
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.83	0.60
12:L:222:GLY:CA	12:L:229:LEU:HD11	2.26	0.60
12:L:542:LEU:HD11	55:L:702:3PE:H261	1.83	0.60
13:M:207:MET:HG3	13:M:239:GLY:HA3	1.83	0.60
13:M:269:MET:HE3	13:M:399:ASN:CB	2.32	0.60
13:M:422:HIS:CE1	38:m:56:ARG:HH22	2.19	0.60
15:O:264:GLU:O	15:O:266:PRO:HD3	2.01	0.60
16:P:136:THR:CG2	16:P:139:PHE:HB2	2.31	0.60
18:R:72:VAL:CG1	18:R:77:ILE:HD12	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:97:LYS:HD2	18:R:100:LYS:HB2	1.84	0.60
33:h:129:PRO:HG3	41:p:66:ARG:CZ	2.32	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
8:H:42:PRO:HG3	42:q:28:PHE:CE1	2.36	0.60
8:H:70:LEU:HD13	10:J:27:TYR:HE1	1.67	0.60
13:M:190:TRP:CE2	24:Y:89:PRO:HG2	2.36	0.60
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.84	0.60
21:V:35:LEU:HA	21:V:38:PHE:HD1	1.65	0.60
47:AC:146:ILE:HD11	68:AC:405:U10:C3M	2.31	0.60
46:Ab:40:PHE:CE1	46:Ab:406:TYR:HB2	2.36	0.60
46:Ab:261:GLN:NE2	46:Ab:443:ASN:HA	2.17	0.60
47:Ac:98:VAL:HG22	67:Ac:402:HEM:HBC2	1.82	0.60
48:Ad:138:VAL:HG12	48:Ad:139:CYS:SG	2.42	0.60
49:Ae:115:TYR:CD1	62:Ae:301:PC1:H122	2.37	0.60
49:Ae:244:ASP:HB3	49:Ae:250:ARG:HH11	1.65	0.60
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.67	0.60
6:F:414:GLU:OE1	43:r:50:SER:HA	2.02	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
12:L:204:SER:HA	12:L:207:ASN:HD22	1.67	0.60
13:M:77:LEU:HD23	13:M:99:LEU:HD12	1.83	0.60
13:M:264:LEU:HD23	38:m:98:LEU:HD11	1.84	0.60
33:h:73:PHE:HD2	33:h:74:TYR:CD1	2.20	0.60
47:AC:302:ALA:O	47:AC:305:PRO:HD2	2.02	0.60
48:AD:218:TYR:CD1	48:AD:246:PRO:HG3	2.36	0.60
49:AE:223:VAL:HG23	47:Ac:141:TRP:CH2	2.36	0.60
46:Ab:85:LEU:HD23	49:Ai:68:VAL:HG21	1.83	0.60
2:B:101:ALA:HB1	58:D:501:UQ1:H112	1.83	0.60
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.32	0.60
8:H:136:VAL:CG1	10:J:69:TYR:HE1	2.13	0.60
12:L:56:HIS:O	40:o:71:ARG:HG3	2.02	0.60
14:N:224:SER:HB2	14:N:229:SER:CB	2.32	0.60
14:N:258:THR:CG2	14:N:336:THR:HG22	2.32	0.60
16:P:217:PHE:HA	16:P:220:TYR:CD2	2.36	0.60
19:S:19:ILE:HD12	19:S:94:VAL:HG11	1.83	0.60
30:e:89:GLU:HB2	30:e:91:LYS:HG2	1.82	0.60
33:h:102:PRO:HD2	33:h:105:TYR:CB	2.32	0.60
41:p:40:VAL:HG13	41:p:41:VAL:HG23	1.84	0.60
45:AA:225:LYS:HE3	45:AA:256:VAL:HA	1.83	0.60
49:AE:207:LYS:HD2	49:AE:210:TRP:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:295:GLY:O	45:Aa:301:ASN:ND2	2.35	0.60
4:D:49:GLY:O	14:N:173:THR:HG21	2.02	0.60
5:E:63:GLU:O	5:E:67:LYS:HG3	2.02	0.60
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.36	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
12:L:334:PHE:HZ	62:L:701:PC1:H121	1.67	0.60
13:M:158:ILE:CG2	14:N:283:ALA:HB1	2.31	0.60
13:M:458:THR:HG22	41:p:148:ALA:HB1	1.83	0.60
20:U:90:TYR:CZ	20:U:92:LYS:HD2	2.35	0.60
45:AA:341:PHE:HE2	45:AA:372:LEU:HD13	1.67	0.60
45:AA:469:ASN:ND2	47:AC:223:TYR:CZ	2.70	0.60
46:AB:138:LEU:CD2	46:AB:238:LEU:HG	2.32	0.60
46:AB:253:TYR:CE2	46:AB:435:LYS:HG3	2.36	0.60
48:AD:155:GLN:HA	48:AD:166:MET:HA	1.82	0.60
50:AF:108:TRP:HA	50:AF:111:LYS:NZ	2.17	0.60
1:A:51:PHE:HZ	11:K:79:VAL:CG1	2.15	0.59
2:B:169:GLY:O	2:B:170:TYR:C	2.44	0.59
5:E:70:PRO:HB3	44:s:60:PRO:HG3	1.82	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
22:W:42:TRP:CZ2	22:W:93:LEU:HA	2.37	0.59
23:X:37:ASP:HA	23:X:40:ASN:HB2	1.84	0.59
24:Y:87:ASP:HA	24:Y:128:LYS:HZ1	1.66	0.59
38:m:101:TRP:CH2	55:m:201:3PE:H2A1	2.37	0.59
52:AH:51:CYS:O	52:AH:55:VAL:HG23	2.01	0.59
45:Aa:62:GLU:CB	45:Aa:413:ILE:HD11	2.31	0.59
45:Aa:120:LEU:HD23	46:Ab:299:ILE:HG12	1.83	0.59
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.59
11:K:20:LEU:O	12:L:588:PHE:HB3	2.02	0.59
12:L:123:LEU:HD22	12:L:150:MET:CG	2.32	0.59
12:L:247:LEU:HD12	12:L:248:HIS:CG	2.36	0.59
13:M:294:MET:HE3	13:M:319:HIS:CD2	2.37	0.59
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.85	0.59
14:N:276:LEU:C	14:N:276:LEU:HD12	2.27	0.59
25:Z:110:VAL:HG11	30:e:71:LYS:CB	2.32	0.59
29:d:106:LYS:HB3	41:p:79:GLU:HB3	1.84	0.59
56:d:201:CDL:H602	56:d:201:CDL:H641	1.83	0.59
33:h:73:PHE:CD2	33:h:74:TYR:CD1	2.90	0.59
46:AB:117:GLU:OE2	46:AB:331:SER:N	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:321:TYR:HB2	50:AF:61:PHE:CD1	2.37	0.59
49:AE:132:VAL:HA	49:AE:135:GLN:NE2	2.17	0.59
51:Ag:19:LEU:CD2	51:Ag:24:GLN:HB3	2.29	0.59
1:A:53:MET:CE	10:J:170:THR:HB	2.31	0.59
3:C:141:ARG:NH1	4:D:410:TYR:HE1	2.00	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:114:GLU:OE2	43:r:54:TYR:N	2.31	0.59
7:G:117:MET:HE3	7:G:143:SER:CA	2.32	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:614:GLY:HA2	16:P:41:ILE:HD12	1.84	0.59
7:G:617:ARG:NH1	22:W:128:GLY:C	2.59	0.59
10:J:70:THR:HA	10:J:73:MET:HE2	1.84	0.59
10:J:82:TRP:CZ3	16:P:360:ARG:HB2	2.36	0.59
11:K:93:LEU:HD23	14:N:54:GLU:HG2	1.84	0.59
13:M:115:LEU:O	13:M:118:PHE:HB3	2.02	0.59
13:M:344:MET:HE1	38:m:59:HIS:NE2	2.17	0.59
24:Y:137:LEU:CD2	24:Y:138:PHE:CD2	2.84	0.59
30:e:41:ILE:HG12	33:h:174:PRO:HB2	1.83	0.59
46:AB:313:VAL:HG21	46:AB:323:VAL:HG21	1.83	0.59
50:Af:108:TRP:HA	50:Af:111:LYS:NZ	2.17	0.59
4:D:65:PRO:HG3	4:D:70:ASP:OD1	2.02	0.59
5:E:226:PRO:HG2	5:E:231:THR:H	1.67	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.38	0.59
8:H:306:SER:HG	8:H:310:PHE:HE2	1.32	0.59
9:I:72:MET:HE1	43:r:16:SER:HB2	1.84	0.59
9:I:80:GLU:HG3	26:a:1:MET:SD	2.42	0.59
12:L:81:LYS:HB2	12:L:135:ASN:OD1	2.02	0.59
12:L:145:GLU:HB3	13:M:370:PRO:HG2	1.83	0.59
12:L:173:LEU:CD2	55:L:702:3PE:H322	2.32	0.59
56:M:503:CDL:H542	29:d:32:VAL:HG11	1.84	0.59
21:V:90:LEU:HD21	21:V:94:MET:CE	2.33	0.59
33:h:69:ARG:O	33:h:73:PHE:HB2	2.02	0.59
47:AC:15:ASN:OD1	47:AC:19:ILE:HB	2.03	0.59
47:Ac:302:ALA:O	47:Ac:305:PRO:HD2	2.02	0.59
2:B:95:PHE:CE1	2:B:145:LEU:HD12	2.36	0.59
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.83	0.59
6:F:418:GLN:HE22	7:G:111:LYS:HG3	1.65	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
13:M:368:ALA:O	13:M:375:LEU:HD12	2.02	0.59
14:N:223:ASN:HB3	15:O:306:ASN:HD21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:343:TYR:HE1	15:O:355:LYS:HB2	1.66	0.59
18:R:45:ARG:HA	18:R:48:PHE:HD2	1.67	0.59
19:S:16:LEU:HD11	19:S:19:ILE:CD1	2.32	0.59
21:V:31:THR:HG22	21:V:88:LEU:HD13	1.84	0.59
29:d:116:PHE:HE1	41:p:146:LEU:HD23	1.66	0.59
39:n:61:THR:CG2	45:Aa:262:VAL:HG21	2.32	0.59
45:AA:403:LEU:HD21	45:AA:423:ARG:HH22	1.66	0.59
46:AB:286:PHE:CE1	46:AB:427:ALA:HB1	2.38	0.59
49:AE:163:LYS:O	49:AE:177:ARG:HG3	2.02	0.59
50:Af:106:GLU:O	50:Af:110:LYS:HG3	2.03	0.59
52:Ah:51:CYS:O	52:Ah:55:VAL:HG23	2.02	0.59
4:D:207:ARG:O	4:D:211:PHE:HD1	1.84	0.59
6:F:270:ASN:HD21	6:F:340:ASP:H	1.50	0.59
6:F:318:ILE:CG1	6:F:355:ILE:HB	2.32	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:127:TYR:CE1	8:H:207:LEU:CD2	2.84	0.59
9:I:188:GLU:OE1	18:R:56:ASN:HB2	2.01	0.59
12:L:149:ILE:HG21	13:M:364:LEU:CD2	2.33	0.59
12:L:312:LEU:CD2	12:L:395:ILE:HG21	2.33	0.59
13:M:209:LEU:HD23	13:M:211:GLY:H	1.67	0.59
27:b:8:PHE:HA	27:b:11:ASN:ND2	2.18	0.59
27:b:20:VAL:HG22	55:b:201:3PE:H261	1.84	0.59
48:AD:308:ARG:HD3	51:AG:27:PHE:CE2	2.38	0.59
49:Ae:132:VAL:HA	49:Ae:135:GLN:NE2	2.17	0.59
49:Ai:62:ARG:HB2	49:Ai:78:PHE:C	2.28	0.59
6:F:314:LEU:O	6:F:329:LYS:HB2	2.03	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
12:L:605:ASN:O	12:L:606:LEU:C	2.46	0.59
13:M:14:LEU:HD21	13:M:26:ASN:HB2	1.84	0.59
15:O:72:LYS:O	15:O:76:GLU:HG2	2.02	0.59
32:g:140:PHE:HZ	41:p:152:ALA:HB1	1.68	0.59
40:o:105:GLU:O	40:o:106:ARG:C	2.44	0.59
47:AC:179:PHE:HE2	47:Ac:179:PHE:HE2	1.49	0.59
47:Ac:220:PHE:CE2	69:Ac:405:UQ6:H4M2	2.38	0.59
48:Ad:215:LEU:CD1	70:Ad:401:HEC:CMB	2.73	0.59
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.38	0.59
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.36	0.59
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.67	0.59
6:F:87:GLY:HA3	6:F:92:GLY:HA2	1.84	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:J:71:THR:HG23	10:J:75:THR:HG21	1.84	0.59
12:L:302:ILE:CG2	12:L:340:PHE:CE2	2.80	0.59
12:L:358:LYS:CG	39:n:80:TYR:CE2	2.78	0.59
14:N:200:LEU:HD22	14:N:269:GLU:HG3	1.84	0.59
15:O:250:SER:HA	15:O:255:VAL:HG23	1.85	0.59
15:O:352:ILE:HG21	29:d:52:PRO:HG2	1.85	0.59
16:P:318:LYS:HG2	16:P:322:ILE:HD11	1.84	0.59
32:g:139:TYR:HD2	32:g:140:PHE:CD1	2.20	0.59
33:h:57:VAL:HG12	39:n:99:VAL:HG21	1.83	0.59
45:AA:55:ASN:HB3	45:AA:226:ALA:HB1	1.84	0.59
45:Aa:279:ASP:OD1	51:Ag:12:ARG:NE	2.35	0.59
46:Ab:322:ASP:OD2	49:Ai:59:ALA:HB2	2.02	0.59
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.84	0.59
1:A:73:LEU:HD11	10:J:57:LEU:HD23	1.84	0.59
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.59
4:D:170:ILE:HD13	4:D:236:LEU:HD11	1.84	0.59
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.67	0.59
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.83	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
10:J:166:ILE:CD1	11:K:76:ALA:CB	2.77	0.59
14:N:300:THR:HG23	14:N:301:SER:N	2.16	0.59
14:N:313:MET:CG	15:O:305:LEU:HD22	2.33	0.59
18:R:32:THR:OG1	18:R:36:GLN:HB3	2.03	0.59
27:b:6:SER:O	27:b:9:LEU:HB3	2.03	0.59
33:h:95:GLU:HB3	33:h:114:LYS:HG2	1.85	0.59
39:n:111:GLU:O	39:n:114:MET:HG2	2.03	0.59
44:s:57:LEU:HG	44:s:58:PRO:HD2	1.84	0.59
45:AA:120:LEU:HD23	46:AB:299:ILE:HG12	1.85	0.59
45:AA:172:MET:HE1	45:AA:205:SER:HA	1.84	0.59
48:AD:233:PHE:HA	48:AD:240:GLN:O	2.02	0.59
3:C:100:ARG:NH1	21:V:86:LYS:NZ	2.51	0.59
3:C:242:PRO:O	3:C:243:ALA:C	2.45	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.59
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.85	0.59
6:F:318:ILE:HG12	6:F:355:ILE:HB	1.85	0.59
12:L:193:MET:CE	38:m:125:PHE:CD2	2.85	0.59
12:L:466:PHE:CE1	12:L:470:TYR:HE2	2.21	0.59
12:L:520:SER:O	12:L:524:THR:N	2.36	0.59
12:L:570:HIS:O	12:L:571:THR:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:210:TYR:O	13:M:213:HIS:CD2	2.56	0.59
15:O:114:LEU:HA	15:O:131:LEU:HD21	1.84	0.59
16:P:178:SER:O	16:P:182:ARG:HG2	2.02	0.59
23:X:120:PRO:HB2	23:X:125:LEU:HD11	1.85	0.59
23:X:124:GLN:HA	23:X:127:LYS:HE3	1.83	0.59
30:e:38:LYS:HG2	33:h:179:ILE:CG2	2.32	0.59
41:p:36:ALA:O	41:p:40:VAL:HG12	2.03	0.59
43:r:20:LEU:C	43:r:20:LEU:HD12	2.27	0.59
45:AA:113:VAL:CG1	46:AB:299:ILE:HD11	2.33	0.59
48:AD:248:ILE:HD11	70:AD:401:HEC:HBB1	1.85	0.59
51:AG:19:LEU:CD2	51:AG:24:GLN:HB3	2.29	0.59
46:Ab:104:GLU:HG3	49:Ai:70:LEU:HD21	1.84	0.59
48:Ad:106:ASP:O	48:Ad:110:ILE:HG13	2.03	0.59
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD1	2.38	0.59
1:A:89:ILE:HD11	56:A:402:CDL:C54	2.30	0.58
4:D:326:CYS:CB	4:D:453:THR:HG21	2.32	0.58
6:F:267:ARG:HH12	6:F:340:ASP:HB3	1.68	0.58
10:J:154:VAL:HG22	11:K:66:PHE:CZ	2.38	0.58
13:M:127:ILE:HG12	14:N:254:LEU:CD2	2.31	0.58
13:M:275:ILE:HD11	13:M:288:TYR:CB	2.33	0.58
15:O:93:TYR:CG	15:O:93:TYR:O	2.57	0.58
19:S:63:PRO:HB2	19:S:79:LEU:HB2	1.85	0.58
20:U:105:MET:SD	20:U:139:MET:HE1	2.42	0.58
33:h:57:VAL:HG12	39:n:99:VAL:CG2	2.33	0.58
42:q:66:THR:HG22	42:q:67:GLU:OE2	2.03	0.58
47:AC:345:HIS:CE1	47:AC:346:PRO:HB3	2.38	0.58
46:Ab:85:LEU:CD2	49:Ai:68:VAL:HG11	2.33	0.58
46:Ab:286:PHE:CE1	46:Ab:427:ALA:HB1	2.38	0.58
49:Ae:264:GLU:HB3	49:Ae:272:VAL:HB	1.85	0.58
1:A:90:MET:HE2	10:J:152:MET:HB3	1.84	0.58
2:B:99:CYS:HB3	4:D:141:TYR:CB	2.33	0.58
4:D:51:VAL:HG21	4:D:58:THR:HG22	1.83	0.58
6:F:225:LEU:N	17:Q:160:TYR:HE2	1.95	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
11:K:19:THR:HG23	11:K:29:THR:HG23	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:46:ASP:HA	32:g:112:MET:HG3	1.85	0.58
13:M:396:MET:HG3	13:M:396:MET:O	2.03	0.58
14:N:77:ASN:OD1	14:N:81:LEU:HD12	2.04	0.58
23:X:151:ASN:ND2	30:e:51:ARG:HH11	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:97:ILE:HD12	30:e:79:ILE:CG2	2.32	0.58
27:b:27:GLY:O	27:b:30:ILE:HG22	2.02	0.58
51:AG:72:ARG:NH1	52:AH:67:GLU:HB2	2.18	0.58
45:Aa:118:ALA:O	46:Ab:298:HIS:CD2	2.55	0.58
46:Ab:312:SER:O	46:Ab:313:VAL:C	2.46	0.58
1:A:77:TRP:CH2	10:J:50:PHE:HD2	2.21	0.58
4:D:37:TRP:CZ2	4:D:39:PRO:HA	2.38	0.58
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.87	0.58
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.32	0.58
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.85	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
12:L:407:TRP:CZ3	12:L:410:LEU:HD11	2.38	0.58
13:M:123:GLU:CG	14:N:255:PRO:HG2	2.33	0.58
14:N:179:MET:CG	14:N:216:PHE:HE1	2.16	0.58
16:P:57:THR:HG23	16:P:123:SER:CB	2.33	0.58
19:S:65:LEU:HB2	19:S:79:LEU:HD11	1.84	0.58
23:X:123:GLY:HA2	25:Z:66:GLU:OE2	2.03	0.58
37:l:105:ILE:HG23	37:l:109:LEU:HD22	1.84	0.58
42:q:59:HIS:CE1	42:q:60:ARG:CG	2.83	0.58
45:AA:285:ALA:O	45:AA:360:CYS:N	2.36	0.58
49:AE:152:ILE:HD13	49:AE:169:TRP:CD1	2.38	0.58
50:AF:106:GLU:O	50:AF:110:LYS:HG3	2.03	0.58
54:AK:37:ASP:O	54:AK:39:ARG:HG3	2.03	0.58
4:D:97:LEU:CD2	4:D:111:PRO:HB3	2.33	0.58
6:F:270:ASN:ND2	6:F:340:ASP:H	2.00	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
12:L:404:THR:HG22	12:L:405:ASN:N	2.19	0.58
12:L:441:ILE:HG21	35:j:48:PRO:HD3	1.85	0.58
12:L:598:ILE:HD11	14:N:153:ILE:HD13	1.84	0.58
20:U:119:ILE:HD11	20:U:138:LEU:HB2	1.85	0.58
26:a:36:LYS:HA	26:a:59:ARG:HH22	1.68	0.58
29:d:14:LEU:HD12	29:d:14:LEU:C	2.27	0.58
30:e:38:LYS:NZ	33:h:181:HIS:HD2	2.02	0.58
37:l:113:ILE:HG12	37:l:114:ARG:H	1.67	0.58
41:p:128:GLU:O	41:p:131:GLN:N	2.37	0.58
54:AK:10:TYR:CD1	50:Af:110:LYS:HA	2.38	0.58
48:Ad:156:ASP:HB2	48:Ad:167:ARG:HG3	1.85	0.58
49:Ae:159:ILE:O	49:Ae:210:TRP:HH2	1.86	0.58
12:L:261:VAL:C	12:L:264:HIS:HD2	2.12	0.58
16:P:57:THR:HG23	16:P:123:SER:HB2	1.86	0.58
22:W:104:THR:O	22:W:108:ARG:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:70:PHE:O	34:i:71:ALA:C	2.47	0.58
38:m:75:ASN:O	38:m:75:ASN:OD1	2.20	0.58
49:AE:156:LEU:HD13	49:AE:210:TRP:NE1	2.19	0.58
49:Ae:146:VAL:HA	49:Ae:149:MET:HE3	1.86	0.58
49:Ae:163:LYS:O	49:Ae:177:ARG:HG3	2.03	0.58
51:Ag:11:ILE:HG22	51:Ag:12:ARG:N	2.18	0.58
6:F:51:TRP:CB	6:F:133:HIS:O	2.52	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:119:GLU:OE1	6:F:125:CYS:HA	2.03	0.58
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.38	0.58
6:F:303:HIS:O	6:F:304:ALA:C	2.45	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:267:THR:HB	17:Q:115:ALA:HB2	1.86	0.58
12:L:436:ARG:HA	36:k:58:ARG:NH1	2.18	0.58
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.33	0.58
14:N:147:PRO:HB2	14:N:148:LEU:HD12	1.86	0.58
20:U:105:MET:CG	20:U:139:MET:HE1	2.33	0.58
31:f:47:GLU:HG2	31:f:47:GLU:O	2.03	0.58
41:p:31:THR:O	41:p:35:LYS:HG3	2.03	0.58
49:AE:160:PRO:O	49:AE:178:HIS:HB3	2.03	0.58
45:Aa:92:PHE:HD1	45:Aa:168:ILE:HD12	1.66	0.58
45:Aa:172:MET:HE1	45:Aa:205:SER:HA	1.85	0.58
47:Ac:345:HIS:CE1	47:Ac:346:PRO:HB3	2.38	0.58
49:Ae:156:LEU:HB2	49:Ae:269:ASP:CA	2.34	0.58
4:D:112:HIS:HE1	22:W:100:TRP:CD1	2.22	0.58
4:D:203:MET:HE2	4:D:258:VAL:HG13	1.86	0.58
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.81	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.66	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
12:L:542:LEU:HD21	37:l:116:ARG:HD2	1.86	0.58
24:Y:71:MET:HG3	24:Y:102:THR:HG21	1.85	0.58
42:q:125:VAL:HG23	42:q:125:VAL:O	2.03	0.58
48:AD:218:TYR:CG	48:AD:246:PRO:HG3	2.38	0.58
49:AE:156:LEU:HB2	49:AE:269:ASP:C	2.28	0.58
52:AH:58:ARG:HD3	52:AH:61:THR:HB	1.86	0.58
49:Ae:160:PRO:O	49:Ae:178:HIS:HB3	2.03	0.58
4:D:94:VAL:HB	4:D:115:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.34	0.58
4:D:217:VAL:HG22	4:D:226:TYR:CE1	2.39	0.58
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.19	0.58
10:J:78:TYR:CE2	10:J:82:TRP:HA	2.38	0.58
12:L:15:LEU:O	12:L:18:PRO:HD2	2.03	0.58
12:L:425:ARG:HG3	12:L:429:PHE:CE2	2.39	0.58
12:L:446:ASN:HD21	35:j:51:THR:HG21	1.69	0.58
12:L:446:ASN:ND2	35:j:51:THR:HG21	2.18	0.58
12:L:466:PHE:HE1	35:j:72:ARG:CZ	2.14	0.58
13:M:73:LEU:HB2	13:M:103:GLN:OE1	2.02	0.58
13:M:196:TRP:HZ3	13:M:261:PHE:CE2	2.21	0.58
14:N:26:LEU:O	14:N:27:MET:C	2.46	0.58
23:X:167:PHE:HB3	23:X:170:TRP:CD1	2.39	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
45:Aa:220:LEU:O	45:Aa:224:TYR:HB2	2.04	0.58
45:Aa:251:SER:O	45:Aa:252:SER:HB3	2.02	0.58
47:Ac:138:MET:HE1	47:Ac:268:ILE:CA	2.31	0.58
48:Ad:152:VAL:HG21	48:Ad:176:PRO:CG	2.34	0.58
1:A:63:LEU:CG	10:J:66:VAL:HG21	2.34	0.58
4:D:121:GLU:HG2	4:D:424:ILE:HD12	1.86	0.58
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.58
8:H:17:MET:CE	8:H:225:MET:HG2	2.34	0.58
12:L:427:ILE:HD11	36:k:69:PHE:HE1	1.66	0.58
20:T:90:TYR:CE2	20:T:110:LEU:HD11	2.39	0.58
23:X:145:ARG:HH11	30:e:58:ILE:HB	1.68	0.58
38:m:25:VAL:O	45:Aa:261:ALA:HB1	2.02	0.58
45:AA:286:HIS:CD2	45:AA:359:VAL:HG13	2.38	0.58
45:AA:295:GLY:O	45:AA:301:ASN:ND2	2.35	0.58
49:AE:159:ILE:O	49:AE:210:TRP:HH2	1.86	0.58
54:Ak:39:ARG:HH22	54:Ak:50:GLY:H	1.52	0.58
1:A:94:LEU:HD22	10:J:152:MET:CE	2.34	0.58
4:D:145:MET:HA	4:D:148:GLU:CG	2.34	0.58
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.58
13:M:109:THR:HG22	13:M:121:LEU:CB	2.34	0.58
14:N:33:LEU:HD11	14:N:141:ILE:HD12	1.86	0.58
14:N:149:LEU:HD11	14:N:195:PRO:HG3	1.84	0.58
15:O:117:PHE:CD1	15:O:128:SER:CB	2.87	0.58
32:g:121:GLU:HA	32:g:124:VAL:HG22	1.86	0.58
52:AH:49:GLU:HA	52:AH:52:ASP:OD2	2.04	0.58
45:Aa:70:THR:O	45:Aa:410:CYS:SG	2.60	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:171:GLU:O	45:Aa:175:ASN:N	2.37	0.58
46:Ab:170:GLN:HB2	49:Ai:78:PHE:CZ	2.39	0.58
49:Ae:88:PHE:O	49:Ae:92:ARG:HG3	2.04	0.58
6:F:297:LYS:O	6:F:301:GLU:HG2	2.03	0.57
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.12	0.57
12:L:232:TRP:CZ3	12:L:233:LEU:HD21	2.38	0.57
12:L:556:ILE:CG2	38:m:80:PHE:CE2	2.86	0.57
16:P:245:VAL:O	16:P:249:ILE:HG13	2.04	0.57
20:U:100:VAL:C	20:U:141:PRO:HG2	2.28	0.57
21:V:28:TYR:HE2	21:V:59:VAL:HG21	1.69	0.57
51:AG:35:ILE:HB	51:AG:36:PRO:HD3	1.86	0.57
45:Aa:87:ASN:HD21	45:Aa:199:GLN:HB2	1.69	0.57
47:Ac:150:LEU:HD13	47:Ac:164:ILE:HD12	1.86	0.57
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.57
1:A:80:GLN:NE2	8:H:315:PRO:O	2.37	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.04	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.86	0.57
12:L:592:LEU:O	12:L:596:ILE:HG12	2.04	0.57
13:M:172:GLY:C	13:M:173:THR:HG23	2.28	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	1.68	0.57
16:P:363:SER:O	22:W:51:HIS:CD2	2.58	0.57
17:Q:77:VAL:HG12	17:Q:101:PHE:HA	1.86	0.57
18:R:37:VAL:O	18:R:37:VAL:HG13	2.03	0.57
45:AA:171:GLU:O	45:AA:175:ASN:N	2.37	0.57
46:Ab:47:LEU:HA	46:Ab:218:MET:O	2.04	0.57
4:D:159:LEU:HG	4:D:391:VAL:HG12	1.86	0.57
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.68	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:17:MET:SD	8:H:225:MET:O	2.62	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
12:L:510:LYS:HE3	12:L:512:SER:HB2	1.84	0.57
24:Y:63:PHE:HE2	24:Y:106:ARG:HE	1.53	0.57
24:Y:108:HIS:CE1	55:Ag:103:3PE:C39	2.80	0.57
30:e:14:LEU:HD12	30:e:15:ASP:CB	2.33	0.57
34:i:70:PHE:CD2	34:i:74:HIS:CD2	2.92	0.57
47:AC:150:LEU:HD13	47:AC:164:ILE:HD12	1.86	0.57
48:AD:120:VAL:O	70:AD:401:HEC:HMC3	2.04	0.57
45:Aa:338:CYS:HB2	45:Aa:368:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:104:SER:HB2	48:Ad:283:ASP:CG	2.29	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
5:E:107:PRO:HB2	5:E:110:ARG:HG2	1.87	0.57
6:F:291:GLU:HG2	6:F:292:MET:O	2.05	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
7:G:608:VAL:HG23	17:Q:103:THR:HG1	1.66	0.57
7:G:632:ILE:HG13	7:G:632:ILE:O	2.04	0.57
12:L:424:MET:HE2	12:L:502:LEU:HB2	1.85	0.57
12:L:588:PHE:CZ	14:N:61:VAL:HG12	2.40	0.57
13:M:127:ILE:CD1	14:N:256:PRO:HG2	2.31	0.57
13:M:230:ILE:HG13	13:M:235:LEU:HG	1.87	0.57
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.86	0.57
14:N:154:ILE:HG12	14:N:195:PRO:HG2	1.86	0.57
18:R:52:GLN:NE2	18:R:54:GLU:HA	2.19	0.57
33:h:188:ASP:O	33:h:189:ASN:C	2.48	0.57
38:m:127:ILE:CG2	41:p:136:THR:HG23	2.33	0.57
48:AD:249:TYR:CE2	48:AD:252:VAL:HA	2.39	0.57
50:AF:107:GLU:OE2	50:AF:111:LYS:HD3	2.05	0.57
55:Aa:501:3PE:H32	47:Ac:221:HIS:CE1	2.40	0.57
47:Ac:147:THR:HG21	47:Ac:165:TRP:CD1	2.40	0.57
52:Ah:58:ARG:HD3	52:Ah:61:THR:HB	1.86	0.57
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.34	0.57
3:C:67:ILE:HD12	21:V:44:TYR:HA	1.85	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
8:H:180:PRO:HD3	25:Z:43:LEU:HD21	1.87	0.57
12:L:227:PHE:CD2	12:L:283:LEU:HD21	2.38	0.57
13:M:73:LEU:HD22	13:M:103:GLN:NE2	2.18	0.57
13:M:447:LEU:HD21	13:M:454:ILE:CD1	2.33	0.57
14:N:253:GLY:N	14:N:290:LEU:HD11	2.19	0.57
14:N:284:MET:O	14:N:287:LEU:HB2	2.04	0.57
15:O:132:GLN:NE2	63:O:401:ADP:HN62	2.02	0.57
31:f:37:PHE:CE2	33:h:141:GLN:OE1	2.57	0.57
38:m:45:ARG:HG2	38:m:49:LEU:HD13	1.87	0.57
38:m:97:PRO:CB	55:m:201:3PE:H2G2	2.34	0.57
46:AB:162:LYS:NZ	46:AB:194:ASP:OD1	2.38	0.57
48:AD:284:HIS:NE2	48:AD:288:MET:HE3	2.19	0.57
45:Aa:120:LEU:HD23	46:Ab:299:ILE:HG23	1.86	0.57
48:Ad:120:VAL:O	70:Ad:401:HEC:HMC3	2.04	0.57
49:Ae:93:ARG:HD2	49:Ae:110:ARG:HD2	1.85	0.57
51:Ag:27:PHE:HB3	51:Ag:30:TYR:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Aj:11:TYR:CZ	53:Aj:16:ARG:HB2	2.39	0.57
2:B:106:HIS:HE1	4:D:207:ARG:HB3	1.69	0.57
4:D:92:HIS:CD2	58:D:501:UQ1:C2	2.87	0.57
4:D:170:ILE:CD1	4:D:236:LEU:HD13	2.34	0.57
4:D:320:ILE:O	4:D:320:ILE:HG13	2.03	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
8:H:136:VAL:CG1	10:J:69:TYR:CE1	2.87	0.57
10:J:63:MET:CE	11:K:68:ALA:CA	2.83	0.57
13:M:297:VAL:O	13:M:301:ILE:HG12	2.03	0.57
13:M:444:LEU:O	13:M:448:THR:HG23	2.04	0.57
15:O:167:PHE:CZ	15:O:244:THR:CG2	2.88	0.57
20:U:93:ILE:HD11	20:U:110:LEU:HD11	1.86	0.57
21:V:31:THR:O	21:V:35:LEU:HG	2.05	0.57
25:Z:59:ARG:NH2	27:b:84:LEU:HB3	2.18	0.57
37:l:166:LEU:HB2	37:l:170:ARG:NH2	2.19	0.57
40:o:39:MET:CE	40:o:58:TYR:HA	2.35	0.57
45:AA:87:ASN:HD21	45:AA:199:GLN:HB2	1.69	0.57
46:AB:322:ASP:OD2	49:AI:59:ALA:CB	2.53	0.57
48:Ad:213:SER:HB3	48:Ad:236:TYR:CD2	2.40	0.57
2:B:202:LEU:HD23	9:I:86:TYR:CB	2.34	0.57
4:D:280:ALA:CB	21:V:11:LEU:CG	2.83	0.57
4:D:320:ILE:HG12	9:I:36:TYR:HD2	1.69	0.57
6:F:87:GLY:N	6:F:92:GLY:HA2	2.19	0.57
6:F:270:ASN:HD22	6:F:338:ASP:CG	2.13	0.57
6:F:296:LEU:O	6:F:297:LYS:C	2.47	0.57
8:H:14:LEU:HG	61:H:401:UQ9:H23	1.86	0.57
8:H:65:THR:HG22	16:P:359:TYR:HD1	1.64	0.57
8:H:175:LEU:HD21	62:I:301:PC1:H2C1	1.86	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
12:L:425:ARG:HG3	12:L:429:PHE:HE2	1.68	0.57
13:M:388:TRP:CD1	38:m:109:ARG:HD2	2.40	0.57
14:N:179:MET:HG3	14:N:216:PHE:CE1	2.39	0.57
27:b:23:PHE:HE1	55:b:201:3PE:H3A2	1.69	0.57
32:g:147:LEU:HD11	41:p:163:MET:CB	2.28	0.57
38:m:49:LEU:HD12	39:n:166:LEU:HD11	1.85	0.57
38:m:97:PRO:HG3	55:m:201:3PE:C2G	2.34	0.57
42:q:86:TRP:CG	42:q:98:PRO:HG2	2.39	0.57
42:q:129:THR:O	42:q:129:THR:HG22	2.03	0.57
52:Ah:49:GLU:HA	52:Ah:52:ASP:OD2	2.04	0.57
2:B:112:TYR:CZ	2:B:199:GLU:HG2	2.40	0.57
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.35	0.57
13:M:42:LEU:HD11	13:M:67:ILE:CD1	2.34	0.57
14:N:273:ASN:O	14:N:274:ASN:HB2	2.05	0.57
17:Q:125:VAL:HG23	17:Q:125:VAL:O	2.05	0.57
55:i:201:3PE:H292	55:i:201:3PE:H332	1.86	0.57
49:AE:207:LYS:HB3	49:AE:209:GLU:OE1	2.05	0.57
46:Ab:51:SER:HB2	46:Ab:230:LEU:CD1	2.33	0.57
46:Ab:297:PRO:CA	46:Ab:304:ASN:OD1	2.52	0.57
48:Ad:249:TYR:CE2	48:Ad:252:VAL:HA	2.40	0.57
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.86	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
13:M:12:LEU:HB2	13:M:13:PRO:HD3	1.85	0.57
13:M:165:ILE:HG21	14:N:268:THR:HA	1.86	0.57
15:O:38:TYR:HB3	15:O:299:GLN:HE22	1.70	0.57
20:U:130:ILE:HG23	20:U:147:TYR:CE2	2.40	0.57
34:i:87:LYS:HG2	34:i:87:LYS:O	2.05	0.57
47:AC:147:THR:HG21	47:AC:165:TRP:CD1	2.40	0.57
47:AC:378:LYS:HE3	50:AF:89:PHE:HE2	1.69	0.57
47:Ac:21:LEU:HD13	69:Ac:405:UQ6:O2	2.05	0.57
50:Af:107:GLU:OE2	50:Af:111:LYS:HD3	2.05	0.57
1:A:51:PHE:CZ	11:K:79:VAL:CG1	2.88	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
3:C:149:LEU:HD11	22:W:80:ARG:HH21	1.64	0.57
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.87	0.57
6:F:382:CYS:HA	7:G:74:ASN:O	2.05	0.57
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.57
8:H:17:MET:SD	8:H:225:MET:CA	2.93	0.57
12:L:60:GLU:CG	12:L:83:ASP:HA	2.35	0.57
12:L:88:LEU:HD23	12:L:326:PHE:HE2	1.69	0.57
12:L:229:LEU:HD12	12:L:229:LEU:C	2.28	0.57
12:L:253:VAL:CG2	12:L:310:LEU:HD11	2.35	0.57
13:M:14:LEU:HD11	13:M:26:ASN:HB3	1.87	0.57
13:M:154:LEU:HB3	14:N:287:LEU:HD22	1.86	0.57
13:M:269:MET:HE3	13:M:399:ASN:HB2	1.86	0.57
15:O:91:ILE:O	15:O:134:TRP:NE1	2.37	0.57
16:P:55:VAL:HA	16:P:79:GLN:HB3	1.85	0.57
33:h:175:GLU:HB3	33:h:177:GLU:HG2	1.86	0.57
45:AA:338:CYS:HB2	45:AA:368:MET:SD	2.45	0.57
48:Ad:98:HIS:HB3	48:Ad:105:LEU:HD23	1.87	0.57
49:Ae:156:LEU:HD13	49:Ae:210:TRP:NE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Ak:10:TYR:HA	54:Ak:13:LEU:HD12	1.87	0.57
3:C:209:LEU:HD21	22:W:108:ARG:NH1	2.20	0.56
5:E:73:HIS:HB3	6:F:236:PHE:CE1	2.40	0.56
12:L:9:LEU:HD11	55:i:201:3PE:H2A1	1.85	0.56
15:O:173:MET:HE2	15:O:179:ILE:HG23	1.87	0.56
29:d:100:ASP:HB3	33:h:159:LEU:HD21	1.87	0.56
29:d:101:PHE:CZ	33:h:156:VAL:HG22	2.40	0.56
38:m:45:ARG:O	38:m:49:LEU:HD13	2.05	0.56
39:n:81:ILE:CD1	39:n:87:GLY:O	2.53	0.56
51:AG:33:LYS:C	51:AG:36:PRO:HD2	2.30	0.56
49:Ae:218:THR:HG21	49:Ae:256:LEU:C	2.30	0.56
6:F:69:LEU:HD11	6:F:143:LEU:HD21	1.87	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.13	0.56
10:J:116:ASN:HD22	10:J:123:TRP:HE1	1.51	0.56
13:M:310:MET:O	13:M:314:MET:HG3	2.04	0.56
14:N:226:THR:HG22	14:N:228:ASN:H	1.70	0.56
15:O:125:ASP:OD1	15:O:126:GLY:N	2.38	0.56
15:O:320:GLY:HA2	32:g:53:TRP:HZ3	1.68	0.56
23:X:5:VAL:HG13	23:X:7:LEU:HG	1.87	0.56
31:f:49:ARG:HB2	31:f:50:PRO:HD2	1.87	0.56
45:Aa:222:ARG:CZ	45:Aa:263:PRO:HB3	2.35	0.56
1:A:64:LEU:CD1	10:J:163:ILE:HG12	2.35	0.56
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.87	0.56
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.85	0.56
2:B:110:PRO:HB3	8:H:33:LEU:O	2.05	0.56
2:B:154:GLU:O	2:B:155:PRO:C	2.48	0.56
2:B:164:CYS:SG	57:B:301:SF4:S3	3.03	0.56
6:F:278:ILE:CD1	6:F:304:ALA:HB1	2.35	0.56
7:G:362:ASP:HB2	19:S:71:PHE:CD1	2.39	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:625:ALA:O	7:G:629:ILE:HG12	2.04	0.56
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.69	0.56
9:I:88:PHE:CZ	42:q:30:ALA:HA	2.40	0.56
10:J:135:LEU:CA	11:K:54:MET:HE1	2.34	0.56
13:M:78:MET:O	13:M:432:ARG:HD2	2.05	0.56
13:M:282:LEU:HD13	13:M:342:MET:HE2	1.87	0.56
14:N:254:LEU:CD1	14:N:255:PRO:HD2	2.35	0.56
15:O:81:LEU:N	15:O:81:LEU:CD1	2.69	0.56
18:R:44:ARG:HG2	18:R:47:ARG:HH12	1.70	0.56
23:X:53:PRO:HD3	25:Z:116:TRP:CD1	2.40	0.56
23:X:168:PHE:O	23:X:169:PHE:CD1	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:92:TYR:CE1	24:Y:128:LYS:HD3	2.40	0.56
25:Z:8:GLN:HG3	43:r:41:LEU:HD12	1.86	0.56
25:Z:127:LEU:CD2	30:e:80:LYS:HG2	2.34	0.56
30:e:38:LYS:HG2	33:h:179:ILE:HG23	1.86	0.56
34:i:70:PHE:HA	34:i:74:HIS:HD2	1.70	0.56
45:AA:68:THR:HG22	45:AA:136:LEU:CD2	2.35	0.56
47:AC:171:ASP:CG	47:AC:172:LYS:H	2.13	0.56
49:AE:219:HIS:HB2	49:AE:254:ALA:HA	1.88	0.56
50:AF:22:TYR:CD2	50:AF:84:TYR:HB2	2.41	0.56
54:AK:10:TYR:HA	54:AK:13:LEU:HD12	1.87	0.56
45:Aa:384:THR:HG21	54:Ak:9:ARG:HG2	1.87	0.56
47:Ac:141:TRP:CD1	47:Ac:265:PRO:HD2	2.41	0.56
47:Ac:171:ASP:CG	47:Ac:172:LYS:H	2.13	0.56
50:Af:22:TYR:CD2	50:Af:84:TYR:HB2	2.41	0.56
54:Ak:6:LEU:HD12	54:Ak:11:ARG:HH12	1.71	0.56
3:C:123:ASN:HD22	21:V:108:PRO:HG2	1.69	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
7:G:62:ARG:H	7:G:142:GLN:HE22	1.53	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.56
8:H:4:ILE:O	8:H:8:THR:HG23	2.05	0.56
11:K:73:VAL:HG21	14:N:38:LEU:HD22	1.87	0.56
12:L:573:MET:HE1	56:Y:202:CDL:H312	1.86	0.56
13:M:118:PHE:O	13:M:122:PHE:CB	2.54	0.56
13:M:127:ILE:HG13	14:N:254:LEU:HD21	1.86	0.56
15:O:149:HIS:CE1	15:O:153:THR:HG21	2.39	0.56
15:O:204:VAL:CG2	15:O:255:VAL:HG22	2.36	0.56
21:V:95:LEU:HA	21:V:100:TRP:CH2	2.40	0.56
23:X:103:GLN:HA	23:X:106:LYS:HD3	1.88	0.56
23:X:122:LEU:HD23	27:b:82:LYS:HG2	1.88	0.56
37:l:38:PRO:C	38:m:75:ASN:ND2	2.64	0.56
47:AC:18:PHE:CD1	69:AC:406:UQ6:H1M2	2.40	0.56
47:AC:264:THR:CG2	49:Ae:225:ILE:CD1	2.70	0.56
49:AE:152:ILE:HG13	49:AE:154:ILE:CD1	2.35	0.56
49:AE:218:THR:HG21	49:AE:256:LEU:C	2.30	0.56
45:Aa:186:TYR:CE1	49:Ae:80:HIS:HB2	2.40	0.56
46:Ab:300:LYS:HG2	46:Ab:301:ARG:HG3	1.86	0.56
1:A:56:PHE:HA	10:J:73:MET:HE1	1.88	0.56
55:A:401:3PE:C24	10:J:41:LEU:HD22	2.36	0.56
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.06	0.56
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.35	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:SER:HB3	13:M:113:THR:HG22	1.88	0.56
16:P:64:PHE:HE1	16:P:209:ARG:O	1.88	0.56
16:P:315:THR:HG22	16:P:317:ASP:H	1.69	0.56
16:P:323:HIS:ND1	16:P:323:HIS:O	2.39	0.56
28:c:68:GLU:HB2	29:d:19:ARG:HD2	1.87	0.56
45:AA:190:THR:CG2	45:AA:275:ILE:HG22	2.36	0.56
45:AA:280:ASP:OD2	51:AG:10:ARG:HA	2.05	0.56
46:AB:297:PRO:CA	46:AB:304:ASN:OD1	2.52	0.56
47:AC:9:PRO:O	47:AC:12:LYS:HB3	2.05	0.56
47:AC:56:THR:HG21	47:Ac:58:ASP:HB2	1.86	0.56
46:Ab:162:LYS:NZ	46:Ab:194:ASP:OD1	2.38	0.56
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.36	0.56
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.40	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
13:M:4:ILE:CG2	13:M:107:ILE:HD13	2.30	0.56
56:M:503:CDL:OA4	56:M:503:CDL:H752	2.06	0.56
14:N:120:GLN:O	14:N:176:ARG:CZ	2.54	0.56
14:N:149:LEU:CD1	14:N:154:ILE:HG21	2.35	0.56
15:O:114:LEU:O	15:O:117:PHE:HB3	2.06	0.56
30:e:14:LEU:HD12	30:e:14:LEU:C	2.31	0.56
32:g:106:TYR:OH	33:h:86:ILE:HD12	2.06	0.56
39:n:50:GLU:HG2	39:n:51:HIS:N	2.20	0.56
56:q:201:CDL:H141	56:q:201:CDL:H321	1.87	0.56
49:AE:197:ASP:HB3	49:AE:257:ASN:OD1	2.06	0.56
50:Af:15:ASP:OD2	50:Af:19:LYS:NZ	2.39	0.56
51:Ag:33:LYS:C	51:Ag:36:PRO:HD2	2.30	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:127:TYR:CD1	8:H:207:LEU:HD23	2.36	0.56
10:J:50:PHE:CE1	10:J:54:MET:HG3	2.41	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
14:N:196:TYR:HB3	14:N:273:ASN:OD1	2.05	0.56
14:N:253:GLY:H	14:N:290:LEU:HD11	1.71	0.56
14:N:321:LYS:HD2	29:d:49:ARG:NE	2.20	0.56
27:b:67:PRO:HB3	27:b:74:LEU:HB2	1.87	0.56
32:g:140:PHE:CZ	41:p:74:ILE:HG22	2.41	0.56
41:p:38:ASP:HA	41:p:42:ASP:HB2	1.87	0.56
48:AD:213:SER:HB3	48:AD:236:TYR:CD2	2.40	0.56
51:AG:27:PHE:HB3	51:AG:30:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:128:PHE:CD1	68:Ac:404:U10:H4M2	2.41	0.56
51:Ag:35:ILE:HB	51:Ag:36:PRO:HD3	1.86	0.56
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.87	0.56
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.71	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.56
7:G:615:LEU:HG	16:P:41:ILE:HG23	1.86	0.56
7:G:651:PRO:HG3	19:S:57:GLU:N	2.19	0.56
9:I:82:ALA:HA	43:r:26:LEU:HD21	1.88	0.56
10:J:99:GLU:HA	10:J:102:LEU:HB3	1.87	0.56
10:J:150:TRP:HA	10:J:153:VAL:HG22	1.87	0.56
14:N:109:ALA:HB3	14:N:110:PRO:CD	2.34	0.56
40:o:4:HIS:HA	40:o:7:ARG:HH11	1.71	0.56
43:r:106:LEU:HD21	43:r:111:PRO:CB	2.36	0.56
45:AA:407:THR:O	45:AA:408:PRO:C	2.46	0.56
46:AB:51:SER:HB2	46:AB:230:LEU:CD1	2.33	0.56
46:AB:300:LYS:HG2	46:AB:301:ARG:HG3	1.86	0.56
54:AK:45:VAL:HG11	54:AK:48:ILE:HG22	1.88	0.56
45:Aa:58:ARG:HD2	45:Aa:417:LEU:HD12	1.88	0.56
48:Ad:116:VAL:HA	48:Ad:253:LEU:HD21	1.88	0.56
3:C:240:ALA:HB1	43:r:61:ARG:CD	2.34	0.56
4:D:271:ARG:NH1	8:H:279:ARG:O	2.38	0.56
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.36	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
12:L:142:ILE:HA	13:M:370:PRO:CB	2.35	0.56
12:L:357:ARG:NH1	39:n:78:GLN:O	2.38	0.56
14:N:258:THR:OG1	14:N:336:THR:HG22	2.06	0.56
25:Z:85:GLN:O	25:Z:89:GLU:HG3	2.06	0.56
25:Z:120:LEU:HD11	30:e:69:ARG:HG2	1.88	0.56
39:n:140:LEU:CD1	39:n:165:PRO:CB	2.57	0.56
46:AB:236:GLN:HG3	46:AB:237:PHE:CD2	2.41	0.56
47:AC:211:LEU:HD21	50:AF:37:THR:HA	1.87	0.56
51:Ag:78:TYR:CE1	52:Ah:63:GLU:HG3	2.41	0.56
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.35	0.56
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.87	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.56
8:H:65:THR:O	8:H:124:ASN:HB2	2.05	0.56
13:M:73:LEU:CD2	13:M:103:GLN:CD	2.79	0.56
14:N:193:ILE:HD11	14:N:269:GLU:HB2	1.88	0.56
16:P:375:VAL:HG12	16:P:377:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:68:SER:O	34:i:72:VAL:HG22	2.06	0.56
37:l:111:MET:HE3	37:l:112:TYR:CZ	2.41	0.56
48:AD:215:LEU:CD1	70:AD:401:HEC:CMB	2.73	0.56
48:AD:295:MET:HG2	53:AJ:36:PHE:CZ	2.41	0.56
49:AE:156:LEU:HD22	49:AE:210:TRP:CE2	2.41	0.56
49:AE:177:ARG:HB3	49:AE:211:VAL:HG13	1.88	0.56
54:AK:9:ARG:NH1	54:AK:13:LEU:HD11	2.21	0.56
47:Ac:153:ILE:HB	47:Ac:157:GLY:CA	2.36	0.56
49:Ae:191:GLU:H	49:Ae:191:GLU:CD	2.14	0.56
49:Ae:207:LYS:HB3	49:Ae:209:GLU:OE1	2.05	0.56
49:Ae:219:HIS:HB2	49:Ae:254:ALA:HA	1.88	0.56
54:Ak:9:ARG:NH1	54:Ak:13:LEU:HD11	2.20	0.56
1:A:73:LEU:HD11	10:J:57:LEU:CD2	2.36	0.55
12:L:94:LEU:CD2	12:L:125:LEU:HD21	2.35	0.55
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.88	0.55
12:L:538:PRO:O	12:L:542:LEU:HD13	2.06	0.55
13:M:134:THR:OG1	14:N:302:LEU:HD13	2.06	0.55
15:O:168:VAL:HG11	15:O:241:TYR:CD1	2.41	0.55
18:R:58:ASN:HB3	18:R:63:LEU:HD11	1.88	0.55
20:T:93:ILE:HA	20:T:108:LEU:HD21	1.88	0.55
23:X:124:GLN:C	23:X:125:LEU:HD12	2.31	0.55
38:m:97:PRO:CG	55:m:201:3PE:H2I3	2.36	0.55
39:n:57:MET:HE2	39:n:57:MET:HA	1.87	0.55
43:r:106:LEU:HD21	43:r:111:PRO:HB2	1.86	0.55
45:AA:183:VAL:HG21	45:AA:286:HIS:HB2	1.88	0.55
46:AB:167:GLN:HE22	49:AI:46:LYS:HA	1.71	0.55
46:AB:366:LEU:HD21	46:AB:425:VAL:HG22	1.87	0.55
47:AC:277:ALA:HB1	68:AC:405:U10:H1M2	1.87	0.55
49:AE:248:ARG:HA	49:AE:257:ASN:CG	2.32	0.55
45:Aa:50:VAL:HG11	45:Aa:417:LEU:HD11	1.89	0.55
47:Ac:97:HIS:CE1	47:Ac:100:ARG:HH21	2.24	0.55
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.35	0.55
1:A:77:TRP:CH2	10:J:50:PHE:CD2	2.94	0.55
56:A:402:CDL:H582	27:b:30:ILE:HD11	1.86	0.55
5:E:231:THR:HG21	6:F:303:HIS:HA	1.88	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.45	0.55
11:K:66:PHE:CE1	14:N:35:PHE:CZ	2.93	0.55
13:M:158:ILE:HG12	14:N:287:LEU:HD11	1.86	0.55
13:M:309:PHE:O	13:M:313:THR:HG23	2.06	0.55
16:P:140:ASP:OD1	16:P:142:GLU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:47:ARG:NH2	23:X:53:PRO:HG3	2.21	0.55
24:Y:137:LEU:HD23	24:Y:138:PHE:CD2	2.41	0.55
29:d:119:VAL:O	29:d:120:ARG:C	2.49	0.55
56:h:201:CDL:H511	55:i:201:3PE:H32	1.88	0.55
38:m:97:PRO:HG3	55:m:201:3PE:H2G2	1.88	0.55
41:p:74:ILE:CD1	41:p:85:ILE:HG13	2.36	0.55
49:AE:132:VAL:O	49:AE:135:GLN:HG2	2.06	0.55
49:Ae:122:THR:HG21	53:Aj:25:ILE:HD13	1.88	0.55
53:Aj:46:HIS:HA	53:Aj:49:GLU:CG	2.35	0.55
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.25	0.55
3:C:62:GLU:O	3:C:66:GLU:HG3	2.06	0.55
3:C:151:PRO:HG2	22:W:23:ILE:HG13	1.86	0.55
4:D:128:THR:HG22	4:D:131:GLN:CD	2.31	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.36	0.55
12:L:598:ILE:HD11	14:N:153:ILE:CD1	2.35	0.55
13:M:4:ILE:H	13:M:4:ILE:HD12	1.70	0.55
14:N:325:MET:HE3	14:N:329:LEU:HD11	1.88	0.55
16:P:145:PHE:O	16:P:149:PRO:HG2	2.05	0.55
23:X:142:TYR:HA	25:Z:115:ARG:HD3	1.86	0.55
27:b:69:HIS:HB3	27:b:72:ASP:OD1	2.05	0.55
34:i:123:PHE:HB3	40:o:40:VAL:HG11	1.87	0.55
39:n:55:LYS:HB3	45:Aa:255:ARG:NH1	2.21	0.55
48:Ad:245:ALA:O	48:Ad:246:PRO:C	2.49	0.55
48:Ad:284:HIS:NE2	48:Ad:288:MET:HE3	2.20	0.55
49:Ae:156:LEU:HD22	49:Ae:210:TRP:CE2	2.42	0.55
49:Ae:177:ARG:HB3	49:Ae:211:VAL:HG13	1.88	0.55
4:D:57:GLU:HA	4:D:60:HIS:CD2	2.41	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
12:L:54:PHE:O	12:L:58:ASN:CA	2.55	0.55
12:L:556:ILE:HD11	38:m:76:ILE:HG22	1.88	0.55
12:L:561:THR:O	12:L:565:SER:HB2	2.07	0.55
15:O:170:LEU:HG	15:O:179:ILE:HD13	1.87	0.55
15:O:201:PRO:HD2	15:O:249:MET:HE1	1.87	0.55
20:T:146:ASP:O	20:T:149:ALA:HB3	2.06	0.55
23:X:39:THR:HG23	23:X:40:ASN:N	2.20	0.55
23:X:169:PHE:CD2	23:X:169:PHE:O	2.59	0.55
40:o:69:CYS:O	40:o:69:CYS:SG	2.65	0.55
47:AC:153:ILE:HB	47:AC:157:GLY:CA	2.37	0.55
48:AD:215:LEU:CD1	70:AD:401:HEC:HMB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:222:PRO:O	48:AD:225:VAL:HG12	2.06	0.55
48:AD:253:LEU:HD12	48:AD:253:LEU:C	2.32	0.55
50:AF:15:ASP:OD2	50:AF:19:LYS:NZ	2.39	0.55
4:D:375:MET:HE1	7:G:126:LEU:CA	2.35	0.55
12:L:186:MET:HE1	13:M:379:LEU:HD21	1.89	0.55
12:L:336:LYS:O	12:L:340:PHE:HD2	1.89	0.55
12:L:407:TRP:HE1	37:l:140:MET:CE	2.19	0.55
12:L:441:ILE:HD12	35:j:46:GLU:O	2.06	0.55
56:L:703:CDL:H122	33:h:71:MET:HE1	1.87	0.55
13:M:143:LEU:HD21	14:N:303:THR:HG23	1.86	0.55
19:S:27:SER:N	19:S:34:ARG:HH22	2.05	0.55
19:S:41:TYR:HE1	19:S:53:ILE:HG23	1.70	0.55
23:X:17:GLU:CB	30:e:104:PRO:HG2	2.37	0.55
48:AD:321:TYR:HB2	50:AF:61:PHE:CE1	2.42	0.55
55:Ac:403:3PE:H12	56:Ag:101:CDL:OB3	2.06	0.55
4:D:189:THR:HG21	58:D:501:UQ1:HM32	1.89	0.55
4:D:217:VAL:CG2	4:D:226:TYR:CZ	2.89	0.55
4:D:264:ASN:O	9:I:65:GLU:OE1	2.25	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.88	0.55
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.89	0.55
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.89	0.55
9:I:68:ARG:HH21	25:Z:26:PRO:HD2	1.72	0.55
12:L:230:HIS:N	12:L:231:PRO:HD3	2.22	0.55
13:M:151:PHE:CZ	14:N:291:PHE:CB	2.87	0.55
14:N:230:ILE:O	14:N:233:LEU:HB2	2.07	0.55
14:N:237:THR:O	14:N:237:THR:CG2	2.55	0.55
56:Y:202:CDL:H371	56:Y:202:CDL:H561	1.89	0.55
30:e:14:LEU:HD12	30:e:15:ASP:N	2.21	0.55
37:l:88:PRO:HB2	39:n:86:PRO:CB	2.37	0.55
42:q:3:LEU:O	42:q:7:LEU:HG	2.07	0.55
49:AE:152:ILE:HD13	49:AE:169:TRP:CG	2.42	0.55
52:AH:58:ARG:CD	52:AH:61:THR:HB	2.36	0.55
46:Ab:60:ARG:HG3	46:Ab:124:GLU:HB3	1.89	0.55
46:Ab:366:LEU:HD21	46:Ab:425:VAL:HG22	1.87	0.55
48:Ad:222:PRO:O	48:Ad:225:VAL:HG12	2.06	0.55
48:Ad:253:LEU:C	48:Ad:253:LEU:HD12	2.32	0.55
49:Ae:132:VAL:O	49:Ae:135:GLN:HG2	2.06	0.55
2:B:91:TRP:CZ3	61:H:401:UQ9:H1MA	2.42	0.55
2:B:194:CYS:HB2	9:I:153:ILE:O	2.07	0.55
6:F:51:TRP:CZ3	6:F:168:ASN:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:K:51:SER:HA	30:e:32:ARG:HD3	1.87	0.55
12:L:69:VAL:HG11	12:L:71:MET:HE2	1.89	0.55
13:M:453:LEU:HD12	13:M:454:ILE:CG2	2.34	0.55
14:N:25:ASN:HB3	30:e:15:ASP:OD2	2.06	0.55
14:N:224:SER:HB2	14:N:229:SER:HB3	1.89	0.55
16:P:217:PHE:HA	16:P:220:TYR:HD2	1.71	0.55
26:a:1:MET:HB2	26:a:3:PHE:CZ	2.42	0.55
30:e:95:PRO:HD2	30:e:98:HIS:CE1	2.42	0.55
37:l:152:SER:HA	40:o:5:LEU:CD2	2.37	0.55
38:m:127:ILE:HG22	41:p:136:THR:HG23	1.89	0.55
47:AC:97:HIS:CE1	47:AC:100:ARG:HH21	2.23	0.55
47:AC:268:ILE:HG13	49:Ae:238:CYS:SG	2.46	0.55
45:Aa:168:ILE:O	45:Aa:171:GLU:HG2	2.06	0.55
48:Ad:215:LEU:CD1	70:Ad:401:HEC:HMB3	2.36	0.55
3:C:240:ALA:HB1	43:r:61:ARG:HH11	1.71	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
5:E:247:GLY:C	6:F:64:LYS:HE2	2.30	0.55
6:F:147:ARG:CD	6:F:191:TYR:CE2	2.90	0.55
12:L:258:PHE:HE1	12:L:262:ARG:HH21	1.55	0.55
13:M:62:SER:C	13:M:64:PRO:HD2	2.32	0.55
20:T:141:PRO:O	20:T:145:VAL:HG23	2.06	0.55
20:U:83:VAL:O	20:U:87:LEU:HG	2.07	0.55
22:W:53:MET:HB2	22:W:55:LEU:HG	1.89	0.55
27:b:8:PHE:CG	27:b:9:LEU:N	2.74	0.55
46:AB:262:ASN:HA	46:Ab:195:TYR:CD1	2.42	0.55
55:Aa:501:3PE:H32	47:Ac:221:HIS:HE1	1.71	0.55
47:Ac:14:ILE:HG22	47:Ac:19:ILE:HG13	1.88	0.55
47:Ac:197:LEU:HD11	67:Ac:402:HEM:HMA1	1.89	0.55
49:Ae:192:VAL:HA	49:Ae:195:LEU:CD1	2.37	0.55
1:A:104:TYR:HE1	14:N:2:ASN:HD22	1.53	0.55
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.42	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:114:TYR:CE1	10:J:33:ILE:HD11	2.42	0.55
8:H:183:MET:HE2	62:I:301:PC1:H271	1.88	0.55
12:L:25:ASN:HB2	33:h:72:LYS:NZ	2.21	0.55
12:L:162:THR:O	12:L:166:THR:HG23	2.06	0.55
13:M:231:LEU:CA	13:M:235:LEU:HD12	2.36	0.55
16:P:273:LEU:O	16:P:277:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:59:LEU:HD21	22:W:80:ARG:HH12	1.71	0.55
20:T:85:TYR:O	20:T:89:LEU:HD13	2.07	0.55
34:i:83:HIS:HE1	34:i:87:LYS:HD2	1.71	0.55
36:k:30:ILE:CD1	36:k:39:GLN:HB2	2.33	0.55
42:q:56:PHE:HD2	43:r:27:ARG:HH11	1.53	0.55
50:AF:102:ARG:HH21	50:AF:103:LYS:HE3	1.72	0.55
54:AK:6:LEU:HD12	54:AK:11:ARG:HH12	1.71	0.55
46:Ab:300:LYS:HG2	46:Ab:301:ARG:CG	2.37	0.55
52:Ah:58:ARG:CD	52:Ah:61:THR:HB	2.36	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HD3	2.37	0.55
6:F:425:CYS:HG	57:F:502:SF4:FE1	0.48	0.55
8:H:9:LEU:O	8:H:13:ILE:HG12	2.06	0.55
8:H:70:LEU:CD1	10:J:27:TYR:HE1	2.20	0.55
11:K:45:SER:O	11:K:49:LEU:HG	2.07	0.55
12:L:389:PHE:CZ	35:j:79:ALA:HB1	2.41	0.55
12:L:427:ILE:CD1	36:k:69:PHE:CE1	2.90	0.55
12:L:578:THR:CG2	14:N:168:GLY:HA2	2.37	0.55
16:P:237:LYS:HE3	16:P:322:ILE:O	2.07	0.55
18:R:43:TYR:O	18:R:46:VAL:HG22	2.07	0.55
20:U:79:ILE:HD11	20:U:148:ILE:CG2	2.36	0.55
26:a:31:ASN:HD21	26:a:36:LYS:HB2	1.71	0.55
46:Ab:39:GLU:HB2	46:Ab:227:HIS:HD1	1.70	0.55
49:Ae:125:VAL:HG21	62:Ae:301:PC1:C36	2.37	0.55
49:Ae:248:ARG:HA	49:Ae:257:ASN:CG	2.32	0.55
53:Aj:11:TYR:HA	53:Aj:15:PHE:HB2	1.89	0.55
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.71	0.54
18:R:45:ARG:HA	18:R:48:PHE:CD2	2.41	0.54
24:Y:83:ARG:NH1	24:Y:90:LEU:HB3	2.18	0.54
25:Z:24:ASN:OD1	25:Z:24:ASN:O	2.24	0.54
25:Z:92:GLU:O	25:Z:96:ILE:HG13	2.07	0.54
27:b:38:TYR:HA	27:b:41:TYR:CD2	2.42	0.54
28:c:55:TRP:CE2	29:d:66:THR:HG22	2.41	0.54
33:h:73:PHE:CD2	33:h:74:TYR:CE1	2.94	0.54
34:i:16:ARG:O	34:i:20:ARG:HG2	2.08	0.54
45:AA:87:ASN:H	45:AA:207:ASN:HD22	1.53	0.54
45:AA:118:ALA:O	46:AB:298:HIS:CD2	2.60	0.54
47:AC:183:PHE:CD1	47:Ac:183:PHE:CD1	2.94	0.54
46:Ab:236:GLN:HG3	46:Ab:237:PHE:CD2	2.41	0.54
47:Ac:264:THR:HG23	47:Ac:268:ILE:HD11	1.89	0.54
49:Ae:195:LEU:HD11	49:Ae:248:ARG:HH11	1.72	0.54
49:Ai:72:VAL:HG23	49:Ai:73:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:MET:CG	2:B:196:PRO:HG2	2.37	0.54
3:C:98:PHE:HB2	21:V:94:MET:CE	2.37	0.54
4:D:293:LEU:HD22	4:D:300:TRP:HB3	1.89	0.54
7:G:617:ARG:HH12	22:W:128:GLY:C	2.15	0.54
8:H:307:LEU:HD11	25:Z:47:TYR:CG	2.42	0.54
12:L:54:PHE:O	12:L:58:ASN:HA	2.08	0.54
12:L:141:PHE:CD1	12:L:182:PHE:CE2	2.94	0.54
13:M:415:GLN:O	13:M:416:ARG:HG3	2.08	0.54
15:O:132:GLN:CD	63:O:401:ADP:HN62	2.14	0.54
16:P:44:GLY:H	17:Q:105:GLU:CD	2.15	0.54
16:P:236:VAL:HG13	16:P:270:ARG:HH21	1.71	0.54
25:Z:40:ILE:O	25:Z:44:ILE:HG12	2.07	0.54
47:AC:30:TRP:HB3	47:AC:100:ARG:HD3	1.90	0.54
49:AI:72:VAL:HG23	49:AI:73:PRO:HD3	1.88	0.54
45:Aa:53:LEU:HD11	45:Aa:57:LEU:HD23	1.89	0.54
48:Ad:235:PRO:HA	48:Ad:240:GLN:HG3	1.89	0.54
2:B:166:ASN:O	2:B:166:ASN:OD1	2.25	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.36	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
9:I:49:ASP:O	9:I:50:MET:C	2.50	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:J:70:THR:C	10:J:72:ALA:H	2.13	0.54
12:L:232:TRP:O	12:L:236:ALA:N	2.40	0.54
13:M:6:LEU:HB3	13:M:7:PRO:HD3	1.88	0.54
13:M:255:LYS:NZ	29:d:117:HIS:HB3	2.22	0.54
15:O:211:VAL:HA	15:O:214:VAL:HG22	1.89	0.54
15:O:259:ASP:H	15:O:262:GLU:HG3	1.71	0.54
15:O:305:LEU:O	15:O:305:LEU:CD1	2.55	0.54
17:Q:165:SER:HB2	17:Q:168:LYS:HG2	1.89	0.54
23:X:23:ALA:HB2	23:X:95:GLN:NE2	2.22	0.54
24:Y:143:VAL:O	33:h:158:ARG:NH2	2.41	0.54
45:AA:168:ILE:O	45:AA:171:GLU:HG2	2.06	0.54
45:AA:186:TYR:CE1	49:AE:80:HIS:HB2	2.43	0.54
47:AC:346:PRO:HG3	51:AG:66:GLU:HG2	1.89	0.54
49:AE:161:GLU:HA	49:AE:178:HIS:CD2	2.43	0.54
45:Aa:87:ASN:H	45:Aa:207:ASN:HD22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:177:LEU:HD11	46:Ab:272:VAL:HG22	1.89	0.54
47:Ac:312:GLN:HE21	50:Af:37:THR:CB	2.21	0.54
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.54
56:A:402:CDL:C77	56:A:402:CDL:HB62	2.37	0.54
4:D:58:THR:HG23	4:D:61:TRP:CZ3	2.41	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:655:ARG:NH1	19:S:59:SER:CB	2.70	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:43:TYR:CE2	42:q:27:PHE:HZ	2.25	0.54
12:L:362:ILE:HA	12:L:365:ILE:HG13	1.90	0.54
12:L:424:MET:HE2	12:L:502:LEU:CB	2.37	0.54
12:L:551:THR:HA	12:L:555:LEU:HD12	1.89	0.54
20:U:131:PRO:HG2	20:U:134:ASP:HB2	1.90	0.54
26:a:58:ASN:HB2	26:a:61:TYR:CD2	2.43	0.54
31:f:37:PHE:HZ	41:p:83:LEU:HD13	1.70	0.54
42:q:50:GLU:HA	42:q:59:HIS:O	2.07	0.54
45:AA:281:ALA:HB2	51:AG:10:ARG:HH22	1.71	0.54
47:AC:287:LYS:HZ1	49:Ae:255:PRO:HG2	1.72	0.54
49:AE:195:LEU:HD11	49:AE:248:ARG:HH11	1.72	0.54
49:AE:207:LYS:CD	49:AE:210:TRP:HD1	2.20	0.54
45:Aa:58:ARG:HH21	45:Aa:417:LEU:C	2.15	0.54
47:Ac:119:LEU:HD22	67:Ac:402:HEM:HBB2	1.88	0.54
47:Ac:140:PHE:CE2	47:Ac:261:PRO:HA	2.41	0.54
48:Ad:214:LEU:CD1	48:Ad:237:PHE:HB2	2.38	0.54
49:Ae:197:ASP:HB3	49:Ae:257:ASN:OD1	2.06	0.54
49:Ai:43:LEU:O	49:Ai:44:ASP:C	2.51	0.54
4:D:150:ALA:HB2	4:D:400:ILE:HG12	1.89	0.54
4:D:189:THR:HB	58:D:501:UQ1:HM21	1.82	0.54
4:D:310:VAL:HG23	4:D:310:VAL:O	2.06	0.54
6:F:286:CYS:SG	6:F:304:ALA:HA	2.47	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:655:ARG:NH1	19:S:59:SER:HB3	2.21	0.54
10:J:29:GLY:N	11:K:31:LEU:HD21	2.22	0.54
11:K:62:THR:O	11:K:66:PHE:CD2	2.60	0.54
12:L:190:SER:HB2	12:L:196:TRP:NE1	2.22	0.54
13:M:79:ALA:HB1	13:M:225:ILE:HD13	1.90	0.54
15:O:170:LEU:HG	15:O:179:ILE:CD1	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
19:S:47:ALA:O	19:S:49:PRO:HD3	2.08	0.54
20:T:84:LEU:O	20:T:88:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:124:GLN:O	27:b:70:PRO:HB2	2.08	0.54
24:Y:141:PRO:HB2	33:h:161:ARG:NH1	2.22	0.54
31:f:38:ARG:HH12	31:f:54:VAL:HB	1.71	0.54
35:j:99:ILE:HD12	40:o:107:ARG:HB2	1.87	0.54
47:AC:222:PRO:HG2	47:AC:223:TYR:CD2	2.43	0.54
49:AE:152:ILE:HG13	49:AE:154:ILE:HD11	1.89	0.54
49:AE:190:VAL:HG11	49:AE:195:LEU:HD21	1.90	0.54
51:AG:39:LEU:O	51:AG:42:THR:HG22	2.08	0.54
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CE2	2.43	0.54
50:Af:102:ARG:HH21	50:Af:103:LYS:HE3	1.72	0.54
3:C:104:ASN:ND2	43:r:94:ALA:HB1	2.22	0.54
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.90	0.54
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.38	0.54
6:F:297:LYS:HD3	6:F:333:GLU:HB2	1.89	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:62:ARG:H	7:G:142:GLN:NE2	2.05	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
11:K:93:LEU:HD13	14:N:57:THR:HG21	1.90	0.54
12:L:232:TRP:CH2	12:L:233:LEU:HD21	2.42	0.54
13:M:1:MET:HE2	13:M:52:PHE:CE2	2.42	0.54
15:O:61:THR:HB	15:O:160:GLU:O	2.08	0.54
15:O:63:ASP:CG	15:O:241:TYR:CE1	2.86	0.54
15:O:180:ARG:NH2	32:g:51:MET:SD	2.80	0.54
15:O:230:THR:HG22	15:O:232:ALA:H	1.72	0.54
16:P:58:VAL:O	16:P:83:PRO:HD2	2.08	0.54
16:P:172:ALA:H	16:P:202:ARG:NH2	2.06	0.54
18:R:48:PHE:CD1	18:R:53:LYS:HB2	2.43	0.54
20:T:115:GLN:O	20:T:119:ILE:HG12	2.08	0.54
23:X:64:ASN:O	23:X:68:LEU:HG	2.07	0.54
23:X:121:ASP:O	23:X:122:LEU:C	2.50	0.54
25:Z:143:TYR:O	25:Z:144:THR:HB	2.08	0.54
29:d:116:PHE:CE1	41:p:146:LEU:HD23	2.42	0.54
62:l:201:PC1:H2A1	62:l:201:PC1:C3A	2.31	0.54
49:AE:136:PHE:O	49:AE:137:VAL:C	2.51	0.54
49:AE:153:GLU:C	49:AE:154:ILE:HD12	2.32	0.54
45:Aa:384:THR:HA	54:Ak:12:GLU:CD	2.33	0.54
47:Ac:211:LEU:HD21	50:Af:37:THR:HA	1.89	0.54
51:Ag:39:LEU:O	51:Ag:42:THR:HG22	2.08	0.54
2:B:100:CYS:CB	2:B:134:ALA:HB1	2.34	0.54
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:278:ILE:HG12	6:F:304:ALA:CB	2.38	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
12:L:515:LYS:O	12:L:518:PRO:HD3	2.08	0.54
13:M:160:LEU:HD23	13:M:164:LEU:HD13	1.89	0.54
13:M:373:ILE:HD11	13:M:454:ILE:HD11	1.88	0.54
14:N:307:THR:CG2	14:N:308:ASN:H	2.19	0.54
15:O:215:GLN:NE2	15:O:231:SER:HB3	2.22	0.54
16:P:306:GLY:HA2	16:P:312:PRO:HB3	1.90	0.54
20:U:155:TYR:OH	33:h:52:LYS:HD2	2.08	0.54
25:Z:120:LEU:HB2	25:Z:123:GLU:HG3	1.89	0.54
38:m:101:TRP:HZ2	55:m:201:3PE:H2C2	1.73	0.54
38:m:109:ARG:O	38:m:113:GLU:HG2	2.08	0.54
45:AA:136:LEU:HD21	46:AB:380:ALA:HA	1.90	0.54
47:AC:277:ALA:CB	68:AC:405:U10:H1M2	2.37	0.54
48:AD:116:VAL:HG22	48:AD:253:LEU:HD21	1.89	0.54
49:AE:122:THR:HG21	53:AJ:25:ILE:HG21	1.90	0.54
45:Aa:68:THR:HG21	46:Ab:384:MET:HG3	1.89	0.54
48:Ad:300:LEU:HG	56:Ag:102:CDL:H552	1.89	0.54
49:Ae:136:PHE:O	49:Ae:137:VAL:C	2.51	0.54
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.43	0.54
4:D:202:TRP:HH2	4:D:261:MET:HG3	1.73	0.54
5:E:84:LEU:HD12	44:s:46:LEU:CD1	2.34	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
9:I:132:ALA:O	9:I:133:GLU:HG3	2.08	0.54
12:L:131:LEU:CD1	12:L:140:LEU:CD1	2.78	0.54
12:L:247:LEU:HD11	12:L:248:HIS:CE1	2.43	0.54
13:M:31:SER:HA	13:M:34:ILE:HG12	1.90	0.54
13:M:231:LEU:O	13:M:236:LEU:HG	2.06	0.54
13:M:276:CYS:HB3	13:M:285:LEU:HG	1.89	0.54
14:N:109:ALA:HB1	14:N:110:PRO:CD	2.38	0.54
17:Q:117:THR:HG22	17:Q:119:ASP:H	1.73	0.54
19:S:79:LEU:HA	19:S:82:LEU:CD1	2.24	0.54
25:Z:54:ASN:O	25:Z:58:ARG:HG2	2.08	0.54
27:b:8:PHE:O	27:b:9:LEU:C	2.50	0.54
34:i:88:TYR:CE2	41:p:49:ARG:HB2	2.42	0.54
38:m:8:PRO:HB3	38:m:14:LEU:N	2.23	0.54
40:o:93:LEU:O	40:o:97:LYS:HG2	2.07	0.54
41:p:40:VAL:O	41:p:44:PRO:CG	2.44	0.54
42:q:88:ARG:HD2	42:q:94:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:71:ARG:NH2	48:AD:277:ALA:O	2.40	0.54
47:AC:72:ASP:OD1	48:AD:133:ARG:NH2	2.38	0.54
47:AC:163:TRP:HZ2	49:Ae:140:MET:HE1	1.73	0.54
48:AD:214:LEU:CD1	48:AD:237:PHE:HB2	2.38	0.54
45:Aa:183:VAL:HG21	45:Aa:286:HIS:HB2	1.90	0.54
54:Ak:45:VAL:HB	54:Ak:48:ILE:HB	1.88	0.54
1:A:69:ILE:O	1:A:73:LEU:HG	2.08	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
10:J:1:MET:SD	25:Z:142:TRP:CH2	3.01	0.54
12:L:74:MET:HE3	13:M:307:TRP:HH2	1.73	0.54
12:L:264:HIS:HA	12:L:267:THR:HG23	1.90	0.54
14:N:239:ALA:HB1	29:d:47:MET:HG2	1.89	0.54
38:m:17:THR:O	38:m:18:LEU:HB2	2.08	0.54
43:r:54:TYR:CZ	43:r:58:ASP:HB3	2.42	0.54
45:AA:118:ALA:O	46:AB:298:HIS:HB3	2.08	0.54
46:AB:60:ARG:CZ	46:AB:390:GLU:HB3	2.37	0.54
47:Ac:117:VAL:HG21	47:Ac:302:ALA:HB2	1.89	0.54
47:Ac:222:PRO:HG2	47:Ac:223:TYR:CD2	2.43	0.54
50:Af:24:ALA:O	51:Ag:48:ARG:NH2	2.38	0.54
5:E:116:THR:O	7:G:199:GLY:HA2	2.07	0.54
5:E:133:VAL:HA	5:E:185:VAL:HG12	1.90	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
55:H:402:3PE:H2E2	62:I:301:PC1:H2A2	1.90	0.54
13:M:283:LYS:HG3	13:M:327:PHE:CE1	2.43	0.54
15:O:206:TYR:HB3	15:O:257:VAL:HG22	1.89	0.54
20:U:86:VAL:CB	20:U:122:MET:HE1	2.37	0.54
39:n:125:TRP:CE3	39:n:128:LEU:HD12	2.42	0.54
46:AB:60:ARG:HG3	46:AB:124:GLU:HB3	1.88	0.54
49:AE:191:GLU:CD	49:AE:191:GLU:H	2.14	0.54
46:Ab:50:ALA:HB3	46:Ab:221:VAL:HG22	1.90	0.54
4:D:446:ASP:OD2	8:H:281:ARG:NH2	2.41	0.53
5:E:62:ILE:HD11	5:E:84:LEU:HD22	1.90	0.53
6:F:87:GLY:CA	6:F:92:GLY:HA2	2.37	0.53
6:F:102:MET:SD	6:F:149:MET:HB2	2.48	0.53
6:F:119:GLU:OE1	6:F:125:CYS:CA	2.56	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
12:L:66:TRP:CZ3	12:L:68:TRP:CD1	2.96	0.53
14:N:179:MET:HE2	14:N:216:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:114:LEU:HA	15:O:131:LEU:HD22	1.91	0.53
16:P:231:LEU:HD13	16:P:292:PRO:CD	2.37	0.53
17:Q:82:PRO:O	17:Q:94:THR:HG23	2.08	0.53
22:W:23:ILE:HG23	22:W:24:PHE:N	2.22	0.53
25:Z:12:PRO:HD3	25:Z:16:TYR:CE1	2.43	0.53
32:g:140:PHE:HB3	41:p:75:THR:HG21	1.89	0.53
40:o:57:ASP:CG	40:o:59:CYS:H	2.16	0.53
43:r:36:GLN:HB3	43:r:37:PRO:HD2	1.90	0.53
45:AA:255:ARG:O	45:AA:255:ARG:CG	2.51	0.53
46:AB:50:ALA:HB3	46:AB:221:VAL:HG22	1.90	0.53
46:AB:300:LYS:HG2	46:AB:301:ARG:CG	2.37	0.53
47:AC:18:PHE:HE1	69:AC:406:UQ6:C8	2.20	0.53
47:AC:377:LEU:HB3	50:AF:34:ARG:HD2	1.90	0.53
48:AD:116:VAL:HA	48:AD:253:LEU:HD21	1.88	0.53
45:Aa:258:GLU:H	45:Aa:258:GLU:CD	2.16	0.53
47:Ac:164:ILE:O	47:Ac:177:ARG:HD2	2.08	0.53
48:Ad:255:TYR:HB3	48:Ad:257:ASP:OD1	2.08	0.53
49:Ae:161:GLU:HA	49:Ae:178:HIS:CD2	2.43	0.53
1:A:63:LEU:CD2	10:J:62:GLY:O	2.55	0.53
1:A:90:MET:HE1	10:J:153:VAL:HG13	1.91	0.53
5:E:52:PHE:CD2	5:E:96:ALA:HA	2.43	0.53
5:E:91:TRP:CZ2	5:E:125:PRO:HD3	2.43	0.53
6:F:293:SER:HA	6:F:336:LEU:HD13	1.89	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
10:J:9:SER:OG	11:K:7:ASN:HB2	2.08	0.53
10:J:37:PHE:HA	10:J:56:PHE:HE1	1.73	0.53
12:L:41:LYS:NZ	62:L:701:PC1:H2B1	2.22	0.53
12:L:183:ILE:HD13	13:M:400:ILE:HD13	1.90	0.53
13:M:264:LEU:HD23	38:m:98:LEU:HD21	1.89	0.53
15:O:40:LEU:HG	15:O:292:HIS:CE1	2.44	0.53
15:O:48:LYS:HD2	15:O:288:ASP:HB2	1.91	0.53
16:P:275:HIS:HB3	16:P:372:ALA:HB1	1.90	0.53
20:T:93:ILE:HG23	20:T:108:LEU:CD1	2.38	0.53
29:d:119:VAL:HG21	41:p:147:GLY:HA2	1.90	0.53
42:q:49:TYR:HB2	42:q:61:TRP:CE2	2.42	0.53
49:AE:204:ARG:HB3	49:AE:260:VAL:CG2	2.25	0.53
50:AF:110:LYS:O	54:Ak:8:PRO:HD2	2.08	0.53
48:Ad:116:VAL:HG22	48:Ad:253:LEU:HD21	1.89	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
10:J:63:MET:HE1	11:K:68:ALA:HA	1.90	0.53
11:K:93:LEU:HA	14:N:54:GLU:OE2	2.08	0.53
12:L:149:ILE:CG2	13:M:364:LEU:HD21	2.38	0.53
12:L:226:GLN:OE1	12:L:284:THR:HG21	2.07	0.53
13:M:278:ARG:HH22	37:l:108:ASP:CB	2.21	0.53
16:P:142:GLU:HA	16:P:146:VAL:HG12	1.90	0.53
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.53
33:h:111:GLU:O	41:p:63:TYR:HA	2.08	0.53
42:q:31:ASN:HD21	62:q:202:PC1:H151	1.73	0.53
46:Ab:167:GLN:HG3	49:Ai:43:LEU:HD13	1.86	0.53
50:Af:108:TRP:HA	50:Af:111:LYS:HZ2	1.72	0.53
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.38	0.53
4:D:140:ASP:CB	4:D:147:ASN:HD21	2.07	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
10:J:19:LEU:HD11	10:J:32:LEU:HB2	1.90	0.53
11:K:1:MET:SD	11:K:50:ASN:ND2	2.77	0.53
12:L:79:SER:CB	12:L:135:ASN:HB2	2.35	0.53
12:L:145:GLU:CG	13:M:370:PRO:HD3	2.39	0.53
12:L:386:LEU:HD11	35:j:69:ILE:HD11	1.91	0.53
12:L:559:GLU:HG2	12:L:564:LYS:HD3	1.90	0.53
13:M:131:ILE:HD12	14:N:302:LEU:HD21	1.91	0.53
15:O:140:LEU:HD11	15:O:198:TYR:OH	2.08	0.53
15:O:164:TYR:CE1	15:O:195:LEU:HD21	2.43	0.53
16:P:283:MET:HE3	16:P:357:ARG:HH11	1.73	0.53
16:P:363:SER:CB	22:W:51:HIS:CE1	2.84	0.53
24:Y:57:ARG:O	24:Y:58:VAL:C	2.52	0.53
25:Z:105:LYS:HD2	25:Z:105:LYS:N	2.24	0.53
31:f:16:VAL:O	31:f:17:PRO:C	2.49	0.53
39:n:30:TRP:CD2	39:n:76:HIS:CD2	2.95	0.53
41:p:103:MET:CE	41:p:135:VAL:HG12	2.38	0.53
47:AC:128:PHE:CE1	68:AC:405:U10:H4M2	2.43	0.53
55:AC:404:3PE:H12	56:AG:101:CDL:OB3	2.08	0.53
48:AD:321:TYR:HB2	50:AF:61:PHE:CG	2.43	0.53
49:AE:192:VAL:HA	49:AE:195:LEU:CD1	2.37	0.53
50:Af:53:GLU:OE2	51:Ag:12:ARG:NH1	2.41	0.53
54:Ak:14:ALA:O	54:Ak:18:ILE:HG12	2.08	0.53
1:A:66:ASP:OD2	10:J:58:ILE:HA	2.09	0.53
2:B:182:ASP:OD1	2:B:183:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:VAL:HG21	4:D:58:THR:CG2	2.38	0.53
4:D:92:HIS:HB2	4:D:458:PHE:HE2	1.73	0.53
4:D:172:VAL:HG21	4:D:310:VAL:HG23	1.90	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:17:MET:SD	8:H:225:MET:CB	2.96	0.53
8:H:180:PRO:CD	25:Z:43:LEU:HD21	2.39	0.53
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.53
10:J:143:ALA:O	10:J:148:ALA:N	2.42	0.53
10:J:160:PHE:HE2	14:N:8:ILE:HD12	1.74	0.53
12:L:362:ILE:HD12	12:L:430:VAL:HG13	1.87	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	1.74	0.53
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.43	0.53
13:M:269:MET:CE	13:M:396:MET:HA	2.36	0.53
14:N:120:GLN:HE22	14:N:174:GLN:CB	2.21	0.53
21:V:114:TRP:O	21:V:115:PRO:C	2.52	0.53
23:X:17:GLU:HG3	23:X:64:ASN:HD22	1.73	0.53
34:i:77:ILE:HB	34:i:78:PRO:HD3	1.90	0.53
45:AA:393:ASN:HB3	46:AB:106:VAL:O	2.08	0.53
47:Ac:30:TRP:HB3	47:Ac:100:ARG:HD3	1.90	0.53
47:Ac:223:TYR:CE1	48:Ad:314:LEU:HG	2.44	0.53
1:A:64:LEU:HD13	10:J:163:ILE:CG1	2.39	0.53
3:C:101:ASP:OD1	21:V:86:LYS:HE3	2.08	0.53
5:E:118:TYR:HE1	6:F:206:CYS:SG	2.31	0.53
7:G:617:ARG:HH12	22:W:129:HIS:N	2.06	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.39	0.53
9:I:54:THR:HG22	27:b:13:TRP:HE1	1.74	0.53
12:L:124:PHE:HZ	12:L:252:MET:HB2	1.74	0.53
12:L:141:PHE:CE2	13:M:375:LEU:CD1	2.66	0.53
12:L:362:ILE:CD1	12:L:430:VAL:CG1	2.82	0.53
13:M:55:MET:HG3	13:M:56:PHE:CD2	2.44	0.53
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.91	0.53
13:M:73:LEU:HD23	13:M:103:GLN:NE2	2.23	0.53
15:O:172:ALA:HB1	15:O:236:ASP:HB2	1.90	0.53
15:O:225:HIS:O	15:O:226:GLU:C	2.50	0.53
15:O:323:GLN:HE21	32:g:55:GLU:HA	1.73	0.53
16:P:164:PHE:CE2	16:P:166:HIS:HB2	2.44	0.53
16:P:353:LEU:HA	16:P:356:HIS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:82:LEU:HD13	19:S:86:GLU:OE1	2.08	0.53
20:U:125:GLU:OE2	35:j:44:TYR:OH	2.26	0.53
22:W:42:TRP:CZ2	22:W:93:LEU:CA	2.91	0.53
23:X:70:PHE:O	23:X:74:ILE:HG13	2.09	0.53
39:n:56:ASP:O	39:n:57:MET:C	2.50	0.53
46:AB:237:PHE:O	46:AB:238:LEU:HB2	2.07	0.53
46:AB:322:ASP:OD2	49:AI:59:ALA:HB3	2.08	0.53
47:AC:218:ILE:HG21	48:AD:314:LEU:HD11	1.91	0.53
47:Ac:141:TRP:NE1	47:Ac:263:ASN:O	2.40	0.53
49:Ae:207:LYS:CD	49:Ae:210:TRP:HD1	2.20	0.53
1:A:63:LEU:CD2	10:J:63:MET:HA	2.38	0.53
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.44	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53
4:D:136:PHE:HZ	4:D:422:CYS:HG	1.56	0.53
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.53
5:E:177:GLY:O	5:E:178:ALA:HB3	2.08	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
10:J:63:MET:HE1	11:K:68:ALA:CA	2.39	0.53
11:K:22:PHE:HZ	14:N:61:VAL:HG11	1.74	0.53
12:L:63:ILE:HG23	34:i:97:ILE:CD1	2.39	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.53
12:L:361:ASN:HA	12:L:431:THR:O	2.09	0.53
13:M:371:PRO:HG2	55:M:502:3PE:H2D1	1.91	0.53
20:U:142:GLN:O	20:U:143:GLU:C	2.50	0.53
22:W:42:TRP:CD2	22:W:93:LEU:HD13	2.44	0.53
23:X:171:THR:O	23:X:172:VAL:C	2.52	0.53
24:Y:50:SER:HB3	24:Y:53:GLU:HG2	1.91	0.53
25:Z:140:PHE:HD1	26:a:45:TRP:HB2	1.72	0.53
30:e:40:TRP:CG	30:e:40:TRP:O	2.61	0.53
33:h:86:ILE:HG22	56:h:201:CDL:H121	1.91	0.53
40:o:39:MET:HE1	40:o:57:ASP:O	2.08	0.53
46:AB:148:ARG:NH2	50:Af:50:ARG:O	2.42	0.53
45:Aa:341:PHE:HE2	45:Aa:372:LEU:HD13	1.67	0.53
49:Ae:190:VAL:HG11	49:Ae:195:LEU:HD21	1.90	0.53
54:Ak:38:TRP:CD2	54:Ak:41:ILE:HD13	2.44	0.53
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.90	0.53
6:F:86:ARG:NH1	6:F:339:PHE:HB2	2.24	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
12:L:20:LEU:C	12:L:20:LEU:CD1	2.81	0.53
12:L:197:GLU:HB2	41:p:111:LYS:HE3	1.90	0.53
12:L:588:PHE:HZ	14:N:61:VAL:HG12	1.73	0.53
13:M:47:GLU:OE2	41:p:93:ARG:HB3	2.08	0.53
13:M:314:MET:HE1	13:M:380:PHE:CD2	2.44	0.53
14:N:227:ILE:HA	14:N:230:ILE:CG2	2.38	0.53
15:O:65:ASN:CG	15:O:66:ILE:H	2.17	0.53
15:O:170:LEU:HD13	15:O:187:TYR:CD2	2.44	0.53
16:P:275:HIS:HA	16:P:278:LYS:HG2	1.91	0.53
25:Z:64:ASP:OD1	25:Z:65:LEU:N	2.42	0.53
33:h:156:VAL:CG1	33:h:160:MET:HE3	2.39	0.53
39:n:39:TYR:CZ	39:n:43:LEU:HD11	2.44	0.53
46:AB:117:GLU:OE2	46:AB:330:TYR:HB3	2.09	0.53
47:AC:164:ILE:O	47:AC:177:ARG:HD2	2.08	0.53
49:AE:207:LYS:HD2	49:AE:210:TRP:CD1	2.44	0.53
46:Ab:117:GLU:OE2	46:Ab:331:SER:N	2.30	0.53
46:Ab:180:VAL:HB	46:Ab:258:ILE:HG13	1.90	0.53
47:Ac:312:GLN:HE21	50:Af:37:THR:HB	1.74	0.53
48:Ad:228:ARG:HG2	48:Ad:231:LEU:HD12	1.91	0.53
49:Ae:115:TYR:HB3	53:Aj:21:PHE:HE1	1.74	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
56:A:402:CDL:H162	10:J:153:VAL:HG11	1.89	0.53
2:B:199:GLU:HB2	9:I:173:PHE:HE2	1.74	0.53
4:D:289:SER:HA	4:D:293:LEU:HD13	1.91	0.53
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
8:H:172:MET:HE1	25:Z:46:GLY:CA	2.39	0.53
10:J:63:MET:HE1	11:K:68:ALA:HB2	1.91	0.53
11:K:73:VAL:HG21	14:N:38:LEU:CD2	2.39	0.53
13:M:57:SER:CB	13:M:113:THR:HG22	2.39	0.53
13:M:354:LEU:O	13:M:357:THR:N	2.41	0.53
13:M:453:LEU:HD12	13:M:453:LEU:C	2.33	0.53
24:Y:84:GLU:O	24:Y:86:PRO:HD3	2.09	0.53
25:Z:59:ARG:HH21	27:b:84:LEU:HB3	1.72	0.53
27:b:28:LEU:HA	27:b:31:ILE:HG22	1.91	0.53
28:c:55:TRP:HZ2	29:d:66:THR:HG22	1.67	0.53
37:l:55:TYR:O	37:l:104:PRO:HG3	2.09	0.53
39:n:114:MET:O	39:n:115:TYR:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:142:ARG:O	41:p:143:TYR:CD1	2.62	0.53
45:AA:55:ASN:HB3	45:AA:226:ALA:CB	2.38	0.53
46:AB:348:GLY:HA2	46:AB:448:PRO:HD3	1.91	0.53
48:AD:255:TYR:HB3	48:AD:257:ASP:OD1	2.08	0.53
49:AI:62:ARG:HB2	49:AI:78:PHE:C	2.33	0.53
53:AJ:43:ILE:O	53:AJ:47:ILE:HG13	2.09	0.53
54:AK:8:PRO:HG2	50:Af:111:LYS:HA	1.91	0.53
46:Ab:226:SER:O	46:Ab:229:VAL:HG22	2.09	0.53
47:Ac:346:PRO:HG3	51:Ag:66:GLU:HG2	1.89	0.53
48:Ad:299:LEU:HD21	49:Ae:124:GLY:HA3	1.90	0.53
3:C:51:ASP:OD1	3:C:54:HIS:HB3	2.08	0.53
3:C:102:HIS:CE1	21:V:44:TYR:HE1	2.27	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:671:LEU:HD21	19:S:45:LYS:HG2	1.90	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
10:J:63:MET:HE2	11:K:68:ALA:CB	2.38	0.53
12:L:108:MET:HB2	12:L:114:ILE:HD13	1.90	0.53
12:L:128:MET:CG	12:L:251:THR:HB	2.36	0.53
12:L:247:LEU:O	12:L:252:MET:HB3	2.09	0.53
13:M:59:ASP:O	13:M:60:PRO:C	2.49	0.53
13:M:310:MET:HG3	13:M:455:THR:CA	2.39	0.53
13:M:348:LEU:HD12	13:M:415:GLN:NE2	2.24	0.53
13:M:447:LEU:HD11	13:M:454:ILE:HG23	1.90	0.53
16:P:336:GLU:CG	16:P:342:PRO:HD3	2.38	0.53
26:a:42:GLN:O	26:a:43:TYR:C	2.50	0.53
32:g:139:TYR:CD2	32:g:140:PHE:CD1	2.96	0.53
34:i:22:TRP:CZ2	39:n:172:THR:HG22	2.44	0.53
42:q:44:TYR:OH	42:q:112:ASN:CG	2.52	0.53
43:r:6:ARG:O	43:r:10:LYS:HG3	2.09	0.53
45:AA:341:PHE:HZ	45:AA:372:LEU:HD13	1.72	0.53
47:AC:18:PHE:HE1	69:AC:406:UQ6:C7	2.22	0.53
47:AC:170:VAL:HG23	47:AC:174:THR:CB	2.39	0.53
49:AE:180:THR:N	49:AE:183:GLU:HB2	2.23	0.53
50:AF:20:TRP:HZ2	55:AG:103:3PE:H3E1	1.73	0.53
47:Ac:265:PRO:O	47:Ac:268:ILE:HG13	2.08	0.53
48:Ad:152:VAL:HG22	48:Ad:153:GLU:N	2.24	0.53
48:Ad:290:LEU:O	48:Ad:294:LEU:HG	2.09	0.53
49:Ae:180:THR:N	49:Ae:183:GLU:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD12	10:J:54:MET:SD	2.49	0.52
3:C:63:TYR:HE1	21:V:47:TYR:CG	2.26	0.52
7:G:275:PRO:HB2	17:Q:86:ASN:ND2	2.24	0.52
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.52
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.91	0.52
12:L:450:LEU:HG	12:L:454:ILE:HD12	1.91	0.52
13:M:15:THR:HG21	13:M:100:ILE:HD12	1.90	0.52
13:M:51:ASN:ND2	33:h:136:THR:HG23	2.24	0.52
13:M:73:LEU:HD21	13:M:100:ILE:HG12	1.90	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
15:O:279:ASN:O	15:O:284:LEU:HD11	2.09	0.52
15:O:336:GLY:N	15:O:344:ASN:ND2	2.56	0.52
18:R:43:TYR:O	18:R:46:VAL:HG13	2.09	0.52
20:U:86:VAL:HG13	36:k:54:ASN:ND2	2.24	0.52
21:V:48:THR:HA	21:V:51:ILE:HD12	1.90	0.52
24:Y:65:ALA:O	24:Y:68:ILE:HG12	2.09	0.52
35:j:87:PRO:HG3	40:o:96:VAL:HG23	1.89	0.52
38:m:85:LYS:O	38:m:85:LYS:HG2	2.09	0.52
41:p:6:ASP:O	41:p:9:VAL:HG22	2.09	0.52
47:AC:202:GLU:CD	47:Ac:9:PRO:HG3	2.34	0.52
48:AD:227:LEU:HD12	48:AD:227:LEU:C	2.34	0.52
48:AD:255:TYR:HH	48:AD:266:VAL:HA	1.74	0.52
55:Aa:501:3PE:H341	55:Aa:501:3PE:H222	1.91	0.52
46:Ab:47:LEU:HD12	46:Ab:218:MET:O	2.09	0.52
46:Ab:170:GLN:CB	49:Ai:78:PHE:CZ	2.92	0.52
47:Ac:28:SER:HB2	56:Ag:101:CDL:HA21	1.90	0.52
47:Ac:71:ARG:NH2	48:Ad:277:ALA:O	2.39	0.52
47:Ac:334:ILE:HD11	51:Ag:56:VAL:HG22	1.90	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
1:A:103:ALA:O	1:A:107:THR:HG23	2.09	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
8:H:153:VAL:HG11	8:H:241:ILE:HG23	1.90	0.52
8:H:311:THR:O	25:Z:51:MET:HG3	2.08	0.52
11:K:25:HIS:HD2	11:K:88:ASP:OD1	1.91	0.52
11:K:89:TYR:HB3	11:K:91:GLN:OE1	2.09	0.52
12:L:536:ILE:HG23	12:L:537:THR:N	2.25	0.52
13:M:188:ALA:H	13:M:253:LEU:HD11	1.75	0.52
14:N:25:ASN:ND2	30:e:18:PHE:CE2	2.78	0.52
14:N:324:LEU:CD1	29:d:64:PHE:HZ	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:310:ILE:HG13	15:O:311:PRO:HD2	1.91	0.52
17:Q:53:ILE:O	22:W:20:VAL:HG22	2.09	0.52
17:Q:58:LYS:O	17:Q:59:LEU:C	2.49	0.52
22:W:23:ILE:HG23	22:W:24:PHE:H	1.74	0.52
48:AD:248:ILE:CG2	48:AD:263:MET:HG3	2.40	0.52
47:Ac:378:LYS:HE3	50:Af:89:PHE:HE2	1.74	0.52
67:Ac:402:HEM:HBA1	69:Ac:405:UQ6:O4	2.10	0.52
48:Ad:262:THR:HG22	52:Ah:24:LEU:HG	1.91	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:161:GLU:O	7:G:163:LYS:HE3	2.10	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:287:HIS:HE1	55:H:402:3PE:HN1	1.55	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
10:J:144:MET:C	10:J:148:ALA:O	2.52	0.52
11:K:38:LEU:HG	11:K:42:ILE:CD1	2.39	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	2.40	0.52
14:N:23:SER:HB2	30:e:15:ASP:OD2	2.08	0.52
15:O:121:PRO:C	15:O:122:LYS:HG2	2.33	0.52
17:Q:72:ILE:HD13	17:Q:143:TRP:NE1	2.24	0.52
38:m:123:ARG:O	41:p:140:GLN:NE2	2.39	0.52
55:m:201:3PE:H392	55:m:201:3PE:H241	1.91	0.52
45:Aa:191:ALA:O	45:Aa:271:THR:N	2.41	0.52
45:Aa:207:ASN:O	45:Aa:211:LEU:HG	2.09	0.52
46:Ab:138:LEU:CD2	46:Ab:238:LEU:HG	2.38	0.52
47:Ac:170:VAL:HG23	47:Ac:174:THR:CB	2.39	0.52
48:Ad:125:HIS:CE1	48:Ad:195:PRO:HD2	2.42	0.52
2:B:163:SER:HA	2:B:166:ASN:OD1	2.10	0.52
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.36	0.52
3:C:195:HIS:HE1	22:W:88:LYS:NZ	2.07	0.52
4:D:348:LEU:O	25:Z:11:PRO:HB3	2.09	0.52
7:G:284:GLU:OE2	17:Q:84:ARG:NH2	2.42	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
10:J:21:LEU:HD23	55:J:201:3PE:H271	1.90	0.52
11:K:57:MET:N	11:K:58:PRO:HD2	2.24	0.52
11:K:93:LEU:HD22	14:N:54:GLU:HA	1.91	0.52
12:L:228:GLY:O	12:L:229:LEU:CG	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:265:PHE:HD1	16:P:334:GLY:HA3	1.74	0.52
18:R:40:GLU:HA	18:R:45:ARG:HH12	1.75	0.52
25:Z:129:THR:HB	25:Z:132:GLU:HG3	1.91	0.52
29:d:109:TYR:HA	29:d:112:ILE:CG2	2.38	0.52
36:k:47:LEU:HD12	39:n:43:LEU:HD23	1.90	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
49:AE:127:TYR:HE1	53:AJ:33:GLU:HG3	1.74	0.52
54:AK:14:ALA:O	54:AK:18:ILE:HG12	2.08	0.52
45:Aa:80:ARG:CD	45:Aa:265:LEU:HD11	2.39	0.52
48:Ad:155:GLN:HA	48:Ad:166:MET:HG2	1.90	0.52
2:B:115:ASP:OD1	8:H:25:ARG:NH2	2.42	0.52
3:C:63:TYR:HB2	43:r:95:VAL:CG2	2.40	0.52
3:C:120:THR:OG1	17:Q:128:PHE:HA	2.10	0.52
4:D:139:LEU:O	4:D:459:GLY:C	2.53	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:65:THR:HG22	16:P:359:TYR:CD1	2.41	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
10:J:22:LYS:HD3	11:K:23:ARG:HG2	1.90	0.52
10:J:77:GLU:O	10:J:78:TYR:C	2.52	0.52
10:J:115:ILE:O	10:J:116:ASN:C	2.50	0.52
10:J:126:TYR:HB3	25:Z:120:LEU:HD22	1.92	0.52
10:J:143:ALA:O	10:J:148:ALA:O	2.27	0.52
12:L:141:PHE:CE2	13:M:370:PRO:HG3	2.44	0.52
13:M:403:THR:HA	13:M:406:TYR:CE2	2.44	0.52
14:N:175:MET:HG2	14:N:219:LEU:CD2	2.40	0.52
23:X:57:LEU:HG	23:X:61:LYS:HZ1	1.74	0.52
26:a:4:GLU:O	26:a:7:PRO:HD2	2.09	0.52
26:a:64:LYS:HG3	26:a:66:LEU:H	1.75	0.52
29:d:1:MET:HG3	29:d:2:MET:N	2.24	0.52
45:AA:165:ARG:HE	45:AA:209:ARG:HA	1.74	0.52
47:AC:107:TYR:HB2	47:AC:305:PRO:HG3	1.92	0.52
47:AC:287:LYS:NZ	49:Ae:255:PRO:HG2	2.24	0.52
51:AG:73:LYS:NZ	52:AH:63:GLU:HG2	2.24	0.52
45:Aa:171:GLU:O	45:Aa:174:GLU:HG2	2.10	0.52
48:Ad:227:LEU:HD12	48:Ad:227:LEU:C	2.34	0.52
3:C:64:VAL:HG11	3:C:85:ILE:CD1	2.32	0.52
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.28	0.52
6:F:109:ARG:HB3	6:F:238:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
10:J:56:PHE:HD1	10:J:60:LEU:HD13	1.75	0.52
11:K:59:ILE:HD12	14:N:27:MET:HG2	1.90	0.52
12:L:123:LEU:HD22	12:L:150:MET:HG3	1.91	0.52
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.90	0.52
13:M:68:LEU:HG	13:M:234:ILE:HD11	1.92	0.52
14:N:175:MET:HG2	14:N:219:LEU:HD22	1.91	0.52
24:Y:141:PRO:HB2	33:h:161:ARG:CZ	2.40	0.52
26:a:6:LEU:O	26:a:7:PRO:C	2.52	0.52
30:e:103:GLU:O	30:e:104:PRO:C	2.53	0.52
48:AD:112:ARG:HD3	48:AD:257:ASP:OD2	2.09	0.52
49:AI:43:LEU:O	49:AI:44:ASP:C	2.51	0.52
45:Aa:165:ARG:HE	45:Aa:209:ARG:HA	1.74	0.52
1:A:93:ILE:HD11	56:A:402:CDL:C59	2.29	0.52
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.73	0.52
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.52
8:H:70:LEU:CD1	10:J:27:TYR:CE1	2.92	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
10:J:67:PHE:CZ	11:K:34:GLU:CG	2.92	0.52
12:L:594:ASN:HD21	14:N:110:PRO:HB2	1.73	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
14:N:10:TYR:O	14:N:13:ILE:HG22	2.09	0.52
28:c:55:TRP:NE1	29:d:66:THR:CG2	2.72	0.52
39:n:37:TYR:C	39:n:39:TYR:N	2.67	0.52
47:Ac:110:MET:CE	47:Ac:306:PHE:CE1	2.93	0.52
49:Ae:207:LYS:HD2	49:Ae:210:TRP:CD1	2.44	0.52
49:Ae:241:SER:OG	49:Ae:253:PRO:HD2	2.10	0.52
55:A:401:3PE:H332	10:J:53:LEU:HD21	1.91	0.52
2:B:199:GLU:HB2	9:I:173:PHE:CE2	2.44	0.52
3:C:149:LEU:CD1	22:W:80:ARG:NH2	2.61	0.52
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.91	0.52
6:F:414:GLU:OE2	43:r:51:ASN:N	2.29	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
10:J:92:LEU:O	10:J:96:VAL:HG23	2.10	0.52
12:L:483:PRO:HG2	12:L:486:LEU:HD13	1.91	0.52
12:L:578:THR:HG21	14:N:168:GLY:HA2	1.90	0.52
13:M:103:GLN:O	13:M:107:ILE:HB	2.10	0.52
14:N:3:PRO:HG2	15:O:289:TRP:CH2	2.45	0.52
14:N:29:MET:HE2	14:N:141:ILE:HG12	1.92	0.52
15:O:170:LEU:HD13	15:O:187:TYR:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:275:TYR:CE1	21:V:23:ARG:NH2	2.76	0.52
16:P:236:VAL:HG11	16:P:270:ARG:HH21	1.75	0.52
20:T:90:TYR:CD2	20:T:93:ILE:HG12	2.38	0.52
20:T:130:ILE:HG23	20:T:147:TYR:HE2	1.75	0.52
20:U:128:PHE:CE1	20:U:148:ILE:HG23	2.45	0.52
25:Z:126:GLY:HA2	25:Z:133:MET:HE2	1.91	0.52
29:d:93:TYR:CD2	33:h:156:VAL:HG13	2.44	0.52
30:e:69:ARG:HG3	30:e:72:THR:OG1	2.10	0.52
37:l:169:GLU:C	37:l:171:GLY:N	2.55	0.52
45:AA:279:ASP:OD1	51:AG:12:ARG:NE	2.42	0.52
46:AB:226:SER:O	46:AB:229:VAL:HG22	2.09	0.52
52:AH:51:CYS:SG	52:AH:54:ARG:NH2	2.83	0.52
45:Aa:70:THR:HG21	45:Aa:407:THR:HA	1.91	0.52
2:B:95:PHE:O	4:D:93:GLY:HA2	2.09	0.52
2:B:161:MET:HE2	2:B:196:PRO:HD2	1.92	0.52
4:D:193:ASP:O	8:H:205:SER:OG	2.27	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
11:K:59:ILE:O	11:K:60:PRO:C	2.49	0.52
12:L:108:MET:HB2	12:L:114:ILE:CD1	2.39	0.52
12:L:563:PRO:HG3	13:M:152:TYR:OH	2.09	0.52
13:M:171:VAL:HG11	13:M:179:LEU:CD2	2.35	0.52
14:N:81:LEU:HD23	30:e:60:PHE:HE1	1.75	0.52
20:U:133:ILE:HG23	20:U:134:ASP:N	2.25	0.52
27:b:23:PHE:CD2	55:b:201:3PE:H281	2.40	0.52
35:j:92:TRP:O	35:j:93:THR:C	2.53	0.52
39:n:168:TRP:HD1	39:n:169:HIS:CE1	2.27	0.52
42:q:138:VAL:HG23	42:q:139:PRO:HD2	1.92	0.52
46:AB:325:ALA:O	49:AI:61:ALA:HB1	2.09	0.52
55:AC:404:3PE:H112	56:AG:101:CDL:PB2	2.49	0.52
49:AE:155:LYS:O	49:AE:158:ASP:HB2	2.09	0.52
50:AF:108:TRP:HA	50:AF:111:LYS:HZ2	1.75	0.52
54:AK:38:TRP:HE1	54:AK:40:LEU:HD12	1.74	0.52
47:Ac:20:ASP:O	47:Ac:21:LEU:C	2.52	0.52
1:A:59:ALA:HB1	10:J:66:VAL:HG13	1.92	0.52
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.90	0.52
2:B:101:ALA:O	2:B:104:MET:HG2	2.10	0.52
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.52
5:E:179:CYS:HA	59:E:301:FES:S1	2.50	0.52
6:F:192:ASP:HB3	44:s:57:LEU:CD1	2.38	0.52
6:F:288:VAL:HG11	6:F:303:HIS:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:81:GLU:O	7:G:103:LEU:HB2	2.09	0.52
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.52
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.91	0.52
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.92	0.52
13:M:139:GLN:HB3	13:M:222:GLU:CG	2.40	0.52
15:O:326:ARG:NH2	32:g:56:ASP:OD1	2.43	0.52
16:P:305:PHE:HB2	16:P:314:THR:HG22	1.92	0.52
18:R:50:ASP:O	18:R:51:ARG:HG3	2.10	0.52
23:X:137:LEU:HA	27:b:58:ARG:HH22	1.75	0.52
27:b:48:ALA:O	27:b:49:THR:C	2.53	0.52
27:b:82:LYS:O	27:b:83:ASN:C	2.52	0.52
40:o:17:PRO:HG3	40:o:106:ARG:HA	1.92	0.52
41:p:164:LEU:O	41:p:168:LYS:N	2.42	0.52
46:AB:70:ARG:NH2	46:AB:332:ASP:OD2	2.42	0.52
46:AB:100:THR:HG23	49:AI:70:LEU:CD1	2.40	0.52
46:AB:170:GLN:HG3	46:AB:339:TYR:OH	2.10	0.52
49:AE:242:HIS:CD2	49:AE:251:LYS:HB3	2.45	0.52
48:Ad:215:LEU:HD21	70:Ad:401:HEC:C1B	2.40	0.52
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.45	0.51
3:C:124:ARG:HD2	17:Q:140:LYS:NZ	2.25	0.51
4:D:36:GLN:HE22	13:M:135:ARG:HH22	1.58	0.51
4:D:303:ARG:HH11	4:D:401:GLU:HG2	1.75	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.92	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
10:J:79:PRO:HA	10:J:82:TRP:CH2	2.45	0.51
12:L:533:ILE:HG23	12:L:534:HIS:HD2	1.74	0.51
13:M:115:LEU:HD21	13:M:176:LEU:CD2	2.37	0.51
14:N:168:GLY:O	14:N:172:GLN:HG2	2.10	0.51
15:O:121:PRO:HB3	15:O:178:TYR:CE1	2.45	0.51
21:V:62:GLU:HB3	21:V:68:LEU:HD13	1.92	0.51
29:d:87:ASP:O	29:d:88:HIS:C	2.51	0.51
30:e:44:ALA:HA	30:e:47:ILE:HG12	1.92	0.51
41:p:32:TYR:HA	41:p:35:LYS:HZ2	1.75	0.51
42:q:101:ASN:OD1	42:q:101:ASN:O	2.28	0.51
49:AE:241:SER:OG	49:AE:253:PRO:HD2	2.10	0.51
56:A:402:CDL:HB31	56:A:402:CDL:H801	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.75	0.51
4:D:97:LEU:HD23	4:D:111:PRO:HB3	1.91	0.51
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.74	0.51
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.51
8:H:99:ASN:OD1	26:a:40:ARG:HG3	2.11	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
10:J:169:ILE:HG23	14:N:45:ILE:CD1	2.37	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:286:LEU:HG	12:L:290:ILE:CD1	2.40	0.51
12:L:569:LEU:O	12:L:573:MET:HG2	2.10	0.51
13:M:129:THR:CG2	13:M:235:LEU:HD11	2.39	0.51
13:M:168:GLN:O	13:M:172:GLY:N	2.44	0.51
13:M:423:MET:SD	38:m:59:HIS:NE2	2.83	0.51
15:O:96:THR:HA	15:O:101:GLY:CA	2.39	0.51
16:P:45:LYS:HB2	17:Q:118:ALA:CB	2.41	0.51
20:T:104:PHE:CE1	20:T:115:GLN:CG	2.94	0.51
22:W:42:TRP:CE3	22:W:93:LEU:HD13	2.45	0.51
29:d:62:LEU:O	29:d:66:THR:OG1	2.22	0.51
33:h:144:SER:HB2	41:p:82:VAL:HG21	1.91	0.51
47:AC:36:LEU:HD11	56:AG:102:CDL:H732	1.92	0.51
47:AC:221:HIS:O	47:AC:225:THR:HB	2.10	0.51
48:AD:138:VAL:HG11	48:AD:276:TRP:NE1	2.25	0.51
48:AD:213:SER:HB3	48:AD:236:TYR:CE2	2.46	0.51
49:AE:248:ARG:HG2	49:AE:257:ASN:ND2	2.25	0.51
50:AF:97:GLU:HA	50:AF:100:ARG:HH11	1.75	0.51
54:AK:45:VAL:HB	54:AK:48:ILE:HG22	1.91	0.51
46:Ab:173:ILE:HG21	46:Ab:339:TYR:HE1	1.75	0.51
49:Ae:155:LYS:O	49:Ae:158:ASP:HB2	2.10	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.92	0.51
6:F:288:VAL:HG11	6:F:303:HIS:HB3	1.91	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:200:LEU:O	8:H:201:THR:C	2.52	0.51
10:J:150:TRP:O	10:J:154:VAL:HG12	2.10	0.51
16:P:157:LYS:O	16:P:158:GLU:C	2.53	0.51
21:V:12:VAL:CG1	21:V:13:GLY:N	2.72	0.51
25:Z:69:ILE:CG2	27:b:54:PRO:HD3	2.40	0.51
31:f:37:PHE:HA	31:f:40:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:56:TRP:CD1	33:h:134:GLU:OE1	2.63	0.51
39:n:140:LEU:HD21	39:n:166:LEU:HG	1.93	0.51
45:AA:171:GLU:O	45:AA:174:GLU:HG2	2.10	0.51
45:AA:225:LYS:HD2	45:AA:256:VAL:H	1.75	0.51
47:AC:150:LEU:HB2	47:AC:161:VAL:HG22	1.93	0.51
47:Ac:147:THR:HG21	47:Ac:165:TRP:NE1	2.25	0.51
48:Ad:248:ILE:CG2	48:Ad:263:MET:HG3	2.40	0.51
50:Af:97:GLU:HA	50:Af:100:ARG:HH11	1.75	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.40	0.51
4:D:179:ARG:HG2	4:D:183:HIS:CD2	2.46	0.51
7:G:614:GLY:HA2	16:P:41:ILE:HG21	1.91	0.51
9:I:88:PHE:O	42:q:62:VAL:HG12	2.10	0.51
9:I:152:CYS:SG	57:I:302:SF4:S3	3.09	0.51
12:L:552:LEU:HD21	38:m:90:GLY:CA	2.32	0.51
13:M:251:ASP:N	13:M:252:PRO:HD2	2.25	0.51
14:N:240:MET:HE2	14:N:326:PHE:CZ	2.45	0.51
16:P:315:THR:HB	16:P:318:LYS:HB2	1.92	0.51
17:Q:85:ASN:N	17:Q:85:ASN:OD1	2.41	0.51
20:U:79:ILE:HG13	20:U:126:PHE:CE2	2.45	0.51
25:Z:86:ILE:HA	25:Z:128:ARG:HH21	1.74	0.51
31:f:56:TRP:CE3	33:h:131:LYS:HG3	2.44	0.51
32:g:106:TYR:CE2	33:h:86:ILE:HD12	2.46	0.51
33:h:52:LYS:O	33:h:53:ARG:C	2.53	0.51
34:i:83:HIS:CE1	34:i:87:LYS:HD2	2.46	0.51
40:o:89:TYR:O	40:o:90:CYS:C	2.52	0.51
45:AA:207:ASN:O	45:AA:211:LEU:HG	2.09	0.51
46:Ab:232:GLN:O	46:Ab:235:GLU:HG3	2.11	0.51
47:Ac:221:HIS:O	47:Ac:225:THR:HB	2.09	0.51
48:Ad:213:SER:HB3	48:Ad:236:TYR:CE2	2.46	0.51
52:Ah:51:CYS:SG	52:Ah:54:ARG:NH2	2.83	0.51
54:Ak:39:ARG:NH2	54:Ak:50:GLY:H	2.09	0.51
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.46	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
6:F:267:ARG:HD3	6:F:338:ASP:OD2	2.10	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.93	0.51
9:I:210:LEU:HD22	43:r:39:PRO:HD2	1.92	0.51
10:J:69:TYR:O	10:J:72:ALA:HB3	2.10	0.51
12:L:434:LYS:NZ	36:k:66:ASN:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:L:701:PC1:H371	62:L:701:PC1:H2C1	1.93	0.51
13:M:165:ILE:HD12	23:X:168:PHE:CZ	2.46	0.51
15:O:221:LYS:HE3	15:O:226:GLU:OE2	2.10	0.51
16:P:272:LEU:HG	16:P:375:VAL:CG2	2.26	0.51
20:T:141:PRO:HD2	20:T:142:GLN:H	1.75	0.51
34:i:10:LEU:HA	34:i:13:GLN:HB3	1.92	0.51
34:i:74:HIS:O	34:i:78:PRO:HG2	2.11	0.51
40:o:76:ASN:HB2	41:p:26:LEU:HD12	1.91	0.51
42:q:8:LYS:O	42:q:12:GLN:HG2	2.10	0.51
47:AC:140:PHE:CE1	47:AC:170:VAL:HG13	2.45	0.51
47:AC:238:ILE:HD12	56:AG:102:CDL:H772	1.92	0.51
48:AD:162:GLY:HA2	48:Ad:183:GLU:CB	2.40	0.51
50:AF:20:TRP:CZ2	55:AG:103:3PE:H3E1	2.45	0.51
45:Aa:148:ALA:HA	45:Aa:250:LEU:HD21	1.92	0.51
45:Aa:257:TYR:CZ	45:Aa:263:PRO:HD2	2.46	0.51
46:Ab:297:PRO:CA	46:Ab:304:ASN:CG	2.83	0.51
47:Ac:140:PHE:CE1	47:Ac:170:VAL:HG13	2.45	0.51
49:Ae:242:HIS:CD2	49:Ae:251:LYS:HB3	2.45	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.92	0.51
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.91	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
13:M:20:PRO:HB3	13:M:89:ASN:ND2	2.25	0.51
13:M:31:SER:HA	13:M:34:ILE:CG1	2.41	0.51
17:Q:77:VAL:HG12	17:Q:101:PHE:CG	2.46	0.51
22:W:65:LYS:HE3	22:W:69:MET:HE2	1.92	0.51
23:X:168:PHE:C	23:X:169:PHE:CD1	2.89	0.51
25:Z:143:TYR:HD1	25:Z:144:THR:N	2.04	0.51
34:i:85:TYR:CE2	34:i:90:MET:HE3	2.46	0.51
38:m:20:PRO:HA	39:n:65:ARG:HH21	1.76	0.51
42:q:88:ARG:HG3	42:q:89:TRP:N	2.26	0.51
45:AA:73:VAL:HG23	45:AA:147:LEU:HD13	1.93	0.51
46:AB:167:GLN:HE21	49:AI:43:LEU:HB2	1.69	0.51
47:AC:107:TYR:HE1	47:AC:308:HIS:HB2	1.76	0.51
47:AC:327:ILE:HG23	55:AG:103:3PE:H2B1	1.91	0.51
49:AE:165:MET:O	49:AE:176:VAL:N	2.44	0.51
49:AE:196:ARG:HD2	49:AE:249:ILE:CG2	2.41	0.51
46:Ab:267:VAL:CG2	46:Ab:344:ALA:HA	2.41	0.51
47:Ac:100:ARG:HH12	67:Ac:402:HEM:CBD	2.23	0.51
47:Ac:277:ALA:HB1	68:Ac:404:U10:H1M2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:346:PRO:O	47:Ac:349:ILE:HG22	2.10	0.51
48:Ad:112:ARG:HD3	48:Ad:257:ASP:OD2	2.09	0.51
1:A:81:THR:O	27:b:46:ASN:ND2	2.44	0.51
4:D:320:ILE:CD1	9:I:36:TYR:CD2	2.93	0.51
5:E:68:ASN:ND2	44:s:49:ASN:HD21	2.07	0.51
5:E:183:PRO:HG2	5:E:194:ASP:HA	1.92	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.10	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.10	0.51
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.41	0.51
8:H:17:MET:CE	8:H:225:MET:CB	2.88	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
12:L:60:GLU:HG3	12:L:83:ASP:HA	1.93	0.51
12:L:161:ARG:NE	12:L:163:ASP:HB2	2.26	0.51
12:L:404:THR:HG22	12:L:405:ASN:H	1.75	0.51
12:L:441:ILE:HD13	35:j:48:PRO:HD3	1.92	0.51
12:L:530:PRO:O	12:L:534:HIS:HB2	2.11	0.51
12:L:595:ILE:O	12:L:599:ILE:HG13	2.11	0.51
32:g:53:TRP:H	32:g:53:TRP:HD1	1.55	0.51
36:k:34:PRO:HD2	36:k:59:TYR:CG	2.46	0.51
62:l:201:PC1:H3A2	62:l:201:PC1:C2A	2.31	0.51
42:q:88:ARG:HB2	42:q:93:MET:HB2	1.92	0.51
48:AD:237:PHE:CG	48:AD:242:ILE:HB	2.46	0.51
48:AD:321:TYR:CD2	48:AD:323:PRO:HD3	2.44	0.51
53:Aj:22:ALA:HB1	54:AK:27:VAL:HG11	1.92	0.51
47:Ac:199:PHE:O	47:Ac:202:GLU:HG2	2.11	0.51
47:Ac:272:TRP:CE2	47:Ac:273:TYR:HD2	2.29	0.51
48:Ad:232:TYR:O	48:Ad:241:ALA:HA	2.10	0.51
49:Ae:184:ILE:HG21	49:Ae:208:PRO:HB3	1.93	0.51
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.92	0.51
2:B:114:MET:HE3	2:B:119:VAL:CG1	2.40	0.51
5:E:180:VAL:HG11	5:E:224:CYS:HB3	1.92	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.51
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.76	0.51
7:G:239:THR:HA	9:I:132:ALA:O	2.11	0.51
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.51
12:L:439:PRO:HA	36:k:57:TRP:CH2	2.46	0.51
12:L:525:LEU:HD21	39:n:77:PRO:CB	2.39	0.51
13:M:11:LEU:O	13:M:15:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:304:GLN:HA	13:M:309:PHE:CE1	2.45	0.51
14:N:344:ILE:HD13	23:X:167:PHE:CE1	2.46	0.51
17:Q:91:VAL:HG13	17:Q:95:LYS:NZ	2.26	0.51
20:U:84:LEU:HD11	20:U:100:VAL:HG12	1.93	0.51
31:f:11:TRP:O	31:f:14:ILE:HG22	2.11	0.51
37:l:183:HIS:O	40:o:37:ARG:HG2	2.10	0.51
38:m:49:LEU:CD1	39:n:166:LEU:HD11	2.41	0.51
41:p:9:VAL:O	41:p:109:ARG:NH2	2.44	0.51
47:AC:197:LEU:HD11	69:AC:406:UQ6:C6	2.41	0.51
48:AD:201:VAL:HG22	48:AD:278:SER:CB	2.41	0.51
49:Ae:248:ARG:HG2	49:Ae:257:ASN:ND2	2.25	0.51
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.41	0.51
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.40	0.51
6:F:42:PHE:CE2	6:F:275:LEU:HD11	2.46	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.92	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
10:J:135:LEU:HB3	30:e:29:ASN:ND2	2.25	0.51
11:K:96:LEU:HD13	14:N:117:GLU:O	2.11	0.51
12:L:141:PHE:CD2	13:M:370:PRO:HG3	2.46	0.51
12:L:152:PHE:HE1	13:M:412:ILE:HD11	1.76	0.51
12:L:364:LYS:CE	36:k:67:ILE:HD11	2.37	0.51
13:M:336:ARG:HH12	13:M:433:GLU:CD	2.19	0.51
14:N:45:ILE:HA	14:N:52:SER:OG	2.11	0.51
16:P:234:LYS:HG2	16:P:234:LYS:O	2.10	0.51
18:R:43:TYR:C	18:R:45:ARG:N	2.69	0.51
24:Y:14:VAL:HG13	24:Y:15:PRO:HD2	1.93	0.51
25:Z:111:PHE:CE1	25:Z:117:VAL:HG21	2.45	0.51
29:d:28:ASP:O	29:d:29:PRO:C	2.53	0.51
33:h:73:PHE:CE2	33:h:74:TYR:CE1	2.98	0.51
33:h:159:LEU:HD23	33:h:163:ARG:HH12	1.75	0.51
42:q:65:THR:OG1	42:q:66:THR:N	2.44	0.51
45:AA:50:VAL:HG11	45:AA:417:LEU:HD11	1.93	0.51
48:AD:160:ASP:C	48:AD:162:GLY:H	2.18	0.51
49:AE:238:CYS:SG	47:Ac:268:ILE:HD12	2.51	0.51
46:Ab:170:GLN:HG3	46:Ab:339:TYR:OH	2.11	0.51
46:Ab:237:PHE:O	46:Ab:238:LEU:HB2	2.11	0.51
48:Ad:244:MET:HB2	70:Ad:401:HEC:C1D	2.41	0.51
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.51
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.46	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:20:ALA:C	10:J:22:LYS:H	2.19	0.51
12:L:451:MET:O	12:L:452:ASN:C	2.53	0.51
12:L:536:ILE:HD11	12:L:540:LYS:HD2	1.93	0.51
13:M:275:ILE:CD1	13:M:288:TYR:CG	2.85	0.51
13:M:354:LEU:O	13:M:355:MET:C	2.52	0.51
23:X:56:CYS:HA	23:X:135:ARG:HH12	1.76	0.51
25:Z:72:MET:SD	27:b:53:TYR:HB2	2.51	0.51
27:b:11:ASN:OD1	27:b:12:ALA:N	2.44	0.51
31:f:41:SER:O	31:f:45:GLN:HB2	2.11	0.51
32:g:115:TRP:HA	32:g:118:ARG:HH11	1.75	0.51
34:i:83:HIS:HD2	41:p:37:TYR:CE2	2.28	0.51
41:p:49:ARG:O	41:p:52:ILE:HB	2.10	0.51
41:p:113:CYS:O	41:p:113:CYS:SG	2.69	0.51
47:AC:147:THR:HG21	47:AC:165:TRP:NE1	2.25	0.51
45:Aa:53:LEU:HD12	45:Aa:57:LEU:HB3	1.92	0.51
45:Aa:259:GLU:C	45:Aa:261:ALA:N	2.65	0.51
47:Ac:28:SER:HB2	56:Ag:101:CDL:OA4	2.10	0.51
47:Ac:150:LEU:HB2	47:Ac:161:VAL:HG22	1.93	0.51
49:Ae:242:HIS:HD2	49:Ae:251:LYS:HB3	1.76	0.51
53:Aj:30:LEU:CD2	54:Ak:48:ILE:HG13	2.41	0.51
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.93	0.50
4:D:54:PRO:HB2	4:D:59:ALA:HB2	1.94	0.50
4:D:274:ASP:H	4:D:325:ASP:CB	2.24	0.50
6:F:109:ARG:HH21	6:F:239:PRO:HG3	1.75	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.42	0.50
6:F:279:SER:O	6:F:355:ILE:HA	2.11	0.50
6:F:280:GLY:O	6:F:356:VAL:HB	2.11	0.50
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.42	0.50
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.46	0.50
11:K:36:MET:HE3	14:N:68:MET:HG3	1.93	0.50
12:L:362:ILE:CD1	12:L:430:VAL:HG13	2.41	0.50
13:M:249:ILE:HG22	13:M:250:LEU:N	2.26	0.50
15:O:182:GLN:O	15:O:183:CYS:C	2.54	0.50
15:O:289:TRP:HA	15:O:289:TRP:CE3	2.46	0.50
16:P:348:LYS:HB3	16:P:351:GLU:OE2	2.11	0.50
22:W:103:ARG:O	22:W:104:THR:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:28:ARG:HG3	25:Z:28:ARG:O	2.11	0.50
28:c:32:ARG:HB2	28:c:32:ARG:NH2	2.27	0.50
28:c:46:LEU:O	28:c:50:ALA:HB2	2.12	0.50
32:g:147:LEU:HD21	41:p:163:MET:HB2	1.91	0.50
45:AA:148:ALA:HA	45:AA:250:LEU:HD21	1.92	0.50
45:AA:226:ALA:HB2	45:AA:253:VAL:HB	1.93	0.50
46:AB:261:GLN:HG3	46:Ab:195:TYR:OH	2.11	0.50
46:AB:429:LYS:HA	46:AB:432:VAL:HG12	1.93	0.50
46:Ab:227:HIS:HD2	46:Ab:231:LYS:HE2	1.76	0.50
47:Ac:291:VAL:O	47:Ac:295:ILE:HG12	2.11	0.50
48:Ad:201:VAL:HG22	48:Ad:278:SER:CB	2.41	0.50
4:D:179:ARG:NH2	4:D:303:ARG:HD3	2.25	0.50
7:G:35:PHE:O	7:G:101:ASN:HA	2.10	0.50
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:J:56:PHE:CE1	10:J:60:LEU:HD22	2.46	0.50
10:J:146:SER:OG	10:J:147:CYS:N	2.41	0.50
12:L:349:SER:HB2	12:L:443:ILE:HG23	1.93	0.50
12:L:395:ILE:O	12:L:399:ILE:HG13	2.10	0.50
12:L:424:MET:HG2	12:L:501:ALA:HB3	1.93	0.50
13:M:4:ILE:HD11	13:M:41:LEU:HD21	1.92	0.50
13:M:294:MET:HE3	13:M:319:HIS:HD2	1.75	0.50
14:N:36:SER:HB2	14:N:134:GLN:HE22	1.76	0.50
14:N:175:MET:O	14:N:179:MET:HG2	2.12	0.50
14:N:248:LEU:CD1	14:N:296:LEU:HD23	2.41	0.50
16:P:65:LEU:HD23	16:P:129:LEU:HD22	1.93	0.50
20:U:122:MET:HA	20:U:122:MET:HE2	1.91	0.50
23:X:9:THR:HG23	23:X:12:GLU:H	1.77	0.50
40:o:71:ARG:HB3	40:o:71:ARG:NH1	2.27	0.50
45:AA:70:THR:HG21	45:AA:407:THR:HA	1.93	0.50
46:AB:305:THR:CG2	46:AB:306:THR:N	2.60	0.50
47:AC:334:ILE:HD12	55:AG:103:3PE:H2F2	1.92	0.50
48:AD:215:LEU:HD21	70:AD:401:HEC:C1B	2.40	0.50
45:Aa:117:GLY:CA	46:Ab:377:LYS:HG2	2.32	0.50
45:Aa:310:ILE:HG21	45:Aa:379:LEU:HD21	1.91	0.50
51:Ag:74:ASN:O	51:Ag:77:MET:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:PHE:HB3	2:B:97:LEU:HD13	1.92	0.50
4:D:55:SER:HB3	4:D:58:THR:HB	1.94	0.50
6:F:78:GLY:O	6:F:82:THR:HG23	2.12	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:643:ARG:O	7:G:644:ASN:C	2.55	0.50
12:L:21:ILE:HG12	12:L:27:ILE:HG23	1.93	0.50
12:L:187:VAL:HG13	13:M:383:MET:HA	1.93	0.50
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.45	0.50
12:L:554:ASP:OD2	13:M:213:HIS:HE1	1.94	0.50
16:P:300:TRP:O	16:P:304:LEU:HG	2.11	0.50
17:Q:75:ARG:HH12	17:Q:104:ARG:HG2	1.76	0.50
23:X:38:LYS:O	23:X:42:GLU:HG3	2.11	0.50
24:Y:114:ALA:O	24:Y:115:MET:C	2.52	0.50
46:AB:40:PHE:CZ	46:AB:406:TYR:HB2	2.46	0.50
46:AB:113:THR:OG1	49:AI:65:VAL:CG1	2.59	0.50
46:AB:174:ILE:HG21	49:AI:64:LEU:HD13	1.93	0.50
46:AB:425:VAL:HG12	46:AB:429:LYS:HZ1	1.76	0.50
48:AD:116:VAL:HA	48:AD:253:LEU:CD2	2.41	0.50
49:AE:127:TYR:CE1	53:AJ:33:GLU:HG3	2.46	0.50
49:AE:155:LYS:HA	49:AE:270:VAL:HG22	1.93	0.50
49:AE:242:HIS:HD2	49:AE:251:LYS:HB3	1.76	0.50
54:AK:37:ASP:O	54:AK:38:TRP:C	2.51	0.50
45:Aa:68:THR:O	45:Aa:406:THR:HG21	2.11	0.50
48:Ad:146:LYS:N	48:Ad:171:LEU:HD21	2.27	0.50
4:D:263:THR:HG22	4:D:263:THR:O	2.11	0.50
5:E:120:MET:HE2	6:F:201:ALA:HA	1.94	0.50
5:E:235:GLU:HB2	5:E:236:PRO:HD2	1.93	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:8:THR:O	8:H:12:PRO:HG2	2.11	0.50
8:H:85:LEU:CD2	8:H:108:THR:HB	2.41	0.50
9:I:58:ALA:HB2	25:Z:36:PHE:CZ	2.45	0.50
10:J:56:PHE:CD1	10:J:60:LEU:HD22	2.47	0.50
10:J:154:VAL:CG2	14:N:35:PHE:CE2	2.94	0.50
10:J:155:ALA:HB1	11:K:65:VAL:HG11	1.94	0.50
12:L:365:ILE:CD1	12:L:366:MET:HE2	2.42	0.50
12:L:383:MET:CB	12:L:386:LEU:HD12	2.30	0.50
14:N:313:MET:HG3	15:O:305:LEU:HD22	1.93	0.50
15:O:233:TYR:CE2	15:O:237:ILE:HD11	2.46	0.50
16:P:69:VAL:HG21	16:P:129:LEU:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:150:ARG:O	16:P:151:ALA:C	2.54	0.50
18:R:38:TYR:CE1	18:R:44:ARG:HD2	2.47	0.50
21:V:7:LYS:O	21:V:8:THR:OG1	2.29	0.50
21:V:44:TYR:O	21:V:48:THR:HG22	2.11	0.50
32:g:74:TYR:CE2	32:g:85:MET:HB3	2.47	0.50
37:l:87:ASP:OD1	37:l:88:PRO:HD2	2.11	0.50
45:AA:127:GLU:OE2	45:AA:348:TYR:HB3	2.11	0.50
45:AA:478:LEU:HA	53:AJ:18:THR:HG21	1.93	0.50
46:AB:227:HIS:HD2	46:AB:231:LYS:HE2	1.76	0.50
48:AD:214:LEU:HD12	48:AD:234:ASN:CG	2.36	0.50
48:AD:232:TYR:HD1	48:AD:242:ILE:O	1.93	0.50
49:AE:156:LEU:H	49:AE:270:VAL:HA	1.75	0.50
56:AG:101:CDL:HA32	56:AG:101:CDL:H512	1.93	0.50
45:Aa:73:VAL:HG23	45:Aa:147:LEU:HD13	1.93	0.50
45:Aa:101:THR:HG21	45:Aa:149:ASP:HB3	1.94	0.50
46:Ab:425:VAL:HG12	46:Ab:429:LYS:HZ1	1.76	0.50
48:Ad:154:VAL:HG11	48:Ad:173:ASP:OD1	2.11	0.50
49:Ae:196:ARG:HD2	49:Ae:249:ILE:CG2	2.40	0.50
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.29	0.50
4:D:189:THR:CB	58:D:501:UQ1:CM2	2.64	0.50
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:277:MET:HE1	17:Q:153:PRO:HD3	1.94	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.50
7:G:621:LYS:HZ3	22:W:131:PRO:HD3	1.76	0.50
11:K:1:MET:HA	11:K:4:THR:HB	1.94	0.50
12:L:117:PHE:HE1	12:L:243:VAL:CG2	2.24	0.50
12:L:552:LEU:CD2	38:m:90:GLY:HA2	2.34	0.50
13:M:118:PHE:O	13:M:122:PHE:HB2	2.11	0.50
13:M:309:PHE:HB2	13:M:458:THR:HG21	1.93	0.50
14:N:189:TRP:HB2	14:N:204:ASN:HD21	1.77	0.50
14:N:258:THR:HG23	14:N:336:THR:HG22	1.93	0.50
15:O:132:GLN:HE22	63:O:401:ADP:HN62	1.59	0.50
15:O:218:ILE:HD13	15:O:229:VAL:HG11	1.93	0.50
16:P:209:ARG:N	16:P:352:VAL:HG22	2.26	0.50
21:V:90:LEU:HD21	21:V:94:MET:HE3	1.93	0.50
25:Z:110:VAL:CG1	30:e:71:LYS:CB	2.86	0.50
30:e:69:ARG:O	30:e:73:MET:HG3	2.11	0.50
34:i:10:LEU:HD12	34:i:13:GLN:HB3	1.94	0.50
34:i:83:HIS:CD2	41:p:37:TYR:CE2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:108:ASP:HB3	37:l:111:MET:HE2	1.92	0.50
43:r:48:LYS:HB2	43:r:52:ASN:HD22	1.76	0.50
46:AB:297:PRO:HB3	46:AB:304:ASN:ND2	2.25	0.50
47:AC:264:THR:HB	49:Ac:223:VAL:HB	1.92	0.50
47:AC:291:VAL:O	47:AC:295:ILE:HG12	2.11	0.50
48:AD:242:ILE:CD1	48:AD:244:MET:HE2	2.41	0.50
49:AE:93:ARG:HD2	49:AE:110:ARG:CD	2.38	0.50
50:AF:53:GLU:OE2	51:AG:12:ARG:NH1	2.45	0.50
46:Ab:429:LYS:HA	46:Ab:432:VAL:HG12	1.93	0.50
48:Ad:255:TYR:HH	48:Ad:266:VAL:HA	1.76	0.50
1:A:106:TRP:HD1	1:A:111:LEU:HD12	1.76	0.50
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.26	0.50
5:E:180:VAL:HG13	5:E:181:ASN:H	1.77	0.50
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.47	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.50
12:L:44:PHE:HE1	62:L:701:PC1:H143	1.76	0.50
12:L:60:GLU:O	12:L:61:TYR:CD1	2.65	0.50
12:L:385:PHE:HE2	35:j:73:PHE:HD1	1.59	0.50
12:L:553:LEU:HD21	38:m:94:GLY:N	2.25	0.50
12:L:586:LEU:CD2	24:Y:47:PRO:HD3	2.42	0.50
13:M:63:THR:N	13:M:64:PRO:HD2	2.27	0.50
13:M:231:LEU:CD1	13:M:235:LEU:CD1	2.85	0.50
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.52	0.50
24:Y:90:LEU:O	24:Y:91:ASN:C	2.53	0.50
25:Z:66:GLU:HA	25:Z:69:ILE:HG12	1.93	0.50
26:a:14:VAL:O	26:a:18:ILE:HG13	2.10	0.50
26:a:53:ARG:HB3	30:e:102:GLU:CB	2.36	0.50
36:k:34:PRO:CG	36:k:59:TYR:CD1	2.94	0.50
43:r:48:LYS:O	43:r:49:LEU:HB2	2.12	0.50
46:AB:375:LYS:NZ	46:AB:419:VAL:O	2.36	0.50
48:AD:91:PRO:HG3	48:AD:236:TYR:CD1	2.47	0.50
48:AD:323:PRO:HG2	48:AD:325:LYS:CD	2.41	0.50
45:Aa:393:ASN:O	45:Aa:397:ASN:ND2	2.44	0.50
46:Ab:297:PRO:HB3	46:Ab:304:ASN:ND2	2.26	0.50
47:Ac:72:ASP:OD1	48:Ad:133:ARG:NH1	2.45	0.50
47:Ac:140:PHE:HE1	47:Ac:170:VAL:HG13	1.77	0.50
2:B:104:MET:HE1	2:B:132:ILE:HD12	1.92	0.50
6:F:270:ASN:HD22	6:F:338:ASP:HB2	1.76	0.50
6:F:297:LYS:CD	6:F:333:GLU:HB2	2.42	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
10:J:166:ILE:HD11	11:K:76:ALA:CB	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:196:TRP:HZ2	13:M:383:MET:SD	2.34	0.50
12:L:474:PRO:HD2	40:o:67:LEU:HD21	1.93	0.50
56:L:703:CDL:H762	13:M:371:PRO:HG3	1.94	0.50
13:M:248:ILE:HG13	13:M:249:ILE:N	2.26	0.50
14:N:239:ALA:HA	29:d:47:MET:HE2	1.93	0.50
16:P:205:ASP:OD1	16:P:205:ASP:O	2.30	0.50
16:P:207:PHE:HE1	16:P:214:LEU:HD22	1.76	0.50
20:T:82:ARG:HD2	20:T:125:GLU:OE2	2.10	0.50
20:U:79:ILE:HG23	20:U:145:VAL:HG13	1.91	0.50
20:U:90:TYR:HD2	20:U:93:ILE:H	1.59	0.50
23:X:57:LEU:HD12	23:X:57:LEU:O	2.12	0.50
37:l:49:ALA:HA	37:l:59:VAL:HG13	1.93	0.50
38:m:124:LYS:HE2	38:m:125:PHE:CE2	2.47	0.50
40:o:26:PRO:HB2	40:o:29:LEU:HB2	1.93	0.50
46:AB:176:ASN:O	46:AB:258:ILE:HD11	2.12	0.50
46:AB:232:GLN:O	46:AB:235:GLU:HG3	2.11	0.50
46:AB:297:PRO:CA	46:AB:304:ASN:CG	2.83	0.50
45:Aa:400:VAL:CB	46:Ab:58:LEU:HG	2.40	0.50
46:Ab:267:VAL:HG23	46:Ab:344:ALA:HA	1.94	0.50
47:Ac:277:ALA:CB	68:Ac:404:U10:H1M2	2.42	0.50
48:Ad:91:PRO:HG3	48:Ad:236:TYR:CD1	2.47	0.50
3:C:104:ASN:O	43:r:97:PRO:HD3	2.12	0.50
3:C:210:ARG:CD	16:P:48:ARG:HD3	2.42	0.50
4:D:333:ARG:HH12	4:D:453:THR:HA	1.77	0.50
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
7:G:617:ARG:NH1	22:W:129:HIS:N	2.60	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
11:K:1:MET:H3	11:K:2:PRO:HD2	1.75	0.50
12:L:109:HIS:O	12:L:110:SER:HB2	2.11	0.50
12:L:302:ILE:CB	12:L:340:PHE:CE1	2.95	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
20:T:97:LYS:NZ	20:T:107:ASP:C	2.69	0.50
24:Y:12:HIS:NE2	24:Y:127:PHE:HZ	2.09	0.50
30:e:103:GLU:HG3	30:e:104:PRO:HD2	1.93	0.50
37:l:88:PRO:HB2	39:n:86:PRO:HB2	1.93	0.50
47:AC:18:PHE:CZ	69:AC:406:UQ6:H1M2	2.45	0.50
47:AC:218:ILE:HB	47:AC:219:PRO:HD2	1.94	0.50
47:AC:294:LEU:CG	68:AC:405:U10:H1M3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:334:ILE:CD1	55:AG:103:3PE:H2F2	2.41	0.50
48:AD:249:TYR:O	48:AD:250:THR:C	2.55	0.50
49:AE:155:LYS:HZ3	49:AE:157:SER:HB3	1.76	0.50
49:AE:195:LEU:HD11	49:AE:248:ARG:NH1	2.26	0.50
45:Aa:55:ASN:O	45:Aa:227:PRO:HG3	2.11	0.50
48:Ad:181:ASN:HB2	48:Ad:182:PRO:HD2	1.94	0.50
49:Ae:165:MET:O	49:Ae:176:VAL:N	2.44	0.50
49:Ae:179:ARG:HA	49:Ae:183:GLU:OE1	2.12	0.50
4:D:36:GLN:HG3	4:D:38:GLN:HE21	1.77	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.50
6:F:42:PHE:HE2	6:F:275:LEU:HD11	1.75	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:173:TRP:CZ2	8:H:262:GLU:OE2	2.65	0.50
9:I:36:TYR:HE2	9:I:38:TYR:CZ	2.29	0.50
10:J:106:LEU:HA	10:J:109:TYR:CD2	2.47	0.50
11:K:38:LEU:HG	11:K:42:ILE:HD11	1.93	0.50
12:L:123:LEU:CD2	12:L:150:MET:HG3	2.42	0.50
13:M:122:PHE:CE1	13:M:238:LEU:HG	2.46	0.50
13:M:432:ARG:HA	13:M:435:THR:HG22	1.94	0.50
13:M:441:MET:HG3	13:M:445:ILE:HD12	1.94	0.50
14:N:133:TRP:CG	14:N:133:TRP:O	2.63	0.50
14:N:175:MET:HE1	14:N:227:ILE:HG22	1.94	0.50
14:N:190:MET:HB3	14:N:201:THR:HG23	1.94	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
23:X:70:PHE:CE2	23:X:74:ILE:HD11	2.46	0.50
23:X:78:CYS:C	23:X:81:PRO:HD2	2.36	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
30:e:74:ARG:O	30:e:75:ARG:C	2.55	0.50
37:l:33:THR:O	37:l:36:MET:HG2	2.12	0.50
38:m:124:LYS:HB3	38:m:124:LYS:HZ3	1.76	0.50
45:AA:65:SER:O	45:AA:66:HIS:C	2.55	0.50
45:AA:101:THR:HG21	45:AA:149:ASP:HB3	1.94	0.50
48:Ad:167:ARG:CZ	48:Ad:170:LYS:HE2	2.42	0.50
48:Ad:214:LEU:HD12	48:Ad:234:ASN:CG	2.36	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.94	0.49
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.94	0.49
5:E:247:GLY:O	6:F:64:LYS:HE2	2.12	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.94	0.49
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.90	0.49
7:G:136:GLU:CD	17:Q:87:MET:HG3	2.36	0.49
9:I:181:GLU:HB2	42:q:126:PRO:CG	2.41	0.49
10:J:18:GLY:O	10:J:23:PRO:HD3	2.12	0.49
10:J:32:LEU:HB3	10:J:64:LEU:HD21	1.94	0.49
12:L:445:GLU:CB	12:L:450:LEU:HD23	2.37	0.49
13:M:51:ASN:O	33:h:135:LYS:HD2	2.12	0.49
13:M:388:TRP:NE1	38:m:109:ARG:CD	2.75	0.49
15:O:170:LEU:HD21	15:O:184:VAL:HG22	1.94	0.49
16:P:135:GLU:CG	16:P:140:ASP:HA	2.41	0.49
16:P:172:ALA:H	16:P:202:ARG:HH21	1.59	0.49
16:P:346:GLU:H	16:P:346:GLU:CD	2.20	0.49
16:P:350:ILE:HB	16:P:366:ILE:HG23	1.94	0.49
23:X:119:ARG:HD2	23:X:120:PRO:HD2	1.94	0.49
37:l:119:THR:HG23	38:m:11:LEU:HA	1.92	0.49
41:p:74:ILE:O	41:p:75:THR:C	2.54	0.49
45:AA:405:GLY:C	45:AA:408:PRO:HD2	2.37	0.49
48:AD:155:GLN:HA	48:AD:165:PHE:O	2.12	0.49
49:AE:184:ILE:HG21	49:AE:208:PRO:HB3	1.93	0.49
45:Aa:400:VAL:CG1	46:Ab:58:LEU:HG	2.41	0.49
47:Ac:215:ALA:HB2	50:Af:60:MET:HE3	1.94	0.49
48:Ad:111:ARG:HG3	48:Ad:140:TYR:CE2	2.47	0.49
48:Ad:249:TYR:O	48:Ad:250:THR:C	2.55	0.49
49:Ae:152:ILE:HB	49:Ae:169:TRP:CD1	2.47	0.49
49:Ae:197:ASP:HB3	49:Ae:257:ASN:ND2	2.27	0.49
2:B:166:ASN:CB	2:B:190:TYR:HD2	2.24	0.49
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.47	0.49
6:F:204:TYR:CE1	60:F:501:FMN:H6	2.47	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:17:MET:HE1	8:H:225:MET:CB	2.42	0.49
8:H:70:LEU:HD13	10:J:27:TYR:CE1	2.46	0.49
10:J:116:ASN:O	10:J:117:LEU:C	2.55	0.49
10:J:154:VAL:HG22	11:K:66:PHE:HZ	1.76	0.49
12:L:385:PHE:CD1	35:j:72:ARG:CG	2.95	0.49
13:M:184:HIS:CD2	13:M:249:ILE:HG23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:207:MET:SD	13:M:240:SER:HA	2.52	0.49
13:M:277:LEU:O	37:l:116:ARG:NH2	2.40	0.49
14:N:239:ALA:CB	29:d:47:MET:HG2	2.42	0.49
16:P:238:GLN:HB2	16:P:270:ARG:HG2	1.94	0.49
16:P:375:VAL:C	16:P:377:TYR:H	2.19	0.49
21:V:31:THR:HA	21:V:88:LEU:HD13	1.92	0.49
21:V:39:PRO:HB2	21:V:42:ALA:HB2	1.94	0.49
25:Z:90:ASN:O	25:Z:94:GLU:HB2	2.12	0.49
25:Z:110:VAL:HG23	30:e:65:GLU:CG	2.31	0.49
37:l:184:TYR:HA	40:o:36:GLU:HA	1.93	0.49
39:n:96:CYS:SG	39:n:97:TYR:CZ	3.05	0.49
39:n:163:LEU:O	39:n:164:PRO:C	2.54	0.49
42:q:55:PHE:CD2	43:r:26:LEU:HD22	2.47	0.49
42:q:85:GLU:HG2	42:q:98:PRO:HB3	1.94	0.49
47:AC:141:TRP:CD1	47:AC:265:PRO:HD3	2.47	0.49
47:AC:199:PHE:CZ	47:Ac:10:LEU:HB2	2.47	0.49
2:B:95:PHE:CD2	2:B:141:MET:HE3	2.47	0.49
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.23	0.49
8:H:127:TYR:HE1	8:H:207:LEU:HD23	1.75	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:J:82:TRP:HE3	16:P:360:ARG:HB2	1.77	0.49
11:K:93:LEU:HD22	14:N:54:GLU:HG2	1.94	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
12:L:477:ILE:HG13	40:o:91:GLU:OE1	2.12	0.49
62:L:701:PC1:H2B2	62:L:701:PC1:H351	1.94	0.49
13:M:177:MET:CE	33:h:140:LEU:HD21	2.42	0.49
13:M:177:MET:HB3	33:h:140:LEU:HD21	1.93	0.49
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.47	0.49
15:O:126:GLY:HA3	32:g:51:MET:HE1	1.94	0.49
15:O:143:TYR:CZ	15:O:164:TYR:HE2	2.30	0.49
16:P:275:HIS:CE1	16:P:373:LYS:HG2	2.47	0.49
27:b:23:PHE:CE2	55:b:201:3PE:H252	2.47	0.49
38:m:30:ARG:HG3	45:Aa:259:GLU:HB2	1.92	0.49
45:AA:271:THR:HG23	51:AG:23:GLU:HG2	1.94	0.49
45:AA:361:ASP:N	45:AA:361:ASP:OD1	2.45	0.49
47:AC:140:PHE:HE1	47:AC:170:VAL:HG13	1.77	0.49
47:AC:220:PHE:HE2	69:AC:406:UQ6:H4M2	1.75	0.49
49:AE:153:GLU:HA	49:AE:272:VAL:HG12	1.93	0.49
45:Aa:53:LEU:HD12	45:Aa:57:LEU:HD23	1.94	0.49
1:A:51:PHE:CD2	10:J:73:MET:HB2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:TYR:O	16:P:137:ARG:NH1	2.45	0.49
3:C:97:THR:O	21:V:90:LEU:HD12	2.12	0.49
3:C:124:ARG:HD2	17:Q:140:LYS:HZ1	1.78	0.49
4:D:35:ARG:O	4:D:36:GLN:C	2.54	0.49
4:D:209:LYS:HG2	43:r:27:ARG:NH2	2.27	0.49
4:D:324:GLY:O	4:D:329:ARG:NH1	2.45	0.49
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.93	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
7:G:611:THR:CG2	17:Q:105:GLU:HA	2.22	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
9:I:54:THR:CG2	27:b:13:TRP:HE1	2.26	0.49
11:K:73:VAL:CG2	14:N:38:LEU:HD22	2.43	0.49
12:L:217:LEU:HD13	12:L:273:ILE:HG23	1.94	0.49
12:L:334:PHE:CZ	62:L:701:PC1:H121	2.47	0.49
13:M:88:ASN:O	13:M:89:ASN:HB3	2.12	0.49
13:M:348:LEU:HD12	13:M:415:GLN:HE22	1.77	0.49
56:M:503:CDL:H141	56:M:503:CDL:OA7	2.12	0.49
14:N:24:THR:HB	30:e:2:PRO:HG3	1.93	0.49
14:N:230:ILE:HG21	14:N:296:LEU:HD11	1.94	0.49
14:N:342:GLN:HE21	29:d:30:ARG:HH11	1.60	0.49
16:P:235:THR:O	16:P:236:VAL:C	2.56	0.49
20:U:120:MET:HE1	39:n:24:LEU:HD12	1.93	0.49
21:V:12:VAL:CG1	21:V:13:GLY:H	2.22	0.49
23:X:165:THR:OG1	23:X:172:VAL:HG11	2.12	0.49
56:h:201:CDL:H321	34:i:84:TYR:CD2	2.47	0.49
34:i:90:MET:O	34:i:91:ALA:C	2.53	0.49
39:n:177:ARG:C	39:n:179:THR:N	2.67	0.49
40:o:117:LEU:HD23	40:o:118:LYS:HG2	1.92	0.49
46:AB:64:PHE:HZ	46:AB:394:SER:HA	1.77	0.49
47:AC:197:LEU:HD11	69:AC:406:UQ6:H72	1.93	0.49
50:AF:111:LYS:HA	54:Ak:8:PRO:HG2	1.93	0.49
45:Aa:338:CYS:SG	45:Aa:359:VAL:C	2.96	0.49
46:Ab:167:GLN:HG2	49:Ai:43:LEU:CD1	2.22	0.49
48:Ad:116:VAL:HA	48:Ad:253:LEU:CD2	2.41	0.49
49:Ae:195:LEU:HD11	49:Ae:248:ARG:NH1	2.26	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
3:C:73:GLN:NE2	21:V:112:TRP:HE1	2.09	0.49
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:632:ILE:O	7:G:632:ILE:CG1	2.60	0.49
10:J:151:MET:HE1	14:N:28:LEU:CD1	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:139:GLN:HG3	13:M:140:THR:N	2.27	0.49
13:M:420:THR:HG21	13:M:423:MET:HG2	1.93	0.49
14:N:231:SER:HA	14:N:300:THR:HA	1.93	0.49
15:O:100:ASP:HB3	15:O:102:ARG:HH11	1.77	0.49
15:O:273:ILE:HA	15:O:276:LEU:HG	1.95	0.49
16:P:40:VAL:HB	16:P:53:GLY:HA2	1.93	0.49
16:P:197:GLU:HB3	16:P:259:VAL:HG23	1.93	0.49
23:X:166:ARG:HH22	29:d:87:ASP:CG	2.20	0.49
24:Y:98:ALA:O	24:Y:102:THR:HG23	2.13	0.49
29:d:109:TYR:HB3	41:p:156:LEU:HD21	1.94	0.49
34:i:123:PHE:HZ	40:o:65:ARG:HD2	1.77	0.49
37:l:81:ARG:HD3	37:l:85:GLU:OE2	2.13	0.49
46:AB:297:PRO:HB3	46:AB:304:ASN:OD1	2.12	0.49
2:B:170:TYR:O	2:B:171:TYR:CB	2.60	0.49
6:F:278:ILE:HG22	6:F:354:VAL:HB	1.94	0.49
6:F:297:LYS:HE2	6:F:333:GLU:HB2	1.94	0.49
7:G:643:ARG:O	7:G:646:LEU:N	2.46	0.49
12:L:67:HIS:HE2	12:L:69:VAL:C	2.20	0.49
12:L:316:THR:CG2	12:L:325:ALA:CB	2.89	0.49
13:M:285:LEU:HD22	13:M:410:MET:SD	2.53	0.49
16:P:318:LYS:O	16:P:322:ILE:HG13	2.13	0.49
25:Z:58:ARG:CB	27:b:45:ILE:HD11	2.42	0.49
30:e:34:HIS:CE1	33:h:184:LYS:NZ	2.80	0.49
38:m:88:LEU:HG	55:m:202:3PE:H3C2	1.94	0.49
39:n:20:TYR:CE2	39:n:24:LEU:CD1	2.91	0.49
43:r:45:PRO:O	43:r:46:SER:HB2	2.13	0.49
46:AB:176:ASN:CA	46:AB:258:ILE:HD11	2.43	0.49
54:AK:48:ILE:HG12	54:AK:48:ILE:O	2.12	0.49
46:Ab:297:PRO:HB3	46:Ab:304:ASN:OD1	2.12	0.49
47:Ac:278:TYR:CZ	47:Ac:282:ARG:HD2	2.48	0.49
51:Ag:73:LYS:NZ	52:Ah:64:ASP:O	2.45	0.49
5:E:131:ILE:HA	5:E:187:ILE:HA	1.93	0.49
6:F:117:ALA:HB1	6:F:131:MET:SD	2.53	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:240:ALA:HA	9:I:117:LYS:HZ3	1.77	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
10:J:24:SER:HB3	10:J:27:TYR:CD2	2.35	0.49
10:J:97:ILE:O	10:J:100:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:264:HIS:HA	12:L:267:THR:OG1	2.13	0.49
12:L:510:LYS:O	12:L:512:SER:N	2.45	0.49
13:M:5:ILE:HG13	13:M:6:LEU:N	2.28	0.49
13:M:248:ILE:CG1	13:M:249:ILE:HD12	2.39	0.49
13:M:263:LEU:HD13	38:m:102:TYR:HB2	1.93	0.49
56:M:503:CDL:HB4	31:f:26:LEU:HD21	1.94	0.49
15:O:267:THR:O	15:O:271:GLU:HG3	2.13	0.49
25:Z:110:VAL:HG21	30:e:65:GLU:CD	2.37	0.49
29:d:99:GLU:HG2	29:d:100:ASP:OD1	2.12	0.49
38:m:97:PRO:CD	55:m:201:3PE:H2I3	2.43	0.49
40:o:50:GLN:OE1	41:p:120:ASN:ND2	2.45	0.49
45:AA:338:CYS:SG	45:AA:359:VAL:C	2.96	0.49
51:AG:41:ARG:HH21	56:AG:101:CDL:PB2	2.35	0.49
51:AG:48:ARG:HE	55:AG:103:3PE:C31	2.26	0.49
48:Ad:214:LEU:HD21	48:Ad:242:ILE:HD12	1.94	0.49
49:Ae:184:ILE:CG2	49:Ae:208:PRO:HB3	2.42	0.49
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.49
3:C:121:ARG:NH2	21:V:114:TRP:HA	2.28	0.49
4:D:249:LYS:HA	25:Z:19:ILE:HG23	1.95	0.49
4:D:378:LEU:HD21	7:G:129:PRO:HD2	1.95	0.49
6:F:170:GLN:HB3	44:s:48:LEU:HD22	1.95	0.49
9:I:79:ARG:CZ	43:r:20:LEU:HD22	2.43	0.49
12:L:477:ILE:HG13	40:o:91:GLU:CD	2.38	0.49
16:P:61:ALA:HB3	16:P:82:ILE:HG23	1.94	0.49
16:P:64:PHE:CZ	16:P:211:ASP:HB3	2.47	0.49
23:X:20:VAL:HG13	23:X:24:VAL:HB	1.94	0.49
23:X:44:MET:O	23:X:48:TRP:CD1	2.66	0.49
31:f:8:ARG:O	31:f:9:GLU:HB2	2.13	0.49
36:k:55:GLU:OE1	39:n:38:ARG:HB2	2.13	0.49
42:q:74:PHE:HD2	42:q:75:TRP:CD2	2.31	0.49
47:AC:215:ALA:HA	51:AG:11:ILE:HD11	1.94	0.49
49:AE:179:ARG:HA	49:AE:183:GLU:OE1	2.12	0.49
49:AE:184:ILE:CG2	49:AE:208:PRO:HB3	2.42	0.49
47:Ac:281:LEU:HD12	47:Ac:290:GLY:HA3	1.95	0.49
48:Ad:153:GLU:OE2	48:Ad:166:MET:SD	2.70	0.49
4:D:260:GLU:OE2	9:I:68:ARG:HG2	2.13	0.49
5:E:77:ALA:C	5:E:80:PRO:HD2	2.38	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.94	0.49
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.94	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:240:ALA:HA	9:I:117:LYS:NZ	2.28	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:9:LEU:HD11	8:H:86:TRP:HB3	1.93	0.49
10:J:105:VAL:O	10:J:108:TYR:HB3	2.13	0.49
12:L:68:TRP:CE3	12:L:76:LEU:HD21	2.47	0.49
12:L:73:SER:CB	41:p:100:GLN:HE21	2.24	0.49
12:L:586:LEU:HD21	24:Y:47:PRO:HD3	1.95	0.49
13:M:1:MET:HB2	13:M:52:PHE:CE2	2.47	0.49
13:M:193:ASN:HA	13:M:253:LEU:HD23	1.94	0.49
14:N:243:MET:CG	29:d:44:MET:HE2	2.41	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
18:R:81:GLY:HA2	18:R:88:HIS:CD2	2.47	0.49
23:X:168:PHE:O	23:X:170:TRP:NE1	2.45	0.49
28:c:70:LYS:O	28:c:75:LEU:HA	2.13	0.49
34:i:72:VAL:HG23	34:i:73:SER:N	2.26	0.49
34:i:79:MET:O	34:i:80:TRP:C	2.54	0.49
38:m:75:ASN:OD1	38:m:79:ASN:ND2	2.46	0.49
39:n:114:MET:HG3	39:n:115:TYR:HD2	1.78	0.49
46:AB:47:LEU:CD2	46:AB:234:ALA:HB1	2.43	0.49
47:AC:187:PHE:CZ	67:AC:402:HEM:HBB1	2.47	0.49
48:AD:167:ARG:NH1	48:AD:169:GLY:HA2	2.28	0.49
46:Ab:346:ALA:HA	46:Ab:349:GLU:OE2	2.13	0.49
47:Ac:361:ILE:HA	47:Ac:365:LEU:HB2	1.95	0.49
49:Ae:153:GLU:C	49:Ae:154:ILE:HD12	2.38	0.49
51:Ag:73:LYS:HB3	52:Ah:67:GLU:CD	2.37	0.49
2:B:144:ALA:O	2:B:145:LEU:C	2.55	0.49
4:D:43:TRP:CZ2	13:M:143:LEU:HD12	2.48	0.49
4:D:43:TRP:CZ2	13:M:143:LEU:CD1	2.96	0.49
4:D:199:PRO:HG3	4:D:262:LEU:HD11	1.95	0.49
6:F:233:VAL:CG1	17:Q:164:PHE:HB2	2.43	0.49
6:F:295:PRO:HA	6:F:336:LEU:CB	2.43	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
8:H:26:LYS:HB3	26:a:5:ILE:HG22	1.94	0.49
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.43	0.49
10:J:107:ASN:HA	10:J:115:ILE:HG13	1.95	0.49
12:L:227:PHE:CD2	12:L:283:LEU:HD23	2.48	0.49
12:L:353:GLU:CD	39:n:80:TYR:OH	2.55	0.49
12:L:480:LEU:HD22	35:j:84:PHE:HD2	1.74	0.49
13:M:6:LEU:HD21	31:f:22:PHE:HD2	1.78	0.49
13:M:134:THR:O	13:M:142:ARG:CD	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:348:LEU:HB2	13:M:415:GLN:OE1	2.13	0.49
15:O:275:TYR:HE1	21:V:23:ARG:NH2	2.11	0.49
16:P:59:PHE:CB	16:P:130:ILE:HD11	2.42	0.49
20:T:116:VAL:HG12	20:T:120:MET:HE2	1.94	0.49
20:U:118:ILE:O	20:U:119:ILE:C	2.55	0.49
23:X:47:ARG:CZ	23:X:53:PRO:HG3	2.42	0.49
24:Y:141:PRO:HB2	33:h:161:ARG:NE	2.28	0.49
35:j:40:ILE:O	35:j:41:GLN:C	2.55	0.49
39:n:20:TYR:OH	39:n:45:ARG:HB2	2.12	0.49
40:o:42:THR:O	40:o:43:GLN:C	2.55	0.49
41:p:54:ARG:O	41:p:58:LYS:HG3	2.12	0.49
42:q:48:TYR:OH	42:q:83:PRO:HD2	2.13	0.49
48:AD:200:ILE:HG12	70:AD:401:HEC:HMA3	1.95	0.49
45:Aa:339:GLN:HB3	49:Ai:45:VAL:HG22	1.95	0.49
55:Aa:501:3PE:O32	56:Aa:502:CDL:H312	2.13	0.49
1:A:77:TRP:HZ3	10:J:50:PHE:CD2	2.25	0.48
2:B:68:ARG:NH1	2:B:70:ARG:HB3	2.28	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
3:C:210:ARG:HD2	16:P:48:ARG:HD3	1.94	0.48
4:D:203:MET:HE2	4:D:258:VAL:CG1	2.43	0.48
4:D:274:ASP:H	4:D:325:ASP:HB2	1.78	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
7:G:612:PRO:HG2	22:W:129:HIS:CD2	2.48	0.48
8:H:196:ALA:HA	8:H:199:ASP:HB2	1.95	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
11:K:19:THR:HG23	11:K:29:THR:CG2	2.43	0.48
12:L:41:LYS:HG3	12:L:98:TRP:CH2	2.44	0.48
12:L:144:TRP:HH2	12:L:256:GLY:HA2	1.78	0.48
13:M:173:THR:HG22	33:h:150:ARG:NH1	2.27	0.48
13:M:216:LEU:HD12	13:M:236:LEU:CD2	2.38	0.48
13:M:227:GLY:HA2	13:M:230:ILE:HG22	1.95	0.48
14:N:109:ALA:HB3	14:N:110:PRO:HD3	1.94	0.48
16:P:278:LYS:HB3	16:P:288:PHE:CE2	2.48	0.48
16:P:298:TYR:HA	16:P:301:ILE:HG12	1.95	0.48
16:P:318:LYS:HA	16:P:321:ARG:HH12	1.78	0.48
23:X:53:PRO:CD	25:Z:116:TRP:CD1	2.96	0.48
29:d:30:ARG:NH1	29:d:76:LEU:HD11	2.27	0.48
36:k:49:ASP:OD2	39:n:38:ARG:HG3	2.13	0.48
37:l:162:PRO:HG3	40:o:39:MET:HE3	1.95	0.48
38:m:122:ASP:O	38:m:123:ARG:C	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:7:VAL:HG13	43:r:8:ILE:N	2.28	0.48
49:AE:192:VAL:O	49:AE:195:LEU:HB2	2.13	0.48
47:Ac:141:TRP:HB3	47:Ac:268:ILE:HD11	1.95	0.48
47:Ac:218:ILE:HB	47:Ac:219:PRO:HD2	1.94	0.48
48:Ad:300:LEU:HB3	48:Ad:301:PRO:HD3	1.93	0.48
49:Ae:217:CYS:O	49:Ae:218:THR:C	2.56	0.48
53:Aj:34:ARG:HG3	54:Ak:47:TYR:CZ	2.49	0.48
1:A:75:LEU:HD23	10:J:145:TYR:CE2	2.49	0.48
1:A:75:LEU:HD23	10:J:145:TYR:CZ	2.47	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.74	0.48
7:G:614:GLY:CA	16:P:41:ILE:HG21	2.43	0.48
7:G:617:ARG:NH1	22:W:129:HIS:HA	2.25	0.48
8:H:42:PRO:HB3	42:q:27:PHE:CE2	2.47	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.12	0.48
9:I:210:LEU:HD23	43:r:39:PRO:O	2.13	0.48
12:L:138:PHE:HZ	13:M:376:MET:HG2	1.78	0.48
12:L:550:LEU:HD11	13:M:279:GLN:NE2	2.28	0.48
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.47	0.48
13:M:105:LEU:HD11	56:d:201:CDL:H472	1.95	0.48
55:M:501:3PE:H121	24:Y:135:TRP:HD1	1.77	0.48
14:N:313:MET:HG2	15:O:305:LEU:HD22	1.95	0.48
17:Q:111:LEU:HA	18:R:47:ARG:NH1	2.29	0.48
20:T:93:ILE:HG23	20:T:108:LEU:HD11	1.95	0.48
22:W:46:VAL:N	22:W:47:PRO:HD2	2.29	0.48
23:X:69:ASN:O	23:X:70:PHE:C	2.56	0.48
32:g:109:ASP:HB2	32:g:114:GLU:HB3	1.94	0.48
37:l:167:TYR:OH	37:l:176:LYS:O	2.15	0.48
38:m:26:SER:HB2	38:m:27:PRO:HD2	1.94	0.48
39:n:51:HIS:HB3	39:n:63:LEU:HD13	1.95	0.48
56:Aa:502:CDL:H342	47:Ac:221:HIS:HD1	1.78	0.48
47:Ac:373:GLU:HG2	50:Af:21:TYR:OH	2.14	0.48
48:Ad:200:ILE:HG12	70:Ad:401:HEC:HMA3	1.95	0.48
48:Ad:302:LEU:O	48:Ad:305:ALA:N	2.44	0.48
49:Ae:204:ARG:O	49:Ae:260:VAL:HG11	2.13	0.48
49:Ae:263:TYR:HB3	49:Ae:273:VAL:HG22	1.94	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:49:VAL:HG13	7:G:102:ILE:HD13	1.94	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
8:H:138:GLN:HG3	8:H:285:LEU:HD21	1.94	0.48
12:L:101:MET:HE1	12:L:121:LEU:CB	2.43	0.48
12:L:316:THR:HG21	12:L:325:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:372:CYS:SG	12:L:454:ILE:HG22	2.54	0.48
14:N:31:VAL:HB	14:N:35:PHE:CE2	2.48	0.48
15:O:54:HIS:O	15:O:55:GLU:C	2.55	0.48
15:O:250:SER:HA	15:O:255:VAL:CG2	2.43	0.48
16:P:375:VAL:C	16:P:377:TYR:N	2.69	0.48
21:V:90:LEU:HD23	21:V:94:MET:HG2	1.94	0.48
26:a:18:ILE:N	26:a:19:PRO:CD	2.76	0.48
33:h:73:PHE:O	33:h:77:LEU:N	2.46	0.48
38:m:101:TRP:CZ2	55:m:201:3PE:H2A1	2.49	0.48
39:n:81:ILE:HD12	39:n:87:GLY:O	2.12	0.48
40:o:104:ARG:O	40:o:105:GLU:C	2.56	0.48
47:AC:278:TYR:CZ	47:AC:282:ARG:HD2	2.48	0.48
45:Aa:361:ASP:OD1	45:Aa:361:ASP:N	2.45	0.48
46:Ab:388:THR:HG23	46:Ab:391:GLY:H	1.78	0.48
47:Ac:213:SER:HA	50:Af:67:LEU:HD11	1.94	0.48
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CD2	2.48	0.48
49:Ae:192:VAL:O	49:Ae:195:LEU:HB2	2.13	0.48
3:C:203:LEU:HD21	4:D:123:LEU:HD23	1.93	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:166:ARG:HH22	25:Z:10:MET:HG2	1.78	0.48
6:F:394:LYS:HB2	7:G:155:GLU:HG2	1.95	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
8:H:85:LEU:HD23	8:H:105:ILE:HA	1.93	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
9:I:105:ARG:HH12	18:R:58:ASN:HB2	1.78	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:L:74:MET:CE	13:M:307:TRP:HH2	2.27	0.48
12:L:350:LEU:HD23	12:L:443:ILE:HD11	1.96	0.48
12:L:361:ASN:O	12:L:361:ASN:CG	2.54	0.48
13:M:311:GLY:HA2	13:M:314:MET:CE	2.42	0.48
13:M:313:THR:HA	13:M:316:MET:CE	2.43	0.48
16:P:328:MET:HE1	16:P:377:TYR:C	2.39	0.48
21:V:35:LEU:HD13	21:V:48:THR:HG23	1.95	0.48
23:X:151:ASN:CG	30:e:51:ARG:HH11	2.21	0.48
24:Y:46:ASN:ND2	56:Y:202:CDL:HB22	2.28	0.48
28:c:62:HIS:O	28:c:66:VAL:HG23	2.12	0.48
33:h:73:PHE:HE2	33:h:74:TYR:HE1	1.62	0.48
39:n:44:MET:O	39:n:45:ARG:C	2.54	0.48
42:q:56:PHE:O	42:q:59:HIS:CD2	2.67	0.48
56:q:201:CDL:OB9	56:q:201:CDL:H311	2.13	0.48
46:AB:388:THR:HG23	46:AB:391:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:163:TRP:CZ2	49:Ae:140:MET:CE	2.96	0.48
47:AC:266:PRO:O	49:Ae:237:PRO:HB2	2.13	0.48
46:Ab:109:LYS:O	46:Ab:123:VAL:HA	2.13	0.48
49:Ae:263:TYR:CA	49:Ae:273:VAL:HA	2.42	0.48
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.49	0.48
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.96	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.48
6:F:261:TRP:CE2	6:F:265:PHE:HE2	2.31	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
7:G:638:THR:O	7:G:639:LEU:C	2.56	0.48
9:I:107:PRO:HG3	42:q:106:ARG:HH11	1.75	0.48
10:J:124:LEU:H	10:J:124:LEU:HD22	1.79	0.48
11:K:93:LEU:CD1	14:N:57:THR:HG21	2.44	0.48
12:L:375:ILE:HG12	35:j:65:MET:SD	2.53	0.48
12:L:402:CYS:SG	12:L:403:ASN:N	2.87	0.48
13:M:166:LEU:HD21	13:M:170:HIS:CE1	2.48	0.48
14:N:146:TYR:CE1	14:N:198:PRO:HG2	2.48	0.48
14:N:227:ILE:CA	14:N:230:ILE:HG22	2.38	0.48
15:O:277:LYS:O	15:O:278:TYR:C	2.53	0.48
21:V:11:LEU:HD23	21:V:14:LEU:HD13	1.95	0.48
26:a:37:ARG:CB	26:a:48:MET:HE2	2.43	0.48
27:b:78:LEU:HA	27:b:80:TRP:CD1	2.49	0.48
30:e:47:ILE:HG13	30:e:47:ILE:O	2.12	0.48
34:i:123:PHE:CE2	40:o:65:ARG:HD2	2.47	0.48
36:k:41:LYS:C	36:k:43:ALA:N	2.64	0.48
37:l:48:ARG:CZ	37:l:64:PRO:HD2	2.44	0.48
40:o:117:LEU:HD22	40:o:118:LYS:CE	2.40	0.48
42:q:64:TYR:CD2	42:q:81:MET:HB2	2.48	0.48
45:AA:80:ARG:NH2	45:AA:268:CYS:SG	2.87	0.48
45:AA:276:ARG:NH2	45:AA:465:LEU:O	2.38	0.48
47:AC:32:ASN:ND2	47:AC:228:ASP:OD1	2.47	0.48
47:AC:177:ARG:HB3	47:Ac:53:MET:HB3	1.94	0.48
47:AC:185:LEU:HD23	47:AC:188:ILE:HD12	1.95	0.48
47:AC:270:PRO:HG3	68:AC:405:U10:O3	2.12	0.48
47:AC:304:MET:HA	47:AC:307:LEU:HD12	1.96	0.48
47:AC:361:ILE:HA	47:AC:365:LEU:HB2	1.95	0.48
49:AE:197:ASP:HB3	49:AE:257:ASN:ND2	2.27	0.48
45:Aa:80:ARG:HD3	45:Aa:265:LEU:HD11	1.96	0.48
45:Aa:393:ASN:HB3	46:Ab:106:VAL:O	2.14	0.48
46:Ab:43:LEU:HB3	46:Ab:44:PRO:HD2	1.95	0.48
47:Ac:96:LEU:HD23	55:Ac:403:3PE:H292	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:206:ASN:N	67:Ac:402:HEM:O2D	2.40	0.48
3:C:98:PHE:HB2	21:V:94:MET:HE3	1.96	0.48
4:D:41:ILE:HD11	32:g:53:TRP:HB3	1.94	0.48
4:D:42:GLU:HA	4:D:45:GLU:HG2	1.96	0.48
5:E:147:ILE:O	5:E:151:LEU:HD13	2.14	0.48
6:F:106:SER:HB2	6:F:111:LYS:HZ2	1.79	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:572:HIS:HB2	7:G:699:SER:OG	2.13	0.48
8:H:196:ALA:C	8:H:198:PHE:N	2.70	0.48
8:H:199:ASP:HB3	8:H:279:ARG:HD2	1.95	0.48
8:H:316:PRO:HA	25:Z:58:ARG:NH1	2.22	0.48
9:I:72:MET:CE	43:r:16:SER:HB2	2.43	0.48
10:J:29:GLY:HA2	11:K:31:LEU:HD21	1.94	0.48
10:J:134:MET:HE3	10:J:139:ILE:HD12	1.96	0.48
12:L:433:THR:HG21	12:L:436:ARG:NH2	2.29	0.48
13:M:159:PRO:HG2	55:M:501:3PE:H3B2	1.94	0.48
13:M:307:TRP:CE3	13:M:383:MET:CE	2.97	0.48
14:N:164:MET:CE	56:Y:202:CDL:H592	2.40	0.48
14:N:338:PRO:O	23:X:170:TRP:HZ3	1.97	0.48
20:T:93:ILE:HD13	20:T:108:LEU:HD22	1.95	0.48
20:U:85:TYR:CE2	35:j:44:TYR:HE2	2.31	0.48
23:X:48:TRP:HH2	33:h:185:ALA:O	1.96	0.48
23:X:80:GLU:O	23:X:81:PRO:C	2.55	0.48
25:Z:53:TRP:CE2	25:Z:57:ARG:HD2	2.48	0.48
25:Z:120:LEU:CD1	30:e:69:ARG:HG2	2.44	0.48
30:e:45:HIS:CD2	33:h:176:LYS:HZ2	2.31	0.48
39:n:155:PRO:HG2	39:n:165:PRO:HG2	1.95	0.48
45:AA:113:VAL:HG13	46:AB:299:ILE:HD11	1.94	0.48
46:AB:109:LYS:O	46:AB:123:VAL:HA	2.14	0.48
56:AG:101:CDL:H511	56:AG:101:CDL:H112	1.95	0.48
47:Ac:32:ASN:ND2	47:Ac:228:ASP:OD1	2.47	0.48
49:Ae:143:SER:HB2	49:Ae:145:ASP:OD1	2.13	0.48
49:Ae:218:THR:OG1	49:Ae:254:ALA:HB1	2.13	0.48
1:A:50:PRO:HA	4:D:80:MET:HE2	1.96	0.48
55:A:401:3PE:H2A2	10:J:37:PHE:CE1	2.48	0.48
2:B:170:TYR:O	2:B:171:TYR:HB2	2.14	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
5:E:142:ARG:HG3	5:E:182:ALA:CB	2.44	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
9:I:35:THR:CG2	43:r:107:SER:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:89:GLU:OE1	42:q:58:ARG:HD2	2.14	0.48
10:J:123:TRP:CZ2	30:e:73:MET:HG2	2.48	0.48
12:L:274:LEU:O	12:L:277:MET:HG2	2.14	0.48
12:L:296:ASN:ND2	12:L:425:ARG:HH21	2.12	0.48
13:M:269:MET:HE3	13:M:399:ASN:HB3	1.96	0.48
14:N:4:ILE:HG23	14:N:5:THR:N	2.29	0.48
15:O:206:TYR:OH	15:O:241:TYR:HB3	2.14	0.48
16:P:221:ARG:CD	16:P:286:ARG:HD3	2.43	0.48
22:W:42:TRP:O	22:W:46:VAL:HG23	2.14	0.48
22:W:87:ILE:O	22:W:91:MET:HG3	2.12	0.48
25:Z:58:ARG:NH2	27:b:46:ASN:HA	2.29	0.48
25:Z:94:GLU:OE2	30:e:75:ARG:NH2	2.45	0.48
25:Z:126:GLY:HA3	30:e:76:MET:HE3	1.96	0.48
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
40:o:87:TRP:NE1	40:o:91:GLU:OE1	2.45	0.48
45:AA:64:SER:OG	45:AA:235:GLY:HA2	2.13	0.48
46:AB:286:PHE:CZ	46:AB:427:ALA:HB1	2.49	0.48
47:AC:58:ASP:HB2	47:Ac:56:THR:CG2	2.44	0.48
47:AC:77:TRP:HZ2	48:AD:284:HIS:CD2	2.32	0.48
47:AC:237:LEU:HD22	48:AD:300:LEU:HD11	1.95	0.48
49:AE:143:SER:HB2	49:AE:145:ASP:OD1	2.13	0.48
49:AE:178:HIS:HD2	49:AE:179:ARG:N	2.11	0.48
49:AE:204:ARG:O	49:AE:260:VAL:HG11	2.13	0.48
49:AE:218:THR:OG1	49:AE:254:ALA:HB1	2.13	0.48
45:Aa:120:LEU:HD23	46:Ab:299:ILE:CG2	2.44	0.48
45:Aa:273:SER:HB2	51:Ag:18:SER:O	2.14	0.48
45:Aa:286:HIS:CD2	45:Aa:359:VAL:HG13	2.48	0.48
47:Ac:304:MET:HA	47:Ac:307:LEU:HD12	1.95	0.48
51:Ag:72:ARG:HD3	51:Ag:73:LYS:H	1.77	0.48
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.48	0.48
2:B:112:TYR:CE1	9:I:84:ILE:HD11	2.48	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.14	0.48
8:H:17:MET:SD	8:H:225:MET:HA	2.54	0.48
10:J:70:THR:C	10:J:72:ALA:N	2.72	0.48
10:J:102:LEU:HD23	10:J:102:LEU:C	2.39	0.48
11:K:23:ARG:HG3	11:K:23:ARG:O	2.14	0.48
12:L:319:MET:O	12:L:319:MET:HG2	2.13	0.48
12:L:434:LYS:NZ	36:k:66:ASN:HD22	2.11	0.48
15:O:73:LEU:CD2	15:O:207:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:267:THR:O	15:O:268:LYS:C	2.56	0.48
15:O:314:LEU:HD12	15:O:315:PRO:HD3	1.93	0.48
16:P:81:ILE:HD11	18:R:46:VAL:HG11	1.96	0.48
25:Z:114:THR:O	25:Z:114:THR:CG2	2.60	0.48
28:c:65:ASP:O	28:c:66:VAL:C	2.56	0.48
30:e:45:HIS:CD2	33:h:176:LYS:HD3	2.49	0.48
32:g:106:TYR:OH	33:h:86:ILE:HG23	2.14	0.48
36:k:41:LYS:O	36:k:42:LEU:C	2.50	0.48
37:l:48:ARG:HH21	37:l:63:GLU:HA	1.78	0.48
38:m:25:VAL:HG21	38:m:30:ARG:NH2	2.29	0.48
46:AB:177:LEU:HD11	46:AB:272:VAL:HG22	1.94	0.48
47:AC:327:ILE:HD11	55:AG:103:3PE:H272	1.96	0.48
49:AE:231:PHE:HD2	49:AE:250:ARG:NH1	2.11	0.48
49:AI:62:ARG:HB3	49:AI:63:PRO:HD2	1.96	0.48
45:Aa:274:GLU:HB2	45:Aa:468:TYR:HD1	1.79	0.48
46:Ab:90:THR:HG23	46:Ab:95:SER:HA	1.95	0.48
46:Ab:253:TYR:CE2	46:Ab:435:LYS:HG3	2.48	0.48
46:Ab:254:ARG:HG3	46:Ab:255:GLY:N	2.28	0.48
46:Ab:286:PHE:CZ	46:Ab:427:ALA:HB1	2.49	0.48
47:Ac:185:LEU:HD23	47:Ac:188:ILE:HD12	1.95	0.48
48:Ad:95:PRO:HG2	52:Ah:85:PHE:HB2	1.95	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
5:E:109:MET:HE2	7:G:196:GLY:HA3	1.96	0.48
6:F:102:MET:CG	6:F:149:MET:HB2	2.43	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:140:GLN:HG3	7:G:141:ASP:N	2.28	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.38	0.48
9:I:123:CYS:SG	57:I:302:SF4:S3	3.12	0.48
12:L:31:ASN:HD22	12:L:34:LEU:HB2	1.79	0.48
13:M:422:HIS:CE1	13:M:425:ASN:OD1	2.67	0.48
14:N:189:TRP:CZ3	14:N:282:MET:HE3	2.49	0.48
15:O:77:ILE:O	15:O:81:LEU:HD13	2.14	0.48
17:Q:82:PRO:HG2	17:Q:93:ASN:O	2.14	0.48
18:R:60:ALA:O	18:R:61:ILE:C	2.56	0.48
19:S:27:SER:H	19:S:34:ARG:HH22	1.62	0.48
19:S:79:LEU:CA	19:S:82:LEU:HD12	2.26	0.48
20:U:113:LEU:HD23	39:n:17:LEU:HD23	1.95	0.48
56:d:201:CDL:H531	56:d:201:CDL:H711	1.94	0.48
32:g:123:LEU:CD1	41:p:98:VAL:HG11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:124:LYS:C	38:m:126:ASN:N	2.70	0.48
45:AA:310:ILE:HG21	45:AA:379:LEU:HD21	1.96	0.48
45:AA:362:ALA:HB2	45:AA:461:PRO:HB2	1.95	0.48
47:AC:244:LEU:HA	48:AD:285:ARG:HD2	1.96	0.48
48:AD:242:ILE:HD11	48:AD:244:MET:HE2	1.95	0.48
47:Ac:153:ILE:HG23	47:Ac:154:PRO:HD2	1.96	0.48
48:Ad:179:TYR:HB3	48:Ad:184:ALA:HB3	1.96	0.48
49:Ae:176:VAL:HG13	49:Ae:212:ILE:HG12	1.95	0.48
51:Ag:78:TYR:CD2	52:Ah:63:GLU:HB2	2.49	0.48
6:F:50:ASP:CG	6:F:52:ARG:HB2	2.39	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
10:J:29:GLY:CA	11:K:31:LEU:HD21	2.44	0.48
10:J:134:MET:HE3	10:J:139:ILE:CD1	2.44	0.48
12:L:385:PHE:CE1	35:j:72:ARG:HG3	2.48	0.48
13:M:4:ILE:HG22	13:M:107:ILE:CD1	2.32	0.48
13:M:42:LEU:HG	13:M:67:ILE:CD1	2.42	0.48
19:S:37:ILE:HD12	19:S:55:ILE:HD12	1.95	0.48
22:W:120:ASP:OD1	22:W:121:PHE:N	2.46	0.48
23:X:80:GLU:HB3	23:X:81:PRO:HD3	1.96	0.48
31:f:41:SER:OG	33:h:134:GLU:HG2	2.13	0.48
34:i:90:MET:SD	34:i:97:ILE:HD11	2.54	0.48
36:k:52:ALA:O	36:k:53:ARG:C	2.56	0.48
38:m:23:TYR:HB3	39:n:65:ARG:HD2	1.95	0.48
39:n:37:TYR:O	39:n:39:TYR:N	2.47	0.48
39:n:81:ILE:HD11	39:n:87:GLY:O	2.14	0.48
46:AB:90:THR:HG23	46:AB:95:SER:HA	1.95	0.48
46:AB:173:ILE:HD11	46:AB:439:ALA:C	2.39	0.48
46:AB:261:GLN:O	46:Ab:195:TYR:CE1	2.67	0.48
47:AC:323:ILE:HD11	55:AG:103:3PE:H12	1.96	0.48
49:AE:217:CYS:O	49:AE:218:THR:C	2.57	0.48
50:AF:50:ARG:HD3	46:Ab:149:TRP:CE2	2.49	0.48
45:Aa:56:GLY:HA3	45:Aa:227:PRO:HA	1.96	0.48
46:Ab:167:GLN:HE21	49:Ai:43:LEU:CD1	2.27	0.48
51:Ag:11:ILE:CG2	51:Ag:12:ARG:N	2.77	0.48
51:Ag:29:SER:CB	51:Ag:32:SER:HB2	2.38	0.48
1:A:53:MET:HE2	10:J:170:THR:HB	1.96	0.47
4:D:300:TRP:HE1	4:D:302:LEU:HD21	1.79	0.47
6:F:293:SER:CA	6:F:338:ASP:HB3	2.42	0.47
6:F:297:LYS:HB2	6:F:333:GLU:CA	2.44	0.47
8:H:3:PHE:O	8:H:4:ILE:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:170:THR:O	10:J:171:ARG:C	2.56	0.47
12:L:145:GLU:HB3	13:M:370:PRO:CD	2.44	0.47
13:M:25:THR:HG22	32:g:84:ASN:CG	2.39	0.47
13:M:94:LEU:O	13:M:98:MET:HG2	2.14	0.47
13:M:176:LEU:HD13	13:M:245:ARG:HH11	1.79	0.47
13:M:192:ASN:C	13:M:194:LEU:N	2.72	0.47
13:M:310:MET:CE	13:M:459:MET:SD	3.02	0.47
15:O:165:SER:HB3	15:O:245:PHE:CZ	2.49	0.47
17:Q:99:MET:SD	17:Q:128:PHE:HE2	2.36	0.47
20:U:128:PHE:HZ	20:U:148:ILE:HD12	1.76	0.47
43:r:32:ALA:HB1	43:r:36:GLN:HE21	1.78	0.47
43:r:54:TYR:HA	43:r:57:ARG:HG2	1.96	0.47
47:AC:281:LEU:HD12	47:AC:290:GLY:HA3	1.95	0.47
47:Ac:146:ILE:CD1	68:Ac:404:U10:C3	2.90	0.47
49:Ae:204:ARG:HB3	49:Ae:260:VAL:CG2	2.25	0.47
49:Ae:231:PHE:HD2	49:Ae:250:ARG:NH1	2.12	0.47
56:A:402:CDL:HA21	56:A:402:CDL:H831	1.96	0.47
2:B:224:ARG:HG3	16:P:85:ARG:HH12	1.79	0.47
4:D:142:VAL:HG11	4:D:185:MET:CG	2.44	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
6:F:261:TRP:CE2	6:F:265:PHE:CE2	3.02	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.47
8:H:187:ILE:CD1	55:H:402:3PE:H242	2.44	0.47
9:I:54:THR:HA	27:b:13:TRP:HE1	1.79	0.47
10:J:124:LEU:CB	25:Z:137:ASN:HD21	2.12	0.47
56:L:703:CDL:H322	13:M:361:MET:HE1	1.95	0.47
14:N:246:LEU:HD11	56:d:201:CDL:H402	1.95	0.47
15:O:350:LYS:O	15:O:351:TRP:HB2	2.12	0.47
16:P:335:LEU:O	16:P:336:GLU:HB2	2.14	0.47
18:R:46:VAL:HA	18:R:49:VAL:HG23	1.96	0.47
20:T:100:VAL:O	20:T:141:PRO:HD2	2.15	0.47
20:T:104:PHE:CD1	20:T:110:LEU:CB	2.94	0.47
20:U:102:SER:C	20:U:141:PRO:HD3	2.39	0.47
24:Y:7:PHE:HE1	24:Y:22:ARG:NH1	2.11	0.47
24:Y:61:TYR:CD1	56:Y:202:CDL:H112	2.49	0.47
25:Z:110:VAL:HG12	30:e:71:LYS:HB3	1.95	0.47
25:Z:129:THR:HB	25:Z:132:GLU:CG	2.43	0.47
27:b:46:ASN:OD1	27:b:47:LYS:N	2.47	0.47
30:e:41:ILE:HD11	33:h:174:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:42:MET:HB2	41:p:87:GLU:OE1	2.14	0.47
33:h:59:PRO:HD3	39:n:99:VAL:HG11	1.96	0.47
34:i:103:ARG:O	41:p:18:PRO:HG3	2.14	0.47
46:AB:64:PHE:CZ	46:AB:394:SER:HA	2.48	0.47
47:AC:272:TRP:HA	47:AC:275:LEU:HG	1.96	0.47
49:AE:176:VAL:HG13	49:AE:212:ILE:HG12	1.95	0.47
45:Aa:362:ALA:HB2	45:Aa:461:PRO:HB2	1.95	0.47
49:Ae:178:HIS:HD2	49:Ae:179:ARG:N	2.11	0.47
1:A:113:TRP:CH2	8:H:287:HIS:CD2	3.02	0.47
55:A:401:3PE:H341	10:J:56:PHE:CE2	2.46	0.47
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.28	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
10:J:20:ALA:C	10:J:22:LYS:N	2.69	0.47
12:L:41:LYS:HZ3	62:L:701:PC1:H2B1	1.79	0.47
12:L:54:PHE:CZ	12:L:84:PHE:HB2	2.49	0.47
12:L:313:MET:O	12:L:316:THR:HG22	2.13	0.47
12:L:363:THR:HG21	36:k:72:VAL:HG22	1.96	0.47
12:L:560:LYS:NZ	55:Y:201:3PE:H32	2.29	0.47
14:N:25:ASN:HB3	30:e:15:ASP:CG	2.40	0.47
15:O:59:VAL:HG22	15:O:157:VAL:CG2	2.44	0.47
15:O:225:HIS:HA	15:O:228:LYS:HE3	1.95	0.47
15:O:320:GLY:HA2	32:g:53:TRP:CZ3	2.48	0.47
16:P:311:GLU:O	16:P:312:PRO:C	2.57	0.47
19:S:50:ASN:O	19:S:51:LEU:C	2.57	0.47
23:X:8:PRO:HB3	23:X:12:GLU:CD	2.39	0.47
55:Y:201:3PE:H261	56:Y:202:CDL:H311	1.96	0.47
32:g:125:LYS:CE	41:p:8:ASP:HB2	2.45	0.47
35:j:97:LEU:HB3	40:o:104:ARG:HB2	1.95	0.47
39:n:96:CYS:SG	39:n:97:TYR:CE1	3.04	0.47
39:n:156:PRO:HD2	39:n:158:ARG:NH1	2.29	0.47
46:AB:312:SER:OG	46:AB:357:GLN:NE2	2.40	0.47
47:AC:297:SER:O	47:AC:300:ILE:HG22	2.13	0.47
52:AH:67:GLU:HG3	52:AH:68:GLU:N	2.30	0.47
54:AK:41:ILE:HD12	54:AK:41:ILE:N	2.29	0.47
1:A:83:LYS:HG3	10:J:146:SER:HB2	1.97	0.47
56:A:402:CDL:HB62	56:A:402:CDL:H772	1.96	0.47
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.95	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.47
8:H:318:MET:CE	10:J:133:VAL:HG12	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.96	0.47
10:J:71:THR:HG22	10:J:71:THR:O	2.15	0.47
10:J:78:TYR:N	10:J:79:PRO:HD3	2.29	0.47
11:K:69:CYS:O	11:K:70:GLU:C	2.57	0.47
12:L:277:MET:SD	12:L:318:GLY:HA2	2.54	0.47
12:L:356:ILE:HA	12:L:359:MET:HG2	1.96	0.47
12:L:433:THR:CG2	12:L:434:LYS:N	2.78	0.47
12:L:564:LYS:HG2	38:m:77:TYR:OH	2.14	0.47
12:L:576:LEU:HA	12:L:579:ASN:ND2	2.29	0.47
13:M:409:TYR:CZ	37:l:116:ARG:NH2	2.78	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
16:P:170:LEU:HG	16:P:171:ASN:N	2.28	0.47
16:P:237:LYS:HZ2	16:P:322:ILE:HG23	1.79	0.47
20:U:93:ILE:HD11	20:U:118:ILE:HD11	1.97	0.47
24:Y:142:LYS:O	24:Y:143:VAL:C	2.57	0.47
30:e:41:ILE:CD1	33:h:174:PRO:HB2	2.44	0.47
38:m:124:LYS:C	38:m:126:ASN:H	2.21	0.47
45:AA:383:ALA:O	45:AA:442:ARG:NH1	2.48	0.47
53:AJ:31:PHE:CD1	54:AK:47:TYR:HD2	2.33	0.47
47:Ac:100:ARG:HH12	67:Ac:402:HEM:HBD2	1.79	0.47
47:Ac:297:SER:O	47:Ac:300:ILE:HG22	2.13	0.47
48:Ad:207:GLY:O	48:Ad:208:GLU:C	2.58	0.47
2:B:174:SER:HA	3:C:203:LEU:CD2	2.45	0.47
3:C:221:GLU:OE1	22:W:114:GLU:HB2	2.14	0.47
4:D:240:LEU:HG	4:D:244:ILE:HD11	1.96	0.47
6:F:61:ASP:O	6:F:140:GLU:OE1	2.32	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
11:K:75:LEU:O	11:K:79:VAL:HG23	2.15	0.47
12:L:3:ILE:HG22	12:L:49:LEU:HD21	1.97	0.47
12:L:121:LEU:HD22	12:L:246:LEU:CD2	2.24	0.47
12:L:496:LEU:C	12:L:496:LEU:HD12	2.39	0.47
12:L:552:LEU:HD22	12:L:553:LEU:HD12	1.97	0.47
13:M:78:MET:HG2	13:M:432:ARG:HG3	1.97	0.47
13:M:122:PHE:HZ	13:M:206:LYS:HD3	1.75	0.47
14:N:1:MET:O	14:N:2:ASN:C	2.54	0.47
15:O:91:ILE:HD11	15:O:131:LEU:CD1	2.40	0.47
15:O:116:LYS:HA	15:O:119:ASP:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:150:ARG:NE	16:P:190:GLU:HG2	2.27	0.47
23:X:5:VAL:O	23:X:6:GLU:C	2.54	0.47
23:X:137:LEU:HA	27:b:58:ARG:NH2	2.30	0.47
24:Y:71:MET:HG3	24:Y:102:THR:CG2	2.43	0.47
29:d:8:HIS:O	29:d:10:PRO:HD3	2.14	0.47
29:d:110:ALA:O	41:p:160:LYS:NZ	2.40	0.47
40:o:122:VAL:O	40:o:123:ALA:C	2.55	0.47
43:r:25:GLN:H	43:r:25:GLN:CD	2.21	0.47
46:AB:306:THR:O	46:AB:307:SER:C	2.58	0.47
48:AD:259:THR:HG23	52:AH:89:LYS:HE2	1.95	0.47
47:Ac:152:ALA:CB	47:Ac:287:LYS:HD2	2.45	0.47
48:Ad:96:TRP:HD1	48:Ad:99:ARG:NH2	2.09	0.47
48:Ad:157:GLY:O	48:Ad:164:MET:HA	2.15	0.47
52:Ah:26:ASP:O	52:Ah:27:PRO:C	2.58	0.47
1:A:106:TRP:HZ3	27:b:19:LEU:HD21	1.78	0.47
56:A:402:CDL:HB62	56:A:402:CDL:H771	1.96	0.47
4:D:185:MET:SD	4:D:204:PHE:HZ	2.37	0.47
4:D:362:LYS:HG3	43:r:54:TYR:CZ	2.50	0.47
58:D:501:UQ1:O1	58:D:501:UQ1:C8	2.50	0.47
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.47
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:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.95	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:642:VAL:O	7:G:645:ARG:HB3	2.14	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:J:78:TYR:HD2	10:J:82:TRP:CD1	2.32	0.47
12:L:138:PHE:CZ	13:M:376:MET:HG2	2.49	0.47
13:M:305:THR:O	13:M:306:PRO:C	2.58	0.47
17:Q:129:SER:HB2	21:V:116:ILE:HD12	1.97	0.47
20:T:134:ASP:HA	20:T:137:LYS:NZ	2.29	0.47
22:W:46:VAL:O	22:W:50:VAL:HG23	2.14	0.47
24:Y:102:THR:O	24:Y:103:LEU:C	2.57	0.47
29:d:73:TYR:O	29:d:77:LYS:HB2	2.14	0.47
30:e:22:SER:HA	30:e:34:HIS:HD2	1.79	0.47
31:f:37:PHE:O	31:f:38:ARG:C	2.57	0.47
39:n:177:ARG:C	39:n:179:THR:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:8:ARG:HB2	40:o:16:GLU:CG	2.23	0.47
44:s:55:PHE:O	44:s:56:ARG:C	2.57	0.47
45:AA:395:LEU:O	45:AA:399:LEU:HG	2.14	0.47
47:AC:18:PHE:CE1	69:AC:406:UQ6:H71	2.49	0.47
49:AE:156:LEU:HD12	49:AE:268:ASP:HA	1.95	0.47
51:AG:11:ILE:CG2	51:AG:12:ARG:N	2.77	0.47
45:Aa:152:GLN:O	45:Aa:153:ASN:HB2	2.15	0.47
45:Aa:341:PHE:HZ	45:Aa:372:LEU:CD1	2.28	0.47
67:Ac:402:HEM:HMA1	69:Ac:405:UQ6:O5	2.14	0.47
48:Ad:156:ASP:HB2	48:Ad:167:ARG:CG	2.43	0.47
1:A:63:LEU:CD1	10:J:66:VAL:HG21	2.45	0.47
2:B:75:VAL:HG13	2:B:218:LEU:HB3	1.95	0.47
3:C:66:GLU:O	3:C:69:PRO:HD3	2.14	0.47
3:C:67:ILE:CD1	21:V:47:TYR:HD2	2.24	0.47
4:D:320:ILE:HD11	9:I:36:TYR:CE2	2.49	0.47
5:E:114:VAL:HG13	5:E:118:TYR:CE2	2.50	0.47
5:E:180:VAL:CG1	5:E:181:ASN:N	2.78	0.47
5:E:190:ASN:HB3	5:E:215:PRO:HB3	1.96	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:254:ILE:O	6:F:258:GLY:N	2.48	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.47	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
7:G:106:SER:O	7:G:107:GLU:C	2.57	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:94:PRO:CG	8:H:97:ASN:HB3	2.39	0.47
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.27	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.02	0.47
10:J:63:MET:HE2	11:K:68:ALA:CA	2.42	0.47
10:J:87:LEU:HD21	10:J:91:PHE:HE2	1.75	0.47
10:J:133:VAL:HG23	25:Z:68:ARG:CZ	2.44	0.47
11:K:29:THR:O	11:K:30:LEU:C	2.54	0.47
12:L:403:ASN:HA	37:l:152:SER:O	2.15	0.47
12:L:460:GLY:HA2	62:L:701:PC1:O14	2.15	0.47
13:M:29:SER:CB	32:g:91:PHE:HD2	2.20	0.47
13:M:57:SER:OG	13:M:113:THR:HG22	2.15	0.47
13:M:231:LEU:CD1	13:M:235:LEU:HD12	2.42	0.47
55:M:501:3PE:H121	24:Y:135:TRP:CD1	2.49	0.47
14:N:26:LEU:O	14:N:29:MET:N	2.47	0.47
14:N:120:GLN:O	14:N:176:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:86:TYR:HB3	15:O:142:GLN:HE21	1.80	0.47
15:O:135:LEU:HB3	15:O:139:ARG:NH1	2.26	0.47
15:O:161:ARG:NH2	63:O:401:ADP:O2A	2.47	0.47
15:O:209:VAL:HA	15:O:210:PRO:HD3	1.64	0.47
16:P:212:ARG:O	16:P:213:PHE:C	2.55	0.47
17:Q:99:MET:SD	17:Q:128:PHE:CE2	3.08	0.47
19:S:48:HIS:HE1	19:S:95:LEU:CD2	2.25	0.47
19:S:58:CYS:HB2	19:S:61:VAL:CG1	2.43	0.47
20:T:90:TYR:CE2	20:T:92:LYS:HB2	2.49	0.47
20:T:134:ASP:O	20:T:138:LEU:HG	2.14	0.47
21:V:116:ILE:HG23	21:V:116:ILE:O	2.15	0.47
22:W:32:LYS:O	22:W:36:ARG:HG3	2.15	0.47
22:W:97:ILE:HG13	22:W:98:LYS:H	1.78	0.47
23:X:39:THR:CG2	23:X:40:ASN:N	2.77	0.47
23:X:48:TRP:CH2	33:h:185:ALA:O	2.68	0.47
23:X:82:PHE:HB2	23:X:107:PHE:CE1	2.50	0.47
24:Y:143:VAL:HG21	33:h:169:TYR:CE2	2.50	0.47
25:Z:97:ILE:HG13	25:Z:98:MET:HE3	1.95	0.47
25:Z:125:TYR:HA	25:Z:128:ARG:HB2	1.95	0.47
26:a:22:SER:O	26:a:23:THR:C	2.57	0.47
28:c:38:LYS:HA	28:c:39:PRO:HD3	1.58	0.47
31:f:39:ASN:ND2	31:f:55:THR:HG21	2.30	0.47
32:g:53:TRP:CD1	32:g:53:TRP:N	2.83	0.47
33:h:57:VAL:CG1	39:n:99:VAL:HG23	2.45	0.47
37:l:32:MET:HG2	37:l:36:MET:HE2	1.97	0.47
37:l:101:TRP:HE1	38:m:62:ASP:HA	1.79	0.47
45:AA:152:GLN:O	45:AA:153:ASN:HB2	2.15	0.47
48:AD:242:ILE:HG12	48:AD:244:MET:H	1.80	0.47
50:AF:29:LYS:HA	50:AF:81:TRP:CD1	2.50	0.47
54:AK:6:LEU:HD12	54:AK:11:ARG:NH1	2.30	0.47
45:Aa:152:GLN:OE1	45:Aa:253:VAL:HG22	2.14	0.47
47:Ac:294:LEU:O	47:Ac:297:SER:HB3	2.15	0.47
47:Ac:296:LEU:O	47:Ac:300:ILE:N	2.45	0.47
48:Ad:302:LEU:O	48:Ad:303:THR:C	2.56	0.47
49:Ae:88:PHE:C	49:Ae:92:ARG:HG3	2.40	0.47
49:Ae:156:LEU:HD11	49:Ae:265:PHE:CE1	2.50	0.47
49:Ae:166:ALA:HA	49:Ae:174:LEU:O	2.15	0.47
51:Ag:76:ALA:O	51:Ag:79:GLU:HG2	2.13	0.47
3:C:203:LEU:CD2	4:D:123:LEU:HD21	2.32	0.47
5:E:153:ARG:HG3	5:E:154:LYS:N	2.29	0.47
5:E:153:ARG:NH2	5:E:154:LYS:HE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:297:LYS:HB2	6:F:333:GLU:HB2	1.94	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:292:ASN:O	27:b:18:VAL:HG11	2.14	0.47
11:K:57:MET:C	11:K:60:PRO:HD2	2.39	0.47
16:P:272:LEU:CG	16:P:375:VAL:HG21	2.25	0.47
20:U:130:ILE:HG21	20:U:138:LEU:HD11	1.97	0.47
23:X:25:LEU:O	23:X:29:ALA:N	2.48	0.47
25:Z:53:TRP:O	25:Z:57:ARG:HG3	2.15	0.47
25:Z:58:ARG:HH21	27:b:46:ASN:HA	1.78	0.47
31:f:43:LEU:HD21	41:p:68:TYR:CD1	2.49	0.47
35:j:99:ILE:CD1	40:o:107:ARG:HB2	2.44	0.47
37:l:44:THR:CG2	37:l:47:GLU:HG3	2.45	0.47
39:n:61:THR:HG21	45:Aa:262:VAL:CG2	2.43	0.47
40:o:103:GLU:O	40:o:104:ARG:C	2.56	0.47
45:AA:102:LYS:HZ3	45:AA:153:ASN:HA	1.77	0.47
45:AA:463:GLU:OE1	51:AG:8:LEU:HB2	2.15	0.47
46:AB:100:THR:HG23	49:AI:70:LEU:HD11	1.97	0.47
47:AC:128:PHE:CD1	68:AC:405:U10:H4M2	2.50	0.47
47:AC:220:PHE:CE2	69:AC:406:UQ6:H4M2	2.50	0.47
47:AC:294:LEU:O	47:AC:297:SER:HB3	2.15	0.47
46:Ab:284:ASN:HB3	46:Ab:419:VAL:CG2	2.45	0.47
47:Ac:242:LEU:HD21	47:Ac:250:LEU:CD1	2.44	0.47
1:A:51:PHE:CE2	11:K:79:VAL:HG13	2.49	0.47
1:A:65:PHE:O	1:A:69:ILE:HG13	2.14	0.47
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.96	0.47
4:D:159:LEU:HD22	43:r:60:ARG:HG3	1.97	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
9:I:54:THR:HA	27:b:13:TRP:NE1	2.30	0.47
10:J:44:LEU:HD23	10:J:48:GLY:O	2.15	0.47
12:L:9:LEU:HG	55:i:201:3PE:H2C2	1.95	0.47
12:L:237:MET:HE1	12:L:248:HIS:HB2	1.97	0.47
12:L:446:ASN:HD21	35:j:51:THR:CG2	2.28	0.47
13:M:196:TRP:HD1	13:M:250:LEU:HB2	1.80	0.47
15:O:129:TYR:CE2	15:O:183:CYS:HB3	2.50	0.47
15:O:201:PRO:HD2	15:O:249:MET:HE2	1.96	0.47
15:O:239:ASN:HB3	15:O:243:LYS:CD	2.41	0.47
16:P:116:ILE:HG21	16:P:152:ILE:HA	1.96	0.47
16:P:245:VAL:HA	16:P:265:PHE:CD2	2.49	0.47
16:P:318:LYS:O	16:P:319:VAL:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:333:PRO:HB2	16:P:337:ASP:CB	2.36	0.47
26:a:2:TRP:O	26:a:5:ILE:HG12	2.14	0.47
28:c:46:LEU:O	28:c:50:ALA:CB	2.63	0.47
37:l:153:TYR:OH	40:o:8:ARG:HD3	2.15	0.47
39:n:57:MET:O	39:n:58:MET:C	2.58	0.47
41:p:65:HIS:O	41:p:66:ARG:C	2.57	0.47
45:AA:390:ARG:HG3	46:AB:104:GLU:O	2.15	0.47
47:AC:16:HIS:NE2	47:AC:201:HIS:CD2	2.82	0.47
47:AC:140:PHE:CE1	47:AC:170:VAL:CG1	2.98	0.47
47:AC:245:PHE:CE1	48:AD:102:LEU:CD2	2.97	0.47
48:AD:160:ASP:C	48:AD:162:GLY:N	2.71	0.47
47:Ac:140:PHE:CE1	47:Ac:170:VAL:CG1	2.98	0.47
50:Af:83:LYS:HB3	50:Af:85:GLU:OE2	2.15	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
9:I:93:LEU:O	42:q:93:MET:CG	2.63	0.47
10:J:82:TRP:HB2	16:P:360:ARG:NH1	2.30	0.47
10:J:138:GLY:O	10:J:139:ILE:C	2.57	0.47
12:L:190:SER:OG	13:M:307:TRP:HZ3	1.98	0.47
16:P:55:VAL:HG12	16:P:123:SER:HA	1.96	0.47
16:P:192:ARG:HH21	16:P:200:ILE:HG12	1.80	0.47
16:P:221:ARG:HD3	16:P:286:ARG:HD3	1.97	0.47
16:P:276:LEU:O	16:P:280:ILE:HG13	2.15	0.47
19:S:16:LEU:CD2	19:S:19:ILE:HD11	2.44	0.47
19:S:27:SER:O	19:S:34:ARG:NH2	2.48	0.47
19:S:40:ARG:HH12	19:S:84:ALA:HB1	1.79	0.47
20:T:103:HIS:CD2	20:T:106:LYS:HD2	2.50	0.47
20:U:133:ILE:CD1	39:n:7:PRO:HD3	2.44	0.47
22:W:94:GLN:HG3	22:W:98:LYS:NZ	2.29	0.47
23:X:120:PRO:HB3	23:X:125:LEU:HD11	1.94	0.47
29:d:51:ARG:O	29:d:52:PRO:C	2.55	0.47
38:m:14:LEU:HD12	38:m:15:PRO:HD2	1.96	0.47
45:AA:120:LEU:HD23	46:AB:299:ILE:HG23	1.96	0.47
45:AA:287:VAL:HB	45:AA:358:PHE:CE2	2.50	0.47
47:AC:227:LYS:HG3	48:AD:307:LYS:HE3	1.97	0.47
48:AD:260:PRO:HD2	52:AH:89:LYS:HE3	1.97	0.47
53:AJ:34:ARG:HG2	54:AK:48:ILE:HA	1.97	0.47
51:Ag:31:PHE:CD1	56:Ag:102:CDL:H312	2.50	0.47
1:A:104:TYR:CE2	10:J:167:ILE:HD12	2.44	0.46
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.50	0.46
6:F:424:ILE:HG13	7:G:76:ARG:HD3	1.97	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
8:H:186:PHE:CZ	8:H:270:PHE:HD1	2.32	0.46
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.46	0.46
9:I:188:GLU:OE2	18:R:33:HIS:NE2	2.47	0.46
11:K:22:PHE:HD2	12:L:584:ILE:CG2	2.26	0.46
12:L:86:SER:OG	12:L:133:SER:HB3	2.15	0.46
12:L:123:LEU:HD21	56:L:703:CDL:C74	2.42	0.46
12:L:277:MET:CG	12:L:318:GLY:HA2	2.44	0.46
13:M:4:ILE:HD12	13:M:4:ILE:N	2.30	0.46
13:M:380:PHE:N	13:M:380:PHE:CD1	2.82	0.46
15:O:351:TRP:CZ3	28:c:41:TRP:HH2	2.33	0.46
16:P:76:MET:HE1	16:P:254:LYS:CE	2.45	0.46
22:W:97:ILE:CG1	22:W:98:LYS:N	2.75	0.46
24:Y:143:VAL:HG23	33:h:157:ARG:O	2.14	0.46
26:a:49:GLU:CD	26:a:52:ARG:HH11	2.22	0.46
29:d:59:HIS:CE1	29:d:60:ARG:HG3	2.50	0.46
29:d:78:ARG:O	29:d:81:TYR:N	2.48	0.46
38:m:50:GLN:HG2	38:m:60:ILE:HD12	1.97	0.46
39:n:133:TRP:O	39:n:137:VAL:HG22	2.14	0.46
46:AB:284:ASN:HB3	46:AB:419:VAL:CG2	2.45	0.46
47:AC:182:HIS:HE1	67:AC:402:HEM:C4C	2.33	0.46
47:AC:221:HIS:NE2	55:AC:401:3PE:O12	2.46	0.46
47:AC:296:LEU:O	47:AC:300:ILE:N	2.45	0.46
49:AE:140:MET:CE	47:Ac:163:TRP:HZ2	2.28	0.46
49:AE:166:ALA:HA	49:AE:174:LEU:O	2.15	0.46
49:AE:231:PHE:CD2	49:AE:250:ARG:HG3	2.50	0.46
54:AK:45:VAL:CB	54:AK:48:ILE:HG22	2.45	0.46
45:Aa:383:ALA:O	45:Aa:442:ARG:NH1	2.48	0.46
47:Ac:128:PHE:CE1	68:Ac:404:U10:C4M	2.98	0.46
48:Ad:156:ASP:N	48:Ad:165:PHE:O	2.43	0.46
49:Ae:226:ALA:HB2	49:Ae:234:TYR:HE1	1.80	0.46
50:Af:85:GLU:CD	50:Af:85:GLU:H	2.24	0.46
4:D:58:THR:HA	4:D:61:TRP:CE2	2.50	0.46
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.43	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
7:G:75:CYS:SG	59:G:803:FES:S1	3.13	0.46
7:G:639:LEU:O	7:G:640:ASP:C	2.58	0.46
10:J:154:VAL:HG13	10:J:155:ALA:N	2.30	0.46
12:L:373:LEU:CD2	12:L:427:ILE:HG22	2.45	0.46
12:L:421:MET:HE2	12:L:500:ILE:HB	1.98	0.46
12:L:491:LEU:CD1	35:j:80:VAL:HG22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:581:LYS:HB2	12:L:586:LEU:HD22	1.97	0.46
13:M:213:HIS:O	13:M:217:PRO:CD	2.63	0.46
13:M:232:ALA:HA	13:M:236:LEU:HD12	1.98	0.46
13:M:380:PHE:N	13:M:380:PHE:HD1	2.13	0.46
15:O:66:ILE:HG13	15:O:234:LEU:CD2	2.45	0.46
15:O:96:THR:CA	15:O:101:GLY:HA2	2.44	0.46
16:P:209:ARG:O	16:P:210:GLU:HB2	2.15	0.46
23:X:41:LYS:O	23:X:42:GLU:C	2.59	0.46
37:l:127:ASP:O	37:l:128:VAL:C	2.59	0.46
39:n:50:GLU:O	39:n:51:HIS:C	2.56	0.46
42:q:137:TRP:CH2	42:q:140:PRO:HD3	2.51	0.46
43:r:50:SER:O	43:r:51:ASN:C	2.58	0.46
45:AA:341:PHE:HZ	45:AA:372:LEU:CD1	2.28	0.46
47:AC:146:ILE:CD1	68:AC:405:U10:C3	2.91	0.46
47:AC:153:ILE:HG23	47:AC:154:PRO:HD2	1.96	0.46
48:AD:244:MET:HB2	70:AD:401:HEC:C4D	2.46	0.46
48:AD:318:LYS:HD2	49:AE:86:PRO:HB2	1.95	0.46
49:AE:156:LEU:HD11	49:AE:265:PHE:CE1	2.50	0.46
45:Aa:99:LYS:HD2	45:Aa:160:GLN:HE21	1.80	0.46
45:Aa:118:ALA:O	46:Ab:298:HIS:HD2	1.97	0.46
47:Ac:141:TRP:HB3	47:Ac:268:ILE:CD1	2.46	0.46
48:Ad:312:SER:O	48:Ad:313:VAL:C	2.59	0.46
49:Ae:93:ARG:HG2	51:Ag:23:GLU:O	2.15	0.46
49:Ae:246:SER:HB3	49:Ae:248:ARG:HE	1.79	0.46
50:Af:29:LYS:HA	50:Af:81:TRP:CD1	2.50	0.46
52:Ah:67:GLU:HG3	52:Ah:68:GLU:N	2.29	0.46
5:E:163:THR:HB	5:E:164:PRO:HD2	1.97	0.46
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.97	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:544:MET:HE3	7:G:565:PHE:CE2	2.42	0.46
8:H:312:ALA:HB2	27:b:41:TYR:HB2	1.98	0.46
10:J:124:LEU:HD23	25:Z:137:ASN:ND2	2.31	0.46
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.46
12:L:172:ILE:O	12:L:176:ARG:HG2	2.16	0.46
56:M:503:CDL:H421	56:M:503:CDL:H452	1.79	0.46
14:N:17:PRO:HG2	14:N:133:TRP:NE1	2.30	0.46
15:O:62:VAL:HG13	15:O:62:VAL:O	2.15	0.46
15:O:201:PRO:CD	15:O:249:MET:HE2	2.45	0.46
16:P:207:PHE:CD2	16:P:241:TYR:HD1	2.33	0.46
18:R:38:TYR:OH	18:R:47:ARG:NH2	2.48	0.46
21:V:22:GLU:O	21:V:26:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:120:PRO:HB2	23:X:125:LEU:CD1	2.44	0.46
23:X:154:ILE:HG12	33:h:167:PRO:HG2	1.98	0.46
29:d:109:TYR:HB3	41:p:156:LEU:CD2	2.45	0.46
34:i:34:VAL:HB	39:n:114:MET:HA	1.98	0.46
34:i:94:PRO:HD3	41:p:5:TRP:HB3	1.97	0.46
45:AA:118:ALA:O	46:AB:298:HIS:HD2	1.98	0.46
45:AA:169:LEU:HD11	45:AA:209:ARG:HG2	1.97	0.46
47:AC:100:ARG:HH12	67:AC:403:HEM:CGD	2.28	0.46
49:AE:205:VAL:HG12	49:AE:211:VAL:HG23	1.98	0.46
48:Ad:146:LYS:NZ	48:Ad:170:LYS:HA	2.30	0.46
49:Ae:231:PHE:CD2	49:Ae:250:ARG:HG3	2.50	0.46
1:A:104:TYR:CE2	10:J:167:ILE:HD13	2.39	0.46
3:C:73:GLN:HG2	21:V:103:LEU:HD21	1.96	0.46
4:D:92:HIS:HB2	4:D:458:PHE:CE2	2.49	0.46
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.50	0.46
13:M:29:SER:HB3	32:g:91:PHE:CE2	2.48	0.46
13:M:114:GLU:HG3	23:X:169:PHE:HB3	1.97	0.46
13:M:139:GLN:HG3	13:M:141:GLU:H	1.80	0.46
13:M:151:PHE:HZ	14:N:291:PHE:CA	2.28	0.46
14:N:154:ILE:HG12	14:N:195:PRO:CG	2.45	0.46
15:O:221:LYS:NZ	63:O:401:ADP:O2B	2.48	0.46
23:X:35:GLN:HG3	23:X:70:PHE:HE1	1.80	0.46
24:Y:7:PHE:HE1	24:Y:22:ARG:HH12	1.64	0.46
29:d:13:PHE:O	29:d:78:ARG:NE	2.43	0.46
33:h:94:GLY:HA3	41:p:56:HIS:CD2	2.51	0.46
34:i:105:PHE:HB3	34:i:106:PRO:HD2	1.97	0.46
35:j:51:THR:O	35:j:52:ARG:C	2.53	0.46
35:j:74:TRP:HB2	36:k:84:PHE:HZ	1.81	0.46
42:q:56:PHE:HA	42:q:59:HIS:HD2	1.81	0.46
44:s:52:LEU:HB3	44:s:56:ARG:HH11	1.81	0.46
46:AB:85:LEU:HD21	49:AI:68:VAL:HG11	1.97	0.46
46:AB:278:ILE:HB	46:AB:331:SER:HA	1.98	0.46
48:AD:290:LEU:CD2	53:AJ:44:TYR:HB2	2.46	0.46
53:AJ:31:PHE:HD1	54:AK:47:TYR:HD2	1.63	0.46
46:Ab:49:ILE:HD13	46:Ab:220:LEU:HB3	1.97	0.46
46:Ab:225:VAL:HG22	46:Ab:229:VAL:CG2	2.46	0.46
46:Ab:426:LYS:HA	46:Ab:429:LYS:HZ3	1.80	0.46
2:B:100:CYS:HB2	2:B:134:ALA:CB	2.37	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:23:MET:HE1	56:L:703:CDL:H362	1.98	0.46
12:L:193:MET:HE1	38:m:125:PHE:CE2	2.51	0.46
12:L:225:ALA:CB	12:L:233:LEU:HD12	2.45	0.46
12:L:466:PHE:HB2	35:j:68:TRP:CH2	2.47	0.46
13:M:435:THR:O	13:M:436:LEU:C	2.59	0.46
16:P:331:ASP:O	16:P:332:LEU:C	2.59	0.46
21:V:72:LEU:CD1	21:V:72:LEU:C	2.89	0.46
22:W:50:VAL:HA	22:W:55:LEU:HD12	1.97	0.46
23:X:54:ARG:NH2	25:Z:116:TRP:HB2	2.31	0.46
23:X:94:MET:O	23:X:95:GLN:C	2.59	0.46
38:m:97:PRO:CG	55:m:201:3PE:H2G2	2.45	0.46
39:n:136:GLU:O	39:n:139:GLN:N	2.49	0.46
42:q:117:VAL:HB	42:q:122:GLU:HB3	1.96	0.46
47:AC:49:LEU:HD22	47:Ac:184:ILE:HD13	1.97	0.46
47:AC:152:ALA:O	47:AC:153:ILE:C	2.58	0.46
49:AE:214:ILE:HG12	49:AE:261:PRO:HD3	1.98	0.46
49:AE:246:SER:HB3	49:AE:248:ARG:HE	1.79	0.46
47:Ac:326:TRP:CE2	51:Ag:49:VAL:HG22	2.50	0.46
48:Ad:309:HIS:CE1	51:Ag:21:PRO:HB2	2.50	0.46
2:B:82:ILE:CA	8:H:57:MET:HE1	2.41	0.46
4:D:137:ASP:O	4:D:223:HIS:CE1	2.68	0.46
4:D:278:VAL:O	21:V:12:VAL:HG11	2.15	0.46
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.98	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.15	0.46
6:F:270:ASN:HD21	6:F:340:ASP:N	2.13	0.46
8:H:14:LEU:O	8:H:17:MET:HB3	2.15	0.46
10:J:142:ALA:C	10:J:144:MET:N	2.71	0.46
12:L:21:ILE:HG12	12:L:27:ILE:CG2	2.45	0.46
12:L:31:ASN:ND2	12:L:34:LEU:HB2	2.31	0.46
12:L:261:VAL:CA	12:L:264:HIS:HD2	2.29	0.46
12:L:264:HIS:HA	12:L:267:THR:CG2	2.45	0.46
12:L:500:ILE:O	12:L:504:LEU:HG	2.16	0.46
55:L:702:3PE:H222	37:l:116:ARG:O	2.15	0.46
13:M:348:LEU:O	13:M:351:VAL:N	2.38	0.46
15:O:38:TYR:CE1	15:O:292:HIS:HD2	2.34	0.46
15:O:168:VAL:HG21	15:O:241:TYR:CE1	2.50	0.46
33:h:69:ARG:O	33:h:73:PHE:CB	2.63	0.46
34:i:116:VAL:O	34:i:117:ILE:C	2.58	0.46
40:o:5:LEU:H	40:o:5:LEU:HD12	1.81	0.46
45:AA:99:LYS:HD2	45:AA:160:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:426:LYS:HA	46:AB:429:LYS:HZ3	1.79	0.46
46:AB:429:LYS:O	46:AB:432:VAL:HG12	2.16	0.46
47:AC:240:MET:C	48:AD:292:MET:HE2	2.41	0.46
48:AD:213:SER:O	48:AD:217:GLY:N	2.49	0.46
47:Ac:14:ILE:O	47:Ac:18:PHE:N	2.47	0.46
47:Ac:319:PRO:HB3	51:Ag:48:ARG:NH2	2.31	0.46
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.42	0.46
3:C:217:ARG:HH12	22:W:112:GLU:CB	2.27	0.46
4:D:139:LEU:HD13	4:D:424:ILE:HG21	1.98	0.46
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.15	0.46
6:F:224:ARG:HD3	17:Q:164:PHE:CE1	2.51	0.46
7:G:648:GLU:HG2	19:S:66:TRP:CZ2	2.50	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:89:LEU:CD1	8:H:233:LEU:CD1	2.77	0.46
12:L:101:MET:HE1	12:L:121:LEU:HB2	1.98	0.46
12:L:306:THR:HA	12:L:336:LYS:NZ	2.27	0.46
12:L:407:TRP:HE1	37:l:140:MET:HE1	1.81	0.46
12:L:529:PHE:CZ	12:L:533:ILE:HG21	2.50	0.46
12:L:589:MET:O	12:L:592:LEU:HB3	2.16	0.46
13:M:10:MET:C	13:M:13:PRO:HD2	2.41	0.46
13:M:49:TYR:CD1	13:M:59:ASP:HB2	2.51	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
16:P:288:PHE:CZ	16:P:290:PRO:HB3	2.51	0.46
18:R:38:TYR:CD2	18:R:48:PHE:HE2	2.33	0.46
23:X:46:CYS:HB3	23:X:56:CYS:SG	2.56	0.46
34:i:64:ALA:HB3	34:i:69:LEU:HD22	1.97	0.46
38:m:25:VAL:CG2	38:m:30:ARG:HD3	2.45	0.46
47:AC:17:SER:HB2	69:AC:406:UQ6:H1M3	1.98	0.46
47:AC:271:GLU:OE1	47:AC:273:TYR:OH	2.32	0.46
47:AC:312:GLN:HE21	50:AF:37:THR:CB	2.28	0.46
47:AC:334:ILE:HD11	51:AG:56:VAL:HG22	1.97	0.46
49:AE:154:ILE:O	49:AE:270:VAL:HG13	2.16	0.46
49:AE:265:PHE:CD1	49:AE:271:VAL:HB	2.51	0.46
50:AF:83:LYS:HB3	50:AF:85:GLU:OE2	2.15	0.46
49:AI:43:LEU:HD12	49:AI:46:LYS:NZ	2.31	0.46
48:Ad:223:THR:HG23	52:Ah:55:VAL:HG21	1.98	0.46
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.97	0.46
4:D:259:GLU:HB3	25:Z:25:LEU:HD21	1.97	0.46
6:F:77:LEU:O	6:F:81:LYS:HG2	2.16	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:318:ILE:HG22	6:F:326:LEU:CA	2.45	0.46
9:I:155:CYS:SG	57:I:302:SF4:S2	3.14	0.46
10:J:57:LEU:HG	10:J:58:ILE:HD13	1.97	0.46
10:J:94:LEU:HD23	10:J:94:LEU:C	2.41	0.46
12:L:141:PHE:CB	12:L:182:PHE:CE2	2.96	0.46
13:M:15:THR:HG21	13:M:100:ILE:CD1	2.46	0.46
13:M:300:SER:HB2	13:M:308:SER:HB3	1.97	0.46
13:M:319:HIS:CA	13:M:322:THR:HG22	2.40	0.46
14:N:37:LEU:HD21	14:N:60:PHE:CD1	2.51	0.46
14:N:123:PRO:HG2	14:N:126:MET:CG	2.40	0.46
15:O:75:LYS:O	15:O:79:GLN:HG3	2.16	0.46
18:R:51:ARG:HD2	42:q:125:VAL:CG1	2.46	0.46
19:S:65:LEU:HD23	19:S:65:LEU:O	2.16	0.46
24:Y:74:LEU:HD23	24:Y:74:LEU:C	2.41	0.46
33:h:95:GLU:OE1	33:h:114:LYS:HD3	2.15	0.46
36:k:69:PHE:CZ	36:k:73:ILE:HG13	2.51	0.46
38:m:9:ALA:O	38:m:10:PRO:C	2.56	0.46
38:m:15:PRO:HG2	38:m:18:LEU:HB2	1.97	0.46
45:AA:168:ILE:HA	45:AA:171:GLU:HG2	1.98	0.46
47:AC:150:LEU:CD1	47:AC:164:ILE:HD12	2.46	0.46
53:Aj:11:TYR:HA	53:Aj:15:PHE:HB2	1.97	0.46
54:Ak:39:ARG:HH22	54:Ak:50:GLY:N	2.13	0.46
1:A:73:LEU:N	1:A:74:PRO:HD2	2.31	0.46
3:C:70:LYS:O	21:V:104:VAL:N	2.47	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
7:G:643:ARG:HA	7:G:646:LEU:HD12	1.98	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.46
8:H:200:LEU:HD12	8:H:201:THR:N	2.31	0.46
10:J:100:VAL:O	10:J:103:ILE:HG13	2.16	0.46
12:L:496:LEU:O	12:L:500:ILE:HG13	2.16	0.46
13:M:208:PRO:CD	13:M:236:LEU:HD22	2.38	0.46
14:N:22:SER:HB2	30:e:6:ILE:HG22	1.98	0.46
15:O:203:ALA:HA	15:O:254:GLU:O	2.16	0.46
16:P:66:GLY:O	16:P:69:VAL:N	2.49	0.46
24:Y:120:MET:HE2	24:Y:120:MET:HB3	1.89	0.46
25:Z:36:PHE:O	25:Z:40:ILE:HG12	2.16	0.46
25:Z:54:ASN:HA	25:Z:57:ARG:HD3	1.96	0.46
27:b:45:ILE:CA	27:b:80:TRP:HH2	2.28	0.46
29:d:54:MET:HE2	29:d:54:MET:HB3	1.89	0.46
31:f:6:LEU:C	31:f:7:LEU:HD12	2.41	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
34:i:70:PHE:HA	34:i:74:HIS:CD2	2.50	0.46
37:l:38:PRO:CB	38:m:75:ASN:ND2	2.71	0.46
39:n:61:THR:O	39:n:65:ARG:HG3	2.15	0.46
47:AC:265:PRO:CD	47:AC:268:ILE:HD11	2.43	0.46
48:AD:237:PHE:CD1	48:AD:238:PRO:HD2	2.51	0.46
49:AE:226:ALA:HB2	49:AE:234:TYR:HE1	1.80	0.46
45:Aa:74:TRP:CZ2	45:Aa:411:GLU:HA	2.51	0.46
45:Aa:340:SER:CB	49:Ai:45:VAL:HG11	2.45	0.46
48:Ad:144:GLU:O	48:Ad:147:ALA:HB3	2.16	0.46
53:Aj:43:ILE:O	53:Aj:47:ILE:HG13	2.16	0.46
2:B:166:ASN:O	2:B:166:ASN:CG	2.59	0.46
4:D:55:SER:HB3	4:D:58:THR:CB	2.46	0.46
4:D:58:THR:HG23	4:D:61:TRP:CH2	2.51	0.46
5:E:176:LEU:HD13	5:E:186:GLN:HB2	1.98	0.46
6:F:88:ARG:HB2	6:F:247:THR:OG1	2.16	0.46
6:F:93:PHE:O	6:F:94:PRO:C	2.58	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.50	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
10:J:87:LEU:CD2	10:J:91:PHE:CE2	2.95	0.46
11:K:57:MET:O	11:K:58:PRO:C	2.59	0.46
12:L:550:LEU:O	12:L:554:ASP:HB3	2.16	0.46
13:M:422:HIS:CE1	38:m:56:ARG:NH2	2.83	0.46
14:N:300:THR:CG2	14:N:301:SER:N	2.78	0.46
15:O:40:LEU:O	15:O:44:ILE:HG13	2.16	0.46
15:O:140:LEU:HD11	15:O:198:TYR:CE2	2.51	0.46
15:O:332:ARG:NH1	29:d:50:MET:HE1	2.31	0.46
16:P:55:VAL:HG22	16:P:79:GLN:HB3	1.97	0.46
21:V:50:GLN:HE22	43:r:93:LYS:HG3	1.80	0.46
23:X:5:VAL:CG1	23:X:7:LEU:HG	2.46	0.46
23:X:78:CYS:SG	23:X:114:LYS:HD2	2.56	0.46
25:Z:70:ALA:O	25:Z:73:PRO:HD2	2.16	0.46
26:a:58:ASN:HB2	26:a:61:TYR:CE2	2.51	0.46
36:k:52:ALA:O	36:k:55:GLU:N	2.49	0.46
42:q:59:HIS:HE1	42:q:60:ARG:NE	2.14	0.46
43:r:91:GLU:OE1	43:r:91:GLU:HA	2.15	0.46
47:AC:30:TRP:HZ3	47:AC:96:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:163:TRP:CZ2	49:Ae:140:MET:HE1	2.51	0.46
48:AD:223:THR:HG21	52:AH:52:ASP:CA	2.30	0.46
53:AJ:30:LEU:CD1	54:AK:34:TRP:HB2	2.45	0.46
47:Ac:18:PHE:CE1	69:Ac:405:UQ6:H1M3	2.51	0.46
47:Ac:152:ALA:O	47:Ac:153:ILE:C	2.58	0.46
48:Ad:146:LYS:O	48:Ad:147:ALA:C	2.58	0.46
54:Ak:6:LEU:HD12	54:Ak:11:ARG:NH1	2.30	0.46
6:F:120:GLY:O	6:F:121:GLU:C	2.59	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
7:G:301:ARG:HA	7:G:572:HIS:CD2	2.52	0.45
7:G:593:SER:O	7:G:643:ARG:NH2	2.46	0.45
9:I:178:GLU:OE2	42:q:119:ALA:HB2	2.15	0.45
10:J:116:ASN:O	10:J:119:GLY:N	2.49	0.45
10:J:164:PHE:HB3	14:N:5:THR:HG23	1.97	0.45
12:L:12:PHE:O	12:L:16:LEU:HG	2.15	0.45
12:L:60:GLU:HG2	12:L:83:ASP:HA	1.98	0.45
12:L:324:LEU:HA	12:L:327:LEU:HD12	1.97	0.45
12:L:339:LEU:HD11	12:L:376:GLY:HA3	1.99	0.45
12:L:371:SER:HB2	35:j:62:SER:OG	2.16	0.45
12:L:475:THR:O	12:L:476:SER:HB2	2.16	0.45
12:L:539:MET:SD	38:m:11:LEU:HD21	2.56	0.45
13:M:56:PHE:CE1	13:M:108:MET:HG2	2.47	0.45
13:M:186:LEU:HD22	13:M:250:LEU:HA	1.97	0.45
13:M:207:MET:O	13:M:208:PRO:C	2.59	0.45
14:N:241:LEU:O	14:N:244:ILE:HG22	2.15	0.45
15:O:126:GLY:CA	32:g:51:MET:HE1	2.46	0.45
15:O:258:TYR:CE2	15:O:269:VAL:HG13	2.51	0.45
15:O:306:ASN:O	15:O:309:THR:HG22	2.15	0.45
16:P:157:LYS:O	16:P:160:GLY:N	2.49	0.45
16:P:220:TYR:HA	16:P:223:PHE:CD2	2.51	0.45
16:P:261:LYS:HB2	16:P:263:PHE:CE1	2.51	0.45
18:R:104:CYS:C	18:R:106:TYR:N	2.73	0.45
23:X:131:VAL:N	27:b:59:ASP:OD1	2.49	0.45
23:X:168:PHE:O	23:X:169:PHE:CG	2.69	0.45
27:b:19:LEU:HD22	55:b:201:3PE:H221	1.98	0.45
27:b:28:LEU:O	27:b:32:MET:HG2	2.15	0.45
27:b:38:TYR:O	27:b:39:THR:C	2.58	0.45
27:b:45:ILE:N	27:b:80:TRP:HH2	2.14	0.45
29:d:94:ILE:HD13	33:h:152:LYS:HE3	1.98	0.45
31:f:49:ARG:NH2	33:h:106:ILE:HG22	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:77:ASP:HA	32:g:78:PRO:HD3	1.70	0.45
34:i:75:VAL:C	34:i:78:PRO:HD2	2.42	0.45
37:l:57:MET:HE2	37:l:57:MET:HB3	1.75	0.45
37:l:166:LEU:HD12	37:l:170:ARG:HH22	1.81	0.45
46:AB:47:LEU:HD11	46:AB:238:LEU:HD13	1.99	0.45
49:AE:188:ALA:HA	49:AE:200:HIS:HE2	1.80	0.45
53:AJ:9:ARG:O	53:AJ:13:LEU:HD23	2.15	0.45
45:Aa:273:SER:O	45:Aa:455:ALA:HA	2.16	0.45
47:Ac:30:TRP:HZ3	47:Ac:96:LEU:HD22	1.81	0.45
47:Ac:138:MET:CE	47:Ac:268:ILE:HA	2.36	0.45
47:Ac:146:ILE:CD1	68:Ac:404:U10:H3M2	2.42	0.45
47:Ac:150:LEU:CD1	47:Ac:164:ILE:HD12	2.46	0.45
49:Ae:207:LYS:HE3	49:Ae:265:PHE:CG	2.51	0.45
49:Ae:231:PHE:CE2	49:Ae:250:ARG:HB3	2.51	0.45
49:Ai:65:VAL:C	49:Ai:76:VAL:HG23	2.41	0.45
4:D:194:ILE:HD12	4:D:268:TRP:CZ3	2.51	0.45
4:D:293:LEU:CD2	4:D:300:TRP:HB3	2.46	0.45
5:E:222:PHE:H	5:E:225:GLU:CD	2.24	0.45
6:F:261:TRP:CD2	6:F:265:PHE:HE2	2.34	0.45
7:G:165:ILE:O	7:G:213:MET:HA	2.16	0.45
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.45
8:H:137:ALA:HA	8:H:140:ILE:HG12	1.98	0.45
9:I:107:PRO:HB3	42:q:106:ARG:HD2	1.98	0.45
10:J:106:LEU:HA	10:J:109:TYR:HD2	1.81	0.45
12:L:204:SER:HA	12:L:207:ASN:ND2	2.31	0.45
12:L:277:MET:HG3	12:L:318:GLY:CA	2.46	0.45
12:L:591:PHE:N	12:L:591:PHE:CD1	2.83	0.45
13:M:122:PHE:CZ	13:M:206:LYS:CD	2.95	0.45
13:M:393:ILE:O	13:M:397:GLY:N	2.49	0.45
14:N:277:ILE:HG22	14:N:278:MET:H	1.79	0.45
14:N:316:HIS:HA	15:O:331:PHE:HZ	1.80	0.45
15:O:54:HIS:CD2	15:O:57:SER:HB3	2.51	0.45
15:O:344:ASN:OD1	15:O:346:GLU:HG2	2.15	0.45
20:T:144:ILE:O	20:T:148:ILE:HG12	2.15	0.45
21:V:32:LEU:O	21:V:36:LYS:HG2	2.16	0.45
22:W:43:TYR:CE1	22:W:63:ARG:HD3	2.50	0.45
22:W:83:ASP:O	22:W:87:ILE:HG12	2.17	0.45
28:c:35:VAL:HG23	28:c:36:ASN:OD1	2.16	0.45
29:d:11:LEU:HB2	30:e:9:LYS:HB2	1.98	0.45
34:i:29:SER:O	34:i:32:GLU:HB2	2.17	0.45
35:j:94:ASP:HB2	35:j:99:ILE:CB	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:25:VAL:CG2	45:Aa:261:ALA:HA	2.31	0.45
41:p:173:GLU:O	41:p:174:ALA:C	2.59	0.45
43:r:20:LEU:HD12	43:r:21:GLN:N	2.31	0.45
45:AA:409:VAL:O	45:AA:410:CYS:C	2.58	0.45
49:AE:155:LYS:HZ3	49:AE:157:SER:CB	2.28	0.45
49:AE:264:GLU:HB3	49:AE:272:VAL:O	2.16	0.45
45:Aa:311:ILE:HG22	45:Aa:341:PHE:CE1	2.50	0.45
46:Ab:297:PRO:HA	46:Ab:304:ASN:ND2	2.28	0.45
47:Ac:312:GLN:HG2	50:Af:37:THR:O	2.16	0.45
48:Ad:321:TYR:HB2	50:Af:61:PHE:CG	2.51	0.45
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.98	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.97	0.45
4:D:292:MET:HA	4:D:329:ARG:HD3	1.97	0.45
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.85	0.45
6:F:394:LYS:HD3	7:G:155:GLU:HB3	1.98	0.45
7:G:43:VAL:HB	7:G:47:THR:HG21	1.99	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
8:H:194:ASN:ND2	8:H:201:THR:HG21	2.31	0.45
11:K:29:THR:O	11:K:32:CYS:N	2.49	0.45
12:L:135:ASN:O	12:L:198:LEU:HD13	2.16	0.45
12:L:381:THR:HG21	12:L:498:PHE:CE2	2.50	0.45
12:L:532:ILE:HG23	12:L:533:ILE:N	2.31	0.45
13:M:22:LYS:HG2	13:M:22:LYS:O	2.17	0.45
13:M:61:LEU:C	13:M:64:PRO:HD2	2.42	0.45
13:M:65:LEU:O	13:M:66:ILE:C	2.59	0.45
13:M:309:PHE:O	13:M:312:ALA:HB3	2.16	0.45
13:M:350:MET:HE2	39:n:96:CYS:HA	1.98	0.45
13:M:453:LEU:CD1	13:M:454:ILE:CG2	2.84	0.45
14:N:133:TRP:CE3	14:N:136:ILE:HD12	2.51	0.45
15:O:204:VAL:O	15:O:205:ILE:C	2.60	0.45
16:P:295:LEU:O	16:P:296:PHE:C	2.59	0.45
17:Q:77:VAL:HG21	17:Q:99:MET:HE3	1.97	0.45
18:R:72:VAL:HG21	18:R:77:ILE:CD1	2.46	0.45
18:R:101:THR:HG22	18:R:112:LYS:HB2	1.99	0.45
22:W:71:MET:C	22:W:73:ASN:N	2.70	0.45
23:X:48:TRP:HZ3	33:h:186:THR:O	1.98	0.45
24:Y:121:GLY:O	24:Y:122:THR:C	2.59	0.45
34:i:72:VAL:O	34:i:76:LEU:HB3	2.16	0.45
39:n:58:MET:HE1	45:Aa:264:GLY:HA2	1.98	0.45
40:o:63:LEU:O	40:o:64:ILE:C	2.59	0.45
45:AA:400:VAL:HG11	46:AB:57:PRO:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:322:ARG:O	51:AG:13:HIS:HB3	2.16	0.45
49:AE:231:PHE:CE2	49:AE:250:ARG:HB3	2.51	0.45
45:Aa:64:SER:OG	45:Aa:235:GLY:HA2	2.16	0.45
45:Aa:168:ILE:HA	45:Aa:171:GLU:HG2	1.98	0.45
48:Ad:213:SER:O	48:Ad:217:GLY:N	2.49	0.45
49:Ae:188:ALA:HA	49:Ae:200:HIS:HE2	1.80	0.45
49:Ae:241:SER:OG	49:Ae:254:ALA:HB2	2.17	0.45
53:Aj:34:ARG:NH1	53:Aj:38:GLN:HB2	2.31	0.45
2:B:95:PHE:HE1	2:B:131:MET:CE	2.28	0.45
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.98	0.45
4:D:88:HIS:CE1	4:D:90:ALA:HB3	2.52	0.45
4:D:201:PHE:HB2	8:H:32:GLN:HB3	1.98	0.45
4:D:301:ASP:HB2	4:D:318:VAL:HG21	1.98	0.45
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.16	0.45
6:F:45:LEU:O	6:F:46:TYR:HB2	2.16	0.45
6:F:270:ASN:HD22	6:F:338:ASP:CB	2.29	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:J:101:PHE:O	10:J:105:VAL:HG23	2.17	0.45
12:L:177:ILE:HA	13:M:401:ILE:HD11	1.99	0.45
12:L:403:ASN:OD1	37:l:153:TYR:HB3	2.15	0.45
12:L:591:PHE:N	12:L:591:PHE:HD1	2.14	0.45
13:M:42:LEU:HD11	13:M:67:ILE:HD12	1.99	0.45
13:M:42:LEU:HD21	13:M:67:ILE:HD12	1.97	0.45
13:M:282:LEU:HD11	13:M:410:MET:HE3	1.96	0.45
15:O:323:GLN:HB2	32:g:56:ASP:OD1	2.17	0.45
15:O:342:GLY:O	15:O:355:LYS:NZ	2.50	0.45
20:T:99:SER:O	20:T:141:PRO:HG2	2.16	0.45
20:T:123:GLU:HG2	20:T:130:ILE:CD1	2.47	0.45
24:Y:39:SER:HB2	24:Y:58:VAL:HA	1.98	0.45
31:f:47:GLU:O	31:f:48:LEU:C	2.60	0.45
33:h:73:PHE:HD2	33:h:74:TYR:CE1	2.33	0.45
33:h:144:SER:HB2	41:p:82:VAL:CG2	2.46	0.45
36:k:26:ARG:O	36:k:27:GLN:C	2.57	0.45
40:o:73:SER:HA	41:p:24:THR:OG1	2.16	0.45
41:p:107:GLN:O	41:p:111:LYS:HG3	2.15	0.45
46:Ab:38:LEU:HA	46:Ab:51:SER:O	2.15	0.45
46:Ab:429:LYS:O	46:Ab:432:VAL:HG12	2.16	0.45
47:Ac:264:THR:O	47:Ac:265:PRO:C	2.58	0.45
47:Ac:377:LEU:HB3	50:Af:34:ARG:HD2	1.97	0.45
49:Ae:123:VAL:HG13	53:Aj:29:ALA:CA	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:155:LYS:HB3	49:Ae:158:ASP:OD2	2.17	0.45
49:Ae:267:SER:C	49:Ae:269:ASP:H	2.24	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
3:C:70:LYS:O	21:V:103:LEU:HA	2.16	0.45
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.52	0.45
4:D:243:ASP:OD2	43:r:31:ILE:HG13	2.16	0.45
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.98	0.45
4:D:362:LYS:O	4:D:384:LEU:HD21	2.17	0.45
6:F:47:GLY:O	6:F:48:ARG:HB2	2.17	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.81	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
10:J:96:VAL:O	10:J:100:VAL:HG23	2.16	0.45
10:J:115:ILE:HA	11:K:3:SER:OG	2.16	0.45
12:L:47:SER:O	12:L:50:PRO:HD2	2.16	0.45
12:L:74:MET:HE3	12:L:74:MET:HB2	1.76	0.45
12:L:247:LEU:HD12	12:L:247:LEU:C	2.41	0.45
12:L:434:LYS:HZ2	36:k:66:ASN:HA	1.80	0.45
12:L:495:VAL:O	12:L:499:LEU:HG	2.17	0.45
62:L:701:PC1:H3B2	62:L:701:PC1:H381	1.70	0.45
13:M:177:MET:HE1	41:p:86:TYR:CE1	2.51	0.45
14:N:155:LEU:O	14:N:159:ILE:HG22	2.16	0.45
14:N:215:MET:SD	14:N:244:ILE:HD11	2.56	0.45
15:O:231:SER:HA	15:O:234:LEU:HD12	1.98	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
21:V:8:THR:CG2	21:V:9:THR:N	2.79	0.45
30:e:18:PHE:O	30:e:18:PHE:CD2	2.69	0.45
30:e:19:MET:HE2	30:e:19:MET:HB3	1.85	0.45
40:o:31:PHE:CG	40:o:34:ARG:HB3	2.51	0.45
42:q:68:MET:O	42:q:69:ASN:C	2.57	0.45
56:q:201:CDL:H341	56:q:201:CDL:H171	1.99	0.45
46:AB:171:THR:HG23	49:AI:64:LEU:HD23	1.98	0.45
46:AB:322:ASP:OD2	49:AI:59:ALA:HB2	2.17	0.45
54:AK:10:TYR:HE1	50:Af:110:LYS:CA	2.19	0.45
46:Ab:171:THR:HA	49:AI:64:LEU:HD21	1.97	0.45
48:Ad:214:LEU:O	48:Ad:234:ASN:ND2	2.46	0.45
49:Ae:154:ILE:HD13	49:Ae:273:VAL:HG23	1.99	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.46	0.45
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:ASN:O	5:E:62:ILE:HG12	2.16	0.45
5:E:226:PRO:HB2	5:E:229:GLY:O	2.17	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.45
9:I:180:HIS:CE1	16:P:100:LEU:HD21	2.52	0.45
10:J:13:LEU:HD11	11:K:10:MET:SD	2.57	0.45
11:K:22:PHE:CD2	12:L:584:ILE:HG21	2.52	0.45
12:L:23:MET:CE	56:L:703:CDL:H521	2.47	0.45
12:L:195:SER:O	12:L:201:ILE:HD11	2.16	0.45
12:L:241:THR:N	12:L:242:PRO:HD2	2.31	0.45
12:L:366:MET:SD	12:L:443:ILE:HG21	2.57	0.45
12:L:594:ASN:CG	14:N:110:PRO:HB2	2.41	0.45
13:M:51:ASN:ND2	33:h:136:THR:CG2	2.80	0.45
13:M:249:ILE:O	13:M:250:LEU:CG	2.47	0.45
13:M:255:LYS:CE	29:d:117:HIS:HB3	2.47	0.45
14:N:26:LEU:HG	14:N:85:MET:SD	2.57	0.45
21:V:99:PRO:HD2	21:V:100:TRP:CE3	2.51	0.45
25:Z:85:GLN:OE1	30:e:103:GLU:OE2	2.35	0.45
29:d:11:LEU:HD12	29:d:11:LEU:HA	1.69	0.45
39:n:101:GLU:HG2	39:n:122:ARG:HH12	1.81	0.45
42:q:55:PHE:HD1	42:q:55:PHE:H	1.64	0.45
46:AB:225:VAL:HG22	46:AB:229:VAL:CG2	2.46	0.45
47:AC:213:SER:HA	50:AF:67:LEU:HD11	1.98	0.45
49:AE:207:LYS:HE3	49:AE:265:PHE:CG	2.51	0.45
53:AJ:34:ARG:NH1	53:AJ:38:GLN:HB2	2.31	0.45
46:Ab:418:SER:O	46:Ab:419:VAL:C	2.59	0.45
49:Ae:205:VAL:HG12	49:Ae:211:VAL:HG23	1.97	0.45
49:Ae:214:ILE:HG12	49:Ae:261:PRO:HD3	1.98	0.45
2:B:96:GLY:O	4:D:93:GLY:HA3	2.16	0.45
2:B:98:ALA:HA	4:D:116:LEU:HD21	1.99	0.45
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.45
3:C:203:LEU:CD1	4:D:123:LEU:CD2	2.84	0.45
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.85	0.45
6:F:72:GLY:O	6:F:76:ILE:HG13	2.17	0.45
6:F:87:GLY:H	6:F:92:GLY:CA	2.29	0.45
7:G:136:GLU:HB3	17:Q:87:MET:HB3	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
10:J:9:SER:HB3	11:K:7:ASN:ND2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:88:ILE:HD11	11:K:23:ARG:NH1	2.31	0.45
55:L:702:3PE:H352	55:L:702:3PE:H381	1.84	0.45
13:M:272:THR:O	13:M:275:ILE:HG13	2.17	0.45
13:M:283:LYS:HG3	13:M:327:PHE:HE1	1.78	0.45
14:N:293:TYR:O	14:N:297:ILE:HG12	2.17	0.45
15:O:258:TYR:HB3	15:O:262:GLU:CB	2.36	0.45
16:P:218:ALA:HB2	16:P:280:ILE:CG2	2.47	0.45
18:R:70:ASN:HB2	18:R:111:PHE:HD2	1.81	0.45
19:S:40:ARG:HD2	19:S:88:THR:OG1	2.16	0.45
20:T:100:VAL:O	20:T:142:GLN:HB2	2.15	0.45
22:W:23:ILE:CD1	22:W:84:LEU:HD21	2.47	0.45
22:W:67:ARG:HD2	22:W:71:MET:SD	2.57	0.45
23:X:9:THR:O	23:X:12:GLU:HB3	2.17	0.45
29:d:13:PHE:CE2	29:d:14:LEU:HD23	2.52	0.45
32:g:67:LYS:O	32:g:68:ASN:C	2.60	0.45
39:n:45:ARG:O	39:n:49:GLU:N	2.37	0.45
42:q:68:MET:HG2	42:q:115:PHE:HE2	1.82	0.45
45:AA:274:GLU:OE2	45:AA:276:ARG:NH1	2.45	0.45
46:AB:167:GLN:NE2	49:AI:43:LEU:CB	2.72	0.45
46:AB:180:VAL:HG21	46:AB:257:GLU:CA	2.46	0.45
46:AB:253:TYR:HE2	46:AB:435:LYS:HG3	1.82	0.45
47:AC:33:PHE:HE1	56:AG:102:CDL:H782	1.82	0.45
49:AE:155:LYS:HB3	49:AE:158:ASP:OD2	2.17	0.45
50:AF:85:GLU:H	50:AF:85:GLU:CD	2.24	0.45
45:Aa:393:ASN:HB3	46:Ab:106:VAL:C	2.42	0.45
46:Ab:43:LEU:HB2	46:Ab:45:ASN:OD1	2.17	0.45
47:Ac:137:GLN:HG3	47:Ac:265:PRO:HD3	1.98	0.45
51:Ag:12:ARG:HB3	51:Ag:13:HIS:CD2	2.52	0.45
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.82	0.45
4:D:37:TRP:CE3	13:M:140:THR:HA	2.52	0.45
4:D:179:ARG:HH22	4:D:303:ARG:HD3	1.82	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
8:H:224:PHE:CZ	61:H:401:UQ9:H12A	2.52	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:J:136:GLU:O	10:J:137:GLY:C	2.58	0.45
12:L:100:ILE:O	12:L:104:SER:N	2.42	0.45
12:L:210:LEU:HD23	12:L:210:LEU:C	2.41	0.45
12:L:246:LEU:C	12:L:246:LEU:CD1	2.90	0.45
12:L:387:THR:HA	12:L:465:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:602:TYR:HB2	14:N:96:ASN:ND2	2.32	0.45
14:N:217:MET:HA	14:N:220:MET:SD	2.56	0.45
16:P:238:GLN:HB3	16:P:326:ASP:OD2	2.17	0.45
23:X:165:THR:N	23:X:172:VAL:HG11	2.32	0.45
25:Z:53:TRP:NE1	25:Z:57:ARG:HD2	2.31	0.45
25:Z:135:ASN:O	25:Z:139:GLY:HA3	2.16	0.45
33:h:73:PHE:CE2	33:h:74:TYR:HE1	2.35	0.45
33:h:120:TRP:NE1	33:h:124:ASN:ND2	2.64	0.45
36:k:57:TRP:O	36:k:58:ARG:C	2.59	0.45
42:q:4:VAL:HA	42:q:7:LEU:HD12	1.99	0.45
45:AA:284:LEU:HD11	49:AI:44:ASP:O	2.16	0.45
47:AC:341:GLN:HE21	47:AC:342:PRO:HD2	1.82	0.45
48:AD:234:ASN:O	48:AD:235:PRO:C	2.59	0.45
49:AE:241:SER:OG	49:AE:254:ALA:HB2	2.17	0.45
51:AG:12:ARG:HB3	51:AG:13:HIS:CD2	2.52	0.45
49:AI:71:ASN:HB2	49:AI:73:PRO:HD2	1.97	0.45
45:Aa:74:TRP:HB3	45:Aa:418:LEU:HD11	1.98	0.45
46:Ab:167:GLN:HE21	49:AI:43:LEU:HB2	1.66	0.45
49:AI:71:ASN:HB2	49:AI:73:PRO:HD2	1.97	0.45
2:B:92:PRO:HA	2:B:130:VAL:O	2.16	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.45
6:F:61:ASP:O	6:F:256:ARG:NH2	2.50	0.45
6:F:227:PRO:HB3	7:G:95:PRO:HD2	1.98	0.45
7:G:160:VAL:O	7:G:174:THR:HG22	2.17	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
7:G:401:LEU:CD1	7:G:462:PHE:CE2	2.88	0.45
8:H:17:MET:CE	8:H:225:MET:CG	2.94	0.45
8:H:63:PRO:O	8:H:66:THR:HG22	2.17	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.45
9:I:67:ILE:HG13	62:I:301:PC1:H231	1.98	0.45
9:I:88:PHE:CE2	42:q:30:ALA:HA	2.51	0.45
10:J:32:LEU:CG	10:J:64:LEU:HD21	2.46	0.45
12:L:357:ARG:HH12	39:n:79:PRO:C	2.24	0.45
12:L:527:GLY:O	12:L:528:PHE:HB2	2.17	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:HD11	2.43	0.45
13:M:129:THR:CG2	13:M:235:LEU:CD1	2.95	0.45
13:M:131:ILE:HD13	14:N:302:LEU:HD21	1.99	0.45
14:N:153:ILE:O	14:N:154:ILE:C	2.58	0.45
14:N:214:PRO:HB2	14:N:247:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:343:TYR:HB3	29:d:52:PRO:HD3	1.99	0.45
17:Q:65:THR:HG23	17:Q:67:VAL:HG23	1.99	0.45
17:Q:77:VAL:CG1	17:Q:101:PHE:CD2	3.00	0.45
20:T:87:LEU:HA	20:T:87:LEU:HD23	1.72	0.45
20:U:116:VAL:HG12	20:U:120:MET:HE2	1.98	0.45
25:Z:66:GLU:HA	25:Z:69:ILE:CG1	2.46	0.45
26:a:1:MET:HG3	56:q:201:CDL:HB21	1.99	0.45
28:c:61:THR:HG21	29:d:74:PHE:CE1	2.51	0.45
29:d:109:TYR:CZ	41:p:153:ARG:HD3	2.52	0.45
31:f:37:PHE:HZ	41:p:83:LEU:CD1	2.29	0.45
31:f:38:ARG:HD3	31:f:56:TRP:NE1	2.32	0.45
35:j:45:ARG:O	36:k:28:TRP:HH2	2.00	0.45
40:o:31:PHE:CD2	40:o:34:ARG:HD2	2.52	0.45
41:p:110:LEU:O	41:p:111:LYS:C	2.58	0.45
41:p:132:PHE:O	41:p:136:THR:OG1	2.17	0.45
43:r:54:TYR:CE2	43:r:58:ASP:HB3	2.51	0.45
47:AC:182:HIS:CE1	67:AC:402:HEM:C4C	3.05	0.45
47:AC:211:LEU:CD2	50:AF:37:THR:HA	2.47	0.45
49:AE:156:LEU:HD23	49:AE:156:LEU:HA	1.62	0.45
49:AE:178:HIS:CD2	49:AE:209:GLU:O	2.70	0.45
45:Aa:285:ALA:O	45:Aa:360:CYS:N	2.46	0.45
47:Ac:141:TRP:CD1	47:Ac:265:PRO:CD	3.00	0.45
47:Ac:341:GLN:HE21	47:Ac:342:PRO:HD2	1.82	0.45
62:Ae:301:PC1:H151	53:Aj:18:THR:OG1	2.17	0.45
54:Ak:23:MET:O	54:Ak:27:VAL:HG23	2.17	0.45
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.96	0.45
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.96	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:136:GLU:OE1	17:Q:87:MET:HG3	2.17	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
7:G:649:VAL:HA	19:S:20:ARG:NE	2.31	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
8:H:30:TYR:CE1	26:a:1:MET:C	2.95	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.45
9:I:184:LEU:HD23	17:Q:114:TRP:CH2	2.51	0.45
9:I:188:GLU:OE1	18:R:56:ASN:CB	2.65	0.45
10:J:63:MET:HE1	11:K:68:ALA:CB	2.46	0.45

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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	0.45
12:L:81:LYS:CA	12:L:135:ASN:HD21	2.29	0.45
12:L:231:PRO:C	12:L:234:PRO:HD2	2.41	0.45
12:L:295:GLN:NE2	12:L:524:THR:O	2.50	0.45
13:M:6:LEU:HD21	31:f:22:PHE:CD2	2.52	0.45
13:M:42:LEU:CG	13:M:67:ILE:CD1	2.95	0.45
13:M:87:ASP:HB3	13:M:91:LEU:HB2	1.99	0.45
14:N:154:ILE:CD1	14:N:195:PRO:HG2	2.47	0.45
14:N:220:MET:O	14:N:221:LEU:C	2.60	0.45
15:O:112:CYS:HB3	15:O:131:LEU:HA	1.98	0.45
15:O:129:TYR:CD2	15:O:183:CYS:HB3	2.52	0.45
16:P:170:LEU:HD12	16:P:171:ASN:H	1.81	0.45
16:P:315:THR:O	16:P:316:LYS:C	2.58	0.45
19:S:74:GLU:OE1	19:S:74:GLU:N	2.49	0.45
23:X:28:ALA:HB2	23:X:82:PHE:CZ	2.52	0.45
25:Z:127:LEU:CD2	30:e:80:LYS:CG	2.94	0.45
32:g:64:VAL:HG11	32:g:71:PHE:CE1	2.52	0.45
41:p:30:ILE:O	41:p:34:THR:HG23	2.17	0.45
44:s:52:LEU:O	44:s:56:ARG:HG2	2.17	0.45
45:AA:373:GLN:NE2	45:AA:471:ILE:O	2.49	0.45
46:AB:39:GLU:HG3	46:AB:227:HIS:ND1	2.32	0.45
46:AB:297:PRO:HA	46:AB:304:ASN:ND2	2.28	0.45
45:Aa:127:GLU:OE2	45:Aa:348:TYR:HB3	2.16	0.45
47:Ac:218:ILE:HD11	47:Ac:224:TYR:CE2	2.52	0.45
48:Ad:259:THR:O	48:Ad:260:PRO:C	2.60	0.45
49:Ae:217:CYS:C	49:Ae:219:HIS:N	2.72	0.45
2:B:120:VAL:HG21	61:H:401:UQ9:H1M	1.99	0.44
3:C:98:PHE:HE1	21:V:44:TYR:CD1	2.34	0.44
3:C:203:LEU:CD2	4:D:123:LEU:CD2	2.88	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:55:SER:OG	4:D:56:LYS:N	2.49	0.44
4:D:301:ASP:OD2	4:D:318:VAL:HG22	2.16	0.44
5:E:55:THR:O	5:E:56:PRO:C	2.59	0.44
5:E:62:ILE:O	5:E:66:VAL:HG23	2.17	0.44
6:F:75:TRP:O	6:F:79:GLU:HG2	2.17	0.44
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.44
7:G:126:LEU:CD1	18:R:89:PRO:CB	2.93	0.44
12:L:226:GLN:HG3	12:L:314:MET:HE2	1.98	0.44
13:M:187:ASP:H	13:M:192:ASN:ND2	2.15	0.44
56:M:503:CDL:H311	23:X:170:TRP:CZ3	2.52	0.44
14:N:163:PHE:CZ	14:N:285:MET:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:250:SER:O	14:N:259:GLY:HA3	2.17	0.44
16:P:55:VAL:HA	16:P:79:GLN:O	2.18	0.44
16:P:209:ARG:CA	16:P:352:VAL:HG22	2.47	0.44
17:Q:99:MET:HG2	17:Q:128:PHE:HE2	1.82	0.44
22:W:71:MET:O	22:W:72:LYS:C	2.59	0.44
25:Z:68:ARG:O	25:Z:69:ILE:C	2.60	0.44
27:b:59:ASP:OD1	27:b:59:ASP:N	2.49	0.44
28:c:32:ARG:O	28:c:33:GLU:C	2.58	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
45:AA:286:HIS:ND1	45:AA:359:VAL:HG22	2.31	0.44
45:AA:467:ASP:OD2	47:AC:223:TYR:CE2	2.70	0.44
46:AB:418:SER:O	46:AB:419:VAL:C	2.59	0.44
50:AF:86:GLU:O	50:AF:87:ASP:C	2.60	0.44
54:AK:29:ALA:O	54:AK:33:VAL:HG23	2.18	0.44
45:Aa:169:LEU:HD11	45:Aa:209:ARG:HG2	1.97	0.44
46:Ab:155:ARG:HD2	46:Ab:198:GLY:H	1.83	0.44
49:Ae:178:HIS:CD2	49:Ae:209:GLU:O	2.70	0.44
49:Ae:201:ASP:OD1	49:Ae:202:LEU:N	2.50	0.44
50:Af:86:GLU:O	50:Af:87:ASP:C	2.60	0.44
4:D:47:PHE:CD1	14:N:227:ILE:HD11	2.52	0.44
5:E:242:PHE:O	6:F:257:ARG:NH1	2.50	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:113:VAL:HG21	8:H:136:VAL:HG23	1.99	0.44
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.52	0.44
8:H:196:ALA:O	8:H:198:PHE:N	2.51	0.44
10:J:20:ALA:O	10:J:22:LYS:HG3	2.17	0.44
10:J:21:LEU:HB3	10:J:88:ILE:HG23	1.98	0.44
10:J:136:GLU:HG3	10:J:139:ILE:HG12	1.99	0.44
11:K:1:MET:N	11:K:2:PRO:CD	2.81	0.44
13:M:158:ILE:CG2	14:N:283:ALA:CB	2.94	0.44
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.81	0.44
13:M:263:LEU:CD1	38:m:102:TYR:CD1	2.95	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
15:O:336:GLY:HA2	15:O:344:ASN:HB3	1.99	0.44
16:P:225:ALA:HB1	16:P:291:TYR:CD1	2.52	0.44
19:S:51:LEU:HA	19:S:52:PRO:HD3	1.86	0.44
19:S:62:GLN:HB2	19:S:80:ASN:CG	2.42	0.44
23:X:134:ASP:O	23:X:135:ARG:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:90:LEU:HD12	24:Y:93:PHE:HB3	1.98	0.44
30:e:93:THR:O	30:e:94:PRO:C	2.56	0.44
32:g:123:LEU:CD1	41:p:98:VAL:CG1	2.96	0.44
33:h:55:PHE:C	33:h:55:PHE:CD1	2.94	0.44
34:i:36:PRO:O	34:i:37:PRO:C	2.60	0.44
39:n:35:ASP:OD1	39:n:35:ASP:N	2.51	0.44
39:n:136:GLU:OE2	39:n:167:TRP:CD1	2.70	0.44
40:o:17:PRO:HG3	40:o:106:ARG:CA	2.46	0.44
40:o:49:ALA:O	40:o:50:GLN:C	2.60	0.44
42:q:3:LEU:HD12	42:q:6:VAL:CG2	2.48	0.44
42:q:44:TYR:CD1	42:q:68:MET:HG3	2.52	0.44
45:AA:197:LEU:HD22	45:AA:268:CYS:SG	2.58	0.44
48:AD:207:GLY:O	48:AD:208:GLU:C	2.58	0.44
54:AK:23:MET:O	54:AK:27:VAL:HG23	2.16	0.44
45:Aa:340:SER:HB2	49:Ai:45:VAL:HG21	1.98	0.44
48:Ad:242:ILE:HG12	48:Ad:244:MET:H	1.82	0.44
1:A:74:PRO:HG2	10:J:145:TYR:CE2	2.52	0.44
55:A:401:3PE:H372	10:J:37:PHE:HZ	1.82	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.17	0.44
2:B:114:MET:HE3	2:B:119:VAL:HG12	1.97	0.44
5:E:243:GLY:O	6:F:257:ARG:HD2	2.17	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
8:H:60:PRO:HG2	8:H:62:ARG:HH22	1.82	0.44
9:I:203:ALA:CB	42:q:88:ARG:NH1	2.80	0.44
12:L:2:ASN:O	12:L:3:ILE:C	2.59	0.44
12:L:117:PHE:CE1	12:L:243:VAL:CG2	3.00	0.44
12:L:366:MET:SD	12:L:443:ILE:CG2	3.06	0.44
13:M:22:LYS:HG2	13:M:26:ASN:ND2	2.33	0.44
13:M:73:LEU:HB3	13:M:103:GLN:OE1	2.16	0.44
13:M:424:ILE:O	13:M:424:ILE:CG2	2.65	0.44
55:M:502:3PE:O22	56:h:201:CDL:H541	2.17	0.44
56:M:503:CDL:H202	56:M:503:CDL:H172	1.73	0.44
14:N:122:ILE:HD11	14:N:127:GLY:HA2	1.98	0.44
14:N:258:THR:CB	14:N:333:SER:O	2.64	0.44
15:O:167:PHE:CZ	15:O:244:THR:HG22	2.52	0.44
15:O:223:ASP:O	15:O:227:MET:HG3	2.17	0.44
15:O:233:TYR:CZ	15:O:237:ILE:HD11	2.52	0.44
15:O:351:TRP:O	15:O:355:LYS:HG2	2.16	0.44
16:P:298:TYR:C	16:P:300:TRP:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:15:PRO:HG2	38:m:17:THR:O	2.18	0.44
40:o:117:LEU:CD2	40:o:118:LYS:HE3	2.40	0.44
47:AC:170:VAL:HG13	47:AC:170:VAL:O	2.16	0.44
47:AC:218:ILE:HD11	47:AC:224:TYR:CE2	2.52	0.44
49:AE:243:TYR:CD2	49:AE:258:LEU:HG	2.52	0.44
52:AH:26:ASP:O	52:AH:27:PRO:C	2.58	0.44
45:Aa:259:GLU:O	45:Aa:261:ALA:N	2.50	0.44
47:Ac:170:VAL:HG13	47:Ac:170:VAL:O	2.16	0.44
48:Ad:201:VAL:HG22	48:Ad:278:SER:OG	2.18	0.44
48:Ad:323:PRO:HG2	48:Ad:325:LYS:CG	2.47	0.44
1:A:65:PHE:HE2	8:H:294:LEU:HD21	1.76	0.44
2:B:167:GLY:HA3	9:I:150:THR:HB	1.99	0.44
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.44
4:D:159:LEU:O	4:D:161:ILE:HG23	2.17	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
6:F:48:ARG:HA	6:F:48:ARG:NH1	2.29	0.44
6:F:51:TRP:HB3	6:F:133:HIS:O	2.17	0.44
6:F:273:THR:HA	6:F:292:MET:H	1.82	0.44
6:F:292:MET:O	6:F:293:SER:HB2	2.17	0.44
6:F:379:CYS:SG	57:F:502:SF4:S2	3.16	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:144:MET:HG3	7:G:144:MET:O	2.17	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.47	0.44
8:H:196:ALA:CB	8:H:274:ARG:HA	2.45	0.44
10:J:3:ASN:O	10:J:4:TYR:C	2.60	0.44
10:J:42:MET:HB2	10:J:42:MET:HE3	1.71	0.44
12:L:155:ILE:HG12	12:L:248:HIS:CE1	2.53	0.44
12:L:493:ILE:HA	12:L:496:LEU:HG	1.99	0.44
13:M:200:MET:HE2	13:M:250:LEU:HD21	2.00	0.44
14:N:45:ILE:O	14:N:45:ILE:CG1	2.58	0.44
14:N:273:ASN:HD21	24:Y:143:VAL:HA	1.82	0.44
14:N:312:LYS:HE3	15:O:319:ILE:HG21	2.00	0.44
15:O:233:TYR:O	15:O:237:ILE:HG13	2.17	0.44
15:O:251:GLU:O	15:O:280:LYS:HD2	2.18	0.44
16:P:82:ILE:HD12	16:P:105:PHE:CE1	2.52	0.44
19:S:42:VAL:O	19:S:46:LYS:HG3	2.18	0.44
22:W:45:GLU:O	22:W:46:VAL:C	2.58	0.44
56:Y:202:CDL:H142	56:Y:202:CDL:H111	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:113:THR:HG23	30:e:62:ASP:OD2	2.17	0.44
36:k:38:VAL:CG1	39:n:39:TYR:HB2	2.47	0.44
37:l:119:THR:HG22	38:m:13:THR:HG23	1.99	0.44
38:m:82:PRO:O	55:m:202:3PE:H32	2.18	0.44
42:q:23:LEU:HD11	42:q:33:ILE:HD13	1.99	0.44
42:q:44:TYR:CE1	42:q:68:MET:HE3	2.51	0.44
46:AB:305:THR:O	46:AB:311:GLN:HG3	2.17	0.44
47:AC:256:TYR:OH	48:AD:202:ARG:NH1	2.50	0.44
49:AE:111:LYS:HE3	53:AJ:11:TYR:CZ	2.52	0.44
49:AE:140:MET:CE	47:Ac:163:TRP:CZ2	3.00	0.44
49:AE:154:ILE:HG22	49:AE:155:LYS:N	2.32	0.44
51:AG:38:VAL:HA	51:AG:41:ARG:HD3	1.99	0.44
45:Aa:78:GLY:H	45:Aa:81:TYR:HD2	1.65	0.44
46:Ab:138:LEU:CD1	46:Ab:233:VAL:HB	2.47	0.44
46:Ab:306:THR:O	46:Ab:307:SER:C	2.58	0.44
46:Ab:375:LYS:NZ	46:Ab:419:VAL:O	2.36	0.44
47:Ac:201:HIS:HE1	69:Ac:405:UQ6:C2	2.30	0.44
47:Ac:256:TYR:OH	48:Ad:202:ARG:NH1	2.50	0.44
47:Ac:294:LEU:CG	68:Ac:404:U10:H1M3	2.47	0.44
50:Af:20:TRP:HH2	55:Ag:103:3PE:O11	2.00	0.44
3:C:73:GLN:HE21	21:V:112:TRP:HE1	1.65	0.44
4:D:121:GLU:OE2	4:D:463:ARG:HD2	2.18	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44
4:D:250:ASN:HA	43:r:23:LYS:HE3	1.99	0.44
5:E:62:ILE:HG23	5:E:81:VAL:HG22	2.00	0.44
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.46	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:593:SER:OG	7:G:639:LEU:HD22	2.18	0.44
8:H:17:MET:HE1	8:H:225:MET:CG	2.48	0.44
11:K:33:LEU:HA	11:K:36:MET:HE2	2.00	0.44
12:L:54:PHE:CB	12:L:87:ILE:HD11	2.47	0.44
12:L:283:LEU:CD1	37:l:140:MET:HE2	2.48	0.44
12:L:537:THR:N	12:L:538:PRO:HD2	2.32	0.44
13:M:18:SER:OG	13:M:26:ASN:ND2	2.51	0.44
13:M:24:TRP:CE3	13:M:81:GLN:HG2	2.52	0.44
13:M:123:GLU:CD	14:N:255:PRO:HG2	2.43	0.44
14:N:87:GLN:O	14:N:88:GLN:C	2.59	0.44
14:N:275:CYS:SG	24:Y:139:PRO:HD2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:324:LEU:HD13	29:d:45:ASP:OD2	2.17	0.44
16:P:358:THR:O	16:P:359:TYR:C	2.60	0.44
19:S:83:SER:O	19:S:87:VAL:HG23	2.17	0.44
20:U:88:LYS:HG3	20:U:98:LEU:HD23	1.98	0.44
23:X:26:LYS:HE2	23:X:26:LYS:HB3	1.74	0.44
23:X:153:VAL:O	23:X:155:GLU:HG3	2.18	0.44
29:d:27:ASN:O	29:d:28:ASP:C	2.60	0.44
30:e:96:PRO:O	30:e:99:SER:N	2.47	0.44
31:f:39:ASN:CG	31:f:55:THR:HG21	2.41	0.44
34:i:15:LEU:CD2	39:n:164:PRO:HB2	2.40	0.44
42:q:86:TRP:CD2	42:q:98:PRO:HG2	2.52	0.44
47:AC:223:TYR:CE1	48:AD:314:LEU:HG	2.52	0.44
49:AE:127:TYR:CD2	53:AJ:32:PHE:HE2	2.36	0.44
49:AE:178:HIS:NE2	49:AE:209:GLU:HB2	2.33	0.44
49:AE:178:HIS:HA	49:AE:209:GLU:O	2.18	0.44
48:Ad:248:ILE:HD12	48:Ad:266:VAL:HG11	2.00	0.44
49:Ae:115:TYR:HB3	53:Aj:21:PHE:CE1	2.53	0.44
49:Ae:161:GLU:HA	49:Ae:178:HIS:HB3	2.00	0.44
49:Ae:178:HIS:HA	49:Ae:209:GLU:O	2.18	0.44
2:B:97:LEU:HD23	2:B:136:THR:O	2.18	0.44
4:D:47:PHE:CD1	14:N:227:ILE:CD1	3.00	0.44
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.53	0.44
5:E:181:ASN:OD1	5:E:221:ARG:HD2	2.17	0.44
6:F:297:LYS:CE	6:F:333:GLU:HB2	2.48	0.44
6:F:383:THR:HG23	7:G:120:LEU:HD23	1.98	0.44
7:G:68:ARG:O	7:G:189:ILE:HD11	2.18	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.44
8:H:184:MET:SD	8:H:296:LEU:HD23	2.58	0.44
9:I:79:ARG:NE	43:r:20:LEU:HD22	2.33	0.44
12:L:66:TRP:CZ3	12:L:68:TRP:HD1	2.34	0.44
12:L:529:PHE:O	12:L:533:ILE:HG22	2.16	0.44
12:L:557:TRP:CE3	55:m:202:3PE:H291	2.53	0.44
14:N:23:SER:C	30:e:2:PRO:HG2	2.42	0.44
15:O:66:ILE:HG13	15:O:234:LEU:HD23	2.00	0.44
16:P:59:PHE:CD1	16:P:83:PRO:HG2	2.52	0.44
16:P:156:SER:HB2	16:P:161:VAL:CG2	2.47	0.44
16:P:275:HIS:CB	16:P:372:ALA:HB1	2.48	0.44
16:P:345:LEU:C	16:P:345:LEU:HD23	2.43	0.44
17:Q:62:THR:HG22	17:Q:141:ASN:O	2.18	0.44
17:Q:101:PHE:CE1	17:Q:124:MET:HE3	2.53	0.44
19:S:24:CYS:SG	19:S:61:VAL:O	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:132:ASP:O	20:T:133:ILE:C	2.60	0.44
23:X:58:LYS:O	23:X:59:GLU:C	2.59	0.44
24:Y:4:VAL:O	24:Y:4:VAL:CG1	2.63	0.44
24:Y:7:PHE:CZ	24:Y:26:ILE:HG12	2.52	0.44
26:a:37:ARG:HB2	26:a:48:MET:HE2	1.99	0.44
34:i:14:GLN:HE22	39:n:157:ALA:HB3	1.83	0.44
37:l:122:THR:O	38:m:6:TYR:CE1	2.70	0.44
41:p:140:GLN:HG2	41:p:144:LEU:CD1	2.47	0.44
46:AB:297:PRO:CB	46:AB:304:ASN:CG	2.91	0.44
46:AB:312:SER:HA	46:AB:315:LYS:HE3	2.00	0.44
47:AC:264:THR:HG21	49:Ae:225:ILE:HD11	1.86	0.44
47:AC:373:GLU:HG2	50:AF:21:TYR:OH	2.17	0.44
48:AD:167:ARG:HH12	48:AD:170:LYS:H	1.65	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:HB3	2.00	0.44
45:Aa:479:ARG:O	54:Ak:20:THR:HG21	2.17	0.44
49:Ae:243:TYR:CD2	49:Ae:258:LEU:HG	2.52	0.44
54:Ak:48:ILE:O	54:Ak:49:ASN:C	2.59	0.44
2:B:81:LEU:CD1	8:H:53:MET:HE1	2.47	0.44
2:B:138:THR:HG21	4:D:116:LEU:HA	2.00	0.44
2:B:170:TYR:O	2:B:171:TYR:CD2	2.71	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:621:LYS:NZ	22:W:131:PRO:HD3	2.33	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.48	0.44
8:H:303:TRP:CZ3	27:b:28:LEU:HG	2.52	0.44
10:J:123:TRP:O	10:J:124:LEU:C	2.57	0.44
12:L:491:LEU:HD13	35:j:80:VAL:HG22	1.99	0.44
12:L:516:ALA:O	12:L:517:ASN:C	2.61	0.44
12:L:560:LYS:HZ1	55:Y:201:3PE:H32	1.83	0.44
13:M:42:LEU:CD1	13:M:67:ILE:CD1	2.96	0.44
13:M:186:LEU:HD13	13:M:250:LEU:HA	2.00	0.44
14:N:146:TYR:CD1	14:N:198:PRO:HG2	2.53	0.44
14:N:227:ILE:HG13	14:N:228:ASN:N	2.32	0.44
15:O:135:LEU:HD13	63:O:401:ADP:C5	2.52	0.44
16:P:245:VAL:HA	16:P:265:PHE:HD2	1.82	0.44
16:P:298:TYR:O	16:P:299:SER:C	2.60	0.44
21:V:56:LEU:O	21:V:57:ASP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:40:ASN:O	23:X:41:LYS:C	2.58	0.44
28:c:61:THR:HG22	28:c:65:ASP:OD2	2.18	0.44
28:c:73:ASN:OD1	28:c:75:LEU:N	2.50	0.44
31:f:8:ARG:HB3	31:f:10:HIS:CE1	2.53	0.44
45:AA:78:GLY:H	45:AA:81:TYR:HD2	1.65	0.44
49:AE:152:ILE:HG21	49:AE:273:VAL:HB	1.98	0.44
49:AE:161:GLU:HA	49:AE:178:HIS:CB	2.48	0.44
49:AE:168:LYS:HZ3	49:AE:171:GLY:HA2	1.83	0.44
49:AE:217:CYS:C	49:AE:219:HIS:N	2.72	0.44
45:Aa:463:GLU:OE1	51:Ag:8:LEU:HB2	2.17	0.44
48:Ad:144:GLU:O	48:Ad:148:LEU:HG	2.16	0.44
48:Ad:234:ASN:O	48:Ad:235:PRO:C	2.59	0.44
48:Ad:298:LEU:C	48:Ad:298:LEU:HD23	2.43	0.44
49:Ae:161:GLU:HA	49:Ae:178:HIS:CB	2.48	0.44
53:Aj:9:ARG:O	53:Aj:13:LEU:HD23	2.18	0.44
53:Aj:30:LEU:HD23	54:Ak:48:ILE:HG13	2.00	0.44
1:A:55:PHE:HB3	10:J:69:TYR:CE2	2.52	0.44
2:B:202:LEU:HD21	9:I:86:TYR:HB2	1.94	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:82:LEU:HD12	8:H:126:LYS:CD	2.44	0.44
4:D:158:LEU:O	4:D:392:PRO:HG2	2.18	0.44
7:G:36:VAL:HG22	7:G:102:ILE:HD12	1.98	0.44
7:G:127:ASP:OD1	7:G:127:ASP:C	2.59	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
8:H:307:LEU:HD11	25:Z:47:TYR:CD1	2.52	0.44
55:J:201:3PE:H322	55:J:201:3PE:H351	1.83	0.44
11:K:41:PHE:CD1	11:K:60:PRO:O	2.71	0.44
13:M:126:LEU:HD11	13:M:153:THR:HG21	2.00	0.44
13:M:264:LEU:HD23	38:m:98:LEU:CD1	2.47	0.44
13:M:423:MET:C	13:M:424:ILE:O	2.56	0.44
15:O:91:ILE:HA	15:O:134:TRP:HD1	1.82	0.44
16:P:72:HIS:HB2	16:P:250:VAL:HG21	2.00	0.44
17:Q:77:VAL:HG21	17:Q:99:MET:CE	2.48	0.44
17:Q:91:VAL:HG22	17:Q:91:VAL:O	2.18	0.44
19:S:16:LEU:HD13	19:S:69:TYR:CE1	2.52	0.44
24:Y:41:TYR:CD1	56:Y:202:CDL:H712	2.53	0.44
25:Z:69:ILE:CG2	27:b:54:PRO:CD	2.96	0.44
29:d:57:GLY:O	29:d:60:ARG:N	2.51	0.44
38:m:30:ARG:HH11	45:Aa:260:ASP:HB2	1.81	0.44
38:m:87:SER:HB2	55:m:202:3PE:H271	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:m:201:3PE:H381	55:m:201:3PE:H222	1.99	0.44
41:p:9:VAL:HG23	41:p:10:TYR:CD2	2.53	0.44
41:p:13:PRO:HD2	41:p:116:ARG:CZ	2.48	0.44
45:AA:110:GLU:HB2	46:AB:299:ILE:CD1	2.45	0.44
45:AA:338:CYS:SG	45:AA:358:PHE:HB2	2.58	0.44
45:AA:393:ASN:HB3	46:AB:106:VAL:C	2.43	0.44
49:AE:140:MET:HE1	47:Ac:163:TRP:HZ2	1.83	0.44
51:AG:25:ARG:NH2	51:AG:29:SER:H	2.16	0.44
55:AG:103:3PE:H372	55:AG:103:3PE:H3C2	2.00	0.44
45:Aa:110:GLU:HB2	46:Ab:299:ILE:CD1	2.47	0.44
45:Aa:373:GLN:NE2	45:Aa:471:ILE:O	2.49	0.44
51:Ag:19:LEU:HG	51:Ag:20:SER:N	2.33	0.44
4:D:198:THR:HG21	8:H:275:ALA:HB1	2.00	0.44
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.40	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.44
7:G:557:ARG:HD3	42:q:144:TYR:CZ	2.53	0.44
55:J:201:3PE:C39	24:Y:43:VAL:HG12	2.46	0.44
11:K:22:PHE:CE2	12:L:584:ILE:HG21	2.53	0.44
11:K:57:MET:O	11:K:60:PRO:HD2	2.18	0.44
12:L:35:TYR:CD1	34:i:70:PHE:HE2	2.36	0.44
12:L:68:TRP:HE3	12:L:76:LEU:HD21	1.83	0.44
13:M:321:LEU:HD23	13:M:321:LEU:HA	1.81	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
14:N:120:GLN:HE22	14:N:174:GLN:HB3	1.83	0.44
14:N:321:LYS:HD2	29:d:49:ARG:CD	2.47	0.44
15:O:92:GLN:C	15:O:94:SER:H	2.25	0.44
15:O:100:ASP:HB3	15:O:102:ARG:NH1	2.33	0.44
16:P:130:ILE:N	16:P:130:ILE:HD12	2.33	0.44
16:P:269:ASN:ND2	16:P:271:TYR:OH	2.51	0.44
19:S:51:LEU:CD1	19:S:95:LEU:HD12	2.46	0.44
23:X:137:LEU:O	23:X:138:PRO:C	2.58	0.44
41:p:27:PRO:HB2	41:p:32:TYR:CE2	2.53	0.44
41:p:165:GLU:C	41:p:167:ARG:H	2.26	0.44
45:AA:478:LEU:O	54:AK:24:TRP:CZ2	2.70	0.44
46:AB:411:THR:O	46:AB:414:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:148:ASN:OD1	49:Ae:220:LEU:C	2.61	0.44
47:AC:245:PHE:CZ	48:AD:102:LEU:HD21	2.53	0.44
48:AD:112:ARG:HB3	48:AD:255:TYR:CE1	2.53	0.44
48:AD:262:THR:O	48:AD:263:MET:C	2.61	0.44
48:AD:263:MET:HB3	52:AH:26:ASP:OD2	2.17	0.44
48:AD:321:TYR:HB2	50:AF:61:PHE:CZ	2.52	0.44
56:AG:101:CDL:O1	56:AG:101:CDL:HA4	2.18	0.44
45:Aa:222:ARG:NH1	45:Aa:263:PRO:HB3	2.32	0.44
46:Ab:38:LEU:HG	46:Ab:396:ILE:HD13	2.00	0.44
46:Ab:170:GLN:HB3	49:Ai:78:PHE:CE1	2.53	0.44
47:Ac:149:LEU:HG	47:Ac:291:VAL:HG22	2.00	0.44
47:Ac:243:VAL:O	47:Ac:247:PRO:HG3	2.18	0.44
48:Ad:100:GLY:O	48:Ad:101:LEU:C	2.61	0.44
48:Ad:323:PRO:HG2	48:Ad:325:LYS:HD2	2.00	0.44
1:A:89:ILE:CD1	56:A:402:CDL:C54	2.91	0.43
2:B:223:ARG:C	16:P:138:ASN:HD21	2.25	0.43
3:C:78:SER:C	3:C:80:LEU:H	2.26	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:267:ILE:HD13	8:H:280:PHE:CE1	2.53	0.43
4:D:390:GLN:OE1	7:G:145:MET:HE1	2.18	0.43
5:E:117:PHE:HB2	6:F:220:GLN:HE21	1.83	0.43
6:F:67:GLU:O	6:F:71:LYS:HG2	2.18	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.99	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
7:G:339:ALA:O	7:G:545:LEU:HD12	2.18	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.53	0.43
10:J:154:VAL:HG23	14:N:35:PHE:CE2	2.52	0.43
12:L:152:PHE:HD2	12:L:153:LEU:HD12	1.83	0.43
12:L:305:SER:OG	12:L:336:LYS:HE2	2.18	0.43
13:M:8:SER:O	13:M:11:LEU:HB2	2.18	0.43
14:N:146:TYR:O	14:N:147:PRO:C	2.53	0.43
14:N:323:ASN:N	14:N:323:ASN:OD1	2.49	0.43
15:O:135:LEU:HD13	63:O:401:ADP:C6	2.53	0.43
16:P:327:VAL:HG22	16:P:328:MET:N	2.32	0.43
19:S:19:ILE:CD1	19:S:94:VAL:HG11	2.48	0.43
20:T:140:CYS:SG	20:T:143:GLU:CB	3.03	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:140:ASN:HD21	23:X:144:SER:N	2.16	0.43
24:Y:12:HIS:CD2	24:Y:131:LYS:HE2	2.53	0.43
25:Z:98:MET:HB3	25:Z:104:TRP:CD1	2.53	0.43
34:i:22:TRP:CE3	39:n:172:THR:HG22	2.53	0.43
34:i:69:LEU:HG	34:i:69:LEU:O	2.17	0.43
34:i:123:PHE:HB3	40:o:40:VAL:HG21	2.00	0.43
62:l:201:PC1:H261	62:l:201:PC1:H332	1.98	0.43
38:m:50:GLN:HG2	38:m:60:ILE:CD1	2.48	0.43
42:q:92:CYS:O	43:r:34:ARG:HG3	2.18	0.43
46:AB:63:LEU:HD12	46:AB:220:LEU:HD13	2.00	0.43
46:AB:233:VAL:HA	46:AB:236:GLN:CG	2.47	0.43
46:AB:254:ARG:NH2	46:Ab:257:GLU:HG3	2.33	0.43
47:AC:99:GLY:HA3	55:AC:404:3PE:H272	2.00	0.43
47:AC:105:GLY:HA3	47:AC:313:ARG:O	2.18	0.43
48:AD:201:VAL:HG22	48:AD:278:SER:HB2	2.00	0.43
55:Aa:501:3PE:O32	56:Aa:502:CDL:H341	2.17	0.43
46:Ab:63:LEU:HD12	46:Ab:220:LEU:HD13	1.99	0.43
46:Ab:297:PRO:HB3	46:Ab:304:ASN:CG	2.43	0.43
47:Ac:120:LEU:HD23	47:Ac:298:ILE:HG23	2.00	0.43
47:Ac:137:GLN:NE2	47:Ac:263:ASN:O	2.50	0.43
50:Af:97:GLU:HA	50:Af:100:ARG:NH1	2.33	0.43
49:Ai:72:VAL:N	49:Ai:73:PRO:HD2	2.34	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
3:C:70:LYS:HG2	21:V:104:VAL:HG23	2.00	0.43
4:D:95:LEU:HD21	4:D:97:LEU:HD11	1.99	0.43
4:D:133:LEU:O	4:D:134:PRO:C	2.60	0.43
4:D:232:VAL:O	4:D:356:ILE:HD12	2.19	0.43
4:D:268:TRP:CE2	4:D:272:THR:HG21	2.53	0.43
5:E:231:THR:CG2	6:F:303:HIS:HA	2.47	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
8:H:199:ASP:HB3	8:H:279:ARG:CD	2.48	0.43
8:H:287:HIS:CE1	55:H:402:3PE:N	2.81	0.43
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
12:L:226:GLN:OE1	12:L:284:THR:CG2	2.66	0.43
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.43
14:N:12:THR:CG2	14:N:39:ALA:HB2	2.48	0.43
15:O:97:THR:HG22	28:c:32:ARG:HH12	1.82	0.43
16:P:126:VAL:HG23	16:P:161:VAL:HG11	2.00	0.43
16:P:164:PHE:HE2	16:P:166:HIS:HB2	1.82	0.43
18:R:104:CYS:C	18:R:106:TYR:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:90:TYR:CD1	36:k:51:TRP:CE2	3.06	0.43
20:U:143:GLU:OE2	34:i:9:LYS:HD3	2.18	0.43
21:V:19:THR:N	21:V:20:PRO:CD	2.81	0.43
22:W:71:MET:O	22:W:74:ALA:N	2.39	0.43
24:Y:7:PHE:O	24:Y:8:PHE:C	2.61	0.43
56:Y:202:CDL:H391	56:Y:202:CDL:H581	2.00	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
37:l:142:PHE:O	37:l:145:TRP:N	2.51	0.43
38:m:87:SER:OG	55:m:202:3PE:H351	2.18	0.43
41:p:75:THR:HG22	41:p:156:LEU:HD13	2.00	0.43
56:q:201:CDL:HB61	56:q:201:CDL:OA9	2.18	0.43
45:AA:225:LYS:HG3	45:AA:256:VAL:HG12	2.00	0.43
46:AB:138:LEU:CD1	46:AB:233:VAL:HB	2.47	0.43
47:AC:317:PHE:CD1	50:AF:27:PHE:HB3	2.53	0.43
48:AD:201:VAL:HG22	48:AD:278:SER:OG	2.18	0.43
49:AE:195:LEU:HD13	49:AE:248:ARG:HD2	1.99	0.43
46:Ab:230:LEU:O	46:Ab:233:VAL:HG22	2.19	0.43
47:Ac:317:PHE:HB3	50:Af:27:PHE:HD2	1.83	0.43
55:Ac:403:3PE:H262	55:Ac:403:3PE:H231	1.88	0.43
49:Ae:178:HIS:NE2	49:Ae:209:GLU:HB2	2.33	0.43
49:Ae:195:LEU:HD13	49:Ae:248:ARG:HD2	1.99	0.43
51:Ag:38:VAL:HA	51:Ag:41:ARG:HD3	1.99	0.43
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
2:B:112:TYR:OH	9:I:91:GLY:HA3	2.19	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:97:ASN:OD1	8:H:97:ASN:O	2.36	0.43
13:M:348:LEU:O	13:M:349:GLN:C	2.60	0.43
14:N:254:LEU:HA	14:N:255:PRO:HD3	1.61	0.43
14:N:279:ALA:HA	14:N:282:MET:HE2	2.00	0.43
15:O:65:ASN:O	15:O:66:ILE:C	2.61	0.43
15:O:167:PHE:HZ	15:O:244:THR:HB	1.83	0.43
17:Q:59:LEU:O	17:Q:140:LYS:HA	2.18	0.43
24:Y:26:ILE:O	24:Y:30:LEU:HG	2.17	0.43
24:Y:74:LEU:O	24:Y:78:VAL:HG12	2.18	0.43
24:Y:115:MET:HE3	24:Y:115:MET:HB3	1.80	0.43
56:Y:202:CDL:H581	56:Y:202:CDL:H612	1.66	0.43
29:d:78:ARG:HG2	29:d:82:LEU:HD23	2.00	0.43
34:i:69:LEU:O	34:i:73:SER:HB2	2.19	0.43
38:m:129:TYR:CZ	41:p:144:LEU:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:131:GLU:O	39:n:131:GLU:HG2	2.17	0.43
40:o:31:PHE:CG	40:o:34:ARG:HD2	2.53	0.43
41:p:5:TRP:HZ3	41:p:10:TYR:O	2.02	0.43
41:p:27:PRO:HB2	41:p:32:TYR:HE2	1.83	0.43
46:AB:297:PRO:HB3	46:AB:304:ASN:CG	2.43	0.43
47:AC:248:ASP:OD2	48:AD:202:ARG:NH1	2.51	0.43
48:AD:214:LEU:O	48:AD:234:ASN:ND2	2.46	0.43
49:AE:155:LYS:HE2	49:AE:157:SER:HB3	1.99	0.43
49:AI:72:VAL:N	49:AI:73:PRO:HD2	2.34	0.43
45:Aa:279:ASP:HA	51:Ag:12:ARG:HA	1.98	0.43
45:Aa:311:ILE:HG22	45:Aa:341:PHE:HE1	1.83	0.43
48:Ad:189:ASN:O	48:Ad:190:ASN:C	2.61	0.43
2:B:170:TYR:OH	4:D:131:GLN:O	2.36	0.43
3:C:224:GLU:OE2	16:P:45:LYS:HD3	2.18	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.01	0.43
5:E:232:SER:HB2	6:F:37:ASP:OD1	2.18	0.43
6:F:317:VAL:HG22	6:F:356:VAL:HG22	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:70:LEU:HD11	10:J:27:TYR:CE1	2.53	0.43
10:J:95:GLY:O	10:J:98:MET:HE3	2.19	0.43
12:L:22:SER:HA	12:L:27:ILE:HG21	2.00	0.43
12:L:53:MET:HE2	12:L:53:MET:HB3	1.78	0.43
12:L:70:THR:O	12:L:75:GLU:HA	2.17	0.43
12:L:172:ILE:HD13	12:L:172:ILE:HA	1.88	0.43
12:L:186:MET:CE	13:M:379:LEU:HD21	2.48	0.43
14:N:175:MET:HE2	14:N:175:MET:HB2	1.84	0.43
14:N:186:HIS:O	14:N:190:MET:HG3	2.18	0.43
14:N:324:LEU:HD21	29:d:64:PHE:CZ	2.53	0.43
15:O:91:ILE:HA	15:O:134:TRP:CD1	2.54	0.43
16:P:168:SER:O	16:P:202:ARG:HA	2.17	0.43
17:Q:99:MET:O	17:Q:99:MET:HG3	2.18	0.43
23:X:37:ASP:OD2	27:b:70:PRO:HD2	2.17	0.43
23:X:142:TYR:HE1	30:e:35:ALA:HA	1.84	0.43
32:g:106:TYR:CZ	33:h:86:ILE:HD12	2.53	0.43
35:j:70:LEU:HD13	36:k:81:PHE:HA	2.00	0.43
37:l:41:TYR:HD2	37:l:43:ARG:HD3	1.82	0.43
37:l:97:LEU:O	37:l:98:ARG:C	2.60	0.43
46:AB:180:VAL:HG21	46:AB:257:GLU:N	2.34	0.43
49:AE:235:TYR:CE1	49:AE:240:GLY:HA2	2.53	0.43
47:Ac:102:LEU:HD12	55:Ac:403:3PE:H2E1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:120:LEU:CD2	47:Ac:298:ILE:HG23	2.49	0.43
48:Ad:112:ARG:HB3	48:Ad:255:TYR:CE1	2.53	0.43
1:A:95:VAL:HG11	8:H:302:MET:CG	2.48	0.43
2:B:99:CYS:HB3	4:D:141:TYR:HB2	2.00	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:47:PHE:CG	14:N:227:ILE:HD11	2.54	0.43
4:D:65:PRO:HD2	14:N:51:ARG:NH1	2.33	0.43
4:D:220:ALA:HB3	4:D:224:ALA:HA	2.00	0.43
7:G:141:ASP:O	7:G:145:MET:HG2	2.18	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:346:VAL:HG21	7:G:548:LEU:HD21	2.00	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
8:H:92:PRO:HG3	8:H:247:TYR:HE1	1.84	0.43
8:H:142:TYR:O	8:H:146:MET:HB2	2.18	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
10:J:82:TRP:HB2	16:P:360:ARG:HH11	1.82	0.43
12:L:92:VAL:HG21	12:L:330:CYS:HB3	2.00	0.43
13:M:73:LEU:HD23	13:M:103:GLN:HE22	1.83	0.43
13:M:154:LEU:HA	13:M:154:LEU:HD23	1.84	0.43
14:N:240:MET:O	14:N:240:MET:HG2	2.18	0.43
15:O:169:PHE:CD2	63:O:401:ADP:N6	2.87	0.43
15:O:172:ALA:CB	15:O:236:ASP:HB2	2.48	0.43
23:X:46:CYS:SG	23:X:135:ARG:HD3	2.58	0.43
23:X:151:ASN:HD22	33:h:165:ASP:HA	1.84	0.43
27:b:15:LYS:O	27:b:15:LYS:HG3	2.18	0.43
34:i:106:PRO:HD2	40:o:64:ILE:CG2	2.48	0.43
38:m:45:ARG:HG2	38:m:45:ARG:O	2.18	0.43
38:m:49:LEU:HD11	39:n:140:LEU:HD23	2.00	0.43
41:p:103:MET:HE1	41:p:135:VAL:HG12	1.99	0.43
47:AC:100:ARG:HH12	67:AC:403:HEM:HBD2	1.82	0.43
45:Aa:60:ALA:O	45:Aa:232:ALA:HA	2.18	0.43
46:Ab:130:ILE:HA	46:Ab:133:LEU:HB2	2.01	0.43
46:Ab:173:ILE:CG2	46:Ab:339:TYR:HE1	2.32	0.43
46:Ab:300:LYS:HE2	46:Ab:301:ARG:HH11	1.83	0.43
48:Ad:167:ARG:NH1	48:Ad:169:GLY:HA2	2.33	0.43
4:D:240:LEU:CG	4:D:244:ILE:HD11	2.49	0.43
5:E:247:GLY:O	6:F:64:LYS:CD	2.67	0.43
6:F:381:GLN:HG3	7:G:74:ASN:OD1	2.19	0.43
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.18	0.43
55:H:402:3PE:H331	55:H:402:3PE:H362	1.68	0.43
10:J:32:LEU:HG	10:J:64:LEU:HD21	1.99	0.43
10:J:71:THR:HG22	10:J:75:THR:HG21	2.00	0.43
10:J:146:SER:O	10:J:149:THR:HG23	2.18	0.43
11:K:4:THR:O	11:K:4:THR:HG22	2.19	0.43
12:L:81:LYS:HD3	12:L:262:ARG:NH1	2.34	0.43
12:L:246:LEU:HD12	12:L:247:LEU:CB	2.49	0.43
12:L:427:ILE:HG13	12:L:428:TYR:N	2.33	0.43
12:L:446:ASN:O	12:L:447:ASP:C	2.57	0.43
12:L:564:LYS:HG2	38:m:77:TYR:CZ	2.54	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.19	0.43
14:N:105:LYS:HE3	14:N:105:LYS:HB3	1.79	0.43
14:N:317:GLN:HE21	15:O:98:THR:CG2	2.31	0.43
18:R:40:GLU:HG3	18:R:41:LYS:HG2	2.00	0.43
19:S:18:GLU:O	19:S:19:ILE:HD13	2.19	0.43
19:S:30:SER:O	19:S:31:GLN:C	2.59	0.43
23:X:154:ILE:CG1	33:h:167:PRO:HG2	2.48	0.43
34:i:73:SER:O	34:i:77:ILE:HB	2.19	0.43
41:p:49:ARG:O	41:p:50:GLU:C	2.59	0.43
41:p:118:GLY:O	41:p:119:GLU:HB2	2.18	0.43
45:AA:175:ASN:C	45:AA:177:ALA:N	2.76	0.43
45:AA:182:VAL:HA	49:AE:80:HIS:CD2	2.54	0.43
46:AB:378:LEU:HD23	46:AB:416:ILE:CG2	2.49	0.43
47:AC:48:GLY:HA3	67:AC:402:HEM:C1B	2.54	0.43
47:AC:133:LEU:HD23	47:AC:133:LEU:HA	1.85	0.43
51:AG:29:SER:CB	51:AG:32:SER:HB2	2.38	0.43
54:AK:48:ILE:O	54:AK:49:ASN:C	2.61	0.43
49:Ae:222:CYS:HB2	49:Ae:236:CYS:SG	2.59	0.43
52:Ah:52:ASP:OD1	52:Ah:53:ASN:N	2.52	0.43
1:A:10:ASN:ND2	8:H:84:SER:OG	2.51	0.43
1:A:77:TRP:HH2	10:J:50:PHE:HD2	1.65	0.43
2:B:172:HIS:CE1	2:B:179:ARG:HD3	2.54	0.43
3:C:70:LYS:HA	21:V:102:PRO:C	2.44	0.43
4:D:261:MET:HE3	4:D:261:MET:HB3	1.74	0.43
4:D:378:LEU:HD22	7:G:126:LEU:HD13	2.01	0.43
4:D:384:LEU:HD23	7:G:144:MET:HE1	2.00	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:639:LEU:HD21	7:G:643:ARG:NH2	2.34	0.43
8:H:132:ALA:O	8:H:136:VAL:HG12	2.18	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
10:J:149:THR:O	10:J:150:TRP:C	2.61	0.43
12:L:60:GLU:C	12:L:61:TYR:CD1	2.97	0.43
12:L:296:ASN:HD21	12:L:425:ARG:HH21	1.65	0.43
12:L:327:LEU:HD21	12:L:472:ILE:HD13	2.00	0.43
62:L:701:PC1:H332	62:L:701:PC1:H281	2.01	0.43
13:M:1:MET:HB3	13:M:1:MET:HE3	1.72	0.43
13:M:63:THR:N	13:M:64:PRO:CD	2.81	0.43
13:M:135:ARG:HE	56:d:201:CDL:H311	1.84	0.43
13:M:207:MET:SD	13:M:240:SER:CA	3.06	0.43
13:M:304:GLN:HA	13:M:309:PHE:HE1	1.83	0.43
14:N:219:LEU:CD2	14:N:230:ILE:HD12	2.49	0.43
15:O:71:ASN:ND2	15:O:75:LYS:HE3	2.34	0.43
16:P:170:LEU:O	16:P:171:ASN:CG	2.61	0.43
17:Q:55:VAL:HG21	22:W:78:ASP:OD1	2.18	0.43
22:W:120:ASP:HB3	22:W:123:SER:OG	2.18	0.43
24:Y:14:VAL:HG21	24:Y:19:GLN:OE1	2.18	0.43
25:Z:98:MET:HE2	25:Z:98:MET:HA	2.01	0.43
25:Z:121:ILE:HA	25:Z:124:MET:HE2	1.99	0.43
33:h:90:ASN:OD1	33:h:115:HIS:NE2	2.52	0.43
33:h:127:ASP:OD1	33:h:127:ASP:C	2.61	0.43
39:n:37:TYR:O	39:n:38:ARG:C	2.61	0.43
40:o:18:ASP:O	40:o:19:PRO:C	2.61	0.43
46:AB:155:ARG:HD2	46:AB:198:GLY:H	1.83	0.43
47:AC:181:PHE:HA	47:AC:184:ILE:HG22	2.00	0.43
47:AC:218:ILE:HG21	48:AD:314:LEU:CD1	2.48	0.43
47:AC:317:PHE:HB3	50:AF:27:PHE:HD2	1.84	0.43
49:AE:154:ILE:HD12	49:AE:154:ILE:N	2.32	0.43
46:Ab:378:LEU:HD23	46:Ab:416:ILE:CG2	2.49	0.43
46:Ab:411:THR:O	46:Ab:414:GLN:HG2	2.19	0.43
49:Ae:263:TYR:CB	49:Ae:273:VAL:HA	2.49	0.43
51:Ag:25:ARG:NH2	51:Ag:29:SER:H	2.16	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:52:MET:O	4:D:54:PRO:HD3	2.19	0.43
5:E:38:PHE:O	7:G:205:GLN:NE2	2.52	0.43
6:F:394:LYS:CB	7:G:155:GLU:HG2	2.48	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:TYR:CE2	42:q:27:PHE:CZ	3.06	0.43
8:H:127:TYR:HD1	8:H:207:LEU:CD2	2.15	0.43
8:H:272:TRP:CZ2	9:I:74:LEU:HB2	2.54	0.43
9:I:50:MET:CE	27:b:10:LYS:HG2	2.49	0.43
10:J:1:MET:SD	25:Z:142:TRP:HH2	2.42	0.43
12:L:61:TYR:HA	34:i:98:VAL:O	2.18	0.43
12:L:217:LEU:CD1	12:L:273:ILE:HG23	2.49	0.43
12:L:386:LEU:HA	35:j:68:TRP:HZ3	1.83	0.43
12:L:389:PHE:CZ	35:j:79:ALA:CB	3.02	0.43
12:L:553:LEU:CD1	38:m:93:ALA:CB	2.89	0.43
56:L:703:CDL:HB62	56:L:703:CDL:H511	2.01	0.43
13:M:14:LEU:HD21	13:M:26:ASN:CB	2.49	0.43
13:M:369:LEU:CD2	13:M:371:PRO:CD	2.84	0.43
14:N:154:ILE:HD12	14:N:155:LEU:N	2.33	0.43
14:N:193:ILE:HD12	14:N:266:ILE:HA	2.01	0.43
16:P:76:MET:HE1	16:P:254:LYS:HE2	2.01	0.43
29:d:99:GLU:HG2	29:d:100:ASP:N	2.33	0.43
30:e:69:ARG:CD	30:e:72:THR:HG21	2.49	0.43
56:h:201:CDL:H772	56:h:201:CDL:H731	2.01	0.43
38:m:19:ASP:O	38:m:20:PRO:C	2.61	0.43
42:q:79:GLY:O	42:q:82:VAL:HG22	2.19	0.43
43:r:54:TYR:C	43:r:56:THR:N	2.76	0.43
45:AA:61:SER:HB3	45:AA:242:LEU:HD22	2.01	0.43
47:AC:50:PHE:CE2	49:AE:140:MET:HE2	2.54	0.43
48:AD:315:LYS:O	50:AF:72:ARG:NH1	2.48	0.43
49:AE:166:ALA:HB2	49:AE:175:PHE:HD1	1.84	0.43
49:AE:222:CYS:HB2	49:AE:236:CYS:SG	2.59	0.43
45:Aa:175:ASN:C	45:Aa:177:ALA:N	2.76	0.43
45:Aa:338:CYS:SG	45:Aa:358:PHE:HB2	2.58	0.43
46:Ab:36:GLN:OE1	46:Ab:36:GLN:N	2.52	0.43
47:Ac:103:TYR:O	47:Ac:315:LEU:HG	2.19	0.43
68:Ac:404:U10:H1M1	68:Ac:404:U10:H72	1.79	0.43
48:Ad:302:LEU:C	48:Ad:304:TYR:N	2.75	0.43
49:Ai:64:LEU:CD1	49:Ai:78:PHE:HD1	2.32	0.43
2:B:92:PRO:HD2	2:B:120:VAL:O	2.19	0.43
3:C:97:THR:O	21:V:90:LEU:CD1	2.67	0.43
4:D:72:LEU:O	4:D:72:LEU:HD12	2.19	0.43
4:D:152:SER:HA	4:D:229:PRO:HA	2.00	0.43
6:F:46:TYR:O	6:F:48:ARG:HG2	2.19	0.43
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.43
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:THR:O	12:L:41:LYS:HB3	2.19	0.43
12:L:72:ASN:ND2	13:M:459:MET:HG2	2.34	0.43
12:L:358:LYS:CG	39:n:80:TYR:CE1	2.84	0.43
12:L:428:TYR:OH	39:n:33:HIS:CE1	2.71	0.43
13:M:119:TYR:HD1	13:M:160:LEU:HD22	1.80	0.43
13:M:208:PRO:HG2	13:M:216:LEU:CD1	2.44	0.43
14:N:11:PHE:O	14:N:15:LEU:N	2.50	0.43
14:N:39:ALA:O	14:N:42:PRO:HD2	2.19	0.43
14:N:272:LYS:HG2	33:h:154:GLN:HE21	1.84	0.43
14:N:338:PRO:HG2	29:d:33:TYR:CZ	2.54	0.43
15:O:303:GLU:O	15:O:304:VAL:C	2.59	0.43
16:P:316:LYS:O	16:P:320:GLU:HG2	2.19	0.43
17:Q:52:LEU:HD23	22:W:19:SER:O	2.19	0.43
19:S:75:LYS:HE2	19:S:75:LYS:HA	2.01	0.43
20:U:119:ILE:HD13	20:U:119:ILE:HA	1.81	0.43
20:U:125:GLU:OE2	35:j:44:TYR:CZ	2.71	0.43
21:V:8:THR:HG22	21:V:9:THR:N	2.34	0.43
22:W:38:LEU:HG	22:W:70:PHE:HZ	1.84	0.43
23:X:115:LEU:HD13	23:X:117:TRP:CH2	2.53	0.43
23:X:120:PRO:HG3	27:b:71:GLN:NE2	2.34	0.43
26:a:4:GLU:C	26:a:7:PRO:HD2	2.44	0.43
27:b:42:ALA:HA	27:b:45:ILE:HG22	2.01	0.43
31:f:37:PHE:O	33:h:134:GLU:HB3	2.19	0.43
35:j:99:ILE:HG23	40:o:108:LEU:HD23	2.01	0.43
37:l:156:VAL:HG11	40:o:95:TYR:CE1	2.54	0.43
46:AB:162:LYS:HG3	46:AB:191:TYR:HB3	2.00	0.43
47:AC:171:ASP:CG	47:AC:172:LYS:N	2.76	0.43
47:AC:208:PRO:HB2	47:AC:316:MET:HE3	2.01	0.43
48:AD:312:SER:O	48:AD:313:VAL:C	2.59	0.43
49:AE:83:VAL:HG22	49:AE:84:LYS:N	2.34	0.43
49:AE:249:ILE:HG12	49:AE:254:ALA:HB3	2.01	0.43
51:AG:73:LYS:HZ3	52:AH:63:GLU:HG2	1.83	0.43
54:AK:33:VAL:CG1	54:AK:42:LEU:HG	2.45	0.43
47:Ac:48:GLY:C	67:Ac:401:HEM:HMB3	2.43	0.43
48:Ad:224:GLY:HA3	52:Ah:64:ASP:HA	1.99	0.43
49:Ae:83:VAL:HG22	49:Ae:84:LYS:N	2.34	0.43
49:Ae:264:GLU:O	49:Ae:272:VAL:N	2.47	0.43
2:B:81:LEU:HD11	62:q:202:PC1:H361	2.00	0.43
2:B:114:MET:HB2	2:B:119:VAL:HB	2.01	0.43
2:B:166:ASN:HB2	2:B:190:TYR:CD2	2.45	0.43
4:D:47:PHE:CE2	14:N:305:PHE:HZ	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:ALA:HB1	4:D:95:LEU:HB3	2.01	0.43
4:D:203:MET:HE1	4:D:255:ILE:HA	2.01	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.50	0.43
4:D:303:ARG:CG	4:D:401:GLU:HB3	2.48	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
6:F:398:ARG:HH22	7:G:155:GLU:CD	2.26	0.43
7:G:401:LEU:HD21	7:G:466:LEU:HD11	2.01	0.43
11:K:96:LEU:O	11:K:97:GLN:C	2.61	0.43
12:L:110:SER:HB3	39:n:179:THR:HG22	2.01	0.43
12:L:253:VAL:HG21	12:L:310:LEU:HD11	1.99	0.43
12:L:283:LEU:HD12	37:l:140:MET:HE2	2.00	0.43
13:M:367:LEU:C	13:M:367:LEU:HD12	2.44	0.43
14:N:309:ASN:HA	15:O:319:ILE:CG2	2.49	0.43
15:O:117:PHE:HD1	15:O:128:SER:CA	2.31	0.43
15:O:238:GLU:O	15:O:241:TYR:HB2	2.19	0.43
16:P:197:GLU:HB3	16:P:259:VAL:HG22	1.99	0.43
24:Y:83:ARG:NH1	24:Y:90:LEU:HD23	2.34	0.43
25:Z:69:ILE:HG23	27:b:54:PRO:CD	2.46	0.43
25:Z:111:PHE:CE2	25:Z:117:VAL:HG21	2.52	0.43
26:a:55:SER:O	26:a:56:GLY:C	2.61	0.43
30:e:49:GLY:O	30:e:50:THR:C	2.61	0.43
31:f:43:LEU:HD21	41:p:68:TYR:HD1	1.83	0.43
36:k:28:TRP:CE3	36:k:60:MET:HG2	2.53	0.43
40:o:57:ASP:OD2	40:o:59:CYS:HB2	2.19	0.43
42:q:34:ARG:HD3	42:q:54:GLN:OE1	2.18	0.43
50:AF:95:LEU:O	50:AF:96:LYS:C	2.62	0.43
50:AF:97:GLU:HA	50:AF:100:ARG:NH1	2.32	0.43
52:AH:52:ASP:OD1	52:AH:53:ASN:N	2.52	0.43
46:Ab:64:PHE:HZ	46:Ab:394:SER:HA	1.84	0.43
46:Ab:261:GLN:HE22	46:Ab:443:ASN:HA	1.84	0.43
47:Ac:83:HIS:CD2	67:Ac:401:HEM:ND	2.86	0.43
47:Ac:181:PHE:HA	47:Ac:184:ILE:HG22	2.00	0.43
47:Ac:270:PRO:HG3	47:Ac:278:TYR:HB2	2.00	0.43
49:Ae:156:LEU:HD23	49:Ae:156:LEU:HA	1.62	0.43
1:A:70:ALA:HB2	10:J:58:ILE:CD1	2.49	0.42
3:C:104:ASN:HD22	43:r:94:ALA:HB1	1.83	0.42
5:E:142:ARG:HG3	5:E:182:ALA:HB3	2.00	0.42
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.54	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.42
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
10:J:82:TRP:HE3	16:P:360:ARG:HD3	1.84	0.42
10:J:146:SER:O	10:J:147:CYS:C	2.62	0.42
11:K:50:ASN:C	11:K:50:ASN:OD1	2.62	0.42
12:L:5:THR:O	12:L:6:THR:C	2.62	0.42
13:M:72:LEU:HD12	13:M:234:ILE:HG12	2.01	0.42
14:N:12:THR:HG22	14:N:39:ALA:HB2	2.00	0.42
14:N:170:LEU:HD12	14:N:292:PHE:CD2	2.54	0.42
14:N:193:ILE:HD11	14:N:269:GLU:CB	2.49	0.42
15:O:297:LEU:C	15:O:297:LEU:HD23	2.43	0.42
20:U:103:HIS:CD2	20:U:140:CYS:HG	2.36	0.42
21:V:35:LEU:HA	21:V:38:PHE:CE1	2.54	0.42
23:X:10:LEU:H	23:X:10:LEU:HD12	1.84	0.42
30:e:44:ALA:HA	30:e:47:ILE:CG1	2.49	0.42
33:h:59:PRO:O	33:h:61:LEU:HG	2.19	0.42
39:n:81:ILE:HD12	39:n:87:GLY:C	2.44	0.42
40:o:10:LEU:HD12	40:o:10:LEU:N	2.34	0.42
45:AA:167:VAL:O	45:AA:170:ARG:HG2	2.19	0.42
46:AB:39:GLU:OE2	46:AB:227:HIS:HB2	2.19	0.42
46:AB:130:ILE:HA	46:AB:133:LEU:HB2	2.00	0.42
46:AB:230:LEU:O	46:AB:233:VAL:HG22	2.18	0.42
47:AC:197:LEU:HD11	69:AC:406:UQ6:C7	2.49	0.42
48:AD:159:ASN:OD1	48:AD:160:ASP:N	2.52	0.42
48:AD:252:VAL:HG13	48:AD:253:LEU:N	2.33	0.42
48:AD:321:TYR:HB2	50:AF:61:PHE:CD2	2.54	0.42
49:AE:196:ARG:HD2	49:AE:249:ILE:HG23	2.01	0.42
56:AG:102:CDL:H742	56:AG:102:CDL:H781	2.01	0.42
46:Ab:60:ARG:CZ	46:Ab:390:GLU:HB3	2.48	0.42
46:Ab:64:PHE:CZ	46:Ab:394:SER:HA	2.54	0.42
46:Ab:173:ILE:HD11	46:Ab:439:ALA:C	2.44	0.42
46:Ab:225:VAL:HG22	46:Ab:229:VAL:HG21	2.01	0.42
46:Ab:297:PRO:CB	46:Ab:304:ASN:CG	2.91	0.42
47:Ac:256:TYR:CD2	48:Ad:202:ARG:HB3	2.54	0.42
47:Ac:263:ASN:OD1	47:Ac:264:THR:N	2.52	0.42
48:Ad:262:THR:O	48:Ad:263:MET:C	2.61	0.42
49:Ae:235:TYR:CE1	49:Ae:240:GLY:HA2	2.53	0.42
53:Aj:19:SER:HB2	54:Ak:23:MET:HB3	2.01	0.42
54:Ak:48:ILE:HD13	54:Ak:48:ILE:HA	1.87	0.42
1:A:93:ILE:CD1	56:A:402:CDL:C62	2.97	0.42
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:225:LEU:HB2	17:Q:160:TYR:CE2	2.54	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
12:L:246:LEU:CD1	12:L:247:LEU:N	2.68	0.42
12:L:275:THR:HG23	12:L:276:THR:N	2.34	0.42
12:L:475:THR:HA	40:o:55:GLN:HE22	1.78	0.42
12:L:526:LEU:HD12	12:L:526:LEU:N	2.34	0.42
12:L:589:MET:HE3	12:L:589:MET:HB2	1.90	0.42
12:L:591:PHE:O	12:L:595:ILE:HG13	2.19	0.42
13:M:100:ILE:O	13:M:103:GLN:HG2	2.19	0.42
13:M:214:LEU:C	13:M:217:PRO:HD2	2.44	0.42
14:N:80:GLN:O	14:N:81:LEU:HG	2.19	0.42
14:N:219:LEU:HD23	14:N:230:ILE:HD12	2.01	0.42
14:N:241:LEU:HG	14:N:301:SER:OG	2.19	0.42
15:O:121:PRO:HB3	15:O:178:TYR:HE1	1.83	0.42
15:O:256:LEU:HD21	15:O:276:LEU:HD21	2.01	0.42
15:O:269:VAL:O	15:O:273:ILE:HG13	2.19	0.42
16:P:259:VAL:N	16:P:261:LYS:HG2	2.33	0.42
17:Q:51:GLN:HB3	22:W:26:ARG:HH22	1.84	0.42
18:R:43:TYR:C	18:R:45:ARG:H	2.27	0.42
20:U:100:VAL:HA	20:U:141:PRO:HG2	2.01	0.42
23:X:69:ASN:O	23:X:73:GLN:HG3	2.19	0.42
24:Y:8:PHE:CD1	24:Y:30:LEU:HD21	2.53	0.42
27:b:31:ILE:HG23	27:b:32:MET:N	2.34	0.42
29:d:11:LEU:HD11	30:e:4:LEU:HD12	2.00	0.42
32:g:125:LYS:HE3	41:p:8:ASP:OD2	2.19	0.42
37:l:89:TRP:CE2	39:n:86:PRO:HD2	2.53	0.42
38:m:5:LYS:HB2	38:m:5:LYS:HE3	1.73	0.42
39:n:45:ARG:O	39:n:46:ALA:C	2.61	0.42
40:o:46:MET:HE2	40:o:60:ALA:HB3	2.00	0.42
41:p:73:ASP:O	41:p:74:ILE:C	2.59	0.42
42:q:125:VAL:O	42:q:125:VAL:CG2	2.67	0.42
48:AD:259:THR:O	48:AD:260:PRO:C	2.60	0.42
49:AE:205:VAL:CG1	49:AE:211:VAL:HG23	2.49	0.42
45:Aa:74:TRP:HB3	45:Aa:418:LEU:CD1	2.49	0.42
45:Aa:117:GLY:HA3	46:Ab:377:LYS:HA	1.99	0.42
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HG13	2.00	0.42
69:Ac:405:UQ6:H171	69:Ac:405:UQ6:H151	1.68	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:109:LYS:HD2	1:A:112:GLU:HB2	2.00	0.42
2:B:93:MET:SD	2:B:125:PRO:HG3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:CYS:HB2	9:I:153:ILE:C	2.43	0.42
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.82	0.42
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.54	0.42
5:E:162:THR:HG22	5:E:163:THR:N	2.34	0.42
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.48	0.42
5:E:180:VAL:CG1	5:E:181:ASN:H	2.32	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:31:LEU:HA	7:G:31:LEU:HD23	1.79	0.42
8:H:136:VAL:O	8:H:140:ILE:HG23	2.19	0.42
61:H:401:UQ9:H1M	61:H:401:UQ9:H7A	1.83	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
11:K:19:THR:O	11:K:22:PHE:HE1	2.02	0.42
11:K:93:LEU:HD13	14:N:57:THR:CG2	2.48	0.42
12:L:60:GLU:N	12:L:60:GLU:OE2	2.53	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	2.34	0.42
12:L:546:LEU:HD23	37:I:108:ASP:OD1	2.18	0.42
13:M:200:MET:CE	13:M:247:SER:HB2	2.46	0.42
14:N:174:GLN:O	14:N:178:ILE:HG13	2.18	0.42
15:O:146:ALA:CB	15:O:159:LEU:HD21	2.49	0.42
16:P:64:PHE:CE1	16:P:209:ARG:O	2.69	0.42
16:P:235:THR:HG21	16:P:323:HIS:CD2	2.55	0.42
21:V:37:HIS:O	21:V:38:PHE:C	2.63	0.42
23:X:47:ARG:NH1	33:h:187:PRO:HB2	2.35	0.42
30:e:41:ILE:HD11	33:h:174:PRO:N	2.35	0.42
33:h:129:PRO:HD2	33:h:130:GLU:OE1	2.19	0.42
34:i:93:LYS:HE3	34:i:96:THR:HG21	2.01	0.42
34:i:95:TYR:CE2	41:p:10:TYR:HB3	2.54	0.42
40:o:35:LYS:HG3	40:o:36:GLU:O	2.20	0.42
41:p:43:TRP:NE1	41:p:47:LEU:HD11	2.33	0.42
46:AB:45:ASN:ND2	46:AB:239:ASN:CA	2.74	0.42
46:AB:286:PHE:CD1	46:AB:427:ALA:HB1	2.54	0.42
47:AC:138:MET:HE1	47:AC:268:ILE:HA	2.01	0.42
48:AD:248:ILE:HD12	48:AD:266:VAL:HG11	2.00	0.42
50:AF:111:LYS:HA	54:Ak:8:PRO:CG	2.50	0.42
52:AH:39:GLU:HA	52:AH:42:VAL:HG12	2.01	0.42
45:Aa:464:GLN:HA	51:Ag:5:PHE:HB3	2.02	0.42
46:Ab:162:LYS:HG3	46:Ab:191:TYR:HB3	2.00	0.42
46:Ab:396:ILE:HG12	46:Ab:406:TYR:HE1	1.84	0.42
47:Ac:169:SER:O	47:Ac:170:VAL:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:154:VAL:HG21	48:Ad:173:ASP:CG	2.44	0.42
3:C:49:ARG:HH21	3:C:54:HIS:CG	2.37	0.42
4:D:79:ASN:O	4:D:80:MET:C	2.62	0.42
4:D:381:HIS:HE1	9:I:161:ALA:O	2.02	0.42
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.34	0.42
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.02	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:409:ILE:HG12	6:F:446:LEU:HD23	1.96	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
12:L:197:GLU:HG3	41:p:111:LYS:HE2	2.01	0.42
12:L:405:ASN:HB2	12:L:408:ALA:HB3	2.01	0.42
13:M:25:THR:HG22	32:g:84:ASN:OD1	2.20	0.42
13:M:68:LEU:HD23	13:M:234:ILE:CD1	2.50	0.42
14:N:80:GLN:O	14:N:80:GLN:HG2	2.19	0.42
15:O:93:TYR:OH	15:O:142:GLN:HA	2.19	0.42
15:O:167:PHE:CE2	15:O:244:THR:HG21	2.55	0.42
15:O:263:ALA:O	15:O:264:GLU:C	2.60	0.42
15:O:310:ILE:HG23	15:O:312:VAL:HG23	2.01	0.42
26:a:17:VAL:O	26:a:18:ILE:C	2.62	0.42
30:e:22:SER:HB2	30:e:34:HIS:CD2	2.54	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
34:i:85:TYR:HB2	55:i:201:3PE:H261	2.00	0.42
34:i:120:MET:O	34:i:121:ARG:C	2.63	0.42
35:j:74:TRP:HB2	36:k:84:PHE:CZ	2.54	0.42
37:l:57:MET:HG2	37:l:104:PRO:CG	2.49	0.42
43:r:113:LEU:HD13	43:r:113:LEU:HA	1.92	0.42
47:AC:331:ASN:HB3	55:AG:103:3PE:H2G1	2.01	0.42
48:AD:318:LYS:CD	49:AE:86:PRO:HB2	2.49	0.42
52:AH:42:VAL:HG23	52:AH:45:ARG:HH21	1.84	0.42
45:Aa:480:PHE:HB3	54:Ak:20:THR:HG21	2.01	0.42
46:Ab:142:THR:HA	46:Ab:241:ARG:NH2	2.35	0.42
49:Ae:112:GLY:O	49:Ae:116:LEU:HB2	2.19	0.42
49:Ae:122:THR:O	49:Ae:123:VAL:C	2.61	0.42
52:Ah:39:GLU:HA	52:Ah:42:VAL:HG12	2.01	0.42
1:A:92:PHE:HZ	8:H:306:SER:HB2	1.83	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:THR:CG2	58:D:501:UQ1:HM23	2.49	0.42
4:D:266:ARG:HH21	9:I:63:TRP:HA	1.85	0.42
4:D:280:ALA:HB1	21:V:11:LEU:CG	2.44	0.42
4:D:280:ALA:HB3	21:V:11:LEU:HD23	2.01	0.42
5:E:101:ALA:HA	5:E:106:VAL:HG22	2.01	0.42
5:E:110:ARG:HD3	5:E:110:ARG:HA	1.81	0.42
5:E:114:VAL:O	5:E:118:TYR:HD2	2.02	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
9:I:113:CYS:SG	57:I:303:SF4:S4	3.17	0.42
10:J:124:LEU:CG	25:Z:138:PHE:HZ	2.32	0.42
10:J:160:PHE:HE2	14:N:8:ILE:CD1	2.32	0.42
12:L:335:PHE:O	12:L:339:LEU:HD13	2.19	0.42
12:L:532:ILE:HG21	37:l:133:LEU:HD22	2.00	0.42
13:M:210:TYR:O	13:M:213:HIS:HD2	2.01	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
13:M:388:TRP:CD2	38:m:109:ARG:HD2	2.54	0.42
13:M:428:PRO:HD3	39:n:106:TYR:CG	2.54	0.42
55:M:501:3PE:O22	14:N:276:LEU:HD13	2.19	0.42
15:O:170:LEU:HD21	15:O:184:VAL:HG13	2.00	0.42
16:P:220:TYR:CG	16:P:226:VAL:HG13	2.55	0.42
18:R:76:ILE:HD11	18:R:92:TYR:CB	2.48	0.42
20:T:108:LEU:HD23	20:T:108:LEU:C	2.44	0.42
20:U:91:ASP:OD2	36:k:48:ARG:NH1	2.50	0.42
24:Y:45:LEU:O	24:Y:46:ASN:C	2.61	0.42
24:Y:61:TYR:CE1	56:Y:202:CDL:H112	2.54	0.42
25:Z:98:MET:HA	25:Z:101:VAL:HG23	2.01	0.42
29:d:114:GLU:OE2	41:p:153:ARG:HB3	2.20	0.42
33:h:62:TYR:N	39:n:111:GLU:OE2	2.53	0.42
35:j:44:TYR:CE2	35:j:45:ARG:HG3	2.54	0.42
37:l:62:TYR:CE2	37:l:64:PRO:HG3	2.55	0.42
39:n:139:GLN:HA	39:n:142:GLU:HG2	2.01	0.42
43:r:54:TYR:HA	43:r:57:ARG:CG	2.48	0.42
43:r:54:TYR:HD1	43:r:57:ARG:HG3	1.83	0.42
46:AB:177:LEU:HD21	46:AB:272:VAL:CG1	2.49	0.42
48:AD:199:TYR:HA	48:AD:278:SER:OG	2.20	0.42
45:Aa:167:VAL:O	45:Aa:170:ARG:HG2	2.19	0.42
45:Aa:467:ASP:OD2	47:Ac:223:TYR:HE2	1.98	0.42
46:Ab:41:THR:OG1	46:Ab:49:ILE:HB	2.19	0.42
46:Ab:177:LEU:HD21	46:Ab:272:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:349:GLU:O	46:Ab:350:VAL:C	2.63	0.42
47:Ac:270:PRO:HB2	47:Ac:274:PHE:HB2	2.01	0.42
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.42	0.42
58:D:501:UQ1:HM23	58:D:501:UQ1:HM32	2.00	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
7:G:360:LYS:HE3	7:G:632:ILE:CB	2.38	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:49:PHE:HB3	62:q:202:PC1:H381	2.01	0.42
9:I:78:PHE:HB3	43:r:8:ILE:CG2	2.48	0.42
62:I:301:PC1:H221	25:Z:35:MET:HE2	2.00	0.42
10:J:19:LEU:HD11	10:J:32:LEU:HD13	2.02	0.42
12:L:189:PHE:CZ	12:L:212:PRO:HB2	2.55	0.42
13:M:206:LYS:HA	13:M:215:TRP:CZ2	2.54	0.42
13:M:207:MET:HE3	13:M:240:SER:HB2	2.02	0.42
13:M:395:LEU:HD11	38:m:101:TRP:CD2	2.54	0.42
14:N:108:LEU:O	14:N:109:ALA:HB3	2.20	0.42
14:N:226:THR:HG22	14:N:228:ASN:N	2.34	0.42
14:N:272:LYS:HG2	33:h:154:GLN:NE2	2.35	0.42
16:P:242:VAL:HG13	16:P:243:ALA:N	2.35	0.42
16:P:265:PHE:CD1	16:P:334:GLY:HA3	2.55	0.42
16:P:280:ILE:HG23	16:P:353:LEU:HD22	2.01	0.42
18:R:77:ILE:HG12	18:R:78:ALA:N	2.34	0.42
19:S:64:LYS:HE2	19:S:66:TRP:CZ2	2.55	0.42
22:W:120:ASP:OD1	22:W:120:ASP:C	2.61	0.42
24:Y:57:ARG:HG2	24:Y:60:ARG:HH21	1.83	0.42
25:Z:65:LEU:CB	27:b:50:PRO:O	2.63	0.42
27:b:32:MET:N	27:b:33:PRO:CD	2.82	0.42
28:c:69:TYR:O	28:c:73:ASN:ND2	2.53	0.42
29:d:93:TYR:OH	33:h:163:ARG:HD2	2.18	0.42
32:g:119:GLU:OE1	32:g:122:ARG:NH1	2.53	0.42
37:l:38:PRO:HD2	38:m:70:TYR:CD2	2.55	0.42
37:l:109:LEU:HG	37:l:109:LEU:O	2.20	0.42
37:l:167:TYR:CG	37:l:178:PRO:HG3	2.55	0.42
39:n:85:SER:O	39:n:86:PRO:C	2.61	0.42
45:AA:278:ARG:CZ	45:AA:463:GLU:HB2	2.50	0.42
46:AB:300:LYS:HE2	46:AB:301:ARG:HH11	1.83	0.42
47:AC:33:PHE:O	47:AC:36:LEU:HB2	2.19	0.42
47:AC:51:LEU:HG	67:AC:402:HEM:HBA1	2.00	0.42
47:AC:153:ILE:HB	47:AC:157:GLY:HA2	2.02	0.42
47:AC:163:TRP:HZ2	49:Ae:140:MET:CE	2.31	0.42
47:AC:179:PHE:HE2	47:Ac:179:PHE:CE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:278:TYR:CE2	47:AC:282:ARG:HD2	2.54	0.42
48:AD:131:ALA:HA	48:AD:174:TYR:HA	2.02	0.42
49:AE:195:LEU:CD1	49:AE:248:ARG:HD2	2.50	0.42
51:AG:19:LEU:HG	51:AG:20:SER:N	2.33	0.42
45:Aa:278:ARG:NH1	51:Ag:11:ILE:HD13	2.35	0.42
45:Aa:358:PHE:CD2	45:Aa:368:MET:HG2	2.54	0.42
47:Ac:33:PHE:CE1	56:Ag:102:CDL:H761	2.55	0.42
48:Ad:242:ILE:HD11	48:Ad:244:MET:HE2	2.02	0.42
49:Ae:177:ARG:HB3	49:Ae:211:VAL:CG1	2.49	0.42
50:Af:95:LEU:O	50:Af:96:LYS:C	2.62	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:81:LEU:HD11	8:H:53:MET:HE1	2.01	0.42
2:B:202:LEU:HD21	9:I:86:TYR:HB3	1.99	0.42
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.50	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
7:G:612:PRO:HG2	22:W:129:HIS:HD2	1.83	0.42
8:H:24:GLU:CD	8:H:195:ARG:HH22	2.27	0.42
8:H:121:TRP:HH2	10:J:27:TYR:HH	1.64	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
9:I:135:ARG:NH1	18:R:61:ILE:HG23	2.27	0.42
10:J:65:VAL:HG13	10:J:66:VAL:N	2.35	0.42
11:K:32:CYS:O	11:K:33:LEU:C	2.60	0.42
12:L:23:MET:HE1	56:L:703:CDL:C36	2.49	0.42
12:L:220:ALA:HB2	12:L:260:LEU:CD1	2.49	0.42
12:L:277:MET:CG	12:L:318:GLY:CA	2.98	0.42
12:L:568:THR:O	12:L:569:LEU:C	2.61	0.42
13:M:77:LEU:O	13:M:81:GLN:HG3	2.19	0.42
13:M:142:ARG:NH2	14:N:303:THR:CG2	2.74	0.42
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.42
14:N:314:MET:CB	15:O:305:LEU:HD11	2.47	0.42
14:N:315:THR:O	14:N:316:HIS:C	2.61	0.42
15:O:49:THR:HG21	15:O:151:LEU:HG	2.01	0.42
15:O:195:LEU:N	15:O:196:PRO:HD2	2.34	0.42
18:R:81:GLY:CA	18:R:88:HIS:CD2	3.02	0.42
23:X:91:TYR:OH	26:a:28:LYS:HE2	2.19	0.42
23:X:143:HIS:ND1	25:Z:115:ARG:HA	2.35	0.42
24:Y:76:THR:CG2	24:Y:92:TYR:HA	2.48	0.42
27:b:45:ILE:HG23	27:b:46:ASN:N	2.34	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CD2	2.55	0.42
39:n:110:SER:O	39:n:113:ALA:HB3	2.20	0.42
39:n:132:SER:O	39:n:133:TRP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:407:MET:HE1	46:AB:415:GLN:CD	2.45	0.42
49:AE:122:THR:CG2	53:AJ:25:ILE:HG21	2.49	0.42
49:AE:178:HIS:CD2	49:AE:179:ARG:N	2.88	0.42
53:AJ:19:SER:HA	54:AK:24:TRP:CH2	2.55	0.42
47:Ac:211:LEU:CD2	50:Af:37:THR:HA	2.49	0.42
48:Ad:231:LEU:HD22	48:Ad:241:ALA:O	2.20	0.42
49:Ae:166:ALA:HB2	49:Ae:175:PHE:HD1	1.84	0.42
53:Aj:21:PHE:O	53:Aj:24:THR:HG22	2.20	0.42
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.49	0.42
2:B:104:MET:HE3	2:B:104:MET:HB2	1.61	0.42
3:C:64:VAL:HG21	3:C:85:ILE:HD11	2.01	0.42
3:C:232:PHE:CE1	7:G:244:GLU:HG3	2.55	0.42
4:D:420:TYR:CD2	21:V:114:TRP:HH2	2.37	0.42
5:E:64:ALA:HA	5:E:67:LYS:HD3	2.02	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:51:TRP:HB2	6:F:133:HIS:O	2.19	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.93	0.42
8:H:113:VAL:HG22	8:H:136:VAL:HG23	2.02	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
55:J:201:3PE:H322	55:J:201:3PE:H381	2.02	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:68:TRP:CZ2	13:M:448:THR:O	2.73	0.42
12:L:81:LYS:HD3	12:L:262:ARG:HH11	1.83	0.42
12:L:396:ILE:HD13	12:L:396:ILE:HA	1.89	0.42
12:L:556:ILE:HG23	38:m:80:PHE:CD2	2.54	0.42
55:L:704:3PE:H322	55:L:704:3PE:H351	1.78	0.42
13:M:118:PHE:HE2	13:M:203:PHE:CE1	2.37	0.42
13:M:123:GLU:OE2	13:M:154:LEU:HD21	2.20	0.42
13:M:162:ILE:HD13	14:N:280:THR:HG23	2.00	0.42
13:M:230:ILE:HG23	13:M:235:LEU:HD11	2.01	0.42
13:M:301:ILE:HG22	13:M:301:ILE:O	2.19	0.42
14:N:154:ILE:HD11	14:N:155:LEU:HG	2.02	0.42
14:N:331:ILE:HG23	14:N:335:MET:HE3	2.01	0.42
14:N:340:ALA:N	14:N:341:PRO:CD	2.83	0.42
16:P:263:PHE:CD2	16:P:333:PRO:O	2.66	0.42
16:P:283:MET:SD	16:P:369:THR:HG21	2.60	0.42
17:Q:75:ARG:NH1	17:Q:104:ARG:HG2	2.34	0.42
19:S:16:LEU:CD1	19:S:19:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:70:LYS:HB3	28:c:75:LEU:HD12	2.02	0.42
32:g:140:PHE:CE2	41:p:74:ILE:HG21	2.52	0.42
34:i:123:PHE:HZ	40:o:65:ARG:HH11	1.67	0.42
38:m:25:VAL:O	45:Aa:261:ALA:CA	2.68	0.42
44:s:53:SER:HA	44:s:56:ARG:HG2	2.02	0.42
48:AD:300:LEU:HB3	56:AG:102:CDL:H552	2.01	0.42
49:AE:112:GLY:O	49:AE:116:LEU:HB2	2.19	0.42
53:AJ:19:SER:HA	54:AK:24:TRP:CZ2	2.55	0.42
45:Aa:58:ARG:CD	45:Aa:417:LEU:HD12	2.50	0.42
46:Ab:163:ALA:HB1	49:Ai:43:LEU:CD2	2.42	0.42
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG23	2.01	0.42
52:Ah:42:VAL:HG23	52:Ah:45:ARG:HH21	1.84	0.42
49:Ai:62:ARG:HB3	49:Ai:63:PRO:HD2	2.00	0.42
49:Ai:71:ASN:OD1	49:Ai:71:ASN:O	2.38	0.42
54:Ak:6:LEU:HA	54:Ak:11:ARG:NH1	2.27	0.42
2:B:70:ARG:HG3	2:B:72:GLU:H	1.85	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:37:TRP:CE3	4:D:37:TRP:O	2.73	0.42
4:D:193:ASP:O	8:H:205:SER:CB	2.67	0.42
4:D:207:ARG:O	4:D:211:PHE:CD1	2.69	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
5:E:226:PRO:HA	6:F:286:CYS:HB3	2.02	0.42
6:F:102:MET:SD	6:F:241:THR:OG1	2.74	0.42
6:F:268:GLU:HG2	6:F:269:ARG:N	2.34	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:65:THR:HG22	16:P:359:TYR:CB	2.50	0.42
8:H:206:GLU:O	8:H:207:LEU:HB2	2.20	0.42
10:J:11:LEU:HD13	10:J:11:LEU:HA	1.93	0.42
11:K:90:VAL:O	11:K:91:GLN:C	2.62	0.42
12:L:21:ILE:HG23	12:L:27:ILE:CG2	2.50	0.42
12:L:203:PHE:CE2	41:p:110:LEU:HD11	2.54	0.42
12:L:346:ILE:HG21	12:L:362:ILE:HD11	2.02	0.42
12:L:365:ILE:CD1	12:L:366:MET:HG3	2.24	0.42
12:L:436:ARG:HB3	39:n:34:ARG:HH11	1.85	0.42
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.01	0.42
13:M:151:PHE:HZ	14:N:291:PHE:HB2	1.75	0.42
13:M:191:SER:O	13:M:194:LEU:HB2	2.20	0.42
14:N:108:LEU:HD22	14:N:191:LEU:HD22	2.02	0.42
14:N:271:MET:HE1	14:N:276:LEU:HB3	2.02	0.42
14:N:314:MET:HB2	15:O:305:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:338:PRO:O	23:X:170:TRP:CZ3	2.73	0.42
15:O:206:TYR:OH	15:O:241:TYR:CB	2.67	0.42
15:O:256:LEU:HD11	15:O:276:LEU:HD21	2.02	0.42
17:Q:58:LYS:O	17:Q:58:LYS:HG3	2.20	0.42
20:T:133:ILE:HG23	20:T:134:ASP:N	2.35	0.42
22:W:28:LEU:O	22:W:32:LYS:HG3	2.20	0.42
27:b:11:ASN:O	27:b:15:LYS:HG2	2.20	0.42
55:b:201:3PE:H2E1	55:b:201:3PE:H2B2	1.80	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CE2	2.54	0.42
32:g:136:GLU:O	41:p:142:ARG:NH1	2.53	0.42
33:h:57:VAL:CG1	39:n:99:VAL:CG2	2.97	0.42
33:h:163:ARG:CG	33:h:165:ASP:HB2	2.33	0.42
33:h:178:PHE:O	33:h:179:ILE:C	2.63	0.42
37:l:48:ARG:NE	37:l:64:PRO:HD2	2.35	0.42
37:l:59:VAL:O	37:l:59:VAL:HG12	2.19	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
43:r:109:ASP:OD1	43:r:110:GLN:N	2.51	0.42
46:AB:272:VAL:HA	46:AB:337:GLY:HA3	2.02	0.42
46:AB:346:ALA:O	46:AB:347:ALA:C	2.62	0.42
46:AB:396:ILE:HG12	46:AB:406:TYR:HE1	1.85	0.42
47:AC:244:LEU:C	48:AD:285:ARG:HH11	2.27	0.42
47:AC:312:GLN:HE21	50:AF:37:THR:HB	1.85	0.42
48:AD:308:ARG:HD3	51:AG:27:PHE:CZ	2.55	0.42
48:AD:317:ARG:HD2	48:AD:319:LEU:HD21	2.02	0.42
49:AE:177:ARG:HB3	49:AE:211:VAL:CG1	2.49	0.42
49:AE:201:ASP:OD1	49:AE:202:LEU:N	2.49	0.42
56:AG:102:CDL:H732	56:AG:102:CDL:H761	1.93	0.42
45:Aa:45:VAL:O	45:Aa:46:PRO:C	2.62	0.42
45:Aa:48:THR:HB	45:Aa:423:ARG:HG2	2.02	0.42
45:Aa:178:SER:OG	45:Aa:181:ASN:ND2	2.53	0.42
46:Ab:39:GLU:HB2	46:Ab:227:HIS:ND1	2.33	0.42
47:Ac:33:PHE:O	47:Ac:36:LEU:HB2	2.19	0.42
47:Ac:242:LEU:HD21	47:Ac:250:LEU:HD11	2.01	0.42
48:Ad:199:TYR:HA	48:Ad:278:SER:OG	2.20	0.42
49:Ae:195:LEU:CD1	49:Ae:248:ARG:HD2	2.50	0.42
49:Ae:249:ILE:HG12	49:Ae:254:ALA:HB3	2.01	0.42
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.42
3:C:224:GLU:OE1	17:Q:118:ALA:HB2	2.20	0.42
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.42
4:D:354:GLY:O	43:r:42:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:361:ALA:HB3	7:G:149:ASP:HB3	2.01	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.42
9:I:123:CYS:SG	57:I:302:SF4:S2	3.17	0.42
10:J:80:GLU:HA	16:P:360:ARG:CG	2.50	0.42
11:K:1:MET:O	11:K:5:PHE:HB2	2.20	0.42
12:L:117:PHE:HZ	12:L:242:PRO:HG2	1.85	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
13:M:150:LEU:CD2	14:N:294:THR:HG21	2.50	0.42
14:N:215:MET:SD	14:N:244:ILE:CD1	3.08	0.42
15:O:207:ILE:HA	15:O:258:TYR:O	2.20	0.42
16:P:99:ASP:HB3	16:P:102:GLN:CD	2.45	0.42
16:P:207:PHE:O	16:P:241:TYR:HA	2.20	0.42
16:P:243:ALA:O	16:P:244:ASP:C	2.62	0.42
16:P:284:THR:HG22	16:P:286:ARG:HG3	2.02	0.42
20:T:138:LEU:HD11	20:T:147:TYR:CD2	2.54	0.42
20:U:113:LEU:HD23	39:n:17:LEU:HD21	2.02	0.42
24:Y:101:LEU:O	24:Y:102:THR:C	2.63	0.42
26:a:64:LYS:CE	26:a:66:LEU:HD12	2.31	0.42
27:b:15:LYS:O	27:b:16:GLU:HB2	2.20	0.42
29:d:24:PRO:HD2	29:d:73:TYR:CE2	2.55	0.42
33:h:55:PHE:HE1	33:h:57:VAL:HA	1.85	0.42
37:l:169:GLU:OE2	40:o:43:GLN:HG2	2.20	0.42
39:n:149:ILE:HD12	39:n:149:ILE:N	2.31	0.42
45:AA:358:PHE:CD2	45:AA:368:MET:HG2	2.54	0.42
48:AD:202:ARG:HG3	48:AD:278:SER:HB3	2.02	0.42
46:Ab:70:ARG:NH2	46:Ab:332:ASP:OD2	2.53	0.42
46:Ab:346:ALA:O	46:Ab:347:ALA:C	2.61	0.42
47:Ac:133:LEU:HD23	47:Ac:133:LEU:HA	1.85	0.42
49:Ae:160:PRO:C	49:Ae:178:HIS:HB3	2.45	0.42
49:Ae:205:VAL:CG1	49:Ae:211:VAL:HG23	2.49	0.42
1:A:48:ARG:HG2	10:J:77:GLU:OE1	2.19	0.41
4:D:170:ILE:CD1	4:D:236:LEU:HD11	2.49	0.41
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.55	0.41
5:E:131:ILE:HD13	5:E:151:LEU:HD21	2.02	0.41
6:F:69:LEU:CD1	6:F:143:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.54	0.41
8:H:196:ALA:O	8:H:279:ARG:HG2	2.19	0.41
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.41
10:J:14:VAL:O	10:J:15:GLY:C	2.63	0.41
12:L:489:THR:O	12:L:492:ILE:HG13	2.20	0.41
13:M:216:LEU:CG	13:M:220:HIS:CE1	2.88	0.41
13:M:263:LEU:CD1	38:m:102:TYR:HB2	2.50	0.41
55:M:501:3PE:H362	55:M:501:3PE:H331	1.82	0.41
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.50	0.41
14:N:180:ALA:O	14:N:184:ILE:HG13	2.20	0.41
15:O:43:ALA:O	15:O:48:LYS:HE3	2.20	0.41
15:O:165:SER:HB3	15:O:245:PHE:CE2	2.55	0.41
20:U:93:ILE:CD1	20:U:110:LEU:HD11	2.49	0.41
21:V:36:LYS:HA	21:V:36:LYS:HD3	1.89	0.41
22:W:23:ILE:CG2	22:W:83:ASP:HB2	2.50	0.41
22:W:53:MET:SD	22:W:106:VAL:HG21	2.60	0.41
22:W:78:ASP:HA	22:W:79:PRO:HD3	1.94	0.41
23:X:141:PRO:C	23:X:143:HIS:H	2.27	0.41
27:b:31:ILE:O	27:b:32:MET:C	2.63	0.41
27:b:69:HIS:HB3	27:b:72:ASP:CG	2.45	0.41
56:d:201:CDL:H551	56:d:201:CDL:H731	2.02	0.41
40:o:59:CYS:SG	40:o:91:GLU:HG2	2.60	0.41
41:p:31:THR:HG23	41:p:32:TYR:N	2.35	0.41
56:q:201:CDL:H511	43:r:8:ILE:HD11	2.01	0.41
45:AA:48:THR:CB	45:AA:423:ARG:HG2	2.50	0.41
45:AA:479:ARG:O	54:AK:20:THR:HG21	2.20	0.41
47:AC:18:PHE:CE1	69:AC:406:UQ6:C7	3.03	0.41
47:AC:141:TRP:CH2	49:Ae:223:VAL:HG23	2.55	0.41
47:AC:148:ASN:OD1	49:Ae:221:GLY:CA	2.65	0.41
48:AD:95:PRO:HG2	52:AH:85:PHE:HB2	2.02	0.41
48:AD:323:PRO:HB2	48:AD:325:LYS:HG3	2.02	0.41
49:AE:156:LEU:N	49:AE:269:ASP:O	2.53	0.41
45:Aa:204:PRO:O	45:Aa:205:SER:C	2.63	0.41
45:Aa:340:SER:O	45:Aa:358:PHE:HA	2.20	0.41
48:Ad:146:LYS:NZ	48:Ad:169:GLY:O	2.48	0.41
50:Af:102:ARG:HA	50:Af:105:ARG:CZ	2.49	0.41
51:Ag:78:TYR:CD1	52:Ah:63:GLU:HG3	2.55	0.41
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.34	0.41
4:D:159:LEU:CD2	43:r:60:ARG:HG3	2.50	0.41
4:D:211:PHE:O	4:D:212:GLU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:ILE:HD13	5:E:84:LEU:HD13	2.01	0.41
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:360:LYS:HB3	7:G:632:ILE:HB	2.01	0.41
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
10:J:114:VAL:HG12	11:K:3:SER:OG	2.21	0.41
10:J:125:MET:C	25:Z:121:ILE:HD11	2.45	0.41
11:K:1:MET:SD	14:N:79:LYS:HD2	2.60	0.41
12:L:44:PHE:CE1	62:L:701:PC1:H143	2.54	0.41
12:L:293:LEU:O	12:L:425:ARG:HD2	2.20	0.41
12:L:390:TYR:CE2	35:j:68:TRP:HH2	2.39	0.41
12:L:407:TRP:CE3	12:L:410:LEU:HD21	2.55	0.41
13:M:105:LEU:CD2	56:M:503:CDL:H411	2.48	0.41
13:M:270:ILE:HD12	13:M:395:LEU:HD22	2.02	0.41
13:M:442:ILE:HG23	56:h:201:CDL:H832	2.01	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
16:P:279:TYR:O	16:P:280:ILE:C	2.62	0.41
20:T:93:ILE:CD1	20:T:108:LEU:HD22	2.49	0.41
20:U:128:PHE:HZ	20:U:148:ILE:CD1	2.33	0.41
23:X:48:TRP:NE1	27:b:55:VAL:HG22	2.32	0.41
32:g:117:ARG:NH2	41:p:108:GLU:OE1	2.53	0.41
33:h:182:SER:O	33:h:184:LYS:HE3	2.20	0.41
34:i:20:ARG:HH11	34:i:20:ARG:HG3	1.84	0.41
35:j:44:TYR:CD2	35:j:45:ARG:HG3	2.55	0.41
37:l:159:LYS:HE3	37:l:161:TYR:HE1	1.86	0.41
38:m:8:PRO:HD3	38:m:14:LEU:HD13	2.03	0.41
39:n:56:ASP:O	39:n:59:ARG:N	2.53	0.41
39:n:114:MET:HG3	39:n:115:TYR:CD2	2.55	0.41
41:p:11:PRO:HD2	41:p:109:ARG:NE	2.35	0.41
41:p:30:ILE:CG1	41:p:31:THR:N	2.81	0.41
46:AB:138:LEU:HD22	46:AB:238:LEU:HG	2.01	0.41
49:AE:231:PHE:CD2	49:AE:250:ARG:NH1	2.88	0.41
45:Aa:80:ARG:NH2	45:Aa:268:CYS:SG	2.93	0.41
45:Aa:338:CYS:SG	45:Aa:359:VAL:O	2.79	0.41
46:Ab:185:ALA:HB3	46:Ab:251:ALA:HB2	2.01	0.41
47:Ac:284:ILE:HG21	47:Ac:289:GLY:HA3	2.02	0.41
48:Ad:223:THR:OG1	52:Ah:55:VAL:HB	2.20	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:VAL:O	3:C:56:GLN:HG3	2.20	0.41
4:D:144:MET:SD	4:D:144:MET:N	2.93	0.41
4:D:179:ARG:CG	4:D:183:HIS:CD2	3.04	0.41
5:E:183:PRO:O	5:E:194:ASP:N	2.53	0.41
6:F:102:MET:HG3	6:F:149:MET:HB2	2.02	0.41
6:F:268:GLU:CG	6:F:269:ARG:H	2.32	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
7:G:639:LEU:C	7:G:641:GLN:N	2.77	0.41
7:G:639:LEU:O	7:G:641:GLN:N	2.54	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.55	0.41
8:H:312:ALA:CB	27:b:41:TYR:HB2	2.50	0.41
9:I:48:VAL:CG1	9:I:53:ALA:HB2	2.50	0.41
9:I:184:LEU:CD2	17:Q:114:TRP:CH2	3.03	0.41
12:L:231:PRO:O	12:L:234:PRO:HD2	2.19	0.41
13:M:85:LYS:O	13:M:85:LYS:HG2	2.21	0.41
13:M:258:ALA:O	13:M:259:TYR:C	2.62	0.41
13:M:270:ILE:HD11	13:M:395:LEU:HA	2.03	0.41
14:N:218:ALA:CB	14:N:240:MET:SD	3.08	0.41
14:N:285:MET:HE1	14:N:288:LEU:HD22	2.03	0.41
15:O:60:ILE:O	15:O:158:VAL:HA	2.19	0.41
16:P:214:LEU:HD23	16:P:352:VAL:HG12	2.01	0.41
16:P:230:SER:O	16:P:231:LEU:C	2.63	0.41
16:P:255:ASP:OD1	16:P:256:PRO:HD2	2.21	0.41
16:P:283:MET:HE3	16:P:357:ARG:NH1	2.35	0.41
25:Z:10:MET:HB3	25:Z:10:MET:HE2	1.75	0.41
25:Z:104:TRP:CH2	30:e:75:ARG:HG2	2.55	0.41
26:a:49:GLU:OE2	26:a:49:GLU:HA	2.20	0.41
28:c:74:GLY:O	28:c:75:LEU:HB2	2.20	0.41
34:i:22:TRP:CE3	39:n:125:TRP:CD1	3.08	0.41
55:i:201:3PE:O22	55:i:201:3PE:H11	2.20	0.41
36:k:42:LEU:HG	39:n:39:TYR:HD1	1.85	0.41
38:m:53:ASP:C	38:m:54:PRO:O	2.63	0.41
40:o:5:LEU:HD12	40:o:5:LEU:N	2.35	0.41
40:o:31:PHE:HA	40:o:32:PRO:HD3	1.98	0.41
40:o:53:LEU:HD23	40:o:56:ARG:NE	2.34	0.41
45:AA:148:ALA:O	45:AA:152:GLN:HG2	2.20	0.41
45:AA:338:CYS:SG	45:AA:359:VAL:O	2.78	0.41
47:AC:18:PHE:CZ	69:AC:406:UQ6:C1M	3.03	0.41
47:AC:256:TYR:CD2	48:AD:202:ARG:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:316:MET:HE2	55:AC:404:3PE:H122	2.03	0.41
48:AD:210:TYR:O	48:AD:211:VAL:C	2.63	0.41
48:AD:299:LEU:HD22	49:AE:121:THR:HG23	2.01	0.41
49:AE:105:GLU:H	49:AE:105:GLU:HG3	1.69	0.41
49:AE:115:TYR:HB3	53:AJ:21:PHE:HE1	1.85	0.41
49:AE:172:LYS:HE2	49:AE:172:LYS:HA	2.02	0.41
50:AF:108:TRP:CE2	46:Ab:101:ARG:HB3	2.55	0.41
51:AG:28:PRO:O	51:AG:29:SER:C	2.63	0.41
52:AH:26:ASP:C	52:AH:28:LEU:N	2.77	0.41
47:Ac:153:ILE:HB	47:Ac:157:GLY:HA2	2.01	0.41
48:Ad:159:ASN:HB2	48:Ad:163:GLU:O	2.20	0.41
48:Ad:201:VAL:HG22	48:Ad:278:SER:HB2	2.00	0.41
48:Ad:210:TYR:O	48:Ad:211:VAL:C	2.63	0.41
48:Ad:252:VAL:HG13	48:Ad:253:LEU:N	2.34	0.41
49:Ae:154:ILE:HD12	49:Ae:154:ILE:N	2.34	0.41
49:Ae:155:LYS:HB3	49:Ae:158:ASP:CG	2.45	0.41
51:Ag:73:LYS:HB3	52:Ah:67:GLU:OE2	2.20	0.41
1:A:4:TYR:HH	10:J:4:TYR:HE1	1.67	0.41
1:A:72:LEU:HB3	8:H:151:LEU:HD21	2.02	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
4:D:179:ARG:HG3	4:D:183:HIS:NE2	2.34	0.41
4:D:267:ILE:CD1	8:H:280:PHE:CE1	3.03	0.41
4:D:353:PRO:HB3	25:Z:10:MET:SD	2.60	0.41
6:F:77:LEU:HD13	6:F:100:SER:HA	2.03	0.41
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.36	0.41
6:F:147:ARG:HD3	6:F:191:TYR:HD2	1.72	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:53:CYS:SG	7:G:102:ILE:HG21	2.60	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:282:ASN:HB2	7:G:285:TRP:O	2.20	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.56	0.41
9:I:79:ARG:NH2	43:r:20:LEU:HD22	2.34	0.41
10:J:52:GLY:O	10:J:55:VAL:N	2.54	0.41
10:J:99:GLU:O	10:J:100:VAL:C	2.62	0.41
12:L:286:LEU:HG	12:L:290:ILE:HD11	2.01	0.41
13:M:173:THR:CG2	33:h:147:ALA:CA	2.99	0.41
13:M:319:HIS:HA	13:M:322:THR:CG2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:64:GLY:O	15:O:161:ARG:NH1	2.53	0.41
19:S:23:LEU:O	19:S:57:GLU:HA	2.20	0.41
19:S:36:PHE:HZ	19:S:44:LEU:HD12	1.86	0.41
20:T:133:ILE:HG13	20:T:137:LYS:NZ	2.36	0.41
23:X:132:LYS:HB3	23:X:132:LYS:HE2	1.84	0.41
24:Y:10:SER:O	24:Y:11:TYR:C	2.63	0.41
27:b:25:VAL:O	27:b:26:TRP:C	2.64	0.41
30:e:75:ARG:O	30:e:79:ILE:HG13	2.20	0.41
32:g:140:PHE:HB3	41:p:75:THR:CG2	2.49	0.41
35:j:52:ARG:HG2	35:j:56:ILE:HD12	2.02	0.41
38:m:42:ARG:O	38:m:43:LEU:C	2.62	0.41
40:o:21:LYS:O	40:o:24:SER:HB3	2.20	0.41
42:q:87:HIS:O	42:q:91:HIS:HD2	2.04	0.41
43:r:41:LEU:N	43:r:41:LEU:HD22	2.35	0.41
46:AB:38:LEU:HD13	46:AB:52:LEU:HB2	2.02	0.41
47:AC:77:TRP:CD2	48:AD:281:GLU:HG3	2.55	0.41
69:AC:406:UQ6:H171	69:AC:406:UQ6:H151	1.68	0.41
48:AD:99:ARG:HA	48:AD:99:ARG:HD3	1.94	0.41
47:Ac:171:ASP:CG	47:Ac:172:LYS:N	2.76	0.41
48:Ad:202:ARG:HG3	48:Ad:278:SER:HB3	2.02	0.41
48:Ad:297:GLY:O	48:Ad:301:PRO:HG2	2.20	0.41
1:A:104:TYR:HA	1:A:107:THR:OG1	2.21	0.41
2:B:144:ALA:O	2:B:147:LYS:N	2.54	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.49	0.41
4:D:149:GLN:NE2	4:D:309:ASP:OD2	2.53	0.41
6:F:54:LYS:HG3	6:F:55:GLY:H	1.85	0.41
6:F:427:LEU:HB2	60:F:501:FMN:HM71	2.02	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
8:H:13:ILE:HD13	8:H:13:ILE:HA	1.87	0.41
8:H:23:VAL:HG11	26:a:9:LEU:HD21	2.02	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:41:LYS:HD3	43:r:112:TYR:HE2	1.85	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
9:I:140:ARG:O	9:I:141:ARG:HG2	2.21	0.41
12:L:202:MET:HE3	12:L:265:PRO:CB	2.50	0.41
13:M:4:ILE:CD1	13:M:41:LEU:HD21	2.51	0.41
13:M:175:ASN:CB	33:h:143:GLU:HG2	2.50	0.41
13:M:247:SER:OG	13:M:304:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:THR:HG22	14:N:84:TRP:N	2.35	0.41
15:O:80:GLN:HG3	15:O:270:VAL:HG21	2.02	0.41
15:O:206:TYR:CG	15:O:246:LEU:HD21	2.56	0.41
15:O:211:VAL:O	15:O:214:VAL:HG22	2.20	0.41
16:P:295:LEU:O	16:P:298:TYR:N	2.53	0.41
17:Q:59:LEU:HD23	17:Q:59:LEU:HA	1.84	0.41
18:R:38:TYR:CD2	18:R:48:PHE:CE2	3.08	0.41
20:T:93:ILE:HD13	20:T:108:LEU:CD2	2.51	0.41
22:W:86:VAL:O	22:W:87:ILE:C	2.61	0.41
23:X:17:GLU:HG3	23:X:64:ASN:ND2	2.34	0.41
23:X:41:LYS:HD2	27:b:56:PRO:HG3	2.01	0.41
23:X:90:ASP:OD2	26:a:62:VAL:HG11	2.21	0.41
26:a:49:GLU:O	26:a:50:ARG:C	2.62	0.41
27:b:78:LEU:O	27:b:81:LEU:N	2.53	0.41
29:d:93:TYR:HD2	33:h:156:VAL:HG13	1.86	0.41
32:g:69:PRO:HB2	39:n:109:PRO:CD	2.50	0.41
32:g:71:PHE:CE2	32:g:73:GLY:HA2	2.55	0.41
37:l:48:ARG:NH2	37:l:64:PRO:HD2	2.36	0.41
37:l:122:THR:HG22	37:l:124:VAL:H	1.85	0.41
38:m:124:LYS:O	38:m:126:ASN:N	2.54	0.41
41:p:71:VAL:HB	41:p:72:PRO:CD	2.50	0.41
42:q:110:TRP:HB2	42:q:113:HIS:CE1	2.55	0.41
47:AC:295:ILE:HG22	47:AC:299:LEU:HD12	2.02	0.41
50:AF:105:ARG:HA	46:Ab:97:PHE:CE2	2.56	0.41
45:Aa:120:LEU:CD2	46:Ab:299:ILE:HG23	2.48	0.41
45:Aa:388:VAL:HG21	45:Aa:438:ALA:HA	2.02	0.41
46:Ab:138:LEU:HD22	46:Ab:238:LEU:HG	2.02	0.41
46:Ab:286:PHE:CD1	46:Ab:427:ALA:HB1	2.54	0.41
47:Ac:295:ILE:HG22	47:Ac:299:LEU:HD12	2.02	0.41
49:Ae:173:PRO:HG2	49:Ae:223:VAL:CG2	2.45	0.41
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.55	0.41
3:C:232:PHE:HE2	9:I:126:GLN:OE1	2.04	0.41
4:D:70:ASP:OD2	11:K:95:LEU:HD13	2.20	0.41
4:D:71:ILE:O	4:D:72:LEU:C	2.62	0.41
4:D:268:TRP:O	4:D:269:ARG:C	2.63	0.41
5:E:167:LEU:HB3	5:E:168:PHE:CD1	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
7:G:126:LEU:HD11	18:R:89:PRO:CB	2.47	0.41
7:G:161:GLU:OE2	18:R:96:ASP:N	2.53	0.41
7:G:617:ARG:NH1	22:W:129:HIS:CA	2.84	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:PRO:HD3	8:H:273:ILE:HG22	2.03	0.41
9:I:82:ALA:CA	43:r:26:LEU:HD21	2.50	0.41
12:L:368:PHE:HB3	12:L:445:GLU:OE1	2.20	0.41
13:M:177:MET:HB3	13:M:177:MET:HE3	1.70	0.41
13:M:198:ALA:HB2	55:M:501:3PE:H331	2.03	0.41
14:N:159:ILE:HB	14:N:278:MET:HE1	2.01	0.41
14:N:168:GLY:HA3	14:N:181:TYR:CE1	2.56	0.41
15:O:54:HIS:CE1	15:O:56:TYR:H	2.39	0.41
15:O:143:TYR:HD1	15:O:159:LEU:HD22	1.85	0.41
15:O:200:PRO:HG3	15:O:282:PRO:CD	2.47	0.41
15:O:263:ALA:C	15:O:265:ASP:N	2.77	0.41
21:V:94:MET:SD	21:V:99:PRO:HG3	2.60	0.41
23:X:120:PRO:HG3	27:b:71:GLN:HE21	1.86	0.41
27:b:49:THR:HA	27:b:50:PRO:HD3	1.89	0.41
30:e:49:GLY:O	30:e:52:ALA:N	2.53	0.41
33:h:175:GLU:HB2	33:h:178:PHE:CE2	2.55	0.41
37:l:32:MET:HG2	37:l:36:MET:CE	2.51	0.41
41:p:91:GLN:O	41:p:91:GLN:HG2	2.21	0.41
45:AA:478:LEU:O	54:AK:24:TRP:HZ2	2.04	0.41
47:AC:77:TRP:HZ2	48:AD:284:HIS:HD2	1.68	0.41
47:AC:284:ILE:HG21	47:AC:289:GLY:HA3	2.02	0.41
49:AE:160:PRO:C	49:AE:178:HIS:HB3	2.45	0.41
45:Aa:281:ALA:HA	51:Ag:10:ARG:HH12	1.85	0.41
46:Ab:407:MET:HE1	46:Ab:415:GLN:CD	2.45	0.41
48:Ad:247:PRO:O	48:Ad:248:ILE:HD13	2.21	0.41
49:Ae:172:LYS:HA	49:Ae:172:LYS:HE2	2.02	0.41
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG21	2.03	0.41
49:Ae:244:ASP:OD2	49:Ae:248:ARG:NE	2.54	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.91	0.41
2:B:154:GLU:O	2:B:156:ARG:N	2.52	0.41
4:D:50:ALA:C	4:D:51:VAL:HG13	2.45	0.41
4:D:270:ASN:HB2	8:H:284:GLN:OE1	2.20	0.41
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.21	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:66:LYS:NZ	6:F:189:SER:CA	2.79	0.41
6:F:384:PRO:HA	7:G:119:PHE:CD2	2.54	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:667:GLN:HB3	19:S:42:VAL:HG13	2.01	0.41
8:H:14:LEU:HD13	8:H:83:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:MET:SD	8:H:225:MET:C	3.03	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
9:I:92:PRO:HB3	42:q:92:CYS:HB2	2.02	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:162:CYS:SG	57:I:303:SF4:S2	3.19	0.41
12:L:253:VAL:HB	12:L:310:LEU:CD1	2.50	0.41
12:L:571:THR:O	12:L:574:THR:HG22	2.20	0.41
13:M:22:LYS:HE3	13:M:26:ASN:HD21	1.86	0.41
13:M:142:ARG:HG3	13:M:143:LEU:N	2.36	0.41
13:M:177:MET:HE2	33:h:140:LEU:HD21	2.02	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.02	0.41
13:M:250:LEU:HD12	13:M:250:LEU:C	2.39	0.41
14:N:191:LEU:HG	14:N:191:LEU:O	2.20	0.41
15:O:117:PHE:CZ	15:O:173:MET:HE3	2.55	0.41
15:O:354:LEU:HD12	15:O:354:LEU:HA	1.95	0.41
20:T:93:ILE:HG23	20:T:108:LEU:HD13	2.03	0.41
21:V:96:LYS:HE2	21:V:96:LYS:HB2	1.95	0.41
23:X:37:ASP:OD1	23:X:37:ASP:C	2.62	0.41
23:X:142:TYR:OH	33:h:189:ASN:HB2	2.21	0.41
23:X:142:TYR:O	23:X:143:HIS:C	2.62	0.41
33:h:141:GLN:HB2	41:p:83:LEU:HD21	2.02	0.41
40:o:117:LEU:CD2	40:o:118:LYS:CE	2.99	0.41
45:AA:340:SER:O	45:AA:358:PHE:HA	2.20	0.41
46:AB:261:GLN:HG2	46:Ab:77:LEU:HD12	2.02	0.41
47:AC:354:ALA:HA	55:AG:103:3PE:H2H2	2.02	0.41
49:AE:159:ILE:HG23	49:AE:163:LYS:HB3	2.03	0.41
54:AK:45:VAL:HB	54:AK:48:ILE:CG2	2.50	0.41
46:Ab:426:LYS:HA	46:Ab:429:LYS:NZ	2.36	0.41
47:Ac:220:PHE:CD2	69:Ac:405:UQ6:H3M3	2.55	0.41
47:Ac:278:TYR:CE2	47:Ac:282:ARG:HD2	2.55	0.41
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HB3	2.03	0.41
51:Ag:28:PRO:O	51:Ag:29:SER:C	2.63	0.41
49:Ai:71:ASN:C	49:Ai:73:PRO:HD2	2.45	0.41
2:B:92:PRO:HG3	2:B:119:VAL:HG12	2.02	0.41
2:B:95:PHE:HD2	2:B:141:MET:HE3	1.86	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG22	2.00	0.41
4:D:326:CYS:SG	4:D:453:THR:HG21	2.61	0.41
5:E:176:LEU:HB3	5:E:191:TYR:OH	2.20	0.41
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.86	0.41
6:F:69:LEU:HD11	6:F:143:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:102:ILE:O	7:G:103:LEU:C	2.60	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:J:122:ASP:OD1	10:J:123:TRP:CD1	2.74	0.41
11:K:25:HIS:CD2	11:K:88:ASP:OD1	2.70	0.41
12:L:258:PHE:O	12:L:261:VAL:HG22	2.21	0.41
12:L:321:GLN:NE2	12:L:324:LEU:HD13	2.36	0.41
12:L:570:HIS:O	12:L:573:MET:N	2.54	0.41
13:M:178:ILE:O	13:M:179:LEU:C	2.60	0.41
13:M:350:MET:HE3	13:M:350:MET:HB2	1.80	0.41
14:N:175:MET:O	14:N:176:ARG:C	2.63	0.41
14:N:307:THR:CG2	14:N:308:ASN:N	2.79	0.41
15:O:287:ASP:HB3	15:O:290:THR:HG23	2.02	0.41
15:O:323:GLN:HE21	32:g:55:GLU:CA	2.31	0.41
16:P:88:VAL:HG12	16:P:92:MET:HE2	2.02	0.41
18:R:44:ARG:O	18:R:47:ARG:HB2	2.21	0.41
20:U:142:GLN:C	20:U:144:ILE:N	2.78	0.41
23:X:45:LEU:HD21	27:b:58:ARG:HE	1.86	0.41
28:c:55:TRP:NE1	29:d:66:THR:HG22	2.34	0.41
29:d:25:LYS:HE3	29:d:27:ASN:OD1	2.21	0.41
34:i:110:ILE:HD11	34:i:117:ILE:HD11	2.03	0.41
35:j:47:PHE:O	35:j:48:PRO:C	2.62	0.41
35:j:92:TRP:CE3	40:o:100:LYS:HA	2.53	0.41
40:o:113:LYS:O	40:o:117:LEU:HB2	2.21	0.41
42:q:120:THR:HA	42:q:121:PRO:HD3	1.83	0.41
43:r:54:TYR:CD1	43:r:57:ARG:HG3	2.56	0.41
45:AA:178:SER:OG	45:AA:181:ASN:ND2	2.53	0.41
45:AA:388:VAL:HG21	45:AA:438:ALA:HA	2.02	0.41
67:AC:403:HEM:HBA1	69:AC:406:UQ6:O4	2.20	0.41
48:AD:115:GLN:HE22	48:AD:256:ASP:CG	2.29	0.41
48:AD:235:PRO:HA	48:AD:240:GLN:CG	2.50	0.41
50:AF:108:TRP:CH2	46:Ab:101:ARG:HB3	2.55	0.41
51:AG:26:ALA:C	51:AG:28:PRO:HD3	2.46	0.41
49:AI:71:ASN:C	49:AI:73:PRO:HD2	2.45	0.41
45:Aa:384:THR:HA	54:Ak:12:GLU:OE2	2.20	0.41
56:Aa:502:CDL:H362	56:Aa:502:CDL:H332	1.90	0.41
46:Ab:233:VAL:HA	46:Ab:236:GLN:CG	2.47	0.41
46:Ab:297:PRO:CB	46:Ab:304:ASN:OD1	2.69	0.41
47:Ac:105:GLY:HA3	47:Ac:313:ARG:O	2.21	0.41
47:Ac:128:PHE:CD1	68:Ac:404:U10:C4M	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:317:PHE:CD1	50:Af:27:PHE:HB3	2.55	0.41
47:Ac:326:TRP:NE1	51:Ag:49:VAL:HG22	2.36	0.41
49:Ae:231:PHE:CD2	49:Ae:250:ARG:NH1	2.88	0.41
54:Ak:12:GLU:HA	54:Ak:15:ARG:HD3	2.02	0.41
54:Ak:41:ILE:HD12	54:Ak:41:ILE:N	2.36	0.41
1:A:67:LEU:O	1:A:70:ALA:HB3	2.21	0.41
2:B:71:ALA:O	2:B:75:VAL:HG23	2.21	0.41
3:C:216:LYS:HG3	16:P:209:ARG:HH11	1.85	0.41
3:C:241:PHE:HB3	3:C:242:PRO:HD2	2.03	0.41
4:D:216:ARG:NH2	4:D:240:LEU:HA	2.36	0.41
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.41
4:D:322:SER:OG	4:D:323:ARG:HG3	2.20	0.41
5:E:182:ALA:O	5:E:183:PRO:C	2.59	0.41
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.41
6:F:309:GLY:HA3	6:F:313:ASN:HD22	1.85	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:544:MET:HE2	7:G:546:PHE:CZ	2.55	0.41
7:G:674:LEU:HD11	19:S:46:LYS:HE2	2.03	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.49	0.41
8:H:130:PHE:HD2	8:H:207:LEU:HD11	1.86	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41
55:H:402:3PE:H342	9:I:63:TRP:CZ2	2.55	0.41
10:J:28:GLY:C	11:K:31:LEU:HD21	2.46	0.41
10:J:124:LEU:HD23	25:Z:137:ASN:HD21	1.86	0.41
12:L:58:ASN:HA	12:L:58:ASN:HD22	1.65	0.41
12:L:211:ILE:N	12:L:212:PRO:CD	2.82	0.41
12:L:525:LEU:CD2	39:n:77:PRO:HB3	2.45	0.41
55:L:704:3PE:O31	55:L:704:3PE:H232	2.21	0.41
13:M:6:LEU:O	13:M:7:PRO:C	2.60	0.41
13:M:71:TRP:CZ3	32:g:96:VAL:HG11	2.55	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:278:ARG:NH2	37:l:108:ASP:CB	2.84	0.41
13:M:329:LEU:HD23	13:M:437:MET:CE	2.49	0.41
13:M:388:TRP:CD1	38:m:109:ARG:CD	3.04	0.41
14:N:109:ALA:O	14:N:112:HIS:ND1	2.52	0.41
14:N:125:HIS:CE1	14:N:129:ILE:HD11	2.56	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)
14:N:308:ASN:HB3	15:O:317:ILE:HG22	2.03	0.41
14:N:316:HIS:HA	15:O:331:PHE:CZ	2.55	0.41
15:O:105:ASP:OD1	15:O:106:ILE:N	2.54	0.41
15:O:248:LYS:O	15:O:252:MET:HE2	2.21	0.41
15:O:332:ARG:O	15:O:338:LYS:HA	2.21	0.41
16:P:265:PHE:CD1	16:P:265:PHE:N	2.87	0.41
16:P:359:TYR:HA	16:P:362:LEU:HG	2.02	0.41
18:R:79:CYS:O	18:R:88:HIS:CE1	2.74	0.41
20:T:110:LEU:HG	20:T:114:ASP:HB3	1.98	0.41
20:U:155:TYR:HB3	34:i:23:LEU:HB2	2.02	0.41
23:X:20:VAL:CG1	23:X:24:VAL:HB	2.51	0.41
24:Y:5:LYS:C	24:Y:7:PHE:N	2.77	0.41
24:Y:87:ASP:OD1	24:Y:87:ASP:N	2.49	0.41
56:Y:202:CDL:CB5	56:Y:202:CDL:H541	2.50	0.41
56:Y:202:CDL:H761	56:Y:202:CDL:H722	2.03	0.41
25:Z:142:TRP:C	25:Z:143:TYR:CD2	2.99	0.41
27:b:16:GLU:N	27:b:17:PRO:HD3	2.35	0.41
30:e:38:LYS:HG2	33:h:179:ILE:HG21	2.03	0.41
30:e:49:GLY:HA2	30:e:52:ALA:HB3	2.02	0.41
31:f:36:ALA:O	31:f:37:PHE:C	2.61	0.41
31:f:39:ASN:HA	33:h:134:GLU:OE2	2.21	0.41
36:k:20:MET:HE2	36:k:20:MET:HB3	1.98	0.41
37:l:44:THR:HG23	37:l:46:GLU:HG2	2.03	0.41
37:l:63:GLU:O	37:l:64:PRO:C	2.64	0.41
37:l:155:PRO:HG3	40:o:4:HIS:CG	2.56	0.41
37:l:184:TYR:CD1	40:o:34:ARG:HG3	2.55	0.41
38:m:23:TYR:HB2	39:n:65:ARG:HE	1.86	0.41
39:n:157:ALA:O	39:n:158:ARG:HB2	2.21	0.41
40:o:20:GLU:O	40:o:21:LYS:HB2	2.21	0.41
40:o:71:ARG:NH1	40:o:72:ASP:OD1	2.54	0.41
40:o:75:PRO:CD	41:p:28:ASN:OD1	2.52	0.41
41:p:73:ASP:OD1	41:p:91:GLN:CD	2.64	0.41
42:q:78:ASP:OD1	42:q:78:ASP:O	2.39	0.41
45:AA:62:GLU:OE1	45:AA:423:ARG:NH1	2.45	0.41
45:AA:384:THR:HG21	54:AK:9:ARG:CG	2.51	0.41
46:AB:225:VAL:HG22	46:AB:229:VAL:HG21	2.01	0.41
47:AC:275:LEU:O	47:AC:276:PHE:C	2.64	0.41
47:AC:378:LYS:HE3	50:AF:89:PHE:CE2	2.51	0.41
49:AE:244:ASP:OD2	49:AE:248:ARG:NE	2.54	0.41
51:AG:35:ILE:O	51:AG:36:PRO:C	2.63	0.41
49:AI:71:ASN:OD1	49:AI:71:ASN:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AK:6:LEU:HA	54:AK:11:ARG:NH1	2.27	0.41
45:Aa:170:ARG:HG3	45:Aa:171:GLU:N	2.36	0.41
47:Ac:227:LYS:HG3	48:Ad:307:LYS:HE3	2.02	0.41
48:Ad:110:ILE:HB	48:Ad:139:CYS:SG	2.61	0.41
48:Ad:125:HIS:HB3	48:Ad:197:LEU:HG	2.03	0.41
48:Ad:242:ILE:CD1	48:Ad:244:MET:HE2	2.51	0.41
49:Ae:115:TYR:CE1	62:Ae:301:PC1:H122	2.55	0.41
49:Ae:156:LEU:HD12	49:Ae:268:ASP:HA	2.03	0.41
49:Ae:178:HIS:CD2	49:Ae:179:ARG:N	2.88	0.41
49:Ae:216:VAL:HG13	49:Ae:221:GLY:HA2	2.03	0.41
50:Af:101:GLU:O	50:Af:105:ARG:HG3	2.21	0.41
51:Ag:26:ALA:C	51:Ag:28:PRO:HD3	2.46	0.41
51:Ag:57:TYR:O	51:Ag:61:THR:HG23	2.21	0.41
52:Ah:26:ASP:C	52:Ah:28:LEU:N	2.77	0.41
56:A:402:CDL:H822	56:A:402:CDL:OB4	2.21	0.41
4:D:92:HIS:CD2	58:D:501:UQ1:C3	3.04	0.41
4:D:398:THR:O	4:D:398:THR:HG23	2.20	0.41
6:F:303:HIS:O	6:F:304:ALA:HB3	2.20	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
6:F:418:GLN:NE2	43:r:53:TYR:OH	2.53	0.41
7:G:44:GLU:O	7:G:47:THR:HG23	2.21	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:127:ASP:HA	18:R:106:TYR:OH	2.20	0.41
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.26	0.41
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.41
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
8:H:295:PRO:HG3	55:b:201:3PE:H382	2.02	0.41
9:I:75:SER:O	43:r:12:ARG:HG2	2.22	0.41
12:L:68:TRP:HZ2	13:M:448:THR:O	2.04	0.41
14:N:106:LEU:HD21	14:N:138:PRO:HB2	2.02	0.41
14:N:331:ILE:HD12	14:N:335:MET:HE3	2.03	0.41
15:O:76:GLU:O	15:O:77:ILE:C	2.63	0.41
15:O:78:ALA:HB1	15:O:83:MET:O	2.20	0.41
15:O:239:ASN:HB3	15:O:243:LYS:NZ	2.36	0.41
16:P:143:ASP:OD1	16:P:147:ASN:ND2	2.54	0.41
16:P:350:ILE:HB	16:P:366:ILE:CG2	2.51	0.41
20:U:128:PHE:CZ	20:U:148:ILE:CD1	3.04	0.41
20:U:133:ILE:HD13	39:n:7:PRO:HD3	2.01	0.41
20:U:133:ILE:CG2	20:U:134:ASP:N	2.84	0.41
23:X:136:PRO:O	23:X:137:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:98:MET:HB3	25:Z:104:TRP:HD1	1.86	0.41
26:a:48:MET:HE3	26:a:48:MET:HB2	1.77	0.41
29:d:45:ASP:O	29:d:46:ASN:C	2.62	0.41
36:k:57:TRP:HA	36:k:60:MET:HB3	2.02	0.41
37:l:122:THR:CG2	37:l:129:MET:HE1	2.45	0.41
37:l:159:LYS:HE3	37:l:161:TYR:CE1	2.56	0.41
38:m:59:HIS:O	38:m:60:ILE:C	2.64	0.41
38:m:90:GLY:O	55:m:202:3PE:H2B2	2.21	0.41
39:n:41:ALA:C	39:n:43:LEU:N	2.78	0.41
40:o:22:ILE:HD12	40:o:102:PHE:HD1	1.86	0.41
46:AB:65:VAL:HG22	46:AB:218:MET:HG2	2.03	0.41
47:AC:10:LEU:O	47:AC:14:ILE:HG12	2.20	0.41
47:AC:346:PRO:HG3	51:AG:66:GLU:CG	2.51	0.41
48:AD:181:ASN:ND2	48:Ad:158:PRO:HB3	2.36	0.41
51:AG:57:TYR:O	51:AG:61:THR:HG23	2.21	0.41
45:Aa:469:ASN:ND2	47:Ac:223:TYR:CZ	2.89	0.41
47:Ac:29:SER:OG	56:Ag:101:CDL:HA61	2.21	0.41
47:Ac:334:ILE:CD1	51:Ag:56:VAL:HG22	2.51	0.41
48:Ad:107:HIS:ND1	48:Ad:138:VAL:O	2.54	0.41
48:Ad:250:THR:HG23	48:Ad:262:THR:HA	2.03	0.41
49:Ae:249:ILE:HG23	49:Ae:249:ILE:O	2.22	0.41
1:A:78:ALA:HB2	10:J:142:ALA:HB1	2.02	0.40
2:B:98:ALA:O	4:D:141:TYR:CE2	2.75	0.40
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.40
4:D:145:MET:HG2	4:D:148:GLU:OE2	2.22	0.40
5:E:109:MET:HE1	7:G:198:THR:CG2	2.51	0.40
5:E:184:MET:HE3	5:E:184:MET:HB3	1.95	0.40
6:F:80:MET:O	6:F:83:SER:HB3	2.20	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.40
7:G:176:CYS:SG	57:G:802:SF4:S1	3.19	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.40
8:H:182:ALA:HB1	55:H:402:3PE:H2H1	2.03	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
55:H:402:3PE:H272	55:H:402:3PE:H241	1.58	0.40
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.40
10:J:64:LEU:O	10:J:65:VAL:C	2.62	0.40
10:J:66:VAL:O	10:J:67:PHE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:52:LEU:O	12:L:53:MET:C	2.62	0.40
12:L:68:TRP:CE3	12:L:76:LEU:CD2	3.04	0.40
12:L:150:MET:HE1	56:L:703:CDL:OB9	2.20	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:178:ILE:HG12	41:p:82:VAL:HG11	2.03	0.40
13:M:218:LYS:HE3	13:M:218:LYS:HB3	1.58	0.40
13:M:303:ILE:HG13	13:M:385:LEU:HD23	2.03	0.40
14:N:146:TYR:CG	14:N:147:PRO:N	2.88	0.40
14:N:215:MET:HE3	14:N:215:MET:HB3	1.97	0.40
15:O:281:GLY:HA2	15:O:282:PRO:HD3	1.99	0.40
16:P:135:GLU:HG3	16:P:140:ASP:HA	2.03	0.40
16:P:203:PRO:HG2	64:P:401:NDP:C6N	2.51	0.40
19:S:17:ARG:O	19:S:52:PRO:HD2	2.21	0.40
23:X:167:PHE:HD2	23:X:170:TRP:HE1	1.65	0.40
24:Y:116:GLY:O	24:Y:117:CYS:C	2.63	0.40
56:Y:202:CDL:H391	56:Y:202:CDL:C58	2.51	0.40
30:e:65:GLU:CD	30:e:71:LYS:HB2	2.47	0.40
30:e:95:PRO:HB2	30:e:97:HIS:ND1	2.36	0.40
33:h:87:THR:O	33:h:91:ILE:HG13	2.21	0.40
35:j:92:TRP:CZ3	40:o:100:LYS:CA	2.96	0.40
35:j:101:PRO:O	35:j:102:ASP:C	2.64	0.40
55:m:202:3PE:C31	55:m:202:3PE:H11	2.52	0.40
40:o:52:THR:O	40:o:53:LEU:C	2.62	0.40
45:AA:48:THR:HB	45:AA:423:ARG:HG2	2.02	0.40
45:AA:117:GLY:HA3	46:AB:377:LYS:HA	2.02	0.40
45:AA:120:LEU:HB3	46:AB:299:ILE:HG13	2.01	0.40
45:AA:454:PRO:O	45:AA:468:TYR:OH	2.34	0.40
47:AC:53:MET:HA	47:Ac:177:ARG:HA	2.02	0.40
47:AC:244:LEU:HD13	48:AD:289:GLY:HA2	2.02	0.40
47:AC:323:ILE:HD13	55:AG:103:3PE:H232	2.02	0.40
49:AE:123:VAL:HG13	53:AJ:29:ALA:CA	2.41	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:CZ	2.49	0.40
54:AK:12:GLU:HA	54:AK:15:ARG:HD3	2.02	0.40
48:Ad:127:MET:HE1	48:Ad:198:SER:HA	2.02	0.40
51:Ag:10:ARG:NH2	51:Ag:12:ARG:HD2	2.36	0.40
54:Ak:23:MET:HE2	54:Ak:23:MET:HB2	1.92	0.40
4:D:391:VAL:HG23	4:D:413:SER:OG	2.21	0.40
5:E:68:ASN:ND2	44:s:56:ARG:NH2	2.68	0.40
6:F:53:LEU:O	6:F:54:LYS:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
6:F:276:PHE:CE2	6:F:290:GLU:HB3	2.56	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:664:TYR:OH	19:S:23:LEU:HD21	2.21	0.40
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.55	0.40
9:I:105:ARG:HH12	18:R:58:ASN:CB	2.34	0.40
10:J:14:VAL:O	10:J:17:LEU:HB3	2.22	0.40
10:J:92:LEU:C	10:J:92:LEU:HD23	2.46	0.40
12:L:3:ILE:HG22	12:L:49:LEU:CD2	2.52	0.40
12:L:22:SER:HA	12:L:27:ILE:CG2	2.52	0.40
12:L:141:PHE:O	12:L:142:ILE:C	2.62	0.40
12:L:210:LEU:HD12	12:L:270:ASN:HD21	1.86	0.40
12:L:324:LEU:HB3	12:L:395:ILE:CD1	2.51	0.40
12:L:357:ARG:HG2	39:n:32:ILE:CG1	2.48	0.40
12:L:556:ILE:HG21	38:m:80:PHE:CD1	2.52	0.40
13:M:53:SER:O	13:M:54:ASN:C	2.63	0.40
13:M:71:TRP:CG	55:M:502:3PE:H3B2	2.56	0.40
13:M:190:TRP:HB3	24:Y:129:ILE:HG23	2.04	0.40
13:M:248:ILE:HG13	13:M:249:ILE:H	1.85	0.40
13:M:259:TYR:HB2	13:M:260:PRO:HD3	2.03	0.40
13:M:277:LEU:O	37:l:116:ARG:NH1	2.53	0.40
13:M:435:THR:HG23	13:M:436:LEU:N	2.36	0.40
56:M:503:CDL:HA31	23:X:172:VAL:H	1.87	0.40
14:N:59:TYR:O	14:N:63:GLN:HG2	2.21	0.40
14:N:224:SER:HB2	14:N:229:SER:HB2	2.01	0.40
15:O:117:PHE:CE1	15:O:128:SER:CB	2.96	0.40
15:O:117:PHE:HE1	15:O:173:MET:HE1	1.80	0.40
15:O:231:SER:HA	15:O:234:LEU:CD1	2.51	0.40
16:P:169:HIS:ND1	64:P:401:NDP:H5N	2.36	0.40
20:U:93:ILE:CG1	20:U:110:LEU:HD11	2.51	0.40
21:V:114:TRP:O	21:V:116:ILE:HG22	2.21	0.40
22:W:23:ILE:HG21	22:W:83:ASP:HB2	2.02	0.40
22:W:27:ASP:O	22:W:28:LEU:C	2.64	0.40
23:X:21:SER:O	23:X:22:SER:C	2.63	0.40
23:X:25:LEU:HD11	26:a:50:ARG:NH2	2.36	0.40
23:X:115:LEU:HB3	23:X:117:TRP:CE2	2.55	0.40
25:Z:55:GLN:O	25:Z:59:ARG:HG3	2.21	0.40
27:b:23:PHE:HE2	55:b:201:3PE:H252	1.85	0.40
32:g:112:MET:HE3	32:g:115:TRP:CE3	2.56	0.40
39:n:139:GLN:O	39:n:140:LEU:C	2.64	0.40
42:q:17:HIS:HE1	42:q:34:ARG:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:44:TYR:HE1	42:q:69:ASN:OD1	2.05	0.40
45:AA:73:VAL:HG11	45:AA:151:VAL:HG11	2.03	0.40
45:AA:170:ARG:HG3	45:AA:171:GLU:N	2.36	0.40
46:AB:297:PRO:CB	46:AB:304:ASN:OD1	2.69	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
47:AC:83:HIS:CD2	67:AC:402:HEM:C4D	3.10	0.40
47:AC:294:LEU:C	47:AC:294:LEU:HD23	2.46	0.40
48:AD:127:MET:HE1	48:AD:198:SER:HA	2.03	0.40
48:AD:159:ASN:O	48:AD:162:GLY:N	2.47	0.40
49:AE:196:ARG:HD2	49:AE:249:ILE:HG21	2.03	0.40
51:AG:48:ARG:HH21	55:AG:103:3PE:H322	1.86	0.40
53:AJ:21:PHE:O	53:AJ:24:THR:HG22	2.20	0.40
45:Aa:463:GLU:CD	51:Ag:8:LEU:HB2	2.46	0.40
52:Ah:67:GLU:HG3	52:Ah:68:GLU:H	1.86	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.40
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.51	0.40
2:B:91:TRP:CD1	2:B:120:VAL:HG23	2.56	0.40
3:C:66:GLU:OE1	21:V:47:TYR:CE2	2.74	0.40
3:C:97:THR:HG21	21:V:97:TRP:HH2	1.86	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:J:63:MET:O	10:J:66:VAL:HB	2.22	0.40
10:J:93:VAL:O	10:J:97:ILE:HG12	2.21	0.40
10:J:135:LEU:O	10:J:135:LEU:HG	2.21	0.40
12:L:59:MET:HE2	12:L:59:MET:HB3	1.89	0.40
12:L:67:HIS:HD2	12:L:76:LEU:O	2.05	0.40
12:L:390:TYR:HE2	35:j:68:TRP:CH2	2.40	0.40
12:L:399:ILE:HG22	12:L:409:LEU:CD1	2.51	0.40
13:M:173:THR:HG23	33:h:147:ALA:CA	2.49	0.40
13:M:177:MET:HE3	33:h:140:LEU:HD21	2.02	0.40
13:M:313:THR:HG21	13:M:456:GLY:CA	2.47	0.40
13:M:394:ILE:O	13:M:398:ILE:HG13	2.22	0.40
14:N:211:LEU:CD2	14:N:333:SER:HB2	2.45	0.40
15:O:170:LEU:CD2	15:O:184:VAL:HG13	2.51	0.40
15:O:209:VAL:HG23	15:O:214:VAL:HG12	2.03	0.40
17:Q:57:GLU:O	17:Q:58:LYS:C	2.65	0.40
20:T:97:LYS:NZ	20:T:108:LEU:N	2.66	0.40
20:T:104:PHE:CE1	20:T:105:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:48:TRP:CZ2	27:b:55:VAL:CG2	2.98	0.40
24:Y:61:TYR:HA	56:Y:202:CDL:H131	2.02	0.40
24:Y:64:THR:O	24:Y:68:ILE:HG23	2.20	0.40
25:Z:104:TRP:O	25:Z:105:LYS:C	2.64	0.40
29:d:58:LEU:HD23	29:d:58:LEU:HA	1.90	0.40
30:e:80:LYS:O	30:e:81:LYS:C	2.63	0.40
33:h:148:GLU:O	33:h:152:LYS:HG3	2.21	0.40
34:i:99:SER:O	34:i:100:SER:C	2.64	0.40
37:l:129:MET:HE3	37:l:129:MET:HB2	1.89	0.40
38:m:87:SER:HB2	55:m:202:3PE:C27	2.52	0.40
38:m:125:PHE:CD1	41:p:132:PHE:CE2	3.09	0.40
39:n:167:TRP:CD1	39:n:167:TRP:H	2.38	0.40
40:o:15:VAL:HG12	40:o:110:GLN:HA	2.02	0.40
41:p:43:TRP:HB3	41:p:44:PRO:HD3	2.03	0.40
43:r:28:TYR:O	43:r:30:GLU:HG3	2.21	0.40
46:AB:160:ILE:HG23	49:AI:44:ASP:HB2	2.02	0.40
46:AB:262:ASN:C	46:Ab:195:TYR:CD2	2.99	0.40
47:AC:33:PHE:CE1	56:AG:102:CDL:H782	2.56	0.40
47:AC:268:ILE:CG1	49:Ae:238:CYS:SG	3.09	0.40
52:AH:67:GLU:HG3	52:AH:68:GLU:H	1.87	0.40
47:Ac:77:TRP:HZ2	48:Ad:284:HIS:CD2	2.38	0.40
48:Ad:138:VAL:HG21	48:Ad:276:TRP:CZ2	2.55	0.40
48:Ad:175:PHE:HA	48:Ad:176:PRO:HD3	1.96	0.40
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CZ	2.56	0.40
49:Ae:127:TYR:HA	54:Ak:34:TRP:CH2	2.57	0.40
51:Ag:19:LEU:HD12	51:Ag:20:SER:H	1.86	0.40
53:Aj:10:LEU:O	53:Aj:11:TYR:C	2.64	0.40
2:B:120:VAL:HG11	61:H:401:UQ9:C1M	2.51	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.42	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
6:F:281:HIS:HB2	6:F:356:VAL:O	2.21	0.40
7:G:114:GLU:OE2	43:r:53:TYR:CA	2.60	0.40
7:G:355:LYS:HB2	7:G:366:LEU:CD2	2.52	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:316:PRO:HG3	25:Z:57:ARG:CB	2.49	0.40
10:J:151:MET:HE2	10:J:151:MET:HA	2.04	0.40
11:K:53:SER:HB2	30:e:21:LEU:HD22	2.03	0.40
12:L:300:LYS:O	12:L:304:PHE:HD2	2.05	0.40
12:L:598:ILE:HG12	14:N:100:MET:SD	2.62	0.40
13:M:197:LEU:O	13:M:201:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:321:LYS:HD2	29:d:49:ARG:HD3	2.04	0.40
15:O:104:LEU:HD23	15:O:104:LEU:HA	1.90	0.40
16:P:80:VAL:HB	16:P:103:LEU:HD22	2.04	0.40
16:P:120:VAL:O	16:P:121:GLN:C	2.64	0.40
16:P:140:ASP:O	16:P:141:PHE:C	2.65	0.40
18:R:36:GLN:O	18:R:36:GLN:HG3	2.22	0.40
24:Y:102:THR:OG1	24:Y:103:LEU:N	2.54	0.40
56:h:201:CDL:C11	56:h:201:CDL:HA32	2.50	0.40
38:m:41:ALA:HA	39:n:152:GLU:HG2	2.04	0.40
38:m:124:LYS:HG2	38:m:125:PHE:CD2	2.57	0.40
39:n:94:TYR:CE2	39:n:177:ARG:NH1	2.90	0.40
40:o:27:PRO:O	40:o:34:ARG:HD3	2.22	0.40
40:o:121:ARG:O	40:o:121:ARG:HG2	2.21	0.40
44:s:41:ASN:HD21	44:s:43:TYR:HB2	1.87	0.40
45:AA:412:ASP:O	45:AA:416:SER:OG	2.32	0.40
46:AB:303:ASN:O	46:AB:304:ASN:C	2.63	0.40
47:AC:30:TRP:CB	47:AC:100:ARG:HD3	2.52	0.40
47:AC:146:ILE:CD1	68:AC:405:U10:H3M2	2.49	0.40
47:AC:376:MET:CE	50:AF:18:ARG:HG2	2.51	0.40
49:AE:159:ILE:O	49:AE:210:TRP:CH2	2.71	0.40
49:AE:168:LYS:NZ	49:AE:171:GLY:HA2	2.36	0.40
51:AG:10:ARG:NH2	51:AG:12:ARG:HD2	2.36	0.40
45:Aa:73:VAL:HG11	45:Aa:151:VAL:HG11	2.03	0.40
45:Aa:454:PRO:O	45:Aa:468:TYR:OH	2.34	0.40
46:Ab:270:ALA:HB2	46:Ab:339:TYR:CD1	2.50	0.40
47:Ac:294:LEU:HD23	47:Ac:294:LEU:C	2.46	0.40
47:Ac:296:LEU:O	47:Ac:297:SER:C	2.64	0.40
49:Ae:162:GLY:N	49:Ae:178:HIS:O	2.54	0.40
50:Af:36:ASP:OD1	50:Af:90:TYR:OH	2.38	0.40
53:Aj:7:PRO:O	53:Aj:10:LEU:HB2	2.21	0.40
1:A:87:MET:HB3	1:A:87:MET:HE3	1.84	0.40
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.90	0.40
3:C:68:LEU:HD13	3:C:95:THR:HA	2.03	0.40
4:D:182:ASN:O	4:D:185:MET:HB3	2.22	0.40
4:D:255:ILE:CG1	4:D:337:MET:HE2	2.47	0.40
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.57	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:297:LYS:CB	6:F:333:GLU:HB2	2.51	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.03	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
10:J:84:SER:C	10:J:86:TRP:N	2.79	0.40
12:L:62:MET:HB3	34:i:98:VAL:CG1	2.52	0.40
12:L:78:MET:HA	56:h:201:CDL:H672	2.03	0.40
12:L:190:SER:OG	13:M:383:MET:SD	2.65	0.40
12:L:277:MET:HG3	12:L:318:GLY:HA3	2.04	0.40
12:L:381:THR:HG22	12:L:420:ALA:HA	2.04	0.40
12:L:553:LEU:HD21	38:m:94:GLY:CA	2.52	0.40
13:M:5:ILE:CG1	13:M:6:LEU:N	2.85	0.40
13:M:62:SER:HB2	13:M:110:PHE:O	2.22	0.40
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.51	0.40
13:M:186:LEU:CB	13:M:253:LEU:HD13	2.52	0.40
13:M:230:ILE:HG23	13:M:235:LEU:CD1	2.51	0.40
13:M:336:ARG:NH2	13:M:429:SER:HA	2.36	0.40
13:M:430:HIS:HB3	32:g:73:GLY:HA3	2.04	0.40
14:N:122:ILE:CD1	14:N:127:GLY:HA2	2.52	0.40
14:N:139:LEU:HD23	14:N:139:LEU:HA	1.86	0.40
14:N:223:ASN:OD1	14:N:223:ASN:O	2.39	0.40
14:N:246:LEU:HD11	56:d:201:CDL:C40	2.51	0.40
14:N:272:LYS:HE3	33:h:154:GLN:HG2	2.03	0.40
14:N:297:ILE:O	14:N:298:TYR:C	2.63	0.40
16:P:56:ALA:HA	16:P:125:VAL:O	2.21	0.40
16:P:146:VAL:HG13	16:P:147:ASN:OD1	2.21	0.40
16:P:227:PRO:O	16:P:228:LEU:HD23	2.21	0.40
16:P:302:GLY:HA2	16:P:314:THR:CG2	2.50	0.40
17:Q:129:SER:HB2	21:V:116:ILE:CD1	2.52	0.40
19:S:59:SER:O	19:S:60:GLU:C	2.63	0.40
35:j:71:TRP:HZ3	35:j:72:ARG:NH2	2.19	0.40
36:k:56:ALA:O	36:k:60:MET:N	2.53	0.40
38:m:123:ARG:NH2	41:p:144:LEU:HD21	2.36	0.40
55:m:201:3PE:H231	55:m:201:3PE:H262	1.92	0.40
41:p:45:VAL:O	41:p:46:THR:C	2.64	0.40
41:p:128:GLU:OE2	41:p:128:GLU:N	2.52	0.40
42:q:64:TYR:CE2	42:q:82:VAL:HG13	2.56	0.40
47:AC:99:GLY:HA3	55:AC:404:3PE:H2A1	2.03	0.40
47:AC:128:PHE:CE1	68:AC:405:U10:C4M	3.04	0.40
48:AD:110:ILE:HG23	48:AD:273:PHE:HA	2.04	0.40
45:Aa:148:ALA:HB2	45:Aa:250:LEU:HG	2.04	0.40
45:Aa:384:THR:HG21	54:Ak:9:ARG:CD	2.51	0.40
46:Ab:65:VAL:HG22	46:Ab:218:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:149:LEU:HD21	47:Ac:294:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	83 (94%)	5 (6%)	0	100	100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	9	41
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	420/463 (91%)	401 (96%)	19 (4%)	0	100	100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	409 (96%)	15 (4%)	0	100	100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100	100
8	H	313/318 (98%)	298 (95%)	14 (4%)	1 (0%)	36	71
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	J	165/172 (96%)	157 (95%)	8 (5%)	0	100	100
11	K	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
12	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
16	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36	71
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
23	X	167/172 (97%)	154 (92%)	13 (8%)	0	100	100
24	Y	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
25	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
26	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
27	b	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
28	c	45/76 (59%)	45 (100%)	0	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	99/151 (66%)	93 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	96/128 (75%)	87 (91%)	9 (9%)	0	100	100
35	j	66/105 (63%)	60 (91%)	6 (9%)	0	100	100
36	k	74/104 (71%)	71 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	123/129 (95%)	116 (94%)	7 (6%)	0	100	100
39	n	176/179 (98%)	167 (95%)	8 (4%)	1 (1%)	21	58
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
41	p	170/176 (97%)	157 (92%)	13 (8%)	0	100	100
42	q	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
43	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11	45
44	s	20/104 (19%)	20 (100%)	0	0	100	100
45	AA	397/480 (83%)	388 (98%)	9 (2%)	0	100	100
45	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
46	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
46	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
48	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
48	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
49	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	Ai	24/274 (9%)	23 (96%)	1 (4%)	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%)	74 (100%)	0	0	100	100
52	AH	66/89 (74%)	66 (100%)	0	0	100	100
52	Ah	66/89 (74%)	66 (100%)	0	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	46 (100%)	0	0	100	100
54	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
54	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	11921/14392 (83%)	11425 (96%)	489 (4%)	7 (0%)	49	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
8	H	88	PRO
16	P	329	PRO
2	B	171	TYR
43	r	39	PRO
39	n	156	PRO
2	B	195	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
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	364 (100%)	2 (0%)	81	81
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	279/280 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/138 (99%)	135 (99%)	1 (1%)	76	78
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	415/415 (100%)	414 (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	296/325 (91%)	295 (100%)	1 (0%)	86	84
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	70
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	80/135 (59%)	80 (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%)	151 (99%)	1 (1%)	76	78
24	Y	105/107 (98%)	105 (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	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	94/120 (78%)	94 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	59/78 (76%)	59 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	80
40	o	112/121 (93%)	112 (100%)	0	100	100
41	p	156/158 (99%)	156 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	85/96 (88%)	84 (99%)	1 (1%)	63	73
44	s	22/95 (23%)	22 (100%)	0	100	100
45	AA	341/398 (86%)	339 (99%)	2 (1%)	78	80
45	Aa	349/398 (88%)	347 (99%)	2 (1%)	78	80
46	AB	328/356 (92%)	327 (100%)	1 (0%)	86	84
46	Ab	324/356 (91%)	323 (100%)	1 (0%)	86	84
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	205/260 (79%)	205 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	158/224 (70%)	157 (99%)	1 (1%)	78	80
49	AI	23/224 (10%)	22 (96%)	1 (4%)	26	48
49	Ae	158/224 (70%)	157 (99%)	1 (1%)	78	80
49	Ai	22/224 (10%)	20 (91%)	2 (9%)	9	29
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	AH	65/83 (78%)	65 (100%)	0	100	100
52	Ah	65/83 (78%)	65 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	39/46 (85%)	39 (100%)	0	100	100
54	Ak	39/46 (85%)	39 (100%)	0	100	100
All	All	10476/12261 (85%)	10445 (100%)	31 (0%)	84	84

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	170	TYR
4	D	127	LYS
4	D	142	VAL
5	E	124	LYS
7	G	271	MET
10	J	124	LEU
12	L	3	ILE
12	L	69	VAL
13	M	218	LYS
14	N	159	ILE
16	P	316	LYS
17	Q	96	LYS
18	R	76	ILE
19	S	68	ARG
23	X	57	LEU
25	Z	6	VAL
39	n	98	LYS
43	r	92	LYS
45	AA	249	HIS
45	AA	403	LEU
46	AB	435	LYS
47	AC	294	LEU
49	AE	135	GLN
49	AI	45	VAL
45	Aa	222	ARG
45	Aa	249	HIS
46	Ab	435	LYS
47	Ac	294	LEU
49	Ae	135	GLN

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Mol	Chain	Res	Type
49	Ai	45	VAL
49	Ai	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) 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	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	60	HIS
4	D	79	ASN
4	D	83	ASN
4	D	88	HIS
4	D	92	HIS
4	D	112	HIS
4	D	117	HIS
4	D	147	ASN
4	D	160	ASN
4	D	168	GLN
4	D	182	ASN
4	D	270	ASN
4	D	381	HIS
4	D	454	GLN
5	E	68	ASN
5	E	132	GLN
5	E	245	GLN
6	F	44	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	281	HIS
6	F	303	HIS
6	F	313	ASN
6	F	346	GLN

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Mol	Chain	Res	Type
6	F	418	GLN
7	G	74	ASN
7	G	205	GLN
7	G	260	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	514	ASN
7	G	571	HIS
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	124	ASN
8	H	169	GLN
8	H	258	ASN
8	H	287	HIS
8	H	292	ASN
10	J	85	ASN
10	J	107	ASN
11	K	7	ASN
11	K	25	HIS
12	L	2	ASN
12	L	25	ASN
12	L	58	ASN
12	L	135	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	446	ASN
12	L	452	ASN

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Mol	Chain	Res	Type
12	L	514	ASN
12	L	572	ASN
12	L	579	ASN
12	L	605	ASN
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN
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	374	ASN
13	M	415	GLN
14	N	120	GLN
14	N	134	GLN
14	N	174	GLN
14	N	273	ASN
14	N	289	ASN
14	N	310	ASN
14	N	317	GLN
15	O	54	HIS
15	O	71	ASN
15	O	80	GLN
15	O	142	GLN
15	O	175	ASN
15	O	219	GLN
15	O	286	GLN
15	O	292	HIS
15	O	306	ASN
15	O	323	GLN
16	P	43	HIS
16	P	79	GLN
16	P	102	GLN
16	P	166	HIS
16	P	216	HIS
16	P	251	ASN
16	P	269	ASN
16	P	275	HIS
16	P	323	HIS

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Mol	Chain	Res	Type
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	86	ASN
17	Q	88	GLN
18	R	58	ASN
19	S	25	GLN
19	S	48	HIS
21	V	41	HIS
22	W	54	GLN
22	W	94	GLN
22	W	105	HIS
23	X	77	HIS
23	X	140	ASN
24	Y	46	ASN
24	Y	81	GLN
24	Y	91	ASN
24	Y	108	HIS
25	Z	135	ASN
25	Z	137	ASN
26	a	31	ASN
27	b	83	ASN
29	d	59	HIS
31	f	10	HIS
31	f	13	HIS
32	g	146	GLN
33	h	154	GLN
33	h	170	GLN
33	h	181	HIS
34	i	74	HIS
34	i	83	HIS
35	j	39	HIS
35	j	41	GLN
36	k	39	GLN
36	k	66	ASN
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	12	HIS

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Mol	Chain	Res	Type
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	76	HIS
40	o	110	GLN
41	p	23	GLN
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	31	ASN
42	q	52	ASN
42	q	87	HIS
42	q	91	HIS
42	q	113	HIS
42	q	116	ASN
43	r	21	GLN
43	r	29	GLN
43	r	52	ASN
43	r	110	GLN
44	s	59	GLN
45	AA	87	ASN
45	AA	160	GLN
45	AA	173	GLN
45	AA	181	ASN
45	AA	207	ASN
45	AA	240	GLN
45	AA	342	GLN
45	AA	402	HIS
46	AB	167	GLN
46	AB	284	ASN
46	AB	298	HIS
46	AB	304	ASN
46	AB	357	GLN
46	AB	365	ASN
46	AB	415	GLN
46	AB	443	ASN
47	AC	32	ASN

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Mol	Chain	Res	Type
47	AC	260	ASN
47	AC	312	GLN
48	AD	115	GLN
48	AD	155	GLN
48	AD	181	ASN
48	AD	189	ASN
49	AE	227	ASN
49	AE	242	HIS
50	AF	80	GLN
49	AI	71	ASN
54	AK	16	ASN
45	Aa	55	ASN
45	Aa	87	ASN
45	Aa	128	HIS
45	Aa	160	GLN
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	207	ASN
45	Aa	240	GLN
45	Aa	342	GLN
45	Aa	397	ASN
46	Ab	167	GLN
46	Ab	284	ASN
46	Ab	298	HIS
46	Ab	304	ASN
46	Ab	357	GLN
46	Ab	415	GLN
46	Ab	443	ASN
47	Ac	32	ASN
47	Ac	201	HIS
47	Ac	312	GLN
48	Ad	115	GLN
48	Ad	190	ASN
49	Ae	227	ASN
49	Ae	242	HIS
50	Af	39	HIS
50	Af	80	GLN
51	Ag	65	GLN
54	Ak	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 61 ligands modelled in this entry, 1 is monoatomic - leaving 60 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$
56	CDL	L	703	-	73,73,99	1.06	4 (5%)	79,85,111	1.15	5 (6%)
57	SF4	G	802	7	0,12,12	-	-	-		
56	CDL	A	402	-	91,91,99	0.95	4 (4%)	97,103,111	1.09	6 (6%)
63	ADP	O	401	-	27,29,29	1.33	4 (14%)	42,45,45	1.99	10 (23%)
55	3PE	m	201	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	4 (7%)
62	PC1	Ae	301	-	34,34,53	1.17	2 (5%)	40,42,61	1.18	4 (10%)
55	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.14	3 (8%)
55	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.21	3 (8%)
56	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
68	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
69	UQ6	AC	406	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.09	3 (5%)
67	HEM	AC	402	47	50,50,50	1.31	7 (14%)	66,82,82	1.68	15 (22%)
55	3PE	b	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.10	3 (6%)
55	3PE	M	501	-	36,36,50	1.06	2 (5%)	39,41,55	1.07	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	CDL	Y	202	-	80,80,99	1.01	4 (5%)	86,92,111	1.13	6 (6%)
56	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.35	6 (12%)
55	3PE	Y	201	-	38,38,50	1.03	2 (5%)	41,43,55	1.11	3 (7%)
57	SF4	G	801	7	0,12,12	-	-	-	-	-
56	CDL	h	201	-	92,92,99	0.94	4 (4%)	98,104,111	1.12	6 (6%)
62	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.10	3 (5%)
56	CDL	d	201	-	83,83,99	1.00	4 (4%)	89,95,111	1.10	5 (5%)
66	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
64	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.67	11 (16%)
66	EHZ	n	201	-	27,31,37	1.88	7 (25%)	37,41,47	1.69	8 (21%)
55	3PE	J	201	-	45,45,50	0.96	2 (4%)	48,50,55	1.08	3 (6%)
55	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.73	1 (4%)
57	SF4	B	301	2	0,12,12	-	-	-	-	-
69	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
59	FES	G	803	7	0,4,4	-	-	-	-	-
60	FMN	F	501	-	33,33,33	1.38	5 (15%)	48,50,50	1.23	7 (14%)
56	CDL	AG	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.33	6 (12%)
55	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
67	HEM	AC	403	47	50,50,50	1.34	6 (12%)	66,82,82	1.66	16 (24%)
57	SF4	F	502	6	0,12,12	-	-	-	-	-
55	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.20	2 (8%)
62	PC1	l	201	-	49,49,53	0.96	2 (4%)	55,57,61	1.01	4 (7%)
67	HEM	Ac	401	47	50,50,50	1.30	7 (14%)	66,82,82	1.67	15 (22%)
61	UQ9	H	401	-	35,35,58	0.84	3 (8%)	42,45,73	0.63	1 (2%)
67	HEM	Ac	402	47	50,50,50	1.32	5 (10%)	66,82,82	1.66	16 (24%)
62	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.20	4 (10%)
56	CDL	M	503	-	78,78,99	1.02	4 (5%)	84,90,111	1.11	6 (7%)
55	3PE	H	402	-	45,45,50	0.92	2 (4%)	48,50,55	1.33	5 (10%)
57	SF4	I	303	9	0,12,12	-	-	-	-	-
56	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.25	6 (9%)
55	3PE	A	401	-	45,45,50	1.11	5 (11%)	48,50,55	1.27	3 (6%)
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.08	3 (5%)
55	3PE	i	201	-	39,39,50	1.05	2 (5%)	42,44,55	1.03	2 (4%)
70	HEC	AD	401	48	50,50,50	1.72	5 (10%)	68,82,82	1.35	7 (10%)
55	3PE	L	704	-	37,37,50	1.05	2 (5%)	40,42,55	1.18	4 (10%)
55	3PE	m	202	-	40,40,50	1.01	2 (5%)	43,45,55	1.21	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
56	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.26	6 (9%)
59	FES	E	301	5	0,4,4	-	-	-	-	-
70	HEC	Ad	401	48	50,50,50	1.73	5 (10%)	68,82,82	1.36	8 (11%)
62	PC1	L	701	-	47,47,53	0.99	2 (4%)	53,55,61	1.09	3 (5%)
56	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.36	6 (11%)
58	UQ1	D	501	-	18,18,18	1.32	3 (16%)	22,25,25	1.61	5 (22%)
68	U10	AC	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.10	7 (25%)
57	SF4	I	302	9	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	CDL	L	703	-	-	18/84/84/110	-
57	SF4	G	802	7	-	-	0/6/5/5
56	CDL	A	402	-	-	24/102/102/110	-
63	ADP	O	401	-	-	3/16/32/32	0/3/3/3
55	3PE	m	201	-	-	14/54/54/54	-
62	PC1	Ae	301	-	-	7/38/38/57	-
55	3PE	AC	404	-	-	1/38/38/54	-
55	3PE	Ac	403	-	-	3/38/38/54	-
56	CDL	Ag	102	-	-	13/66/66/110	-
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
69	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
55	3PE	L	702	-	-	14/52/52/54	-
67	HEM	AC	402	47	-	9/14/54/54	-
55	3PE	b	201	-	-	10/49/49/54	-
55	3PE	M	501	-	-	11/40/40/54	-
56	CDL	Y	202	-	-	24/91/91/110	-
56	CDL	Ag	101	-	-	7/52/52/110	-
55	3PE	Y	201	-	-	5/42/42/54	-
57	SF4	G	801	7	-	-	0/6/5/5
56	CDL	h	201	-	-	27/103/103/110	-
62	PC1	I	301	-	-	10/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	CDL	d	201	-	-	17/94/94/110	-
66	EHZ	W	201	-	-	12/39/39/45	-
64	NDP	P	401	-	-	2/34/77/77	0/5/5/5
66	EHZ	n	201	-	-	19/39/39/45	-
55	3PE	J	201	-	-	12/49/49/54	-
55	3PE	AC	401	-	-	7/26/26/54	-
57	SF4	B	301	2	-	-	0/6/5/5
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
59	FES	G	803	7	-	-	0/1/1/1
60	FMN	F	501	-	-	0/18/18/18	0/3/3/3
56	CDL	AG	101	-	-	8/52/52/110	-
55	3PE	Ag	103	-	-	10/54/54/54	-
67	HEM	AC	403	47	-	8/14/54/54	-
62	PC1	l	201	-	-	8/53/53/57	-
55	3PE	Aa	501	-	-	7/26/26/54	-
67	HEM	Ac	401	47	-	9/14/54/54	-
57	SF4	F	502	6	-	-	0/6/5/5
61	UQ9	H	401	-	-	15/30/54/81	0/1/1/1
67	HEM	Ac	402	47	-	8/14/54/54	-
62	PC1	q	202	-	-	14/38/38/57	-
56	CDL	M	503	-	-	26/89/89/110	-
55	3PE	H	402	-	-	11/49/49/54	-
57	SF4	I	303	9	-	-	0/6/5/5
56	CDL	AG	102	-	-	15/66/66/110	-
55	3PE	A	401	-	-	18/49/49/54	-
55	3PE	M	502	-	-	13/54/54/54	-
55	3PE	i	201	-	-	13/43/43/54	-
70	HEC	AD	401	48	1/1/3/7	0/14/54/54	-
55	3PE	L	704	-	-	7/41/41/54	-
55	3PE	m	202	-	-	8/44/44/54	-
55	3PE	AG	103	-	-	9/54/54/54	-
56	CDL	q	201	-	-	15/67/67/110	-
59	FES	E	301	5	-	-	0/1/1/1
70	HEC	Ad	401	48	1/1/3/7	0/14/54/54	-
62	PC1	L	701	-	-	11/51/51/57	-
56	CDL	Aa	502	-	-	13/56/56/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	UQ1	D	501	-	-	6/9/33/33	0/1/1/1
68	U10	AC	405	-	-	6/15/39/87	0/1/1/1
57	SF4	I	302	9	-	-	0/6/5/5

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	Ad	401	HEC	C3D-C2D	8.07	1.53	1.36
70	AD	401	HEC	C3D-C2D	7.98	1.53	1.36
66	n	201	EHZ	C15-N2	5.33	1.45	1.33
66	n	201	EHZ	C12-N1	5.19	1.45	1.33
66	W	201	EHZ	C15-N2	5.15	1.44	1.33
66	W	201	EHZ	C12-N1	5.03	1.44	1.33
60	F	501	FMN	C9A-C5A	4.80	1.49	1.41
62	L	701	PC1	O31-C31	4.34	1.46	1.33
62	Ae	301	PC1	O31-C31	4.33	1.46	1.33
56	A	402	CDL	OA8-CA7	4.29	1.45	1.33
63	O	401	ADP	C5-C4	4.27	1.47	1.39
55	i	201	3PE	O31-C31	4.26	1.45	1.33
55	b	201	3PE	O31-C31	4.26	1.45	1.33
55	M	501	3PE	O31-C31	4.25	1.45	1.33
56	M	503	CDL	OA8-CA7	4.24	1.45	1.33
56	Y	202	CDL	OB8-CB7	4.24	1.45	1.33
56	Aa	502	CDL	OA8-CA7	4.24	1.45	1.33
55	i	201	3PE	O21-C21	4.24	1.46	1.34
56	h	201	CDL	OA8-CA7	4.24	1.45	1.33
56	d	201	CDL	OA8-CA7	4.24	1.45	1.33
56	Aa	502	CDL	OB8-CB7	4.24	1.45	1.33
56	AG	101	CDL	OA8-CA7	4.24	1.45	1.33
55	AC	404	3PE	O31-C31	4.23	1.45	1.33
55	m	201	3PE	O31-C31	4.23	1.45	1.33
64	P	401	NDP	C5A-C4A	4.22	1.46	1.39
55	Aa	501	3PE	O31-C31	4.22	1.45	1.33
55	Ac	403	3PE	O31-C31	4.22	1.45	1.33
62	l	201	PC1	O31-C31	4.21	1.45	1.33
55	J	201	3PE	O31-C31	4.21	1.45	1.33
55	AG	103	3PE	O31-C31	4.21	1.45	1.33
56	L	703	CDL	OB6-CB5	4.21	1.46	1.34
56	Y	202	CDL	OA8-CA7	4.20	1.45	1.33
56	Ag	101	CDL	OB8-CB7	4.20	1.45	1.33
55	m	202	3PE	O31-C31	4.20	1.45	1.33
56	L	703	CDL	OA8-CA7	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	L	704	3PE	O31-C31	4.18	1.45	1.33
56	M	503	CDL	OB8-CB7	4.18	1.45	1.33
56	d	201	CDL	OB8-CB7	4.17	1.45	1.33
55	Y	201	3PE	O31-C31	4.17	1.45	1.33
56	A	402	CDL	OB8-CB7	4.17	1.45	1.33
56	A	402	CDL	OA6-CA5	4.17	1.46	1.34
62	I	301	PC1	O31-C31	4.17	1.45	1.33
56	Ag	101	CDL	OA8-CA7	4.16	1.45	1.33
56	AG	101	CDL	OB8-CB7	4.16	1.45	1.33
56	h	201	CDL	OB8-CB7	4.16	1.45	1.33
56	AG	102	CDL	OB8-CB7	4.16	1.45	1.33
56	q	201	CDL	OB8-CB7	4.15	1.45	1.33
56	AG	102	CDL	OA8-CA7	4.15	1.45	1.33
55	Aa	501	3PE	O21-C21	4.14	1.46	1.34
55	AG	103	3PE	O21-C21	4.14	1.46	1.34
56	L	703	CDL	OB8-CB7	4.13	1.45	1.33
56	d	201	CDL	OB6-CB5	4.13	1.45	1.34
56	Aa	502	CDL	OB6-CB5	4.11	1.45	1.34
56	q	201	CDL	OA8-CA7	4.11	1.45	1.33
55	M	502	3PE	O31-C31	4.11	1.45	1.33
62	Ae	301	PC1	O21-C21	4.10	1.45	1.34
55	L	702	3PE	O31-C31	4.10	1.45	1.33
56	AG	101	CDL	OA6-CA5	4.10	1.45	1.34
56	d	201	CDL	OA6-CA5	4.07	1.45	1.34
56	Y	202	CDL	OA6-CA5	4.06	1.45	1.34
62	q	202	PC1	O31-C31	4.06	1.45	1.33
55	M	502	3PE	O21-C21	4.06	1.45	1.34
56	q	201	CDL	OA6-CA5	4.06	1.45	1.34
62	q	202	PC1	O21-C21	4.05	1.45	1.34
56	Ag	101	CDL	OA6-CA5	4.05	1.45	1.34
56	L	703	CDL	OA6-CA5	4.05	1.45	1.34
55	b	201	3PE	O21-C21	4.04	1.45	1.34
55	Y	201	3PE	O21-C21	4.04	1.45	1.34
56	AG	101	CDL	OB6-CB5	4.04	1.45	1.34
56	Ag	101	CDL	OB6-CB5	4.03	1.45	1.34
56	h	201	CDL	OA6-CA5	4.03	1.45	1.34
55	L	704	3PE	O21-C21	4.03	1.45	1.34
55	m	202	3PE	O21-C21	4.02	1.45	1.34
62	I	301	PC1	O21-C21	4.02	1.45	1.34
56	Y	202	CDL	OB6-CB5	4.01	1.45	1.34
56	AG	102	CDL	OA6-CA5	4.01	1.45	1.34
56	Aa	502	CDL	OA6-CA5	4.01	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	q	201	CDL	OB6-CB5	4.00	1.45	1.34
56	M	503	CDL	OB6-CB5	4.00	1.45	1.34
62	l	201	PC1	O21-C21	4.00	1.45	1.34
55	m	201	3PE	O21-C21	3.99	1.45	1.34
56	A	402	CDL	OB6-CB5	3.97	1.45	1.34
55	J	201	3PE	O21-C21	3.95	1.45	1.34
56	M	503	CDL	OA6-CA5	3.94	1.45	1.34
55	AC	404	3PE	O21-C21	3.94	1.45	1.34
55	L	702	3PE	O21-C21	3.94	1.45	1.34
55	M	501	3PE	O21-C21	3.93	1.45	1.34
55	Ac	403	3PE	O21-C21	3.93	1.45	1.34
62	L	701	PC1	O21-C21	3.92	1.45	1.34
56	AG	102	CDL	OB6-CB5	3.92	1.45	1.34
58	D	501	UQ1	C2-C1	-3.91	1.37	1.48
56	h	201	CDL	OB6-CB5	3.88	1.45	1.34
55	H	402	3PE	O21-C21	3.84	1.45	1.34
67	AC	403	HEM	C4D-ND	-3.81	1.33	1.40
70	AD	401	HEC	FE-ND	3.76	2.06	1.94
70	Ad	401	HEC	FE-ND	3.75	2.06	1.94
67	Ac	402	HEM	C4D-ND	-3.73	1.33	1.40
55	H	402	3PE	O31-C31	3.71	1.44	1.33
67	AC	402	HEM	C4D-ND	-3.67	1.34	1.40
67	Ac	401	HEM	C4D-ND	-3.59	1.34	1.40
70	Ad	401	HEC	FE-NB	3.58	2.05	1.94
70	AD	401	HEC	FE-NB	3.56	2.05	1.94
55	A	401	3PE	O21-C21	3.26	1.43	1.34
67	AC	403	HEM	C1B-NB	-3.26	1.34	1.40
64	P	401	NDP	C6N-C5N	3.23	1.39	1.33
67	Ac	402	HEM	C1B-NB	-3.21	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.06	1.35	1.40
67	Ac	401	HEM	C1B-NB	-3.06	1.35	1.40
67	Ac	402	HEM	C1C-C2C	-3.01	1.39	1.45
55	A	401	3PE	O31-C31	3.00	1.42	1.33
60	F	501	FMN	C8-C7	2.99	1.48	1.40
67	AC	403	HEM	C1C-C2C	-2.98	1.39	1.45
69	Ac	405	UQ6	O2-C2	-2.96	1.30	1.37
69	AC	406	UQ6	O2-C2	-2.95	1.30	1.37
68	AC	405	U10	C6-C5	-2.93	1.38	1.46
68	Ac	404	U10	C6-C5	-2.92	1.38	1.46
70	Ad	401	HEC	FE-NA	2.91	2.05	1.95
68	Ac	404	U10	C4-C3	2.90	1.48	1.36
68	AC	405	U10	C4-C3	2.89	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	AD	401	HEC	FE-NA	2.88	2.04	1.95
61	H	401	UQ9	C3-C2	-2.80	1.40	1.48
67	AC	403	HEM	C1D-ND	-2.72	1.33	1.38
67	Ac	402	HEM	C1D-ND	-2.69	1.33	1.38
67	AC	402	HEM	C1C-C2C	-2.67	1.40	1.45
70	AD	401	HEC	FE-NC	2.66	2.04	1.95
67	Ac	401	HEM	C1C-C2C	-2.66	1.40	1.45
70	Ad	401	HEC	FE-NC	2.65	2.04	1.95
66	n	201	EHZ	P1-O7	2.62	1.64	1.54
63	O	401	ADP	C5-C6	2.60	1.48	1.41
64	P	401	NDP	C5A-C6A	2.60	1.48	1.41
60	F	501	FMN	C4-N3	-2.59	1.34	1.38
67	AC	402	HEM	C1D-ND	-2.55	1.33	1.38
61	H	401	UQ9	C4-C5	-2.52	1.41	1.48
68	Ac	404	U10	C3-C2	-2.50	1.41	1.48
68	AC	405	U10	C3-C2	-2.47	1.41	1.48
58	D	501	UQ1	C3-C4	-2.46	1.41	1.48
67	Ac	401	HEM	C1D-ND	-2.45	1.33	1.38
66	n	201	EHZ	C9-S1	2.44	1.82	1.76
66	W	201	EHZ	O4-C15	-2.44	1.18	1.23
64	P	401	NDP	C8A-N7A	2.41	1.36	1.31
63	O	401	ADP	C8-N7	2.41	1.36	1.31
66	n	201	EHZ	O4-C15	-2.39	1.18	1.23
66	W	201	EHZ	O3-C12	-2.38	1.18	1.23
64	P	401	NDP	C5A-N7A	-2.34	1.34	1.39
58	D	501	UQ1	C3-C2	2.33	1.45	1.36
67	AC	402	HEM	FE-NB	2.32	2.02	1.94
67	Ac	401	HEM	FE-NB	2.32	2.02	1.94
67	AC	403	HEM	FE-NB	2.29	2.01	1.94
61	H	401	UQ9	C6-C5	-2.28	1.40	1.46
67	Ac	402	HEM	FE-NB	2.28	2.01	1.94
67	AC	402	HEM	FE-ND	2.28	2.01	1.94
66	n	201	EHZ	P1-OP3	-2.26	1.46	1.54
66	n	201	EHZ	O3-C12	-2.25	1.18	1.23
67	Ac	401	HEM	C3C-C4C	-2.25	1.42	1.46
67	Ac	401	HEM	FE-ND	2.24	2.01	1.94
63	O	401	ADP	C5-N7	-2.24	1.34	1.39
67	AC	402	HEM	C3C-C4C	-2.22	1.42	1.46
60	F	501	FMN	C4A-N5	2.20	1.35	1.30
66	W	201	EHZ	C9-S1	2.20	1.81	1.76
55	A	401	3PE	P-O12	-2.12	1.45	1.55
60	F	501	FMN	C5A-N5	-2.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	401	3PE	O21-C2	-2.06	1.41	1.46
55	A	401	3PE	O31-C3	-2.06	1.40	1.45
67	AC	403	HEM	C3C-C4C	-2.02	1.42	1.46

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	AC	405	U10	C6-C1-C2	7.80	125.35	119.18
68	Ac	404	U10	C6-C1-C2	7.71	125.28	119.18
70	Ad	401	HEC	C1D-ND-C4D	6.43	111.71	105.07
70	AD	401	HEC	C1D-ND-C4D	6.42	111.70	105.07
63	O	401	ADP	C5-C4-N3	-6.15	118.72	126.75
64	P	401	NDP	C5A-C4A-N3A	-6.13	118.75	126.75
66	W	201	EHZ	C8-C9-S1	6.05	121.11	113.63
66	n	201	EHZ	C8-C9-S1	5.26	120.14	113.63
63	O	401	ADP	N3-C4-N9	4.90	135.16	127.08
64	P	401	NDP	N3A-C4A-N9A	4.75	134.91	127.08
67	AC	402	HEM	CHC-C4B-NB	4.75	129.58	124.42
55	A	401	3PE	O21-C21-C22	4.72	121.67	111.50
58	D	501	UQ1	O1-C1-C2	-4.70	110.95	120.93
67	Ac	401	HEM	CHC-C4B-NB	4.67	129.49	124.42
55	H	402	3PE	O21-C21-C22	4.64	121.50	111.50
67	AC	403	HEM	C4D-ND-C1D	4.47	109.69	105.07
55	AG	103	3PE	O21-C21-C22	4.44	121.07	111.50
67	Ac	401	HEM	CHD-C4C-NC	4.39	129.19	124.44
67	Ac	402	HEM	C4D-ND-C1D	4.38	109.59	105.07
56	h	201	CDL	OB6-CB5-C51	4.37	120.92	111.50
67	AC	402	HEM	CHD-C4C-NC	4.37	129.16	124.44
62	I	301	PC1	O21-C21-C22	4.37	120.91	111.50
56	q	201	CDL	OA6-CA5-C11	4.36	120.90	111.50
56	L	703	CDL	OB6-CB5-C51	4.33	120.84	111.50
56	d	201	CDL	OA6-CA5-C11	4.33	120.83	111.50
56	A	402	CDL	OB6-CB5-C51	4.29	120.74	111.50
55	m	202	3PE	O21-C21-C22	4.28	120.73	111.50
55	L	704	3PE	O21-C21-C22	4.27	120.70	111.50
62	L	701	PC1	O21-C21-C22	4.22	120.59	111.50
67	AC	403	HEM	CHC-C4B-NB	4.21	128.99	124.42
67	Ac	402	HEM	CHC-C4B-NB	4.21	128.99	124.42
55	M	502	3PE	O21-C21-C22	4.17	120.50	111.50
56	Aa	502	CDL	OA6-CA5-C11	4.17	120.49	111.50
56	h	201	CDL	OA6-CA5-C11	4.15	120.45	111.50
68	AC	405	U10	C1-C6-C5	-4.14	115.69	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	b	201	3PE	O21-C21-C22	4.13	120.41	111.50
68	Ac	404	U10	C1-C6-C5	-4.09	115.73	119.58
55	Ac	403	3PE	O21-C21-C22	4.07	120.27	111.50
62	Ae	301	PC1	O21-C21-C22	4.03	120.19	111.50
62	q	202	PC1	O21-C21-C22	4.02	120.17	111.50
67	Ac	402	HEM	CHB-C1B-NB	4.00	129.31	124.37
55	m	201	3PE	O21-C21-C22	4.00	120.11	111.50
56	M	503	CDL	OA6-CA5-C11	3.98	120.09	111.50
56	AG	102	CDL	OA6-CA5-C11	3.97	120.06	111.50
56	AG	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
67	AC	403	HEM	CHB-C1B-NB	3.96	129.26	124.37
67	Ac	401	HEM	CHB-C1B-NB	3.95	129.24	124.37
63	O	401	ADP	C2-N3-C4	3.94	121.05	111.75
56	AG	101	CDL	OB6-CB5-C51	3.92	119.94	111.50
64	P	401	NDP	PN-O3-PA	-3.90	119.43	132.83
67	Ac	402	HEM	CHD-C4C-NC	3.90	128.66	124.44
63	O	401	ADP	PA-O3A-PB	-3.88	119.50	132.83
67	AC	402	HEM	CHB-C1B-NB	3.88	129.16	124.37
55	M	501	3PE	O21-C21-C22	3.88	119.86	111.50
67	AC	403	HEM	CHD-C4C-NC	3.87	128.63	124.44
55	J	201	3PE	O21-C21-C22	3.86	119.83	111.50
56	Y	202	CDL	OA6-CA5-C11	3.86	119.82	111.50
56	L	703	CDL	OA6-CA5-C11	3.84	119.78	111.50
64	P	401	NDP	C2A-N3A-C4A	3.84	120.82	111.75
55	Y	201	3PE	O21-C21-C22	3.82	119.73	111.50
55	i	201	3PE	O21-C21-C22	3.81	119.71	111.50
56	M	503	CDL	OB6-CB5-C51	3.79	119.68	111.50
55	L	702	3PE	O21-C21-C22	3.78	119.66	111.50
56	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
55	AC	404	3PE	O21-C21-C22	3.70	119.48	111.50
62	l	201	PC1	O21-C21-C22	3.68	119.42	111.50
56	Y	202	CDL	OB6-CB5-C51	3.64	119.35	111.50
56	q	201	CDL	OB6-CB5-C51	3.63	119.32	111.50
56	d	201	CDL	OB6-CB5-C51	3.59	119.24	111.50
56	A	402	CDL	OA6-CA5-C11	3.50	119.04	111.50
56	Ag	101	CDL	OA6-CA5-C11	3.36	120.17	110.80
56	Aa	502	CDL	OB6-CB5-C51	3.34	120.11	110.80
56	Ag	101	CDL	OB8-CB7-C71	3.33	120.12	111.38
66	n	201	EHZ	C14-C13-C12	-3.32	106.82	112.36
58	D	501	UQ1	C3-C2-C1	-3.31	114.18	120.68
67	AC	402	HEM	C4D-ND-C1D	3.29	108.48	105.07
64	P	401	NDP	C4A-C5A-N7A	-3.29	106.61	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Aa	502	CDL	OB8-CB7-C71	3.29	120.00	111.38
68	Ac	404	U10	C4-C3-C2	-3.28	114.23	120.68
55	Aa	501	3PE	O21-C21-C22	3.27	119.92	110.80
68	AC	405	U10	C4-C3-C2	-3.25	114.30	120.68
67	AC	403	HEM	C1B-NB-C4B	3.23	108.41	105.07
67	AC	403	HEM	CHD-C1D-ND	3.23	127.92	124.42
67	Ac	401	HEM	C4D-ND-C1D	3.21	108.39	105.07
67	Ac	402	HEM	C1B-NB-C4B	3.20	108.38	105.07
63	O	401	ADP	N3-C2-N1	-3.20	123.60	128.60
55	H	402	3PE	C3-C2-C1	-3.20	104.22	111.79
67	Ac	402	HEM	CHD-C1D-ND	3.18	127.88	124.42
63	O	401	ADP	C4-C5-N7	-3.12	106.82	110.62
56	AG	101	CDL	OA6-CA5-C11	3.12	119.49	110.80
56	AG	101	CDL	OB8-CB7-C71	3.11	119.53	111.38
67	Ac	401	HEM	C1B-NB-C4B	3.09	108.27	105.07
62	q	202	PC1	O31-C31-C32	3.08	121.56	111.91
64	P	401	NDP	N3A-C2A-N1A	-3.08	123.79	128.60
56	M	503	CDL	CA4-OA6-CA5	-3.07	110.22	117.79
56	A	402	CDL	CB4-OB6-CB5	-3.07	110.23	117.79
67	AC	402	HEM	C1B-NB-C4B	3.07	108.24	105.07
66	n	201	EHZ	C13-C12-N1	2.97	121.42	116.42
56	h	201	CDL	OA8-CA7-C31	2.97	121.23	111.91
62	L	701	PC1	C2-O21-C21	-2.97	110.48	117.79
56	d	201	CDL	OA8-CA7-C31	2.92	121.06	111.91
55	m	202	3PE	O31-C31-C32	2.90	121.02	111.91
67	AC	402	HEM	CHD-C1D-ND	2.88	127.55	124.42
56	AG	102	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
55	i	201	3PE	O31-C31-C32	2.86	120.89	111.91
56	Y	202	CDL	CA4-OA6-CA5	-2.85	110.78	117.79
62	I	301	PC1	O31-C31-C32	2.84	120.83	111.91
67	Ac	401	HEM	CHD-C1D-ND	2.83	127.49	124.42
56	Y	202	CDL	OB8-CB7-C71	2.82	120.74	111.91
63	O	401	ADP	C4-N9-C8	2.81	108.78	105.73
56	A	402	CDL	OA8-CA7-C31	2.81	120.72	111.91
62	I	301	PC1	C2-O21-C21	-2.80	110.89	117.79
64	P	401	NDP	C5A-N7A-C8A	2.80	107.49	103.51
55	J	201	3PE	O31-C31-C32	2.80	120.68	111.91
55	A	401	3PE	O31-C31-C32	2.79	120.66	111.91
56	AG	102	CDL	CB4-OB6-CB5	-2.79	110.93	117.79
55	M	502	3PE	O31-C31-C32	2.78	120.63	111.91
56	h	201	CDL	CB4-OB6-CB5	-2.77	110.98	117.79
56	Y	202	CDL	CB4-OB6-CB5	-2.76	110.99	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	O	401	ADP	C5-N7-C8	2.75	107.42	103.51
55	L	702	3PE	C2-O21-C21	-2.75	111.03	117.79
55	m	202	3PE	C2-O21-C21	-2.73	111.06	117.79
56	Aa	502	CDL	CB4-OB6-CB5	-2.73	111.07	117.79
56	L	703	CDL	OB8-CB7-C71	2.73	120.47	111.91
55	Ac	403	3PE	C2-O21-C21	-2.72	111.08	117.79
64	P	401	NDP	C4A-N9A-C8A	2.71	108.67	105.73
60	F	501	FMN	C4-C4A-N5	2.71	122.09	118.23
67	Ac	402	HEM	C4C-NC-C1C	2.71	108.00	105.35
56	q	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
56	Ag	101	CDL	CA4-OA6-CA5	-2.69	111.16	117.79
55	M	502	3PE	C2-O21-C21	-2.68	111.18	117.79
56	M	503	CDL	OA8-CA7-C31	2.68	120.32	111.91
55	Ac	403	3PE	O31-C31-C32	2.68	120.31	111.91
56	A	402	CDL	OB8-CB7-C71	2.68	120.31	111.91
56	L	703	CDL	OA8-CA7-C31	2.67	120.27	111.91
67	AC	403	HEM	C4C-NC-C1C	2.66	107.96	105.35
55	m	201	3PE	O31-C31-C32	2.66	120.26	111.91
62	Ae	301	PC1	O31-C31-C32	2.66	120.25	111.91
67	AC	402	HEM	CHA-C1A-NA	2.64	128.71	123.85
55	J	201	3PE	C2-O21-C21	-2.64	111.28	117.79
68	AC	405	U10	C7-C6-C5	2.64	121.66	118.48
55	AC	404	3PE	O31-C31-C32	2.63	120.17	111.91
56	q	201	CDL	OA8-CA7-C31	2.63	120.16	111.91
61	H	401	UQ9	C1M-C1-C6	-2.63	120.11	124.40
70	AD	401	HEC	CAA-CBA-CGA	-2.62	107.96	113.60
66	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
56	AG	101	CDL	OA8-CA7-C31	2.62	120.11	111.91
56	Aa	502	CDL	CA4-OA6-CA5	-2.61	111.36	117.79
56	AG	101	CDL	CB4-OB6-CB5	-2.60	111.38	117.79
67	AC	402	HEM	CHA-C4D-ND	2.59	127.57	124.37
68	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
62	Ae	301	PC1	C2-O21-C21	-2.59	111.42	117.79
55	b	201	3PE	C2-O21-C21	-2.58	111.43	117.79
67	Ac	401	HEM	CHA-C1A-NA	2.58	128.60	123.85
56	h	201	CDL	OB8-CB7-C71	2.58	120.01	111.91
70	Ad	401	HEC	CAA-CBA-CGA	-2.58	108.05	113.60
55	b	201	3PE	O31-C31-C32	2.57	119.99	111.91
55	L	704	3PE	C2-O21-C21	-2.57	111.47	117.79
56	M	503	CDL	OB8-CB7-C71	2.56	119.94	111.91
60	F	501	FMN	C4A-C10-N1	-2.55	118.81	124.73
68	Ac	404	U10	O4-C4-C5	-2.55	107.94	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	d	201	CDL	OB8-CB7-C71	2.55	119.90	111.91
68	AC	405	U10	O4-C4-C5	-2.55	107.95	116.56
55	H	402	3PE	O31-C31-C32	2.54	119.88	111.91
55	Aa	501	3PE	O31-C31-C32	2.53	119.85	111.91
55	L	704	3PE	O31-C31-C32	2.52	119.83	111.91
55	Y	201	3PE	O31-C31-C32	2.51	119.77	111.91
66	n	201	EHZ	OP3-P1-O9	-2.50	100.88	110.68
55	L	702	3PE	O31-C31-C32	2.50	119.74	111.91
56	Ag	101	CDL	OA8-CA7-C31	2.49	119.71	111.91
66	W	201	EHZ	C13-C12-N1	2.47	120.58	116.42
67	Ac	401	HEM	CHA-C4D-ND	2.47	127.42	124.37
55	m	201	3PE	C2-O21-C21	-2.47	111.72	117.79
62	l	201	PC1	O31-C31-C32	2.46	119.64	111.91
56	AG	102	CDL	OB8-CB7-C71	2.46	119.61	111.91
56	AG	102	CDL	OA8-CA7-C31	2.45	119.59	111.91
67	Ac	402	HEM	C4A-CHB-C1B	-2.45	120.53	126.34
56	q	201	CDL	CA4-OA6-CA5	-2.44	111.77	117.79
67	AC	403	HEM	C4A-NA-C1A	2.44	107.74	105.35
66	W	201	EHZ	C14-N2-C15	-2.43	118.25	122.59
67	Ac	402	HEM	CHB-C1B-C2B	-2.43	119.98	126.73
55	AG	103	3PE	O31-C31-C32	2.43	119.52	111.91
67	AC	403	HEM	C4A-CHB-C1B	-2.43	120.58	126.34
56	Aa	502	CDL	OA8-CA7-C31	2.42	119.51	111.91
67	AC	403	HEM	CHB-C1B-C2B	-2.42	120.00	126.73
62	L	701	PC1	O31-C31-C32	2.42	119.50	111.91
67	Ac	402	HEM	C4A-NA-C1A	2.42	107.71	105.35
62	Ae	301	PC1	C11-C12-N	-2.41	107.73	115.78
67	Ac	401	HEM	C4B-C3B-C2B	-2.37	105.23	107.11
66	n	201	EHZ	C11-N1-C12	-2.37	118.44	122.84
55	AC	404	3PE	C2-O21-C21	-2.37	111.96	117.79
67	AC	402	HEM	C4B-C3B-C2B	-2.37	105.24	107.11
55	M	501	3PE	O31-C31-C32	2.36	119.33	111.91
55	H	402	3PE	C24-C23-C22	-2.36	104.70	113.19
62	l	201	PC1	C2-O21-C21	-2.36	111.98	117.79
66	W	201	EHZ	O2-C9-S1	-2.35	119.56	122.61
56	Y	202	CDL	OA8-CA7-C31	2.35	119.29	111.91
66	n	201	EHZ	C10-S1-C9	2.35	109.18	101.87
62	q	202	PC1	C2-O21-C21	-2.35	112.01	117.79
67	AC	403	HEM	CHA-C4D-ND	2.32	127.24	124.37
67	Ac	401	HEM	C4A-NA-C1A	2.30	107.60	105.35
56	AG	101	CDL	CA4-OA6-CA5	-2.29	112.16	117.79
67	AC	402	HEM	C4A-NA-C1A	2.29	107.59	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	q	201	CDL	CB4-OB6-CB5	-2.27	112.19	117.79
56	Ag	101	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
56	h	201	CDL	OB6-CB5-OB7	-2.26	118.24	123.70
55	A	401	3PE	O12-P-O14	-2.26	101.08	112.24
67	Ac	402	HEM	CHA-C4D-ND	2.26	127.16	124.37
55	Y	201	3PE	C2-O21-C21	-2.25	112.25	117.79
67	Ac	401	HEM	CHB-C1B-C2B	-2.24	120.50	126.73
67	Ac	402	HEM	CHA-C1A-NA	2.24	127.97	123.85
63	O	401	ADP	N9-C8-N7	-2.24	110.86	113.91
67	Ac	402	HEM	C4C-CHD-C1D	-2.23	121.24	126.06
67	AC	402	HEM	CHB-C1B-C2B	-2.23	120.53	126.73
55	AC	401	3PE	C2-O21-C21	2.23	123.29	117.79
67	Ac	402	HEM	C1C-CHC-C4B	-2.23	121.24	126.06
66	n	201	EHZ	O2-C9-S1	-2.23	119.72	122.61
67	AC	403	HEM	CHA-C1A-NA	2.23	127.95	123.85
67	AC	403	HEM	C4C-CHD-C1D	-2.23	121.25	126.06
55	AG	103	3PE	C2-O21-C21	-2.22	112.31	117.79
67	AC	403	HEM	C1C-CHC-C4B	-2.22	121.27	126.06
60	F	501	FMN	O2-C2-N1	-2.21	118.16	121.83
64	P	401	NDP	C6A-C5A-N7A	2.21	136.13	132.02
67	Ac	401	HEM	C4C-NC-C1C	2.21	107.51	105.35
64	P	401	NDP	N9A-C8A-N7A	-2.20	110.91	113.91
67	AC	402	HEM	C4C-NC-C1C	2.19	107.50	105.35
63	O	401	ADP	C6-C5-N7	2.19	136.10	132.02
60	F	501	FMN	C4A-C10-N10	2.19	119.67	116.48
60	F	501	FMN	O4-C4-C4A	-2.18	120.82	126.60
58	D	501	UQ1	O1-C1-C6	-2.18	117.73	121.55
56	d	201	CDL	CA4-OA6-CA5	-2.18	112.43	117.79
70	AD	401	HEC	CHA-C4D-ND	2.17	126.78	124.42
70	Ad	401	HEC	CHA-C4D-ND	2.17	126.77	124.42
67	AC	403	HEM	C2A-C1A-NA	-2.16	107.73	110.15
62	q	202	PC1	O31-C31-O32	-2.14	118.18	123.59
56	M	503	CDL	OA6-CA5-OA7	-2.14	118.54	123.70
70	Ad	401	HEC	C3C-C4C-NC	-2.13	107.77	110.15
67	Ac	402	HEM	C2A-C1A-NA	-2.13	107.77	110.15
58	D	501	UQ1	CM2-O2-C2	2.11	123.93	116.47
70	AD	401	HEC	C3C-C4C-NC	-2.10	107.80	110.15
66	n	201	EHZ	C14-N2-C15	-2.10	118.84	122.59
55	M	501	3PE	C2-O21-C21	-2.10	112.62	117.79
60	F	501	FMN	C10-N1-C2	2.10	121.10	116.90
67	AC	402	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
55	H	402	3PE	C26-C25-C24	-2.09	103.80	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	m	202	3PE	O21-C21-O22	-2.09	118.65	123.70
67	Ac	401	HEM	C1C-CHC-C4B	-2.09	121.55	126.06
70	AD	401	HEC	C2A-C1A-NA	-2.08	108.30	110.32
70	Ad	401	HEC	C4A-NA-C1A	2.08	107.38	105.35
67	AC	403	HEM	CAD-C3D-C4D	2.07	128.28	124.66
55	m	202	3PE	O31-C31-O32	-2.07	118.38	123.59
70	Ad	401	HEC	C4C-NC-C1C	2.06	107.37	105.35
56	L	703	CDL	OB8-CB7-OB9	-2.05	118.41	123.59
55	L	704	3PE	O21-C21-O22	-2.05	118.75	123.70
64	P	401	NDP	C3D-C2D-C1D	2.05	105.31	101.43
70	AD	401	HEC	C4A-NA-C1A	2.05	107.35	105.35
67	Ac	402	HEM	CAD-C3D-C4D	2.04	128.22	124.66
67	Ac	401	HEM	C4A-CHB-C1B	-2.04	121.50	126.34
56	A	402	CDL	OB6-CB5-OB7	-2.04	118.78	123.70
68	Ac	404	U10	C3M-O3-C3	2.04	123.69	116.47
62	l	201	PC1	C11-C12-N	-2.04	108.98	115.78
58	D	501	UQ1	O2-C2-C3	2.04	131.31	123.64
67	AC	402	HEM	CAA-CBA-CGA	-2.03	109.23	113.60
60	F	501	FMN	C4A-C4-N3	2.03	118.35	113.19
67	Ac	401	HEM	CAA-CBA-CGA	-2.03	109.23	113.60
68	AC	405	U10	C3M-O3-C3	2.03	123.66	116.47
67	AC	402	HEM	C4A-CHB-C1B	-2.03	121.53	126.34
70	Ad	401	HEC	C4B-NB-C1B	2.03	107.17	105.07
70	AD	401	HEC	C4C-NC-C1C	2.02	107.33	105.35
68	AC	405	U10	O4-C4-C3	2.02	131.26	123.64
55	m	201	3PE	O21-C21-O22	-2.01	118.83	123.70
70	Ad	401	HEC	C2A-C1A-NA	-2.01	108.37	110.32
68	Ac	404	U10	O4-C4-C3	2.00	131.20	123.64

All (2) chirality outliers are listed below:

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

All (559) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	O22-C21-O21-C2
55	H	402	3PE	C11-O13-P-O11
55	H	402	3PE	C11-O13-P-O12
55	H	402	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
55	H	402	3PE	O13-C11-C12-N
55	J	201	3PE	C1-O11-P-O12
55	J	201	3PE	C1-O11-P-O13
55	J	201	3PE	C11-O13-P-O12
55	J	201	3PE	C11-O13-P-O14
55	L	702	3PE	C1-O11-P-O12
55	L	702	3PE	C1-O11-P-O14
55	L	702	3PE	O22-C21-O21-C2
55	L	702	3PE	C22-C21-O21-C2
55	L	704	3PE	C1-O11-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-O14
55	M	502	3PE	C11-O13-P-O14
55	Y	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C1-O11-P-O14
55	b	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C1-O11-P-O12
55	i	201	3PE	C1-O11-P-O14
55	m	201	3PE	C11-O13-P-O14
55	m	202	3PE	C11-O13-P-O14
55	AC	401	3PE	C11-O13-P-O12
55	AC	401	3PE	O13-C11-C12-N
55	AG	103	3PE	C1-O11-P-O12
55	AG	103	3PE	C1-O11-P-O13
55	AG	103	3PE	C1-O11-P-O14
55	AG	103	3PE	C11-O13-P-O14
55	Aa	501	3PE	C11-O13-P-O12
55	Ag	103	3PE	C1-O11-P-O12
55	Ag	103	3PE	C1-O11-P-O14
55	Ag	103	3PE	C11-O13-P-O11
55	Ag	103	3PE	O13-C11-C12-N
56	A	402	CDL	CA4-CA3-OA5-PA1
56	A	402	CDL	CB3-OB5-PB2-OB3
56	A	402	CDL	CB3-OB5-PB2-OB4
56	L	703	CDL	CA2-OA2-PA1-OA3
56	L	703	CDL	CB3-OB5-PB2-OB3
56	L	703	CDL	C51-CB5-OB6-CB4
56	M	503	CDL	CA3-OA5-PA1-OA4
56	M	503	CDL	CA4-CA3-OA5-PA1
56	M	503	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
56	M	503	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CB3-OB5-PB2-OB3
56	M	503	CDL	CB3-OB5-PB2-OB4
56	Y	202	CDL	CA3-OA5-PA1-OA2
56	Y	202	CDL	CB2-OB2-PB2-OB4
56	Y	202	CDL	CB3-OB5-PB2-OB4
56	Y	202	CDL	C51-CB5-OB6-CB4
56	d	201	CDL	CA2-OA2-PA1-OA3
56	d	201	CDL	CA2-OA2-PA1-OA4
56	d	201	CDL	C11-CA5-OA6-CA4
56	d	201	CDL	CB2-OB2-PB2-OB3
56	d	201	CDL	CB2-OB2-PB2-OB4
56	d	201	CDL	CB2-OB2-PB2-OB5
56	h	201	CDL	CA2-OA2-PA1-OA4
56	h	201	CDL	C11-CA5-OA6-CA4
56	h	201	CDL	CB2-OB2-PB2-OB3
56	h	201	CDL	OB7-CB5-OB6-CB4
56	q	201	CDL	CA3-OA5-PA1-OA3
56	q	201	CDL	CA3-OA5-PA1-OA4
56	AG	101	CDL	CA2-OA2-PA1-OA4
56	AG	101	CDL	CB2-OB2-PB2-OB3
56	AG	102	CDL	C1-CB2-OB2-PB2
56	AG	102	CDL	CB2-OB2-PB2-OB4
56	AG	102	CDL	CB3-OB5-PB2-OB2
56	AG	102	CDL	CB3-OB5-PB2-OB3
56	AG	102	CDL	CB3-OB5-PB2-OB4
56	Aa	502	CDL	CA2-OA2-PA1-OA5
56	Aa	502	CDL	CA3-OA5-PA1-OA3
56	Aa	502	CDL	CB2-OB2-PB2-OB3
56	Aa	502	CDL	CB2-OB2-PB2-OB4
56	Ag	101	CDL	CB2-OB2-PB2-OB3
56	Ag	101	CDL	CB2-OB2-PB2-OB4
56	Ag	101	CDL	CB2-OB2-PB2-OB5
56	Ag	101	CDL	CB3-OB5-PB2-OB2
56	Ag	101	CDL	CB3-OB5-PB2-OB3
56	Ag	101	CDL	CB3-OB5-PB2-OB4
56	Ag	102	CDL	CB2-OB2-PB2-OB5
56	Ag	102	CDL	CB3-OB5-PB2-OB4
58	D	501	UQ1	C1-C6-C7-C8
58	D	501	UQ1	C5-C6-C7-C8
61	H	401	UQ9	C24-C26-C27-C28
61	H	401	UQ9	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
61	H	401	UQ9	C22-C23-C24-C25
61	H	401	UQ9	C21-C22-C23-C24
61	H	401	UQ9	C19-C21-C22-C23
61	H	401	UQ9	C17-C18-C19-C21
61	H	401	UQ9	C17-C18-C19-C20
62	I	301	PC1	C11-O13-P-O12
62	I	301	PC1	C11-O13-P-O14
62	I	301	PC1	C11-O13-P-O11
62	L	701	PC1	C11-O13-P-O12
62	L	701	PC1	C11-O13-P-O14
62	L	701	PC1	C1-O11-P-O12
62	L	701	PC1	C1-O11-P-O14
62	L	701	PC1	C1-O11-P-O13
62	l	201	PC1	C11-O13-P-O14
62	q	202	PC1	C11-O13-P-O14
62	q	202	PC1	C1-O11-P-O12
62	q	202	PC1	C1-O11-P-O14
62	q	202	PC1	C1-O11-P-O13
62	Ae	301	PC1	C1-O11-P-O12
62	Ae	301	PC1	O13-C11-C12-N
63	O	401	ADP	C5'-O5'-PA-O3A
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	O2-C9-S1-C10
66	W	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C6-C7-C8-C9
66	n	201	EHZ	S1-C10-C11-N1
66	n	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C19
66	n	201	EHZ	C15-C16-C17-C20
66	n	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C19
66	n	201	EHZ	O5-C16-C17-C20
66	n	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C20-O6-P1-OP3
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C2C-C3C-CAC-CBC
67	AC	402	HEM	C4C-C3C-CAC-CBC
67	AC	403	HEM	C2B-C3B-CAB-CBB
67	AC	403	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
67	AC	403	HEM	C2C-C3C-CAC-CBC
67	Ac	401	HEM	C2B-C3B-CAB-CBB
67	Ac	401	HEM	C2C-C3C-CAC-CBC
67	Ac	401	HEM	C4C-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
68	AC	405	U10	C7-C8-C9-C10
68	AC	405	U10	C7-C8-C9-C11
68	Ac	404	U10	C7-C8-C9-C10
68	Ac	404	U10	C7-C8-C9-C11
69	AC	406	UQ6	C1-C6-C7-C8
69	AC	406	UQ6	C7-C8-C9-C10
69	AC	406	UQ6	C7-C8-C9-C11
69	AC	406	UQ6	C12-C13-C14-C15
69	AC	406	UQ6	C12-C13-C14-C16
69	AC	406	UQ6	C13-C14-C16-C17
69	AC	406	UQ6	C15-C14-C16-C17
69	AC	406	UQ6	C17-C18-C19-C20
69	Ac	405	UQ6	C1-C6-C7-C8
69	Ac	405	UQ6	C7-C8-C9-C10
69	Ac	405	UQ6	C7-C8-C9-C11
69	Ac	405	UQ6	C12-C13-C14-C15
69	Ac	405	UQ6	C12-C13-C14-C16
69	Ac	405	UQ6	C13-C14-C16-C17
69	Ac	405	UQ6	C15-C14-C16-C17
69	Ac	405	UQ6	C17-C18-C19-C20
55	H	402	3PE	O32-C31-O31-C3
56	L	703	CDL	OA9-CA7-OA8-CA6
55	m	202	3PE	C2-C3-O31-C31
55	b	201	3PE	C32-C31-O31-C3
56	L	703	CDL	C31-CA7-OA8-CA6
58	D	501	UQ1	C7-C8-C9-C10
58	D	501	UQ1	C7-C8-C9-C11
68	AC	405	U10	C12-C13-C14-C15
68	AC	405	U10	C12-C13-C14-C16
68	Ac	404	U10	C12-C13-C14-C15
68	Ac	404	U10	C12-C13-C14-C16
55	J	201	3PE	O32-C31-O31-C3
55	Y	201	3PE	O32-C31-O31-C3
55	b	201	3PE	O32-C31-O31-C3
55	m	202	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
55	M	502	3PE	O22-C21-O21-C2
56	L	703	CDL	OB7-CB5-OB6-CB4
56	Y	202	CDL	OB7-CB5-OB6-CB4
56	d	201	CDL	OA7-CA5-OA6-CA4
55	H	402	3PE	C32-C31-O31-C3
55	Y	201	3PE	C32-C31-O31-C3
55	m	202	3PE	C32-C31-O31-C3
55	A	401	3PE	C22-C21-O21-C2
55	M	502	3PE	C22-C21-O21-C2
55	Y	201	3PE	C22-C21-O21-C2
55	b	201	3PE	C22-C21-O21-C2
56	h	201	CDL	C51-CB5-OB6-CB4
55	J	201	3PE	C32-C31-O31-C3
56	h	201	CDL	C31-CA7-OA8-CA6
69	AC	406	UQ6	C17-C18-C19-C21
69	Ac	405	UQ6	C17-C18-C19-C21
61	H	401	UQ9	C7-C8-C9-C10
56	M	503	CDL	OB7-CB5-OB6-CB4
56	h	201	CDL	OA7-CA5-OA6-CA4
62	Ae	301	PC1	O32-C31-O31-C3
62	I	301	PC1	C32-C31-O31-C3
55	Aa	501	3PE	C22-C21-O21-C2
56	M	503	CDL	C51-CB5-OB6-CB4
62	Ae	301	PC1	C32-C31-O31-C3
56	h	201	CDL	OA9-CA7-OA8-CA6
62	I	301	PC1	O32-C31-O31-C3
62	L	701	PC1	O32-C31-O31-C3
61	H	401	UQ9	C9-C11-C12-C13
69	AC	406	UQ6	C9-C11-C12-C13
69	AC	406	UQ6	C14-C16-C17-C18
69	Ac	405	UQ6	C9-C11-C12-C13
69	Ac	405	UQ6	C14-C16-C17-C18
62	L	701	PC1	C32-C31-O31-C3
55	Aa	501	3PE	O22-C21-O21-C2
55	m	201	3PE	C32-C31-O31-C3
56	Y	202	CDL	C71-CB7-OB8-CB6
62	l	201	PC1	C32-C31-O31-C3
55	H	402	3PE	C24-C25-C26-C27
55	A	401	3PE	C32-C31-O31-C3
55	Ag	103	3PE	C32-C33-C34-C35
66	n	201	EHZ	C5-C6-C7-O1
56	Y	202	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
62	q	202	PC1	C2-C1-O11-P
56	Y	202	CDL	OB9-CB7-OB8-CB6
55	m	201	3PE	O32-C31-O31-C3
62	l	201	PC1	O32-C31-O31-C3
56	M	503	CDL	C71-CB7-OB8-CB6
55	A	401	3PE	O32-C31-O31-C3
55	L	702	3PE	C33-C34-C35-C36
56	q	201	CDL	C12-C13-C14-C15
56	A	402	CDL	C11-CA5-OA6-CA4
56	A	402	CDL	C51-CB5-OB6-CB4
55	J	201	3PE	C11-O13-P-O11
55	L	702	3PE	C1-O11-P-O13
55	i	201	3PE	C1-O11-P-O13
55	m	201	3PE	C1-O11-P-O13
55	m	201	3PE	C11-O13-P-O11
55	AC	401	3PE	C11-O13-P-O11
55	AG	103	3PE	C11-O13-P-O11
55	Ag	103	3PE	C1-O11-P-O13
56	A	402	CDL	CA3-OA5-PA1-OA2
56	A	402	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CA2-OA2-PA1-OA5
56	M	503	CDL	CA3-OA5-PA1-OA2
56	Y	202	CDL	CB2-OB2-PB2-OB5
56	Y	202	CDL	CB3-OB5-PB2-OB2
56	d	201	CDL	CA2-OA2-PA1-OA5
56	h	201	CDL	CB2-OB2-PB2-OB5
56	h	201	CDL	CB3-OB5-PB2-OB2
56	q	201	CDL	CA3-OA5-PA1-OA2
56	AG	101	CDL	CB2-OB2-PB2-OB5
56	AG	102	CDL	CB2-OB2-PB2-OB5
56	Aa	502	CDL	CB2-OB2-PB2-OB5
56	Aa	502	CDL	CB3-OB5-PB2-OB2
56	Ag	102	CDL	CB3-OB5-PB2-OB2
62	L	701	PC1	C11-O13-P-O11
62	q	202	PC1	C11-O13-P-O11
62	l	201	PC1	C3B-C3C-C3D-C3E
56	A	402	CDL	C71-CB7-OB8-CB6
56	A	402	CDL	OA7-CA5-OA6-CA4
56	A	402	CDL	OB7-CB5-OB6-CB4
55	AG	103	3PE	C32-C33-C34-C35
56	A	402	CDL	C31-CA7-OA8-CA6
55	Ag	103	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
66	W	201	EHZ	C18-C17-C20-O6
66	W	201	EHZ	C19-C17-C20-O6
55	A	401	3PE	C3-C2-O21-C21
56	h	201	CDL	CA3-CA4-OA6-CA5
56	AG	101	CDL	C31-CA7-OA8-CA6
56	Aa	502	CDL	C51-CB5-OB6-CB4
55	Ag	103	3PE	C37-C38-C39-C3A
56	Ag	102	CDL	C74-C75-C76-C77
55	A	401	3PE	O13-C11-C12-N
55	M	501	3PE	C32-C33-C34-C35
56	A	402	CDL	OA9-CA7-OA8-CA6
56	A	402	CDL	OB9-CB7-OB8-CB6
56	h	201	CDL	C71-CB7-OB8-CB6
56	Y	202	CDL	C73-C74-C75-C76
55	L	704	3PE	C22-C21-O21-C2
56	Y	202	CDL	C11-CA5-OA6-CA4
56	M	503	CDL	OB9-CB7-OB8-CB6
55	L	704	3PE	O22-C21-O21-C2
56	Y	202	CDL	OA7-CA5-OA6-CA4
56	Aa	502	CDL	OB7-CB5-OB6-CB4
61	H	401	UQ9	C7-C8-C9-C11
55	AG	103	3PE	C37-C38-C39-C3A
56	h	201	CDL	OB9-CB7-OB8-CB6
56	AG	101	CDL	OA9-CA7-OA8-CA6
56	L	703	CDL	C71-CB7-OB8-CB6
56	AG	102	CDL	C31-CA7-OA8-CA6
55	i	201	3PE	C32-C31-O31-C3
56	AG	102	CDL	C74-C75-C76-C77
55	m	201	3PE	C22-C21-O21-C2
55	H	402	3PE	C39-C3A-C3B-C3C
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	AC	403	HEM	C4C-C3C-CAC-CBC
67	Ac	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4C-C3C-CAC-CBC
55	M	501	3PE	C22-C21-O21-C2
56	AG	102	CDL	C51-CB5-OB6-CB4
56	h	201	CDL	C56-C57-C58-C59
55	m	202	3PE	C11-O13-P-O11
55	Aa	501	3PE	C11-O13-P-O11
56	A	402	CDL	CB2-OB2-PB2-OB5
56	AG	101	CDL	CA2-OA2-PA1-OA5
56	Ag	102	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
66	W	201	EHZ	C3-C4-C5-C6
55	M	502	3PE	C3C-C3D-C3E-C3F
56	q	201	CDL	C11-CA5-OA6-CA4
56	AG	102	CDL	OA9-CA7-OA8-CA6
56	M	503	CDL	C43-C44-C45-C46
55	L	702	3PE	C25-C26-C27-C28
56	L	703	CDL	C12-C13-C14-C15
62	L	701	PC1	C33-C34-C35-C36
56	L	703	CDL	OB9-CB7-OB8-CB6
66	n	201	EHZ	O4-C15-C16-O5
55	A	401	3PE	C27-C28-C29-C2A
66	W	201	EHZ	C5-C6-C7-O1
56	A	402	CDL	CA3-CA4-OA6-CA5
56	M	503	CDL	CB6-CB4-OB6-CB5
56	M	503	CDL	C11-C12-C13-C14
62	Ae	301	PC1	C2-C1-O11-P
55	i	201	3PE	O32-C31-O31-C3
62	l	201	PC1	C33-C34-C35-C36
55	A	401	3PE	O21-C2-C3-O31
55	m	201	3PE	O22-C21-O21-C2
56	M	503	CDL	C31-C32-C33-C34
55	J	201	3PE	C33-C34-C35-C36
66	W	201	EHZ	C5-C6-C7-C8
66	n	201	EHZ	C5-C6-C7-C8
55	L	702	3PE	C32-C31-O31-C3
56	q	201	CDL	C31-CA7-OA8-CA6
55	L	702	3PE	C31-C32-C33-C34
56	Ag	102	CDL	OB5-CB3-CB4-CB6
56	Aa	502	CDL	C71-CB7-OB8-CB6
56	d	201	CDL	C54-C55-C56-C57
55	M	501	3PE	O22-C21-O21-C2
62	q	202	PC1	C32-C31-O31-C3
56	Y	202	CDL	CA4-CA3-OA5-PA1
56	d	201	CDL	C1-CA2-OA2-PA1
64	P	401	NDP	O4D-C1D-N1N-C6N
67	AC	402	HEM	C2A-CAA-CBA-CGA
67	Ac	401	HEM	C2A-CAA-CBA-CGA
56	d	201	CDL	C33-C34-C35-C36
55	L	704	3PE	C1-O11-P-O13
55	M	501	3PE	C11-O13-P-O11
55	M	502	3PE	C11-O13-P-O11
56	A	402	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
56	h	201	CDL	CA2-OA2-PA1-OA5
62	Ae	301	PC1	C1-O11-P-O13
56	M	503	CDL	C34-C35-C36-C37
56	Y	202	CDL	C72-C73-C74-C75
55	A	401	3PE	C37-C38-C39-C3A
56	Ag	102	CDL	OB5-CB3-CB4-OB6
56	AG	102	CDL	OB7-CB5-OB6-CB4
56	q	201	CDL	OB6-CB4-CB6-OB8
55	H	402	3PE	C34-C35-C36-C37
55	M	502	3PE	C36-C37-C38-C39
56	q	201	CDL	OA7-CA5-OA6-CA4
55	L	704	3PE	C2-C1-O11-P
56	AG	102	CDL	C1-CA2-OA2-PA1
62	I	301	PC1	C11-C12-N-C15
55	A	401	3PE	C2B-C2C-C2D-C2E
56	L	703	CDL	C31-C32-C33-C34
55	L	702	3PE	O32-C31-O31-C3
56	q	201	CDL	OA9-CA7-OA8-CA6
56	Y	202	CDL	CB7-C71-C72-C73
66	n	201	EHZ	N2-C15-C16-O5
56	h	201	CDL	C73-C74-C75-C76
55	Aa	501	3PE	C3-C2-O21-C21
56	Aa	502	CDL	OB9-CB7-OB8-CB6
56	d	201	CDL	C60-C61-C62-C63
55	i	201	3PE	C1-C2-C3-O31
56	A	402	CDL	CB4-CB3-OB5-PB2
56	q	201	CDL	CB3-CB4-CB6-OB8
56	AG	102	CDL	CB4-CB3-OB5-PB2
62	q	202	PC1	O32-C31-O31-C3
56	Y	202	CDL	OA5-CA3-CA4-OA6
62	I	301	PC1	C11-C12-N-C13
55	m	201	3PE	C33-C34-C35-C36
62	q	202	PC1	C32-C33-C34-C35
55	A	401	3PE	C22-C23-C24-C25
55	H	402	3PE	C1-O11-P-O13
55	b	201	3PE	C1-O11-P-O13
56	d	201	CDL	CA3-OA5-PA1-OA2
62	I	301	PC1	C1-O11-P-O13
56	A	402	CDL	C1-CA2-OA2-PA1
56	q	201	CDL	CA4-CA3-OA5-PA1
56	Ag	102	CDL	CB4-CB3-OB5-PB2
55	J	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
55	L	704	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O12
55	b	201	3PE	C1-O11-P-O12
55	m	201	3PE	C1-O11-P-O14
55	m	201	3PE	C11-O13-P-O12
55	m	202	3PE	C11-O13-P-O12
55	AC	401	3PE	C11-O13-P-O14
55	AG	103	3PE	C11-O13-P-O12
55	Aa	501	3PE	C11-O13-P-O14
55	Ag	103	3PE	C11-O13-P-O12
56	A	402	CDL	CA3-OA5-PA1-OA3
56	M	503	CDL	CA2-OA2-PA1-OA4
56	Y	202	CDL	CA3-OA5-PA1-OA4
56	h	201	CDL	CA2-OA2-PA1-OA3
56	h	201	CDL	CB2-OB2-PB2-OB4
56	h	201	CDL	CB3-OB5-PB2-OB3
56	AG	101	CDL	CA2-OA2-PA1-OA3
56	AG	101	CDL	CB2-OB2-PB2-OB4
56	Aa	502	CDL	CA2-OA2-PA1-OA4
56	Aa	502	CDL	CB3-OB5-PB2-OB3
56	Aa	502	CDL	CB3-OB5-PB2-OB4
56	Ag	102	CDL	CB2-OB2-PB2-OB4
62	q	202	PC1	C11-O13-P-O12
62	Ae	301	PC1	C1-O11-P-O14
63	O	401	ADP	C5'-O5'-PA-O1A
63	O	401	ADP	C5'-O5'-PA-O2A
58	D	501	UQ1	C1-C2-O2-CM2
56	d	201	CDL	C51-C52-C53-C54
55	i	201	3PE	C32-C33-C34-C35
55	m	202	3PE	C22-C21-O21-C2
66	W	201	EHZ	C2-C3-C4-C5
62	L	701	PC1	O13-C11-C12-N
62	l	201	PC1	O13-C11-C12-N
62	q	202	PC1	O13-C11-C12-N
55	J	201	3PE	O22-C21-O21-C2
55	i	201	3PE	O21-C2-C3-O31
56	M	503	CDL	C1-CB2-OB2-PB2
56	q	201	CDL	C1-CB2-OB2-PB2
66	n	201	EHZ	C3-C4-C5-C6
56	h	201	CDL	C53-C54-C55-C56
66	W	201	EHZ	O4-C15-C16-O5
62	I	301	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
61	H	401	UQ9	C12-C11-C9-C10
55	i	201	3PE	C3-C2-O21-C21
56	L	703	CDL	CB3-CB4-OB6-CB5
55	J	201	3PE	C22-C21-O21-C2
56	q	201	CDL	C1-CA2-OA2-PA1
56	Ag	102	CDL	C1-CA2-OA2-PA1
56	AG	102	CDL	C71-CB7-OB8-CB6
56	AG	102	CDL	OB9-CB7-OB8-CB6
55	A	401	3PE	O11-C1-C2-O21
56	M	503	CDL	C15-C16-C17-C18
55	M	502	3PE	C1-O11-P-O13
55	Y	201	3PE	C1-O11-P-O13
56	L	703	CDL	CA2-OA2-PA1-OA5
56	L	703	CDL	CA3-OA5-PA1-OA2
56	L	703	CDL	CB2-OB2-PB2-OB5
56	L	703	CDL	CB3-OB5-PB2-OB2
56	M	503	CDL	CB2-OB2-PB2-OB5
56	d	201	CDL	CB3-OB5-PB2-OB2
56	q	201	CDL	CB2-OB2-PB2-OB5
62	l	201	PC1	C11-O13-P-O11
55	L	704	3PE	C21-C22-C23-C24
55	A	401	3PE	C1-C2-C3-O31
55	M	501	3PE	C1-C2-C3-O31
55	A	401	3PE	C25-C26-C27-C28
55	Ag	103	3PE	C35-C36-C37-C38
64	P	401	NDP	PN-O3-PA-O2A
55	AG	103	3PE	C35-C36-C37-C38
55	i	201	3PE	C2-C1-O11-P
55	m	202	3PE	O22-C21-O21-C2
55	J	201	3PE	C23-C24-C25-C26
56	M	503	CDL	C17-C18-C19-C20
56	Y	202	CDL	C53-C54-C55-C56
62	q	202	PC1	O11-C1-C2-C3
61	H	401	UQ9	C14-C16-C17-C18
56	L	703	CDL	C74-C75-C76-C77
56	A	402	CDL	C16-C17-C18-C19
56	Ag	101	CDL	C1-CA2-OA2-PA1
68	AC	405	U10	C12-C11-C9-C10
68	Ac	404	U10	C12-C11-C9-C10
56	h	201	CDL	C79-C80-C81-C82
67	AC	403	HEM	CAD-CBD-CGD-O1D
67	Ac	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
55	L	702	3PE	C28-C29-C2A-C2B
56	Y	202	CDL	CA3-CA4-OA6-CA5
55	i	201	3PE	O22-C21-O21-C2
55	b	201	3PE	C25-C26-C27-C28
67	AC	402	HEM	CAD-CBD-CGD-O1D
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAD-CBD-CGD-O2D
56	M	503	CDL	C42-C43-C44-C45
67	AC	402	HEM	CAA-CBA-CGA-O2A
67	Ac	401	HEM	CAA-CBA-CGA-O2A
67	Ac	401	HEM	CAD-CBD-CGD-O1D
56	A	402	CDL	C35-C36-C37-C38
56	Y	202	CDL	OA5-CA3-CA4-CA6
67	AC	403	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O2D
55	A	401	3PE	C21-C22-C23-C24
67	AC	402	HEM	CAA-CBA-CGA-O1A
67	Ac	401	HEM	CAA-CBA-CGA-O1A
56	h	201	CDL	C16-C17-C18-C19
66	n	201	EHZ	C11-C10-S1-C9
56	d	201	CDL	C36-C37-C38-C39
68	AC	405	U10	C12-C11-C9-C8
68	Ac	404	U10	C12-C11-C9-C8
56	L	703	CDL	C53-C54-C55-C56
69	AC	406	UQ6	C5-C6-C7-C8
69	Ac	405	UQ6	C5-C6-C7-C8
62	q	202	PC1	C34-C35-C36-C37
56	Y	202	CDL	C60-C61-C62-C63
56	Ag	102	CDL	C72-C73-C74-C75
61	H	401	UQ9	C12-C11-C9-C8
62	l	201	PC1	C2-C3-O31-C31
67	AC	403	HEM	CAA-CBA-CGA-O2A
67	Ac	402	HEM	CAA-CBA-CGA-O2A
56	Ag	102	CDL	C52-C51-CB5-OB6
55	b	201	3PE	C2B-C2C-C2D-C2E
62	L	701	PC1	C38-C39-C3A-C3B
66	n	201	EHZ	C20-O6-P1-O7
56	h	201	CDL	CB5-C51-C52-C53
56	A	402	CDL	C59-C60-C61-C62
55	M	502	3PE	O32-C31-O31-C3
55	L	702	3PE	C24-C25-C26-C27
56	h	201	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C39-C3A-C3B-C3C
55	L	702	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C38-C39-C3A-C3B
67	Ac	402	HEM	CAA-CBA-CGA-O1A
55	M	502	3PE	C2F-C2G-C2H-C2I
55	H	402	3PE	C2F-C2G-C2H-C2I
67	AC	403	HEM	CAA-CBA-CGA-O1A
56	L	703	CDL	C35-C36-C37-C38
66	n	201	EHZ	O1-C7-C8-C9
55	Ac	403	3PE	C23-C24-C25-C26
55	m	201	3PE	C27-C28-C29-C2A
55	i	201	3PE	O21-C21-C22-C23
55	AC	401	3PE	O31-C31-C32-C33
62	q	202	PC1	C11-C12-N-C15
55	M	502	3PE	C32-C31-O31-C3
56	h	201	CDL	C11-C12-C13-C14
61	H	401	UQ9	C23-C24-C26-C27
56	d	201	CDL	OB7-CB5-OB6-CB4
55	M	501	3PE	C33-C34-C35-C36
56	h	201	CDL	C12-C11-CA5-OA6
69	AC	406	UQ6	C6-C7-C8-C9
69	Ac	405	UQ6	C6-C7-C8-C9
55	L	702	3PE	C2B-C2C-C2D-C2E
55	i	201	3PE	O22-C21-C22-C23
55	M	502	3PE	C2-C1-O11-P
56	M	503	CDL	CB4-CB3-OB5-PB2
56	Y	202	CDL	C1-CA2-OA2-PA1
55	m	201	3PE	C36-C37-C38-C39
55	A	401	3PE	C1-O11-P-O14
55	AC	404	3PE	C11-O13-P-O14
55	Aa	501	3PE	C1-O11-P-O14
55	Ac	403	3PE	C11-O13-P-O14
56	A	402	CDL	CA2-OA2-PA1-OA4
56	A	402	CDL	CB2-OB2-PB2-OB3
56	h	201	CDL	C12-C11-CA5-OA7
55	A	401	3PE	O11-C1-C2-C3
56	M	503	CDL	OA5-CA3-CA4-CA6
55	b	201	3PE	C37-C38-C39-C3A
55	m	201	3PE	C2A-C2B-C2C-C2D
56	M	503	CDL	C73-C74-C75-C76
56	q	201	CDL	C18-C19-C20-C21
55	m	201	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
55	M	502	3PE	C12-C11-O13-P
56	Y	202	CDL	C72-C71-CB7-OB8
56	Ag	102	CDL	CB2-C1-CA2-OA2
61	H	401	UQ9	C25-C24-C26-C27
55	Ac	403	3PE	C22-C23-C24-C25
62	I	301	PC1	C2C-C2D-C2E-C2F
55	AC	401	3PE	O21-C21-C22-C23
55	AC	401	3PE	O32-C31-C32-C33
58	D	501	UQ1	C2-C3-O3-CM3

There are no ring outliers.

57 monomers are involved in 488 short contacts:

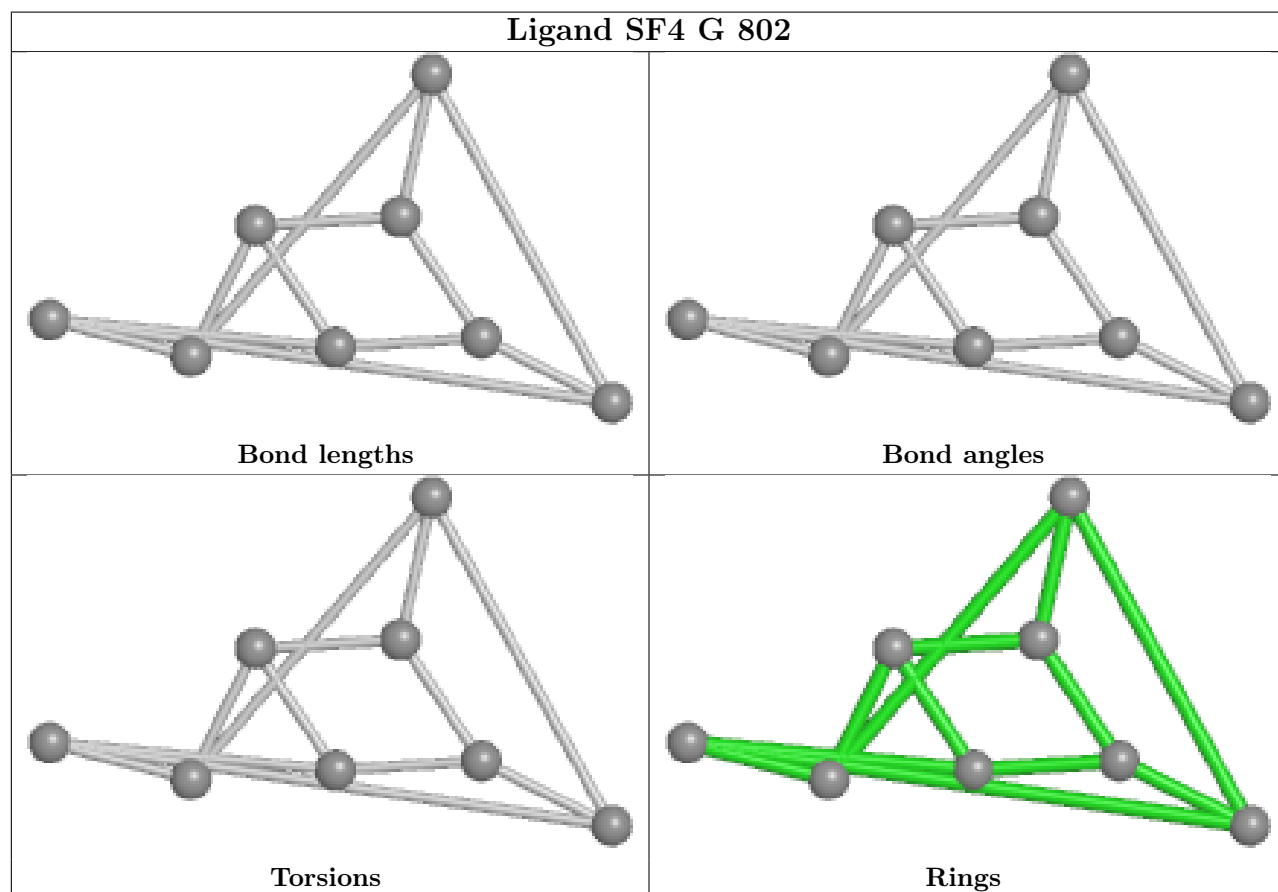
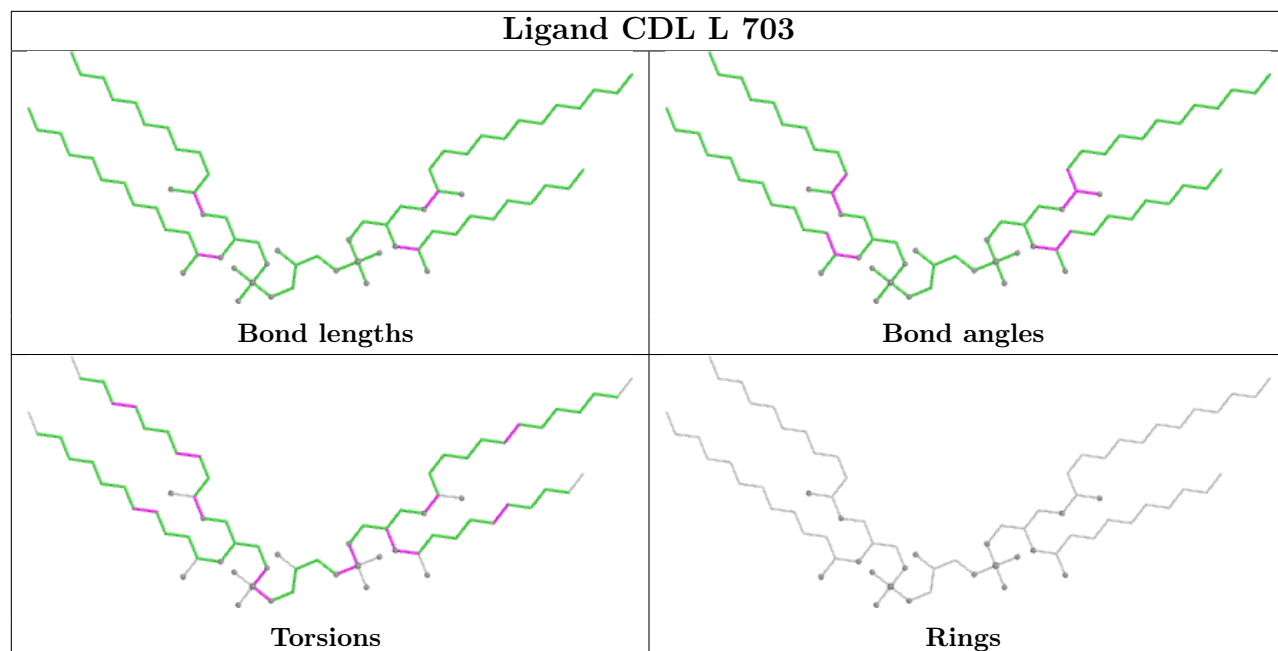
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	L	703	CDL	11	0
57	G	802	SF4	3	0
56	A	402	CDL	21	0
63	O	401	ADP	8	0
55	m	201	3PE	17	0
62	Ae	301	PC1	6	0
55	AC	404	3PE	6	0
55	Ac	403	3PE	4	0
56	Ag	102	CDL	5	0
68	Ac	404	U10	21	0
69	AC	406	UQ6	27	0
55	L	702	3PE	5	0
67	AC	402	HEM	7	0
55	b	201	3PE	13	0
55	M	501	3PE	7	0
56	Y	202	CDL	18	0
56	Ag	101	CDL	4	0
55	Y	201	3PE	4	0
56	h	201	CDL	11	0
62	I	301	PC1	9	0
56	d	201	CDL	11	0
64	P	401	NDP	2	0
55	J	201	3PE	6	0
55	AC	401	3PE	2	0
57	B	301	SF4	2	0
69	Ac	405	UQ6	12	0
59	G	803	FES	6	0
60	F	501	FMN	2	0

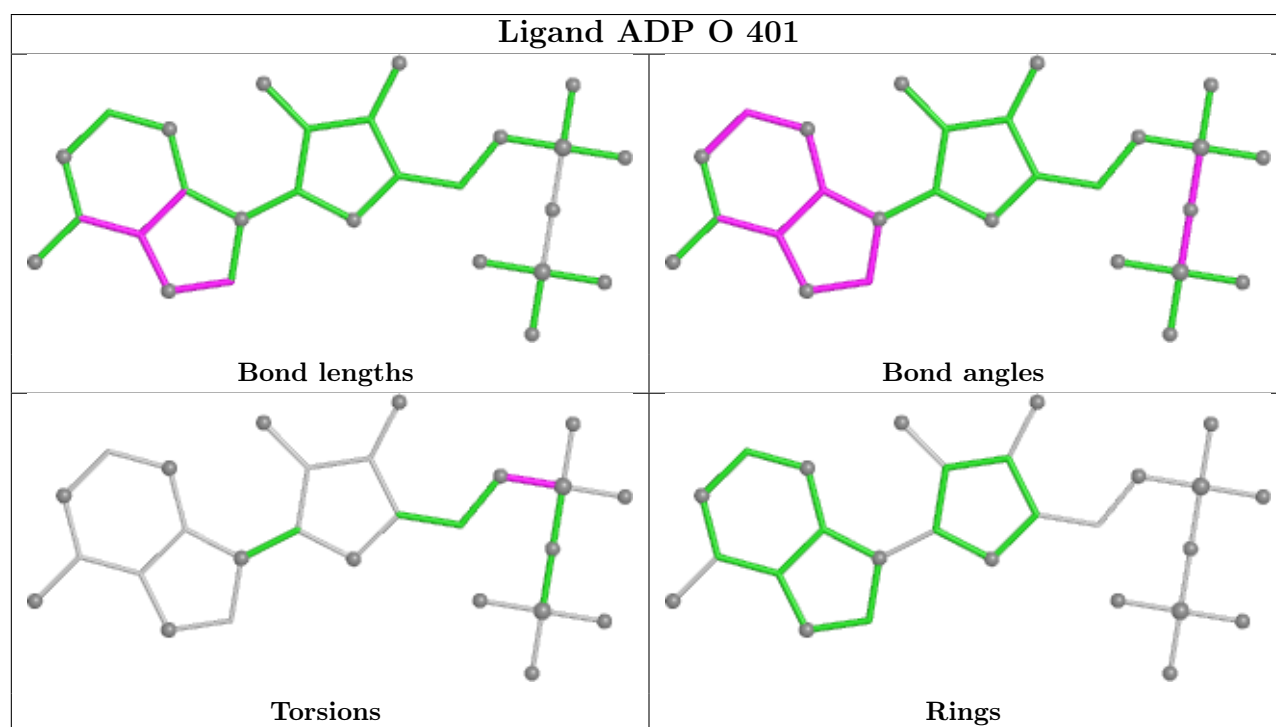
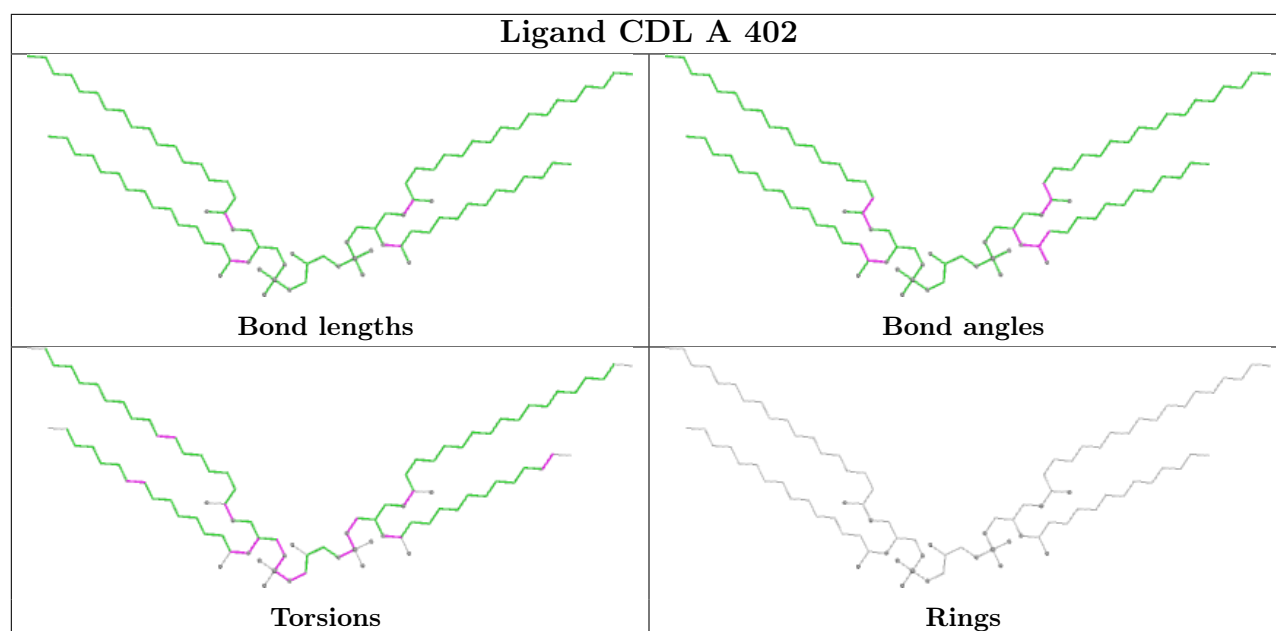
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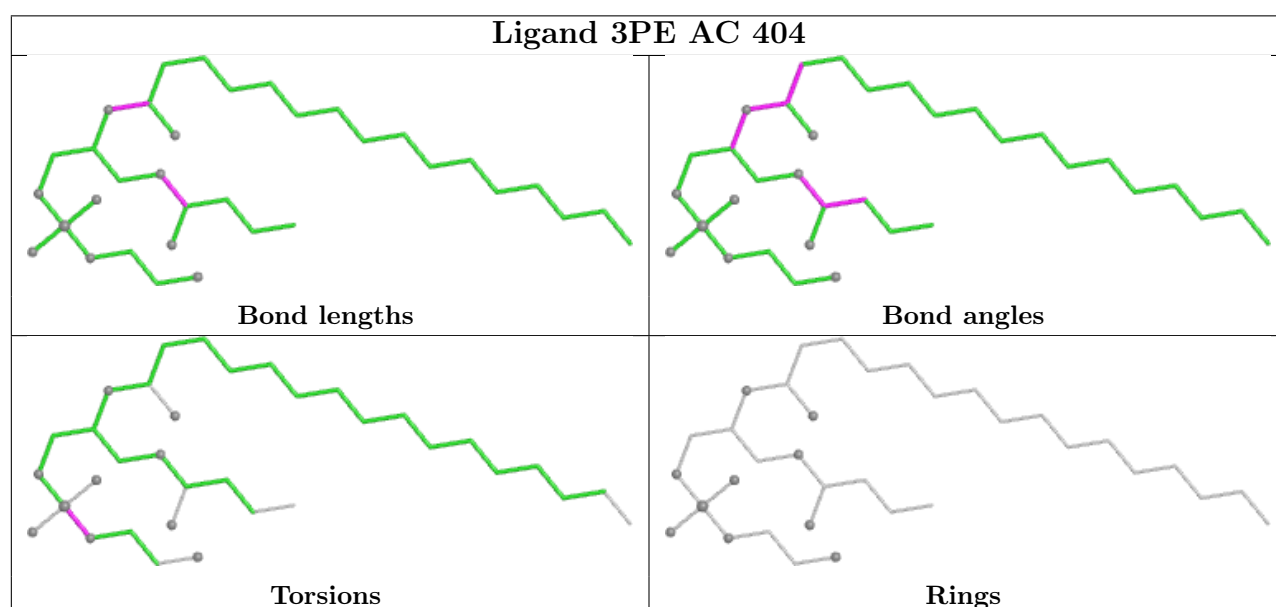
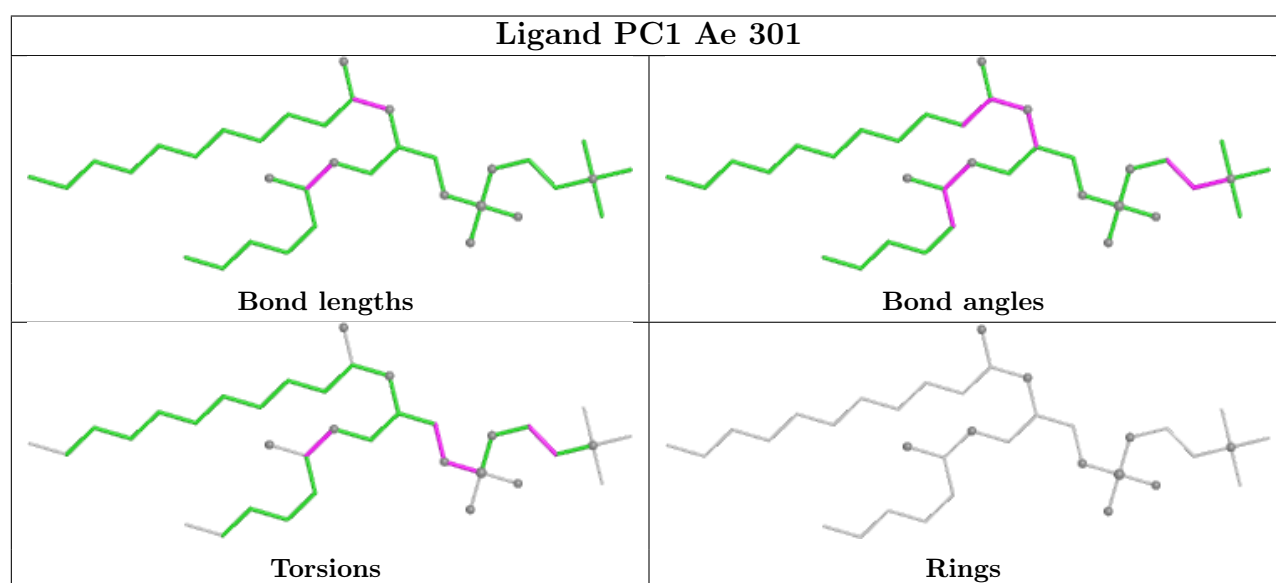
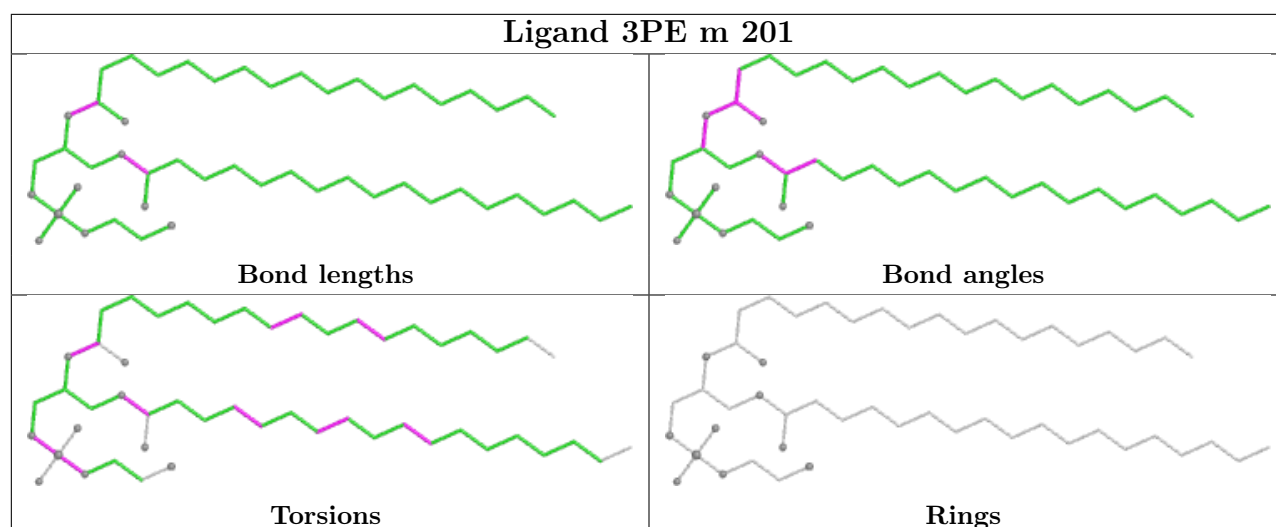
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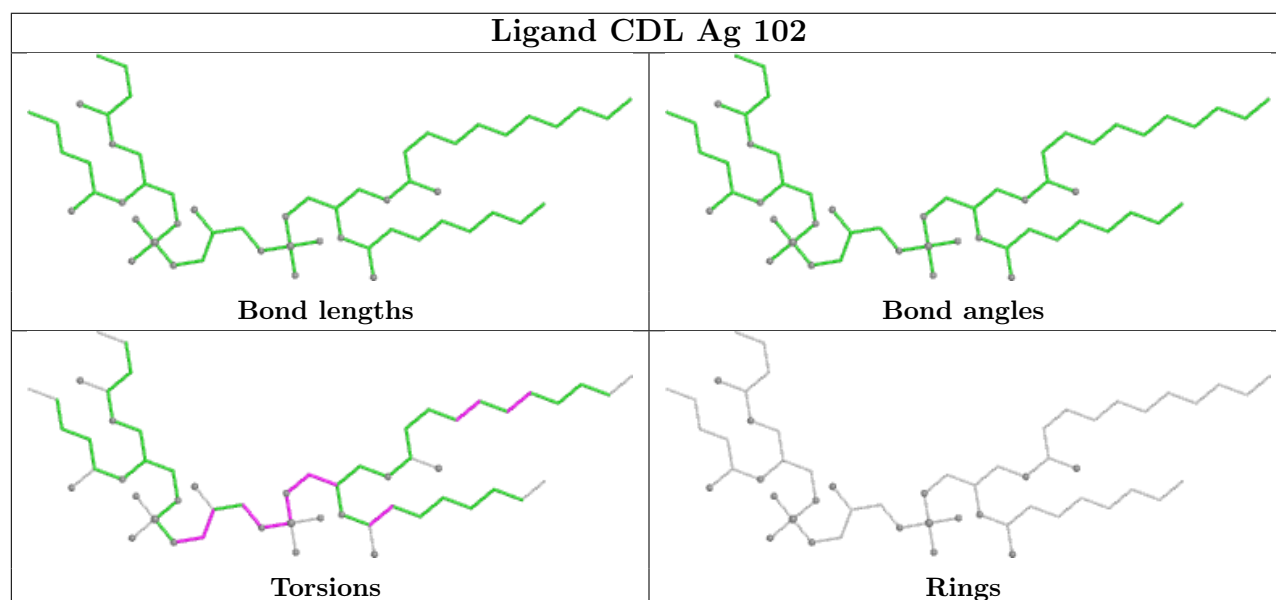
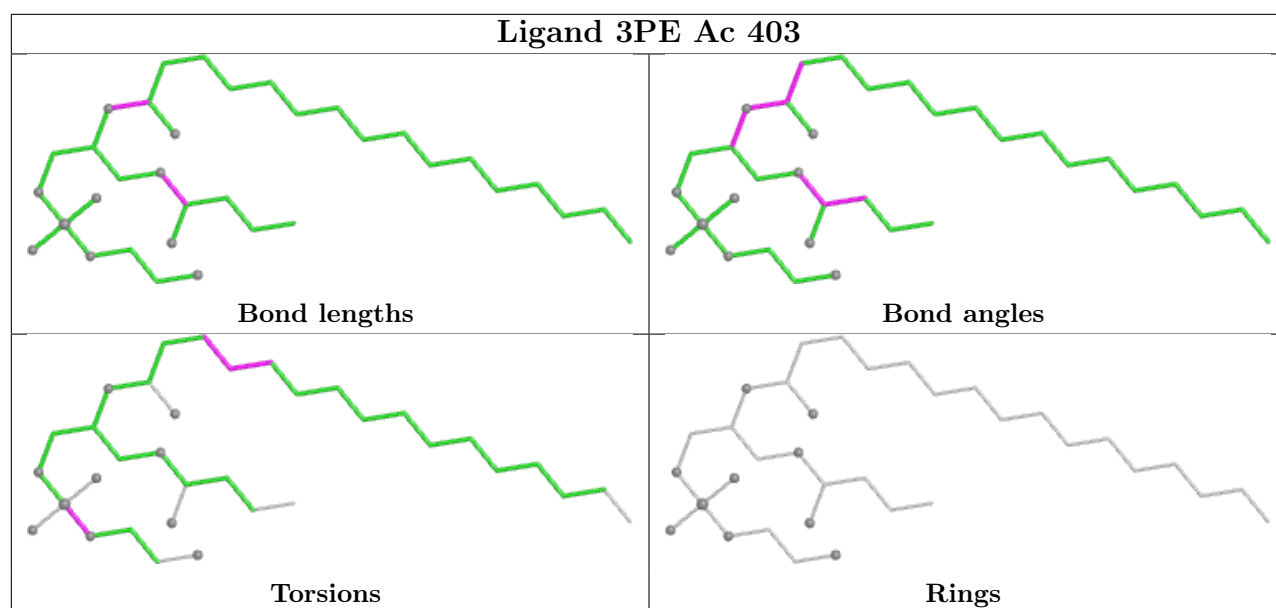
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AG	101	CDL	8	0
55	Ag	103	3PE	5	0
67	AC	403	HEM	8	0
57	F	502	SF4	9	0
55	Aa	501	3PE	7	0
62	l	201	PC1	5	0
67	Ac	401	HEM	3	0
61	H	401	UQ9	10	0
67	Ac	402	HEM	9	0
62	q	202	PC1	6	0
56	M	503	CDL	12	0
55	H	402	3PE	16	0
57	I	303	SF4	6	0
56	AG	102	CDL	8	0
55	A	401	3PE	10	0
55	M	502	3PE	4	0
55	i	201	3PE	9	0
70	AD	401	HEC	12	0
55	L	704	3PE	3	0
55	m	202	3PE	8	0
55	AG	103	3PE	16	0
56	q	201	CDL	8	0
59	E	301	FES	3	0
70	Ad	401	HEC	11	0
62	L	701	PC1	12	0
56	Aa	502	CDL	4	0
58	D	501	UQ1	14	0
68	AC	405	U10	19	0
57	I	302	SF4	10	0

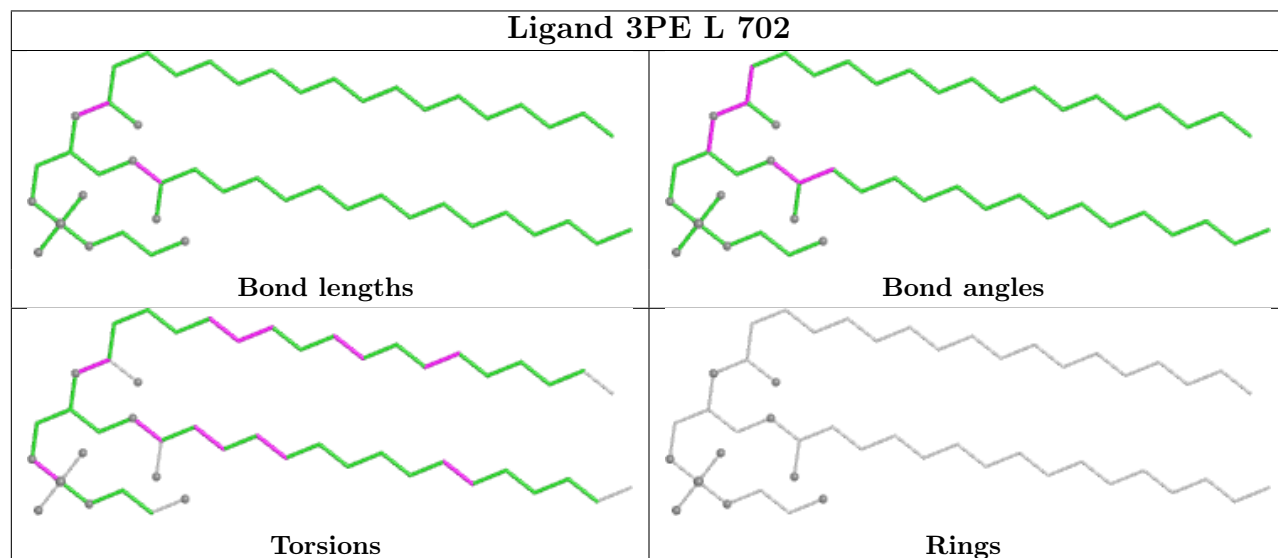
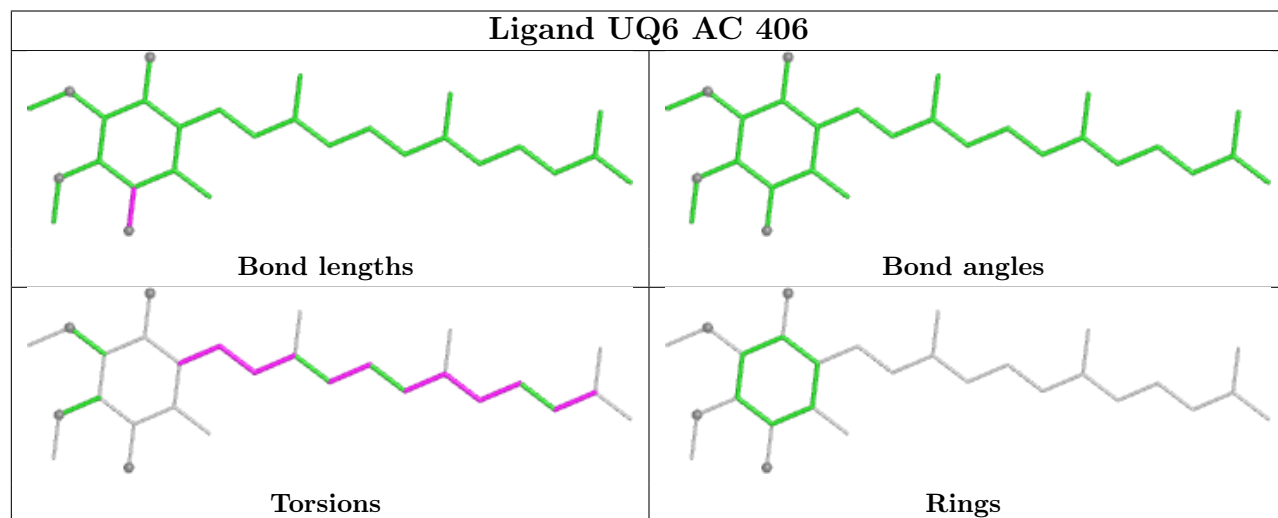
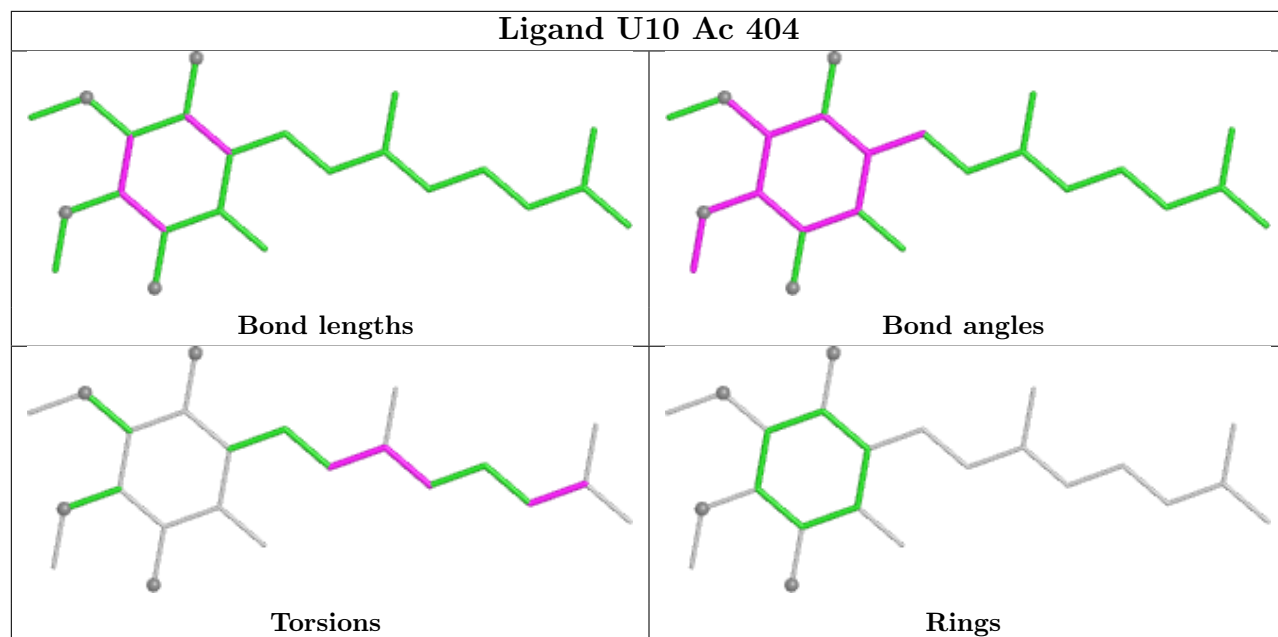
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



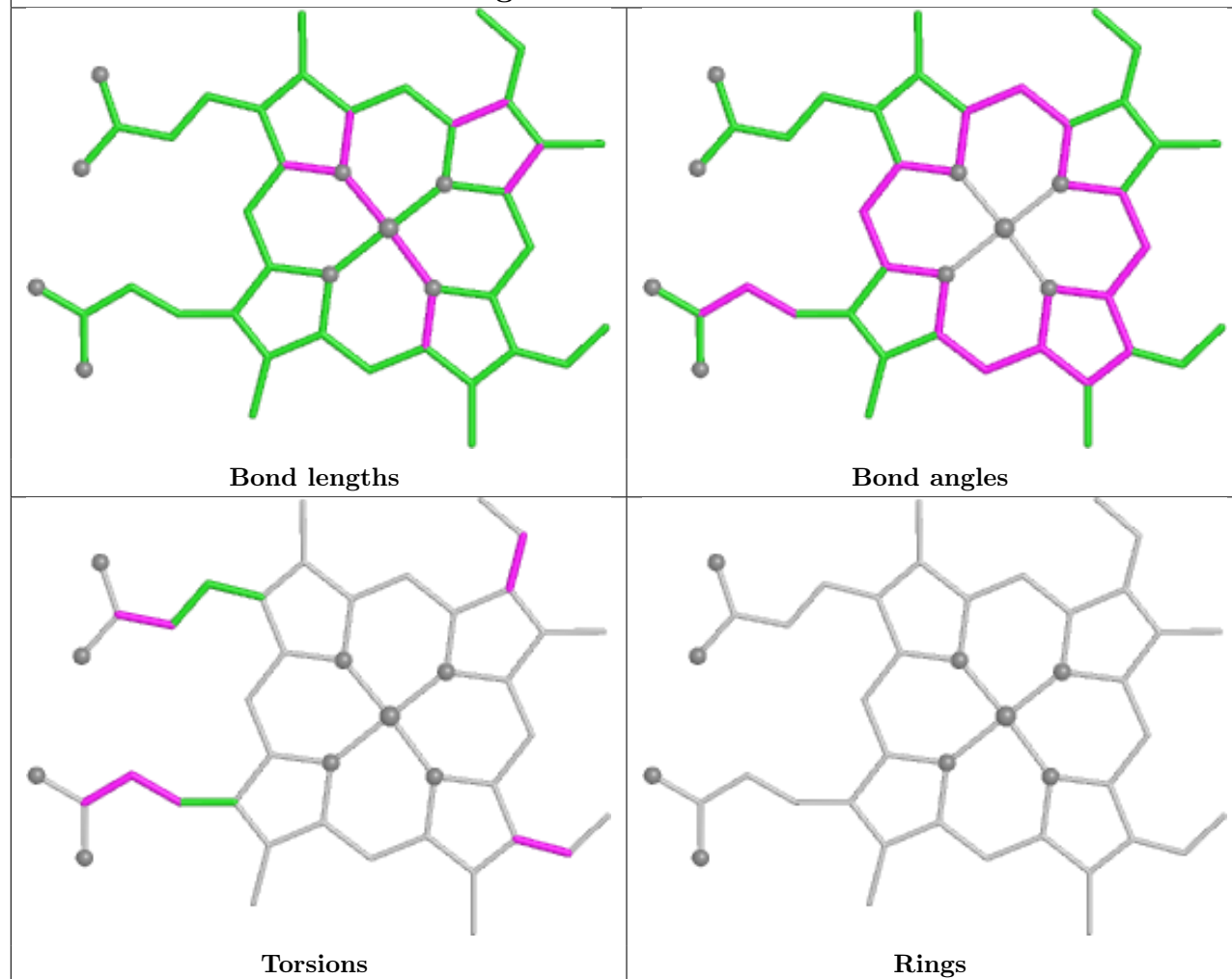




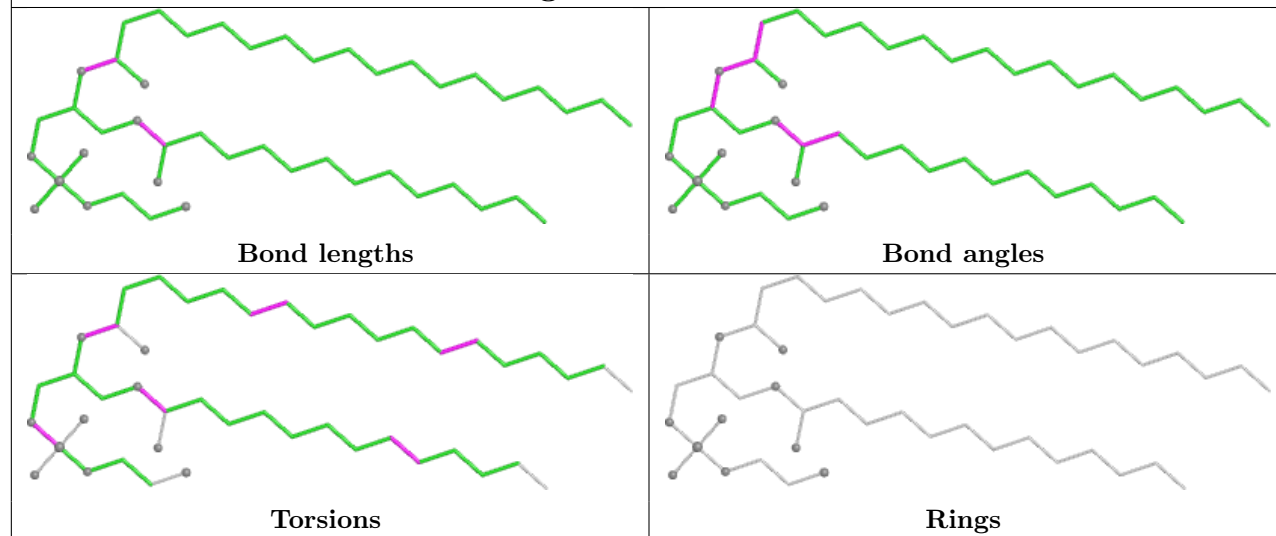


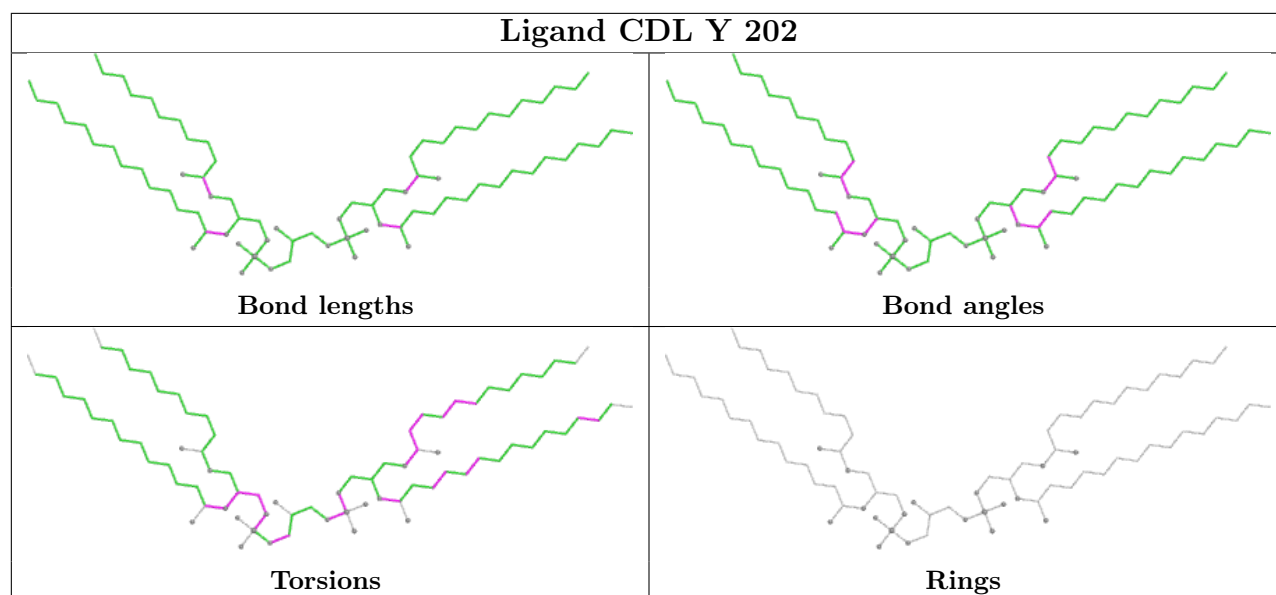
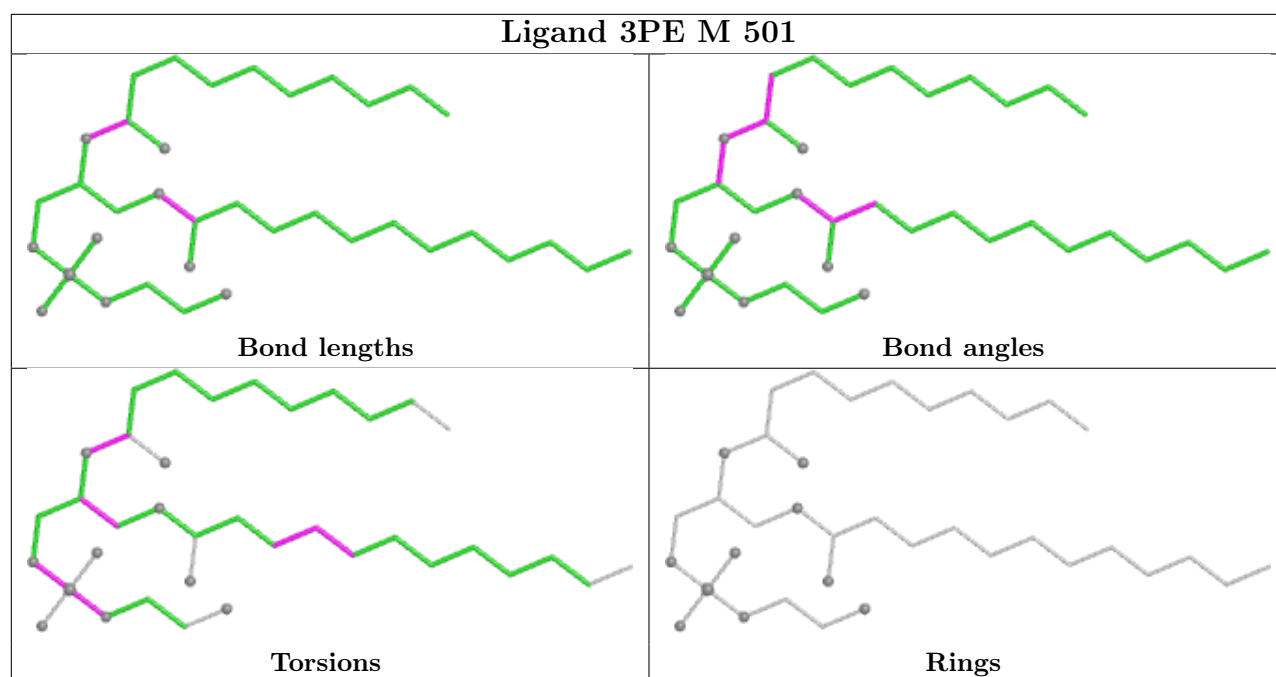


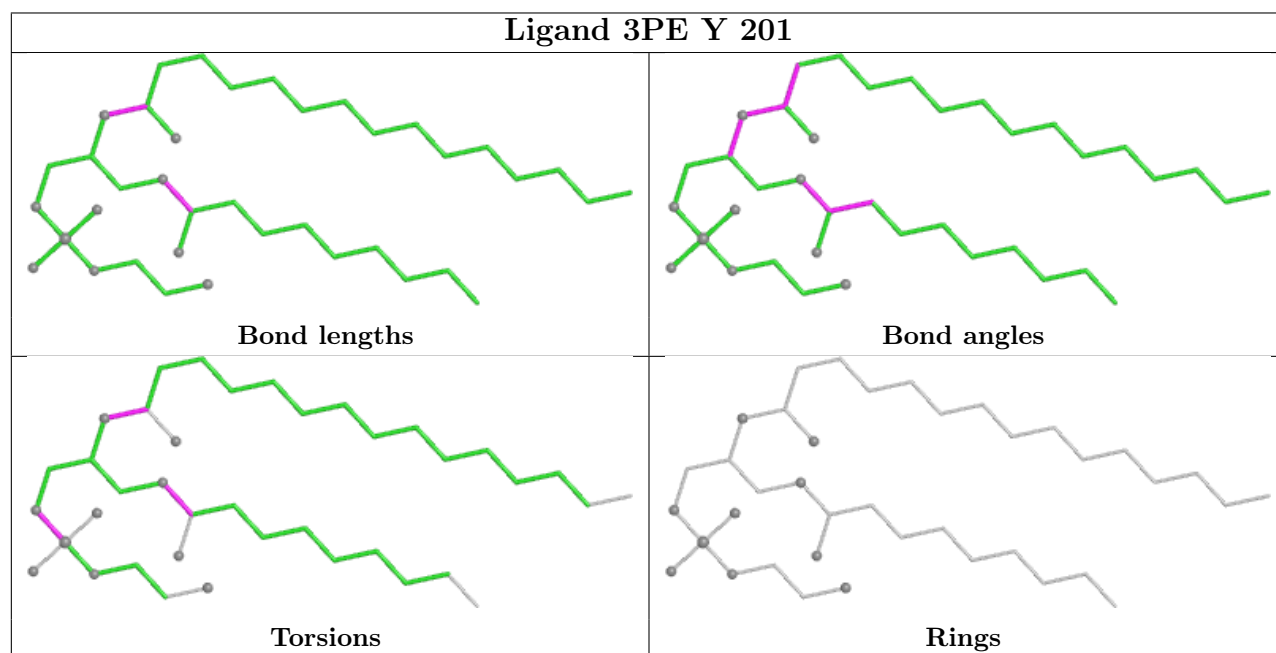
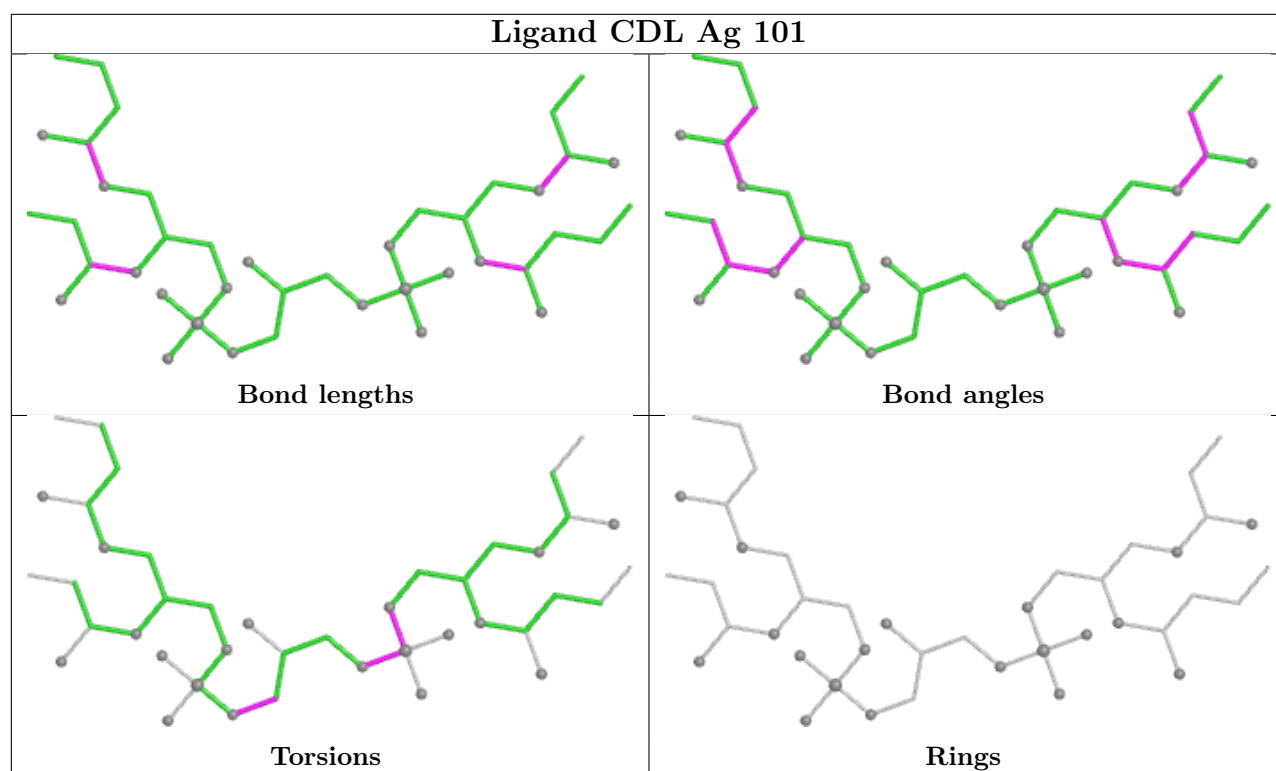
Ligand HEM AC 402

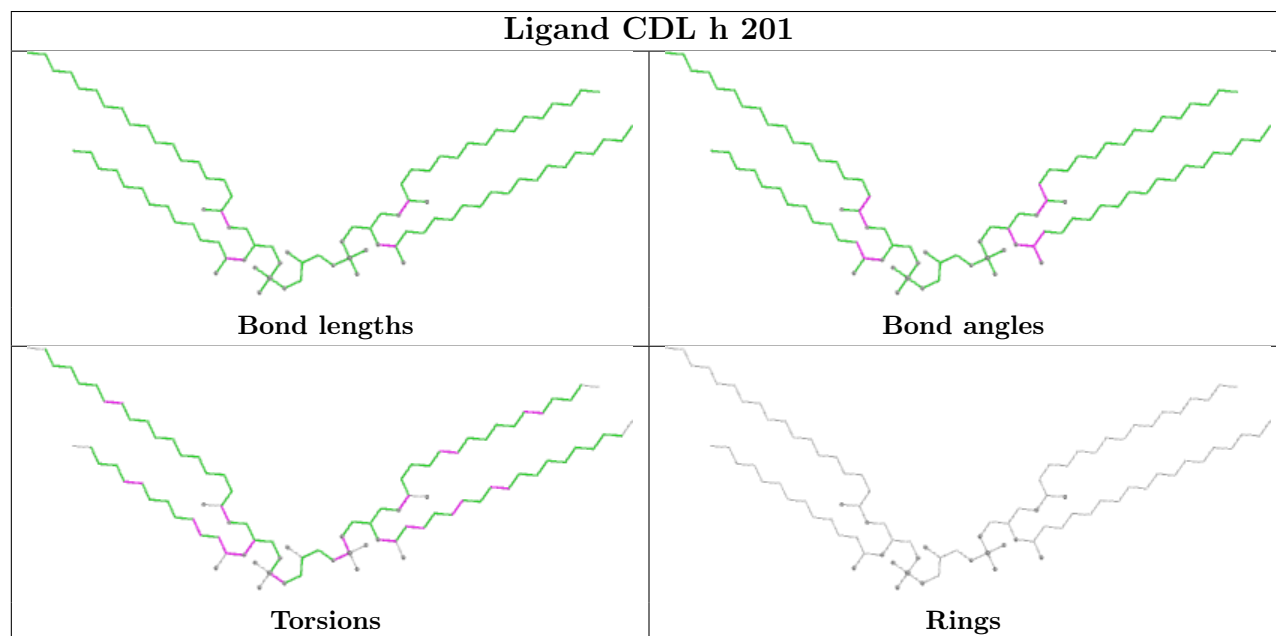
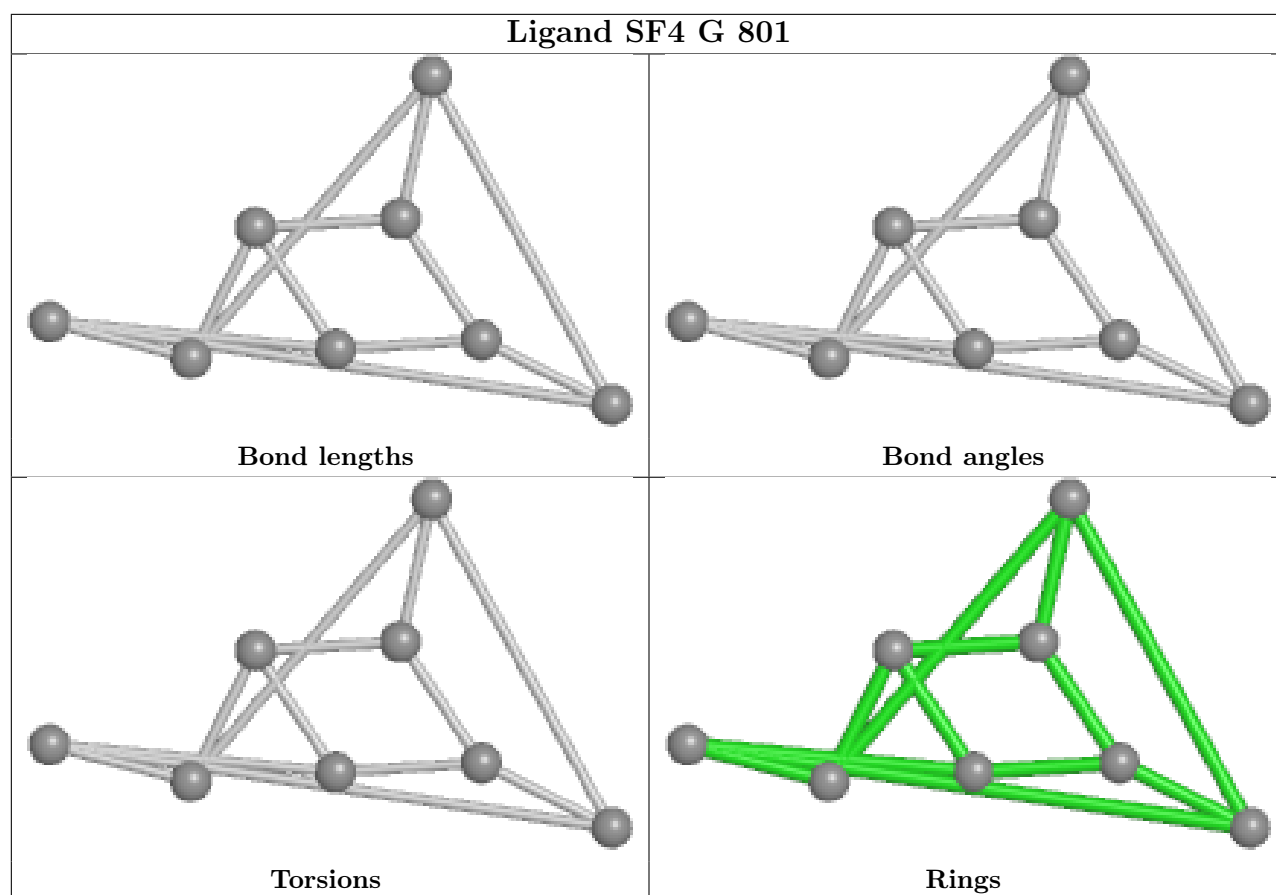


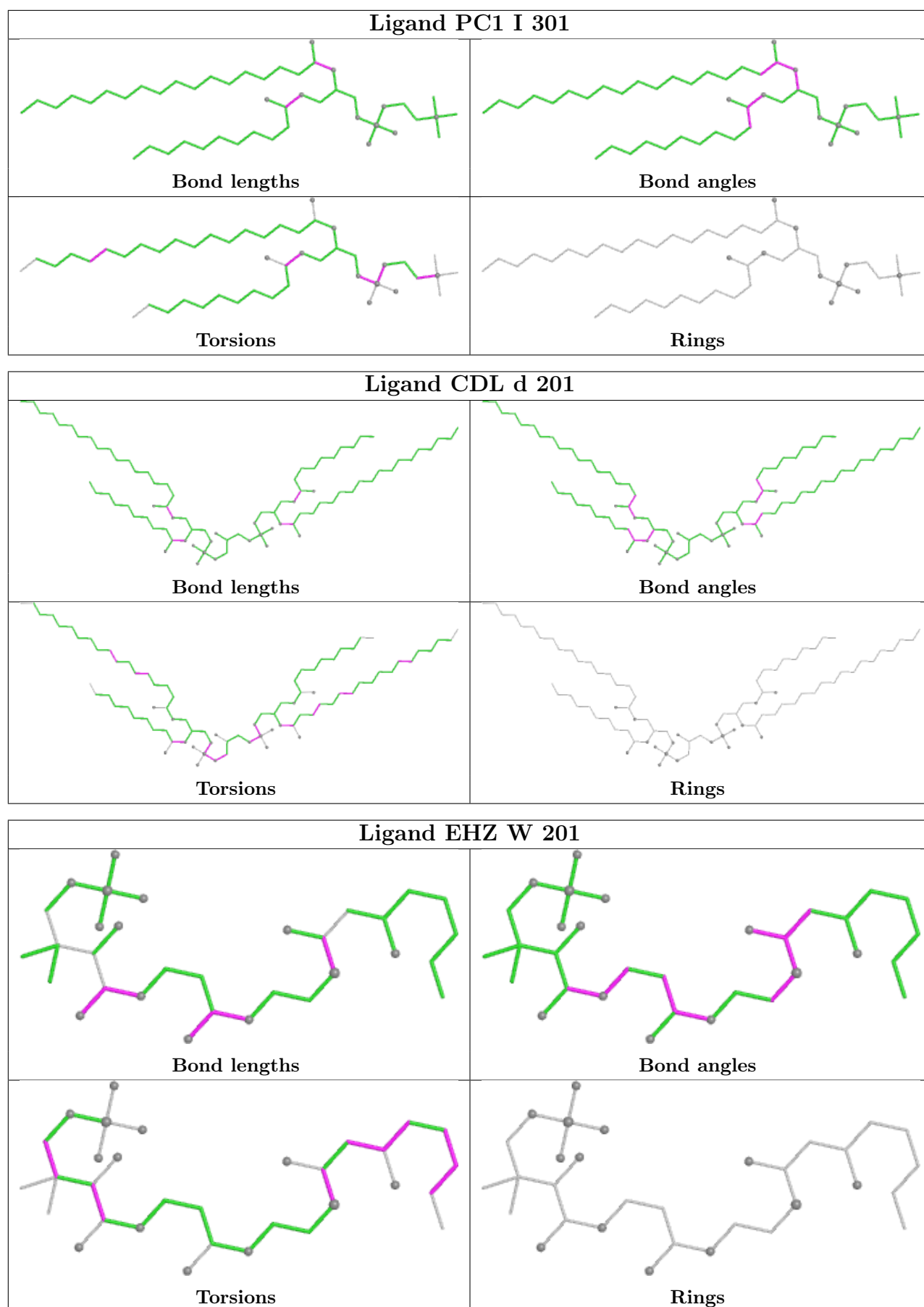
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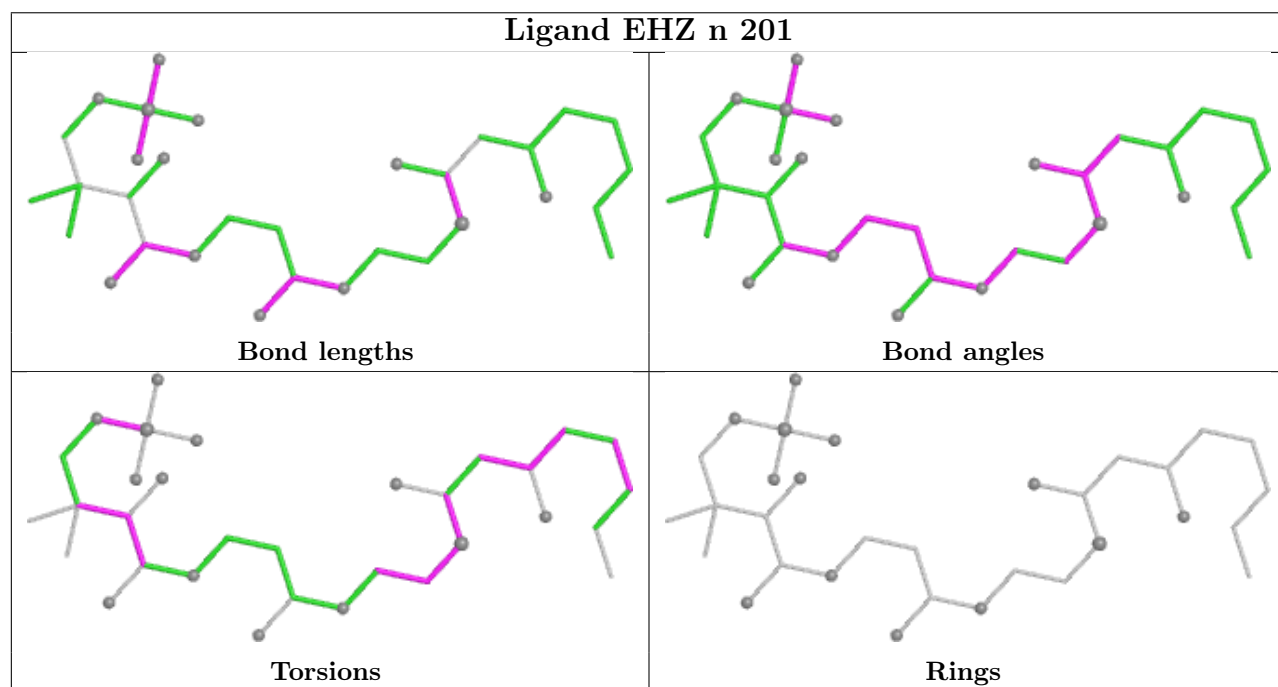
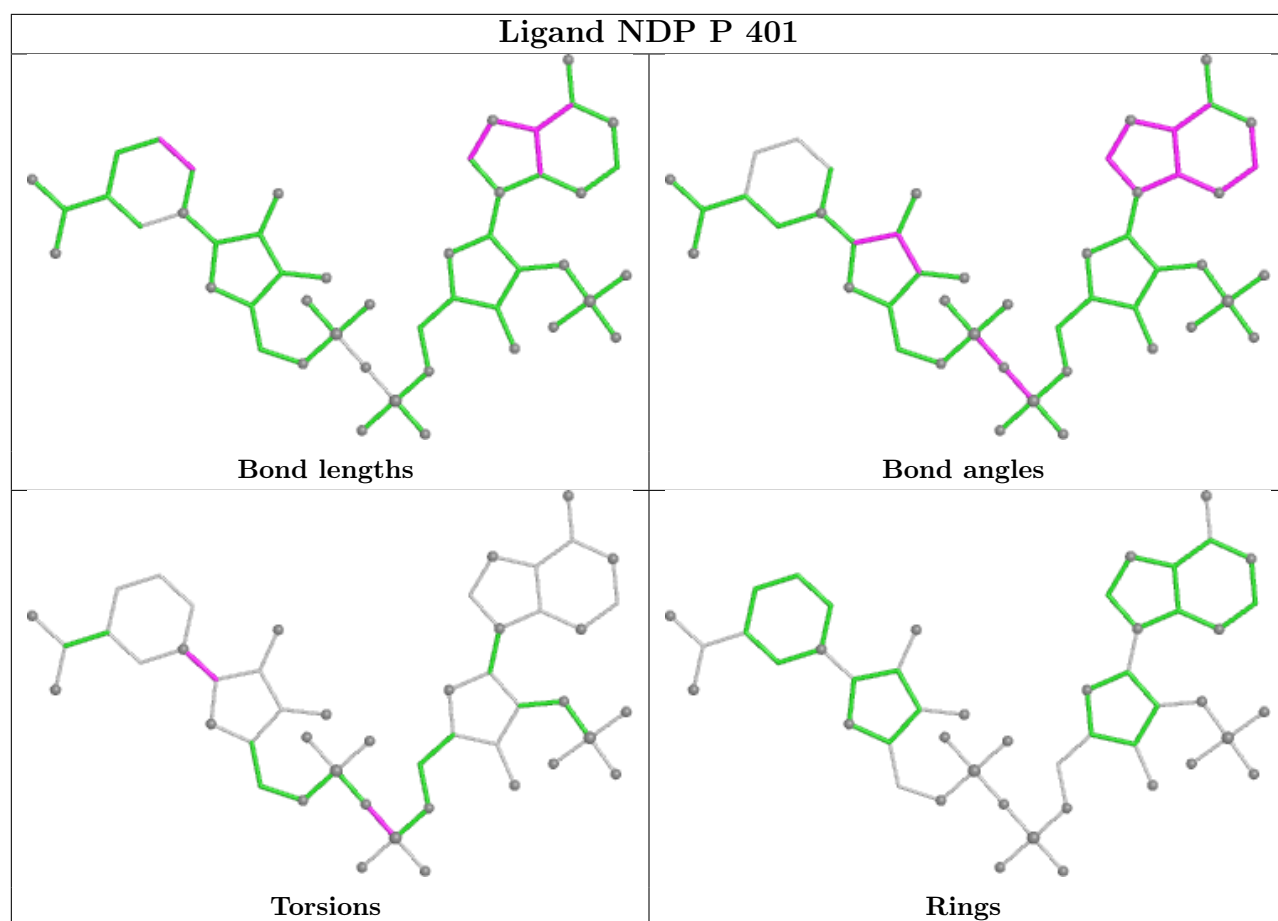


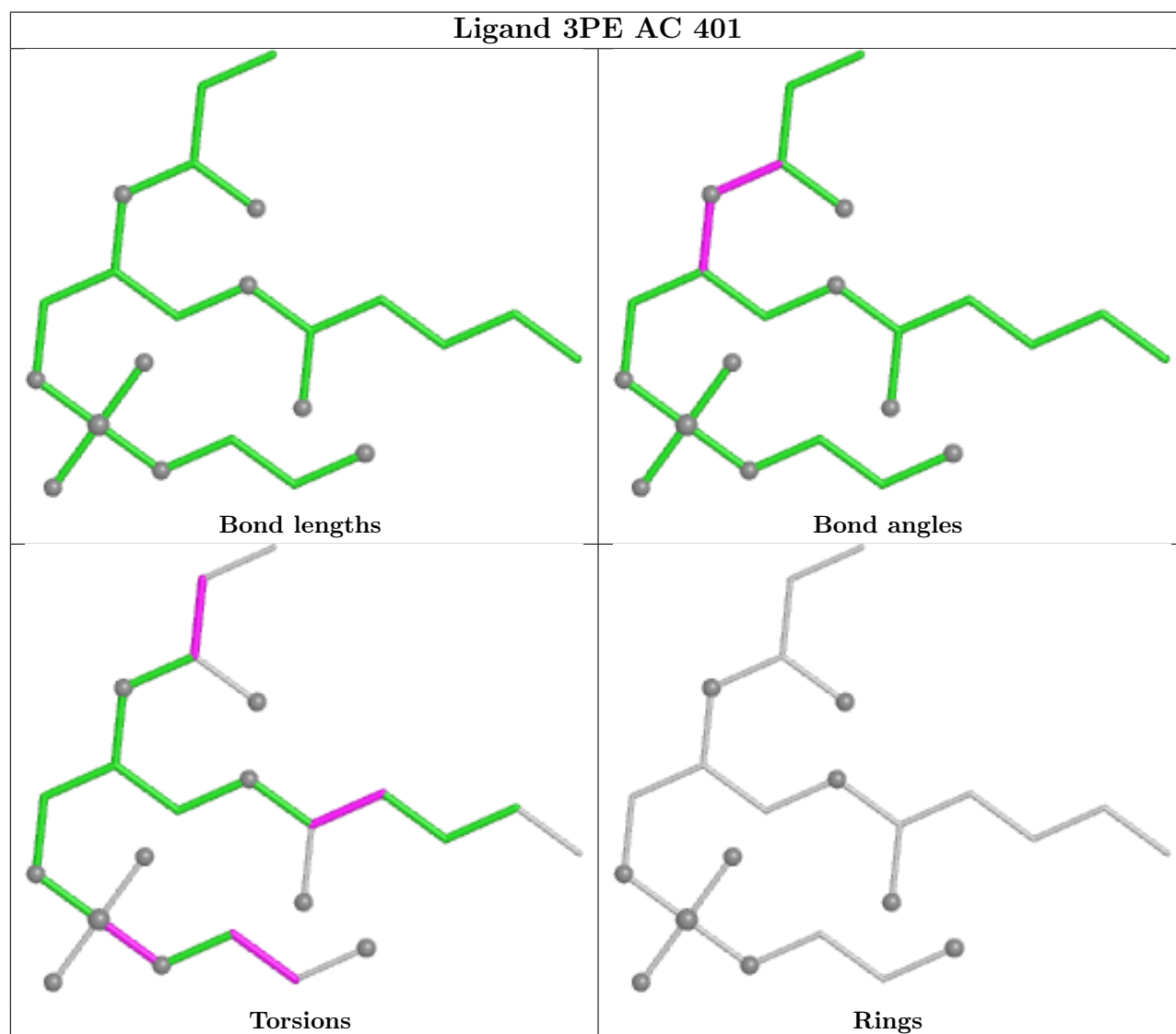
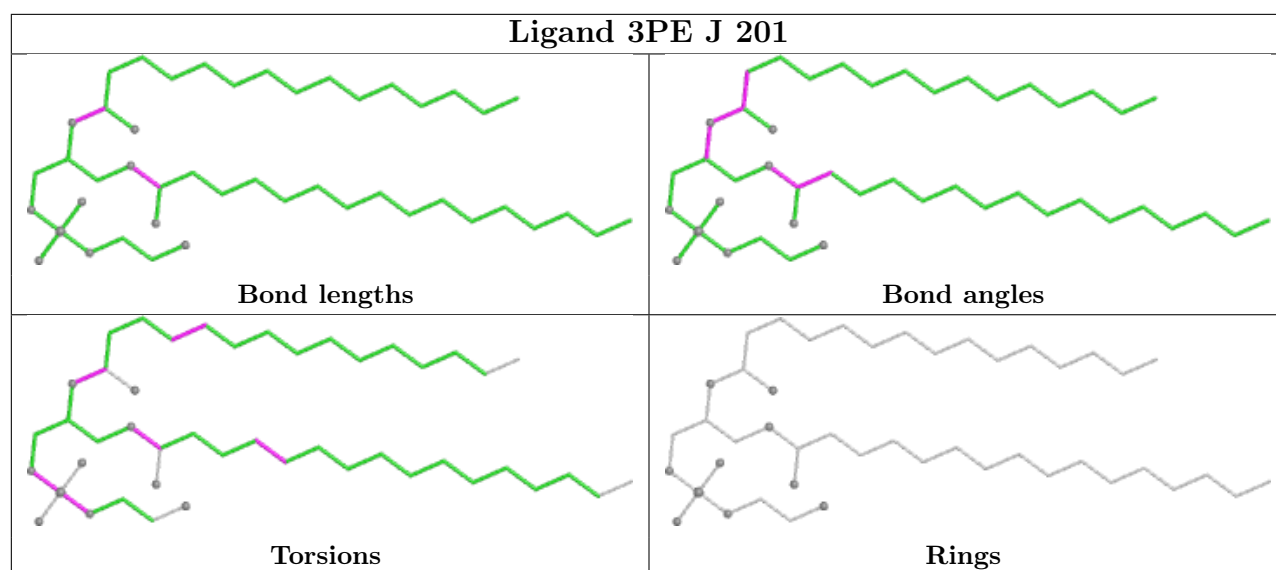


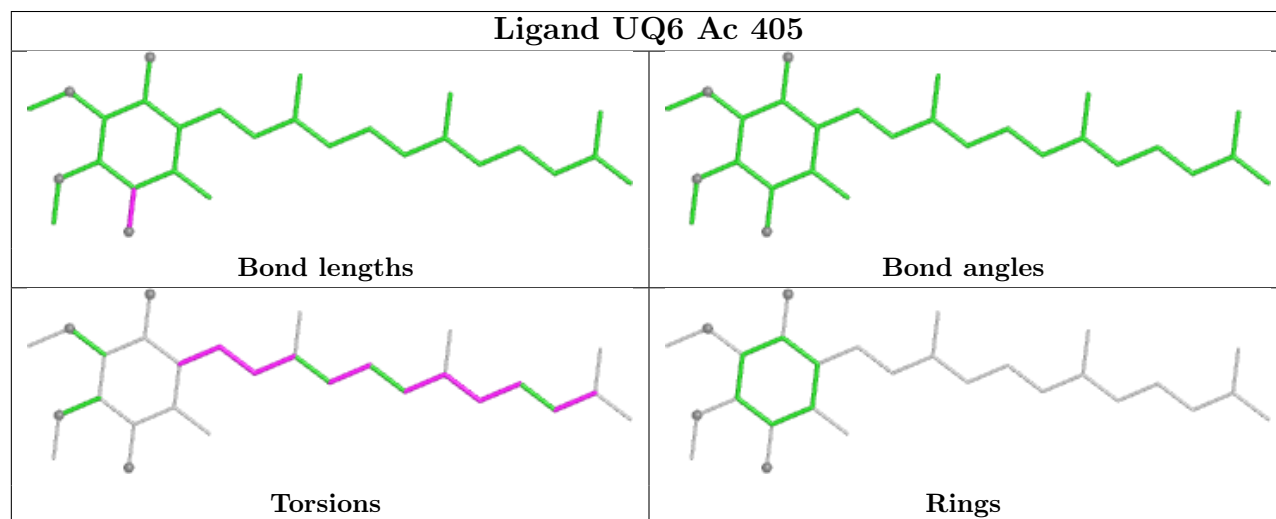
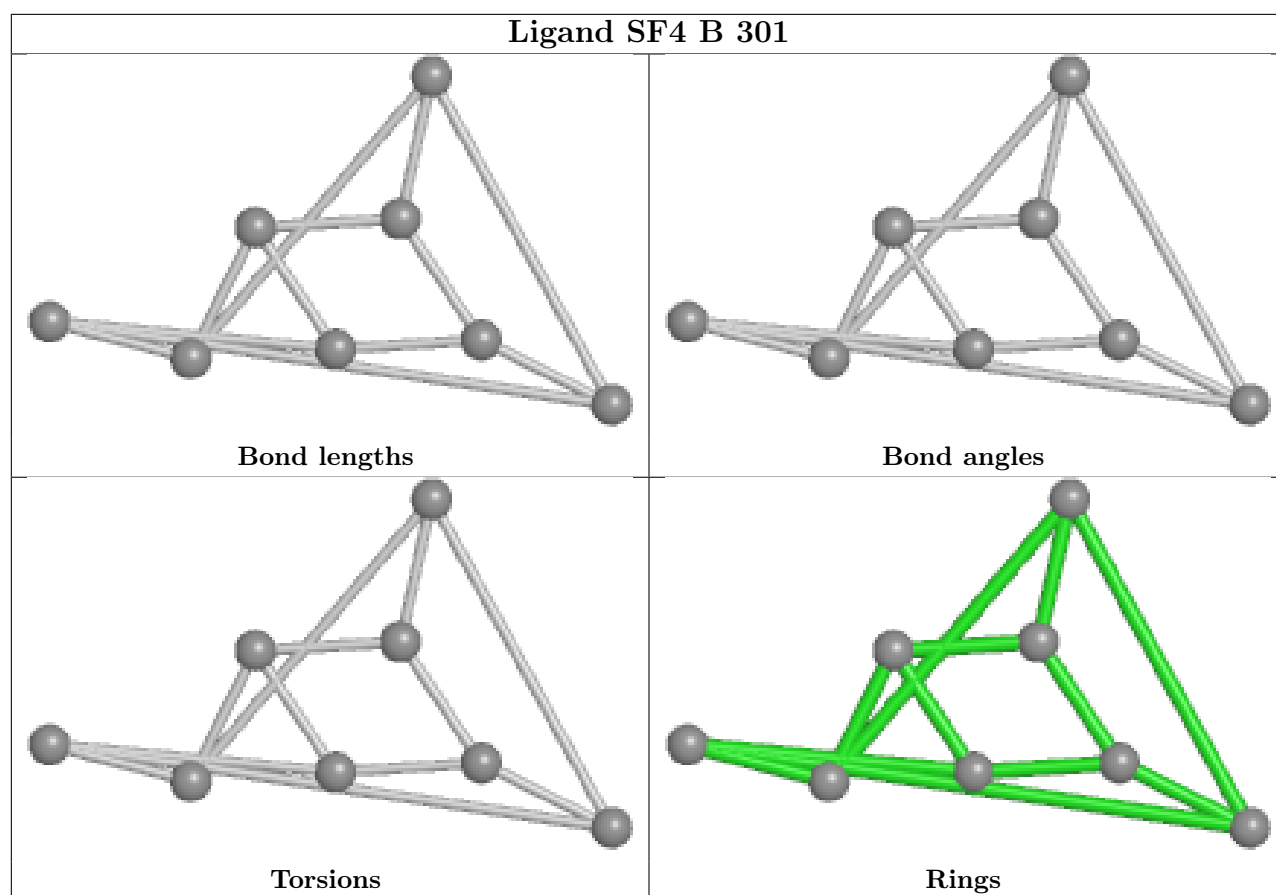


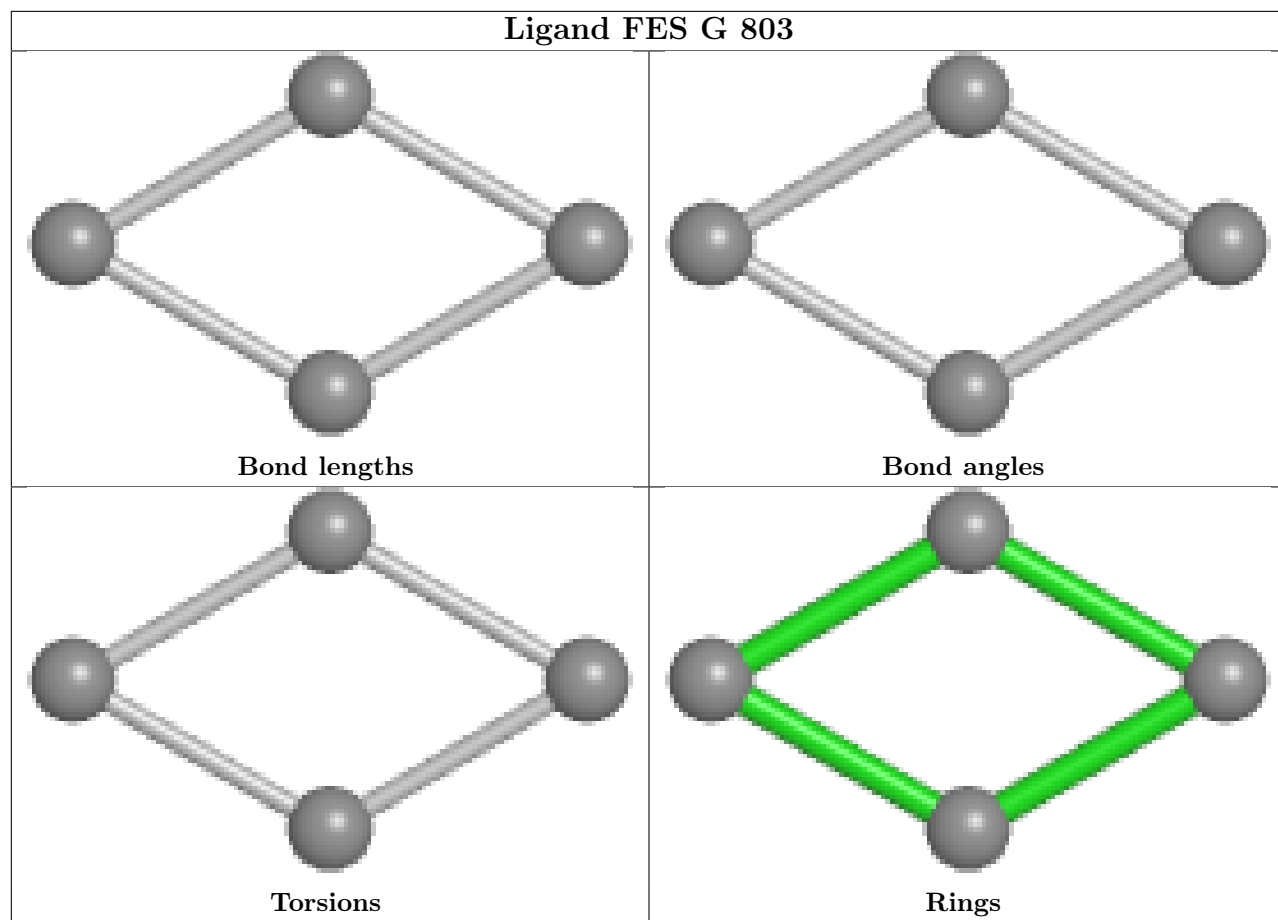


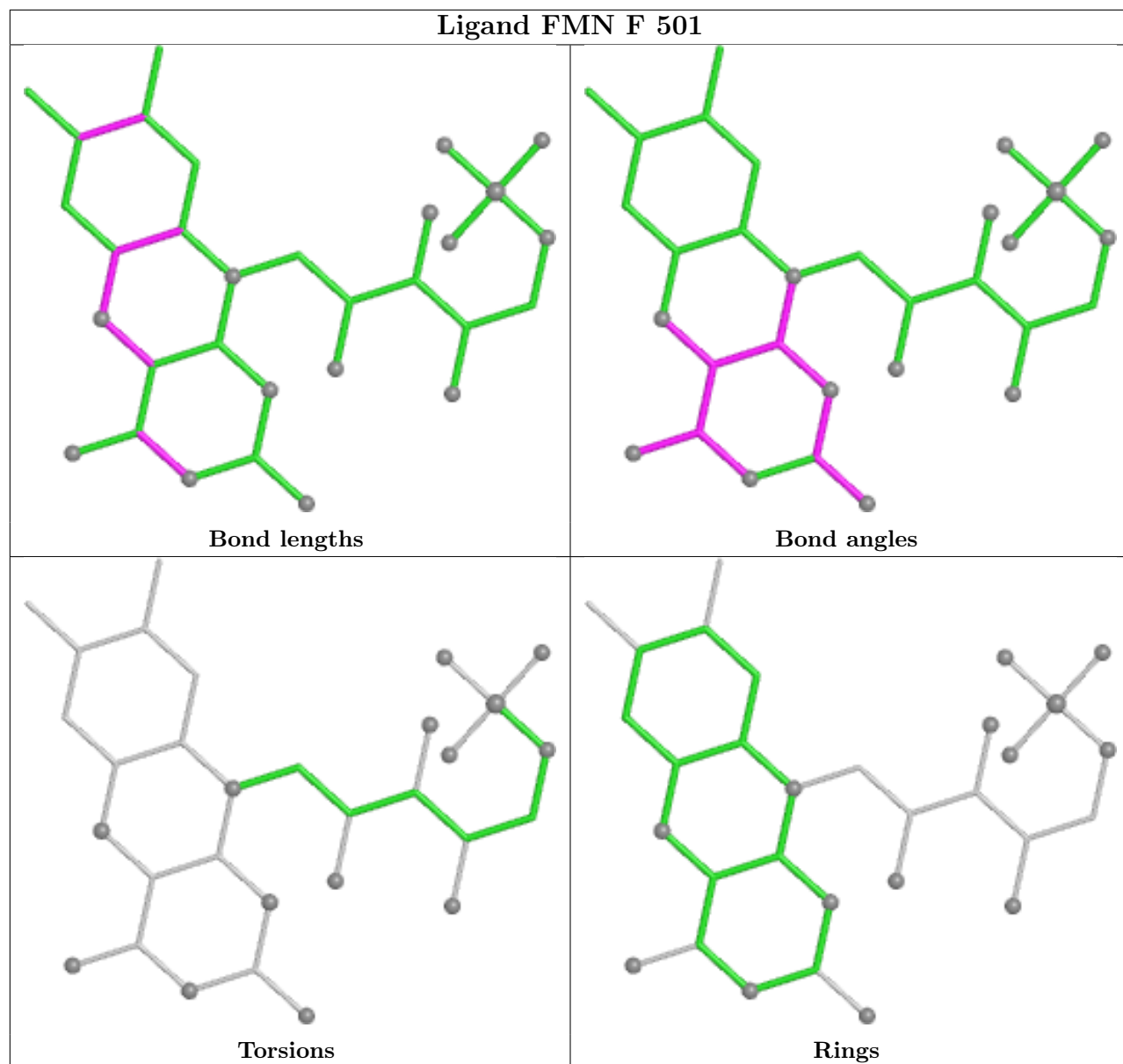


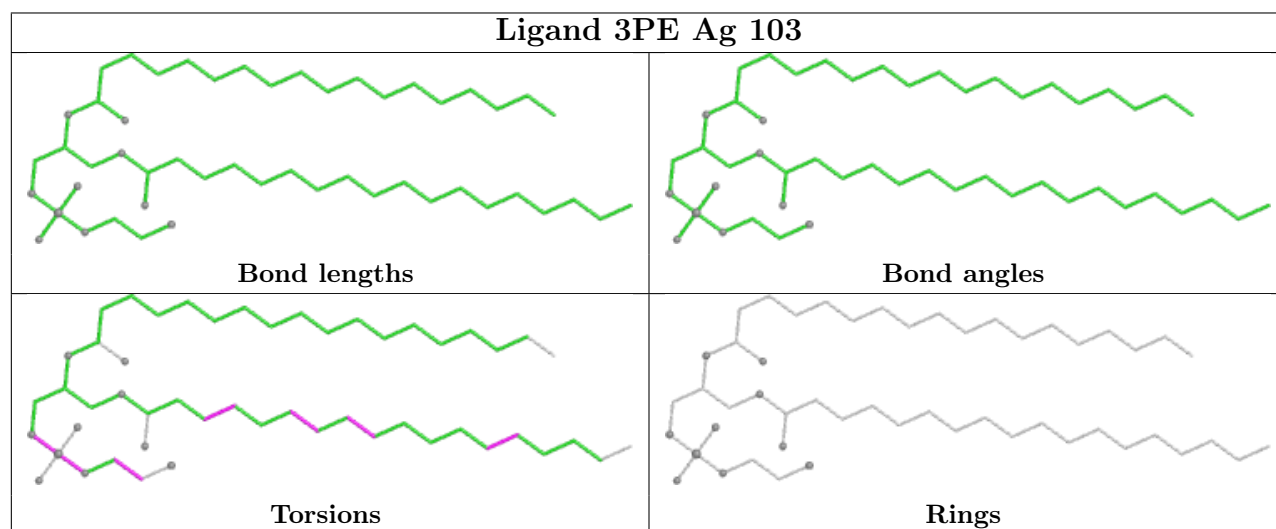
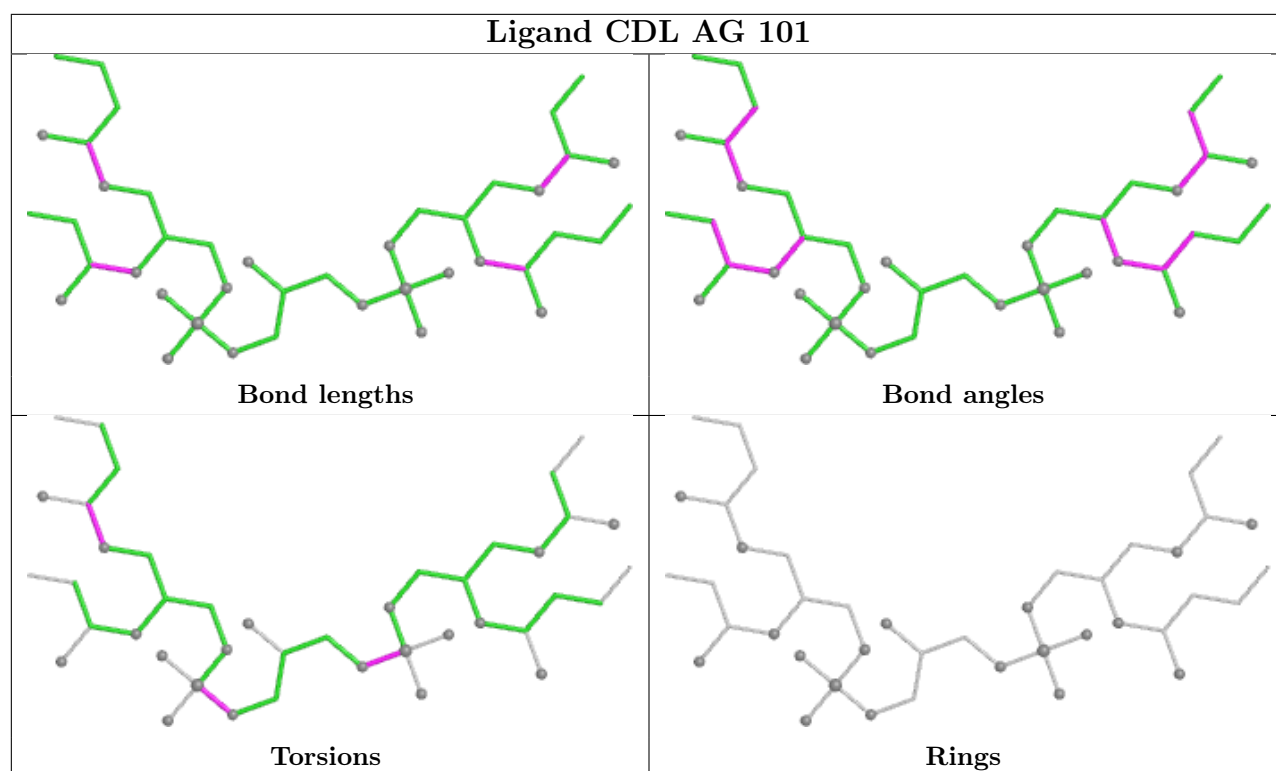




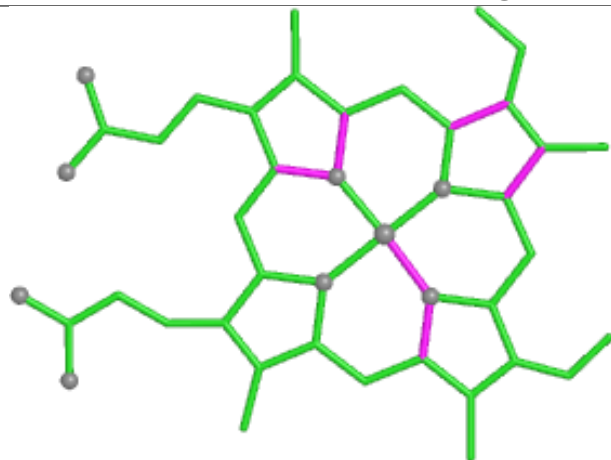




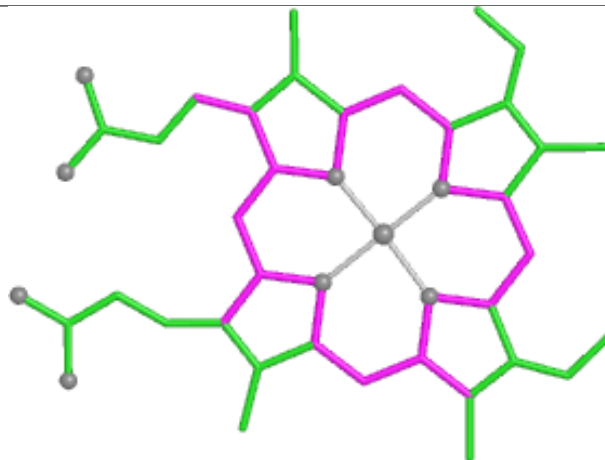




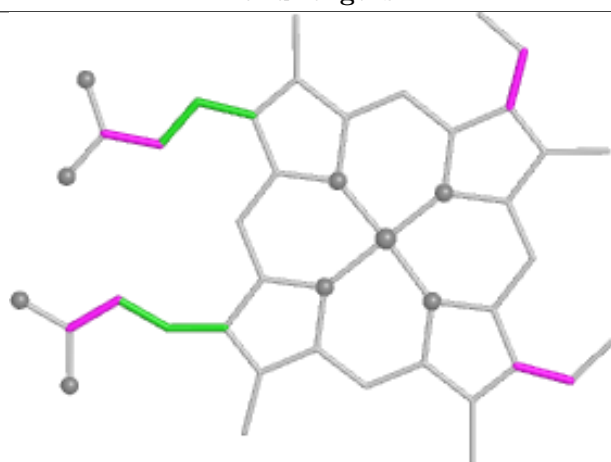
Ligand HEM AC 403



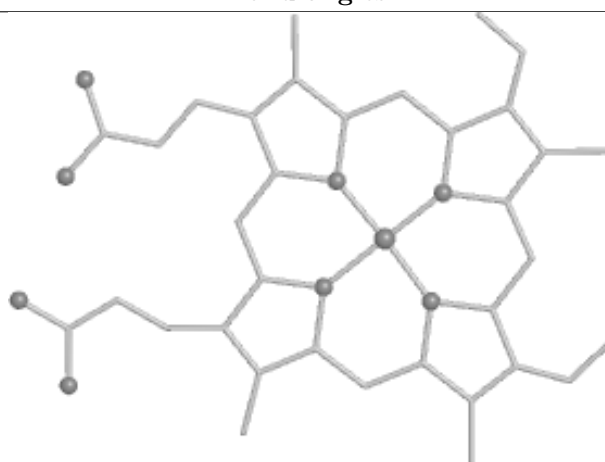
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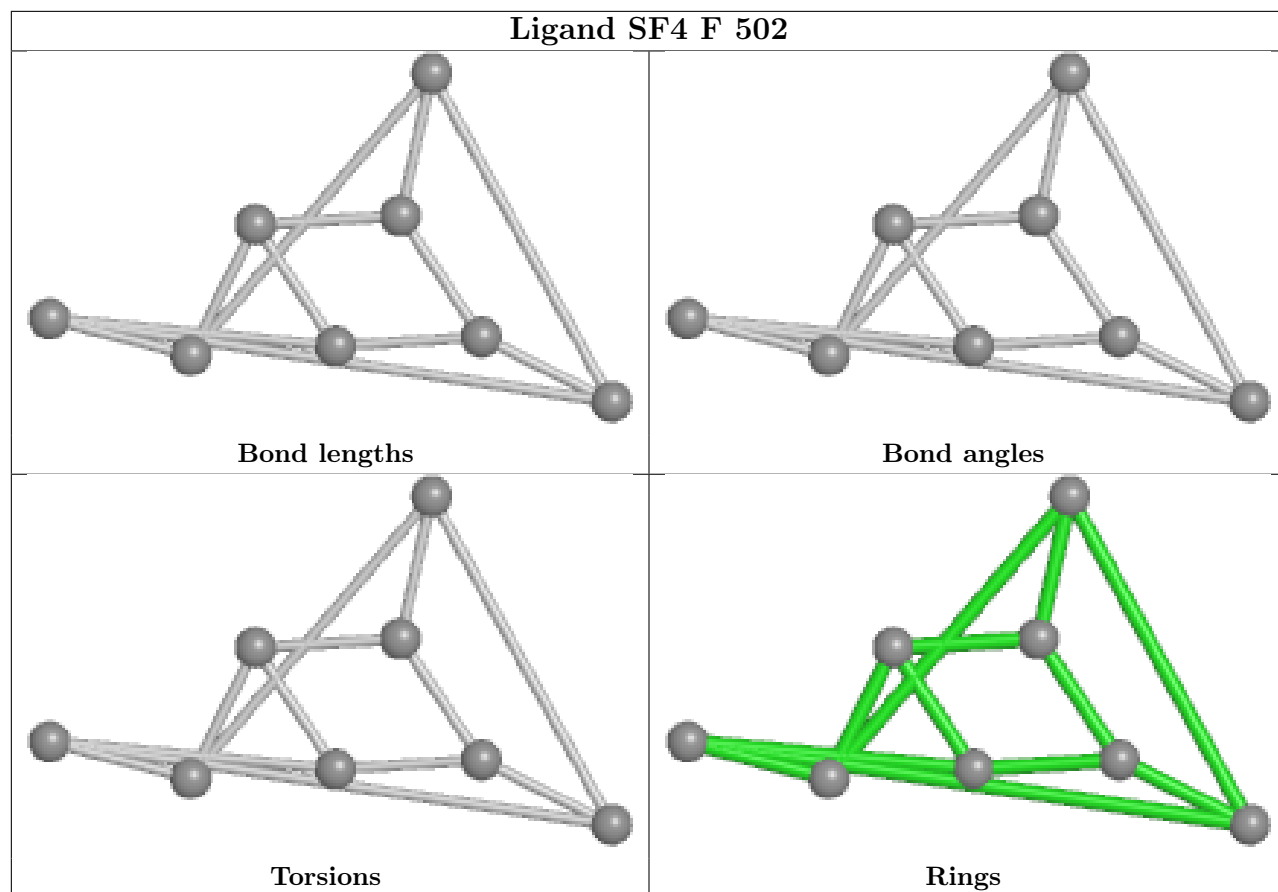
Bond angles

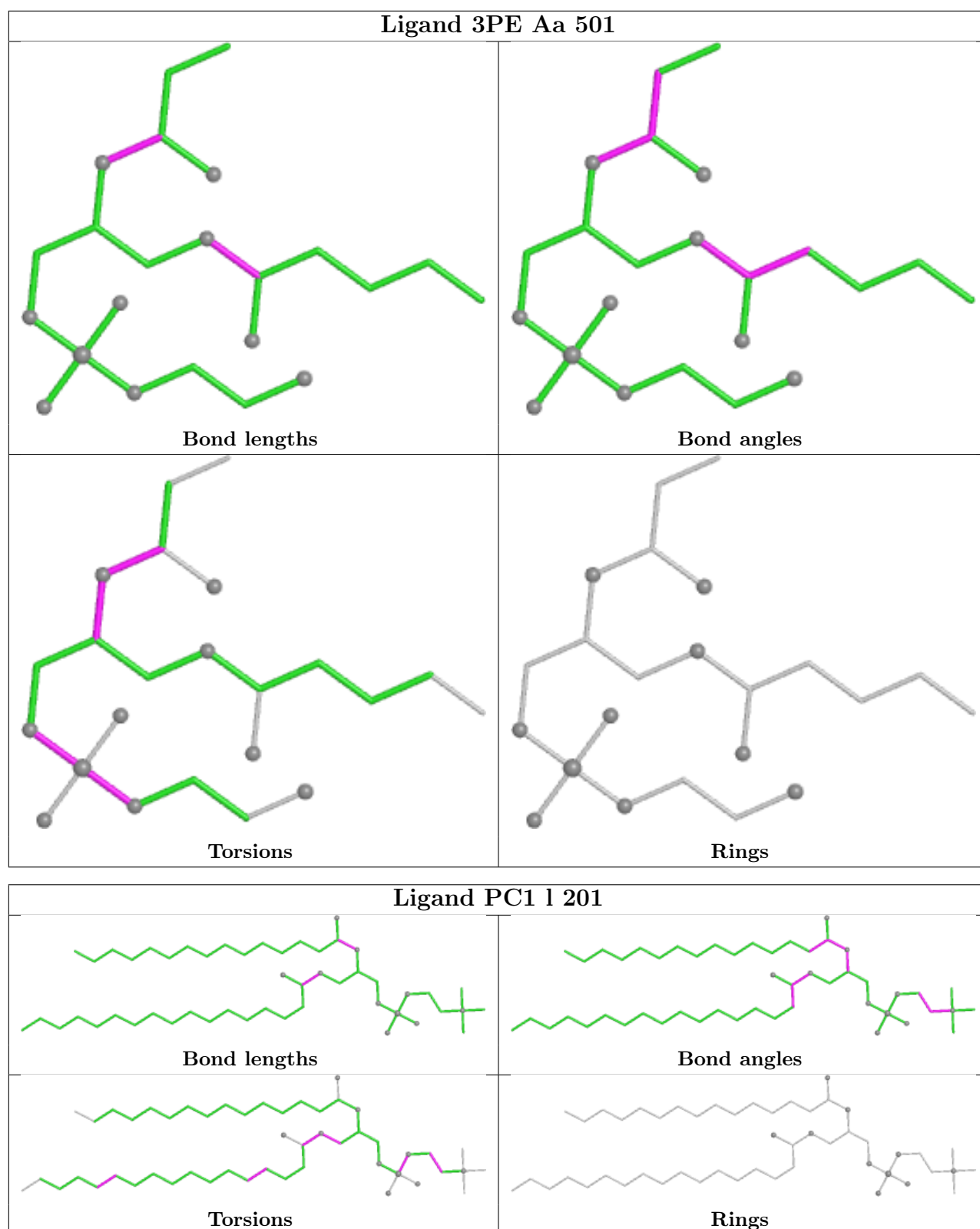


Torsions

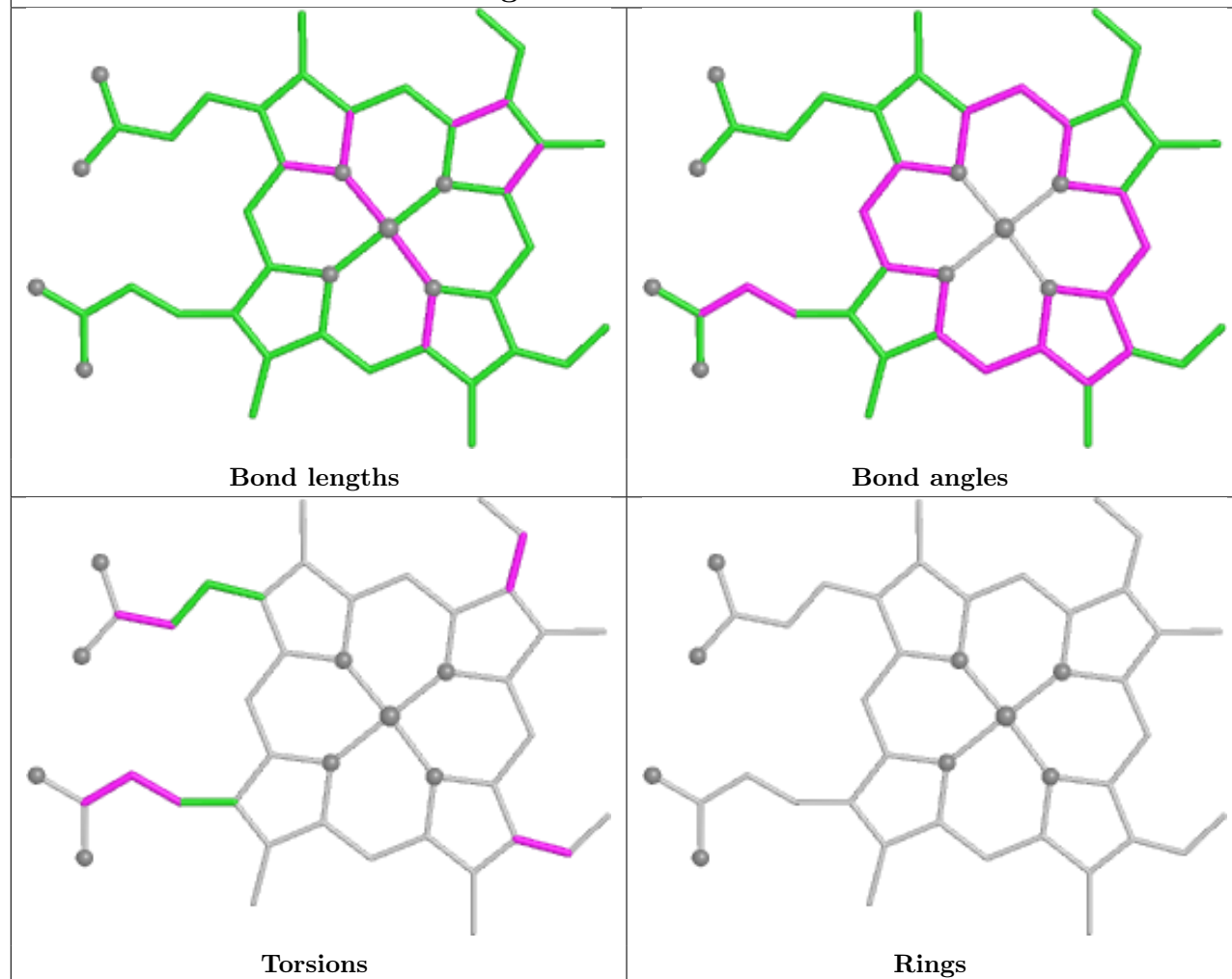


Rings

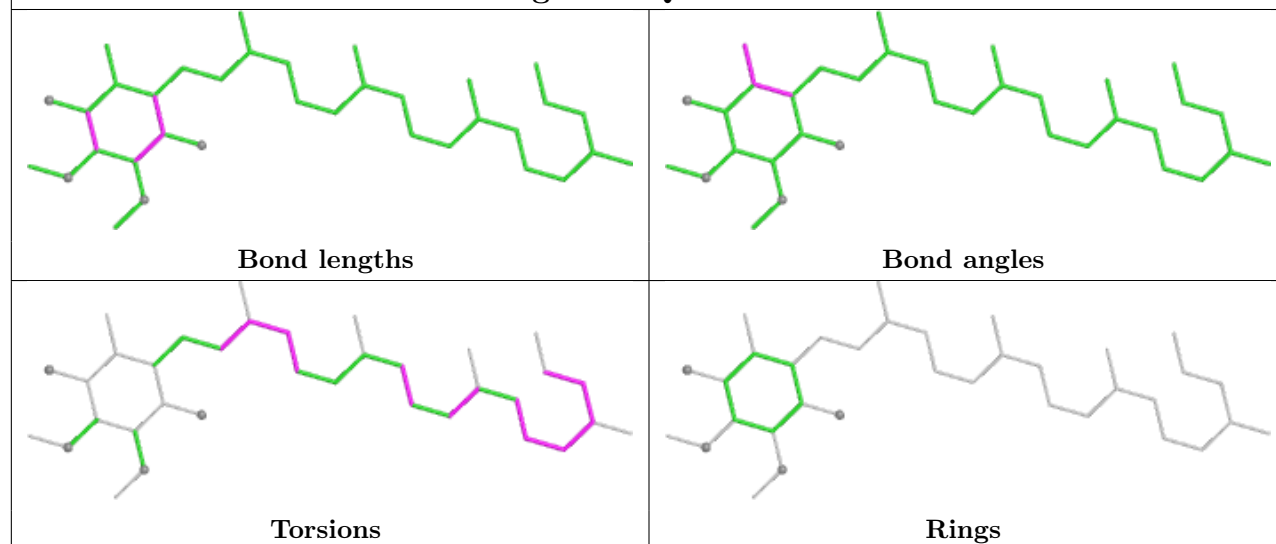




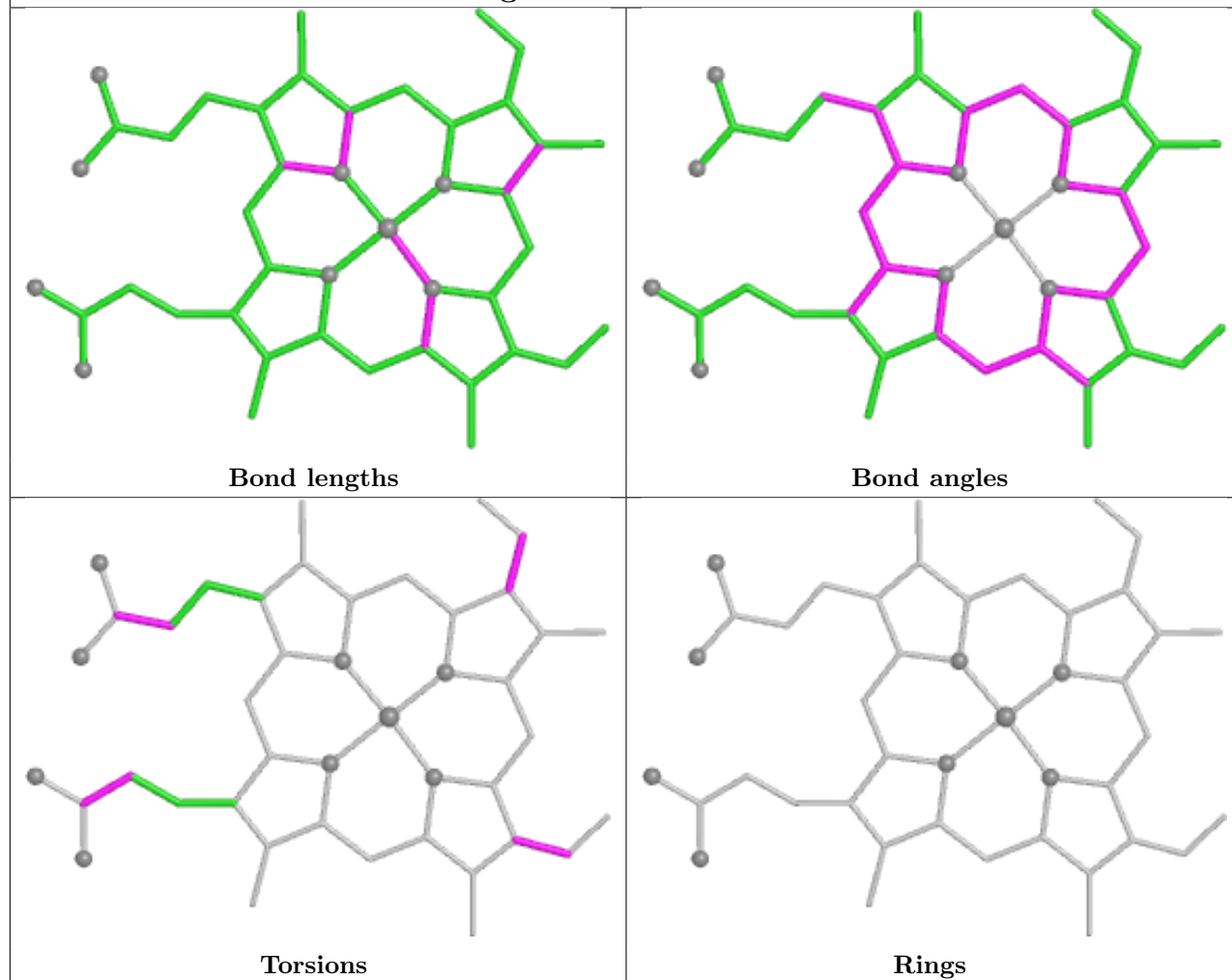
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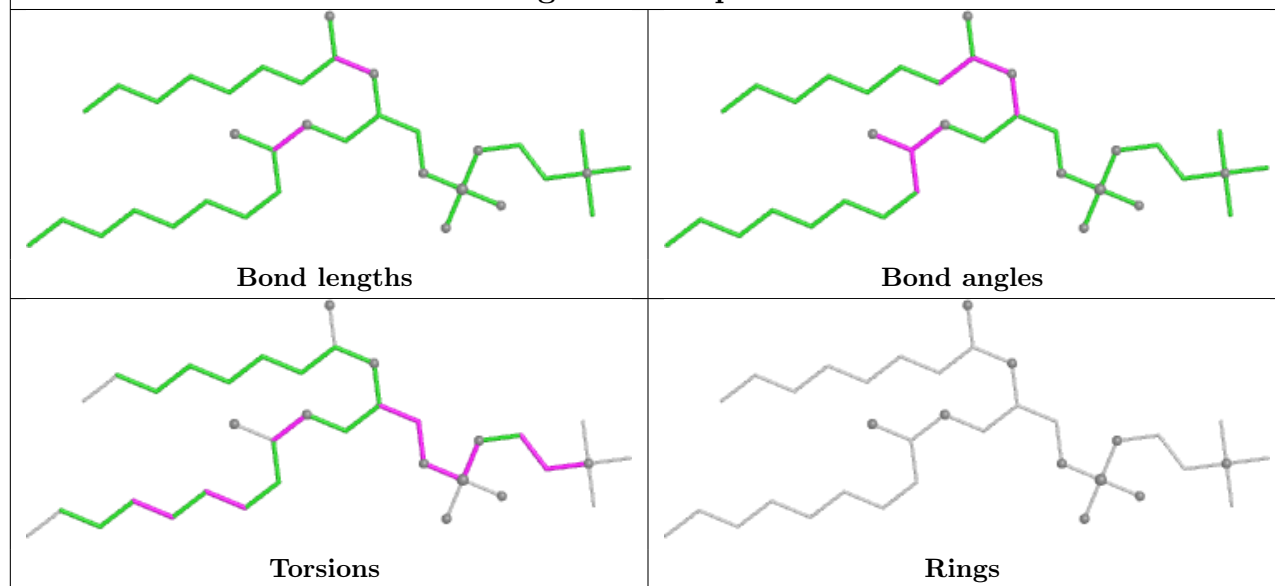
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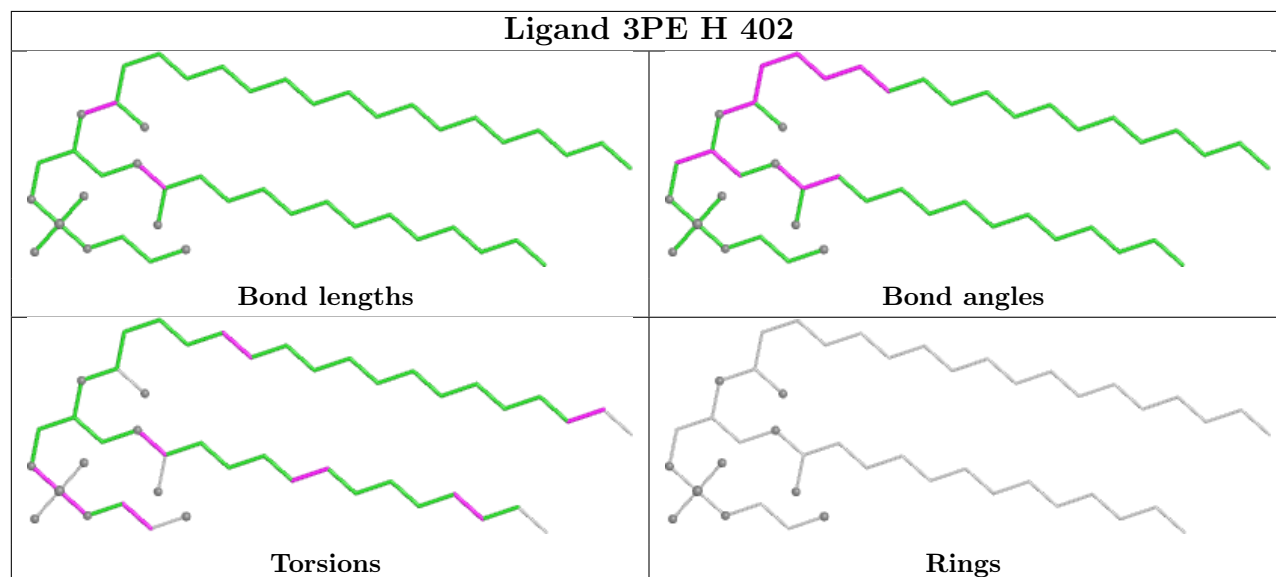
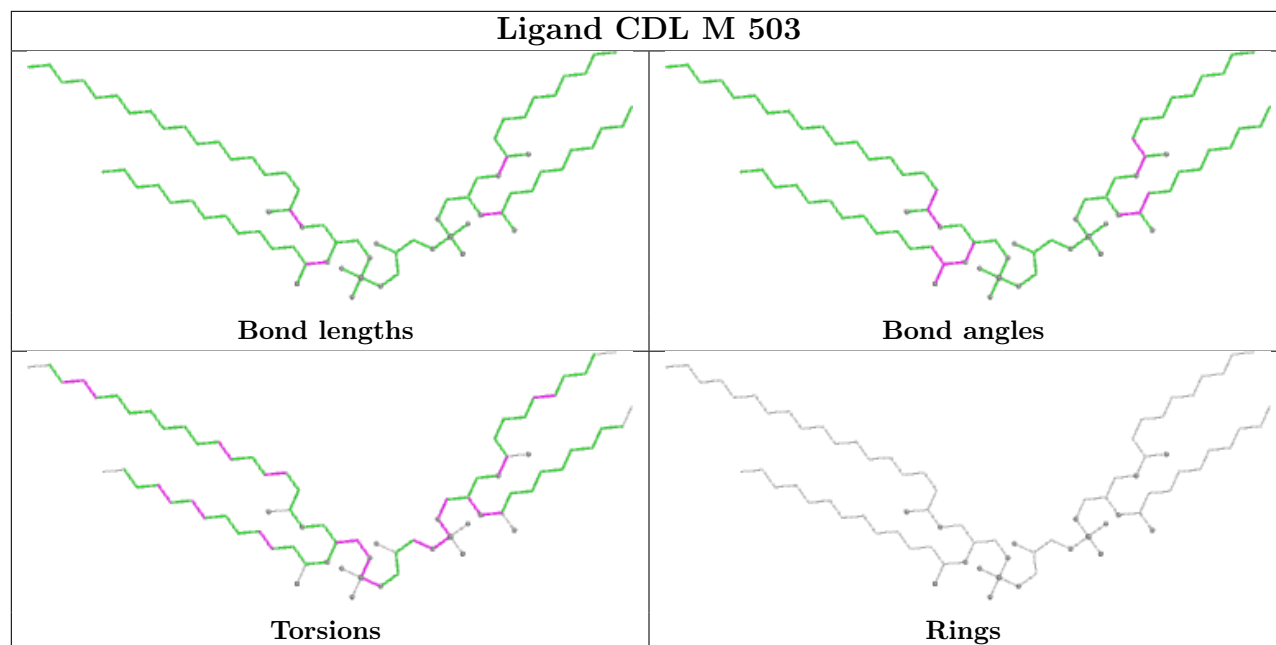


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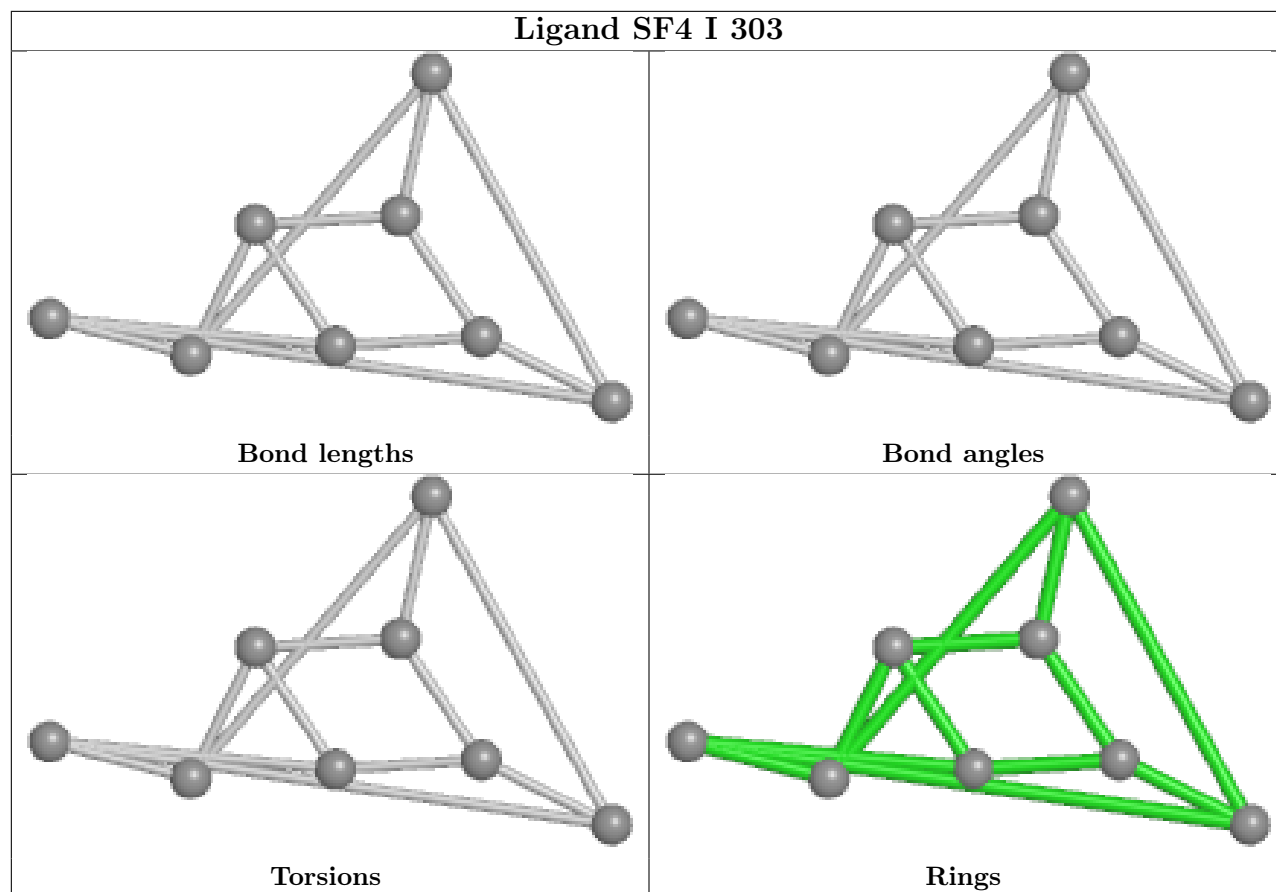


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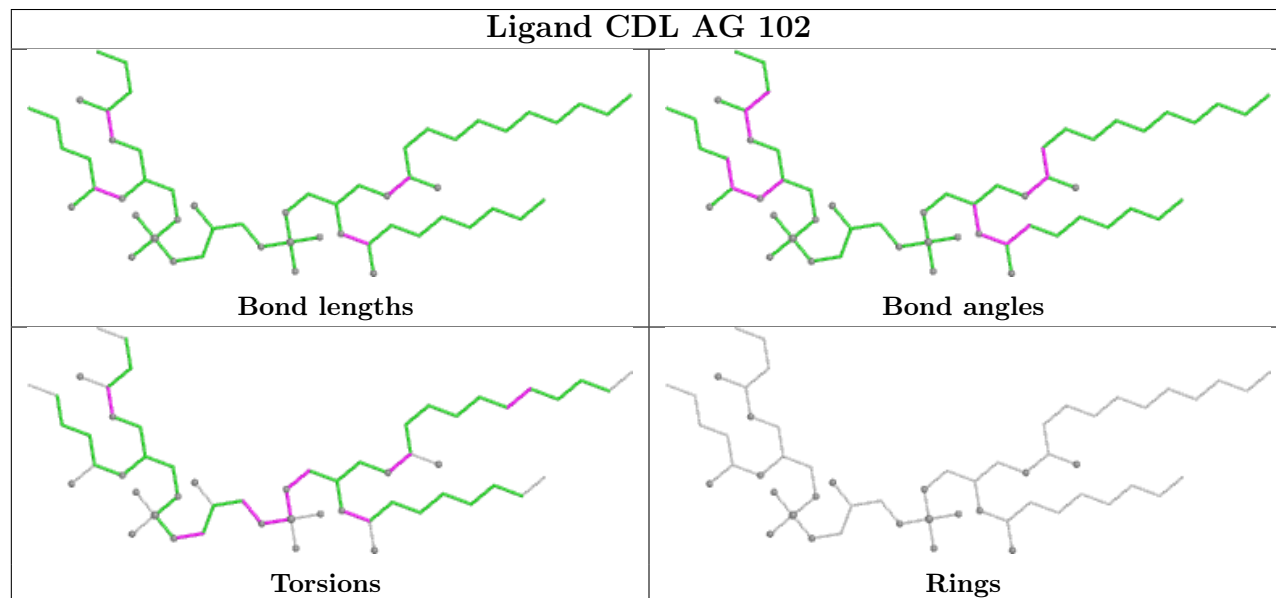


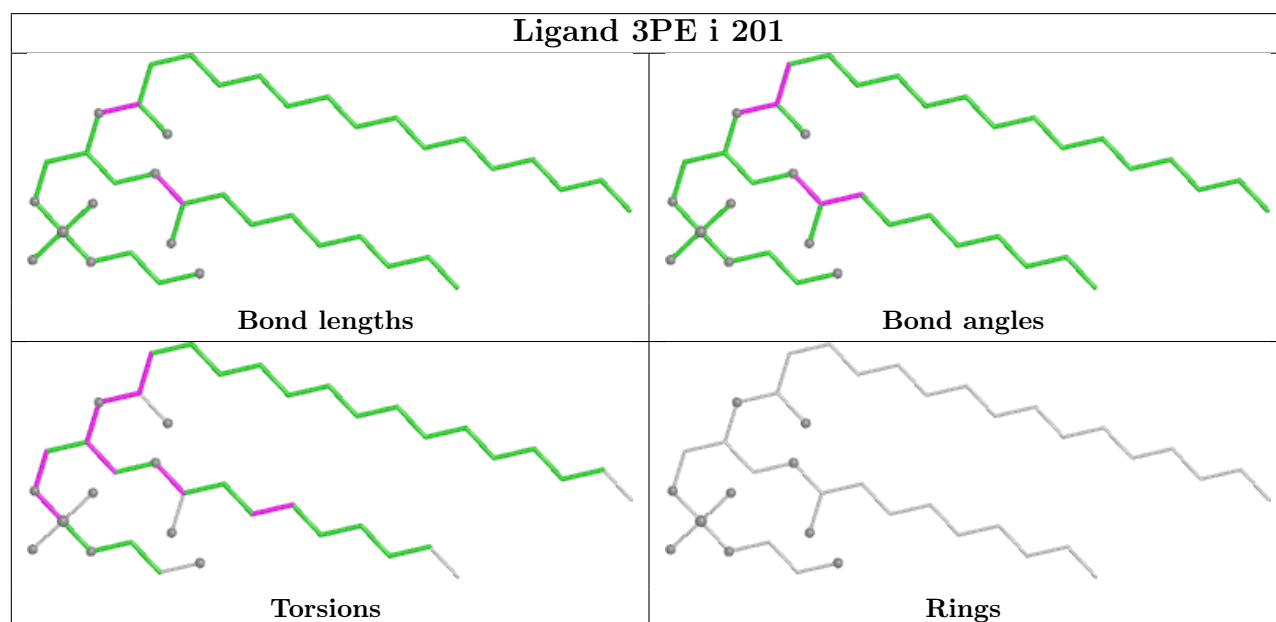
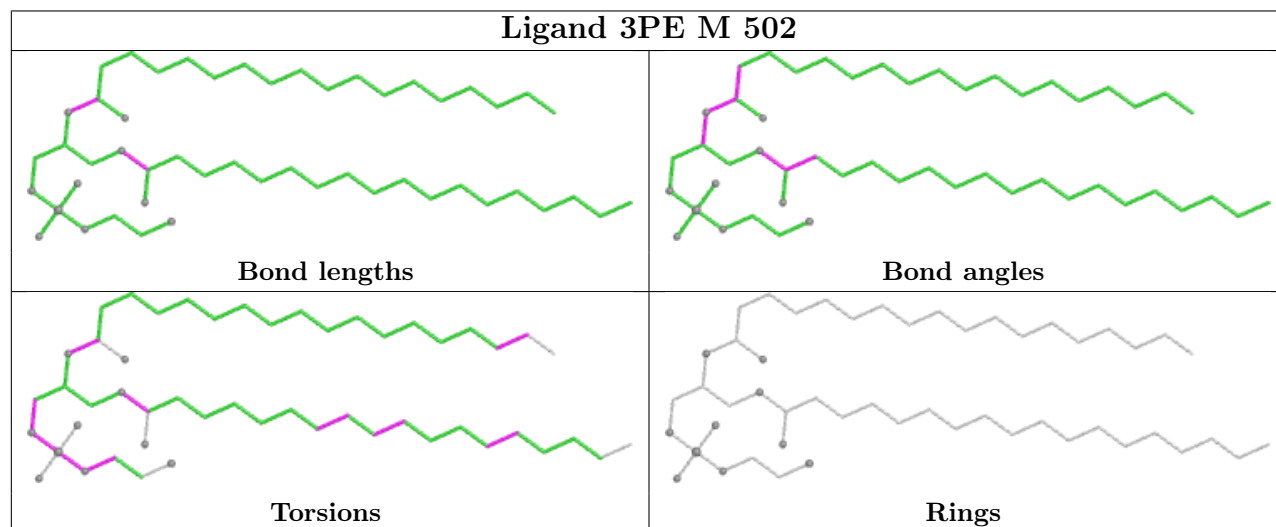
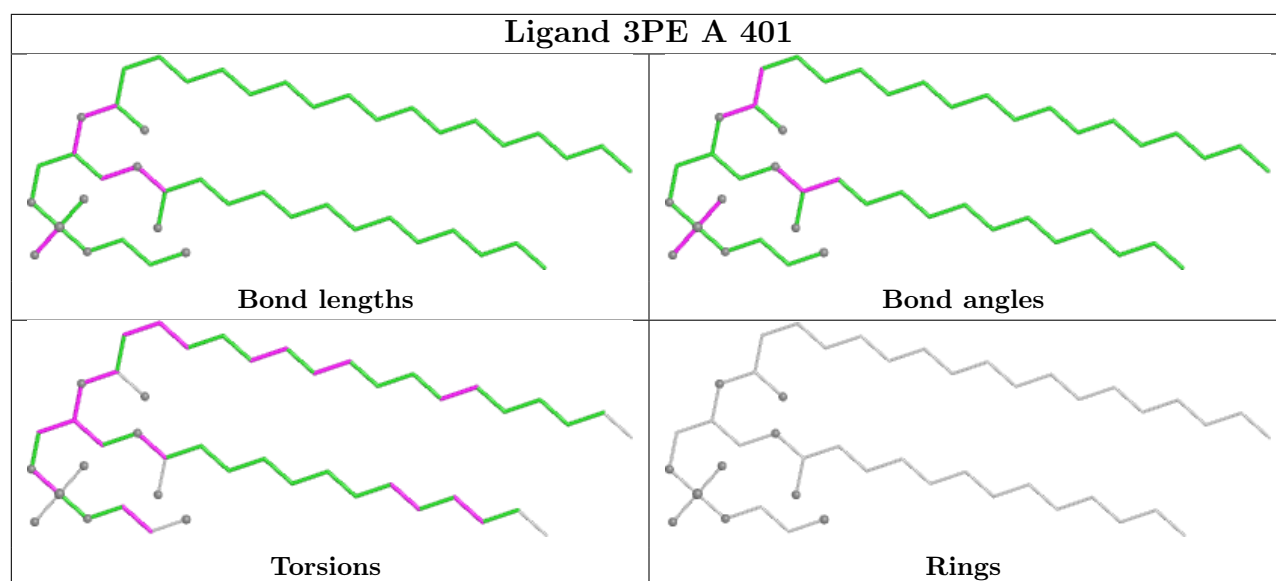


Ligand SF4 I 303

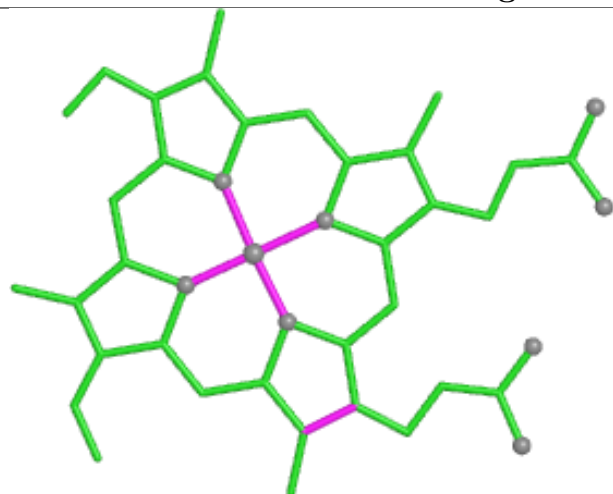


Ligand CDL AG 102

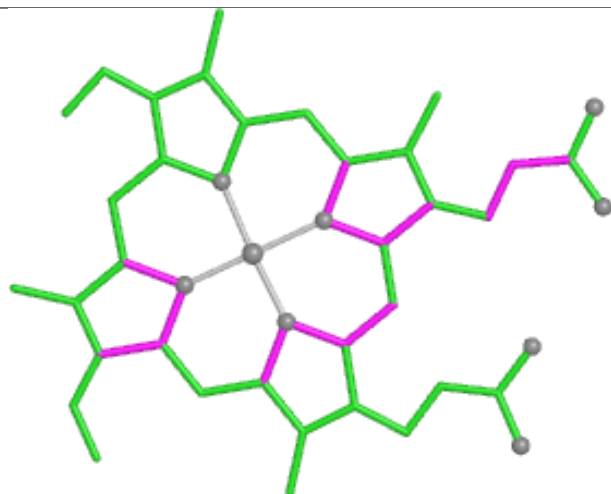




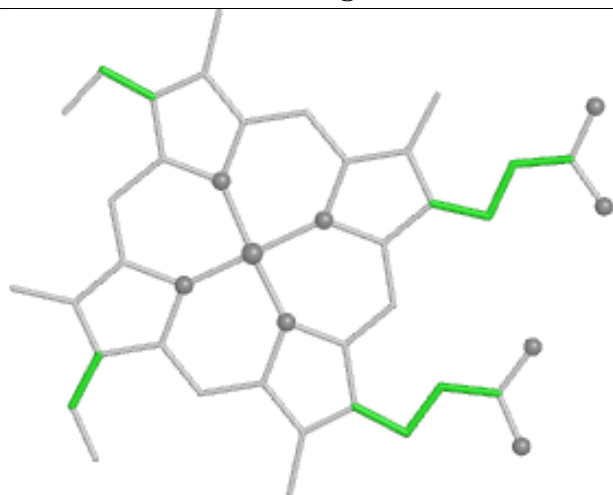
Ligand HEC AD 401



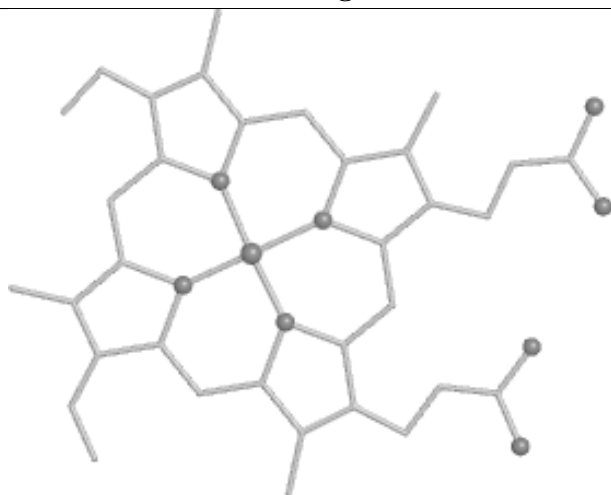
Bond lengths



Bond angles

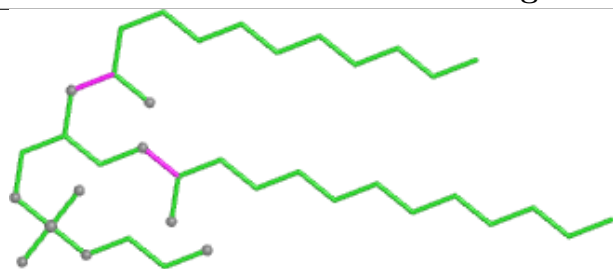


Torsions

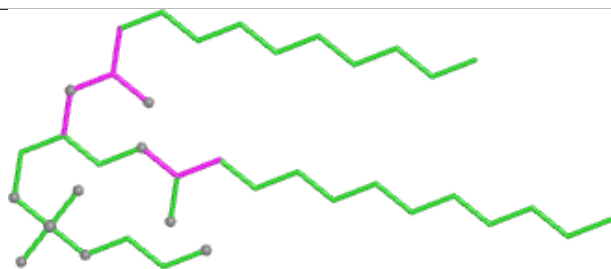


Rings

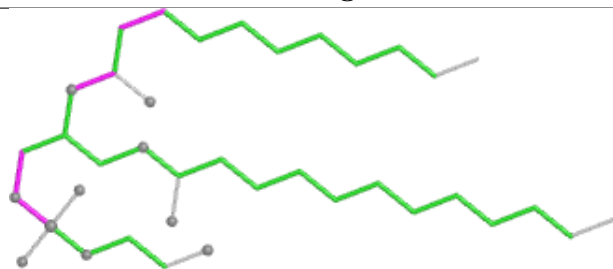
Ligand 3PE L 704



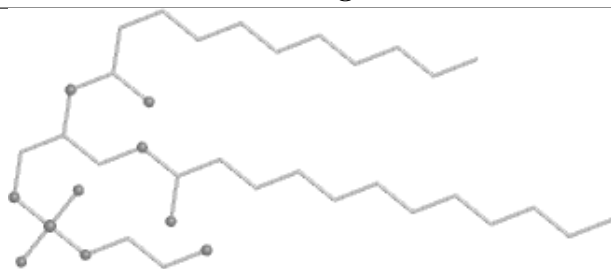
Bond lengths



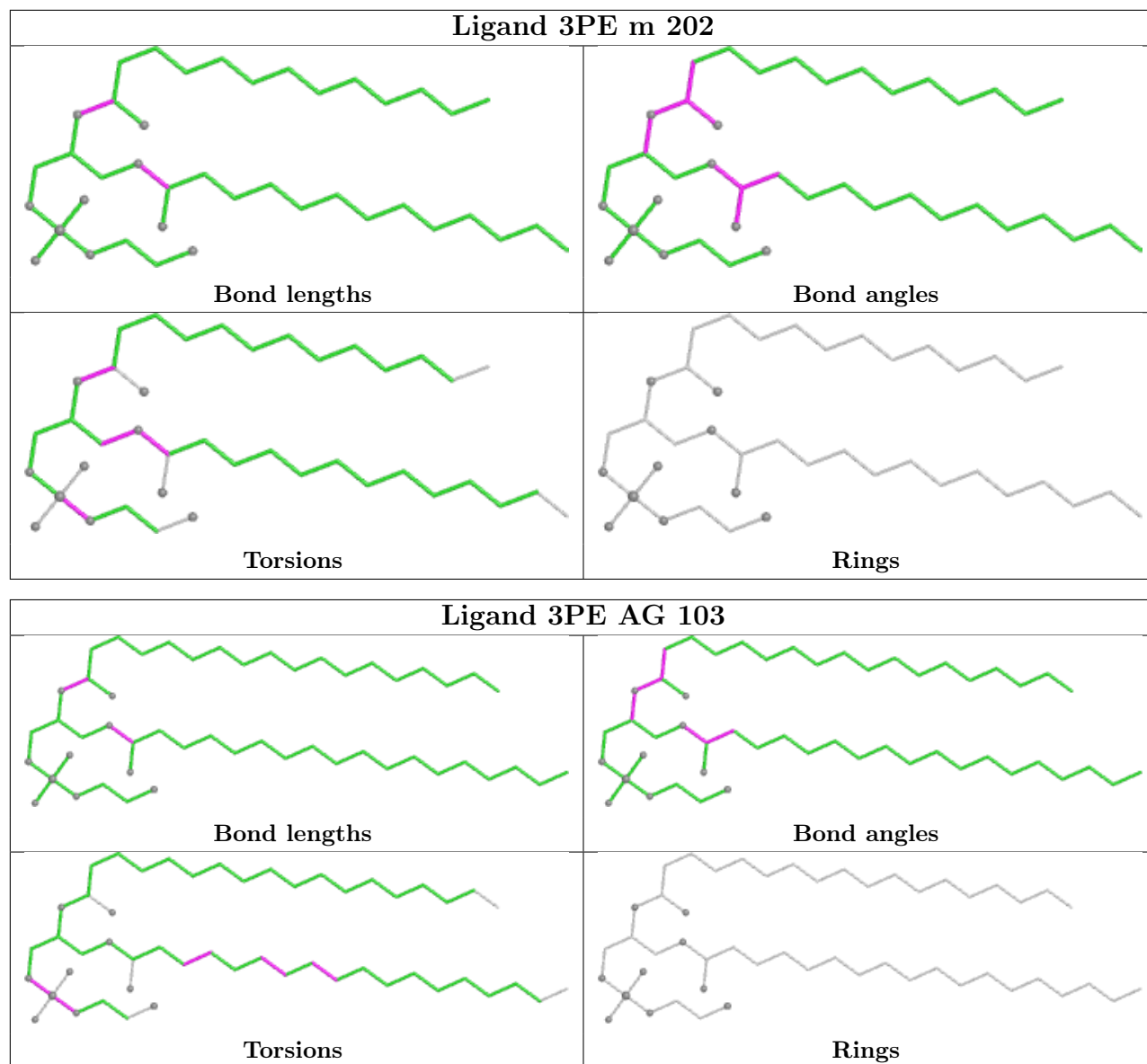
Bond angles

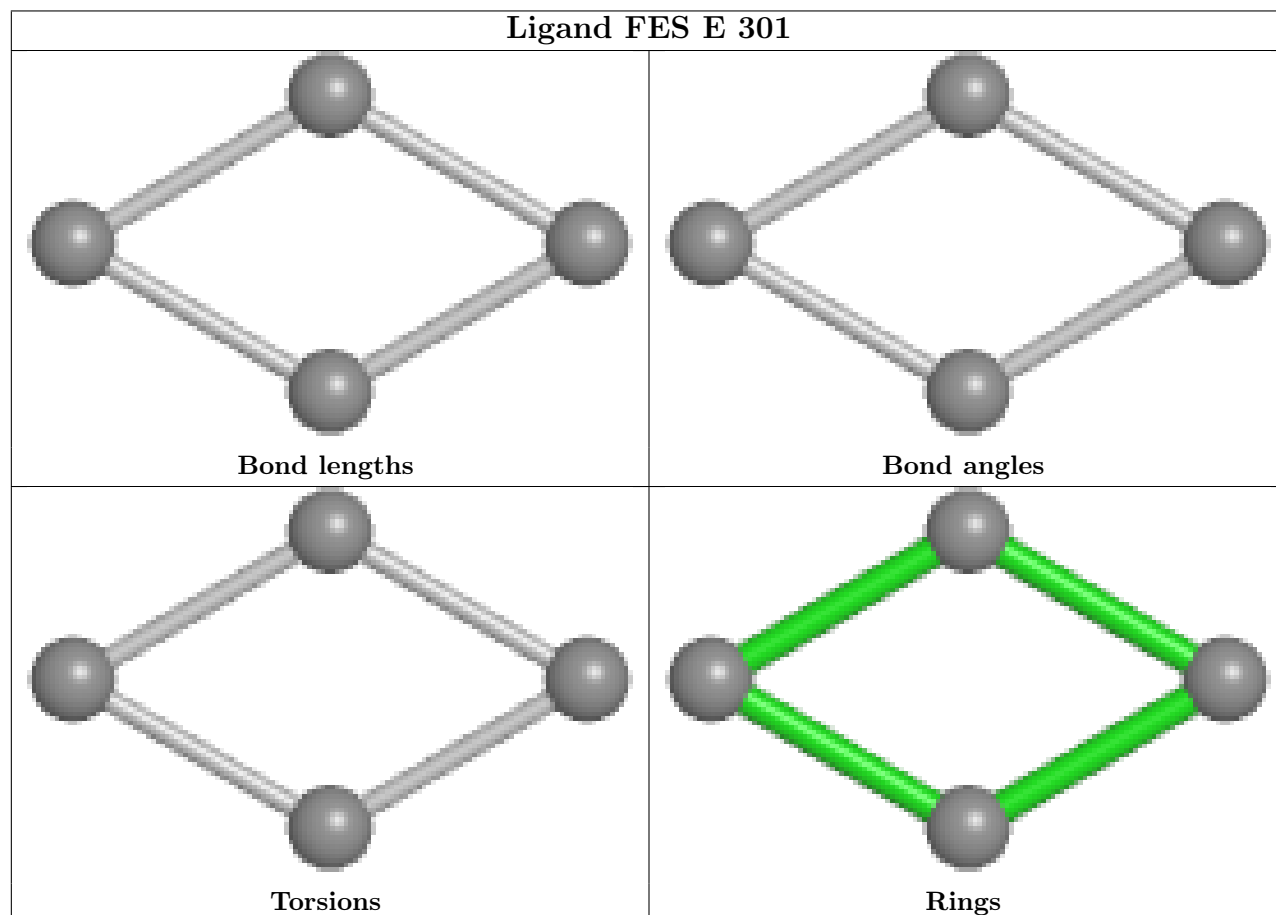
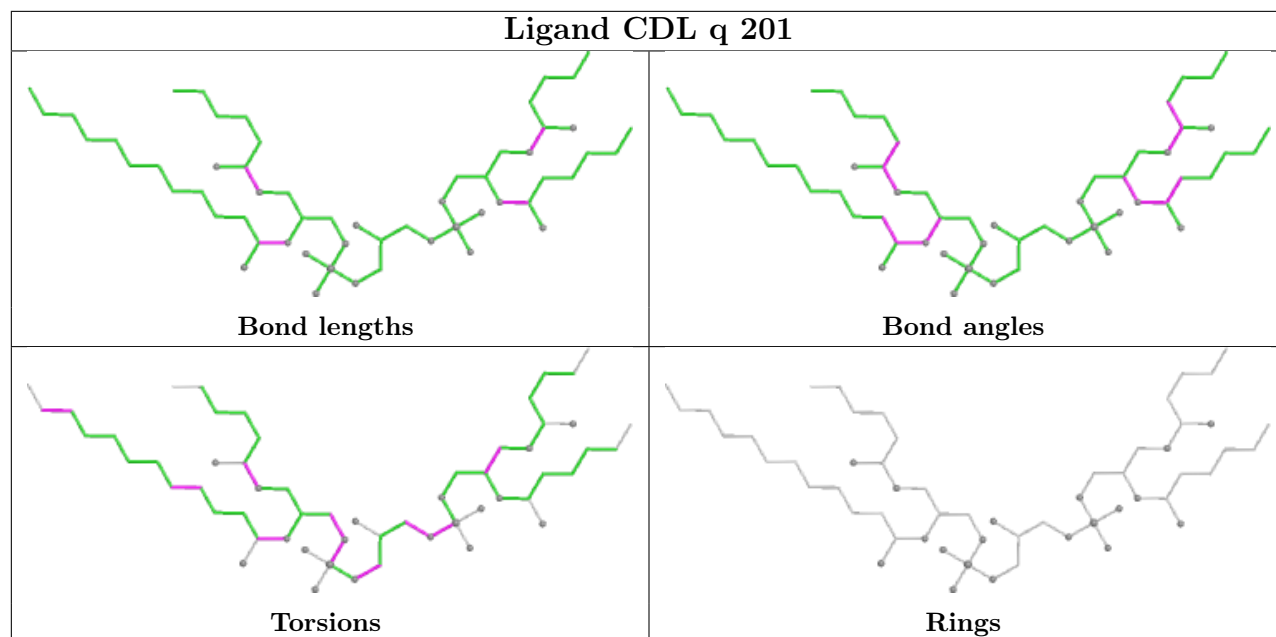


Torsions

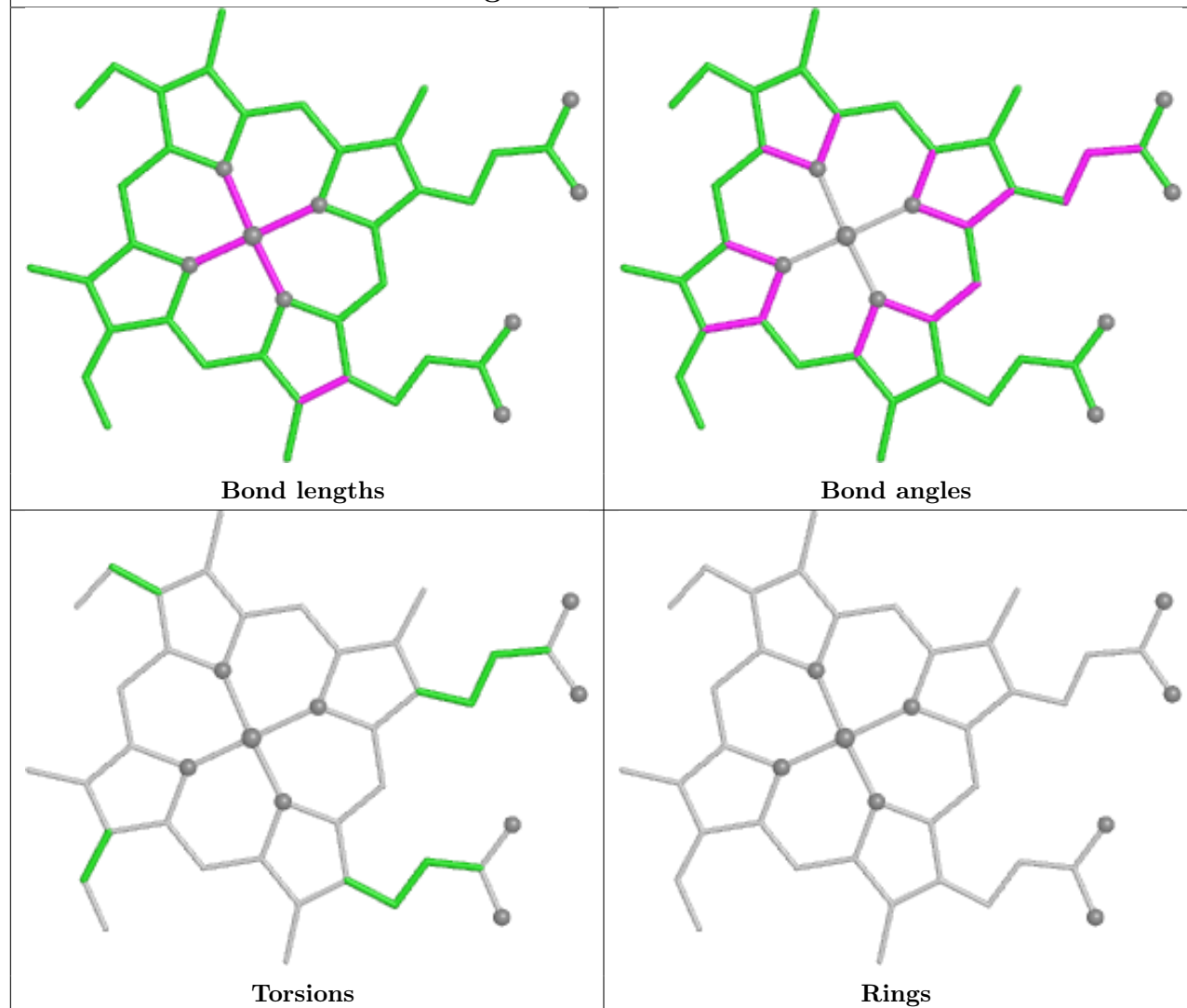


Rings

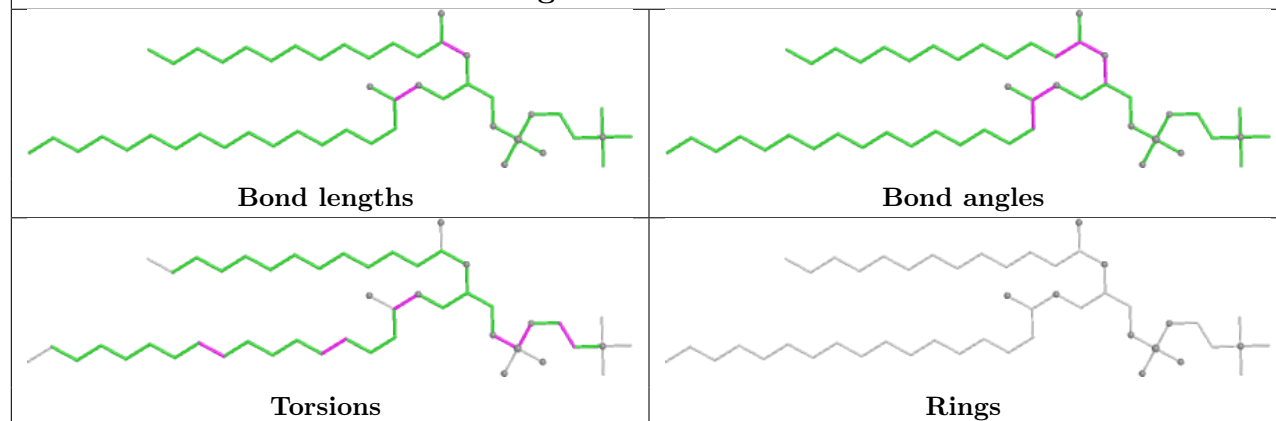


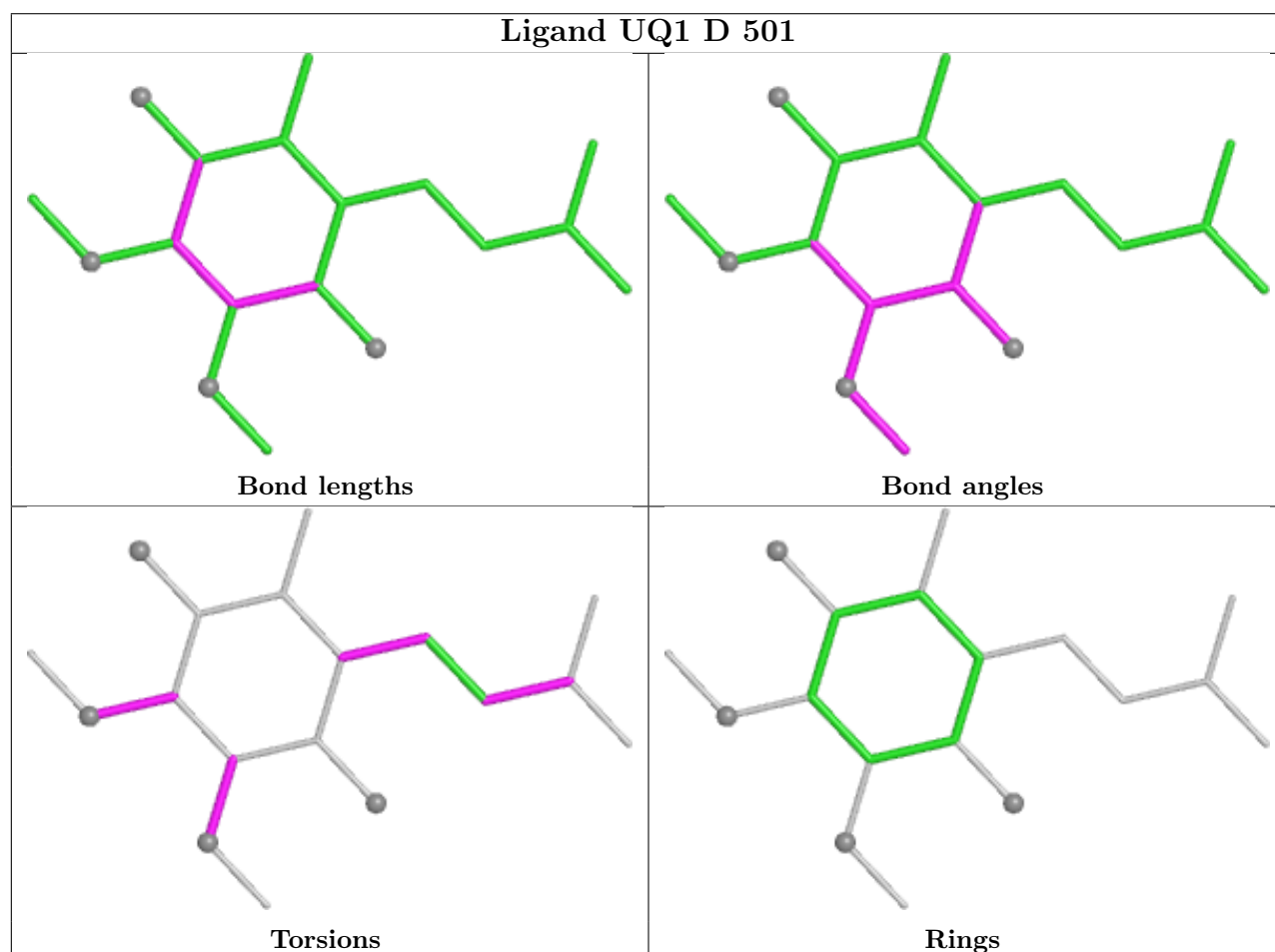
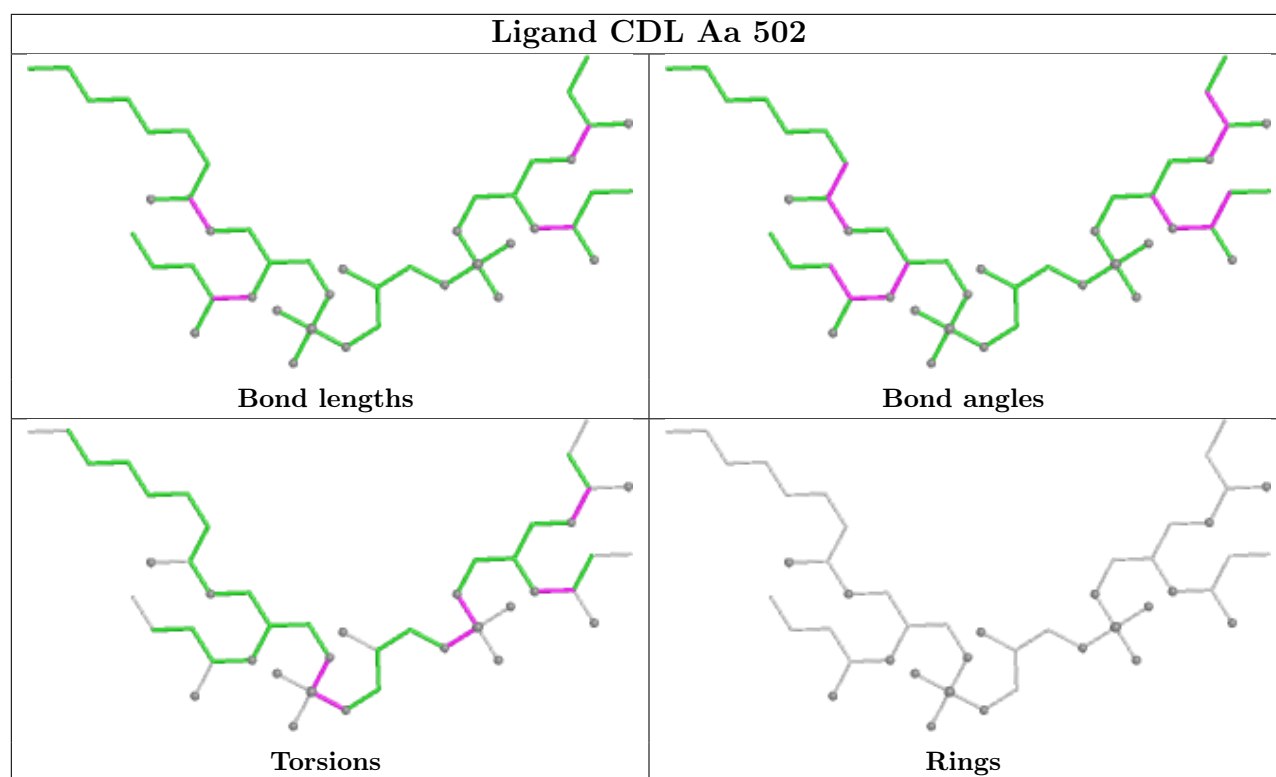


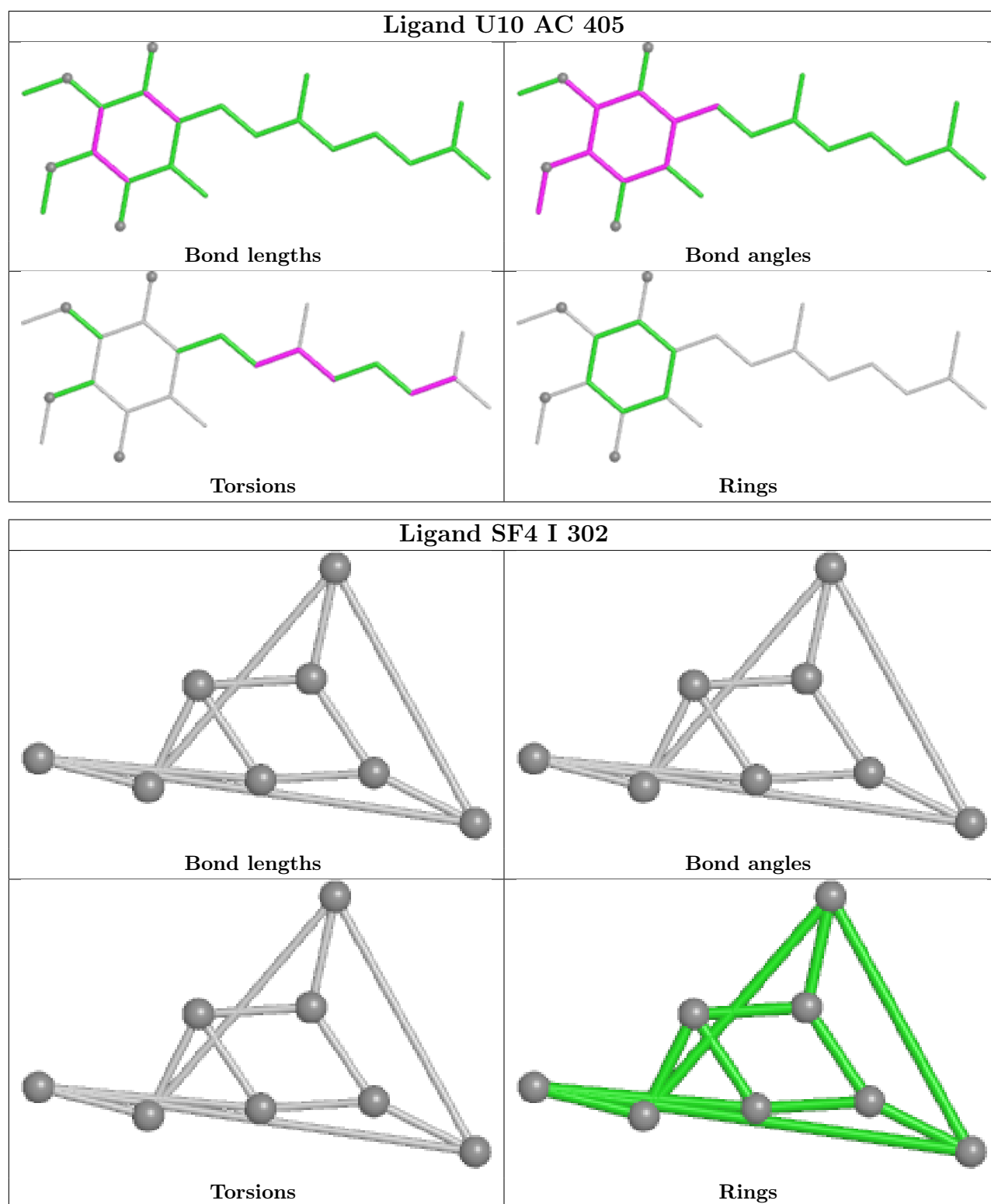
Ligand HEC Ad 401



Ligand PC1 L 701







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

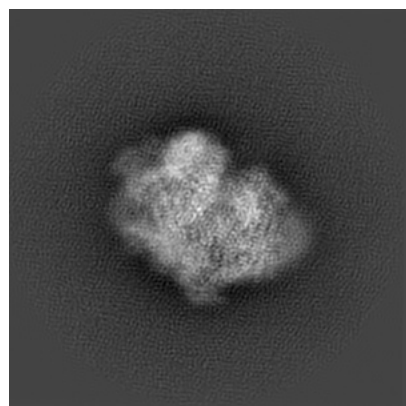
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35313. These allow visual inspection of the internal detail of the map and identification of artifacts.

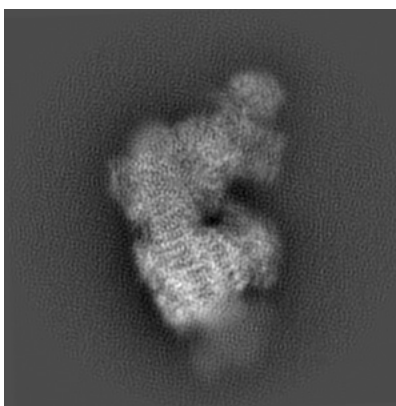
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

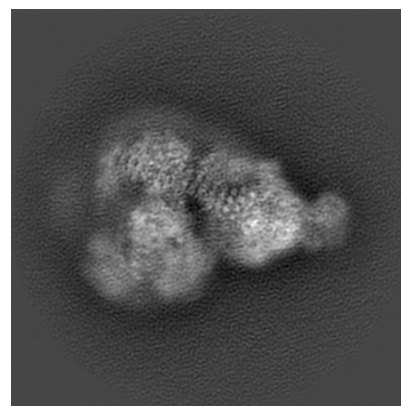
6.1.1 Primary map



X

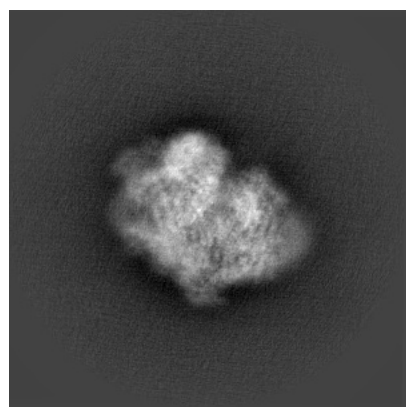


Y

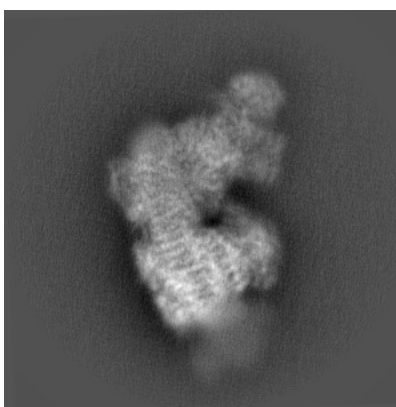


Z

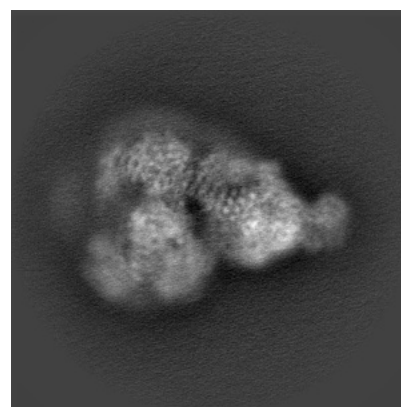
6.1.2 Raw map



X



Y

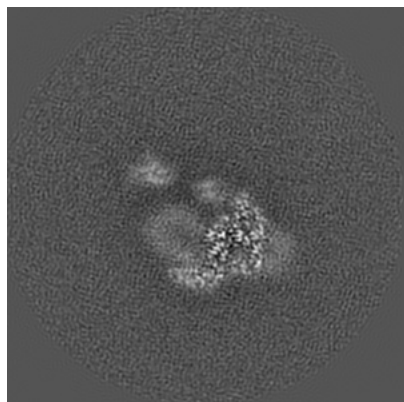


Z

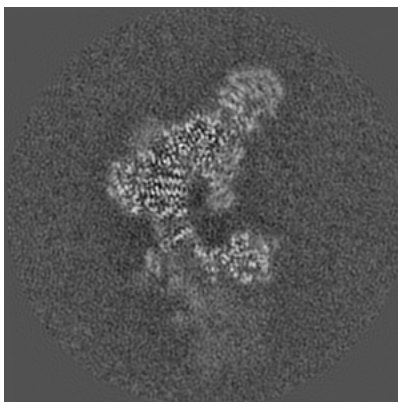
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

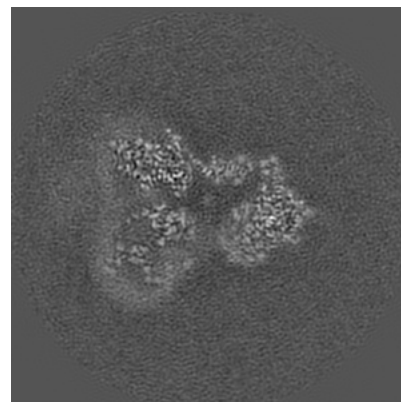
6.2.1 Primary map



X Index: 192

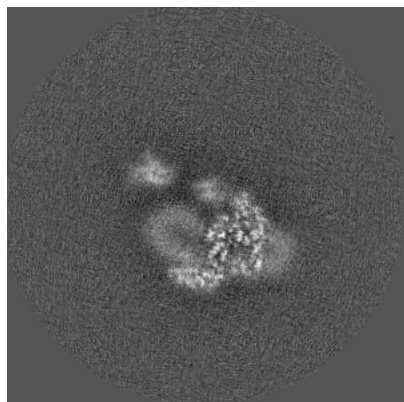


Y Index: 192

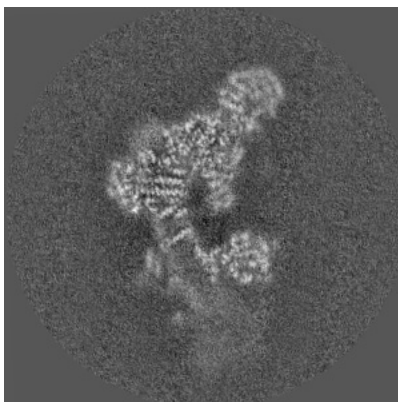


Z Index: 192

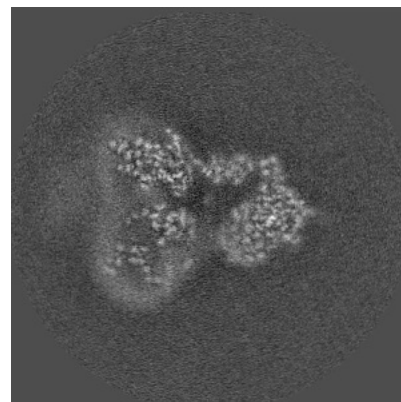
6.2.2 Raw map



X Index: 192



Y Index: 192

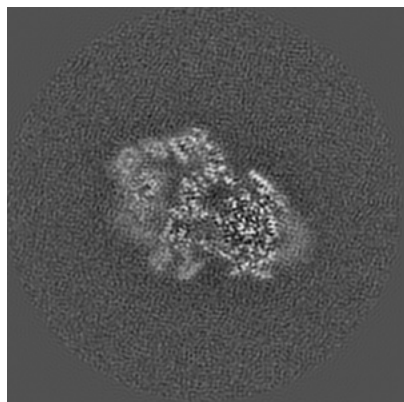


Z Index: 192

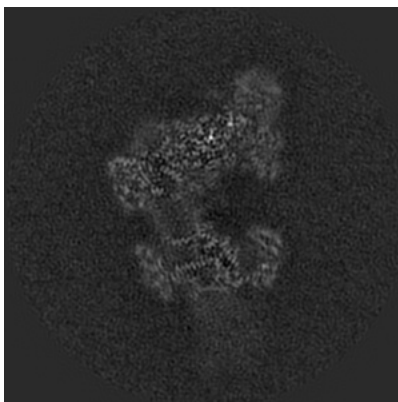
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

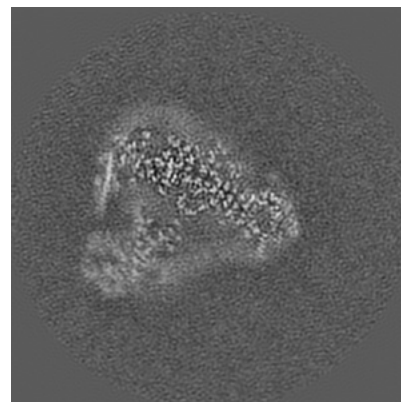
6.3.1 Primary map



X Index: 153

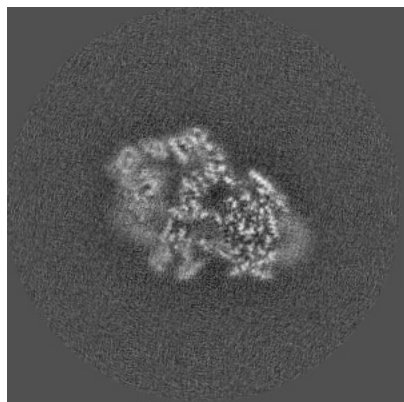


Y Index: 177

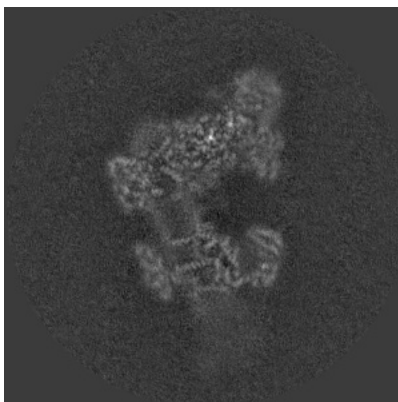


Z Index: 167

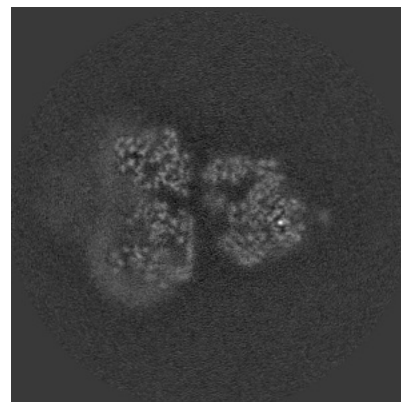
6.3.2 Raw map



X Index: 153



Y Index: 177

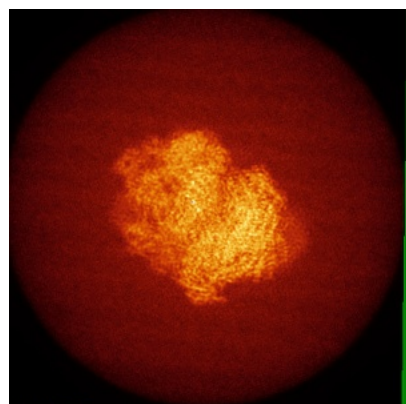


Z Index: 198

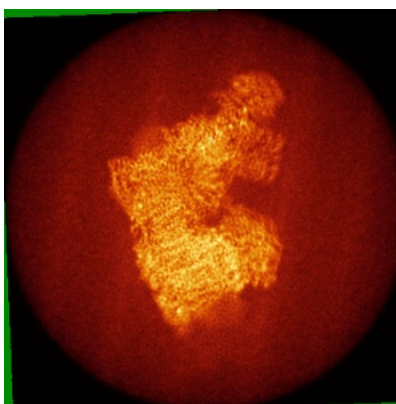
The images above show the largest variance slices of the map in three orthogonal directions.

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

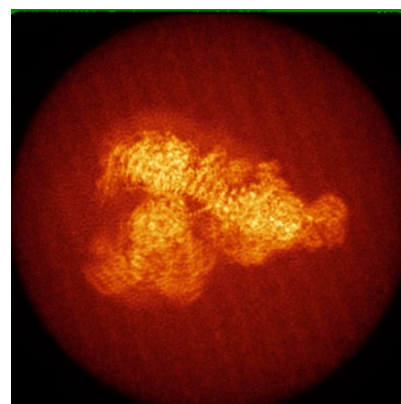
6.4.1 Primary map



X

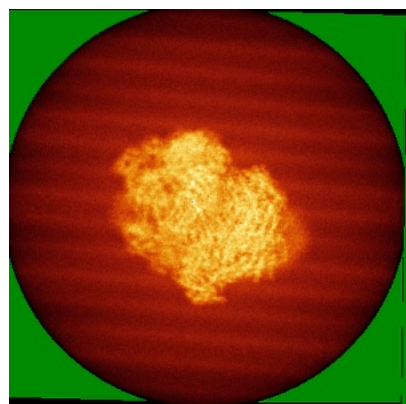


Y

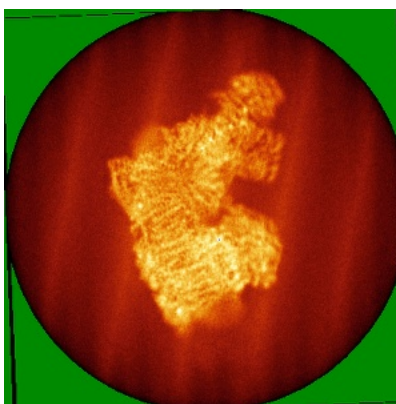


Z

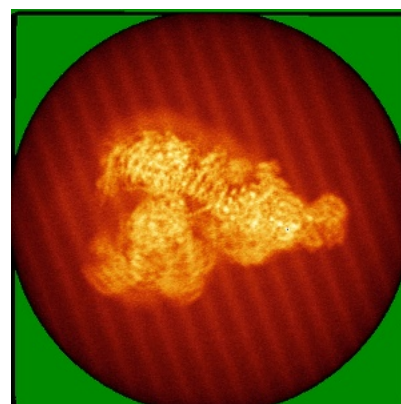
6.4.2 Raw map



X



Y

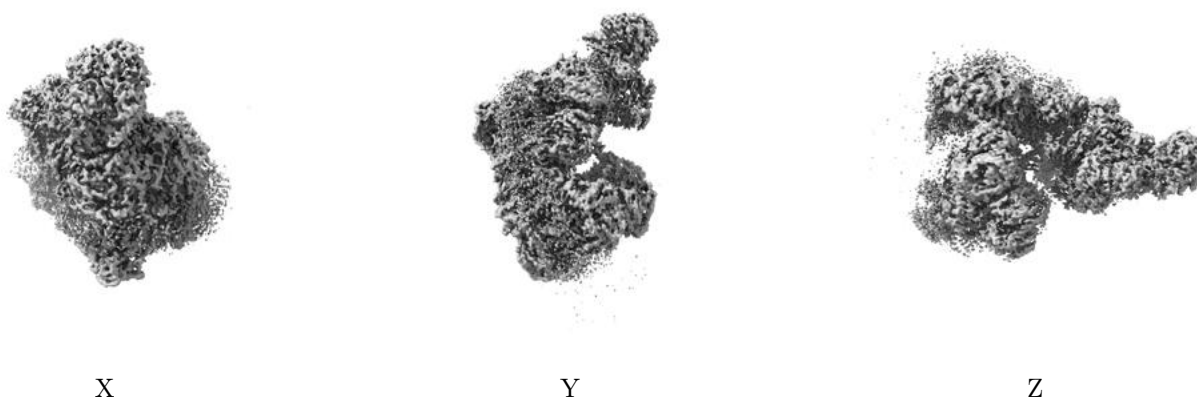


Z

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.

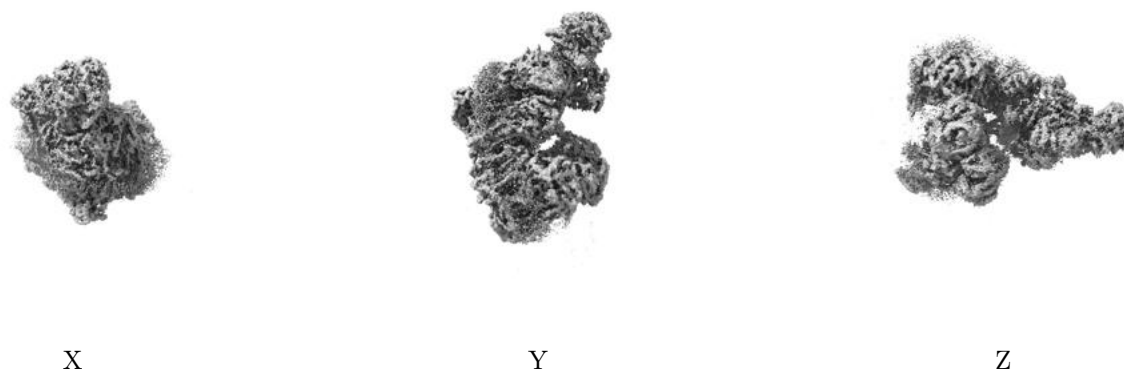
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

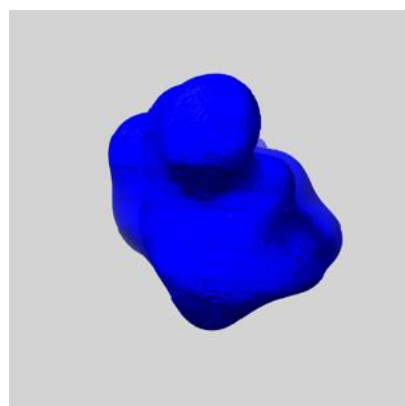
6.6 Mask visualisation [i](#)

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

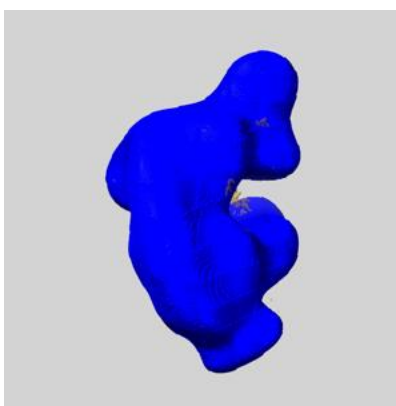
A mask typically either:

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

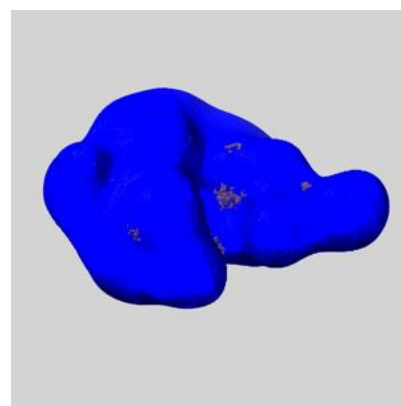
6.6.1 emd_35313_msk_1.map [i](#)



X



Y

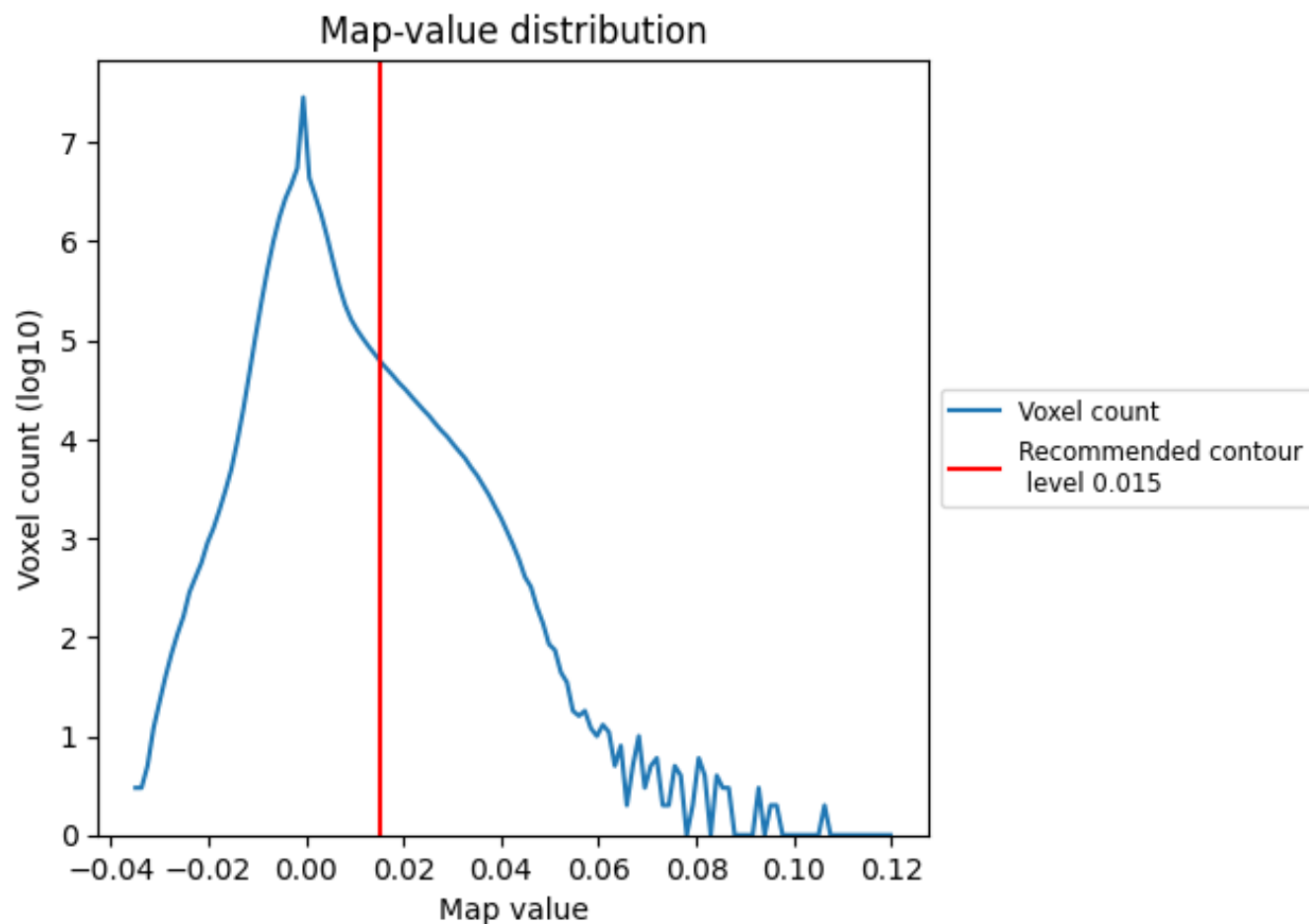


Z

7 Map analysis [i](#)

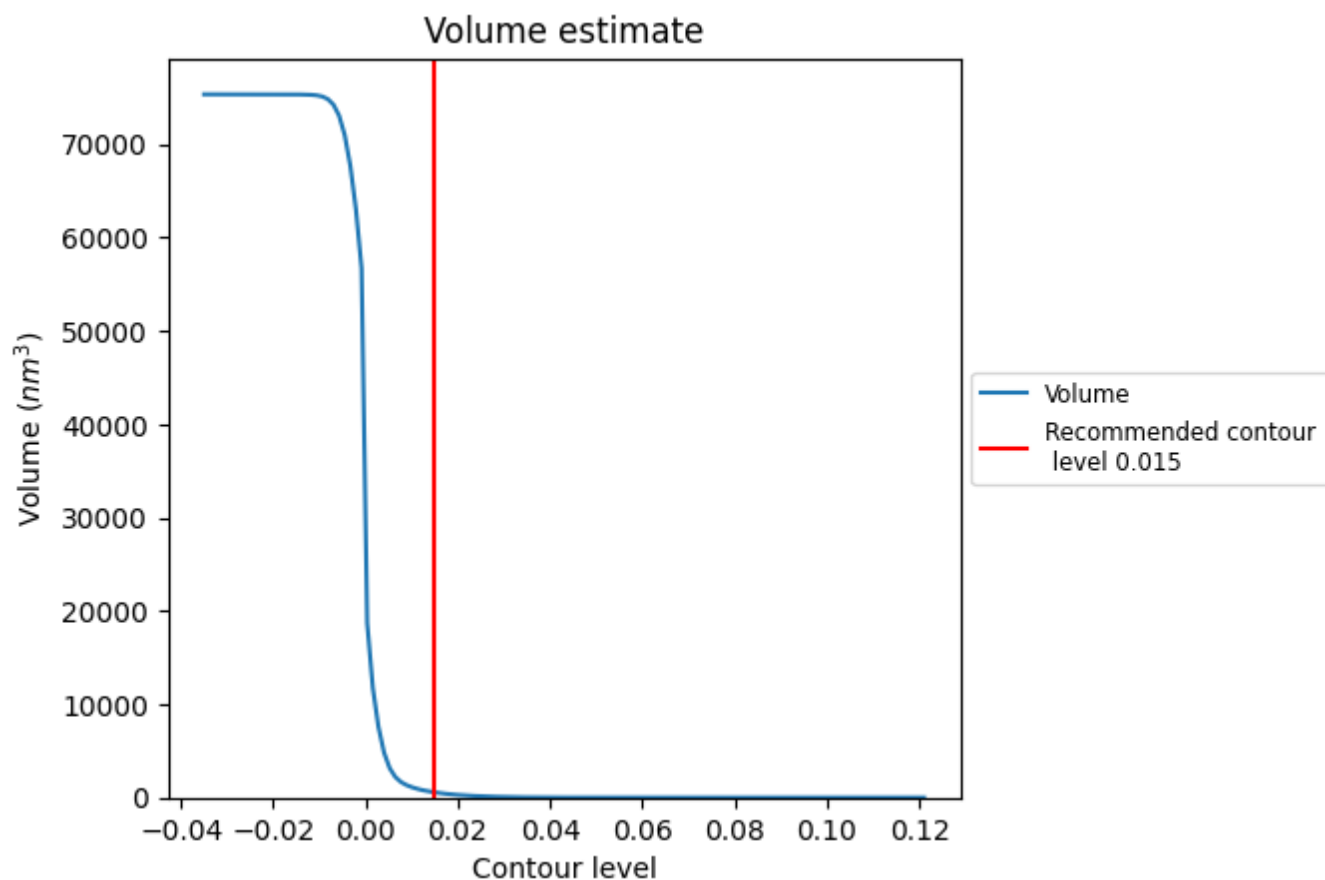
This section contains the results of statistical analysis of the map.

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.

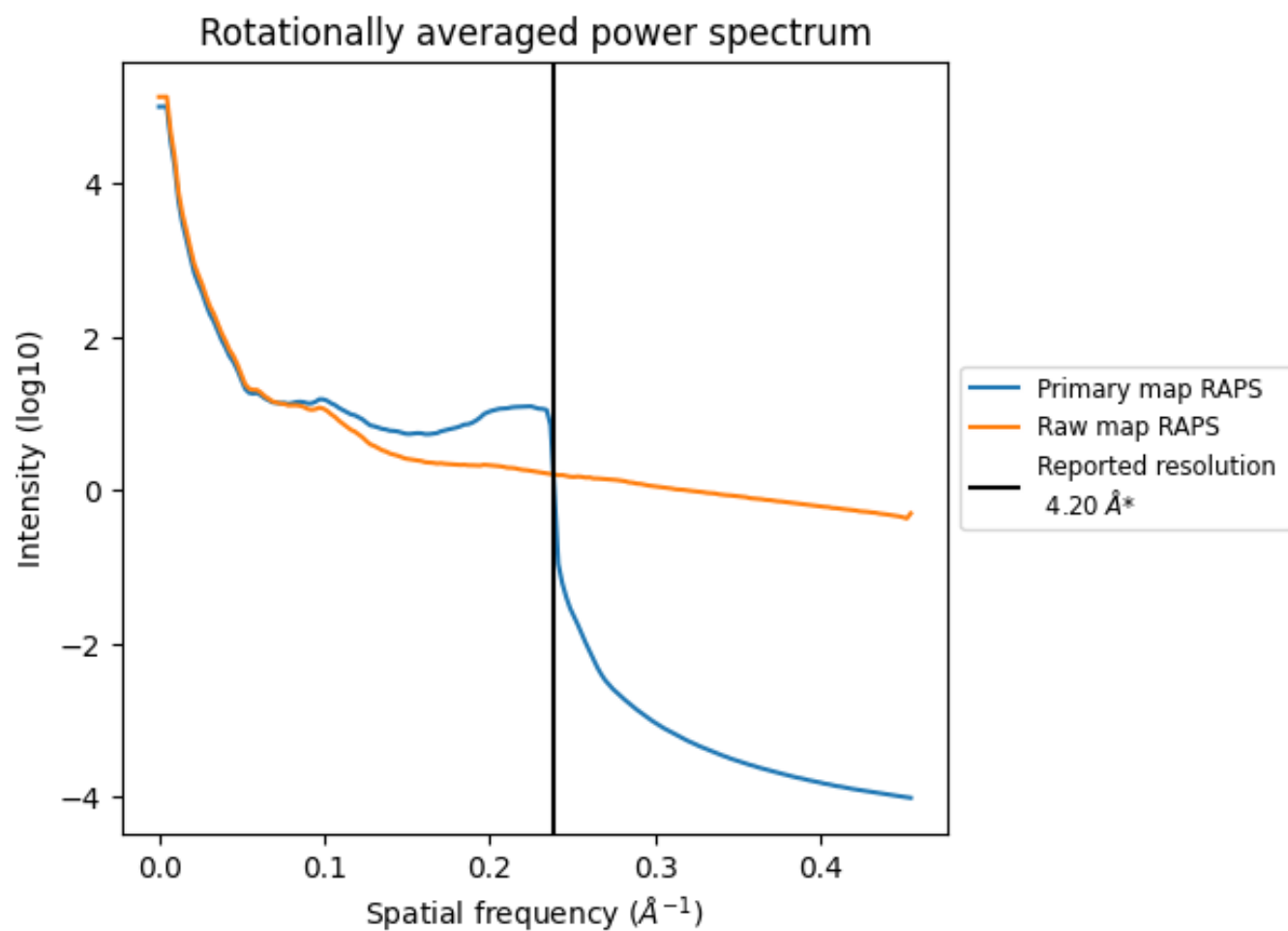
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 556 nm^3 ; this corresponds to an approximate mass of 502 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

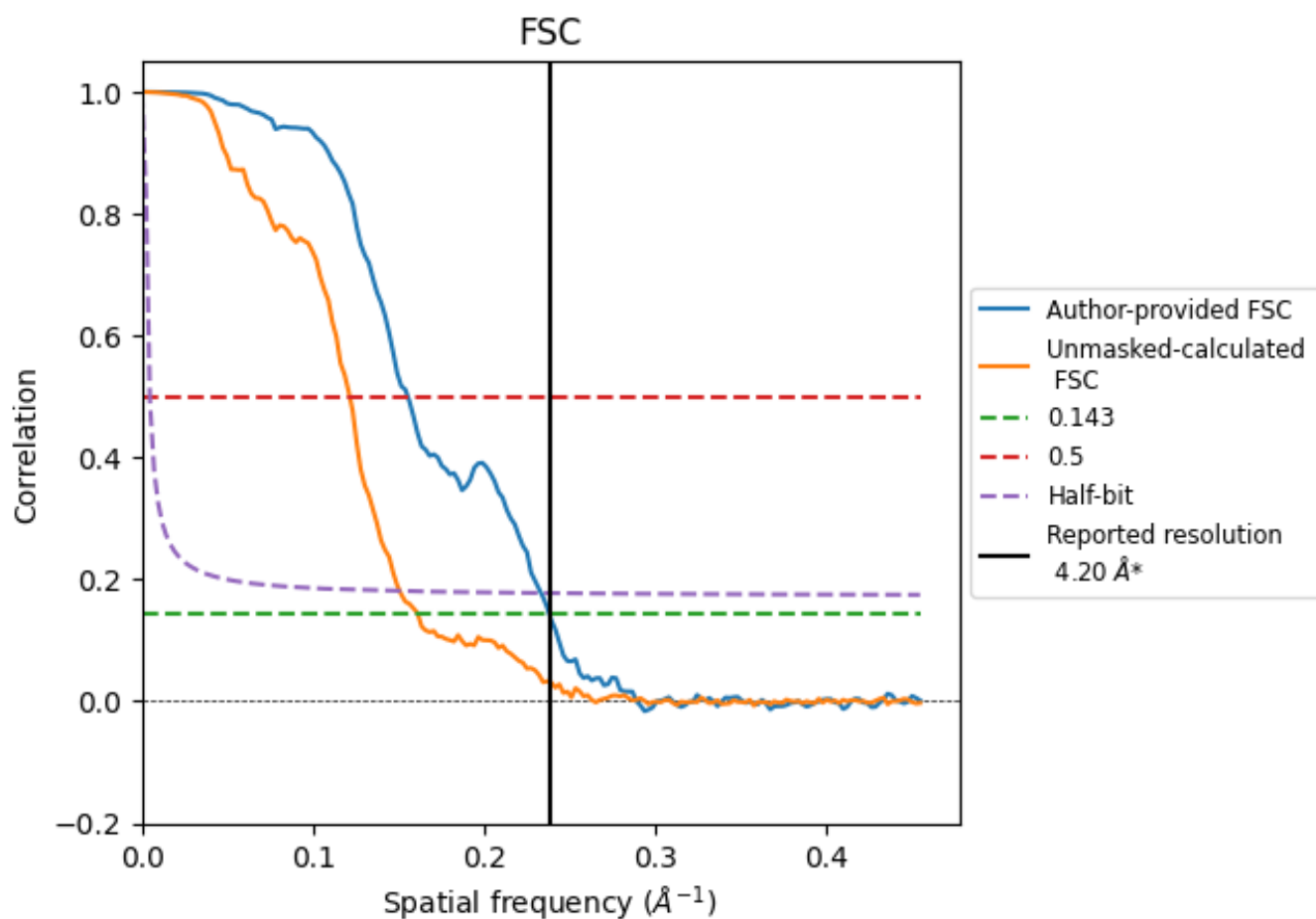


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

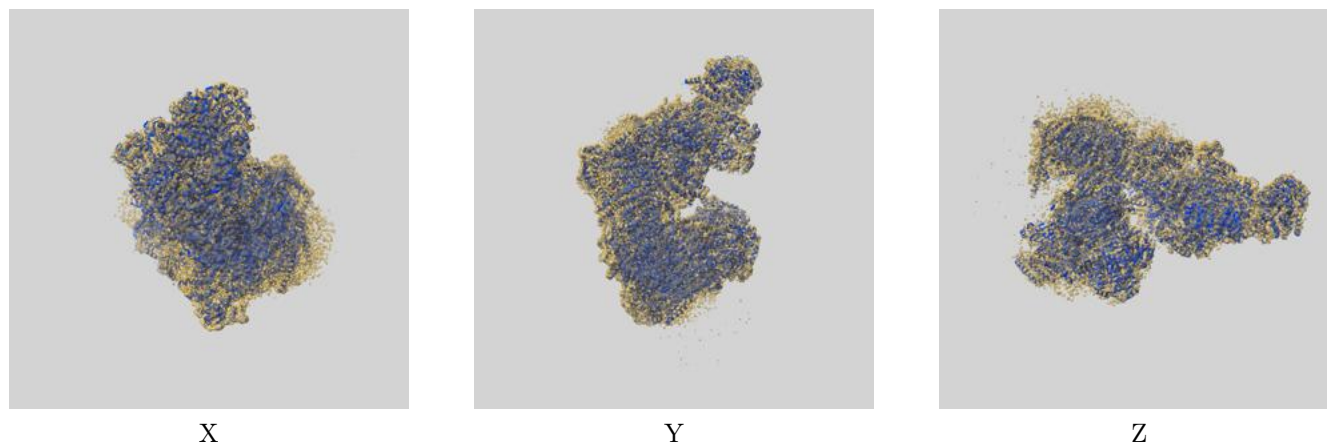
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.44	4.29
Unmasked-calculated*	6.21	8.24	6.64

*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 6.21 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

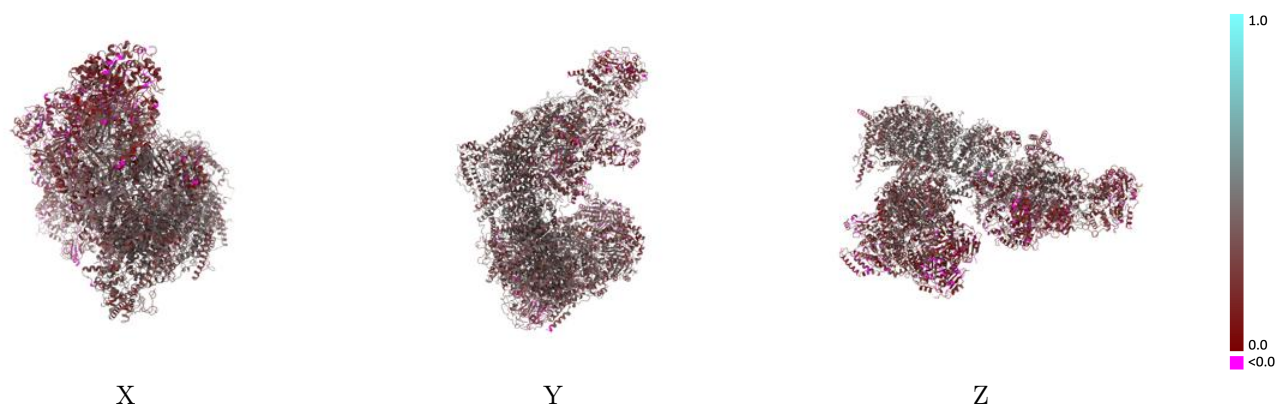
This section contains information regarding the fit between EMDB map EMD-35313 and PDB model 8IAO. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



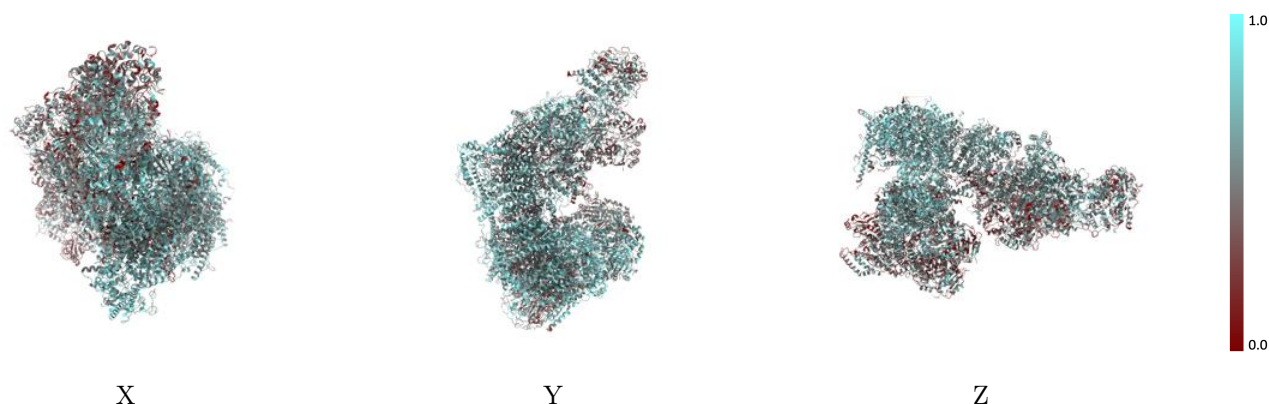
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



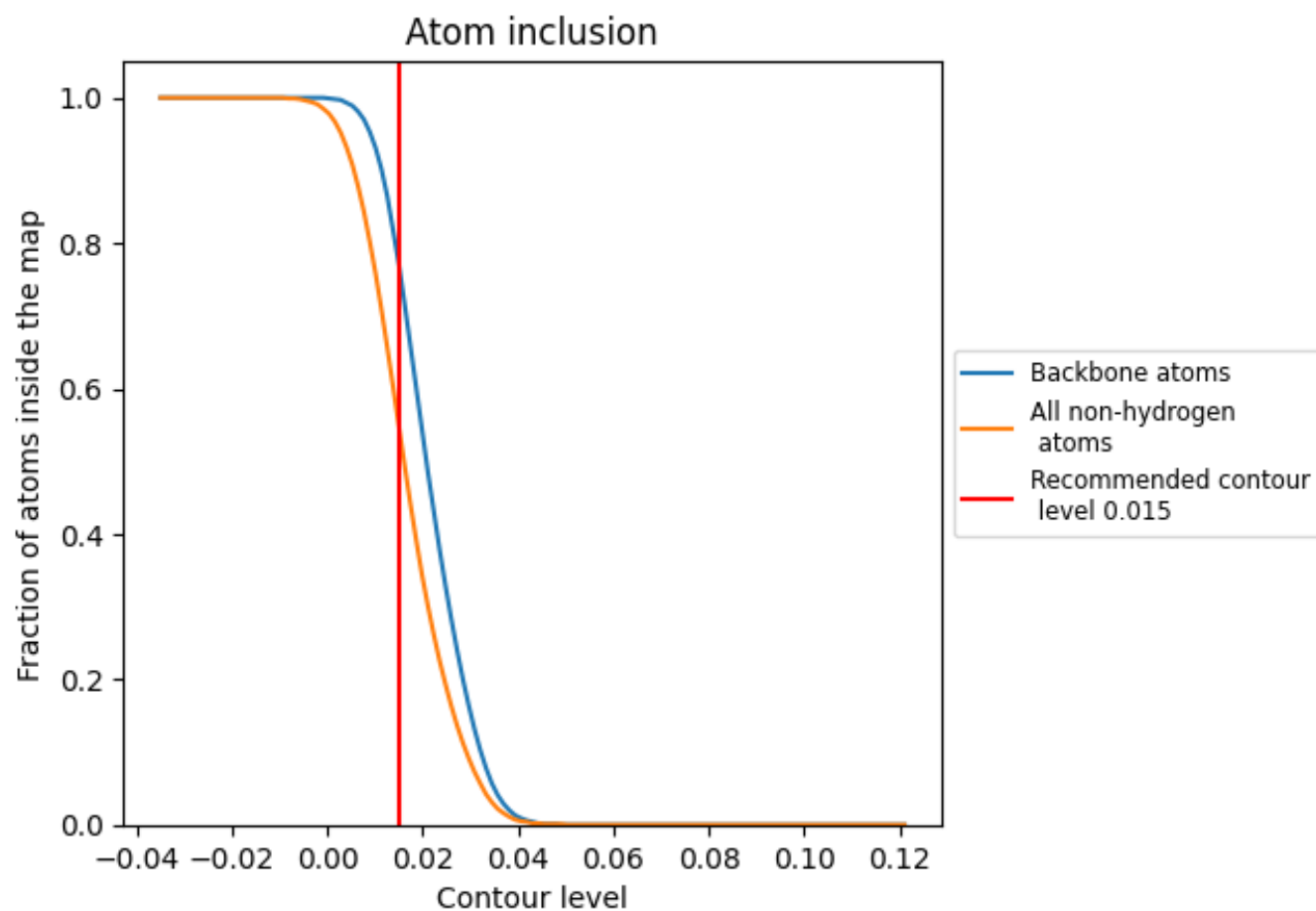
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 55% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5480	 0.2950
A	 0.4860	 0.3410
AA	 0.4790	 0.1900
AB	 0.4570	 0.2030
AC	 0.4580	 0.2680
AD	 0.4900	 0.2020
AE	 0.2500	 0.1680
AF	 0.5790	 0.2560
AG	 0.3290	 0.1880
AH	 0.4340	 0.1150
AI	 0.1140	 0.1520
AJ	 0.3730	 0.2090
AK	 0.2270	 0.1820
Aa	 0.6570	 0.3410
Ab	 0.6130	 0.2800
Ac	 0.5380	 0.3210
Ad	 0.5200	 0.2490
Ae	 0.2530	 0.1840
Af	 0.5570	 0.2980
Ag	 0.4900	 0.3220
Ah	 0.4380	 0.1750
Ai	 0.2340	 0.2550
Aj	 0.3740	 0.2260
Ak	 0.2810	 0.2340
B	 0.6520	 0.3650
C	 0.6110	 0.3230
D	 0.6340	 0.3640
E	 0.4710	 0.2200
F	 0.4780	 0.2120
G	 0.4680	 0.2300
H	 0.5830	 0.3630
I	 0.6470	 0.3510
J	 0.4890	 0.3360
K	 0.6140	 0.3890
L	 0.6360	 0.3700



Continued on next page...

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Chain	Atom inclusion	Q-score
M	 0.6520	 0.4030
N	 0.6470	 0.3960
O	 0.6120	 0.3250
P	 0.3820	 0.1950
Q	 0.4740	 0.2750
R	 0.4820	 0.2780
S	 0.3800	 0.1320
T	 0.2640	 0.1360
U	 0.6950	 0.3650
V	 0.5510	 0.2390
W	 0.4310	 0.2360
X	 0.6940	 0.3350
Y	 0.5540	 0.3560
Z	 0.6820	 0.3230
a	 0.6990	 0.3640
b	 0.6520	 0.3380
c	 0.5850	 0.2880
d	 0.6340	 0.3740
e	 0.6710	 0.3650
f	 0.6220	 0.3180
g	 0.6470	 0.3470
h	 0.6460	 0.3530
i	 0.6530	 0.3580
j	 0.6570	 0.3130
k	 0.7120	 0.3440
l	 0.6680	 0.3680
m	 0.6300	 0.3620
n	 0.7200	 0.3760
o	 0.5940	 0.2710
p	 0.6840	 0.3510
q	 0.5190	 0.3170
r	 0.4450	 0.2750
s	 0.3350	 0.1910