Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 07:19 PM JST

PDB ID	:	8IB9 / pdb_00008ib9
EMDB ID	:	EMD-35336
Title	:	Respiratory complex CI:CIII2, type IB, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	4.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

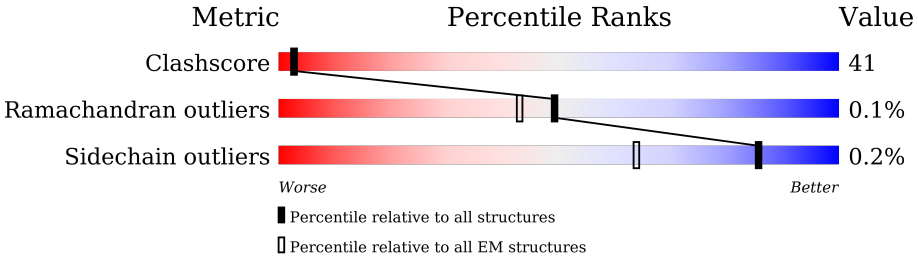
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

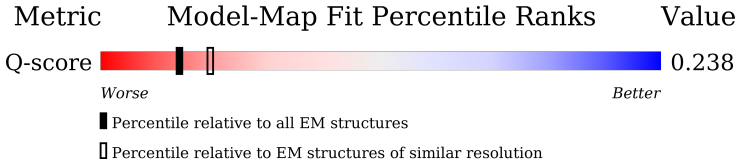
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8%, 25%, 53%, •, 19%
2	B	224	•, 28%, 36%, 5%, 30%
3	C	263	10%, 38%, 33%, •, 25%
4	D	463	8%, 37%, 50%, 5%, 8%

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Mol	Chain	Length	Quality of chain
5	E	248	46% 27% 54% • 15%
6	F	464	47% 31% 54% 6% 8%
7	G	727	36% 38% 50% 7% 6%
8	H	318	6% 31% 57% 11% •
9	I	212	• 37% 40% 6% 18%
10	J	172	12% 32% 54% 5% • 9%
11	K	98	• 39% 58% • •
12	L	607	• 32% 57% 10%
13	M	459	• 29% 59% 13%
14	N	345	34% 57% 8%
15	O	355	15% 35% 51% • 10%
16	P	377	44% 32% 53% 5% 10%
17	Q	175	28% 35% 29% • 33%
18	R	116	47% 24% 38% 9% 28%
19	S	99	46% 31% 46% 6% 16%
20	T	156	31% 13% 29% 6% 52%
20	U	156	• 21% 30% • • 44%
21	V	116	16% 47% 44% 6% •
22	W	131	24% 42% 42% • 13%
23	X	172	• 38% 55% 5% •
24	Y	143	8% 49% 48% • •
25	Z	144	• 36% 56% 5% •
26	a	70	• 34% 57% • •
27	b	84	• 32% 61% • 6%
28	c	76	7% 22% 34% 5% 38%

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Mol	Chain	Length	Quality of chain
29	d	120	7% 39% 58%
30	e	106	40% 57%
31	f	57	5% 42% 37% 12% 9%
32	g	151	35% 25% 7% 34%
33	h	189	33% 39% 27%
34	i	128	30% 35% 7% 28%
35	j	105	30% 32% 5% 33%
36	k	104	31% 28% 11% 31%
37	l	186	45% 33% 6% 16%
38	m	129	50% 41% 6%
39	n	179	40% 53% 6%
40	o	137	12% 34% 50% 13%
41	p	176	45% 47%
42	q	145	67% 32% 43% 8% 17%
43	r	113	27% 22% 17% 5% 56%
44	s	104	23% 12% 12% 75%
45	AA	480	54% 46% 36% 17%
45	Aa	480	20% 52% 30% 16%
46	AB	453	64% 62% 29% 9%
46	Ab	453	37% 60% 30% 9%
47	AC	381	72% 68% 30%
47	Ac	381	46% 58% 38%
48	AD	325	46% 30% 43% 27%
48	Ad	325	39% 30% 42% 27%
49	AE	274	65% 20% 47% 32%

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Mol	Chain	Length	Quality of chain
49	AI	274	17% 9% 9% 81%
49	Ae	274	61% 16% 49% 31%
50	AF	111	50% 61% 27% 12%
50	Af	111	33% 41% 47% 12%
51	AG	82	72% 46% 46% 7%
51	Ag	82	35% 41% 51% 7%
52	AH	89	47% 19% 49% 28%
52	Ah	89	39% 20% 54% 26%
53	AJ	64	59% 30% 30% 41%
53	Aj	64	61% 36% 38% 25%
54	AK	56	55% 20% 41% 39%
54	Ak	56	75% 36% 39% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	SF4	B	301	-	-	X	-
55	SF4	F	502	-	-	X	-
55	SF4	G	802	-	-	X	-
55	SF4	I	303	-	-	X	-
55	SF4	I	304	-	-	X	-
56	UQ1	B	302	-	-	X	-
58	3PE	M	503	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
70	HEC	AD	401	X	-	-	-
70	HEC	Ad	401	X	-	-	-

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 97317 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
			Total	C	N	O	S		
1	A	93	762	528	108	120	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	14	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	425	3423	2188	588	623	24	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	316	2525	1698	382	423	22	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	157	1193	806	169	203	15	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3630	2407	567	616	40	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	75	604	388	89	122	5	0	0
			Total	C	N	O	S		
20	U	87	700	450	103	142	5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	79	620	408	98	110	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	996	651	171	165	9	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	100	842	545	135	158	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	92	773	506	132	132	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	70	587	383	98	105	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	72	578	381	101	94	2	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	177	1534	981	275	267	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	119	1019	642	191	178	8	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	50	413	263	77	72	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	s	26	226	147	38	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AA	399	3117	1943	554	604	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Aa	401	3131	1955	555	605	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AB	414	3107	1954	546	598	9	0	0
			Total	C	N	O	S		
46	Ab	413	3101	1948	543	601	9	0	0

- Molecule 47 is a protein called Cytochrome b.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	AE	185	1427	902	250	268	7	0	0
			Total	C	N	O			
49	AI	51	347	221	65	61		0	0
			Total	C	N	O	S		
49	Ae	188	1451	916	254	274	7	0	0

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AH	64	527	321	98	103	5	0	0
			Total	C	N	O	S		
52	Ah	66	544	333	101	105	5	0	0

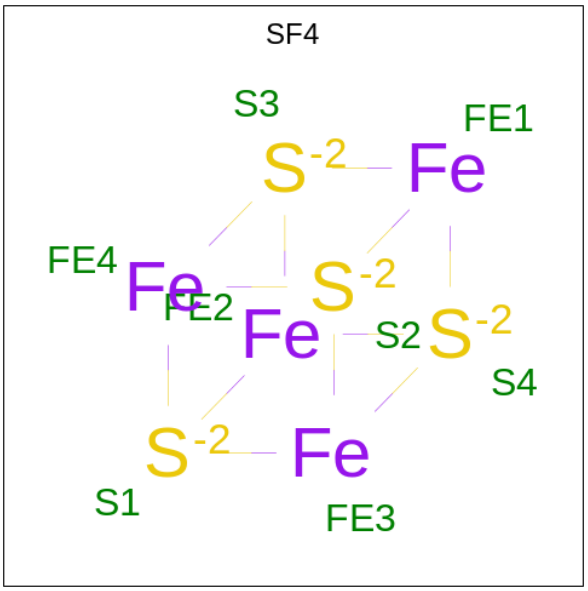
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	AJ	38	307	201	51	55	0	0
			Total	C	N	O		
53	Aj	48	392	257	67	68	0	0

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

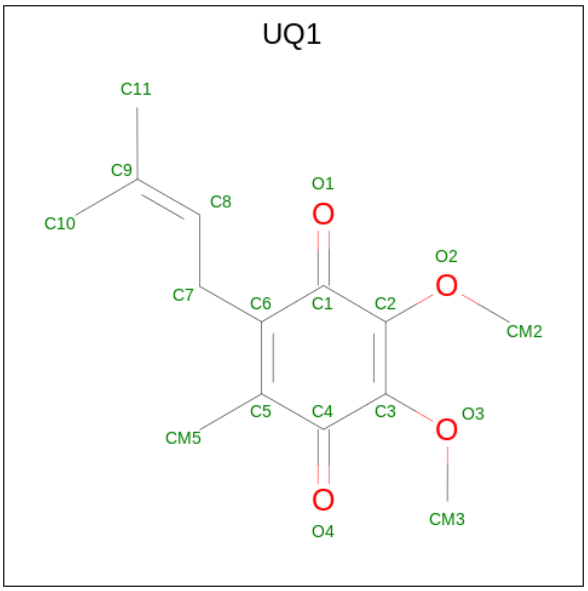
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AK	34	278	183	51	43	1	0	0
			Total	C	N	O	S		
54	Ak	44	357	236	63	57	1	0	0

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



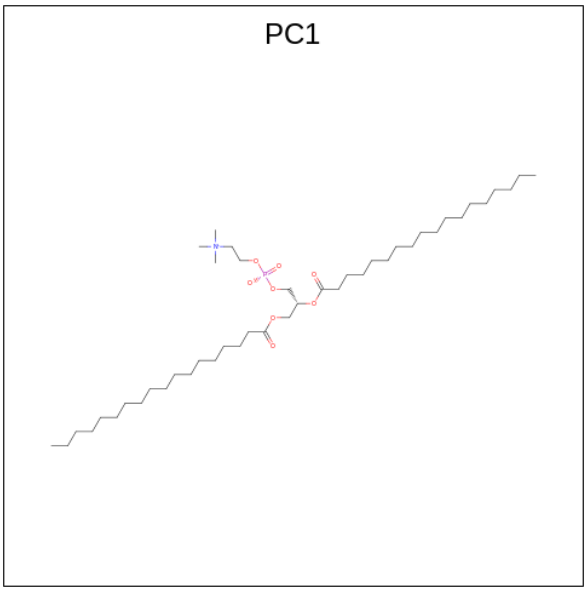
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
55	B	1	8	4	4	0
55	F	1	8	4	4	0
55	G	1	8	4	4	0
55	G	1	8	4	4	0
55	I	1	8	4	4	0
55	I	1	8	4	4	0

- Molecule 56 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
			Total	C	O		
56	B	1	18	14	4		0

- Molecule 57 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	B	1	35	25	1	8	1	0
			Total	C	N	O	P	
57	I	1	47	37	1	8	1	0

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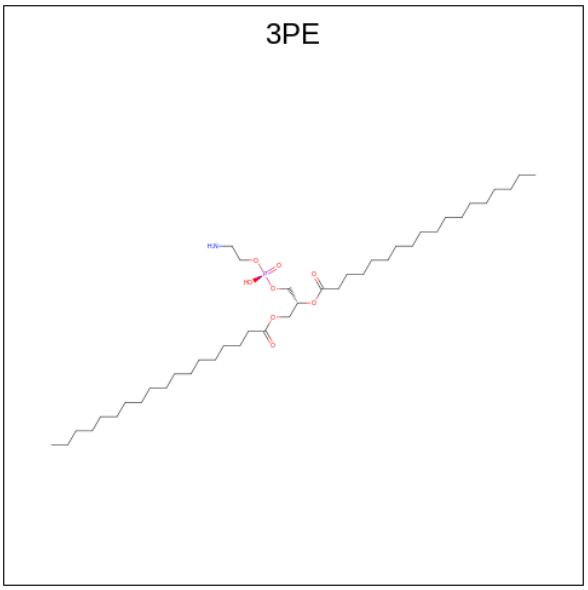
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	L	1	50	40	1	8	1	0

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	D	1	38	28	1	8	1	0
			Total	C	N	O	P	
58	I	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	J	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	K	1	46	36	1	8	1	0
			Total	C	N	O	P	
58	L	1	49	39	1	8	1	0
			Total	C	N	O	P	
58	L	1	39	29	1	8	1	0
			Total	C	N	O	P	
58	L	1	47	37	1	8	1	0
			Total	C	N	O	P	
58	M	1	37	27	1	8	1	0
			Total	C	N	O	P	
58	M	1	51	41	1	8	1	0
			Total	C	N	O	P	
58	M	1	51	41	1	8	1	0

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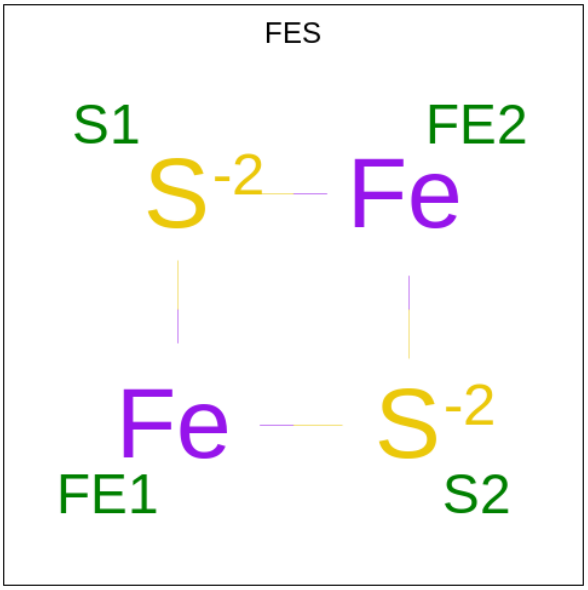
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	O	1	44	34	1	8	1	0
58	b	1	46	36	1	8	1	0
58	i	1	40	30	1	8	1	0
58	j	1	40	30	1	8	1	0
58	m	1	51	41	1	8	1	0
58	m	1	41	31	1	8	1	0
58	AC	1	25	15	1	8	1	0
58	Ac	1	35	25	1	8	1	0

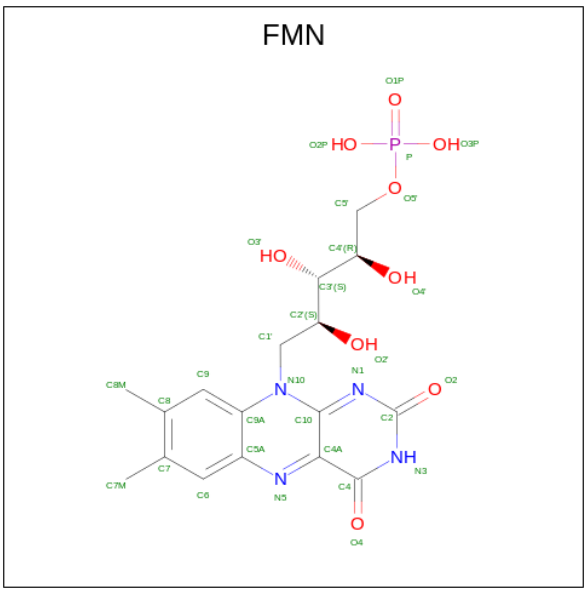
- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

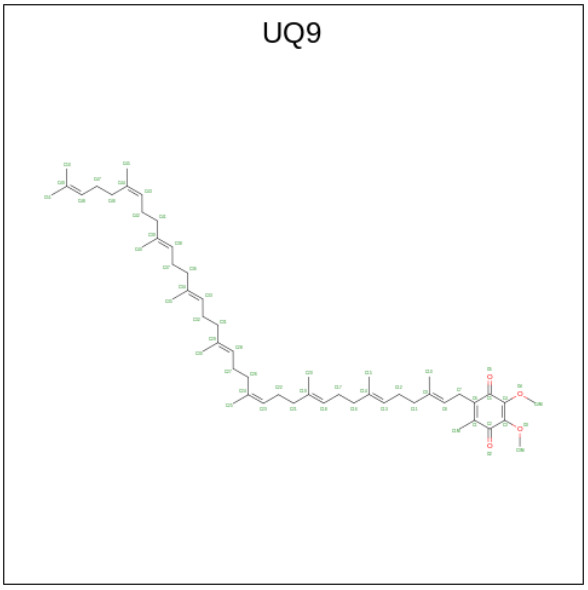
- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$)

(labeled as "Ligand of Interest" by depositor).



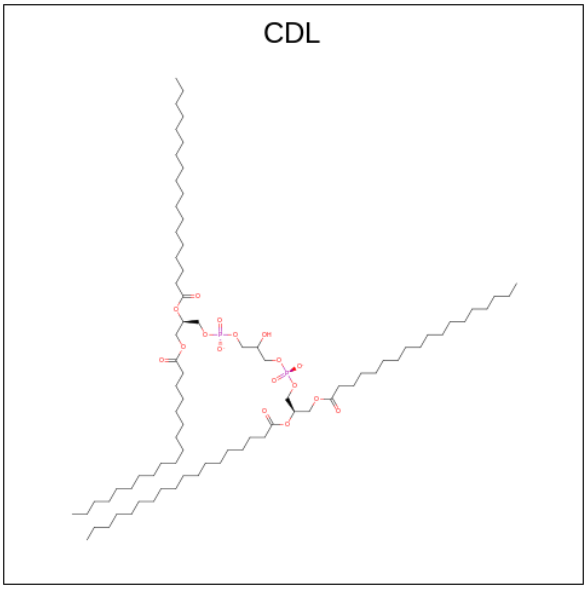
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

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



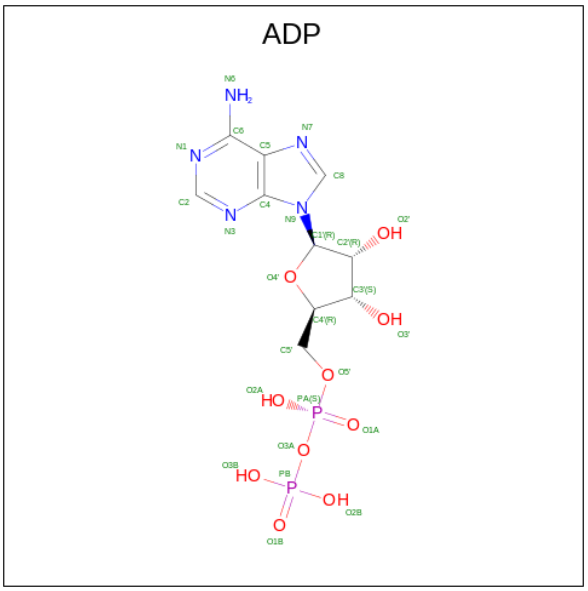
Mol	Chain	Residues	Atoms					AltConf
			Total	C	O			
61	H	1	35	31	4			0

- Molecule 62 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



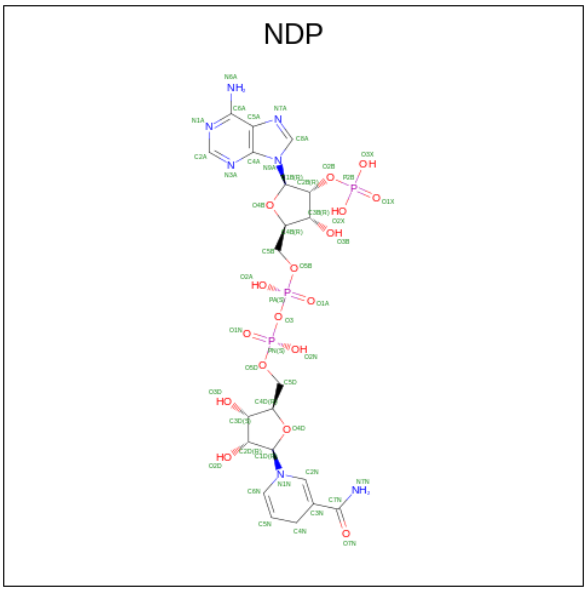
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
62	L	1	77	58	17	2	0
62	L	1	81	62	17	2	0
62	a	1	57	38	17	2	0
62	d	1	67	48	17	2	0
62	h	1	70	51	17	2	0
62	Aa	1	46	27	17	2	0
62	Ac	1	42	23	17	2	0
62	Ag	1	56	37	17	2	0

- 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
			Total	C	N	O	P	
63	O	1	27	10	5	10	2	0

- 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).



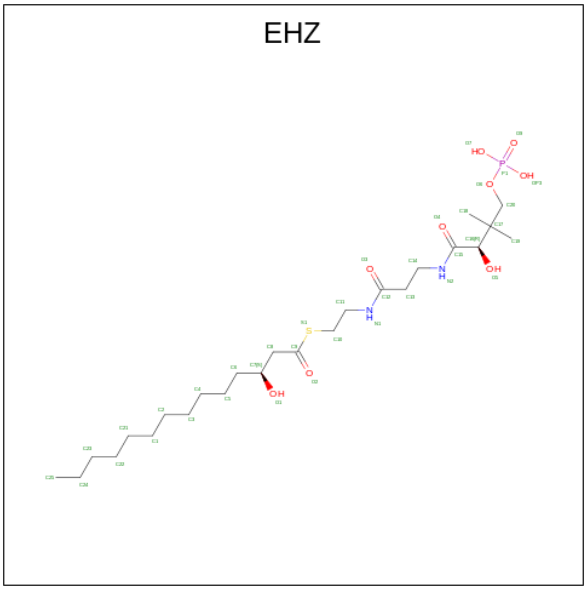
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	P	1	48	21	7	17	3	0

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

depositor).

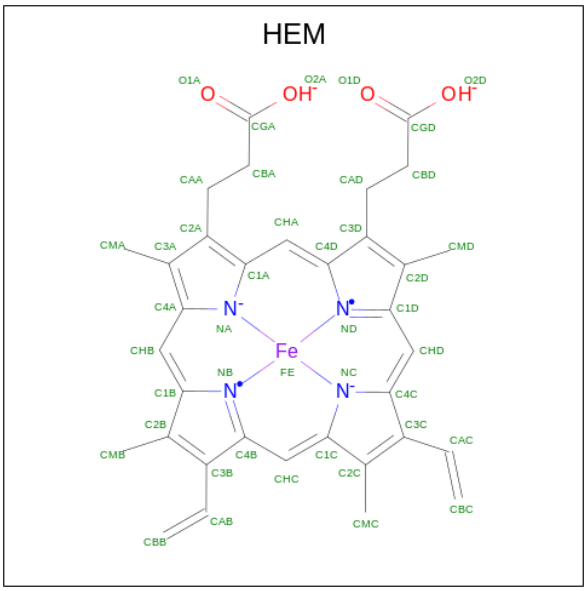
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
65	R	1	1	1	0

- 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: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



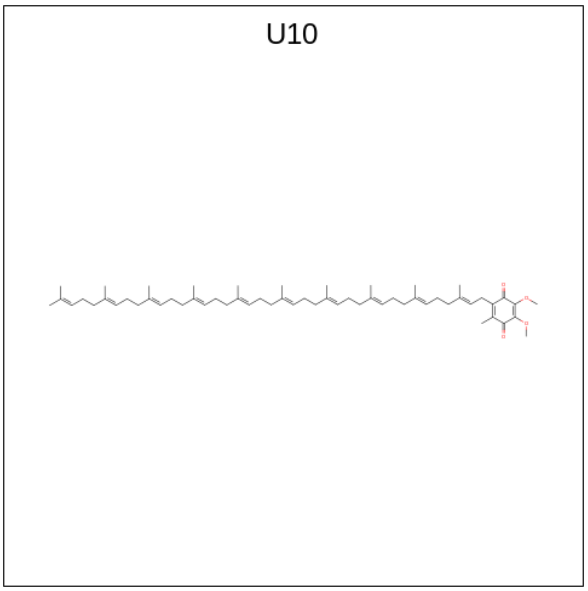
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
66	W	1	32	19	2	9	1	1	0
			Total	C	N	O	P	S	
66	n	1	32	19	2	9	1	1	0

- 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).



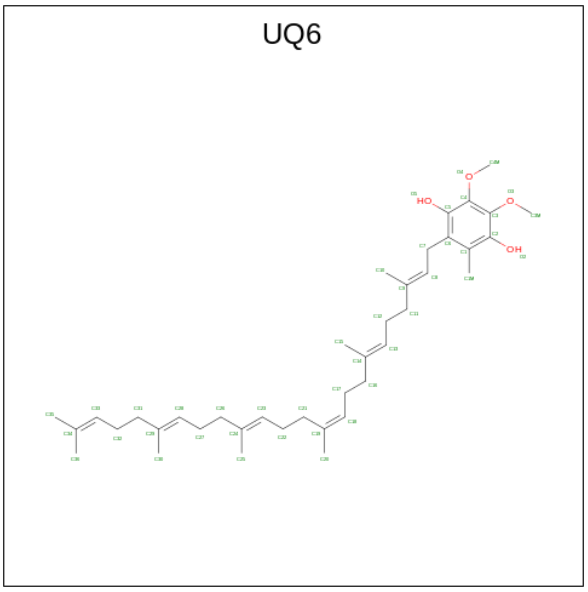
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
67	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	AC	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	Ac	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
67	Ac	1	43	34	1	4	4	0

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



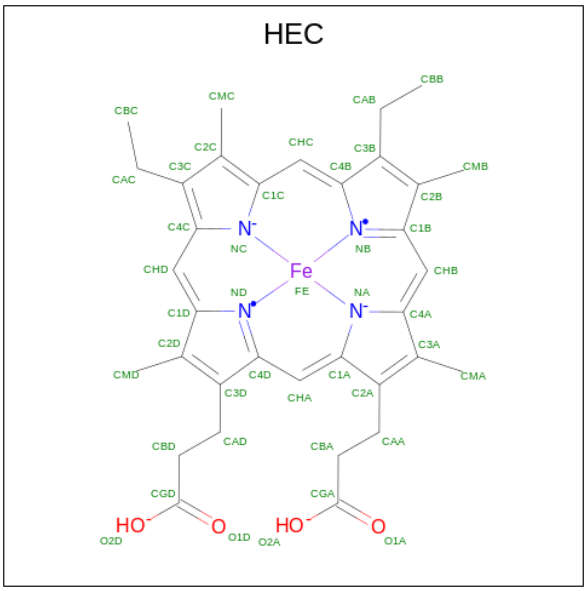
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
68	AC	1	23	19	4	0
68	Ac	1	23	19	4	0

- Molecule 69 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-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
			Total	C	O	
69	AC	1	28	24	4	0
69	Ac	1	28	24	4	0

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



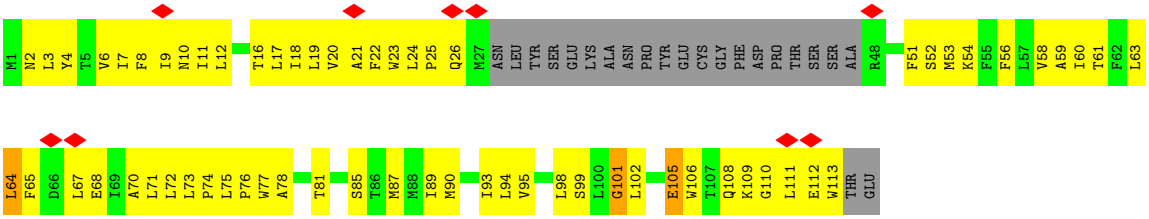
Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

3 Residue-property plots (i)

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

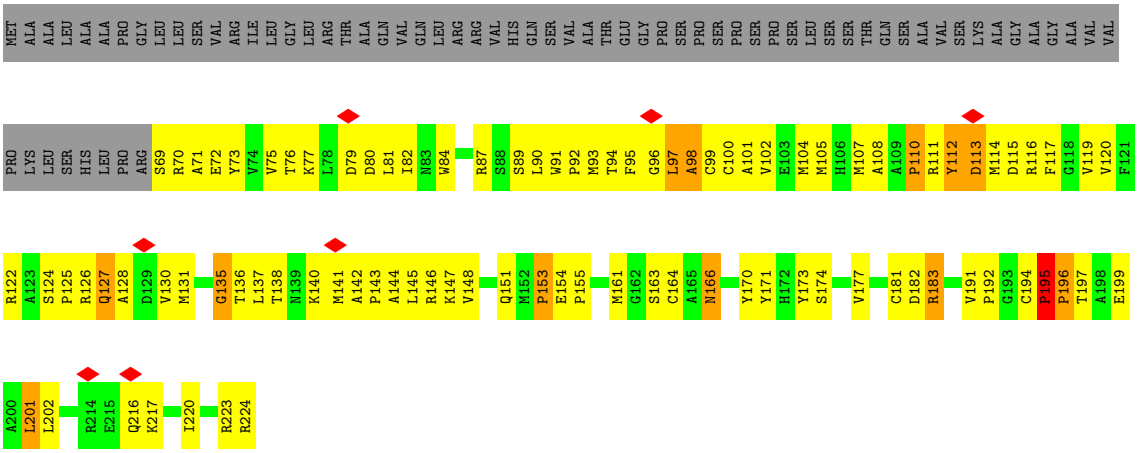
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 8% 25% 53% • 19%



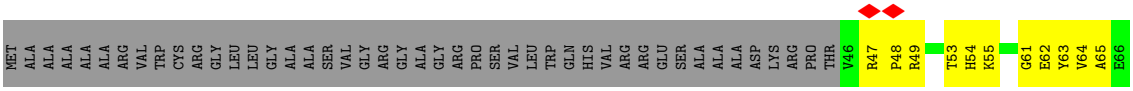
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

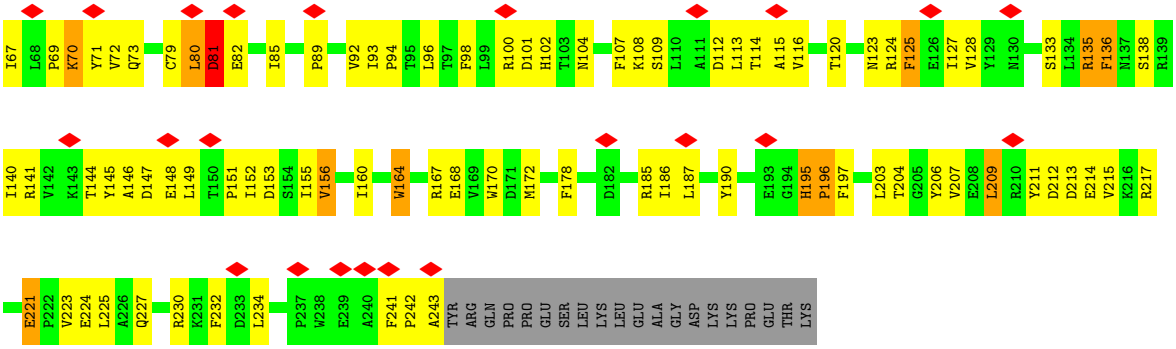
Chain B: • 28% 36% 5% 30%



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

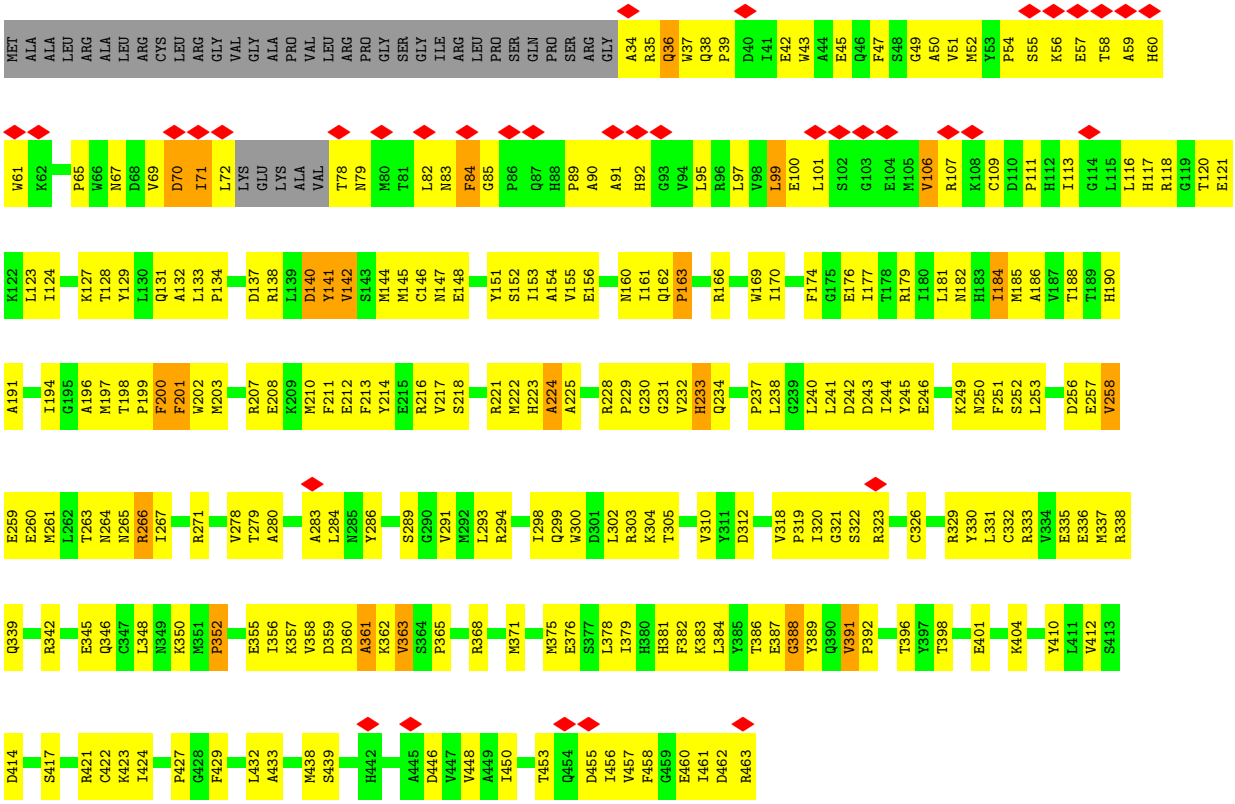
Chain C: 10% 38% 33% • 25%





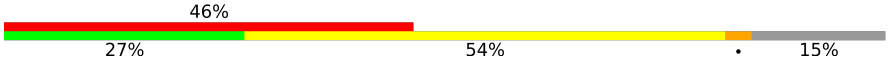
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

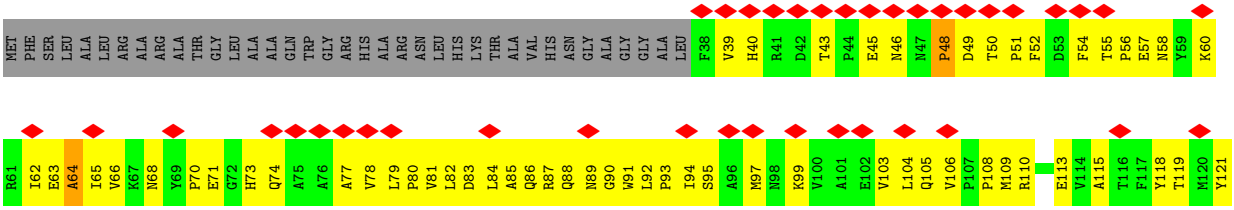
Chain D:

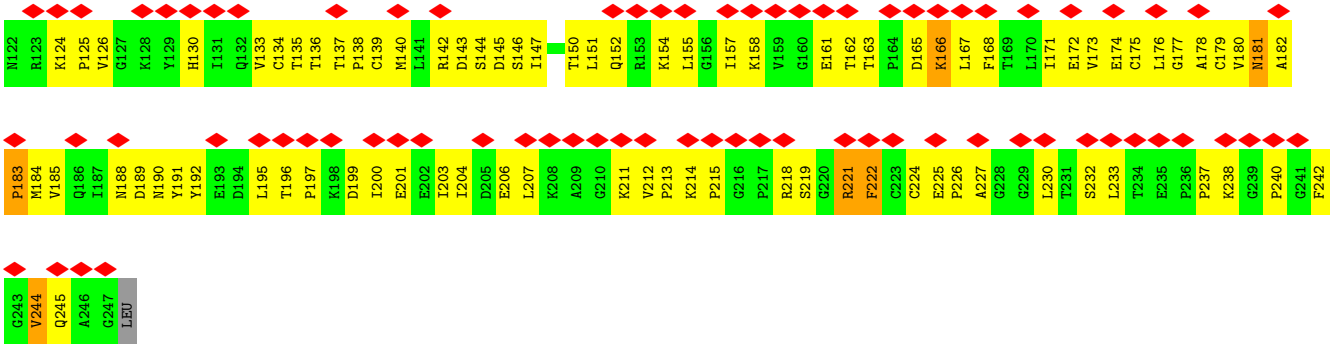


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:

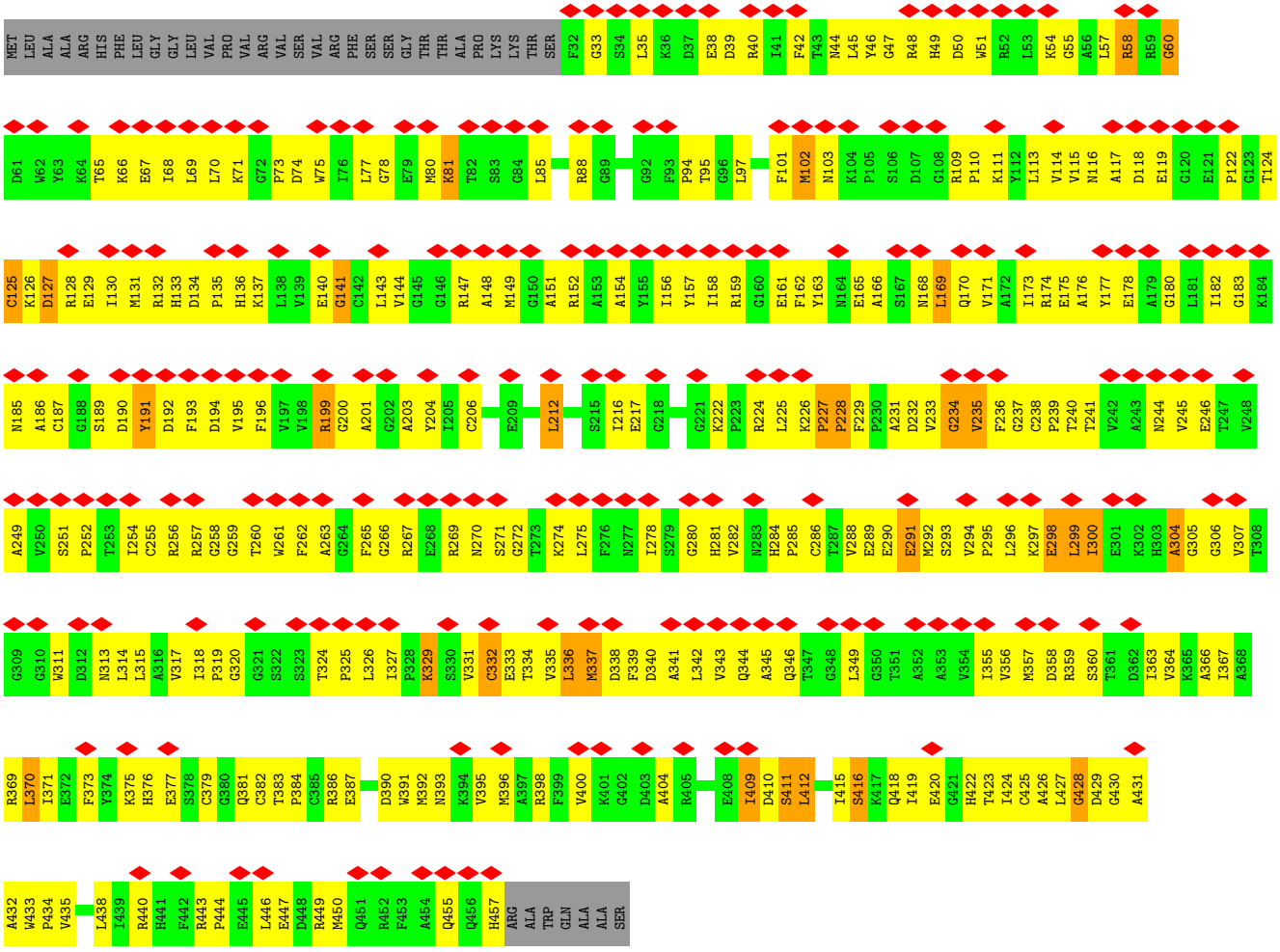






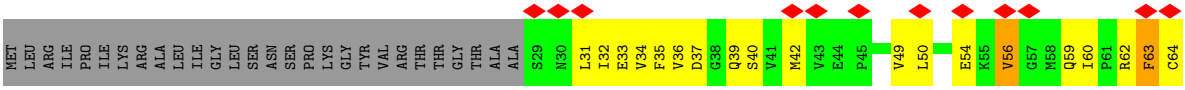
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

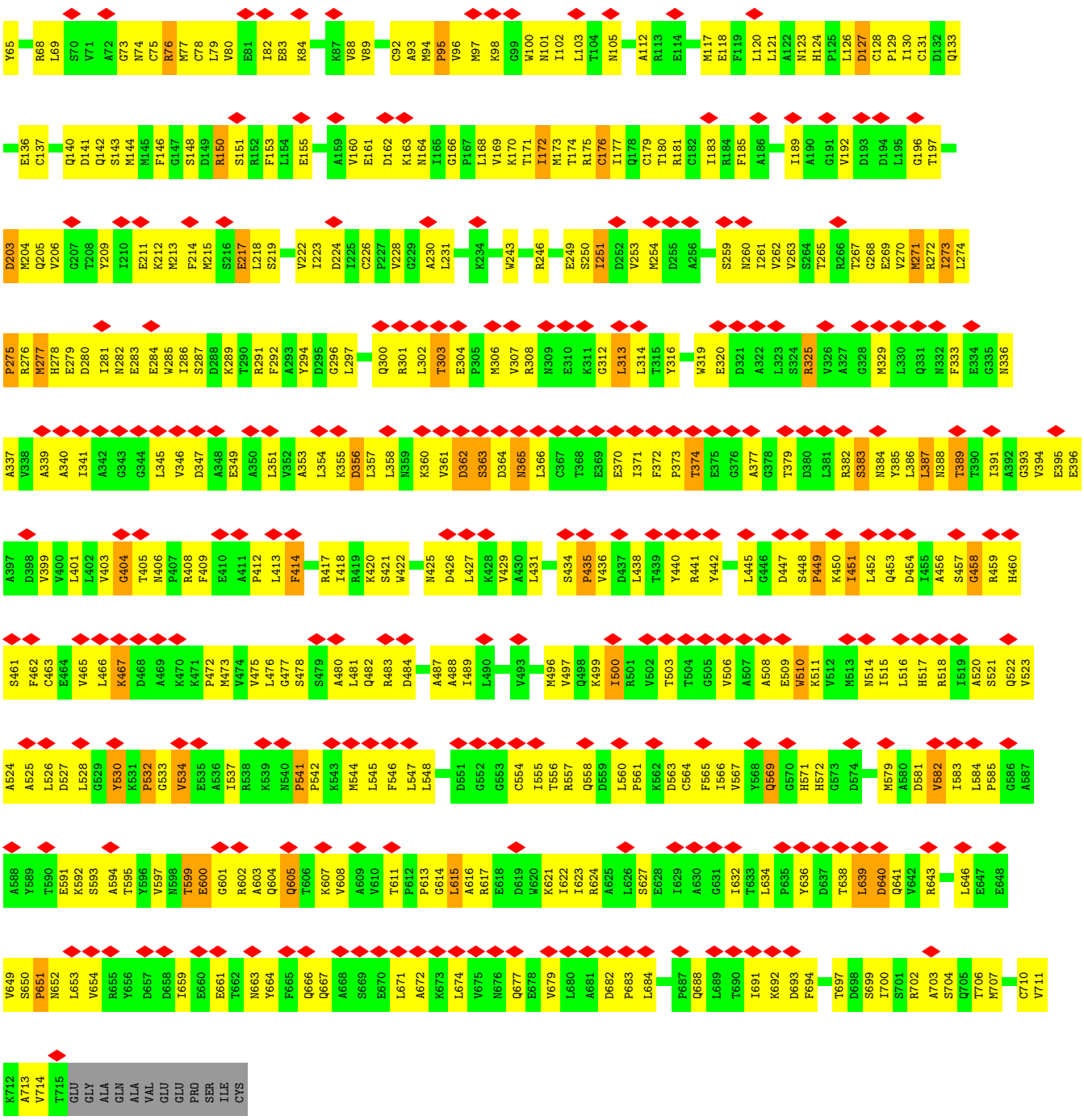
Chain F:



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

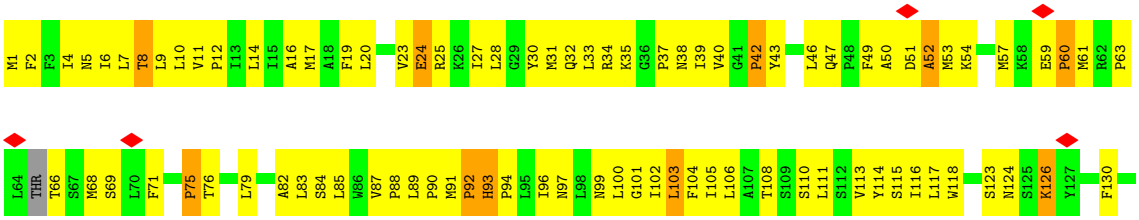
Chain G:

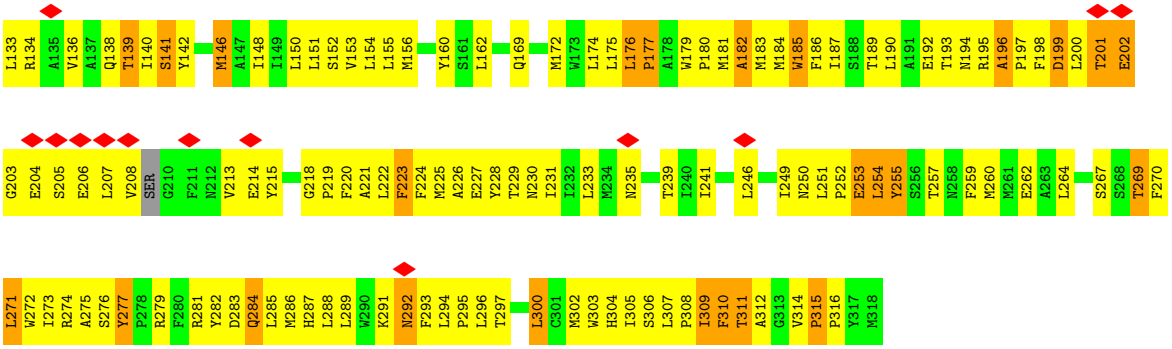




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

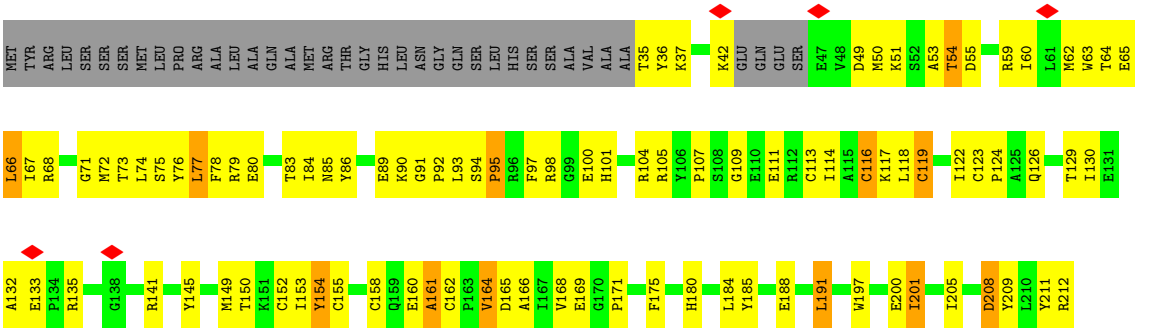
Chain H:





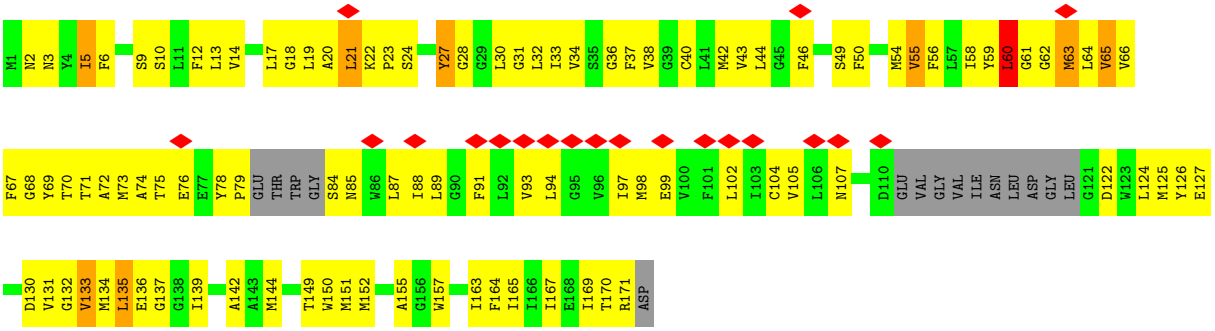
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

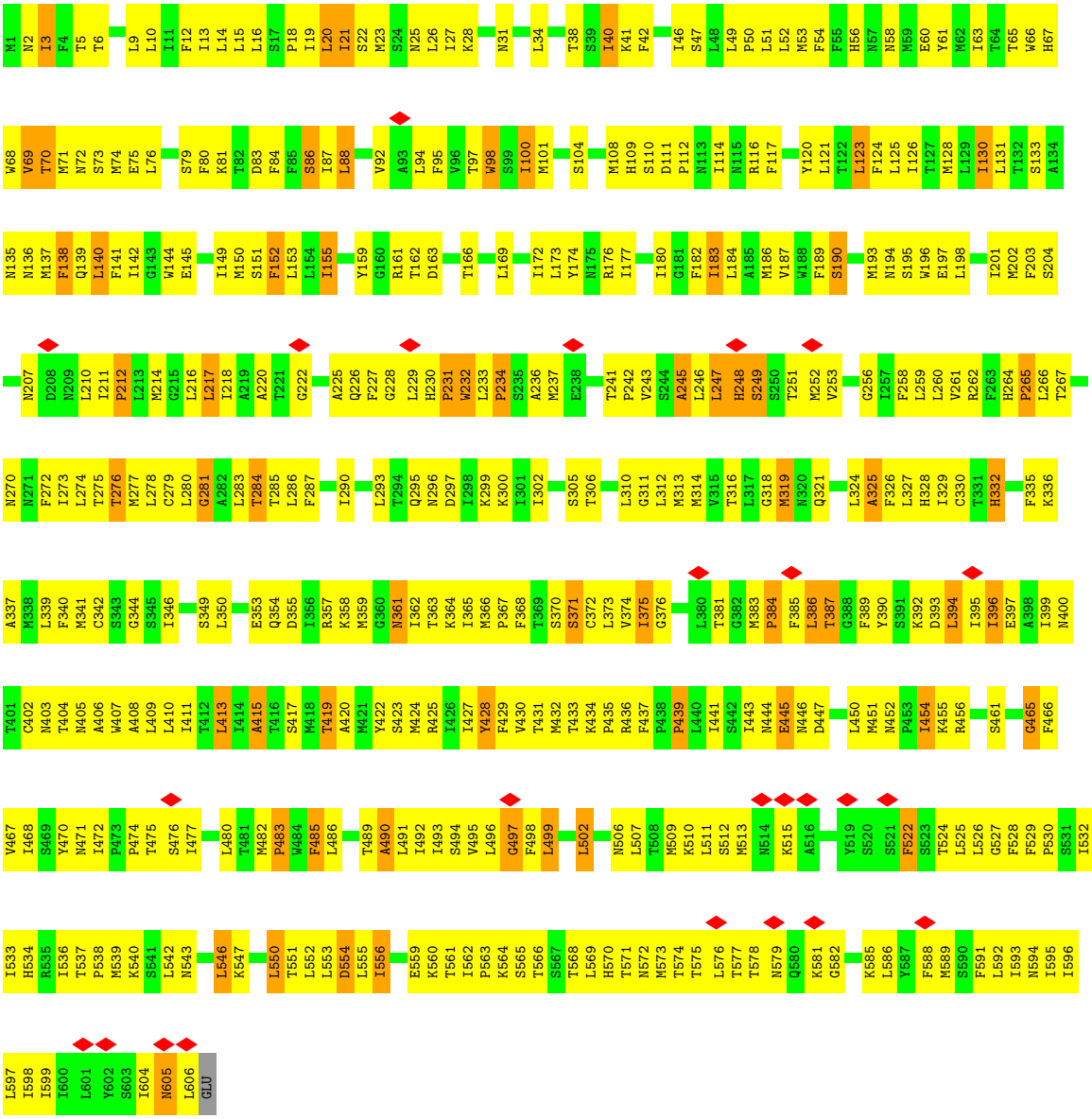


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

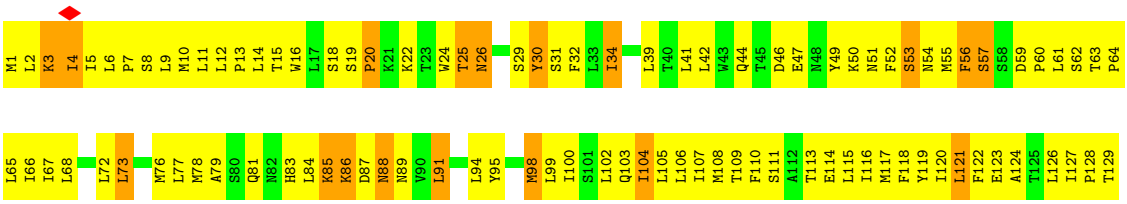
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

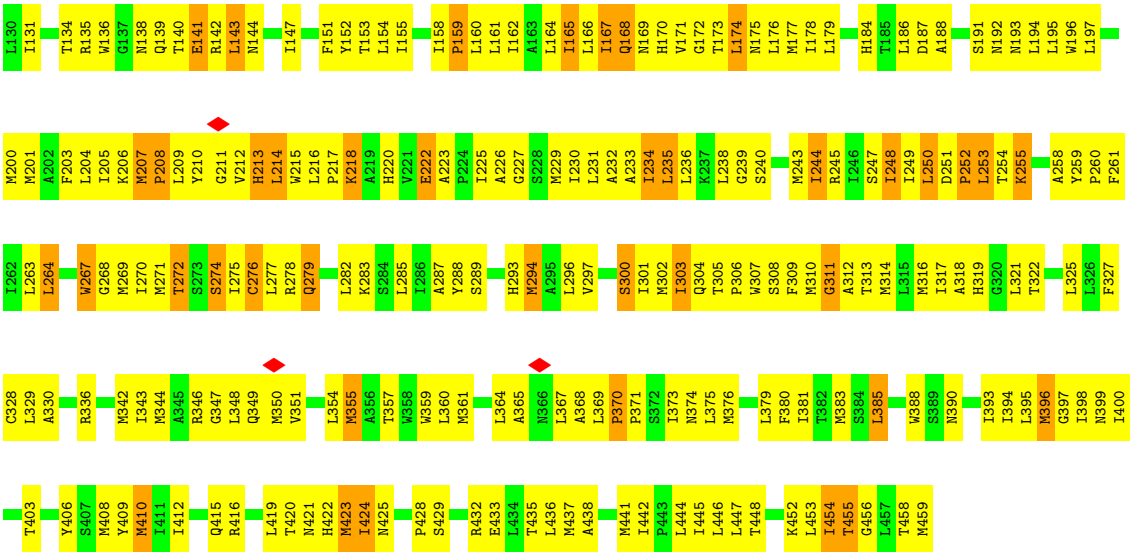
Chain L: 32% 57% 10%



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

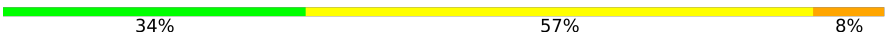
Chain M: 29% 59% 13%

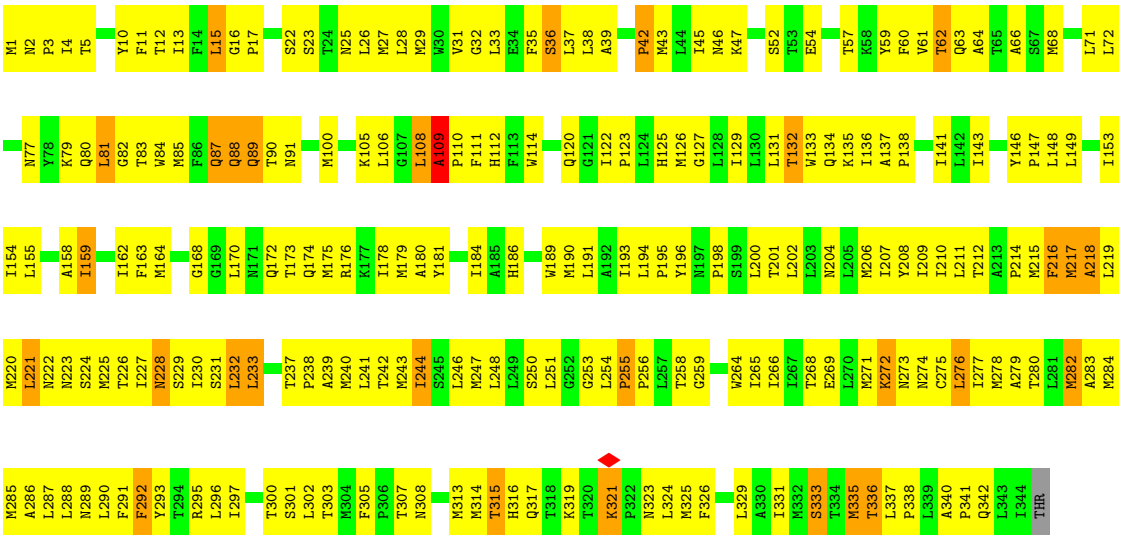




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

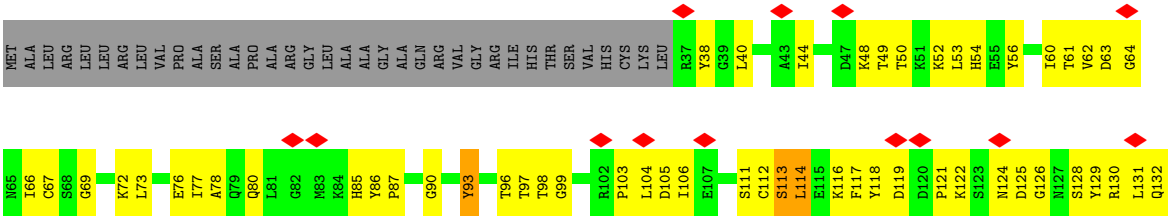
Chain N:

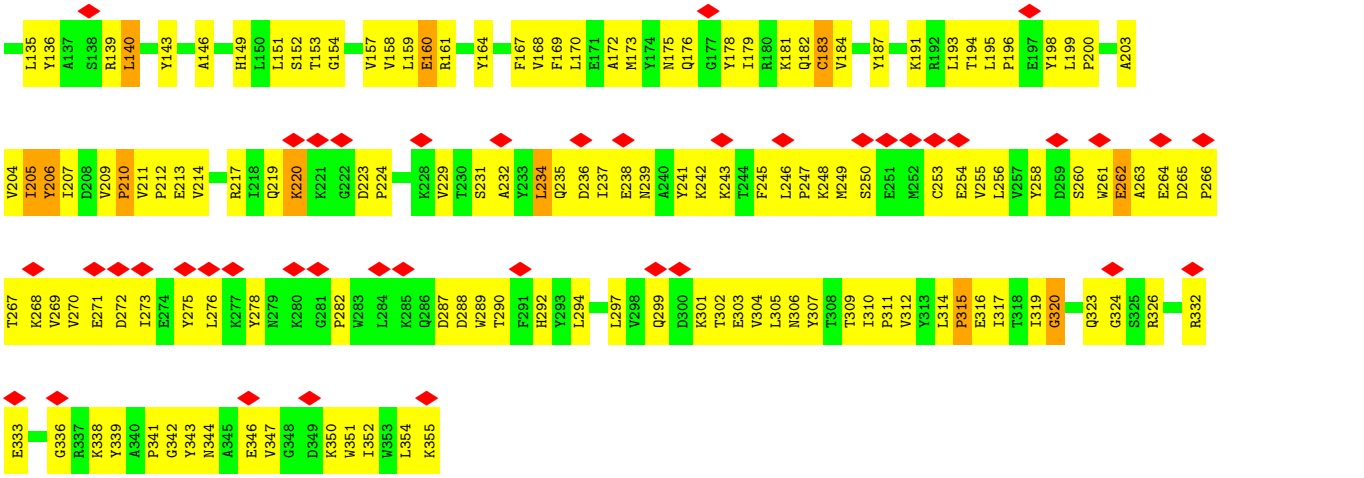




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

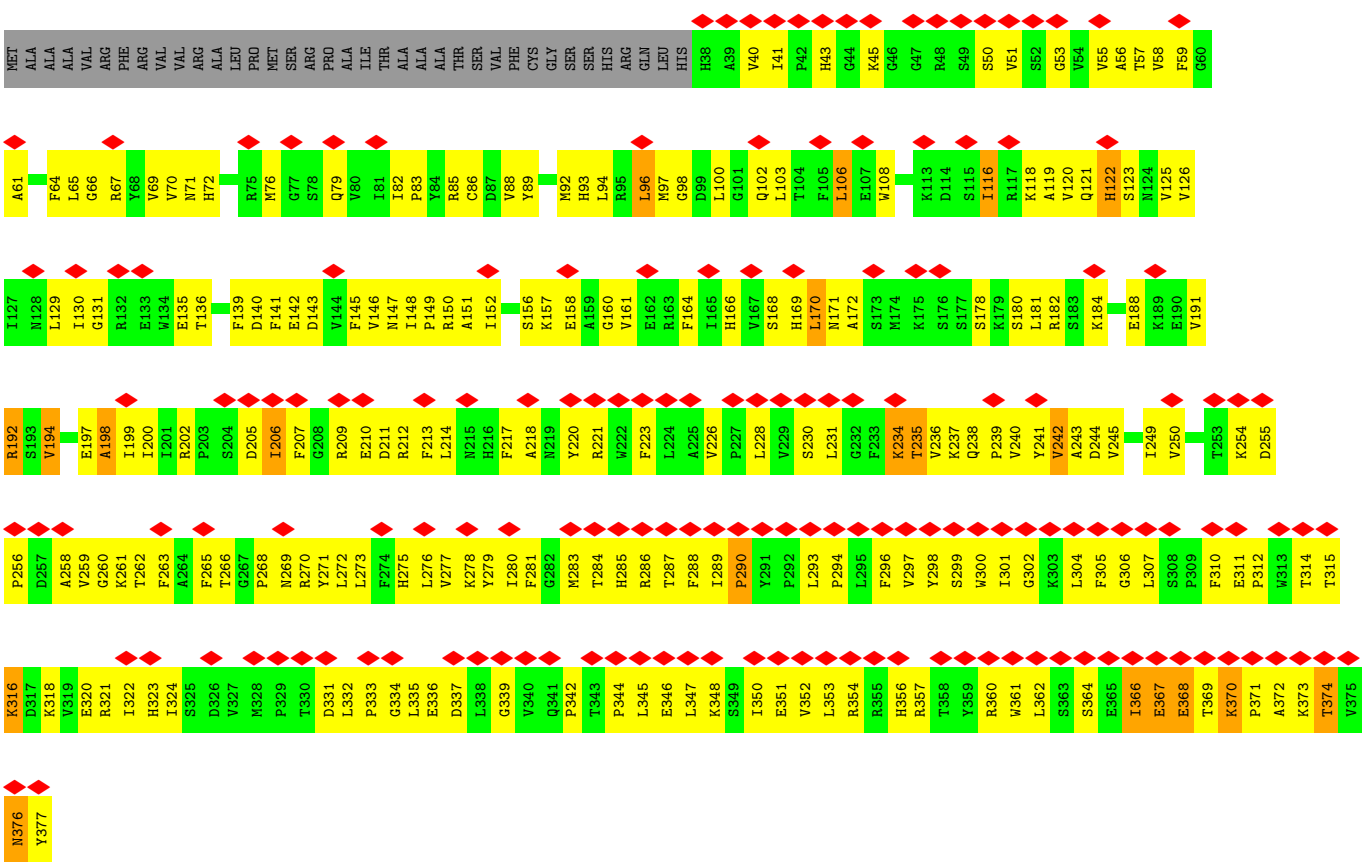
Chain O:





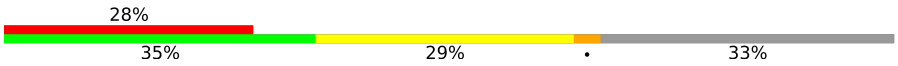
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

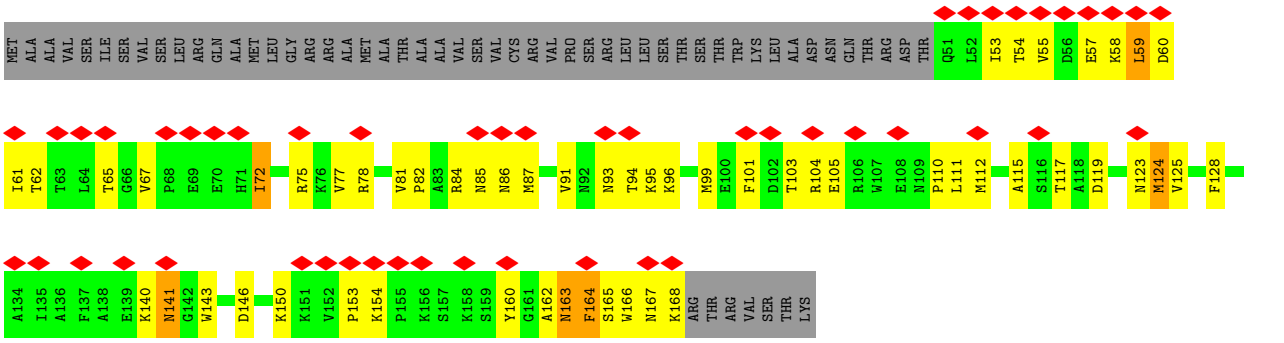
Chain P:



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

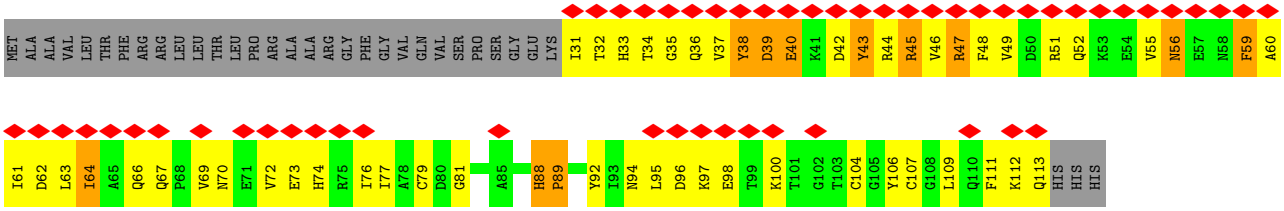
Chain Q:





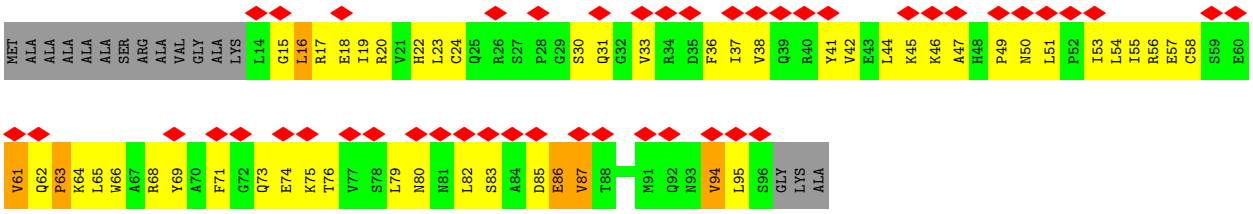
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



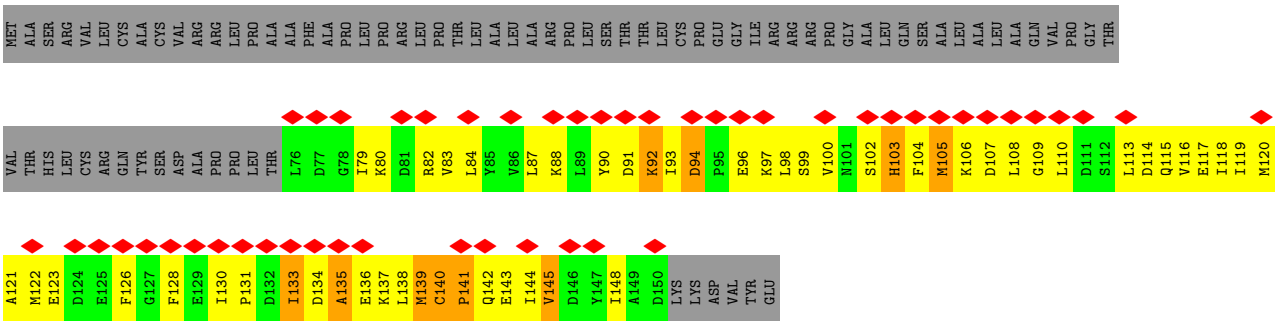
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



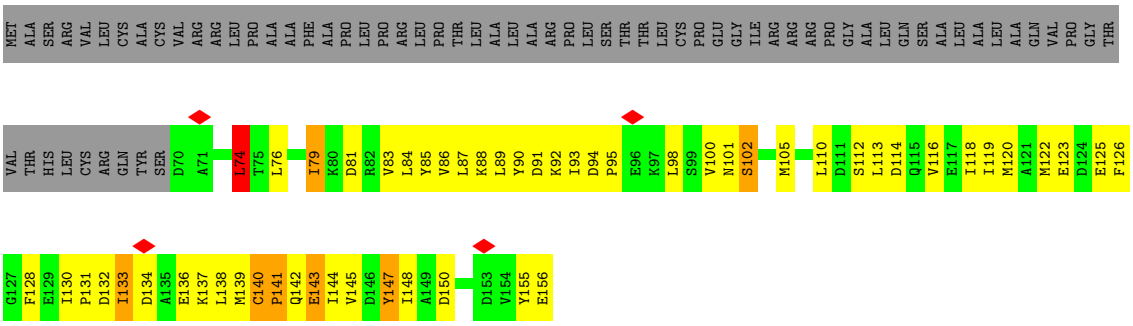
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



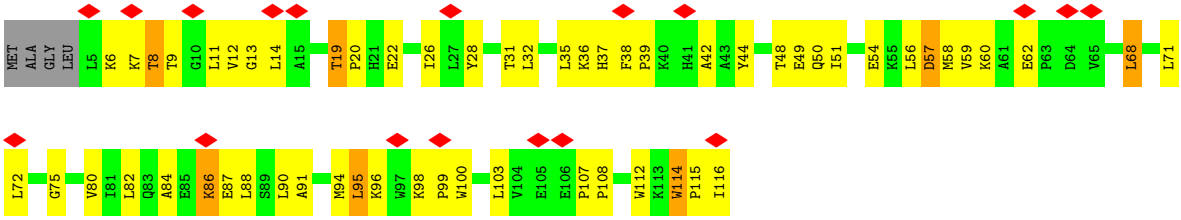
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:



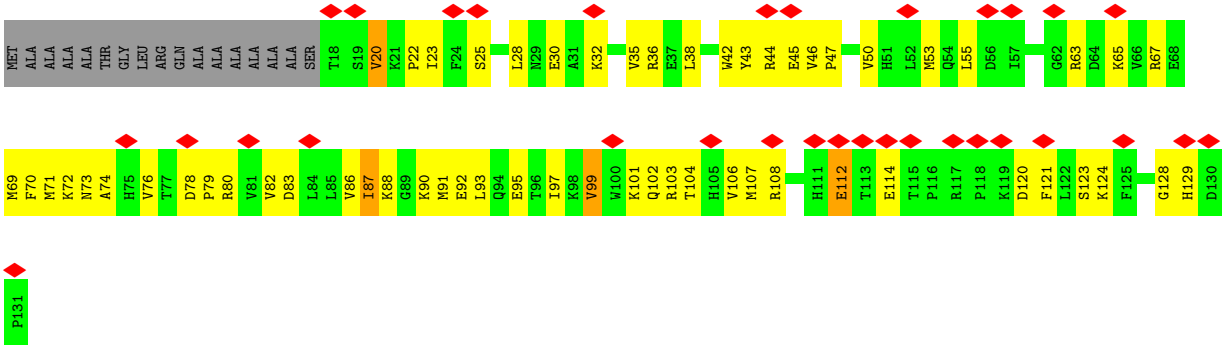
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



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

Chain W:

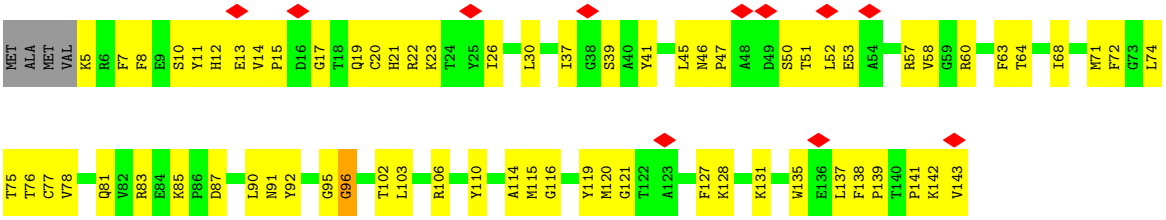


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:

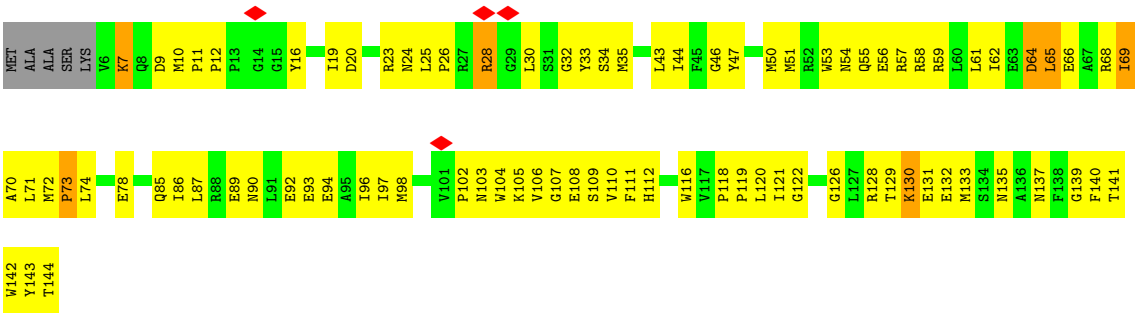
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



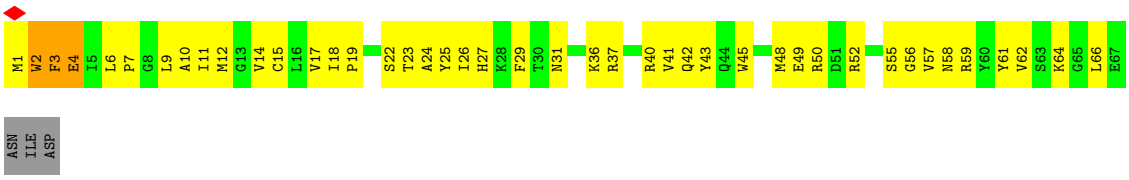
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



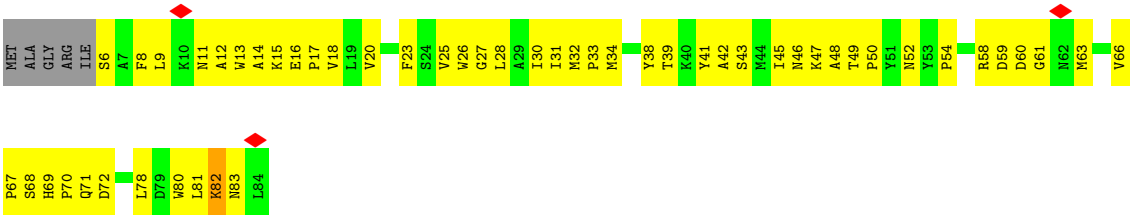
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



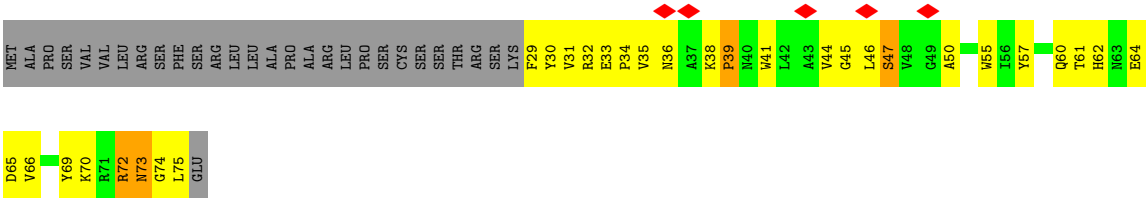
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:



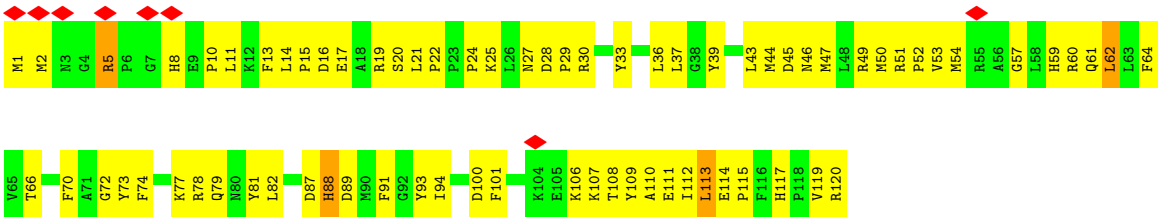
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



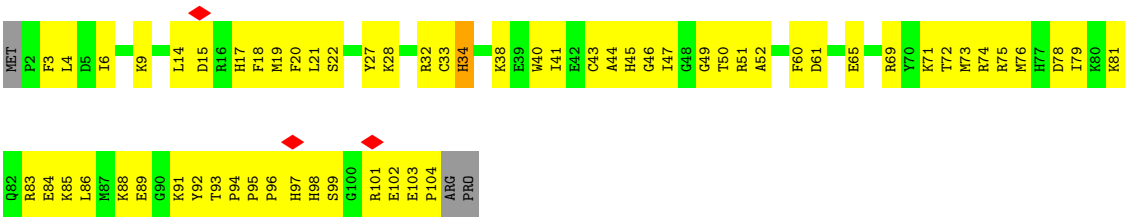
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



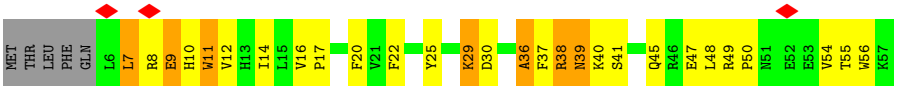
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



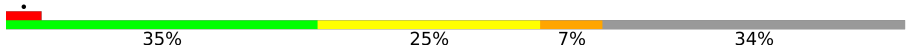
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

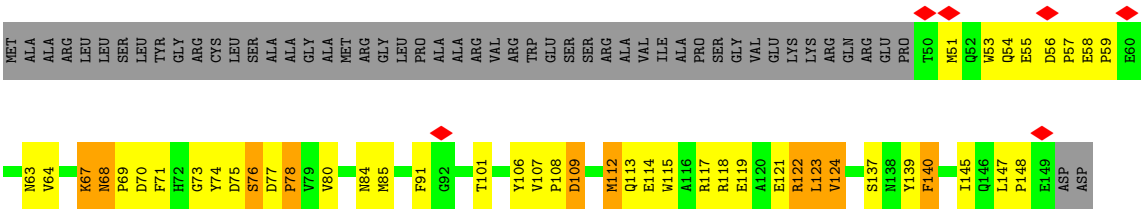
Chain f:



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

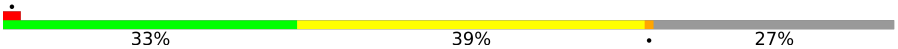
Chain g:

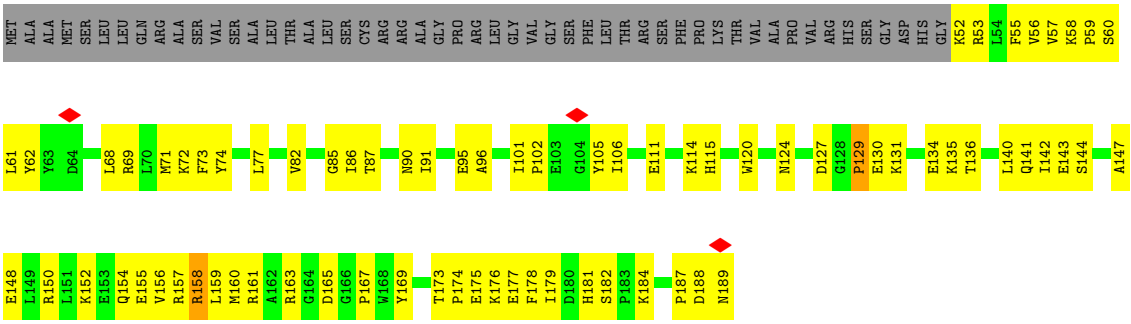




• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

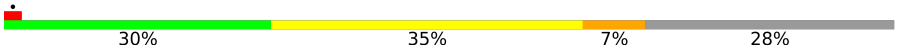
Chain h:

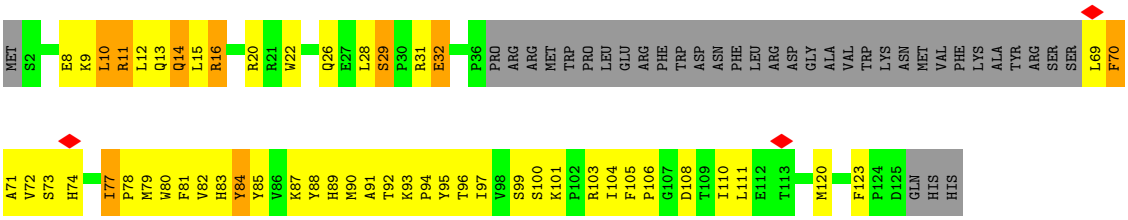




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

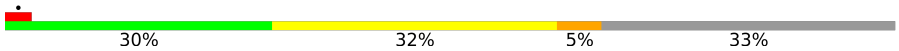
Chain i:

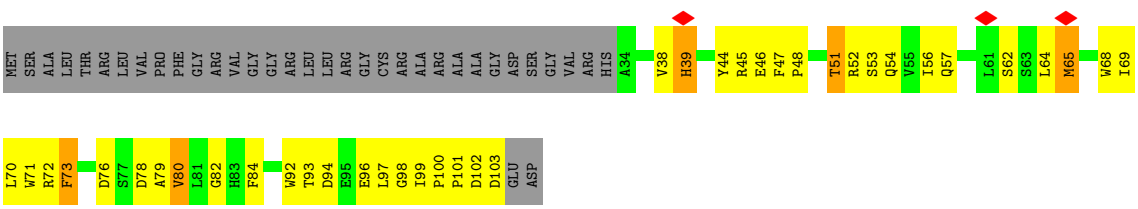




• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

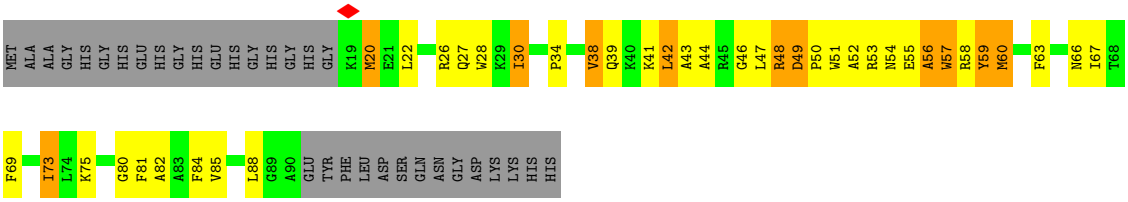
Chain j:





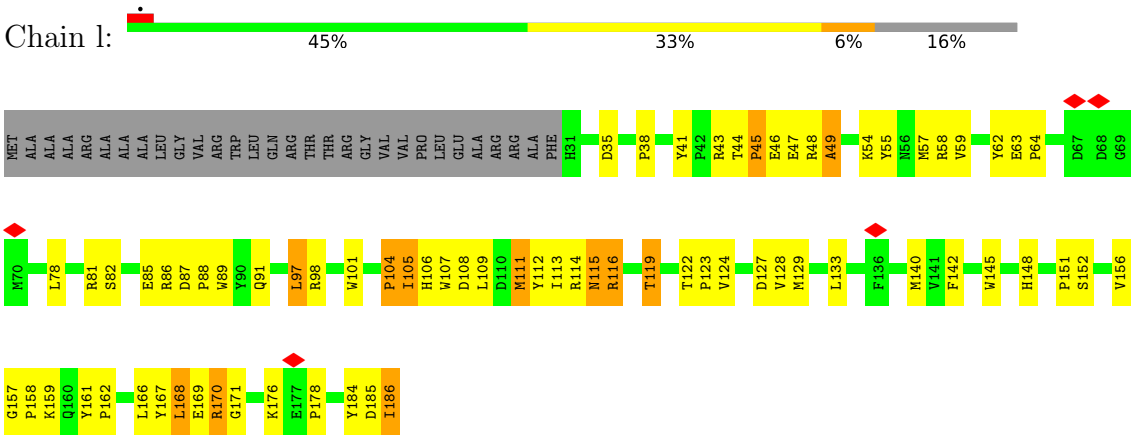
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



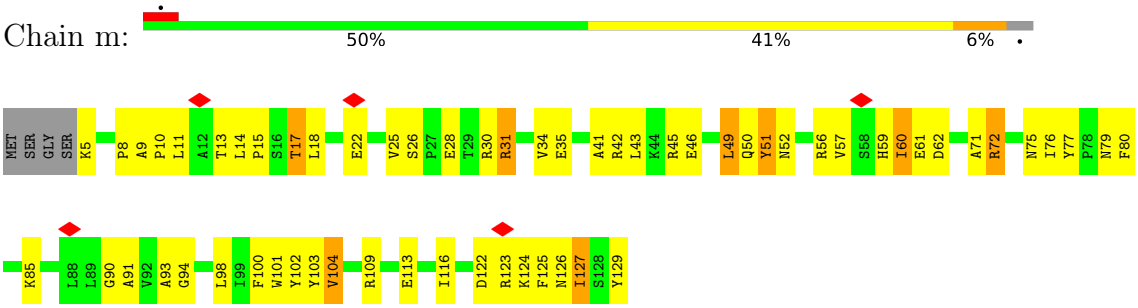
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



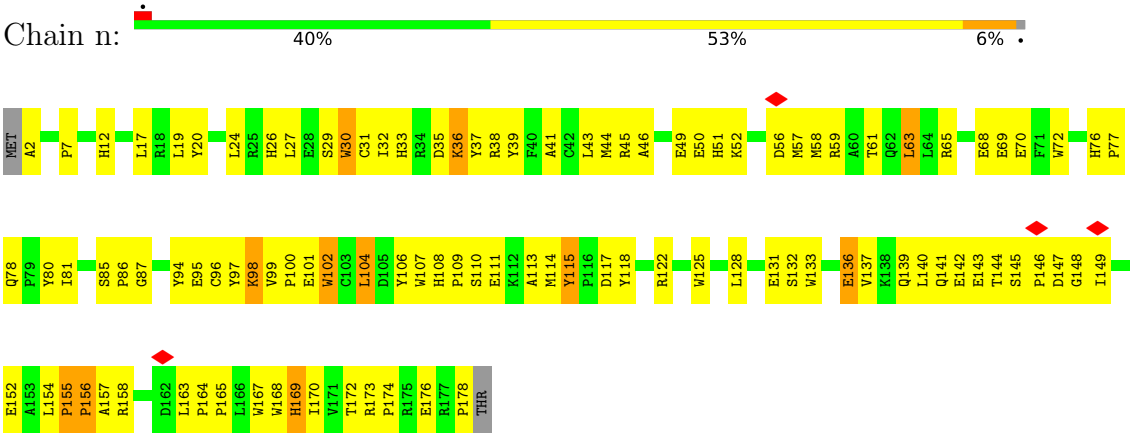
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



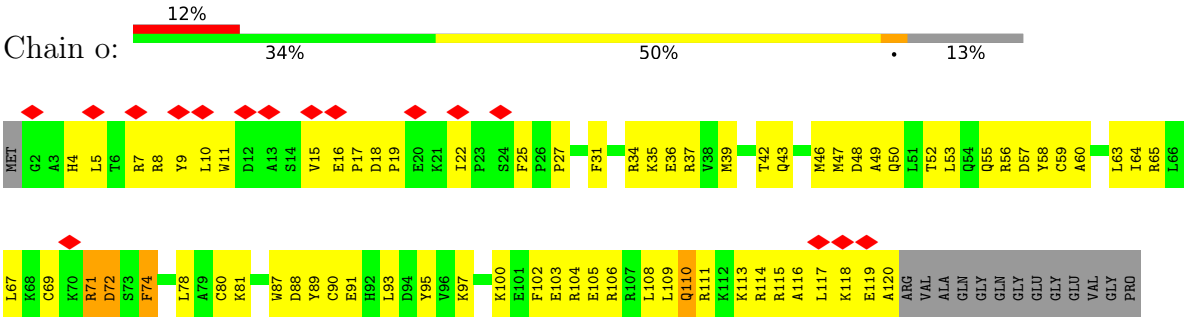
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

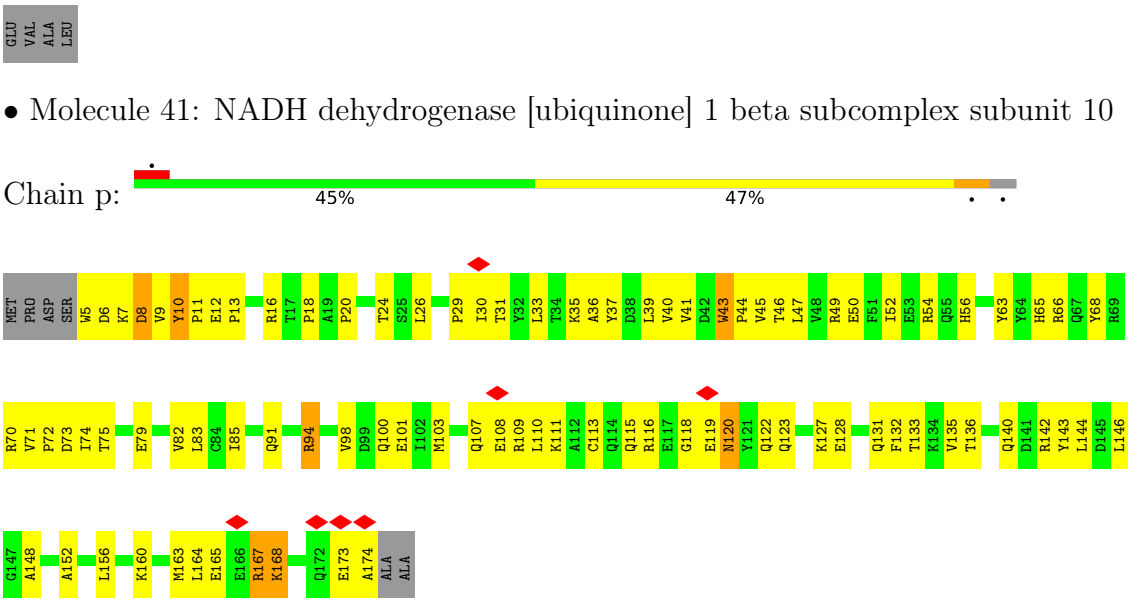
Chain n:



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

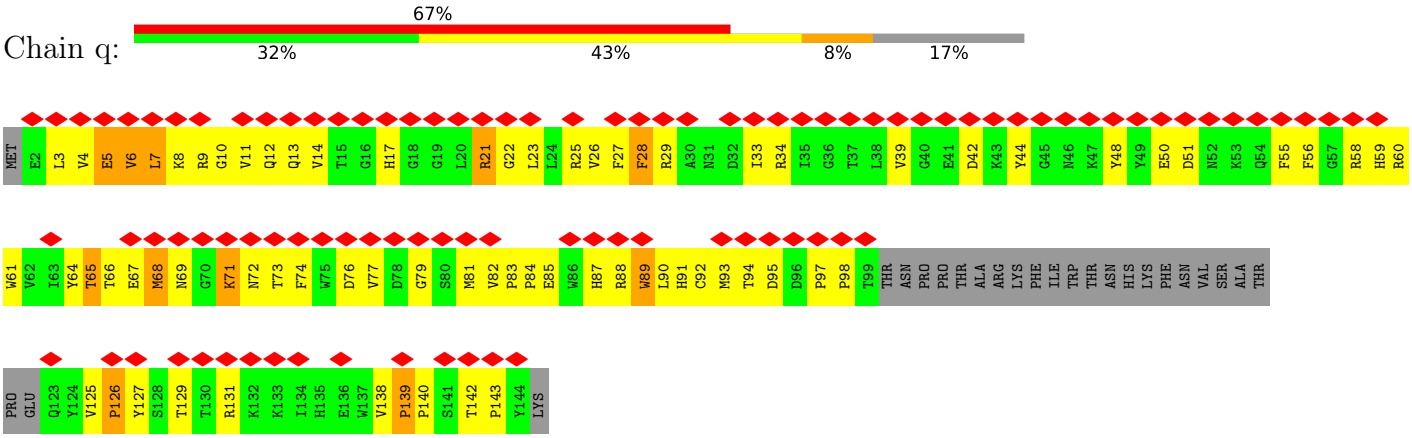
Chain o:



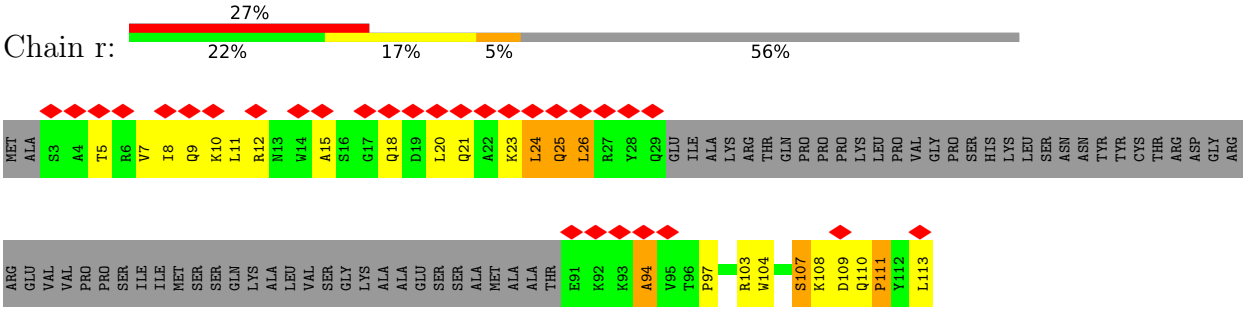


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

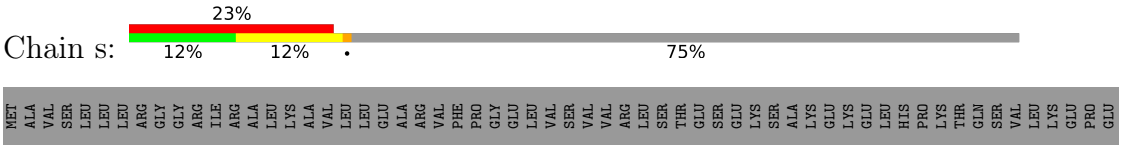
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

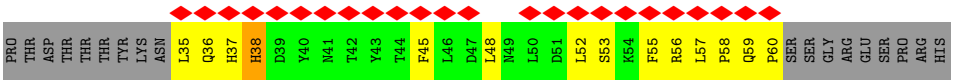


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



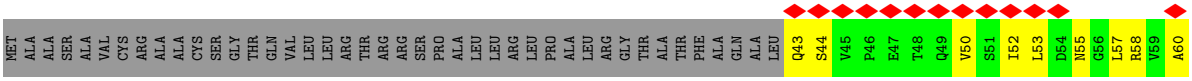
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

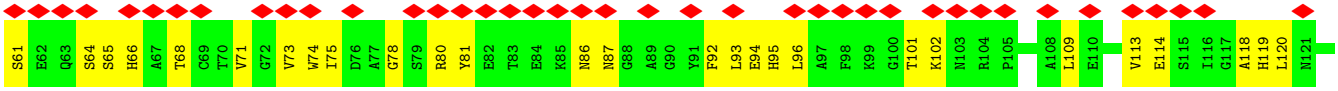


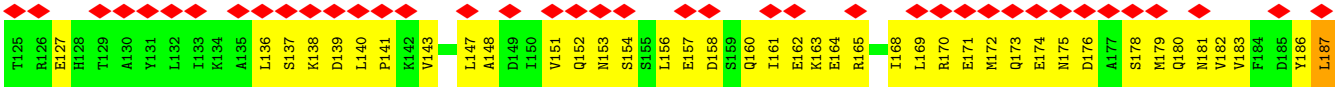


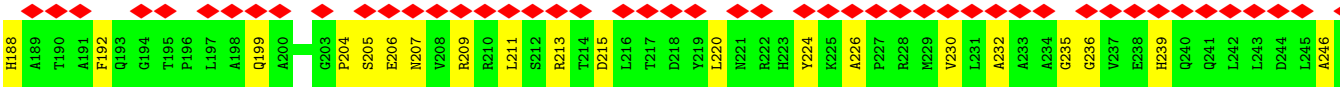
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

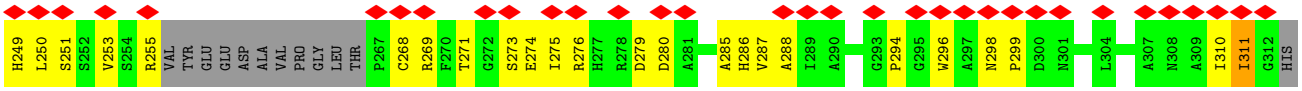
Chain AA:

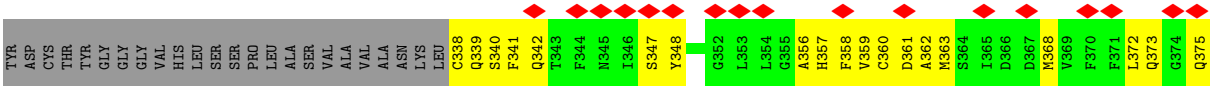


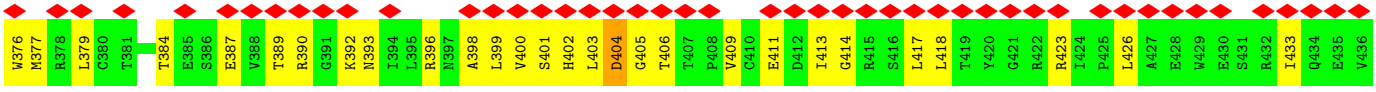


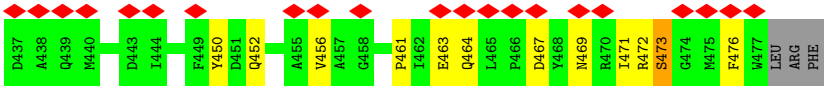






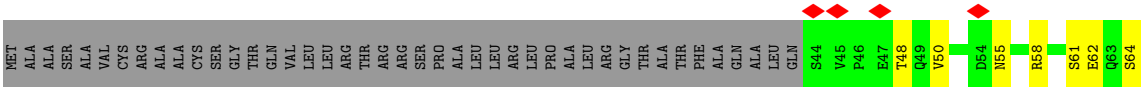


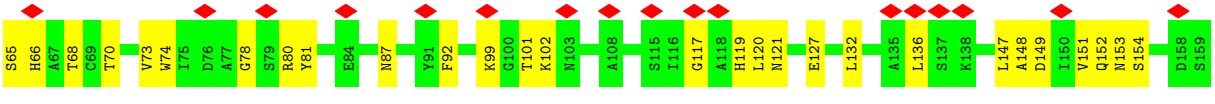


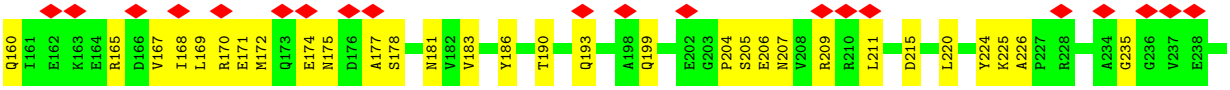


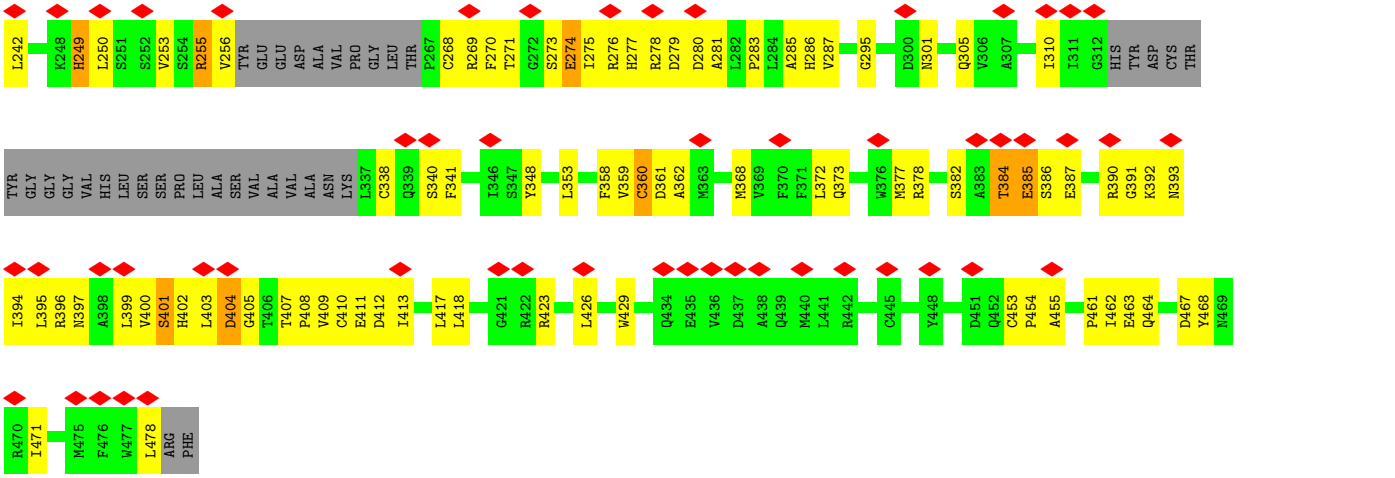
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Aa:



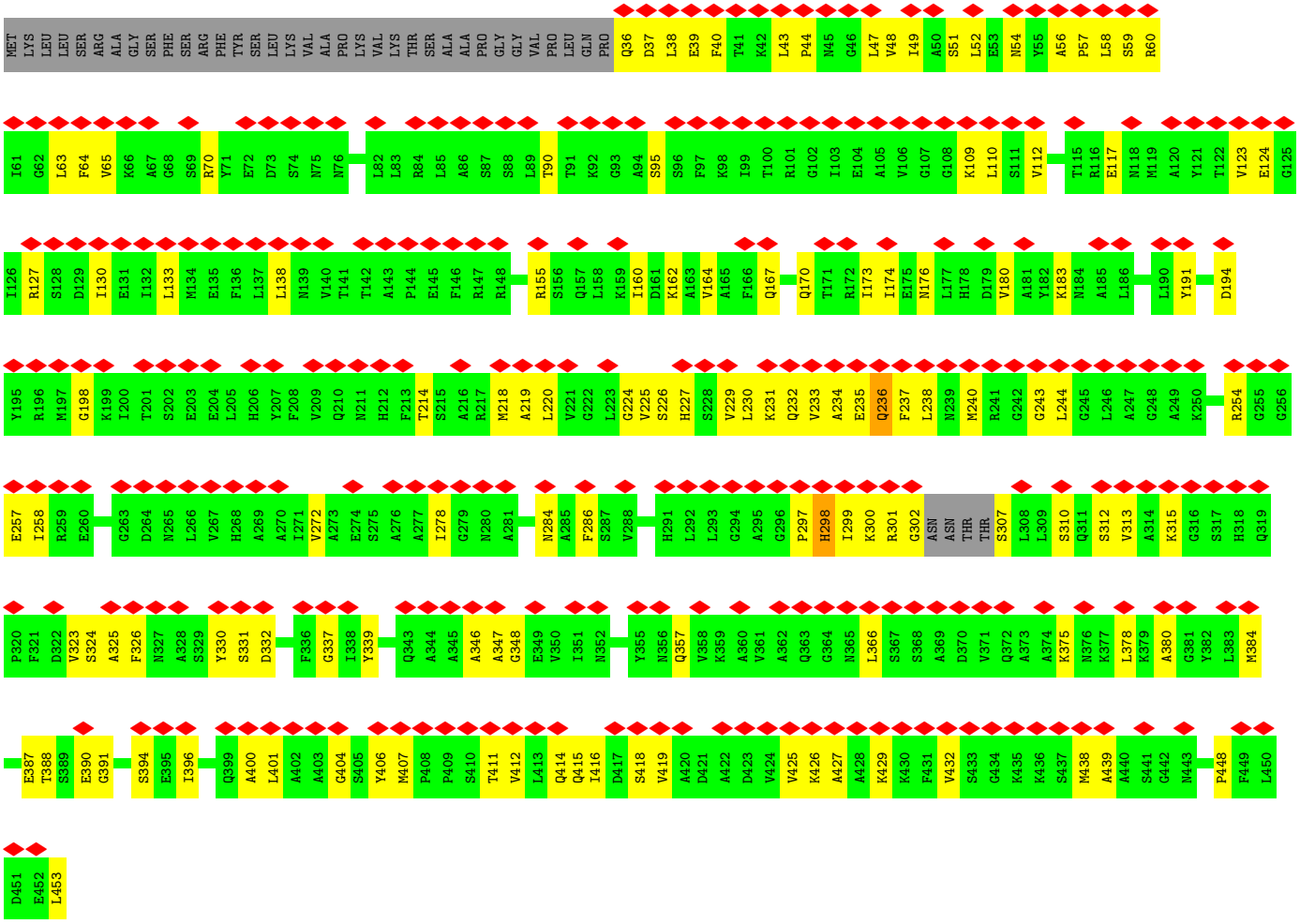






• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:



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

Chain Ab:

MET LYS LEU LEU SER ARG ALA GLY SER PHE SER ARG PHE TYR SER LEU LYS VAL ALA PRO LYS VAL LYS THR SER ALA ALA PRO GLY GLY VAL PRO LEU GLN PRO Q36 D37 L38 E39 F40 T41 P44 N45 G46 L47 V48 I49 A50 S51 N54 Y55 L58 S59 R60 I61 G62 L63

F64 S69 R70 D73 S74 N75 N76 L77 L82 L83 S87 S88 L89 T90 T91 K92 G93 A94 S95 S96 F97 K98 I99 T100 R101 G102 I103 E104 A105 V106 K109 L110 S111 T115 R116 E117 A120 Y121 T122 V123 R127 S128 D129 I130 E131 I132 L133 M134 E135 L138 N139

V140 T141 T142 A143 P144 E145 F146 R147 R148 W149 E150 L154 R155 L158 K159 K162 A163 V164 A165 F166 Q167 N168 S169 Q170 I173 I174 E175 N176 L177 H178 D179 V180 A181 Y182 K183 N184 A185 L186 L190 Y191 C192 P193 D194 M197 G198 K199 S202 E203 Y207 N211

L220 V221 V225 S226 H227 S228 V229 L230 K231 Q232 V233 A234 E235 Q236 F237 L238 N239 M240 R241 G242 G243 L244 G245 L246 A247 G248 A249 K250 A251 K252 Y253 R254 E257 I258 R259 E260 Q261 N262 G263 D264 N265 L266 V267 H268 A269 A270 I271 V272 A273 E274 S275 A276 A277 I278 G279 N280 A281 E282

A283 N284 A285 F286 S287 V288 L293 H298 I299 K300 ARG GLY N303 N304 T305 T306 S307 L308 L309 S310 Q311 S312 VAL ALA LYS G316 S317 H318 Q319 P320 F321 D322 V323 F326 N327 A328 S329 Y330 S331 D332 Y339 T340 Q343 A344 A345 A346 A347 G348 E349 V350 I351 N352 Y355 N356

Q357 V358 K359 A360 V361 A362 Q363 G364 N365 L366 S367 S368 A369 A374 K377 L378 K379 A380 T388 S389 E390 G391 F392 L393 S394 E395 I396 Q399 A400 L401 A402 A403 Y406 M407 T411 V412 L413 Q414 Q415 I416 D417 S418 V419 A422 D423 V424 V425 K426 A427 A428 K429 K430 F431

V432 S433 G434 K435 K436 A439 A440 S441 G442 N443 L444 G445 H446 T447 P448 F449 L450 D451 E452 L453

- Molecule 47: Cytochrome b

Chain AC: 72% 68% 30%

MET THR ASN MET ARG LYS THR H8 P9 L10 F11 K12 I13 I14 N15 H16 S17 F18 I19 D20 L21 P22 A23 N26 W30 W31 N32 F33 G34 S35 L36 L37 G38 V39 C40 L41 M42 I45 I46 T47 G48 L49 F50 L51 A52 M53 T56 S57 D58 T59 M60 T61 A62 R71 D72

W77 L78 I79 R80 Y81 M82 N85 G86 A87 S88 M89 F90 F91 I92 C93 L94 F95 L96 H97 V98 G99 R100 G101 L102 Y103 Y104 G105 S106 Y107 T108 F109 M110 E111 T112 W113 N114 I115 L118 L119 L120 F121 A122 V123 M124 A125 T126 A127 F128 M129 G130 Y131 V132 L133 P134 W135 G136 Q137

M138 S139 F140 W141 G142 A143 T144 V145 I146 T147 N148 L149 L150 S151 A152 I153 P154 Y155 I156 G157 T158 V161 E162 W163 I164 W165 G166 G167 F168 S169 V170 D171 K172 A173 T174 L175 T176 R177 F178 F179 A180 F181 H182 F183 I184 L185 P186 F187 I188 I189 A190 A191 L192 A193 I194 V195 H196 L197 L198

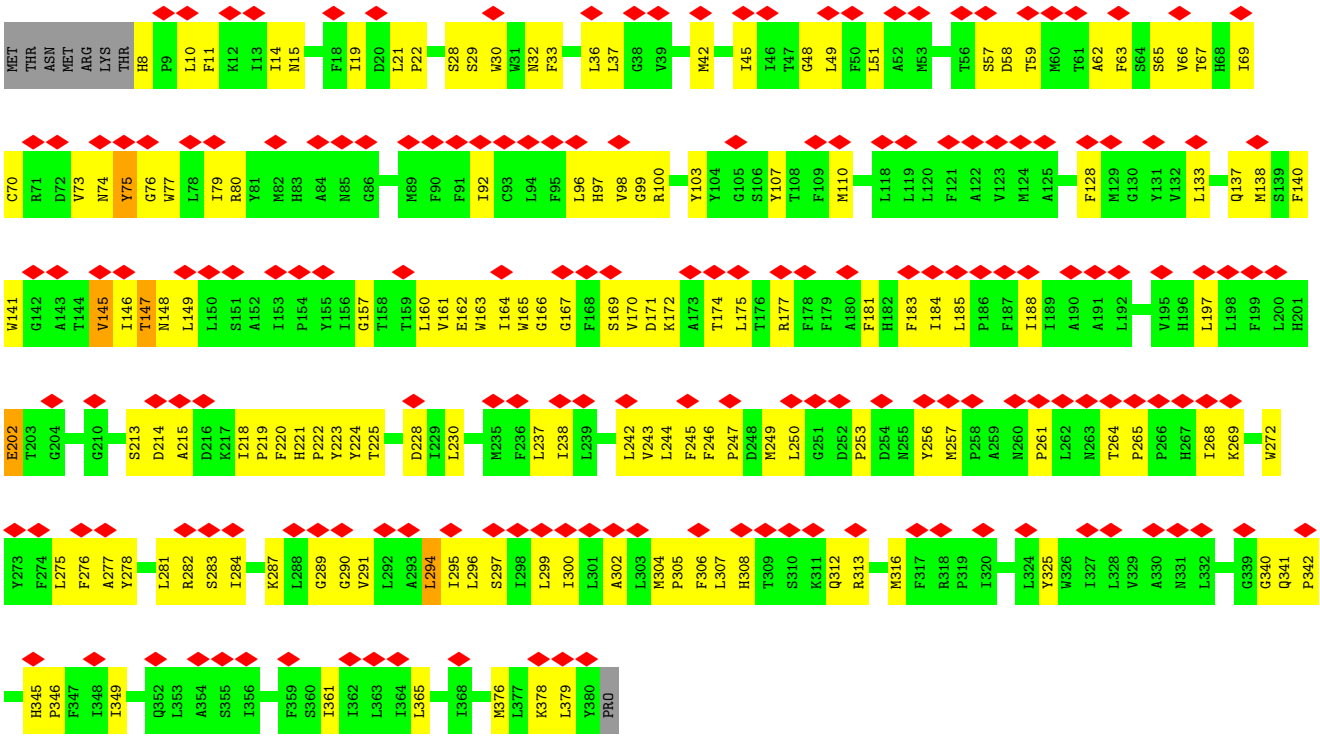
F199 L200 H201 E202 T203 G204 S205 N206 N207 G210 L211 N212 S213 D214 A215 D216 K217 I218 P219 F220 H221 P222 Y223 Y224 T225 I226 K227 D228 I229 L230 G231 T232 L233 I234 M235 F236 L237 I238 L239 M240 T241 L242 V243 L244 F245 F246 M249 L250 G251 D252 P253 D254 N255 Y256 M257 P258 A259 N260

P261 L262 N263 T264 P265 P266 H267 I268 K269 W272 Y273 F274 L275 F276 A277 Y278 A279 I280 L281 R282 S283 I284 P285 N286 K287 L288 G289 G290 V291 L292 A293 L294 I295 L296 S297 I298 L299 I300 L301 A302 L303 M304 P305 F306 L307 H308 T309 S310 K311 Q312 R313 S314 L315 M316 F317 R318 P319 I320 T321

Q322 I323 W326 I327 L328 V329 A330 N331 L332 L333 I334 L335 T336 W337 I338 G339 G340 Q341 P342 V343 E344 H345 P346 F347 I348 I349 I350 G351 Q352 L353 A354 S355 I356 S357 Y358 F359 S360 I361 I362 L363 I364 L365 M366 P367 I368 I371 I372 E373 D374 K375 M376 L377 K378 L379 Y380 PRO

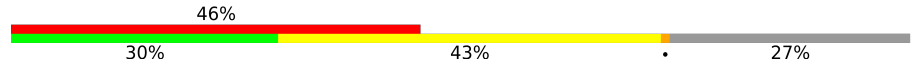
• Molecule 47: Cytochrome b

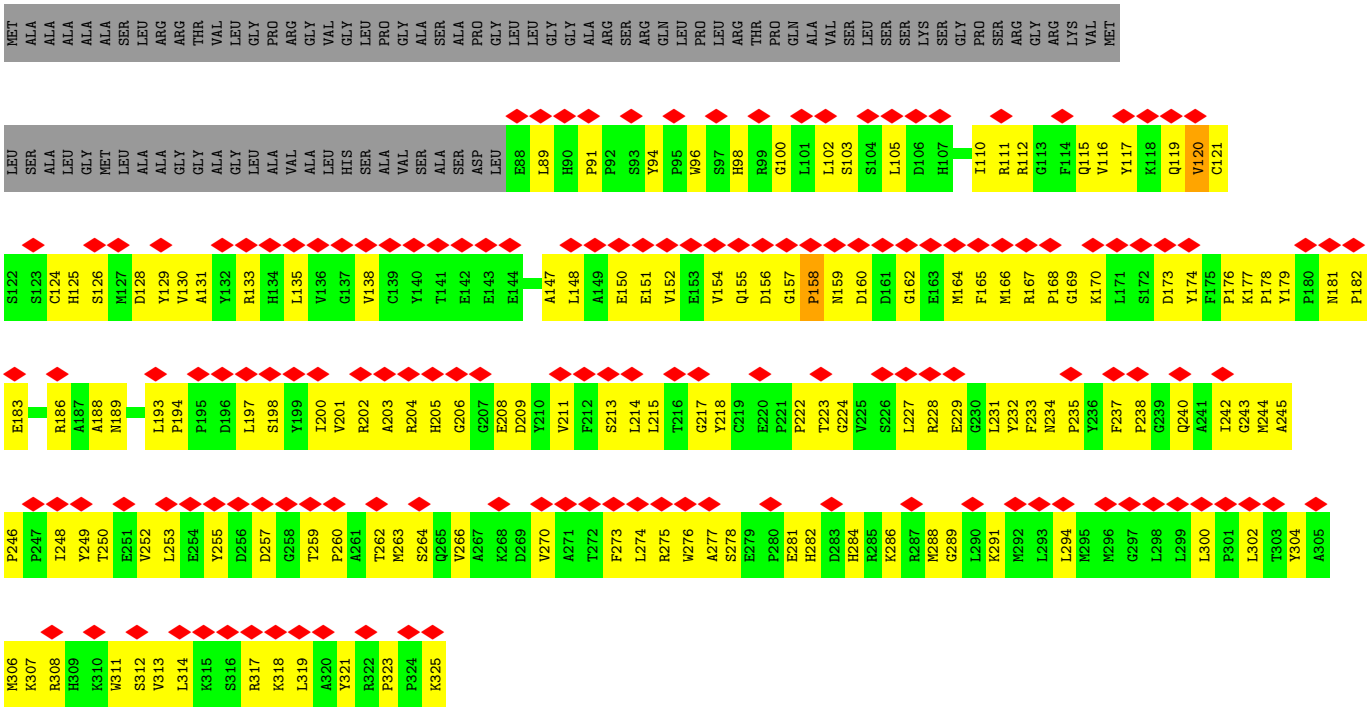
Chain Ac:



• Molecule 48: Cytochrome c1, heme protein, mitochondrial

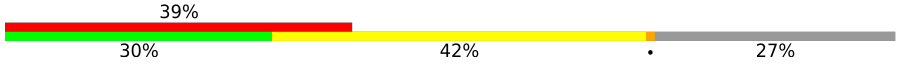
Chain AD:

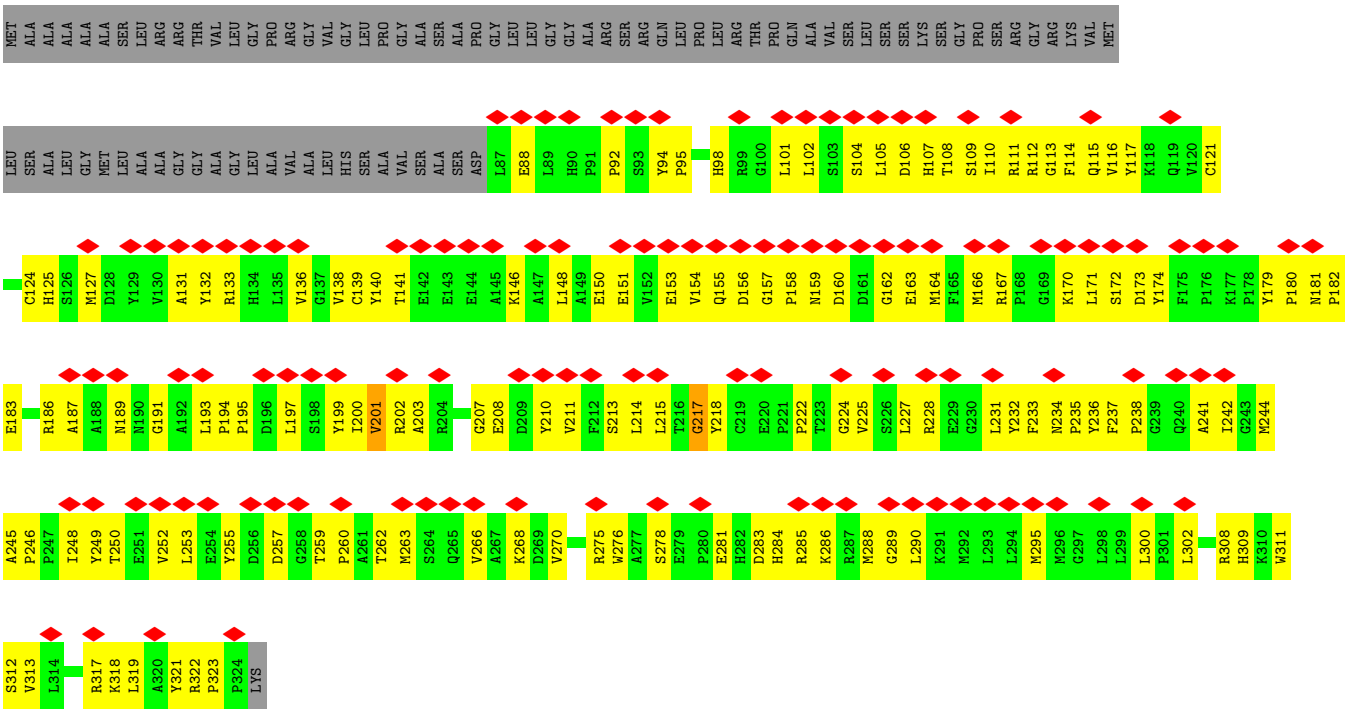




• Molecule 48: Cytochrome c1, heme protein, mitochondrial

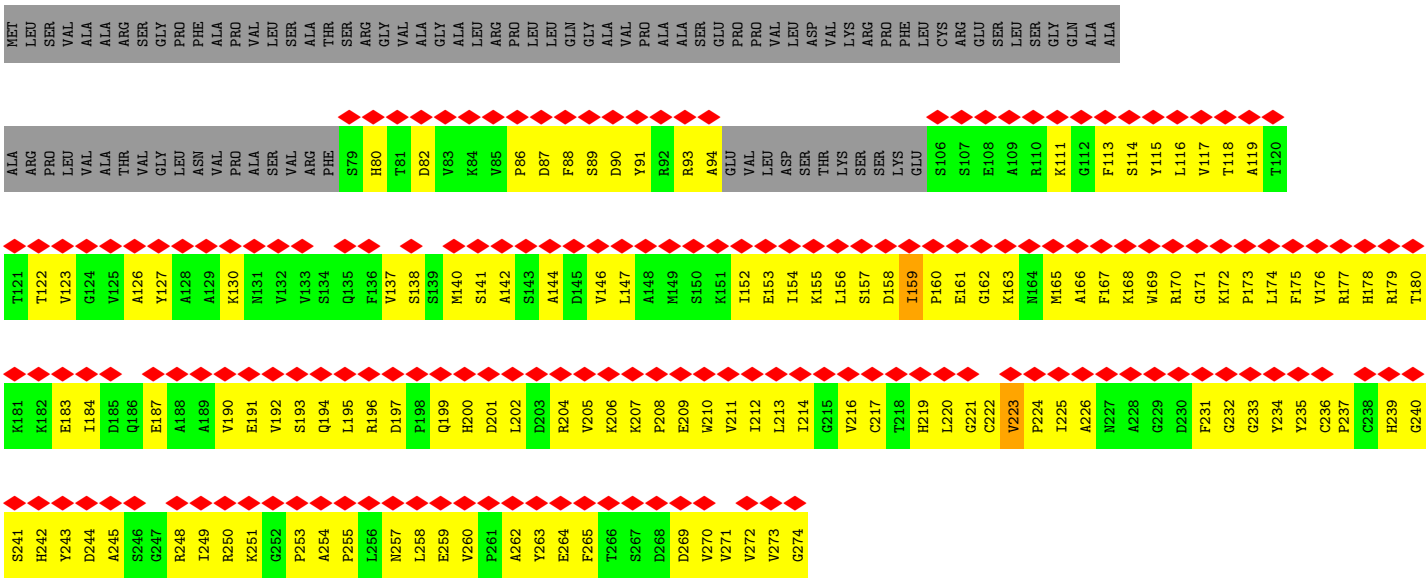
Chain Ad:





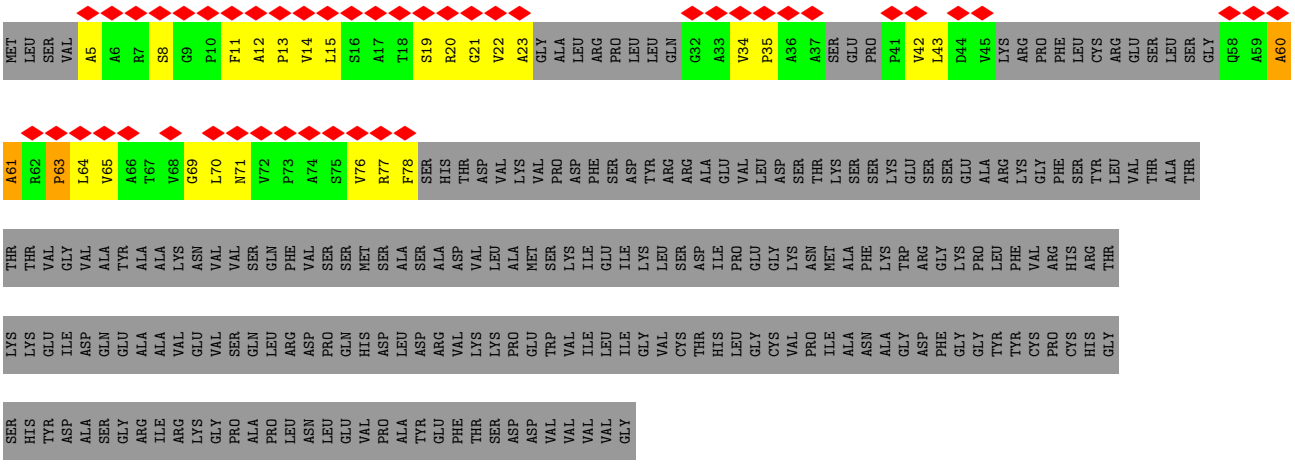
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE:



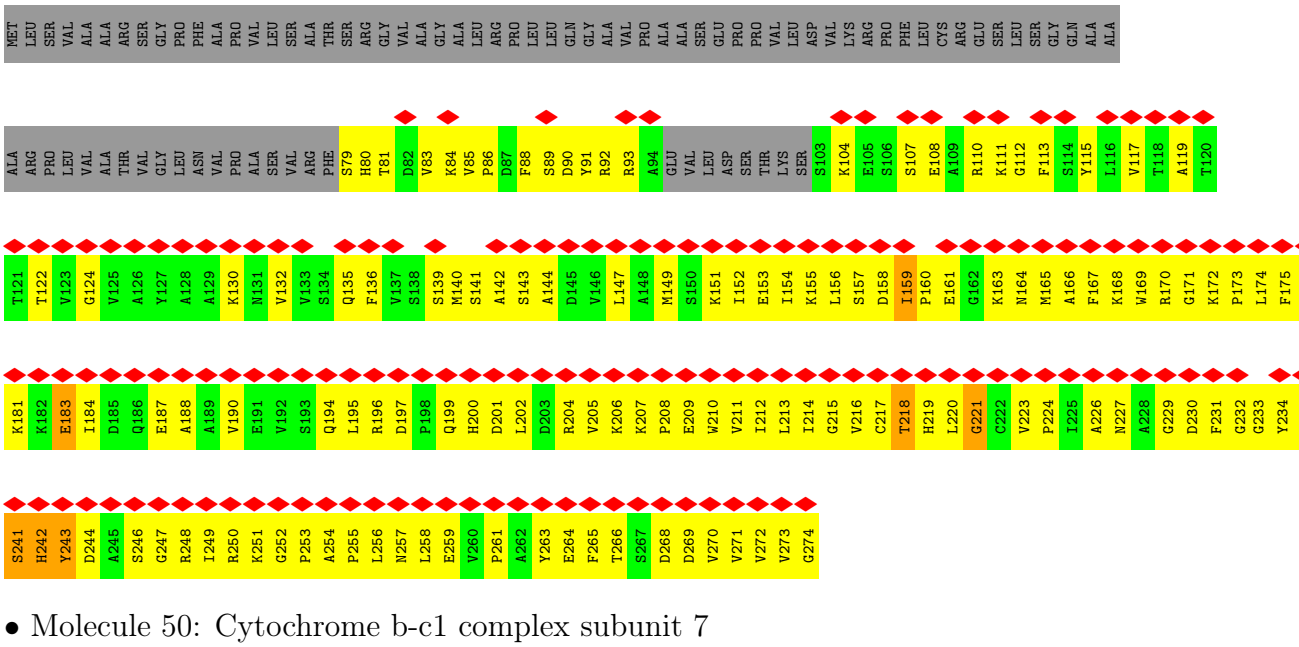
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



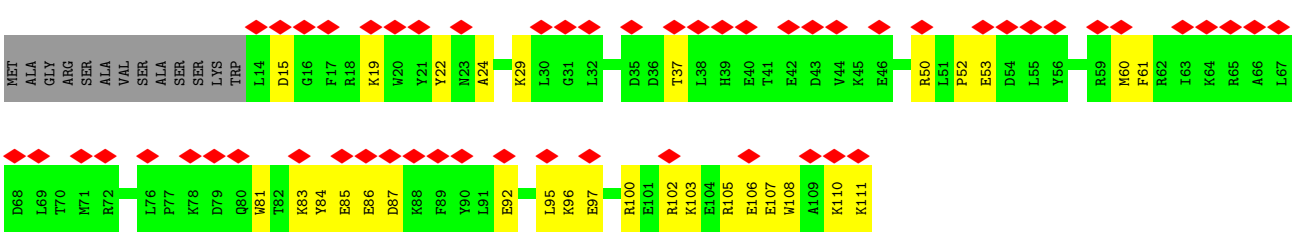
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



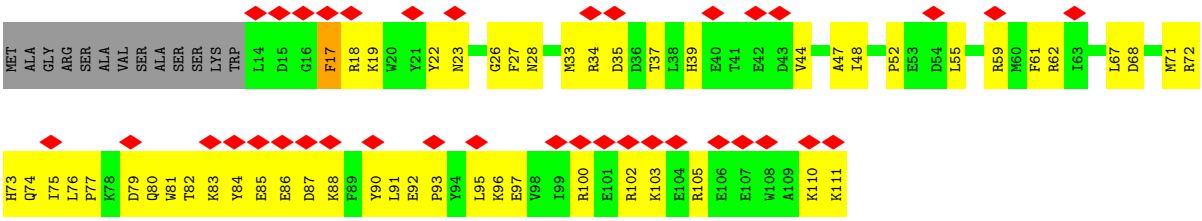
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain AF:



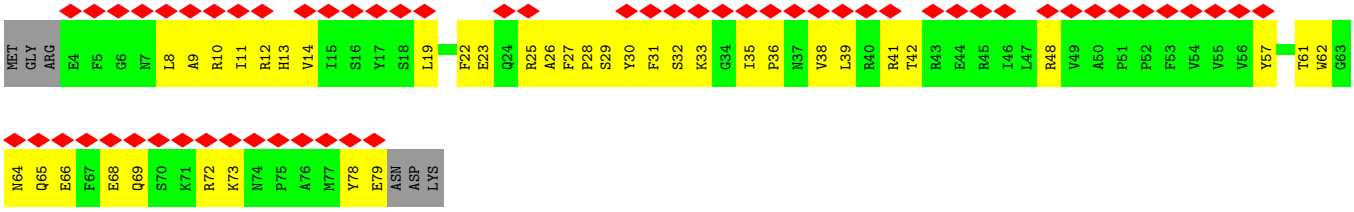
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain Af:



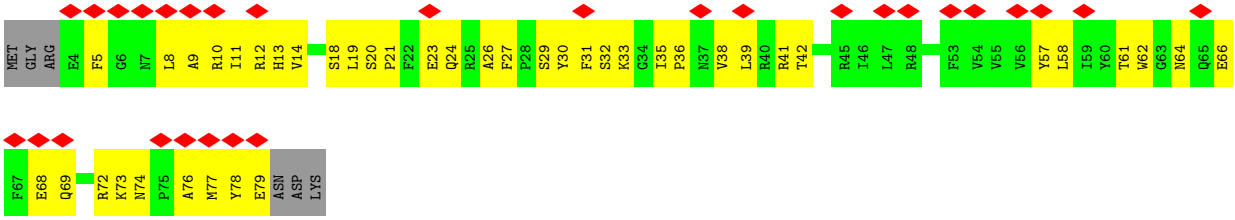
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain AG:



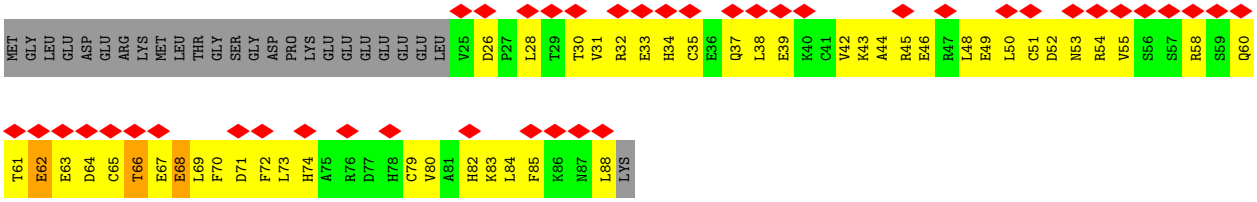
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain Ag:



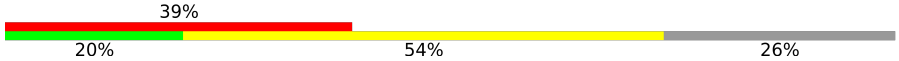
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

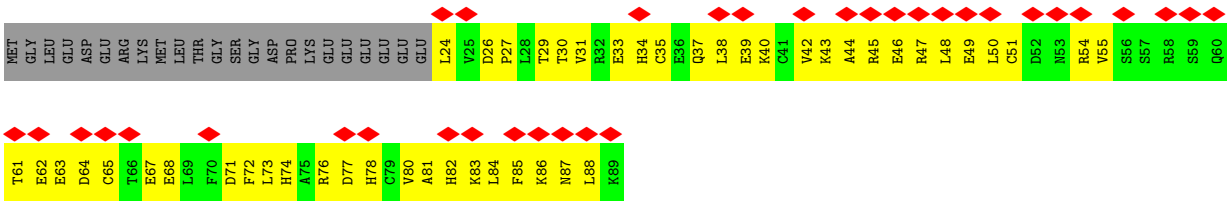
Chain AH:



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

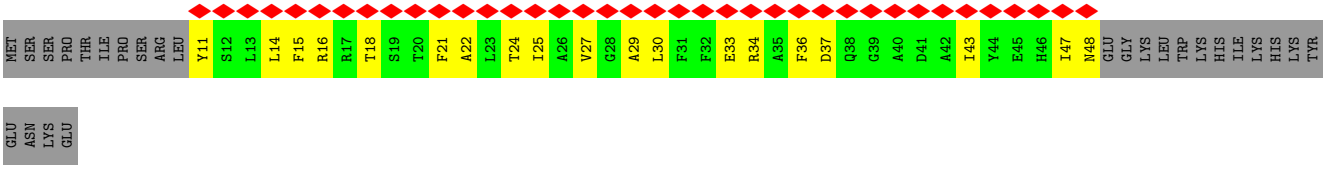
Chain Ah:





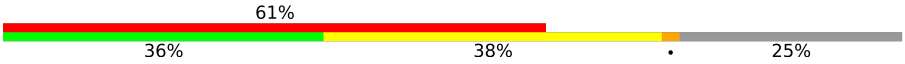
• Molecule 53: Cytochrome b-c1 complex subunit 9

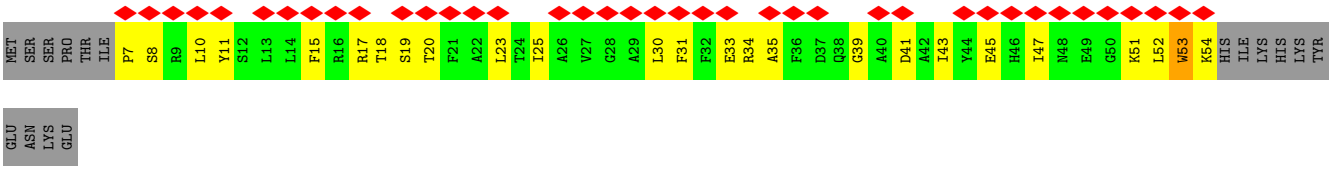
Chain AJ:



• Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj:



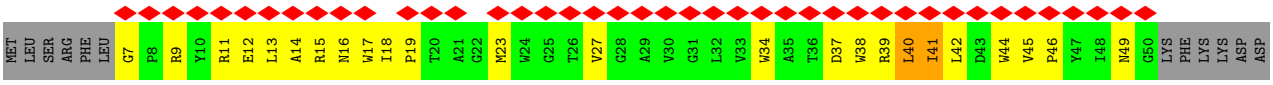


• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain AK:

• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37608	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 ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.81	0/782	1.19	6/1066 (0.6%)
2	B	0.97	1/1278 (0.1%)	1.37	13/1730 (0.8%)
3	C	0.94	2/1687 (0.1%)	1.33	14/2297 (0.6%)
4	D	0.94	7/3512 (0.2%)	1.39	35/4758 (0.7%)
5	E	0.82	2/1675 (0.1%)	1.31	22/2282 (1.0%)
6	F	0.96	6/3363 (0.2%)	1.53	63/4543 (1.4%)
7	G	0.93	10/5374 (0.2%)	1.59	107/7281 (1.5%)
8	H	0.96	3/2600 (0.1%)	1.49	54/3550 (1.5%)
9	I	0.93	1/1427 (0.1%)	1.52	19/1927 (1.0%)
10	J	0.80	0/1221	1.34	16/1656 (1.0%)
11	K	0.91	0/740	1.50	14/1005 (1.4%)
12	L	0.98	5/4921 (0.1%)	1.57	109/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.57	87/5062 (1.7%)
14	N	1.00	4/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.87	6/2666 (0.2%)	1.22	27/3615 (0.7%)
16	P	0.83	3/2804 (0.1%)	1.23	29/3802 (0.8%)
17	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
18	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
19	S	0.90	1/678 (0.1%)	1.47	11/915 (1.2%)
20	T	1.04	1/613 (0.2%)	1.56	12/826 (1.5%)
20	U	1.02	1/712 (0.1%)	1.42	17/962 (1.8%)
21	V	0.86	0/937	1.46	14/1270 (1.1%)
22	W	0.82	1/993 (0.1%)	1.00	3/1335 (0.2%)
23	X	0.79	0/1422	1.31	19/1921 (1.0%)
24	Y	0.87	0/1054	0.97	3/1429 (0.2%)
25	Z	0.82	1/1183 (0.1%)	1.22	12/1597 (0.8%)
26	a	0.88	0/561	1.38	8/755 (1.1%)
27	b	0.74	0/643	0.95	1/884 (0.1%)
28	c	0.96	1/400 (0.2%)	1.34	11/544 (2.0%)
29	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
30	e	0.74	1/881 (0.1%)	1.00	2/1173 (0.2%)
31	f	0.90	1/459 (0.2%)	1.32	11/618 (1.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.88	3/870 (0.3%)	1.36	19/1185 (1.6%)
33	h	0.75	0/1197	1.22	6/1621 (0.4%)
34	i	0.85	0/798	1.38	17/1085 (1.6%)
35	j	0.87	2/612 (0.3%)	1.28	10/837 (1.2%)
36	k	1.12	2/596 (0.3%)	1.55	20/805 (2.5%)
37	l	1.02	4/1367 (0.3%)	1.27	10/1866 (0.5%)
38	m	0.85	1/1073 (0.1%)	1.20	15/1455 (1.0%)
39	n	0.95	1/1589 (0.1%)	1.26	17/2152 (0.8%)
40	o	0.82	0/1044	1.14	7/1401 (0.5%)
41	p	0.73	1/1471 (0.1%)	1.01	13/1988 (0.7%)
42	q	0.98	2/1037 (0.2%)	1.41	17/1408 (1.2%)
43	r	0.94	2/421 (0.5%)	1.37	8/566 (1.4%)
44	s	0.43	0/233	0.75	1/317 (0.3%)
45	AA	0.57	1/3176 (0.0%)	0.85	7/4305 (0.2%)
45	Aa	0.45	0/3190	0.78	9/4325 (0.2%)
46	AB	0.44	1/3156 (0.0%)	0.62	3/4263 (0.1%)
46	Ab	0.44	0/3149	0.69	5/4255 (0.1%)
47	AC	0.41	0/3089	0.72	6/4221 (0.1%)
47	Ac	0.48	0/3089	0.79	5/4221 (0.1%)
48	AD	0.54	0/1955	0.81	1/2655 (0.0%)
48	Ad	0.65	2/1954 (0.1%)	0.86	4/2655 (0.2%)
49	AE	0.50	0/1459	0.94	4/1976 (0.2%)
49	AI	0.96	1/351 (0.3%)	1.34	5/478 (1.0%)
49	Ae	0.56	0/1483	1.04	8/2007 (0.4%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.72	1/884 (0.1%)	0.82	0/1184
51	AG	0.50	0/662	0.87	1/895 (0.1%)
51	Ag	0.54	0/662	0.94	2/895 (0.2%)
52	AH	0.54	0/534	0.95	4/717 (0.6%)
52	Ah	0.65	0/551	0.82	0/739
53	AJ	0.46	0/314	0.60	0/424
53	Aj	0.62	0/402	0.80	1/541 (0.2%)
54	AK	0.49	0/287	0.84	1/393 (0.3%)
54	Ak	0.53	0/371	0.82	2/511 (0.4%)
All	All	0.81	96/97648 (0.1%)	1.22	1053/132394 (0.8%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	89	PRO	N-CD	-15.12	1.26	1.47
29	d	115	PRO	N-CD	-14.11	1.28	1.47
12	L	265	PRO	N-CD	13.82	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	50	PRO	N-CD	-13.63	1.28	1.47
14	N	255	PRO	N-CD	-13.58	1.28	1.47
49	AI	63	PRO	N-CD	-13.53	1.28	1.47
42	q	139	PRO	N-CD	-13.36	1.29	1.47
28	c	39	PRO	N-CD	-13.26	1.29	1.47
16	P	371	PRO	N-CD	12.95	1.65	1.47
7	G	532	PRO	N-CD	-12.57	1.30	1.47
15	O	315	PRO	N-CD	-12.07	1.30	1.47
20	T	141	PRO	N-CD	11.84	1.64	1.47
48	Ad	182	PRO	N-CD	-11.67	1.31	1.47
15	O	210	PRO	N-CD	-11.39	1.31	1.47
12	L	234	PRO	N-CD	11.17	1.63	1.47
8	H	42	PRO	N-CD	10.85	1.62	1.47
13	M	370	PRO	N-CD	-10.60	1.32	1.47
6	F	234	GLY	CA-C	-10.28	1.41	1.52
6	F	227	PRO	N-CD	10.07	1.61	1.47
6	F	235	VAL	N-CA	-9.68	1.34	1.46
16	P	290	PRO	N-CD	9.62	1.61	1.47
36	k	20	MET	C-N	9.61	1.47	1.33
32	g	78	PRO	N-CD	-9.51	1.34	1.47
7	G	275	PRO	N-CD	-9.48	1.34	1.47
29	d	15	PRO	N-CD	-9.38	1.34	1.47
8	H	75	PRO	N-CD	9.22	1.60	1.47
6	F	319	PRO	N-CD	9.07	1.60	1.47
9	I	107	PRO	N-CD	8.59	1.59	1.47
46	AB	240	MET	C-N	8.57	1.45	1.33
13	M	20	PRO	N-CD	8.54	1.59	1.47
4	D	163	PRO	N-CD	-8.41	1.35	1.47
12	L	212	PRO	N-CD	-8.21	1.36	1.47
25	Z	73	PRO	N-CD	8.15	1.59	1.47
39	n	155	PRO	N-CD	8.07	1.59	1.47
4	D	352	PRO	N-CD	-7.95	1.36	1.47
18	R	39	ASP	CA-C	7.91	1.64	1.53
17	Q	53	ILE	C-O	7.90	1.33	1.24
3	C	81	ASP	C-O	-7.88	1.14	1.24
19	S	63	PRO	N-CD	-7.88	1.36	1.47
5	E	218	ARG	CA-C	7.87	1.62	1.53
18	R	40	GLU	N-CA	7.68	1.56	1.46
43	r	111	PRO	N-CD	-7.45	1.37	1.47
37	l	115	ASN	C-N	-7.30	1.24	1.33
37	l	104	PRO	N-CD	-7.21	1.37	1.47
13	M	208	PRO	N-CD	7.15	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	238	PRO	N-CD	-7.00	1.38	1.47
35	j	38	VAL	C-N	6.98	1.43	1.33
15	O	206	TYR	C-N	6.83	1.42	1.33
7	G	449	PRO	N-CD	6.79	1.57	1.47
7	G	541	PRO	N-CD	-6.74	1.38	1.47
6	F	233	VAL	CA-C	-6.71	1.44	1.52
7	G	203	ASP	CA-C	6.71	1.62	1.52
32	g	113	GLN	CA-C	6.62	1.61	1.52
4	D	106	VAL	C-N	-6.54	1.24	1.33
7	G	600	GLU	CA-C	6.48	1.61	1.52
15	O	205	ILE	C-N	6.48	1.42	1.33
4	D	266	ARG	C-O	-6.31	1.16	1.24
12	L	384	PRO	N-CD	6.28	1.56	1.47
7	G	127	ASP	CA-C	6.24	1.62	1.52
41	p	10	TYR	CA-C	-6.23	1.46	1.52
6	F	384	PRO	N-CD	-6.18	1.39	1.47
2	B	110	PRO	C-O	-6.16	1.16	1.24
7	G	76	ARG	CA-C	6.08	1.61	1.53
32	g	137	SER	C-O	-6.04	1.16	1.24
12	L	112	PRO	N-CD	6.01	1.56	1.47
7	G	361	VAL	CA-C	5.89	1.60	1.52
38	m	72	ARG	CA-C	5.89	1.60	1.52
5	E	93	PRO	N-CD	-5.88	1.39	1.47
30	e	34	HIS	C-O	-5.85	1.16	1.24
8	H	60	PRO	N-CD	5.83	1.55	1.47
43	r	25	GLN	CA-C	5.79	1.60	1.52
37	l	45	PRO	N-CD	-5.77	1.39	1.47
18	R	59	PHE	CA-C	-5.76	1.45	1.52
35	j	39	HIS	C-N	-5.73	1.28	1.33
15	O	87	PRO	N-CD	-5.72	1.39	1.47
13	M	454	ILE	CA-C	5.66	1.60	1.52
22	W	22	PRO	N-CD	5.66	1.55	1.47
48	Ad	217	GLY	C-O	-5.62	1.16	1.23
13	M	252	PRO	N-CD	-5.58	1.40	1.47
14	N	333	SER	C-O	-5.57	1.17	1.23
4	D	107	ARG	C-N	5.50	1.40	1.33
4	D	392	PRO	C-O	-5.50	1.20	1.24
7	G	683	PRO	N-CD	-5.41	1.40	1.47
20	U	140	CYS	C-O	-5.41	1.17	1.24
42	q	126	PRO	N-CD	5.33	1.55	1.47
16	P	235	THR	CA-C	5.32	1.59	1.53
50	Af	17	PHE	C-N	-5.30	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	103	PRO	N-CD	-5.24	1.40	1.47
45	AA	311	ILE	C-N	5.18	1.40	1.33
31	f	38	ARG	CA-C	-5.16	1.46	1.52
4	D	266	ARG	CA-C	-5.14	1.45	1.52
37	l	111	MET	C-O	-5.12	1.17	1.24
13	M	424	ILE	CA-C	-5.11	1.45	1.52
3	C	61	GLY	C-N	-5.04	1.27	1.33
13	M	159	PRO	N-CD	5.03	1.54	1.47
14	N	88	GLN	CA-C	5.00	1.59	1.52

All (1053) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	142	VAL	N-CA-CB	19.28	132.44	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-16.87	89.00	114.64
6	F	125	CYS	N-CA-C	-15.62	93.48	113.17
6	F	332	CYS	N-CA-C	15.55	129.99	111.02
13	M	370	PRO	N-CA-C	14.57	128.48	110.70
14	N	255	PRO	N-CA-C	14.49	128.38	110.70
15	O	118	TYR	N-CA-C	13.83	125.86	111.07
42	q	139	PRO	N-CA-CB	-13.57	95.59	103.19
7	G	251	ILE	N-CA-C	13.34	126.84	108.17
7	G	77	MET	N-CA-C	-13.05	97.32	113.38
7	G	500	ILE	N-CA-C	-12.50	98.78	110.53
26	a	3	PHE	CB-CA-C	-12.40	89.60	110.68
16	P	106	LEU	N-CA-C	12.19	128.70	109.07
6	F	171	VAL	N-CA-C	-11.86	99.38	110.53
13	M	424	ILE	N-CA-C	-11.65	94.03	109.30
7	G	204	MET	N-CA-C	-11.62	91.46	109.25
6	F	449	ARG	N-CA-C	-11.61	98.70	111.36
34	i	14	GLN	N-CA-C	11.58	123.90	111.28
13	M	104	ILE	N-CA-C	-11.56	99.09	110.30
6	F	334	THR	N-CA-CB	11.51	127.31	109.82
12	L	194	ASN	N-CA-C	11.47	125.40	109.11
15	O	114	LEU	N-CA-C	-11.46	98.87	111.36
49	Ae	242	HIS	N-CA-C	11.44	125.36	109.11
10	J	5	ILE	N-CA-C	11.42	121.90	110.82
13	M	311	GLY	N-CA-C	-11.38	99.30	112.50
17	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
37	l	116	ARG	N-CA-C	11.32	123.30	110.97
7	G	599	THR	N-CA-C	11.30	126.17	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	244	ILE	N-CA-C	-11.28	99.33	110.72
12	L	278	LEU	N-CA-C	-11.23	99.01	111.14
11	K	83	ASN	N-CA-C	-11.19	100.17	114.04
21	V	57	ASP	N-CA-C	-11.02	99.28	111.07
8	H	259	PHE	N-CA-C	-11.00	99.37	111.36
20	U	79	ILE	N-CA-C	-10.99	102.35	112.90
12	L	582	GLY	N-CA-C	-10.80	99.52	114.64
12	L	556	ILE	N-CA-C	10.70	121.36	110.23
49	AI	63	PRO	N-CA-CB	-10.69	93.84	103.25
12	L	231	PRO	N-CA-C	10.67	127.71	113.84
9	I	164	VAL	N-CA-C	-10.60	100.19	113.22
33	h	101	ILE	N-CA-C	-10.55	98.61	108.95
9	I	77	LEU	N-CA-C	-10.52	99.62	111.71
5	E	68	ASN	N-CA-C	-10.40	99.94	111.07
20	T	139	MET	N-CA-C	-10.39	97.48	113.89
15	O	210	PRO	N-CA-CB	-10.36	94.62	103.32
13	M	276	CYS	N-CA-C	-10.35	99.99	111.28
2	B	195	PRO	N-CA-C	-10.34	98.08	110.70
15	O	96	THR	N-CA-C	-10.32	100.11	111.36
7	G	280	ASP	N-CA-C	10.31	122.52	111.28
3	C	80	LEU	N-CA-C	-10.29	99.83	112.38
4	D	337	MET	N-CA-C	-10.21	100.14	111.07
37	l	170	ARG	N-CA-C	-10.19	101.49	113.21
4	D	140	ASP	CB-CA-C	-10.18	98.08	111.42
16	P	366	ILE	N-CA-C	10.15	120.97	110.62
7	G	414	PHE	N-CA-C	-10.14	101.40	113.88
9	I	161	ALA	N-CA-C	10.14	122.33	111.28
20	T	135	ALA	N-CA-C	-10.08	100.29	111.28
26	a	4	GLU	N-CA-C	10.05	124.80	112.54
39	n	29	SER	N-CA-C	-10.05	101.52	113.88
13	M	117	MET	N-CA-C	-10.04	100.34	111.28
10	J	27	TYR	N-CA-C	-9.91	100.95	113.23
10	J	36	GLY	N-CA-C	-9.89	101.03	112.50
7	G	325	ARG	N-CA-C	-9.87	100.21	110.97
9	I	166	ALA	N-CA-C	-9.84	100.82	113.12
6	F	178	GLU	N-CA-C	-9.84	99.31	111.11
45	AA	187	LEU	N-CA-C	-9.83	100.39	112.38
6	F	103	ASN	N-CA-C	-9.81	101.00	113.16
6	F	141	GLY	N-CA-C	-9.78	101.16	112.50
7	G	654	VAL	N-CA-C	9.74	123.26	111.09
5	E	64	ALA	N-CA-C	-9.73	99.44	111.11
6	F	144	VAL	N-CA-C	-9.72	101.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	Aa	385	GLU	N-CA-C	9.71	121.95	111.36
13	M	423	MET	N-CA-C	-9.71	96.95	110.35
14	N	255	PRO	CA-N-CD	9.70	125.58	112.00
36	k	50	PRO	CA-N-CD	9.69	125.56	112.00
14	N	286	ALA	N-CA-C	-9.68	100.73	111.28
16	P	371	PRO	N-CA-CB	9.66	111.86	103.36
13	M	83	HIS	N-CA-C	-9.64	97.24	110.35
29	d	115	PRO	N-CA-CB	-9.60	95.00	103.35
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
7	G	337	ALA	N-CA-C	-9.57	100.81	114.12
22	W	87	ILE	N-CA-C	-9.57	101.23	110.42
26	a	2	TRP	N-CA-C	-9.56	101.62	113.28
8	H	52	ALA	N-CA-C	-9.54	100.86	111.07
34	i	12	LEU	N-CA-C	-9.51	101.23	113.12
3	C	136	PHE	N-CA-C	-9.50	96.84	110.24
12	L	375	ILE	N-CA-C	-9.50	101.30	110.42
23	X	70	PHE	N-CA-C	-9.49	99.72	111.11
18	R	38	TYR	N-CA-C	-9.46	96.34	110.24
41	p	56	HIS	N-CA-C	9.43	121.56	111.28
4	D	427	PRO	N-CA-C	-9.42	95.71	110.50
23	X	112	LEU	N-CA-C	-9.41	100.97	111.14
14	N	228	ASN	N-CA-C	-9.41	101.00	111.07
42	q	139	PRO	CA-N-CD	9.38	125.14	112.00
29	d	115	PRO	CA-N-CD	9.37	125.12	112.00
31	f	12	VAL	N-CA-CB	9.37	124.01	110.52
13	M	104	ILE	N-CA-CB	9.36	120.82	110.62
36	k	60	MET	N-CA-C	9.33	121.14	110.97
7	G	694	PHE	N-CA-C	9.32	121.44	111.28
20	T	133	ILE	N-CA-C	9.30	119.84	110.82
36	k	56	ALA	N-CA-C	9.29	121.49	111.36
12	L	394	LEU	N-CA-C	-9.29	101.13	111.07
12	L	40	ILE	N-CA-C	-9.29	101.34	110.72
7	G	692	LYS	N-CA-C	-9.28	100.53	112.23
16	P	367	GLU	N-CA-C	9.27	122.57	111.82
16	P	369	THR	N-CA-CB	9.24	123.47	110.17
7	G	640	ASP	N-CA-C	-9.21	101.32	111.36
12	L	483	PRO	N-CA-C	-9.20	96.75	111.38
25	Z	69	ILE	N-CA-C	-9.20	100.70	110.36
49	AI	63	PRO	CA-N-CD	9.15	124.81	112.00
7	G	389	THR	N-CA-C	-9.13	96.26	109.96
28	c	64	GLU	N-CA-C	-9.12	101.31	111.07
14	N	87	GLN	N-CA-C	9.11	123.26	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	85	ALA	N-CA-C	-9.11	101.43	111.36
47	Ac	157	GLY	N-CA-C	9.10	123.06	112.50
12	L	467	VAL	N-CA-C	9.10	119.15	110.42
45	AA	473	SER	N-CA-C	9.07	122.14	111.71
13	M	442	ILE	N-CA-CB	9.06	117.52	110.45
26	a	57	VAL	N-CA-C	-9.04	105.12	113.71
28	c	39	PRO	N-CA-CB	-9.01	95.32	103.25
31	f	12	VAL	N-CA-C	-9.00	102.09	110.82
41	p	115	GLN	N-CA-C	-8.97	102.85	113.88
11	K	70	GLU	N-CA-C	-8.96	100.35	111.11
6	F	411	SER	N-CA-C	-8.86	101.59	111.07
15	O	183	CYS	N-CA-C	-8.86	100.47	111.11
12	L	344	GLY	N-CA-C	-8.86	102.22	112.50
14	N	233	LEU	N-CA-C	-8.82	101.66	111.28
7	G	133	GLN	N-CA-CB	8.80	121.54	110.45
12	L	406	ALA	N-CA-C	-8.80	101.76	111.36
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
40	o	72	ASP	N-CA-C	-8.77	98.96	110.53
39	n	70	GLU	N-CA-C	-8.74	101.71	111.07
14	N	255	PRO	N-CA-CB	-8.74	94.60	103.08
13	M	255	LYS	N-CA-C	-8.72	101.74	111.07
14	N	81	LEU	N-CA-C	-8.72	94.43	108.55
7	G	365	ASN	N-CA-C	-8.69	102.23	112.92
9	I	154	TYR	N-CA-CB	-8.69	99.19	111.62
8	H	60	PRO	N-CA-CB	8.69	108.56	102.65
47	Ac	147	THR	N-CA-C	-8.67	101.77	111.14
22	W	20	VAL	N-CA-C	8.65	120.74	108.36
16	P	96	LEU	N-CA-C	8.64	121.65	111.71
49	AI	61	ALA	N-CA-C	8.60	123.25	112.24
13	M	248	ILE	N-CA-C	-8.58	102.18	110.42
12	L	212	PRO	N-CA-C	8.57	125.73	113.47
26	a	3	PHE	CA-CB-CG	8.54	122.34	113.80
19	S	18	GLU	N-CA-C	8.50	123.25	109.40
12	L	265	PRO	N-CA-C	-8.50	101.32	113.47
15	O	315	PRO	CA-N-CD	8.50	123.90	112.00
19	S	86	GLU	N-CA-C	-8.49	102.10	111.36
3	C	70	LYS	N-CA-C	8.49	121.60	111.33
16	P	373	LYS	N-CA-C	8.48	121.89	110.35
12	L	287	PHE	N-CA-C	-8.46	102.02	111.07
14	N	109	ALA	CA-C-N	-8.45	110.74	120.12
14	N	109	ALA	C-N-CA	-8.45	110.74	120.12
14	N	221	LEU	N-CA-C	-8.43	101.13	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	108	LYS	N-CA-C	8.42	120.08	111.07
12	L	281	GLY	N-CA-C	-8.41	102.75	112.50
14	N	272	LYS	N-CA-C	-8.40	102.12	111.28
48	Ad	182	PRO	CA-N-CD	8.39	123.75	112.00
23	X	99	HIS	N-CA-C	-8.37	102.23	111.36
8	H	141	SER	N-CA-C	-8.36	102.12	111.07
48	Ad	108	THR	N-CA-C	-8.36	102.67	113.12
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
7	G	452	LEU	N-CA-C	-8.33	102.20	111.28
17	Q	54	THR	N-CA-C	8.32	123.28	109.46
39	n	19	LEU	N-CA-C	-8.31	103.27	113.41
7	G	558	GLN	N-CA-C	-8.29	102.20	111.07
36	k	50	PRO	N-CA-CB	-8.27	93.50	102.76
14	N	218	ALA	N-CA-C	-8.25	98.93	111.56
12	L	151	SER	N-CA-C	-8.24	102.38	111.36
8	H	196	ALA	N-CA-C	8.23	127.99	109.81
5	E	218	ARG	CB-CA-C	-8.20	99.81	112.12
13	M	274	SER	N-CA-C	8.20	120.22	111.28
8	H	311	THR	N-CA-C	-8.19	102.60	112.59
10	J	133	VAL	N-CA-C	-8.18	96.73	108.42
7	G	691	ILE	N-CA-C	8.17	123.66	111.89
6	F	298	GLU	N-CA-C	8.16	120.18	111.28
12	L	169	LEU	N-CA-C	-8.16	102.46	111.36
3	C	196	PRO	N-CA-C	8.15	124.86	113.53
4	D	36	GLN	N-CA-C	-8.15	98.53	110.42
12	L	88	LEU	N-CA-C	-8.15	102.34	111.14
13	M	26	ASN	N-CA-C	-8.14	102.35	111.14
6	F	411	SER	N-CA-CB	8.13	121.80	110.01
6	F	191	TYR	N-CA-C	8.12	121.68	110.24
1	A	64	LEU	N-CA-C	-8.11	102.39	111.07
7	G	484	ASP	N-CA-C	8.11	121.03	111.71
36	k	38	VAL	N-CA-C	-8.10	102.54	110.72
7	G	534	VAL	N-CA-C	-8.10	104.70	111.91
14	N	32	GLY	N-CA-C	-8.08	103.12	112.50
47	Ac	147	THR	N-CA-CB	8.07	121.77	110.07
21	V	86	LYS	N-CA-C	-8.06	102.43	111.14
7	G	500	ILE	N-CA-CB	8.06	120.88	110.57
45	AA	360	CYS	N-CA-C	8.06	121.41	109.24
19	S	76	THR	N-CA-C	8.04	122.00	108.90
2	B	110	PRO	N-CA-C	8.03	124.49	113.65
29	d	15	PRO	N-CA-CB	-8.03	96.37	103.35
45	Aa	386	SER	N-CA-C	8.02	120.03	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	219	SER	N-CA-CB	8.02	123.99	111.56
39	n	170	ILE	N-CA-C	-8.02	103.08	111.58
9	I	201	ILE	N-CA-C	-8.01	102.63	110.72
8	H	271	LEU	N-CA-C	-8.01	102.50	111.14
23	X	43	PHE	N-CA-C	-8.01	102.50	111.07
12	L	276	THR	N-CA-CB	8.00	121.62	110.01
10	J	60	LEU	N-CA-C	7.99	120.76	111.02
13	M	385	LEU	N-CA-C	-7.98	102.58	111.28
13	M	205	ILE	N-CA-C	7.98	118.08	110.42
1	A	9	ILE	N-CA-C	-7.96	102.50	110.62
7	G	651	PRO	CB-CA-C	-7.95	98.44	111.56
42	q	67	GLU	CB-CA-C	-7.94	99.60	112.06
16	P	206	ILE	N-CA-C	7.93	120.93	108.87
23	X	46	CYS	N-CA-C	-7.93	102.72	111.36
45	Aa	404	ASP	N-CA-C	-7.92	101.74	111.40
13	M	141	GLU	N-CA-C	7.91	122.77	113.20
28	c	39	PRO	CA-N-CD	7.91	123.07	112.00
28	c	45	GLY	N-CA-C	7.91	123.60	113.24
45	Aa	360	CYS	N-CA-C	7.91	120.92	109.14
21	V	6	LYS	N-CA-C	-7.88	100.12	110.53
12	L	265	PRO	N-CA-CB	7.88	111.66	103.23
8	H	311	THR	N-CA-CB	7.85	123.48	110.92
7	G	270	VAL	N-CA-CB	-7.84	100.67	110.31
9	I	160	GLU	N-CA-C	7.82	124.20	111.37
16	P	235	THR	CB-CA-C	-7.82	100.02	112.07
10	J	3	ASN	N-CA-C	-7.82	101.18	111.74
49	Ae	241	SER	N-CA-C	7.82	123.09	109.96
12	L	111	ASP	N-CA-C	-7.82	100.24	109.93
31	f	30	ASP	N-CA-C	-7.80	103.37	113.12
10	J	137	GLY	N-CA-C	-7.79	103.76	112.33
9	I	74	LEU	N-CA-C	-7.79	102.80	111.28
7	G	389	THR	N-CA-CB	7.77	121.43	109.85
13	M	330	ALA	N-CA-C	-7.77	102.75	111.14
13	M	85	LYS	N-CA-C	-7.77	101.45	113.02
23	X	58	LYS	N-CA-C	-7.76	102.76	111.07
11	K	51	SER	N-CA-C	-7.76	102.90	113.30
12	L	265	PRO	CA-N-CD	-7.76	101.13	112.00
14	N	336	THR	N-CA-C	-7.74	103.36	114.12
4	D	141	TYR	CA-C-N	7.74	130.16	120.72
4	D	141	TYR	C-N-CA	7.74	130.16	120.72
12	L	415	ALA	N-CA-C	-7.72	102.86	111.28
42	q	44	TYR	N-CA-C	-7.70	98.89	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	253	GLU	N-CA-C	7.70	121.93	112.54
18	R	47	ARG	N-CA-C	7.69	120.63	111.33
6	F	334	THR	N-CA-C	-7.68	101.65	111.02
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
7	G	56	VAL	N-CA-C	-7.65	102.99	110.72
5	E	68	ASN	N-CA-CB	7.65	121.11	110.01
42	q	89	TRP	N-CA-C	-7.65	102.88	111.14
2	B	153	PRO	CB-CA-C	-7.62	98.98	111.56
15	O	210	PRO	CA-N-CD	7.61	122.66	112.00
4	D	361	ALA	N-CA-C	-7.59	103.12	112.38
20	U	147	TYR	N-CA-C	-7.59	102.94	111.14
7	G	569	GLN	N-CA-C	7.58	121.97	108.24
5	E	166	LYS	N-CA-C	-7.58	102.20	113.72
8	H	201	THR	N-CA-C	-7.58	102.62	111.03
6	F	171	VAL	N-CA-CB	7.58	120.27	110.57
20	T	141	PRO	N-CA-C	-7.57	103.00	113.53
52	AH	71	ASP	N-CA-C	-7.55	102.65	111.03
18	R	74	HIS	N-CA-C	7.54	121.14	110.50
32	g	124	VAL	N-CA-C	-7.54	103.11	110.72
12	L	245	ALA	N-CA-C	7.52	119.11	111.07
8	H	223	PHE	CB-CA-C	-7.51	99.09	110.88
9	I	119	CYS	N-CA-C	-7.51	103.18	111.36
2	B	183	ARG	N-CA-C	-7.50	104.37	113.97
40	o	81	LYS	N-CA-C	-7.49	104.66	113.88
7	G	277	MET	N-CA-C	7.49	120.60	109.59
11	K	14	LEU	N-CA-C	-7.49	103.20	111.36
30	e	46	GLY	N-CA-C	-7.49	104.94	114.37
7	G	467	LYS	N-CA-C	-7.48	102.27	111.33
25	Z	73	PRO	N-CA-C	-7.47	103.14	113.53
9	I	158	CYS	N-CA-C	-7.44	103.17	111.28
6	F	430	GLY	N-CA-C	7.43	121.64	112.73
12	L	138	PHE	N-CA-C	-7.42	103.19	111.28
12	L	605	ASN	N-CA-CB	7.42	121.23	110.47
35	j	82	GLY	N-CA-C	-7.42	103.51	112.48
7	G	510	TRP	N-CA-CB	7.41	120.90	109.85
47	AC	202	GLU	N-CA-C	-7.41	103.22	111.82
45	AA	471	ILE	N-CA-C	-7.40	103.24	110.72
4	D	350	LYS	CB-CA-C	-7.40	100.98	111.85
4	D	99	LEU	N-CA-C	7.39	120.98	109.07
13	M	250	LEU	N-CA-C	-7.39	103.56	112.58
29	d	113	LEU	N-CA-CB	-7.39	99.93	111.23
12	L	392	LYS	N-CA-C	7.38	118.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Ac	145	VAL	N-CA-C	7.38	117.91	110.23
12	L	123	LEU	N-CA-C	-7.38	103.31	111.36
18	R	39	ASP	N-CA-C	7.37	121.28	110.59
8	H	309	ILE	N-CA-C	7.36	117.44	110.30
7	G	303	THR	N-CA-C	7.35	122.96	113.18
49	AE	119	ALA	N-CA-C	-7.34	103.22	111.07
21	V	57	ASP	N-CA-CB	7.33	120.64	110.01
47	Ac	202	GLU	N-CA-C	-7.33	103.32	111.82
12	L	21	ILE	N-CA-CB	7.33	121.57	110.58
19	S	94	VAL	N-CA-C	7.32	117.45	110.42
13	M	455	THR	N-CA-C	-7.32	100.40	110.35
37	l	97	LEU	N-CA-C	-7.30	103.97	113.17
38	m	72	ARG	N-CA-C	7.30	122.48	113.50
13	M	289	SER	N-CA-C	-7.29	103.27	111.07
7	G	384	ASN	N-CA-C	-7.28	103.38	111.82
12	L	28	LYS	N-CA-C	-7.27	103.35	111.28
7	G	661	GLU	N-CA-C	7.27	118.89	110.97
20	T	105	MET	N-CA-C	7.27	119.28	111.36
3	C	195	HIS	CB-CA-C	7.27	117.36	110.17
47	AC	8	HIS	CA-C-N	7.25	126.95	119.56
47	AC	8	HIS	C-N-CA	7.25	126.95	119.56
49	Ae	221	GLY	N-CA-C	7.25	126.81	113.76
49	AI	61	ALA	CB-CA-C	-7.24	100.07	111.51
12	L	19	ILE	N-CA-C	7.24	117.37	110.42
7	G	374	THR	CB-CA-C	-7.23	99.85	111.28
11	K	24	SER	CB-CA-C	-7.22	107.40	117.23
36	k	73	ILE	N-CA-C	-7.21	103.27	110.62
51	Ag	26	ALA	N-CA-C	7.20	119.21	111.36
11	K	81	VAL	N-CA-C	7.19	117.95	110.62
8	H	139	THR	N-CA-CB	7.18	120.42	110.01
8	H	50	ALA	N-CA-C	7.17	118.74	111.07
20	U	136	GLU	N-CA-C	-7.17	104.52	113.20
21	V	68	LEU	N-CA-C	-7.15	103.48	111.28
41	p	168	LYS	N-CA-C	-7.14	104.19	113.12
8	H	254	LEU	N-CA-C	-7.14	103.53	111.82
7	G	497	VAL	N-CA-C	-7.14	103.34	110.62
12	L	554	ASP	N-CA-CB	7.13	121.26	110.42
13	M	244	ILE	N-CA-C	7.13	117.90	110.62
6	F	73	PRO	N-CA-C	-7.13	103.85	113.40
48	AD	120	VAL	N-CA-C	7.12	118.07	111.45
7	G	461	SER	N-CA-C	7.11	119.94	111.33
20	U	74	LEU	N-CA-C	7.11	119.16	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	f	9	GLU	N-CA-C	7.11	121.70	113.38
6	F	81	LYS	N-CA-C	-7.11	103.61	111.36
7	G	465	VAL	N-CA-CB	7.10	118.39	110.51
7	G	217	GLU	N-CA-C	-7.09	101.69	110.41
11	K	48	SER	N-CA-C	-7.08	103.56	111.28
39	n	102	TRP	N-CA-C	-7.07	105.01	112.93
21	V	95	LEU	N-CA-C	-7.07	103.58	111.28
7	G	148	SER	N-CA-C	7.06	120.91	109.40
6	F	78	GLY	N-CA-C	-7.06	104.26	112.73
13	M	325	LEU	N-CA-C	-7.06	103.52	111.07
17	Q	162	ALA	N-CA-C	7.05	118.96	111.28
7	G	150	ARG	N-CA-C	7.04	119.64	109.14
8	H	176	LEU	CA-C-N	-7.04	113.55	120.52
8	H	176	LEU	C-N-CA	-7.04	113.55	120.52
13	M	34	ILE	N-CA-C	-7.03	103.45	110.62
13	M	365	ALA	N-CA-C	-7.03	103.69	111.36
6	F	455	GLN	N-CA-C	7.03	118.59	111.07
12	L	319	MET	N-CA-C	-7.03	104.70	112.72
35	j	65	MET	N-CA-C	-7.03	103.55	111.07
13	M	264	LEU	N-CA-C	-7.02	103.56	111.07
47	AC	17	SER	N-CA-C	7.02	122.01	113.38
23	X	153	VAL	N-CA-C	7.02	117.97	107.80
6	F	169	LEU	N-CA-C	7.01	118.93	111.28
49	Ae	218	THR	N-CA-C	-7.00	102.78	111.75
16	P	235	THR	CA-C-O	7.00	128.18	121.67
13	M	213	HIS	CB-CA-C	-7.00	96.81	110.11
2	B	166	ASN	N-CA-C	-6.99	103.36	110.97
14	N	132	THR	N-CA-C	6.97	122.90	113.97
18	R	45	ARG	N-CA-C	-6.97	104.65	113.01
25	Z	34	SER	N-CA-C	-6.97	103.61	111.07
7	G	294	TYR	N-CA-C	-6.97	104.59	113.23
6	F	418	GLN	N-CA-CB	6.96	120.16	110.07
8	H	292	ASN	N-CA-C	6.95	118.93	111.36
6	F	428	GLY	N-CA-C	-6.94	103.88	112.77
12	L	546	LEU	N-CA-C	6.94	119.49	111.02
12	L	471	ASN	N-CA-C	6.93	118.92	111.36
13	M	91	LEU	N-CA-C	-6.93	103.81	112.90
34	i	9	LYS	N-CA-C	-6.93	104.81	112.72
6	F	103	ASN	N-CA-CB	6.93	121.05	110.44
7	G	582	VAL	N-CA-C	6.93	118.46	108.48
13	M	235	LEU	N-CA-C	6.93	119.42	111.11
5	E	152	GLN	N-CA-C	-6.92	103.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	100	ILE	N-CA-C	6.90	119.67	111.05
12	L	86	SER	N-CA-C	6.89	118.45	111.07
34	i	11	ARG	N-CA-C	-6.89	104.87	113.28
36	k	59	TYR	N-CA-CB	-6.89	98.83	110.41
6	F	246	GLU	N-CA-C	-6.89	103.77	111.28
7	G	300	GLN	N-CA-CB	6.88	122.47	112.08
12	L	26	LEU	N-CA-C	6.88	119.62	111.71
12	L	522	PHE	N-CA-C	-6.88	103.71	111.07
6	F	233	VAL	O-C-N	6.88	131.14	123.10
6	F	148	ALA	N-CA-C	-6.87	103.87	111.36
11	K	83	ASN	N-CA-CB	6.87	120.98	110.81
13	M	276	CYS	N-CA-CB	6.87	120.22	110.12
7	G	362	ASP	N-CA-C	6.86	125.42	110.80
20	T	145	VAL	N-CA-C	-6.86	103.79	110.72
8	H	300	LEU	N-CA-C	-6.86	104.17	112.54
25	Z	28	ARG	N-CA-C	6.85	119.69	108.52
39	n	117	ASP	N-CA-C	-6.85	103.87	111.82
13	M	442	ILE	N-CA-C	-6.84	104.14	112.35
6	F	329	LYS	N-CA-C	6.83	119.60	111.33
12	L	547	LYS	N-CA-C	6.83	118.73	111.28
7	G	133	GLN	N-CA-C	-6.82	101.20	110.68
7	G	268	GLY	N-CA-C	6.81	124.77	115.30
38	m	49	LEU	N-CA-C	-6.81	104.95	112.72
18	R	56	ASN	N-CA-C	6.81	120.00	108.90
6	F	233	VAL	CA-C-O	-6.81	113.25	120.53
11	K	70	GLU	N-CA-CB	6.79	120.06	109.94
32	g	78	PRO	CA-N-CD	6.79	121.51	112.00
13	M	165	ILE	N-CA-C	-6.78	102.61	111.09
8	H	305	ILE	N-CA-C	-6.77	103.43	113.39
8	H	8	THR	N-CA-C	-6.77	101.14	110.35
15	O	93	TYR	N-CA-C	-6.77	103.98	111.36
6	F	244	ASN	N-CA-C	-6.76	100.97	110.50
38	m	127	ILE	N-CA-C	-6.76	106.21	112.43
10	J	58	ILE	N-CA-C	6.75	117.36	111.56
29	d	88	HIS	N-CA-C	-6.74	103.02	111.11
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
13	M	248	ILE	N-CA-CB	6.74	118.43	110.55
15	O	175	ASN	N-CA-C	-6.73	104.01	111.82
13	M	374	ASN	N-CA-C	-6.72	103.88	111.07
12	L	95	PHE	N-CA-C	-6.72	103.88	111.07
21	V	114	TRP	N-CA-CB	6.72	120.31	110.30
16	P	371	PRO	CA-N-CD	-6.71	102.61	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	86	ARG	N-CA-C	-6.70	99.61	110.20
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
21	V	8	THR	N-CA-C	6.70	119.03	108.79
13	M	410	MET	N-CA-C	-6.69	103.91	111.07
20	U	150	ASP	CB-CA-C	6.69	121.90	110.79
14	N	228	ASN	N-CA-CB	6.69	119.71	110.01
6	F	344	GLN	N-CA-C	-6.68	104.00	111.28
35	j	53	SER	N-CA-C	6.68	119.42	111.33
38	m	51	TYR	N-CA-C	-6.68	105.70	114.31
4	D	184	ILE	N-CA-C	-6.66	103.83	110.62
20	U	140	CYS	CA-C-N	-6.66	114.04	120.83
20	U	140	CYS	C-N-CA	-6.66	114.04	120.83
8	H	93	HIS	CB-CA-C	6.66	117.88	108.76
32	g	76	SER	N-CA-C	6.66	118.19	111.07
45	AA	361	ASP	N-CA-C	-6.65	101.30	110.35
13	M	143	LEU	N-CA-C	-6.65	103.96	111.07
16	P	116	ILE	N-CA-C	-6.65	104.01	110.72
3	C	69	PRO	N-CA-C	-6.64	104.29	113.53
23	X	129	THR	N-CA-C	6.64	120.87	110.17
3	C	125	PHE	N-CA-CB	-6.64	100.60	110.17
15	O	315	PRO	N-CA-CB	-6.64	96.03	103.33
4	D	70	ASP	N-CA-C	6.63	120.69	110.42
7	G	640	ASP	N-CA-CB	6.63	119.97	110.16
20	T	141	PRO	N-CA-CB	6.63	110.62	103.33
7	G	601	GLY	N-CA-C	6.62	124.83	115.30
34	i	8	GLU	N-CA-C	-6.62	104.79	114.39
21	V	86	LYS	N-CA-CB	6.62	119.67	110.07
34	i	70	PHE	N-CA-C	6.62	120.22	111.75
35	j	38	VAL	O-C-N	6.62	128.47	122.65
11	K	76	ALA	N-CA-C	-6.61	104.15	111.36
7	G	287	SER	N-CA-C	6.61	119.26	110.53
36	k	49	ASP	CA-C-N	-6.61	113.40	120.47
36	k	49	ASP	C-N-CA	-6.61	113.40	120.47
39	n	115	TYR	N-CA-CB	6.60	122.11	110.37
13	M	303	ILE	N-CA-C	-6.59	104.06	110.72
6	F	228	PRO	N-CA-C	-6.59	98.89	112.47
5	E	166	LYS	CB-CA-C	6.59	123.49	110.65
17	Q	141	ASN	N-CA-CB	6.58	120.79	110.46
20	U	102	SER	N-CA-C	6.58	119.57	107.99
7	G	435	PRO	N-CA-C	-6.58	100.17	110.50
13	M	161	LEU	N-CA-C	-6.57	104.04	111.07
8	H	267	SER	N-CA-C	-6.57	104.20	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	499	LEU	N-CA-C	-6.57	103.81	110.97
36	k	46	GLY	N-CA-C	-6.57	106.88	114.69
25	Z	65	LEU	N-CA-C	-6.56	104.21	111.36
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
2	B	97	LEU	N-CA-C	-6.55	101.44	110.35
12	L	329	ILE	N-CA-C	-6.55	104.14	110.42
6	F	336	LEU	N-CA-CB	-6.54	101.03	111.43
12	L	130	ILE	N-CA-C	-6.54	103.95	110.62
8	H	223	PHE	N-CA-C	-6.53	104.08	111.07
15	O	140	LEU	N-CA-C	-6.52	104.09	111.07
12	L	232	TRP	N-CA-C	6.52	120.49	112.54
6	F	234	GLY	CA-C-N	-6.51	111.77	120.50
6	F	234	GLY	C-N-CA	-6.51	111.77	120.50
15	O	118	TYR	N-CA-CB	-6.51	100.57	110.01
23	X	98	ARG	N-CA-C	6.51	120.48	112.54
36	k	57	TRP	N-CA-C	-6.51	104.60	112.54
12	L	423	SER	N-CA-C	-6.50	104.11	111.07
10	J	21	LEU	N-CA-C	-6.49	105.67	112.93
7	G	275	PRO	CB-CA-C	-6.48	102.49	110.98
7	G	605	GLN	N-CA-C	6.48	119.08	108.52
9	I	66	LEU	N-CA-C	-6.48	104.30	111.36
20	T	141	PRO	CA-N-CD	-6.47	102.94	112.00
45	AA	215	ASP	N-CA-C	-6.47	103.92	110.97
45	AA	404	ASP	N-CA-C	-6.47	105.11	112.87
19	S	16	LEU	N-CA-C	-6.47	98.36	108.90
7	G	250	SER	N-CA-C	6.47	116.81	108.34
41	p	54	ARG	N-CA-C	-6.47	103.74	111.69
43	r	24	LEU	N-CA-C	6.46	119.61	110.50
4	D	388	GLY	N-CA-C	6.46	119.55	110.38
24	Y	96	GLY	N-CA-C	-6.46	104.50	112.77
15	O	320	GLY	N-CA-C	-6.45	96.59	111.04
4	D	140	ASP	N-CA-C	-6.45	96.47	107.23
8	H	177	PRO	N-CA-C	-6.44	101.53	111.13
14	N	315	THR	N-CA-C	-6.44	104.18	111.07
10	J	139	ILE	N-CA-C	-6.44	102.81	111.44
4	D	84	PHE	N-CA-C	-6.43	104.31	111.71
21	V	49	GLU	N-CA-C	-6.43	104.27	111.28
36	k	42	LEU	N-CA-C	-6.42	103.53	111.75
12	L	325	ALA	N-CA-C	-6.42	104.28	111.28
18	R	81	GLY	N-CA-C	-6.42	106.86	115.21
7	G	275	PRO	CA-N-CD	6.42	120.98	112.00
3	C	125	PHE	N-CA-C	6.41	119.54	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Ak	40	LEU	N-CA-C	-6.41	104.51	112.72
8	H	255	TYR	N-CA-CB	6.41	119.30	110.01
6	F	178	GLU	N-CA-CB	6.41	119.48	109.94
13	M	32	PHE	N-CA-C	-6.40	104.22	111.07
7	G	95	PRO	N-CA-C	-6.40	101.14	110.80
48	Ad	182	PRO	N-CA-CB	-6.40	96.14	103.30
11	K	11	ALA	N-CA-C	-6.40	104.23	111.07
28	c	72	ARG	N-CA-C	-6.40	104.23	111.07
6	F	370	LEU	N-CA-C	-6.39	104.40	111.36
37	l	119	THR	N-CA-C	-6.39	98.13	108.41
45	Aa	215	ASP	N-CA-C	-6.38	104.01	110.97
17	Q	59	LEU	N-CA-C	-6.38	100.73	110.30
6	F	416	SER	N-CA-C	6.37	117.89	111.07
8	H	271	LEU	N-CA-CB	6.36	119.30	110.07
7	G	273	ILE	N-CA-C	-6.35	98.37	107.77
12	L	234	PRO	CA-N-CD	-6.35	103.11	112.00
13	M	317	ILE	N-CA-C	-6.35	104.56	110.53
29	d	15	PRO	CA-N-CD	6.35	120.89	112.00
32	g	112	MET	N-CA-C	6.35	120.81	113.38
9	I	205	ILE	N-CA-C	-6.34	104.31	110.72
7	G	176	CYS	N-CA-C	6.34	119.68	110.42
12	L	439	PRO	N-CA-C	6.34	122.34	113.53
15	O	98	THR	N-CA-C	6.34	120.61	109.96
21	V	71	LEU	N-CA-C	6.34	118.19	111.28
12	L	387	THR	N-CA-C	6.34	119.00	111.71
6	F	144	VAL	N-CA-CB	6.33	118.67	110.57
12	L	70	THR	N-CA-C	-6.33	103.91	111.69
21	V	91	ALA	N-CA-C	-6.31	104.40	111.28
12	L	337	ALA	N-CA-C	-6.30	104.41	111.28
42	q	28	PHE	N-CA-C	6.29	117.80	111.07
13	M	26	ASN	N-CA-CB	6.29	119.19	110.07
34	i	32	GLU	CA-C-N	-6.29	111.98	119.84
34	i	32	GLU	C-N-CA	-6.29	111.98	119.84
6	F	415	ILE	N-CA-C	-6.27	104.39	110.72
23	X	99	HIS	N-CA-CB	6.27	119.44	110.16
12	L	490	ALA	N-CA-C	-6.27	104.36	111.07
15	O	113	SER	N-CA-C	6.27	118.63	108.41
46	Ab	306	THR	N-CA-C	-6.26	104.11	112.94
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
12	L	502	LEU	N-CA-C	-6.26	104.46	111.28
54	AK	39	ARG	N-CA-C	-6.26	104.70	112.90
46	Ab	308	LEU	N-CA-C	-6.25	104.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	337	LEU	CA-C-N	-6.25	113.70	119.82
14	N	337	LEU	C-N-CA	-6.25	113.70	119.82
37	l	105	ILE	CA-C-O	-6.24	115.16	121.59
4	D	233	HIS	N-CA-C	6.24	119.01	111.40
5	E	50	THR	N-CA-CB	6.24	121.47	110.37
7	G	356	ASP	N-CA-CB	6.24	119.29	110.12
35	j	78	ASP	N-CA-C	-6.24	102.82	110.61
26	a	26	ILE	N-CA-C	-6.23	104.59	113.07
14	N	91	ASN	N-CA-CB	6.23	119.13	109.97
28	c	47	SER	N-CA-CB	6.23	120.80	110.33
6	F	255	CYS	N-CA-C	-6.23	104.57	111.36
17	Q	141	ASN	N-CA-C	-6.22	105.69	113.28
1	A	101	GLY	N-CA-C	-6.22	105.28	112.50
52	AH	66	THR	N-CA-C	-6.22	104.42	111.14
4	D	141	TYR	N-CA-C	6.22	120.87	113.16
14	N	89	GLN	N-CA-C	6.22	120.43	112.34
5	E	64	ALA	N-CA-CB	6.22	119.20	109.94
6	F	192	ASP	N-CA-C	6.21	119.07	109.07
39	n	63	LEU	N-CA-C	-6.21	104.05	111.69
2	B	113	ASP	N-CA-CB	6.21	119.46	109.28
43	r	26	LEU	N-CA-CB	-6.21	101.10	110.35
8	H	52	ALA	N-CA-CB	6.21	119.01	110.01
14	N	276	LEU	N-CA-C	-6.20	105.36	113.17
6	F	101	PHE	N-CA-C	6.20	118.83	111.33
7	G	451	ILE	N-CA-C	-6.20	104.94	113.00
8	H	76	THR	N-CA-C	-6.20	104.53	111.28
42	q	69	ASN	N-CA-CB	6.19	121.32	111.66
6	F	409	ILE	N-CA-C	6.19	116.36	110.42
14	N	46	ASN	N-CA-C	-6.19	105.75	113.55
36	k	59	TYR	N-CA-C	6.19	120.67	113.18
25	Z	69	ILE	N-CA-CB	6.18	117.37	110.51
8	H	269	THR	N-CA-C	6.18	118.01	111.28
40	o	110	GLN	N-CA-C	-6.18	104.63	111.36
7	G	420	LYS	N-CA-C	6.17	118.80	111.33
14	N	216	PHE	N-CA-C	6.17	118.08	111.36
16	P	368	GLU	N-CA-CB	6.17	119.80	110.30
19	S	61	VAL	N-CA-C	-6.17	99.60	108.42
32	g	123	LEU	N-CA-CB	6.16	119.01	110.07
7	G	418	ILE	N-CA-C	-6.15	103.42	112.04
4	D	291	VAL	N-CA-C	-6.15	103.40	111.09
12	L	361	ASN	CB-CA-C	-6.14	102.83	111.80
13	M	4	ILE	N-CA-C	-6.14	103.96	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	n	30	TRP	N-CA-C	-6.14	104.14	111.69
25	Z	44	ILE	N-CA-C	-6.14	104.76	110.53
38	m	72	ARG	CA-C-O	6.14	125.89	119.14
16	P	118	LYS	N-CA-C	6.13	118.94	111.82
6	F	212	LEU	N-CA-C	-6.13	104.59	111.28
8	H	202	GLU	N-CA-C	-6.13	105.78	113.20
13	M	121	LEU	N-CA-C	-6.13	104.68	111.36
14	N	47	LYS	N-CA-C	-6.13	104.71	111.82
7	G	325	ARG	N-CA-CB	6.12	118.85	109.91
8	H	276	SER	N-CA-C	6.12	118.92	111.82
12	L	287	PHE	N-CA-CB	6.11	118.87	110.01
31	f	39	ASN	N-CA-C	-6.10	104.00	112.30
36	k	30	ILE	N-CA-C	6.10	118.71	111.09
41	p	127	LYS	N-CA-C	-6.10	104.19	111.69
33	h	101	ILE	N-CA-CB	6.08	115.74	110.08
19	S	87	VAL	N-CA-C	-6.08	104.42	110.62
13	M	57	SER	N-CA-C	6.08	119.11	109.50
38	m	52	ASN	N-CA-C	-6.08	105.17	112.59
49	AE	159	ILE	N-CA-C	6.07	114.10	107.60
7	G	508	ALA	N-CA-C	6.07	117.90	111.28
13	M	213	HIS	N-CA-C	6.07	120.54	113.20
14	N	91	ASN	N-CA-C	-6.07	101.30	110.28
8	H	24	GLU	N-CA-C	-6.05	104.03	112.45
12	L	98	TRP	N-CA-C	-6.05	104.76	111.36
13	M	168	GLN	N-CA-C	-6.05	104.76	111.36
32	g	109	ASP	CA-CB-CG	6.05	118.65	112.60
12	L	140	LEU	N-CA-C	-6.05	104.68	111.28
7	G	353	ALA	N-CA-C	-6.05	104.61	112.23
16	P	370	LYS	N-CA-C	6.05	119.29	108.47
32	g	123	LEU	N-CA-C	-6.05	104.61	111.14
8	H	103	LEU	N-CA-C	-6.04	104.77	111.36
8	H	185	TRP	N-CA-C	-6.04	104.05	112.45
7	G	638	THR	N-CA-C	-6.03	100.14	109.24
49	AE	82	ASP	N-CA-C	6.03	118.62	111.33
8	H	7	LEU	N-CA-C	-6.02	104.35	111.03
25	Z	65	LEU	N-CA-CB	6.02	119.07	110.16
38	m	22	GLU	N-CA-C	-6.02	104.63	111.07
53	Aj	53	TRP	N-CA-C	6.02	117.64	111.14
54	Ak	41	ILE	N-CA-C	-6.02	104.44	111.00
12	L	454	ILE	N-CA-C	-6.01	104.48	110.62
15	O	234	LEU	N-CA-C	-6.01	104.81	111.36
33	h	142	ILE	N-CA-C	-6.01	104.65	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	AG	31	PHE	N-CA-C	-6.01	105.99	113.38
7	G	532	PRO	N-CA-CB	-6.01	97.07	103.38
43	r	108	LYS	N-CA-C	6.01	117.91	111.36
13	M	370	PRO	CA-N-CD	6.01	120.41	112.00
15	O	160	GLU	CB-CA-C	-6.00	109.64	116.54
13	M	396	MET	N-CA-C	-6.00	105.94	113.20
28	c	47	SER	N-CA-C	-6.00	104.70	112.68
15	O	181	LYS	N-CA-C	5.99	117.48	111.07
13	M	253	LEU	N-CA-C	5.98	117.80	111.28
10	J	135	LEU	N-CA-C	-5.98	106.52	113.88
13	M	3	LYS	N-CA-C	-5.98	106.11	113.41
15	O	183	CYS	N-CA-CB	5.98	118.85	109.94
12	L	234	PRO	N-CA-CB	5.98	109.62	103.23
32	g	78	PRO	N-CA-C	5.98	121.84	113.53
2	B	196	PRO	N-CA-C	-5.97	101.84	111.03
13	M	300	SER	N-CA-C	-5.97	106.98	114.56
13	M	222	GLU	N-CA-C	5.97	120.40	113.18
46	Ab	317	SER	N-CA-C	5.97	117.19	107.23
51	Ag	31	PHE	N-CA-C	-5.95	105.97	113.18
10	J	155	ALA	N-CA-C	-5.95	104.88	111.36
12	L	88	LEU	N-CA-CB	5.95	118.69	110.07
46	AB	244	LEU	N-CA-C	-5.95	106.03	113.28
4	D	352	PRO	N-CA-CB	-5.95	97.31	103.08
41	p	8	ASP	N-CA-C	5.94	120.59	113.23
46	AB	298	HIS	N-CA-C	-5.94	105.12	112.90
12	L	112	PRO	CB-CA-C	-5.93	103.02	111.68
13	M	88	ASN	N-CA-C	5.93	120.14	113.02
6	F	291	GLU	N-CA-C	5.93	118.20	110.43
23	X	38	LYS	N-CA-C	-5.93	104.73	111.07
12	L	248	HIS	CB-CA-C	5.92	120.91	110.85
52	AH	62	GLU	N-CA-C	-5.91	105.38	112.59
7	G	387	LEU	CB-CA-C	-5.91	101.75	111.68
14	N	295	ARG	N-CA-C	-5.91	104.84	111.28
12	L	278	LEU	N-CA-CB	5.91	118.63	110.07
13	M	272	THR	N-CA-C	-5.91	104.92	111.36
12	L	247	LEU	N-CA-CB	5.90	120.60	110.34
5	E	66	VAL	N-CA-C	5.89	116.55	110.36
20	U	143	GLU	N-CA-C	-5.89	104.21	111.75
15	O	262	GLU	N-CA-C	-5.89	104.86	111.28
14	N	16	GLY	CA-C-N	-5.89	112.43	118.85
14	N	16	GLY	C-N-CA	-5.89	112.43	118.85
15	O	205	ILE	O-C-N	5.88	129.05	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	127	ASP	N-CA-C	5.88	118.48	111.71
12	L	387	THR	CB-CA-C	-5.88	99.75	110.63
8	H	315	PRO	O-C-N	5.88	123.91	121.15
39	n	27	LEU	N-CA-C	-5.87	106.08	113.72
15	O	130	ARG	N-CA-C	-5.87	104.88	111.28
20	T	94	ASP	N-CA-CB	-5.87	105.14	111.66
7	G	639	LEU	N-CA-C	5.87	118.62	111.82
36	k	82	ALA	N-CA-C	-5.87	104.89	111.28
16	P	122	HIS	N-CA-C	5.86	120.12	112.92
7	G	480	ALA	N-CA-C	-5.85	104.98	111.36
9	I	116	CYS	N-CA-C	-5.85	105.64	112.89
14	N	15	LEU	N-CA-C	-5.85	105.64	112.89
23	X	97	PHE	N-CA-C	5.85	118.60	111.82
40	o	11	TRP	CB-CA-C	-5.84	109.85	116.63
2	B	135	GLY	CA-C-O	-5.84	117.91	122.52
12	L	428	TYR	N-CA-C	-5.83	104.84	111.14
34	i	105	PHE	CA-C-N	-5.83	113.69	119.99
34	i	105	PHE	C-N-CA	-5.83	113.69	119.99
42	q	65	THR	N-CA-C	5.83	119.17	110.14
49	AE	191	GLU	CB-CA-C	-5.82	109.88	116.63
34	i	10	LEU	N-CA-C	-5.82	107.17	114.56
36	k	80	GLY	N-CA-C	-5.82	105.75	112.50
3	C	209	LEU	N-CA-CB	-5.82	100.71	110.83
4	D	258	VAL	N-CA-C	-5.82	103.99	110.62
7	G	672	ALA	N-CA-C	-5.81	104.94	111.28
21	V	19	THR	N-CA-CB	5.81	120.72	110.37
19	S	86	GLU	N-CA-CB	5.81	118.76	110.16
6	F	102	MET	CB-CA-C	-5.81	101.35	110.94
13	M	424	ILE	O-C-N	5.81	128.42	122.79
8	H	116	ILE	N-CA-C	-5.81	104.84	110.42
29	d	62	LEU	N-CA-C	5.81	117.61	111.28
16	P	367	GLU	CB-CA-C	-5.80	99.53	110.67
42	q	7	LEU	N-CA-C	-5.80	104.86	111.07
29	d	53	VAL	N-CA-C	5.80	116.45	110.36
14	N	66	ALA	N-CA-C	-5.79	105.05	111.36
14	N	321	LYS	N-CA-C	5.79	118.54	110.20
17	Q	164	PHE	N-CA-CB	5.79	119.81	110.42
18	R	34	THR	N-CA-C	-5.79	106.83	112.97
26	a	3	PHE	N-CA-CB	5.79	118.75	110.06
12	L	467	VAL	N-CA-CB	-5.79	103.78	110.55
37	l	186	ILE	N-CA-CB	-5.79	101.66	111.50
4	D	414	ASP	N-CA-C	-5.78	101.40	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	177	ILE	N-CA-C	-5.78	104.72	110.62
31	f	36	ALA	N-CA-C	-5.77	103.31	110.41
20	U	101	ASN	N-CA-C	-5.77	106.10	113.02
23	X	36	CYS	CB-CA-C	-5.77	102.57	111.74
11	K	6	PHE	N-CA-C	-5.76	106.38	113.41
36	k	20	MET	CA-C-N	-5.76	111.13	122.02
36	k	20	MET	C-N-CA	-5.76	111.13	122.02
38	m	116	ILE	N-CA-C	-5.76	104.89	110.42
7	G	275	PRO	N-CA-CB	-5.75	97.98	103.33
8	H	252	PRO	N-CA-CB	-5.75	97.99	103.51
39	n	52	LYS	N-CA-C	-5.75	105.93	113.12
13	M	124	ALA	N-CA-C	-5.75	105.10	111.36
32	g	78	PRO	N-CA-CB	-5.74	97.02	103.33
12	L	495	VAL	N-CA-C	5.74	115.93	110.42
20	U	137	LYS	CA-C-N	-5.74	113.56	122.05
20	U	137	LYS	C-N-CA	-5.74	113.56	122.05
38	m	104	VAL	N-CA-C	-5.73	105.50	111.58
35	j	73	PHE	N-CA-C	-5.73	104.94	111.07
16	P	234	LYS	CB-CA-C	-5.73	103.44	111.80
6	F	299	LEU	N-CA-C	5.73	118.46	111.82
49	Ae	183	GLU	N-CA-C	-5.73	104.94	111.07
10	J	27	TYR	N-CA-CB	5.72	119.37	110.44
12	L	419	THR	N-CA-C	-5.72	105.04	111.28
19	S	73	GLN	N-CA-C	-5.72	100.38	109.59
8	H	126	LYS	N-CA-C	5.72	117.52	111.28
13	M	279	GLN	N-CA-C	-5.72	98.57	108.69
16	P	272	LEU	N-CA-C	-5.72	101.81	110.28
7	G	289	LYS	N-CA-C	5.72	117.51	111.28
18	R	35	GLY	N-CA-C	5.71	121.81	113.48
32	g	67	LYS	N-CA-C	-5.70	102.02	110.46
6	F	393	ASN	N-CA-C	-5.69	104.98	111.07
12	L	342	CYS	N-CA-CB	5.69	118.26	110.01
1	A	105	GLU	N-CA-C	-5.69	105.08	111.28
30	e	34	HIS	N-CA-C	-5.68	106.19	113.01
5	E	119	THR	N-CA-C	-5.68	105.85	112.89
4	D	352	PRO	N-CA-C	5.68	117.63	110.70
40	o	71	ARG	N-CA-C	-5.67	104.48	111.40
15	O	220	LYS	N-CA-C	5.67	117.46	111.28
16	P	119	ALA	N-CA-C	-5.67	105.02	111.14
13	M	19	SER	N-CA-C	5.67	117.72	109.84
46	Ab	304	ASN	N-CA-C	5.67	116.87	108.60
6	F	457	HIS	N-CA-CB	-5.66	100.87	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	176	ALA	N-CA-C	5.66	118.18	111.33
7	G	59	GLN	N-CA-C	5.66	118.01	107.99
17	Q	124	MET	CA-C-N	-5.66	114.94	122.98
17	Q	124	MET	C-N-CA	-5.66	114.94	122.98
12	L	214	MET	N-CA-C	-5.65	105.20	111.36
12	L	20	LEU	N-CA-C	5.65	119.89	112.89
12	L	605	ASN	N-CA-C	-5.65	106.24	113.02
18	R	52	GLN	N-CA-C	5.64	117.98	110.53
47	AC	17	SER	N-CA-CB	-5.64	102.12	110.53
7	G	599	THR	CA-C-N	-5.64	114.14	122.83
7	G	599	THR	C-N-CA	-5.64	114.14	122.83
14	N	232	LEU	N-CA-C	-5.64	106.61	112.93
10	J	130	ASP	N-CA-C	5.64	117.43	111.28
13	M	214	LEU	N-CA-C	-5.64	105.66	112.54
31	f	7	LEU	CB-CA-C	-5.64	102.26	111.50
34	i	14	GLN	N-CA-CB	-5.63	101.84	110.12
37	l	49	ALA	N-CA-C	-5.63	106.57	113.50
42	q	140	PRO	N-CA-C	-5.63	102.29	110.80
12	L	371	SER	N-CA-C	-5.63	105.06	111.14
29	d	5	ARG	CA-C-N	-5.63	114.16	119.90
29	d	5	ARG	C-N-CA	-5.63	114.16	119.90
31	f	10	HIS	CB-CA-C	-5.62	100.67	110.17
38	m	31	ARG	N-CA-C	-5.62	106.55	113.41
10	J	132	GLY	N-CA-C	5.61	121.24	111.14
25	Z	64	ASP	N-CA-C	5.61	119.85	112.89
6	F	304	ALA	CB-CA-C	-5.60	110.10	116.54
12	L	151	SER	N-CA-CB	5.60	118.45	110.16
2	B	112	TYR	N-CA-C	5.60	122.73	110.80
34	i	84	TYR	N-CA-C	-5.59	105.18	111.28
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
12	L	445	GLU	CB-CA-C	-5.59	101.96	111.02
23	X	40	ASN	N-CA-C	-5.58	104.88	110.97
5	E	222	PHE	CB-CA-C	-5.58	100.64	109.80
32	g	140	PHE	N-CA-CB	5.58	118.31	109.71
5	E	183	PRO	N-CA-C	-5.58	102.17	111.26
12	L	234	PRO	N-CA-C	-5.58	105.49	113.47
49	Ae	119	ALA	N-CA-C	-5.57	105.11	111.07
12	L	155	ILE	N-CA-C	-5.57	105.30	110.53
41	p	115	GLN	N-CA-CB	5.57	118.00	110.59
42	q	142	THR	N-CA-CB	5.57	119.86	109.68
14	N	251	LEU	N-CA-C	-5.56	105.22	111.28
32	g	107	VAL	N-CA-C	-5.56	102.90	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	64	GLU	N-CA-CB	5.55	118.06	110.01
2	B	201	LEU	N-CA-C	-5.55	105.13	111.07
7	G	530	TYR	N-CA-C	-5.55	102.06	110.28
24	Y	13	GLU	N-CA-C	5.55	117.77	111.11
19	S	63	PRO	CA-N-CD	5.55	119.77	112.00
32	g	113	GLN	CA-C-O	5.55	126.21	119.11
14	N	36	SER	N-CA-C	-5.54	105.24	111.28
38	m	60	ILE	N-CA-C	-5.54	102.04	109.30
38	m	46	GLU	N-CA-C	-5.54	106.52	113.72
6	F	118	ASP	N-CA-C	-5.54	102.08	110.28
42	q	68	MET	N-CA-C	5.54	119.30	112.54
43	r	94	ALA	N-CA-C	-5.54	101.66	109.96
11	K	3	SER	N-CA-C	-5.53	106.43	114.12
49	Ae	243	TYR	N-CA-CB	5.53	118.17	110.26
6	F	294	VAL	CA-C-N	-5.53	114.07	119.76
6	F	294	VAL	C-N-CA	-5.53	114.07	119.76
32	g	122	ARG	N-CA-C	5.52	118.23	111.82
18	R	89	PRO	N-CA-CB	-5.52	98.30	103.27
12	L	370	SER	N-CA-C	-5.51	105.35	111.36
4	D	163	PRO	N-CA-CB	-5.51	97.73	103.08
4	D	200	PHE	CA-CB-CG	5.51	119.31	113.80
41	p	120	ASN	N-CA-C	-5.51	105.19	113.89
12	L	465	GLY	N-CA-C	-5.50	105.72	112.77
39	n	136	GLU	CB-CA-C	5.50	121.37	110.42
7	G	615	LEU	N-CA-C	-5.50	106.34	113.16
31	f	29	LYS	N-CA-C	-5.50	106.16	112.92
42	q	71	LYS	N-CA-C	5.50	119.98	113.16
7	G	127	ASP	CA-C-O	5.50	128.98	121.89
8	H	141	SER	N-CA-CB	5.50	117.98	110.01
13	M	73	LEU	N-CA-C	-5.50	105.28	112.75
35	j	64	LEU	N-CA-C	-5.50	105.45	111.82
4	D	132	ALA	N-CA-C	-5.49	106.58	113.72
26	a	25	TYR	N-CA-C	-5.49	107.83	114.75
12	L	194	ASN	CB-CA-C	-5.49	103.32	111.72
12	L	394	LEU	N-CA-CB	5.49	117.96	110.01
49	AI	60	ALA	N-CA-C	5.49	116.61	108.60
45	Aa	255	ARG	N-CA-C	5.48	118.21	107.57
7	G	363	SER	N-CA-C	-5.47	100.26	109.07
7	G	313	LEU	N-CA-C	5.47	118.47	109.72
13	M	223	ALA	N-CA-CB	5.47	118.10	110.11
13	M	355	MET	N-CA-C	-5.47	104.71	111.33
35	j	80	VAL	CB-CA-C	-5.47	106.25	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	152	PHE	N-CA-C	-5.47	105.22	111.07
31	f	11	TRP	CA-C-O	5.46	125.68	119.18
13	M	370	PRO	N-CA-CB	-5.46	97.78	103.08
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
2	B	98	ALA	CB-CA-C	-5.46	108.69	115.89
16	P	86	CYS	N-CA-C	-5.45	103.19	110.55
20	T	135	ALA	N-CA-CB	5.45	118.13	110.12
43	r	111	PRO	N-CA-C	-5.45	106.44	113.57
4	D	231	GLY	N-CA-C	-5.44	103.09	110.43
14	N	62	THR	N-CA-C	-5.43	105.26	111.07
15	O	154	GLY	N-CA-C	-5.43	107.53	114.37
45	Aa	274	GLU	N-CA-C	5.43	118.30	109.06
7	G	150	ARG	N-CA-CB	-5.43	102.83	111.62
14	N	108	LEU	N-CA-C	5.43	118.09	109.24
34	i	77	ILE	CB-CA-C	-5.43	108.60	114.35
7	G	404	GLY	N-CA-C	5.42	121.39	113.48
7	G	420	LYS	N-CA-CB	-5.42	101.94	110.06
14	N	89	GLN	N-CA-CB	-5.42	100.43	110.18
32	g	137	SER	N-CA-CB	-5.41	101.32	110.41
7	G	682	ASP	CA-C-N	-5.41	114.19	119.76
7	G	682	ASP	C-N-CA	-5.41	114.19	119.76
16	P	374	THR	N-CA-C	5.41	117.55	108.73
23	X	27	ALA	N-CA-C	-5.41	105.03	111.69
46	AB	236	GLN	N-CA-C	-5.41	105.94	112.54
12	L	543	ASN	N-CA-C	-5.40	105.40	111.28
25	Z	50	MET	N-CA-C	-5.39	105.41	111.28
25	Z	55	GLN	N-CA-C	-5.38	105.41	111.28
41	p	94	ARG	N-CA-C	5.38	116.83	111.07
13	M	174	LEU	N-CA-C	-5.38	106.49	112.57
4	D	141	TYR	N-CA-CB	-5.38	102.21	110.44
12	L	386	LEU	N-CA-C	-5.37	100.96	108.96
13	M	117	MET	N-CA-CB	5.37	118.01	110.12
13	M	409	TYR	N-CA-C	-5.37	105.59	111.82
20	T	92	LYS	N-CA-C	-5.37	106.32	112.92
36	k	48	ARG	N-CA-C	-5.37	98.82	108.48
13	M	343	ILE	N-CA-C	5.37	116.09	110.62
5	E	219	SER	N-CA-C	-5.36	100.58	108.79
13	M	234	ILE	N-CA-C	5.36	116.25	111.90
20	U	141	PRO	N-CA-C	-5.36	109.11	114.68
17	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
18	R	88	HIS	CB-CA-C	5.35	117.27	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	48	PRO	N-CA-C	5.35	120.79	113.84
4	D	201	PHE	N-CA-C	-5.35	105.53	111.36
7	G	510	TRP	N-CA-C	-5.35	101.94	109.96
12	L	21	ILE	N-CA-C	-5.35	105.32	110.72
12	L	311	GLY	N-CA-C	-5.34	106.33	112.73
12	L	413	LEU	N-CA-C	5.34	117.10	111.28
13	M	53	SER	N-CA-C	5.34	115.58	108.38
13	M	169	ASN	N-CA-C	-5.33	105.55	111.36
8	H	252	PRO	CA-N-CD	5.33	119.47	112.00
12	L	550	LEU	CA-C-O	-5.33	115.29	120.89
8	H	284	GLN	N-CA-C	-5.33	105.55	111.36
33	h	173	THR	O-C-N	5.33	125.71	121.55
17	Q	164	PHE	N-CA-C	-5.32	106.76	113.20
13	M	294	MET	N-CA-C	-5.32	106.80	113.72
6	F	412	LEU	N-CA-C	-5.32	105.65	111.82
14	N	218	ALA	N-CA-CB	5.31	118.43	110.14
42	q	131	ARG	N-CA-C	5.31	117.68	110.35
5	E	74	GLN	N-CA-C	-5.31	107.46	114.04
32	g	80	VAL	N-CA-C	-5.31	105.32	110.42
39	n	104	LEU	N-CA-C	-5.30	106.84	113.15
8	H	94	PRO	N-CA-C	5.30	118.64	111.22
15	O	264	GLU	N-CA-C	-5.30	107.18	113.38
12	L	415	ALA	N-CA-CB	5.30	117.91	110.12
12	L	183	ILE	N-CA-C	-5.30	105.22	110.62
13	M	25	THR	CB-CA-C	-5.30	100.50	110.67
5	E	221	ARG	N-CA-C	5.29	117.91	110.23
7	G	362	ASP	CA-CB-CG	5.29	117.89	112.60
6	F	199	ARG	N-CA-C	5.29	117.36	109.59
9	I	54	THR	N-CA-C	-5.29	104.93	111.33
16	P	339	GLY	N-CA-C	5.29	122.62	115.00
12	L	231	PRO	CB-CA-C	-5.29	104.34	111.85
39	n	36	LYS	N-CA-C	-5.29	105.52	111.28
4	D	391	VAL	CA-C-N	-5.28	115.86	119.66
4	D	391	VAL	C-N-CA	-5.28	115.86	119.66
7	G	356	ASP	N-CA-C	-5.27	105.53	111.28
12	L	494	SER	N-CA-C	-5.27	105.44	111.14
10	J	65	VAL	N-CA-CB	5.27	116.15	110.62
7	G	449	PRO	N-CA-CB	5.26	109.07	103.39
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
8	H	46	LEU	N-CA-C	-5.26	106.64	113.16
42	q	6	VAL	CB-CA-C	-5.26	105.05	112.14
8	H	199	ASP	CB-CA-C	-5.25	102.63	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	212	VAL	CB-CA-C	-5.25	105.17	112.36
7	G	277	MET	N-CA-CB	-5.25	101.63	109.71
12	L	190	SER	N-CA-C	-5.24	106.73	113.23
23	X	33	GLY	N-CA-C	-5.24	107.81	114.16
32	g	68	ASN	N-CA-CB	5.24	119.01	111.51
33	h	129	PRO	N-CA-C	-5.24	106.70	113.57
13	M	167	ILE	N-CA-C	5.24	117.60	111.05
35	j	76	ASP	CB-CA-C	-5.24	104.60	112.09
17	Q	72	ILE	N-CA-C	-5.24	108.40	113.53
13	M	98	MET	N-CA-C	-5.23	105.47	111.07
35	j	51	THR	O-C-N	-5.23	117.05	122.96
39	n	26	HIS	N-CA-C	-5.23	106.48	112.92
5	E	48	PRO	CB-CA-C	-5.23	104.42	111.85
8	H	146	MET	N-CA-C	-5.23	105.47	111.07
8	H	310	PHE	N-CA-C	5.23	119.29	113.01
12	L	137	MET	N-CA-C	5.23	119.29	113.01
4	D	391	VAL	N-CA-C	5.23	113.88	109.02
6	F	300	ILE	N-CA-CB	5.23	119.29	110.56
42	q	21	ARG	N-CA-C	5.23	117.65	111.33
45	Aa	401	SER	N-CA-C	-5.23	108.16	114.75
39	n	12	HIS	N-CA-C	-5.22	105.03	111.40
19	S	85	ASP	N-CA-C	5.22	117.88	111.82
43	r	111	PRO	CA-N-CD	5.22	119.31	112.00
13	M	317	ILE	N-CA-CB	5.22	117.25	110.57
20	U	133	ILE	CB-CA-C	-5.22	104.08	112.16
43	r	25	GLN	N-CA-C	5.22	118.90	112.54
43	r	107	SER	N-CA-C	-5.21	102.14	109.96
21	V	84	ALA	N-CA-C	5.21	116.65	111.07
7	G	63	PHE	CA-C-O	-5.21	115.02	121.06
7	G	600	GLU	CB-CA-C	-5.21	102.99	111.06
7	G	435	PRO	CB-CA-C	-5.21	105.89	111.56
13	M	20	PRO	N-CA-C	-5.21	106.29	113.53
4	D	363	VAL	N-CA-C	5.20	116.28	111.81
7	G	556	THR	N-CA-C	-5.20	101.50	109.41
20	U	133	ILE	N-CA-C	5.20	117.56	111.05
38	m	17	THR	N-CA-C	-5.20	103.66	110.53
16	P	260	GLY	N-CA-C	-5.20	108.44	115.36
47	AC	16	HIS	N-CA-C	5.20	117.69	111.71
12	L	485	PHE	N-CA-CB	5.19	117.54	110.01
16	P	194	VAL	N-CA-CB	5.19	118.37	110.58
12	L	386	LEU	CA-C-O	-5.19	115.89	121.45
3	C	164	TRP	N-CA-C	5.19	117.01	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	375	ILE	N-CA-CB	5.18	116.62	110.55
8	H	101	GLY	N-CA-C	5.18	118.51	112.50
16	P	316	LYS	N-CA-C	-5.18	104.89	111.11
14	N	335	MET	CB-CA-C	-5.18	104.44	111.95
41	p	167	ARG	CB-CA-C	5.17	117.20	109.13
15	O	206	TYR	CA-C-N	-5.17	115.01	122.45
15	O	206	TYR	C-N-CA	-5.17	115.01	122.45
7	G	458	GLY	N-CA-C	-5.17	108.19	115.32
7	G	713	ALA	N-CA-C	-5.17	105.54	111.07
14	N	222	ASN	N-CA-C	-5.17	106.22	112.88
12	L	332	HIS	N-CA-C	-5.17	105.65	111.28
41	p	43	TRP	CA-C-N	-5.16	113.60	118.97
41	p	43	TRP	C-N-CA	-5.16	113.60	118.97
7	G	172	ILE	N-CA-C	-5.16	98.61	109.34
49	Ae	159	ILE	N-CA-C	5.15	112.25	107.56
16	P	198	ALA	N-CA-C	-5.15	100.12	108.52
7	G	569	GLN	CB-CA-C	-5.15	104.23	112.05
12	L	284	THR	N-CA-C	-5.14	105.75	111.36
31	f	11	TRP	N-CA-C	-5.14	107.00	113.28
14	N	90	THR	N-CA-C	5.14	117.55	110.35
1	A	2	ASN	CA-C-N	-5.14	113.00	120.29
1	A	2	ASN	C-N-CA	-5.14	113.00	120.29
8	H	196	ALA	CA-C-N	-5.14	113.46	119.32
8	H	196	ALA	C-N-CA	-5.14	113.46	119.32
27	b	82	LYS	N-CA-C	-5.14	103.75	110.53
12	L	249	SER	N-CA-C	5.13	116.68	111.14
29	d	37	LEU	N-CA-C	-5.13	105.69	111.28
41	p	13	PRO	O-C-N	5.13	123.56	121.15
45	Aa	384	THR	N-CA-C	5.13	117.43	110.35
12	L	217	LEU	N-CA-C	-5.13	105.69	111.28
24	Y	72	PHE	N-CA-C	-5.13	105.58	111.07
48	Ad	88	GLU	N-CA-C	5.13	117.78	109.06
3	C	156	VAL	N-CA-C	-5.12	104.10	111.17
6	F	337	MET	CB-CA-C	-5.12	103.07	111.68
14	N	225	MET	N-CA-C	-5.12	106.62	112.92
37	l	168	LEU	N-CA-C	-5.12	105.61	111.14
7	G	387	LEU	N-CA-C	-5.12	98.35	107.98
33	h	158	ARG	N-CA-C	-5.12	105.61	111.14
8	H	277	TYR	N-CA-C	5.11	117.92	110.10
12	L	396	ILE	O-C-N	5.11	126.92	121.91
13	M	330	ALA	N-CA-CB	5.11	117.48	110.07
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	497	GLY	N-CA-C	-5.11	106.57	112.50
28	c	60	GLN	N-CA-C	-5.10	105.61	111.07
38	m	26	SER	N-CA-C	-5.10	102.75	109.84
38	m	61	GLU	N-CA-C	5.10	119.58	112.90
14	N	292	PHE	CA-CB-CG	5.10	118.90	113.80
9	I	95	PRO	N-CA-C	5.10	121.20	113.81
23	X	140	ASN	CA-C-N	-5.10	114.53	119.78
23	X	140	ASN	C-N-CA	-5.10	114.53	119.78
13	M	86	LYS	N-CA-C	-5.09	106.31	112.88
4	D	71	ILE	N-CA-C	5.09	118.26	111.44
14	N	42	PRO	CB-CA-C	-5.09	104.97	113.06
36	k	44	ALA	N-CA-C	-5.09	105.73	111.28
42	q	5	GLU	N-CA-C	5.09	116.51	111.07
5	E	181	ASN	N-CA-C	-5.08	99.51	108.20
3	C	109	SER	N-CA-C	5.08	118.09	109.76
28	c	39	PRO	N-CA-C	5.08	119.18	111.15
13	M	234	ILE	CB-CA-C	5.08	116.17	111.30
2	B	98	ALA	N-CA-C	5.07	117.54	109.02
11	K	48	SER	N-CA-CB	5.07	117.57	110.12
14	N	282	MET	N-CA-C	-5.07	105.64	111.07
7	G	280	ASP	N-CA-CB	-5.07	102.67	110.12
7	G	393	GLY	N-CA-C	-5.07	107.75	115.66
8	H	254	LEU	N-CA-CB	5.07	118.14	110.28
16	P	376	ASN	CB-CA-C	-5.07	102.24	110.85
34	i	16	ARG	N-CA-C	-5.07	105.76	111.28
44	s	38	HIS	N-CA-C	5.07	118.56	112.38
3	C	221	GLU	N-CA-C	-5.06	102.38	108.25
13	M	267	TRP	N-CA-C	-5.06	105.84	111.36
13	M	56	PHE	N-CA-C	5.06	116.77	108.52
32	g	137	SER	N-CA-C	5.06	119.30	113.18
23	X	112	LEU	N-CA-CB	5.05	117.40	110.07
16	P	170	LEU	N-CA-C	5.05	117.05	110.43
13	M	229	MET	N-CA-C	-5.04	105.67	111.07
18	R	43	TYR	N-CA-CB	-5.04	103.19	110.70
20	U	132	ASP	N-CA-C	5.04	117.17	111.02
22	W	112	GLU	N-CA-C	5.04	116.86	111.36
46	Ab	233	VAL	N-CA-C	-5.04	107.84	112.83
20	U	81	ASP	N-CA-C	-5.04	106.30	112.90
37	l	45	PRO	N-CA-C	5.04	120.45	113.65
13	M	32	PHE	N-CA-CB	5.03	117.31	110.01
39	n	169	HIS	CB-CA-C	5.03	118.67	110.17
5	E	222	PHE	N-CA-C	5.03	117.80	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	T	140	CYS	CB-CA-C	-5.03	104.12	109.85
34	i	29	SER	CA-C-N	-5.03	114.61	119.78
34	i	29	SER	C-N-CA	-5.03	114.61	119.78
4	D	224	ALA	N-CA-C	5.02	117.14	111.11
12	L	212	PRO	CA-N-CD	5.02	119.03	112.00
14	N	64	ALA	N-CA-C	5.02	116.44	111.07
13	M	30	TYR	N-CA-C	5.02	116.75	111.28
13	M	207	MET	N-CA-CB	5.02	119.31	110.37
52	AH	68	GLU	N-CA-C	-5.02	107.29	113.41
7	G	203	ASP	CA-C-O	5.01	127.14	121.32
14	N	217	MET	N-CA-C	-5.01	107.00	113.01
25	Z	130	LYS	N-CA-C	-5.01	105.71	111.07
9	I	160	GLU	CB-CA-C	5.01	119.15	110.84
28	c	73	ASN	N-CA-C	-5.01	103.44	110.35
32	g	109	ASP	CB-CA-C	5.00	119.00	111.89
12	L	384	PRO	N-CA-CB	5.00	107.70	103.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	823	117	0
2	B	1247	0	1258	156	0
3	C	1641	0	1596	135	0
4	D	3423	0	3364	356	0
5	E	1635	0	1626	166	0
6	F	3288	0	3243	356	0
7	G	5287	0	5323	554	0
8	H	2525	0	2613	380	0
9	I	1398	0	1359	166	0
10	J	1193	0	1215	203	0
11	K	729	0	764	111	0
12	L	4798	0	4986	622	0
13	M	3630	0	3854	550	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	2694	0	2896	348	0
15	O	2599	0	2552	264	0
16	P	2730	0	2747	226	0
17	Q	957	0	949	70	0
18	R	660	0	639	73	0
19	S	667	0	683	71	0
20	T	604	0	596	93	0
20	U	700	0	691	74	0
21	V	915	0	954	80	0
22	W	970	0	991	80	0
23	X	1385	0	1370	137	0
24	Y	1030	0	1015	96	0
25	Z	1152	0	1148	142	0
26	a	548	0	562	56	0
27	b	620	0	617	90	0
28	c	389	0	385	38	0
29	d	996	0	1001	91	0
30	e	859	0	849	105	0
31	f	447	0	444	31	0
32	g	842	0	779	69	0
33	h	1162	0	1163	126	0
34	i	773	0	780	71	0
35	j	587	0	533	71	0
36	k	578	0	581	55	0
37	l	1312	0	1204	100	0
38	m	1044	0	1056	112	0
39	n	1534	0	1463	159	0
40	o	1019	0	1006	108	0
41	p	1438	0	1404	122	0
42	q	1004	0	962	90	0
43	r	413	0	429	45	0
44	s	226	0	214	14	0
45	AA	3117	0	3032	188	0
45	Aa	3131	0	3055	165	0
46	AB	3107	0	3116	148	0
46	Ab	3101	0	3098	134	0
47	AC	2988	0	3045	144	0
47	Ac	2988	0	3045	187	0
48	AD	1896	0	1846	188	0
48	Ad	1895	0	1844	173	0
49	AE	1427	0	1407	230	0
49	AI	347	0	363	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Ae	1451	0	1433	250	0
50	AF	864	0	854	27	0
50	Af	864	0	854	56	0
51	AG	643	0	643	64	0
51	Ag	643	0	643	61	0
52	AH	527	0	507	73	0
52	Ah	544	0	529	56	0
53	AJ	307	0	295	34	0
53	Aj	392	0	388	30	0
54	AK	278	0	278	37	0
54	Ak	357	0	347	25	0
55	B	8	0	0	5	0
55	F	8	0	0	10	0
55	G	16	0	0	5	0
55	I	16	0	0	16	0
56	B	18	0	18	12	0
57	B	35	0	44	3	0
57	I	47	0	71	7	0
57	L	50	0	74	17	0
58	AC	25	0	24	4	0
58	Ac	35	0	44	4	0
58	D	38	0	50	13	0
58	I	46	0	69	10	0
58	J	46	0	69	18	0
58	K	46	0	66	6	0
58	L	135	0	198	35	0
58	M	139	0	212	40	0
58	O	44	0	65	7	0
58	b	46	0	69	11	0
58	i	40	0	54	11	0
58	j	40	0	54	9	0
58	m	92	0	138	16	0
59	E	4	0	0	4	0
59	G	4	0	0	4	0
60	F	31	0	19	3	0
61	H	35	0	43	16	0
62	Aa	46	0	36	3	0
62	Ac	42	0	28	5	0
62	Ag	56	0	56	6	0
62	L	158	0	204	31	0
62	a	57	0	58	15	0
62	d	67	0	81	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	h	70	0	87	13	0
63	O	27	0	12	6	0
64	P	48	0	26	4	0
65	R	1	0	0	0	0
66	W	32	0	0	7	0
66	n	32	0	0	0	0
67	AC	86	0	60	8	0
67	Ac	86	0	60	6	0
68	AC	23	0	23	9	0
68	Ac	23	0	23	12	0
69	AC	28	0	31	7	0
69	Ac	28	0	31	8	0
70	AD	43	0	32	5	0
70	Ad	43	0	32	18	0
All	All	97317	0	97570	7945	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (7945) 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)
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.17	1.28
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
62:L:705:CDL:H111	24:Y:115:MET:SD	1.75	1.27
58:M:503:3PE:HN3	15:O:338:LYS:CE	1.50	1.23
12:L:141:PHE:CE2	13:M:375:LEU:HD21	1.75	1.22
16:P:93:HIS:CD2	16:P:94:LEU:HD12	1.75	1.22
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.20
8:H:251:LEU:HD12	8:H:251:LEU:O	1.41	1.20
20:U:90:TYR:CE2	20:U:92:LYS:HB2	1.76	1.20
12:L:437:PHE:CE1	12:L:441:ILE:HG12	1.77	1.19
49:AE:88:PHE:CB	51:AG:19:LEU:HD11	1.71	1.19
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.40	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
12:L:280:LEU:HD23	57:L:706:PC1:C3H	1.73	1.17
13:M:369:LEU:HD23	13:M:371:PRO:HD2	1.18	1.16
10:J:22:LYS:HD2	11:K:23:ARG:HG2	1.28	1.16
12:L:141:PHE:CE2	13:M:375:LEU:CD2	2.29	1.15
12:L:280:LEU:CD2	57:L:706:PC1:C3H	2.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:SER:CB	11:K:7:ASN:HD22	1.59	1.15
12:L:358:LYS:HG3	39:n:80:TYR:CZ	1.82	1.14
12:L:141:PHE:HE2	13:M:375:LEU:CD2	1.60	1.14
12:L:247:LEU:CD1	12:L:248:HIS:CD2	2.31	1.14
10:J:22:LYS:HD2	11:K:23:ARG:CG	1.77	1.13
58:M:503:3PE:N	15:O:338:LYS:CE	2.10	1.13
6:F:382:CYS:SG	55:F:502:SF4:FE3	1.38	1.12
12:L:261:VAL:O	12:L:264:HIS:CD2	2.01	1.12
46:AB:167:GLN:HE21	49:AI:35:PRO:HD3	1.08	1.12
56:B:302:UQ1:HM33	4:D:185:MET:CE	1.78	1.12
14:N:215:MET:CE	14:N:248:LEU:HD21	1.79	1.12
12:L:437:PHE:HE1	12:L:441:ILE:HG12	0.96	1.12
9:I:123:CYS:SG	55:I:303:SF4:FE1	1.40	1.12
47:Ac:98:VAL:HG22	67:Ac:402:HEM:HBC2	1.25	1.12
49:Ae:239:HIS:CD2	49:Ae:253:PRO:HD2	1.83	1.12
40:o:8:ARG:HB2	40:o:16:GLU:HG2	1.32	1.11
53:Aj:31:PHE:O	53:Aj:34:ARG:HG2	1.47	1.11
29:d:14:LEU:O	29:d:14:LEU:HD12	1.49	1.11
45:AA:43:GLN:NE2	46:AB:57:PRO:HG3	1.66	1.11
12:L:365:ILE:HD12	12:L:366:MET:HG3	1.32	1.11
58:M:503:3PE:HN3	15:O:338:LYS:NZ	1.48	1.11
20:U:90:TYR:OH	20:U:92:LYS:HD2	1.48	1.11
12:L:229:LEU:HD12	12:L:229:LEU:O	1.51	1.10
15:O:80:GLN:HG3	15:O:270:VAL:HG21	1.25	1.10
4:D:47:PHE:HB3	14:N:227:ILE:HD11	1.23	1.10
6:F:379:CYS:SG	55:F:502:SF4:FE4	1.43	1.09
13:M:162:ILE:HG23	14:N:271:MET:HE3	1.33	1.09
12:L:550:LEU:HD12	13:M:275:ILE:HB	1.34	1.09
12:L:121:LEU:HD22	12:L:246:LEU:HD21	1.33	1.09
12:L:141:PHE:HE2	13:M:375:LEU:HD22	1.17	1.09
49:Ae:242:HIS:H	49:Ae:251:LYS:HB3	1.07	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.08
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.08
49:Ae:232:GLY:HA3	49:Ae:244:ASP:HA	1.13	1.08
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.08
10:J:126:TYR:HA	25:Z:120:LEU:HD11	1.36	1.08
12:L:569:LEU:HB2	24:Y:115:MET:HE1	1.36	1.08
23:X:4:ILE:HG22	23:X:5:VAL:H	0.96	1.08
36:k:34:PRO:HG2	36:k:59:TYR:CE1	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:91:GLN:HE21	39:n:2:ALA:HB1	1.13	1.07
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.07
12:L:553:LEU:HD11	38:m:93:ALA:HB3	1.37	1.07
4:D:52:MET:HE3	58:D:501:3PE:N	1.68	1.07
24:Y:21:HIS:CE1	51:Ag:62:TRP:HB2	1.89	1.07
46:AB:48:VAL:CG2	46:AB:219:ALA:HB2	1.85	1.06
8:H:136:VAL:CG1	10:J:69:TYR:HE1	1.67	1.06
51:Ag:11:ILE:HG21	51:Ag:14:VAL:HG21	1.36	1.06
3:C:98:PHE:HA	21:V:90:LEU:HD11	1.31	1.06
9:I:152:CYS:SG	55:I:303:SF4:FE2	1.46	1.06
12:L:16:LEU:HD23	12:L:126:ILE:HD13	1.30	1.06
19:S:23:LEU:HD12	19:S:23:LEU:O	1.54	1.06
20:T:138:LEU:HD12	20:T:138:LEU:O	1.55	1.06
19:S:79:LEU:HA	19:S:82:LEU:HD12	1.38	1.05
49:Ae:224:PRO:HG2	49:Ae:258:LEU:HD21	1.33	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.36	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
12:L:141:PHE:HB2	12:L:182:PHE:CE2	1.92	1.05
56:B:302:UQ1:HM33	4:D:185:MET:HE3	1.34	1.05
7:G:445:LEU:HD22	7:G:460:HIS:CE1	1.87	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
48:Ad:215:LEU:HD11	70:Ad:401:HEC:CMB	1.85	1.05
2:B:82:ILE:HG23	8:H:57:MET:SD	1.97	1.04
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.04
35:j:97:LEU:HB3	40:o:104:ARG:HB2	1.36	1.04
14:N:233:LEU:HD23	14:N:241:LEU:HD12	1.36	1.04
4:D:279:THR:HG23	21:V:13:GLY:HA3	1.33	1.04
5:E:179:CYS:SG	59:E:301:FES:FE2	1.48	1.04
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.40	1.04
52:AH:48:LEU:HD21	52:AH:69:LEU:HD13	1.32	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.04
12:L:141:PHE:CE2	13:M:370:PRO:HG3	1.91	1.03
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.03
13:M:249:ILE:O	13:M:250:LEU:HG	1.58	1.03
51:AG:11:ILE:HG21	51:AG:14:VAL:HG21	1.36	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
12:L:131:LEU:HD12	12:L:140:LEU:HD12	1.36	1.03
48:Ad:155:GLN:HB3	48:Ad:166:MET:HG2	1.41	1.03
49:Ae:263:TYR:HA	49:Ae:273:VAL:HA	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.22	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
40:o:69:CYS:O	40:o:80:CYS:SG	2.17	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.02
13:M:179:LEU:HB3	13:M:249:ILE:HD11	1.42	1.02
22:W:32:LYS:HG2	66:W:201:EHZ:C19	1.90	1.02
49:AI:64:LEU:HD23	49:AI:78:PHE:HA	1.42	1.02
49:Ae:265:PHE:HA	49:Ae:271:VAL:HG23	1.40	1.01
52:AH:48:LEU:HD21	52:AH:69:LEU:CD1	1.89	1.01
48:Ad:215:LEU:HD11	70:Ad:401:HEC:HMB3	1.03	1.01
12:L:228:GLY:O	12:L:229:LEU:HG	1.61	1.01
46:AB:48:VAL:CG2	46:AB:219:ALA:CB	2.39	1.01
30:e:20:PHE:CZ	33:h:178:PHE:HB2	1.95	1.01
49:AE:221:GLY:HA3	47:Ac:148:ASN:HD22	1.25	1.01
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.96	1.01
39:n:97:TYR:HB2	39:n:178:PRO:HG2	1.39	1.01
47:Ac:21:LEU:HD22	69:Ac:405:UQ6:H3M1	1.38	1.01
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
12:L:222:GLY:HA2	12:L:229:LEU:HD11	1.40	1.00
13:M:172:GLY:O	13:M:173:THR:HG23	1.61	1.00
47:Ac:128:PHE:CZ	47:Ac:146:ILE:HD11	1.94	1.00
10:J:60:LEU:HD13	10:J:60:LEU:C	1.86	1.00
21:V:72:LEU:HD11	21:V:80:VAL:HG21	1.40	1.00
42:q:66:THR:HG22	42:q:74:PHE:HB2	1.39	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
9:I:155:CYS:SG	55:I:303:SF4:FE4	1.52	1.00
49:AE:88:PHE:HB2	51:AG:19:LEU:HD11	1.39	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	1.00
12:L:358:LYS:CG	39:n:80:TYR:CZ	2.45	1.00
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	0.99
12:L:466:PHE:HB2	35:j:68:TRP:HZ2	1.27	0.99
58:L:703:3PE:H321	58:m:201:3PE:H342	1.44	0.99
13:M:196:TRP:CD1	13:M:250:LEU:HD13	1.96	0.99
10:J:87:LEU:HG	10:J:91:PHE:CZ	1.97	0.99
58:M:503:3PE:HN3	15:O:338:LYS:HE3	1.23	0.99
5:E:179:CYS:HG	59:E:301:FES:FE2	0.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.44	0.99
14:N:232:LEU:HD23	14:N:307:THR:HG23	1.39	0.99
37:l:38:PRO:HB2	38:m:75:ASN:HD22	1.26	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.98
13:M:127:ILE:CD1	14:N:256:PRO:HG3	1.93	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
2:B:82:ILE:HG12	8:H:57:MET:CE	1.93	0.98
3:C:149:LEU:HD11	22:W:80:ARG:NH2	1.78	0.98
25:Z:89:GLU:CD	30:e:97:HIS:HD2	1.70	0.98
46:AB:164:VAL:HG23	49:AI:34:VAL:CG2	1.93	0.98
46:Ab:142:THR:HG21	46:Ab:237:PHE:HB3	1.44	0.98
8:H:30:TYR:CE1	26:a:1:MET:O	2.16	0.98
58:M:503:3PE:N	15:O:338:LYS:NZ	2.10	0.98
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
12:L:141:PHE:HB2	12:L:182:PHE:HE2	1.27	0.98
22:W:55:LEU:HB3	22:W:107:MET:CE	1.94	0.98
13:M:275:ILE:HD11	13:M:288:TYR:CG	1.98	0.98
11:K:22:PHE:HB2	12:L:585:LYS:HG2	1.40	0.98
15:O:254:GLU:HG2	15:O:276:LEU:HD22	1.45	0.98
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.43	0.97
39:n:57:MET:CG	45:Aa:256:VAL:HG21	1.94	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
23:X:4:ILE:HG22	23:X:5:VAL:N	1.77	0.97
7:G:611:THR:HG21	17:Q:105:GLU:HA	1.47	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
8:H:136:VAL:HG11	10:J:69:TYR:CE1	2.00	0.97
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.45	0.97
24:Y:68:ILE:HD11	24:Y:103:LEU:HB2	1.46	0.97
48:Ad:215:LEU:CD1	70:Ad:401:HEC:HMB3	1.94	0.97
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.44	0.97
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.96
10:J:9:SER:HB3	11:K:7:ASN:HD22	1.26	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
8:H:136:VAL:HG11	10:J:69:TYR:HE1	1.26	0.96
26:a:64:LYS:HE2	26:a:66:LEU:HD12	1.43	0.96
12:L:173:LEU:HD23	58:L:701:3PE:H321	1.46	0.96
12:L:174:TYR:HD2	12:L:232:TRP:CD1	1.82	0.96
1:A:63:LEU:HD21	10:J:62:GLY:C	1.91	0.96
6:F:379:CYS:HG	55:F:502:SF4:FE4	0.73	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:CYS:SG	59:G:803:FES:S1	2.62	0.96
12:L:174:TYR:CD2	12:L:232:TRP:HD1	1.83	0.96
39:n:57:MET:HG2	45:Aa:256:VAL:CG2	1.96	0.96
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.46	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	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
24:Y:21:HIS:HE1	51:Ag:58:LEU:O	1.48	0.96
46:Ab:36:GLN:HG2	46:Ab:37:ASP:H	1.27	0.96
16:P:376:ASN:OD1	16:P:377:TYR:N	1.98	0.96
46:AB:167:GLN:NE2	49:AI:35:PRO:HD3	1.80	0.96
12:L:363:THR:HG23	12:L:431:THR:HB	1.48	0.95
2:B:100:CYS:SG	55:B:301:SF4:FE4	1.59	0.95
12:L:466:PHE:HB2	35:j:68:TRP:CZ2	2.01	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
20:U:90:TYR:HE2	20:U:92:LYS:HB2	1.25	0.95
12:L:174:TYR:HD2	12:L:232:TRP:HD1	1.03	0.95
12:L:319:MET:HE1	12:L:399:ILE:HA	1.47	0.95
19:S:16:LEU:HD11	19:S:51:LEU:HD11	1.46	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
13:M:143:LEU:HD21	14:N:303:THR:CG2	1.96	0.95
54:AK:36:THR:HB	54:AK:38:TRP:CD1	2.00	0.95
48:Ad:249:TYR:CE1	48:Ad:252:VAL:HG23	2.02	0.95
52:Ah:44:ALA:HA	52:Ah:47:ARG:HD3	1.46	0.95
37:l:91:GLN:NE2	39:n:2:ALA:HB1	1.82	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
12:L:247:LEU:HD12	12:L:248:HIS:CD2	1.98	0.95
12:L:466:PHE:CZ	35:j:72:ARG:NH2	2.35	0.95
13:M:4:ILE:HG22	13:M:107:ILE:HD13	1.47	0.95
14:N:31:VAL:O	14:N:35:PHE:CD2	2.18	0.95
18:R:38:TYR:HE2	42:q:127:TYR:HB2	1.30	0.95
39:n:57:MET:CG	45:Aa:256:VAL:CG2	2.44	0.95
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	0.95
4:D:90:ALA:HB2	8:H:205:SER:HA	1.45	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
12:L:302:ILE:CG2	12:L:340:PHE:CZ	2.49	0.94
14:N:307:THR:HB	15:O:319:ILE:CD1	1.97	0.94
1:A:67:LEU:HD11	11:K:68:ALA:CB	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:230:ASP:H	49:Ae:242:HIS:CD2	1.84	0.94
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.44	0.94
9:I:152:CYS:HG	55:I:303:SF4:FE2	0.69	0.94
13:M:216:LEU:HG	13:M:220:HIS:CE1	2.01	0.94
13:M:369:LEU:CD2	13:M:371:PRO:HD2	1.97	0.94
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	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:173:THR:CG2	33:h:147:ALA:HB2	1.96	0.94
24:Y:21:HIS:CE1	51:Ag:58:LEU:O	2.21	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:224:PHE:CE2	61:H:400:UQ9:H13	2.02	0.94
12:L:362:ILE:HD12	12:L:430:VAL:HG12	1.50	0.94
53:AJ:11:TYR:HA	53:AJ:15:PHE:HB2	1.48	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
20:U:140:CYS:HB2	20:U:143:GLU:HG2	1.49	0.94
48:AD:249:TYR:CE1	48:AD:252:VAL:HG23	2.02	0.94
47:Ac:376:MET:CE	50:Af:17:PHE:HD1	1.80	0.94
6:F:382:CYS:HG	55:F:502:SF4:FE3	0.64	0.94
9:I:113:CYS:SG	55:I:304:SF4:FE3	1.59	0.94
16:P:333:PRO:HB2	16:P:337:ASP:HB2	1.47	0.94
13:M:1:MET:HG3	13:M:4:ILE:HD13	1.50	0.93
49:AE:263:TYR:HA	49:AE:273:VAL:HA	1.49	0.93
12:L:247:LEU:HD11	12:L:248:HIS:NE2	1.83	0.93
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
12:L:274:LEU:HA	12:L:277:MET:HE3	1.49	0.93
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.93
30:e:20:PHE:HZ	33:h:178:PHE:HB2	1.28	0.93
13:M:142:ARG:HH21	14:N:303:THR:HG22	1.32	0.93
13:M:453:LEU:CD1	13:M:454:ILE:HG23	1.99	0.93
46:AB:164:VAL:HG23	49:AI:34:VAL:HG22	1.50	0.93
49:AE:234:TYR:HB2	49:AE:243:TYR:HB2	1.48	0.93
47:Ac:137:GLN:HG3	47:Ac:265:PRO:HG3	1.48	0.93
25:Z:98:MET:HE1	30:e:78:ASP:OD2	1.68	0.93
13:M:173:THR:HG21	33:h:147:ALA:HB2	1.48	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.93
7:G:445:LEU:HD23	7:G:460:HIS:CE1	2.00	0.93
16:P:93:HIS:CD2	16:P:94:LEU:CD1	2.52	0.93
16:P:262:THR:H	16:P:332:LEU:HD12	1.34	0.93
12:L:41:LYS:HG3	12:L:98:TRP:CZ2	2.04	0.92
30:e:41:ILE:HG23	33:h:179:ILE:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:98:VAL:HG22	67:AC:402:HEM:HBC2	1.51	0.92
15:O:314:LEU:CD1	15:O:315:PRO:HD2	2.00	0.92
15:O:256:LEU:HD21	15:O:276:LEU:HD23	1.47	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
8:H:136:VAL:CG1	10:J:69:TYR:CE1	2.52	0.92
12:L:136:ASN:HD21	62:h:201:CDL:H273	1.34	0.92
25:Z:86:ILE:HG23	25:Z:128:ARG:HE	1.33	0.92
43:r:9:GLN:HA	43:r:12:ARG:HD3	1.50	0.92
45:AA:43:GLN:HE21	46:AB:57:PRO:HG3	1.24	0.92
7:G:445:LEU:CD2	7:G:460:HIS:HE1	1.82	0.92
23:X:4:ILE:CG2	23:X:5:VAL:H	1.82	0.92
47:Ac:376:MET:CE	50:Af:17:PHE:CD1	2.53	0.92
10:J:12:PHE:CE2	11:K:42:ILE:HD13	2.05	0.92
45:Aa:58:ARG:HE	45:Aa:417:LEU:HD12	1.33	0.92
23:X:37:ASP:OD2	27:b:70:PRO:HD3	1.69	0.91
10:J:12:PHE:CE2	11:K:42:ILE:CD1	2.53	0.91
37:l:158:PRO:HD3	40:o:22:ILE:HB	1.53	0.91
21:V:75:GLY:HA2	43:r:103:ARG:HD2	1.51	0.91
39:n:57:MET:HB2	45:Aa:256:VAL:HG21	1.51	0.91
54:Ak:12:GLU:HA	54:Ak:15:ARG:HD3	1.53	0.91
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.00	0.91
22:W:55:LEU:HB3	22:W:107:MET:HE1	1.52	0.91
8:H:111:LEU:HD21	10:J:60:LEU:CD1	2.00	0.91
8:H:111:LEU:CD2	10:J:60:LEU:HD11	2.01	0.91
12:L:202:MET:HE3	12:L:265:PRO:HG3	1.53	0.91
12:L:560:LYS:HD2	38:m:80:PHE:HE2	1.35	0.91
39:n:57:MET:CB	45:Aa:256:VAL:HG21	1.99	0.91
58:M:503:3PE:H261	58:O:401:3PE:H252	1.52	0.91
15:O:106:ILE:HG12	15:O:111:SER:HA	1.50	0.91
12:L:245:ALA:O	12:L:249:SER:HB3	1.70	0.91
37:l:156:VAL:HG11	40:o:95:TYR:CZ	2.05	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
58:M:503:3PE:HN3	15:O:338:LYS:HZ1	1.19	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
47:AC:137:GLN:HG3	47:AC:265:PRO:HG3	1.50	0.90
13:M:231:LEU:HD12	13:M:235:LEU:CD1	2.00	0.90
15:O:347:VAL:O	15:O:347:VAL:HG12	1.71	0.90
6:F:425:CYS:HG	55:F:502:SF4:FE1	0.62	0.90
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.54	0.90
58:M:503:3PE:N	15:O:338:LYS:HE3	1.78	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:93:HIS:NE2	16:P:94:LEU:CD1	2.35	0.90
7:G:226:CYS:HG	55:G:802:SF4:FE1	0.75	0.90
9:I:80:GLU:HG3	26:a:1:MET:SD	2.11	0.90
12:L:280:LEU:HD21	57:L:706:PC1:C3H	2.00	0.90
13:M:2:LEU:HA	13:M:5:ILE:HG12	1.53	0.89
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
12:L:466:PHE:CB	35:j:68:TRP:HZ2	1.84	0.89
13:M:453:LEU:HD12	13:M:454:ILE:N	1.87	0.89
15:O:314:LEU:CG	15:O:315:PRO:HD2	2.02	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
12:L:123:LEU:HD22	12:L:150:MET:SD	2.12	0.89
45:Aa:273:SER:HB2	51:Ag:18:SER:O	1.71	0.89
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
13:M:380:PHE:HA	13:M:383:MET:HE2	1.55	0.89
34:i:94:PRO:HG3	41:p:10:TYR:CE2	2.07	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
12:L:466:PHE:CE1	35:j:72:ARG:NH2	2.41	0.89
13:M:168:GLN:OE1	23:X:168:PHE:CE1	2.24	0.89
54:AK:36:THR:HB	54:AK:38:TRP:NE1	1.88	0.89
21:V:72:LEU:HD12	21:V:72:LEU:O	1.73	0.89
49:Ae:242:HIS:N	49:Ae:251:LYS:HB3	1.86	0.89
12:L:261:VAL:O	12:L:264:HIS:HD2	1.50	0.89
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.89
12:L:364:LYS:HE2	36:k:67:ILE:CD1	2.03	0.89
10:J:24:SER:HB2	10:J:27:TYR:HD2	1.35	0.88
1:A:63:LEU:HD21	10:J:62:GLY:O	1.72	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
39:n:101:GLU:O	39:n:122:ARG:NH2	2.06	0.88
47:AC:223:TYR:O	48:AD:311:TRP:NE1	2.06	0.88
45:Aa:102:LYS:HZ1	45:Aa:153:ASN:HA	1.36	0.88
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.88	0.88
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.54	0.88
49:AE:168:LYS:HA	49:AE:173:PRO:HA	1.54	0.88
7:G:176:CYS:HG	55:G:802:SF4:FE4	0.62	0.88
13:M:8:SER:HA	13:M:11:LEU:HD13	1.55	0.88
16:P:96:LEU:HD12	16:P:97:MET:N	1.88	0.88
46:AB:48:VAL:HG21	46:AB:400:ALA:HB1	1.53	0.88
49:AI:60:ALA:HB1	46:Ab:339:TYR:CD2	2.08	0.88
4:D:99:LEU:CD2	4:D:109:CYS:SG	2.62	0.88
14:N:307:THR:HB	15:O:319:ILE:HD11	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:MET:HE3	58:D:501:3PE:HN3	1.37	0.88
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.88
2:B:81:LEU:HG	8:H:53:MET:HE1	1.54	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
13:M:310:MET:SD	13:M:455:THR:HB	2.13	0.88
16:P:344:PRO:HB2	16:P:347:LEU:HD13	1.56	0.88
56:B:302:UQ1:CM3	4:D:185:MET:HE3	2.04	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.87
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.87
12:L:428:TYR:HA	12:L:432:MET:HG2	1.56	0.87
13:M:447:LEU:HD11	13:M:454:ILE:HG21	1.55	0.87
16:P:192:ARG:HH22	16:P:198:ALA:HB3	1.36	0.87
19:S:16:LEU:HD22	19:S:19:ILE:HD11	1.53	0.87
12:L:362:ILE:HD12	12:L:430:VAL:CG1	2.03	0.87
12:L:496:LEU:HD12	12:L:497:GLY:N	1.90	0.87
45:Aa:341:PHE:CD2	45:Aa:368:MET:CE	2.56	0.87
10:J:9:SER:CB	11:K:7:ASN:ND2	2.37	0.87
57:L:706:PC1:H3C1	37:l:148:HIS:CE1	2.09	0.87
13:M:368:ALA:HB1	13:M:375:LEU:HD13	1.56	0.87
27:b:60:ASP:OD1	27:b:61:GLY:N	2.07	0.87
49:Ae:239:HIS:CE1	49:Ae:254:ALA:HB2	2.08	0.87
30:e:17:HIS:CD2	30:e:18:PHE:HD1	1.92	0.87
48:Ad:167:ARG:HH12	48:Ad:173:ASP:HB2	1.40	0.87
48:AD:228:ARG:H	48:AD:231:LEU:HD12	1.37	0.87
48:Ad:141:THR:HG22	53:Aj:53:TRP:HZ2	1.38	0.87
13:M:102:LEU:HD13	13:M:230:ILE:HG12	1.57	0.87
12:L:553:LEU:HD11	38:m:93:ALA:CB	2.04	0.87
62:L:705:CDL:C11	24:Y:115:MET:SD	2.63	0.87
20:T:79:ILE:HB	20:T:145:VAL:HG13	1.55	0.87
46:AB:48:VAL:HG22	46:AB:219:ALA:HB2	1.57	0.86
49:AE:167:PHE:HE2	49:AE:176:VAL:HB	1.36	0.86
51:AG:29:SER:HB2	51:AG:32:SER:HB2	1.57	0.86
49:AI:43:LEU:HD13	46:Ab:164:VAL:HG23	1.57	0.86
12:L:79:SER:HB2	12:L:135:ASN:HB2	1.55	0.86
13:M:1:MET:HE1	13:M:111:SER:HB2	1.58	0.86
13:M:127:ILE:CD1	14:N:256:PRO:CG	2.54	0.86
13:M:127:ILE:HD12	14:N:256:PRO:HG3	1.56	0.86
50:Af:22:TYR:HE1	50:Af:28:ASN:HB3	1.38	0.86
2:B:104:MET:HE3	56:B:302:UQ1:H112	1.58	0.86
4:D:52:MET:CE	58:D:501:3PE:H121	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
45:AA:43:GLN:NE2	46:AB:57:PRO:CG	2.37	0.86
46:AB:48:VAL:HG23	46:AB:219:ALA:CB	2.03	0.86
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.57	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
20:T:138:LEU:HD13	20:T:144:ILE:HG12	1.56	0.86
31:f:8:ARG:HG2	31:f:9:GLU:OE1	1.75	0.86
48:AD:117:TYR:HA	48:AD:121:CYS:SG	2.14	0.86
49:AI:8:SER:HB3	49:AI:12:ALA:HB2	1.57	0.86
47:Ac:21:LEU:HD13	69:Ac:405:UQ6:O2	1.75	0.86
19:S:16:LEU:HD12	19:S:16:LEU:O	1.76	0.86
46:AB:164:VAL:CG2	49:AI:34:VAL:CG2	2.54	0.86
32:g:145:ILE:HG23	41:p:160:LYS:HE2	1.57	0.86
46:AB:48:VAL:HG23	46:AB:219:ALA:HB1	1.55	0.86
7:G:78:CYS:SG	59:G:803:FES:FE2	1.68	0.86
47:AC:35:SER:HA	69:AC:405:UQ6:H112	1.58	0.86
3:C:80:LEU:O	3:C:81:ASP:HB2	1.73	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
22:W:55:LEU:HD22	22:W:107:MET:HE2	1.57	0.86
4:D:99:LEU:HD23	4:D:109:CYS:HA	1.57	0.86
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.86
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.86
9:I:162:CYS:SG	55:I:304:SF4:FE4	1.68	0.86
45:AA:55:ASN:HB3	45:AA:226:ALA:HB1	1.58	0.86
45:AA:255:ARG:O	45:AA:255:ARG:HG3	1.75	0.86
47:AC:148:ASN:OD1	49:Ae:221:GLY:HA3	1.76	0.86
23:X:53:PRO:HD2	25:Z:116:TRP:CD1	2.11	0.85
45:AA:400:VAL:HG21	46:AB:58:LEU:HD11	1.58	0.85
51:AG:11:ILE:HG21	51:AG:14:VAL:CG2	2.05	0.85
45:Aa:255:ARG:HG3	45:Aa:255:ARG:O	1.75	0.85
47:Ac:138:MET:HE1	47:Ac:268:ILE:HG12	1.57	0.85
12:L:417:SER:HB3	12:L:493:ILE:HG13	1.58	0.85
37:l:167:TYR:HD2	37:l:168:LEU:HD12	1.41	0.85
18:R:32:THR:HG22	18:R:36:GLN:H	1.40	0.85
4:D:52:MET:HE2	58:D:501:3PE:H121	1.58	0.85
12:L:54:PHE:O	12:L:58:ASN:N	2.10	0.85
49:AE:213:LEU:HD23	49:AE:260:VAL:HG22	1.59	0.85
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.59	0.85
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.85
13:M:175:ASN:HD22	33:h:143:GLU:HG2	1.42	0.85
20:T:110:LEU:HG	20:T:114:ASP:HB2	1.59	0.85
45:Aa:58:ARG:NH2	45:Aa:417:LEU:O	2.10	0.85
12:L:247:LEU:HD11	12:L:248:HIS:CD2	2.11	0.85
12:L:437:PHE:HE1	12:L:441:ILE:CG1	1.85	0.85
45:Aa:66:HIS:HE1	45:Aa:403:LEU:HD22	1.41	0.85
2:B:101:ALA:HB3	56:B:302:UQ1:HM23	1.59	0.84
7:G:78:CYS:HG	59:G:803:FES:FE2	0.55	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.59	0.84
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.59	0.84
16:P:206:ILE:H	64:P:401:NDP:H71N	1.24	0.84
21:V:56:LEU:HD12	21:V:57:ASP:N	1.92	0.84
49:Ae:174:LEU:HD21	49:Ae:273:VAL:HG21	1.58	0.84
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.84
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.84
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
12:L:128:MET:HG2	12:L:251:THR:HB	1.59	0.84
16:P:192:ARG:NH2	16:P:198:ALA:HB3	1.92	0.84
46:AB:174:ILE:HG13	49:AI:14:VAL:HG11	1.59	0.84
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.77	0.84
12:L:302:ILE:HG22	12:L:340:PHE:CE2	2.11	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
15:O:314:LEU:HD12	15:O:315:PRO:HD2	1.56	0.84
47:AC:214:ASP:HB3	51:AG:9:ALA:HB2	1.58	0.84
6:F:300:ILE:HD13	6:F:307:VAL:H	1.41	0.84
8:H:111:LEU:CD2	10:J:60:LEU:CD1	2.55	0.84
62:L:704:CDL:H782	13:M:371:PRO:HG3	1.57	0.84
13:M:447:LEU:HD11	13:M:454:ILE:CG2	2.07	0.84
30:e:14:LEU:HD12	30:e:15:ASP:HB2	1.57	0.84
48:AD:183:GLU:HB3	48:Ad:160:ASP:O	1.78	0.84
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.84
8:H:224:PHE:CE2	61:H:400:UQ9:C13	2.59	0.84
12:L:445:GLU:HB2	12:L:450:LEU:HD23	1.59	0.84
51:Ag:11:ILE:HG21	51:Ag:14:VAL:CG2	2.05	0.84
14:N:215:MET:SD	14:N:248:LEU:HD21	2.18	0.84
37:l:167:TYR:CD2	37:l:168:LEU:HD12	2.13	0.84
45:Aa:281:ALA:HB2	51:Ag:10:ARG:HH22	1.43	0.84
13:M:196:TRP:NE1	13:M:250:LEU:HD13	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:275:HIS:HA	16:P:278:LYS:HE2	1.60	0.84
51:AG:69:GLN:NE2	51:AG:72:ARG:NH2	2.24	0.84
47:Ac:376:MET:HE1	50:Af:17:PHE:HD1	1.39	0.84
12:L:20:LEU:HD12	12:L:21:ILE:N	1.92	0.84
12:L:466:PHE:CE1	35:j:72:ARG:CZ	2.60	0.84
18:R:38:TYR:CE2	42:q:127:TYR:HB2	2.13	0.84
49:AE:175:PHE:HZ	49:AE:223:VAL:HG13	1.43	0.84
38:m:125:PHE:HE1	41:p:133:THR:HG22	1.43	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
62:h:201:CDL:H171	58:i:201:3PE:H372	1.57	0.83
45:AA:64:SER:HB2	45:AA:235:GLY:HA2	1.61	0.83
48:Ad:95:PRO:HG2	52:Ah:85:PHE:CB	2.08	0.83
4:D:67:ASN:HB3	4:D:69:VAL:HG12	1.58	0.83
13:M:373:ILE:HG12	13:M:454:ILE:HD11	1.60	0.83
8:H:187:ILE:HD12	58:I:301:3PE:H251	1.59	0.83
12:L:16:LEU:HD23	12:L:126:ILE:CD1	2.08	0.83
13:M:361:MET:HB3	13:M:441:MET:HE3	1.60	0.83
15:O:314:LEU:HG	15:O:315:PRO:HD2	1.58	0.83
47:Ac:376:MET:HE1	50:Af:17:PHE:CD1	2.11	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
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
12:L:9:LEU:HD21	58:i:201:3PE:H2A2	1.59	0.83
24:Y:143:VAL:HG23	33:h:157:ARG:HG2	1.59	0.83
15:O:347:VAL:HG11	28:c:29:PHE:HA	1.61	0.83
25:Z:89:GLU:CD	30:e:97:HIS:CD2	2.56	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
10:J:126:TYR:CA	25:Z:120:LEU:HD11	2.09	0.83
34:i:15:LEU:HD21	39:n:164:PRO:HB2	1.61	0.83
49:AE:88:PHE:CB	51:AG:19:LEU:CD1	2.55	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.83
15:O:168:VAL:HG11	15:O:241:TYR:CD1	2.14	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.92	0.82
9:I:162:CYS:HG	55:I:304:SF4:FE4	0.53	0.82
12:L:131:LEU:CD1	12:L:140:LEU:HD12	2.09	0.82
12:L:556:ILE:HG21	38:m:80:PHE:CE1	2.14	0.82
13:M:269:MET:HE1	13:M:396:MET:HA	1.61	0.82
48:AD:100:GLY:O	48:AD:286:LYS:NZ	2.13	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:432:MET:HG3	12:L:432:MET:O	1.78	0.82
49:AE:221:GLY:HA3	47:Ac:148:ASN:ND2	1.94	0.82
12:L:222:GLY:HA2	12:L:229:LEU:CD1	2.08	0.82
13:M:151:PHE:CZ	14:N:291:PHE:HB2	2.14	0.82
14:N:335:MET:HG3	14:N:335:MET:O	1.79	0.82
45:AA:55:ASN:HB3	45:AA:226:ALA:CB	2.09	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
13:M:162:ILE:HG23	14:N:271:MET:CE	2.08	0.82
15:O:339:TYR:OH	58:O:401:3PE:H122	1.79	0.82
3:C:217:ARG:NH1	22:W:112:GLU:HB2	1.95	0.82
8:H:183:MET:HE2	57:I:302:PC1:H2A1	1.61	0.82
9:I:171:PRO:HB3	42:q:93:MET:HE1	1.60	0.82
49:Ae:243:TYR:CZ	49:Ae:258:LEU:HD22	2.13	0.82
2:B:89:SER:O	8:H:54:LYS:HD3	1.79	0.82
12:L:493:ILE:HD12	12:L:496:LEU:HD21	1.61	0.82
13:M:29:SER:HB3	32:g:91:PHE:CD2	2.15	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
12:L:364:LYS:HE2	36:k:67:ILE:HD11	1.60	0.82
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.45	0.82
17:Q:146:ASP:OD1	17:Q:146:ASP:O	1.97	0.82
18:R:51:ARG:HH21	42:q:125:VAL:HG12	1.44	0.82
45:Aa:341:PHE:CE2	45:Aa:372:LEU:HD13	2.15	0.82
49:Ae:167:PHE:HE2	49:Ae:176:VAL:CG2	1.93	0.82
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
10:J:65:VAL:HG13	10:J:66:VAL:N	1.92	0.81
49:Ae:242:HIS:H	49:Ae:251:LYS:CB	1.92	0.81
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.61	0.81
36:k:34:PRO:HD2	36:k:59:TYR:CD1	2.15	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
9:I:123:CYS:HG	55:I:303:SF4:FE1	0.53	0.81
12:L:358:LYS:HG3	39:n:80:TYR:OH	1.79	0.81
12:L:552:LEU:HD21	38:m:90:GLY:HA2	1.61	0.81
12:L:572:ASN:OD1	62:L:705:CDL:OA4	1.98	0.81
48:Ad:121:CYS:SG	70:Ad:401:HEC:CAB	2.68	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
15:O:168:VAL:HG21	15:O:241:TYR:CE1	2.15	0.81
42:q:71:LYS:O	42:q:72:ASN:OD1	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:102:LYS:NZ	45:Aa:153:ASN:HA	1.94	0.81
1:A:63:LEU:CD1	10:J:63:MET:HE3	2.10	0.81
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
22:W:55:LEU:CD2	22:W:107:MET:HE2	2.09	0.81
39:n:97:TYR:HB2	39:n:178:PRO:CG	2.10	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
62:L:705:CDL:H351	24:Y:114:ALA:HB1	1.61	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
38:m:125:PHE:CE1	41:p:133:THR:HG22	2.16	0.81
49:AE:123:VAL:HG13	53:AJ:29:ALA:HA	1.63	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
12:L:229:LEU:O	12:L:229:LEU:CD1	2.28	0.81
45:AA:68:THR:HG22	45:AA:136:LEU:HD23	1.63	0.81
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.81
36:k:30:ILE:HD11	36:k:39:GLN:HB2	1.61	0.81
10:J:22:LYS:CD	11:K:23:ARG:HG2	2.10	0.81
12:L:424:MET:HE2	12:L:502:LEU:HB2	1.62	0.81
13:M:172:GLY:O	13:M:173:THR:CG2	2.28	0.81
14:N:277:ILE:CG2	14:N:278:MET:H	1.93	0.81
14:N:277:ILE:HG23	14:N:278:MET:N	1.96	0.81
14:N:307:THR:HG22	14:N:308:ASN:H	1.46	0.81
19:S:36:PHE:HZ	19:S:44:LEU:HD11	1.45	0.81
51:AG:69:GLN:NE2	51:AG:72:ARG:CZ	2.44	0.81
49:Ae:232:GLY:HA3	49:Ae:244:ASP:CA	2.05	0.81
13:M:216:LEU:HD12	13:M:236:LEU:HD21	1.60	0.80
58:M:503:3PE:H3A2	14:N:246:LEU:HD11	1.63	0.80
14:N:200:LEU:HD21	14:N:265:ILE:HG12	1.62	0.80
51:AG:69:GLN:HE22	51:AG:72:ARG:NH1	1.79	0.80
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.63	0.80
8:H:311:THR:HB	25:Z:51:MET:SD	2.21	0.80
27:b:20:VAL:HA	58:b:201:3PE:H282	1.64	0.80
2:B:89:SER:O	8:H:54:LYS:CD	2.29	0.80
6:F:109:ARG:NH1	6:F:237:GLY:O	2.13	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.82	0.80
41:p:6:ASP:HB3	41:p:9:VAL:HG22	1.61	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
13:M:453:LEU:HD12	13:M:454:ILE:HG23	1.63	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
13:M:458:THR:CG2	41:p:148:ALA:HB1	2.12	0.80
49:Ae:167:PHE:HE2	49:Ae:176:VAL:HG21	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:251:LEU:O	8:H:251:LEU:CD1	2.27	0.80
10:J:9:SER:HB2	11:K:7:ASN:ND2	1.96	0.80
39:n:57:MET:HG2	45:Aa:256:VAL:HG21	1.61	0.80
45:AA:400:VAL:HG21	46:AB:58:LEU:CD1	2.10	0.80
46:AB:164:VAL:CG2	49:AI:34:VAL:HG23	2.11	0.80
45:Aa:280:ASP:OD2	51:Ag:10:ARG:HA	1.82	0.80
13:M:168:GLN:OE1	23:X:168:PHE:HE1	1.62	0.80
49:AE:159:ILE:HG23	49:AE:163:LYS:HE3	1.63	0.80
51:AG:73:LYS:NZ	52:AH:63:GLU:HB2	1.95	0.80
4:D:253:LEU:HB2	43:r:23:LYS:HD2	1.63	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
25:Z:93:GLU:CD	30:e:95:PRO:HG3	2.06	0.80
49:AI:42:VAL:HG11	45:Aa:283:PRO:HB2	1.63	0.80
9:I:113:CYS:HG	55:I:304:SF4:FE3	0.52	0.80
45:Aa:341:PHE:CZ	45:Aa:372:LEU:HD13	2.17	0.80
48:Ad:300:LEU:HB3	62:Ag:101:CDL:H552	1.64	0.80
6:F:174:ARG:HA	44:s:52:LEU:HD21	1.64	0.80
15:O:117:PHE:CE1	15:O:173:MET:HE3	2.17	0.80
16:P:106:LEU:HD21	18:R:49:VAL:HG11	1.63	0.80
58:j:700:3PE:H3B2	40:o:78:LEU:HD13	1.63	0.80
48:AD:152:VAL:HG11	48:AD:176:PRO:HG3	1.62	0.80
7:G:73:GLY:HA2	59:G:803:FES:S1	2.21	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
10:J:22:LYS:CD	11:K:23:ARG:CG	2.60	0.79
15:O:199:LEU:HD11	15:O:294:LEU:HD22	1.64	0.79
20:T:87:LEU:HD21	20:T:104:PHE:HZ	1.47	0.79
49:AE:88:PHE:CG	51:AG:19:LEU:HD11	2.16	0.79
4:D:52:MET:CE	58:D:501:3PE:N	2.44	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
20:T:93:ILE:HG21	20:T:110:LEU:HD22	1.63	0.79
21:V:95:LEU:HA	21:V:100:TRP:HH2	1.46	0.79
25:Z:93:GLU:OE2	30:e:95:PRO:HG3	1.81	0.79
45:AA:338:CYS:HB3	45:AA:368:MET:SD	2.22	0.79
46:Ab:259:ARG:HB3	46:Ab:444:LEU:HD13	1.63	0.79
4:D:47:PHE:CB	14:N:227:ILE:HD11	2.08	0.79
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
12:L:16:LEU:CD2	12:L:126:ILE:HD13	2.10	0.79
12:L:130:ILE:HG23	12:L:139:GLN:HE21	1.46	0.79
45:Aa:117:GLY:HA2	46:Ab:377:LYS:HG2	1.65	0.79
47:Ac:376:MET:HE2	50:Af:17:PHE:CD1	2.15	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
10:J:61:GLY:O	10:J:65:VAL:CG1	2.31	0.79
20:U:76:LEU:HD12	20:U:156:GLU:HB2	1.62	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
12:L:73:SER:HB3	41:p:100:GLN:NE2	1.97	0.79
13:M:122:PHE:CZ	13:M:206:LYS:HD3	2.18	0.79
13:M:367:LEU:HD21	13:M:408:MET:HE2	1.64	0.79
4:D:52:MET:CE	58:D:501:3PE:C12	2.61	0.79
30:e:41:ILE:CG2	33:h:179:ILE:HD11	2.13	0.79
49:Ae:229:GLY:HA2	49:Ae:242:HIS:HD2	1.47	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
12:L:131:LEU:HD12	12:L:140:LEU:CD1	2.12	0.79
13:M:29:SER:HB3	32:g:91:PHE:HD2	1.47	0.79
20:T:113:LEU:HD22	22:W:71:MET:HE2	1.63	0.79
23:X:120:PRO:CB	23:X:125:LEU:HD11	2.13	0.79
39:n:20:TYR:CE2	39:n:24:LEU:HD11	2.18	0.79
42:q:55:PHE:CD1	43:r:26:LEU:HD22	2.17	0.79
48:Ad:215:LEU:HD21	70:Ad:401:HEC:C2B	2.12	0.79
49:Ae:204:ARG:HH21	49:Ae:247:GLY:HA3	1.47	0.79
7:G:651:PRO:HD3	19:S:56:ARG:HB3	1.65	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.63	0.79
14:N:123:PRO:HG2	14:N:126:MET:HG2	1.63	0.79
48:AD:291:LYS:HB3	53:AJ:36:PHE:HE2	1.48	0.79
49:Ae:152:ILE:HG13	49:Ae:154:ILE:HD11	1.65	0.79
12:L:565:SER:OG	62:L:705:CDL:H322	1.83	0.79
19:S:20:ARG:HG3	19:S:54:LEU:HB2	1.64	0.79
4:D:280:ALA:CB	21:V:11:LEU:HG	2.13	0.78
10:J:34:VAL:HG13	58:J:401:3PE:H2I2	1.64	0.78
21:V:48:THR:OG1	21:V:87:GLU:OE2	2.01	0.78
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.78
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.65	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.23	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:L:706:PC1:H3C1	37:l:148:HIS:HE1	1.47	0.78
14:N:319:LYS:HA	15:O:302:THR:HG21	1.64	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.78
13:M:370:PRO:HA	13:M:375:LEU:CD2	2.13	0.78
50:AF:52:PRO:HD3	46:Ab:148:ARG:NH2	1.98	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
12:L:302:ILE:CG2	12:L:340:PHE:CE1	2.66	0.78
13:M:248:ILE:HG13	13:M:249:ILE:HD12	1.64	0.78
15:O:117:PHE:HE1	15:O:173:MET:CE	1.96	0.78
12:L:3:ILE:H	12:L:3:ILE:HD12	1.48	0.78
13:M:231:LEU:HD12	13:M:235:LEU:HD13	1.64	0.78
15:O:314:LEU:HD12	15:O:315:PRO:CD	2.13	0.78
30:e:89:GLU:HB2	30:e:91:LYS:HG2	1.65	0.78
50:Af:22:TYR:CE1	50:Af:28:ASN:HB3	2.18	0.78
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.18	0.78
12:L:475:THR:HA	40:o:55:GLN:NE2	1.97	0.78
15:O:250:SER:HA	15:O:255:VAL:HG23	1.66	0.78
20:T:87:LEU:HD22	20:T:104:PHE:CE1	2.19	0.78
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.78
12:L:534:HIS:O	12:L:538:PRO:HG3	1.83	0.78
34:i:69:LEU:HD12	34:i:71:ALA:H	1.48	0.78
11:K:42:ILE:O	11:K:46:VAL:HG23	1.84	0.78
12:L:136:ASN:HA	12:L:197:GLU:HA	1.66	0.78
13:M:9:LEU:HD23	13:M:104:ILE:HD13	1.65	0.78
49:AE:88:PHE:HB3	51:AG:19:LEU:HD11	1.66	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.78
23:X:168:PHE:O	23:X:170:TRP:CD1	2.37	0.78
37:l:44:THR:OG1	37:l:45:PRO:HD2	1.83	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
13:M:319:HIS:HA	13:M:322:THR:HG22	1.66	0.78
14:N:215:MET:CE	14:N:248:LEU:CD2	2.62	0.78
27:b:66:VAL:HG13	27:b:72:ASP:HB2	1.65	0.78
48:Ad:95:PRO:HG2	52:Ah:85:PHE:CG	2.18	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.67	0.77
10:J:67:PHE:CE2	11:K:75:LEU:HD21	2.19	0.77
40:o:31:PHE:HE2	40:o:104:ARG:NH1	1.80	0.77
47:Ac:223:TYR:O	48:Ad:311:TRP:NE1	2.16	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:305:LEU:HD12	15:O:305:LEU:O	1.83	0.77
20:T:83:VAL:CG2	20:T:126:PHE:HZ	1.97	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
2:B:96:GLY:HA2	2:B:101:ALA:HB2	1.67	0.77
13:M:204:LEU:HD22	13:M:209:LEU:HD12	1.65	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
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.66	0.77
8:H:93:HIS:CE1	26:a:24:ALA:HA	2.19	0.77
12:L:174:TYR:HE1	58:L:701:3PE:H362	1.49	0.77
17:Q:81:VAL:HG21	17:Q:150:LYS:HG3	1.65	0.77
38:m:18:LEU:HD21	39:n:69:GLU:HA	1.64	0.77
42:q:9:ARG:HA	42:q:12:GLN:HG2	1.65	0.77
51:AG:11:ILE:CG2	51:AG:14:VAL:CG2	2.62	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
14:N:254:LEU:HD12	14:N:255:PRO:CD	2.14	0.77
30:e:17:HIS:CD2	30:e:18:PHE:CD1	2.72	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
10:J:34:VAL:HG13	58:J:401:3PE:C2I	2.15	0.77
58:M:503:3PE:H3I3	62:d:201:CDL:H651	1.67	0.77
18:R:95:LEU:HD21	18:R:111:PHE:HB3	1.66	0.77
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
13:M:173:THR:HG23	33:h:147:ALA:CB	2.15	0.77
13:M:208:PRO:HG2	13:M:216:LEU:HD13	1.67	0.77
14:N:31:VAL:O	14:N:35:PHE:HD2	1.68	0.77
46:AB:63:LEU:HD11	46:AB:238:LEU:HD21	1.65	0.77
3:C:217:ARG:HH12	22:W:112:GLU:HB2	1.50	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
49:Ae:236:CYS:SG	49:Ae:239:HIS:ND1	2.55	0.77
4:D:99:LEU:HD22	4:D:109:CYS:SG	2.24	0.77
10:J:40:CYS:SG	10:J:56:PHE:HB2	2.25	0.77
10:J:59:TYR:OH	11:K:34:GLU:HB3	1.84	0.77
12:L:594:ASN:ND2	14:N:110:PRO:HB2	1.99	0.77
13:M:98:MET:CE	13:M:128:PRO:HA	2.14	0.77
23:X:124:GLN:O	23:X:125:LEU:HD12	1.85	0.77
37:l:113:ILE:HG23	37:l:115:ASN:H	1.50	0.77
39:n:57:MET:CG	45:Aa:256:VAL:HG23	2.14	0.77
53:Aj:30:LEU:HA	54:Ak:34:TRP:CD1	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.50	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
13:M:42:LEU:HG	13:M:67:ILE:HD11	1.67	0.76
13:M:453:LEU:HD11	13:M:454:ILE:HG23	1.66	0.76
14:N:232:LEU:CD2	14:N:307:THR:HG23	2.15	0.76
23:X:20:VAL:HG22	23:X:24:VAL:HG21	1.66	0.76
37:l:169:GLU:C	37:l:171:GLY:H	1.92	0.76
47:Ac:57:SER:O	47:Ac:175:LEU:HD23	1.85	0.76
51:Ag:11:ILE:CG2	51:Ag:14:VAL:CG2	2.62	0.76
56:B:302:UQ1:HM33	4:D:185:MET:HE2	1.65	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
12:L:419:THR:HA	12:L:422:TYR:CE2	2.20	0.76
51:AG:73:LYS:HZ1	52:AH:63:GLU:HB2	1.50	0.76
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.00	0.76
13:M:60:PRO:O	13:M:64:PRO:HD3	1.85	0.76
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.65	0.76
15:O:339:TYR:OH	58:O:401:3PE:C12	2.34	0.76
20:U:86:VAL:HB	20:U:122:MET:HE1	1.67	0.76
20:U:123:GLU:HG2	20:U:130:ILE:HG12	1.67	0.76
42:q:56:PHE:HA	42:q:59:HIS:HD2	1.50	0.76
49:Ae:161:GLU:HB2	49:Ae:180:THR:HG22	1.68	0.76
49:Ae:212:ILE:HD11	49:Ae:271:VAL:HG11	1.68	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
12:L:302:ILE:HG22	12:L:340:PHE:CE1	2.20	0.76
12:L:496:LEU:HD12	12:L:496:LEU:C	2.09	0.76
13:M:171:VAL:HG11	13:M:179:LEU:HD21	1.65	0.76
19:S:51:LEU:HD13	19:S:95:LEU:HD21	1.67	0.76
20:T:119:ILE:HD12	20:T:138:LEU:HD11	1.67	0.76
42:q:14:VAL:HG13	42:q:23:LEU:HD22	1.68	0.76
2:B:89:SER:O	8:H:54:LYS:HE2	1.85	0.76
3:C:98:PHE:HA	21:V:90:LEU:CD1	2.13	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.76
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.67	0.76
20:T:93:ILE:HG23	20:T:110:LEU:HD13	1.66	0.76
47:AC:137:GLN:HE21	47:AC:265:PRO:HD3	1.50	0.76
46:Ab:407:MET:HG2	46:Ab:411:THR:OG1	1.85	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.86	0.76
49:AE:217:CYS:SG	49:AE:222:CYS:HB2	2.26	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
45:Aa:255:ARG:O	45:Aa:256:VAL:C	2.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:ARG:CZ	6:F:237:GLY:O	2.34	0.76
12:L:232:TRP:CZ3	12:L:233:LEU:CD2	2.69	0.76
12:L:506:ASN:HA	12:L:509:MET:HE2	1.66	0.76
14:N:211:LEU:HD23	14:N:333:SER:HB2	1.68	0.76
16:P:143:ASP:HA	16:P:147:ASN:HB2	1.67	0.76
52:AH:65:CYS:O	52:AH:69:LEU:CB	2.34	0.76
47:Ac:19:ILE:HG23	47:Ac:221:HIS:HB2	1.67	0.76
49:Ae:181:LYS:HA	49:Ae:184:ILE:HD12	1.67	0.76
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	0.76
9:I:184:LEU:HD23	17:Q:112:MET:HG3	1.68	0.76
12:L:605:ASN:OD1	12:L:605:ASN:O	2.04	0.76
52:AH:58:ARG:HB3	52:AH:61:THR:HG22	1.68	0.76
49:AE:167:PHE:CE2	49:AE:176:VAL:HB	2.20	0.76
57:B:303:PC1:H371	8:H:49:PHE:HB3	1.66	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.67	0.75
49:Ae:195:LEU:HD22	49:Ae:248:ARG:HD2	1.67	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
12:L:56:HIS:HA	40:o:74:PHE:CD1	2.21	0.75
15:O:121:PRO:O	15:O:122:LYS:HG2	1.85	0.75
16:P:348:LYS:O	16:P:351:GLU:HG2	1.86	0.75
19:S:19:ILE:HG13	19:S:95:LEU:HD11	1.69	0.75
34:i:110:ILE:HD13	41:p:16:ARG:HD2	1.68	0.75
39:n:20:TYR:CZ	39:n:24:LEU:HD11	2.21	0.75
47:Ac:21:LEU:HD22	69:Ac:405:UQ6:C3M	2.14	0.75
7:G:651:PRO:HG3	19:S:57:GLU:H	1.51	0.75
10:J:60:LEU:C	10:J:60:LEU:CD1	2.59	0.75
10:J:61:GLY:O	10:J:65:VAL:HG12	1.86	0.75
12:L:387:THR:HG23	12:L:461:SER:O	1.85	0.75
26:a:3:PHE:HE2	62:a:101:CDL:HA4	1.50	0.75
33:h:57:VAL:HG22	39:n:104:LEU:HD11	1.69	0.75
34:i:22:TRP:CE2	39:n:172:THR:HG22	2.21	0.75
51:AG:11:ILE:HG22	51:AG:14:VAL:HG22	1.69	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
8:H:316:PRO:HA	25:Z:58:ARG:HH11	1.52	0.75
23:X:29:ALA:HB2	25:Z:71:LEU:HD11	1.67	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.75
12:L:513:MET:HE3	12:L:515:LYS:HG3	1.68	0.75
17:Q:167:ASN:O	17:Q:168:LYS:CD	2.35	0.75
49:AE:161:GLU:HA	49:AE:178:HIS:CG	2.21	0.75
16:P:214:LEU:HG	16:P:353:LEU:HD21	1.68	0.75
18:R:104:CYS:SG	18:R:107:CYS:HB2	2.27	0.75
47:AC:150:LEU:HD21	68:AC:404:U10:O2	1.87	0.75
10:J:63:MET:HE3	10:J:63:MET:HA	1.68	0.75
12:L:393:ASP:OD1	12:L:394:LEU:N	2.19	0.75
46:AB:407:MET:HG2	46:AB:411:THR:OG1	1.85	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
22:W:28:LEU:HG	22:W:32:LYS:HE3	1.69	0.75
45:AA:450:TYR:HE2	53:AJ:16:ARG:O	1.68	0.75
45:Aa:279:ASP:OD1	51:Ag:12:ARG:NE	2.19	0.75
49:Ae:163:LYS:HZ1	49:Ae:165:MET:HB2	1.51	0.75
51:Ag:11:ILE:HG22	51:Ag:14:VAL:HG22	1.68	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
14:N:277:ILE:HG23	14:N:278:MET:H	1.50	0.75
24:Y:71:MET:HG3	24:Y:102:THR:HG21	1.68	0.75
32:g:70:ASP:OD1	39:n:108:HIS:NE2	2.18	0.75
45:AA:53:LEU:HD12	45:AA:57:LEU:HB3	1.67	0.75
46:AB:429:LYS:HA	46:AB:432:VAL:HG12	1.67	0.75
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
10:J:151:MET:HE2	14:N:28:LEU:HD13	1.69	0.74
13:M:314:MET:HA	13:M:454:ILE:HD12	1.69	0.74
14:N:227:ILE:HA	14:N:230:ILE:HG22	1.66	0.74
15:O:333:GLU:O	15:O:333:GLU:CD	2.30	0.74
17:Q:61:ILE:O	17:Q:61:ILE:HD12	1.86	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
12:L:9:LEU:HD11	58:i:201:3PE:H2A1	1.69	0.74
22:W:55:LEU:HB3	22:W:107:MET:HE2	1.66	0.74
27:b:23:PHE:HD2	58:b:201:3PE:H281	1.51	0.74
4:D:99:LEU:HD21	4:D:109:CYS:SG	2.26	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
57:L:706:PC1:H321	57:L:706:PC1:H231	1.70	0.74
14:N:314:MET:HB2	15:O:305:LEU:HD11	1.69	0.74
16:P:336:GLU:HG3	16:P:342:PRO:HD3	1.67	0.74
20:T:117:GLU:HA	20:T:120:MET:HE3	1.67	0.74
1:A:4:TYR:CE2	58:J:401:3PE:H231	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:608:VAL:HG23	17:Q:103:THR:OG1	1.88	0.74
12:L:362:ILE:HG23	12:L:366:MET:HE3	1.68	0.74
28:c:30:TYR:HB2	28:c:34:PRO:HD3	1.69	0.74
49:AE:234:TYR:CB	49:AE:243:TYR:HB2	2.17	0.74
15:O:117:PHE:CE1	15:O:128:SER:HB2	2.22	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
27:b:31:ILE:HA	27:b:34:MET:HE2	1.69	0.74
49:Ae:219:HIS:HB3	49:Ae:239:HIS:CD2	2.23	0.74
4:D:67:ASN:HB2	15:O:193:LEU:HD23	1.69	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.70	0.74
24:Y:76:THR:HG23	24:Y:95:GLY:HA3	1.70	0.74
37:l:38:PRO:HB2	38:m:75:ASN:ND2	2.00	0.74
45:Aa:66:HIS:CE1	45:Aa:403:LEU:HD22	2.22	0.74
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.74
23:X:23:ALA:HB2	23:X:95:GLN:NE2	2.03	0.74
39:n:57:MET:HG2	45:Aa:256:VAL:HG23	1.67	0.74
48:Ad:124:CYS:HA	48:Ad:179:TYR:HE2	1.53	0.74
6:F:425:CYS:SG	55:F:502:SF4:FE1	1.78	0.74
7:G:674:LEU:HD11	19:S:46:LYS:HE2	1.69	0.74
8:H:180:PRO:HD3	25:Z:43:LEU:HD21	1.70	0.74
13:M:173:THR:CG2	33:h:147:ALA:CB	2.65	0.74
13:M:310:MET:HG3	13:M:455:THR:HA	1.70	0.74
17:Q:112:MET:SD	42:q:126:PRO:HB2	2.28	0.74
20:T:88:LYS:HG3	20:T:98:LEU:HD22	1.70	0.74
27:b:20:VAL:HG13	58:b:201:3PE:H2A1	1.69	0.74
49:Ae:104:LYS:HA	49:Ae:107:SER:HB3	1.69	0.74
13:M:1:MET:HB2	13:M:52:PHE:CD2	2.23	0.74
13:M:200:MET:HE1	13:M:247:SER:HB2	1.69	0.74
14:N:202:LEU:O	14:N:206:MET:HG2	1.87	0.74
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.23	0.74
16:P:350:ILE:HB	16:P:366:ILE:HG23	1.70	0.74
20:T:103:HIS:CG	20:T:106:LYS:HD2	2.23	0.74
54:AK:36:THR:HB	54:AK:38:TRP:CE2	2.22	0.74
47:Ac:294:LEU:HD11	68:Ac:404:U10:H1M3	1.69	0.74
2:B:91:TRP:CZ3	61:H:400:UQ9:H1M	2.22	0.73
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
15:O:217:ARG:O	15:O:220:LYS:HG2	1.88	0.73
47:AC:141:TRP:CD1	47:AC:265:PRO:HD3	2.22	0.73
49:AE:225:ILE:HG12	49:AE:237:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AJ:22:ALA:HB1	54:AK:27:VAL:HG11	1.69	0.73
47:Ac:29:SER:HB2	62:Ag:101:CDL:H712	1.69	0.73
25:Z:93:GLU:O	25:Z:97:ILE:HG13	1.88	0.73
48:Ad:244:MET:HB2	70:Ad:401:HEC:C4D	2.18	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
12:L:174:TYR:CD2	12:L:232:TRP:CD1	2.68	0.73
13:M:260:PRO:O	13:M:264:LEU:HG	1.88	0.73
20:T:94:ASP:HB3	20:T:98:LEU:HB2	1.68	0.73
42:q:56:PHE:HD1	42:q:59:HIS:HE2	1.35	0.73
47:AC:269:LYS:HE3	47:AC:340:GLY:HA2	1.70	0.73
4:D:67:ASN:HB2	15:O:193:LEU:CD2	2.17	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73
48:AD:200:ILE:HG21	48:AD:274:LEU:HD13	1.68	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
15:O:117:PHE:HE1	15:O:173:MET:HE3	1.53	0.73
21:V:54:GLU:HG2	21:V:58:MET:HE2	1.70	0.73
23:X:47:ARG:NH1	33:h:187:PRO:HB2	2.04	0.73
46:AB:48:VAL:HG23	46:AB:48:VAL:O	1.88	0.73
2:B:112:TYR:OH	9:I:91:GLY:CA	2.28	0.73
3:C:80:LEU:HG	4:D:396:THR:HG22	1.71	0.73
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.73
12:L:20:LEU:HD12	12:L:20:LEU:C	2.13	0.73
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.12	0.73
12:L:455:LYS:NZ	35:j:57:GLN:OE1	2.21	0.73
13:M:216:LEU:HG	13:M:220:HIS:HE1	1.48	0.73
14:N:275:CYS:SG	24:Y:139:PRO:HG2	2.28	0.73
27:b:69:HIS:HD2	27:b:70:PRO:HD2	1.54	0.73
45:AA:171:GLU:O	45:AA:174:GLU:HG2	1.88	0.73
1:A:94:LEU:HD22	10:J:152:MET:CE	2.18	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
8:H:111:LEU:HD11	10:J:56:PHE:CZ	2.23	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
12:L:232:TRP:CZ3	12:L:233:LEU:HD23	2.23	0.73
12:L:579:ASN:OD1	12:L:579:ASN:O	2.06	0.73
13:M:167:ILE:HD11	13:M:195:LEU:HD21	1.70	0.73
15:O:204:VAL:CG2	15:O:255:VAL:HG22	2.19	0.73
21:V:12:VAL:HG13	21:V:13:GLY:N	2.04	0.73
27:b:23:PHE:HE1	58:b:201:3PE:H371	1.53	0.73
58:m:202:3PE:H261	58:m:202:3PE:H371	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:42:ASP:OD2	42:q:83:PRO:HG2	1.87	0.73
49:AE:155:LYS:HE2	49:AE:157:SER:HB3	1.71	0.73
49:Ae:234:TYR:HB3	49:Ae:243:TYR:CE1	2.24	0.73
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
13:M:122:PHE:CD1	13:M:238:LEU:HG	2.23	0.73
37:l:89:TRP:CZ2	39:n:86:PRO:HD2	2.24	0.73
46:Ab:36:GLN:HG2	46:Ab:37:ASP:N	2.01	0.73
47:Ac:214:ASP:HB3	51:Ag:9:ALA:HB2	1.71	0.73
48:Ad:217:GLY:O	48:Ad:235:PRO:HD2	1.88	0.73
49:Ae:149:MET:HB3	49:Ae:170:ARG:HG2	1.70	0.73
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.70	0.73
22:W:32:LYS:HE2	66:W:201:EHZ:C19	2.18	0.73
24:Y:68:ILE:CD1	24:Y:103:LEU:HB2	2.18	0.73
53:Aj:41:ASP:O	53:Aj:45:GLU:HG2	1.88	0.73
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
10:J:9:SER:HB2	11:K:7:ASN:HD22	1.45	0.72
12:L:141:PHE:CD2	13:M:370:PRO:HB3	2.24	0.72
12:L:153:LEU:HD11	13:M:360:LEU:HD11	1.70	0.72
12:L:358:LYS:HG3	39:n:80:TYR:CE2	2.23	0.72
13:M:441:MET:SD	13:M:444:LEU:HD23	2.29	0.72
13:M:458:THR:HG22	41:p:148:ALA:HB1	1.71	0.72
14:N:215:MET:SD	14:N:248:LEU:CD2	2.77	0.72
17:Q:167:ASN:O	17:Q:168:LYS:HD2	1.88	0.72
19:S:69:TYR:CE2	19:S:75:LYS:HG3	2.24	0.72
25:Z:65:LEU:O	25:Z:69:ILE:HG12	1.89	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
12:L:136:ASN:ND2	62:h:201:CDL:H273	2.03	0.72
41:p:7:LYS:O	41:p:11:PRO:HA	1.89	0.72
42:q:56:PHE:HA	42:q:59:HIS:CD2	2.24	0.72
51:AG:79:GLU:HA	52:AH:58:ARG:NE	2.03	0.72
7:G:126:LEU:CD1	18:R:89:PRO:CB	2.68	0.72
12:L:556:ILE:CG2	38:m:80:PHE:CZ	2.72	0.72
13:M:243:MET:HE1	13:M:302:MET:HE3	1.71	0.72
20:U:79:ILE:HD11	20:U:148:ILE:HG22	1.71	0.72
49:Ae:249:ILE:HG12	49:Ae:254:ALA:HB3	1.69	0.72
4:D:375:MET:HE1	7:G:126:LEU:HA	1.71	0.72
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.69	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
12:L:569:LEU:HB2	24:Y:115:MET:CE	2.17	0.72
15:O:168:VAL:HG21	15:O:241:TYR:CZ	2.24	0.72
16:P:169:HIS:H	16:P:184:LYS:HE3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:34:PRO:HG2	36:k:59:TYR:HE1	1.54	0.72
49:AE:184:ILE:HG23	49:AE:208:PRO:HB2	1.71	0.72
49:Ae:167:PHE:H	49:Ae:174:LEU:H	1.36	0.72
4:D:90:ALA:HB2	8:H:205:SER:CA	2.18	0.72
12:L:316:THR:CG2	12:L:325:ALA:HB2	2.19	0.72
15:O:176:GLN:HB2	15:O:178:TYR:HD2	1.55	0.72
20:U:112:SER:HB2	39:n:17:LEU:HD11	1.72	0.72
47:AC:9:PRO:HG3	47:Ac:202:GLU:OE1	1.88	0.72
47:Ac:148:ASN:OD1	47:Ac:165:TRP:CH2	2.41	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
12:L:553:LEU:HD21	38:m:93:ALA:C	2.15	0.72
15:O:80:GLN:HG3	15:O:270:VAL:CG2	2.11	0.72
45:AA:74:TRP:CZ2	45:AA:411:GLU:HA	2.24	0.72
45:AA:249:HIS:O	45:AA:250:LEU:HB2	1.89	0.72
1:A:63:LEU:HD11	10:J:63:MET:HE3	1.69	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
8:H:111:LEU:HD21	10:J:60:LEU:HD12	1.71	0.72
10:J:165:ILE:HG23	14:N:42:PRO:HG3	1.69	0.72
12:L:576:LEU:HD12	12:L:577:THR:N	2.05	0.72
14:N:59:TYR:CE2	14:N:63:GLN:HG3	2.23	0.72
33:h:96:ALA:HB3	41:p:63:TYR:HD1	1.54	0.72
48:AD:306:MET:SD	49:AE:118:THR:HG22	2.29	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
47:Ac:141:TRP:CD1	47:Ac:265:PRO:HD3	2.24	0.72
50:Af:72:ARG:HG3	50:Af:74:GLN:HB2	1.71	0.72
15:O:238:GLU:HA	15:O:241:TYR:HD2	1.54	0.72
20:T:120:MET:HG2	22:W:44:ARG:HH11	1.54	0.72
33:h:163:ARG:HG2	33:h:165:ASP:CB	2.19	0.72
52:AH:48:LEU:CD2	52:AH:69:LEU:CD1	2.65	0.72
48:Ad:186:ARG:HE	48:Ad:193:LEU:HB2	1.53	0.72
9:I:200:GLU:OE2	42:q:93:MET:SD	2.48	0.72
12:L:141:PHE:HD2	13:M:370:PRO:HB3	1.54	0.72
12:L:299:LYS:HB2	12:L:354:GLN:HE21	1.55	0.72
49:AE:127:TYR:CD1	53:AJ:33:GLU:HA	2.25	0.72
45:Aa:58:ARG:NE	45:Aa:417:LEU:HD12	2.04	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
10:J:87:LEU:HG	10:J:91:PHE:CE2	2.25	0.71
12:L:9:LEU:HD22	34:i:82:VAL:HG13	1.72	0.71
49:AE:162:GLY:HA3	49:AE:180:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Ak:38:TRP:CD1	54:Ak:40:LEU:HB2	2.25	0.71
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.38	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
9:I:53:ALA:HB1	27:b:14:ALA:HB2	1.71	0.71
12:L:247:LEU:HD12	12:L:248:HIS:N	2.04	0.71
13:M:106:LEU:HD13	13:M:234:ILE:HG22	1.71	0.71
13:M:373:ILE:CG1	13:M:454:ILE:HD11	2.19	0.71
15:O:336:GLY:H	15:O:344:ASN:ND2	1.88	0.71
16:P:192:ARG:NH1	16:P:192:ARG:HA	2.05	0.71
49:Ae:207:LYS:NZ	49:Ae:268:ASP:HA	2.05	0.71
49:Ae:248:ARG:HA	49:Ae:257:ASN:CG	2.14	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
4:D:35:ARG:HH22	32:g:56:ASP:C	1.99	0.71
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
14:N:146:TYR:CD1	14:N:147:PRO:HD3	2.26	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:183:MET:HE2	57:I:302:PC1:H271	1.72	0.71
40:o:39:MET:HE1	40:o:58:TYR:HA	1.71	0.71
49:AE:156:LEU:H	49:AE:270:VAL:HA	1.55	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
4:D:249:LYS:HA	25:Z:19:ILE:HG23	1.73	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.72	0.71
57:I:302:PC1:H2D1	57:I:302:PC1:H291	1.71	0.71
12:L:358:LYS:HG2	39:n:80:TYR:CZ	2.26	0.71
13:M:263:LEU:HD11	38:m:102:TYR:HD1	1.54	0.71
14:N:273:ASN:ND2	24:Y:143:VAL:HA	2.04	0.71
37:l:38:PRO:HG2	38:m:71:ALA:HB2	1.73	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
45:AA:310:ILE:HG21	45:AA:379:LEU:HD21	1.73	0.71
48:Ad:95:PRO:HG2	52:Ah:85:PHE:HB3	1.72	0.71
1:A:90:MET:HE2	10:J:152:MET:HB3	1.71	0.71
4:D:52:MET:HE3	58:D:501:3PE:HN1	1.54	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
13:M:313:THR:HG21	13:M:456:GLY:HA3	1.71	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	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:HD23	1.72	0.71
20:U:144:ILE:O	20:U:148:ILE:HG12	1.91	0.71
23:X:93:ASN:OD1	23:X:94:MET:N	2.24	0.71
45:AA:50:VAL:HG13	45:AA:60:ALA:HB2	1.72	0.71
54:AK:10:TYR:CE2	50:Af:110:LYS:HG2	2.26	0.71
46:Ab:39:GLU:O	46:Ab:50:ALA:HA	1.91	0.71
49:Ae:230:ASP:H	49:Ae:242:HIS:CG	2.08	0.71
1:A:67:LEU:HD11	11:K:68:ALA:HB1	1.72	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
8:H:311:THR:O	25:Z:51:MET:HG3	1.91	0.71
25:Z:107:GLY:HA2	30:e:75:ARG:NH2	2.06	0.71
4:D:52:MET:HE2	58:D:501:3PE:C12	2.20	0.71
12:L:368:PHE:HB3	12:L:445:GLU:CD	2.15	0.71
13:M:220:HIS:CE1	13:M:231:LEU:HD23	2.26	0.71
16:P:170:LEU:O	16:P:171:ASN:OD1	2.09	0.71
49:AE:115:TYR:CD2	53:AJ:15:PHE:HB3	2.26	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
20:U:102:SER:O	20:U:141:PRO:HD3	1.91	0.71
38:m:45:ARG:O	38:m:45:ARG:HG2	1.90	0.71
48:AD:121:CYS:HB3	70:AD:401:HEC:CAB	2.21	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.70
13:M:373:ILE:HG12	13:M:454:ILE:CD1	2.20	0.70
14:N:275:CYS:SG	24:Y:139:PRO:CG	2.78	0.70
48:AD:167:ARG:HH12	48:AD:170:LYS:HG3	1.55	0.70
12:L:141:PHE:CD2	13:M:375:LEU:HD21	2.26	0.70
12:L:556:ILE:HG23	38:m:80:PHE:CE2	2.26	0.70
25:Z:69:ILE:HG23	27:b:54:PRO:HD3	1.73	0.70
26:a:3:PHE:CE2	62:a:101:CDL:HA4	2.26	0.70
49:Ae:168:LYS:H	49:Ae:173:PRO:HA	1.55	0.70
49:Ae:207:LYS:HB2	49:Ae:210:TRP:HB2	1.73	0.70
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.74	0.70
8:H:23:VAL:HG11	26:a:9:LEU:HD21	1.72	0.70
9:I:155:CYS:HG	55:I:303:SF4:FE4	1.08	0.70
13:M:388:TRP:CE2	38:m:109:ARG:HD2	2.26	0.70
14:N:237:THR:HG23	14:N:237:THR:O	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:67:GLN:HG2	18:R:109:LEU:CD2	2.21	0.70
38:m:127:ILE:CG2	41:p:136:THR:HG23	2.20	0.70
47:Ac:28:SER:HB2	62:Ac:406:CDL:HA21	1.73	0.70
2:B:116:ARG:O	8:H:39:ILE:HG22	1.91	0.70
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.70
7:G:617:ARG:HH11	22:W:129:HIS:HA	1.55	0.70
12:L:510:LYS:HE3	12:L:512:SER:HB3	1.72	0.70
14:N:313:MET:CG	15:O:305:LEU:HD22	2.22	0.70
14:N:342:GLN:HE21	29:d:30:ARG:HH11	1.38	0.70
22:W:42:TRP:CZ2	22:W:93:LEU:HA	2.26	0.70
49:AE:115:TYR:HD2	53:AJ:15:PHE:HB3	1.57	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
15:O:135:LEU:HB3	15:O:139:ARG:HH12	1.57	0.70
49:Ae:229:GLY:HA2	49:Ae:242:HIS:CD2	2.26	0.70
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.70
12:L:428:TYR:HA	12:L:432:MET:CG	2.20	0.70
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.74	0.70
49:AE:195:LEU:HD21	49:AE:248:ARG:HD2	1.72	0.70
2:B:89:SER:O	8:H:54:LYS:CE	2.40	0.70
12:L:559:GLU:O	12:L:564:LYS:HB2	1.92	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
12:L:25:ASN:HB2	33:h:72:LYS:HZ1	1.55	0.70
13:M:123:GLU:HB3	14:N:255:PRO:HG2	1.74	0.70
13:M:142:ARG:NH2	14:N:303:THR:HG22	2.05	0.70
18:R:70:ASN:HB2	18:R:111:PHE:HD1	1.55	0.70
22:W:32:LYS:CG	66:W:201:EHZ:C19	2.69	0.70
34:i:69:LEU:HD11	34:i:71:ALA:HB3	1.72	0.70
48:AD:183:GLU:HG2	48:Ad:159:ASN:O	1.91	0.70
49:AE:93:ARG:HA	51:AG:25:ARG:HG3	1.72	0.70
45:Aa:382:SER:HA	54:Ak:16:ASN:HD22	1.57	0.70
2:B:82:ILE:HA	8:H:57:MET:HE1	1.74	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.27	0.70
7:G:127:ASP:HA	18:R:106:TYR:OH	1.90	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
12:L:285:THR:HG22	12:L:415:ALA:CB	2.21	0.70
58:M:503:3PE:HN2	15:O:338:LYS:CE	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:12:VAL:HG13	21:V:13:GLY:H	1.56	0.70
46:Ab:36:GLN:CG	46:Ab:37:ASP:H	2.00	0.70
48:Ad:218:TYR:CD1	48:Ad:246:PRO:HG3	2.26	0.70
13:M:134:THR:O	13:M:142:ARG:HD2	1.91	0.70
14:N:254:LEU:HD12	14:N:255:PRO:HD3	1.72	0.70
24:Y:143:VAL:CG2	33:h:157:ARG:HG2	2.22	0.70
25:Z:12:PRO:HD3	25:Z:16:TYR:CZ	2.25	0.70
34:i:22:TRP:CD2	39:n:172:THR:HG22	2.26	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
10:J:144:MET:O	10:J:149:THR:HA	1.92	0.69
21:V:56:LEU:HD12	21:V:56:LEU:C	2.16	0.69
25:Z:86:ILE:HG23	25:Z:128:ARG:NE	2.06	0.69
45:AA:119:HIS:ND1	46:AB:298:HIS:HA	2.06	0.69
45:Aa:68:THR:HG22	45:Aa:136:LEU:HD23	1.73	0.69
49:Ae:235:TYR:CD1	49:Ae:242:HIS:CE1	2.80	0.69
54:Ak:7:GLY:O	54:Ak:11:ARG:HD3	1.92	0.69
2:B:95:PHE:HE2	2:B:131:MET:SD	2.15	0.69
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.69
12:L:142:ILE:HA	13:M:370:PRO:HB2	1.74	0.69
12:L:480:LEU:HD23	12:L:480:LEU:O	1.93	0.69
13:M:424:ILE:HG13	38:m:57:VAL:O	1.92	0.69
13:M:447:LEU:HD21	13:M:454:ILE:HD13	1.73	0.69
49:AE:156:LEU:HD22	49:AE:210:TRP:CE3	2.26	0.69
49:AE:169:TRP:CZ3	49:AE:273:VAL:HG11	2.27	0.69
47:Ac:147:THR:HG22	47:Ac:161:VAL:HG13	1.74	0.69
47:Ac:269:LYS:HE3	47:Ac:340:GLY:HA2	1.74	0.69
49:Ae:239:HIS:CE1	49:Ae:241:SER:CB	2.75	0.69
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.21	0.69
21:V:35:LEU:HA	21:V:38:PHE:CD1	2.27	0.69
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE1	2.27	0.69
46:Ab:305:THR:HG23	46:Ab:311:GLN:HE21	1.57	0.69
13:M:127:ILE:HD11	14:N:256:PRO:CG	2.22	0.69
20:T:100:VAL:HB	20:T:142:GLN:HB2	1.74	0.69
37:l:122:THR:HG21	37:l:129:MET:HE1	1.73	0.69
53:AJ:30:LEU:HA	54:AK:34:TRP:CD1	2.28	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
9:I:68:ARG:NH2	25:Z:26:PRO:HD2	2.08	0.69
42:q:3:LEU:HD12	42:q:6:VAL:CG2	2.22	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
58:L:703:3PE:H291	58:L:703:3PE:H3D1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:248:LEU:HD13	14:N:296:LEU:HD23	1.75	0.69
49:AE:231:PHE:CE1	49:AE:251:LYS:HB2	2.28	0.69
48:Ad:249:TYR:CZ	48:Ad:252:VAL:HA	2.28	0.69
52:Ah:42:VAL:HG13	52:Ah:45:ARG:HH21	1.57	0.69
4:D:35:ARG:O	4:D:36:GLN:C	2.35	0.69
4:D:253:LEU:HB2	43:r:23:LYS:CD	2.23	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.74	0.69
9:I:92:PRO:HA	42:q:91:HIS:O	1.93	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
12:L:353:GLU:OE1	39:n:80:TYR:OH	2.10	0.69
16:P:171:ASN:OD1	16:P:171:ASN:O	2.11	0.69
20:T:87:LEU:HD22	20:T:104:PHE:HE1	1.58	0.69
38:m:25:VAL:HA	38:m:30:ARG:HD3	1.73	0.69
49:Ae:229:GLY:H	49:Ae:233:GLY:HA2	1.57	0.69
49:Ae:265:PHE:CA	49:Ae:271:VAL:HG23	2.20	0.69
4:D:280:ALA:HB1	21:V:11:LEU:HG	1.74	0.69
6:F:225:LEU:H	17:Q:160:TYR:HE2	1.38	0.69
10:J:9:SER:OG	11:K:4:THR:HG23	1.93	0.69
12:L:149:ILE:HG13	13:M:369:LEU:HD12	1.75	0.69
13:M:216:LEU:HD11	13:M:236:LEU:HD11	1.72	0.69
13:M:369:LEU:HD23	13:M:371:PRO:CD	2.12	0.69
15:O:238:GLU:O	15:O:241:TYR:HB2	1.93	0.69
16:P:148:ILE:HB	16:P:149:PRO:HD3	1.74	0.69
40:o:19:PRO:HA	40:o:22:ILE:HD11	1.74	0.69
52:AH:48:LEU:CD2	52:AH:69:LEU:HD12	2.23	0.69
47:Ac:45:ILE:HA	67:Ac:401:HEM:HAB	1.75	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
7:G:126:LEU:HD11	18:R:89:PRO:CB	2.23	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
12:L:332:HIS:NE2	12:L:336:LYS:HG3	2.07	0.69
29:d:106:LYS:HB3	41:p:79:GLU:HB3	1.74	0.69
45:AA:50:VAL:HG22	45:AA:60:ALA:HB1	1.73	0.69
62:Ac:406:CDL:H511	51:Ag:38:VAL:HG13	1.75	0.69
52:Ah:35:CYS:HA	52:Ah:38:LEU:HD13	1.74	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.69
8:H:5:ASN:HD21	26:a:23:THR:HG23	1.58	0.69
8:H:136:VAL:HG13	10:J:69:TYR:CE1	2.28	0.69
12:L:18:PRO:O	12:L:21:ILE:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:138:LEU:HD13	20:T:144:ILE:CG1	2.22	0.69
52:AH:65:CYS:O	52:AH:69:LEU:HB3	1.92	0.69
48:Ad:214:LEU:HD11	48:Ad:237:PHE:HB2	1.75	0.69
49:Ae:230:ASP:N	49:Ae:242:HIS:CD2	2.59	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.23	0.68
12:L:436:ARG:HA	36:k:58:ARG:NH1	2.08	0.68
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.75	0.68
16:P:191:VAL:HA	16:P:194:VAL:HG22	1.73	0.68
36:k:34:PRO:CD	36:k:59:TYR:CD1	2.75	0.68
49:AE:200:HIS:HE1	49:AE:202:LEU:HB2	1.58	0.68
46:Ab:412:VAL:HG13	46:Ab:415:GLN:HE21	1.58	0.68
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.68
12:L:279:CYS:SG	57:L:706:PC1:H3D2	2.33	0.68
14:N:215:MET:HE2	14:N:248:LEU:CD2	2.23	0.68
21:V:72:LEU:HD11	21:V:80:VAL:CG2	2.19	0.68
23:X:50:GLU:HG3	23:X:56:CYS:SG	2.33	0.68
24:Y:77:CYS:SG	24:Y:78:VAL:N	2.66	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
8:H:30:TYR:CZ	26:a:1:MET:O	2.45	0.68
8:H:33:LEU:HD23	43:r:25:GLN:HG2	1.76	0.68
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.68
8:H:114:TYR:OH	10:J:60:LEU:O	2.11	0.68
8:H:224:PHE:CZ	61:H:400:UQ9:H13	2.28	0.68
11:K:66:PHE:HE2	14:N:35:PHE:CZ	2.11	0.68
12:L:279:CYS:SG	57:L:706:PC1:C3D	2.82	0.68
12:L:312:LEU:HD21	12:L:395:ILE:HG21	1.75	0.68
15:O:60:ILE:HD12	15:O:203:ALA:HB3	1.74	0.68
20:T:116:VAL:HG12	20:T:120:MET:HE2	1.75	0.68
37:l:78:LEU:HD11	37:l:104:PRO:HB2	1.74	0.68
49:AE:88:PHE:HB3	51:AG:19:LEU:CD1	2.20	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
12:L:385:PHE:CD1	35:j:72:ARG:HG3	2.29	0.68
58:M:503:3PE:H3D1	58:M:503:3PE:H2B2	1.76	0.68
46:AB:233:VAL:HA	46:AB:236:GLN:HG2	1.76	0.68
48:AD:249:TYR:CZ	48:AD:252:VAL:HA	2.27	0.68
49:AE:161:GLU:HA	49:AE:178:HIS:CD2	2.28	0.68
10:J:65:VAL:CG1	10:J:66:VAL:N	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:73:SER:HB3	41:p:100:GLN:HE21	1.58	0.68
15:O:140:LEU:HG	15:O:304:VAL:HG12	1.74	0.68
16:P:344:PRO:HD2	16:P:347:LEU:HD22	1.74	0.68
24:Y:96:GLY:HA3	24:Y:121:GLY:HA2	1.75	0.68
48:AD:235:PRO:HB3	52:AH:70:PHE:CE1	2.28	0.68
49:AE:221:GLY:O	49:AE:222:CYS:SG	2.51	0.68
49:Ae:219:HIS:CB	49:Ae:239:HIS:CD2	2.76	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
12:L:211:ILE:N	12:L:212:PRO:HD2	2.08	0.68
14:N:243:MET:HG2	29:d:44:MET:HE2	1.75	0.68
26:a:31:ASN:ND2	26:a:36:LYS:HB2	2.08	0.68
37:l:158:PRO:HD3	40:o:22:ILE:CB	2.23	0.68
43:r:20:LEU:C	43:r:20:LEU:HD12	2.18	0.68
45:AA:342:GLN:HE21	45:AA:357:HIS:HB3	1.59	0.68
4:D:34:ALA:HB3	13:M:86:LYS:NZ	2.09	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
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
14:N:215:MET:HE1	14:N:248:LEU:HD21	1.71	0.68
19:S:19:ILE:HD12	19:S:94:VAL:HG11	1.76	0.68
27:b:23:PHE:HZ	58:b:201:3PE:H351	1.58	0.68
40:o:31:PHE:CD1	40:o:34:ARG:HB3	2.29	0.68
46:AB:51:SER:HB2	46:AB:230:LEU:HD12	1.74	0.68
47:AC:16:HIS:CE1	47:AC:201:HIS:NE2	2.62	0.68
45:Aa:101:THR:HG22	45:Aa:154:SER:HA	1.76	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
62:L:704:CDL:HA62	33:h:68:LEU:HD13	1.76	0.68
16:P:192:ARG:NH2	16:P:200:ILE:HD11	2.09	0.68
20:U:100:VAL:O	20:U:141:PRO:HG2	1.94	0.68
49:AE:231:PHE:HE1	49:AE:251:LYS:HB2	1.58	0.68
48:Ad:159:ASN:HB3	48:Ad:162:GLY:O	1.93	0.68
49:Ae:218:THR:OG1	49:Ae:254:ALA:HB1	1.94	0.68
4:D:49:GLY:O	14:N:173:THR:HG21	1.93	0.68
12:L:357:ARG:HG2	39:n:32:ILE:HG12	1.76	0.68
13:M:39:LEU:HD23	13:M:67:ILE:HD13	1.74	0.68
13:M:311:GLY:HA2	13:M:314:MET:HE3	1.76	0.68
37:l:157:GLY:HA2	40:o:22:ILE:HG13	1.76	0.68
47:Ac:242:LEU:HD21	47:Ac:250:LEU:HD11	1.75	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:227:PRO:HG3	7:G:94:MET:SD	2.34	0.68
12:L:228:GLY:C	12:L:229:LEU:HG	2.19	0.68
12:L:358:LYS:HG2	39:n:80:TYR:CE1	2.29	0.68
37:l:122:THR:HG23	37:l:123:PRO:HD2	1.75	0.68
1:A:105:GLU:CG	1:A:111:LEU:HG	2.25	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
13:M:446:LEU:HD13	32:g:101:THR:HG21	1.75	0.67
27:b:23:PHE:HE1	58:b:201:3PE:H3A2	1.59	0.67
45:AA:338:CYS:N	45:AA:368:MET:SD	2.67	0.67
45:AA:384:THR:HB	54:AK:9:ARG:HG3	1.76	0.67
51:AG:11:ILE:CG2	51:AG:14:VAL:HG21	2.18	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
7:G:126:LEU:CD1	18:R:89:PRO:HB3	2.24	0.67
15:O:339:TYR:OH	58:O:401:3PE:N	2.27	0.67
29:d:5:ARG:HD2	29:d:89:ASP:OD2	1.93	0.67
32:g:140:PHE:CE2	41:p:74:ILE:CG2	2.77	0.67
37:l:152:SER:HA	40:o:5:LEU:HD21	1.76	0.67
47:AC:147:THR:HG22	47:AC:161:VAL:HG13	1.75	0.67
47:Ac:66:VAL:HA	47:Ac:69:ILE:HD12	1.76	0.67
2:B:94:THR:HB	2:B:104:MET:HE1	1.74	0.67
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.67
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
12:L:80:PHE:C	12:L:135:ASN:ND2	2.52	0.67
13:M:127:ILE:CG1	14:N:254:LEU:HD21	2.24	0.67
13:M:275:ILE:HD11	13:M:288:TYR:CD1	2.29	0.67
13:M:395:LEU:HD21	38:m:101:TRP:CE2	2.29	0.67
14:N:149:LEU:HD13	14:N:154:ILE:HG21	1.75	0.67
15:O:347:VAL:O	15:O:347:VAL:CG1	2.42	0.67
25:Z:126:GLY:HA3	30:e:76:MET:HE1	1.77	0.67
45:AA:43:GLN:HE22	46:AB:57:PRO:CA	2.07	0.67
48:AD:186:ARG:NE	48:AD:193:LEU:HB2	2.09	0.67
1:A:3:LEU:HD23	58:J:401:3PE:H251	1.75	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
12:L:141:PHE:CE2	13:M:375:LEU:HD22	2.08	0.67
13:M:30:TYR:O	13:M:34:ILE:HG12	1.95	0.67
14:N:26:LEU:HD23	14:N:29:MET:SD	2.35	0.67
15:O:114:LEU:HA	15:O:131:LEU:CD2	2.24	0.67
49:Ae:239:HIS:CD2	49:Ae:253:PRO:CD	2.70	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Af:92:GLU:HG2	50:Af:96:LYS:HE2	1.76	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
9:I:188:GLU:OE2	18:R:56:ASN:HB2	1.94	0.67
12:L:203:PHE:CZ	41:p:110:LEU:HD11	2.30	0.67
58:L:703:3PE:H252	58:L:703:3PE:H3A1	1.76	0.67
13:M:350:MET:HG2	39:n:99:VAL:HG12	1.77	0.67
32:g:109:ASP:CB	32:g:114:GLU:HB3	2.24	0.67
46:AB:51:SER:HB2	46:AB:230:LEU:CD1	2.24	0.67
49:AE:156:LEU:HB2	49:AE:269:ASP:C	2.19	0.67
45:Aa:401:SER:HA	45:Aa:404:ASP:CG	2.19	0.67
1:A:51:PHE:CD2	10:J:73:MET:HE3	2.29	0.67
1:A:67:LEU:CD1	11:K:68:ALA:HB3	2.24	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
9:I:188:GLU:CD	18:R:56:ASN:HB2	2.19	0.67
13:M:11:LEU:HB3	13:M:100:ILE:HD13	1.76	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
21:V:116:ILE:HG23	21:V:116:ILE:O	1.92	0.67
42:q:138:VAL:CG2	42:q:139:PRO:HD2	2.25	0.67
49:AE:153:GLU:HA	49:AE:272:VAL:HG13	1.76	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
8:H:136:VAL:HG13	10:J:69:TYR:HE1	1.59	0.67
12:L:187:VAL:HG22	13:M:383:MET:HG2	1.77	0.67
13:M:44:GLN:HE22	13:M:49:TYR:HA	1.58	0.67
13:M:285:LEU:HD13	13:M:342:MET:HE1	1.75	0.67
14:N:313:MET:HG3	15:O:305:LEU:HD22	1.76	0.67
16:P:197:GLU:HB3	16:P:259:VAL:CG2	2.24	0.67
37:l:106:HIS:HD2	37:l:107:TRP:H	1.43	0.67
53:Aj:30:LEU:HD22	53:Aj:31:PHE:CE1	2.30	0.67
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.05	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.67
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
35:j:47:PHE:HA	36:k:63:PHE:CZ	2.30	0.67
47:Ac:220:PHE:HE2	69:Ac:405:UQ6:H4M2	1.60	0.67
48:Ad:321:TYR:HB2	50:Af:61:PHE:CG	2.29	0.67
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.77	0.67
4:D:36:GLN:HE21	4:D:38:GLN:NE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:81:LYS:N	12:L:135:ASN:ND2	2.43	0.67
12:L:552:LEU:CD2	12:L:553:LEU:HD12	2.25	0.67
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.60	0.67
19:S:16:LEU:HB3	19:S:69:TYR:HD1	1.58	0.67
23:X:18:VAL:HG21	25:Z:74:LEU:HD11	1.75	0.67
29:d:14:LEU:O	29:d:14:LEU:CD1	2.37	0.67
46:AB:412:VAL:HG13	46:AB:415:GLN:HE21	1.58	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
9:I:93:LEU:O	42:q:93:MET:HG2	1.94	0.67
12:L:480:LEU:HD22	35:j:84:PHE:CD2	2.30	0.67
13:M:344:MET:HE1	38:m:59:HIS:NE2	2.10	0.67
16:P:94:LEU:HA	16:P:97:MET:HE3	1.77	0.67
24:Y:71:MET:HG3	24:Y:102:THR:CG2	2.26	0.67
49:AE:152:ILE:HG23	49:AE:274:GLY:N	2.09	0.67
1:A:51:PHE:CE2	10:J:73:MET:CE	2.78	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
9:I:54:THR:HG21	25:Z:33:TYR:CZ	2.29	0.66
12:L:180:ILE:HD11	13:M:400:ILE:HB	1.78	0.66
13:M:166:LEU:HD11	58:M:501:3PE:H11	1.77	0.66
13:M:270:ILE:HG22	13:M:271:MET:HE2	1.76	0.66
13:M:361:MET:CB	13:M:441:MET:HE3	2.25	0.66
16:P:192:ARG:HH22	16:P:198:ALA:CB	2.07	0.66
16:P:288:PHE:CZ	16:P:290:PRO:HB3	2.30	0.66
24:Y:76:THR:HG22	24:Y:92:TYR:HA	1.77	0.66
30:e:14:LEU:CD1	30:e:15:ASP:HB2	2.25	0.66
45:AA:341:PHE:CZ	45:AA:372:LEU:HD13	2.31	0.66
51:AG:11:ILE:CG2	51:AG:14:VAL:HG22	2.25	0.66
48:Ad:95:PRO:CG	52:Ah:85:PHE:HB3	2.25	0.66
49:Ae:272:VAL:HG12	49:Ae:274:GLY:H	1.59	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.74	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
11:K:22:PHE:CB	12:L:585:LYS:HG2	2.21	0.66
12:L:201:ILE:HG22	12:L:266:LEU:HD11	1.76	0.66
20:U:128:PHE:CZ	20:U:148:ILE:HD12	2.30	0.66
33:h:102:PRO:HD2	33:h:105:TYR:HB2	1.78	0.66
49:Ae:239:HIS:CE1	49:Ae:241:SER:HB2	2.30	0.66
15:O:124:ASN:O	32:g:51:MET:HE3	1.95	0.66
40:o:89:TYR:CE2	40:o:93:LEU:HD11	2.30	0.66
48:AD:117:TYR:HA	48:AD:121:CYS:HG	1.60	0.66
52:AH:48:LEU:HD11	52:AH:65:CYS:HB3	1.76	0.66
49:Ae:159:ILE:HG22	49:Ae:178:HIS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.93	0.66
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.60	0.66
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.25	0.66
12:L:522:PHE:O	12:L:527:GLY:N	2.25	0.66
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.78	0.66
58:L:702:3PE:O32	62:L:705:CDL:H812	1.94	0.66
15:O:209:VAL:HG12	15:O:260:SER:HB2	1.76	0.66
47:Ac:257:MET:HG3	48:Ad:203:ALA:HB1	1.78	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
7:G:246:ARG:NH2	17:Q:123:ASN:OD1	2.28	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
12:L:407:TRP:CE3	12:L:410:LEU:HD11	2.29	0.66
13:M:318:ALA:HB2	13:M:373:ILE:HG23	1.75	0.66
15:O:343:TYR:HD1	15:O:352:ILE:HG23	1.59	0.66
46:AB:164:VAL:CG2	49:AI:34:VAL:HG22	2.22	0.66
46:AB:229:VAL:O	46:AB:232:GLN:HG2	1.95	0.66
48:Ad:270:VAL:HG21	70:Ad:401:HEC:HBB3	1.78	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
8:H:207:LEU:O	8:H:208:VAL:C	2.38	0.66
9:I:35:THR:CG2	43:r:107:SER:HA	2.26	0.66
13:M:446:LEU:HD13	32:g:101:THR:CG2	2.26	0.66
20:T:87:LEU:CD2	20:T:104:PHE:CZ	2.78	0.66
20:T:130:ILE:HG23	20:T:131:PRO:HD2	1.77	0.66
58:i:201:3PE:H2B2	58:i:201:3PE:H342	1.76	0.66
51:Ag:19:LEU:HD23	51:Ag:24:GLN:HB3	1.77	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
9:I:80:GLU:OE2	43:r:26:LEU:CD1	2.44	0.66
12:L:174:TYR:CE1	58:L:701:3PE:H331	2.30	0.66
15:O:62:VAL:HA	15:O:205:ILE:O	1.96	0.66
18:R:42:ASP:HB3	18:R:44:ARG:HH11	1.61	0.66
22:W:121:PHE:HA	22:W:124:LYS:HE2	1.75	0.66
4:D:55:SER:HB2	12:L:575:THR:HG23	1.78	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
15:O:205:ILE:HD11	15:O:273:ILE:HG12	1.77	0.66
19:S:24:CYS:SG	19:S:61:VAL:O	2.53	0.66
20:T:83:VAL:HG22	20:T:126:PHE:CZ	2.31	0.66
21:V:72:LEU:HD12	21:V:72:LEU:C	2.19	0.66
40:o:25:PHE:CE2	40:o:109:LEU:HD22	2.31	0.66
41:p:70:ARG:CZ	41:p:91:GLN:HE21	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:CYS:C	3:C:81:ASP:N	2.48	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.74	0.66
10:J:56:PHE:O	10:J:60:LEU:HB3	1.96	0.66
12:L:116:ARG:HG2	12:L:120:TYR:CE2	2.31	0.66
15:O:48:LYS:HD2	15:O:288:ASP:HB2	1.78	0.66
15:O:200:PRO:HG3	15:O:282:PRO:HD2	1.77	0.66
16:P:169:HIS:H	16:P:184:LYS:CE	2.09	0.66
16:P:199:ILE:HD11	16:P:258:ALA:O	1.96	0.66
18:R:97:LYS:HE3	18:R:100:LYS:HD3	1.78	0.66
21:V:72:LEU:O	21:V:72:LEU:CD1	2.42	0.66
24:Y:141:PRO:HB2	33:h:161:ARG:NH1	2.11	0.66
49:AI:61:ALA:HB1	46:Ab:326:PHE:HA	1.77	0.66
47:Ac:57:SER:O	47:Ac:175:LEU:CD2	2.43	0.66
49:Ae:229:GLY:HA3	49:Ae:234:TYR:H	1.60	0.66
1:A:90:MET:CE	10:J:152:MET:HB3	2.26	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
12:L:66:TRP:HZ3	12:L:68:TRP:CD1	2.14	0.66
12:L:552:LEU:HD23	12:L:553:LEU:HD12	1.77	0.66
29:d:113:LEU:HD22	32:g:148:PRO:HG3	1.78	0.66
36:k:34:PRO:CG	36:k:59:TYR:CE1	2.72	0.66
1:A:8:PHE:HE1	58:J:401:3PE:H2C1	1.60	0.65
3:C:98:PHE:CA	21:V:90:LEU:HD11	2.19	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
14:N:25:ASN:ND2	30:e:18:PHE:CE2	2.65	0.65
15:O:38:TYR:HB3	15:O:299:GLN:NE2	2.11	0.65
49:AE:175:PHE:CZ	49:AE:223:VAL:HG13	2.29	0.65
49:AI:77:ARG:O	49:AI:78:PHE:C	2.38	0.65
47:Ac:128:PHE:CE2	47:Ac:146:ILE:HD11	2.30	0.65
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.26	0.65
2:B:91:TRP:CH2	61:H:400:UQ9:H1M	2.31	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
8:H:130:PHE:HD2	8:H:207:LEU:HD21	1.61	0.65
10:J:12:PHE:HE2	11:K:42:ILE:CD1	2.05	0.65
16:P:268:PRO:HG2	16:P:344:PRO:HA	1.76	0.65
20:U:134:ASP:OD2	39:n:2:ALA:N	2.29	0.65
28:c:72:ARG:HD2	29:d:20:SER:HA	1.78	0.65
38:m:15:PRO:CG	38:m:18:LEU:HD12	2.26	0.65
47:AC:38:GLY:O	47:AC:42:MET:HG3	1.96	0.65
45:Aa:478:LEU:HA	53:Aj:18:THR:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:HB1	10:J:66:VAL:HG13	1.78	0.65
1:A:94:LEU:HD22	10:J:152:MET:HE1	1.77	0.65
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.65
8:H:283:ASP:OD1	8:H:284:GLN:N	2.29	0.65
16:P:59:PHE:HB2	16:P:130:ILE:HD11	1.79	0.65
18:R:76:ILE:HD11	18:R:92:TYR:HB3	1.77	0.65
48:Ad:189:ASN:HB3	70:Ad:401:HEC:HMD2	1.77	0.65
52:Ah:27:PRO:HB3	52:Ah:87:ASN:CG	2.21	0.65
6:F:236:PHE:HA	17:Q:166:TRP:CD1	2.30	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.65
12:L:524:THR:HG22	39:n:78:GLN:HG2	1.78	0.65
14:N:220:MET:C	14:N:223:ASN:H	2.04	0.65
14:N:258:THR:HB	14:N:333:SER:O	1.96	0.65
19:S:16:LEU:HB3	19:S:69:TYR:CD1	2.32	0.65
21:V:38:PHE:CD1	21:V:95:LEU:HD21	2.31	0.65
48:AD:228:ARG:N	48:AD:231:LEU:HD12	2.11	0.65
54:AK:36:THR:O	54:AK:38:TRP:CD1	2.50	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
12:L:190:SER:HB2	12:L:196:TRP:HE1	1.61	0.65
12:L:445:GLU:OE2	35:j:54:GLN:HG3	1.97	0.65
12:L:542:LEU:HB3	13:M:278:ARG:HD2	1.77	0.65
62:L:705:CDL:HA22	62:L:705:CDL:H512	1.79	0.65
62:L:705:CDL:H591	24:Y:68:ILE:HD12	1.77	0.65
19:S:58:CYS:HB2	19:S:61:VAL:HG12	1.78	0.65
48:AD:181:ASN:HB2	48:AD:182:PRO:HD2	1.78	0.65
48:AD:202:ARG:HG3	48:AD:278:SER:HB3	1.78	0.65
2:B:93:MET:HE1	2:B:131:MET:HE2	1.78	0.65
4:D:47:PHE:HB3	14:N:227:ILE:CD1	2.13	0.65
13:M:367:LEU:CD2	13:M:408:MET:HE2	2.25	0.65
18:R:70:ASN:HB2	18:R:111:PHE:CD1	2.31	0.65
32:g:108:PRO:O	32:g:109:ASP:OD1	2.13	0.65
35:j:94:ASP:HB3	35:j:99:ILE:HB	1.78	0.65
37:l:82:SER:HA	37:l:112:TYR:HB3	1.79	0.65
45:Aa:279:ASP:HA	51:Ag:12:ARG:HA	1.79	0.65
48:Ad:186:ARG:HB3	48:Ad:191:GLY:HA2	1.78	0.65
51:Ag:11:ILE:CG2	51:Ag:14:VAL:HG22	2.25	0.65
12:L:88:LEU:HD23	12:L:326:PHE:CE2	2.32	0.65
16:P:236:VAL:CG1	16:P:270:ARG:HH21	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:30:TRP:CD2	39:n:76:HIS:HD2	2.15	0.65
45:AA:68:THR:HG21	46:AB:384:MET:HG3	1.79	0.65
45:AA:413:ILE:HG12	45:AA:423:ARG:HD3	1.78	0.65
45:AA:452:GLN:C	45:AA:472:ARG:HH12	2.05	0.65
47:AC:137:GLN:CG	47:AC:265:PRO:HG3	2.27	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
9:I:79:ARG:HG2	43:r:12:ARG:HH21	1.62	0.65
10:J:37:PHE:HZ	58:J:401:3PE:C29	2.10	0.65
12:L:70:THR:HG21	41:p:101:GLU:OE2	1.96	0.65
20:T:118:ILE:HG23	20:T:122:MET:HE3	1.78	0.65
28:c:55:TRP:CZ2	29:d:66:THR:HG22	2.31	0.65
31:f:38:ARG:NH1	31:f:54:VAL:HB	2.11	0.65
37:l:162:PRO:HG3	40:o:39:MET:HE3	1.78	0.65
48:Ad:270:VAL:HG11	70:Ad:401:HEC:CBB	2.26	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
10:J:68:GLY:HA2	10:J:71:THR:HB	1.78	0.65
12:L:387:THR:HG22	12:L:465:GLY:H	1.61	0.65
14:N:23:SER:HB2	30:e:15:ASP:OD2	1.96	0.65
15:O:343:TYR:CE1	15:O:355:LYS:HB2	2.31	0.65
16:P:191:VAL:HG13	16:P:192:ARG:NH2	2.12	0.65
16:P:226:VAL:HG21	16:P:281:PHE:CZ	2.31	0.65
48:AD:270:VAL:HG21	70:AD:401:HEC:HBB3	1.77	0.65
46:Ab:261:GLN:HA	46:Ab:442:GLY:O	1.97	0.65
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.14	0.65
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.78	0.65
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.65
13:M:122:PHE:HD1	13:M:238:LEU:HG	1.62	0.65
13:M:127:ILE:HG12	14:N:254:LEU:HD21	1.77	0.65
15:O:117:PHE:CE1	15:O:173:MET:CE	2.77	0.65
23:X:124:GLN:O	27:b:70:PRO:HB2	1.97	0.65
23:X:162:LYS:HB3	23:X:166:ARG:HH21	1.61	0.65
41:p:24:THR:HG22	41:p:26:LEU:H	1.62	0.65
47:Ac:141:TRP:HD1	47:Ac:265:PRO:HD3	1.62	0.65
48:Ad:170:LYS:HD2	49:Ae:151:LYS:HE2	1.79	0.65
53:Aj:34:ARG:HG3	53:Aj:35:ALA:N	2.11	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.97	0.64
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
12:L:368:PHE:HB3	12:L:445:GLU:OE2	1.97	0.64
32:g:140:PHE:CE2	41:p:74:ILE:HG22	2.32	0.64
58:i:201:3PE:H292	58:i:201:3PE:H332	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:71:ARG:HB3	40:o:71:ARG:HH11	1.61	0.64
46:AB:300:LYS:HG2	46:AB:301:ARG:HG3	1.79	0.64
48:AD:138:VAL:HG11	48:AD:276:TRP:NE1	2.11	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
13:M:119:TYR:CD1	13:M:160:LEU:HD22	2.32	0.64
13:M:307:TRP:CD1	13:M:459:MET:SD	2.91	0.64
15:O:194:THR:HG23	15:O:307:TYR:HB2	1.79	0.64
16:P:88:VAL:HG12	16:P:92:MET:HE2	1.80	0.64
18:R:112:LYS:O	18:R:113:GLN:C	2.40	0.64
33:h:127:ASP:OD1	33:h:127:ASP:O	2.15	0.64
41:p:74:ILE:HD13	41:p:85:ILE:HG13	1.80	0.64
51:Ag:77:MET:HE3	51:Ag:78:TYR:CE2	2.32	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.64
8:H:33:LEU:CD2	43:r:25:GLN:HG2	2.26	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
13:M:167:ILE:O	13:M:171:VAL:HG12	1.98	0.64
13:M:300:SER:HB3	13:M:381:ILE:HG23	1.78	0.64
14:N:307:THR:HG22	14:N:308:ASN:N	2.12	0.64
23:X:167:PHE:HD2	23:X:170:TRP:NE1	1.94	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
45:AA:55:ASN:HD21	45:AA:251:SER:C	2.05	0.64
46:AB:48:VAL:HG22	46:AB:219:ALA:CB	2.21	0.64
47:AC:141:TRP:HD1	47:AC:265:PRO:HD3	1.61	0.64
45:Aa:249:HIS:O	45:Aa:250:LEU:HB2	1.97	0.64
47:Ac:137:GLN:HE21	47:Ac:265:PRO:HD3	1.62	0.64
48:Ad:244:MET:HB2	70:Ad:401:HEC:ND	2.11	0.64
52:Ah:26:ASP:HB3	52:Ah:29:THR:HG23	1.79	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	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
58:M:503:3PE:C12	15:O:338:LYS:HE3	2.28	0.64
15:O:238:GLU:HA	15:O:241:TYR:CD2	2.32	0.64
17:Q:163:ASN:OD1	17:Q:164:PHE:N	2.31	0.64
46:AB:48:VAL:CG2	46:AB:400:ALA:HB1	2.27	0.64
47:Ac:253:PRO:O	48:Ad:203:ALA:HA	1.98	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:22:PHE:O	12:L:585:LYS:HE3	1.97	0.64
12:L:40:ILE:HD13	12:L:97:THR:HG22	1.79	0.64
12:L:366:MET:CG	12:L:443:ILE:HG21	2.28	0.64
29:d:109:TYR:HA	29:d:112:ILE:CG2	2.28	0.64
36:k:38:VAL:HG13	39:n:39:TYR:HB2	1.78	0.64
40:o:105:GLU:O	40:o:106:ARG:C	2.39	0.64
45:AA:341:PHE:CE1	45:AA:372:LEU:HD13	2.32	0.64
48:Ad:112:ARG:HD3	48:Ad:257:ASP:OD2	1.97	0.64
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HA	1.80	0.64
49:Ae:160:PRO:HD2	49:Ae:163:LYS:HE3	1.78	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	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
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.78	0.64
15:O:347:VAL:CG1	28:c:29:PHE:HA	2.28	0.64
20:T:138:LEU:O	20:T:138:LEU:CD1	2.40	0.64
29:d:60:ARG:O	29:d:61:GLN:C	2.40	0.64
34:i:101:LYS:HG2	41:p:116:ARG:O	1.97	0.64
48:AD:218:TYR:CD1	48:AD:246:PRO:HG3	2.32	0.64
49:AE:178:HIS:HD2	49:AE:179:ARG:H	1.43	0.64
52:AH:48:LEU:HD21	52:AH:69:LEU:HD12	1.80	0.64
49:Ae:154:ILE:O	49:Ae:270:VAL:HG13	1.97	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
8:H:172:MET:HE1	25:Z:46:GLY:HA2	1.79	0.64
13:M:175:ASN:ND2	33:h:143:GLU:HG2	2.13	0.64
14:N:37:LEU:HD12	14:N:63:GLN:HB3	1.79	0.64
14:N:179:MET:HG3	14:N:216:PHE:HE1	1.63	0.64
18:R:32:THR:HG22	18:R:36:GLN:N	2.09	0.64
19:S:69:TYR:CD2	19:S:75:LYS:HG3	2.33	0.64
20:T:83:VAL:HG23	20:T:126:PHE:HZ	1.62	0.64
41:p:5:TRP:HH2	41:p:12:GLU:OE1	1.81	0.64
47:AC:148:ASN:OD1	49:Ae:220:LEU:C	2.40	0.64
48:AD:323:PRO:HG2	48:AD:325:LYS:HD2	1.80	0.64
49:AE:200:HIS:CE1	49:AE:202:LEU:HB2	2.32	0.64
49:AI:60:ALA:HA	46:Ab:170:GLN:NE2	2.13	0.64
48:Ad:248:ILE:HG22	48:Ad:263:MET:HG3	1.79	0.64
48:Ad:262:THR:HG22	52:Ah:24:LEU:HG	1.78	0.64
12:L:246:LEU:HD12	12:L:246:LEU:C	2.23	0.64
15:O:323:GLN:HE22	32:g:54:GLN:HB3	1.63	0.64
20:T:87:LEU:HD21	20:T:104:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:65:GLY:HA2	23:X:68:LEU:HD12	1.78	0.64
39:n:31:CYS:SG	39:n:36:LYS:NZ	2.71	0.64
45:AA:92:PHE:CZ	45:AA:161:ILE:HG23	2.33	0.64
48:AD:156:ASP:HB3	48:AD:165:PHE:HD2	1.63	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
12:L:446:ASN:ND2	35:j:51:THR:HG21	2.12	0.64
13:M:160:LEU:HD11	13:M:203:PHE:CZ	2.33	0.64
25:Z:86:ILE:HA	25:Z:128:ARG:HH21	1.62	0.64
36:k:47:LEU:HD12	39:n:43:LEU:HD23	1.79	0.64
48:AD:255:TYR:OH	48:AD:266:VAL:HA	1.98	0.64
49:AE:178:HIS:NE2	49:AE:209:GLU:HB2	2.12	0.64
52:AH:31:VAL:HG21	52:AH:84:LEU:HA	1.79	0.64
49:Ae:161:GLU:HA	49:Ae:178:HIS:HB3	1.80	0.64
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.33	0.64
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.64
8:H:111:LEU:HD22	10:J:60:LEU:HD11	1.77	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
10:J:125:MET:HB2	25:Z:137:ASN:OD1	1.98	0.64
12:L:446:ASN:HD21	35:j:51:THR:HG21	1.63	0.64
14:N:143:ILE:HA	14:N:194:LEU:HD11	1.79	0.64
23:X:37:ASP:OD1	23:X:38:LYS:N	2.31	0.64
34:i:29:SER:HB2	34:i:32:GLU:OE1	1.97	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	2.67	0.64
45:AA:274:GLU:HG3	45:AA:456:VAL:HB	1.80	0.64
46:AB:307:SER:HB2	46:AB:310:SER:HB2	1.78	0.64
49:AE:122:THR:HG21	53:AJ:25:ILE:HD13	1.80	0.64
49:Ae:261:PRO:HB2	49:Ae:273:VAL:CG1	2.27	0.64
2:B:92:PRO:HD2	2:B:120:VAL:HG12	1.80	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.29	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
16:P:333:PRO:HB2	16:P:337:ASP:CB	2.25	0.63
48:AD:167:ARG:HB2	48:AD:168:PRO:HD2	1.79	0.63
46:Ab:426:LYS:O	46:Ab:429:LYS:HG2	1.97	0.63
2:B:94:THR:CB	2:B:104:MET:HE1	2.27	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.32	0.63
14:N:220:MET:HA	14:N:223:ASN:HA	1.79	0.63
16:P:284:THR:HG23	16:P:356:HIS:HB2	1.79	0.63
25:Z:65:LEU:O	25:Z:68:ARG:HG2	1.98	0.63
32:g:147:LEU:HD11	41:p:163:MET:HB3	1.79	0.63
40:o:31:PHE:CE2	40:o:104:ARG:NH1	2.63	0.63
45:AA:96:LEU:HD11	45:AA:161:ILE:HG12	1.79	0.63
45:AA:204:PRO:HB2	45:AA:206:GLU:OE1	1.98	0.63
46:AB:297:PRO:HB3	46:AB:302:GLY:C	2.23	0.63
48:AD:167:ARG:NH2	48:AD:173:ASP:HB2	2.13	0.63
48:Ad:255:TYR:OH	48:Ad:266:VAL:HA	1.98	0.63
1:A:63:LEU:CD1	10:J:63:MET:CE	2.76	0.63
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	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:196:TRP:HZ3	13:M:261:PHE:HE2	1.44	0.63
16:P:180:SER:O	16:P:184:LYS:HG3	1.98	0.63
21:V:38:PHE:CE1	21:V:95:LEU:HD21	2.33	0.63
32:g:75:ASP:OD1	32:g:76:SER:N	2.32	0.63
48:AD:248:ILE:HG22	48:AD:263:MET:HG3	1.79	0.63
49:AE:201:ASP:HB3	49:AE:248:ARG:NH1	2.13	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
12:L:100:ILE:HD13	12:L:341:MET:SD	2.38	0.63
12:L:145:GLU:HB3	13:M:370:PRO:CG	2.28	0.63
12:L:305:SER:HB2	12:L:422:TYR:CE1	2.34	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
13:M:368:ALA:HB1	13:M:375:LEU:CD1	2.25	0.63
13:M:422:HIS:HB3	38:m:51:TYR:CE2	2.33	0.63
15:O:176:GLN:HB2	15:O:178:TYR:CD2	2.32	0.63
19:S:16:LEU:HD12	19:S:16:LEU:C	2.22	0.63
19:S:16:LEU:HA	19:S:69:TYR:HA	1.79	0.63
25:Z:70:ALA:O	25:Z:73:PRO:HD2	1.99	0.63
36:k:34:PRO:HG2	36:k:59:TYR:CD1	2.34	0.63
46:AB:40:PHE:CZ	46:AB:48:VAL:HB	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:402:HIS:CE1	45:Aa:403:LEU:HG	2.33	0.63
45:Aa:405:GLY:O	45:Aa:409:VAL:HG23	1.98	0.63
46:Ab:60:ARG:HD2	46:Ab:393:LEU:HD13	1.81	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
12:L:80:PHE:C	12:L:135:ASN:HD21	2.06	0.63
12:L:381:THR:HG21	12:L:498:PHE:CE2	2.33	0.63
12:L:410:LEU:HD12	12:L:411:ILE:N	2.13	0.63
13:M:118:PHE:O	13:M:122:PHE:N	2.25	0.63
13:M:220:HIS:NE2	13:M:231:LEU:HB3	2.13	0.63
16:P:93:HIS:NE2	16:P:94:LEU:HD11	2.14	0.63
20:T:93:ILE:CG2	20:T:110:LEU:HD13	2.28	0.63
30:e:69:ARG:HD2	30:e:72:THR:HG21	1.80	0.63
39:n:95:GLU:HA	39:n:98:LYS:HG3	1.81	0.63
48:AD:227:LEU:HB3	48:AD:231:LEU:HB2	1.81	0.63
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE3	2.32	0.63
46:Ab:230:LEU:HA	46:Ab:233:VAL:HG22	1.80	0.63
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.79	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
12:L:202:MET:HE3	12:L:265:PRO:CG	2.25	0.63
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.80	0.63
14:N:131:LEU:O	14:N:135:LYS:HG2	1.98	0.63
14:N:149:LEU:HD13	14:N:154:ILE:CG2	2.28	0.63
20:U:140:CYS:SG	20:U:143:GLU:OE2	2.53	0.63
23:X:83:THR:HA	23:X:86:TRP:CD1	2.34	0.63
43:r:109:ASP:O	43:r:110:GLN:HG2	1.99	0.63
49:AE:146:VAL:HG11	47:Ac:167:GLY:HA2	1.80	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.63
8:H:111:LEU:HD21	10:J:60:LEU:HD11	1.69	0.63
35:j:52:ARG:HG3	35:j:56:ILE:HD12	1.78	0.63
45:AA:182:VAL:HG12	45:AA:186:TYR:CE2	2.33	0.63
49:AE:168:LYS:N	49:AE:174:LEU:H	1.96	0.63
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CE2	2.34	0.63
49:Ae:155:LYS:HZ3	49:Ae:157:SER:HB3	1.64	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
12:L:361:ASN:OD1	12:L:361:ASN:O	2.17	0.63
58:L:702:3PE:H361	14:N:164:MET:HE1	1.81	0.63
58:M:502:3PE:H2A1	62:h:201:CDL:H202	1.80	0.63
15:O:305:LEU:HD12	15:O:305:LEU:C	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:326:ARG:HH21	32:g:56:ASP:CG	2.07	0.63
19:S:15:GLY:HA3	19:S:17:ARG:HH22	1.63	0.63
34:i:28:LEU:HD22	34:i:32:GLU:HG2	1.79	0.63
42:q:6:VAL:HA	42:q:9:ARG:HG2	1.79	0.63
46:AB:426:LYS:O	46:AB:429:LYS:HG2	1.97	0.63
48:AD:129:TYR:HD2	48:AD:198:SER:CB	2.12	0.63
52:Ah:82:HIS:HB3	52:Ah:83:LYS:HZ3	1.64	0.63
1:A:56:PHE:HB2	10:J:73:MET:HE1	1.81	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.63
14:N:158:ALA:O	14:N:162:ILE:HG12	1.99	0.63
19:S:16:LEU:CD2	19:S:19:ILE:HD11	2.28	0.63
20:T:103:HIS:CD2	20:T:106:LYS:HD2	2.34	0.63
22:W:55:LEU:CB	22:W:107:MET:CE	2.75	0.63
33:h:155:GLU:O	33:h:159:LEU:HD13	1.99	0.63
48:Ad:106:ASP:O	48:Ad:107:HIS:HB2	1.97	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
9:I:188:GLU:HG3	18:R:55:VAL:HA	1.80	0.62
13:M:129:THR:HG21	13:M:235:LEU:HD13	1.80	0.62
20:U:74:LEU:N	20:U:74:LEU:HD12	2.15	0.62
39:n:141:GLN:O	39:n:144:THR:HG22	1.99	0.62
40:o:18:ASP:OD1	40:o:19:PRO:HD2	1.99	0.62
46:Ab:305:THR:O	46:Ab:305:THR:HG22	1.97	0.62
47:Ac:376:MET:HE2	50:Af:17:PHE:CE1	2.34	0.62
1:A:52:SER:HB2	1:A:54:LYS:HG2	1.78	0.62
58:D:501:3PE:H272	14:N:288:LEU:HD13	1.81	0.62
5:E:230:LEU:HD11	6:F:48:ARG:HE	1.64	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
8:H:195:ARG:O	8:H:199:ASP:HB2	1.99	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:395:LEU:HD21	38:m:101:TRP:CZ2	2.33	0.62
41:p:66:ARG:HD2	41:p:68:TYR:CZ	2.34	0.62
46:Ab:92:LYS:HG2	46:Ab:145:GLU:HG3	1.81	0.62
49:Ae:194:GLN:HB3	49:Ae:250:ARG:HE	1.63	0.62
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	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
38:m:127:ILE:HG22	41:p:136:THR:HG23	1.81	0.62
45:AA:74:TRP:HZ2	45:AA:411:GLU:HA	1.63	0.62
45:AA:80:ARG:NH2	45:AA:268:CYS:SG	2.72	0.62
47:Ac:138:MET:CE	47:Ac:268:ILE:HG23	2.29	0.62
1:A:108:GLN:HE21	10:J:167:ILE:HG21	1.63	0.62
4:D:260:GLU:HG3	25:Z:25:LEU:HD22	1.80	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
12:L:365:ILE:HD11	12:L:366:MET:HE2	1.81	0.62
13:M:16:TRP:HZ2	58:M:503:3PE:H282	1.64	0.62
15:O:61:THR:HB	15:O:160:GLU:O	2.00	0.62
22:W:55:LEU:CB	22:W:107:MET:HE2	2.30	0.62
45:AA:120:LEU:HB3	46:AB:299:ILE:HG13	1.80	0.62
47:Ac:63:PHE:O	47:Ac:67:THR:HG23	1.99	0.62
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.35	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
11:K:51:SER:HA	30:e:32:ARG:HD3	1.80	0.62
13:M:98:MET:SD	58:M:503:3PE:H3C1	2.40	0.62
13:M:307:TRP:CE3	13:M:383:MET:HE3	2.34	0.62
13:M:318:ALA:CB	13:M:373:ILE:HG23	2.29	0.62
20:T:103:HIS:ND1	20:T:140:CYS:SG	2.73	0.62
23:X:115:LEU:HD13	23:X:117:TRP:CH2	2.34	0.62
25:Z:58:ARG:NH2	27:b:49:THR:HG21	2.13	0.62
40:o:17:PRO:HG3	40:o:106:ARG:HA	1.82	0.62
53:AJ:18:THR:HG22	54:AK:24:TRP:HH2	1.64	0.62
49:Ae:214:ILE:HD11	49:Ae:261:PRO:HB3	1.82	0.62
2:B:194:CYS:O	55:B:301:SF4:S2	2.58	0.62
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.62
8:H:25:ARG:HD2	61:H:400:UQ9:H10A	1.80	0.62
11:K:93:LEU:CD2	14:N:54:GLU:HG2	2.30	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
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.64	0.62
16:P:240:VAL:HB	16:P:266:THR:O	2.00	0.62
38:m:129:TYR:CZ	41:p:144:LEU:O	2.53	0.62
39:n:168:TRP:O	39:n:172:THR:OG1	2.18	0.62
40:o:5:LEU:HB3	40:o:9:TYR:CE2	2.34	0.62
47:AC:141:TRP:CH2	49:Ae:223:VAL:HG23	2.35	0.62
45:Aa:204:PRO:HB2	45:Aa:206:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:412:VAL:O	46:Ab:415:GLN:HG2	2.00	0.62
48:Ad:268:LYS:HE3	52:Ah:85:PHE:HE1	1.63	0.62
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.79	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.29	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
58:L:703:3PE:H3C1	58:L:703:3PE:H271	1.81	0.62
13:M:56:PHE:HE1	13:M:108:MET:HG2	1.64	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
16:P:297:VAL:O	16:P:300:TRP:HB3	1.98	0.62
24:Y:64:THR:OG1	24:Y:106:ARG:HG2	2.00	0.62
43:r:20:LEU:HD12	43:r:21:GLN:N	2.14	0.62
45:AA:182:VAL:CG1	45:AA:186:TYR:CE2	2.83	0.62
48:Ad:141:THR:HG22	53:Aj:53:TRP:CZ2	2.28	0.62
48:Ad:189:ASN:HB3	70:Ad:401:HEC:CMD	2.29	0.62
49:Ae:239:HIS:CE1	49:Ae:241:SER:HB3	2.35	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.82	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
12:L:542:LEU:HD21	37:l:116:ARG:HD2	1.81	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	1.65	0.62
46:AB:412:VAL:O	46:AB:415:GLN:HG2	2.00	0.62
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.62
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.48	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
11:K:1:MET:N	11:K:2:PRO:HD2	2.15	0.62
12:L:437:PHE:CE1	12:L:441:ILE:CG1	2.69	0.62
13:M:98:MET:HE3	13:M:128:PRO:HA	1.81	0.62
34:i:69:LEU:HD12	34:i:71:ALA:N	2.14	0.62
38:m:17:THR:O	38:m:18:LEU:HB2	1.99	0.62
45:Aa:382:SER:HB2	54:Ak:13:LEU:HD22	1.82	0.62
45:Aa:463:GLU:OE1	51:Ag:8:LEU:HB2	2.00	0.62
49:Ae:167:PHE:HD2	49:Ae:174:LEU:HB3	1.65	0.62
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:L:550:LEU:HB2	13:M:275:ILE:HG22	1.82	0.62
14:N:109:ALA:CB	14:N:110:PRO:HD3	2.30	0.62
19:S:23:LEU:O	19:S:23:LEU:CD1	2.41	0.62
25:Z:28:ARG:HG3	25:Z:28:ARG:O	1.99	0.62
27:b:11:ASN:O	27:b:15:LYS:N	2.31	0.62
48:AD:235:PRO:HA	48:AD:240:GLN:HG3	1.82	0.62
47:Ac:107:TYR:HB2	47:Ac:305:PRO:HG3	1.80	0.62
48:Ad:124:CYS:SG	70:Ad:401:HEC:CAC	2.88	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.61
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.81	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
7:G:651:PRO:CD	19:S:56:ARG:HB3	2.30	0.61
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.61
8:H:306:SER:HG	8:H:310:PHE:HE2	1.30	0.61
14:N:218:ALA:HB1	14:N:240:MET:SD	2.40	0.61
15:O:140:LEU:HD11	15:O:198:TYR:CZ	2.35	0.61
23:X:164:GLY:O	23:X:165:THR:C	2.41	0.61
27:b:23:PHE:CE1	58:b:201:3PE:H371	2.35	0.61
41:p:5:TRP:CH2	41:p:12:GLU:OE1	2.53	0.61
45:AA:169:LEU:HD11	45:AA:209:ARG:HG2	1.82	0.61
48:Ad:124:CYS:HA	48:Ad:179:TYR:CE2	2.33	0.61
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.65	0.61
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.61
7:G:176:CYS:SG	55:G:802:SF4:FE4	1.78	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
7:G:617:ARG:NH1	22:W:129:HIS:HA	2.14	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
58:K:101:3PE:H3C1	12:L:593:ILE:HD11	1.82	0.61
12:L:10:LEU:HD23	12:L:46:ILE:HG21	1.82	0.61
12:L:141:PHE:CE2	13:M:370:PRO:CG	2.76	0.61
12:L:466:PHE:CB	35:j:68:TRP:CZ2	2.71	0.61
20:U:128:PHE:CZ	20:U:148:ILE:HG23	2.35	0.61
23:X:69:ASN:O	23:X:73:GLN:HG3	2.00	0.61
30:e:95:PRO:HD2	30:e:98:HIS:CE1	2.34	0.61
37:l:57:MET:HG2	37:l:104:PRO:HG2	1.82	0.61
50:AF:108:TRP:CZ2	46:Ab:101:ARG:HB3	2.35	0.61
51:Ag:72:ARG:HD3	51:Ag:73:LYS:H	1.63	0.61
52:Ah:27:PRO:HB2	52:Ah:88:LEU:HD23	1.81	0.61
52:Ah:46:GLU:O	52:Ah:50:LEU:HG	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.36	0.61
3:C:80:LEU:H	3:C:80:LEU:HD22	1.64	0.61
5:E:71:GLU:HB2	44:s:59:GLN:HB3	1.82	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
12:L:149:ILE:HG21	13:M:364:LEU:HD21	1.83	0.61
12:L:556:ILE:HD11	38:m:76:ILE:HG22	1.82	0.61
12:L:559:GLU:HA	12:L:563:PRO:HG2	1.82	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
13:M:151:PHE:CE2	14:N:291:PHE:HB2	2.34	0.61
14:N:175:MET:HE1	14:N:227:ILE:HA	1.80	0.61
15:O:117:PHE:HD1	15:O:128:SER:HA	1.64	0.61
18:R:98:GLU:CD	18:R:98:GLU:H	2.07	0.61
38:m:100:PHE:O	38:m:104:VAL:HG23	2.00	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
62:L:705:CDL:H581	62:L:705:CDL:H762	1.81	0.61
13:M:158:ILE:HG12	14:N:287:LEU:HD11	1.82	0.61
13:M:373:ILE:H	13:M:448:THR:HG22	1.65	0.61
14:N:17:PRO:HG2	14:N:133:TRP:CE2	2.35	0.61
15:O:213:GLU:O	15:O:217:ARG:HG3	2.00	0.61
33:h:106:ILE:O	33:h:106:ILE:HG22	1.99	0.61
40:o:5:LEU:HB3	40:o:9:TYR:CD2	2.36	0.61
40:o:22:ILE:HA	40:o:105:GLU:OE2	2.00	0.61
40:o:111:ARG:NH1	40:o:115:ARG:HD3	2.14	0.61
42:q:71:LYS:O	42:q:72:ASN:CG	2.43	0.61
50:Af:110:LYS:O	50:Af:111:LYS:C	2.43	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
12:L:468:ILE:O	12:L:472:ILE:HG23	2.00	0.61
62:L:704:CDL:H571	62:L:704:CDL:H792	1.82	0.61
13:M:139:GLN:HB3	13:M:222:GLU:HG3	1.83	0.61
13:M:422:HIS:NE2	13:M:425:ASN:OD1	2.33	0.61
13:M:433:GLU:O	13:M:437:MET:HG2	2.01	0.61
58:M:501:3PE:H112	14:N:276:LEU:HD21	1.81	0.61
42:q:3:LEU:HD12	42:q:6:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:253:PRO:HG3	48:AD:205:HIS:HA	1.82	0.61
48:AD:156:ASP:HB3	48:AD:165:PHE:CD2	2.36	0.61
49:AE:156:LEU:HD22	49:AE:210:TRP:CD2	2.35	0.61
45:Aa:193:GLN:OE1	45:Aa:271:THR:HG21	1.99	0.61
2:B:93:MET:HB2	2:B:128:ALA:CB	2.30	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	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
13:M:98:MET:HE1	13:M:128:PRO:HA	1.83	0.61
13:M:143:LEU:HD21	14:N:303:THR:HG23	1.80	0.61
13:M:318:ALA:HB2	13:M:373:ILE:CG2	2.30	0.61
14:N:342:GLN:NE2	29:d:30:ARG:HH11	1.99	0.61
15:O:140:LEU:HD21	15:O:304:VAL:O	2.00	0.61
16:P:191:VAL:HG13	16:P:192:ARG:HH21	1.66	0.61
20:T:138:LEU:HD12	20:T:138:LEU:C	2.24	0.61
27:b:23:PHE:CE1	58:b:201:3PE:H3A2	2.35	0.61
30:e:32:ARG:O	30:e:33:CYS:HB2	1.99	0.61
37:l:62:TYR:CZ	37:l:64:PRO:HG3	2.36	0.61
39:n:149:ILE:H	39:n:149:ILE:HD12	1.65	0.61
46:AB:176:ASN:O	46:AB:258:ILE:HD11	2.00	0.61
47:AC:138:MET:CE	47:AC:268:ILE:HG23	2.31	0.61
49:AE:172:LYS:HE3	47:Ac:169:SER:CB	2.31	0.61
45:Aa:405:GLY:C	45:Aa:408:PRO:HD2	2.25	0.61
49:Ae:111:LYS:O	49:Ae:115:TYR:HD1	1.84	0.61
1:A:63:LEU:HD13	10:J:63:MET:HE3	1.83	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
8:H:172:MET:HE1	25:Z:46:GLY:CA	2.31	0.61
12:L:560:LYS:HD2	38:m:80:PHE:CE2	2.26	0.61
16:P:41:ILE:HB	16:P:43:HIS:CE1	2.35	0.61
20:U:138:LEU:HB3	20:U:144:ILE:HG12	1.83	0.61
40:o:69:CYS:C	40:o:80:CYS:SG	2.82	0.61
52:AH:45:ARG:O	52:AH:49:GLU:HG2	2.00	0.61
47:Ac:220:PHE:CE2	69:Ac:405:UQ6:H4M2	2.36	0.61
48:Ad:232:TYR:CZ	48:Ad:245:ALA:HB2	2.35	0.61
51:Ag:64:ASN:O	51:Ag:68:GLU:HG2	2.01	0.61
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.61
9:I:53:ALA:CB	27:b:14:ALA:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:SER:O	10:J:27:TYR:N	2.32	0.61
12:L:424:MET:HE2	12:L:502:LEU:CB	2.31	0.61
13:M:1:MET:CE	13:M:111:SER:HB2	2.29	0.61
16:P:156:SER:HB2	16:P:161:VAL:HG21	1.81	0.61
16:P:169:HIS:HD2	16:P:181:LEU:HD11	1.65	0.61
17:Q:167:ASN:O	17:Q:168:LYS:CG	2.48	0.61
45:AA:384:THR:O	45:AA:387:GLU:HG2	2.00	0.61
47:AC:119:LEU:HD22	67:AC:402:HEM:HBB2	1.83	0.61
51:AG:69:GLN:HE22	51:AG:72:ARG:CZ	2.11	0.61
53:AJ:21:PHE:CE2	53:AJ:25:ILE:HD11	2.36	0.61
46:Ab:262:ASN:OD1	46:Ab:442:GLY:HA2	2.01	0.61
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
12:L:302:ILE:HB	12:L:340:PHE:CE1	2.36	0.61
20:T:79:ILE:CB	20:T:145:VAL:HG13	2.28	0.61
23:X:160:PRO:HG3	29:d:22:PRO:HD3	1.83	0.61
24:Y:68:ILE:CG2	24:Y:120:MET:HE1	2.31	0.61
46:Ab:40:PHE:HA	46:Ab:49:ILE:O	2.01	0.61
48:Ad:155:GLN:HA	48:Ad:166:MET:HA	1.83	0.61
2:B:101:ALA:HB1	56:B:302:UQ1:O1	2.01	0.61
3:C:133:SER:OG	3:C:136:PHE:O	2.16	0.61
4:D:35:ARG:HE	32:g:59:PRO:CD	2.13	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	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:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
12:L:174:TYR:HE1	58:L:701:3PE:H331	1.64	0.61
12:L:182:PHE:CE2	12:L:186:MET:SD	2.94	0.61
12:L:594:ASN:CG	14:N:110:PRO:HB2	2.26	0.61
13:M:109:THR:HG22	13:M:121:LEU:HB3	1.82	0.61
31:f:38:ARG:NH1	31:f:56:TRP:O	2.34	0.61
32:g:109:ASP:HB3	32:g:114:GLU:HB3	1.82	0.61
40:o:50:GLN:OE1	41:p:120:ASN:ND2	2.34	0.61
50:AF:92:GLU:HG2	50:AF:96:LYS:HE2	1.82	0.61
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
10:J:71:THR:HA	11:K:27:MET:HE3	1.82	0.60
10:J:87:LEU:CG	10:J:91:PHE:CZ	2.81	0.60
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.35	0.60
11:K:66:PHE:CE2	14:N:35:PHE:CZ	2.89	0.60
13:M:209:LEU:HD23	13:M:210:TYR:N	2.16	0.60
14:N:59:TYR:CZ	14:N:63:GLN:HG3	2.36	0.60
16:P:192:ARG:HA	16:P:192:ARG:CZ	2.30	0.60
42:q:34:ARG:NE	42:q:58:ARG:NH2	2.48	0.60
47:AC:16:HIS:NE2	47:AC:201:HIS:NE2	2.49	0.60
49:AE:88:PHE:CG	51:AG:19:LEU:CD1	2.84	0.60
49:AE:167:PHE:HB2	49:AE:174:LEU:HB3	1.83	0.60
49:AE:244:ASP:HB3	49:AE:250:ARG:HH11	1.66	0.60
45:Aa:80:ARG:NH2	45:Aa:268:CYS:SG	2.73	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
13:M:423:MET:O	13:M:424:ILE:C	2.44	0.60
16:P:263:PHE:HD2	16:P:333:PRO:O	1.84	0.60
16:P:268:PRO:CG	16:P:344:PRO:HA	2.30	0.60
18:R:32:THR:HA	18:R:55:VAL:HG23	1.84	0.60
42:q:3:LEU:O	42:q:6:VAL:HG22	2.01	0.60
47:AC:265:PRO:HD2	47:AC:268:ILE:HD11	1.81	0.60
49:AE:235:TYR:CE1	49:AE:240:GLY:HA2	2.36	0.60
51:AG:64:ASN:O	51:AG:68:GLU:HG2	2.01	0.60
52:AH:50:LEU:O	52:AH:54:ARG:HG2	2.01	0.60
45:Aa:397:ASN:O	45:Aa:400:VAL:HB	2.01	0.60
46:Ab:183:LYS:HG3	46:Ab:254:ARG:HB3	1.82	0.60
47:Ac:8:HIS:CE1	47:Ac:10:LEU:HB3	2.35	0.60
7:G:126:LEU:CD1	18:R:89:PRO:HB2	2.31	0.60
12:L:40:ILE:HD12	12:L:101:MET:HG3	1.82	0.60
12:L:180:ILE:HG21	58:L:703:3PE:H3G2	1.84	0.60
14:N:100:MET:HE3	14:N:111:PHE:HZ	1.66	0.60
16:P:299:SER:HB3	16:P:316:LYS:HE3	1.83	0.60
20:T:103:HIS:HB2	20:T:106:LYS:HB2	1.83	0.60
45:AA:101:THR:HG22	45:AA:154:SER:HA	1.83	0.60
45:AA:373:GLN:O	45:AA:377:MET:HG2	2.01	0.60
46:Ab:97:PHE:CZ	46:Ab:101:ARG:HG3	2.35	0.60
49:Ae:179:ARG:HH21	49:Ae:208:PRO:HA	1.67	0.60
52:Ah:40:LYS:HA	52:Ah:43:LYS:HE2	1.82	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
19:S:19:ILE:HG13	19:S:95:LEU:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:82:LEU:O	21:V:86:LYS:HG3	2.00	0.60
25:Z:143:TYR:O	25:Z:144:THR:C	2.45	0.60
45:AA:362:ALA:HB2	45:AA:461:PRO:HB2	1.81	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.63	0.60
12:L:42:PHE:O	12:L:46:ILE:HG12	2.01	0.60
12:L:556:ILE:HG21	38:m:80:PHE:CZ	2.34	0.60
16:P:315:THR:O	16:P:316:LYS:C	2.45	0.60
23:X:159:LYS:O	23:X:160:PRO:C	2.43	0.60
29:d:16:ASP:O	29:d:19:ARG:HG3	2.01	0.60
32:g:63:ASN:OD1	39:n:106:TYR:HE1	1.85	0.60
45:AA:341:PHE:HB2	45:AA:368:MET:HE1	1.84	0.60
45:AA:341:PHE:HE1	45:AA:356:ALA:HB1	1.66	0.60
48:AD:131:ALA:HB2	48:AD:174:TYR:CD2	2.36	0.60
49:Ae:197:ASP:C	49:Ae:199:GLN:H	2.08	0.60
49:Ae:207:LYS:HD2	49:Ae:210:TRP:HD1	1.66	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	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:239:THR:O	8:H:239:THR:HG22	2.01	0.60
9:I:80:GLU:OE2	43:r:26:LEU:HD11	2.01	0.60
10:J:122:ASP:O	25:Z:122:GLY:HA3	2.01	0.60
12:L:222:GLY:CA	12:L:229:LEU:HD11	2.26	0.60
12:L:594:ASN:HD21	14:N:110:PRO:HB2	1.66	0.60
16:P:217:PHE:HA	16:P:220:TYR:CD2	2.37	0.60
39:n:57:MET:HG3	45:Aa:256:VAL:CG2	2.30	0.60
45:AA:168:ILE:O	45:AA:171:GLU:HG2	2.01	0.60
45:AA:450:TYR:CE2	53:AJ:16:ARG:O	2.53	0.60
47:AC:150:LEU:HD21	68:AC:404:U10:C1M	2.31	0.60
47:AC:302:ALA:O	47:AC:305:PRO:HD2	2.02	0.60
49:AE:154:ILE:HB	49:AE:271:VAL:O	2.02	0.60
49:AI:60:ALA:CB	46:Ab:339:TYR:CD2	2.83	0.60
50:Af:23:ASN:HA	50:Af:28:ASN:HD21	1.66	0.60
53:Aj:53:TRP:O	53:Aj:54:LYS:C	2.43	0.60
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.67	0.60
12:L:56:HIS:O	40:o:71:ARG:HG3	2.02	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
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:224:SER:HB2	14:N:229:SER:CB	2.32	0.60
15:O:76:GLU:HG3	15:O:266:PRO:HG2	1.83	0.60
15:O:249:MET:HB3	15:O:253:CYS:SG	2.40	0.60
2:B:97:LEU:CD2	2:B:141:MET:HG2	2.30	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
12:L:173:LEU:CD2	58:L:701:3PE:H321	2.27	0.60
62:L:705:CDL:H541	62:L:705:CDL:H142	1.82	0.60
13:M:178:ILE:HD12	33:h:143:GLU:HG3	1.84	0.60
13:M:370:PRO:HA	13:M:375:LEU:HD22	1.83	0.60
16:P:136:THR:CG2	16:P:139:PHE:HB2	2.31	0.60
19:S:16:LEU:CB	19:S:69:TYR:HD1	2.14	0.60
21:V:35:LEU:HA	21:V:38:PHE:HD1	1.65	0.60
37:l:38:PRO:CB	38:m:75:ASN:HD22	2.09	0.60
37:l:184:TYR:CD1	40:o:36:GLU:HA	2.36	0.60
48:AD:217:GLY:O	48:AD:235:PRO:HD2	2.01	0.60
48:AD:244:MET:HB2	70:AD:401:HEC:C1D	2.31	0.60
49:AE:115:TYR:HE2	53:AJ:11:TYR:HE1	1.50	0.60
49:AE:155:LYS:HB3	49:AE:158:ASP:CG	2.26	0.60
49:AI:5:ALA:N	49:AI:8:SER:HG	1.99	0.60
54:AK:36:THR:HG1	54:AK:38:TRP:CG	2.20	0.60
46:Ab:117:GLU:OE2	46:Ab:331:SER:N	2.24	0.60
47:Ac:70:CYS:SG	47:Ac:80:ARG:HD3	2.42	0.60
52:Ah:39:GLU:O	52:Ah:43:LYS:HG3	2.01	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
10:J:68:GLY:O	10:J:69:TYR:C	2.45	0.60
12:L:204:SER:HA	12:L:207:ASN:HD22	1.67	0.60
13:M:144:ASN:HA	13:M:147:ILE:HD12	1.82	0.60
16:P:262:THR:N	16:P:332:LEU:HD12	2.12	0.60
20:T:83:VAL:HG22	20:T:126:PHE:HZ	1.66	0.60
33:h:73:PHE:HD2	33:h:74:TYR:CD1	2.20	0.60
39:n:143:GLU:OE1	39:n:155:PRO:HB3	2.02	0.60
48:AD:159:ASN:HB3	48:AD:162:GLY:CA	2.31	0.60
49:AE:166:ALA:HA	49:AE:174:LEU:O	2.02	0.60
50:AF:108:TRP:HA	50:AF:111:LYS:NZ	2.17	0.60
46:Ab:138:LEU:HB3	46:Ab:237:PHE:CD2	2.36	0.60
49:Ae:239:HIS:NE2	49:Ae:254:ALA:HB2	2.16	0.60
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.37	0.60
7:G:304:GLU:OE2	16:P:41:ILE:HG12	2.01	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
13:M:77:LEU:HD23	13:M:99:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:M:503:3PE:H251	14:N:242:THR:HG21	1.84	0.60
15:O:256:LEU:HD11	15:O:276:LEU:CD2	2.32	0.60
23:X:37:ASP:HA	23:X:40:ASN:HB2	1.84	0.60
24:Y:137:LEU:CD2	24:Y:138:PHE:CD2	2.84	0.60
33:h:102:PRO:HD2	33:h:105:TYR:CB	2.32	0.60
34:i:69:LEU:CD1	34:i:71:ALA:HB3	2.31	0.60
49:AE:214:ILE:HG12	49:AE:259:GLU:OE1	2.01	0.60
49:Ae:201:ASP:H	49:Ae:248:ARG:NH1	1.99	0.60
52:Ah:65:CYS:HA	52:Ah:68:GLU:OE1	2.02	0.60
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.37	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
12:L:123:LEU:HD22	12:L:150:MET:CG	2.32	0.59
12:L:145:GLU:HG2	13:M:370:PRO:HD3	1.84	0.59
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.84	0.59
14:N:258:THR:CG2	14:N:336:THR:HG22	2.32	0.59
14:N:276:LEU:C	14:N:276:LEU:HD12	2.27	0.59
18:R:42:ASP:HB3	18:R:44:ARG:NH1	2.17	0.59
23:X:20:VAL:HG12	23:X:25:LEU:HD21	1.84	0.59
23:X:133:THR:HG23	27:b:58:ARG:HH12	1.65	0.59
33:h:73:PHE:CD2	33:h:74:TYR:CD1	2.90	0.59
39:n:176:GLU:O	39:n:178:PRO:HD3	2.02	0.59
45:Aa:295:GLY:O	45:Aa:301:ASN:ND2	2.35	0.59
47:Ac:302:ALA:O	47:Ac:305:PRO:HD2	2.01	0.59
1:A:101:GLY:HA3	10:J:163:ILE:CD1	2.32	0.59
3:C:70:LYS:O	21:V:103:LEU:HD12	2.02	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
10:J:9:SER:HB3	11:K:7:ASN:ND2	2.05	0.59
58:L:703:3PE:H232	58:m:201:3PE:H3B1	1.84	0.59
13:M:126:LEU:HD21	13:M:153:THR:HB	1.83	0.59
15:O:54:HIS:HB2	15:O:56:TYR:CE1	2.37	0.59
20:U:90:TYR:CZ	20:U:92:LYS:HD2	2.35	0.59
23:X:158:LEU:HB3	29:d:21:LEU:HD21	1.84	0.59
47:AC:45:ILE:HA	67:AC:401:HEM:HAB	1.83	0.59
49:AE:226:ALA:HB2	49:AE:234:TYR:CE1	2.37	0.59
48:Ad:138:VAL:HG12	48:Ad:139:CYS:SG	2.42	0.59
49:Ae:164:ASN:HD22	49:Ae:226:ALA:HB2	1.65	0.59
49:Ae:239:HIS:NE2	49:Ae:254:ALA:N	2.50	0.59
4:D:95:LEU:HG	4:D:97:LEU:HG	1.84	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:81:LYS:HB2	12:L:135:ASN:OD1	2.02	0.59
12:L:247:LEU:HD12	12:L:248:HIS:CG	2.36	0.59
13:M:115:LEU:O	13:M:118:PHE:HB3	2.02	0.59
34:i:104:ILE:HG13	40:o:48:ASP:HB3	1.84	0.59
46:AB:138:LEU:CD2	46:AB:238:LEU:HG	2.32	0.59
48:Ad:309:HIS:CE1	51:Ag:21:PRO:HB2	2.38	0.59
48:Ad:318:LYS:CD	49:Ae:86:PRO:HB2	2.33	0.59
10:J:134:MET:HE2	30:e:27:TYR:CZ	2.37	0.59
13:M:294:MET:HE3	13:M:319:HIS:CD2	2.37	0.59
15:O:126:GLY:HA3	32:g:51:MET:HE1	1.84	0.59
15:O:167:PHE:HE1	15:O:245:PHE:HB2	1.67	0.59
15:O:343:TYR:HE1	15:O:355:LYS:HB2	1.66	0.59
27:b:8:PHE:HA	27:b:11:ASN:ND2	2.18	0.59
33:h:69:ARG:O	33:h:73:PHE:HB2	2.02	0.59
49:AE:212:ILE:O	49:AE:260:VAL:HG13	2.01	0.59
45:Aa:225:LYS:HE3	45:Aa:256:VAL:HA	1.83	0.59
48:Ad:186:ARG:NE	48:Ad:193:LEU:HB2	2.17	0.59
4:D:34:ALA:HB3	13:M:86:LYS:HZ3	1.67	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
12:L:302:ILE:CG2	12:L:340:PHE:CE2	2.80	0.59
12:L:313:MET:HE2	12:L:328:HIS:CE1	2.38	0.59
16:P:318:LYS:O	16:P:322:ILE:HG13	2.02	0.59
16:P:350:ILE:HB	16:P:366:ILE:CG2	2.32	0.59
21:V:90:LEU:HD21	21:V:94:MET:CE	2.33	0.59
25:Z:54:ASN:O	25:Z:58:ARG:HG2	2.02	0.59
33:h:87:THR:HA	62:h:201:CDL:H512	1.83	0.59
37:l:38:PRO:C	38:m:75:ASN:ND2	2.60	0.59
46:AB:39:GLU:O	46:AB:227:HIS:CE1	2.56	0.59
46:AB:313:VAL:HG21	46:AB:323:VAL:HG21	1.83	0.59
47:Ac:138:MET:HE1	47:Ac:268:ILE:CG1	2.32	0.59
4:D:65:PRO:HG3	4:D:70:ASP:OD1	2.02	0.59
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
8:H:111:LEU:CD2	10:J:60:LEU:HD12	2.29	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
10:J:19:LEU:HD21	10:J:31:GLY:HA3	1.83	0.59
12:L:227:PHE:CD2	12:L:283:LEU:CD2	2.86	0.59
13:M:14:LEU:HD21	13:M:26:ASN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:209:LEU:HD23	13:M:211:GLY:H	1.67	0.59
14:N:200:LEU:HD22	14:N:269:GLU:HG3	1.84	0.59
45:AA:50:VAL:HG22	45:AA:60:ALA:CB	2.33	0.59
46:AB:286:PHE:CE1	46:AB:427:ALA:HB1	2.38	0.59
52:AH:35:CYS:HA	52:AH:38:LEU:HD13	1.84	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
2:B:91:TRP:CH2	61:H:400:UQ9:C1M	2.86	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.37	0.59
10:J:12:PHE:CZ	11:K:42:ILE:CD1	2.86	0.59
12:L:312:LEU:CD2	12:L:395:ILE:HG21	2.33	0.59
12:L:605:ASN:O	12:L:606:LEU:C	2.46	0.59
13:M:255:LYS:NZ	29:d:117:HIS:HB3	2.18	0.59
13:M:388:TRP:NE1	38:m:109:ARG:HD2	2.18	0.59
16:P:96:LEU:HD12	16:P:96:LEU:C	2.28	0.59
25:Z:98:MET:HB2	25:Z:104:TRP:NE1	2.18	0.59
25:Z:107:GLY:HA2	30:e:75:ARG:HH22	1.66	0.59
45:AA:186:TYR:HB3	45:AA:275:ILE:HG21	1.84	0.59
49:AE:212:ILE:HD11	49:AE:271:VAL:HG21	1.84	0.59
46:Ab:90:THR:HG23	46:Ab:95:SER:HA	1.83	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
62:L:704:CDL:H322	33:h:71:MET:HE1	1.83	0.59
14:N:324:LEU:HD11	29:d:64:PHE:CZ	2.37	0.59
16:P:178:SER:O	16:P:182:ARG:HG2	2.02	0.59
19:S:63:PRO:HB2	19:S:79:LEU:HB2	1.85	0.59
32:g:139:TYR:HD2	32:g:140:PHE:CD1	2.20	0.59
42:q:51:ASP:O	42:q:59:HIS:HB2	2.02	0.59
44:s:57:LEU:HG	44:s:58:PRO:HD2	1.84	0.59
48:AD:94:TYR:HB3	52:AH:85:PHE:CE2	2.38	0.59
48:AD:233:PHE:HA	48:AD:240:GLN:O	2.03	0.59
48:AD:264:SER:HB2	52:AH:88:LEU:HD11	1.84	0.59
49:AE:152:ILE:HG23	49:AE:274:GLY:H	1.67	0.59
45:Aa:281:ALA:HA	51:Ag:10:ARG:HH12	1.67	0.59
4:D:375:MET:HE1	7:G:126:LEU:CA	2.33	0.59
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	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)
15:O:114:LEU:HA	15:O:131:LEU:HD21	1.84	0.59
16:P:357:ARG:HD3	16:P:361:TRP:O	2.03	0.59
18:R:40:GLU:HA	18:R:45:ARG:CZ	2.32	0.59
20:U:105:MET:SD	20:U:139:MET:HE1	2.42	0.59
21:V:31:THR:HG22	21:V:88:LEU:HD13	1.85	0.59
22:W:93:LEU:HG	22:W:97:ILE:CD1	2.33	0.59
25:Z:105:LYS:O	25:Z:106:VAL:C	2.46	0.59
27:b:6:SER:O	27:b:9:LEU:HB3	2.03	0.59
27:b:27:GLY:O	27:b:30:ILE:HG22	2.02	0.59
33:h:95:GLU:HB3	33:h:114:LYS:HG2	1.85	0.59
48:AD:154:VAL:O	48:AD:167:ARG:N	2.36	0.59
48:Ad:146:LYS:HD3	48:Ad:171:LEU:HG	1.83	0.59
49:Ae:190:VAL:HG13	49:Ae:194:GLN:OE1	2.01	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.59
4:D:51:VAL:HG21	4:D:58:THR:HG22	1.83	0.59
58:D:501:3PE:H361	12:L:566:THR:HG21	1.85	0.59
8:H:310:PHE:O	27:b:38:TYR:HB2	2.02	0.59
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.59
10:J:21:LEU:HA	58:K:101:3PE:H252	1.85	0.59
12:L:466:PHE:CE1	12:L:470:TYR:HE2	2.21	0.59
13:M:263:LEU:CD1	38:m:102:TYR:HD1	2.16	0.59
13:M:275:ILE:HD11	13:M:288:TYR:CB	2.33	0.59
13:M:396:MET:HG3	13:M:396:MET:O	2.03	0.59
15:O:242:LYS:HA	15:O:246:LEU:HD12	1.84	0.59
20:T:123:GLU:OE1	22:W:44:ARG:NH1	2.36	0.59
23:X:78:CYS:SG	23:X:110:CYS:HB3	2.42	0.59
23:X:120:PRO:HB2	23:X:125:LEU:HD11	1.85	0.59
35:j:71:TRP:CH2	58:j:700:3PE:H3B1	2.38	0.59
37:l:113:ILE:HG12	37:l:114:ARG:H	1.67	0.59
39:n:97:TYR:HB2	39:n:178:PRO:CB	2.32	0.59
39:n:111:GLU:O	39:n:114:MET:HG2	2.03	0.59
45:AA:92:PHE:CE2	45:AA:161:ILE:HG23	2.38	0.59
46:AB:174:ILE:HG13	49:AI:14:VAL:CG1	2.31	0.59
48:AD:197:LEU:HA	48:AD:200:ILE:HB	1.84	0.59
46:Ab:60:ARG:CG	46:Ab:393:LEU:HD13	2.33	0.59
47:Ac:36:LEU:HD11	62:Ag:101:CDL:H732	1.84	0.59
48:Ad:268:LYS:HE3	52:Ah:85:PHE:CE1	2.38	0.59
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.84	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:230:HIS:N	12:L:231:PRO:CD	2.66	0.58
13:M:210:TYR:O	13:M:213:HIS:CD2	2.56	0.58
14:N:77:ASN:OD1	14:N:81:LEU:HD12	2.03	0.58
14:N:179:MET:CG	14:N:216:PHE:HE1	2.16	0.58
14:N:300:THR:HG23	14:N:301:SER:N	2.17	0.58
23:X:124:GLN:HA	23:X:127:LYS:HE3	1.83	0.58
30:e:101:ARG:CZ	30:e:102:GLU:H	2.16	0.58
46:AB:110:LEU:HB3	49:AI:22:VAL:CG2	2.33	0.58
50:AF:24:ALA:O	51:AG:48:ARG:NH2	2.35	0.58
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.33	0.58
1:A:53:MET:HE2	10:J:170:THR:HB	1.84	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.84	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.86	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
11:K:19:THR:HG23	11:K:29:THR:HG23	1.85	0.58
12:L:417:SER:HB3	12:L:493:ILE:CG1	2.31	0.58
14:N:109:ALA:CB	14:N:110:PRO:CD	2.81	0.58
19:S:47:ALA:O	19:S:49:PRO:HD3	2.03	0.58
23:X:134:ASP:O	23:X:135:ARG:C	2.45	0.58
23:X:151:ASN:ND2	30:e:51:ARG:HH11	2.01	0.58
25:Z:122:GLY:O	25:Z:126:GLY:N	2.34	0.58
41:p:37:TYR:CZ	41:p:41:VAL:HG11	2.38	0.58
46:AB:47:LEU:HA	46:AB:218:MET:O	2.03	0.58
46:AB:170:GLN:HG3	46:AB:339:TYR:OH	2.03	0.58
49:AE:93:ARG:HG2	51:AG:23:GLU:O	2.03	0.58
45:Aa:92:PHE:HD1	45:Aa:168:ILE:HD12	1.66	0.58
48:Ad:113:GLY:O	48:Ad:116:VAL:HB	2.03	0.58
4:D:99:LEU:CD2	4:D:109:CYS:HA	2.32	0.58
6:F:382:CYS:SG	55:F:502:SF4:S1	3.02	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.85	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.86	0.58
14:N:307:THR:C	15:O:319:ILE:HG12	2.29	0.58
16:P:122:HIS:CB	18:R:46:VAL:HG12	2.33	0.58
20:U:119:ILE:HD11	20:U:138:LEU:HB2	1.85	0.58
37:l:105:ILE:HG23	37:l:109:LEU:HD22	1.84	0.58
48:AD:126:SER:HB3	48:AD:178:PRO:CD	2.33	0.58
48:AD:147:ALA:O	48:AD:150:GLU:HG2	2.02	0.58
47:Ac:345:HIS:CE1	47:Ac:346:PRO:HB3	2.37	0.58
48:Ad:215:LEU:HD13	70:Ad:401:HEC:HBB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.84	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
11:K:70:GLU:HA	14:N:38:LEU:HD21	1.84	0.58
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.34	0.58
14:N:308:ASN:C	15:O:319:ILE:HG23	2.29	0.58
16:P:57:THR:HG23	16:P:123:SER:CB	2.33	0.58
16:P:66:GLY:O	16:P:67:ARG:C	2.42	0.58
22:W:104:THR:O	22:W:108:ARG:HG3	2.02	0.58
26:a:36:LYS:HA	26:a:59:ARG:HH22	1.68	0.58
45:AA:452:GLN:C	45:AA:472:ARG:NH1	2.61	0.58
49:AE:172:LYS:HE3	47:Ac:169:SER:HB2	1.85	0.58
45:Aa:172:MET:HE1	45:Aa:205:SER:HA	1.85	0.58
45:Aa:467:ASP:OD2	47:Ac:223:TYR:CE2	2.57	0.58
51:Ag:11:ILE:HG22	51:Ag:12:ARG:N	2.18	0.58
4:D:37:TRP:CZ2	4:D:39:PRO:HA	2.38	0.58
4:D:99:LEU:HB3	4:D:101:LEU:CD1	2.34	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
8:H:316:PRO:HG3	25:Z:57:ARG:HB3	1.85	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
12:L:407:TRP:CZ3	12:L:410:LEU:HD11	2.38	0.58
19:S:65:LEU:HB2	19:S:79:LEU:HD11	1.84	0.58
20:U:105:MET:CG	20:U:139:MET:HE1	2.33	0.58
62:a:101:CDL:HB4	42:q:3:LEU:HD13	1.86	0.58
29:d:14:LEU:HD12	29:d:14:LEU:C	2.27	0.58
33:h:96:ALA:HB3	41:p:63:TYR:CD1	2.37	0.58
38:m:75:ASN:O	38:m:75:ASN:OD1	2.20	0.58
41:p:128:GLU:O	41:p:131:GLN:N	2.37	0.58
47:AC:233:LEU:HD23	48:AD:300:LEU:HA	1.84	0.58
47:AC:345:HIS:CE1	47:AC:346:PRO:HB3	2.38	0.58
48:AD:284:HIS:NE2	48:AD:288:MET:HE3	2.18	0.58
49:AE:264:GLU:HB3	49:AE:272:VAL:O	2.03	0.58
49:AI:64:LEU:CD2	49:AI:78:PHE:HA	2.25	0.58
45:Aa:55:ASN:HB3	45:Aa:226:ALA:HB1	1.84	0.58
46:Ab:286:PHE:CE1	46:Ab:427:ALA:HB1	2.38	0.58
46:Ab:305:THR:HG23	46:Ab:311:GLN:NE2	2.19	0.58
48:Ad:95:PRO:CG	52:Ah:85:PHE:CB	2.79	0.58
49:Ae:218:THR:HG21	49:Ae:256:LEU:C	2.28	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
8:H:201:THR:OG1	8:H:202:GLU:N	2.36	0.58
10:J:33:ILE:HG23	10:J:60:LEU:HD21	1.85	0.58
12:L:15:LEU:O	12:L:18:PRO:HD2	2.03	0.58
12:L:261:VAL:C	12:L:264:HIS:HD2	2.12	0.58
12:L:404:THR:HG22	12:L:405:ASN:N	2.19	0.58
15:O:49:THR:O	15:O:53:LEU:HG	2.04	0.58
16:P:57:THR:HG23	16:P:123:SER:HB2	1.86	0.58
30:e:41:ILE:HG12	33:h:174:PRO:HB2	1.84	0.58
31:f:37:PHE:CE2	33:h:141:GLN:OE1	2.56	0.58
45:AA:118:ALA:O	46:AB:298:HIS:HB3	2.03	0.58
46:AB:117:GLU:OE2	46:AB:331:SER:N	2.25	0.58
47:AC:18:PHE:CE1	69:AC:405:UQ6:H1M2	2.38	0.58
50:AF:106:GLU:O	50:AF:110:LYS:HG3	2.03	0.58
48:Ad:284:HIS:NE2	48:Ad:288:MET:HE3	2.19	0.58
49:Ae:168:LYS:NZ	49:Ae:171:GLY:HA2	2.18	0.58
54:Ak:23:MET:O	54:Ak:27:VAL:HG23	2.04	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
12:L:477:ILE:HG13	40:o:91:GLU:CD	2.29	0.58
13:M:154:LEU:HD13	14:N:287:LEU:CD2	2.33	0.58
13:M:196:TRP:HZ3	13:M:261:PHE:CE2	2.21	0.58
25:Z:135:ASN:O	25:Z:139:GLY:HA3	2.04	0.58
28:c:65:ASP:OD2	29:d:73:TYR:OH	2.18	0.58
29:d:113:LEU:O	29:d:113:LEU:HG	2.02	0.58
31:f:47:GLU:HG2	31:f:47:GLU:O	2.03	0.58
44:s:35:LEU:HB3	44:s:38:HIS:HB2	1.85	0.58
45:Aa:171:GLU:O	45:Aa:175:ASN:N	2.37	0.58
52:Ah:45:ARG:O	52:Ah:49:GLU:HG2	2.04	0.58
2:B:101:ALA:CB	56:B:302:UQ1:O1	2.52	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
12:L:466:PHE:HE1	35:j:72:ARG:CZ	2.13	0.58
13:M:398:ILE:HD12	58:m:201:3PE:H2G1	1.86	0.58
14:N:26:LEU:O	14:N:27:MET:C	2.46	0.58
14:N:147:PRO:HB2	14:N:148:LEU:HD12	1.86	0.58
14:N:314:MET:CB	15:O:305:LEU:HD11	2.33	0.58
22:W:42:TRP:CH2	22:W:93:LEU:HA	2.39	0.58
23:X:90:ASP:OD2	26:a:62:VAL:HG11	2.04	0.58
45:AA:220:LEU:O	45:AA:224:TYR:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:255:PRO:HG2	47:Ac:287:LYS:NZ	2.19	0.58
51:AG:11:ILE:HG22	51:AG:12:ARG:N	2.18	0.58
62:Aa:501:CDL:OB6	62:Aa:501:CDL:H112	2.03	0.58
47:Ac:162:GLU:O	47:Ac:166:GLY:N	2.36	0.58
47:Ac:163:TRP:O	47:Ac:177:ARG:NH1	2.37	0.58
51:Ag:78:TYR:HB3	52:Ah:61:THR:OG1	2.04	0.58
2:B:115:ASP:HA	2:B:119:VAL:O	2.04	0.58
3:C:120:THR:OG1	17:Q:128:PHE:HA	2.04	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
12:L:65:THR:HA	34:i:90:MET:HE2	1.86	0.58
12:L:542:LEU:HD11	58:L:701:3PE:H261	1.86	0.58
15:O:76:GLU:HG3	15:O:266:PRO:CG	2.34	0.58
23:X:122:LEU:HD23	27:b:82:LYS:HG2	1.85	0.58
23:X:141:PRO:O	23:X:142:TYR:HB2	2.04	0.58
25:Z:62:ILE:HG12	27:b:49:THR:HA	1.85	0.58
25:Z:129:THR:HB	25:Z:132:GLU:HG3	1.86	0.58
34:i:95:TYR:OH	41:p:11:PRO:O	2.20	0.58
45:AA:43:GLN:NE2	46:AB:57:PRO:CB	2.66	0.58
45:AA:363:MET:HA	45:AA:464:GLN:OE1	2.04	0.58
45:Aa:220:LEU:O	45:Aa:224:TYR:HB2	2.03	0.58
46:Ab:142:THR:HG21	46:Ab:237:PHE:CB	2.28	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.86	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
12:L:425:ARG:HG3	12:L:429:PHE:CE2	2.39	0.58
13:M:73:LEU:HB2	13:M:103:GLN:OE1	2.02	0.58
13:M:109:THR:HG22	13:M:121:LEU:CB	2.34	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
16:P:245:VAL:O	16:P:249:ILE:HG13	2.04	0.58
16:P:275:HIS:HB3	16:P:372:ALA:HB1	1.86	0.58
20:U:155:TYR:OH	33:h:52:LYS:HD2	2.04	0.58
23:X:167:PHE:HB3	23:X:170:TRP:CD1	2.39	0.58
32:g:121:GLU:HA	32:g:124:VAL:HG22	1.86	0.58
45:Aa:70:THR:HG21	45:Aa:407:THR:HA	1.85	0.58
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD1	2.39	0.58
1:A:51:PHE:CD2	10:J:73:MET:CE	2.86	0.57
1:A:63:LEU:CD2	10:J:62:GLY:C	2.71	0.57
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.57
7:G:671:LEU:HD21	19:S:45:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
12:L:232:TRP:CZ3	12:L:233:LEU:HD21	2.37	0.57
12:L:592:LEU:O	12:L:596:ILE:HG12	2.04	0.57
13:M:154:LEU:HD13	14:N:287:LEU:HD22	1.85	0.57
58:M:503:3PE:H382	14:N:246:LEU:CD1	2.34	0.57
20:U:100:VAL:C	20:U:141:PRO:HG2	2.28	0.57
51:AG:35:ILE:HB	51:AG:36:PRO:HD3	1.86	0.57
46:Ab:177:LEU:HD11	46:Ab:272:VAL:HG22	1.85	0.57
48:Ad:302:LEU:HD22	49:Ae:117:VAL:HG13	1.86	0.57
51:Ag:76:ALA:O	51:Ag:79:GLU:HG3	2.04	0.57
1:A:51:PHE:CZ	11:K:79:VAL:HG13	2.40	0.57
2:B:164:CYS:SG	55:B:301:SF4:S4	3.02	0.57
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.39	0.57
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.39	0.57
12:L:456:ARG:HG2	58:j:700:3PE:H241	1.86	0.57
14:N:33:LEU:HD11	14:N:141:ILE:HD12	1.86	0.57
16:P:214:LEU:HD23	16:P:352:VAL:CG1	2.34	0.57
17:Q:77:VAL:HG12	17:Q:101:PHE:HA	1.86	0.57
20:T:90:TYR:CE2	20:T:92:LYS:HB3	2.39	0.57
20:U:113:LEU:HD23	39:n:17:LEU:CD2	2.34	0.57
21:V:28:TYR:HE2	21:V:59:VAL:HG21	1.69	0.57
47:AC:141:TRP:NE1	47:AC:264:THR:HA	2.19	0.57
47:AC:150:LEU:HD13	47:AC:164:ILE:HD12	1.86	0.57
49:AE:190:VAL:O	49:AE:194:GLN:HB3	2.03	0.57
45:Aa:269:ARG:HD2	49:Ae:92:ARG:NH2	2.19	0.57
47:Ac:128:PHE:CD1	68:Ac:404:U10:H4M2	2.39	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
10:J:65:VAL:HG13	10:J:66:VAL:H	1.66	0.57
12:L:358:LYS:CG	39:n:80:TYR:CE2	2.83	0.57
12:L:441:ILE:HG21	35:j:48:PRO:HD3	1.86	0.57
13:M:172:GLY:C	13:M:173:THR:HG23	2.28	0.57
16:P:220:TYR:HA	16:P:223:PHE:HD2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:90:TYR:CE2	20:T:92:LYS:CB	2.87	0.57
33:h:188:ASP:O	33:h:189:ASN:C	2.48	0.57
47:AC:215:ALA:HA	51:AG:11:ILE:HD11	1.85	0.57
48:AD:197:LEU:O	48:AD:198:SER:C	2.44	0.57
45:Aa:463:GLU:CD	51:Ag:8:LEU:HB2	2.29	0.57
48:Ad:92:PRO:HG2	48:Ad:94:TYR:CE1	2.40	0.57
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.57
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
57:L:706:PC1:H2B2	57:L:706:PC1:H352	1.87	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:253:GLY:N	14:N:290:LEU:HD11	2.19	0.57
24:Y:63:PHE:HE2	24:Y:106:ARG:HE	1.53	0.57
30:e:14:LEU:HD12	30:e:15:ASP:CB	2.33	0.57
46:AB:162:LYS:NZ	46:AB:194:ASP:OD1	2.38	0.57
50:AF:107:GLU:OE2	50:AF:111:LYS:HD3	2.05	0.57
45:Aa:87:ASN:HD21	45:Aa:199:GLN:HB2	1.69	0.57
45:Aa:410:CYS:SG	45:Aa:411:GLU:N	2.77	0.57
47:Ac:128:PHE:CE1	68:Ac:404:U10:H4M2	2.39	0.57
48:Ad:104:SER:HB2	48:Ad:283:ASP:CG	2.29	0.57
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.02	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
8:H:307:LEU:HD11	25:Z:47:TYR:CG	2.39	0.57
11:K:96:LEU:O	11:K:97:GLN:C	2.47	0.57
12:L:227:PHE:CD2	12:L:283:LEU:HD21	2.38	0.57
12:L:425:ARG:HG3	12:L:429:PHE:HE2	1.68	0.57
13:M:73:LEU:HD22	13:M:103:GLN:NE2	2.18	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
14:N:154:ILE:HG12	14:N:195:PRO:HG2	1.87	0.57
14:N:179:MET:HG3	14:N:216:PHE:CE1	2.39	0.57
14:N:284:MET:O	14:N:287:LEU:HB2	2.04	0.57
16:P:55:VAL:HA	16:P:79:GLN:HB3	1.85	0.57
16:P:192:ARG:CZ	16:P:198:ALA:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:37:VAL:O	18:R:38:TYR:C	2.44	0.57
25:Z:89:GLU:CG	30:e:97:HIS:CD2	2.86	0.57
27:b:69:HIS:CD2	27:b:70:PRO:HD2	2.36	0.57
32:g:123:LEU:HD12	41:p:98:VAL:CG1	2.35	0.57
45:AA:158:ASP:HA	45:AA:161:ILE:HD12	1.86	0.57
49:AE:190:VAL:HG23	49:AE:250:ARG:NH2	2.20	0.57
47:Ac:376:MET:HE2	50:Af:17:PHE:HD1	1.57	0.57
48:Ad:167:ARG:NH1	48:Ad:170:LYS:H	2.03	0.57
2:B:110:PRO:HB3	8:H:33:LEU:O	2.03	0.57
2:B:170:TYR:OH	4:D:131:GLN:O	2.22	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
11:K:20:LEU:HA	12:L:588:PHE:HD2	1.70	0.57
12:L:145:GLU:HB3	13:M:370:PRO:HG2	1.85	0.57
13:M:447:LEU:HD21	13:M:454:ILE:CD1	2.33	0.57
21:V:31:THR:O	21:V:35:LEU:HG	2.05	0.57
45:AA:87:ASN:HD21	45:AA:199:GLN:HB2	1.69	0.57
45:AA:158:ASP:O	45:AA:162:GLU:HG2	2.05	0.57
46:AB:324:SER:HG	49:AI:11:PHE:HZ	1.53	0.57
47:AC:137:GLN:HG3	47:AC:265:PRO:CG	2.31	0.57
48:Ad:136:VAL:HA	48:Ad:140:TYR:O	2.05	0.57
49:Ae:168:LYS:HA	49:Ae:172:LYS:C	2.28	0.57
49:Ae:239:HIS:NE2	49:Ae:253:PRO:HD2	2.19	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
7:G:136:GLU:CD	17:Q:87:MET:HG3	2.29	0.57
7:G:267:THR:HB	17:Q:115:ALA:HB2	1.86	0.57
12:L:141:PHE:CD2	13:M:370:PRO:HG3	2.38	0.57
14:N:273:ASN:O	14:N:274:ASN:HB2	2.05	0.57
20:U:93:ILE:HD11	20:U:110:LEU:HD11	1.86	0.57
39:n:57:MET:HG3	45:Aa:256:VAL:HG23	1.86	0.57
39:n:98:LYS:HG2	39:n:178:PRO:HG3	1.86	0.57
42:q:13:GLN:HB3	42:q:33:ILE:HG22	1.87	0.57
47:AC:148:ASN:OD1	49:Ae:221:GLY:CA	2.49	0.57
49:AE:200:HIS:O	49:AE:204:ARG:HG2	2.04	0.57
45:Aa:286:HIS:CD2	45:Aa:359:VAL:HG13	2.38	0.57
49:Ae:197:ASP:HB3	49:Ae:199:GLN:HG3	1.86	0.57
51:Ag:74:ASN:HD21	51:Ag:76:ALA:HB3	1.70	0.57
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.66	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ASP:HA	6:F:261:TRP:HZ2	1.70	0.57
8:H:19:PHE:CE1	26:a:11:ILE:HD12	2.40	0.57
9:I:62:MET:SD	25:Z:35:MET:HG2	2.45	0.57
12:L:246:LEU:HD12	12:L:247:LEU:CA	2.34	0.57
12:L:407:TRP:HE1	37:l:140:MET:CE	2.18	0.57
13:M:4:ILE:CG2	13:M:107:ILE:HD13	2.29	0.57
13:M:14:LEU:HD11	13:M:26:ASN:HB3	1.87	0.57
15:O:38:TYR:HB3	15:O:299:GLN:HE22	1.70	0.57
17:Q:125:VAL:HG23	17:Q:125:VAL:O	2.05	0.57
19:S:16:LEU:HD11	19:S:51:LEU:CD1	2.29	0.57
20:U:130:ILE:HG23	20:U:147:TYR:CE2	2.40	0.57
25:Z:110:VAL:HG11	30:e:72:THR:CG2	2.34	0.57
31:f:8:ARG:C	31:f:9:GLU:OE1	2.48	0.57
34:i:87:LYS:HG2	34:i:87:LYS:O	2.05	0.57
37:l:166:LEU:HB2	37:l:170:ARG:NH2	2.19	0.57
40:o:39:MET:CE	40:o:58:TYR:HA	2.35	0.57
42:q:65:THR:HG22	42:q:66:THR:N	2.20	0.57
42:q:68:MET:SD	42:q:81:MET:HB3	2.44	0.57
47:AC:56:THR:HG21	47:Ac:58:ASP:HB2	1.87	0.57
47:AC:150:LEU:HD21	68:AC:404:U10:H1M1	1.87	0.57
45:Aa:338:CYS:HB2	45:Aa:368:MET:SD	2.45	0.57
48:Ad:249:TYR:CE2	48:Ad:252:VAL:HA	2.39	0.57
1:A:78:ALA:HB2	10:J:142:ALA:HB1	1.87	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
5:E:222:PHE:H	5:E:225:GLU:CD	2.13	0.57
9:I:89:GLU:HG3	42:q:61:TRP:HB3	1.87	0.57
10:J:169:ILE:CD1	14:N:42:PRO:HA	2.35	0.57
13:M:12:LEU:HB2	13:M:13:PRO:HD3	1.85	0.57
13:M:282:LEU:HD13	13:M:342:MET:HE2	1.86	0.57
15:O:80:GLN:CG	15:O:270:VAL:HG21	2.18	0.57
15:O:167:PHE:CE1	15:O:245:PHE:HB2	2.40	0.57
15:O:258:TYR:HB3	15:O:262:GLU:HB2	1.86	0.57
23:X:52:ASP:OD2	23:X:55:ARG:HG3	2.03	0.57
42:q:129:THR:O	42:q:129:THR:HG22	2.03	0.57
45:AA:402:HIS:HB2	45:AA:426:LEU:HD11	1.86	0.57
51:AG:33:LYS:C	51:AG:36:PRO:HD2	2.30	0.57
45:Aa:68:THR:HG22	45:Aa:136:LEU:CD2	2.35	0.57
53:Aj:7:PRO:HB2	53:Aj:10:LEU:HG	1.87	0.57
1:A:60:ILE:O	1:A:61:THR:C	2.46	0.57
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.57
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.57
12:L:25:ASN:HB2	33:h:72:LYS:NZ	2.20	0.57
12:L:88:LEU:HD23	12:L:326:PHE:HE2	1.69	0.57
12:L:253:VAL:CG2	12:L:310:LEU:HD11	2.35	0.57
13:M:42:LEU:HD11	13:M:67:ILE:CD1	2.34	0.57
13:M:264:LEU:HD23	38:m:98:LEU:HD11	1.87	0.57
13:M:278:ARG:HH22	37:l:108:ASP:CG	2.13	0.57
14:N:109:ALA:HB1	14:N:110:PRO:HD3	1.86	0.57
15:O:323:GLN:HB2	32:g:56:ASP:OD1	2.05	0.57
16:P:320:GLU:O	16:P:324:ILE:HG12	2.05	0.57
22:W:42:TRP:CZ2	66:W:201:EHZ:O1	2.58	0.57
24:Y:57:ARG:HG2	24:Y:60:ARG:HH21	1.68	0.57
32:g:140:PHE:CZ	41:p:74:ILE:HG22	2.40	0.57
52:AH:35:CYS:HB3	52:AH:79:CYS:SG	2.45	0.57
52:AH:42:VAL:O	52:AH:46:GLU:HG3	2.05	0.57
2:B:100:CYS:HG	55:B:301:SF4:FE4	1.22	0.56
4:D:36:GLN:HE22	13:M:135:ARG:NH2	2.02	0.56
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.56
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.20	0.56
4:D:348:LEU:O	25:Z:11:PRO:HB3	2.05	0.56
8:H:69:SER:C	8:H:71:PHE:H	2.12	0.56
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.56
10:J:22:LYS:CD	11:K:23:ARG:HG3	2.35	0.56
12:L:60:GLU:CG	12:L:83:ASP:HA	2.35	0.56
13:M:269:MET:HE3	13:M:399:ASN:HB2	1.86	0.56
14:N:226:THR:HG22	14:N:228:ASN:H	1.70	0.56
16:P:188:GLU:O	16:P:192:ARG:HG2	2.05	0.56
23:X:5:VAL:HG13	23:X:7:LEU:HG	1.87	0.56
33:h:175:GLU:HB3	33:h:177:GLU:HG2	1.86	0.56
47:AC:147:THR:HG21	47:AC:165:TRP:CD1	2.40	0.56
49:Ae:166:ALA:HA	49:Ae:174:LEU:O	2.05	0.56
53:Aj:31:PHE:HB3	53:Aj:34:ARG:HE	1.69	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
13:M:310:MET:O	13:M:314:MET:HG3	2.04	0.56
58:M:501:3PE:H221	24:Y:135:TRP:CH2	2.40	0.56
15:O:125:ASP:OD1	15:O:126:GLY:N	2.38	0.56
15:O:209:VAL:HG23	15:O:209:VAL:O	2.05	0.56
31:f:49:ARG:HB2	31:f:50:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:92:ILE:HG13	47:AC:272:TRP:HH2	1.70	0.56
46:Ab:38:LEU:HB3	46:Ab:40:PHE:HE1	1.70	0.56
47:Ac:164:ILE:O	47:Ac:177:ARG:HD2	2.06	0.56
48:Ad:222:PRO:O	48:Ad:225:VAL:HG12	2.05	0.56
49:Ae:163:LYS:O	49:Ae:177:ARG:HA	2.04	0.56
1:A:71:LEU:HB3	10:J:152:MET:HE1	1.87	0.56
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.58	0.56
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.56
7:G:161:GLU:OE1	18:R:97:LYS:HE2	2.05	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
12:L:229:LEU:HD12	12:L:229:LEU:C	2.28	0.56
12:L:247:LEU:CD1	12:L:248:HIS:NE2	2.52	0.56
12:L:279:CYS:SG	57:L:706:PC1:H3D1	2.45	0.56
12:L:367:PRO:HB3	36:k:75:LYS:NZ	2.20	0.56
58:L:703:3PE:N	58:L:703:3PE:H2	2.19	0.56
13:M:264:LEU:CD2	38:m:98:LEU:HD21	2.34	0.56
15:O:173:MET:HE2	15:O:179:ILE:HG23	1.87	0.56
17:Q:59:LEU:HD21	22:W:80:ARG:HH12	1.70	0.56
18:R:59:PHE:O	18:R:63:LEU:HG	2.06	0.56
18:R:62:ASP:O	18:R:66:GLN:HG3	2.06	0.56
23:X:168:PHE:O	23:X:169:PHE:CD1	2.58	0.56
24:Y:92:TYR:CE1	24:Y:128:LYS:HD3	2.40	0.56
25:Z:7:LYS:HB2	25:Z:7:LYS:NZ	2.20	0.56
25:Z:92:GLU:O	25:Z:96:ILE:HG13	2.05	0.56
34:i:108:ASP:OD2	41:p:18:PRO:CB	2.52	0.56
39:n:81:ILE:CD1	39:n:87:GLY:O	2.53	0.56
46:AB:117:GLU:OE2	46:AB:330:TYR:HB3	2.05	0.56
47:AC:138:MET:HE1	47:AC:268:ILE:HA	1.87	0.56
47:AC:171:ASP:CG	47:AC:172:LYS:H	2.13	0.56
48:AD:157:GLY:HA2	48:AD:165:PHE:H	1.71	0.56
52:AH:48:LEU:CD1	52:AH:65:CYS:HB3	2.35	0.56
47:Ac:171:ASP:CG	47:Ac:172:LYS:H	2.13	0.56
48:Ad:92:PRO:HG3	52:Ah:77:ASP:HB3	1.87	0.56
49:Ae:235:TYR:CE1	49:Ae:242:HIS:CE1	2.93	0.56
51:Ag:35:ILE:HB	51:Ag:36:PRO:HD3	1.86	0.56
54:Ak:14:ALA:O	54:Ak:18:ILE:HG12	2.04	0.56
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.87	0.56
1:A:113:TRP:HH2	8:H:287:HIS:CD2	2.23	0.56
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:ASP:OD2	61:H:400:UQ9:H12	2.06	0.56
8:H:312:ALA:HB2	27:b:38:TYR:HB3	1.87	0.56
13:M:57:SER:HB3	13:M:113:THR:HG22	1.87	0.56
13:M:78:MET:O	13:M:432:ARG:HD2	2.05	0.56
13:M:118:PHE:O	13:M:122:PHE:CB	2.54	0.56
13:M:196:TRP:HE1	13:M:250:LEU:HD13	1.69	0.56
14:N:120:GLN:O	14:N:176:ARG:CZ	2.54	0.56
14:N:254:LEU:CD1	14:N:255:PRO:HD2	2.35	0.56
15:O:149:HIS:CE1	15:O:153:THR:HG21	2.40	0.56
20:T:134:ASP:OD1	20:T:134:ASP:O	2.23	0.56
20:U:91:ASP:OD2	36:k:48:ARG:NH2	2.38	0.56
23:X:130:LYS:HE3	27:b:67:PRO:HB3	1.86	0.56
34:i:93:LYS:HD3	58:i:201:3PE:H121	1.88	0.56
37:l:88:PRO:HB2	39:n:86:PRO:CB	2.35	0.56
38:m:15:PRO:HG3	38:m:18:LEU:HD12	1.86	0.56
41:p:39:LEU:O	41:p:44:PRO:HD3	2.06	0.56
48:AD:147:ALA:O	48:AD:151:GLU:HG3	2.05	0.56
49:AE:190:VAL:HG11	49:AE:248:ARG:NH1	2.20	0.56
50:AF:22:TYR:CD2	50:AF:84:TYR:HB2	2.41	0.56
49:Ae:204:ARG:NH2	49:Ae:213:LEU:HD22	2.20	0.56
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.87	0.56
2:B:93:MET:HE1	2:B:95:PHE:CE2	2.40	0.56
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.56
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.36	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.40	0.56
8:H:19:PHE:HB3	26:a:12:MET:HG3	1.87	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
15:O:114:LEU:O	15:O:117:PHE:HB3	2.06	0.56
20:T:90:TYR:HE2	20:T:92:LYS:CB	2.19	0.56
23:X:137:LEU:HD23	23:X:138:PRO:O	2.05	0.56
30:e:14:LEU:HD12	30:e:14:LEU:C	2.31	0.56
39:n:50:GLU:HG2	39:n:51:HIS:N	2.20	0.56
47:AC:107:TYR:HB2	47:AC:305:PRO:HG3	1.86	0.56
49:AE:146:VAL:HG11	47:Ac:167:GLY:CA	2.35	0.56
51:AG:27:PHE:HB3	51:AG:30:TYR:HB2	1.87	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:667:GLN:NE2	19:S:38:VAL:HA	2.21	0.56
10:J:169:ILE:HD13	14:N:42:PRO:HA	1.87	0.56
12:L:295:GLN:NE2	12:L:524:THR:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:196:TYR:HB3	14:N:273:ASN:OD1	2.05	0.56
14:N:314:MET:HB2	15:O:305:LEU:CD1	2.34	0.56
15:O:256:LEU:CD2	15:O:276:LEU:HD23	2.30	0.56
17:Q:167:ASN:O	17:Q:168:LYS:HG2	2.05	0.56
20:T:83:VAL:CG2	20:T:126:PHE:CZ	2.83	0.56
20:T:130:ILE:HD11	20:T:148:ILE:HD11	1.86	0.56
20:U:125:GLU:OE2	35:j:44:TYR:HE1	1.89	0.56
62:a:101:CDL:H141	62:a:101:CDL:H321	1.86	0.56
32:g:140:PHE:HB3	41:p:75:THR:HG21	1.87	0.56
46:AB:40:PHE:CE1	46:AB:48:VAL:HB	2.40	0.56
47:AC:272:TRP:HA	47:AC:275:LEU:HG	1.87	0.56
49:AE:152:ILE:HD13	49:AE:169:TRP:HB2	1.87	0.56
49:AE:155:LYS:CE	49:AE:157:SER:HB3	2.35	0.56
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.40	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
10:J:38:VAL:O	10:J:42:MET:HG3	2.05	0.56
12:L:397:GLU:HB2	12:L:482:MET:SD	2.46	0.56
14:N:149:LEU:CD1	14:N:154:ILE:HG21	2.35	0.56
14:N:253:GLY:H	14:N:290:LEU:HD11	1.71	0.56
40:o:15:VAL:HG11	40:o:113:LYS:HD3	1.87	0.56
45:AA:53:LEU:HD11	45:AA:246:ALA:HB1	1.86	0.56
48:AD:249:TYR:CE2	48:AD:252:VAL:HA	2.39	0.56
49:AE:200:HIS:H	49:AE:204:ARG:NH2	2.03	0.56
47:Ac:51:LEU:HD12	47:Ac:69:ILE:HD13	1.86	0.56
47:Ac:138:MET:HE1	47:Ac:268:ILE:HG23	1.86	0.56
4:D:338:ARG:NH1	25:Z:23:ARG:HA	2.21	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.56
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.56
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.56
8:H:202:GLU:O	8:H:203:GLY:C	2.49	0.56
14:N:258:THR:OG1	14:N:336:THR:HG22	2.05	0.56
26:a:14:VAL:O	26:a:18:ILE:HG13	2.06	0.56
27:b:52:ASN:ND2	30:e:28:LYS:CE	2.69	0.56
28:c:55:TRP:HE1	29:d:66:THR:HG21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:69:LEU:HD11	34:i:71:ALA:CB	2.35	0.56
35:j:52:ARG:HG3	35:j:56:ILE:CD1	2.36	0.56
35:j:92:TRP:CZ3	40:o:100:LYS:HA	2.41	0.56
37:l:185:ASP:OD1	40:o:37:ARG:HA	2.05	0.56
40:o:4:HIS:HA	40:o:7:ARG:HH11	1.71	0.56
46:AB:236:GLN:HG3	46:AB:237:PHE:CD2	2.41	0.56
48:AD:102:LEU:HD13	53:AJ:47:ILE:HD13	1.86	0.56
48:AD:321:TYR:HB2	50:AF:61:PHE:CZ	2.41	0.56
46:Ab:162:LYS:NZ	46:Ab:194:ASP:OD1	2.38	0.56
49:Ae:207:LYS:HB3	49:Ae:209:GLU:OE1	2.05	0.56
51:Ag:33:LYS:C	51:Ag:36:PRO:HD2	2.30	0.56
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.87	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
12:L:427:ILE:CD1	36:k:69:PHE:HE1	2.18	0.56
13:M:73:LEU:CD2	13:M:103:GLN:CD	2.79	0.56
13:M:370:PRO:CA	13:M:375:LEU:CD2	2.83	0.56
14:N:193:ILE:HD11	14:N:269:GLU:HB2	1.88	0.56
17:Q:165:SER:HB3	17:Q:168:LYS:O	2.06	0.56
18:R:77:ILE:HD11	18:R:111:PHE:CG	2.41	0.56
30:e:85:LYS:O	30:e:88:LYS:HB3	2.06	0.56
46:AB:366:LEU:HD21	46:AB:425:VAL:HG22	1.87	0.56
49:AI:76:VAL:HG23	49:AI:78:PHE:CE2	2.41	0.56
54:AK:36:THR:HB	54:AK:38:TRP:CG	2.39	0.56
47:Ac:65:SER:O	47:Ac:69:ILE:HG13	2.06	0.56
49:Ae:168:LYS:N	49:Ae:173:PRO:HA	2.21	0.56
52:Ah:82:HIS:HB3	52:Ah:83:LYS:NZ	2.20	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
2:B:97:LEU:HD21	2:B:141:MET:HG2	1.88	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
16:P:64:PHE:HE1	16:P:209:ARG:O	1.88	0.56
16:P:140:ASP:OD1	16:P:142:GLU:HB2	2.05	0.56
17:Q:110:PRO:HB3	18:R:43:TYR:OH	2.06	0.56
23:X:160:PRO:HG3	29:d:22:PRO:CD	2.35	0.56
24:Y:76:THR:CG2	24:Y:95:GLY:HA3	2.34	0.56
36:k:42:LEU:HG	39:n:39:TYR:HD1	1.71	0.56
37:l:111:MET:HE3	37:l:112:TYR:CZ	2.41	0.56
40:o:25:PHE:CZ	40:o:109:LEU:HD13	2.40	0.56
41:p:74:ILE:CD1	41:p:85:ILE:HG13	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AF:15:ASP:OD2	50:AF:19:LYS:NZ	2.39	0.56
54:AK:23:MET:O	54:AK:27:VAL:HG23	2.05	0.56
48:Ad:318:LYS:HD2	49:Ae:86:PRO:HB2	1.87	0.56
2:B:95:PHE:CE2	2:B:131:MET:SD	2.99	0.55
2:B:154:GLU:O	16:P:89:TYR:OH	2.21	0.55
4:D:266:ARG:HD3	58:I:301:3PE:O14	2.05	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
7:G:382:ARG:HD2	19:S:56:ARG:CD	2.36	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
11:K:59:ILE:HD12	14:N:27:MET:HG2	1.88	0.55
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.88	0.55
12:L:597:LEU:HD21	24:Y:37:ILE:HD12	1.87	0.55
13:M:309:PHE:O	13:M:313:THR:HG23	2.06	0.55
16:P:61:ALA:HB3	16:P:82:ILE:HG23	1.88	0.55
23:X:158:LEU:HD13	29:d:17:GLU:HG3	1.88	0.55
25:Z:69:ILE:CG2	27:b:54:PRO:HD3	2.37	0.55
33:h:129:PRO:HG3	41:p:66:ARG:CZ	2.37	0.55
46:AB:326:PHE:CZ	49:AI:15:LEU:HD21	2.41	0.55
45:Aa:310:ILE:HA	45:Aa:390:ARG:NH1	2.21	0.55
46:Ab:307:SER:HB2	46:Ab:310:SER:HB2	1.86	0.55
47:Ac:294:LEU:CD1	68:Ac:404:U10:H1M3	2.36	0.55
48:Ad:116:VAL:HA	48:Ad:253:LEU:HD21	1.88	0.55
4:D:238:LEU:HA	25:Z:9:ASP:HB2	1.86	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
10:J:126:TYR:C	25:Z:120:LEU:HD11	2.32	0.55
12:L:94:LEU:CD2	12:L:125:LEU:HD21	2.35	0.55
12:L:385:PHE:CD1	35:j:72:ARG:CG	2.89	0.55
12:L:538:PRO:O	12:L:542:LEU:HD13	2.06	0.55
62:L:704:CDL:H171	13:M:361:MET:HE1	1.89	0.55
13:M:267:TRP:HZ3	58:m:201:3PE:H2F1	1.72	0.55
14:N:325:MET:HE3	14:N:329:LEU:HD11	1.88	0.55
15:O:316:GLU:HG3	32:g:51:MET:HE2	1.87	0.55
23:X:169:PHE:CD2	23:X:169:PHE:O	2.59	0.55
24:Y:71:MET:CG	24:Y:102:THR:HG21	2.37	0.55
47:AC:233:LEU:CD2	48:AD:300:LEU:HA	2.37	0.55
48:AD:321:TYR:HB2	50:AF:61:PHE:CE1	2.40	0.55
49:AE:168:LYS:H	49:AE:174:LEU:H	1.53	0.55
49:AE:205:VAL:HG21	49:AE:208:PRO:HA	1.89	0.55
52:AH:49:GLU:HA	52:AH:52:ASP:OD2	2.07	0.55
45:Aa:407:THR:HB	45:Aa:408:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:43:LYS:HA	52:Ah:46:GLU:CD	2.31	0.55
54:Ak:42:LEU:O	54:Ak:45:VAL:HB	2.06	0.55
1:A:102:LEU:CD1	1:A:111:LEU:HD11	2.37	0.55
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.72	0.55
4:D:266:ARG:NH2	9:I:59:ARG:O	2.39	0.55
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
8:H:175:LEU:HD21	57:I:302:PC1:H2C1	1.88	0.55
10:J:65:VAL:CG1	10:J:66:VAL:H	2.19	0.55
16:P:122:HIS:HB2	18:R:46:VAL:HG12	1.88	0.55
24:Y:137:LEU:HD23	24:Y:138:PHE:CD2	2.41	0.55
39:n:57:MET:HE2	39:n:57:MET:HA	1.87	0.55
46:AB:43:LEU:HB3	46:AB:44:PRO:HD2	1.88	0.55
45:Aa:74:TRP:CZ2	45:Aa:411:GLU:HA	2.42	0.55
49:Ae:167:PHE:CE2	49:Ae:176:VAL:HG21	2.34	0.55
4:D:57:GLU:HA	4:D:60:HIS:CD2	2.41	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
10:J:2:ASN:HB2	25:Z:130:LYS:NZ	2.22	0.55
12:L:336:LYS:O	12:L:340:PHE:HD2	1.89	0.55
12:L:578:THR:CG2	14:N:168:GLY:HA2	2.36	0.55
13:M:4:ILE:H	13:M:4:ILE:HD12	1.70	0.55
13:M:421:ASN:HB2	38:m:51:TYR:OH	2.06	0.55
20:T:103:HIS:HD1	20:T:140:CYS:HG	1.49	0.55
23:X:124:GLN:C	23:X:125:LEU:HD12	2.32	0.55
40:o:69:CYS:O	40:o:69:CYS:SG	2.65	0.55
45:AA:74:TRP:HB3	45:AA:418:LEU:HD11	1.89	0.55
46:AB:36:GLN:O	46:AB:52:LEU:HD13	2.07	0.55
47:AC:97:HIS:CE1	47:AC:100:ARG:HH21	2.24	0.55
47:AC:138:MET:HE1	47:AC:268:ILE:HG23	1.89	0.55
49:Ae:235:TYR:HA	49:Ae:241:SER:O	2.06	0.55
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.55
4:D:279:THR:HA	21:V:12:VAL:HG13	1.87	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
15:O:66:ILE:HD12	15:O:67:CYS:SG	2.46	0.55
16:P:145:PHE:O	16:P:149:PRO:HG2	2.05	0.55
23:X:39:THR:HG23	23:X:40:ASN:N	2.20	0.55
25:Z:89:GLU:OE1	30:e:97:HIS:CD2	2.60	0.55
49:Ae:242:HIS:O	49:Ae:250:ARG:HB2	2.07	0.55
50:Af:35:ASP:HB2	50:Af:90:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:PHE:HB2	4:D:97:LEU:HB2	1.87	0.55
4:D:89:PRO:HG2	8:H:204:GLU:HG3	1.88	0.55
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.07	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
8:H:249:ILE:HD13	23:X:99:HIS:CG	2.42	0.55
10:J:55:VAL:HB	11:K:41:PHE:CE2	2.42	0.55
11:K:93:LEU:HD13	14:N:57:THR:HG21	1.88	0.55
12:L:54:PHE:O	12:L:58:ASN:CA	2.55	0.55
12:L:69:VAL:HG11	12:L:71:MET:HE2	1.89	0.55
12:L:162:THR:O	12:L:166:THR:HG23	2.06	0.55
12:L:230:HIS:N	12:L:231:PRO:HD3	2.22	0.55
12:L:561:THR:O	12:L:565:SER:HB2	2.07	0.55
58:M:501:3PE:O22	14:N:276:LEU:HD13	2.07	0.55
14:N:224:SER:HB2	14:N:229:SER:HB3	1.89	0.55
14:N:237:THR:O	14:N:237:THR:CG2	2.55	0.55
15:O:135:LEU:HD13	63:O:402:ADP:C6	2.41	0.55
15:O:170:LEU:HG	15:O:179:ILE:HD13	1.87	0.55
20:U:89:LEU:HA	36:k:53:ARG:HH22	1.71	0.55
24:Y:68:ILE:HG21	24:Y:120:MET:HE1	1.87	0.55
25:Z:53:TRP:O	25:Z:57:ARG:HG3	2.06	0.55
42:q:6:VAL:HG23	42:q:7:LEU:N	2.21	0.55
43:r:9:GLN:O	43:r:12:ARG:HB2	2.06	0.55
47:AC:153:ILE:HB	47:AC:157:GLY:CA	2.36	0.55
48:AD:253:LEU:HD12	48:AD:253:LEU:C	2.32	0.55
45:Aa:168:ILE:O	45:Aa:171:GLU:HG2	2.06	0.55
48:Ad:181:ASN:HB3	48:Ad:183:GLU:OE1	2.07	0.55
49:Ae:194:GLN:HB3	49:Ae:250:ARG:NE	2.21	0.55
6:F:382:CYS:SG	55:F:502:SF4:S4	3.05	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
9:I:75:SER:O	43:r:12:ARG:HG2	2.07	0.55
14:N:230:ILE:O	14:N:233:LEU:HB2	2.07	0.55
17:Q:163:ASN:OD1	17:Q:163:ASN:C	2.49	0.55
22:W:23:ILE:HG13	22:W:80:ARG:HG2	1.87	0.55
30:e:14:LEU:HD12	30:e:15:ASP:N	2.21	0.55
35:j:97:LEU:O	40:o:104:ARG:NH1	2.39	0.55
49:AE:226:ALA:HA	49:AE:234:TYR:HA	1.88	0.55
53:AJ:43:ILE:O	53:AJ:47:ILE:HG13	2.07	0.55
47:Ac:97:HIS:CE1	47:Ac:100:ARG:HH21	2.23	0.55
49:Ae:195:LEU:CD2	49:Ae:248:ARG:HD2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:170:GLN:HB3	44:s:48:LEU:HD22	1.89	0.55
10:J:75:THR:OG1	11:K:25:HIS:CD2	2.59	0.55
12:L:441:ILE:HD12	35:j:46:GLU:O	2.06	0.55
62:L:704:CDL:H341	33:h:71:MET:HE1	1.89	0.55
13:M:62:SER:C	13:M:64:PRO:HD2	2.32	0.55
15:O:319:ILE:HG13	15:O:320:GLY:H	1.72	0.55
16:P:217:PHE:HA	16:P:220:TYR:HD2	1.71	0.55
16:P:376:ASN:OD1	16:P:376:ASN:C	2.50	0.55
20:U:120:MET:HE1	39:n:24:LEU:HD12	1.88	0.55
22:W:25:SER:HB3	22:W:30:GLU:HB3	1.88	0.55
23:X:20:VAL:HG13	23:X:24:VAL:HB	1.87	0.55
23:X:132:LYS:HB3	27:b:59:ASP:HB3	1.87	0.55
27:b:8:PHE:CG	27:b:9:LEU:N	2.74	0.55
34:i:69:LEU:CD1	34:i:71:ALA:CB	2.85	0.55
45:AA:139:ASP:O	45:AA:143:VAL:HG23	2.07	0.55
47:AC:49:LEU:HD22	47:Ac:184:ILE:HD13	1.88	0.55
49:AE:127:TYR:HD1	53:AJ:33:GLU:HA	1.72	0.55
48:Ad:95:PRO:HG2	52:Ah:85:PHE:CD2	2.41	0.55
48:Ad:107:HIS:CE1	48:Ad:138:VAL:HG13	2.41	0.55
48:Ad:253:LEU:C	48:Ad:253:LEU:HD12	2.32	0.55
49:Ae:168:LYS:HZ3	49:Ae:171:GLY:HA2	1.72	0.55
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.55
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.55
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.55
6:F:48:ARG:HA	6:F:48:ARG:HH11	1.72	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
10:J:34:VAL:CG1	58:J:401:3PE:C2I	2.84	0.55
12:L:197:GLU:HB2	41:p:111:LYS:HE3	1.88	0.55
13:M:231:LEU:CA	13:M:235:LEU:HD12	2.36	0.55
13:M:453:LEU:HD12	13:M:454:ILE:CG2	2.34	0.55
20:U:83:VAL:O	20:U:87:LEU:HG	2.07	0.55
22:W:35:VAL:HG21	66:W:201:EHZ:N2	2.22	0.55
22:W:53:MET:HB2	22:W:55:LEU:HG	1.89	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
43:r:7:VAL:O	43:r:11:LEU:HG	2.06	0.55
45:AA:87:ASN:H	45:AA:207:ASN:HD22	1.53	0.55
45:AA:120:LEU:N	46:AB:298:HIS:O	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:135:LEU:HD23	48:AD:276:TRP:CH2	2.41	0.55
50:AF:102:ARG:HH21	50:AF:103:LYS:HE3	1.72	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.32	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
8:H:69:SER:C	8:H:71:PHE:N	2.61	0.55
8:H:130:PHE:CD2	8:H:207:LEU:HD11	2.41	0.55
11:K:45:SER:O	11:K:49:LEU:HG	2.07	0.55
12:L:258:PHE:HE1	12:L:262:ARG:HH21	1.55	0.55
12:L:586:LEU:HD21	24:Y:47:PRO:HD3	1.89	0.55
58:M:503:3PE:C3A	14:N:246:LEU:HD11	2.35	0.55
14:N:273:ASN:HD21	24:Y:143:VAL:HA	1.72	0.55
16:P:98:GLY:HA3	16:P:103:LEU:HG	1.87	0.55
16:P:236:VAL:HG13	16:P:270:ARG:HH21	1.71	0.55
16:P:273:LEU:O	16:P:277:VAL:HG23	2.06	0.55
20:U:79:ILE:HD11	20:U:148:ILE:CG2	2.37	0.55
20:U:125:GLU:OE2	35:j:44:TYR:CE1	2.60	0.55
25:Z:56:GLU:HA	25:Z:59:ARG:HH11	1.72	0.55
27:b:38:TYR:HA	27:b:41:TYR:CD2	2.42	0.55
31:f:56:TRP:CD1	33:h:134:GLU:OE1	2.60	0.55
34:i:108:ASP:OD2	41:p:18:PRO:HB2	2.07	0.55
47:AC:272:TRP:CE2	47:AC:273:TYR:HD2	2.25	0.55
46:Ab:89:LEU:HD11	46:Ab:154:LEU:HD12	1.89	0.55
49:Ae:167:PHE:CE2	49:Ae:176:VAL:CG2	2.83	0.55
1:A:108:GLN:HG3	10:J:167:ILE:HD13	1.88	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.89	0.54
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.54
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.54
8:H:11:VAL:O	8:H:12:PRO:C	2.50	0.54
10:J:126:TYR:C	25:Z:120:LEU:CD1	2.80	0.54
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.43	0.54
12:L:477:ILE:HG13	40:o:91:GLU:OE1	2.07	0.54
16:P:71:ASN:HA	16:P:97:MET:SD	2.47	0.54
20:T:87:LEU:HD22	20:T:104:PHE:CZ	2.41	0.54
20:T:128:PHE:CE2	20:T:130:ILE:HG13	2.42	0.54
25:Z:24:ASN:OD1	25:Z:24:ASN:O	2.24	0.54
31:f:38:ARG:HH12	31:f:54:VAL:HB	1.71	0.54
31:f:56:TRP:CE3	33:h:131:LYS:HG3	2.41	0.54
45:AA:186:TYR:OH	49:AE:80:HIS:HB2	2.07	0.54
46:AB:60:ARG:CZ	46:AB:390:GLU:HB3	2.37	0.54
49:AE:93:ARG:CA	51:AG:25:ARG:HG3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:312:GLN:HG2	50:Af:37:THR:O	2.07	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
9:I:123:CYS:SG	55:I:303:SF4:S3	3.06	0.54
10:J:22:LYS:HD2	11:K:23:ARG:CD	2.35	0.54
12:L:54:PHE:O	12:L:58:ASN:HA	2.08	0.54
13:M:415:GLN:O	13:M:416:ARG:HG3	2.08	0.54
15:O:49:THR:HG21	15:O:151:LEU:HG	1.89	0.54
26:a:31:ASN:HD21	26:a:36:LYS:HB2	1.71	0.54
31:f:49:ARG:NH2	33:h:106:ILE:HG22	2.23	0.54
33:h:73:PHE:CD2	33:h:74:TYR:CE1	2.94	0.54
35:j:71:TRP:CZ3	58:j:700:3PE:H3B1	2.42	0.54
40:o:103:GLU:OE2	40:o:106:ARG:HD2	2.07	0.54
47:AC:30:TRP:HB3	47:AC:100:ARG:HD3	1.90	0.54
52:AH:58:ARG:HB3	52:AH:61:THR:CG2	2.38	0.54
45:Aa:87:ASN:H	45:Aa:207:ASN:HD22	1.53	0.54
46:Ab:366:LEU:HD21	46:Ab:425:VAL:HG22	1.87	0.54
48:Ad:214:LEU:CD1	48:Ad:237:PHE:HB2	2.38	0.54
49:Ae:236:CYS:SG	49:Ae:239:HIS:HB3	2.47	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:617:ARG:HH12	22:W:128:GLY:C	2.16	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
10:J:12:PHE:CZ	11:K:42:ILE:HD12	2.42	0.54
10:J:37:PHE:CZ	58:J:401:3PE:H2A2	2.42	0.54
12:L:190:SER:HB2	12:L:196:TRP:NE1	2.22	0.54
15:O:63:ASP:OD2	15:O:241:TYR:CE1	2.60	0.54
23:X:121:ASP:O	23:X:122:LEU:C	2.50	0.54
23:X:158:LEU:HD13	29:d:17:GLU:CG	2.38	0.54
26:a:58:ASN:HB2	26:a:61:TYR:CD2	2.43	0.54
29:d:100:ASP:HB3	33:h:159:LEU:HD21	1.89	0.54
30:e:38:LYS:HG2	33:h:179:ILE:CG2	2.36	0.54
34:i:16:ARG:O	34:i:20:ARG:HG2	2.08	0.54
34:i:69:LEU:CD1	34:i:71:ALA:H	2.18	0.54
48:AD:228:ARG:HG3	48:AD:229:GLU:HG3	1.89	0.54
45:Aa:121:ASN:OD1	46:Ab:300:LYS:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:136:LEU:HD21	46:Ab:380:ALA:HA	1.89	0.54
45:Aa:183:VAL:HG21	45:Aa:286:HIS:HB2	1.88	0.54
51:Ag:72:ARG:HD3	51:Ag:73:LYS:N	2.23	0.54
1:A:77:TRP:NE1	10:J:136:GLU:OE2	2.40	0.54
3:C:124:ARG:HD2	17:Q:140:LYS:NZ	2.23	0.54
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:445:LEU:HD23	7:G:460:HIS:HE1	1.55	0.54
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
10:J:164:PHE:HE2	14:N:4:ILE:HG12	1.73	0.54
12:L:232:TRP:O	12:L:236:ALA:N	2.40	0.54
12:L:385:PHE:CE1	35:j:72:ARG:HG3	2.42	0.54
12:L:551:THR:HA	12:L:555:LEU:HD12	1.89	0.54
13:M:6:LEU:HB3	13:M:7:PRO:HD3	1.88	0.54
13:M:25:THR:HG22	32:g:84:ASN:CG	2.33	0.54
15:O:305:LEU:O	15:O:305:LEU:CD1	2.55	0.54
16:P:300:TRP:O	16:P:304:LEU:HG	2.08	0.54
21:V:50:GLN:HE22	43:r:94:ALA:H	1.56	0.54
23:X:17:GLU:HG2	30:e:104:PRO:HD3	1.88	0.54
42:q:17:HIS:NE2	42:q:33:ILE:HG23	2.23	0.54
49:AE:199:GLN:HB3	49:AE:204:ARG:HH21	1.72	0.54
49:AE:248:ARG:HA	49:AE:257:ASN:CG	2.33	0.54
53:AJ:14:LEU:HD22	53:AJ:24:THR:HB	1.89	0.54
45:Aa:285:ALA:O	45:Aa:360:CYS:N	2.36	0.54
45:Aa:384:THR:CG2	45:Aa:387:GLU:HG2	2.38	0.54
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.43	0.54
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
10:J:60:LEU:HD13	10:J:61:GLY:N	2.21	0.54
11:K:93:LEU:HA	14:N:54:GLU:OE2	2.06	0.54
12:L:131:LEU:CD1	12:L:140:LEU:CD1	2.78	0.54
12:L:362:ILE:HA	12:L:365:ILE:HG13	1.90	0.54
62:L:704:CDL:H211	62:L:704:CDL:H532	1.90	0.54
13:M:423:MET:SD	38:m:59:HIS:NE2	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:131:PRO:HG2	20:U:134:ASP:HB2	1.90	0.54
23:X:64:ASN:O	23:X:68:LEU:HG	2.07	0.54
48:AD:214:LEU:C	48:AD:217:GLY:H	2.16	0.54
49:AE:196:ARG:HH11	49:AE:249:ILE:HG13	1.73	0.54
54:AK:36:THR:O	54:AK:38:TRP:HD1	1.90	0.54
46:Ab:159:LYS:HB2	46:Ab:197:MET:SD	2.47	0.54
49:Ae:93:ARG:HD2	49:Ae:110:ARG:HD3	1.90	0.54
50:Af:47:ALA:HB1	50:Af:91:LEU:HD11	1.90	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
2:B:126:ARG:HG3	8:H:213:VAL:O	2.08	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:445:LEU:HD21	7:G:460:HIS:CE1	2.34	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
12:L:123:LEU:HD21	62:L:704:CDL:H741	1.90	0.54
12:L:232:TRP:CH2	12:L:233:LEU:HD21	2.42	0.54
12:L:539:MET:SD	38:m:11:LEU:HD21	2.48	0.54
13:M:231:LEU:O	13:M:236:LEU:HG	2.06	0.54
14:N:223:ASN:HB3	15:O:306:ASN:HD21	1.73	0.54
15:O:69:GLY:HA2	15:O:72:LYS:HZ3	1.72	0.54
15:O:170:LEU:HG	15:O:179:ILE:CD1	2.37	0.54
15:O:209:VAL:HG23	15:O:214:VAL:HG13	1.88	0.54
16:P:239:PRO:HG2	16:P:345:LEU:HD12	1.90	0.54
16:P:316:LYS:O	16:P:320:GLU:HG2	2.08	0.54
17:Q:160:TYR:CZ	17:Q:164:PHE:HZ	2.26	0.54
32:g:147:LEU:HD21	41:p:163:MET:HB2	1.90	0.54
58:m:201:3PE:H2D2	58:m:201:3PE:H2H1	1.89	0.54
45:AA:187:LEU:HD22	45:AA:288:ALA:HB1	1.89	0.54
47:AC:141:TRP:CD1	47:AC:265:PRO:CD	2.90	0.54
47:AC:222:PRO:HG2	47:AC:223:TYR:CD2	2.43	0.54
49:AE:93:ARG:HD2	51:AG:22:PHE:O	2.07	0.54
51:AG:39:LEU:O	51:AG:42:THR:HG22	2.08	0.54
52:AH:58:ARG:HG2	52:AH:61:THR:H	1.72	0.54
45:Aa:55:ASN:HB3	45:Aa:226:ALA:CB	2.38	0.54
48:Ad:157:GLY:HA2	48:Ad:164:MET:HA	1.88	0.54
50:Af:102:ARG:HH21	50:Af:103:LYS:HE3	1.73	0.54
52:Ah:67:GLU:HG3	52:Ah:68:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:ARG:HH12	22:W:112:GLU:CB	2.19	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
8:H:43:TYR:CE2	42:q:27:PHE:HZ	2.26	0.54
58:L:702:3PE:C2F	14:N:100:MET:HE1	2.38	0.54
13:M:31:SER:HA	13:M:34:ILE:HG12	1.90	0.54
13:M:79:ALA:HB1	13:M:225:ILE:HD13	1.90	0.54
15:O:60:ILE:O	15:O:158:VAL:HA	2.07	0.54
15:O:237:ILE:HG22	15:O:241:TYR:CE2	2.43	0.54
16:P:207:PHE:CE1	16:P:214:LEU:HD22	2.43	0.54
30:e:83:ARG:HD3	30:e:92:TYR:CD2	2.43	0.54
31:f:37:PHE:CZ	41:p:83:LEU:HD13	2.43	0.54
38:m:8:PRO:HB3	38:m:14:LEU:N	2.23	0.54
38:m:109:ARG:O	38:m:113:GLU:HG2	2.08	0.54
39:n:20:TYR:CE2	39:n:24:LEU:CD1	2.91	0.54
40:o:39:MET:HE1	40:o:57:ASP:O	2.07	0.54
40:o:93:LEU:O	40:o:97:LYS:HG2	2.07	0.54
46:AB:160:ILE:HG23	49:AI:34:VAL:HG21	1.89	0.54
49:AE:168:LYS:HZ3	49:AE:171:GLY:HA2	1.72	0.54
49:AE:179:ARG:HB3	49:AE:183:GLU:HB2	1.89	0.54
4:D:58:THR:HG23	4:D:61:TRP:CZ3	2.41	0.54
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.54
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.54
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:179:CYS:HG	55:G:802:SF4:FE3	1.23	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
11:K:1:MET:SD	11:K:50:ASN:ND2	2.77	0.54
12:L:264:HIS:HA	12:L:267:THR:HG23	1.89	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	1.89	0.54
16:P:172:ALA:H	16:P:202:ARG:NH2	2.06	0.54
20:T:97:LYS:HG3	20:T:97:LYS:O	2.08	0.54
20:T:140:CYS:HB2	20:T:143:GLU:HG2	1.90	0.54
20:U:85:TYR:CE2	35:j:44:TYR:HE2	2.25	0.54
23:X:133:THR:O	27:b:58:ARG:NH1	2.40	0.54
25:Z:53:TRP:NE1	25:Z:57:ARG:HD2	2.23	0.54
62:a:101:CDL:H511	43:r:8:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:8:PHE:O	27:b:9:LEU:C	2.50	0.54
33:h:57:VAL:HG12	39:n:99:VAL:HG21	1.89	0.54
34:i:103:ARG:O	41:p:18:PRO:HG3	2.08	0.54
45:AA:43:GLN:HE22	46:AB:57:PRO:HA	1.72	0.54
46:Ab:38:LEU:HB3	46:Ab:40:PHE:CE1	2.43	0.54
48:Ad:125:HIS:HE1	48:Ad:195:PRO:HD2	1.73	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.89	0.54
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:80:GLU:CB	43:r:26:LEU:HD11	2.38	0.54
9:I:109:GLY:O	18:R:63:LEU:HD12	2.08	0.54
12:L:247:LEU:HD11	12:L:248:HIS:CE1	2.43	0.54
12:L:427:ILE:HD11	36:k:69:PHE:CE1	2.43	0.54
12:L:507:LEU:O	12:L:510:LYS:HG2	2.07	0.54
13:M:158:ILE:HG21	14:N:283:ALA:HB1	1.90	0.54
13:M:276:CYS:HB3	13:M:285:LEU:HG	1.89	0.54
13:M:283:LYS:HG3	13:M:327:PHE:CE1	2.43	0.54
14:N:307:THR:CG2	14:N:308:ASN:H	2.19	0.54
16:P:142:GLU:HA	16:P:146:VAL:HG12	1.90	0.54
17:Q:117:THR:HG22	17:Q:119:ASP:H	1.73	0.54
33:h:57:VAL:HG12	39:n:99:VAL:CG2	2.38	0.54
42:q:88:ARG:HD2	42:q:94:THR:OG1	2.08	0.54
49:AE:118:THR:HG1	53:AJ:21:PHE:HZ	1.55	0.54
47:Ac:222:PRO:HG2	47:Ac:223:TYR:CD2	2.43	0.54
1:A:110:GLY:O	1:A:111:LEU:HB2	2.08	0.54
4:D:259:GLU:HB3	25:Z:25:LEU:HD11	1.89	0.54
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
13:M:1:MET:HE2	13:M:52:PHE:CE2	2.42	0.54
38:m:28:GLU:HG2	38:m:31:ARG:HH22	1.73	0.54
48:AD:154:VAL:HG12	48:AD:155:GLN:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:159:ASN:HB3	48:AD:162:GLY:HA3	1.90	0.54
49:AE:234:TYR:HB2	49:AE:243:TYR:CB	2.30	0.54
51:AG:69:GLN:NE2	51:AG:72:ARG:HH22	2.06	0.54
45:Aa:341:PHE:HE2	45:Aa:372:LEU:HD13	1.67	0.54
45:Aa:400:VAL:HG21	46:Ab:58:LEU:HG	1.90	0.54
46:Ab:50:ALA:HB3	46:Ab:221:VAL:HG22	1.90	0.54
49:Ae:154:ILE:HD13	49:Ae:271:VAL:O	2.08	0.54
49:Ae:184:ILE:CG2	49:Ae:208:PRO:HB3	2.38	0.54
3:C:80:LEU:HG	4:D:396:THR:CG2	2.37	0.53
3:C:100:ARG:HH12	21:V:86:LYS:NZ	2.06	0.53
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.73	0.53
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.51	0.53
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.53
10:J:20:ALA:O	58:K:101:3PE:H242	2.08	0.53
12:L:193:MET:HE1	38:m:125:PHE:CD2	2.43	0.53
12:L:362:ILE:CD1	12:L:430:VAL:CG1	2.82	0.53
16:P:58:VAL:O	16:P:83:PRO:HD2	2.09	0.53
20:U:86:VAL:CB	20:U:122:MET:HE1	2.37	0.53
26:a:2:TRP:HH2	62:a:101:CDL:H522	1.73	0.53
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.53
40:o:57:ASP:CG	40:o:59:CYS:H	2.16	0.53
41:p:31:THR:O	41:p:35:LYS:HG3	2.07	0.53
47:AC:233:LEU:HD23	48:AD:300:LEU:HD23	1.90	0.53
48:AD:126:SER:HB2	48:AD:128:ASP:OD1	2.07	0.53
49:AE:184:ILE:HG12	49:AE:209:GLU:HA	1.90	0.53
46:Ab:320:PRO:HG2	46:Ab:343:GLN:HE21	1.73	0.53
49:Ae:264:GLU:N	49:Ae:272:VAL:O	2.39	0.53
51:Ag:39:LEU:O	51:Ag:42:THR:HG22	2.08	0.53
4:D:35:ARG:HH21	32:g:59:PRO:HD3	1.73	0.53
4:D:253:LEU:HD11	43:r:18:GLN:HG3	1.90	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
11:K:62:THR:HG23	11:K:66:PHE:CE1	2.43	0.53
12:L:149:ILE:HG21	13:M:364:LEU:CD2	2.38	0.53
13:M:173:THR:HB	33:h:143:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:M:501:3PE:H342	14:N:280:THR:HG21	1.90	0.53
14:N:179:MET:HE2	14:N:216:PHE:CE1	2.43	0.53
15:O:40:LEU:HG	15:O:292:HIS:CE1	2.44	0.53
17:Q:82:PRO:O	17:Q:94:THR:HG23	2.08	0.53
20:T:118:ILE:HG23	20:T:122:MET:CE	2.37	0.53
22:W:88:LYS:O	22:W:92:GLU:HG2	2.08	0.53
34:i:22:TRP:CZ2	39:n:172:THR:HG22	2.43	0.53
39:n:30:TRP:CD2	39:n:76:HIS:CD2	2.95	0.53
46:AB:59:SER:OG	46:AB:130:ILE:HG21	2.08	0.53
48:AD:121:CYS:HB3	70:AD:401:HEC:HAB	1.89	0.53
48:AD:231:LEU:HD23	48:AD:243:GLY:HA2	1.90	0.53
49:AE:168:LYS:HA	49:AE:173:PRO:CA	2.34	0.53
47:Ac:146:ILE:O	47:Ac:149:LEU:HB3	2.07	0.53
49:Ae:175:PHE:N	49:Ae:213:LEU:O	2.41	0.53
49:Ae:248:ARG:HA	49:Ae:257:ASN:ND2	2.22	0.53
4:D:36:GLN:HE22	13:M:135:ARG:HH22	1.57	0.53
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.73	0.53
12:L:559:GLU:HG2	12:L:564:LYS:HD3	1.90	0.53
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.90	0.53
15:O:114:LEU:HA	15:O:131:LEU:HD22	1.91	0.53
15:O:164:TYR:CE1	15:O:195:LEU:HD21	2.43	0.53
15:O:332:ARG:NH1	29:d:50:MET:HE1	2.23	0.53
25:Z:12:PRO:HD3	25:Z:16:TYR:CE1	2.43	0.53
30:e:38:LYS:NZ	33:h:181:HIS:HD2	2.06	0.53
33:h:55:PHE:HB2	34:i:28:LEU:HD21	1.91	0.53
39:n:125:TRP:CE3	39:n:128:LEU:HD12	2.43	0.53
45:AA:136:LEU:HD21	46:AB:380:ALA:HA	1.91	0.53
45:AA:170:ARG:HG3	45:AA:171:GLU:N	2.22	0.53
46:AB:237:PHE:O	46:AB:238:LEU:HB2	2.07	0.53
48:AD:154:VAL:HG12	48:AD:155:GLN:H	1.74	0.53
48:AD:234:ASN:O	48:AD:240:GLN:HA	2.08	0.53
47:Ac:30:TRP:HB3	47:Ac:100:ARG:HD3	1.90	0.53
48:Ad:255:TYR:HB3	48:Ad:257:ASP:OD1	2.08	0.53
53:Aj:31:PHE:O	53:Aj:34:ARG:CG	2.39	0.53
54:Ak:19:PRO:O	54:Ak:23:MET:HG2	2.08	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.73	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
7:G:617:ARG:NH1	22:W:128:GLY:C	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:124:LEU:HB3	25:Z:137:ASN:HD21	1.71	0.53
12:L:226:GLN:OE1	12:L:284:THR:HG21	2.07	0.53
12:L:362:ILE:HD12	12:L:430:VAL:HG13	1.88	0.53
12:L:387:THR:HG22	12:L:465:GLY:N	2.24	0.53
12:L:586:LEU:CD2	24:Y:47:PRO:HD3	2.37	0.53
13:M:263:LEU:HD11	38:m:102:TYR:CD1	2.39	0.53
15:O:140:LEU:HD11	15:O:198:TYR:OH	2.08	0.53
15:O:319:ILE:HG13	15:O:320:GLY:N	2.22	0.53
16:P:85:ARG:HE	64:P:401:NDP:C2A	2.21	0.53
18:R:94:ASN:OD1	18:R:96:ASP:HB2	2.08	0.53
19:S:30:SER:O	19:S:31:GLN:C	2.49	0.53
19:S:79:LEU:HA	19:S:82:LEU:CD1	2.24	0.53
19:S:82:LEU:HD13	19:S:86:GLU:OE1	2.08	0.53
26:a:7:PRO:HD3	62:a:101:CDL:H181	1.90	0.53
27:b:59:ASP:HA	27:b:63:MET:HE2	1.89	0.53
47:AC:77:TRP:CD2	48:AD:281:GLU:HG3	2.44	0.53
51:AG:79:GLU:HA	52:AH:58:ARG:HE	1.73	0.53
45:Aa:384:THR:HG22	45:Aa:387:GLU:HG2	1.91	0.53
48:Ad:116:VAL:HG22	48:Ad:253:LEU:HD21	1.89	0.53
48:Ad:197:LEU:HA	48:Ad:200:ILE:HB	1.90	0.53
48:Ad:214:LEU:HA	48:Ad:234:ASN:HD21	1.73	0.53
49:Ae:155:LYS:NZ	49:Ae:157:SER:HB3	2.23	0.53
49:Ae:241:SER:HB2	49:Ae:251:LYS:O	2.07	0.53
49:Ae:243:TYR:CD2	49:Ae:247:GLY:HA2	2.43	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
4:D:51:VAL:HG21	4:D:58:THR:CG2	2.38	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
9:I:67:ILE:HG13	57:I:302:PC1:H251	1.89	0.53
12:L:79:SER:CB	12:L:135:ASN:HB2	2.35	0.53
12:L:400:ASN:HD21	12:L:413:LEU:HD11	1.74	0.53
58:L:701:3PE:H222	37:l:116:ARG:O	2.09	0.53
58:M:503:3PE:H382	14:N:246:LEU:HD11	1.91	0.53
16:P:370:LYS:HG3	16:P:370:LYS:O	2.08	0.53
18:R:98:GLU:HA	18:R:113:GLN:CD	2.33	0.53
19:S:16:LEU:HD13	19:S:19:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:74:LEU:N	20:U:74:LEU:CD1	2.72	0.53
32:g:106:TYR:CE2	33:h:86:ILE:HD12	2.44	0.53
41:p:103:MET:CE	41:p:135:VAL:HG12	2.38	0.53
45:AA:255:ARG:O	45:AA:255:ARG:CG	2.51	0.53
46:AB:47:LEU:HD11	46:AB:238:LEU:HD13	1.91	0.53
46:AB:60:ARG:HG3	46:AB:124:GLU:HB3	1.89	0.53
46:AB:257:GLU:HA	46:AB:438:MET:O	2.09	0.53
48:AD:224:GLY:HA3	52:AH:64:ASP:OD1	2.08	0.53
48:AD:232:TYR:CD1	48:AD:246:PRO:HD3	2.43	0.53
49:AE:206:LYS:HZ2	49:AE:265:PHE:HB2	1.73	0.53
52:AH:65:CYS:O	52:AH:69:LEU:HB2	2.08	0.53
45:Aa:464:GLN:HA	51:Ag:5:PHE:HB3	1.91	0.53
48:Ad:213:SER:O	48:Ad:217:GLY:N	2.42	0.53
49:Ae:207:LYS:CD	49:Ae:210:TRP:HD1	2.20	0.53
49:Ae:266:THR:HB	49:Ae:269:ASP:O	2.08	0.53
1:A:112:GLU:C	1:A:113:TRP:CG	2.86	0.53
2:B:122:ARG:HH21	4:D:89:PRO:HB3	1.74	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:80:GLU:OE2	43:r:26:LEU:HD13	2.08	0.53
10:J:22:LYS:HD2	11:K:23:ARG:HG3	1.80	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.53
12:L:124:PHE:HZ	12:L:252:MET:HB2	1.74	0.53
13:M:269:MET:CE	13:M:396:MET:HA	2.36	0.53
16:P:164:PHE:CE2	16:P:166:HIS:HB2	2.44	0.53
21:V:114:TRP:O	21:V:115:PRO:C	2.52	0.53
29:d:109:TYR:O	29:d:110:ALA:C	2.50	0.53
30:e:40:TRP:CG	30:e:40:TRP:O	2.61	0.53
38:m:17:THR:HB	39:n:68:GLU:OE1	2.08	0.53
48:AD:111:ARG:O	48:AD:115:GLN:HG3	2.09	0.53
49:AE:111:LYS:HB3	49:AE:115:TYR:CE2	2.44	0.53
46:Ab:304:ASN:O	46:Ab:305:THR:C	2.50	0.53
49:Ae:144:ALA:HA	49:Ae:147:LEU:HB2	1.91	0.53
1:A:53:MET:HE1	10:J:170:THR:HG22	1.90	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
12:L:20:LEU:C	12:L:20:LEU:CD1	2.81	0.53
58:L:703:3PE:H382	58:L:703:3PE:H231	1.91	0.53
13:M:55:MET:HG3	13:M:56:PHE:CD2	2.44	0.53
13:M:57:SER:CB	13:M:113:THR:HG22	2.39	0.53
13:M:422:HIS:CE1	38:m:56:ARG:HH22	2.26	0.53
15:O:97:THR:HG22	28:c:32:ARG:HH12	1.73	0.53
20:T:87:LEU:HD23	20:T:122:MET:HE1	1.91	0.53
24:Y:50:SER:HB3	24:Y:53:GLU:HG2	1.91	0.53
31:f:16:VAL:O	31:f:17:PRO:C	2.49	0.53
33:h:156:VAL:CG1	33:h:160:MET:HE3	2.39	0.53
39:n:56:ASP:O	39:n:57:MET:C	2.50	0.53
40:o:15:VAL:CG1	40:o:113:LYS:HD3	2.39	0.53
42:q:73:THR:HA	42:q:76:ASP:OD1	2.09	0.53
46:AB:348:GLY:HA2	46:AB:448:PRO:HD3	1.91	0.53
45:Aa:310:ILE:HA	45:Aa:390:ARG:HH12	1.74	0.53
49:Ae:235:TYR:HE1	49:Ae:240:GLY:O	1.92	0.53
2:B:126:ARG:NH1	8:H:61:MET:SD	2.76	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.90	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.91	0.53
8:H:292:ASN:O	27:b:18:VAL:HG11	2.09	0.53
12:L:361:ASN:HA	12:L:431:THR:O	2.09	0.53
13:M:15:THR:HG21	13:M:100:ILE:HD12	1.90	0.53
14:N:120:GLN:HE22	14:N:174:GLN:CB	2.21	0.53
16:P:353:LEU:HA	16:P:356:HIS:HD2	1.74	0.53
18:R:95:LEU:HD21	18:R:111:PHE:CB	2.37	0.53
23:X:133:THR:HG23	27:b:58:ARG:NH1	2.23	0.53
23:X:171:THR:O	23:X:172:VAL:C	2.52	0.53
25:Z:65:LEU:HB3	27:b:50:PRO:O	2.09	0.53
47:AC:170:VAL:HG23	47:AC:174:THR:CB	2.39	0.53
48:AD:284:HIS:CE1	48:AD:288:MET:HE3	2.43	0.53
45:Aa:281:ALA:HB2	51:Ag:10:ARG:NH2	2.19	0.53
48:Ad:133:ARG:HD3	48:Ad:172:SER:HA	1.89	0.53
49:Ae:176:VAL:HG22	49:Ae:212:ILE:HG23	1.90	0.53
49:Ae:235:TYR:CE1	49:Ae:240:GLY:C	2.87	0.53
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.90	0.53
3:C:149:LEU:CD1	22:W:80:ARG:NH2	2.64	0.53
4:D:338:ARG:HH12	25:Z:23:ARG:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
10:J:68:GLY:HA2	10:J:71:THR:CB	2.39	0.53
12:L:128:MET:CG	12:L:251:THR:HB	2.36	0.53
12:L:450:LEU:HG	12:L:454:ILE:HD12	1.91	0.53
13:M:73:LEU:HD23	13:M:103:GLN:NE2	2.23	0.53
13:M:310:MET:HG3	13:M:455:THR:CA	2.39	0.53
13:M:314:MET:HE1	13:M:380:PHE:CD2	2.44	0.53
13:M:348:LEU:HD12	13:M:415:GLN:NE2	2.24	0.53
13:M:453:LEU:HD12	13:M:453:LEU:C	2.33	0.53
15:O:170:LEU:HD13	15:O:187:TYR:CD2	2.44	0.53
32:g:139:TYR:CD2	32:g:140:PHE:CD1	2.96	0.53
37:l:55:TYR:O	37:l:104:PRO:HG3	2.09	0.53
38:m:18:LEU:HD11	39:n:72:TRP:CG	2.44	0.53
38:m:85:LYS:O	38:m:85:LYS:HG2	2.09	0.53
41:p:142:ARG:O	41:p:143:TYR:CD1	2.62	0.53
42:q:9:ARG:HA	42:q:12:GLN:CG	2.37	0.53
47:AC:164:ILE:O	47:AC:177:ARG:HD2	2.08	0.53
52:AH:50:LEU:HD22	52:AH:54:ARG:HH22	1.72	0.53
46:Ab:229:VAL:HA	46:Ab:232:GLN:HG2	1.89	0.53
47:Ac:148:ASN:OD1	47:Ac:165:TRP:HH2	1.89	0.53
50:Af:88:LYS:NZ	50:Af:90:TYR:HB3	2.23	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
7:G:126:LEU:HD13	18:R:89:PRO:HB3	1.90	0.53
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
13:M:59:ASP:O	13:M:60:PRO:C	2.49	0.53
13:M:213:HIS:O	13:M:217:PRO:HD3	2.09	0.53
13:M:313:THR:HA	13:M:316:MET:HE3	1.89	0.53
13:M:354:LEU:O	13:M:357:THR:N	2.41	0.53
14:N:227:ILE:HA	14:N:230:ILE:CG2	2.38	0.53
16:P:265:PHE:HD1	16:P:334:GLY:HA3	1.74	0.53
16:P:275:HIS:HA	16:P:278:LYS:HG2	1.91	0.53
18:R:69:VAL:HG12	18:R:112:LYS:N	2.24	0.53
21:V:48:THR:HA	21:V:51:ILE:HD12	1.90	0.53
27:b:28:LEU:HA	27:b:31:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:106:TYR:OH	33:h:86:ILE:HD12	2.09	0.53
45:AA:52:ILE:HG12	45:AA:53:LEU:N	2.24	0.53
45:Aa:255:ARG:O	45:Aa:255:ARG:CG	2.51	0.53
46:Ab:226:SER:O	46:Ab:229:VAL:HG22	2.09	0.53
52:Ah:29:THR:O	52:Ah:33:GLU:HG3	2.09	0.53
3:C:135:ARG:O	3:C:136:PHE:C	2.47	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
8:H:249:ILE:HG21	23:X:99:HIS:CE1	2.45	0.52
9:I:80:GLU:HB3	43:r:26:LEU:HD11	1.90	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
12:L:108:MET:HB2	12:L:114:ILE:HD13	1.90	0.52
12:L:247:LEU:O	12:L:252:MET:HB3	2.09	0.52
14:N:307:THR:HB	15:O:319:ILE:CG1	2.39	0.52
39:n:39:TYR:CZ	39:n:43:LEU:HD11	2.44	0.52
40:o:116:ALA:O	40:o:119:GLU:HB3	2.09	0.52
42:q:55:PHE:CG	43:r:26:LEU:HD22	2.43	0.52
48:AD:227:LEU:HB3	48:AD:231:LEU:CB	2.38	0.52
51:AG:69:GLN:HE21	51:AG:72:ARG:NH2	2.07	0.52
67:Ac:401:HEM:HHA	67:Ac:401:HEM:O2A	2.09	0.52
48:Ad:107:HIS:NE2	48:Ad:283:ASP:OD2	2.41	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.90	0.52
3:C:80:LEU:O	3:C:81:ASP:CB	2.52	0.52
3:C:102:HIS:CE1	21:V:44:TYR:HE1	2.27	0.52
3:C:149:LEU:HD11	22:W:80:ARG:HH21	1.69	0.52
4:D:166:ARG:HH22	25:Z:10:MET:HG2	1.73	0.52
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
10:J:37:PHE:HZ	58:J:401:3PE:C2A	2.23	0.52
11:K:38:LEU:HG	11:K:42:ILE:CD1	2.39	0.52
11:K:89:TYR:HB3	11:K:91:GLN:OE1	2.09	0.52
12:L:400:ASN:HB3	12:L:486:LEU:HD22	1.90	0.52
12:L:480:LEU:HD22	35:j:84:PHE:HD2	1.72	0.52
12:L:536:ILE:HG23	12:L:537:THR:N	2.25	0.52
58:L:703:3PE:C32	58:m:201:3PE:H342	2.30	0.52
13:M:73:LEU:HD21	13:M:100:ILE:HG12	1.91	0.52
13:M:188:ALA:H	13:M:253:LEU:HD11	1.75	0.52
16:P:305:PHE:CG	16:P:314:THR:HG22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:58:LYS:O	17:Q:59:LEU:C	2.49	0.52
24:Y:141:PRO:HB2	33:h:161:ARG:CZ	2.39	0.52
25:Z:89:GLU:OE1	30:e:97:HIS:HD2	1.90	0.52
26:a:42:GLN:O	26:a:43:TYR:C	2.50	0.52
38:m:103:TYR:HB3	58:m:201:3PE:H112	1.89	0.52
45:AA:64:SER:N	45:AA:235:GLY:O	2.38	0.52
47:AC:9:PRO:HG3	47:Ac:202:GLU:CD	2.34	0.52
48:AD:125:HIS:HB3	48:AD:197:LEU:HG	1.91	0.52
48:AD:255:TYR:HB3	48:AD:257:ASP:OD1	2.08	0.52
52:AH:80:VAL:O	52:AH:84:LEU:N	2.41	0.52
48:Ad:157:GLY:HA2	48:Ad:163:GLU:O	2.09	0.52
49:Ae:143:SER:O	49:Ae:147:LEU:HG	2.09	0.52
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.91	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.75	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
9:I:54:THR:HG22	27:b:13:TRP:HE1	1.74	0.52
11:K:25:HIS:HD2	11:K:88:ASP:OD1	1.91	0.52
12:L:332:HIS:CD2	12:L:336:LYS:HG3	2.44	0.52
12:L:496:LEU:C	12:L:496:LEU:CD1	2.79	0.52
12:L:604:ILE:O	24:Y:5:LYS:HD2	2.09	0.52
57:L:706:PC1:H252	57:L:706:PC1:H341	1.90	0.52
13:M:160:LEU:CD2	13:M:164:LEU:HD13	2.40	0.52
13:M:447:LEU:HD11	13:M:454:ILE:HG23	1.90	0.52
14:N:81:LEU:HD23	30:e:60:PHE:HE1	1.74	0.52
15:O:121:PRO:C	15:O:122:LYS:HG2	2.33	0.52
15:O:310:ILE:HG13	15:O:311:PRO:HD2	1.91	0.52
15:O:336:GLY:N	15:O:344:ASN:ND2	2.56	0.52
16:P:283:MET:HE2	16:P:366:ILE:HG22	1.92	0.52
22:W:93:LEU:HG	22:W:97:ILE:HD12	1.92	0.52
24:Y:90:LEU:O	24:Y:91:ASN:C	2.51	0.52
27:b:66:VAL:HG11	27:b:70:PRO:HA	1.92	0.52
37:l:169:GLU:C	37:l:171:GLY:N	2.55	0.52
42:q:29:ARG:HD3	42:q:74:PHE:CE1	2.44	0.52
45:AA:398:ALA:O	45:AA:399:LEU:C	2.51	0.52
46:AB:48:VAL:HG21	46:AB:219:ALA:HB2	1.86	0.52
48:AD:91:PRO:HB3	48:AD:213:SER:OG	2.09	0.52
52:AH:33:GLU:O	52:AH:37:GLN:HG2	2.08	0.52
52:AH:35:CYS:O	52:AH:38:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ag:29:SER:HB3	51:Ag:32:SER:HB2	1.90	0.52
3:C:104:ASN:O	43:r:97:PRO:HD3	2.10	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
11:K:20:LEU:O	12:L:588:PHE:HB3	2.08	0.52
13:M:196:TRP:HE1	13:M:254:THR:HB	1.75	0.52
13:M:403:THR:HA	13:M:406:TYR:CE2	2.44	0.52
14:N:313:MET:HG2	15:O:305:LEU:HD22	1.91	0.52
17:Q:72:ILE:HD13	17:Q:143:TRP:NE1	2.24	0.52
20:T:130:ILE:CG2	20:T:131:PRO:HD2	2.40	0.52
23:X:80:GLU:HB3	23:X:81:PRO:HD3	1.91	0.52
28:c:47:SER:HB2	29:d:59:HIS:HD2	1.74	0.52
30:e:38:LYS:HG2	33:h:179:ILE:HG23	1.90	0.52
39:n:173:ARG:O	39:n:174:PRO:C	2.52	0.52
46:AB:226:SER:O	46:AB:229:VAL:HG22	2.09	0.52
48:AD:248:ILE:CG2	48:AD:263:MET:HG3	2.40	0.52
45:Aa:410:CYS:O	45:Aa:413:ILE:N	2.43	0.52
47:Ac:170:VAL:HG23	47:Ac:174:THR:CB	2.39	0.52
48:Ad:215:LEU:HD21	70:Ad:401:HEC:CMB	2.39	0.52
50:Af:19:LYS:HG2	50:Af:84:TYR:CG	2.44	0.52
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.40	0.52
4:D:381:HIS:HE1	9:I:161:ALA:O	1.93	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
11:K:57:MET:N	11:K:58:PRO:HD2	2.24	0.52
11:K:73:VAL:HG21	14:N:38:LEU:HD22	1.90	0.52
12:L:123:LEU:HD22	12:L:150:MET:HG3	1.91	0.52
12:L:427:ILE:HD11	36:k:69:PHE:HE1	1.75	0.52
12:L:446:ASN:HD21	35:j:51:THR:CG2	2.23	0.52
13:M:55:MET:HE1	62:d:201:CDL:H511	1.92	0.52
13:M:84:LEU:HD21	13:M:95:TYR:HB3	1.90	0.52
14:N:10:TYR:O	14:N:13:ILE:HG22	2.09	0.52
14:N:175:MET:HG2	14:N:219:LEU:CD2	2.40	0.52
16:P:336:GLU:CG	16:P:342:PRO:HD3	2.38	0.52
21:V:95:LEU:HA	21:V:100:TRP:CH2	2.35	0.52
25:Z:64:ASP:OD1	25:Z:65:LEU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
42:q:125:VAL:HG23	42:q:125:VAL:O	2.08	0.52
45:AA:207:ASN:O	45:AA:211:LEU:HG	2.09	0.52
45:AA:339:GLN:HB2	45:AA:359:VAL:O	2.10	0.52
47:AC:346:PRO:O	47:AC:349:ILE:HG22	2.10	0.52
49:AE:115:TYR:HE2	53:AJ:11:TYR:CE1	2.27	0.52
49:AE:206:LYS:NZ	49:AE:265:PHE:HB2	2.25	0.52
45:Aa:165:ARG:HE	45:Aa:209:ARG:HA	1.74	0.52
45:Aa:276:ARG:HB3	45:Aa:462:ILE:HD12	1.90	0.52
48:Ad:244:MET:HB2	70:Ad:401:HEC:C1D	2.39	0.52
48:Ad:321:TYR:CD2	48:Ad:323:PRO:HD3	2.44	0.52
1:A:113:TRP:CH2	8:H:287:HIS:CD2	2.98	0.52
5:E:177:GLY:O	59:E:301:FES:S1	2.68	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.52
8:H:23:VAL:HG11	26:a:9:LEU:CD2	2.39	0.52
10:J:127:GLU:HG3	25:Z:120:LEU:CD1	2.40	0.52
11:K:93:LEU:HD23	14:N:54:GLU:HG2	1.91	0.52
12:L:123:LEU:HD21	62:L:704:CDL:C74	2.40	0.52
12:L:297:ASP:HB3	12:L:300:LYS:CG	2.40	0.52
12:L:441:ILE:HD13	35:j:48:PRO:HD3	1.91	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
15:O:170:LEU:HD13	15:O:187:TYR:CG	2.44	0.52
23:X:172:VAL:HG23	29:d:30:ARG:NH1	2.25	0.52
62:h:201:CDL:H721	34:i:84:TYR:CD2	2.45	0.52
42:q:56:PHE:HD1	42:q:59:HIS:NE2	2.06	0.52
45:AA:384:THR:HG21	54:AK:9:ARG:HD2	1.91	0.52
49:Ae:270:VAL:O	49:Ae:270:VAL:HG12	2.09	0.52
1:A:113:TRP:CH2	8:H:287:HIS:HD2	2.27	0.52
4:D:101:LEU:HG	4:D:106:VAL:HA	1.91	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
12:L:228:GLY:O	12:L:229:LEU:CG	2.47	0.52
62:L:704:CDL:H111	62:L:704:CDL:H161	1.91	0.52
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.92	0.52
14:N:29:MET:HE2	14:N:141:ILE:HG12	1.92	0.52
16:P:236:VAL:HG11	16:P:270:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:77:HIS:HD2	23:X:115:LEU:HD21	1.75	0.52
25:Z:110:VAL:HG21	30:e:72:THR:HG23	1.90	0.52
26:a:6:LEU:O	26:a:7:PRO:C	2.52	0.52
30:e:81:LYS:O	30:e:84:GLU:HB3	2.10	0.52
34:i:31:ARG:O	34:i:32:GLU:C	2.51	0.52
34:i:88:TYR:CE2	41:p:49:ARG:HB2	2.44	0.52
42:q:138:VAL:HG23	42:q:139:PRO:HD2	1.92	0.52
47:AC:326:TRP:CZ2	58:AC:403:3PE:H222	2.44	0.52
48:AD:112:ARG:HD3	48:AD:257:ASP:OD2	2.09	0.52
48:AD:233:PHE:CD1	48:AD:240:GLN:HB3	2.45	0.52
49:AE:242:HIS:CD2	49:AE:251:LYS:HB3	2.45	0.52
50:AF:108:TRP:HA	50:AF:111:LYS:HZ2	1.75	0.52
45:Aa:171:GLU:O	45:Aa:174:GLU:HG2	2.10	0.52
45:Aa:207:ASN:O	45:Aa:211:LEU:HG	2.09	0.52
49:Ae:204:ARG:HH21	49:Ae:213:LEU:HD22	1.74	0.52
52:Ah:35:CYS:O	52:Ah:38:LEU:HB2	2.09	0.52
53:Aj:34:ARG:CG	53:Aj:35:ALA:N	2.72	0.52
2:B:127:GLN:H	2:B:127:GLN:CD	2.18	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:617:ARG:HH12	22:W:129:HIS:N	2.07	0.52
12:L:108:MET:HB2	12:L:114:ILE:CD1	2.39	0.52
13:M:346:ARG:O	13:M:419:LEU:HA	2.09	0.52
15:O:172:ALA:HA	15:O:236:ASP:HB3	1.91	0.52
20:T:79:ILE:CG2	20:T:145:VAL:HG13	2.40	0.52
20:U:128:PHE:CE1	20:U:148:ILE:HG23	2.45	0.52
26:a:1:MET:HG3	62:a:101:CDL:HB21	1.92	0.52
27:b:82:LYS:O	27:b:83:ASN:C	2.52	0.52
45:AA:170:ARG:HA	45:AA:173:GLN:CD	2.34	0.52
49:AE:168:LYS:CA	49:AE:174:LEU:H	2.23	0.52
49:AE:255:PRO:HG2	47:Ac:287:LYS:HZ1	1.73	0.52
51:AG:73:LYS:HZ3	52:AH:63:GLU:HB2	1.74	0.52
52:AH:69:LEU:HG	52:AH:73:LEU:HD11	1.92	0.52
47:Ac:275:LEU:O	47:Ac:276:PHE:C	2.51	0.52
49:Ae:239:HIS:ND1	49:Ae:241:SER:HB3	2.25	0.52
1:A:102:LEU:HD11	1:A:111:LEU:HD11	1.91	0.52
3:C:73:GLN:NE2	21:V:112:TRP:HE1	2.07	0.52
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.98	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:23:MET:HE3	62:L:704:CDL:H522	1.92	0.52
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.90	0.52
58:L:703:3PE:C23	58:m:201:3PE:H3B1	2.39	0.52
13:M:115:LEU:HD21	13:M:176:LEU:CD2	2.37	0.52
13:M:171:VAL:HG11	13:M:179:LEU:CD2	2.35	0.52
15:O:326:ARG:NH2	32:g:56:ASP:OD1	2.43	0.52
18:R:113:GLN:CD	18:R:113:GLN:N	2.66	0.52
20:U:133:ILE:HG23	20:U:134:ASP:N	2.25	0.52
24:Y:21:HIS:NE2	51:Ag:62:TRP:HB2	2.22	0.52
27:b:48:ALA:O	27:b:49:THR:C	2.53	0.52
30:e:69:ARG:HG3	30:e:72:THR:OG1	2.10	0.52
39:n:37:TYR:C	39:n:39:TYR:N	2.67	0.52
39:n:168:TRP:HD1	39:n:169:HIS:CE1	2.27	0.52
47:AC:221:HIS:O	47:AC:225:THR:HB	2.09	0.52
52:AH:65:CYS:O	52:AH:69:LEU:N	2.38	0.52
46:Ab:60:ARG:CD	46:Ab:393:LEU:HD13	2.40	0.52
46:Ab:60:ARG:HG2	46:Ab:393:LEU:HD13	1.90	0.52
49:Ae:207:LYS:HD2	49:Ae:210:TRP:CD1	2.43	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
2:B:81:LEU:HD22	57:B:303:PC1:H262	1.92	0.52
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.43	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:126:LEU:HD11	18:R:89:PRO:HB3	1.91	0.52
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
9:I:155:CYS:SG	55:I:303:SF4:S2	3.08	0.52
12:L:533:ILE:HG23	12:L:534:HIS:HD2	1.74	0.52
13:M:103:GLN:O	13:M:107:ILE:HB	2.10	0.52
13:M:139:GLN:HB3	13:M:222:GLU:CG	2.40	0.52
13:M:168:GLN:O	13:M:172:GLY:N	2.43	0.52
15:O:121:PRO:HB3	15:O:178:TYR:CE1	2.45	0.52
21:V:12:VAL:CG1	21:V:13:GLY:N	2.72	0.52
24:Y:19:GLN:HE21	24:Y:22:ARG:HB2	1.75	0.52
37:l:156:VAL:HG11	40:o:95:TYR:CE1	2.43	0.52
42:q:60:ARG:HH12	42:q:95:ASP:HA	1.75	0.52
47:AC:200:LEU:CD2	67:AC:402:HEM:HAA1	2.39	0.52
49:AE:241:SER:OG	49:AE:253:PRO:HD2	2.10	0.52
46:Ab:70:ARG:NH2	46:Ab:332:ASP:OD2	2.43	0.52
46:Ab:95:SER:O	46:Ab:99:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:68:GLU:HA	52:Ah:71:ASP:OD2	2.09	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.51
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
10:J:60:LEU:CD1	10:J:61:GLY:N	2.72	0.51
11:K:1:MET:SD	14:N:79:LYS:HD2	2.50	0.51
12:L:52:LEU:HB2	41:p:30:ILE:HD11	1.91	0.51
12:L:286:LEU:HG	12:L:290:ILE:CD1	2.40	0.51
12:L:386:LEU:HD11	35:j:69:ILE:HD11	1.92	0.51
14:N:338:PRO:HG3	62:d:201:CDL:H611	1.92	0.51
16:P:192:ARG:NH1	16:P:198:ALA:HB3	2.25	0.51
24:Y:17:GLY:O	24:Y:81:GLN:HG2	2.09	0.51
25:Z:61:LEU:O	25:Z:64:ASP:OD1	2.29	0.51
29:d:87:ASP:O	29:d:88:HIS:C	2.50	0.51
30:e:44:ALA:HA	30:e:47:ILE:HG12	1.92	0.51
35:j:98:GLY:O	35:j:100:PRO:HD3	2.11	0.51
36:k:49:ASP:OD2	39:n:38:ARG:HG3	2.10	0.51
41:p:164:LEU:O	41:p:168:LYS:N	2.42	0.51
50:AF:97:GLU:HA	50:AF:100:ARG:HH11	1.75	0.51
46:Ab:293:LEU:O	46:Ab:307:SER:HB3	2.10	0.51
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	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
11:K:59:ILE:O	11:K:60:PRO:C	2.49	0.51
12:L:569:LEU:O	12:L:573:MET:HG2	2.11	0.51
14:N:168:GLY:O	14:N:172:GLN:HG2	2.10	0.51
25:Z:110:VAL:HG11	30:e:72:THR:CA	2.40	0.51
42:q:29:ARG:HD3	42:q:74:PHE:CD1	2.44	0.51
42:q:65:THR:CG2	42:q:66:THR:N	2.72	0.51
45:AA:180:GLN:HG3	45:AA:181:ASN:N	2.25	0.51
47:AC:148:ASN:OD1	49:Ae:220:LEU:O	2.28	0.51
48:AD:155:GLN:HA	48:AD:166:MET:HA	1.91	0.51
46:Ab:348:GLY:HA2	46:Ab:448:PRO:HD3	1.91	0.51
47:Ac:110:MET:HE1	47:Ac:306:PHE:CE1	2.45	0.51
47:Ac:146:ILE:HA	47:Ac:149:LEU:HB2	1.92	0.51
48:Ad:218:TYR:CG	48:Ad:246:PRO:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HG3	1:A:111:LEU:HG	1.91	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.51
7:G:136:GLU:HB3	17:Q:87:MET:HB3	1.92	0.51
7:G:275:PRO:HB2	17:Q:86:ASN:ND2	2.25	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:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	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	2.32	0.51
13:M:173:THR:HG22	33:h:150:ARG:NH1	2.25	0.51
13:M:388:TRP:CD1	38:m:109:ARG:HD2	2.46	0.51
15:O:204:VAL:HG21	15:O:255:VAL:HG22	1.90	0.51
19:S:16:LEU:O	19:S:16:LEU:CD1	2.51	0.51
21:V:62:GLU:HB3	21:V:68:LEU:HD13	1.92	0.51
29:d:62:LEU:O	29:d:66:THR:OG1	2.22	0.51
34:i:77:ILE:HD13	34:i:80:TRP:CZ3	2.46	0.51
39:n:143:GLU:O	39:n:143:GLU:HG2	2.10	0.51
45:AA:392:LYS:HE3	45:AA:433:ILE:O	2.11	0.51
47:AC:77:TRP:HZ2	48:AD:284:HIS:CD2	2.28	0.51
47:AC:141:TRP:CD1	47:AC:264:THR:HA	2.45	0.51
49:AE:220:LEU:O	47:Ac:145:VAL:HA	2.10	0.51
49:AI:61:ALA:HA	46:Ab:326:PHE:HD1	1.76	0.51
46:Ab:229:VAL:O	46:Ab:232:GLN:HG2	2.10	0.51
47:Ac:140:PHE:CE1	47:Ac:170:VAL:HG13	2.45	0.51
48:Ad:146:LYS:O	48:Ad:150:GLU:HG2	2.10	0.51
48:Ad:248:ILE:CG2	48:Ad:263:MET:HG3	2.40	0.51
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.91	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.25	0.51
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.51
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.74	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
11:K:1:MET:H3	11:K:2:PRO:HD2	1.74	0.51
13:M:129:THR:CG2	13:M:235:LEU:HD11	2.40	0.51
13:M:154:LEU:HD22	14:N:287:LEU:HD21	1.93	0.51
13:M:251:ASP:N	13:M:252:PRO:HD2	2.26	0.51
14:N:240:MET:HE2	14:N:326:PHE:CZ	2.45	0.51
23:X:17:GLU:HG2	30:e:104:PRO:CD	2.40	0.51
24:Y:143:VAL:HG21	33:h:169:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:37:PHE:HA	31:f:40:LYS:HB2	1.93	0.51
47:AC:150:LEU:HB2	47:AC:161:VAL:HG22	1.93	0.51
48:AD:201:VAL:HG21	48:AD:275:ARG:HA	1.92	0.51
49:AE:93:ARG:HA	51:AG:25:ARG:CG	2.40	0.51
52:AH:42:VAL:HG13	52:AH:45:ARG:HH21	1.76	0.51
45:Aa:148:ALA:HA	45:Aa:250:LEU:HD21	1.92	0.51
46:Ab:307:SER:HB2	46:Ab:310:SER:H	1.75	0.51
47:Ac:221:HIS:O	47:Ac:225:THR:HB	2.10	0.51
49:Ae:179:ARG:NH2	49:Ae:205:VAL:HG21	2.26	0.51
49:Ae:204:ARG:HD3	49:Ae:248:ARG:HG2	1.92	0.51
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.51
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.51
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.35	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
13:M:177:MET:CE	33:h:140:LEU:HD21	2.41	0.51
15:O:132:GLN:CD	63:O:402:ADP:HN62	2.19	0.51
16:P:157:LYS:O	16:P:158:GLU:C	2.53	0.51
23:X:168:PHE:C	23:X:169:PHE:CD1	2.88	0.51
33:h:52:LYS:O	33:h:53:ARG:C	2.53	0.51
37:l:151:PRO:HD2	40:o:9:TYR:OH	2.10	0.51
40:o:89:TYR:O	40:o:90:CYS:C	2.52	0.51
45:AA:338:CYS:SG	45:AA:339:GLN:N	2.84	0.51
46:AB:425:VAL:HG12	46:AB:429:LYS:HZ1	1.76	0.51
48:AD:304:TYR:CZ	48:AD:308:ARG:HD2	2.45	0.51
48:AD:318:LYS:CD	49:AE:86:PRO:HB2	2.40	0.51
45:Aa:274:GLU:HG2	51:Ag:18:SER:HB2	1.92	0.51
47:Ac:28:SER:CB	62:Ac:406:CDL:HA21	2.40	0.51
48:Ad:228:ARG:HG2	48:Ad:231:LEU:CD1	2.40	0.51
50:Af:97:GLU:HA	50:Af:100:ARG:HH11	1.75	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.93	0.51
1:A:106:TRP:CD1	1:A:111:LEU:HD12	2.45	0.51
4:D:299:GLN:HB3	43:r:104:TRP:CE3	2.45	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
10:J:61:GLY:O	10:J:65:VAL:HG11	2.08	0.51
11:K:66:PHE:CE2	14:N:31:VAL:HB	2.46	0.51
12:L:161:ARG:NE	12:L:163:ASP:HB2	2.26	0.51
12:L:530:PRO:O	12:L:534:HIS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:595:ILE:O	12:L:599:ILE:HG13	2.11	0.51
13:M:11:LEU:O	13:M:15:THR:HG23	2.10	0.51
13:M:31:SER:HA	13:M:34:ILE:CG1	2.41	0.51
13:M:201:MET:HG2	58:M:501:3PE:H3B1	1.91	0.51
20:U:79:ILE:HG13	20:U:126:PHE:CE2	2.45	0.51
23:X:25:LEU:O	23:X:29:ALA:N	2.44	0.51
62:a:101:CDL:HA62	42:q:10:GLY:HA3	1.93	0.51
34:i:10:LEU:HA	34:i:13:GLN:HB3	1.91	0.51
34:i:83:HIS:CE1	34:i:87:LYS:HD2	2.46	0.51
34:i:85:TYR:CE2	34:i:90:MET:HE3	2.46	0.51
42:q:88:ARG:HG3	42:q:89:TRP:N	2.26	0.51
45:AA:160:GLN:HA	45:AA:163:LYS:HZ3	1.76	0.51
47:AC:269:LYS:CE	47:AC:340:GLY:HA2	2.39	0.51
48:AD:237:PHE:CG	48:AD:242:ILE:HB	2.46	0.51
49:AE:190:VAL:HG11	49:AE:248:ARG:HH12	1.75	0.51
50:AF:50:ARG:O	46:Ab:148:ARG:NH2	2.44	0.51
49:AI:69:GLY:HA2	46:Ab:111:SER:HA	1.91	0.51
46:Ab:142:THR:HG21	46:Ab:238:LEU:H	1.74	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.51
9:I:71:GLY:O	43:r:15:ALA:HB1	2.11	0.51
12:L:60:GLU:HG3	12:L:83:ASP:HA	1.93	0.51
13:M:20:PRO:HB3	13:M:89:ASN:ND2	2.25	0.51
13:M:336:ARG:HH12	13:M:433:GLU:CD	2.19	0.51
17:Q:77:VAL:HG12	17:Q:101:PHE:CG	2.46	0.51
20:T:140:CYS:HB2	20:T:143:GLU:CG	2.40	0.51
34:i:70:PHE:O	34:i:73:SER:HB2	2.10	0.51
36:k:34:PRO:HD2	36:k:59:TYR:CG	2.46	0.51
42:q:88:ARG:HB2	42:q:93:MET:HB2	1.92	0.51
45:AA:169:LEU:O	45:AA:173:GLN:HG3	2.11	0.51
46:AB:56:ALA:O	46:AB:127:ARG:HD2	2.10	0.51
47:Ac:346:PRO:O	47:Ac:349:ILE:HG22	2.10	0.51
48:Ad:106:ASP:HA	53:Aj:51:LYS:HB3	1.92	0.51
49:Ae:201:ASP:O	49:Ae:205:VAL:HG22	2.10	0.51
2:B:81:LEU:CG	8:H:53:MET:HE1	2.34	0.51
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
11:K:93:LEU:HD22	14:N:54:GLU:HG2	1.93	0.51
12:L:66:TRP:CZ3	12:L:68:TRP:CD1	2.96	0.51
12:L:536:ILE:HD11	12:L:540:LYS:HD2	1.93	0.51
14:N:45:ILE:HA	14:N:52:SER:OG	2.11	0.51
15:O:289:TRP:HA	15:O:289:TRP:CE3	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
22:W:65:LYS:HE3	22:W:69:MET:HE2	1.92	0.51
25:Z:98:MET:SD	30:e:79:ILE:HA	2.51	0.51
62:a:101:CDL:H311	42:q:7:LEU:HD23	1.91	0.51
29:d:28:ASP:O	29:d:29:PRO:C	2.53	0.51
45:AA:71:VAL:HG21	45:AA:140:LEU:HD12	1.93	0.51
45:AA:73:VAL:HG23	45:AA:147:LEU:HD13	1.93	0.51
47:AC:190:ALA:HB1	69:AC:405:UQ6:C21	2.41	0.51
48:AD:102:LEU:HB3	53:AJ:47:ILE:HG21	1.92	0.51
49:AI:70:LEU:HD11	46:Ab:100:THR:HG23	1.92	0.51
54:AK:33:VAL:HG21	54:AK:42:LEU:HD12	1.92	0.51
67:Ac:402:HEM:HHA	67:Ac:402:HEM:HBA1	1.93	0.51
49:Ae:201:ASP:HA	49:Ae:246:SER:OG	2.11	0.51
4:D:47:PHE:CE2	14:N:305:PHE:HZ	2.28	0.51
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.51
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.51
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
6:F:217:GLU:CD	17:Q:166:TRP:HE1	2.18	0.51
10:J:104:CYS:HA	10:J:107:ASN:CG	2.36	0.51
12:L:383:MET:CB	12:L:386:LEU:HD12	2.30	0.51
12:L:451:MET:O	12:L:452:ASN:C	2.53	0.51
12:L:563:PRO:HG3	13:M:152:TYR:OH	2.10	0.51
13:M:304:GLN:HA	13:M:309:PHE:CE1	2.45	0.51
14:N:321:LYS:HD2	29:d:49:ARG:NE	2.26	0.51
16:P:374:THR:HG23	16:P:374:THR:O	2.11	0.51
25:Z:118:PRO:HG3	33:h:188:ASP:OD2	2.10	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
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
47:AC:140:PHE:CE1	47:AC:170:VAL:HG13	2.45	0.51
48:AD:321:TYR:CD2	48:AD:323:PRO:HD3	2.44	0.51
49:AE:152:ILE:HB	49:AE:169:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:152:ILE:HD13	49:Ae:169:TRP:HB2	1.92	0.51
1:A:11:ILE:CD1	58:J:401:3PE:H2D1	2.41	0.51
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.51
4:D:304:LYS:HE2	9:I:35:THR:N	2.25	0.51
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.51
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
12:L:141:PHE:CD2	13:M:370:PRO:CG	2.94	0.51
12:L:598:ILE:HG21	14:N:100:MET:HE2	1.93	0.51
58:L:703:3PE:H361	58:L:703:3PE:H222	1.93	0.51
62:L:705:CDL:H351	24:Y:114:ALA:CB	2.37	0.51
13:M:354:LEU:O	13:M:355:MET:C	2.52	0.51
16:P:305:PHE:HB2	16:P:314:THR:HG22	1.92	0.51
18:R:72:VAL:HG12	18:R:73:GLU:N	2.26	0.51
20:T:87:LEU:HD23	20:T:122:MET:CE	2.41	0.51
20:U:89:LEU:HA	36:k:53:ARG:NH2	2.25	0.51
24:Y:14:VAL:HG13	24:Y:15:PRO:HD2	1.93	0.51
29:d:108:THR:HG23	29:d:110:ALA:HB3	1.93	0.51
35:j:97:LEU:HB3	40:o:104:ARG:CB	2.25	0.51
41:p:113:CYS:O	41:p:113:CYS:SG	2.69	0.51
45:AA:109:LEU:O	45:AA:113:VAL:HG12	2.11	0.51
45:AA:148:ALA:HA	45:AA:250:LEU:HD21	1.92	0.51
46:AB:227:HIS:HD2	46:AB:231:LYS:HE2	1.76	0.51
47:AC:18:PHE:HE1	69:AC:405:UQ6:C8	2.24	0.51
47:AC:253:PRO:HB2	48:AD:203:ALA:O	2.10	0.51
47:AC:316:MET:HG3	58:AC:403:3PE:O14	2.11	0.51
48:AD:244:MET:HB2	70:AD:401:HEC:ND	2.26	0.51
48:AD:291:LYS:HB3	53:AJ:36:PHE:CE2	2.36	0.51
45:Aa:193:GLN:HG2	49:Ae:85:VAL:HG21	1.93	0.51
45:Aa:225:LYS:HD2	45:Aa:256:VAL:H	1.75	0.51
46:Ab:185:ALA:HB3	46:Ab:251:ALA:HB2	1.93	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.50
2:B:125:PRO:HB3	2:B:148:VAL:HG13	1.93	0.50
3:C:195:HIS:HE1	22:W:88:LYS:NZ	2.08	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:639:LEU:HD23	7:G:639:LEU:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:307:LEU:HD11	25:Z:47:TYR:CD1	2.46	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
12:L:362:ILE:CD1	12:L:430:VAL:HG13	2.41	0.50
12:L:404:THR:HG22	12:L:405:ASN:H	1.75	0.50
13:M:249:ILE:HG22	13:M:250:LEU:N	2.26	0.50
13:M:275:ILE:CD1	13:M:288:TYR:CG	2.84	0.50
16:P:69:VAL:HG21	16:P:129:LEU:HD11	1.91	0.50
20:U:86:VAL:HG13	36:k:54:ASN:ND2	2.26	0.50
23:X:137:LEU:HG	23:X:138:PRO:HD2	1.92	0.50
24:Y:83:ARG:HH12	24:Y:90:LEU:HB3	1.76	0.50
25:Z:97:ILE:HG21	30:e:83:ARG:HB2	1.93	0.50
28:c:72:ARG:HD2	29:d:20:SER:CA	2.40	0.50
32:g:115:TRP:HA	32:g:118:ARG:HH11	1.75	0.50
45:AA:226:ALA:HB2	45:AA:253:VAL:HB	1.94	0.50
47:AC:291:VAL:O	47:AC:295:ILE:HG12	2.11	0.50
45:Aa:73:VAL:HG23	45:Aa:147:LEU:HD13	1.93	0.50
47:Ac:215:ALA:HA	51:Ag:11:ILE:HD11	1.93	0.50
47:Ac:291:VAL:O	47:Ac:295:ILE:HG12	2.11	0.50
48:Ad:309:HIS:NE2	51:Ag:21:PRO:HB2	2.26	0.50
49:Ae:141:SER:O	49:Ae:142:ALA:C	2.54	0.50
49:Ae:224:PRO:CB	49:Ae:243:TYR:HE1	2.23	0.50
1:A:56:PHE:HD1	10:J:70:THR:HG1	1.50	0.50
4:D:345:GLU:HB2	25:Z:19:ILE:HD12	1.93	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	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:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.50
10:J:133:VAL:HG12	26:a:41:VAL:HG21	1.93	0.50
12:L:173:LEU:HD23	58:L:701:3PE:C32	2.30	0.50
12:L:349:SER:HB2	12:L:443:ILE:HG23	1.93	0.50
13:M:4:ILE:HD11	13:M:41:LEU:HD21	1.92	0.50
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.41	0.50
14:N:36:SER:HB2	14:N:134:GLN:HE22	1.76	0.50
15:O:182:GLN:O	15:O:183:CYS:C	2.54	0.50
16:P:65:LEU:HD23	16:P:129:LEU:HD22	1.93	0.50
16:P:108:TRP:CZ2	64:P:401:NDP:H2A	2.46	0.50
16:P:209:ARG:N	16:P:352:VAL:HG22	2.26	0.50
16:P:234:LYS:HG2	16:P:234:LYS:O	2.10	0.50
16:P:348:LYS:HB3	16:P:351:GLU:OE2	2.11	0.50
20:T:105:MET:HB2	20:T:139:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:74:LEU:CD1	20:U:74:LEU:H	2.24	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
23:X:130:LYS:CE	27:b:67:PRO:HB3	2.42	0.50
28:c:32:ARG:HB2	28:c:32:ARG:NH2	2.27	0.50
41:p:49:ARG:O	41:p:52:ILE:HB	2.11	0.50
45:AA:401:SER:O	45:AA:409:VAL:HG22	2.11	0.50
46:AB:38:LEU:H	46:AB:38:LEU:HD22	1.76	0.50
46:AB:432:VAL:HG22	46:AB:432:VAL:O	2.09	0.50
47:AC:147:THR:HG21	47:AC:165:TRP:NE1	2.26	0.50
47:AC:163:TRP:HH2	68:AC:404:U10:H152	1.76	0.50
48:AD:323:PRO:HG2	48:AD:325:LYS:CD	2.41	0.50
45:Aa:127:GLU:OE2	45:Aa:348:TYR:HB3	2.11	0.50
47:Ac:92:ILE:HG13	47:Ac:272:TRP:CH2	2.46	0.50
47:Ac:128:PHE:CZ	47:Ac:146:ILE:CD1	2.83	0.50
48:Ad:237:PHE:CG	48:Ad:242:ILE:HB	2.46	0.50
48:Ad:255:TYR:HH	48:Ad:266:VAL:HA	1.76	0.50
49:Ae:271:VAL:O	49:Ae:271:VAL:HG13	2.11	0.50
51:Ag:74:ASN:HB3	51:Ag:77:MET:HB2	1.92	0.50
1:A:90:MET:HE3	10:J:152:MET:CG	2.42	0.50
3:C:190:TYR:HB3	22:W:101:LYS:HG2	1.94	0.50
4:D:54:PRO:HB2	4:D:59:ALA:HB2	1.94	0.50
7:G:651:PRO:HD2	19:S:56:ARG:HD2	1.94	0.50
12:L:21:ILE:HG12	12:L:27:ILE:HG23	1.93	0.50
12:L:145:GLU:CG	13:M:370:PRO:HD3	2.42	0.50
12:L:395:ILE:O	12:L:399:ILE:HG13	2.11	0.50
12:L:424:MET:HE2	12:L:502:LEU:HA	1.93	0.50
13:M:294:MET:HE3	13:M:319:HIS:HD2	1.76	0.50
13:M:370:PRO:CA	13:M:375:LEU:HD22	2.40	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
21:V:7:LYS:O	21:V:8:THR:OG1	2.29	0.50
24:Y:57:ARG:HG2	24:Y:60:ARG:NH2	2.27	0.50
28:c:46:LEU:O	28:c:50:ALA:HB2	2.12	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:114:GLU:HG2	46:AB:299:ILE:CD1	2.41	0.50
48:AD:94:TYR:HB2	48:AD:96:TRP:NE1	2.26	0.50
48:AD:126:SER:HB3	48:AD:178:PRO:HD2	1.94	0.50
48:AD:159:ASN:O	48:AD:160:ASP:C	2.52	0.50
49:AE:155:LYS:HB3	49:AE:158:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:236:CYS:HB3	49:AE:241:SER:HB2	1.93	0.50
49:AE:242:HIS:HD2	49:AE:251:LYS:HB3	1.76	0.50
54:AK:14:ALA:O	54:AK:18:ILE:HG12	2.11	0.50
45:Aa:101:THR:HG21	45:Aa:149:ASP:HB3	1.94	0.50
48:Ad:186:ARG:O	48:Ad:187:ALA:C	2.54	0.50
49:Ae:122:THR:HG21	53:Aj:25:ILE:HD13	1.94	0.50
49:Ae:207:LYS:HZ3	49:Ae:268:ASP:HA	1.77	0.50
4:D:359:ASP:O	7:G:150:ARG:NH2	2.44	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
10:J:164:PHE:HD2	14:N:5:THR:HA	1.77	0.50
12:L:117:PHE:HE1	12:L:243:VAL:CG2	2.24	0.50
12:L:365:ILE:CD1	12:L:366:MET:HE2	2.42	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
16:P:212:ARG:O	16:P:213:PHE:C	2.55	0.50
17:Q:75:ARG:HH12	17:Q:104:ARG:HG2	1.76	0.50
17:Q:167:ASN:C	17:Q:168:LYS:HG2	2.36	0.50
18:R:55:VAL:HG22	18:R:56:ASN:H	1.77	0.50
20:T:90:TYR:CE2	20:T:92:LYS:HB2	2.46	0.50
20:T:130:ILE:HG23	20:T:131:PRO:CD	2.40	0.50
21:V:44:TYR:O	21:V:48:THR:HG22	2.11	0.50
23:X:17:GLU:HG2	30:e:104:PRO:CG	2.42	0.50
23:X:17:GLU:HB3	30:e:104:PRO:HG3	1.93	0.50
40:o:71:ARG:HB3	40:o:71:ARG:NH1	2.27	0.50
41:p:5:TRP:HZ3	41:p:10:TYR:O	1.94	0.50
46:AB:232:GLN:O	46:AB:235:GLU:HG3	2.11	0.50
46:AB:375:LYS:NZ	46:AB:419:VAL:O	2.36	0.50
48:AD:242:ILE:CD1	48:AD:244:MET:HE2	2.41	0.50
49:AE:178:HIS:CD2	49:AE:179:ARG:H	2.27	0.50
45:Aa:50:VAL:HG11	45:Aa:417:LEU:HD11	1.93	0.50
46:Ab:40:PHE:CZ	46:Ab:406:TYR:HB2	2.45	0.50
46:Ab:180:VAL:O	46:Ab:254:ARG:HG3	2.12	0.50
46:Ab:429:LYS:HA	46:Ab:432:VAL:HG12	1.93	0.50
48:Ad:146:LYS:CD	48:Ad:171:LEU:HG	2.41	0.50
48:Ad:201:VAL:HG22	48:Ad:278:SER:CB	2.41	0.50
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CD2	2.46	0.50
49:Ae:161:GLU:HA	49:Ae:178:HIS:CB	2.42	0.50
52:Ah:48:LEU:CD1	52:Ah:65:CYS:HB3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLY:HA3	10:J:163:ILE:HD13	1.92	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
4:D:55:SER:HB3	4:D:58:THR:HB	1.94	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
12:L:109:HIS:O	12:L:110:SER:HB2	2.11	0.50
20:U:79:ILE:HG23	20:U:145:VAL:HG13	1.91	0.50
23:X:38:LYS:O	23:X:42:GLU:HG3	2.11	0.50
30:e:69:ARG:O	30:e:73:MET:HG3	2.11	0.50
36:k:34:PRO:CG	36:k:59:TYR:CD1	2.94	0.50
49:AE:114:SER:HB2	51:AG:22:PHE:HE2	1.76	0.50
49:AE:152:ILE:HD11	49:AE:154:ILE:HD11	1.94	0.50
49:AI:76:VAL:HG23	49:AI:78:PHE:CD2	2.46	0.50
45:Aa:402:HIS:HB2	45:Aa:426:LEU:HD11	1.94	0.50
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.94	0.50
6:F:49:HIS:O	6:F:50:ASP:C	2.54	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
8:H:230:ASN:O	8:H:231:ILE:C	2.53	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
10:J:9:SER:HB3	11:K:7:ASN:HB2	1.93	0.50
10:J:98:MET:O	10:J:102:LEU:HG	2.11	0.50
10:J:127:GLU:HG3	25:Z:120:LEU:HD13	1.92	0.50
12:L:336:LYS:O	12:L:340:PHE:CD2	2.65	0.50
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.52	0.50
58:M:503:3PE:HN2	15:O:338:LYS:HE2	1.77	0.50
14:N:189:TRP:HB2	14:N:204:ASN:HD21	1.77	0.50
16:P:205:ASP:OD1	16:P:205:ASP:O	2.30	0.50
20:U:90:TYR:HD2	20:U:93:ILE:H	1.59	0.50
21:V:90:LEU:HD21	21:V:94:MET:HE3	1.94	0.50
32:g:106:TYR:OH	33:h:86:ILE:HG23	2.12	0.50
34:i:10:LEU:HD12	34:i:13:GLN:HB3	1.94	0.50
36:k:55:GLU:OE1	39:n:38:ARG:HB2	2.12	0.50
37:l:49:ALA:HA	37:l:59:VAL:HG13	1.93	0.50
37:l:108:ASP:HB3	37:l:111:MET:HE2	1.92	0.50
37:l:119:THR:HG23	38:m:11:LEU:HA	1.92	0.50
47:AC:218:ILE:HB	47:AC:219:PRO:HD2	1.94	0.50
49:AE:223:VAL:HG23	47:Ac:141:TRP:CH2	2.46	0.50
52:AH:44:ALA:HB3	52:AH:72:PHE:HD1	1.76	0.50
45:Aa:401:SER:HA	45:Aa:404:ASP:OD2	2.11	0.50
47:Ac:21:LEU:C	47:Ac:21:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:140:PHE:HE1	47:Ac:170:VAL:HG13	1.76	0.50
49:Ae:161:GLU:HA	49:Ae:178:HIS:CG	2.47	0.50
49:Ae:235:TYR:OH	49:Ae:240:GLY:HA2	2.12	0.50
51:Ag:19:LEU:HD11	51:Ag:23:GLU:CG	2.42	0.50
62:Ag:101:CDL:O1	62:Ag:101:CDL:HA4	2.12	0.50
54:Ak:39:ARG:NH1	54:Ak:49:ASN:HB2	2.26	0.50
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.76	0.50
4:D:89:PRO:HG2	8:H:204:GLU:CG	2.42	0.50
5:E:70:PRO:HB3	44:s:60:PRO:HG3	1.92	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
9:I:63:TRP:CZ2	58:I:301:3PE:H321	2.46	0.50
11:K:1:MET:HA	11:K:4:THR:HB	1.94	0.50
12:L:141:PHE:CD2	13:M:370:PRO:CB	2.94	0.50
12:L:193:MET:CE	38:m:125:PHE:CD2	2.94	0.50
12:L:354:GLN:O	12:L:354:GLN:HG2	2.12	0.50
12:L:589:MET:O	12:L:592:LEU:N	2.45	0.50
15:O:352:ILE:HG21	29:d:52:PRO:HG2	1.94	0.50
20:U:142:GLN:O	20:U:145:VAL:N	2.43	0.50
27:b:38:TYR:HA	27:b:41:TYR:HD2	1.76	0.50
62:h:201:CDL:H132	62:h:201:CDL:H172	1.92	0.50
39:n:114:MET:O	39:n:115:TYR:C	2.52	0.50
40:o:114:ARG:HG3	40:o:115:ARG:N	2.27	0.50
45:AA:400:VAL:HG12	45:AA:402:HIS:HB3	1.94	0.50
49:AE:177:ARG:HB3	49:AE:211:VAL:HG13	1.92	0.50
49:AE:233:GLY:O	49:AE:234:TYR:CG	2.64	0.50
49:AI:12:ALA:HB3	49:AI:13:PRO:HD3	1.93	0.50
46:Ab:89:LEU:HD22	46:Ab:150:GLU:HB3	1.93	0.50
49:Ae:235:TYR:HE1	49:Ae:240:GLY:C	2.20	0.50
52:Ah:54:ARG:HH21	52:Ah:55:VAL:CG2	2.25	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
12:L:60:GLU:O	12:L:61:TYR:CD1	2.65	0.50
13:M:63:THR:N	13:M:64:PRO:HD2	2.27	0.50
13:M:432:ARG:HA	13:M:435:THR:HG22	1.94	0.50
14:N:258:THR:HG23	14:N:336:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:136:TYR:OH	15:O:191:LYS:HA	2.11	0.50
16:P:150:ARG:O	16:P:151:ALA:C	2.55	0.50
16:P:207:PHE:HE1	16:P:214:LEU:HD22	1.76	0.50
20:T:140:CYS:O	20:T:144:ILE:HG13	2.12	0.50
24:Y:12:HIS:NE2	24:Y:127:PHE:HZ	2.09	0.50
27:b:28:LEU:HA	27:b:31:ILE:CG2	2.42	0.50
35:j:84:PHE:HE2	40:o:88:ASP:HB3	1.77	0.50
38:m:91:ALA:HB2	58:m:202:3PE:H272	1.93	0.50
38:m:124:LYS:HE2	38:m:125:PHE:CE2	2.47	0.50
46:AB:70:ARG:NH2	46:AB:332:ASP:OD2	2.45	0.50
46:AB:173:ILE:HD11	46:AB:439:ALA:C	2.37	0.50
49:AE:196:ARG:HB3	49:AE:249:ILE:O	2.11	0.50
47:Ac:378:LYS:HG3	50:Af:18:ARG:HH12	1.75	0.50
48:Ad:242:ILE:CD1	48:Ad:244:MET:HE2	2.41	0.50
51:Ag:78:TYR:CE2	52:Ah:62:GLU:HB2	2.46	0.50
3:C:79:CYS:C	3:C:81:ASP:H	2.18	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	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
12:L:123:LEU:CD2	12:L:150:MET:HG3	2.42	0.50
12:L:302:ILE:CB	12:L:340:PHE:CE1	2.95	0.50
12:L:357:ARG:NH1	39:n:78:GLN:O	2.45	0.50
13:M:248:ILE:HG13	13:M:249:ILE:N	2.26	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
16:P:70:VAL:HG12	16:P:97:MET:SD	2.52	0.50
18:R:70:ASN:HD22	18:R:111:PHE:HE1	1.60	0.50
21:V:31:THR:HA	21:V:88:LEU:HD13	1.92	0.50
24:Y:114:ALA:HB2	58:m:202:3PE:H231	1.94	0.50
25:Z:129:THR:HG22	25:Z:131:GLU:H	1.77	0.50
45:AA:171:GLU:O	45:AA:175:ASN:N	2.45	0.50
47:AC:140:PHE:HE1	47:AC:170:VAL:HG13	1.76	0.50
48:AD:249:TYR:O	48:AD:250:THR:C	2.55	0.50
49:AE:219:HIS:O	49:AE:239:HIS:CE1	2.65	0.50
52:AH:58:ARG:NE	52:AH:60:GLN:HB2	2.26	0.50
48:Ad:116:VAL:HA	48:Ad:253:LEU:CD2	2.41	0.50
52:Ah:86:LYS:HG3	52:Ah:87:ASN:N	2.27	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
10:J:55:VAL:HG13	10:J:56:PHE:H	1.77	0.49
11:K:38:LEU:HG	11:K:42:ILE:HD11	1.93	0.49
12:L:14:LEU:HD21	34:i:74:HIS:O	2.12	0.49
58:L:703:3PE:H222	58:L:703:3PE:H332	1.94	0.49
13:M:184:HIS:CD2	13:M:249:ILE:HG23	2.47	0.49
13:M:441:MET:HG3	13:M:445:ILE:HD12	1.94	0.49
14:N:133:TRP:CG	14:N:133:TRP:O	2.63	0.49
15:O:276:LEU:HD11	15:O:278:TYR:CE2	2.47	0.49
15:O:319:ILE:HD12	15:O:324:GLY:HA3	1.94	0.49
16:P:192:ARG:CZ	16:P:200:ILE:HD11	2.42	0.49
20:T:138:LEU:HD13	20:T:144:ILE:CD1	2.42	0.49
24:Y:141:PRO:HB2	33:h:161:ARG:HH11	1.77	0.49
25:Z:66:GLU:HA	25:Z:69:ILE:HG12	1.93	0.49
45:AA:50:VAL:HA	45:AA:60:ALA:HA	1.94	0.49
45:AA:55:ASN:ND2	45:AA:251:SER:C	2.70	0.49
46:AB:176:ASN:CA	46:AB:258:ILE:HD11	2.42	0.49
47:AC:211:LEU:HD21	50:AF:37:THR:HA	1.94	0.49
49:AE:88:PHE:CD2	51:AG:19:LEU:HG	2.47	0.49
49:AE:219:HIS:CD2	49:AE:253:PRO:HG2	2.47	0.49
1:A:51:PHE:HZ	11:K:79:VAL:CG1	2.25	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.49
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
6:F:427:LEU:HB2	60:F:501:FMN:C7M	2.43	0.49
8:H:30:TYR:HE1	26:a:1:MET:O	1.87	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
12:L:142:ILE:HA	13:M:370:PRO:CB	2.42	0.49
12:L:393:ASP:OD1	12:L:393:ASP:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:PHE:CE1	13:M:238:LEU:HG	2.46	0.49
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.47	0.49
16:P:135:GLU:CG	16:P:140:ASP:HA	2.41	0.49
19:S:24:CYS:N	19:S:58:CYS:SG	2.85	0.49
21:V:12:VAL:CG1	21:V:13:GLY:H	2.22	0.49
23:X:119:ARG:HD2	23:X:120:PRO:HD2	1.94	0.49
25:Z:140:PHE:O	25:Z:141:THR:C	2.55	0.49
26:a:4:GLU:O	26:a:7:PRO:HD2	2.11	0.49
62:a:101:CDL:OB3	43:r:5:THR:N	2.34	0.49
30:e:45:HIS:CD2	33:h:176:LYS:HD3	2.47	0.49
33:h:96:ALA:O	41:p:63:TYR:HE1	1.94	0.49
47:AC:164:ILE:CD1	68:AC:404:U10:H1M2	2.42	0.49
48:AD:167:ARG:HH22	48:AD:173:ASP:HB2	1.76	0.49
49:AE:93:ARG:HG2	51:AG:23:GLU:C	2.37	0.49
52:AH:26:ASP:OD2	52:AH:28:LEU:HB3	2.12	0.49
45:Aa:226:ALA:HB2	45:Aa:253:VAL:HB	1.93	0.49
48:Ad:157:GLY:N	48:Ad:158:PRO:HD2	2.27	0.49
50:Af:44:VAL:O	50:Af:48:ILE:HG13	2.12	0.49
52:Ah:30:THR:HA	52:Ah:33:GLU:CD	2.36	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
12:L:578:THR:HG21	14:N:168:GLY:HA2	1.94	0.49
13:M:88:ASN:O	13:M:89:ASN:HB3	2.12	0.49
13:M:166:LEU:CD1	58:M:501:3PE:H11	2.41	0.49
13:M:207:MET:SD	13:M:240:SER:HA	2.52	0.49
14:N:313:MET:HG3	15:O:305:LEU:CD2	2.41	0.49
15:O:170:LEU:HD21	15:O:184:VAL:HG22	1.95	0.49
15:O:351:TRP:HB3	28:c:39:PRO:HG3	1.94	0.49
19:S:42:VAL:O	19:S:46:LYS:HG3	2.12	0.49
21:V:39:PRO:HB2	21:V:42:ALA:HB2	1.94	0.49
23:X:33:GLY:CA	25:Z:70:ALA:HB1	2.43	0.49
23:X:49:GLU:HB3	23:X:138:PRO:HG3	1.93	0.49
58:j:700:3PE:C3B	40:o:78:LEU:HD13	2.40	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
41:p:74:ILE:O	41:p:75:THR:C	2.54	0.49
49:AE:205:VAL:CG1	49:AE:211:VAL:HA	2.42	0.49
46:Ab:425:VAL:HG12	46:Ab:429:LYS:HZ1	1.76	0.49
48:Ad:95:PRO:HD2	52:Ah:85:PHE:HB2	1.95	0.49
52:Ah:73:LEU:O	52:Ah:74:HIS:C	2.55	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
10:J:59:TYR:HH	11:K:34:GLU:C	2.19	0.49
12:L:217:LEU:HD13	12:L:273:ILE:HG23	1.94	0.49
12:L:399:ILE:HG22	12:L:409:LEU:HD13	1.93	0.49
12:L:542:LEU:CD2	37:l:116:ARG:HD2	2.43	0.49
13:M:285:LEU:HD22	13:M:410:MET:SD	2.53	0.49
13:M:348:LEU:HD12	13:M:415:GLN:HE22	1.77	0.49
58:M:502:3PE:O22	62:h:201:CDL:H141	2.13	0.49
14:N:230:ILE:HG21	14:N:296:LEU:HD11	1.94	0.49
16:P:172:ALA:H	16:P:202:ARG:HH21	1.59	0.49
16:P:238:GLN:HB2	16:P:270:ARG:HG2	1.94	0.49
16:P:367:GLU:HG2	16:P:368:GLU:N	2.26	0.49
18:R:67:GLN:HG2	18:R:109:LEU:HD21	1.95	0.49
29:d:11:LEU:HB2	30:e:9:LYS:HB2	1.94	0.49
34:i:90:MET:O	34:i:91:ALA:C	2.53	0.49
45:AA:113:VAL:HG13	46:AB:299:ILE:HD11	1.94	0.49
45:AA:158:ASP:OD1	45:AA:213:ARG:HD2	2.11	0.49
45:AA:285:ALA:O	45:AA:359:VAL:HA	2.12	0.49
45:AA:341:PHE:HE1	45:AA:356:ALA:CB	2.26	0.49
49:AI:43:LEU:HB2	46:Ab:167:GLN:NE2	2.28	0.49
54:AK:10:TYR:CZ	50:Af:110:LYS:HG2	2.47	0.49
45:Aa:338:CYS:SG	45:Aa:359:VAL:C	2.96	0.49
46:Ab:304:ASN:O	46:Ab:306:THR:HG23	2.12	0.49
47:Ac:99:GLY:HA3	58:Ac:403:3PE:H2A1	1.94	0.49
47:Ac:238:ILE:HD12	62:Ag:101:CDL:H772	1.94	0.49
48:Ad:213:SER:HB3	48:Ad:236:TYR:CE1	2.47	0.49
48:Ad:249:TYR:O	48:Ad:250:THR:C	2.55	0.49
54:Ak:13:LEU:HB3	54:Ak:17:TRP:CH2	2.47	0.49
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.46	0.49
3:C:73:GLN:HE21	21:V:112:TRP:HE1	1.60	0.49
3:C:224:GLU:OE2	16:P:45:LYS:HB3	2.13	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.31	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.93	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:12:PRO:O	26:a:15:CYS:HB3	2.13	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
58:J:401:3PE:O14	58:J:401:3PE:N	2.38	0.49
12:L:439:PRO:HA	36:k:57:TRP:CZ2	2.47	0.49
12:L:445:GLU:CB	12:L:450:LEU:HD23	2.37	0.49
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
15:O:143:TYR:CZ	15:O:164:TYR:HE2	2.30	0.49
15:O:354:LEU:HD21	28:c:44:VAL:HG11	1.94	0.49
16:P:346:GLU:H	16:P:346:GLU:CD	2.20	0.49
22:W:32:LYS:CD	66:W:201:EHZ:C19	2.90	0.49
23:X:73:GLN:OE1	23:X:117:TRP:HZ2	1.96	0.49
23:X:165:THR:OG1	23:X:172:VAL:HG11	2.12	0.49
29:d:109:TYR:HB3	41:p:156:LEU:HD21	1.94	0.49
45:AA:101:THR:O	45:AA:102:LYS:C	2.55	0.49
45:AA:387:GLU:HB2	45:AA:390:ARG:HH22	1.78	0.49
45:AA:400:VAL:HG21	46:AB:58:LEU:HD12	1.90	0.49
52:AH:35:CYS:SG	52:AH:80:VAL:HA	2.52	0.49
49:AI:76:VAL:HG11	46:Ab:165:ALA:HA	1.93	0.49
47:Ac:107:TYR:HE1	47:Ac:308:HIS:HB2	1.77	0.49
47:Ac:213:SER:HA	50:Af:67:LEU:HD11	1.94	0.49
49:Ae:174:LEU:HD11	49:Ae:261:PRO:HG3	1.95	0.49
53:Aj:30:LEU:CD2	53:Aj:31:PHE:CE1	2.94	0.49
1:A:54:LYS:O	1:A:58:VAL:HG23	2.12	0.49
4:D:259:GLU:C	4:D:261:MET:N	2.68	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:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
12:L:316:THR:CG2	12:L:325:ALA:CB	2.89	0.49
13:M:131:ILE:HD12	14:N:302:LEU:HD21	1.93	0.49
14:N:231:SER:HA	14:N:300:THR:HA	1.93	0.49
16:P:40:VAL:HB	16:P:53:GLY:HA2	1.93	0.49
20:T:88:LYS:NZ	20:T:96:GLU:H	2.11	0.49
32:g:53:TRP:H	32:g:53:TRP:HE3	1.58	0.49
62:h:201:CDL:C17	58:i:201:3PE:H372	2.36	0.49
37:l:81:ARG:HD3	37:l:85:GLU:OE2	2.13	0.49
49:AE:168:LYS:H	49:AE:174:LEU:N	2.11	0.49
49:AE:179:ARG:HB3	49:AE:183:GLU:CB	2.43	0.49
45:Aa:277:HIS:NE2	51:Ag:13:HIS:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:278:TYR:CZ	47:Ac:282:ARG:HD2	2.48	0.49
49:Ae:196:ARG:NE	49:Ae:196:ARG:HA	2.28	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.26	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
8:H:93:HIS:CE1	26:a:24:ALA:CA	2.94	0.49
12:L:67:HIS:HE2	12:L:69:VAL:C	2.20	0.49
12:L:183:ILE:HD13	13:M:400:ILE:HD13	1.94	0.49
12:L:296:ASN:OD1	12:L:357:ARG:NH1	2.45	0.49
12:L:405:ASN:OD1	37:l:148:HIS:CE1	2.66	0.49
12:L:477:ILE:HG13	40:o:91:GLU:OE2	2.13	0.49
13:M:193:ASN:HA	13:M:253:LEU:HD23	1.94	0.49
13:M:248:ILE:CG1	13:M:249:ILE:HD12	2.39	0.49
15:O:260:SER:O	15:O:263:ALA:HB3	2.13	0.49
16:P:64:PHE:CZ	16:P:211:ASP:HB3	2.48	0.49
16:P:235:THR:O	16:P:236:VAL:C	2.56	0.49
32:g:121:GLU:OE2	41:p:10:TYR:CZ	2.66	0.49
33:h:111:GLU:O	41:p:63:TYR:HA	2.12	0.49
37:l:88:PRO:HB2	39:n:86:PRO:HB2	1.94	0.49
38:m:50:GLN:O	38:m:60:ILE:HD11	2.13	0.49
39:n:145:SER:HB2	39:n:146:PRO:HD2	1.94	0.49
48:AD:98:HIS:HB3	48:AD:105:LEU:HD23	1.95	0.49
48:AD:105:LEU:HB3	48:AD:110:ILE:HD11	1.95	0.49
48:AD:128:ASP:OD1	48:AD:177:LYS:HD2	2.11	0.49
48:AD:218:TYR:CE2	48:AD:246:PRO:HA	2.47	0.49
49:AE:196:ARG:HD2	49:AE:249:ILE:O	2.12	0.49
46:Ab:261:GLN:NE2	46:Ab:444:LEU:HB2	2.28	0.49
47:Ac:242:LEU:HD21	47:Ac:250:LEU:CD1	2.41	0.49
47:Ac:281:LEU:HD12	47:Ac:290:GLY:HA3	1.95	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
10:J:68:GLY:O	10:J:71:THR:N	2.46	0.49
10:J:76:GLU:HG2	10:J:76:GLU:O	2.12	0.49
12:L:496:LEU:HA	12:L:499:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:114:GLU:HG3	23:X:169:PHE:HB3	1.95	0.49
13:M:227:GLY:HA2	13:M:230:ILE:HG22	1.95	0.49
16:P:315:THR:H	16:P:318:LYS:HB3	1.76	0.49
20:U:133:ILE:CD1	39:n:7:PRO:HD3	2.42	0.49
21:V:56:LEU:HA	21:V:59:VAL:HB	1.94	0.49
23:X:4:ILE:CG2	23:X:5:VAL:N	2.50	0.49
23:X:115:LEU:HD13	23:X:117:TRP:CZ3	2.48	0.49
27:b:52:ASN:HD21	30:e:28:LYS:CE	2.25	0.49
28:c:62:HIS:O	28:c:66:VAL:HG23	2.12	0.49
38:m:129:TYR:HE2	41:p:146:LEU:O	1.95	0.49
39:n:20:TYR:OH	39:n:45:ARG:HB2	2.12	0.49
45:AA:186:TYR:C	45:AA:188:HIS:N	2.68	0.49
45:AA:358:PHE:CD1	45:AA:368:MET:HG2	2.48	0.49
46:AB:49:ILE:CD1	46:AB:220:LEU:HB3	2.42	0.49
48:AD:233:PHE:CE2	48:AD:235:PRO:HD3	2.47	0.49
49:AE:206:LYS:HB3	49:AE:265:PHE:CD2	2.47	0.49
51:AG:69:GLN:HE22	51:AG:72:ARG:HH12	1.57	0.49
54:AK:36:THR:CB	54:AK:38:TRP:CD1	2.86	0.49
47:Ac:146:ILE:HG12	68:Ac:404:U10:H4M2	1.94	0.49
49:Ae:241:SER:OG	49:Ae:249:ILE:HD11	2.13	0.49
50:Af:68:ASP:O	50:Af:71:MET:HB3	2.12	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
4:D:279:THR:HA	21:V:12:VAL:CG1	2.43	0.49
58:D:501:3PE:H3A2	13:M:155:ILE:HD13	1.94	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
6:F:379:CYS:SG	55:F:502:SF4:S1	3.11	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	0.49
8:H:303:TRP:CZ3	27:b:28:LEU:HG	2.48	0.49
10:J:99:GLU:HA	10:J:102:LEU:HD12	1.93	0.49
12:L:68:TRP:CE3	12:L:76:LEU:HD21	2.47	0.49
12:L:264:HIS:HA	12:L:267:THR:OG1	2.13	0.49
12:L:316:THR:HG23	12:L:325:ALA:CB	2.32	0.49
13:M:4:ILE:HG22	13:M:107:ILE:CD1	2.32	0.49
13:M:5:ILE:HG13	13:M:6:LEU:N	2.28	0.49
13:M:51:ASN:ND2	33:h:136:THR:HG23	2.27	0.49
13:M:178:ILE:HG12	41:p:82:VAL:HG11	1.94	0.49
32:g:140:PHE:HZ	41:p:152:ALA:HB1	1.78	0.49
39:n:114:MET:HG3	39:n:115:TYR:HD2	1.78	0.49
49:AE:178:HIS:CD2	49:AE:209:GLU:HB2	2.48	0.49
52:AH:70:PHE:HA	52:AH:73:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:63:LEU:HD11	46:Ab:238:LEU:HD21	1.95	0.49
46:Ab:142:THR:CG2	46:Ab:237:PHE:HB3	2.30	0.49
47:Ac:218:ILE:HB	47:Ac:219:PRO:HD2	1.94	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
9:I:114:ILE:HD13	18:R:106:TYR:CD1	2.48	0.49
10:J:150:TRP:CD1	14:N:28:LEU:HD21	2.47	0.49
12:L:511:LEU:HD12	39:n:36:LYS:HA	1.94	0.49
58:L:703:3PE:H2	58:L:703:3PE:HN1	1.77	0.49
13:M:348:LEU:HB2	13:M:415:GLN:OE1	2.13	0.49
14:N:335:MET:CB	62:d:201:CDL:H642	2.43	0.49
15:O:78:ALA:HB2	15:O:85:HIS:HB2	1.95	0.49
19:S:36:PHE:CZ	19:S:44:LEU:HD11	2.36	0.49
20:U:118:ILE:O	20:U:119:ILE:C	2.55	0.49
23:X:168:PHE:O	23:X:170:TRP:NE1	2.45	0.49
25:Z:69:ILE:HG23	27:b:54:PRO:CD	2.41	0.49
37:l:101:TRP:HE1	38:m:62:ASP:HA	1.77	0.49
37:l:167:TYR:OH	37:l:176:LYS:O	2.14	0.49
38:m:75:ASN:OD1	38:m:79:ASN:ND2	2.46	0.49
39:n:81:ILE:HD12	39:n:87:GLY:O	2.12	0.49
45:AA:296:TRP:NE1	45:AA:347:SER:O	2.45	0.49
47:AC:92:ILE:HG13	47:AC:272:TRP:CH2	2.48	0.49
47:AC:223:TYR:CE1	48:AD:314:LEU:HG	2.48	0.49
47:AC:244:LEU:HD13	48:AD:289:GLY:HA2	1.94	0.49
48:AD:116:VAL:HA	48:AD:253:LEU:CD2	2.43	0.49
52:AH:43:LYS:HA	52:AH:46:GLU:CD	2.38	0.49
45:Aa:361:ASP:OD1	45:Aa:361:ASP:N	2.45	0.49
49:Ae:89:SER:O	49:Ae:90:ASP:C	2.54	0.49
50:Af:85:GLU:CD	50:Af:85:GLU:H	2.21	0.49
2:B:127:GLN:NE2	8:H:215:TYR:O	2.46	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:35:ARG:HE	32:g:59:PRO:HD2	1.77	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
12:L:227:PHE:CD2	12:L:283:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1:MET:HB2	13:M:52:PHE:CE2	2.47	0.48
13:M:216:LEU:HD12	13:M:236:LEU:CD2	2.38	0.48
15:O:135:LEU:HD13	63:O:402:ADP:C5	2.48	0.48
18:R:32:THR:CG2	18:R:36:GLN:H	2.18	0.48
23:X:112:LEU:HD13	23:X:118:VAL:HG22	1.95	0.48
28:c:72:ARG:NH1	29:d:19:ARG:HD3	2.28	0.48
32:g:109:ASP:HB2	32:g:114:GLU:HB3	1.94	0.48
38:m:45:ARG:CZ	39:n:140:LEU:HD11	2.43	0.48
38:m:122:ASP:O	38:m:123:ARG:C	2.53	0.48
45:AA:280:ASP:OD2	51:AG:10:ARG:HA	2.13	0.48
48:AD:157:GLY:N	48:AD:158:PRO:HD3	2.27	0.48
49:AE:118:THR:OG1	53:AJ:21:PHE:HZ	1.95	0.48
47:Ac:313:ARG:HB2	50:Af:39:HIS:ND1	2.28	0.48
48:Ad:222:PRO:HD3	48:Ad:233:PHE:CZ	2.47	0.48
48:Ad:295:MET:HE1	49:Ae:124:GLY:HA2	1.94	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
4:D:36:GLN:HG3	4:D:38:GLN:HE21	1.78	0.48
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
8:H:66:THR:HA	8:H:124:ASN:OD1	2.13	0.48
57:I:302:PC1:H133	25:Z:30:LEU:O	2.13	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:101:MET:HE1	12:L:121:LEU:CB	2.43	0.48
12:L:144:TRP:HH2	12:L:256:GLY:HA2	1.78	0.48
12:L:350:LEU:HD23	12:L:443:ILE:HD11	1.96	0.48
12:L:556:ILE:HG23	38:m:80:PHE:CZ	2.47	0.48
13:M:134:THR:O	13:M:142:ARG:CD	2.59	0.48
16:P:59:PHE:CB	16:P:130:ILE:HD11	2.42	0.48
16:P:228:LEU:HD11	16:P:288:PHE:HZ	1.78	0.48
16:P:298:TYR:HA	16:P:301:ILE:HG12	1.95	0.48
20:T:90:TYR:HE2	20:T:92:LYS:HB3	1.78	0.48
20:U:90:TYR:CD1	36:k:51:TRP:CE2	3.01	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
40:o:42:THR:O	40:o:43:GLN:C	2.56	0.48
45:AA:279:ASP:OD1	51:AG:12:ARG:NE	2.46	0.48
45:AA:402:HIS:C	45:AA:404:ASP:N	2.71	0.48
47:AC:278:TYR:CZ	47:AC:282:ARG:HD2	2.48	0.48
49:AE:138:SER:HA	49:AE:141:SER:HB3	1.94	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:361:ILE:HA	47:Ac:365:LEU:HB2	1.95	0.48
48:Ad:159:ASN:HB3	48:Ad:162:GLY:C	2.38	0.48
49:Ae:179:ARG:HG3	49:Ae:211:VAL:HG12	1.96	0.48
49:Ae:217:CYS:O	49:Ae:218:THR:C	2.56	0.48
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
8:H:42:PRO:HB3	42:q:27:PHE:CE2	2.47	0.48
12:L:361:ASN:O	12:L:361:ASN:CG	2.54	0.48
12:L:372:CYS:SG	12:L:454:ILE:HG22	2.54	0.48
12:L:390:TYR:CE2	35:j:68:TRP:HH2	2.32	0.48
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.47	0.48
13:M:311:GLY:HA2	13:M:314:MET:CE	2.42	0.48
14:N:31:VAL:HB	14:N:35:PHE:CE2	2.48	0.48
17:Q:72:ILE:HD13	17:Q:143:TRP:HE1	1.76	0.48
23:X:151:ASN:CG	30:e:51:ARG:HH11	2.21	0.48
24:Y:68:ILE:HG12	24:Y:102:THR:OG1	2.13	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
36:k:41:LYS:C	36:k:43:ALA:N	2.64	0.48
39:n:44:MET:O	39:n:45:ARG:C	2.53	0.48
39:n:51:HIS:HB3	39:n:63:LEU:HD13	1.95	0.48
40:o:8:ARG:HB2	40:o:16:GLU:CG	2.23	0.48
47:AC:32:ASN:ND2	47:AC:228:ASP:OD1	2.47	0.48
48:AD:103:SER:HA	53:AJ:48:ASN:OD1	2.14	0.48
48:AD:307:LYS:O	48:AD:311:TRP:HB2	2.13	0.48
46:Ab:109:LYS:O	46:Ab:123:VAL:HA	2.13	0.48
46:Ab:307:SER:HB2	46:Ab:310:SER:CB	2.43	0.48
49:Ae:83:VAL:HG22	49:Ae:84:LYS:N	2.28	0.48
1:A:109:LYS:HD2	1:A:112:GLU:OE2	2.14	0.48
3:C:234:LEU:O	4:D:387:GLU:HG3	2.13	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:L:74:MET:HE3	13:M:307:TRP:HH2	1.78	0.48
12:L:141:PHE:HD1	12:L:182:PHE:CD2	2.31	0.48
12:L:316:THR:HG21	12:L:325:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:402:CYS:SG	12:L:403:ASN:N	2.87	0.48
62:L:704:CDL:OB7	62:L:704:CDL:HB32	2.13	0.48
13:M:25:THR:HG22	32:g:84:ASN:OD1	2.13	0.48
13:M:166:LEU:HD21	13:M:170:HIS:CE1	2.48	0.48
13:M:313:THR:HA	13:M:316:MET:CE	2.43	0.48
21:V:90:LEU:HD23	21:V:94:MET:HG2	1.94	0.48
26:a:37:ARG:CB	26:a:48:MET:HE2	2.43	0.48
28:c:70:LYS:O	28:c:75:LEU:HA	2.12	0.48
30:e:47:ILE:HG13	30:e:47:ILE:O	2.12	0.48
30:e:83:ARG:HD3	30:e:92:TYR:CE2	2.48	0.48
33:h:62:TYR:N	39:n:111:GLU:OE2	2.47	0.48
36:k:47:LEU:CD1	39:n:43:LEU:HD23	2.43	0.48
45:AA:400:VAL:O	45:AA:401:SER:C	2.54	0.48
46:AB:312:SER:OG	46:AB:357:GLN:NE2	2.40	0.48
48:AD:115:GLN:O	48:AD:119:GLN:HG3	2.13	0.48
49:AE:168:LYS:CA	49:AE:173:PRO:HA	2.36	0.48
46:Ab:92:LYS:HE2	46:Ab:143:ALA:HB1	1.96	0.48
48:Ad:98:HIS:HB3	48:Ad:105:LEU:HD23	1.95	0.48
1:A:113:TRP:CH2	8:H:287:HIS:HB2	2.49	0.48
8:H:42:PRO:HG3	42:q:28:PHE:HE1	1.79	0.48
8:H:118:TRP:CZ2	10:J:30:LEU:CD2	2.96	0.48
8:H:224:PHE:CZ	61:H:400:UQ9:C13	2.94	0.48
10:J:24:SER:O	10:J:28:GLY:N	2.44	0.48
12:L:296:ASN:ND2	12:L:425:ARG:HH21	2.12	0.48
12:L:424:MET:HE2	12:L:502:LEU:CA	2.43	0.48
13:M:127:ILE:CD1	14:N:256:PRO:HG2	2.42	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
16:P:197:GLU:HB3	16:P:259:VAL:HG23	1.93	0.48
20:U:94:ASP:OD1	20:U:95:PRO:HD2	2.13	0.48
21:V:11:LEU:HD23	21:V:14:LEU:HD13	1.95	0.48
27:b:23:PHE:CD2	58:b:201:3PE:H281	2.40	0.48
33:h:73:PHE:HE2	33:h:74:TYR:HE1	1.62	0.48
37:l:48:ARG:CZ	37:l:64:PRO:HD2	2.44	0.48
41:p:5:TRP:CZ3	41:p:10:TYR:O	2.66	0.48
47:AC:304:MET:HA	47:AC:307:LEU:HD12	1.96	0.48
49:AE:111:LYS:HE2	53:AJ:11:TYR:CE1	2.48	0.48
47:Ac:74:ASN:HB2	49:Ae:139:SER:HA	1.95	0.48
47:Ac:316:MET:HE2	58:Ac:403:3PE:H111	1.95	0.48
48:Ad:295:MET:HE1	49:Ae:124:GLY:CA	2.43	0.48
49:Ae:152:ILE:HG21	49:Ae:273:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.96	0.48
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.49	0.48
3:C:79:CYS:O	3:C:80:LEU:C	2.55	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
8:H:136:VAL:HG11	10:J:69:TYR:CD1	2.48	0.48
9:I:55:ASP:OD1	25:Z:32:GLY:N	2.43	0.48
11:K:21:MET:HB2	58:K:101:3PE:H231	1.94	0.48
12:L:319:MET:O	12:L:319:MET:HG2	2.13	0.48
12:L:433:THR:HG21	12:L:436:ARG:NH2	2.29	0.48
13:M:42:LEU:HG	13:M:67:ILE:CD1	2.42	0.48
13:M:123:GLU:CG	14:N:255:PRO:HG2	2.43	0.48
14:N:4:ILE:HG23	14:N:5:THR:N	2.29	0.48
16:P:79:GLN:NE2	16:P:102:GLN:O	2.47	0.48
16:P:221:ARG:CD	16:P:286:ARG:HD3	2.43	0.48
21:V:35:LEU:HD13	21:V:48:THR:HG23	1.96	0.48
25:Z:85:GLN:O	25:Z:89:GLU:HG3	2.14	0.48
28:c:57:TYR:HD2	29:d:70:PHE:CZ	2.30	0.48
34:i:14:GLN:HE22	39:n:157:ALA:HB3	1.79	0.48
39:n:144:THR:HG23	39:n:144:THR:O	2.13	0.48
39:n:155:PRO:HG2	39:n:165:PRO:HG2	1.95	0.48
46:AB:388:THR:HG23	46:AB:391:GLY:H	1.78	0.48
48:AD:167:ARG:HG3	48:AD:169:GLY:H	1.77	0.48
47:Ac:32:ASN:ND2	47:Ac:228:ASP:OD1	2.47	0.48
47:Ac:304:MET:HA	47:Ac:307:LEU:HD12	1.95	0.48
51:Ag:11:ILE:CG2	51:Ag:12:ARG:N	2.77	0.48
54:Ak:45:VAL:HG13	54:Ak:46:PRO:HD2	1.95	0.48
1:A:11:ILE:HD11	58:J:401:3PE:H2D1	1.95	0.48
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.96	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
12:L:149:ILE:CG2	13:M:364:LEU:HD21	2.43	0.48
12:L:197:GLU:HG3	41:p:111:LYS:HE2	1.94	0.48
12:L:274:LEU:O	12:L:277:MET:HG2	2.14	0.48
12:L:496:LEU:HD12	12:L:497:GLY:CA	2.44	0.48
13:M:6:LEU:HD21	31:f:22:PHE:HD2	1.79	0.48
13:M:307:TRP:CE3	13:M:383:MET:CE	2.97	0.48
16:P:191:VAL:CG1	16:P:192:ARG:HH21	2.26	0.48
20:T:104:PHE:CZ	20:T:118:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:22:TRP:CE3	39:n:172:THR:HG22	2.49	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:341:PHE:HB2	45:AA:368:MET:CE	2.43	0.48
45:AA:402:HIS:C	45:AA:404:ASP:H	2.21	0.48
46:AB:109:LYS:O	46:AB:123:VAL:HA	2.14	0.48
46:AB:176:ASN:C	46:AB:258:ILE:HD11	2.39	0.48
49:AE:154:ILE:O	49:AE:270:VAL:HG13	2.13	0.48
46:Ab:227:HIS:CD2	46:Ab:231:LYS:HG3	2.49	0.48
49:Ae:160:PRO:O	49:Ae:178:HIS:HB3	2.13	0.48
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.95	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:42:GLU:HA	4:D:45:GLU:HG2	1.96	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
8:H:20:LEU:HA	26:a:12:MET:SD	2.53	0.48
8:H:272:TRP:HH2	57:I:302:PC1:H381	1.79	0.48
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.48
10:J:5:ILE:CG2	11:K:4:THR:HG21	2.44	0.48
11:K:22:PHE:HZ	14:N:61:VAL:HG11	1.79	0.48
12:L:186:MET:HE1	13:M:379:LEU:HD21	1.96	0.48
12:L:389:PHE:CZ	35:j:79:ALA:HB1	2.48	0.48
13:M:269:MET:HE3	13:M:399:ASN:HB3	1.96	0.48
13:M:422:HIS:CE1	13:M:425:ASN:OD1	2.67	0.48
14:N:307:THR:CB	15:O:319:ILE:HD11	2.37	0.48
15:O:76:GLU:HB2	15:O:266:PRO:HB3	1.95	0.48
15:O:76:GLU:O	15:O:77:ILE:C	2.57	0.48
17:Q:82:PRO:HG2	17:Q:93:ASN:O	2.14	0.48
19:S:79:LEU:CA	19:S:82:LEU:HD12	2.26	0.48
20:T:119:ILE:HG13	20:T:135:ALA:HB1	1.95	0.48
20:U:128:PHE:HZ	20:U:148:ILE:HD12	1.76	0.48
22:W:103:ARG:O	22:W:104:THR:C	2.56	0.48
23:X:17:GLU:HB3	23:X:19:LYS:HG3	1.96	0.48
27:b:78:LEU:HA	27:b:80:TRP:CD1	2.49	0.48
36:k:41:LYS:O	36:k:42:LEU:C	2.50	0.48
36:k:69:PHE:CE1	36:k:73:ILE:HD11	2.48	0.48
45:AA:68:THR:O	45:AA:406:THR:HG21	2.14	0.48
45:AA:403:LEU:C	45:AA:405:GLY:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:390:ARG:O	45:Aa:394:ILE:HG13	2.14	0.48
47:Ac:297:SER:O	47:Ac:300:ILE:HG22	2.13	0.48
48:Ad:148:LEU:HA	48:Ad:151:GLU:CD	2.39	0.48
48:Ad:242:ILE:HD11	48:Ad:244:MET:HE2	1.95	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:100:ARG:HH12	21:V:86:LYS:HZ1	1.62	0.48
3:C:151:PRO:HG2	22:W:23:ILE:HG23	1.96	0.48
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.49	0.48
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.48	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
9:I:171:PRO:HB3	42:q:93:MET:CE	2.38	0.48
11:K:29:THR:O	11:K:30:LEU:C	2.54	0.48
13:M:177:MET:HE2	33:h:140:LEU:HD21	1.96	0.48
58:M:503:3PE:H231	29:d:47:MET:HE1	1.95	0.48
14:N:82:GLY:HA3	30:e:21:LEU:HG	1.96	0.48
14:N:308:ASN:HB3	15:O:317:ILE:HG22	1.96	0.48
16:P:294:PRO:HB3	16:P:296:PHE:HD1	1.79	0.48
23:X:5:VAL:O	23:X:6:GLU:C	2.54	0.48
27:b:68:SER:O	27:b:69:HIS:C	2.56	0.48
29:d:119:VAL:O	29:d:120:ARG:C	2.55	0.48
34:i:90:MET:SD	34:i:97:ILE:HD11	2.54	0.48
37:l:48:ARG:HH21	37:l:63:GLU:HA	1.78	0.48
46:AB:299:ILE:HD12	46:AB:299:ILE:N	2.29	0.48
47:AC:185:LEU:HD23	47:AC:188:ILE:HD12	1.95	0.48
47:AC:326:TRP:HZ2	58:AC:403:3PE:H222	1.76	0.48
48:AD:94:TYR:HB3	52:AH:85:PHE:CZ	2.48	0.48
48:AD:242:ILE:HD11	48:AD:244:MET:HE2	1.95	0.48
49:AE:179:ARG:HD2	49:AE:245:ALA:HB1	1.96	0.48
52:AH:69:LEU:HG	52:AH:73:LEU:CD1	2.44	0.48
45:Aa:64:SER:OG	45:Aa:235:GLY:HA2	2.13	0.48
49:Ae:166:ALA:HB1	49:Ae:173:PRO:HB3	1.96	0.48
1:A:102:LEU:HG	1:A:106:TRP:HE1	1.79	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:35:ARG:HE	32:g:59:PRO:HD3	1.77	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:667:GLN:HE21	19:S:38:VAL:HA	1.79	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
9:I:54:THR:HG21	25:Z:33:TYR:CE2	2.49	0.48
10:J:18:GLY:O	10:J:23:PRO:HD3	2.14	0.48
12:L:152:PHE:HE1	13:M:412:ILE:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:LEU:O	13:M:98:MET:HG2	2.14	0.48
13:M:310:MET:CE	13:M:459:MET:SD	3.02	0.48
14:N:189:TRP:CZ3	14:N:282:MET:HE3	2.49	0.48
15:O:314:LEU:HD12	15:O:315:PRO:HD3	1.93	0.48
18:R:79:CYS:O	18:R:88:HIS:CE1	2.67	0.48
19:S:50:ASN:O	19:S:51:LEU:C	2.57	0.48
27:b:69:HIS:HD2	27:b:70:PRO:CD	2.26	0.48
35:j:45:ARG:HD3	36:k:57:TRP:CD1	2.49	0.48
36:k:52:ALA:O	36:k:53:ARG:C	2.56	0.48
37:l:184:TYR:CD1	40:o:36:GLU:CA	2.97	0.48
38:m:124:LYS:C	38:m:126:ASN:N	2.70	0.48
39:n:37:TYR:O	39:n:39:TYR:N	2.47	0.48
45:AA:338:CYS:CB	45:AA:368:MET:SD	2.97	0.48
47:AC:361:ILE:HA	47:AC:365:LEU:HB2	1.95	0.48
45:Aa:273:SER:O	45:Aa:455:ALA:HA	2.13	0.48
46:Ab:426:LYS:HA	46:Ab:429:LYS:HZ3	1.79	0.48
49:Ae:200:HIS:ND1	49:Ae:202:LEU:HG	2.29	0.48
2:B:115:ASP:O	2:B:116:ARG:C	2.55	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.47
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	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
10:J:65:VAL:O	10:J:66:VAL:C	2.54	0.47
12:L:554:ASP:OD2	13:M:213:HIS:HE1	1.97	0.47
62:L:705:CDL:H342	24:Y:115:MET:HG3	1.95	0.47
13:M:192:ASN:C	13:M:194:LEU:N	2.72	0.47
58:M:501:3PE:H321	58:M:501:3PE:C21	2.44	0.47
17:Q:99:MET:SD	17:Q:128:PHE:HE2	2.36	0.47
20:U:102:SER:C	20:U:141:PRO:HD3	2.39	0.47
35:j:44:TYR:CG	36:k:22:LEU:HD22	2.49	0.47
36:k:42:LEU:HG	39:n:39:TYR:CD1	2.49	0.47
38:m:45:ARG:NE	39:n:140:LEU:HD11	2.29	0.47
39:n:81:ILE:HD11	39:n:87:GLY:O	2.14	0.47
39:n:156:PRO:HD2	39:n:158:ARG:NH1	2.29	0.47
40:o:22:ILE:HD12	40:o:102:PHE:HD1	1.79	0.47
40:o:111:ARG:HG2	40:o:115:ARG:HG3	1.96	0.47
45:AA:65:SER:O	45:AA:66:HIS:C	2.57	0.47
45:AA:96:LEU:HD23	45:AA:164:GLU:HG3	1.94	0.47
45:AA:160:GLN:HA	45:AA:163:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:90:THR:HG23	46:AB:95:SER:HA	1.95	0.47
46:AB:286:PHE:CZ	46:AB:427:ALA:HB1	2.49	0.47
46:AB:429:LYS:HA	46:AB:432:VAL:CG1	2.40	0.47
47:AC:281:LEU:HD12	47:AC:290:GLY:HA3	1.95	0.47
48:AD:208:GLU:O	48:AD:209:ASP:C	2.57	0.47
49:AE:223:VAL:HG23	47:Ac:141:TRP:CZ2	2.49	0.47
45:Aa:65:SER:O	45:Aa:66:HIS:C	2.55	0.47
45:Aa:396:ARG:O	45:Aa:400:VAL:HG23	2.13	0.47
46:Ab:176:ASN:HB3	46:Ab:258:ILE:HD11	1.95	0.47
46:Ab:286:PHE:CZ	46:Ab:427:ALA:HB1	2.49	0.47
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.95	0.47
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:284:GLU:OE2	17:Q:84:ARG:NH2	2.48	0.47
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:J:102:LEU:O	10:J:105:VAL:HB	2.14	0.47
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.49	0.47
12:L:31:ASN:HD22	12:L:34:LEU:HB2	1.79	0.47
12:L:54:PHE:CZ	12:L:84:PHE:HB2	2.49	0.47
62:L:705:CDL:H312	24:Y:115:MET:SD	2.54	0.47
16:P:335:LEU:O	16:P:336:GLU:HB2	2.15	0.47
16:P:360:ARG:HD3	16:P:360:ARG:O	2.15	0.47
23:X:53:PRO:HD2	25:Z:116:TRP:HD1	1.75	0.47
23:X:80:GLU:O	23:X:81:PRO:C	2.56	0.47
23:X:123:GLY:HA2	25:Z:66:GLU:OE2	2.14	0.47
27:b:46:ASN:OD1	27:b:47:LYS:N	2.47	0.47
29:d:8:HIS:O	29:d:10:PRO:HD3	2.14	0.47
36:k:84:PHE:CZ	36:k:88:LEU:HD22	2.49	0.47
43:r:113:LEU:HD12	43:r:113:LEU:HA	1.77	0.47
47:AC:119:LEU:HD22	67:AC:402:HEM:CBB	2.44	0.47
67:AC:402:HEM:O2A	67:AC:402:HEM:C2A	2.68	0.47
49:AE:155:LYS:HA	49:AE:270:VAL:HA	1.97	0.47
49:AE:199:GLN:HB3	49:AE:204:ARG:NH2	2.29	0.47
47:Ac:243:VAL:O	47:Ac:247:PRO:HB3	2.13	0.47
47:Ac:265:PRO:HD2	47:Ac:268:ILE:HD11	1.95	0.47
47:Ac:277:ALA:CB	68:Ac:404:U10:H1M2	2.44	0.47
1:A:51:PHE:CZ	11:K:79:VAL:CG1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:HG3	16:P:85:ARG:HH22	1.79	0.47
3:C:209:LEU:HD21	22:W:108:ARG:NH1	2.29	0.47
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
10:J:66:VAL:O	10:J:69:TYR:HB3	2.14	0.47
10:J:104:CYS:HA	10:J:107:ASN:ND2	2.29	0.47
11:K:36:MET:HE3	14:N:68:MET:HG3	1.96	0.47
12:L:3:ILE:HG22	12:L:49:LEU:HD21	1.96	0.47
12:L:121:LEU:HD22	12:L:246:LEU:CD2	2.24	0.47
12:L:482:MET:HE2	12:L:486:LEU:HB3	1.96	0.47
12:L:483:PRO:HG2	12:L:486:LEU:HD12	1.96	0.47
57:L:706:PC1:H2D2	57:L:706:PC1:H371	1.96	0.47
13:M:176:LEU:HD13	13:M:245:ARG:HH11	1.79	0.47
58:M:503:3PE:H3I1	58:M:503:3PE:H2G1	1.96	0.47
15:O:242:LYS:O	15:O:247:PRO:HD3	2.14	0.47
15:O:341:PRO:HB2	28:c:34:PRO:HB3	1.95	0.47
16:P:304:LEU:O	16:P:307:LEU:HB3	2.14	0.47
22:W:120:ASP:OD1	22:W:121:PHE:N	2.46	0.47
34:i:79:MET:O	34:i:80:TRP:C	2.57	0.47
49:AE:213:LEU:HD13	49:AE:258:LEU:HD12	1.96	0.47
52:AH:58:ARG:HD3	52:AH:61:THR:HB	1.95	0.47
54:AK:18:ILE:N	54:AK:19:PRO:HD2	2.28	0.47
45:Aa:362:ALA:HB2	45:Aa:461:PRO:HB2	1.95	0.47
47:Ac:185:LEU:HD23	47:Ac:188:ILE:HD12	1.95	0.47
48:Ad:207:GLY:O	48:Ad:208:GLU:C	2.58	0.47
1:A:53:MET:SD	11:K:79:VAL:HG11	2.55	0.47
1:A:63:LEU:HD13	10:J:63:MET:CE	2.42	0.47
55:B:301:SF4:S4	4:D:138:ARG:HD3	2.54	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
7:G:136:GLU:OE1	17:Q:87:MET:HG3	2.15	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.96	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
10:J:170:THR:O	10:J:171:ARG:C	2.57	0.47
12:L:277:MET:SD	12:L:318:GLY:HA2	2.54	0.47
12:L:433:THR:CG2	12:L:434:LYS:N	2.78	0.47
58:L:703:3PE:H231	58:L:703:3PE:H361	1.96	0.47
14:N:1:MET:HE1	14:N:43:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:89:GLN:H	14:N:89:GLN:CD	2.22	0.47
15:O:116:LYS:HA	15:O:119:ASP:OD1	2.13	0.47
15:O:343:TYR:CE1	15:O:355:LYS:CB	2.96	0.47
15:O:350:LYS:O	15:O:351:TRP:HB2	2.13	0.47
25:Z:85:GLN:OE1	30:e:103:GLU:OE2	2.31	0.47
31:f:37:PHE:O	31:f:38:ARG:C	2.57	0.47
40:o:15:VAL:HB	40:o:110:GLN:HG2	1.96	0.47
41:p:6:ASP:C	41:p:8:ASP:N	2.69	0.47
45:AA:137:SER:HB3	45:AA:236:GLY:O	2.15	0.47
45:AA:138:LYS:O	45:AA:141:PRO:HD2	2.14	0.47
45:AA:172:MET:HA	45:AA:175:ASN:ND2	2.30	0.47
45:AA:469:ASN:ND2	47:AC:223:TYR:CZ	2.83	0.47
49:AE:155:LYS:HG3	49:AE:269:ASP:O	2.13	0.47
51:AG:11:ILE:CG2	51:AG:12:ARG:N	2.77	0.47
48:Ad:110:ILE:O	48:Ad:111:ARG:C	2.57	0.47
49:Ae:252:GLY:C	49:Ae:254:ALA:H	2.21	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
3:C:70:LYS:HB2	21:V:99:PRO:O	2.14	0.47
4:D:36:GLN:HA	13:M:138:ASN:HA	1.97	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
10:J:24:SER:HB2	10:J:27:TYR:CD2	2.28	0.47
10:J:59:TYR:OH	11:K:34:GLU:O	2.29	0.47
11:K:69:CYS:O	11:K:70:GLU:C	2.57	0.47
12:L:390:TYR:HE2	35:j:68:TRP:CH2	2.33	0.47
12:L:474:PRO:HD2	40:o:67:LEU:HD21	1.96	0.47
12:L:513:MET:SD	39:n:36:LYS:NZ	2.86	0.47
12:L:576:LEU:HA	12:L:579:ASN:ND2	2.29	0.47
13:M:78:MET:HG2	13:M:432:ARG:HG3	1.97	0.47
14:N:1:MET:O	14:N:2:ASN:C	2.54	0.47
16:P:311:GLU:O	16:P:312:PRO:C	2.57	0.47
20:U:93:ILE:HD11	20:U:118:ILE:HD11	1.97	0.47
22:W:46:VAL:O	22:W:50:VAL:HG23	2.14	0.47
30:e:22:SER:HA	30:e:34:HIS:HD2	1.79	0.47
38:m:124:LYS:C	38:m:126:ASN:H	2.21	0.47
45:AA:109:LEU:HD21	45:AA:120:LEU:HD21	1.95	0.47
47:AC:297:SER:O	47:AC:300:ILE:HG22	2.13	0.47
50:AF:29:LYS:HA	50:AF:81:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AI:63:PRO:HG3	46:Ab:328:ALA:HB2	1.95	0.47
49:Ae:177:ARG:NH1	49:Ae:227:ASN:OD1	2.48	0.47
52:Ah:84:LEU:HD11	52:Ah:88:LEU:HD21	1.96	0.47
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.50	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:425:CYS:SG	55:F:502:SF4:S4	3.13	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
10:J:85:ASN:O	10:J:89:LEU:HG	2.15	0.47
11:K:75:LEU:O	11:K:79:VAL:HG23	2.15	0.47
11:K:93:LEU:HD22	14:N:54:GLU:HA	1.97	0.47
12:L:420:ALA:HB1	12:L:498:PHE:CD2	2.50	0.47
13:M:50:LYS:HE2	13:M:52:PHE:HE1	1.80	0.47
13:M:57:SER:OG	13:M:113:THR:HG22	2.15	0.47
13:M:122:PHE:HZ	13:M:206:LYS:HD3	1.75	0.47
13:M:264:LEU:HD23	38:m:98:LEU:HD21	1.96	0.47
14:N:26:LEU:O	14:N:29:MET:N	2.47	0.47
19:S:58:CYS:HB2	19:S:61:VAL:CG1	2.43	0.47
23:X:122:LEU:HD21	27:b:81:LEU:HD23	1.95	0.47
23:X:139:GLU:O	23:X:140:ASN:C	2.57	0.47
24:Y:142:LYS:O	24:Y:143:VAL:C	2.57	0.47
29:d:101:PHE:CZ	33:h:159:LEU:HD22	2.50	0.47
42:q:55:PHE:CD1	43:r:26:LEU:CD2	2.95	0.47
47:AC:227:LYS:HE2	48:AD:307:LYS:HE2	1.96	0.47
49:AE:165:MET:HG3	49:AE:167:PHE:CZ	2.49	0.47
49:AE:183:GLU:O	49:AE:187:GLU:HB2	2.15	0.47
49:AE:199:GLN:CD	49:AE:257:ASN:HD22	2.22	0.47
52:AH:39:GLU:O	52:AH:43:LYS:HG3	2.15	0.47
45:Aa:152:GLN:O	45:Aa:153:ASN:HB2	2.15	0.47
47:Ac:51:LEU:CD1	47:Ac:69:ILE:HG21	2.44	0.47
47:Ac:275:LEU:O	47:Ac:278:TYR:N	2.48	0.47
49:Ae:190:VAL:HG11	49:Ae:195:LEU:HD21	1.97	0.47
1:A:108:GLN:C	1:A:110:GLY:N	2.72	0.47
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.45	0.47
4:D:279:THR:HG23	21:V:13:GLY:CA	2.23	0.47
4:D:280:ALA:CB	21:V:11:LEU:CG	2.90	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	2.48	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	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:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:93:HIS:HE1	26:a:24:ALA:HA	1.74	0.47
8:H:224:PHE:CZ	61:H:400:UQ9:H11	2.49	0.47
8:H:310:PHE:HB3	27:b:33:PRO:HA	1.96	0.47
9:I:188:GLU:OE1	18:R:56:ASN:CB	2.63	0.47
10:J:46:PHE:CE2	11:K:46:VAL:HG13	2.50	0.47
12:L:237:MET:HE1	12:L:248:HIS:HB2	1.96	0.47
12:L:353:GLU:CD	39:n:80:TYR:OH	2.57	0.47
12:L:386:LEU:HA	35:j:68:TRP:HZ3	1.79	0.47
12:L:428:TYR:OH	39:n:33:HIS:CE1	2.68	0.47
12:L:552:LEU:HD22	12:L:553:LEU:HD12	1.97	0.47
13:M:16:TRP:CZ2	58:M:503:3PE:H282	2.47	0.47
13:M:231:LEU:CD1	13:M:235:LEU:HD12	2.42	0.47
13:M:305:THR:O	13:M:306:PRO:C	2.58	0.47
13:M:370:PRO:CA	13:M:375:LEU:HD23	2.42	0.47
14:N:120:GLN:O	14:N:176:ARG:NH2	2.48	0.47
16:P:55:VAL:HG12	16:P:123:SER:HA	1.96	0.47
16:P:76:MET:HE1	16:P:254:LYS:CE	2.45	0.47
16:P:170:LEU:HG	16:P:171:ASN:N	2.28	0.47
17:Q:99:MET:SD	17:Q:128:PHE:CE2	3.08	0.47
21:V:116:ILE:O	21:V:116:ILE:CG2	2.61	0.47
22:W:32:LYS:O	22:W:36:ARG:HG3	2.15	0.47
23:X:39:THR:CG2	23:X:40:ASN:N	2.77	0.47
25:Z:144:THR:HA	26:a:45:TRP:HZ3	1.79	0.47
26:a:22:SER:O	26:a:23:THR:C	2.57	0.47
27:b:69:HIS:CD2	27:b:71:GLN:H	2.33	0.47
29:d:73:TYR:O	29:d:77:LYS:HB2	2.14	0.47
30:e:85:LYS:O	30:e:89:GLU:HG2	2.15	0.47
37:l:44:THR:CG2	37:l:47:GLU:HG3	2.45	0.47
38:m:14:LEU:HD12	38:m:15:PRO:HD2	1.96	0.47
39:n:96:CYS:SG	39:n:97:TYR:CE1	3.04	0.47
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:71:VAL:O	45:AA:147:LEU:HD11	2.15	0.47
45:AA:339:GLN:O	45:AA:340:SER:C	2.56	0.47
46:AB:429:LYS:CA	46:AB:432:VAL:HG12	2.43	0.47
47:AC:140:PHE:CE1	47:AC:170:VAL:CG1	2.98	0.47
47:AC:294:LEU:O	47:AC:297:SER:HB3	2.15	0.47
68:AC:404:U10:H1M3	68:AC:404:U10:H71	1.77	0.47
48:AD:217:GLY:O	48:AD:218:TYR:C	2.57	0.47
49:AE:88:PHE:O	49:AE:89:SER:C	2.58	0.47
49:AE:190:VAL:HG21	49:AE:195:LEU:HD13	1.96	0.47
49:AE:214:ILE:CG2	49:AE:216:VAL:HG22	2.44	0.47
50:AF:53:GLU:OE2	51:AG:12:ARG:NH1	2.47	0.47
52:AH:55:VAL:HG13	52:AH:63:GLU:O	2.14	0.47
52:AH:70:PHE:HD1	52:AH:73:LEU:HD12	1.80	0.47
49:AI:43:LEU:HD13	46:Ab:164:VAL:CG2	2.37	0.47
49:AI:71:ASN:HD21	46:Ab:109:LYS:HA	1.79	0.47
45:Aa:341:PHE:HZ	45:Aa:372:LEU:CD1	2.28	0.47
45:Aa:410:CYS:O	45:Aa:411:GLU:C	2.56	0.47
46:Ab:142:THR:HA	46:Ab:241:ARG:HH22	1.80	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
47:Ac:346:PRO:HG3	51:Ag:66:GLU:HG2	1.96	0.47
49:Ae:197:ASP:C	49:Ae:199:GLN:N	2.71	0.47
49:Ae:266:THR:OG1	49:Ae:272:VAL:HG23	2.15	0.47
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.47	0.47
4:D:35:ARG:NH2	32:g:57:PRO:C	2.72	0.47
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
11:K:57:MET:C	11:K:60:PRO:HD2	2.39	0.47
13:M:196:TRP:HD1	13:M:250:LEU:HB2	1.80	0.47
13:M:428:PRO:HD3	39:n:106:TYR:CG	2.49	0.47
58:M:503:3PE:H122	15:O:338:LYS:HE3	1.96	0.47
14:N:25:ASN:HB3	30:e:15:ASP:CG	2.40	0.47
14:N:317:GLN:HG2	15:O:301:LYS:HB3	1.96	0.47
15:O:78:ALA:CB	15:O:85:HIS:HB2	2.45	0.47
15:O:135:LEU:HB3	15:O:139:ARG:NH1	2.26	0.47
16:P:221:ARG:HD3	16:P:286:ARG:HD3	1.97	0.47
20:U:130:ILE:HG21	20:U:138:LEU:HD11	1.97	0.47
25:Z:87:LEU:HD21	25:Z:119:PRO:HG3	1.97	0.47
29:d:51:ARG:O	29:d:52:PRO:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:65:HIS:O	41:p:66:ARG:C	2.57	0.47
45:AA:74:TRP:C	45:AA:75:ILE:HG13	2.40	0.47
45:AA:375:GLN:O	45:AA:376:TRP:C	2.58	0.47
47:AC:16:HIS:NE2	47:AC:201:HIS:CD2	2.82	0.47
47:AC:218:ILE:HG21	48:AD:314:LEU:HD11	1.97	0.47
48:AD:159:ASN:ND2	48:AD:162:GLY:H	2.13	0.47
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HG13	1.97	0.47
46:Ab:47:LEU:CD2	46:Ab:234:ALA:HB1	2.45	0.47
47:Ac:73:VAL:HA	49:Ae:143:SER:OG	2.15	0.47
47:Ac:140:PHE:CE1	47:Ac:170:VAL:CG1	2.98	0.47
48:Ad:227:LEU:HD13	48:Ad:231:LEU:HB2	1.97	0.47
53:Aj:43:ILE:O	53:Aj:47:ILE:HG12	2.15	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.47
1:A:51:PHE:CE2	10:J:73:MET:HE2	2.50	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.47
4:D:299:GLN:OE1	43:r:104:TRP:HB2	2.14	0.47
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.97	0.47
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
9:I:63:TRP:HZ2	58:I:301:3PE:H321	1.80	0.47
12:L:63:ILE:HG23	34:i:97:ILE:CD1	2.45	0.47
58:L:703:3PE:H351	13:M:390:ASN:HB2	1.96	0.47
13:M:127:ILE:HG12	14:N:254:LEU:CD2	2.44	0.47
15:O:129:TYR:CE2	15:O:183:CYS:HB3	2.50	0.47
15:O:232:ALA:O	15:O:235:GLN:HB3	2.14	0.47
16:P:287:THR:HG23	16:P:289:ILE:HD11	1.97	0.47
17:Q:85:ASN:N	17:Q:85:ASN:OD1	2.48	0.47
21:V:56:LEU:HD12	21:V:57:ASP:CA	2.44	0.47
23:X:8:PRO:HB3	23:X:12:GLU:CD	2.39	0.47
23:X:120:PRO:HB3	23:X:125:LEU:HD11	1.94	0.47
23:X:151:ASN:HD22	33:h:165:ASP:HA	1.80	0.47
23:X:154:ILE:HG12	33:h:167:PRO:HG2	1.97	0.47
25:Z:89:GLU:HG2	30:e:97:HIS:CD2	2.49	0.47
28:c:46:LEU:O	28:c:50:ALA:CB	2.63	0.47
31:f:39:ASN:ND2	31:f:55:THR:HG21	2.30	0.47
39:n:57:MET:O	39:n:58:MET:C	2.58	0.47
44:s:55:PHE:O	44:s:56:ARG:C	2.57	0.47
45:AA:152:GLN:O	45:AA:153:ASN:HB2	2.15	0.47
45:AA:341:PHE:CZ	45:AA:372:LEU:CD1	2.98	0.47
48:AD:242:ILE:HG12	48:AD:244:MET:H	1.80	0.47
48:Ad:242:ILE:HG12	48:Ad:244:MET:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:206:LYS:HD2	49:Ae:263:TYR:HE1	1.79	0.47
49:Ae:235:TYR:CD1	49:Ae:242:HIS:NE2	2.83	0.47
53:Aj:39:GLY:O	53:Aj:43:ILE:HG13	2.15	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
7:G:496:MET:O	7:G:500:ILE:HG13	2.14	0.47
8:H:180:PRO:CD	25:Z:43:LEU:HD21	2.43	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
10:J:37:PHE:HD1	10:J:56:PHE:CE1	2.33	0.47
18:R:72:VAL:HG21	18:R:77:ILE:HG21	1.97	0.47
23:X:7:LEU:CD1	25:Z:87:LEU:HB3	2.45	0.47
25:Z:110:VAL:HG11	30:e:72:THR:N	2.30	0.47
29:d:93:TYR:OH	33:h:163:ARG:HD2	2.15	0.47
29:d:93:TYR:CD2	33:h:156:VAL:HG13	2.49	0.47
31:f:41:SER:OG	33:h:134:GLU:HG2	2.14	0.47
37:l:127:ASP:O	37:l:128:VAL:C	2.58	0.47
39:n:50:GLU:O	39:n:51:HIS:C	2.55	0.47
41:p:29:PRO:O	41:p:33:LEU:HD13	2.14	0.47
42:q:14:VAL:HA	42:q:23:LEU:HD13	1.97	0.47
45:AA:74:TRP:CD2	45:AA:414:GLY:HA3	2.50	0.47
46:AB:183:LYS:HG3	46:AB:254:ARG:HB3	1.96	0.47
46:AB:284:ASN:HB3	46:AB:419:VAL:CG2	2.45	0.47
49:AE:220:LEU:O	47:Ac:148:ASN:HB2	2.15	0.47
49:AI:22:VAL:O	49:AI:23:ALA:C	2.58	0.47
47:Ac:162:GLU:HA	47:Ac:165:TRP:HB2	1.97	0.47
48:Ad:154:VAL:HG21	48:Ad:173:ASP:CG	2.39	0.47
50:Af:59:ARG:HA	50:Af:62:ARG:CZ	2.45	0.47
52:Ah:67:GLU:HG3	52:Ah:68:GLU:N	2.30	0.47
53:Aj:17:ARG:HG2	53:Aj:19:SER:OG	2.14	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.14	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
9:I:79:ARG:HG2	43:r:12:ARG:NH2	2.29	0.46
11:K:73:VAL:HG21	14:N:38:LEU:CD2	2.45	0.46
58:L:702:3PE:H231	58:L:702:3PE:H261	1.83	0.46
13:M:232:ALA:HA	13:M:236:LEU:HD12	1.97	0.46
13:M:348:LEU:O	13:M:351:VAL:N	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:50:THR:OG1	15:O:288:ASP:HB3	2.15	0.46
16:P:207:PHE:CD2	16:P:241:TYR:HD1	2.33	0.46
18:R:33:HIS:HE1	18:R:56:ASN:HD22	1.63	0.46
22:W:42:TRP:CZ2	22:W:93:LEU:CA	2.95	0.46
23:X:20:VAL:CG2	23:X:24:VAL:HG21	2.40	0.46
24:Y:116:GLY:O	24:Y:120:MET:HB2	2.15	0.46
37:l:119:THR:HG22	38:m:13:THR:HG23	1.96	0.46
39:n:133:TRP:O	39:n:137:VAL:HG22	2.15	0.46
42:q:8:LYS:HG2	42:q:12:GLN:HE21	1.79	0.46
43:r:109:ASP:O	43:r:110:GLN:OE1	2.32	0.46
52:AH:79:CYS:O	52:AH:82:HIS:HB3	2.15	0.46
54:AK:9:ARG:NH2	54:AK:10:TYR:HE1	2.14	0.46
45:Aa:399:LEU:HD21	45:Aa:429:TRP:HB3	1.97	0.46
46:Ab:228:SER:HA	46:Ab:231:LYS:CE	2.45	0.46
46:Ab:228:SER:HA	46:Ab:231:LYS:HE2	1.97	0.46
47:Ac:10:LEU:O	47:Ac:14:ILE:HG12	2.15	0.46
49:Ae:163:LYS:NZ	49:Ae:165:MET:HB2	2.28	0.46
4:D:264:ASN:O	9:I:65:GLU:OE1	2.32	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.97	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:1:MET:HE3	26:a:29:PHE:CE1	2.50	0.46
10:J:75:THR:HG23	10:J:75:THR:O	2.14	0.46
12:L:86:SER:OG	12:L:133:SER:HB3	2.15	0.46
12:L:277:MET:CG	12:L:318:GLY:HA2	2.44	0.46
12:L:482:MET:HE2	12:L:486:LEU:CB	2.45	0.46
13:M:213:HIS:O	13:M:217:PRO:CD	2.63	0.46
14:N:17:PRO:HG2	14:N:133:TRP:NE1	2.30	0.46
16:P:116:ILE:HG21	16:P:152:ILE:HA	1.96	0.46
16:P:209:ARG:O	16:P:210:GLU:HB2	2.15	0.46
19:S:19:ILE:HD12	19:S:94:VAL:CG1	2.44	0.46
23:X:115:LEU:HD13	23:X:117:TRP:CZ2	2.51	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
32:g:147:LEU:HD11	41:p:163:MET:HE2	1.97	0.46
34:i:103:ARG:NH1	40:o:67:LEU:HD22	2.31	0.46
41:p:6:ASP:OD1	41:p:8:ASP:HB2	2.15	0.46
41:p:43:TRP:O	41:p:44:PRO:C	2.58	0.46
45:AA:341:PHE:CE1	45:AA:356:ALA:HB1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:212:ILE:CD1	49:AE:271:VAL:HG21	2.45	0.46
49:AE:216:VAL:HA	49:AE:222:CYS:O	2.16	0.46
54:AK:36:THR:O	54:AK:37:ASP:C	2.56	0.46
47:Ac:30:TRP:CE2	58:Ac:403:3PE:H232	2.51	0.46
52:Ah:80:VAL:CG1	52:Ah:84:LEU:HB2	2.45	0.46
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.46
2:B:116:ARG:HA	8:H:37:PRO:HA	1.97	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
10:J:33:ILE:HG23	10:J:60:LEU:CD2	2.45	0.46
10:J:74:ALA:O	10:J:75:THR:C	2.56	0.46
10:J:135:LEU:O	11:K:54:MET:CE	2.64	0.46
12:L:172:ILE:O	12:L:176:ARG:HG2	2.16	0.46
12:L:367:PRO:HB3	36:k:75:LYS:HZ1	1.81	0.46
13:M:123:GLU:CB	14:N:255:PRO:HG2	2.42	0.46
15:O:62:VAL:HG13	15:O:62:VAL:O	2.15	0.46
15:O:258:TYR:HE2	15:O:272:ASP:OD2	1.98	0.46
21:V:22:GLU:O	21:V:26:ILE:HG12	2.16	0.46
23:X:35:GLN:HG3	23:X:70:PHE:HE1	1.80	0.46
23:X:120:PRO:HB2	23:X:125:LEU:CD1	2.44	0.46
25:Z:110:VAL:HG11	30:e:72:THR:HA	1.98	0.46
30:e:34:HIS:CE1	33:h:184:LYS:NZ	2.83	0.46
34:i:89:HIS:ND1	58:i:201:3PE:H112	2.31	0.46
35:j:97:LEU:O	40:o:104:ARG:HG3	2.16	0.46
38:m:125:PHE:HE1	41:p:133:THR:CG2	2.21	0.46
47:AC:35:SER:HA	69:AC:405:UQ6:C11	2.39	0.46
47:AC:296:LEU:O	47:AC:300:ILE:N	2.45	0.46
52:AH:53:ASN:HB3	52:AH:54:ARG:HH11	1.80	0.46
53:AJ:33:GLU:HB2	54:AK:34:TRP:HZ2	1.79	0.46
47:Ac:74:ASN:C	47:Ac:76:GLY:N	2.72	0.46
48:Ad:312:SER:O	48:Ad:313:VAL:C	2.59	0.46
49:Ae:183:GLU:O	49:Ae:187:GLU:HG2	2.16	0.46
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:58:THR:HA	4:D:61:TRP:CE2	2.50	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	0.46
8:H:118:TRP:CZ2	10:J:30:LEU:HD23	2.50	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
10:J:135:LEU:O	11:K:54:MET:HE2	2.15	0.46
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.46
12:L:373:LEU:CD2	12:L:427:ILE:HG22	2.45	0.46
13:M:4:ILE:HD12	13:M:4:ILE:N	2.30	0.46
13:M:380:PHE:HD1	13:M:380:PHE:N	2.13	0.46
13:M:380:PHE:N	13:M:380:PHE:CD1	2.82	0.46
13:M:435:THR:O	13:M:436:LEU:C	2.59	0.46
14:N:275:CYS:SG	24:Y:139:PRO:HD2	2.56	0.46
16:P:276:LEU:O	16:P:280:ILE:HG13	2.15	0.46
22:W:50:VAL:HA	22:W:55:LEU:HD12	1.97	0.46
23:X:94:MET:O	23:X:95:GLN:C	2.59	0.46
25:Z:98:MET:HE1	30:e:78:ASP:CG	2.37	0.46
33:h:73:PHE:HD2	33:h:74:TYR:CE1	2.33	0.46
37:l:38:PRO:CB	38:m:75:ASN:ND2	2.73	0.46
39:n:136:GLU:O	39:n:139:GLN:N	2.49	0.46
46:AB:38:LEU:HD13	46:AB:52:LEU:HB2	1.96	0.46
46:AB:278:ILE:HB	46:AB:331:SER:HA	1.98	0.46
47:AC:152:ALA:O	47:AC:153:ILE:C	2.58	0.46
47:AC:169:SER:HB3	49:Ae:172:LYS:HD2	1.97	0.46
49:AE:219:HIS:CD2	49:AE:253:PRO:HB2	2.50	0.46
49:AE:233:GLY:O	49:AE:234:TYR:CD2	2.68	0.46
52:AH:48:LEU:HD22	52:AH:69:LEU:HD12	1.97	0.46
47:Ac:146:ILE:CG2	68:Ac:404:U10:H3M2	2.46	0.46
49:Ae:204:ARG:HD3	49:Ae:248:ARG:CG	2.46	0.46
2:B:93:MET:HB2	2:B:128:ALA:HB2	1.97	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.80	0.46
6:F:51:TRP:HZ2	44:s:36:GLN:HG3	1.80	0.46
9:I:64:THR:HG21	25:Z:35:MET:HE1	1.97	0.46
12:L:21:ILE:HG12	12:L:27:ILE:CG2	2.46	0.46
12:L:225:ALA:CB	12:L:233:LEU:HD12	2.45	0.46
12:L:264:HIS:HA	12:L:267:THR:CG2	2.45	0.46
12:L:581:LYS:HB2	12:L:586:LEU:HD22	1.97	0.46
58:L:703:3PE:H251	58:L:703:3PE:H221	1.48	0.46
13:M:10:MET:C	13:M:13:PRO:HD2	2.41	0.46
13:M:139:GLN:HG3	13:M:141:GLU:H	1.80	0.46
13:M:300:SER:HB2	13:M:308:SER:HB3	1.97	0.46
14:N:25:ASN:HB3	30:e:15:ASP:OD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:38:TYR:CE1	15:O:292:HIS:HD2	2.34	0.46
15:O:135:LEU:CD1	63:O:402:ADP:C6	2.99	0.46
18:R:38:TYR:CD1	18:R:44:ARG:HB2	2.51	0.46
20:T:87:LEU:CD2	20:T:104:PHE:HZ	2.12	0.46
20:T:114:ASP:OD1	22:W:67:ARG:NH1	2.48	0.46
25:Z:72:MET:N	25:Z:73:PRO:CD	2.78	0.46
27:b:52:ASN:ND2	30:e:28:LYS:NZ	2.64	0.46
40:o:111:ARG:HA	40:o:114:ARG:HG2	1.98	0.46
41:p:6:ASP:O	41:p:8:ASP:N	2.49	0.46
44:s:52:LEU:HB3	44:s:56:ARG:HH11	1.81	0.46
47:AC:153:ILE:HG23	47:AC:154:PRO:HD2	1.96	0.46
48:AD:233:PHE:HZ	52:AH:70:PHE:HE1	1.63	0.46
48:AD:302:LEU:HD22	49:AE:117:VAL:HG13	1.97	0.46
49:AE:168:LYS:NZ	49:AE:171:GLY:HA2	2.30	0.46
45:Aa:99:LYS:HD2	45:Aa:160:GLN:HE21	1.80	0.46
48:Ad:98:HIS:CB	48:Ad:105:LEU:HD23	2.46	0.46
48:Ad:214:LEU:O	48:Ad:234:ASN:ND2	2.49	0.46
48:Ad:236:TYR:O	48:Ad:237:PHE:C	2.58	0.46
52:Ah:80:VAL:HG12	52:Ah:84:LEU:HB2	1.98	0.46
2:B:94:THR:HB	2:B:104:MET:CE	2.45	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
6:F:109:ARG:NH2	6:F:232:ASP:O	2.45	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
10:J:32:LEU:HG	10:J:64:LEU:HD21	1.97	0.46
12:L:261:VAL:CA	12:L:264:HIS:HD2	2.29	0.46
12:L:598:ILE:HD11	14:N:153:ILE:HG12	1.97	0.46
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.98	0.46
14:N:154:ILE:HG12	14:N:195:PRO:CG	2.45	0.46
16:P:55:VAL:HG22	16:P:79:GLN:HB3	1.97	0.46
16:P:235:THR:HG22	16:P:323:HIS:O	2.15	0.46
20:T:117:GLU:HG2	22:W:43:TYR:CZ	2.51	0.46
21:V:72:LEU:C	21:V:72:LEU:CD1	2.89	0.46
22:W:32:LYS:CE	66:W:201:EHZ:C19	2.90	0.46
33:h:69:ARG:O	33:h:73:PHE:CB	2.63	0.46
40:o:31:PHE:CG	40:o:34:ARG:HB3	2.51	0.46
42:q:48:TYR:OH	42:q:83:PRO:HD2	2.15	0.46
48:AD:130:VAL:HG21	48:AD:277:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:205:HIS:CG	48:AD:206:GLY:N	2.83	0.46
49:AE:172:LYS:HE3	47:Ac:169:SER:HB3	1.98	0.46
50:AF:83:LYS:HB3	50:AF:85:GLU:OE2	2.15	0.46
53:AJ:33:GLU:OE1	54:AK:34:TRP:NE1	2.49	0.46
46:Ab:225:VAL:HG22	46:Ab:229:VAL:CG2	2.46	0.46
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CD2	2.51	0.46
48:Ad:218:TYR:CE2	48:Ad:246:PRO:HA	2.51	0.46
48:Ad:270:VAL:HG11	70:Ad:401:HEC:HBB2	1.95	0.46
49:Ae:229:GLY:N	49:Ae:233:GLY:HA2	2.27	0.46
50:Af:77:PRO:HB2	50:Af:79:ASP:OD1	2.16	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
10:J:5:ILE:HG13	10:J:124:LEU:HD11	1.97	0.46
12:L:13:ILE:HD11	58:i:201:3PE:H2A2	1.98	0.46
12:L:306:THR:HA	12:L:336:LYS:NZ	2.27	0.46
12:L:466:PHE:CE2	58:j:700:3PE:H361	2.50	0.46
12:L:529:PHE:CZ	12:L:533:ILE:HG21	2.50	0.46
12:L:556:ILE:HD11	38:m:76:ILE:CG2	2.44	0.46
13:M:15:THR:HG21	13:M:100:ILE:CD1	2.46	0.46
14:N:123:PRO:HG2	14:N:126:MET:CG	2.40	0.46
14:N:239:ALA:HB1	29:d:47:MET:HG2	1.98	0.46
14:N:319:LYS:HA	15:O:302:THR:CG2	2.40	0.46
16:P:131:GLY:HA3	64:P:401:NDP:O3D	2.15	0.46
18:R:32:THR:HA	18:R:55:VAL:CG2	2.45	0.46
23:X:33:GLY:HA3	25:Z:70:ALA:HB1	1.98	0.46
32:g:77:ASP:HA	32:g:78:PRO:HD3	1.70	0.46
33:h:95:GLU:OE1	33:h:114:LYS:HD3	2.15	0.46
37:l:184:TYR:HD1	40:o:36:GLU:HA	1.78	0.46
39:n:61:THR:O	39:n:65:ARG:HG3	2.15	0.46
45:AA:183:VAL:HG21	45:AA:286:HIS:HB2	1.96	0.46
45:AA:393:ASN:HA	45:AA:396:ARG:NH1	2.31	0.46
48:AD:102:LEU:CB	53:AJ:47:ILE:HG21	2.46	0.46
49:AE:153:GLU:HG3	49:AE:272:VAL:HG13	1.98	0.46
49:AE:210:TRP:HB2	49:AE:265:PHE:HZ	1.79	0.46
49:AI:20:ARG:O	49:AI:21:GLY:C	2.58	0.46
45:Aa:287:VAL:HB	45:Aa:358:PHE:CE2	2.50	0.46
47:Ac:15:ASN:OD1	47:Ac:19:ILE:HB	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:160:LEU:O	47:Ac:163:TRP:HB3	2.15	0.46
49:Ae:165:MET:HG3	49:Ae:167:PHE:CE1	2.51	0.46
49:Ae:243:TYR:CE2	49:Ae:247:GLY:HA2	2.51	0.46
2:B:96:GLY:HA3	56:B:302:UQ1:O1	2.15	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.46
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
8:H:186:PHE:HB2	58:I:301:3PE:H2G1	1.98	0.46
12:L:31:ASN:ND2	12:L:34:LEU:HB2	2.31	0.46
12:L:101:MET:HE1	12:L:121:LEU:HB2	1.98	0.46
14:N:37:LEU:HD21	14:N:60:PHE:CD1	2.51	0.46
16:P:157:LYS:O	16:P:160:GLY:N	2.49	0.46
16:P:245:VAL:HA	16:P:265:PHE:CD2	2.49	0.46
18:R:39:ASP:CG	18:R:40:GLU:N	2.74	0.46
20:T:87:LEU:CD2	20:T:122:MET:HE1	2.46	0.46
21:V:56:LEU:HD13	21:V:60:LYS:HE2	1.98	0.46
23:X:5:VAL:CG1	23:X:7:LEU:HG	2.46	0.46
24:Y:74:LEU:HD23	24:Y:74:LEU:C	2.41	0.46
25:Z:86:ILE:CG2	25:Z:128:ARG:HE	2.16	0.46
27:b:45:ILE:CA	27:b:80:TRP:HH2	2.28	0.46
28:c:38:LYS:HA	28:c:39:PRO:HD3	1.58	0.46
29:d:108:THR:O	29:d:109:TYR:C	2.55	0.46
33:h:59:PRO:HD3	39:n:99:VAL:HG11	1.98	0.46
35:j:84:PHE:CE2	40:o:88:ASP:HB3	2.50	0.46
35:j:92:TRP:O	35:j:93:THR:C	2.59	0.46
38:m:15:PRO:HG2	38:m:18:LEU:HD12	1.97	0.46
45:AA:74:TRP:CE2	45:AA:414:GLY:HA3	2.50	0.46
47:AC:30:TRP:HZ3	47:AC:96:LEU:HD22	1.81	0.46
48:AD:318:LYS:HD3	49:AE:86:PRO:HB2	1.96	0.46
49:AE:195:LEU:HD22	49:AE:248:ARG:NH1	2.30	0.46
49:AE:209:GLU:HG2	49:AE:210:TRP:N	2.31	0.46
49:AE:235:TYR:CE2	49:AE:237:PRO:HA	2.51	0.46
45:Aa:387:GLU:O	45:Aa:390:ARG:HB3	2.15	0.46
49:Ae:229:GLY:CA	49:Ae:242:HIS:HD2	2.24	0.46
49:Ae:243:TYR:OH	49:Ae:258:LEU:HD22	2.14	0.46
4:D:279:THR:CG2	21:V:13:GLY:HA3	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:140:ILE:HG13	8:H:141:SER:N	2.30	0.46
9:I:80:GLU:N	26:a:1:MET:HE1	2.31	0.46
10:J:94:LEU:HD23	10:J:94:LEU:C	2.40	0.46
12:L:324:LEU:HA	12:L:327:LEU:HD12	1.97	0.46
12:L:427:ILE:CD1	36:k:69:PHE:CE1	2.99	0.46
13:M:208:PRO:CD	13:M:236:LEU:HD22	2.38	0.46
13:M:319:HIS:CA	13:M:322:THR:HG22	2.41	0.46
15:O:231:SER:O	15:O:234:LEU:N	2.48	0.46
23:X:54:ARG:HD3	25:Z:116:TRP:CE3	2.51	0.46
25:Z:62:ILE:CG1	27:b:49:THR:HG22	2.44	0.46
26:a:58:ASN:HB2	26:a:61:TYR:CE2	2.50	0.46
27:b:45:ILE:N	27:b:80:TRP:HH2	2.14	0.46
33:h:82:VAL:O	33:h:85:GLY:N	2.49	0.46
36:k:52:ALA:O	36:k:55:GLU:N	2.49	0.46
42:q:71:LYS:HB2	42:q:73:THR:HG23	1.97	0.46
48:AD:321:TYR:HB2	50:AF:61:PHE:CD1	2.51	0.46
49:AE:175:PHE:CE2	49:AE:224:PRO:HD2	2.51	0.46
54:AK:36:THR:HB	54:AK:38:TRP:CD2	2.50	0.46
48:Ad:237:PHE:CD1	48:Ad:238:PRO:HD2	2.51	0.46
49:Ae:241:SER:HA	49:Ae:251:LYS:HG3	1.98	0.46
52:Ah:84:LEU:O	52:Ah:88:LEU:HG	2.16	0.46
4:D:58:THR:HG23	4:D:61:TRP:CH2	2.51	0.46
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.46
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.31	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.46
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.46
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.46
9:I:123:CYS:SG	55:I:303:SF4:S4	3.13	0.46
58:I:301:3PE:H362	58:I:301:3PE:H331	1.75	0.46
11:K:57:MET:O	11:K:58:PRO:C	2.58	0.46
12:L:390:TYR:CE2	35:j:68:TRP:CH2	3.05	0.46
13:M:122:PHE:CZ	13:M:206:LYS:CD	2.95	0.46
15:O:140:LEU:HD11	15:O:198:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:261:LYS:HB2	16:P:263:PHE:CE1	2.51	0.46
19:S:65:LEU:HD23	19:S:65:LEU:O	2.16	0.46
23:X:168:PHE:O	23:X:169:PHE:CG	2.69	0.46
24:Y:143:VAL:HG21	33:h:169:TYR:CZ	2.51	0.46
28:c:55:TRP:HE1	29:d:66:THR:CG2	2.28	0.46
29:d:54:MET:HE2	29:d:54:MET:HB3	1.89	0.46
36:k:69:PHE:CZ	36:k:73:ILE:HG13	2.51	0.46
37:l:35:ASP:O	37:l:54:LYS:HD3	2.15	0.46
37:l:38:PRO:CG	38:m:71:ALA:HB2	2.43	0.46
38:m:9:ALA:O	38:m:10:PRO:C	2.56	0.46
45:AA:287:VAL:HB	45:AA:358:PHE:CZ	2.50	0.46
47:AC:150:LEU:CD1	47:AC:164:ILE:HD12	2.46	0.46
48:AD:237:PHE:CD1	48:AD:238:PRO:HD2	2.51	0.46
49:AE:167:PHE:HB2	49:AE:174:LEU:HD23	1.98	0.46
49:AE:168:LYS:O	49:AE:168:LYS:HG2	2.16	0.46
49:AE:200:HIS:H	49:AE:204:ARG:HH22	1.64	0.46
45:Aa:280:ASP:HB2	51:Ag:10:ARG:HG3	1.98	0.46
46:Ab:429:LYS:O	46:Ab:432:VAL:HG12	2.16	0.46
48:Ad:114:PHE:O	48:Ad:115:GLN:C	2.58	0.46
48:Ad:159:ASN:HD22	48:Ad:162:GLY:HA3	1.81	0.46
50:Af:92:GLU:N	50:Af:93:PRO:HD2	2.30	0.46
52:Ah:34:HIS:HA	52:Ah:37:GLN:CD	2.41	0.46
4:D:55:SER:HB3	4:D:58:THR:CB	2.46	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.45
7:G:611:THR:HG21	17:Q:105:GLU:CA	2.30	0.45
9:I:90:LYS:HG2	42:q:90:LEU:HD21	1.97	0.45
10:J:74:ALA:O	10:J:75:THR:HG22	2.16	0.45
12:L:12:PHE:O	12:L:16:LEU:HG	2.15	0.45
12:L:74:MET:HE3	12:L:74:MET:HB2	1.76	0.45
12:L:339:LEU:HD11	12:L:376:GLY:HA3	1.99	0.45
12:L:550:LEU:O	12:L:554:ASP:HB3	2.16	0.45
13:M:56:PHE:CE1	13:M:108:MET:HG2	2.47	0.45
13:M:61:LEU:C	13:M:64:PRO:HD2	2.41	0.45
13:M:116:ILE:HD12	13:M:119:TYR:HB3	1.98	0.45
14:N:241:LEU:O	14:N:244:ILE:HG22	2.15	0.45
14:N:277:ILE:HG22	14:N:278:MET:H	1.79	0.45
15:O:40:LEU:O	15:O:44:ILE:HG13	2.16	0.45
15:O:126:GLY:CA	32:g:51:MET:HE1	2.45	0.45
15:O:344:ASN:OD1	15:O:346:GLU:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:28:LEU:O	27:b:32:MET:HG2	2.15	0.45
27:b:38:TYR:O	27:b:39:THR:C	2.59	0.45
28:c:35:VAL:HG23	28:c:36:ASN:OD1	2.16	0.45
28:c:57:TYR:CD2	29:d:70:PHE:HZ	2.34	0.45
54:AK:33:VAL:HG13	54:AK:41:ILE:O	2.16	0.45
46:Ab:177:LEU:HD21	46:Ab:272:VAL:CG1	2.46	0.45
49:Ae:130:LYS:HD3	53:Aj:33:GLU:OE1	2.16	0.45
49:Ae:152:ILE:HG13	49:Ae:154:ILE:CD1	2.41	0.45
49:Ae:205:VAL:HG12	49:Ae:211:VAL:HG23	1.98	0.45
49:Ae:214:ILE:HB	49:Ae:259:GLU:HB3	1.97	0.45
49:Ae:244:ASP:HB3	49:Ae:250:ARG:HH11	1.80	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
7:G:176:CYS:SG	55:G:802:SF4:S1	3.14	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
9:I:60:ILE:HG23	58:I:301:3PE:O14	2.16	0.45
10:J:12:PHE:HE2	11:K:42:ILE:HD11	1.77	0.45
11:K:51:SER:HA	30:e:32:ARG:CD	2.46	0.45
12:L:60:GLU:HG2	12:L:83:ASP:HA	1.98	0.45
12:L:277:MET:HG3	12:L:318:GLY:CA	2.46	0.45
12:L:475:THR:O	12:L:476:SER:HB2	2.16	0.45
12:L:550:LEU:HD11	13:M:279:GLN:NE2	2.31	0.45
13:M:186:LEU:HD22	13:M:250:LEU:HA	1.98	0.45
13:M:282:LEU:HD11	13:M:410:MET:HE3	1.96	0.45
13:M:309:PHE:O	13:M:312:ALA:HB3	2.16	0.45
13:M:393:ILE:O	13:M:397:GLY:N	2.49	0.45
14:N:300:THR:CG2	14:N:301:SER:N	2.79	0.45
15:O:204:VAL:O	15:O:205:ILE:C	2.59	0.45
16:P:66:GLY:O	16:P:69:VAL:N	2.48	0.45
16:P:285:HIS:CE1	16:P:364:SER:HB3	2.51	0.45
20:T:119:ILE:CD1	20:T:138:LEU:HD11	2.43	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
24:Y:39:SER:HB2	24:Y:58:VAL:HA	1.98	0.45
30:e:89:GLU:HB3	30:e:91:LYS:HE2	1.98	0.45
36:k:38:VAL:CG1	39:n:39:TYR:HB2	2.46	0.45
37:l:166:LEU:HD12	37:l:170:ARG:HH22	1.81	0.45
58:m:201:3PE:H252	58:m:201:3PE:H3C1	1.97	0.45
40:o:5:LEU:H	40:o:5:LEU:HD12	1.81	0.45
41:p:24:THR:HG22	41:p:26:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:144:ALA:HA	49:AE:147:LEU:HD12	1.98	0.45
45:Aa:270:PHE:HE2	45:Aa:353:LEU:HD23	1.81	0.45
46:Ab:267:VAL:HA	46:Ab:441:SER:O	2.17	0.45
49:Ae:217:CYS:C	49:Ae:219:HIS:N	2.72	0.45
49:Ae:234:TYR:HB3	49:Ae:243:TYR:CZ	2.50	0.45
50:Af:33:MET:O	50:Af:34:ARG:C	2.58	0.45
54:Ak:9:ARG:O	54:Ak:13:LEU:HG	2.17	0.45
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
4:D:43:TRP:CZ2	13:M:143:LEU:CD1	2.98	0.45
4:D:92:HIS:O	4:D:458:PHE:CE2	2.70	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.99	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
10:J:44:LEU:CD2	10:J:49:SER:HA	2.47	0.45
10:J:84:SER:O	10:J:88:ILE:HG12	2.16	0.45
12:L:135:ASN:O	12:L:198:LEU:HD13	2.16	0.45
12:L:195:SER:O	12:L:201:ILE:HD11	2.16	0.45
12:L:204:SER:HA	12:L:207:ASN:ND2	2.31	0.45
12:L:366:MET:SD	12:L:443:ILE:HG21	2.57	0.45
13:M:22:LYS:HG2	13:M:22:LYS:O	2.17	0.45
13:M:458:THR:HG21	41:p:148:ALA:HB1	1.93	0.45
14:N:133:TRP:CE3	14:N:136:ILE:HD12	2.51	0.45
14:N:308:ASN:ND2	15:O:310:ILE:O	2.49	0.45
15:O:306:ASN:O	15:O:309:THR:HG22	2.16	0.45
16:P:315:THR:HB	16:P:318:LYS:HB2	1.98	0.45
21:V:56:LEU:HD11	21:V:57:ASP:OD1	2.17	0.45
22:W:83:ASP:O	22:W:87:ILE:HG12	2.17	0.45
23:X:147:ARG:HD2	30:e:43:CYS:HA	1.98	0.45
24:Y:75:THR:HB	24:Y:95:GLY:HA2	1.98	0.45
30:e:19:MET:HE2	30:e:19:MET:HB3	1.85	0.45
41:p:107:GLN:O	41:p:111:LYS:HG3	2.15	0.45
41:p:173:GLU:O	41:p:174:ALA:C	2.59	0.45
45:AA:52:ILE:HG12	45:AA:53:LEU:H	1.81	0.45
45:AA:74:TRP:HB3	45:AA:418:LEU:CD1	2.46	0.45
45:AA:140:LEU:O	45:AA:141:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:387:GLU:HB2	45:AA:390:ARG:NH2	2.30	0.45
49:AE:93:ARG:O	49:AE:94:ALA:C	2.59	0.45
45:Aa:286:HIS:ND1	45:Aa:359:VAL:HG22	2.31	0.45
46:Ab:267:VAL:HG13	46:Ab:444:LEU:CD2	2.46	0.45
46:Ab:319:GLN:HB3	46:Ab:320:PRO:HD2	1.97	0.45
47:Ac:59:THR:HG23	47:Ac:172:LYS:HA	1.98	0.45
47:Ac:379:LEU:HG	50:Af:34:ARG:HD2	1.97	0.45
48:Ad:109:SER:O	48:Ad:110:ILE:C	2.58	0.45
49:Ae:172:LYS:HA	49:Ae:172:LYS:HE2	1.97	0.45
3:C:85:ILE:CD1	3:C:140:ILE:HD11	2.47	0.45
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.98	0.45
4:D:36:GLN:OE1	13:M:136:TRP:HA	2.17	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
11:K:29:THR:O	11:K:32:CYS:N	2.49	0.45
12:L:241:THR:N	12:L:242:PRO:HD2	2.31	0.45
12:L:444:ASN:ND2	35:j:39:HIS:HB2	2.32	0.45
58:L:703:3PE:H112	58:L:703:3PE:H11	1.99	0.45
13:M:42:LEU:HD21	13:M:67:ILE:HD12	1.97	0.45
13:M:65:LEU:O	13:M:66:ILE:C	2.59	0.45
13:M:131:ILE:HD12	58:M:503:3PE:H362	1.97	0.45
14:N:26:LEU:HG	14:N:85:MET:SD	2.56	0.45
15:O:265:ASP:O	15:O:266:PRO:C	2.58	0.45
15:O:342:GLY:O	15:O:355:LYS:NZ	2.50	0.45
16:P:218:ALA:HB2	16:P:280:ILE:CG2	2.47	0.45
17:Q:77:VAL:HG21	17:Q:99:MET:HE3	1.97	0.45
62:h:201:CDL:H162	62:h:201:CDL:H191	1.75	0.45
34:i:123:PHE:CD1	40:o:65:ARG:NH2	2.85	0.45
36:k:26:ARG:O	36:k:27:GLN:C	2.57	0.45
45:AA:92:PHE:HZ	45:AA:161:ILE:HG23	1.81	0.45
45:AA:174:GLU:C	45:AA:176:ASP:N	2.73	0.45
45:AA:274:GLU:OE2	45:AA:276:ARG:NH1	2.45	0.45
48:AD:294:LEU:HB2	53:AJ:36:PHE:CZ	2.51	0.45
49:Ae:167:PHE:CD2	49:Ae:174:LEU:HD23	2.51	0.45
49:Ae:180:THR:OG1	49:Ae:183:GLU:HG3	2.17	0.45
49:Ae:217:CYS:SG	49:Ae:239:HIS:ND1	2.89	0.45
49:Ae:224:PRO:HA	49:Ae:236:CYS:HA	1.98	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:355:LYS:NZ	7:G:528:LEU:O	2.47	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
9:I:92:PRO:HB3	42:q:92:CYS:HB2	1.98	0.45
9:I:188:GLU:OE1	18:R:56:ASN:HB2	2.16	0.45
10:J:33:ILE:HA	10:J:64:LEU:HD23	1.99	0.45
10:J:169:ILE:HG23	14:N:45:ILE:HD11	1.98	0.45
12:L:47:SER:O	12:L:50:PRO:HD2	2.16	0.45
12:L:532:ILE:HG23	12:L:533:ILE:N	2.31	0.45
13:M:42:LEU:HD11	13:M:67:ILE:HD12	1.99	0.45
13:M:207:MET:O	13:M:208:PRO:C	2.59	0.45
13:M:453:LEU:CD1	13:M:454:ILE:CG2	2.84	0.45
14:N:3:PRO:HG2	15:O:289:TRP:CH2	2.52	0.45
14:N:215:MET:SD	14:N:244:ILE:HD11	2.56	0.45
16:P:170:LEU:HD12	16:P:171:ASN:H	1.81	0.45
16:P:220:TYR:HA	16:P:223:PHE:CD2	2.50	0.45
20:T:87:LEU:CD2	20:T:104:PHE:CE1	2.94	0.45
20:T:117:GLU:HA	20:T:120:MET:CE	2.41	0.45
20:U:90:TYR:HD1	36:k:51:TRP:CE2	2.34	0.45
24:Y:83:ARG:NH1	24:Y:90:LEU:HD23	2.31	0.45
25:Z:69:ILE:CG2	27:b:54:PRO:CD	2.94	0.45
29:d:11:LEU:HD12	29:d:11:LEU:HA	1.69	0.45
40:o:63:LEU:O	40:o:64:ILE:C	2.59	0.45
47:AC:138:MET:HE1	47:AC:268:ILE:CD1	2.47	0.45
48:AD:116:VAL:HA	48:AD:253:LEU:HD21	1.99	0.45
48:AD:167:ARG:NH1	48:AD:170:LYS:HG3	2.28	0.45
49:AE:271:VAL:O	49:AE:271:VAL:HG13	2.17	0.45
52:AH:45:ARG:HG2	52:AH:49:GLU:HG2	1.98	0.45
45:Aa:186:TYR:HB3	45:Aa:275:ILE:CG2	2.47	0.45
47:Ac:170:VAL:HG13	47:Ac:170:VAL:O	2.16	0.45
47:Ac:246:PHE:HB3	47:Ac:249:MET:HE3	1.99	0.45
49:Ae:212:ILE:HG22	49:Ae:261:PRO:HG3	1.99	0.45
50:Af:86:GLU:O	50:Af:87:ASP:C	2.59	0.45
53:Aj:17:ARG:HH12	54:Ak:19:PRO:HB2	1.81	0.45
53:Aj:34:ARG:HG3	53:Aj:35:ALA:H	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.51	0.45
2:B:126:ARG:C	2:B:128:ALA:H	2.24	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:382:ARG:HD2	19:S:56:ARG:HD3	1.99	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
58:J:401:3PE:H262	58:J:401:3PE:H352	1.98	0.45
12:L:210:LEU:HD23	12:L:210:LEU:C	2.41	0.45
12:L:247:LEU:HD12	12:L:247:LEU:C	2.41	0.45
12:L:310:LEU:HA	12:L:313:MET:HB2	1.99	0.45
12:L:385:PHE:HE2	35:j:73:PHE:HD1	1.64	0.45
12:L:591:PHE:N	12:L:591:PHE:CD1	2.83	0.45
12:L:591:PHE:N	12:L:591:PHE:HD1	2.15	0.45
13:M:162:ILE:HD13	14:N:280:THR:HG23	1.97	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
16:P:318:LYS:HA	16:P:321:ARG:NH1	2.32	0.45
19:S:74:GLU:OE1	19:S:74:GLU:N	2.49	0.45
20:U:113:LEU:HD23	39:n:17:LEU:HD23	1.97	0.45
24:Y:83:ARG:O	24:Y:85:LYS:HG2	2.17	0.45
28:c:57:TYR:CD2	29:d:70:PHE:CZ	3.04	0.45
30:e:18:PHE:O	30:e:18:PHE:CD2	2.69	0.45
30:e:41:ILE:CD1	33:h:174:PRO:HB2	2.46	0.45
32:g:67:LYS:O	32:g:68:ASN:C	2.60	0.45
33:h:144:SER:HB2	41:p:82:VAL:HG21	1.98	0.45
39:n:101:GLU:HG2	39:n:122:ARG:HH12	1.81	0.45
45:AA:286:HIS:CG	45:AA:359:VAL:HG22	2.51	0.45
46:AB:326:PHE:CE1	49:AI:15:LEU:HD21	2.52	0.45
47:AC:346:PRO:HG3	51:AG:66:GLU:HG2	1.99	0.45
48:AD:229:GLU:C	48:AD:231:LEU:N	2.75	0.45
49:AE:214:ILE:HG21	49:AE:216:VAL:HG22	1.99	0.45
51:AG:12:ARG:HB3	51:AG:13:HIS:CD2	2.52	0.45
45:Aa:190:THR:O	45:Aa:273:SER:OG	2.34	0.45
62:Ac:406:CDL:HA22	50:Af:73:HIS:CE1	2.52	0.45
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CG	2.52	0.45
49:Ae:168:LYS:HA	49:Ae:173:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:188:ALA:HA	49:Ae:200:HIS:HE1	1.81	0.45
50:Af:77:PRO:HD2	50:Af:80:GLN:NE2	2.31	0.45
54:Ak:15:ARG:NH1	54:Ak:15:ARG:HB2	2.32	0.45
1:A:108:GLN:HE21	10:J:167:ILE:CG2	2.29	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.74	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:163:LYS:HE2	18:R:97:LYS:NZ	2.31	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:CD1	2.47	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
10:J:78:TYR:O	10:J:79:PRO:C	2.60	0.45
12:L:387:THR:HA	12:L:465:GLY:HA3	1.98	0.45
58:L:701:3PE:H362	58:L:701:3PE:H331	1.45	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:155:LEU:O	14:N:159:ILE:HG22	2.16	0.45
15:O:112:CYS:HB3	15:O:131:LEU:HA	1.97	0.45
19:S:42:VAL:HB	19:S:46:LYS:HE3	1.98	0.45
20:T:83:VAL:HG21	20:T:145:VAL:HG22	1.99	0.45
23:X:53:PRO:HG2	25:Z:116:TRP:NE1	2.32	0.45
29:d:13:PHE:CE2	29:d:14:LEU:HD23	2.52	0.45
32:g:121:GLU:OE2	41:p:10:TYR:CE2	2.69	0.45
36:k:57:TRP:O	36:k:58:ARG:C	2.59	0.45
37:l:57:MET:HE2	37:l:57:MET:HB3	1.75	0.45
39:n:45:ARG:O	39:n:49:GLU:N	2.37	0.45
40:o:27:PRO:O	40:o:34:ARG:NH1	2.42	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
42:q:21:ARG:O	42:q:25:ARG:HG3	2.17	0.45
46:AB:426:LYS:HA	46:AB:429:LYS:HZ3	1.80	0.45
47:AC:341:GLN:HE21	47:AC:342:PRO:HD2	1.82	0.45
48:AD:186:ARG:HE	48:AD:193:LEU:HB2	1.80	0.45
48:AD:227:LEU:CB	48:AD:231:LEU:HB2	2.47	0.45
48:AD:232:TYR:CE1	48:AD:245:ALA:HA	2.51	0.45
49:AE:195:LEU:HG	49:AE:197:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:241:SER:OG	49:AE:254:ALA:HB2	2.16	0.45
49:AE:262:ALA:C	49:AE:273:VAL:HG13	2.42	0.45
52:AH:65:CYS:HA	52:AH:68:GLU:OE1	2.17	0.45
49:AI:76:VAL:CG1	46:Ab:165:ALA:HA	2.46	0.45
45:Aa:168:ILE:HA	45:Aa:171:GLU:HG2	1.98	0.45
45:Aa:169:LEU:HD11	45:Aa:209:ARG:HG2	1.97	0.45
49:Ae:175:PHE:HZ	49:Ae:223:VAL:HG13	1.81	0.45
49:Ae:187:GLU:OE2	49:Ae:244:ASP:HB2	2.16	0.45
50:Af:83:LYS:O	50:Af:84:TYR:C	2.59	0.45
3:C:123:ASN:ND2	21:V:108:PRO:HG2	2.32	0.45
4:D:91:ALA:O	4:D:92:HIS:C	2.58	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
9:I:93:LEU:O	42:q:93:MET:CG	2.65	0.45
12:L:246:LEU:C	12:L:246:LEU:CD1	2.90	0.45
58:L:702:3PE:H122	24:Y:46:ASN:HD22	1.81	0.45
62:L:704:CDL:H161	62:L:704:CDL:C11	2.46	0.45
13:M:3:LYS:HA	13:M:7:PRO:HD2	1.99	0.45
13:M:87:ASP:HB3	13:M:91:LEU:HB2	1.99	0.45
13:M:452:LYS:NZ	58:M:502:3PE:O14	2.49	0.45
14:N:293:TYR:O	14:N:297:ILE:HG12	2.17	0.45
17:Q:65:THR:HG23	17:Q:67:VAL:HG23	1.99	0.45
20:T:90:TYR:O	20:T:91:ASP:HB2	2.17	0.45
20:T:130:ILE:CG2	20:T:131:PRO:CD	2.95	0.45
21:V:8:THR:CG2	21:V:9:THR:N	2.79	0.45
22:W:71:MET:C	22:W:73:ASN:N	2.70	0.45
23:X:7:LEU:HD13	25:Z:87:LEU:HB3	1.98	0.45
23:X:165:THR:N	23:X:172:VAL:HG11	2.32	0.45
25:Z:66:GLU:HA	25:Z:69:ILE:CG1	2.46	0.45
28:c:32:ARG:O	28:c:33:GLU:C	2.58	0.45
35:j:71:TRP:CH2	58:j:700:3PE:H392	2.51	0.45
39:n:98:LYS:HD3	39:n:176:GLU:O	2.17	0.45
39:n:146:PRO:O	39:n:147:ASP:C	2.60	0.45
45:AA:294:PRO:HB2	45:AA:298:ASN:HB3	1.98	0.45
46:AB:225:VAL:HG22	46:AB:229:VAL:CG2	2.46	0.45
47:AC:107:TYR:HE1	47:AC:308:HIS:HB2	1.82	0.45
49:AE:169:TRP:NE1	49:AE:170:ARG:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:177:ARG:HH21	49:AE:183:GLU:CD	2.25	0.45
47:Ac:51:LEU:CD1	47:Ac:69:ILE:HD13	2.47	0.45
47:Ac:245:PHE:CZ	48:Ad:289:GLY:C	2.95	0.45
49:Ae:160:PRO:C	49:Ae:178:HIS:HB3	2.42	0.45
49:Ae:167:PHE:HE2	49:Ae:176:VAL:HG23	1.78	0.45
49:Ae:184:ILE:HD13	49:Ae:208:PRO:HB2	1.98	0.45
49:Ae:217:CYS:SG	49:Ae:239:HIS:CG	3.10	0.45
50:Af:92:GLU:O	50:Af:96:LYS:HG3	2.17	0.45
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.52	0.45
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.51	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	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
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.45
12:L:483:PRO:CG	12:L:486:LEU:HD12	2.47	0.45
12:L:527:GLY:O	12:L:528:PHE:HB2	2.17	0.45
62:L:704:CDL:H202	62:L:704:CDL:H511	1.99	0.45
13:M:42:LEU:CG	13:M:67:ILE:HD11	2.43	0.45
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.81	0.45
13:M:388:TRP:NE1	38:m:109:ARG:CD	2.79	0.45
14:N:153:ILE:O	14:N:154:ILE:C	2.58	0.45
16:P:209:ARG:CA	16:P:352:VAL:HG22	2.47	0.45
18:R:97:LYS:CE	18:R:100:LYS:HD3	2.45	0.45
19:S:37:ILE:HD12	19:S:55:ILE:HD12	1.98	0.45
20:T:133:ILE:HG23	20:T:134:ASP:N	2.32	0.45
23:X:166:ARG:HH22	29:d:87:ASP:CG	2.25	0.45
28:c:65:ASP:O	28:c:66:VAL:C	2.56	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
37:l:91:GLN:HG2	39:n:2:ALA:O	2.16	0.45
45:AA:463:GLU:OE1	51:AG:8:LEU:HB2	2.17	0.45
48:AD:154:VAL:N	48:AD:167:ARG:O	2.44	0.45
50:AF:85:GLU:H	50:AF:85:GLU:CD	2.24	0.45
54:AK:33:VAL:HG11	54:AK:42:LEU:HB2	1.98	0.45
45:Aa:278:ARG:NH2	51:Ag:9:ALA:O	2.50	0.45
46:Ab:418:SER:O	46:Ab:419:VAL:C	2.59	0.45
47:Ac:341:GLN:HE21	47:Ac:342:PRO:HD2	1.82	0.45
52:Ah:38:LEU:O	52:Ah:42:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.45
3:C:73:GLN:NE2	21:V:107:PRO:HB3	2.31	0.45
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.98	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
8:H:25:ARG:NH1	61:H:400:UQ9:H10A	2.32	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
12:L:81:LYS:CA	12:L:135:ASN:HD21	2.29	0.45
12:L:226:GLN:HG3	12:L:314:MET:HE2	1.98	0.45
12:L:407:TRP:HE1	37:l:140:MET:HE3	1.82	0.45
12:L:437:PHE:CZ	12:L:441:ILE:HG12	2.43	0.45
13:M:42:LEU:CG	13:M:67:ILE:CD1	2.95	0.45
13:M:129:THR:CG2	13:M:235:LEU:CD1	2.95	0.45
13:M:187:ASP:H	13:M:192:ASN:ND2	2.15	0.45
13:M:249:ILE:O	13:M:250:LEU:CG	2.47	0.45
14:N:109:ALA:HB3	14:N:110:PRO:CD	2.46	0.45
14:N:154:ILE:CD1	14:N:195:PRO:HG2	2.47	0.45
14:N:217:MET:HA	14:N:220:MET:SD	2.57	0.45
14:N:220:MET:O	14:N:221:LEU:C	2.60	0.45
15:O:129:TYR:CD2	15:O:183:CYS:HB3	2.52	0.45
16:P:192:ARG:HH12	16:P:198:ALA:HB3	1.80	0.45
17:Q:77:VAL:CG1	17:Q:101:PHE:CD2	3.00	0.45
17:Q:99:MET:HG2	17:Q:128:PHE:HE2	1.82	0.45
20:U:114:ASP:OD1	39:n:45:ARG:NH2	2.50	0.45
20:U:116:VAL:HG12	20:U:120:MET:HE2	1.98	0.45
28:c:72:ARG:HH11	29:d:19:ARG:HD3	1.82	0.45
32:g:64:VAL:HG11	32:g:71:PHE:CE1	2.52	0.45
34:i:106:PRO:HD2	40:o:64:ILE:CG2	2.46	0.45
39:n:145:SER:O	39:n:146:PRO:C	2.58	0.45
45:AA:139:ASP:O	45:AA:140:LEU:C	2.59	0.45
45:AA:246:ALA:O	45:AA:249:HIS:O	2.34	0.45
68:AC:404:U10:H122	68:AC:404:U10:H101	1.58	0.45
48:AD:211:VAL:O	48:AD:215:LEU:HG	2.16	0.45
48:AD:232:TYR:O	48:AD:233:PHE:C	2.58	0.45
50:AF:86:GLU:O	50:AF:87:ASP:C	2.60	0.45
45:Aa:399:LEU:O	45:Aa:400:VAL:C	2.60	0.45
47:Ac:141:TRP:CD1	47:Ac:265:PRO:CD	2.97	0.45
47:Ac:218:ILE:HD11	47:Ac:224:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:153:GLU:OE2	48:Ad:166:MET:HB3	2.16	0.45
48:Ad:259:THR:O	48:Ad:260:PRO:C	2.60	0.45
49:Ae:156:LEU:HB2	49:Ae:269:ASP:HA	1.99	0.45
1:A:109:LYS:HA	1:A:112:GLU:CD	2.42	0.44
2:B:124:SER:HB3	2:B:125:PRO:HD2	2.00	0.44
3:C:98:PHE:HB2	21:V:94:MET:CE	2.47	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	0.44
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.31	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:16:ALA:HB2	26:a:15:CYS:HB2	1.99	0.44
8:H:295:PRO:HB3	58:b:201:3PE:H382	1.98	0.44
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.44
11:K:66:PHE:HE2	14:N:35:PHE:CE2	2.35	0.44
11:K:93:LEU:CD1	14:N:57:THR:HG21	2.47	0.44
12:L:100:ILE:O	12:L:104:SER:N	2.42	0.44
12:L:371:SER:HB2	35:j:62:SER:OG	2.17	0.44
12:L:375:ILE:HG12	35:j:65:MET:SD	2.57	0.44
13:M:73:LEU:HB3	13:M:103:GLN:OE1	2.16	0.44
14:N:163:PHE:CZ	14:N:285:MET:HG3	2.52	0.44
14:N:214:PRO:HB2	14:N:247:MET:SD	2.56	0.44
14:N:250:SER:O	14:N:259:GLY:HA3	2.17	0.44
15:O:250:SER:HA	15:O:255:VAL:CG2	2.41	0.44
16:P:55:VAL:HA	16:P:79:GLN:O	2.18	0.44
16:P:245:VAL:HA	16:P:265:PHE:HD2	1.82	0.44
18:R:39:ASP:H	18:R:42:ASP:CG	2.21	0.44
19:S:20:ARG:HG3	19:S:54:LEU:CB	2.43	0.44
20:T:82:ARG:NH2	20:T:126:PHE:HD1	2.15	0.44
22:W:45:GLU:O	22:W:46:VAL:C	2.58	0.44
22:W:71:MET:O	22:W:72:LYS:C	2.59	0.44
23:X:115:LEU:HB3	23:X:117:TRP:CE2	2.52	0.44
24:Y:20:CYS:O	24:Y:21:HIS:C	2.60	0.44
24:Y:21:HIS:CE1	51:Ag:62:TRP:CB	2.81	0.44
25:Z:68:ARG:O	25:Z:69:ILE:C	2.60	0.44
25:Z:98:MET:HB2	25:Z:104:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:110:VAL:HG11	30:e:72:THR:HG23	1.97	0.44
28:c:73:ASN:OD1	28:c:75:LEU:N	2.50	0.44
31:f:38:ARG:HD3	31:f:56:TRP:NE1	2.32	0.44
33:h:55:PHE:C	33:h:55:PHE:CD1	2.94	0.44
33:h:56:VAL:O	33:h:58:LYS:HG3	2.16	0.44
62:h:201:CDL:HB61	34:i:84:TYR:CE2	2.51	0.44
40:o:110:GLN:O	40:o:111:ARG:C	2.59	0.44
41:p:6:ASP:HB3	41:p:9:VAL:CG2	2.39	0.44
45:AA:43:GLN:O	45:AA:44:SER:C	2.60	0.44
45:AA:92:PHE:HE1	45:AA:165:ARG:N	2.14	0.44
46:AB:39:GLU:O	46:AB:227:HIS:HE1	2.01	0.44
46:AB:214:THR:OG1	46:AB:243:GLY:O	2.34	0.44
46:AB:418:SER:O	46:AB:419:VAL:C	2.59	0.44
48:AD:222:PRO:O	48:AD:223:THR:C	2.59	0.44
48:Ad:179:TYR:O	48:Ad:180:PRO:C	2.60	0.44
49:Ae:204:ARG:NH1	49:Ae:257:ASN:HB2	2.32	0.44
53:Aj:34:ARG:CG	53:Aj:35:ALA:H	2.30	0.44
2:B:80:ASP:O	2:B:81:LEU:C	2.59	0.44
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.44
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.44
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.44
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.44
11:K:61:ILE:O	11:K:62:THR:C	2.58	0.44
12:L:231:PRO:C	12:L:234:PRO:HD2	2.41	0.44
12:L:366:MET:SD	12:L:443:ILE:CG2	3.05	0.44
62:L:705:CDL:H591	24:Y:68:ILE:CD1	2.45	0.44
15:O:69:GLY:HA2	15:O:72:LYS:NZ	2.32	0.44
15:O:169:PHE:CD2	63:O:402:ADP:N6	2.85	0.44
15:O:351:TRP:O	15:O:355:LYS:HG2	2.16	0.44
16:P:298:TYR:O	16:P:299:SER:C	2.60	0.44
19:S:62:GLN:HB2	19:S:80:ASN:CG	2.42	0.44
23:X:9:THR:O	23:X:12:GLU:HB3	2.17	0.44
23:X:46:CYS:SG	23:X:135:ARG:NH1	2.90	0.44
29:d:78:ARG:O	29:d:79:GLN:C	2.59	0.44
30:e:92:TYR:OH	30:e:94:PRO:HA	2.16	0.44
38:m:49:LEU:HD12	38:m:49:LEU:HA	1.82	0.44
39:n:136:GLU:OE2	39:n:167:TRP:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:52:LEU:O	44:s:56:ARG:HG2	2.17	0.44
45:AA:162:GLU:HA	45:AA:165:ARG:NH1	2.32	0.44
47:AC:51:LEU:HG	67:AC:401:HEM:O2A	2.18	0.44
47:AC:163:TRP:HE1	49:Ae:140:MET:HE3	1.82	0.44
48:AD:124:CYS:HG	48:AD:179:TYR:HH	1.64	0.44
48:AD:154:VAL:HG21	48:AD:173:ASP:CG	2.42	0.44
48:AD:213:SER:O	48:AD:217:GLY:N	2.50	0.44
49:AE:154:ILE:HG23	49:AE:167:PHE:CZ	2.51	0.44
49:AE:168:LYS:HA	49:AE:174:LEU:H	1.82	0.44
49:AE:179:ARG:NH1	49:AE:187:GLU:HG2	2.32	0.44
45:Aa:78:GLY:H	45:Aa:81:TYR:HD2	1.65	0.44
48:Ad:195:PRO:HG2	70:Ad:401:HEC:HAA2	1.98	0.44
51:Ag:12:ARG:HB3	51:Ag:13:HIS:CD2	2.52	0.44
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.44
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.81	0.44
4:D:55:SER:OG	4:D:56:LYS:N	2.49	0.44
4:D:78:THR:O	4:D:79:ASN:C	2.59	0.44
4:D:100:GLU:C	4:D:101:LEU:HD12	2.41	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	0.44
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
6:F:427:LEU:HB2	60:F:501:FMN:HM73	2.00	0.44
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
10:J:43:VAL:HG13	11:K:49:LEU:HD11	2.00	0.44
11:K:1:MET:N	11:K:2:PRO:CD	2.81	0.44
12:L:485:PHE:CE1	12:L:486:LEU:HG	2.52	0.44
58:L:702:3PE:H122	24:Y:46:ASN:ND2	2.32	0.44
13:M:24:TRP:CE3	13:M:81:GLN:HG2	2.52	0.44
13:M:415:GLN:O	13:M:416:ARG:CG	2.64	0.44
14:N:258:THR:CB	14:N:333:SER:O	2.64	0.44
15:O:336:GLY:HA2	15:O:344:ASN:HB3	1.99	0.44
20:T:79:ILE:O	20:T:83:VAL:HG23	2.17	0.44
20:T:133:ILE:O	20:T:136:GLU:N	2.46	0.44
23:X:154:ILE:CG1	33:h:167:PRO:HG2	2.47	0.44
24:Y:120:MET:HE2	24:Y:120:MET:HB3	1.90	0.44
35:j:39:HIS:ND1	35:j:39:HIS:N	2.65	0.44
38:m:125:PHE:HA	41:p:136:THR:HG21	1.99	0.44
39:n:35:ASP:OD1	39:n:35:ASP:N	2.51	0.44
39:n:97:TYR:HB2	39:n:178:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:49:ALA:O	40:o:50:GLN:C	2.60	0.44
43:r:109:ASP:O	43:r:110:GLN:CG	2.64	0.44
47:AC:138:MET:HE1	47:AC:268:ILE:HD13	1.98	0.44
47:AC:218:ILE:HD11	47:AC:224:TYR:CE2	2.52	0.44
48:AD:167:ARG:NH1	48:AD:170:LYS:HE2	2.31	0.44
48:AD:208:GLU:HG3	48:AD:209:ASP:N	2.32	0.44
48:AD:227:LEU:HD13	48:AD:231:LEU:HB3	2.00	0.44
49:AE:155:LYS:HB3	49:AE:158:ASP:OD1	2.17	0.44
49:AE:192:VAL:HG13	49:AE:193:SER:H	1.82	0.44
46:Ab:229:VAL:O	46:Ab:233:VAL:HG13	2.16	0.44
48:Ad:138:VAL:HG11	48:Ad:276:TRP:NE1	2.33	0.44
49:Ae:244:ASP:OD1	49:Ae:248:ARG:N	2.50	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
10:J:68:GLY:O	10:J:71:THR:HB	2.18	0.44
12:L:2:ASN:O	12:L:3:ILE:C	2.59	0.44
12:L:54:PHE:CB	12:L:87:ILE:HD11	2.47	0.44
12:L:73:SER:CB	41:p:100:GLN:HE21	2.27	0.44
12:L:117:PHE:CE1	12:L:243:VAL:CG2	3.00	0.44
12:L:155:ILE:HG12	12:L:248:HIS:CE1	2.53	0.44
12:L:435:PRO:O	36:k:58:ARG:HD2	2.18	0.44
12:L:537:THR:N	12:L:538:PRO:HD2	2.32	0.44
13:M:200:MET:HE2	13:M:250:LEU:HD21	2.00	0.44
13:M:424:ILE:O	13:M:424:ILE:CG2	2.65	0.44
14:N:87:GLN:O	14:N:88:GLN:C	2.59	0.44
14:N:208:TYR:O	14:N:212:THR:HG22	2.18	0.44
15:O:223:ASP:O	15:O:224:PRO:C	2.60	0.44
16:P:156:SER:HB2	16:P:161:VAL:CG2	2.47	0.44
16:P:305:PHE:CB	16:P:314:THR:HG22	2.47	0.44
17:Q:62:THR:HG22	17:Q:141:ASN:O	2.18	0.44
18:R:32:THR:HG21	42:q:129:THR:HG23	1.98	0.44
19:S:83:SER:O	19:S:87:VAL:HG23	2.17	0.44
34:i:94:PRO:HG3	41:p:10:TYR:CD2	2.50	0.44
39:n:149:ILE:HD12	39:n:149:ILE:N	2.32	0.44
46:AB:138:LEU:CD1	46:AB:233:VAL:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:170:VAL:HG13	47:AC:170:VAL:O	2.16	0.44
49:AE:113:PHE:O	49:AE:117:VAL:HG23	2.16	0.44
49:AE:180:THR:O	49:AE:184:ILE:HG13	2.18	0.44
49:AE:190:VAL:HB	49:AE:248:ARG:HH22	1.81	0.44
49:AE:234:TYR:N	49:AE:243:TYR:O	2.50	0.44
52:AH:34:HIS:HD2	52:AH:83:LYS:HD2	1.83	0.44
52:AH:51:CYS:O	52:AH:55:VAL:HG23	2.18	0.44
47:Ac:77:TRP:CD2	48:Ad:281:GLU:HG3	2.52	0.44
48:Ad:201:VAL:HG22	48:Ad:278:SER:OG	2.18	0.44
48:Ad:248:ILE:HD12	48:Ad:266:VAL:HG11	2.00	0.44
49:Ae:230:ASP:N	49:Ae:242:HIS:HB3	2.32	0.44
49:Ae:231:PHE:HB2	49:Ae:250:ARG:CB	2.47	0.44
50:Af:75:ILE:HD12	50:Af:81:TRP:HZ2	1.81	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.17	0.44
2:B:105:MET:CE	56:B:302:UQ1:C6	2.96	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.44
9:I:78:PHE:HB2	43:r:12:ARG:CG	2.48	0.44
9:I:90:LYS:HG3	42:q:90:LEU:CD2	2.48	0.44
58:I:301:3PE:C27	58:I:301:3PE:H231	2.47	0.44
10:J:133:VAL:O	10:J:134:MET:HB2	2.16	0.44
12:L:56:HIS:CA	40:o:74:PHE:CE1	3.01	0.44
57:L:706:PC1:H371	57:L:706:PC1:C2D	2.47	0.44
13:M:18:SER:OG	13:M:26:ASN:ND2	2.51	0.44
13:M:22:LYS:HG2	13:M:26:ASN:ND2	2.33	0.44
14:N:227:ILE:HG13	14:N:228:ASN:N	2.32	0.44
15:O:262:GLU:HB3	15:O:268:LYS:NZ	2.33	0.44
16:P:122:HIS:HB3	18:R:46:VAL:HG12	1.98	0.44
16:P:345:LEU:C	16:P:345:LEU:HD23	2.43	0.44
22:W:86:VAL:O	22:W:90:LYS:HG3	2.18	0.44
23:X:153:VAL:O	23:X:155:GLU:HG3	2.18	0.44
24:Y:7:PHE:CZ	24:Y:26:ILE:HG12	2.52	0.44
34:i:69:LEU:HD12	34:i:69:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:101:PRO:O	35:j:102:ASP:C	2.59	0.44
37:l:38:PRO:C	38:m:75:ASN:HD21	2.26	0.44
40:o:31:PHE:CG	40:o:34:ARG:HD2	2.53	0.44
43:r:109:ASP:OD1	43:r:110:GLN:N	2.51	0.44
45:AA:311:ILE:CG2	45:AA:341:PHE:CZ	3.01	0.44
46:AB:49:ILE:HD13	46:AB:220:LEU:HB3	1.98	0.44
48:AD:204:ARG:HA	48:AD:204:ARG:HD3	1.72	0.44
49:AE:187:GLU:HG3	49:AE:201:ASP:HB2	1.98	0.44
49:AE:272:VAL:HG12	49:AE:274:GLY:C	2.42	0.44
51:AG:29:SER:CB	51:AG:32:SER:HB2	2.38	0.44
52:AH:66:THR:HG23	52:AH:67:GLU:N	2.33	0.44
47:Ac:28:SER:HB2	62:Ac:406:CDL:OA4	2.17	0.44
48:Ad:102:LEU:CD1	48:Ad:290:LEU:HD13	2.47	0.44
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD2	2.52	0.44
52:Ah:47:ARG:NH1	52:Ah:47:ARG:HB2	2.32	0.44
52:Ah:61:THR:OG1	52:Ah:63:GLU:HG2	2.17	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:607:LYS:HG2	17:Q:78:ARG:HH11	1.82	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.44
11:K:33:LEU:HA	11:K:36:MET:HE2	2.00	0.44
12:L:66:TRP:CZ3	12:L:68:TRP:HD1	2.34	0.44
12:L:68:TRP:HE3	12:L:76:LEU:HD21	1.82	0.44
12:L:529:PHE:O	12:L:533:ILE:HG22	2.16	0.44
62:L:704:CDL:H561	62:L:704:CDL:H531	1.83	0.44
13:M:350:MET:HE2	39:n:96:CYS:HA	1.99	0.44
13:M:445:ILE:HG23	58:M:502:3PE:H292	1.99	0.44
14:N:45:ILE:O	14:N:45:ILE:CG1	2.58	0.44
14:N:338:PRO:HG2	29:d:33:TYR:CZ	2.52	0.44
58:O:401:3PE:H2A2	58:O:401:3PE:H272	1.83	0.44
17:Q:91:VAL:HG22	17:Q:91:VAL:O	2.18	0.44
22:W:95:GLU:HB3	22:W:101:LYS:HG3	2.00	0.44
30:e:74:ARG:O	30:e:75:ARG:C	2.59	0.44
31:f:25:TYR:O	31:f:29:LYS:HG2	2.17	0.44
31:f:39:ASN:CG	31:f:55:THR:HG21	2.41	0.44
46:AB:312:SER:HA	46:AB:315:LYS:HE3	1.99	0.44
47:AC:53:MET:SD	49:AE:140:MET:HG2	2.58	0.44
47:Ac:128:PHE:CE1	68:Ac:404:U10:C4M	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:165:TRP:CE3	47:Ac:169:SER:HA	2.52	0.44
1:A:18:ILE:HG12	8:H:222:LEU:CD2	2.48	0.44
2:B:93:MET:CE	2:B:95:PHE:CE2	3.00	0.44
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.99	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
10:J:74:ALA:C	10:J:75:THR:HG22	2.42	0.44
12:L:594:ASN:OD1	24:Y:41:TYR:OH	2.34	0.44
13:M:131:ILE:HD13	14:N:302:LEU:HD21	2.00	0.44
14:N:122:ILE:HD11	14:N:127:GLY:HA2	1.98	0.44
15:O:272:ASP:O	15:O:275:TYR:HB2	2.18	0.44
16:P:72:HIS:HB2	16:P:250:VAL:HG21	2.00	0.44
16:P:168:SER:O	16:P:202:ARG:HA	2.17	0.44
17:Q:77:VAL:HG21	17:Q:99:MET:CE	2.48	0.44
18:R:47:ARG:HG3	18:R:48:PHE:N	2.32	0.44
23:X:40:ASN:O	23:X:41:LYS:C	2.58	0.44
26:a:37:ARG:HB2	26:a:48:MET:HE2	1.99	0.44
28:c:55:TRP:CE2	29:d:66:THR:HG22	2.53	0.44
28:c:61:THR:HG22	28:c:65:ASP:OD2	2.18	0.44
41:p:140:GLN:HG2	41:p:144:LEU:CD1	2.47	0.44
42:q:3:LEU:O	42:q:6:VAL:CG2	2.66	0.44
45:AA:78:GLY:H	45:AA:81:TYR:HD2	1.65	0.44
46:AB:64:PHE:HZ	46:AB:394:SER:HA	1.83	0.44
46:AB:326:PHE:HZ	49:AI:15:LEU:HD21	1.83	0.44
49:AE:88:PHE:CD2	51:AG:19:LEU:CD1	3.01	0.44
49:AE:130:LYS:NZ	54:AK:34:TRP:O	2.47	0.44
51:AG:38:VAL:HA	51:AG:41:ARG:HD3	1.99	0.44
51:AG:78:TYR:CE1	52:AH:62:GLU:HB2	2.52	0.44
45:Aa:373:GLN:NE2	45:Aa:471:ILE:O	2.49	0.44
45:Aa:384:THR:OG1	45:Aa:385:GLU:N	2.51	0.44
49:Ae:184:ILE:HG23	49:Ae:208:PRO:HB3	1.99	0.44
49:Ae:244:ASP:OD2	49:Ae:248:ARG:HB2	2.18	0.44
51:Ag:38:VAL:HA	51:Ag:41:ARG:HD3	1.98	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:617:ARG:NH1	22:W:129:HIS:CA	2.80	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
13:M:42:LEU:CD1	13:M:67:ILE:CD1	2.96	0.44
13:M:126:LEU:HD11	13:M:153:THR:HG21	2.00	0.44
13:M:186:LEU:HD13	13:M:250:LEU:HA	2.00	0.44
13:M:321:LEU:HD23	13:M:321:LEU:HA	1.81	0.44
14:N:146:TYR:CD1	14:N:198:PRO:HG2	2.53	0.44
14:N:146:TYR:O	14:N:147:PRO:C	2.53	0.44
15:O:206:TYR:CD1	15:O:246:LEU:HD21	2.53	0.44
16:P:130:ILE:N	16:P:130:ILE:HD12	2.33	0.44
17:Q:101:PHE:CE1	17:Q:124:MET:HE3	2.53	0.44
19:S:23:LEU:HB3	19:S:33:VAL:HG12	2.00	0.44
20:U:88:LYS:HG3	20:U:98:LEU:HD23	1.98	0.44
22:W:20:VAL:HG21	22:W:80:ARG:CZ	2.48	0.44
25:Z:97:ILE:CG2	30:e:83:ARG:HB2	2.47	0.44
25:Z:112:HIS:HE1	30:e:61:ASP:OD2	2.01	0.44
25:Z:129:THR:HG22	25:Z:131:GLU:N	2.33	0.44
34:i:92:THR:O	41:p:5:TRP:CD1	2.71	0.44
40:o:118:LYS:HA	40:o:118:LYS:HD2	1.81	0.44
46:AB:63:LEU:HD12	46:AB:220:LEU:HD13	2.00	0.44
46:AB:180:VAL:O	46:AB:254:ARG:HG3	2.18	0.44
47:AC:72:ASP:OD1	48:AD:133:ARG:NH1	2.51	0.44
48:AD:164:MET:O	48:AD:165:PHE:C	2.60	0.44
48:AD:321:TYR:HB2	50:AF:61:PHE:CE2	2.53	0.44
49:AE:260:VAL:CG1	49:AE:263:TYR:HE2	2.30	0.44
52:AH:58:ARG:CB	52:AH:61:THR:HG22	2.43	0.44
46:Ab:173:ILE:HD11	46:Ab:439:ALA:C	2.43	0.44
48:Ad:111:ARG:O	48:Ad:115:GLN:HG3	2.17	0.44
49:Ae:83:VAL:HG22	49:Ae:84:LYS:H	1.83	0.44
49:Ae:108:GLU:OE1	53:Aj:8:SER:HB3	2.17	0.44
49:Ae:174:LEU:CD1	49:Ae:261:PRO:HG3	2.47	0.44
49:Ae:234:TYR:CG	49:Ae:243:TYR:CZ	3.05	0.44
50:Af:26:GLY:O	50:Af:27:PHE:C	2.60	0.44
54:Ak:38:TRP:HD1	54:Ak:40:LEU:HB2	1.76	0.44
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.85	0.44
3:C:70:LYS:O	21:V:103:LEU:HA	2.18	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:271:ARG:CD	8:H:279:ARG:O	2.62	0.44
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.44
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
8:H:63:PRO:HD2	8:H:66:THR:HG21	2.00	0.44
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.52	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
9:I:66:LEU:CD1	58:I:301:3PE:H271	2.48	0.44
12:L:152:PHE:HD2	12:L:153:LEU:HD12	1.83	0.44
12:L:588:PHE:O	12:L:589:MET:C	2.60	0.44
62:L:704:CDL:H1	13:M:357:THR:OG1	2.18	0.44
13:M:8:SER:O	13:M:11:LEU:HB2	2.18	0.44
13:M:158:ILE:CG2	14:N:283:ALA:HB1	2.47	0.44
13:M:277:LEU:O	37:l:116:ARG:NH2	2.44	0.44
13:M:344:MET:HE3	13:M:423:MET:CE	2.48	0.44
13:M:423:MET:C	13:M:424:ILE:O	2.56	0.44
14:N:202:LEU:HD11	30:e:3:PHE:CE1	2.53	0.44
15:O:323:GLN:HE21	32:g:55:GLU:HA	1.83	0.44
20:T:113:LEU:O	20:T:116:VAL:HB	2.17	0.44
22:W:87:ILE:O	22:W:91:MET:HG3	2.18	0.44
24:Y:12:HIS:CD2	24:Y:131:LYS:HE2	2.53	0.44
45:AA:467:ASP:OD2	47:AC:223:TYR:CE2	2.71	0.44
47:AC:220:PHE:CE2	69:AC:405:UQ6:H4M2	2.53	0.44
49:AE:152:ILE:HB	49:AE:169:TRP:CD1	2.53	0.44
49:AE:155:LYS:O	49:AE:158:ASP:HB2	2.18	0.44
51:AG:25:ARG:NH2	51:AG:29:SER:H	2.16	0.44
46:Ab:38:LEU:HA	46:Ab:51:SER:O	2.18	0.44
47:Ac:256:TYR:OH	48:Ad:202:ARG:NH1	2.50	0.44
49:Ae:231:PHE:O	49:Ae:242:HIS:O	2.36	0.44
49:Ae:243:TYR:CE1	49:Ae:258:LEU:HD22	2.52	0.44
52:Ah:27:PRO:O	52:Ah:31:VAL:HG23	2.18	0.44
52:Ah:78:HIS:O	52:Ah:81:ALA:HB3	2.18	0.44
54:Ak:12:GLU:HG3	54:Ak:15:ARG:NH1	2.33	0.44
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
4:D:338:ARG:NH1	25:Z:23:ARG:CA	2.80	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:362:ASP:HB2	19:S:71:PHE:CD1	2.52	0.43
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:78:PHE:HB2	43:r:12:ARG:HG2	2.00	0.43
10:J:40:CYS:O	10:J:44:LEU:HG	2.17	0.43
10:J:44:LEU:HD23	10:J:49:SER:HA	2.00	0.43
10:J:157:TRP:HE1	14:N:11:PHE:HD2	1.65	0.43
10:J:164:PHE:HB3	14:N:5:THR:HG23	1.99	0.43
58:J:401:3PE:H322	58:J:401:3PE:H32	1.85	0.43
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.43
13:M:158:ILE:HG21	14:N:283:ALA:CB	2.48	0.43
58:M:503:3PE:H2I2	62:d:201:CDL:H602	2.00	0.43
14:N:31:VAL:C	14:N:35:PHE:CD2	2.91	0.43
14:N:120:GLN:HE22	14:N:174:GLN:HB3	1.83	0.43
16:P:126:VAL:HG23	16:P:161:VAL:HG11	2.00	0.43
17:Q:59:LEU:O	17:Q:140:LYS:HA	2.18	0.43
24:Y:7:PHE:O	24:Y:8:PHE:C	2.61	0.43
29:d:57:GLY:O	29:d:60:ARG:N	2.51	0.43
29:d:72:GLY:O	29:d:73:TYR:C	2.60	0.43
30:e:92:TYR:CG	30:e:93:THR:N	2.86	0.43
41:p:165:GLU:C	41:p:167:ARG:H	2.26	0.43
43:r:110:GLN:HA	43:r:111:PRO:HD2	1.85	0.43
45:AA:183:VAL:HG21	45:AA:286:HIS:CB	2.48	0.43
45:AA:389:THR:O	45:AA:390:ARG:C	2.59	0.43
46:AB:324:SER:OG	49:AI:11:PHE:HZ	1.99	0.43
46:AB:411:THR:O	46:AB:414:GLN:HG2	2.18	0.43
49:AE:111:LYS:HE2	53:AJ:11:TYR:CZ	2.53	0.43
46:Ab:236:GLN:HG3	46:Ab:237:PHE:CD2	2.53	0.43
48:Ad:112:ARG:HB3	48:Ad:255:TYR:CE1	2.53	0.43
48:Ad:167:ARG:HD2	48:Ad:167:ARG:O	2.18	0.43
49:Ae:156:LEU:HD12	49:Ae:268:ASP:C	2.43	0.43
51:Ag:19:LEU:HG	51:Ag:20:SER:N	2.33	0.43
51:Ag:27:PHE:HB3	51:Ag:30:TYR:HB2	2.00	0.43
1:A:56:PHE:CD1	10:J:70:THR:OG1	2.69	0.43
2:B:96:GLY:CA	2:B:101:ALA:HB2	2.40	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.33	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.83	0.43
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.43
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.43
8:H:200:LEU:HD21	8:H:282:TYR:HD1	1.84	0.43
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:MET:HB2	58:K:101:3PE:C23	2.48	0.43
11:K:57:MET:O	11:K:60:PRO:HD2	2.18	0.43
12:L:226:GLN:OE1	12:L:284:THR:CG2	2.66	0.43
12:L:305:SER:OG	12:L:336:LYS:HE2	2.18	0.43
13:M:151:PHE:HZ	14:N:291:PHE:HB2	1.78	0.43
14:N:12:THR:CG2	14:N:39:ALA:HB2	2.48	0.43
16:P:197:GLU:HB3	16:P:259:VAL:HG22	1.99	0.43
16:P:269:ASN:ND2	16:P:271:TYR:OH	2.51	0.43
24:Y:19:GLN:OE1	24:Y:19:GLN:HA	2.17	0.43
34:i:94:PRO:CB	41:p:10:TYR:CD2	3.02	0.43
58:i:201:3PE:H11	58:i:201:3PE:O22	2.18	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:142:PHE:O	37:l:145:TRP:N	2.51	0.43
38:m:45:ARG:O	38:m:45:ARG:CG	2.61	0.43
39:n:131:GLU:O	39:n:131:GLU:HG2	2.17	0.43
45:AA:52:ILE:HA	45:AA:58:ARG:HA	1.99	0.43
45:AA:172:MET:HE1	45:AA:205:SER:HA	2.00	0.43
48:AD:112:ARG:HB3	48:AD:255:TYR:CE1	2.53	0.43
48:AD:159:ASN:OD1	48:AD:160:ASP:N	2.51	0.43
48:AD:262:THR:O	48:AD:263:MET:C	2.61	0.43
49:AE:163:LYS:O	49:AE:177:ARG:HG3	2.17	0.43
49:AE:179:ARG:HH12	49:AE:187:GLU:HG2	1.83	0.43
45:Aa:132:LEU:HD11	45:Aa:407:THR:HG23	2.00	0.43
45:Aa:453:CYS:SG	51:Ag:20:SER:OG	2.71	0.43
46:Ab:130:ILE:HA	46:Ab:133:LEU:HB2	2.00	0.43
53:Aj:11:TYR:HA	53:Aj:15:PHE:HD2	1.82	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.19	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:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HD1	2.31	0.43
8:H:200:LEU:C	8:H:200:LEU:HD12	2.43	0.43
10:J:55:VAL:HG13	10:J:56:PHE:N	2.33	0.43
12:L:564:LYS:HG2	38:m:77:TYR:OH	2.18	0.43
12:L:589:MET:O	12:L:592:LEU:HB3	2.18	0.43
13:M:278:ARG:HH22	37:l:108:ASP:CB	2.31	0.43
13:M:348:LEU:O	13:M:349:GLN:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:72:LYS:O	15:O:76:GLU:HG2	2.18	0.43
15:O:211:VAL:HB	15:O:212:PRO:HD3	2.00	0.43
19:S:30:SER:O	19:S:33:VAL:N	2.51	0.43
21:V:19:THR:N	21:V:20:PRO:CD	2.81	0.43
23:X:48:TRP:CH2	33:h:184:LYS:O	2.71	0.43
24:Y:26:ILE:O	24:Y:30:LEU:HG	2.17	0.43
25:Z:53:TRP:CE2	25:Z:57:ARG:HD2	2.53	0.43
27:b:23:PHE:CZ	58:b:201:3PE:H351	2.46	0.43
34:i:32:GLU:OE2	39:n:118:TYR:N	2.50	0.43
37:l:58:ARG:HD2	38:m:35:GLU:OE1	2.18	0.43
38:m:17:THR:O	38:m:18:LEU:CB	2.66	0.43
38:m:34:VAL:O	38:m:34:VAL:HG12	2.16	0.43
45:AA:473:SER:HA	45:AA:476:PHE:CE1	2.53	0.43
54:AK:41:ILE:O	54:AK:42:LEU:C	2.61	0.43
47:Ac:79:ILE:HG12	49:Ae:136:PHE:CE1	2.54	0.43
47:Ac:378:LYS:CG	50:Af:18:ARG:HH12	2.31	0.43
49:Ae:195:LEU:HD11	49:Ae:248:ARG:NH1	2.32	0.43
49:Ae:204:ARG:HD2	49:Ae:257:ASN:HD22	1.83	0.43
49:Ae:243:TYR:CE1	49:Ae:258:LEU:CD2	3.02	0.43
50:Af:76:LEU:HD22	50:Af:80:GLN:NE2	2.33	0.43
1:A:56:PHE:HD1	10:J:70:THR:OG1	2.02	0.43
1:A:112:GLU:O	1:A:113:TRP:C	2.58	0.43
2:B:104:MET:HE3	56:B:302:UQ1:C11	2.40	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.60	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
9:I:197:TRP:CZ3	42:q:84:PRO:HA	2.53	0.43
12:L:496:LEU:CD1	12:L:497:GLY:N	2.73	0.43
12:L:564:LYS:HG2	38:m:77:TYR:CZ	2.54	0.43
13:M:154:LEU:HA	13:M:154:LEU:HD23	1.84	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
14:N:307:THR:HB	15:O:319:ILE:HG12	2.00	0.43
14:N:323:ASN:N	14:N:323:ASN:OD1	2.49	0.43
15:O:210:PRO:O	15:O:213:GLU:N	2.51	0.43
15:O:256:LEU:HD11	15:O:276:LEU:HD22	1.99	0.43
16:P:76:MET:HE1	16:P:254:LYS:HE2	2.01	0.43
16:P:310:PHE:O	16:P:311:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:92:LYS:O	20:T:92:LYS:HG2	2.16	0.43
21:V:56:LEU:CD1	21:V:57:ASP:OD1	2.67	0.43
24:Y:19:GLN:O	24:Y:23:LYS:HG2	2.19	0.43
24:Y:143:VAL:O	33:h:158:ARG:NH2	2.52	0.43
27:b:82:LYS:HB3	27:b:82:LYS:HE2	1.81	0.43
29:d:78:ARG:HG2	29:d:82:LEU:HD23	2.00	0.43
32:g:58:GLU:CD	32:g:59:PRO:HD2	2.44	0.43
58:m:201:3PE:H2I3	58:m:201:3PE:H2F2	1.87	0.43
45:AA:398:ALA:O	45:AA:400:VAL:HG23	2.18	0.43
48:AD:189:ASN:ND2	48:AD:194:PRO:HG3	2.33	0.43
45:Aa:478:LEU:H	62:Aa:501:CDL:PB2	2.41	0.43
46:Ab:97:PHE:CE2	46:Ab:101:ARG:HG3	2.53	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
3:C:221:GLU:OE1	22:W:114:GLU:HB2	2.18	0.43
4:D:36:GLN:NE2	4:D:38:GLN:NE2	2.62	0.43
4:D:99:LEU:HB3	4:D:101:LEU:HD11	2.00	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:292:ASN:HD21	58:I:301:3PE:H121	1.84	0.43
12:L:246:LEU:HD12	12:L:247:LEU:CB	2.49	0.43
12:L:407:TRP:HE1	37:l:140:MET:HE1	1.84	0.43
12:L:427:ILE:HG13	12:L:428:TYR:N	2.33	0.43
14:N:175:MET:HE2	14:N:175:MET:HB2	1.85	0.43
14:N:186:HIS:O	14:N:190:MET:HG3	2.18	0.43
14:N:240:MET:O	14:N:240:MET:HG2	2.18	0.43
14:N:324:LEU:CD1	29:d:64:PHE:HZ	2.30	0.43
16:P:64:PHE:CE1	16:P:209:ARG:O	2.69	0.43
16:P:298:TYR:C	16:P:300:TRP:N	2.71	0.43
19:S:24:CYS:SG	19:S:61:VAL:HG12	2.58	0.43
22:W:71:MET:O	22:W:74:ALA:N	2.39	0.43
33:h:57:VAL:HG13	39:n:104:LEU:HG	2.01	0.43
37:l:97:LEU:O	37:l:98:ARG:C	2.60	0.43
41:p:75:THR:HG22	41:p:156:LEU:HD13	2.00	0.43
46:AB:54:ASN:OD1	46:AB:224:GLY:HA2	2.18	0.43
47:AC:71:ARG:NH2	48:AD:277:ALA:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:232:TYR:CE1	48:AD:246:PRO:HD3	2.54	0.43
49:AE:160:PRO:HD2	49:AE:163:LYS:CE	2.48	0.43
49:AE:207:LYS:HB3	49:AE:209:GLU:OE2	2.18	0.43
45:Aa:225:LYS:HG3	45:Aa:256:VAL:HG12	2.00	0.43
46:Ab:282:GLU:OE2	46:Ab:430:LYS:HD2	2.18	0.43
48:Ad:98:HIS:O	48:Ad:286:LYS:NZ	2.51	0.43
49:Ae:235:TYR:CE2	49:Ae:237:PRO:HA	2.53	0.43
51:Ag:69:GLN:O	51:Ag:72:ARG:HB3	2.17	0.43
53:Aj:17:ARG:HB3	53:Aj:20:THR:HG23	2.00	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.01	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:166:ALA:HB1	44:s:45:PHE:HD2	1.84	0.43
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.18	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
8:H:43:TYR:CE2	42:q:27:PHE:CZ	3.06	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.43
8:H:306:SER:OG	27:b:33:PRO:HG3	2.19	0.43
10:J:67:PHE:O	10:J:68:GLY:C	2.59	0.43
12:L:22:SER:HA	12:L:27:ILE:HG21	2.00	0.43
12:L:81:LYS:HD3	12:L:262:ARG:NH1	2.34	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
13:M:73:LEU:HD23	13:M:103:GLN:HE22	1.84	0.43
14:N:105:LYS:HE3	14:N:105:LYS:HB3	1.79	0.43
15:O:99:GLY:O	28:c:31:VAL:N	2.36	0.43
15:O:239:ASN:HB3	15:O:243:LYS:NZ	2.33	0.43
15:O:303:GLU:O	15:O:304:VAL:C	2.59	0.43
16:P:164:PHE:HE2	16:P:166:HIS:HB2	1.82	0.43
16:P:170:LEU:O	16:P:171:ASN:CG	2.61	0.43
17:Q:99:MET:O	17:Q:99:MET:HG3	2.18	0.43
24:Y:115:MET:O	24:Y:119:TYR:HD2	2.02	0.43
24:Y:141:PRO:CB	33:h:161:ARG:NH1	2.81	0.43
27:b:15:LYS:O	27:b:15:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:42:ALA:HA	27:b:45:ILE:HG22	2.01	0.43
30:e:41:ILE:HD11	33:h:174:PRO:O	2.18	0.43
38:m:28:GLU:HA	38:m:31:ARG:NH2	2.33	0.43
46:AB:162:LYS:HG3	46:AB:191:TYR:HB3	2.00	0.43
48:AD:152:VAL:HG11	48:AD:176:PRO:CG	2.43	0.43
48:AD:231:LEU:HD23	48:AD:242:ILE:C	2.44	0.43
48:AD:231:LEU:HD23	48:AD:243:GLY:N	2.34	0.43
49:AE:126:ALA:HB1	54:AK:34:TRP:CZ3	2.54	0.43
49:AE:219:HIS:O	49:AE:220:LEU:HB2	2.18	0.43
46:Ab:63:LEU:HD12	46:Ab:220:LEU:HD13	2.00	0.43
46:Ab:378:LEU:HD23	46:Ab:416:ILE:CG2	2.49	0.43
48:Ad:125:HIS:CE1	48:Ad:194:PRO:HB3	2.54	0.43
48:Ad:157:GLY:O	48:Ad:158:PRO:C	2.59	0.43
49:Ae:80:HIS:CD2	49:Ae:81:THR:HG23	2.53	0.43
49:Ae:169:TRP:CD1	49:Ae:170:ARG:HG3	2.53	0.43
49:Ae:175:PHE:CZ	49:Ae:224:PRO:HD2	2.54	0.43
50:Af:47:ALA:CB	50:Af:91:LEU:HD11	2.48	0.43
50:Af:97:GLU:HA	50:Af:100:ARG:NH1	2.33	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:105:MET:HE2	56:B:302:UQ1:C8	2.48	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
7:G:279:GLU:HG3	17:Q:154:LYS:HG3	2.00	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
10:J:30:LEU:O	10:J:31:GLY:C	2.59	0.43
10:J:144:MET:HB3	10:J:152:MET:HB2	2.01	0.43
11:K:4:THR:O	11:K:4:THR:HG22	2.19	0.43
12:L:60:GLU:C	12:L:61:TYR:CD1	2.97	0.43
12:L:70:THR:O	12:L:75:GLU:HA	2.18	0.43
12:L:172:ILE:HD13	12:L:172:ILE:HA	1.89	0.43
12:L:446:ASN:O	12:L:447:ASP:C	2.57	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.19	0.43
13:M:119:TYR:HD1	13:M:160:LEU:HD22	1.79	0.43
13:M:208:PRO:HG2	13:M:216:LEU:CD1	2.44	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
14:N:275:CYS:SG	24:Y:139:PRO:CD	3.07	0.43
17:Q:104:ARG:HA	17:Q:104:ARG:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:111:LEU:HD11	42:q:126:PRO:HG2	2.00	0.43
18:R:72:VAL:HG11	18:R:77:ILE:HG22	2.01	0.43
20:T:109:GLY:O	20:T:110:LEU:C	2.61	0.43
21:V:56:LEU:C	21:V:56:LEU:CD1	2.85	0.43
23:X:29:ALA:CB	25:Z:71:LEU:HD11	2.43	0.43
24:Y:22:ARG:O	24:Y:26:ILE:HG13	2.19	0.43
25:Z:28:ARG:O	25:Z:28:ARG:CG	2.64	0.43
25:Z:86:ILE:HA	25:Z:128:ARG:NH2	2.33	0.43
31:f:11:TRP:O	31:f:14:ILE:HG22	2.18	0.43
33:h:127:ASP:OD1	33:h:127:ASP:C	2.61	0.43
37:l:186:ILE:HG23	40:o:100:LYS:HZ1	1.84	0.43
39:n:37:TYR:O	39:n:38:ARG:C	2.61	0.43
41:p:103:MET:HE1	41:p:135:VAL:HG12	1.99	0.43
42:q:4:VAL:HG23	42:q:5:GLU:N	2.33	0.43
42:q:79:GLY:O	42:q:82:VAL:HG22	2.19	0.43
46:AB:155:ARG:HD2	46:AB:198:GLY:H	1.83	0.43
49:AE:152:ILE:HB	49:AE:169:TRP:NE1	2.33	0.43
45:Aa:378:ARG:O	45:Aa:382:SER:N	2.40	0.43
46:Ab:92:LYS:HA	46:Ab:145:GLU:OE1	2.18	0.43
46:Ab:411:THR:O	46:Ab:414:GLN:HG2	2.18	0.43
47:Ac:181:PHE:HA	47:Ac:184:ILE:HG22	2.00	0.43
68:Ac:404:U10:H1M1	68:Ac:404:U10:H72	1.79	0.43
49:Ae:115:TYR:HB3	53:Aj:15:PHE:CD1	2.54	0.43
49:Ae:195:LEU:HD13	49:Ae:200:HIS:HA	2.00	0.43
49:Ae:212:ILE:HG22	49:Ae:261:PRO:CG	2.48	0.43
52:Ah:71:ASP:OD1	52:Ah:72:PHE:N	2.52	0.43
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:123:SER:HB3	8:H:214:GLU:HG3	2.00	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
10:J:13:LEU:HD11	11:K:10:MET:SD	2.58	0.43
12:L:92:VAL:HG21	12:L:330:CYS:HB3	2.00	0.43
12:L:184:LEU:HD22	58:L:703:3PE:H3C2	2.01	0.43
12:L:187:VAL:HG13	13:M:383:MET:HA	2.00	0.43
12:L:196:TRP:HZ2	13:M:383:MET:SD	2.41	0.43
12:L:353:GLU:CD	39:n:80:TYR:HH	2.26	0.43
12:L:493:ILE:O	12:L:496:LEU:HG	2.19	0.43
13:M:63:THR:N	13:M:64:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:207:MET:SD	13:M:240:SER:CA	3.06	0.43
14:N:11:PHE:O	14:N:15:LEU:N	2.49	0.43
14:N:154:ILE:HD12	14:N:155:LEU:N	2.33	0.43
15:O:76:GLU:CB	15:O:266:PRO:HB3	2.49	0.43
19:S:75:LYS:HE2	19:S:75:LYS:HA	2.01	0.43
22:W:120:ASP:HB3	22:W:123:SER:OG	2.18	0.43
31:f:39:ASN:HA	33:h:134:GLU:OE2	2.18	0.43
38:m:129:TYR:CE2	41:p:146:LEU:O	2.72	0.43
39:n:81:ILE:HD12	39:n:87:GLY:C	2.44	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	2.19	0.43
42:q:22:GLY:O	42:q:26:VAL:HG23	2.18	0.43
45:AA:61:SER:OG	45:AA:239:HIS:ND1	2.51	0.43
45:AA:403:LEU:C	45:AA:405:GLY:H	2.26	0.43
46:AB:233:VAL:HA	46:AB:236:GLN:CG	2.47	0.43
47:AC:35:SER:HB3	69:AC:405:UQ6:O5	2.19	0.43
47:AC:326:TRP:CZ2	58:AC:403:3PE:H322	2.54	0.43
48:AD:89:LEU:HD13	52:AH:74:HIS:HB2	2.01	0.43
50:AF:95:LEU:O	50:AF:96:LYS:C	2.62	0.43
52:AH:30:THR:O	52:AH:33:GLU:HB3	2.18	0.43
62:Aa:501:CDL:H342	62:Aa:501:CDL:H311	1.76	0.43
46:Ab:283:ALA:O	46:Ab:284:ASN:C	2.60	0.43
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.49	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
4:D:47:PHE:CD1	14:N:227:ILE:CD1	3.01	0.43
4:D:52:MET:O	4:D:54:PRO:HD3	2.19	0.43
4:D:72:LEU:O	4:D:72:LEU:HD12	2.18	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.43
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
6:F:409:ILE:HG12	6:F:446:LEU:HD23	1.96	0.43
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.43
6:F:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:617:ARG:NH1	22:W:129:HIS:N	2.67	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.43
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.43
12:L:38:THR:O	12:L:41:LYS:HB3	2.19	0.43
12:L:53:MET:HE2	12:L:53:MET:HB3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:145:GLU:HB3	13:M:370:PRO:CD	2.48	0.43
12:L:217:LEU:CD1	12:L:273:ILE:HG23	2.49	0.43
13:M:46:ASP:OD1	13:M:47:GLU:N	2.52	0.43
14:N:12:THR:HG22	14:N:39:ALA:HB2	2.00	0.43
14:N:39:ALA:O	14:N:42:PRO:HD2	2.19	0.43
14:N:193:ILE:HD12	14:N:266:ILE:HA	2.01	0.43
18:R:72:VAL:HG11	18:R:77:ILE:CG2	2.49	0.43
20:T:87:LEU:HD11	20:T:141:PRO:HB3	2.01	0.43
20:U:133:ILE:HD13	39:n:7:PRO:HD3	1.99	0.43
21:V:8:THR:HG22	21:V:9:THR:N	2.34	0.43
26:a:12:MET:HE2	26:a:12:MET:HB3	1.90	0.43
30:e:69:ARG:CD	30:e:72:THR:HG21	2.49	0.43
33:h:90:ASN:OD1	33:h:115:HIS:NE2	2.52	0.43
37:l:184:TYR:CE1	40:o:36:GLU:HB3	2.54	0.43
42:q:14:VAL:HG13	42:q:23:LEU:CD2	2.43	0.43
45:AA:53:LEU:HD12	45:AA:57:LEU:CB	2.45	0.43
45:AA:93:LEU:HD21	45:AA:156:LEU:HD11	1.99	0.43
45:AA:230:VAL:HG21	45:AA:417:LEU:HB3	2.00	0.43
46:AB:130:ILE:HA	46:AB:133:LEU:HB2	2.01	0.43
49:AE:249:ILE:HG12	49:AE:254:ALA:HB3	2.01	0.43
45:Aa:61:SER:HB3	45:Aa:242:LEU:HD22	2.01	0.43
49:Ae:104:LYS:HA	49:Ae:107:SER:CB	2.44	0.43
2:B:82:ILE:CG1	8:H:57:MET:CE	2.82	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
8:H:179:TRP:CD1	25:Z:43:LEU:HD21	2.54	0.43
9:I:152:CYS:SG	55:I:303:SF4:S3	3.17	0.43
10:J:20:ALA:C	10:J:22:LYS:H	2.26	0.43
11:K:50:ASN:C	11:K:50:ASN:OD1	2.62	0.43
12:L:491:LEU:CD1	35:j:80:VAL:HG22	2.49	0.43
12:L:522:PHE:CD2	12:L:527:GLY:HA2	2.54	0.43
13:M:6:LEU:HD21	31:f:22:PHE:CD2	2.54	0.43
13:M:100:ILE:O	13:M:103:GLN:HG2	2.19	0.43
13:M:263:LEU:HD13	38:m:102:TYR:HB2	2.00	0.43
13:M:367:LEU:C	13:M:367:LEU:HD12	2.44	0.43
14:N:193:ILE:HD11	14:N:269:GLU:CB	2.49	0.43
14:N:272:LYS:HE3	33:h:154:GLN:HG2	2.00	0.43
16:P:237:LYS:HE3	16:P:322:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:280:ILE:HG23	16:P:353:LEU:HD22	2.00	0.43
16:P:283:MET:HE3	16:P:357:ARG:HH11	1.83	0.43
16:P:306:GLY:HA2	16:P:312:PRO:HB3	2.01	0.43
22:W:38:LEU:HG	22:W:70:PHE:HZ	1.84	0.43
22:W:99:VAL:O	22:W:99:VAL:HG12	2.19	0.43
22:W:102:GLN:O	22:W:103:ARG:C	2.60	0.43
24:Y:8:PHE:CD1	24:Y:30:LEU:HD21	2.53	0.43
26:a:4:GLU:C	26:a:7:PRO:HD2	2.44	0.43
26:a:55:SER:O	26:a:56:GLY:C	2.61	0.43
30:e:96:PRO:O	30:e:97:HIS:C	2.62	0.43
31:f:37:PHE:HZ	41:p:83:LEU:HD13	1.83	0.43
33:h:59:PRO:O	33:h:61:LEU:HG	2.19	0.43
39:n:45:ARG:O	39:n:46:ALA:C	2.61	0.43
46:AB:47:LEU:HD12	46:AB:218:MET:O	2.18	0.43
47:AC:48:GLY:HA3	67:AC:401:HEM:C2B	2.53	0.43
47:AC:181:PHE:HA	47:AC:184:ILE:HG22	2.00	0.43
48:AD:223:THR:HG23	52:AH:55:VAL:HG11	2.00	0.43
48:AD:231:LEU:HD23	48:AD:243:GLY:CA	2.48	0.43
48:AD:248:ILE:HD12	48:AD:266:VAL:HG11	2.00	0.43
48:AD:264:SER:OG	52:AH:88:LEU:HD21	2.19	0.43
48:AD:312:SER:O	48:AD:313:VAL:C	2.59	0.43
49:AE:91:TYR:CD2	51:AG:28:PRO:HG2	2.54	0.43
52:AH:31:VAL:HG13	52:AH:83:LYS:HG3	2.01	0.43
45:Aa:167:VAL:O	45:Aa:170:ARG:HG2	2.19	0.43
45:Aa:338:CYS:SG	45:Aa:358:PHE:HB2	2.58	0.43
49:Ae:79:SER:OG	49:Ae:80:HIS:N	2.51	0.43
52:Ah:26:ASP:O	52:Ah:27:PRO:C	2.61	0.43
1:A:73:LEU:O	8:H:160:TYR:OH	2.25	0.42
4:D:83:ASN:C	4:D:85:GLY:N	2.74	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
4:D:198:THR:HG23	8:H:275:ALA:O	2.18	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
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
8:H:33:LEU:HD21	43:r:25:GLN:HG2	2.01	0.42
9:I:162:CYS:SG	55:I:304:SF4:S2	3.17	0.42
10:J:50:PHE:O	10:J:54:MET:HG2	2.20	0.42
12:L:466:PHE:HB2	35:j:68:TRP:CH2	2.50	0.42
12:L:553:LEU:HD21	38:m:94:GLY:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:569:LEU:CB	24:Y:115:MET:HE1	2.26	0.42
13:M:123:GLU:CD	14:N:255:PRO:HG2	2.44	0.42
13:M:214:LEU:C	13:M:217:PRO:HD2	2.44	0.42
14:N:170:LEU:HD12	14:N:292:PHE:CD2	2.54	0.42
15:O:117:PHE:HD1	15:O:128:SER:CA	2.31	0.42
15:O:209:VAL:HG23	15:O:214:VAL:CG1	2.49	0.42
16:P:259:VAL:N	16:P:261:LYS:HG2	2.33	0.42
20:T:93:ILE:HD11	20:T:118:ILE:HD11	2.00	0.42
20:U:100:VAL:HA	20:U:141:PRO:HG2	2.00	0.42
20:U:142:GLN:O	20:U:143:GLU:C	2.60	0.42
23:X:10:LEU:H	23:X:10:LEU:HD12	1.84	0.42
29:d:94:ILE:HD13	33:h:152:LYS:HE3	2.01	0.42
40:o:57:ASP:OD2	40:o:59:CYS:HB2	2.19	0.42
40:o:111:ARG:HA	40:o:114:ARG:NH1	2.34	0.42
43:r:12:ARG:HB3	43:r:20:LEU:CD2	2.49	0.42
45:AA:94:GLU:CD	46:AB:301:ARG:HH12	2.27	0.42
49:AE:89:SER:O	49:AE:90:ASP:C	2.60	0.42
49:AE:116:LEU:HD23	49:AE:116:LEU:C	2.44	0.42
49:AE:159:ILE:CG2	49:AE:178:HIS:HB2	2.49	0.42
49:AE:190:VAL:HG11	49:AE:248:ARG:NH2	2.34	0.42
49:AE:207:LYS:HB2	49:AE:210:TRP:HD1	1.83	0.42
49:AE:221:GLY:O	47:Ac:145:VAL:HG22	2.19	0.42
50:AF:97:GLU:HA	50:AF:100:ARG:NH1	2.33	0.42
52:AH:52:ASP:N	52:AH:65:CYS:SG	2.92	0.42
54:AK:10:TYR:N	54:AK:10:TYR:CD1	2.87	0.42
54:AK:12:GLU:HA	54:AK:15:ARG:HH11	1.84	0.42
54:AK:36:THR:C	54:AK:38:TRP:N	2.74	0.42
47:Ac:230:LEU:HD21	62:Ag:101:CDL:H522	2.01	0.42
48:Ad:201:VAL:HG22	48:Ad:278:SER:HB2	2.00	0.42
48:Ad:262:THR:O	48:Ad:263:MET:C	2.61	0.42
49:Ae:88:PHE:O	49:Ae:89:SER:C	2.61	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
5:E:137:THR:HG22	6:F:370:LEU:HD21	2.02	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.42
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.42
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.42
8:H:93:HIS:CD2	26:a:27:HIS:ND1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:THR:HG22	43:r:107:SER:HA	1.97	0.42
12:L:5:THR:O	12:L:6:THR:C	2.62	0.42
12:L:60:GLU:N	12:L:60:GLU:OE2	2.52	0.42
12:L:197:GLU:HG3	41:p:111:LYS:CE	2.49	0.42
12:L:275:THR:HG23	12:L:276:THR:N	2.34	0.42
12:L:526:LEU:HD12	12:L:526:LEU:N	2.34	0.42
12:L:591:PHE:O	12:L:595:ILE:HG13	2.19	0.42
13:M:369:LEU:CD2	13:M:371:PRO:CD	2.84	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:86:TYR:HE1	15:O:157:VAL:HG12	1.82	0.42
15:O:323:GLN:HE21	32:g:55:GLU:CA	2.32	0.42
16:P:169:HIS:CD2	16:P:181:LEU:HD11	2.52	0.42
21:V:35:LEU:HA	21:V:38:PHE:CE1	2.54	0.42
21:V:37:HIS:O	21:V:38:PHE:C	2.62	0.42
27:b:52:ASN:HD21	30:e:28:LYS:NZ	2.17	0.42
30:e:44:ALA:HA	30:e:47:ILE:CG1	2.50	0.42
30:e:49:GLY:O	30:e:50:THR:C	2.61	0.42
30:e:101:ARG:NE	30:e:101:ARG:HA	2.34	0.42
33:h:129:PRO:HD2	33:h:130:GLU:OE1	2.18	0.42
34:i:32:GLU:HG3	39:n:115:TYR:HA	2.00	0.42
36:k:28:TRP:CE3	36:k:60:MET:HG2	2.54	0.42
40:o:10:LEU:HD12	40:o:10:LEU:N	2.34	0.42
41:p:73:ASP:O	41:p:74:ILE:C	2.59	0.42
45:AA:172:MET:HA	45:AA:175:ASN:CG	2.44	0.42
45:AA:178:SER:O	45:AA:179:MET:C	2.60	0.42
46:AB:286:PHE:CD1	46:AB:427:ALA:HB1	2.54	0.42
46:AB:378:LEU:HD23	46:AB:416:ILE:CG2	2.49	0.42
48:AD:120:VAL:HG23	48:AD:253:LEU:HD23	2.00	0.42
49:AE:159:ILE:HG22	49:AE:178:HIS:HB2	2.01	0.42
49:AE:162:GLY:HA3	49:AE:180:THR:CG2	2.45	0.42
49:AE:205:VAL:HG12	49:AE:211:VAL:HA	2.01	0.42
52:AH:53:ASN:HB3	52:AH:54:ARG:NH1	2.35	0.42
52:AH:68:GLU:OE1	52:AH:68:GLU:N	2.51	0.42
47:Ac:256:TYR:CD2	48:Ad:202:ARG:HB3	2.54	0.42
47:Ac:277:ALA:HB1	68:Ac:404:U10:H1M2	2.00	0.42
49:Ae:112:GLY:O	49:Ae:113:PHE:C	2.62	0.42
49:Ae:199:GLN:O	49:Ae:248:ARG:HG2	2.19	0.42
49:Ae:251:LYS:HG3	49:Ae:252:GLY:N	2.34	0.42
1:A:73:LEU:N	1:A:74:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ASP:OD1	21:V:86:LYS:HE3	2.19	0.42
3:C:124:ARG:HD2	17:Q:140:LYS:HZ1	1.84	0.42
3:C:133:SER:OG	3:C:133:SER:O	2.32	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.42
7:G:664:TYR:OH	19:S:23:LEU:HD11	2.20	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:J:131:VAL:HG13	26:a:43:TYR:HD1	1.82	0.42
12:L:253:VAL:HG21	12:L:310:LEU:HD11	2.00	0.42
13:M:1:MET:HB3	13:M:1:MET:HE3	1.73	0.42
13:M:14:LEU:HD21	13:M:26:ASN:CB	2.50	0.42
13:M:68:LEU:HD23	13:M:234:ILE:CD1	2.50	0.42
13:M:72:LEU:HD12	13:M:234:ILE:HG12	2.01	0.42
13:M:210:TYR:O	13:M:213:HIS:HD2	2.01	0.42
15:O:121:PRO:HB3	15:O:178:TYR:HE1	1.83	0.42
15:O:170:LEU:HD21	15:O:184:VAL:HG13	2.00	0.42
15:O:256:LEU:N	15:O:256:LEU:HD12	2.34	0.42
15:O:297:LEU:C	15:O:297:LEU:HD23	2.43	0.42
15:O:310:ILE:HG23	15:O:312:VAL:HG23	2.01	0.42
58:O:401:3PE:H351	58:O:401:3PE:H391	2.01	0.42
16:P:376:ASN:O	16:P:377:TYR:C	2.61	0.42
18:R:45:ARG:HA	18:R:48:PHE:HE1	1.83	0.42
18:R:48:PHE:CD2	42:q:125:VAL:HG21	2.54	0.42
19:S:16:LEU:HD13	19:S:19:ILE:HD11	2.02	0.42
19:S:30:SER:HB3	19:S:63:PRO:HG3	2.00	0.42
23:X:75:LYS:O	23:X:79:ALA:HB2	2.19	0.42
25:Z:74:LEU:O	25:Z:78:GLU:HG3	2.20	0.42
27:b:31:ILE:HG23	27:b:32:MET:N	2.34	0.42
27:b:32:MET:N	27:b:33:PRO:CD	2.82	0.42
29:d:27:ASN:O	29:d:28:ASP:C	2.60	0.42
29:d:114:GLU:O	29:d:114:GLU:HG2	2.18	0.42
30:e:22:SER:HB2	30:e:34:HIS:CD2	2.54	0.42
34:i:93:LYS:HE3	34:i:96:THR:HG21	2.01	0.42
40:o:46:MET:HE2	40:o:60:ALA:HB3	2.00	0.42
41:p:36:ALA:O	41:p:37:TYR:C	2.60	0.42
45:AA:74:TRP:CZ3	45:AA:232:ALA:HB3	2.54	0.42
46:AB:332:ASP:OD1	46:AB:332:ASP:N	2.52	0.42
47:AC:33:PHE:O	47:AC:36:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:171:ASP:CG	47:AC:172:LYS:N	2.76	0.42
48:AD:240:GLN:HG2	52:AH:70:PHE:HZ	1.85	0.42
48:AD:284:HIS:HE2	48:AD:288:MET:HE3	1.83	0.42
49:AI:65:VAL:HG11	49:AI:77:ARG:HH22	1.84	0.42
46:Ab:332:ASP:OD1	46:Ab:332:ASP:N	2.52	0.42
46:Ab:396:ILE:HG12	46:Ab:406:TYR:HE1	1.85	0.42
48:Ad:156:ASP:O	48:Ad:164:MET:HA	2.20	0.42
53:Aj:23:LEU:HA	54:Ak:27:VAL:HG22	2.01	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.42
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
61:H:400:UQ9:H15B	61:H:400:UQ9:H17	1.80	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
11:K:32:CYS:O	11:K:33:LEU:C	2.60	0.42
12:L:141:PHE:CB	12:L:182:PHE:CE2	2.81	0.42
12:L:220:ALA:HB2	12:L:260:LEU:CD1	2.49	0.42
12:L:335:PHE:O	12:L:339:LEU:HD13	2.19	0.42
12:L:489:THR:HG23	12:L:490:ALA:N	2.33	0.42
13:M:77:LEU:O	13:M:81:GLN:HG3	2.19	0.42
13:M:173:THR:HG23	33:h:147:ALA:HB2	1.78	0.42
13:M:200:MET:CE	13:M:247:SER:HB2	2.45	0.42
13:M:231:LEU:CD1	13:M:235:LEU:CD1	2.85	0.42
14:N:174:GLN:O	14:N:178:ILE:HG13	2.19	0.42
15:O:73:LEU:HD22	15:O:207:ILE:HD11	2.02	0.42
15:O:146:ALA:CB	15:O:159:LEU:HD21	2.49	0.42
20:U:119:ILE:HD13	20:U:119:ILE:HA	1.81	0.42
24:Y:87:ASP:HA	24:Y:128:LYS:NZ	2.34	0.42
25:Z:108:GLU:O	25:Z:109:SER:C	2.61	0.42
28:c:69:TYR:O	28:c:73:ASN:ND2	2.53	0.42
34:i:11:ARG:HD2	39:n:154:LEU:O	2.20	0.42
34:i:22:TRP:O	34:i:26:GLN:HG2	2.19	0.42
37:l:57:MET:HG2	37:l:104:PRO:CG	2.49	0.42
41:p:6:ASP:C	41:p:8:ASP:H	2.27	0.42
41:p:43:TRP:NE1	41:p:47:LEU:HD11	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:150:LEU:CD2	68:AC:404:U10:O2	2.62	0.42
48:AD:252:VAL:HG13	48:AD:253:LEU:N	2.34	0.42
49:AE:202:LEU:C	49:AE:204:ARG:N	2.75	0.42
53:AJ:27:VAL:HG22	54:AK:30:VAL:HG11	2.01	0.42
45:Aa:175:ASN:C	45:Aa:177:ALA:N	2.76	0.42
45:Aa:401:SER:O	45:Aa:404:ASP:HB2	2.19	0.42
46:Ab:284:ASN:HB3	46:Ab:419:VAL:CG2	2.49	0.42
46:Ab:284:ASN:HB3	46:Ab:419:VAL:HG21	2.01	0.42
49:Ae:206:LYS:HD2	49:Ae:265:PHE:HD2	1.85	0.42
54:Ak:38:TRP:CG	54:Ak:41:ILE:HG12	2.54	0.42
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.42	0.42
2:B:91:TRP:CE3	61:H:400:UQ9:H1M	2.54	0.42
3:C:64:VAL:HG11	3:C:85:ILE:HD13	2.02	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:78:PHE:HD1	26:a:2:TRP:CD1	2.37	0.42
12:L:272:PHE:O	12:L:275:THR:HG22	2.20	0.42
13:M:165:ILE:HD12	23:X:168:PHE:CZ	2.55	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:422:HIS:CB	38:m:51:TYR:CE2	3.01	0.42
14:N:80:GLN:O	14:N:80:GLN:HG2	2.19	0.42
15:O:211:VAL:O	15:O:214:VAL:HG22	2.19	0.42
16:P:207:PHE:O	16:P:241:TYR:HA	2.19	0.42
16:P:220:TYR:CG	16:P:226:VAL:HG13	2.55	0.42
16:P:300:TRP:NE1	16:P:304:LEU:HD21	2.35	0.42
22:W:120:ASP:OD1	22:W:120:ASP:C	2.61	0.42
23:X:26:LYS:HD3	23:X:95:GLN:OE1	2.19	0.42
26:a:17:VAL:O	26:a:18:ILE:C	2.62	0.42
28:c:70:LYS:HB3	28:c:75:LEU:HD12	2.01	0.42
35:j:44:TYR:CE2	35:j:45:ARG:HG3	2.54	0.42
38:m:5:LYS:HB2	38:m:5:LYS:HE3	1.73	0.42
39:n:110:SER:O	39:n:113:ALA:HB3	2.20	0.42
40:o:35:LYS:HG3	40:o:36:GLU:O	2.19	0.42
45:AA:271:THR:HG22	45:AA:273:SER:OG	2.18	0.42
46:AB:230:LEU:O	46:AB:233:VAL:HG22	2.19	0.42
47:AC:148:ASN:HB3	49:Ae:220:LEU:HA	2.02	0.42
47:AC:153:ILE:HB	47:AC:157:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:201:ASP:HB3	49:AE:248:ARG:CZ	2.49	0.42
46:Ab:155:ARG:HD2	46:Ab:198:GLY:H	1.84	0.42
47:Ac:62:ALA:O	47:Ac:63:PHE:C	2.63	0.42
48:Ad:252:VAL:HG13	48:Ad:253:LEU:N	2.34	0.42
52:Ah:47:ARG:HA	52:Ah:50:LEU:HD12	2.01	0.42
53:Aj:51:LYS:O	53:Aj:52:LEU:HG	2.19	0.42
1:A:52:SER:O	1:A:53:MET:C	2.61	0.42
2:B:94:THR:OG1	2:B:104:MET:HE1	2.20	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:68:ARG:HH22	25:Z:26:PRO:HD2	1.83	0.42
10:J:13:LEU:C	10:J:13:LEU:HD23	2.45	0.42
10:J:55:VAL:O	10:J:56:PHE:C	2.62	0.42
11:K:19:THR:O	11:K:22:PHE:HE1	2.02	0.42
12:L:81:LYS:HD3	12:L:262:ARG:HH11	1.83	0.42
13:M:29:SER:CB	32:g:91:PHE:HD2	2.27	0.42
14:N:315:THR:O	14:N:316:HIS:C	2.61	0.42
14:N:331:ILE:HG23	14:N:335:MET:HE3	2.01	0.42
15:O:229:VAL:HG21	15:O:234:LEU:HD21	2.02	0.42
16:P:279:TYR:O	16:P:280:ILE:C	2.62	0.42
16:P:354:ARG:HG3	16:P:362:LEU:CD2	2.48	0.42
18:R:44:ARG:C	18:R:46:VAL:N	2.73	0.42
24:Y:83:ARG:NH1	24:Y:90:LEU:HB3	2.34	0.42
31:f:37:PHE:O	33:h:134:GLU:HB3	2.20	0.42
32:g:106:TYR:CZ	33:h:86:ILE:HD12	2.54	0.42
32:g:119:GLU:OE1	32:g:122:ARG:NH1	2.53	0.42
33:h:57:VAL:CG1	39:n:99:VAL:HG23	2.50	0.42
34:i:81:PHE:O	34:i:82:VAL:C	2.60	0.42
37:l:62:TYR:CE2	37:l:64:PRO:HG3	2.55	0.42
44:s:35:LEU:HA	44:s:37:HIS:CE1	2.55	0.42
45:AA:342:GLN:HE21	45:AA:357:HIS:CB	2.31	0.42
46:AB:64:PHE:HB3	46:AB:401:LEU:HD11	2.01	0.42
48:AD:147:ALA:HA	48:AD:150:GLU:CD	2.44	0.42
46:Ab:162:LYS:HG3	46:Ab:191:TYR:HB3	2.00	0.42
46:Ab:312:SER:OG	46:Ab:357:GLN:NE2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:169:SER:O	47:Ac:170:VAL:C	2.62	0.42
50:Af:95:LEU:O	50:Af:96:LYS:C	2.61	0.42
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.49	0.42
2:B:126:ARG:O	2:B:128:ALA:N	2.50	0.42
4:D:43:TRP:CZ2	13:M:143:LEU:HD12	2.54	0.42
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.42
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.68	0.42
8:H:68:MET:HG3	8:H:68:MET:O	2.19	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:179:TRP:HE1	25:Z:43:LEU:HG	1.85	0.42
10:J:21:LEU:O	10:J:22:LYS:C	2.62	0.42
10:J:55:VAL:HG23	10:J:59:TYR:HB3	2.02	0.42
10:J:74:ALA:O	10:J:75:THR:CG2	2.68	0.42
11:K:59:ILE:HB	11:K:60:PRO:HD3	2.01	0.42
12:L:189:PHE:CZ	12:L:212:PRO:HB2	2.55	0.42
12:L:226:GLN:OE1	12:L:281:GLY:HA2	2.20	0.42
12:L:277:MET:CG	12:L:318:GLY:CA	2.98	0.42
12:L:396:ILE:HD13	12:L:396:ILE:HA	1.89	0.42
12:L:405:ASN:HB2	12:L:408:ALA:HB3	2.01	0.42
12:L:525:LEU:O	12:L:526:LEU:C	2.61	0.42
12:L:534:HIS:O	12:L:538:PRO:CG	2.60	0.42
58:L:703:3PE:H271	58:L:703:3PE:C3C	2.48	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: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:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.42
14:N:154:ILE:HD11	14:N:155:LEU:HG	2.02	0.42
14:N:226:THR:HG22	14:N:228:ASN:N	2.34	0.42
14:N:340:ALA:N	14:N:341:PRO:CD	2.83	0.42
15:O:48:LYS:O	15:O:52:LYS:HE3	2.19	0.42
15:O:258:TYR:CZ	15:O:269:VAL:HG13	2.55	0.42
15:O:272:ASP:HA	15:O:275:TYR:HD2	1.85	0.42
58:O:401:3PE:H3A2	29:d:36:LEU:HD11	2.01	0.42
16:P:242:VAL:HG13	16:P:243:ALA:N	2.35	0.42
17:Q:55:VAL:HG21	22:W:78:ASP:OD1	2.19	0.42
19:S:19:ILE:O	19:S:53:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:41:LYS:O	23:X:42:GLU:C	2.59	0.42
24:Y:45:LEU:O	24:Y:46:ASN:C	2.62	0.42
24:Y:76:THR:CG2	24:Y:92:TYR:HA	2.48	0.42
27:b:45:ILE:HG23	27:b:46:ASN:N	2.34	0.42
32:g:147:LEU:O	32:g:148:PRO:C	2.61	0.42
34:i:15:LEU:CD2	39:n:164:PRO:HB2	2.41	0.42
34:i:89:HIS:HB3	58:i:201:3PE:H122	2.02	0.42
35:j:52:ARG:HA	35:j:52:ARG:HD3	1.88	0.42
35:j:96:GLU:HG2	35:j:97:LEU:HD23	2.00	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
39:n:132:SER:O	39:n:133:TRP:C	2.62	0.42
39:n:139:GLN:HA	39:n:142:GLU:HG2	2.01	0.42
40:o:104:ARG:O	40:o:108:LEU:HG	2.20	0.42
41:p:6:ASP:O	41:p:7:LYS:C	2.63	0.42
44:s:53:SER:HA	44:s:56:ARG:HG2	2.02	0.42
45:AA:157:GLU:O	45:AA:161:ILE:HG13	2.19	0.42
46:AB:37:ASP:O	46:AB:38:LEU:C	2.60	0.42
46:AB:396:ILE:HG12	46:AB:406:TYR:HE1	1.84	0.42
46:AB:407:MET:HE1	46:AB:415:GLN:CD	2.45	0.42
49:AE:123:VAL:HG13	53:AJ:29:ALA:CA	2.40	0.42
49:AE:232:GLY:O	49:AE:244:ASP:HA	2.20	0.42
53:AJ:34:ARG:NH1	53:AJ:37:ASP:HB2	2.35	0.42
45:Aa:373:GLN:O	45:Aa:377:MET:HG2	2.19	0.42
46:Ab:225:VAL:HG22	46:Ab:229:VAL:HG21	2.02	0.42
46:Ab:346:ALA:O	46:Ab:347:ALA:C	2.62	0.42
47:Ac:33:PHE:O	47:Ac:36:LEU:HB2	2.19	0.42
47:Ac:133:LEU:HD23	47:Ac:133:LEU:HA	1.85	0.42
48:Ad:231:LEU:HD13	48:Ad:241:ALA:HB1	2.01	0.42
48:Ad:317:ARG:HD2	48:Ad:319:LEU:HD21	2.02	0.42
49:Ae:158:ASP:O	49:Ae:160:PRO:HD3	2.20	0.42
49:Ae:159:ILE:HD12	49:Ae:159:ILE:N	2.35	0.42
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.83	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
3:C:133:SER:OG	3:C:138:SER:N	2.53	0.42
4:D:35:ARG:NH2	32:g:57:PRO:O	2.53	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:227:PRO:HB3	7:G:95:PRO:HD3	2.01	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:104:PHE:CE2	58:J:401:3PE:H362	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.42
10:J:23:PRO:O	10:J:24:SER:C	2.61	0.42
12:L:51:LEU:HA	12:L:87:ILE:HD12	2.02	0.42
12:L:246:LEU:CD1	12:L:247:LEU:N	2.68	0.42
12:L:346:ILE:HG21	12:L:362:ILE:HD11	2.02	0.42
13:M:51:ASN:ND2	33:h:136:THR:CG2	2.83	0.42
13:M:191:SER:O	13:M:194:LEU:HB2	2.20	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:109:ALA:HB3	14:N:110:PRO:HD3	2.01	0.42
14:N:338:PRO:O	23:X:170:TRP:HZ3	2.03	0.42
15:O:258:TYR:OH	15:O:272:ASP:HB2	2.20	0.42
15:O:343:TYR:HB3	29:d:52:PRO:HD3	2.02	0.42
19:S:64:LYS:HE2	19:S:66:TRP:CZ2	2.55	0.42
21:V:36:LYS:HA	21:V:36:LYS:HD3	1.89	0.42
23:X:132:LYS:HB3	23:X:132:LYS:HE2	1.84	0.42
25:Z:120:LEU:HD12	25:Z:121:ILE:H	1.85	0.42
27:b:11:ASN:O	27:b:15:LYS:HG2	2.20	0.42
32:g:117:ARG:NH2	41:p:10:TYR:OH	2.53	0.42
32:g:123:LEU:CD1	41:p:98:VAL:HG11	2.50	0.42
33:h:55:PHE:HE1	33:h:57:VAL:HA	1.84	0.42
33:h:163:ARG:CG	33:h:165:ASP:HB2	2.32	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:109:LEU:HG	37:l:109:LEU:O	2.20	0.42
37:l:184:TYR:HD1	40:o:36:GLU:CA	2.32	0.42
38:m:15:PRO:HG2	38:m:18:LEU:HB2	2.01	0.42
38:m:125:PHE:CE1	41:p:133:THR:CG2	2.98	0.42
39:n:100:PRO:HB2	39:n:102:TRP:NE1	2.35	0.42
42:q:5:GLU:HG3	42:q:9:ARG:HE	1.84	0.42
46:AB:138:LEU:HD22	46:AB:238:LEU:HG	2.01	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
47:AC:42:MET:HG3	47:AC:42:MET:H	1.64	0.42
47:AC:184:ILE:HD13	47:Ac:49:LEU:HD22	2.02	0.42
47:AC:233:LEU:HD21	48:AD:300:LEU:N	2.35	0.42
48:AD:323:PRO:HB2	48:AD:325:LYS:HG3	2.02	0.42
49:AE:165:MET:HG3	49:AE:167:PHE:CE2	2.54	0.42
52:AH:28:LEU:HD11	52:AH:32:ARG:HE	1.85	0.42
45:Aa:48:THR:HB	45:Aa:423:ARG:HG2	2.02	0.42
47:Ac:74:ASN:O	47:Ac:75:TYR:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:146:ILE:HG12	68:Ac:404:U10:C4M	2.50	0.42
48:Ad:199:TYR:HA	48:Ad:278:SER:OG	2.20	0.42
49:Ae:167:PHE:CD2	49:Ae:174:LEU:HB3	2.49	0.42
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.42
2:B:94:THR:CB	2:B:104:MET:CE	2.97	0.42
4:D:37:TRP:O	4:D:37:TRP:CE3	2.73	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	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:365:ILE:CD1	12:L:366:MET:HG3	2.24	0.42
12:L:466:PHE:HE2	58:j:700:3PE:H361	1.84	0.42
12:L:491:LEU:HD13	35:j:80:VAL:HG22	2.01	0.42
12:L:552:LEU:HD21	38:m:90:GLY:CA	2.41	0.42
12:L:568:THR:O	12:L:569:LEU:C	2.61	0.42
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.01	0.42
14:N:108:LEU:HD22	14:N:191:LEU:HD22	2.02	0.42
14:N:239:ALA:HA	29:d:47:MET:HE2	2.02	0.42
14:N:243:MET:CG	29:d:44:MET:HE2	2.47	0.42
14:N:317:GLN:HG2	15:O:301:LYS:CB	2.49	0.42
17:Q:58:LYS:O	17:Q:58:LYS:HG3	2.20	0.42
17:Q:59:LEU:HD23	17:Q:59:LEU:HA	1.84	0.42
17:Q:75:ARG:NH1	17:Q:104:ARG:HG2	2.34	0.42
18:R:31:ILE:HG22	18:R:55:VAL:HG21	2.02	0.42
20:T:80:LYS:O	20:T:84:LEU:HG	2.20	0.42
23:X:52:ASP:O	23:X:53:PRO:C	2.61	0.42
27:b:15:LYS:O	27:b:16:GLU:HB2	2.20	0.42
27:b:59:ASP:HA	27:b:63:MET:CE	2.50	0.42
29:d:24:PRO:HD2	29:d:73:TYR:CE2	2.55	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CE2	2.54	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CD2	2.55	0.42
32:g:145:ILE:CG2	41:p:160:LYS:HE2	2.39	0.42
37:l:59:VAL:O	37:l:59:VAL:HG12	2.19	0.42
43:r:18:GLN:OE1	43:r:18:GLN:N	2.53	0.42
45:AA:174:GLU:C	45:AA:176:ASP:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:137:VAL:HA	49:AE:140:MET:HE3	2.01	0.42
49:AE:248:ARG:O	49:AE:250:ARG:HG2	2.20	0.42
45:Aa:74:TRP:HB3	45:Aa:418:LEU:HD11	2.02	0.42
45:Aa:305:GLN:HB3	45:Aa:395:LEU:HD11	2.01	0.42
45:Aa:358:PHE:CD2	45:Aa:368:MET:HG2	2.55	0.42
47:Ac:8:HIS:HB3	47:Ac:11:PHE:HD2	1.85	0.42
47:Ac:197:LEU:HD11	69:Ac:405:UQ6:H72	2.02	0.42
49:Ae:219:HIS:CG	49:Ae:239:HIS:HD2	2.38	0.42
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.20	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.67	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42
5:E:136:THR:HB	59:E:301:FES:S2	2.60	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	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:138:PHE:HZ	13:M:376:MET:HG2	1.85	0.42
12:L:390:TYR:HE2	35:j:68:TRP:HH2	1.67	0.42
57:L:706:PC1:H341	57:L:706:PC1:C25	2.50	0.42
14:N:180:ALA:O	14:N:184:ILE:HG13	2.20	0.42
15:O:195:LEU:N	15:O:196:PRO:HD2	2.35	0.42
20:U:120:MET:HE1	39:n:24:LEU:CD1	2.49	0.42
22:W:28:LEU:O	22:W:32:LYS:HG3	2.20	0.42
22:W:53:MET:SD	22:W:106:VAL:HG21	2.60	0.42
25:Z:102:PRO:O	25:Z:103:ASN:C	2.62	0.42
28:c:74:GLY:O	28:c:75:LEU:HB2	2.20	0.42
30:e:45:HIS:CD2	33:h:176:LYS:HZ2	2.36	0.42
35:j:71:TRP:HH2	58:j:700:3PE:C3A	2.33	0.42
38:m:8:PRO:HD3	38:m:14:LEU:HD13	2.02	0.42
40:o:59:CYS:SG	40:o:91:GLU:HG2	2.60	0.42
41:p:9:VAL:O	41:p:109:ARG:NH2	2.51	0.42
41:p:132:PHE:O	41:p:136:THR:OG1	2.17	0.42
42:q:25:ARG:O	42:q:26:VAL:C	2.62	0.42
42:q:39:VAL:HG21	42:q:89:TRP:CZ2	2.55	0.42
43:r:10:LYS:O	43:r:11:LEU:C	2.62	0.42
45:AA:400:VAL:O	45:AA:426:LEU:HD21	2.20	0.42
47:AC:148:ASN:OD1	49:Ae:221:GLY:N	2.52	0.42
47:AC:278:TYR:CE2	47:AC:282:ARG:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:259:THR:O	48:AD:260:PRO:C	2.60	0.42
51:AG:28:PRO:O	51:AG:29:SER:C	2.63	0.42
45:Aa:119:HIS:CE1	46:Ab:298:HIS:CD2	3.08	0.42
45:Aa:178:SER:OG	45:Aa:181:ASN:ND2	2.53	0.42
45:Aa:204:PRO:O	45:Aa:205:SER:C	2.63	0.42
45:Aa:340:SER:O	45:Aa:358:PHE:HA	2.20	0.42
46:Ab:286:PHE:CD1	46:Ab:427:ALA:HB1	2.54	0.42
47:Ac:237:LEU:HD22	48:Ad:300:LEU:HD11	2.02	0.42
49:Ae:154:ILE:N	49:Ae:154:ILE:HD12	2.35	0.42
50:Af:91:LEU:O	50:Af:92:GLU:C	2.62	0.42
52:Ah:48:LEU:O	52:Ah:51:CYS:HB3	2.20	0.42
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
1:A:81:THR:O	27:b:46:ASN:ND2	2.53	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	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
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
8:H:311:THR:O	25:Z:51:MET:CG	2.66	0.41
10:J:37:PHE:HD1	10:J:56:PHE:HE1	1.66	0.41
10:J:43:VAL:HG13	11:K:49:LEU:CD1	2.50	0.41
12:L:52:LEU:CB	41:p:30:ILE:HD11	2.50	0.41
12:L:407:TRP:CE3	12:L:410:LEU:HD21	2.55	0.41
12:L:489:THR:O	12:L:492:ILE:HG13	2.20	0.41
12:L:524:THR:HG22	39:n:78:GLN:CG	2.49	0.41
12:L:525:LEU:HD21	39:n:77:PRO:HB3	2.02	0.41
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.50	0.41
14:N:215:MET:SD	14:N:244:ILE:CD1	3.08	0.41
14:N:239:ALA:CB	29:d:47:MET:HG2	2.50	0.41
16:P:214:LEU:HD23	16:P:352:VAL:HG12	2.01	0.41
16:P:331:ASP:CG	16:P:332:LEU:H	2.28	0.41
20:T:90:TYR:CD2	20:T:92:LYS:HB3	2.54	0.41
20:U:128:PHE:HZ	20:U:148:ILE:CD1	2.33	0.41
22:W:76:VAL:HG13	22:W:82:VAL:HG22	2.02	0.41
22:W:78:ASP:HA	22:W:79:PRO:HD3	1.94	0.41
23:X:47:ARG:CZ	33:h:187:PRO:HB2	2.48	0.41
24:Y:10:SER:O	24:Y:11:TYR:C	2.62	0.41
62:a:101:CDL:HA22	42:q:6:VAL:HG12	2.01	0.41
38:m:41:ALA:HA	39:n:152:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:114:MET:HG3	39:n:115:TYR:CD2	2.55	0.41
49:AE:156:LEU:C	49:AE:158:ASP:N	2.76	0.41
49:AE:213:LEU:CD2	49:AE:260:VAL:HG22	2.40	0.41
49:AE:243:TYR:CD2	49:AE:258:LEU:HG	2.55	0.41
47:Ac:37:LEU:HD22	67:Ac:402:HEM:HBB2	2.02	0.41
49:Ae:168:LYS:HA	49:Ae:173:PRO:N	2.35	0.41
49:Ae:219:HIS:CG	49:Ae:239:HIS:CD2	3.08	0.41
49:Ae:241:SER:HA	49:Ae:251:LYS:CG	2.50	0.41
50:Af:52:PRO:HG2	50:Af:55:LEU:HG	2.02	0.41
1:A:112:GLU:O	1:A:113:TRP:CD1	2.73	0.41
2:B:146:ARG:NH2	3:C:211:TYR:CE2	2.89	0.41
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.41
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
57:B:303:PC1:H372	8:H:53:MET:SD	2.60	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
3:C:82:GLU:OE1	3:C:141:ARG:NH2	2.53	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:266:ARG:CA	9:I:65:GLU:OE2	2.68	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:19:PHE:CB	26:a:12:MET:HG3	2.49	0.41
9:I:152:CYS:SG	55:I:303:SF4:S1	3.17	0.41
10:J:10:SER:O	10:J:14:VAL:HG23	2.20	0.41
10:J:37:PHE:CE2	58:J:401:3PE:H2A2	2.55	0.41
10:J:59:TYR:OH	11:K:34:GLU:C	2.63	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:179:ILE:HD12	15:O:184:VAL:HG22	2.02	0.41
16:P:228:LEU:HD11	16:P:288:PHE:CZ	2.54	0.41
16:P:255:ASP:OD1	16:P:256:PRO:HD2	2.21	0.41
16:P:284:THR:HG22	16:P:286:ARG:HG3	2.02	0.41
20:T:115:GLN:O	20:T:116:VAL:C	2.63	0.41
20:U:93:ILE:CD1	20:U:110:LEU:HD11	2.49	0.41
23:X:70:PHE:CE1	23:X:117:TRP:CZ3	3.08	0.41
28:c:61:THR:HG21	29:d:74:PHE:CE1	2.55	0.41
33:h:182:SER:O	33:h:184:LYS:HE3	2.20	0.41
35:j:100:PRO:O	35:j:101:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:102:ASP:O	35:j:103:ASP:HB2	2.20	0.41
37:l:159:LYS:HE3	37:l:161:TYR:HE1	1.86	0.41
40:o:47:MET:HE1	41:p:123:GLN:NE2	2.35	0.41
42:q:64:TYR:CD1	42:q:77:VAL:HG11	2.54	0.41
45:AA:271:THR:HG23	51:AG:23:GLU:HG2	2.02	0.41
46:AB:325:ALA:O	49:AI:11:PHE:CE2	2.73	0.41
48:AD:201:VAL:HG23	48:AD:202:ARG:N	2.35	0.41
48:AD:317:ARG:HD2	48:AD:319:LEU:HD21	2.02	0.41
49:AI:61:ALA:CA	46:Ab:326:PHE:HD1	2.32	0.41
47:Ac:96:LEU:HD23	58:Ac:403:3PE:H292	2.01	0.41
49:Ae:200:HIS:CE1	49:Ae:201:ASP:OD1	2.73	0.41
49:Ae:204:ARG:NH2	49:Ae:247:GLY:HA3	2.27	0.41
54:Ak:41:ILE:HA	54:Ak:44:TRP:CZ3	2.55	0.41
2:B:91:TRP:CZ2	61:H:400:UQ9:C1M	3.03	0.41
3:C:170:TRP:HE1	22:W:91:MET:HE1	1.86	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.02	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.56	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.81	0.41
12:L:293:LEU:O	12:L:425:ARG:HD2	2.20	0.41
12:L:355:ASP:O	12:L:359:MET:HG3	2.20	0.41
13:M:165:ILE:HG21	14:N:268:THR:HA	2.01	0.41
13:M:258:ALA:O	13:M:259:TYR:C	2.62	0.41
15:O:179:ILE:CD1	15:O:184:VAL:HG22	2.50	0.41
15:O:267:THR:O	15:O:271:GLU:HG3	2.19	0.41
18:R:72:VAL:HG12	18:R:73:GLU:H	1.85	0.41
20:T:123:GLU:HG2	20:T:130:ILE:HD12	2.02	0.41
26:a:64:LYS:CE	26:a:66:LEU:HD12	2.31	0.41
27:b:61:GLY:O	27:b:63:MET:HG3	2.20	0.41
62:h:201:CDL:H732	34:i:84:TYR:HB2	2.01	0.41
34:i:20:ARG:HH11	34:i:20:ARG:HG3	1.84	0.41
34:i:111:LEU:HD11	41:p:20:PRO:HD3	2.02	0.41
39:n:56:ASP:O	39:n:59:ARG:N	2.54	0.41
45:AA:148:ALA:O	45:AA:152:GLN:HG2	2.20	0.41
45:AA:152:GLN:NE2	45:AA:250:LEU:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:192:PHE:HD1	45:AA:269:ARG:O	2.04	0.41
47:AC:145:VAL:HA	49:Ae:220:LEU:O	2.21	0.41
49:AE:168:LYS:HE2	47:Ac:261:PRO:HG2	2.01	0.41
49:AE:272:VAL:O	49:AE:273:VAL:C	2.59	0.41
45:Aa:338:CYS:SG	45:Aa:359:VAL:O	2.79	0.41
45:Aa:391:GLY:O	45:Aa:392:LYS:C	2.64	0.41
46:Ab:232:GLN:O	46:Ab:235:GLU:HG3	2.20	0.41
48:Ad:202:ARG:HG3	48:Ad:278:SER:HB3	2.02	0.41
49:Ae:184:ILE:HG21	49:Ae:208:PRO:HB3	2.01	0.41
2:B:95:PHE:HE2	2:B:131:MET:CE	2.33	0.41
4:D:67:ASN:HB3	4:D:69:VAL:CG1	2.41	0.41
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.41
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.41
4:D:448:VAL:HG11	8:H:205:SER:HB2	2.02	0.41
58:D:501:3PE:H272	14:N:288:LEU:CD1	2.49	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	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:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:50:MET:O	9:I:54:THR:N	2.37	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
9:I:89:GLU:CG	42:q:61:TRP:HB3	2.50	0.41
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.41
10:J:55:VAL:HB	11:K:41:PHE:HE2	1.86	0.41
58:J:401:3PE:H2E1	58:J:401:3PE:H2H2	1.83	0.41
58:K:101:3PE:H261	58:K:101:3PE:H232	1.92	0.41
12:L:159:TYR:CZ	39:n:96:CYS:HB2	2.55	0.41
12:L:218:ILE:HD11	58:L:703:3PE:H2A2	2.02	0.41
12:L:286:LEU:HG	12:L:290:ILE:HD11	2.01	0.41
13:M:7:PRO:HG3	31:f:20:PHE:HA	2.01	0.41
13:M:85:LYS:O	13:M:85:LYS:HG2	2.21	0.41
13:M:142:ARG:HG3	13:M:143:LEU:N	2.36	0.41
13:M:247:SER:OG	13:M:304:GLN:NE2	2.53	0.41
15:O:64:GLY:O	15:O:161:ARG:NH1	2.53	0.41
15:O:231:SER:O	15:O:232:ALA:C	2.62	0.41
15:O:239:ASN:HB3	15:O:243:LYS:HD3	2.02	0.41
16:P:243:ALA:O	16:P:244:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:87:LEU:CD2	20:T:122:MET:CE	2.98	0.41
20:T:100:VAL:O	20:T:141:PRO:HD2	2.20	0.41
20:T:118:ILE:HD13	20:T:118:ILE:HA	1.83	0.41
24:Y:141:PRO:HB2	33:h:161:ARG:NE	2.35	0.41
26:a:49:GLU:OE2	26:a:49:GLU:HA	2.20	0.41
27:b:25:VAL:O	27:b:26:TRP:C	2.64	0.41
27:b:31:ILE:O	27:b:32:MET:C	2.63	0.41
27:b:78:LEU:O	27:b:81:LEU:N	2.53	0.41
31:f:7:LEU:HG	31:f:11:TRP:HB3	2.02	0.41
32:g:69:PRO:HB2	39:n:109:PRO:CD	2.49	0.41
32:g:71:PHE:CE2	32:g:73:GLY:HA2	2.55	0.41
37:l:122:THR:HG22	37:l:124:VAL:H	1.85	0.41
38:m:42:ARG:O	38:m:43:LEU:C	2.62	0.41
42:q:87:HIS:O	42:q:91:HIS:HD2	2.04	0.41
45:AA:92:PHE:HD1	45:AA:168:ILE:HD12	1.86	0.41
47:AC:128:PHE:CD2	68:AC:404:U10:O5	2.74	0.41
47:AC:287:LYS:NZ	49:Ae:255:PRO:HG2	2.35	0.41
45:Aa:269:ARG:NH1	45:Aa:271:THR:OG1	2.53	0.41
45:Aa:278:ARG:CZ	45:Aa:463:GLU:HB2	2.50	0.41
47:Ac:48:GLY:HA3	67:Ac:401:HEM:C2B	2.55	0.41
47:Ac:128:PHE:CD1	68:Ac:404:U10:C4M	3.02	0.41
47:Ac:171:ASP:CG	47:Ac:172:LYS:N	2.76	0.41
47:Ac:220:PHE:CD2	69:Ac:405:UQ6:H3M3	2.56	0.41
47:Ac:264:THR:O	47:Ac:265:PRO:C	2.62	0.41
47:Ac:295:ILE:HG22	47:Ac:299:LEU:HD12	2.02	0.41
48:Ad:154:VAL:HG21	48:Ad:173:ASP:OD2	2.20	0.41
49:Ae:168:LYS:CA	49:Ae:173:PRO:HA	2.49	0.41
49:Ae:241:SER:HB2	49:Ae:252:GLY:HA3	2.02	0.41
1:A:90:MET:HE2	10:J:152:MET:CB	2.45	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.36	0.41
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.41
4:D:47:PHE:CD1	14:N:227:ILE:HD11	2.55	0.41
4:D:71:ILE:O	4:D:72:LEU:C	2.62	0.41
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.17	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
8:H:206:GLU:O	8:H:207:LEU:HB2	2.20	0.41
10:J:17:LEU:O	10:J:21:LEU:HG	2.20	0.41
11:K:25:HIS:CD2	11:K:88:ASP:OD1	2.70	0.41
12:L:74:MET:CE	13:M:307:TRP:HH2	2.34	0.41
12:L:546:LEU:HD22	38:m:72:ARG:NH2	2.35	0.41
13:M:216:LEU:CG	13:M:220:HIS:CE1	2.88	0.41
13:M:270:ILE:HD11	13:M:395:LEU:HA	2.03	0.41
13:M:270:ILE:HD12	13:M:395:LEU:HD22	2.02	0.41
13:M:350:MET:HE3	13:M:350:MET:HB2	1.80	0.41
14:N:83:THR:HG22	14:N:84:TRP:N	2.35	0.41
14:N:159:ILE:HB	14:N:278:MET:HE1	2.01	0.41
14:N:191:LEU:HG	14:N:191:LEU:O	2.20	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:261:TRP:H	15:O:261:TRP:HE3	1.68	0.41
15:O:263:ALA:C	15:O:265:ASP:N	2.77	0.41
16:P:230:SER:O	16:P:231:LEU:C	2.63	0.41
16:P:316:LYS:C	16:P:316:LYS:HD3	2.46	0.41
17:Q:85:ASN:C	17:Q:87:MET:N	2.76	0.41
18:R:64:ILE:HD12	18:R:64:ILE:HA	1.95	0.41
19:S:20:ARG:HD2	19:S:22:HIS:NE2	2.35	0.41
24:Y:21:HIS:NE2	51:Ag:62:TRP:N	2.69	0.41
26:a:49:GLU:O	26:a:50:ARG:C	2.62	0.41
33:h:144:SER:HB2	41:p:82:VAL:CG2	2.49	0.41
33:h:175:GLU:HB2	33:h:178:PHE:CE2	2.55	0.41
35:j:44:TYR:CD2	35:j:45:ARG:HG3	2.56	0.41
38:m:18:LEU:HD11	39:n:72:TRP:CB	2.50	0.41
38:m:124:LYS:O	38:m:126:ASN:N	2.54	0.41
40:o:53:LEU:HD23	40:o:56:ARG:NE	2.34	0.41
40:o:117:LEU:O	40:o:120:ALA:N	2.52	0.41
45:AA:204:PRO:O	45:AA:205:SER:C	2.63	0.41
45:AA:298:ASN:OD1	45:AA:299:PRO:HD2	2.20	0.41
47:AC:215:ALA:HB2	50:AF:60:MET:HE3	2.02	0.41
47:AC:264:THR:O	47:AC:265:PRO:C	2.59	0.41
47:AC:295:ILE:HG22	47:AC:299:LEU:HD12	2.02	0.41
49:AE:190:VAL:HG11	49:AE:248:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AH:66:THR:CG2	52:AH:67:GLU:N	2.83	0.41
53:AJ:30:LEU:HA	54:AK:34:TRP:CG	2.56	0.41
47:Ac:284:ILE:HG21	47:Ac:289:GLY:HA3	2.02	0.41
48:Ad:157:GLY:CA	48:Ad:164:MET:HA	2.50	0.41
48:Ad:163:GLU:O	48:Ad:164:MET:HB3	2.20	0.41
48:Ad:167:ARG:NH1	48:Ad:173:ASP:HB2	2.21	0.41
48:Ad:224:GLY:HA3	52:Ah:64:ASP:OD1	2.21	0.41
49:Ae:132:VAL:HA	49:Ae:135:GLN:OE1	2.20	0.41
54:Ak:18:ILE:N	54:Ak:19:PRO:HD2	2.34	0.41
2:B:224:ARG:HG3	16:P:85:ARG:HH12	1.84	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.18	0.41
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.51	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
6:F:119:GLU:CD	60:F:501:FMN:HN3	2.28	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
10:J:32:LEU:HD12	10:J:32:LEU:HA	1.86	0.41
12:L:202:MET:HE3	12:L:265:PRO:CB	2.50	0.41
12:L:231:PRO:O	12:L:234:PRO:HD2	2.20	0.41
13:M:263:LEU:CD1	38:m:102:TYR:CD1	3.00	0.41
15:O:262:GLU:O	15:O:265:ASP:HB3	2.21	0.41
15:O:355:LYS:O	29:d:59:HIS:HE1	2.04	0.41
16:P:265:PHE:N	16:P:265:PHE:CD1	2.87	0.41
20:T:134:ASP:HA	20:T:137:LYS:NZ	2.35	0.41
20:U:89:LEU:HD12	35:j:45:ARG:HH12	1.86	0.41
22:W:86:VAL:O	22:W:87:ILE:C	2.62	0.41
62:a:101:CDL:HA62	42:q:10:GLY:CA	2.51	0.41
30:e:41:ILE:HD11	33:h:174:PRO:N	2.36	0.41
30:e:49:GLY:O	30:e:52:ALA:N	2.54	0.41
35:j:99:ILE:HA	40:o:108:LEU:HD21	2.03	0.41
37:l:48:ARG:NH2	37:l:64:PRO:HD2	2.36	0.41
37:l:63:GLU:O	37:l:64:PRO:C	2.63	0.41
40:o:111:ARG:HG3	40:o:114:ARG:HH11	1.85	0.41
41:p:71:VAL:HB	41:p:72:PRO:CD	2.50	0.41
41:p:73:ASP:OD1	41:p:73:ASP:N	2.54	0.41
42:q:50:GLU:HA	42:q:59:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:109:LEU:HD21	45:AA:120:LEU:CD2	2.51	0.41
46:AB:65:VAL:HG22	46:AB:218:MET:HG2	2.03	0.41
47:AC:284:ILE:HG21	47:AC:289:GLY:HA3	2.02	0.41
48:AD:148:LEU:HA	48:AD:151:GLU:CD	2.46	0.41
52:AH:39:GLU:HG2	52:AH:43:LYS:HE2	2.03	0.41
45:Aa:62:GLU:OE1	45:Aa:423:ARG:NH1	2.45	0.41
45:Aa:410:CYS:C	45:Aa:412:ASP:N	2.78	0.41
47:Ac:278:TYR:CE2	47:Ac:282:ARG:HD2	2.54	0.41
47:Ac:378:LYS:HG3	50:Af:18:ARG:NH1	2.36	0.41
48:Ad:114:PHE:O	48:Ad:117:TYR:N	2.54	0.41
49:Ae:153:GLU:C	49:Ae:154:ILE:HD12	2.45	0.41
52:Ah:33:GLU:O	52:Ah:37:GLN:HG3	2.20	0.41
52:Ah:76:ARG:O	52:Ah:80:VAL:HG23	2.21	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
4:D:50:ALA:C	4:D:51:VAL:HG13	2.45	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
10:J:5:ILE:O	10:J:6:PHE:C	2.63	0.41
10:J:60:LEU:O	10:J:64:LEU:HB2	2.20	0.41
12:L:258:PHE:O	12:L:261:VAL:HG22	2.21	0.41
13:M:4:ILE:CD1	13:M:41:LEU:HD21	2.51	0.41
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.55	0.41
13:M:319:HIS:HA	13:M:322:THR:CG2	2.44	0.41
14:N:168:GLY:HA3	14:N:181:TYR:CE1	2.56	0.41
15:O:117:PHE:CZ	15:O:173:MET:HE3	2.54	0.41
15:O:229:VAL:HG13	15:O:229:VAL:O	2.21	0.41
19:S:16:LEU:CB	19:S:69:TYR:CD1	2.97	0.41
23:X:26:LYS:HE2	23:X:26:LYS:HB3	1.85	0.41
23:X:70:PHE:O	23:X:74:ILE:HG13	2.21	0.41
25:Z:90:ASN:O	25:Z:94:GLU:HB2	2.21	0.41
26:a:48:MET:HE3	26:a:48:MET:HB2	1.77	0.41
41:p:91:GLN:O	41:p:91:GLN:HG2	2.21	0.41
45:AA:341:PHE:O	45:AA:341:PHE:CG	2.74	0.41
47:AC:133:LEU:HD23	47:AC:133:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:119:GLN:OE1	48:AD:253:LEU:HB2	2.20	0.41
48:AD:157:GLY:HA2	48:AD:165:PHE:HB3	2.03	0.41
48:AD:235:PRO:HB3	52:AH:70:PHE:HE1	1.80	0.41
49:AE:154:ILE:HG22	49:AE:155:LYS:N	2.34	0.41
49:AE:169:TRP:CD1	49:AE:170:ARG:HG3	2.55	0.41
49:Ae:147:LEU:HD23	49:Ae:147:LEU:HA	1.94	0.41
54:Ak:39:ARG:NE	54:Ak:39:ARG:HA	2.36	0.41
1:A:8:PHE:CE1	58:J:401:3PE:H2C1	2.48	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.86	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:42:PHE:HE1	6:F:249:ALA:HB1	1.86	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.02	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:75:PRO:HB2	8:H:222:LEU:HB2	2.03	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:172:MET:HE1	25:Z:46:GLY:HA3	2.01	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
10:J:72:ALA:O	10:J:76:GLU:HB2	2.21	0.41
12:L:253:VAL:HB	12:L:310:LEU:CD1	2.51	0.41
12:L:368:PHE:HB3	12:L:445:GLU:OE1	2.20	0.41
12:L:482:MET:CE	12:L:486:LEU:HB3	2.51	0.41
12:L:571:THR:O	12:L:574:THR:HG22	2.20	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:177:MET:HE3	13:M:177:MET:HB3	1.70	0.41
15:O:105:ASP:OD1	15:O:106:ILE:N	2.53	0.41
15:O:287:ASP:HB3	15:O:290:THR:HG23	2.02	0.41
15:O:332:ARG:O	15:O:338:LYS:HA	2.21	0.41
18:R:60:ALA:O	18:R:61:ILE:C	2.63	0.41
20:T:87:LEU:HD11	20:T:141:PRO:HG3	2.03	0.41
27:b:16:GLU:N	27:b:17:PRO:HD3	2.35	0.41
33:h:96:ALA:CB	41:p:63:TYR:HD1	2.29	0.41
36:k:20:MET:HE2	36:k:20:MET:HB3	1.98	0.41
36:k:81:PHE:O	36:k:85:VAL:HG23	2.21	0.41
37:l:129:MET:HE3	37:l:129:MET:HB2	1.89	0.41
42:q:64:TYR:CE2	42:q:81:MET:HB2	2.56	0.41
42:q:85:GLU:HG2	42:q:98:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:37:ASP:N	46:AB:37:ASP:OD1	2.52	0.41
46:AB:176:ASN:CB	46:AB:258:ILE:HD11	2.51	0.41
48:AD:318:LYS:HE3	49:AE:87:ASP:O	2.21	0.41
51:AG:26:ALA:C	51:AG:28:PRO:HD3	2.46	0.41
51:AG:35:ILE:O	51:AG:36:PRO:C	2.63	0.41
45:Aa:48:THR:CB	45:Aa:423:ARG:HG2	2.50	0.41
45:Aa:401:SER:O	45:Aa:402:HIS:C	2.64	0.41
48:Ad:322:ARG:O	51:Ag:13:HIS:HB3	2.20	0.41
49:Ae:239:HIS:HD1	49:Ae:241:SER:HB3	1.86	0.41
49:Ae:272:VAL:HG12	49:Ae:273:VAL:N	2.35	0.41
50:Af:82:THR:HG22	50:Af:83:LYS:N	2.36	0.41
51:Ag:19:LEU:HD11	51:Ag:23:GLU:HG2	2.03	0.41
1:A:90:MET:SD	10:J:149:THR:OG1	2.79	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
2:B:111:ARG:NE	4:D:208:GLU:HG2	2.35	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41
3:C:47:ARG:HG3	4:D:160:ASN:HA	2.03	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.36	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.41
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.33	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:163:LYS:HD3	7:G:163:LYS:HA	1.84	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.41
8:H:25:ARG:HD2	61:H:400:UQ9:C10	2.48	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.41
8:H:224:PHE:CD2	61:H:400:UQ9:H13	2.50	0.41
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.41
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
10:J:72:ALA:O	10:J:73:MET:C	2.64	0.41
10:J:93:VAL:O	10:J:97:ILE:HG12	2.20	0.41
10:J:122:ASP:HA	25:Z:133:MET:SD	2.61	0.41
11:K:93:LEU:HD13	14:N:57:THR:CG2	2.50	0.41
12:L:58:ASN:HA	12:L:58:ASN:HD22	1.65	0.41
12:L:68:TRP:CE3	12:L:76:LEU:CD2	3.04	0.41
12:L:211:ILE:N	12:L:212:PRO:CD	2.82	0.41
12:L:321:GLN:NE2	12:L:324:LEU:HD13	2.36	0.41
12:L:511:LEU:CD1	39:n:36:LYS:HA	2.50	0.41
12:L:570:HIS:O	12:L:573:MET:N	2.54	0.41
62:L:705:CDL:H581	62:L:705:CDL:H741	2.02	0.41
13:M:22:LYS:HE3	13:M:26:ASN:HD21	1.86	0.41
13:M:51:ASN:O	33:h:135:LYS:HD2	2.21	0.41
13:M:53:SER:O	13:M:54:ASN:C	2.63	0.41
13:M:178:ILE:O	13:M:179:LEU:C	2.60	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.03	0.41
13:M:218:LYS:HE3	13:M:218:LYS:HB3	1.58	0.41
13:M:250:LEU:HD12	13:M:250:LEU:C	2.40	0.41
13:M:329:LEU:HD23	13:M:437:MET:CE	2.49	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:175:MET:O	14:N:176:ARG:C	2.63	0.41
14:N:215:MET:HE3	14:N:215:MET:HB3	1.96	0.41
14:N:233:LEU:CD2	14:N:241:LEU:HD12	2.26	0.41
14:N:307:THR:CG2	14:N:308:ASN:N	2.79	0.41
14:N:307:THR:O	15:O:319:ILE:N	2.50	0.41
14:N:331:ILE:HD12	14:N:335:MET:HE3	2.03	0.41
15:O:52:LYS:HD3	15:O:152:SER:O	2.20	0.41
15:O:90:GLY:H	15:O:93:TYR:HB2	1.85	0.41
15:O:104:LEU:HD23	15:O:104:LEU:HA	1.90	0.41
15:O:132:GLN:OE1	63:O:402:ADP:N6	2.45	0.41
15:O:254:GLU:OE2	15:O:276:LEU:HB2	2.21	0.41
15:O:354:LEU:HD12	15:O:354:LEU:HA	1.95	0.41
16:P:135:GLU:HG3	16:P:140:ASP:HA	2.03	0.41
16:P:362:LEU:HA	16:P:362:LEU:HD23	1.88	0.41
18:R:55:VAL:HG22	18:R:56:ASN:N	2.35	0.41
20:U:128:PHE:CZ	20:U:148:ILE:CD1	3.04	0.41
21:V:96:LYS:HE2	21:V:96:LYS:HB2	1.95	0.41
21:V:98:LYS:HG2	21:V:100:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:37:ASP:OD1	23:X:37:ASP:C	2.62	0.41
25:Z:19:ILE:HG22	25:Z:20:ASP:N	2.36	0.41
25:Z:62:ILE:HG13	27:b:49:THR:HG22	2.02	0.41
26:a:2:TRP:CH2	62:a:101:CDL:H522	2.55	0.41
27:b:49:THR:HA	27:b:50:PRO:HD3	1.89	0.41
28:c:55:TRP:NE1	29:d:66:THR:CG2	2.84	0.41
29:d:25:LYS:HE3	29:d:27:ASN:OD1	2.21	0.41
30:e:65:GLU:CD	30:e:71:LYS:HB2	2.46	0.41
30:e:96:PRO:O	30:e:99:SER:N	2.53	0.41
30:e:101:ARG:HA	30:e:101:ARG:HE	1.86	0.41
31:f:47:GLU:O	31:f:48:LEU:C	2.60	0.41
32:g:117:ARG:NH2	41:p:108:GLU:OE1	2.54	0.41
34:i:29:SER:O	34:i:32:GLU:HB2	2.21	0.41
34:i:74:HIS:O	34:i:78:PRO:HG2	2.20	0.41
37:l:44:THR:HG23	37:l:46:GLU:HG2	2.03	0.41
37:l:156:VAL:CG1	40:o:95:TYR:CZ	2.91	0.41
39:n:94:TYR:HB3	39:n:178:PRO:HD2	2.03	0.41
40:o:5:LEU:HD12	40:o:5:LEU:N	2.35	0.41
40:o:17:PRO:HG3	40:o:106:ARG:CA	2.48	0.41
40:o:53:LEU:HD11	41:p:122:GLN:HG3	2.03	0.41
40:o:71:ARG:NH1	40:o:72:ASP:OD1	2.54	0.41
41:p:40:VAL:O	41:p:44:PRO:HG2	2.21	0.41
46:AB:64:PHE:CZ	46:AB:394:SER:HA	2.56	0.41
46:AB:112:VAL:HB	49:AI:19:SER:OG	2.20	0.41
47:AC:49:LEU:HD13	47:Ac:184:ILE:HD12	2.03	0.41
48:AD:165:PHE:CE2	48:AD:167:ARG:HB3	2.56	0.41
48:AD:318:LYS:HD2	49:AE:86:PRO:HB2	2.03	0.41
49:AE:235:TYR:HA	49:AE:241:SER:O	2.21	0.41
50:AF:102:ARG:HA	50:AF:105:ARG:CZ	2.49	0.41
51:AG:57:TYR:O	51:AG:61:THR:HG23	2.21	0.41
45:Aa:73:VAL:HG11	45:Aa:151:VAL:HG11	2.03	0.41
45:Aa:74:TRP:HH2	45:Aa:410:CYS:SG	2.43	0.41
45:Aa:418:LEU:HD23	45:Aa:418:LEU:HA	1.95	0.41
46:Ab:64:PHE:HZ	46:Ab:394:SER:HA	1.86	0.41
46:Ab:227:HIS:HD2	46:Ab:231:LYS:HE2	1.85	0.41
46:Ab:407:MET:HE1	46:Ab:415:GLN:CD	2.45	0.41
46:Ab:426:LYS:HA	46:Ab:429:LYS:NZ	2.36	0.41
47:Ac:21:LEU:O	47:Ac:22:PRO:C	2.63	0.41
47:Ac:69:ILE:HA	47:Ac:73:VAL:CG2	2.51	0.41
47:Ac:103:TYR:HD1	47:Ac:325:TYR:CD2	2.38	0.41
49:Ae:197:ASP:HB2	49:Ae:257:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:216:VAL:HG13	49:Ae:221:GLY:HA2	2.03	0.41
51:Ag:76:ALA:C	51:Ag:79:GLU:HG3	2.46	0.41
52:Ah:34:HIS:HA	52:Ah:37:GLN:OE1	2.20	0.41
1:A:70:ALA:CB	10:J:54:MET:HE1	2.51	0.41
1:A:102:LEU:O	1:A:106:TRP:HD1	2.04	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:79:ASN:HB2	4:D:100:GLU:HB3	2.03	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.21	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.55	0.41
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.41
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.41
8:H:300:LEU:HD23	27:b:25:VAL:HG11	2.02	0.41
9:I:180:HIS:CE1	16:P:100:LEU:HD21	2.55	0.41
10:J:131:VAL:HG12	25:Z:68:ARG:HH11	1.86	0.41
12:L:52:LEU:O	12:L:53:MET:C	2.62	0.41
12:L:56:HIS:N	40:o:74:PHE:CE1	2.88	0.41
13:M:6:LEU:O	13:M:7:PRO:C	2.60	0.41
13:M:72:LEU:O	13:M:76:MET:N	2.45	0.41
58:M:503:3PE:O14	29:d:47:MET:HE3	2.20	0.41
15:O:117:PHE:CE1	15:O:128:SER:CB	2.96	0.41
15:O:268:LYS:HA	15:O:271:GLU:OE1	2.21	0.41
19:S:41:TYR:HE1	19:S:53:ILE:HG23	1.85	0.41
20:T:107:ASP:OD1	20:T:108:LEU:N	2.54	0.41
20:T:120:MET:O	20:T:121:ALA:C	2.63	0.41
20:U:133:ILE:CG2	20:U:134:ASP:N	2.84	0.41
23:X:167:PHE:HD2	23:X:170:TRP:HE1	1.65	0.41
24:Y:5:LYS:C	24:Y:7:PHE:N	2.77	0.41
24:Y:51:THR:HG23	24:Y:52:LEU:N	2.35	0.41
29:d:45:ASP:O	29:d:46:ASN:C	2.62	0.41
31:f:36:ALA:O	31:f:37:PHE:C	2.61	0.41
33:h:60:SER:HB2	39:n:107:TRP:CD1	2.56	0.41
34:i:80:TRP:HE1	41:p:44:PRO:HG2	1.86	0.41
36:k:57:TRP:HA	36:k:60:MET:HB3	2.02	0.41
38:m:59:HIS:O	38:m:60:ILE:C	2.64	0.41
58:m:201:3PE:H362	58:m:201:3PE:H332	1.91	0.41
39:n:139:GLN:O	39:n:140:LEU:C	2.64	0.41
39:n:157:ALA:O	39:n:158:ARG:HB2	2.21	0.41
39:n:167:TRP:CD1	39:n:167:TRP:H	2.38	0.41
45:AA:86:ASN:OD1	45:AA:86:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:95:HIS:HB3	45:AA:164:GLU:OE1	2.21	0.41
45:AA:384:THR:HG22	54:AK:13:LEU:HD21	2.02	0.41
47:AC:275:LEU:O	47:AC:276:PHE:C	2.64	0.41
47:AC:363:LEU:HD23	47:AC:363:LEU:HA	1.95	0.41
48:AD:208:GLU:HG3	48:AD:209:ASP:H	1.86	0.41
48:AD:214:LEU:O	48:AD:217:GLY:N	2.45	0.41
49:AE:141:SER:O	49:AE:142:ALA:C	2.64	0.41
52:AH:32:ARG:HA	52:AH:80:VAL:HG22	2.02	0.41
49:AI:65:VAL:HG13	46:Ab:115:THR:HG22	2.03	0.41
45:Aa:147:LEU:HD23	45:Aa:147:LEU:HA	1.93	0.41
46:Ab:239:ASN:OD1	46:Ab:239:ASN:N	2.53	0.41
47:Ac:8:HIS:CG	47:Ac:11:PHE:HD2	2.38	0.41
47:Ac:42:MET:HG2	69:Ac:405:UQ6:H203	2.03	0.41
48:Ad:117:TYR:CE1	48:Ad:127:MET:HG2	2.56	0.41
48:Ad:250:THR:HG23	48:Ad:262:THR:HA	2.03	0.41
49:Ae:88:PHE:C	49:Ae:92:ARG:HG3	2.46	0.41
49:Ae:175:PHE:CE1	49:Ae:215:GLY:HA3	2.55	0.41
49:Ae:214:ILE:HG12	49:Ae:261:PRO:HD3	2.02	0.41
51:Ag:10:ARG:NH2	51:Ag:12:ARG:HD2	2.36	0.41
51:Ag:57:TYR:O	51:Ag:61:THR:HG23	2.21	0.41
2:B:163:SER:HB2	9:I:150:THR:O	2.20	0.40
3:C:101:ASP:O	21:V:90:LEU:HD13	2.21	0.40
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.41	0.40
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.85	0.40
6:F:225:LEU:HB2	17:Q:160:TYR:CE2	2.57	0.40
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.84	0.40
7:G:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:312:GLY:O	42:q:143:PRO:HA	2.21	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:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
12:L:434:LYS:NZ	36:k:66:ASN:HA	2.36	0.40
57:L:706:PC1:H382	57:L:706:PC1:H351	1.93	0.40
13:M:151:PHE:HZ	14:N:291:PHE:CA	2.34	0.40
15:O:351:TRP:CZ3	28:c:41:TRP:HH2	2.39	0.40
16:P:143:ASP:OD1	16:P:147:ASN:ND2	2.54	0.40
16:P:146:VAL:HG13	16:P:147:ASN:OD1	2.21	0.40
16:P:293:LEU:HD12	16:P:294:PRO:HD2	2.01	0.40
17:Q:55:VAL:HG21	22:W:80:ARG:HH11	1.85	0.40
19:S:22:HIS:CD2	19:S:66:TRP:HD1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:91:ASP:OD2	36:k:48:ARG:NH1	2.53	0.40
25:Z:10:MET:HE2	25:Z:10:MET:HB3	1.72	0.40
62:a:101:CDL:OB7	42:q:3:LEU:HD13	2.21	0.40
33:h:87:THR:O	33:h:91:ILE:HG13	2.21	0.40
33:h:148:GLU:O	33:h:152:LYS:HG3	2.21	0.40
35:j:47:PHE:O	35:j:48:PRO:C	2.62	0.40
37:l:159:LYS:HE3	37:l:161:TYR:CE1	2.56	0.40
38:m:123:ARG:O	41:p:140:GLN:NE2	2.48	0.40
58:m:201:3PE:H2E2	58:m:201:3PE:H2B1	1.70	0.40
39:n:41:ALA:C	39:n:43:LEU:N	2.78	0.40
42:q:39:VAL:CG1	42:q:97:PRO:HB3	2.52	0.40
42:q:68:MET:HE1	42:q:81:MET:O	2.21	0.40
45:AA:127:GLU:OE2	45:AA:348:TYR:HB3	2.21	0.40
47:AC:148:ASN:CB	49:Ae:220:LEU:HA	2.51	0.40
48:AD:147:ALA:HA	48:AD:150:GLU:HG2	2.02	0.40
48:AD:235:PRO:HA	48:AD:240:GLN:CG	2.50	0.40
48:AD:281:GLU:O	48:AD:282:HIS:C	2.64	0.40
45:Aa:148:ALA:HB2	45:Aa:250:LEU:HG	2.03	0.40
45:Aa:148:ALA:O	45:Aa:152:GLN:HG2	2.20	0.40
45:Aa:170:ARG:HG3	45:Aa:171:GLU:N	2.36	0.40
45:Aa:402:HIS:O	45:Aa:403:LEU:C	2.64	0.40
47:Ac:14:ILE:O	47:Ac:15:ASN:C	2.64	0.40
49:Ae:197:ASP:HB2	49:Ae:257:ASN:ND2	2.35	0.40
50:Af:92:GLU:O	50:Af:93:PRO:C	2.63	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40
2:B:138:THR:HG21	4:D:116:LEU:HA	2.02	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
58:D:501:3PE:H322	58:D:501:3PE:H351	1.79	0.40
5:E:109:MET:HE2	7:G:196:GLY:CA	2.51	0.40
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
7:G:277:MET:HE1	17:Q:153:PRO:HD3	2.03	0.40
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
12:L:3:ILE:HG22	12:L:49:LEU:CD2	2.51	0.40
12:L:72:ASN:ND2	13:M:459:MET:HG2	2.36	0.40
12:L:138:PHE:CZ	13:M:376:MET:HG2	2.56	0.40
12:L:141:PHE:CD2	13:M:375:LEU:CD2	2.94	0.40
12:L:210:LEU:HD12	12:L:270:ASN:HD21	1.86	0.40
12:L:210:LEU:O	12:L:211:ILE:C	2.62	0.40
12:L:532:ILE:HG21	37:l:133:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:303:ILE:HG13	13:M:385:LEU:HD23	2.03	0.40
13:M:394:ILE:O	13:M:398:ILE:HG13	2.22	0.40
14:N:22:SER:HB2	30:e:6:ILE:HG22	2.03	0.40
14:N:146:TYR:CG	14:N:147:PRO:N	2.88	0.40
14:N:224:SER:HB2	14:N:229:SER:HB2	2.01	0.40
15:O:219:GLN:NE2	15:O:219:GLN:HA	2.36	0.40
15:O:263:ALA:C	15:O:265:ASP:H	2.30	0.40
16:P:96:LEU:HD12	16:P:97:MET:CA	2.51	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
16:P:191:VAL:HG13	16:P:192:ARG:CZ	2.51	0.40
20:T:99:SER:HB2	20:T:102:SER:HB2	2.03	0.40
23:X:23:ALA:HB2	23:X:95:GLN:HE22	1.82	0.40
30:e:49:GLY:HA2	30:e:52:ALA:HB3	2.02	0.40
32:g:112:MET:HE3	32:g:115:TRP:CE3	2.56	0.40
37:l:122:THR:CG2	37:l:129:MET:HE1	2.45	0.40
38:m:28:GLU:HG2	38:m:31:ARG:NH2	2.37	0.40
38:m:49:LEU:HD11	39:n:137:VAL:HG12	2.03	0.40
39:n:148:GLY:O	39:n:149:ILE:C	2.63	0.40
43:r:24:LEU:HD23	43:r:24:LEU:HA	1.85	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
48:AD:176:PRO:C	48:AD:177:LYS:HD3	2.46	0.40
48:AD:179:TYR:CE1	48:AD:188:ALA:HB3	2.56	0.40
49:AE:192:VAL:HG13	49:AE:193:SER:N	2.37	0.40
49:AE:210:TRP:HB2	49:AE:265:PHE:CZ	2.55	0.40
54:AK:28:GLY:O	54:AK:32:LEU:N	2.48	0.40
46:Ab:282:GLU:O	46:Ab:283:ALA:C	2.64	0.40
47:Ac:244:LEU:HA	48:Ad:285:ARG:HD2	2.02	0.40
47:Ac:294:LEU:HD23	47:Ac:294:LEU:C	2.46	0.40
48:Ad:210:TYR:O	48:Ad:211:VAL:C	2.63	0.40
49:Ae:107:SER:HB2	49:Ae:111:LYS:HZ1	1.85	0.40
49:Ae:229:GLY:HA3	49:Ae:234:TYR:N	2.33	0.40
49:Ae:234:TYR:HB2	49:Ae:243:TYR:O	2.21	0.40
52:Ah:61:THR:HG1	52:Ah:63:GLU:HG2	1.85	0.40
4:D:61:TRP:CD1	4:D:61:TRP:N	2.89	0.40
6:F:196:PHE:HD1	44:s:56:ARG:HH21	1.70	0.40
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:338:ASP:OD1	6:F:341:ALA:HB2	2.20	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
8:H:63:PRO:O	8:H:66:THR:HG22	2.21	0.40
12:L:22:SER:HA	12:L:27:ILE:CG2	2.52	0.40
12:L:56:HIS:CA	40:o:74:PHE:CD1	2.98	0.40
12:L:138:PHE:CD1	62:h:201:CDL:H271	2.56	0.40
12:L:324:LEU:HB3	12:L:395:ILE:CD1	2.51	0.40
12:L:400:ASN:HD22	12:L:409:LEU:HD11	1.85	0.40
57:L:706:PC1:H331	57:L:706:PC1:H362	1.79	0.40
13:M:197:LEU:O	13:M:201:MET:HB2	2.21	0.40
14:N:106:LEU:HD21	14:N:138:PRO:HB2	2.03	0.40
15:O:248:LYS:HE2	15:O:248:LYS:HB3	1.82	0.40
20:T:140:CYS:HB2	20:T:143:GLU:HB2	2.02	0.40
20:U:93:ILE:CG1	20:U:110:LEU:HD11	2.51	0.40
25:Z:58:ARG:CZ	27:b:49:THR:HG21	2.51	0.40
26:a:9:LEU:O	26:a:10:ALA:C	2.64	0.40
29:d:107:LYS:HB3	29:d:111:GLU:HB3	2.04	0.40
32:g:140:PHE:HB3	41:p:75:THR:CG2	2.51	0.40
34:i:99:SER:O	34:i:100:SER:C	2.64	0.40
34:i:106:PRO:HD2	40:o:64:ILE:HG21	2.03	0.40
40:o:52:THR:O	40:o:53:LEU:C	2.62	0.40
41:p:43:TRP:HB3	41:p:44:PRO:HD3	2.03	0.40
43:r:20:LEU:C	43:r:20:LEU:CD1	2.89	0.40
45:AA:43:GLN:NE2	46:AB:57:PRO:CA	2.77	0.40
45:AA:68:THR:OG1	46:AB:387:GLU:OE1	2.39	0.40
45:AA:73:VAL:HG11	45:AA:151:VAL:HG11	2.03	0.40
46:AB:40:PHE:CE1	46:AB:404:GLY:O	2.74	0.40
46:AB:234:ALA:C	46:AB:237:PHE:O	2.65	0.40
49:AE:163:LYS:NZ	49:AE:165:MET:HB2	2.36	0.40
54:AK:17:TRP:O	54:AK:18:ILE:C	2.63	0.40
45:Aa:454:PRO:O	45:Aa:468:TYR:OH	2.34	0.40
47:Ac:245:PHE:CG	48:Ad:101:LEU:HD11	2.56	0.40
47:Ac:296:LEU:O	47:Ac:297:SER:C	2.64	0.40
48:Ad:131:ALA:O	48:Ad:132:TYR:C	2.64	0.40
48:Ad:138:VAL:C	53:Aj:53:TRP:HD1	2.30	0.40
48:Ad:215:LEU:HD21	70:Ad:401:HEC:C1B	2.50	0.40
49:Ae:88:PHE:O	49:Ae:91:TYR:N	2.54	0.40
49:Ae:164:ASN:ND2	49:Ae:234:TYR:HE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Ak:37:ASP:O	54:Ak:38:TRP:C	2.65	0.40
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.40
1:A:102:LEU:HG	1:A:106:TRP:NE1	2.36	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:224:GLU:OE1	16:P:50:SER:OG	2.40	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
7:G:49:VAL:HG13	7:G:102:ILE:HG12	2.03	0.40
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.40
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.04	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.03	0.40
9:I:90:LYS:CG	42:q:90:LEU:CD2	3.00	0.40
12:L:399:ILE:HG22	12:L:409:LEU:CD1	2.51	0.40
13:M:264:LEU:HD23	38:m:98:LEU:CD1	2.51	0.40
13:M:313:THR:HG21	13:M:456:GLY:CA	2.47	0.40
13:M:435:THR:HG23	13:M:436:LEU:N	2.36	0.40
13:M:437:MET:O	13:M:438:ALA:C	2.62	0.40
14:N:59:TYR:O	14:N:63:GLN:HG2	2.21	0.40
14:N:202:LEU:HD21	30:e:3:PHE:CE1	2.56	0.40
14:N:211:LEU:CD2	14:N:333:SER:HB2	2.45	0.40
15:O:117:PHE:HE1	15:O:173:MET:HE1	1.80	0.40
15:O:170:LEU:CD2	15:O:184:VAL:HG13	2.51	0.40
15:O:276:LEU:C	15:O:276:LEU:HD12	2.46	0.40
16:P:315:THR:HB	16:P:318:LYS:H	1.85	0.40
17:Q:57:GLU:O	17:Q:58:LYS:C	2.65	0.40
23:X:53:PRO:HG2	25:Z:116:TRP:HE1	1.87	0.40
24:Y:110:TYR:HB2	58:m:202:3PE:H11	2.02	0.40
29:d:11:LEU:HD11	30:e:4:LEU:HD12	2.02	0.40
35:j:51:THR:O	35:j:52:ARG:C	2.61	0.40
35:j:71:TRP:HZ3	35:j:72:ARG:NH2	2.19	0.40
37:l:119:THR:CG2	38:m:13:THR:HG23	2.52	0.40
40:o:4:HIS:ND1	40:o:106:ARG:NH1	2.70	0.40
40:o:25:PHE:CD2	40:o:108:LEU:HB3	2.56	0.40
42:q:7:LEU:O	42:q:11:VAL:HG23	2.21	0.40
45:AA:402:HIS:HB2	45:AA:426:LEU:CD1	2.50	0.40
46:AB:48:VAL:CG2	46:AB:48:VAL:O	2.59	0.40
48:AD:110:ILE:HG23	48:AD:273:PHE:HA	2.04	0.40
48:AD:306:MET:C	48:AD:308:ARG:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:93:ARG:HB3	51:AG:25:ARG:N	2.37	0.40
49:AE:248:ARG:HG2	49:AE:257:ASN:ND2	2.36	0.40
48:Ad:155:GLN:HE21	48:Ad:166:MET:HG2	1.87	0.40
50:Af:79:ASP:OD1	50:Af:80:GLN:N	2.55	0.40
50:Af:102:ARG:HA	50:Af:105:ARG:NH2	2.37	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:144:MET:HE2	4:D:144:MET:HB2	1.91	0.40
6:F:114:VAL:CG1	6:F:212:LEU:HD23	2.52	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40
8:H:204:GLU:O	8:H:208:VAL:HA	2.21	0.40
9:I:50:MET:HB3	25:Z:33:TYR:OH	2.21	0.40
12:L:277:MET:HG3	12:L:318:GLY:HA3	2.04	0.40
12:L:371:SER:O	12:L:374:VAL:HG12	2.21	0.40
57:L:706:PC1:H3C2	57:L:706:PC1:H391	1.89	0.40
13:M:62:SER:HB2	13:M:110:PHE:O	2.22	0.40
13:M:151:PHE:CZ	14:N:291:PHE:CB	2.97	0.40
13:M:159:PRO:HG2	58:M:501:3PE:H391	2.03	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
14:N:132:THR:HB	14:N:209:ILE:HG12	2.03	0.40
16:P:56:ALA:HA	16:P:125:VAL:O	2.20	0.40
16:P:96:LEU:C	16:P:96:LEU:CD1	2.94	0.40
16:P:302:GLY:HA2	16:P:314:THR:CG2	2.50	0.40
17:Q:166:TRP:O	17:Q:167:ASN:C	2.64	0.40
19:S:23:LEU:HB3	19:S:33:VAL:CG1	2.51	0.40
25:Z:111:PHE:CE1	30:e:65:GLU:HG3	2.56	0.40
25:Z:140:PHE:C	25:Z:142:TRP:N	2.77	0.40
27:b:43:SER:O	27:b:47:LYS:HB2	2.22	0.40
29:d:21:LEU:CD1	29:d:81:TYR:HA	2.51	0.40
30:e:86:LEU:HD23	30:e:86:LEU:HA	1.93	0.40
32:g:112:MET:HE1	41:p:94:ARG:HG3	2.04	0.40
34:i:70:PHE:O	34:i:71:ALA:C	2.65	0.40
34:i:120:MET:SD	34:i:123:PHE:CZ	3.15	0.40
36:k:56:ALA:O	36:k:60:MET:N	2.53	0.40
38:m:124:LYS:HG2	38:m:125:PHE:CD2	2.57	0.40
41:p:45:VAL:O	41:p:46:THR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:225:VAL:HG22	46:AB:229:VAL:HG21	2.01	0.40
47:AC:183:PHE:CD1	47:Ac:183:PHE:CD1	3.10	0.40
47:AC:294:LEU:C	47:AC:294:LEU:HD23	2.46	0.40
49:AE:219:HIS:ND1	49:AE:239:HIS:CG	2.90	0.40
51:AG:10:ARG:NH2	51:AG:12:ARG:HD2	2.37	0.40
51:AG:62:TRP:O	51:AG:65:GLN:HG3	2.22	0.40
45:Aa:384:THR:HA	54:Ak:12:GLU:CD	2.46	0.40
45:Aa:393:ASN:HD22	46:Ab:106:VAL:HA	1.86	0.40
46:Ab:263:GLY:O	46:Ab:264:ASP:C	2.64	0.40
47:Ac:8:HIS:CB	47:Ac:11:PHE:HD2	2.34	0.40
47:Ac:221:HIS:HB3	47:Ac:222:PRO:HD3	2.04	0.40
47:Ac:283:SER:OG	47:Ac:284:ILE:HD12	2.22	0.40
50:Af:71:MET:HB3	50:Af:71:MET:HE2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	89/115 (77%)	82 (92%)	7 (8%)	0	100 100
2	B	154/224 (69%)	142 (92%)	10 (6%)	2 (1%)	9 41
3	C	196/263 (74%)	186 (95%)	8 (4%)	2 (1%)	12 47
4	D	421/463 (91%)	392 (93%)	29 (7%)	0	100 100
5	E	208/248 (84%)	191 (92%)	17 (8%)	0	100 100
6	F	424/464 (91%)	406 (96%)	18 (4%)	0	100 100
7	G	685/727 (94%)	631 (92%)	54 (8%)	0	100 100
8	H	310/318 (98%)	291 (94%)	18 (6%)	1 (0%)	36 71
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100 100
10	J	151/172 (88%)	140 (93%)	11 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
16	P	338/377 (90%)	312 (92%)	26 (8%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	110 (98%)	1 (1%)	1 (1%)	14	49
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	71 (92%)	6 (8%)	0	100	100
28	c	45/76 (59%)	45 (100%)	0	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	f	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	g	98/151 (65%)	92 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	88/128 (69%)	79 (90%)	9 (10%)	0	100	100
35	j	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
36	k	70/104 (67%)	67 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	58
40	o	117/137 (85%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	168/176 (96%)	150 (89%)	18 (11%)	0	100	100
42	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
43	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
44	s	24/104 (23%)	24 (100%)	0	0	100	100
45	AA	393/480 (82%)	378 (96%)	15 (4%)	0	100	100
45	Aa	395/480 (82%)	384 (97%)	11 (3%)	0	100	100
46	AB	410/453 (90%)	400 (98%)	10 (2%)	0	100	100
46	Ab	407/453 (90%)	397 (98%)	10 (2%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	362 (98%)	8 (2%)	1 (0%)	36	71
48	AD	236/325 (73%)	229 (97%)	6 (2%)	1 (0%)	30	66
48	Ad	236/325 (73%)	224 (95%)	12 (5%)	0	100	100
49	AE	181/274 (66%)	168 (93%)	13 (7%)	0	100	100
49	AI	43/274 (16%)	41 (95%)	2 (5%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	12 (6%)	1 (0%)	24	62
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
52	AH	62/89 (70%)	62 (100%)	0	0	100	100
52	Ah	64/89 (72%)	63 (98%)	1 (2%)	0	100	100
53	AJ	36/64 (56%)	36 (100%)	0	0	100	100
53	Aj	46/64 (72%)	45 (98%)	1 (2%)	0	100	100
54	AK	32/56 (57%)	31 (97%)	1 (3%)	0	100	100
54	Ak	42/56 (75%)	41 (98%)	1 (2%)	0	100	100
All	All	11748/14118 (83%)	11208 (95%)	529 (4%)	11 (0%)	49	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	127	GLN
3	C	135	ARG
8	H	92	PRO

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Mol	Chain	Res	Type
14	N	109	ALA
3	C	81	ASP
22	W	99	VAL
47	Ac	75	TYR
48	AD	158	PRO
2	B	195	PRO
39	n	156	PRO
49	Ae	237	PRO

5.3.2 Protein sidechains (i)

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	85/104 (82%)	85 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	367/395 (93%)	367 (100%)	0	100	100
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	278/280 (99%)	278 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	126/138 (91%)	123 (98%)	3 (2%)	43	63
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	297/325 (91%)	295 (99%)	2 (1%)	76	79
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
20	U	80/135 (59%)	79 (99%)	1 (1%)	61	72
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	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
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	91/129 (70%)	91 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	87/120 (72%)	86 (99%)	1 (1%)	65	74
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	55/78 (70%)	55 (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	162/164 (99%)	161 (99%)	1 (1%)	78	80
40	o	109/121 (90%)	109 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	108/131 (82%)	108 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	26/95 (27%)	26 (100%)	0	100	100
45	AA	337/398 (85%)	337 (100%)	0	100	100
45	Aa	339/398 (85%)	338 (100%)	1 (0%)	86	84
46	AB	324/356 (91%)	324 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Ab	325/356 (91%)	324 (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	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	202 (100%)	1 (0%)	81	81
49	AE	155/224 (69%)	154 (99%)	1 (1%)	78	80
49	AI	34/224 (15%)	34 (100%)	0	100	100
49	Ae	158/224 (70%)	158 (100%)	0	100	100
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	30/55 (54%)	30 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	26/46 (56%)	26 (100%)	0	100	100
54	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	10324/12037 (86%)	10299 (100%)	25 (0%)	85	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	244	VAL
7	G	271	MET
10	J	55	VAL
10	J	60	LEU
10	J	63	MET
12	L	3	ILE
12	L	69	VAL
13	M	218	LYS
14	N	159	ILE
16	P	192	ARG
16	P	242	VAL
17	Q	96	LYS
18	R	64	ILE

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Mol	Chain	Res	Type
19	S	68	ARG
20	T	103	HIS
20	U	74	LEU
25	Z	7	LYS
34	i	72	VAL
39	n	98	LYS
47	AC	294	LEU
49	AE	223	VAL
45	Aa	249	HIS
46	Ab	260	GLU
47	Ac	294	LEU
48	Ad	201	VAL

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

Mol	Chain	Res	Type
1	A	10	ASN
1	A	108	GLN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
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	36	GLN
4	D	38	GLN
4	D	60	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN

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Mol	Chain	Res	Type
5	E	152	GLN
5	E	245	GLN
6	F	44	ASN
6	F	49	HIS
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	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	569	GLN
7	G	571	HIS
7	G	605	GLN
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	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	287	HIS
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	136	ASN
12	L	139	GLN

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Mol	Chain	Res	Type
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
12	L	579	ASN
13	M	26	ASN
13	M	44	GLN
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	342	GLN
15	O	80	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	71	ASN

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Mol	Chain	Res	Type
16	P	154	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
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	88	GLN
18	R	33	HIS
21	V	41	HIS
21	V	50	GLN
22	W	54	GLN
23	X	30	HIS
23	X	77	HIS
24	Y	19	GLN
24	Y	91	ASN
25	Z	112	HIS
25	Z	135	ASN
25	Z	137	ASN
26	a	31	ASN
27	b	52	ASN
27	b	69	HIS
27	b	83	ASN
28	c	62	HIS
29	d	59	HIS
29	d	79	GLN
30	e	97	HIS
33	h	109	HIS
33	h	170	GLN
33	h	181	HIS
34	i	83	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
38	m	75	ASN
38	m	79	ASN

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Mol	Chain	Res	Type
39	n	12	HIS
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	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	12	GLN
42	q	31	ASN
42	q	52	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS
43	r	9	GLN
43	r	21	GLN
43	r	110	GLN
44	s	59	GLN
45	AA	43	GLN
45	AA	87	ASN
45	AA	103	ASN
45	AA	173	GLN
45	AA	207	ASN
45	AA	240	GLN
45	AA	277	HIS
45	AA	301	ASN
45	AA	342	GLN
45	AA	345	ASN
45	AA	402	HIS
46	AB	167	GLN
46	AB	284	ASN
46	AB	357	GLN
46	AB	365	ASN
46	AB	415	GLN
47	AC	260	ASN
47	AC	312	GLN

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Mol	Chain	Res	Type
48	AD	98	HIS
48	AD	115	GLN
48	AD	189	ASN
48	AD	190	ASN
50	AF	80	GLN
51	AG	69	GLN
52	AH	37	GLN
52	AH	82	HIS
45	Aa	87	ASN
45	Aa	119	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
46	Ab	167	GLN
46	Ab	227	HIS
46	Ab	284	ASN
46	Ab	298	HIS
46	Ab	304	ASN
46	Ab	311	GLN
46	Ab	343	GLN
46	Ab	357	GLN
46	Ab	365	ASN
46	Ab	415	GLN
46	Ab	443	ASN
47	Ac	32	ASN
47	Ac	148	ASN
47	Ac	260	ASN
47	Ac	312	GLN
48	Ad	107	HIS
48	Ad	115	GLN
48	Ad	155	GLN
48	Ad	190	ASN
49	Ae	242	HIS
50	Af	80	GLN
51	Ag	24	GLN
52	Ah	82	HIS
54	Ak	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 1 is monoatomic - leaving 54 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	$\#\|Z\| > 2$
67	HEM	Ac	401	47	50,50,50	1.59	10 (20%)	66,82,82	1.78	16 (24%)
62	CDL	L	704	-	76,76,99	1.03	4 (5%)	82,88,111	1.17	5 (6%)
58	3PE	L	703	-	46,46,50	0.95	2 (4%)	49,51,55	1.03	3 (6%)
58	3PE	j	700	-	39,39,50	1.02	2 (5%)	42,44,55	1.23	4 (9%)
67	HEM	AC	402	47	50,50,50	1.59	9 (18%)	66,82,82	1.85	16 (24%)
68	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.09	7 (25%)
55	SF4	G	801	7	0,12,12	-	-	-		
62	CDL	Ag	101	62	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
58	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.20	3 (8%)
57	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.13	2 (5%)
63	ADP	O	402	-	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
69	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
58	3PE	K	101	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
57	PC1	L	706	-	49,49,53	0.97	2 (4%)	55,57,61	1.09	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	CDL	Ac	406	62	41,41,99	1.39	4 (9%)	47,53,111	1.45	7 (14%)
58	3PE	AC	403	-	24,24,50	1.30	2 (8%)	27,29,55	1.17	2 (7%)
60	FMN	F	501	-	33,33,33	1.38	4 (12%)	48,50,50	1.21	6 (12%)
59	FES	E	301	5	0,4,4	-	-	-		
59	FES	G	803	7	0,4,4	-	-	-		
67	HEM	AC	401	47	50,50,50	1.59	8 (16%)	66,82,82	1.85	13 (19%)
55	SF4	F	502	6	0,12,12	-	-	-		
58	3PE	M	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.05	4 (7%)
55	SF4	G	802	7	0,12,12	-	-	-		
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
62	CDL	L	705	-	80,80,99	1.01	4 (5%)	86,92,111	1.12	7 (8%)
66	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
58	3PE	m	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.06	4 (7%)
68	U10	AC	404	-	23,23,63	1.75	2 (8%)	28,31,79	1.70	7 (25%)
58	3PE	b	201	-	45,45,50	1.11	5 (11%)	48,50,55	1.23	3 (6%)
66	EHZ	n	201	-	27,31,37	1.85	7 (25%)	37,41,47	1.99	11 (29%)
67	HEM	Ac	402	47	50,50,50	1.56	8 (16%)	66,82,82	1.82	14 (21%)
55	SF4	B	301	2	0,12,12	-	-	-		
57	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.03	3 (5%)
58	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.06	2 (4%)
58	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	3 (5%)
58	3PE	D	501	-	37,37,50	1.05	2 (5%)	40,42,55	1.16	3 (7%)
58	3PE	O	401	-	43,43,50	0.99	2 (4%)	46,48,55	1.04	3 (6%)
70	HEC	Ad	401	48	50,50,50	2.78	25 (50%)	68,82,82	2.48	26 (38%)
58	3PE	L	702	-	38,38,50	1.06	2 (5%)	41,43,55	1.15	2 (4%)
58	3PE	m	202	-	40,40,50	1.00	2 (5%)	43,45,55	1.12	3 (6%)
64	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.66	11 (16%)
70	HEC	AD	401	48	50,50,50	2.82	27 (54%)	68,82,82	2.42	27 (39%)
55	SF4	I	303	9	0,12,12	-	-	-		
69	UQ6	AC	405	-	28,28,43	2.44	6 (21%)	33,37,55	1.65	8 (24%)
58	3PE	M	501	-	36,36,50	1.07	2 (5%)	39,41,55	1.21	3 (7%)
56	UQ1	B	302	-	18,18,18	1.94	2 (11%)	22,25,25	1.35	3 (13%)
55	SF4	I	304	9	0,12,12	-	-	-		
58	3PE	J	401	-	45,45,50	1.12	5 (11%)	48,50,55	1.19	3 (6%)
61	UQ9	H	400	-	35,35,58	0.83	2 (5%)	42,45,73	0.52	0
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	CDL	d	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
62	CDL	Aa	501	-	45,45,99	1.34	4 (8%)	51,57,111	1.32	6 (11%)
58	3PE	L	701	-	48,48,50	0.91	2 (4%)	51,53,55	1.13	4 (7%)
58	3PE	I	301	-	45,45,50	0.98	2 (4%)	48,50,55	1.08	3 (6%)

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
67	HEM	Ac	401	47	-	9/14/54/54	-
62	CDL	L	704	-	-	27/87/87/110	-
58	3PE	L	703	-	-	10/50/50/54	-
58	3PE	j	700	-	-	6/43/43/54	-
67	HEM	AC	402	47	-	9/14/54/54	-
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
55	SF4	G	801	7	-	-	0/6/5/5
62	CDL	Ag	101	62	-	22/66/66/110	-
58	3PE	Ac	403	-	-	3/38/38/54	-
57	PC1	B	303	-	-	8/38/38/57	-
63	ADP	O	402	-	-	1/16/32/32	0/3/3/3
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
58	3PE	K	101	-	-	14/49/49/54	-
57	PC1	L	706	-	-	10/53/53/57	-
62	CDL	Ac	406	62	-	18/52/52/110	-
58	3PE	AC	403	-	-	7/28/28/54	-
60	FMN	F	501	-	-	3/18/18/18	0/3/3/3
59	FES	E	301	5	-	-	0/1/1/1
59	FES	G	803	7	-	-	0/1/1/1
67	HEM	AC	401	47	-	8/14/54/54	-
55	SF4	F	502	6	-	-	0/6/5/5
58	3PE	M	503	-	-	8/54/54/54	-
55	SF4	G	802	7	-	-	0/6/5/5
62	CDL	h	201	-	-	23/80/80/110	-
62	CDL	L	705	-	-	21/91/91/110	-
66	EHZ	W	201	-	-	21/39/39/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	3PE	m	201	-	-	13/54/54/54	-
68	U10	AC	404	-	-	5/15/39/87	0/1/1/1
58	3PE	b	201	-	-	19/49/49/54	-
66	EHZ	n	201	-	-	14/39/39/45	-
67	HEM	Ac	402	47	-	8/14/54/54	-
55	SF4	B	301	2	-	-	0/6/5/5
57	PC1	I	302	-	-	10/50/50/57	-
58	3PE	i	201	-	-	12/43/43/54	-
58	3PE	M	502	-	-	16/54/54/54	-
58	3PE	D	501	-	-	10/41/41/54	-
58	3PE	O	401	-	-	9/47/47/54	-
70	HEC	Ad	401	48	1/1/3/7	8/14/54/54	-
58	3PE	L	702	-	-	16/42/42/54	-
58	3PE	m	202	-	-	7/44/44/54	-
64	NDP	P	401	-	-	3/34/77/77	0/5/5/5
70	HEC	AD	401	48	1/1/3/7	7/14/54/54	-
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
55	SF4	I	303	9	-	-	0/6/5/5
58	3PE	M	501	-	-	8/40/40/54	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
55	SF4	I	304	9	-	-	0/6/5/5
58	3PE	J	401	-	-	18/49/49/54	-
61	UQ9	H	400	-	-	14/30/54/81	0/1/1/1
62	CDL	a	101	-	-	18/67/67/110	-
62	CDL	d	201	-	-	27/77/77/110	-
62	CDL	Aa	501	-	-	12/56/56/110	-
58	3PE	L	701	-	-	13/52/52/54	-
58	3PE	I	301	-	-	12/49/49/54	-

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	B	302	UQ1	C6-C5	7.36	1.48	1.35
68	AC	404	U10	C6-C1	7.36	1.48	1.35
69	AC	405	UQ6	C2-C3	5.91	1.49	1.39
69	AC	405	UQ6	C5-C4	5.85	1.48	1.39
69	AC	405	UQ6	C5-C6	5.74	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	W	201	EHZ	C15-N2	5.38	1.45	1.33
66	n	201	EHZ	C15-N2	5.24	1.45	1.33
67	Ac	401	HEM	FE-NB	5.22	2.11	1.94
66	W	201	EHZ	C12-N1	5.16	1.45	1.33
67	Ac	402	HEM	FE-NB	5.07	2.10	1.94
70	AD	401	HEC	FE-NB	5.04	2.10	1.94
70	AD	401	HEC	FE-ND	5.00	2.10	1.94
70	Ad	401	HEC	C2A-C3A	5.00	1.47	1.36
69	AC	405	UQ6	C6-C1	4.98	1.48	1.40
70	Ad	401	HEC	C3D-C2D	4.97	1.47	1.36
70	AD	401	HEC	C2A-C3A	4.95	1.47	1.36
70	AD	401	HEC	C3B-C2B	4.93	1.47	1.36
66	n	201	EHZ	C12-N1	4.92	1.44	1.33
67	AC	402	HEM	FE-NB	4.92	2.10	1.94
67	AC	401	HEM	FE-NB	4.86	2.09	1.94
60	F	501	FMN	C9A-C5A	4.82	1.49	1.41
70	AD	401	HEC	C3D-C2D	4.80	1.46	1.36
70	AD	401	HEC	CHB-C4A	4.78	1.47	1.38
70	Ad	401	HEC	C3B-C2B	4.77	1.46	1.36
70	AD	401	HEC	CHA-C1A	4.77	1.47	1.38
70	Ad	401	HEC	FE-ND	4.75	2.09	1.94
70	Ad	401	HEC	CHA-C1A	4.72	1.47	1.38
70	Ad	401	HEC	FE-NB	4.66	2.09	1.94
69	AC	405	UQ6	C4-C3	4.58	1.48	1.39
70	Ad	401	HEC	FE-NC	4.57	2.10	1.95
70	Ad	401	HEC	CHD-C1D	4.57	1.47	1.38
70	AD	401	HEC	FE-NC	4.56	2.10	1.95
70	AD	401	HEC	FE-NA	4.55	2.10	1.95
70	Ad	401	HEC	FE-NA	4.54	2.10	1.95
70	Ad	401	HEC	CHB-C4A	4.39	1.46	1.38
70	AD	401	HEC	CHD-C1D	4.38	1.47	1.38
70	Ad	401	HEC	CHC-C4B	4.38	1.47	1.38
70	AD	401	HEC	CHC-C4B	4.34	1.47	1.38
57	L	706	PC1	O31-C31	4.31	1.45	1.33
58	L	702	3PE	O31-C31	4.30	1.45	1.33
58	O	401	3PE	O31-C31	4.30	1.45	1.33
58	i	201	3PE	O31-C31	4.28	1.45	1.33
58	M	501	3PE	O31-C31	4.25	1.45	1.33
58	I	301	3PE	O31-C31	4.25	1.45	1.33
63	O	402	ADP	C5-C4	4.25	1.46	1.39
62	d	201	CDL	OB8-CB7	4.25	1.45	1.33
58	L	703	3PE	O31-C31	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	P	401	NDP	C5A-C4A	4.23	1.46	1.39
62	Aa	501	CDL	OA8-CA7	4.23	1.45	1.33
62	L	704	CDL	OB6-CB5	4.23	1.46	1.34
58	i	201	3PE	O21-C21	4.23	1.46	1.34
62	Ac	406	CDL	OB8-CB7	4.22	1.45	1.33
58	j	700	3PE	O31-C31	4.22	1.45	1.33
58	K	101	3PE	O31-C31	4.21	1.45	1.33
58	Ac	403	3PE	O31-C31	4.20	1.45	1.33
58	I	301	3PE	O21-C21	4.20	1.46	1.34
62	a	101	CDL	OA8-CA7	4.19	1.45	1.33
62	L	705	CDL	OA8-CA7	4.19	1.45	1.33
62	Ag	101	CDL	OB8-CB7	4.19	1.45	1.33
62	Aa	501	CDL	OB8-CB7	4.19	1.45	1.33
58	M	503	3PE	O31-C31	4.19	1.45	1.33
58	m	202	3PE	O31-C31	4.18	1.45	1.33
57	B	303	PC1	O31-C31	4.18	1.45	1.33
62	d	201	CDL	OA8-CA7	4.18	1.45	1.33
58	D	501	3PE	O31-C31	4.18	1.45	1.33
62	h	201	CDL	OA8-CA7	4.17	1.45	1.33
58	m	201	3PE	O31-C31	4.17	1.45	1.33
58	AC	403	3PE	O31-C31	4.17	1.45	1.33
62	a	101	CDL	OB8-CB7	4.17	1.45	1.33
62	L	705	CDL	OB8-CB7	4.17	1.45	1.33
57	I	302	PC1	O31-C31	4.16	1.45	1.33
62	Ag	101	CDL	OA8-CA7	4.14	1.45	1.33
67	AC	401	HEM	FE-NC	4.13	2.09	1.95
62	L	704	CDL	OB8-CB7	4.12	1.45	1.33
58	M	502	3PE	O31-C31	4.11	1.45	1.33
62	h	201	CDL	OB8-CB7	4.10	1.45	1.33
62	h	201	CDL	OB6-CB5	4.10	1.45	1.34
62	Aa	501	CDL	OB6-CB5	4.10	1.45	1.34
58	L	702	3PE	O21-C21	4.10	1.45	1.34
57	B	303	PC1	O21-C21	4.10	1.45	1.34
62	Ac	406	CDL	OA8-CA7	4.10	1.45	1.33
62	Aa	501	CDL	OA6-CA5	4.09	1.45	1.34
69	AC	405	UQ6	C2-C1	4.08	1.48	1.40
62	a	101	CDL	OA6-CA5	4.07	1.45	1.34
57	L	706	PC1	O21-C21	4.07	1.45	1.34
62	L	705	CDL	OA6-CA5	4.07	1.45	1.34
58	L	703	3PE	O21-C21	4.06	1.45	1.34
62	L	704	CDL	OA8-CA7	4.05	1.45	1.33
62	Ac	406	CDL	OA6-CA5	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	a	101	CDL	OB6-CB5	4.05	1.45	1.34
58	L	701	3PE	O31-C31	4.04	1.45	1.33
57	I	302	PC1	O21-C21	4.03	1.45	1.34
62	Ag	101	CDL	OA6-CA5	4.02	1.45	1.34
58	Ac	403	3PE	O21-C21	4.02	1.45	1.34
58	AC	403	3PE	O21-C21	4.01	1.45	1.34
58	M	501	3PE	O21-C21	4.00	1.45	1.34
58	D	501	3PE	O21-C21	3.99	1.45	1.34
62	L	705	CDL	OB6-CB5	3.98	1.45	1.34
62	Ag	101	CDL	OB6-CB5	3.98	1.45	1.34
58	j	700	3PE	O21-C21	3.98	1.45	1.34
62	h	201	CDL	OA6-CA5	3.98	1.45	1.34
62	Ac	406	CDL	OB6-CB5	3.97	1.45	1.34
58	M	502	3PE	O21-C21	3.97	1.45	1.34
62	d	201	CDL	OA6-CA5	3.96	1.45	1.34
58	L	701	3PE	O21-C21	3.95	1.45	1.34
58	m	202	3PE	O21-C21	3.94	1.45	1.34
67	Ac	402	HEM	FE-NC	3.94	2.08	1.95
58	M	503	3PE	O21-C21	3.94	1.45	1.34
67	AC	402	HEM	FE-NC	3.93	2.08	1.95
58	O	401	3PE	O21-C21	3.93	1.45	1.34
62	d	201	CDL	OB6-CB5	3.92	1.45	1.34
58	K	101	3PE	O21-C21	3.91	1.45	1.34
62	L	704	CDL	OA6-CA5	3.89	1.45	1.34
67	AC	402	HEM	C4D-ND	-3.85	1.33	1.40
67	Ac	401	HEM	FE-NC	3.82	2.08	1.95
58	m	201	3PE	O21-C21	3.82	1.45	1.34
67	AC	401	HEM	C1B-NB	-3.79	1.33	1.40
70	Ad	401	HEC	CHC-C1C	3.76	1.47	1.39
70	Ad	401	HEC	CHA-C4D	3.68	1.47	1.39
70	AD	401	HEC	CHB-C1B	3.67	1.47	1.39
70	Ad	401	HEC	CHD-C4C	3.66	1.47	1.39
70	AD	401	HEC	CHD-C4C	3.62	1.47	1.39
70	AD	401	HEC	CHA-C4D	3.58	1.47	1.39
67	Ac	401	HEM	C4D-ND	-3.55	1.34	1.40
70	AD	401	HEC	CHC-C1C	3.52	1.47	1.39
67	Ac	402	HEM	C1B-NB	-3.51	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.47	1.34	1.40
67	AC	401	HEM	C4D-ND	-3.46	1.34	1.40
64	P	401	NDP	C6N-C5N	3.35	1.39	1.33
67	Ac	401	HEM	C1B-NB	-3.28	1.34	1.40
70	Ad	401	HEC	C4B-NB	-3.26	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	AD	401	HEC	C3C-C2C	3.19	1.47	1.38
58	J	401	3PE	O21-C21	3.18	1.43	1.34
67	Ac	402	HEM	C4D-ND	-3.18	1.34	1.40
68	AC	404	U10	C4-C3	3.14	1.49	1.36
58	b	201	3PE	O21-C21	3.13	1.43	1.34
70	Ad	401	HEC	C1D-ND	-3.10	1.35	1.40
60	F	501	FMN	C8-C7	3.08	1.48	1.40
56	B	302	UQ1	C3-C2	3.03	1.48	1.36
58	b	201	3PE	O31-C31	3.01	1.42	1.33
58	J	401	3PE	O31-C31	3.01	1.42	1.33
70	AD	401	HEC	C4B-NB	-3.00	1.35	1.40
70	Ad	401	HEC	C3C-C2C	3.00	1.46	1.38
70	AD	401	HEC	C1D-ND	-2.99	1.35	1.40
67	AC	401	HEM	C1C-C2C	-2.96	1.39	1.45
69	Ac	405	UQ6	O2-C2	-2.92	1.30	1.37
68	Ac	404	U10	C6-C5	-2.92	1.38	1.46
68	Ac	404	U10	C4-C3	2.86	1.48	1.36
61	H	400	UQ9	C3-C2	-2.78	1.40	1.48
70	Ad	401	HEC	CHB-C1B	2.70	1.45	1.39
60	F	501	FMN	C4-N3	-2.67	1.33	1.38
67	AC	402	HEM	FE-ND	-2.64	1.86	1.94
66	n	201	EHZ	P1-O7	2.59	1.64	1.54
66	W	201	EHZ	P1-O7	2.57	1.64	1.54
67	AC	401	HEM	FE-ND	-2.55	1.86	1.94
67	AC	402	HEM	C1C-C2C	-2.55	1.40	1.45
67	Ac	401	HEM	C1C-C2C	-2.53	1.40	1.45
63	O	402	ADP	C5-C6	2.52	1.48	1.41
61	H	400	UQ9	C4-C5	-2.52	1.41	1.48
66	W	201	EHZ	O4-C15	-2.52	1.18	1.23
68	Ac	404	U10	C3-C2	-2.50	1.41	1.48
70	AD	401	HEC	C4C-NC	-2.50	1.34	1.39
67	Ac	402	HEM	FE-ND	-2.50	1.87	1.94
66	n	201	EHZ	O4-C15	-2.48	1.18	1.23
64	P	401	NDP	C5A-C6A	2.48	1.48	1.41
70	Ad	401	HEC	C4A-NA	-2.47	1.35	1.39
70	Ad	401	HEC	C1A-NA	-2.45	1.35	1.39
67	Ac	402	HEM	C1C-C2C	-2.44	1.40	1.45
70	Ad	401	HEC	C4C-NC	-2.43	1.35	1.39
67	Ac	402	HEM	C3C-C4C	-2.43	1.41	1.46
66	W	201	EHZ	C9-S1	2.43	1.82	1.76
70	Ad	401	HEC	C1B-NB	-2.43	1.33	1.38
67	Ac	401	HEM	FE-ND	-2.42	1.87	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	Ad	401	HEC	C1C-C2C	2.42	1.48	1.43
70	AD	401	HEC	C1C-C2C	2.41	1.48	1.43
70	AD	401	HEC	C4A-NA	-2.41	1.35	1.39
63	O	402	ADP	C8-N7	2.39	1.36	1.31
66	W	201	EHZ	O3-C12	-2.39	1.18	1.23
66	n	201	EHZ	O3-C12	-2.39	1.18	1.23
64	P	401	NDP	C5A-N7A	-2.38	1.34	1.39
70	AD	401	HEC	C1B-C2B	2.38	1.49	1.44
64	P	401	NDP	C8A-N7A	2.38	1.36	1.31
67	AC	402	HEM	C3C-C4C	-2.38	1.41	1.46
70	AD	401	HEC	C1A-NA	-2.38	1.35	1.39
67	Ac	401	HEM	C1D-ND	-2.34	1.34	1.38
66	n	201	EHZ	P1-OP3	-2.33	1.45	1.54
66	n	201	EHZ	C9-S1	2.30	1.81	1.76
60	F	501	FMN	C5A-N5	-2.29	1.35	1.39
67	Ac	401	HEM	C3C-C4C	-2.28	1.42	1.46
58	b	201	3PE	O21-C2	-2.27	1.40	1.46
66	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
58	J	401	3PE	O31-C3	-2.20	1.40	1.45
58	J	401	3PE	O21-C2	-2.19	1.41	1.46
67	Ac	401	HEM	C1A-C2A	-2.18	1.40	1.44
70	Ad	401	HEC	C1A-C2A	2.17	1.49	1.45
63	O	402	ADP	C5-N7	-2.17	1.34	1.39
67	Ac	401	HEM	C4B-NB	-2.15	1.34	1.38
58	b	201	3PE	O31-C3	-2.15	1.40	1.45
67	AC	402	HEM	C1D-ND	-2.12	1.34	1.38
58	J	401	3PE	P-O12	-2.12	1.45	1.55
67	AC	401	HEM	C1D-ND	-2.11	1.34	1.38
70	AD	401	HEC	C1D-C2D	2.11	1.48	1.44
70	AD	401	HEC	C1C-NC	-2.11	1.35	1.39
67	AC	401	HEM	C4B-NB	-2.10	1.34	1.38
58	b	201	3PE	P-O12	-2.09	1.45	1.55
70	AD	401	HEC	C4D-C3D	2.07	1.48	1.45
70	Ad	401	HEC	C1C-NC	-2.03	1.35	1.39
67	Ac	402	HEM	C4B-NB	-2.03	1.34	1.38
67	AC	402	HEM	C4B-NB	-2.01	1.34	1.38
70	AD	401	HEC	C1A-C2A	2.01	1.48	1.45

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	Ac	404	U10	C6-C1-C2	7.85	125.39	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
70	Ad	401	HEC	C2B-C1B-NB	6.18	117.29	109.88
64	P	401	NDP	C5A-C4A-N3A	-6.07	118.83	126.75
67	AC	401	HEM	CHC-C4B-NB	6.04	130.98	124.42
63	O	402	ADP	C5-C4-N3	-5.91	119.04	126.75
70	AD	401	HEC	C1B-C2B-C3B	-5.78	100.88	106.96
67	AC	402	HEM	CHC-C4B-NB	5.76	130.67	124.42
70	Ad	401	HEC	C1B-C2B-C3B	-5.73	100.94	106.96
66	n	201	EHZ	C8-C9-S1	5.63	120.59	113.63
67	Ac	402	HEM	CHC-C4B-NB	5.38	130.26	124.42
70	Ad	401	HEC	CHB-C1B-C2B	-5.33	116.65	124.98
70	AD	401	HEC	C1C-C2C-C3C	-5.26	100.68	106.83
67	Ac	401	HEM	CHC-C4B-NB	5.21	130.07	124.42
70	AD	401	HEC	C2A-C1A-NA	5.21	115.39	110.32
70	AD	401	HEC	C2B-C1B-NB	5.13	116.03	109.88
67	Ac	402	HEM	CHD-C1D-ND	5.11	129.97	124.42
70	Ad	401	HEC	C2A-C1A-NA	5.11	115.29	110.32
70	Ad	401	HEC	C1C-C2C-C3C	-5.00	100.98	106.83
66	n	201	EHZ	C14-C13-C12	-4.98	104.06	112.36
70	AD	401	HEC	C3D-C4D-ND	4.96	115.16	110.36
67	AC	401	HEM	CHD-C1D-ND	4.87	129.70	124.42
63	O	402	ADP	N3-C4-N9	4.81	135.01	127.08
64	P	401	NDP	N3A-C4A-N9A	4.76	134.92	127.08
70	Ad	401	HEC	C3D-C4D-ND	4.75	114.95	110.36
67	AC	402	HEM	CHD-C1D-ND	4.73	129.56	124.42
70	AD	401	HEC	C2D-C1D-ND	4.72	115.43	109.84
68	AC	404	U10	C7-C8-C9	-4.63	119.08	126.79
62	Ac	406	CDL	OB6-CB5-C51	4.56	121.32	111.50
58	j	700	3PE	O21-C21-C22	4.54	121.28	111.50
62	d	201	CDL	OA6-CA5-C11	4.50	121.20	111.50
62	h	201	CDL	OB6-CB5-C51	4.45	121.08	111.50
62	L	704	CDL	OB6-CB5-C51	4.43	121.05	111.50
67	AC	401	HEM	CHB-C1B-NB	4.38	129.77	124.37
57	L	706	PC1	O21-C21-C22	4.37	120.91	111.50
58	I	301	3PE	O21-C21-C22	4.36	120.90	111.50
62	d	201	CDL	OB6-CB5-C51	4.32	120.82	111.50
67	Ac	402	HEM	CHA-C4D-ND	4.28	129.65	124.37
67	Ac	401	HEM	CHD-C1D-ND	4.27	129.06	124.42
62	a	101	CDL	OA6-CA5-C11	4.26	120.69	111.50
58	M	501	3PE	O21-C21-C22	4.25	120.66	111.50
58	J	401	3PE	O21-C21-C22	4.25	120.65	111.50
70	Ad	401	HEC	C2D-C1D-ND	4.22	114.83	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	AD	401	HEC	C1D-C2D-C3D	-4.19	102.55	106.96
69	AC	405	UQ6	C7-C8-C9	-4.10	120.89	127.24
57	B	303	PC1	O21-C21-C22	4.08	120.30	111.50
68	Ac	404	U10	C1-C6-C5	-4.07	115.75	119.58
62	Aa	501	CDL	OA6-CA5-C11	4.06	120.26	111.50
62	L	705	CDL	OB6-CB5-C51	4.05	120.24	111.50
58	i	201	3PE	O21-C21-C22	4.05	120.24	111.50
58	b	201	3PE	O21-C21-C22	4.05	120.22	111.50
58	M	502	3PE	O21-C21-C22	4.03	120.19	111.50
58	L	702	3PE	O21-C21-C22	4.03	120.18	111.50
70	AD	401	HEC	C2C-C1C-NC	4.00	116.17	110.08
58	L	701	3PE	O21-C21-C22	3.99	120.11	111.50
58	Ac	403	3PE	O21-C21-C22	3.99	120.11	111.50
62	h	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
62	L	704	CDL	OA6-CA5-C11	3.97	120.05	111.50
57	I	302	PC1	O21-C21-C22	3.97	120.05	111.50
68	AC	404	U10	C1M-C1-C6	-3.95	117.95	124.40
70	Ad	401	HEC	CMB-C2B-C3B	3.95	136.84	126.12
58	D	501	3PE	O21-C21-C22	3.95	120.01	111.50
67	AC	401	HEM	C1B-NB-C4B	3.94	109.14	105.07
67	AC	402	HEM	CHA-C4D-ND	3.91	129.20	124.37
62	a	101	CDL	OB6-CB5-C51	3.90	119.90	111.50
64	P	401	NDP	C2A-N3A-C4A	3.88	120.91	111.75
58	K	101	3PE	O21-C21-C22	3.86	119.83	111.50
70	Ad	401	HEC	C1D-C2D-C3D	-3.86	102.90	106.96
67	AC	402	HEM	C1B-NB-C4B	3.86	109.06	105.07
67	AC	402	HEM	CBD-CAD-C3D	-3.85	101.92	112.63
67	Ac	402	HEM	C1B-NB-C4B	3.85	109.05	105.07
63	O	402	ADP	C2-N3-C4	3.84	120.82	111.75
67	Ac	402	HEM	CHD-C4C-NC	3.83	128.58	124.44
67	AC	401	HEM	CHA-C4D-ND	3.79	129.05	124.37
67	Ac	401	HEM	CHB-C1B-NB	3.76	129.01	124.37
62	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
67	Ac	401	HEM	CHA-C4D-ND	3.74	128.98	124.37
58	O	401	3PE	O21-C21-C22	3.73	119.54	111.50
62	L	705	CDL	OA6-CA5-C11	3.73	119.54	111.50
62	Ag	101	CDL	OA6-CA5-C11	3.73	119.53	111.50
58	m	201	3PE	O21-C21-C22	3.72	119.51	111.50
67	Ac	401	HEM	C1B-NB-C4B	3.71	108.91	105.07
70	Ad	401	HEC	C2C-C1C-NC	3.68	115.69	110.08
58	m	202	3PE	O21-C21-C22	3.66	119.38	111.50
64	P	401	NDP	PN-O3-PA	-3.65	120.29	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	AD	401	HEC	CBB-CAB-C3B	3.64	122.47	112.43
70	Ad	401	HEC	CBC-CAC-C3C	3.63	122.43	112.43
58	M	503	3PE	O21-C21-C22	3.59	119.25	111.50
67	Ac	402	HEM	CHB-C1B-NB	3.58	128.78	124.37
63	O	402	ADP	PA-O3A-PB	-3.57	120.57	132.83
67	AC	402	HEM	CHB-C1B-NB	3.57	128.77	124.37
69	AC	405	UQ6	C12-C13-C14	-3.55	119.12	127.66
66	n	201	EHZ	C13-C12-N1	3.54	122.37	116.42
58	AC	403	3PE	O21-C21-C22	3.49	119.02	111.50
58	L	703	3PE	O21-C21-C22	3.47	118.98	111.50
62	Ac	406	CDL	OB8-CB7-C71	3.46	120.46	111.38
70	AD	401	HEC	C1A-C2A-C3A	-3.42	102.67	107.13
70	Ad	401	HEC	C3A-C4A-NA	3.41	115.99	109.69
70	AD	401	HEC	C3B-C4B-NB	3.40	113.95	110.17
70	Ad	401	HEC	CBB-CAB-C3B	3.39	121.78	112.43
70	Ad	401	HEC	C1A-C2A-C3A	-3.37	102.73	107.13
70	AD	401	HEC	CBC-CAC-C3C	3.36	121.69	112.43
66	n	201	EHZ	C14-N2-C15	-3.34	116.63	122.59
62	Aa	501	CDL	OB6-CB5-C51	3.32	120.07	110.80
62	Aa	501	CDL	OB8-CB7-C71	3.32	120.09	111.38
67	AC	402	HEM	CHD-C4C-NC	3.31	128.02	124.44
70	AD	401	HEC	C3C-C4C-NC	3.30	113.83	110.15
63	O	402	ADP	N3-C2-N1	-3.27	123.49	128.60
62	Ac	406	CDL	CB4-OB6-CB5	-3.24	109.81	117.79
62	Ac	406	CDL	OA6-CA5-C11	3.24	119.83	110.80
69	AC	405	UQ6	C15-C14-C16	3.23	120.70	115.27
68	Ac	404	U10	C4-C3-C2	-3.22	114.35	120.68
64	P	401	NDP	N3A-C2A-N1A	-3.20	123.59	128.60
64	P	401	NDP	C4A-C5A-N7A	-3.19	106.73	110.62
58	M	501	3PE	C2-O21-C21	-3.16	110.02	117.79
66	n	201	EHZ	C11-N1-C12	-3.14	117.00	122.84
58	K	101	3PE	C2-O21-C21	-3.13	110.08	117.79
67	Ac	401	HEM	C4C-NC-C1C	3.13	108.41	105.35
62	d	201	CDL	CA4-OA6-CA5	-3.11	110.15	117.79
58	j	700	3PE	C2-O21-C21	-3.10	110.16	117.79
70	Ad	401	HEC	C4A-C3A-C2A	-3.10	102.42	106.94
63	O	402	ADP	C4-N9-C8	3.10	109.09	105.73
66	W	201	EHZ	C13-C12-N1	3.08	121.60	116.42
70	AD	401	HEC	C3A-C4A-NA	3.06	115.33	109.69
67	Ac	401	HEM	CHD-C4C-NC	3.05	127.74	124.44
63	O	402	ADP	C4-C5-N7	-3.04	106.92	110.62
66	W	201	EHZ	C14-C13-C12	-3.04	107.30	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	L	702	3PE	O31-C31-C32	3.03	121.43	111.91
58	m	202	3PE	C2-O21-C21	-3.02	110.36	117.79
70	Ad	401	HEC	C3C-C4C-NC	3.00	113.50	110.15
67	Ac	402	HEM	C4D-ND-C1D	2.99	108.16	105.07
58	M	502	3PE	C2-O21-C21	-2.95	110.52	117.79
67	AC	401	HEM	C4D-ND-C1D	2.91	108.08	105.07
57	B	303	PC1	O31-C31-C32	2.91	121.04	111.91
66	W	201	EHZ	OP3-P1-O9	-2.89	99.35	110.68
70	AD	401	HEC	C4A-C3A-C2A	-2.88	102.74	106.94
58	m	201	3PE	C2-O21-C21	-2.86	110.75	117.79
66	W	201	EHZ	C7-C8-C9	-2.85	107.37	113.89
62	h	201	CDL	OB8-CB7-C71	2.85	120.84	111.91
67	AC	401	HEM	CHD-C1D-C2D	-2.84	120.54	124.98
58	i	201	3PE	O31-C31-C32	2.83	120.80	111.91
67	Ac	401	HEM	CAD-CBD-CGD	-2.80	107.57	113.60
62	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
70	Ad	401	HEC	C4D-C3D-C2D	-2.79	102.84	106.90
58	Ac	403	3PE	O31-C31-C32	2.78	120.64	111.91
70	Ad	401	HEC	CBD-CAD-C3D	-2.78	104.91	112.63
67	AC	401	HEM	C4C-NC-C1C	2.77	108.06	105.35
67	AC	402	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
56	B	302	UQ1	CM5-C5-C6	-2.77	119.88	124.40
62	a	101	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
67	Ac	402	HEM	C4C-CHD-C1D	-2.77	120.09	126.06
62	L	705	CDL	OB8-CB7-C71	2.76	120.57	111.91
64	P	401	NDP	C4A-N9A-C8A	2.73	108.68	105.73
62	L	704	CDL	OB8-CB7-C71	2.73	120.46	111.91
64	P	401	NDP	C5A-N7A-C8A	2.72	107.38	103.51
68	AC	404	U10	C12-C13-C14	-2.72	118.47	127.75
58	j	700	3PE	O31-C31-C32	2.71	120.42	111.91
62	d	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
63	O	402	ADP	C5-N7-C8	2.69	107.33	103.51
58	K	101	3PE	O31-C31-C32	2.69	120.35	111.91
57	I	302	PC1	C2-O21-C21	-2.69	111.17	117.79
62	L	705	CDL	CA4-OA6-CA5	-2.69	111.17	117.79
62	d	201	CDL	OA8-CA7-C31	2.68	120.32	111.91
56	B	302	UQ1	C11-C9-C10	2.68	120.52	114.60
58	M	502	3PE	O31-C31-C32	2.68	120.31	111.91
70	AD	401	HEC	C4D-C3D-C2D	-2.67	103.00	106.90
62	Ag	101	CDL	CB4-OB6-CB5	-2.66	111.23	117.79
70	AD	401	HEC	CAA-CBA-CGA	-2.66	107.88	113.60
67	AC	402	HEM	C4C-NC-C1C	2.66	107.95	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	AC	404	U10	C10-C9-C11	2.66	119.74	115.27
70	AD	401	HEC	CMD-C2D-C1D	2.66	129.09	125.04
58	m	202	3PE	O31-C31-C32	2.65	120.23	111.91
58	O	401	3PE	C2-O21-C21	-2.65	111.27	117.79
63	O	402	ADP	O4'-C1'-N9	2.65	113.28	108.06
58	M	503	3PE	O31-C31-C32	2.64	120.21	111.91
69	AC	405	UQ6	C10-C9-C11	2.64	119.71	115.27
58	m	201	3PE	O31-C31-C32	2.64	120.18	111.91
66	n	201	EHZ	OP3-P1-O9	-2.63	100.37	110.68
58	L	701	3PE	O31-C31-C32	2.63	120.17	111.91
69	AC	405	UQ6	C6-C7-C8	-2.63	108.01	112.17
62	L	705	CDL	CB4-OB6-CB5	-2.62	111.34	117.79
62	Aa	501	CDL	OA8-CA7-C31	2.62	120.12	111.91
58	M	503	3PE	C2-O21-C21	-2.61	111.37	117.79
67	AC	402	HEM	CHA-C4D-C3D	-2.60	120.44	125.33
62	h	201	CDL	CA4-OA6-CA5	-2.60	111.39	117.79
70	AD	401	HEC	CMC-C2C-C3C	2.59	131.22	125.61
58	Ac	403	3PE	C2-O21-C21	-2.59	111.42	117.79
62	L	705	CDL	OA8-CA7-C31	2.58	120.02	111.91
62	a	101	CDL	OB8-CB7-C71	2.58	120.00	111.91
60	F	501	FMN	C4A-C10-N1	-2.57	118.76	124.73
57	L	706	PC1	O31-C31-C32	2.57	119.97	111.91
68	Ac	404	U10	O4-C4-C5	-2.57	107.88	116.56
67	AC	401	HEM	C4B-C3B-C2B	-2.56	105.08	107.11
58	M	501	3PE	O31-C31-C32	2.56	119.94	111.91
67	Ac	401	HEM	CHD-C1D-C2D	-2.56	120.99	124.98
69	AC	405	UQ6	C21-C19-C20	2.55	120.24	114.60
67	Ac	402	HEM	C4C-NC-C1C	2.55	107.85	105.35
58	AC	403	3PE	O31-C31-C32	2.54	119.89	111.91
62	Ag	101	CDL	OA8-CA7-C31	2.54	119.89	111.91
70	AD	401	HEC	CAD-C3D-C4D	2.54	129.09	124.66
58	O	401	3PE	O31-C31-C32	2.53	119.84	111.91
67	Ac	402	HEM	CHD-C1D-C2D	-2.53	121.03	124.98
58	L	703	3PE	O31-C31-C32	2.52	119.81	111.91
62	L	704	CDL	OA8-CA7-C31	2.52	119.81	111.91
58	J	401	3PE	O31-C31-C32	2.52	119.81	111.91
57	L	706	PC1	C2-O21-C21	-2.51	111.61	117.79
58	D	501	3PE	C2-O21-C21	-2.50	111.63	117.79
58	b	201	3PE	O31-C31-C32	2.50	119.76	111.91
62	L	704	CDL	CA4-OA6-CA5	-2.50	111.64	117.79
68	Ac	404	U10	C7-C6-C5	2.50	121.48	118.48
58	L	703	3PE	C2-O21-C21	-2.49	111.67	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	D	501	3PE	O31-C31-C32	2.49	119.71	111.91
62	h	201	CDL	OA8-CA7-C31	2.47	119.67	111.91
66	n	201	EHZ	C10-S1-C9	2.47	109.56	101.87
58	L	701	3PE	C2-O21-C21	-2.47	111.72	117.79
62	Ac	406	CDL	OA8-CA7-C31	2.46	119.63	111.91
62	h	201	CDL	CB4-OB6-CB5	-2.46	111.74	117.79
67	AC	401	HEM	C3B-C2B-C1B	2.43	108.29	106.49
58	I	301	3PE	C2-O21-C21	-2.43	111.80	117.79
69	AC	405	UQ6	C4M-O4-C4	2.43	121.44	114.78
67	AC	401	HEM	CBD-CAD-C3D	-2.42	105.89	112.63
70	Ad	401	HEC	C3B-C4B-NB	2.42	112.86	110.17
67	Ac	402	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
60	F	501	FMN	O4-C4-C4A	-2.40	120.23	126.60
57	I	302	PC1	O31-C31-C32	2.39	119.41	111.91
60	F	501	FMN	C4-C4A-N5	2.39	121.63	118.23
66	W	201	EHZ	C5-C6-C7	-2.38	107.99	114.85
70	Ad	401	HEC	CMC-C2C-C1C	2.38	128.99	125.37
67	Ac	401	HEM	CAA-CBA-CGA	-2.37	108.51	113.60
62	Aa	501	CDL	CA4-OA6-CA5	-2.36	111.98	117.79
66	n	201	EHZ	O2-C9-S1	-2.36	119.55	122.61
67	AC	402	HEM	C1A-CHA-C4D	-2.36	120.74	126.34
62	a	101	CDL	CB4-OB6-CB5	-2.36	111.99	117.79
67	Ac	401	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
70	AD	401	HEC	CHB-C1B-C2B	-2.35	121.30	124.98
68	AC	404	U10	C16-C14-C15	2.35	119.79	114.60
56	B	302	UQ1	C7-C8-C9	-2.34	119.92	127.26
70	Ad	401	HEC	CAA-C2A-C1A	2.34	129.31	124.89
63	O	402	ADP	N9-C8-N7	-2.34	110.71	113.91
62	Ag	101	CDL	OB8-CB7-C71	2.33	119.22	111.91
67	AC	402	HEM	CHA-C1A-NA	2.28	128.05	123.85
70	Ad	401	HEC	CHA-C4D-C3D	-2.28	121.50	124.84
66	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
62	Aa	501	CDL	CB4-OB6-CB5	-2.25	112.26	117.79
67	Ac	401	HEM	C4D-ND-C1D	2.24	107.39	105.07
70	AD	401	HEC	CHC-C1C-C2C	-2.23	120.92	127.24
67	AC	402	HEM	C4A-NA-C1A	2.23	107.53	105.35
67	AC	402	HEM	C4C-CHD-C1D	-2.23	121.24	126.06
70	AD	401	HEC	CMB-C2B-C1B	2.22	128.43	125.04
67	Ac	402	HEM	CBD-CAD-C3D	-2.22	106.45	112.63
63	O	402	ADP	C6-C5-N7	2.22	136.16	132.02
58	I	301	3PE	O31-C31-C32	2.22	118.89	111.91
60	F	501	FMN	O2-C2-N1	-2.22	118.15	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	n	201	EHZ	O3-C12-N1	-2.22	118.83	123.01
67	Ac	401	HEM	C1A-CHA-C4D	-2.21	121.10	126.34
60	F	501	FMN	C4A-C10-N10	2.21	119.70	116.48
64	P	401	NDP	C3D-C2D-C1D	2.20	105.60	101.43
64	P	401	NDP	C6A-C5A-N7A	2.19	136.11	132.02
70	AD	401	HEC	CBD-CAD-C3D	-2.19	106.54	112.63
70	Ad	401	HEC	CHC-C1C-C2C	-2.19	121.05	127.24
67	Ac	401	HEM	CHA-C1A-NA	2.18	127.86	123.85
66	W	201	EHZ	C11-N1-C12	-2.18	118.79	122.84
58	b	201	3PE	O12-P-O14	-2.17	101.49	112.24
67	AC	401	HEM	C4A-CHB-C1B	-2.17	121.19	126.34
66	W	201	EHZ	O2-C9-S1	-2.17	119.80	122.61
67	AC	402	HEM	C4D-ND-C1D	2.17	107.31	105.07
62	Ag	101	CDL	CA4-OA6-CA5	-2.17	112.46	117.79
69	AC	405	UQ6	C17-C18-C19	-2.16	120.35	127.75
64	P	401	NDP	N9A-C8A-N7A	-2.16	110.96	113.91
62	Ac	406	CDL	OB6-CB5-OB7	-2.16	118.49	123.70
70	AD	401	HEC	CHA-C4D-C3D	-2.14	121.69	124.84
58	m	201	3PE	O21-C21-O22	-2.14	118.54	123.70
70	AD	401	HEC	CMA-C3A-C4A	2.13	128.47	124.71
60	F	501	FMN	C10-N1-C2	2.13	121.16	116.90
67	Ac	401	HEM	CHB-C1B-C2B	-2.12	120.83	126.73
66	W	201	EHZ	O6-P1-O9	2.12	112.42	106.47
62	d	201	CDL	OB6-CB5-OB7	-2.12	118.58	123.70
70	Ad	401	HEC	CHB-C4A-C3A	-2.11	121.05	125.48
62	L	705	CDL	OA6-CA5-OA7	-2.11	118.60	123.70
66	W	201	EHZ	O3-C12-N1	-2.10	119.04	123.01
67	AC	402	HEM	CAA-CBA-CGA	-2.10	109.08	113.60
67	AC	401	HEM	CHB-C1B-C2B	-2.10	120.89	126.73
67	Ac	402	HEM	C1A-CHA-C4D	-2.10	121.35	126.34
68	AC	404	U10	C7-C6-C5	2.08	120.99	118.48
70	AD	401	HEC	CHA-C1A-C2A	-2.08	121.56	124.94
66	n	201	EHZ	C5-C6-C7	-2.08	108.87	114.85
58	L	701	3PE	O21-C21-O22	-2.08	118.68	123.70
58	J	401	3PE	O12-P-O14	-2.06	102.07	112.24
58	j	700	3PE	O21-C21-O22	-2.05	118.74	123.70
70	Ad	401	HEC	CMC-C2C-C3C	2.04	130.03	125.61
67	Ac	402	HEM	CHB-C1B-C2B	-2.04	121.07	126.73
68	Ac	404	U10	O4-C4-C3	2.04	131.32	123.64
58	M	503	3PE	O21-C21-O22	-2.03	118.78	123.70
68	AC	404	U10	C6-C1-C2	2.03	120.79	119.18
66	n	201	EHZ	C16-C15-N2	2.03	120.62	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	Ac	404	U10	C3M-O3-C3	2.02	123.64	116.47
62	d	201	CDL	OA6-CA5-OA7	-2.01	118.84	123.70
62	Ac	406	CDL	CA4-OA6-CA5	-2.01	112.85	117.79
70	Ad	401	HEC	CMA-C3A-C4A	2.01	128.25	124.71
67	Ac	401	HEM	C4C-CHD-C1D	-2.01	121.73	126.06

All (2) chirality outliers are listed below:

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

All (529) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	I	302	PC1	C11-O13-P-O14
57	L	706	PC1	C1-O11-P-O14
57	L	706	PC1	C22-C21-O21-C2
57	L	706	PC1	O32-C31-O31-C3
57	L	706	PC1	C32-C31-O31-C3
58	D	501	3PE	C1-O11-P-O12
58	I	301	3PE	C1-O11-P-O12
58	I	301	3PE	C22-C21-O21-C2
58	J	401	3PE	C11-O13-P-O12
58	J	401	3PE	C11-O13-P-O14
58	J	401	3PE	C12-C11-O13-P
58	J	401	3PE	O32-C31-O31-C3
58	J	401	3PE	C32-C31-O31-C3
58	K	101	3PE	C11-O13-P-O12
58	L	701	3PE	C1-O11-P-O12
58	L	701	3PE	O22-C21-O21-C2
58	L	701	3PE	C22-C21-O21-C2
58	L	702	3PE	C1-O11-P-O13
58	L	702	3PE	C1-O11-P-O14
58	L	702	3PE	C11-O13-P-O11
58	L	702	3PE	C11-O13-P-O12
58	L	702	3PE	C11-O13-P-O14
58	L	702	3PE	O32-C31-O31-C3
58	L	702	3PE	C32-C31-O31-C3
58	L	702	3PE	C22-C21-O21-C2
58	M	502	3PE	C1-O11-P-O12
58	M	502	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
58	M	502	3PE	C1-O11-P-O14
58	M	502	3PE	C11-O13-P-O11
58	M	502	3PE	C11-O13-P-O12
58	M	502	3PE	C11-O13-P-O14
58	b	201	3PE	C1-O11-P-O12
58	b	201	3PE	C1-O11-P-O14
58	b	201	3PE	O22-C21-O21-C2
58	i	201	3PE	C1-O11-P-O12
58	m	201	3PE	C11-O13-P-O12
58	m	202	3PE	C1-O11-P-O12
58	m	202	3PE	C1-O11-P-O14
58	m	202	3PE	C22-C21-O21-C2
58	AC	403	3PE	C1-O11-P-O12
58	Ac	403	3PE	C1-O11-P-O12
60	F	501	FMN	C5'-O5'-P-O2P
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C19-C21-C22-C23
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C18-C19-C21-C22
61	H	400	UQ9	C17-C18-C19-C21
61	H	400	UQ9	C17-C18-C19-C20
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C12-C13-C14-C16
61	H	400	UQ9	C12-C13-C14-C15
62	L	704	CDL	CA2-OA2-PA1-OA3
62	L	704	CDL	CA2-OA2-PA1-OA4
62	L	704	CDL	CA2-OA2-PA1-OA5
62	L	704	CDL	CB2-OB2-PB2-OB3
62	L	704	CDL	C51-CB5-OB6-CB4
62	L	705	CDL	CA2-OA2-PA1-OA3
62	L	705	CDL	CA2-OA2-PA1-OA4
62	L	705	CDL	CB3-OB5-PB2-OB2
62	L	705	CDL	CB3-OB5-PB2-OB3
62	L	705	CDL	CB3-OB5-PB2-OB4
62	a	101	CDL	CA3-OA5-PA1-OA2
62	a	101	CDL	CA3-OA5-PA1-OA3
62	a	101	CDL	CA3-OA5-PA1-OA4
62	d	201	CDL	CA2-C1-CB2-OB2
62	d	201	CDL	CA3-OA5-PA1-OA2
62	d	201	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	CB2-OB2-PB2-OB3
62	d	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
62	d	201	CDL	C51-CB5-OB6-CB4
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB2-OB2-PB2-OB3
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	Aa	501	CDL	CA3-OA5-PA1-OA3
62	Aa	501	CDL	CB2-OB2-PB2-OB4
62	Ac	406	CDL	CA2-OA2-PA1-OA3
62	Ac	406	CDL	CA2-OA2-PA1-OA4
62	Ac	406	CDL	CB2-OB2-PB2-OB3
62	Ac	406	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
64	P	401	NDP	C2B-O2B-P2B-O2X
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C7-C8-C9-S1
66	W	201	EHZ	S1-C10-C11-N1
66	W	201	EHZ	C11-C10-S1-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	C20-O6-P1-O7
66	W	201	EHZ	C20-O6-P1-O9
66	W	201	EHZ	C20-O6-P1-OP3
66	n	201	EHZ	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
67	AC	401	HEM	C2C-C3C-CAC-CBC
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
67	AC	402	HEM	C2C-C3C-CAC-CBC
67	Ac	401	HEM	C2C-C3C-CAC-CBC
67	Ac	402	HEM	C1A-C2A-CAA-CBA
68	Ac	404	U10	C7-C8-C9-C10
68	Ac	404	U10	C7-C8-C9-C11
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
70	AD	401	HEC	C4B-C3B-CAB-CBB
68	Ac	404	U10	C12-C13-C14-C15
68	Ac	404	U10	C12-C13-C14-C16
70	AD	401	HEC	C2B-C3B-CAB-CBB
70	Ad	401	HEC	C4B-C3B-CAB-CBB
57	I	302	PC1	O32-C31-O31-C3
58	K	101	3PE	O32-C31-O31-C3
58	M	503	3PE	O32-C31-O31-C3
58	j	700	3PE	O32-C31-O31-C3
62	Ac	406	CDL	OB9-CB7-OB8-CB6
70	AD	401	HEC	C4C-C3C-CAC-CBC
70	Ad	401	HEC	C4C-C3C-CAC-CBC
70	Ad	401	HEC	C2B-C3B-CAB-CBB
70	AD	401	HEC	C2C-C3C-CAC-CBC
70	Ad	401	HEC	C2C-C3C-CAC-CBC
58	I	301	3PE	O22-C21-O21-C2
58	L	702	3PE	O22-C21-O21-C2
58	m	201	3PE	O22-C21-O21-C2
58	m	202	3PE	O22-C21-O21-C2
62	L	704	CDL	OB7-CB5-OB6-CB4
62	d	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
57	I	302	PC1	C32-C31-O31-C3
58	j	700	3PE	C32-C31-O31-C3
62	L	704	CDL	C31-CA7-OA8-CA6
62	L	705	CDL	C71-CB7-OB8-CB6
62	Ac	406	CDL	C71-CB7-OB8-CB6
58	b	201	3PE	C22-C21-O21-C2
58	m	201	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	Ac	405	UQ6	C17-C18-C19-C21
61	H	400	UQ9	C24-C26-C27-C28
68	AC	404	U10	C12-C11-C9-C10
68	AC	404	U10	C12-C11-C9-C8
58	I	301	3PE	C32-C31-O31-C3
58	K	101	3PE	C32-C31-O31-C3
58	M	503	3PE	C32-C31-O31-C3
61	H	400	UQ9	C22-C23-C24-C25
57	L	706	PC1	O22-C21-O21-C2
61	H	400	UQ9	C22-C23-C24-C26
58	m	202	3PE	O32-C31-O31-C3
62	L	704	CDL	OA9-CA7-OA8-CA6
62	Aa	501	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	O1-C1-CB2-OB2
58	O	401	3PE	C32-C31-O31-C3
58	AC	403	3PE	C32-C31-O31-C3
62	Aa	501	CDL	C71-CB7-OB8-CB6
62	L	705	CDL	OB9-CB7-OB8-CB6
58	D	501	3PE	C22-C21-O21-C2
58	J	401	3PE	C22-C21-O21-C2
58	L	703	3PE	C22-C21-O21-C2
62	L	705	CDL	C11-CA5-OA6-CA4
58	m	202	3PE	C32-C31-O31-C3
62	h	201	CDL	CA4-CA3-OA5-PA1
58	I	301	3PE	O32-C31-O31-C3
58	AC	403	3PE	O32-C31-O31-C3
67	Ac	401	HEM	C2A-CAA-CBA-CGA
61	H	400	UQ9	C13-C14-C16-C17
58	O	401	3PE	O32-C31-O31-C3
61	H	400	UQ9	C9-C11-C12-C13
69	Ac	405	UQ6	C9-C11-C12-C13
69	Ac	405	UQ6	C14-C16-C17-C18
58	L	703	3PE	C32-C31-O31-C3
62	Ac	406	CDL	CB4-CB6-OB8-CB7
58	b	201	3PE	C2B-C2C-C2D-C2E
58	J	401	3PE	O22-C21-O21-C2
58	L	703	3PE	O32-C31-O31-C3
58	b	201	3PE	C32-C31-O31-C3
62	d	201	CDL	C31-CA7-OA8-CA6
62	Aa	501	CDL	C31-CA7-OA8-CA6
58	b	201	3PE	C39-C3A-C3B-C3C
62	d	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
58	L	703	3PE	O22-C21-O21-C2
62	a	101	CDL	C12-C13-C14-C15
58	b	201	3PE	O32-C31-O31-C3
62	d	201	CDL	OA9-CA7-OA8-CA6
62	h	201	CDL	C71-CB7-OB8-CB6
58	m	201	3PE	C32-C31-O31-C3
58	M	501	3PE	C2-C3-O31-C31
58	M	501	3PE	C32-C33-C34-C35
62	Ag	101	CDL	CA4-CA3-OA5-PA1
62	Aa	501	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C14-C16-C17-C18
58	D	501	3PE	O22-C21-O21-C2
62	L	705	CDL	OA7-CA5-OA6-CA4
58	m	201	3PE	O32-C31-O31-C3
58	AC	403	3PE	C22-C21-O21-C2
58	I	301	3PE	C1-O11-P-O13
58	J	401	3PE	C11-O13-P-O11
58	L	701	3PE	C1-O11-P-O13
58	O	401	3PE	C1-O11-P-O13
58	b	201	3PE	C1-O11-P-O13
58	i	201	3PE	C1-O11-P-O13
58	m	201	3PE	C1-O11-P-O13
58	m	201	3PE	C11-O13-P-O11
58	m	202	3PE	C1-O11-P-O13
58	AC	403	3PE	C1-O11-P-O13
62	L	705	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2
62	Aa	501	CDL	CA3-OA5-PA1-OA2
62	Ac	406	CDL	CA2-OA2-PA1-OA5
62	Ac	406	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CA2-OA2-PA1-OA5
62	Ag	101	CDL	CA3-OA5-PA1-OA2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
58	M	501	3PE	C32-C31-O31-C3
62	L	704	CDL	C17-C18-C19-C20
58	M	502	3PE	C22-C21-O21-C2
58	M	501	3PE	C23-C24-C25-C26
62	h	201	CDL	C18-C19-C20-C21
62	h	201	CDL	OB9-CB7-OB8-CB6
58	M	502	3PE	O22-C21-O21-C2
58	AC	403	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
58	L	703	3PE	C21-C22-C23-C24
62	L	704	CDL	C52-C53-C54-C55
58	m	201	3PE	C24-C25-C26-C27
62	L	704	CDL	C12-C13-C14-C15
62	L	704	CDL	C71-CB7-OB8-CB6
58	O	401	3PE	C22-C21-O21-C2
62	L	704	CDL	C11-CA5-OA6-CA4
58	M	501	3PE	O32-C31-O31-C3
62	Ag	101	CDL	C74-C75-C76-C77
62	L	704	CDL	OA7-CA5-OA6-CA4
58	L	703	3PE	C22-C23-C24-C25
67	AC	402	HEM	C2A-CAA-CBA-CGA
57	B	303	PC1	C22-C21-O21-C2
62	L	705	CDL	C51-CB5-OB6-CB4
58	b	201	3PE	C27-C28-C29-C2A
62	L	705	CDL	C72-C73-C74-C75
62	L	704	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	OA7-CA5-OA6-CA4
62	Ac	406	CDL	OA7-CA5-OA6-CA4
62	d	201	CDL	C71-CB7-OB8-CB6
67	Ac	401	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2C-C3C-CAC-CBC
58	M	502	3PE	C3C-C3D-C3E-C3F
58	K	101	3PE	C22-C21-O21-C2
62	d	201	CDL	C11-CA5-OA6-CA4
62	Ac	406	CDL	C11-CA5-OA6-CA4
67	AC	401	HEM	C4C-C3C-CAC-CBC
67	AC	402	HEM	C4C-C3C-CAC-CBC
67	Ac	401	HEM	C4C-C3C-CAC-CBC
57	B	303	PC1	O22-C21-O21-C2
58	O	401	3PE	O22-C21-O21-C2
62	L	705	CDL	OB7-CB5-OB6-CB4
58	K	101	3PE	O22-C21-O21-C2
58	I	301	3PE	C11-O13-P-O11
58	K	101	3PE	C11-O13-P-O11
58	M	501	3PE	C1-O11-P-O13
62	h	201	CDL	CB3-OB5-PB2-OB2
62	Aa	501	CDL	CB2-OB2-PB2-OB5
58	J	401	3PE	C37-C38-C39-C3A
58	K	101	3PE	C22-C23-C24-C25
58	D	501	3PE	C24-C25-C26-C27
62	a	101	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
58	b	201	3PE	C1-C2-C3-O31
62	d	201	CDL	CA3-CA4-CA6-OA8
58	L	701	3PE	C24-C25-C26-C27
62	a	101	CDL	C71-CB7-OB8-CB6
66	n	201	EHZ	C3-C4-C5-C6
58	AC	403	3PE	C23-C24-C25-C26
62	Ag	101	CDL	C31-CA7-OA8-CA6
62	L	705	CDL	C12-C13-C14-C15
58	J	401	3PE	C3-C2-O21-C21
60	F	501	FMN	C5'-O5'-P-O1P
58	i	201	3PE	C32-C33-C34-C35
62	d	201	CDL	OB9-CB7-OB8-CB6
58	M	503	3PE	C24-C25-C26-C27
58	K	101	3PE	C21-C22-C23-C24
58	L	701	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
58	b	201	3PE	O11-C1-C2-C3
58	M	503	3PE	C28-C29-C2A-C2B
58	m	201	3PE	C23-C24-C25-C26
58	L	702	3PE	C2-C1-O11-P
62	d	201	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	CB4-CB3-OB5-PB2
58	L	702	3PE	C34-C35-C36-C37
58	L	702	3PE	C24-C25-C26-C27
58	i	201	3PE	C1-C2-C3-O31
66	W	201	EHZ	N2-C15-C16-C17
58	I	301	3PE	C23-C24-C25-C26
58	M	502	3PE	C23-C24-C25-C26
62	a	101	CDL	OB9-CB7-OB8-CB6
62	Ag	101	CDL	OA9-CA7-OA8-CA6
58	b	201	3PE	C24-C25-C26-C27
57	I	302	PC1	C11-O13-P-O11
62	L	705	CDL	CA3-OA5-PA1-OA2
62	h	201	CDL	CB2-OB2-PB2-OB5
66	W	201	EHZ	C3-C4-C5-C6
62	a	101	CDL	OA9-CA7-OA8-CA6
58	I	301	3PE	C21-C22-C23-C24
66	W	201	EHZ	C5-C6-C7-O1
58	i	201	3PE	O21-C2-C3-O31
57	B	303	PC1	C32-C31-O31-C3
62	d	201	CDL	C52-C53-C54-C55
68	AC	404	U10	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
62	a	101	CDL	OA7-CA5-OA6-CA4
69	AC	405	UQ6	C15-C14-C16-C17
67	Ac	402	HEM	C3A-C2A-CAA-CBA
62	h	201	CDL	C14-C15-C16-C17
62	L	704	CDL	CA4-CA3-OA5-PA1
62	L	705	CDL	CA4-CA3-OA5-PA1
58	M	502	3PE	C32-C31-O31-C3
66	W	201	EHZ	O2-C9-S1-C10
62	Ag	101	CDL	C51-CB5-OB6-CB4
62	L	704	CDL	OB5-CB3-CB4-CB6
58	J	401	3PE	C2A-C2B-C2C-C2D
58	L	702	3PE	C25-C26-C27-C28
62	h	201	CDL	CB3-CB4-OB6-CB5
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
58	J	401	3PE	C2-C1-O11-P
58	O	401	3PE	C2-C1-O11-P
58	i	201	3PE	C2-C1-O11-P
62	a	101	CDL	CB3-CB4-CB6-OB8
62	d	201	CDL	CB4-CB3-OB5-PB2
62	h	201	CDL	CB4-CB3-OB5-PB2
58	b	201	3PE	O11-C1-C2-O21
62	L	704	CDL	OB5-CB3-CB4-OB6
67	Ac	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4C-C3C-CAC-CBC
66	n	201	EHZ	O1-C7-C8-C9
58	L	701	3PE	O32-C31-O31-C3
58	M	502	3PE	O32-C31-O31-C3
62	a	101	CDL	OB6-CB4-CB6-OB8
58	L	701	3PE	C28-C29-C2A-C2B
58	L	702	3PE	C32-C33-C34-C35
62	L	705	CDL	C57-C58-C59-C60
62	Ac	406	CDL	OB7-CB5-OB6-CB4
62	Ag	101	CDL	OB7-CB5-OB6-CB4
57	B	303	PC1	O32-C31-O31-C3
58	O	401	3PE	C36-C37-C38-C39
62	L	704	CDL	C71-C72-C73-C74
62	Ac	406	CDL	C51-CB5-OB6-CB4
57	I	302	PC1	C1-O11-P-O13
58	M	503	3PE	C11-O13-P-O11
58	b	201	3PE	C11-O13-P-O11
62	L	704	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
62	a	101	CDL	CA4-CA3-OA5-PA1
62	Ag	101	CDL	C1-CA2-OA2-PA1
58	I	301	3PE	C11-O13-P-O12
58	I	301	3PE	C11-O13-P-O14
58	K	101	3PE	C11-O13-P-O14
58	O	401	3PE	C1-O11-P-O12
58	O	401	3PE	C1-O11-P-O14
58	b	201	3PE	C11-O13-P-O12
58	m	201	3PE	C1-O11-P-O12
58	m	201	3PE	C1-O11-P-O14
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	Aa	501	CDL	CA3-OA5-PA1-OA4
62	Aa	501	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CA2-OA2-PA1-OA3
62	Ag	101	CDL	CA3-OA5-PA1-OA3
62	Ag	101	CDL	CA3-OA5-PA1-OA4
58	m	201	3PE	C2E-C2F-C2G-C2H
62	Ag	101	CDL	C71-CB7-OB8-CB6
58	L	701	3PE	C25-C26-C27-C28
58	L	703	3PE	C29-C2A-C2B-C2C
64	P	401	NDP	O4D-C1D-N1N-C6N
57	B	303	PC1	C11-C12-N-C15
57	I	302	PC1	C11-C12-N-C15
57	L	706	PC1	O13-C11-C12-N
58	b	201	3PE	O21-C2-C3-O31
58	m	201	3PE	C33-C34-C35-C36
58	j	700	3PE	C22-C21-O21-C2
62	L	705	CDL	C56-C57-C58-C59
66	W	201	EHZ	O4-C15-C16-O5
62	Ag	101	CDL	OB9-CB7-OB8-CB6
58	M	503	3PE	C34-C35-C36-C37
57	L	706	PC1	C3B-C3C-C3D-C3E
66	W	201	EHZ	C19-C17-C20-O6
58	b	201	3PE	C3-C2-O21-C21
62	L	704	CDL	CB6-CB4-OB6-CB5
62	Ac	406	CDL	CA6-CA4-OA6-CA5
58	D	501	3PE	C32-C31-O31-C3
57	I	302	PC1	C11-C12-N-C13
58	j	700	3PE	O22-C21-O21-C2
57	L	706	PC1	C1-O11-P-O13
58	M	503	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
58	j	700	3PE	C1-O11-P-O13
62	L	704	CDL	CA3-OA5-PA1-OA2
62	L	704	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CB2-OB2-PB2-OB5
62	d	201	CDL	CA2-OA2-PA1-OA5
62	d	201	CDL	CB3-OB5-PB2-OB2
62	Aa	501	CDL	CA2-OA2-PA1-OA5
58	D	501	3PE	C32-C33-C34-C35
58	L	701	3PE	C33-C34-C35-C36
66	W	201	EHZ	C2-C3-C4-C5
64	P	401	NDP	PN-O3-PA-O2A
58	j	700	3PE	C2-C1-O11-P
62	Aa	501	CDL	CA4-CA3-OA5-PA1
58	D	501	3PE	O32-C31-O31-C3
58	J	401	3PE	C2B-C2C-C2D-C2E
57	B	303	PC1	C11-C12-N-C14
67	Ac	401	HEM	CAA-CBA-CGA-O1A
58	J	401	3PE	C28-C29-C2A-C2B
67	AC	402	HEM	CAD-CBD-CGD-O1D
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	AC	402	HEM	CAA-CBA-CGA-O2A
67	Ac	402	HEM	CAD-CBD-CGD-O1D
67	AC	401	HEM	CAD-CBD-CGD-O1D
67	AC	402	HEM	CAA-CBA-CGA-O1A
58	i	201	3PE	O22-C21-O21-C2
70	Ad	401	HEC	C3A-C2A-CAA-CBA
58	M	503	3PE	C23-C24-C25-C26
68	Ac	404	U10	C12-C11-C9-C10
67	AC	401	HEM	CAA-CBA-CGA-O2A
58	i	201	3PE	C3-C2-O21-C21
57	B	303	PC1	C11-C12-N-C13
57	I	302	PC1	C11-C12-N-C14
58	M	502	3PE	C39-C3A-C3B-C3C
67	Ac	401	HEM	CAD-CBD-CGD-O2D
62	a	101	CDL	C1-CA2-OA2-PA1
58	J	401	3PE	O11-C1-C2-O21
67	Ac	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAD-CBD-CGD-O1D
62	d	201	CDL	C59-C60-C61-C62
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
66	n	201	EHZ	C11-C10-S1-C9
62	h	201	CDL	C31-CA7-OA8-CA6
70	Ad	401	HEC	C1A-C2A-CAA-CBA
68	Ac	404	U10	C12-C11-C9-C8
58	L	702	3PE	C23-C24-C25-C26
67	AC	401	HEM	CAD-CBD-CGD-O2D
62	L	704	CDL	C14-C15-C16-C17
62	Ac	406	CDL	CA4-CA3-OA5-PA1
69	Ac	405	UQ6	C5-C6-C7-C8
58	J	401	3PE	C25-C26-C27-C28
66	n	201	EHZ	C2-C3-C4-C5
68	AC	404	U10	C1-C6-C7-C8
62	h	201	CDL	OA9-CA7-OA8-CA6
62	L	704	CDL	OA5-CA3-CA4-OA6
57	I	302	PC1	C2C-C2D-C2E-C2F
57	L	706	PC1	C2-C3-O31-C31
58	J	401	3PE	O11-C1-C2-C3
69	AC	405	UQ6	C13-C14-C16-C17
66	W	201	EHZ	N2-C15-C16-O5
70	AD	401	HEC	C3D-CAD-CBD-CGD
58	b	201	3PE	C25-C26-C27-C28
66	W	201	EHZ	C18-C17-C20-O6
57	I	302	PC1	C2E-C2F-C2G-C2H
68	AC	404	U10	C5-C6-C7-C8
58	D	501	3PE	C34-C35-C36-C37
70	AD	401	HEC	CAA-CBA-CGA-O2A
70	Ad	401	HEC	CAA-CBA-CGA-O2A
62	L	705	CDL	C52-C53-C54-C55
58	i	201	3PE	O21-C21-C22-C23
58	K	101	3PE	O11-C1-C2-O21
58	J	401	3PE	C33-C34-C35-C36
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
58	M	502	3PE	C26-C27-C28-C29
66	W	201	EHZ	C15-C16-C17-C18
70	AD	401	HEC	CAA-CBA-CGA-O1A
70	Ad	401	HEC	CAA-CBA-CGA-O1A
66	W	201	EHZ	O5-C16-C17-C18
58	L	701	3PE	C39-C3A-C3B-C3C
58	M	501	3PE	C24-C25-C26-C27
58	K	101	3PE	C24-C25-C26-C27
62	L	705	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
58	M	502	3PE	C36-C37-C38-C39
58	K	101	3PE	C36-C37-C38-C39
62	L	704	CDL	C53-C54-C55-C56
69	AC	405	UQ6	C1-C6-C7-C8
62	a	101	CDL	C32-C31-CA7-OA8
62	d	201	CDL	C12-C11-CA5-OA6
58	K	101	3PE	C23-C24-C25-C26
58	i	201	3PE	O22-C21-C22-C23
69	Ac	405	UQ6	C6-C7-C8-C9
58	L	701	3PE	C34-C35-C36-C37
62	a	101	CDL	C1-CB2-OB2-PB2
62	Ac	406	CDL	C1-CA2-OA2-PA1
58	D	501	3PE	C1-O11-P-O14
58	L	703	3PE	C1-O11-P-O14
58	M	501	3PE	C1-O11-P-O14
58	Ac	403	3PE	C1-O11-P-O14
62	L	705	CDL	CA3-OA5-PA1-OA4
62	d	201	CDL	CA2-OA2-PA1-OA3
62	d	201	CDL	CB3-OB5-PB2-OB3
63	O	402	ADP	C5'-O5'-PA-O1A
62	a	101	CDL	C32-C31-CA7-OA9
62	Ac	406	CDL	C52-C51-CB5-OB6
58	i	201	3PE	C32-C31-O31-C3
58	K	101	3PE	O13-C11-C12-N
58	L	701	3PE	C2B-C2C-C2D-C2E
58	M	502	3PE	C2B-C2C-C2D-C2E
58	D	501	3PE	C12-C11-O13-P
58	I	301	3PE	C1-C2-O21-C21
58	L	703	3PE	C12-C11-O13-P
66	W	201	EHZ	O4-C15-C16-C17
58	i	201	3PE	O32-C31-O31-C3
58	L	702	3PE	O21-C21-C22-C23
58	Ac	403	3PE	C23-C24-C25-C26
57	L	706	PC1	C27-C28-C29-C2A
58	L	703	3PE	C24-C25-C26-C27
57	B	303	PC1	O21-C21-C22-C23
62	h	201	CDL	C72-C71-CB7-OB8
62	d	201	CDL	C11-C12-C13-C14
62	d	201	CDL	C12-C11-CA5-OA7
62	Ac	406	CDL	C52-C51-CB5-OB7

There are no ring outliers.

52 monomers are involved in 442 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Ac	401	HEM	3	0
62	L	704	CDL	16	0
58	L	703	3PE	20	0
58	j	700	3PE	9	0
67	AC	402	HEM	5	0
68	Ac	404	U10	12	0
62	Ag	101	CDL	6	0
58	Ac	403	3PE	4	0
57	B	303	PC1	3	0
63	O	402	ADP	6	0
69	Ac	405	UQ6	8	0
58	K	101	3PE	6	0
57	L	706	PC1	17	0
62	Ac	406	CDL	5	0
58	AC	403	3PE	4	0
60	F	501	FMN	3	0
59	E	301	FES	4	0
59	G	803	FES	4	0
67	AC	401	HEM	3	0
55	F	502	SF4	10	0
58	M	503	3PE	27	0
55	G	802	SF4	5	0
62	h	201	CDL	13	0
62	L	705	CDL	15	0
66	W	201	EHZ	7	0
58	m	201	3PE	12	0
68	AC	404	U10	9	0
58	b	201	3PE	11	0
67	Ac	402	HEM	3	0
55	B	301	SF4	5	0
57	I	302	PC1	7	0
58	i	201	3PE	11	0
58	M	502	3PE	4	0
58	D	501	3PE	13	0
58	O	401	3PE	7	0
70	Ad	401	HEC	18	0
58	L	702	3PE	6	0
58	m	202	3PE	4	0
64	P	401	NDP	4	0
70	AD	401	HEC	5	0
55	I	303	SF4	11	0
69	AC	405	UQ6	7	0

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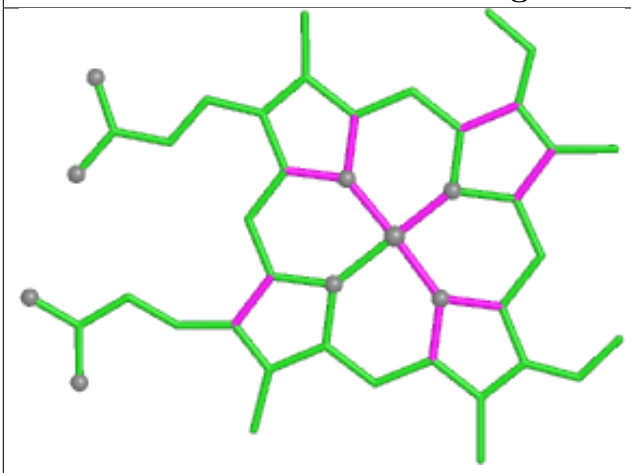
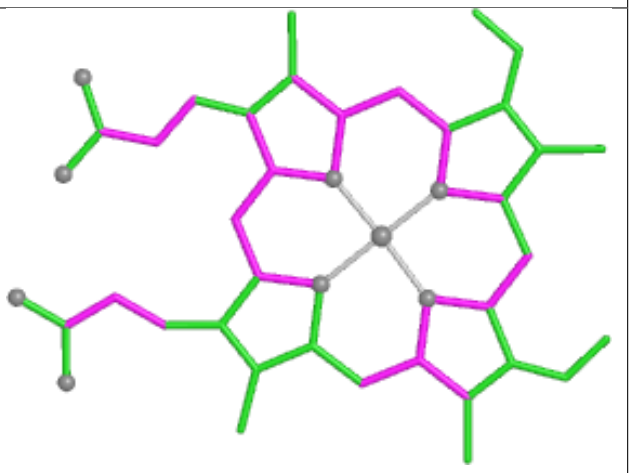
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	M	501	3PE	9	0
56	B	302	UQ1	12	0
55	I	304	SF4	5	0
58	J	401	3PE	18	0
61	H	400	UQ9	16	0
62	a	101	CDL	15	0
62	d	201	CDL	5	0
62	Aa	501	CDL	3	0
58	L	701	3PE	9	0
58	I	301	3PE	10	0

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 then 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.

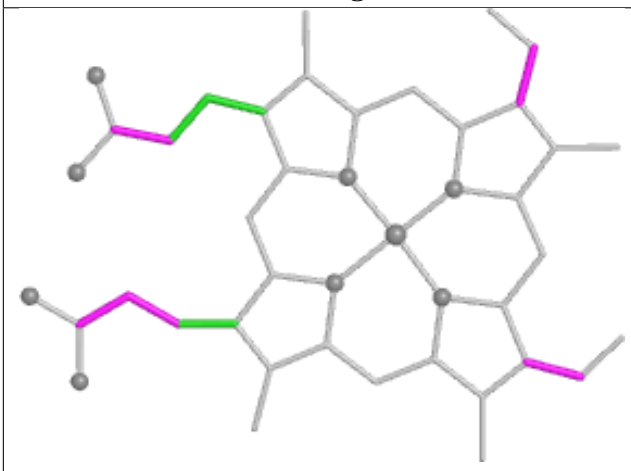
Ligand HEM Ac 401



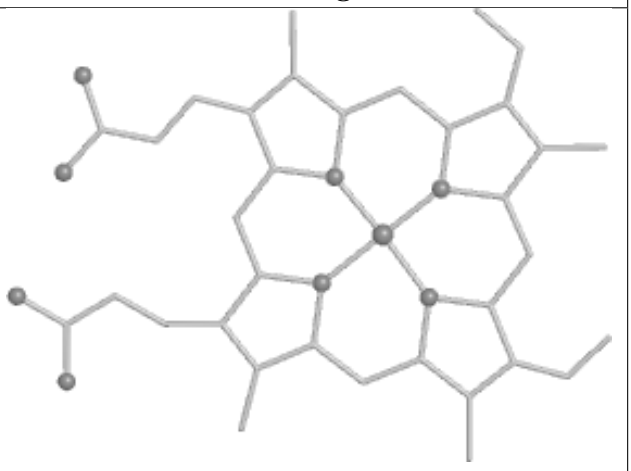
Bond lengths



Bond angles

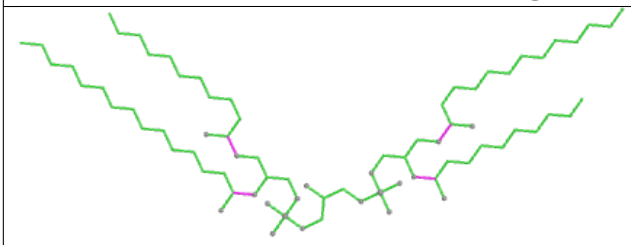


Torsions



Rings

Ligand CDL L 704



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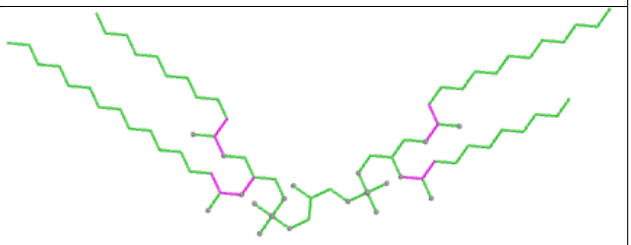

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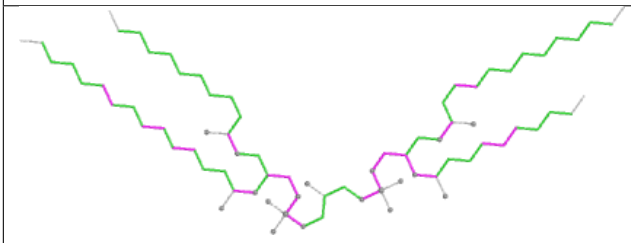
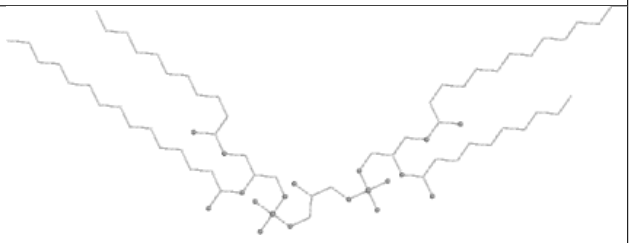
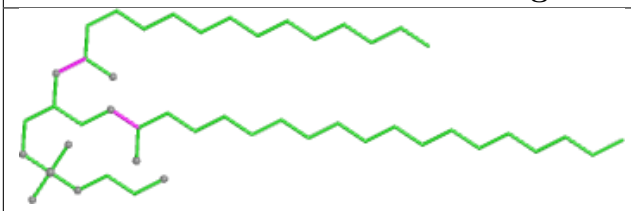
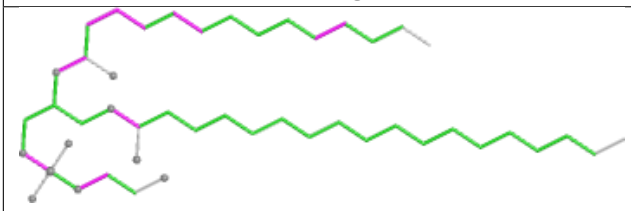
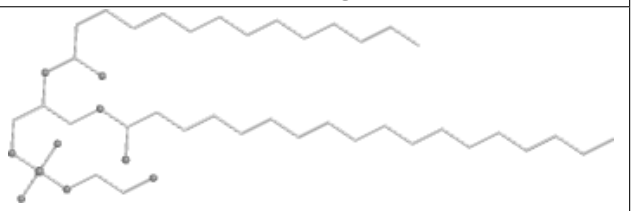
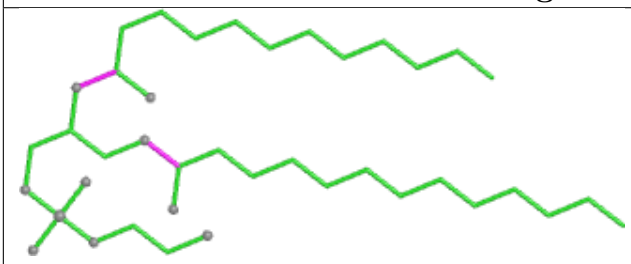
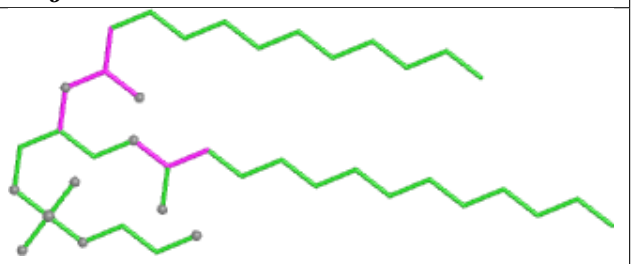
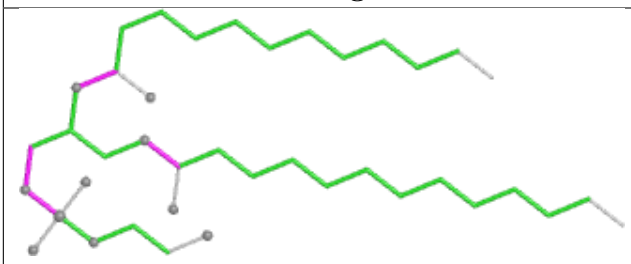
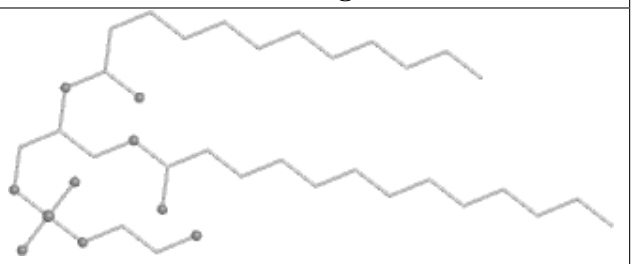


Torsions

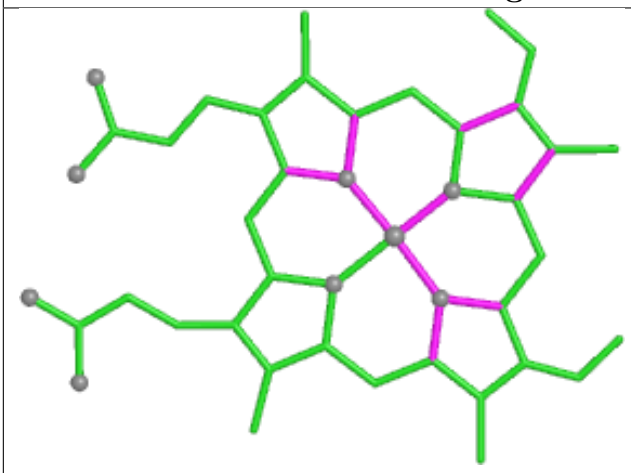


Rings

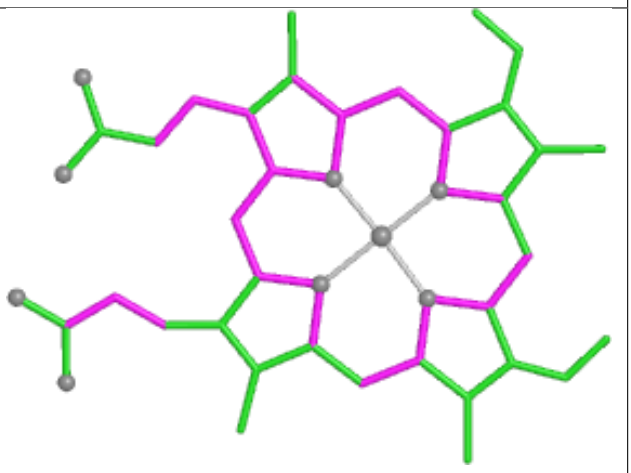
Ligand 3PE L 703	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand 3PE j 700	
 Bond lengths	 Bond angles
 Torsions	 Rings

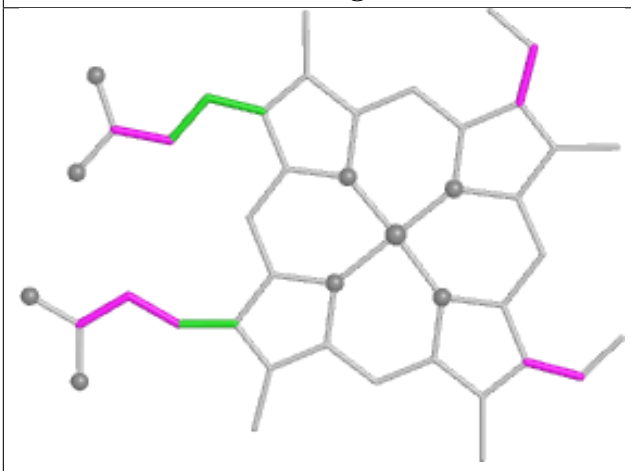
Ligand HEM AC 402



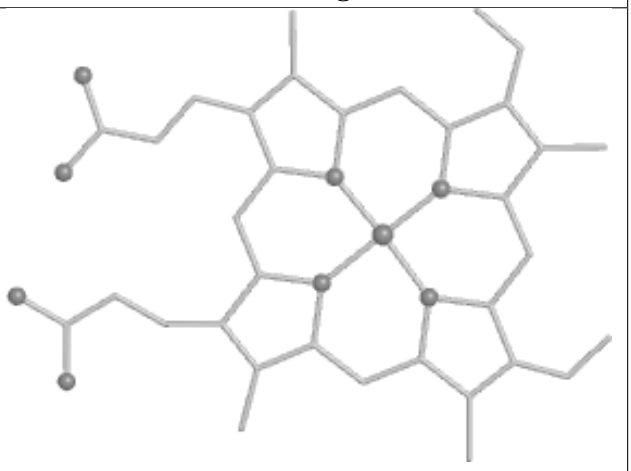
Bond lengths



Bond angles

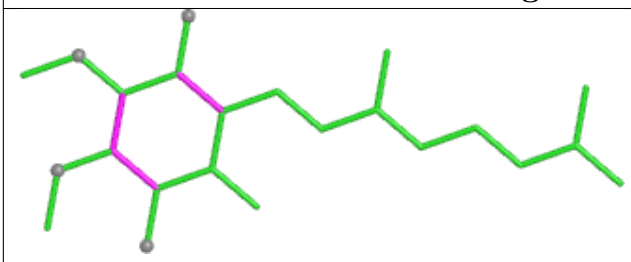


Torsions



Rings

Ligand U10 Ac 404



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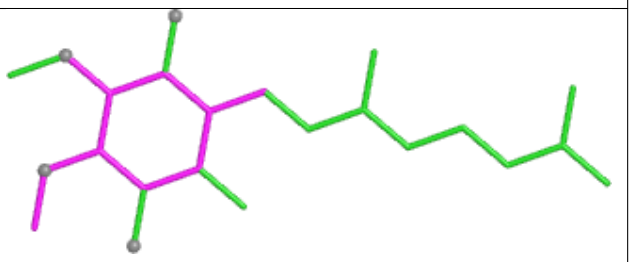
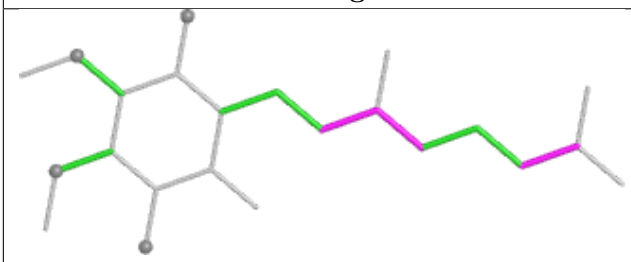
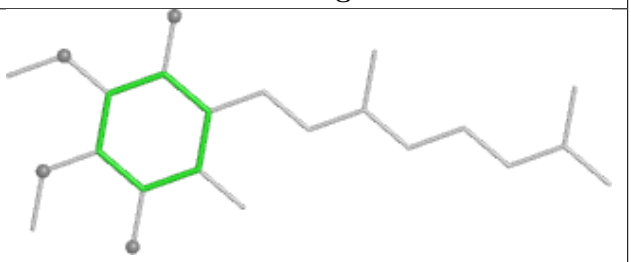


Bond angles

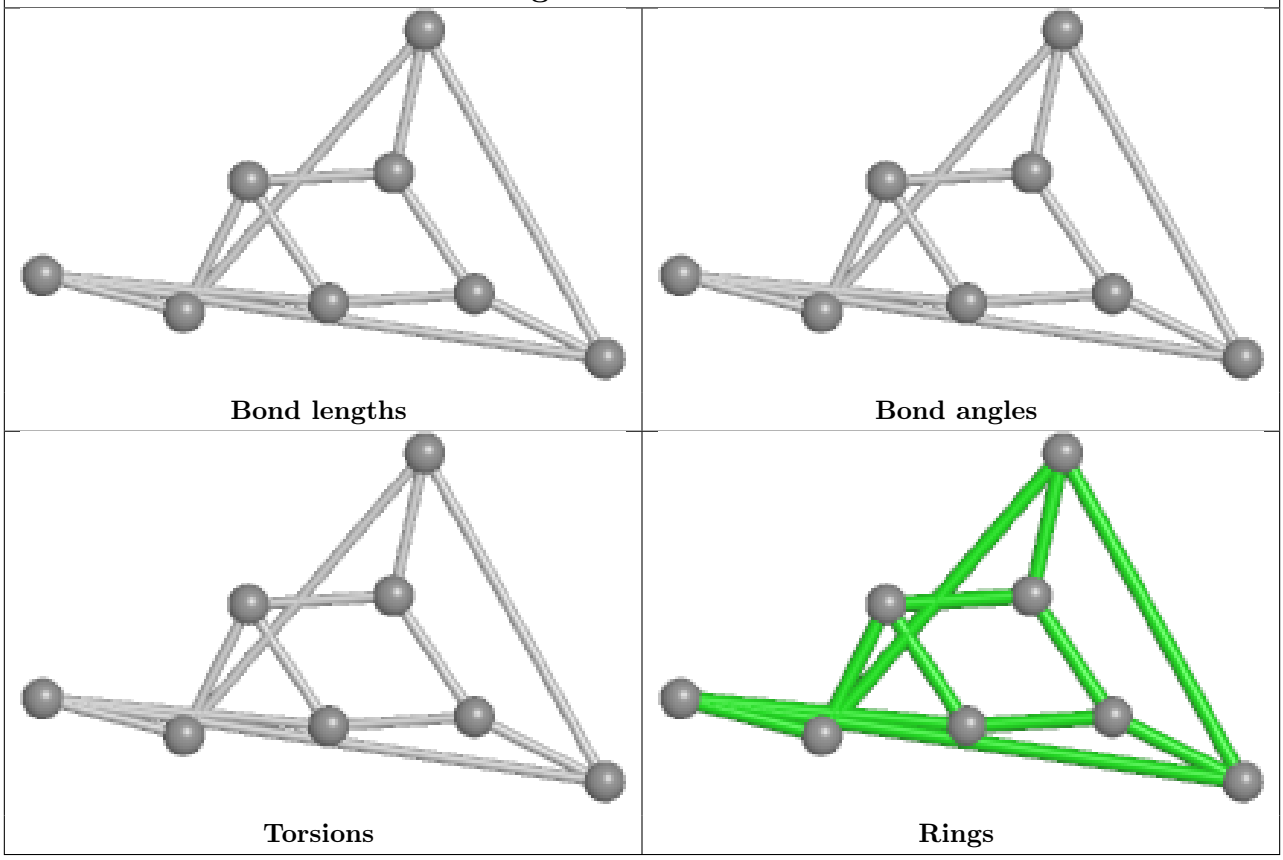


Torsions

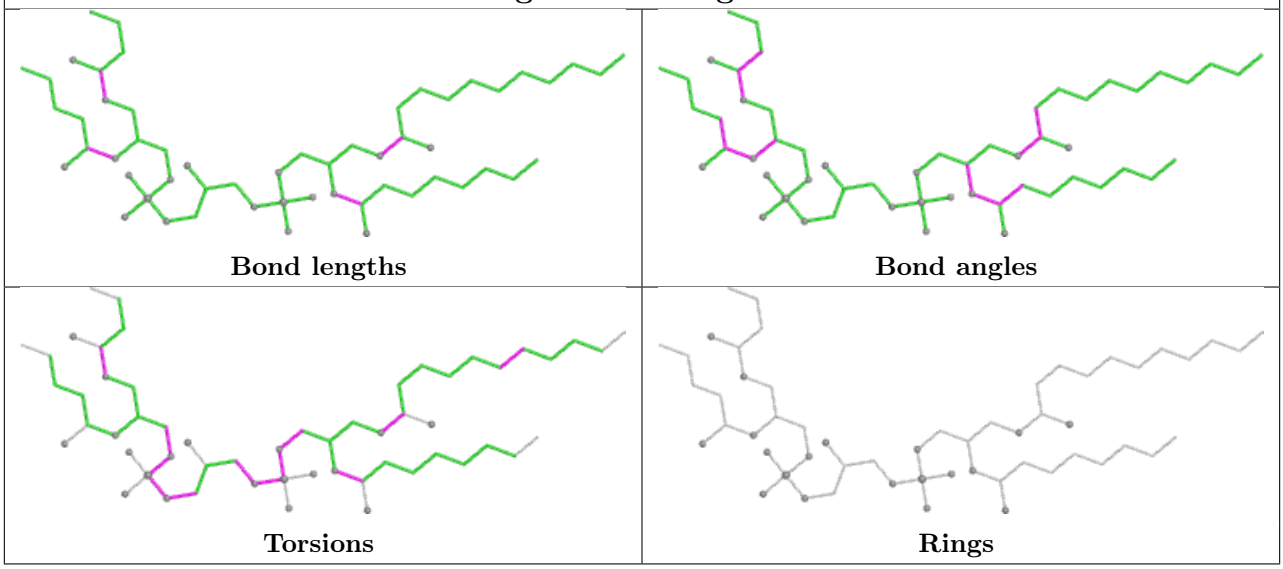


Rings

Ligand SF4 G 801



Ligand CDL Ag 101



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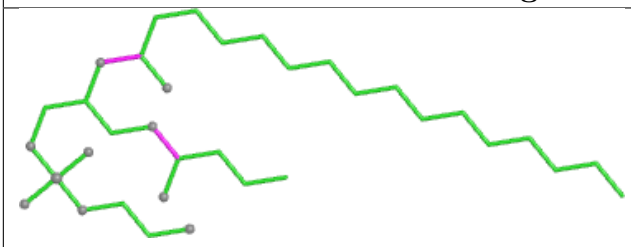
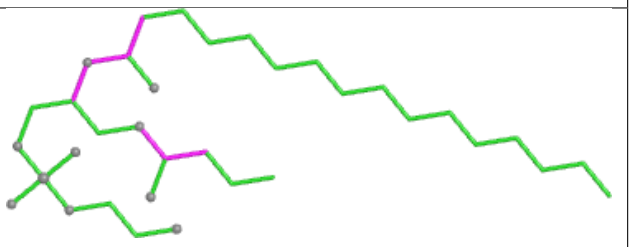
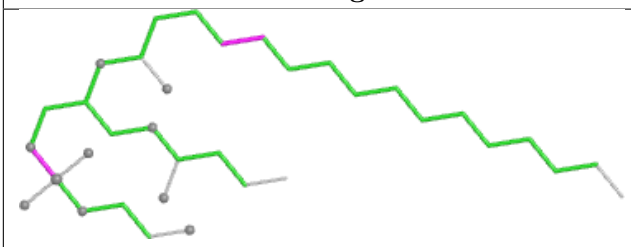
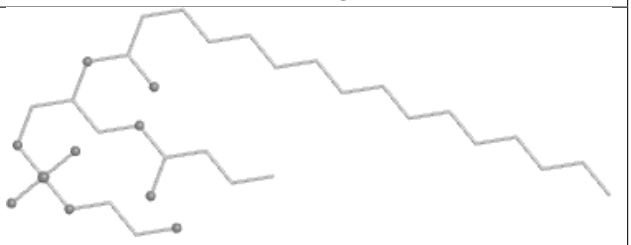
 Bond lengths	 Bond angles
 Torsions	 Rings

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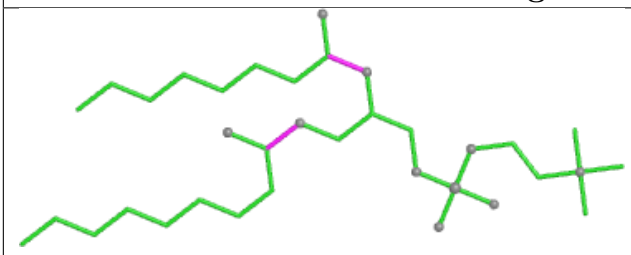
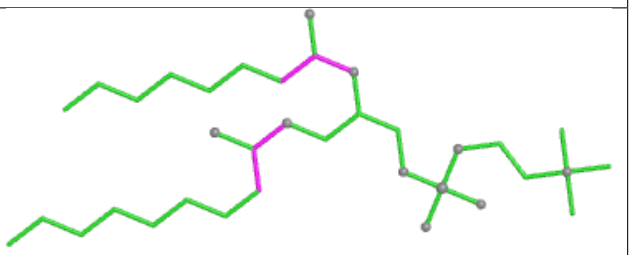
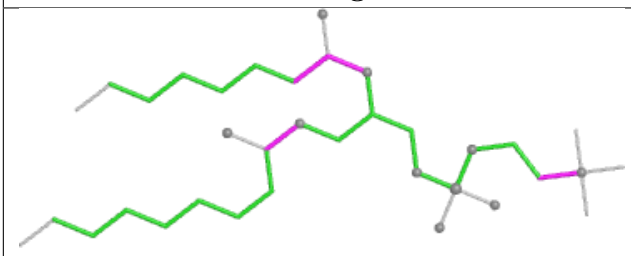
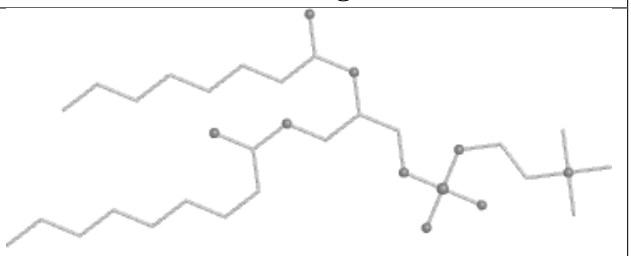
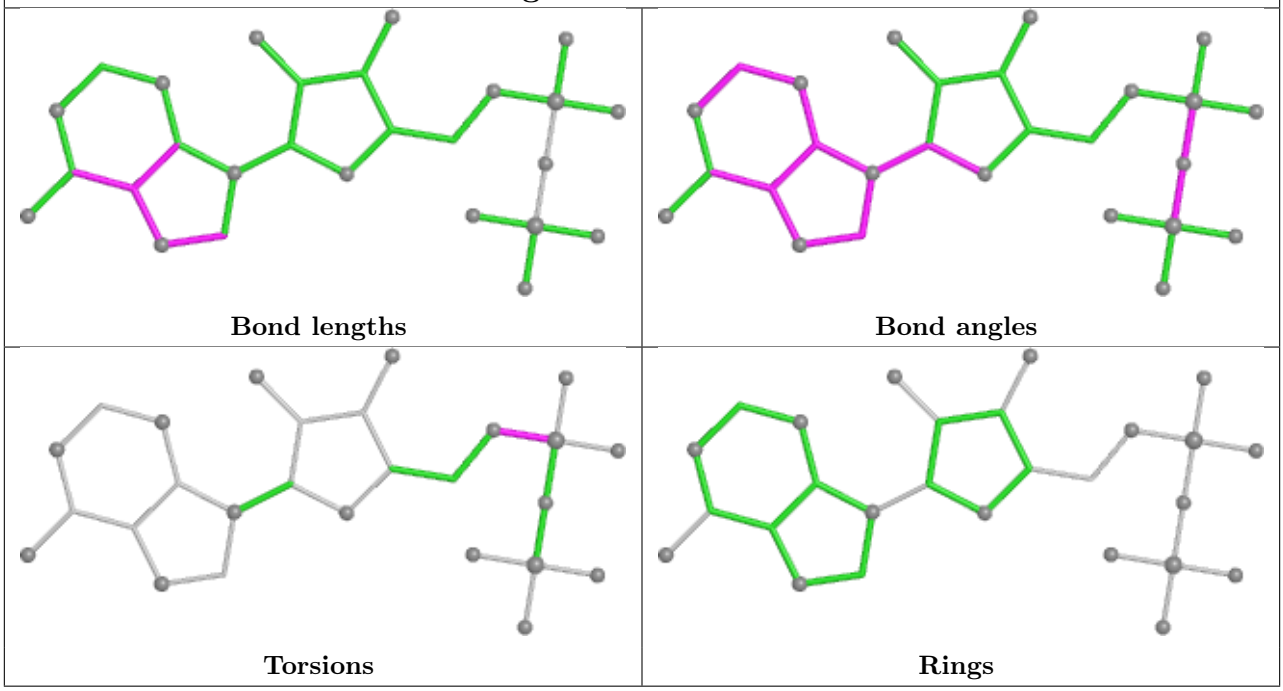
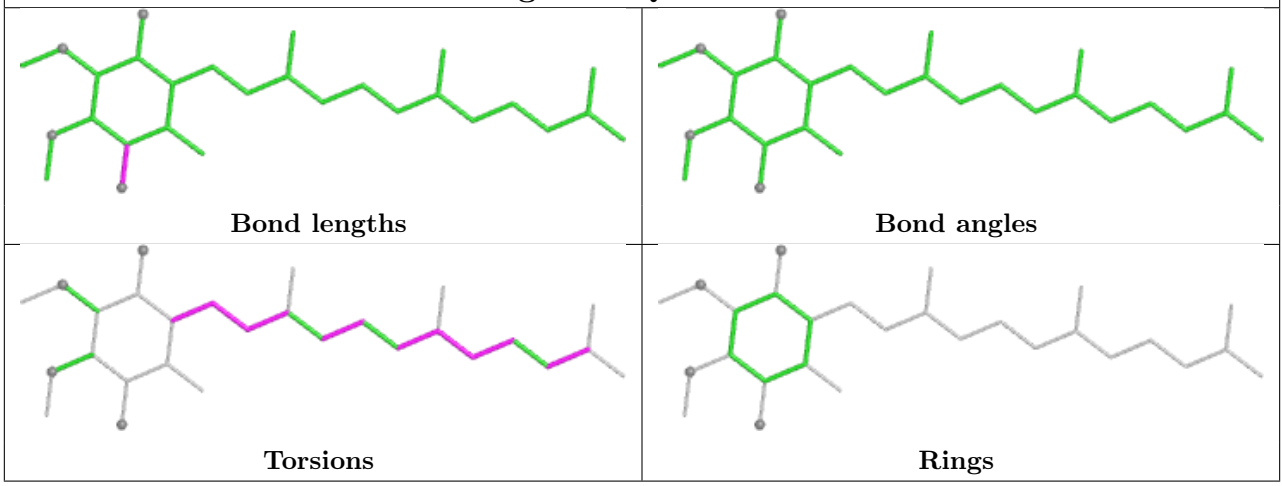
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP O 402



Ligand UQ6 Ac 405



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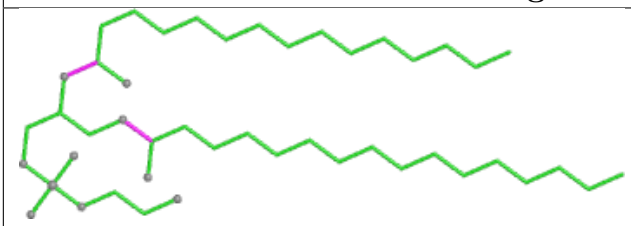
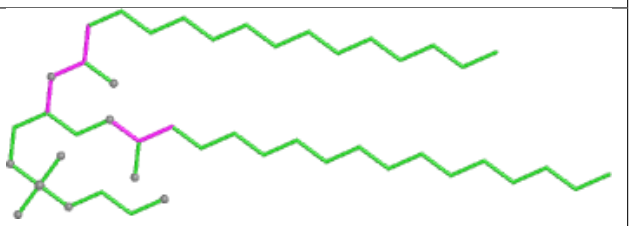
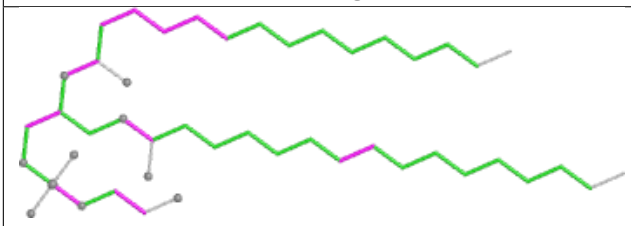
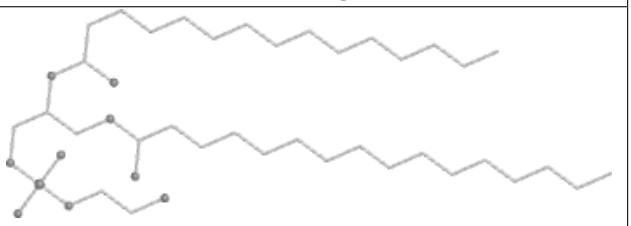
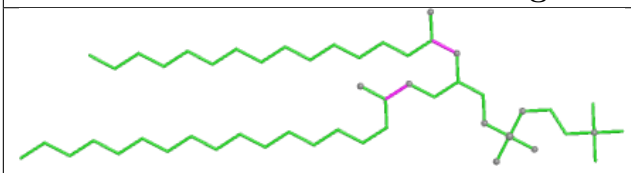
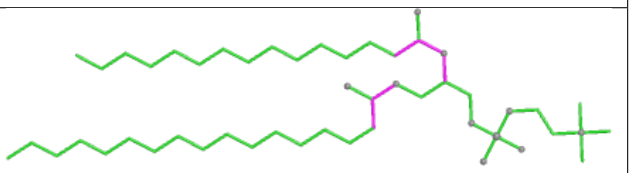
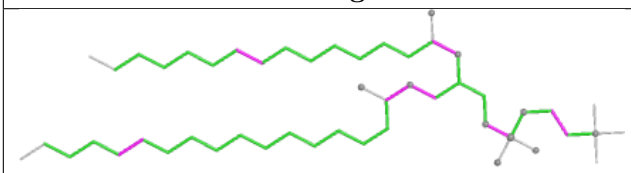
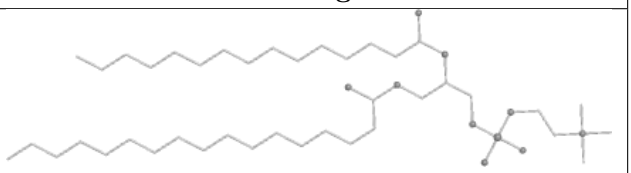
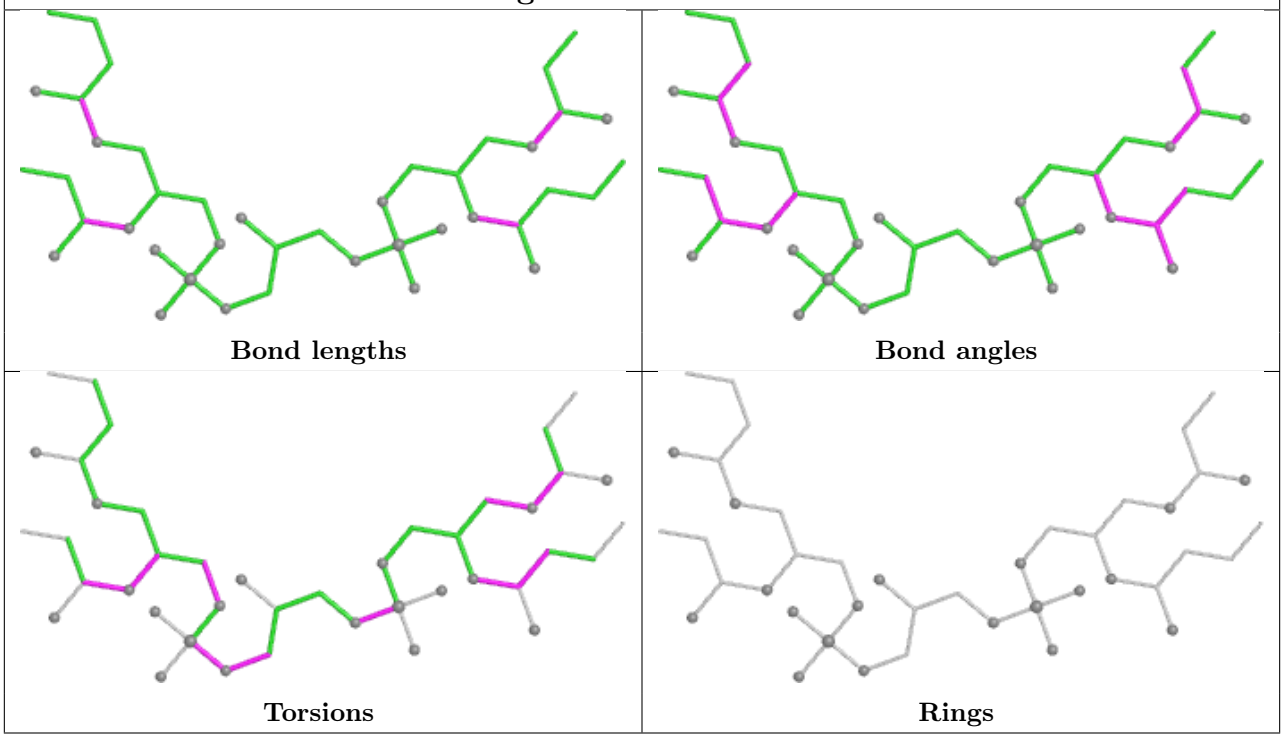
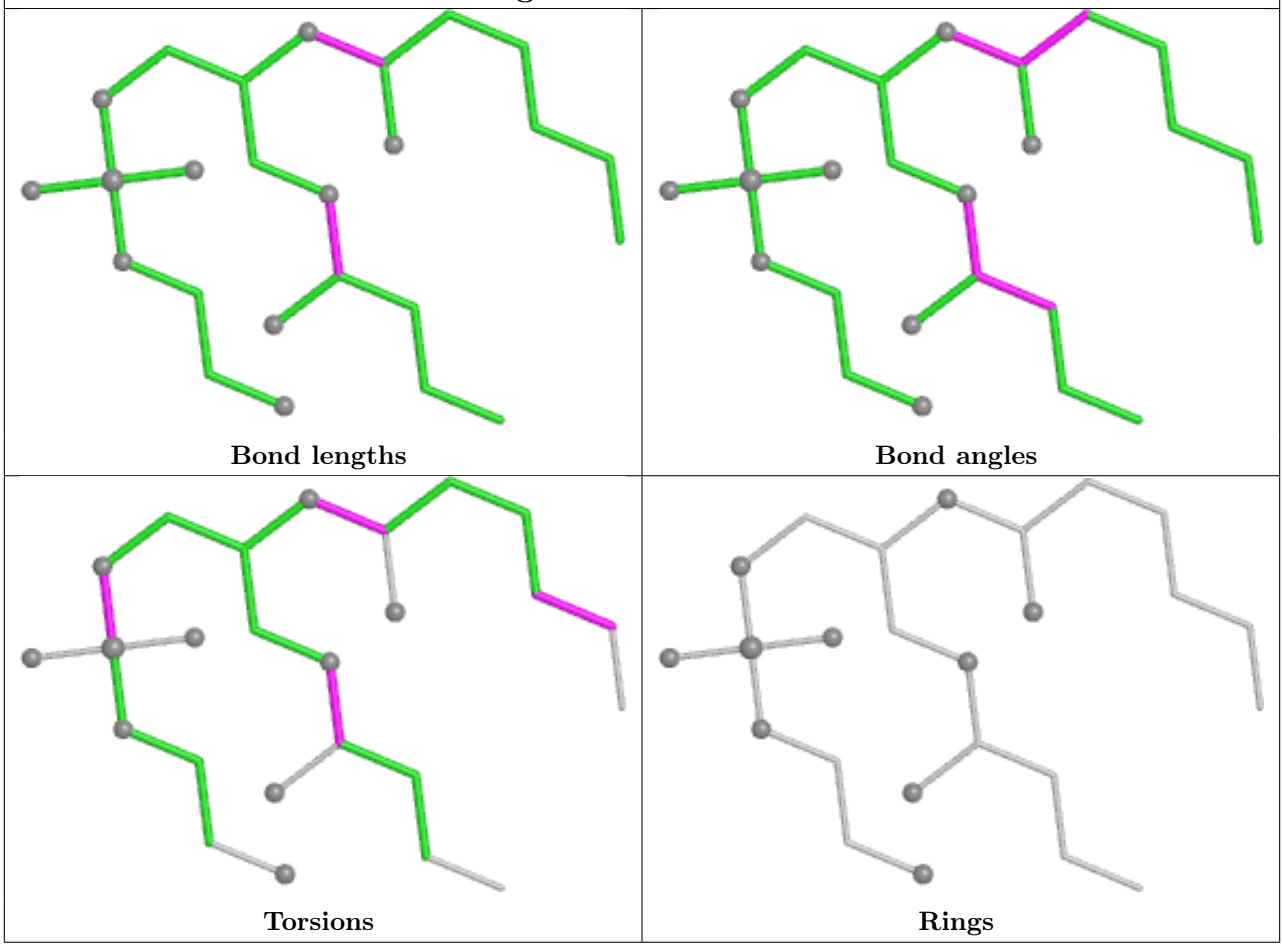
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 L 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

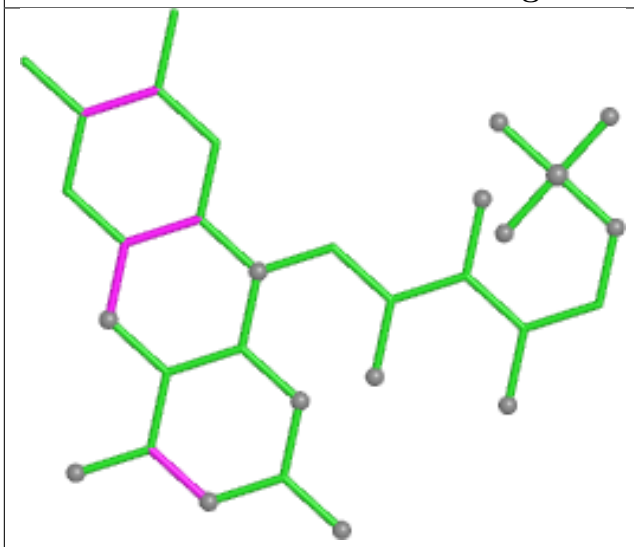
Ligand CDL Ac 406



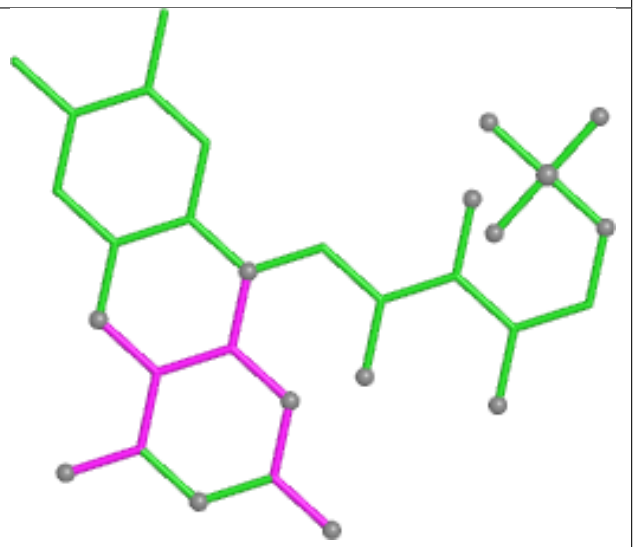
Ligand 3PE AC 403



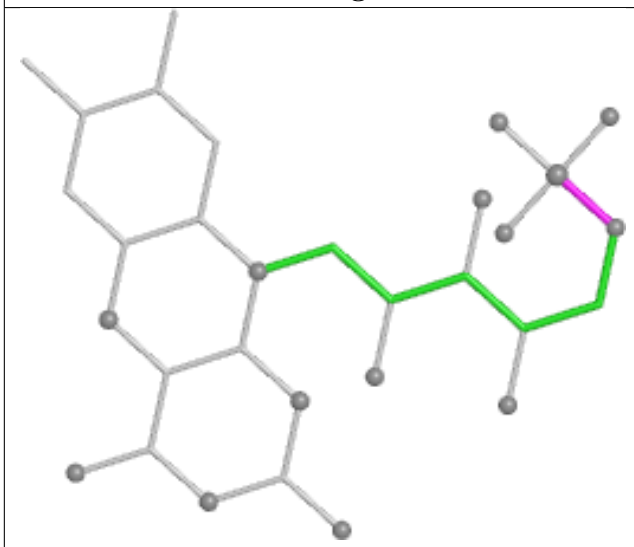
Ligand FMN F 501



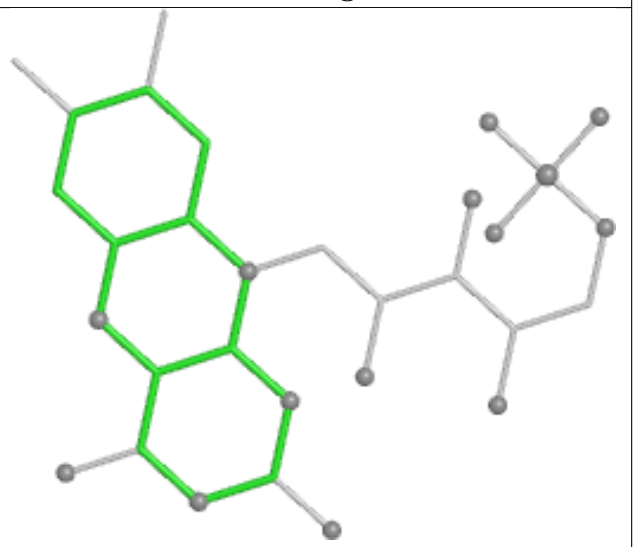
Bond lengths



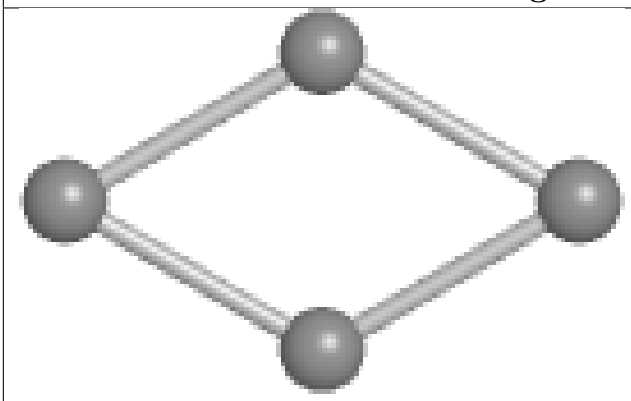
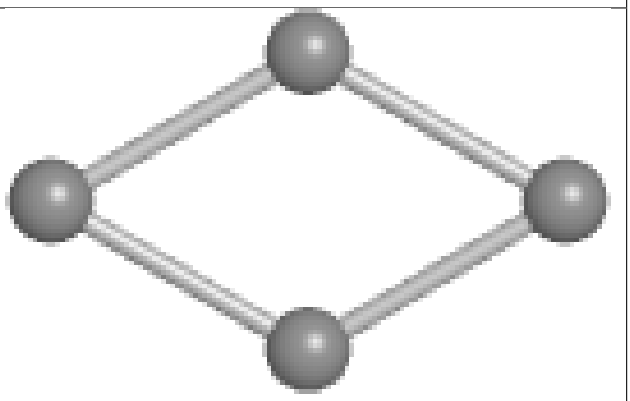
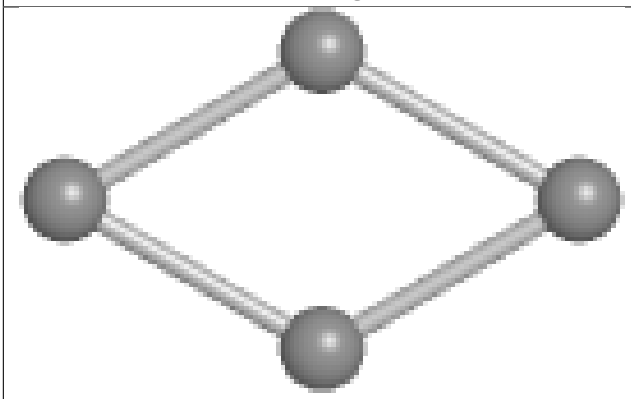
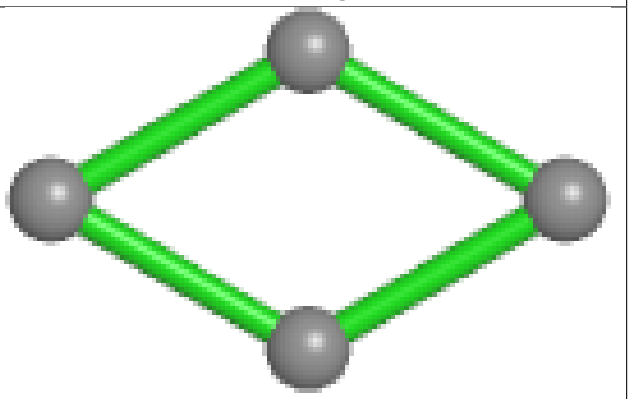
Bond angles



Torsions



Rings

Ligand FES E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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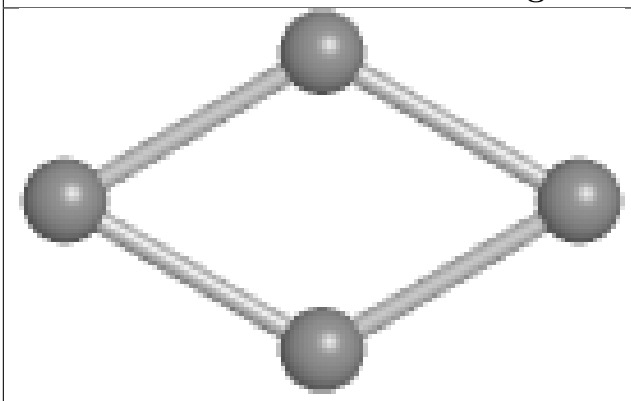
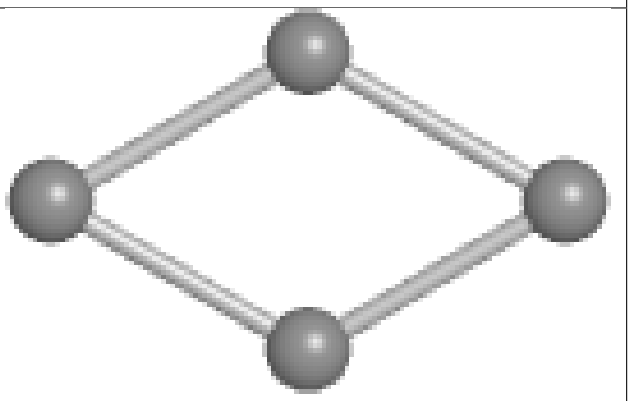
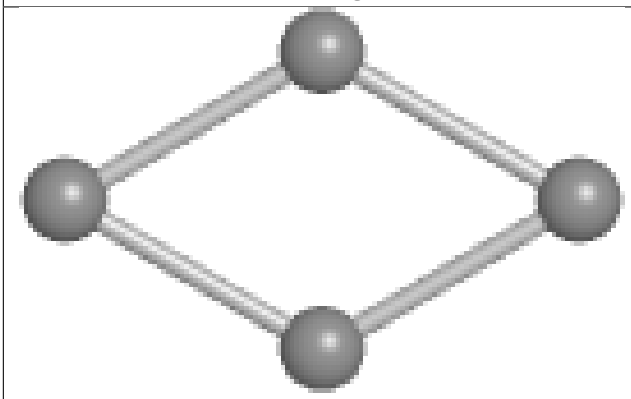
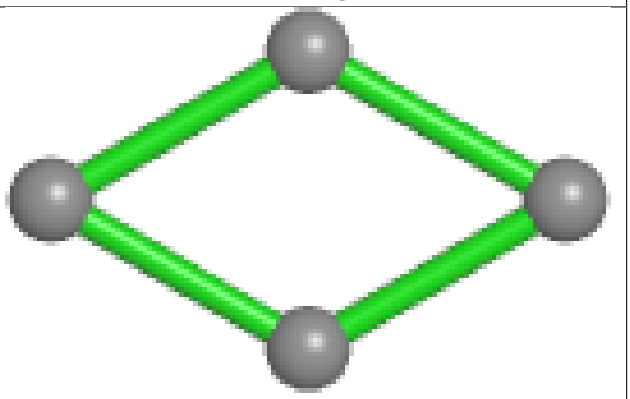
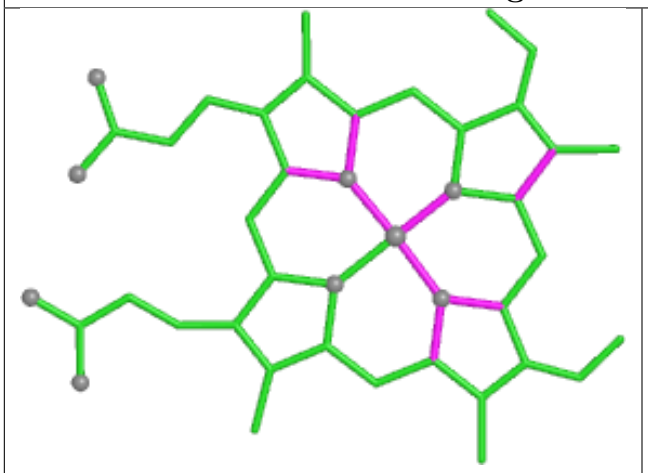
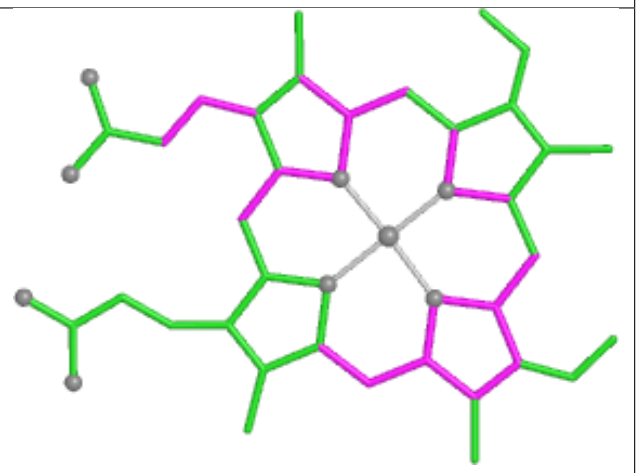
 Bond lengths	 Bond angles
 Torsions	 Rings

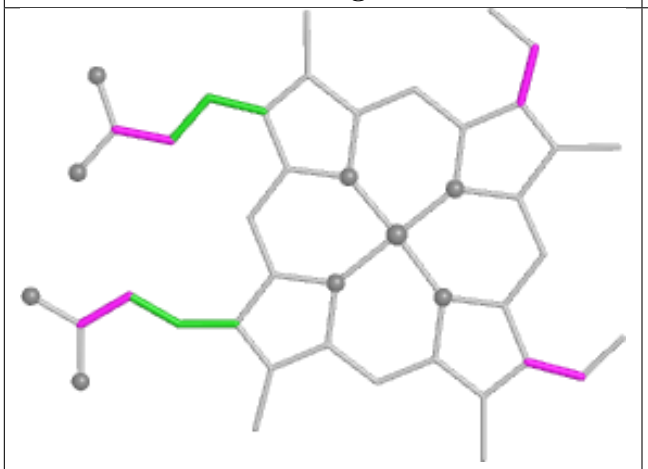
Ligand HEM AC 401



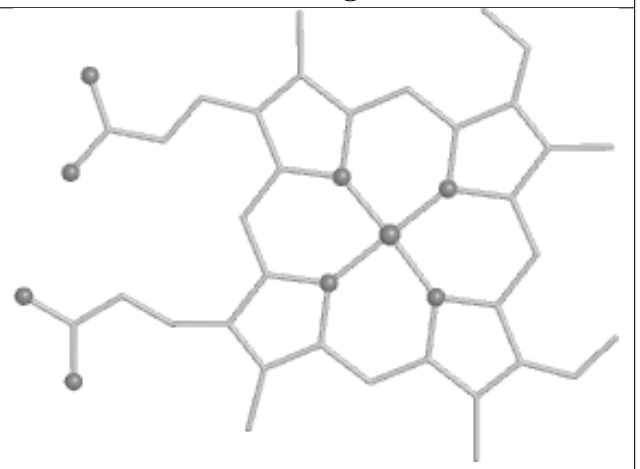
Bond lengths



Bond angles

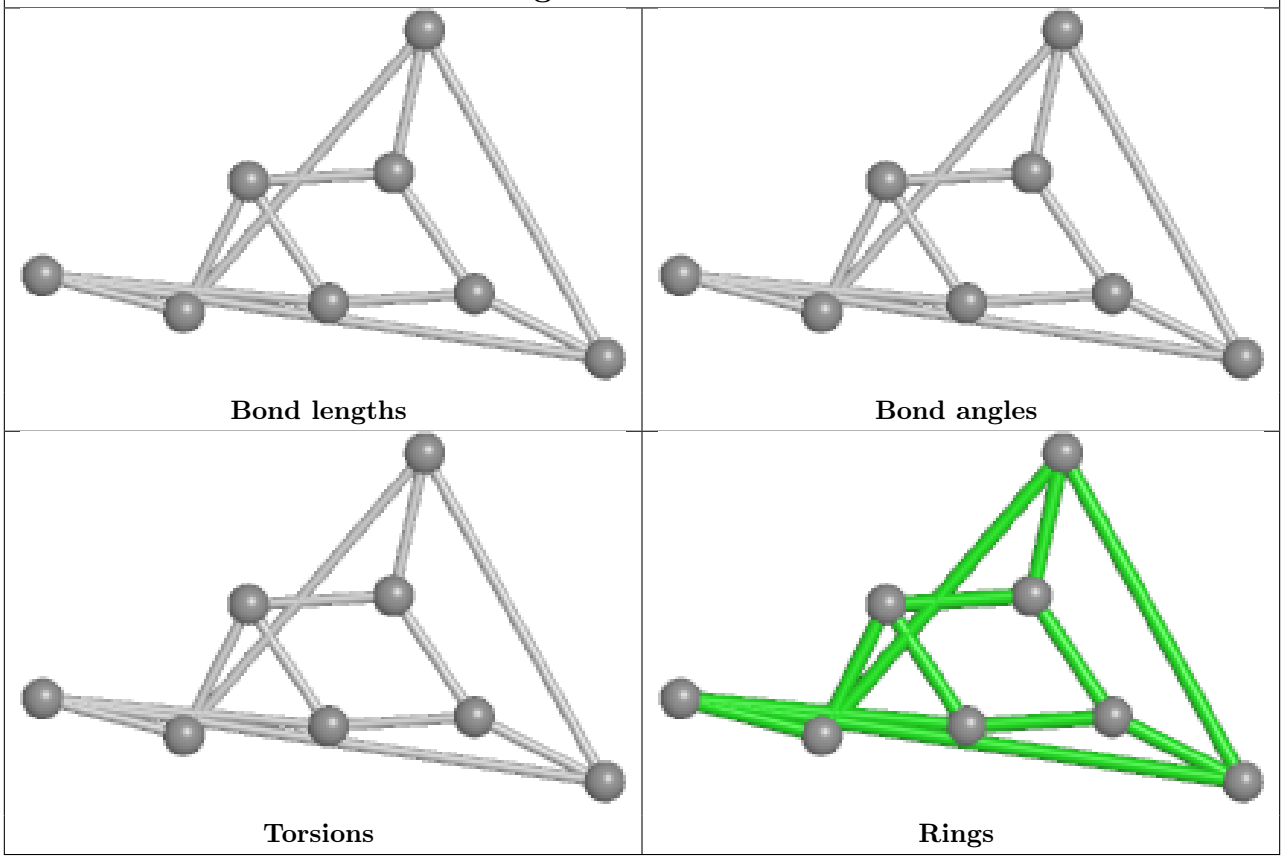


Torsions

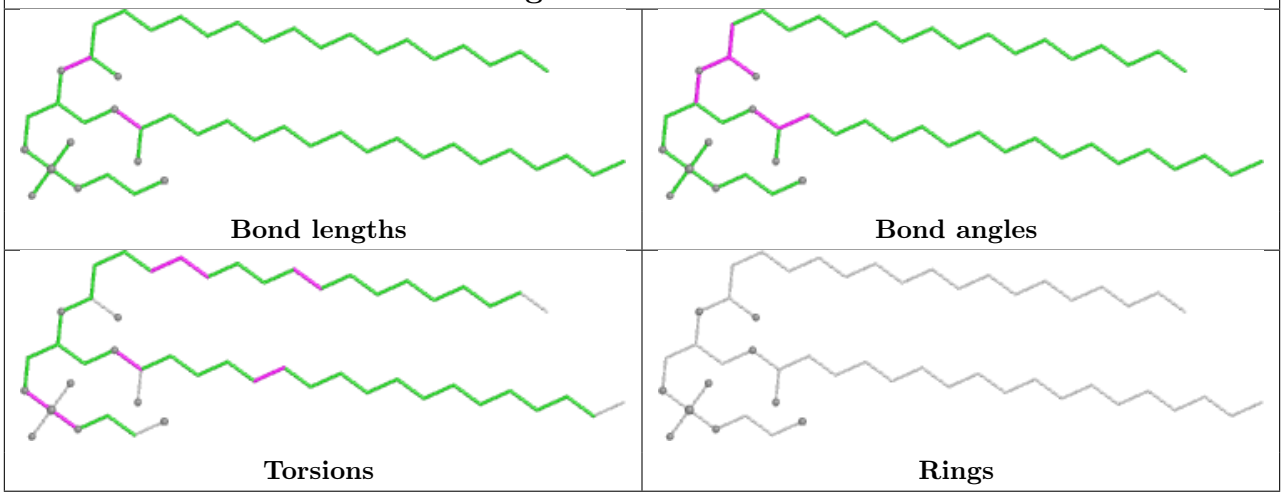


Rings

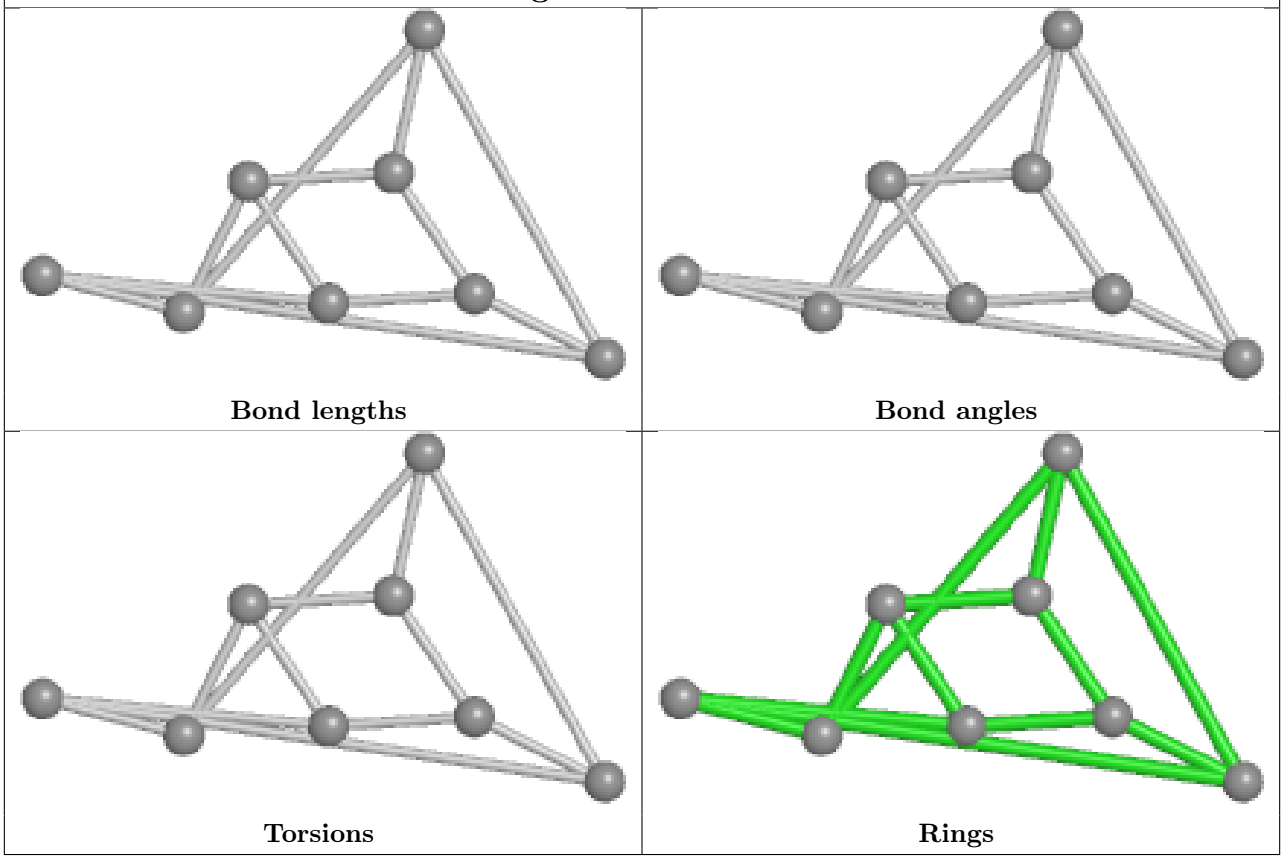
Ligand SF4 F 502



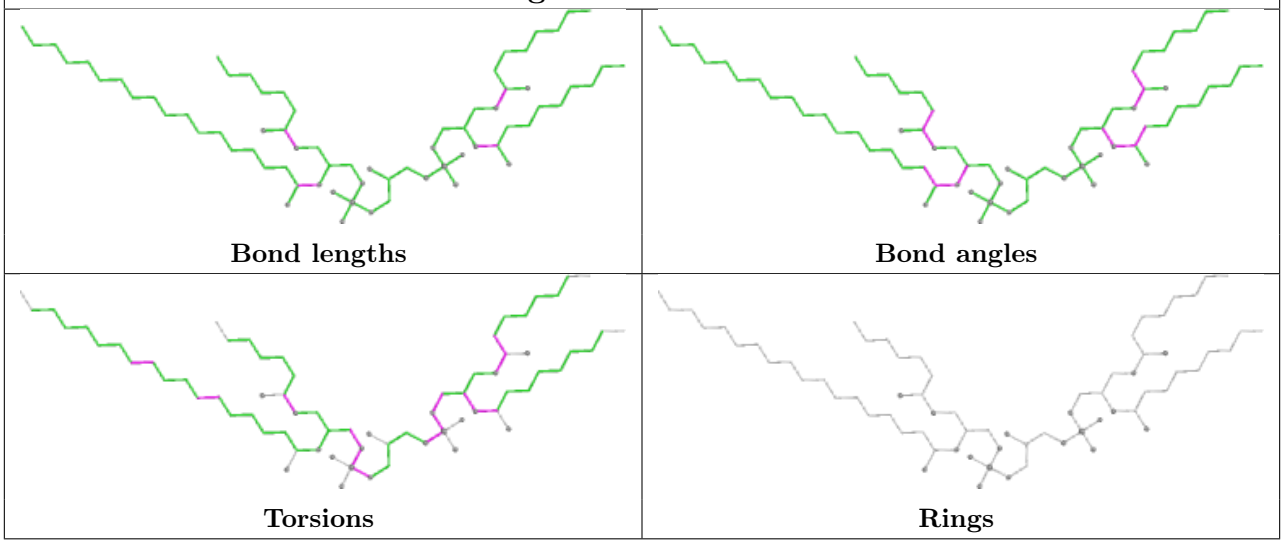
Ligand 3PE M 503



Ligand SF4 G 802



Ligand CDL h 201



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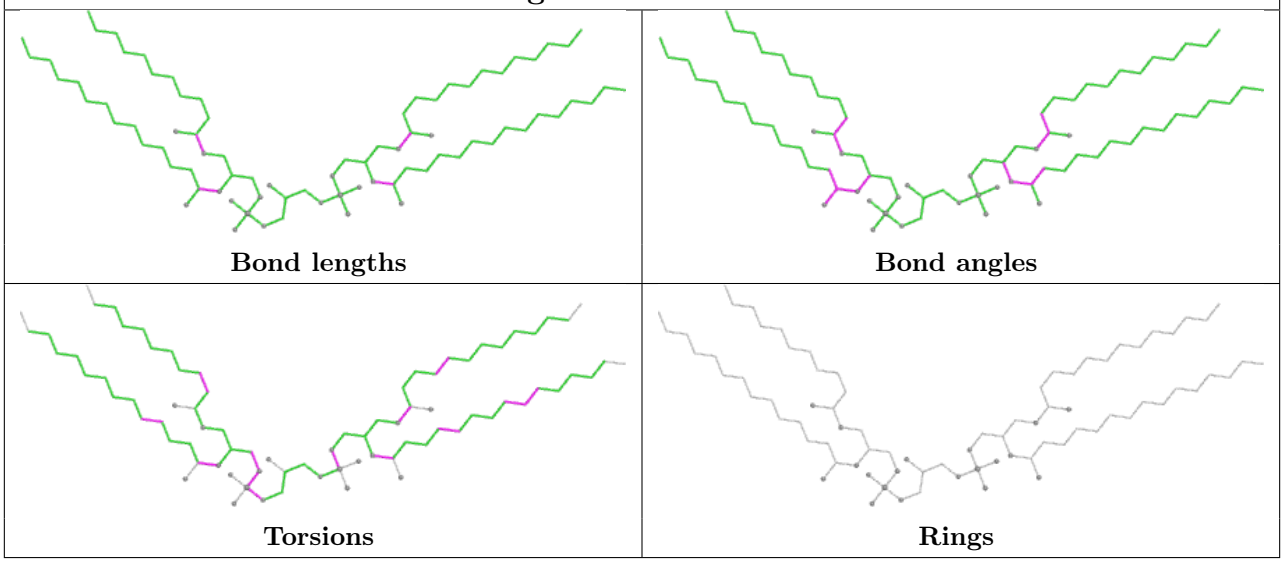

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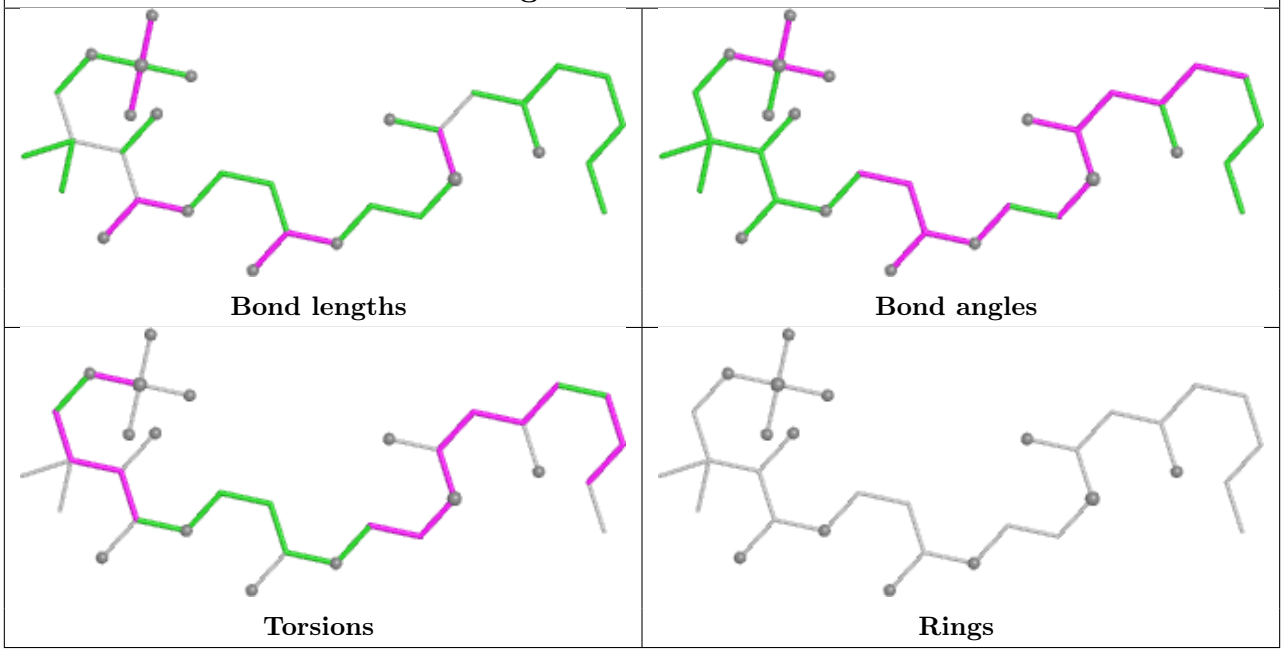

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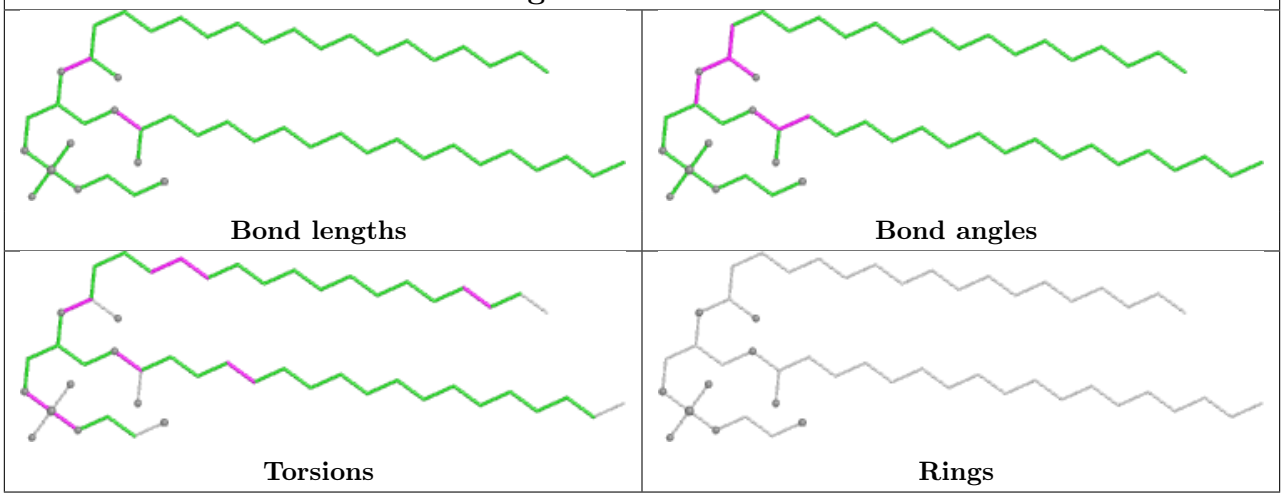
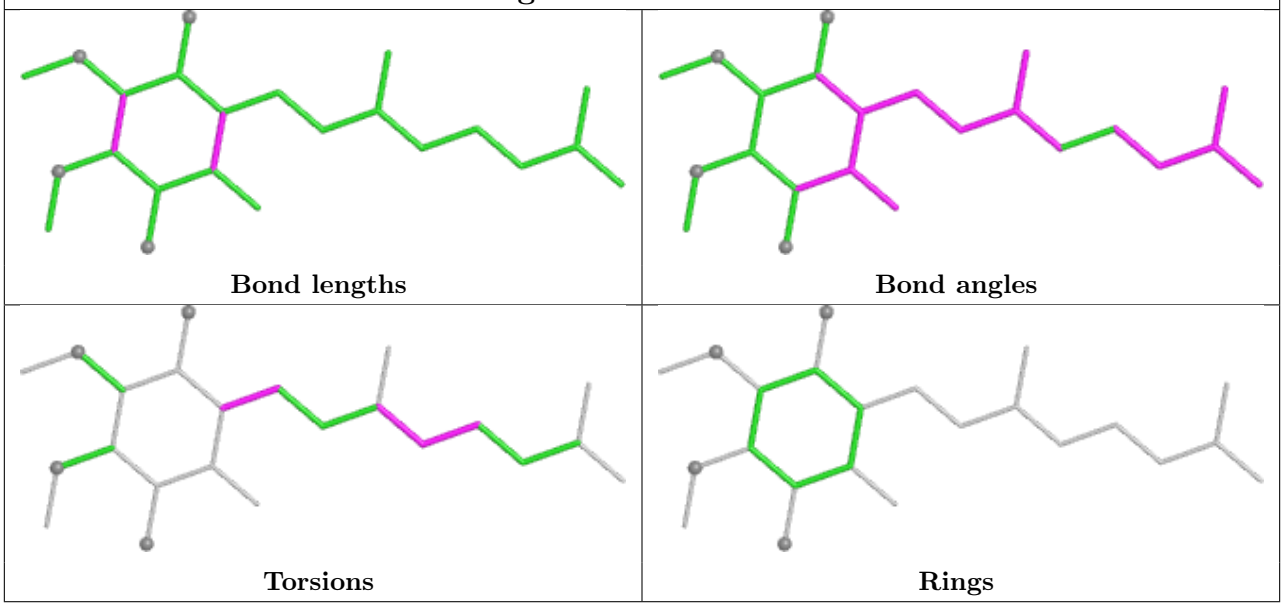
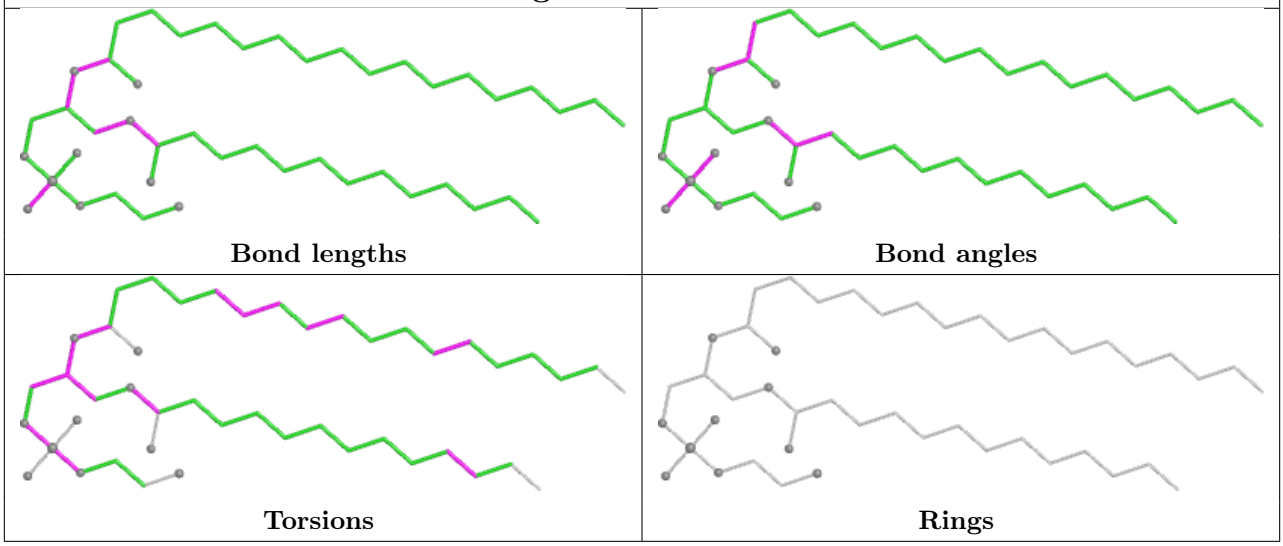


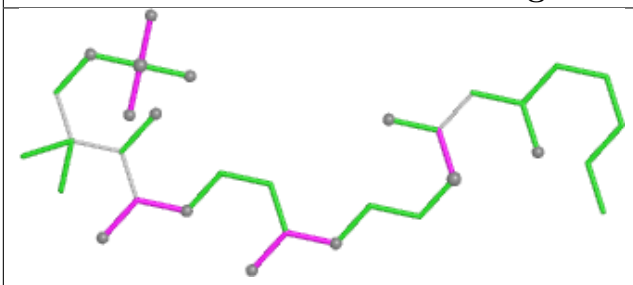
Ligand U10 AC 404



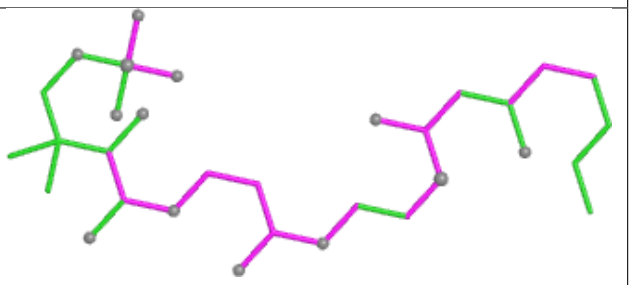
Ligand 3PE b 201



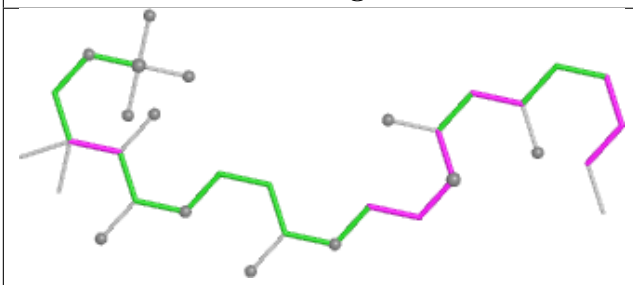
Ligand EHZ n 201



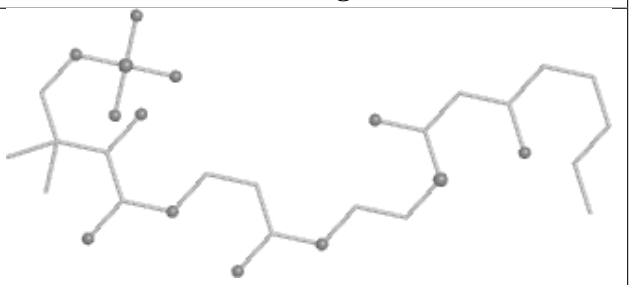
Bond lengths



Bond angles

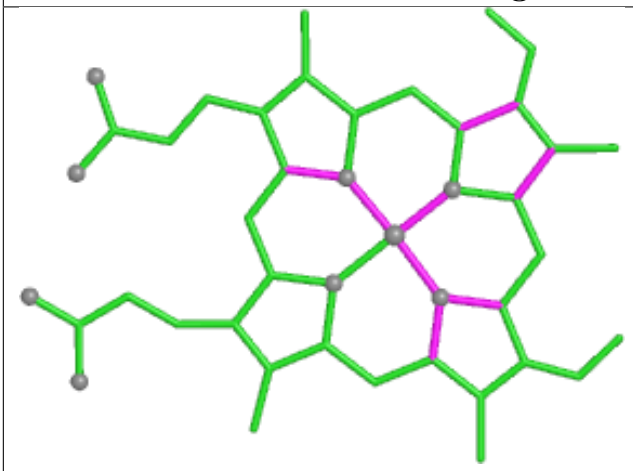


Torsions



Rings

Ligand HEM Ac 402



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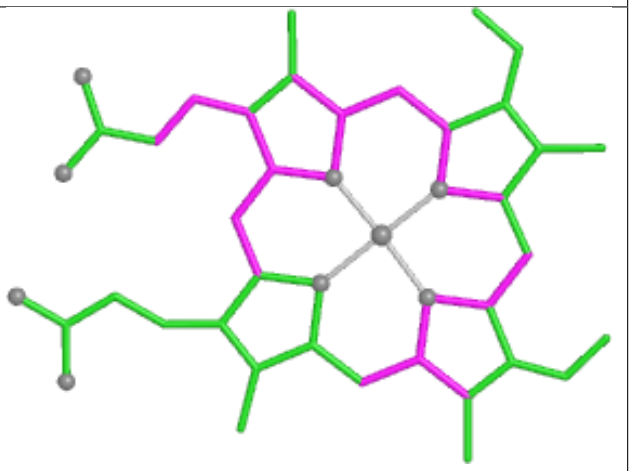
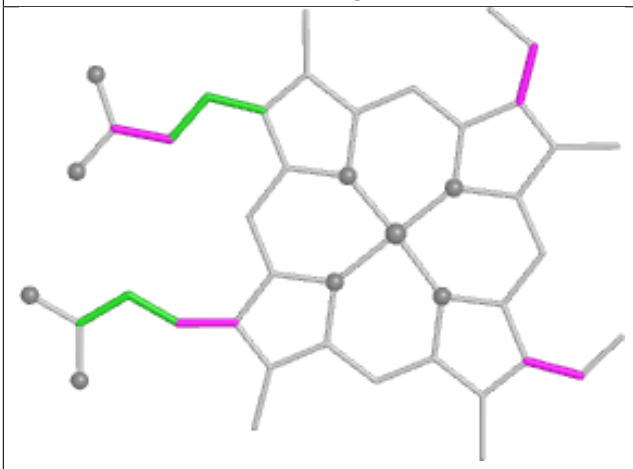


Bond angles



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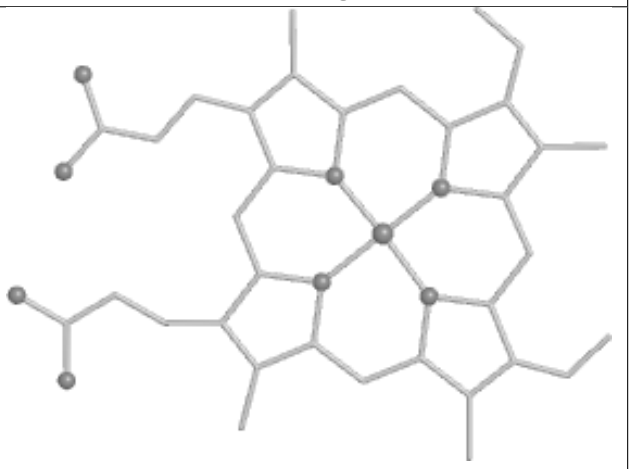
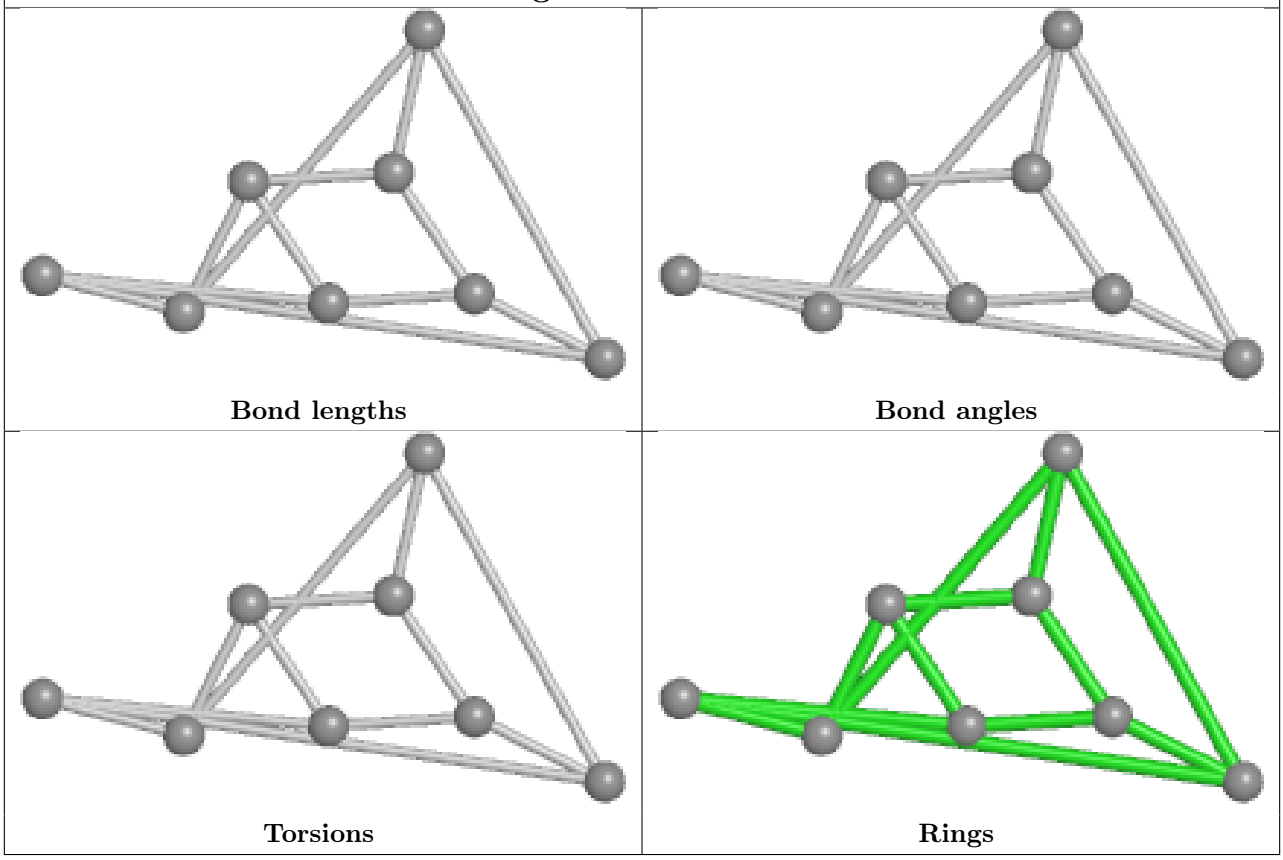
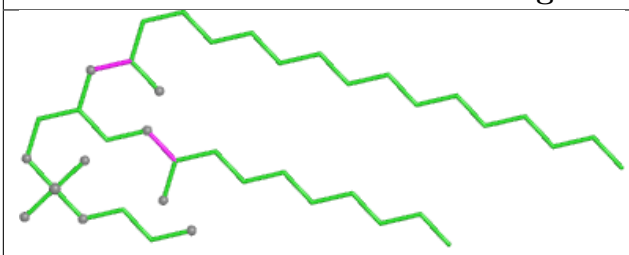
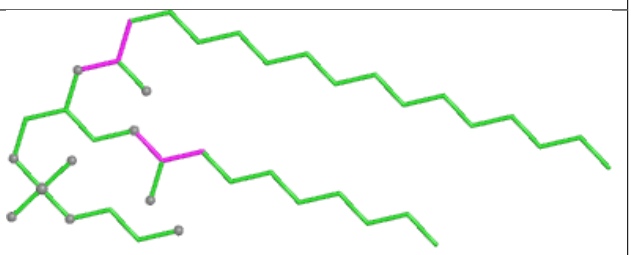
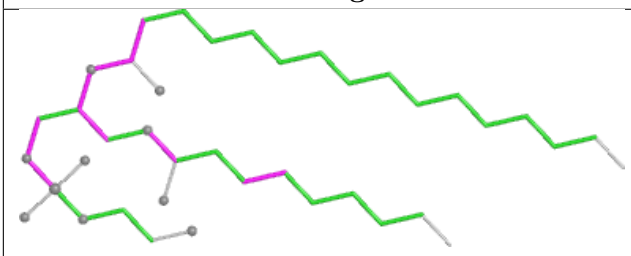
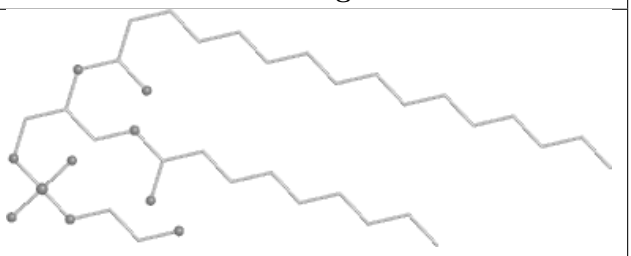


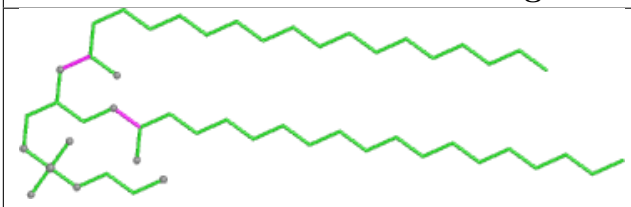
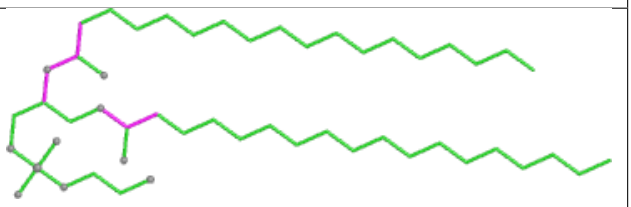
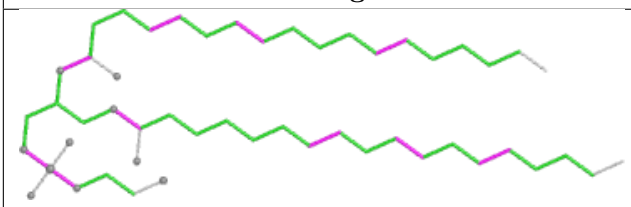
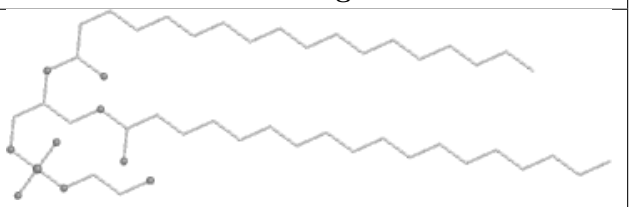
Rings

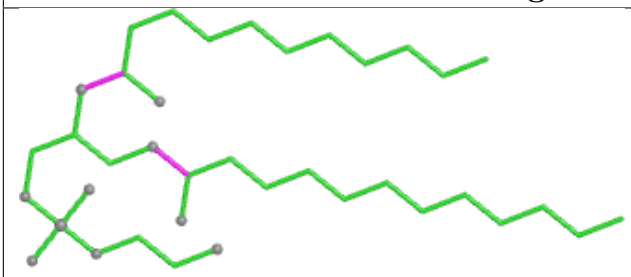
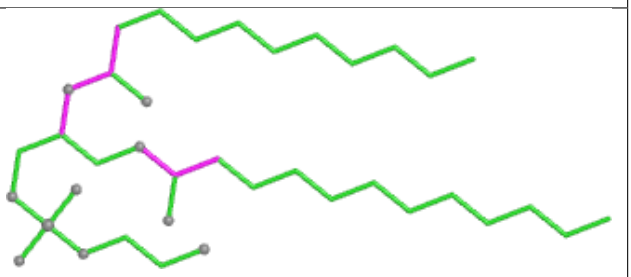
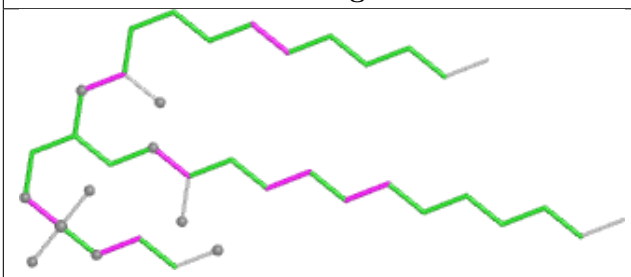
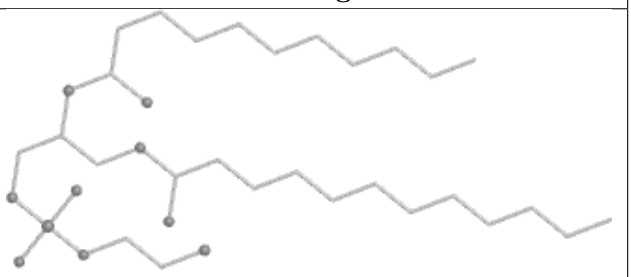
Ligand SF4 B 301

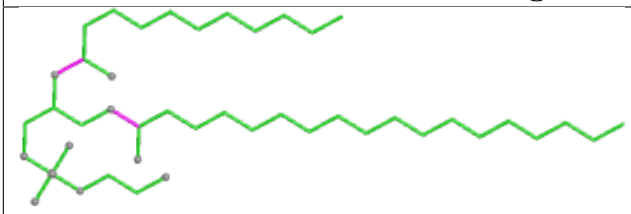
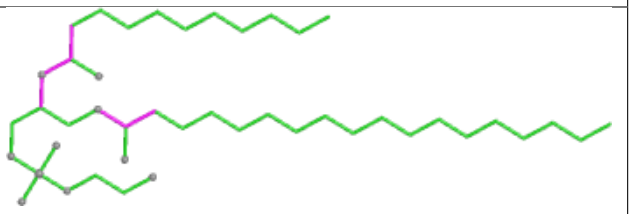
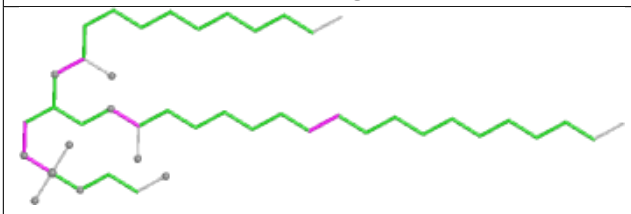
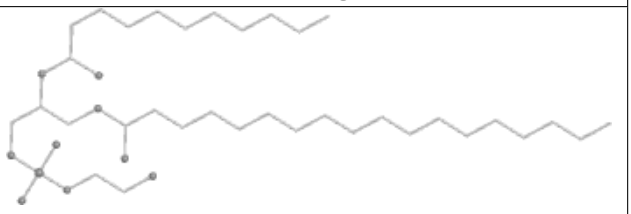


Ligand PC1 I 302

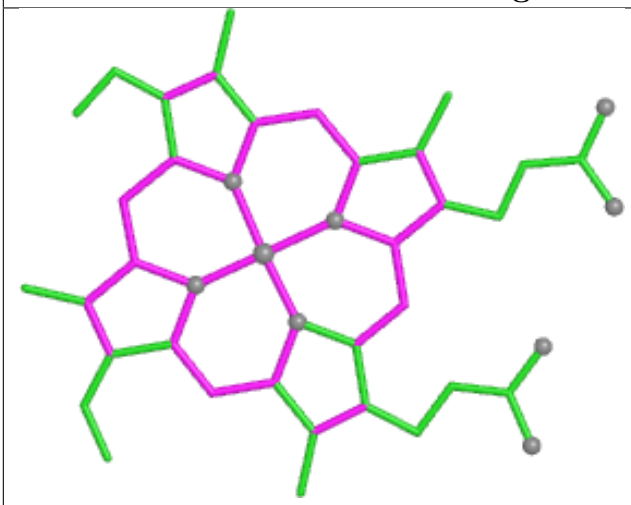
Ligand 3PE i 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE M 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE O 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC Ad 401



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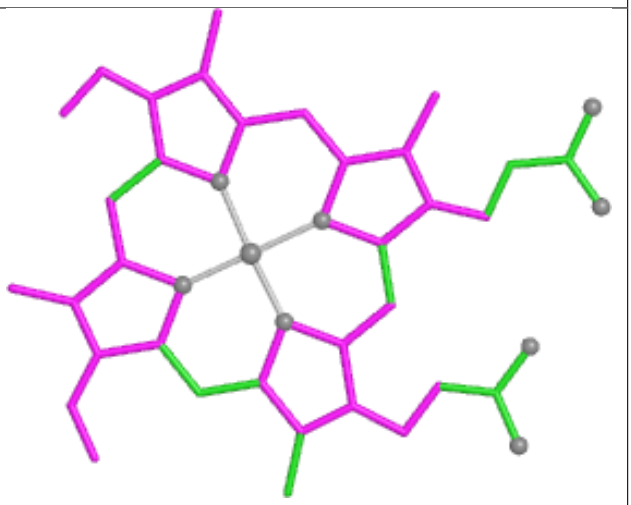

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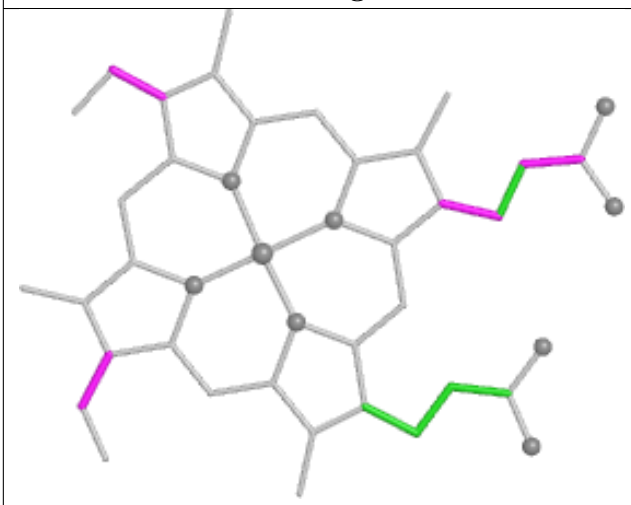

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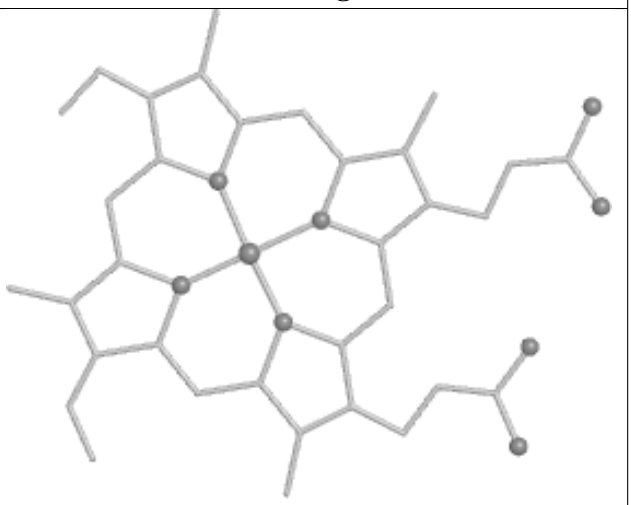
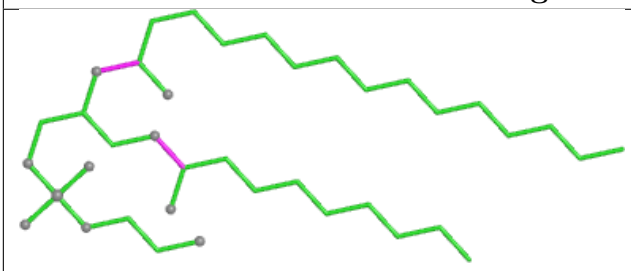


Rings

Ligand 3PE L 702



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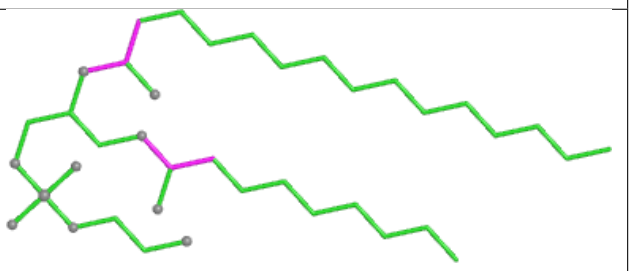

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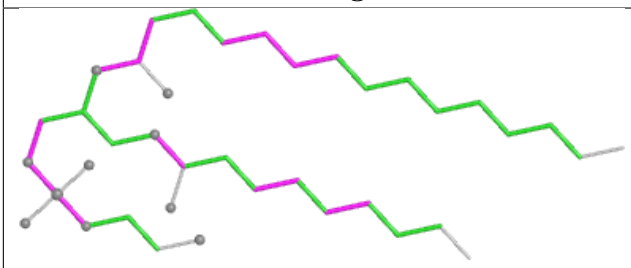

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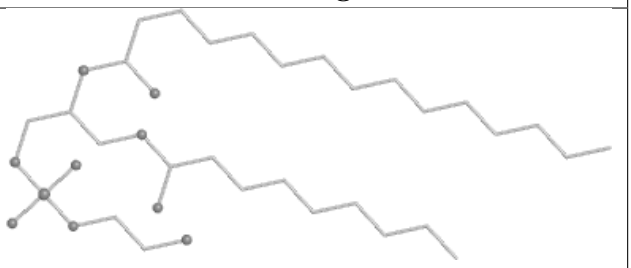
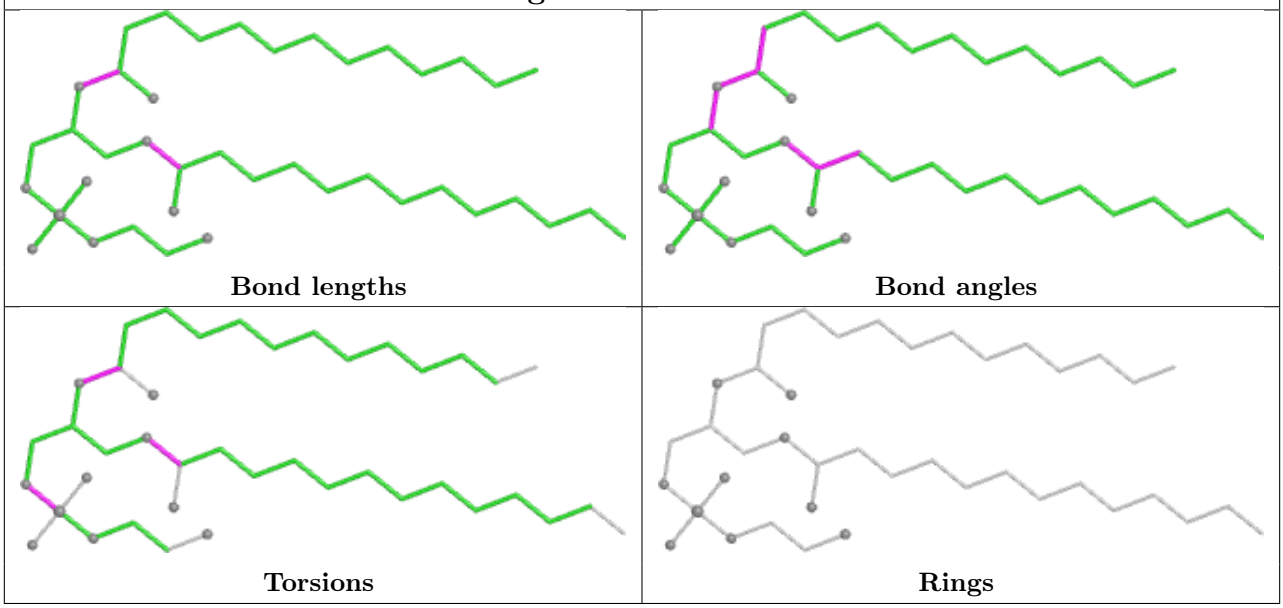
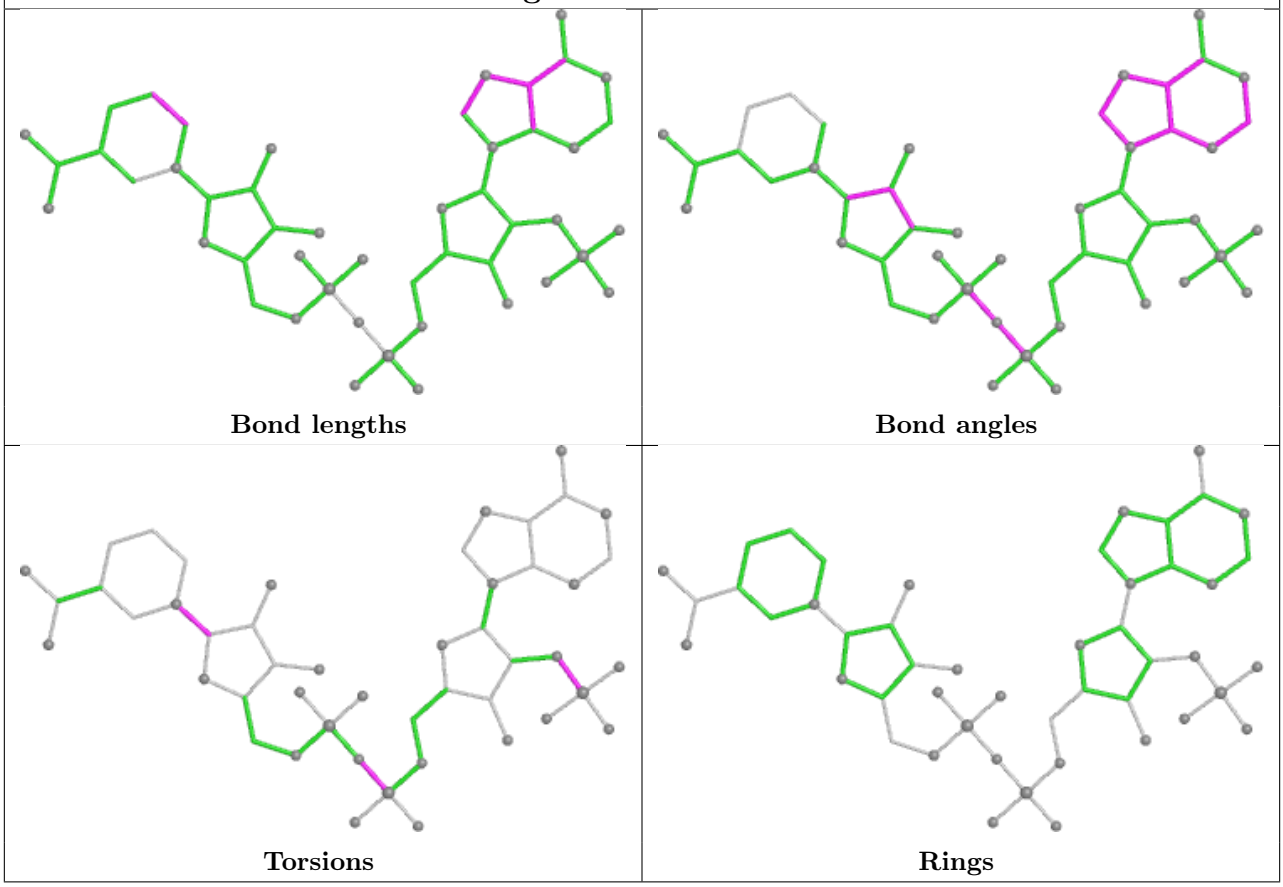


Rings

Ligand 3PE m 202



Ligand NDP P 401



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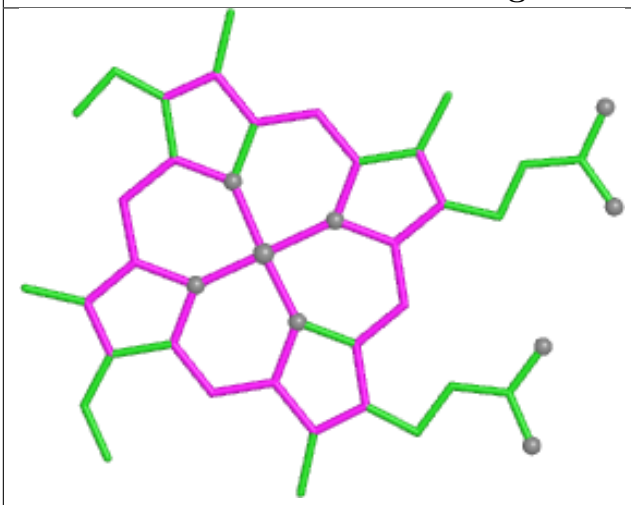

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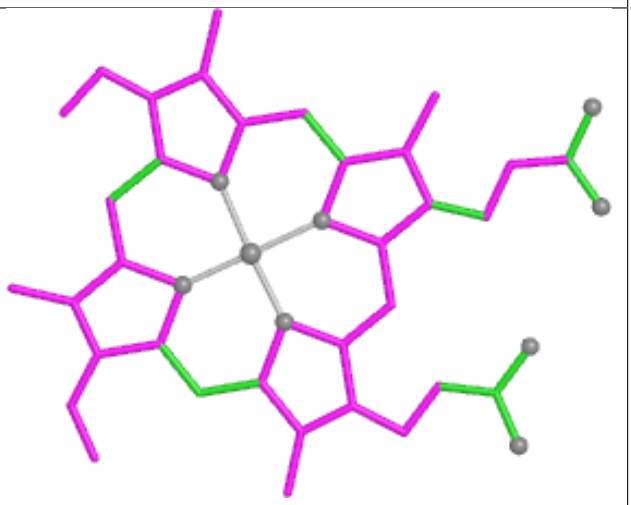
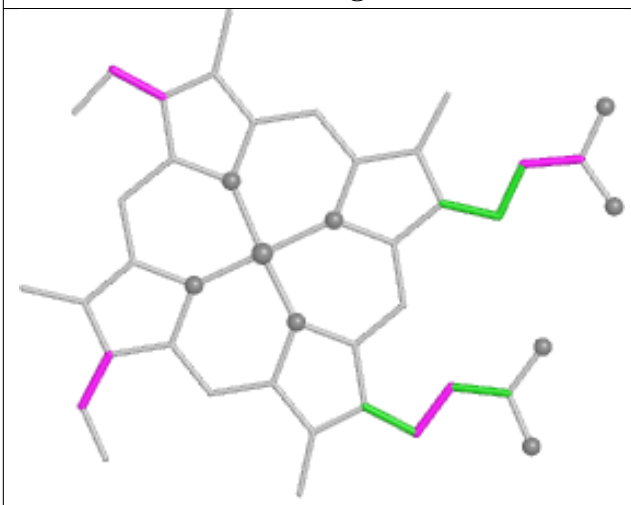


Bond angles



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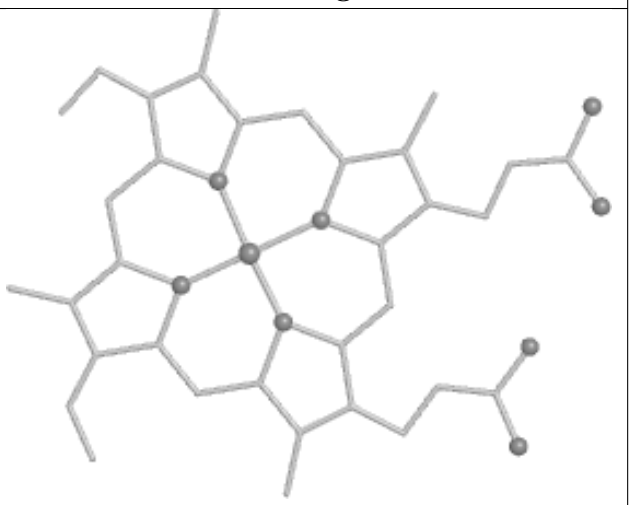
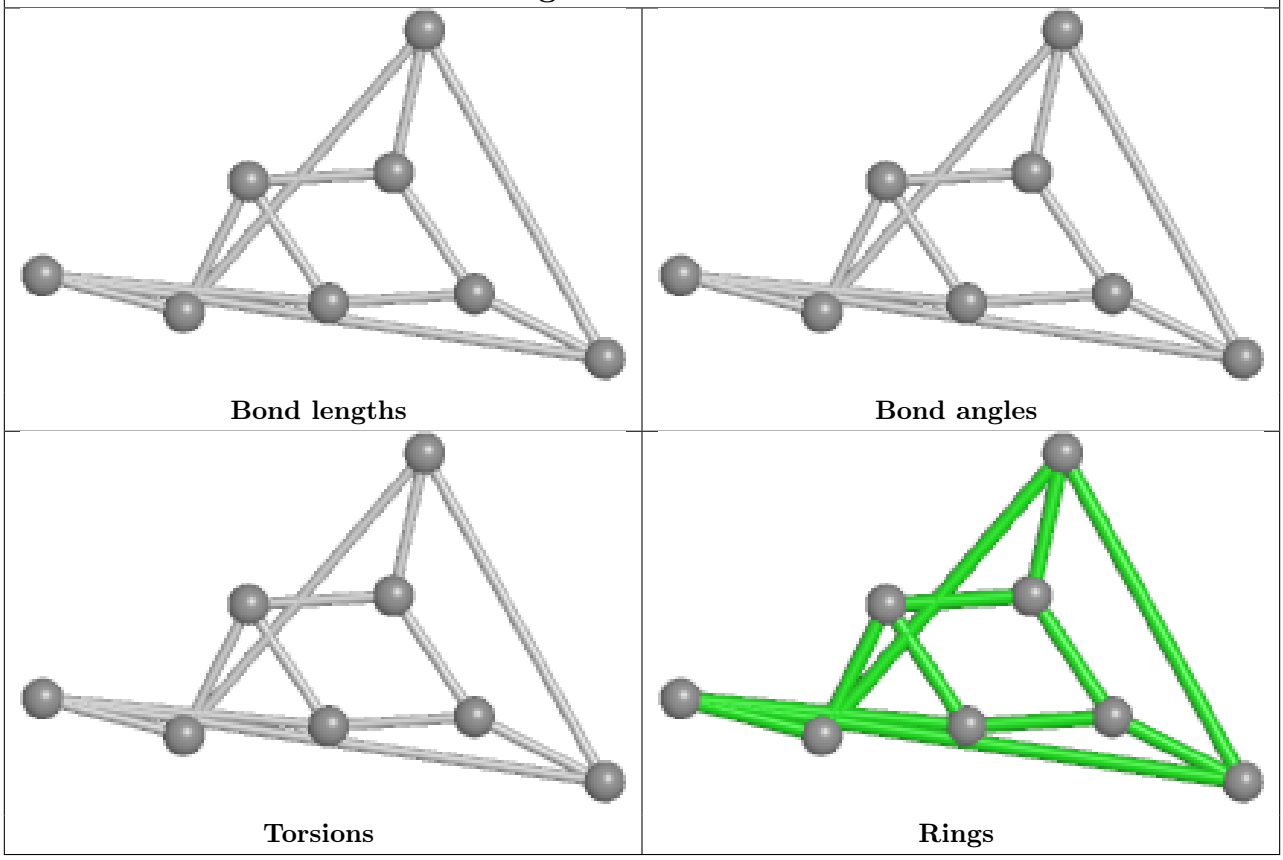
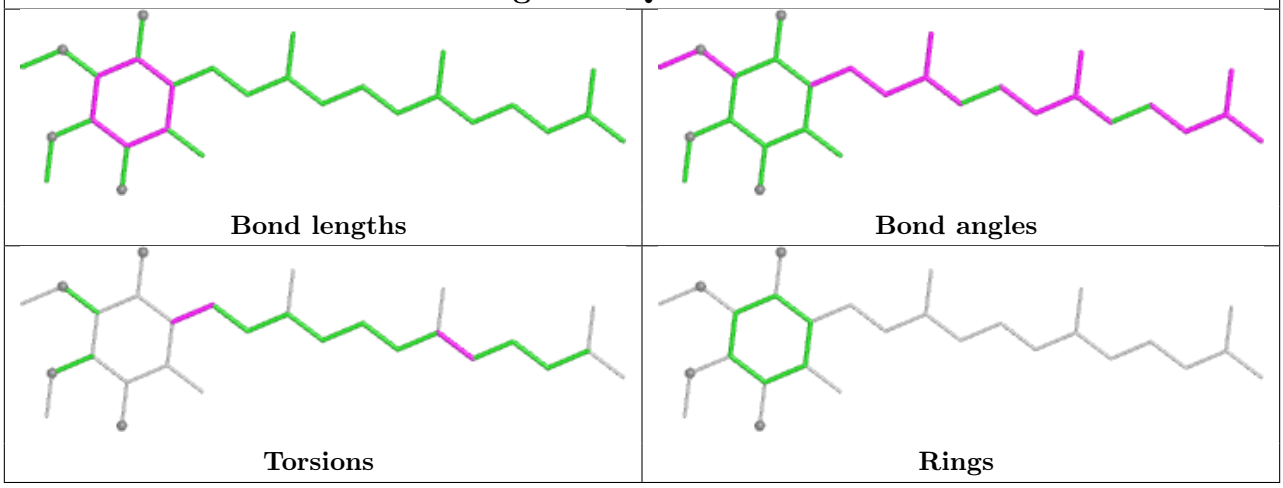


Rings

Ligand SF4 I 303



Ligand UQ6 AC 405



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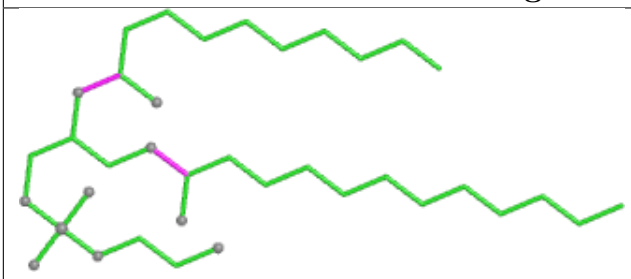
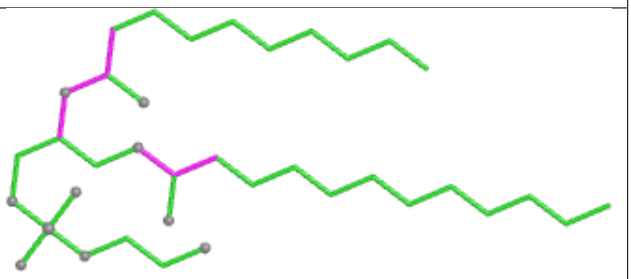
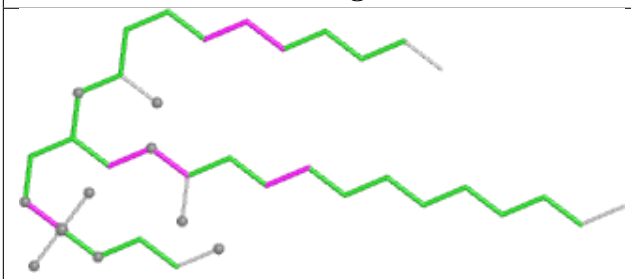
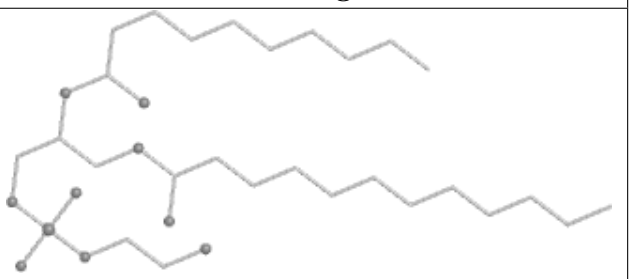
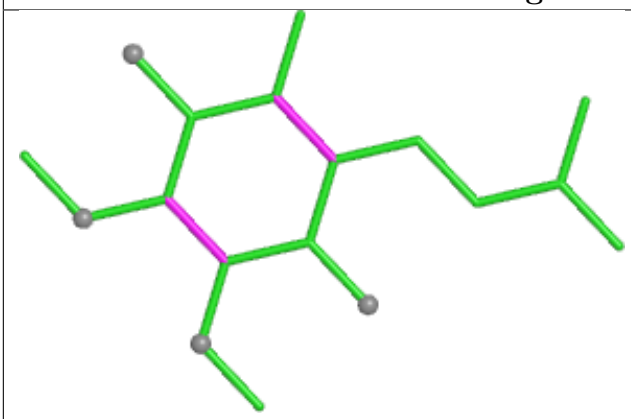
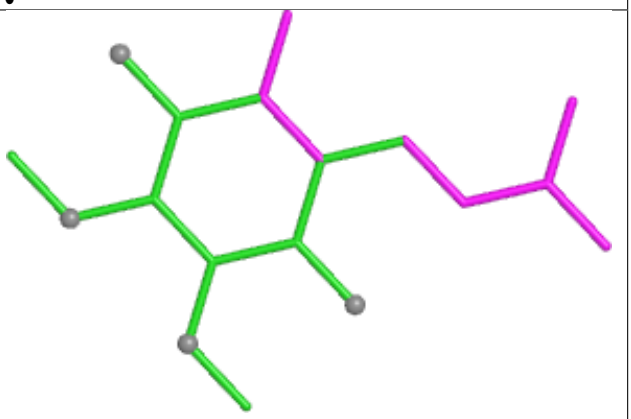
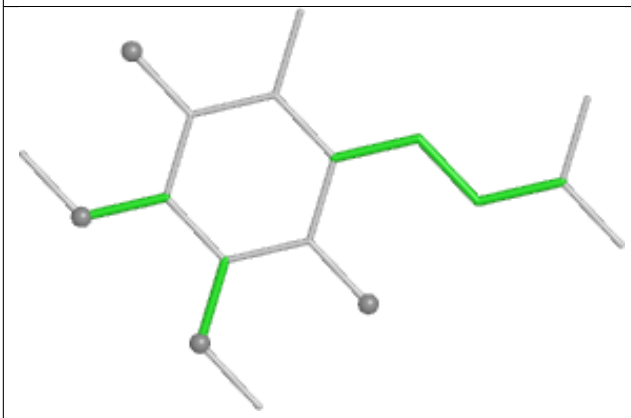
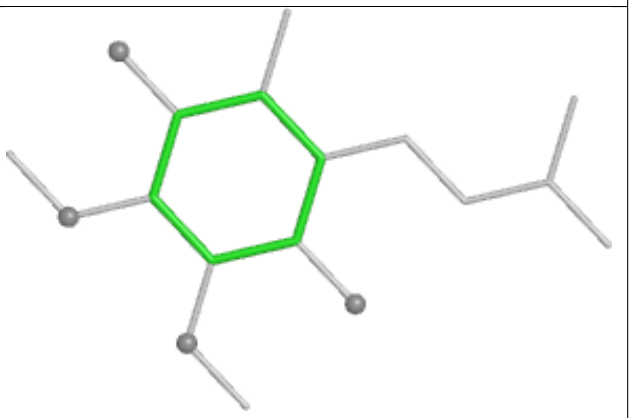
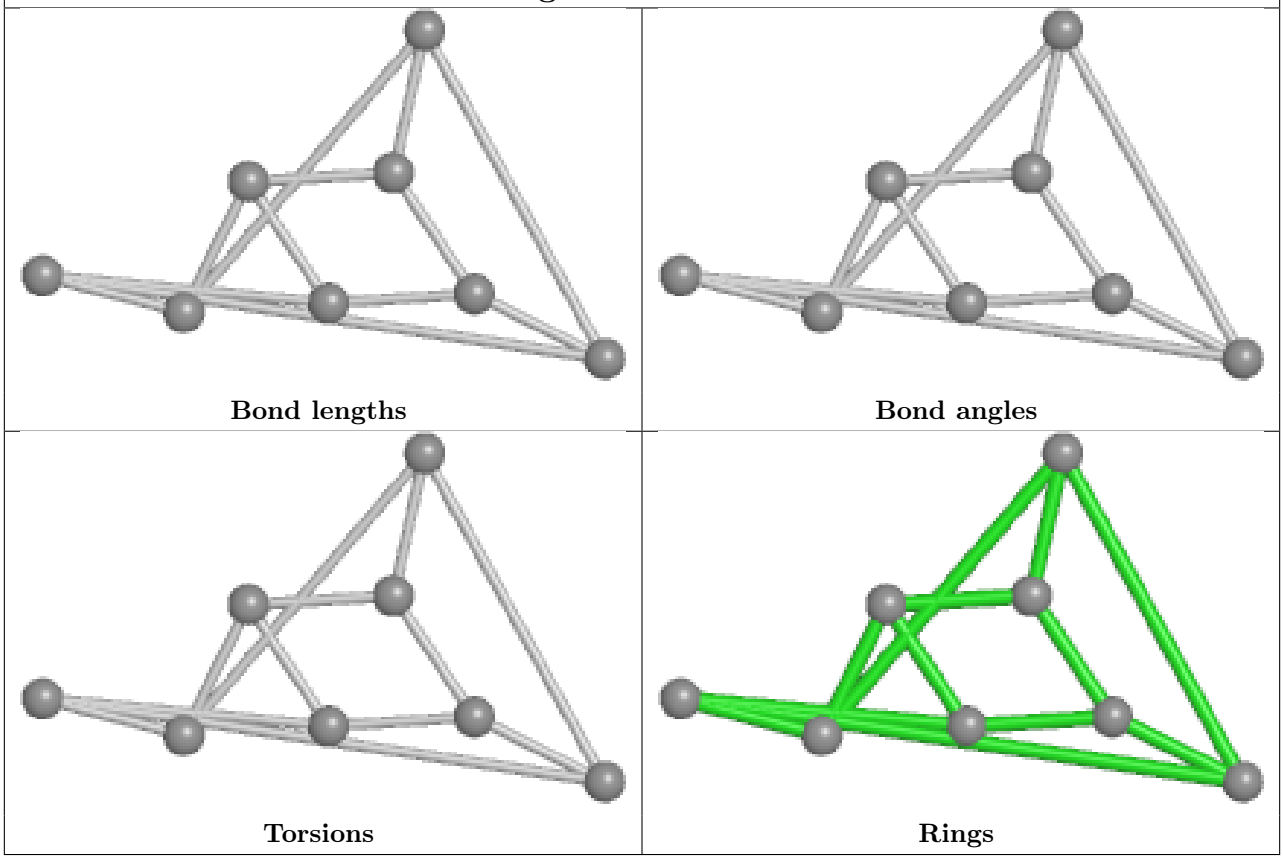
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ1 B 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 I 304



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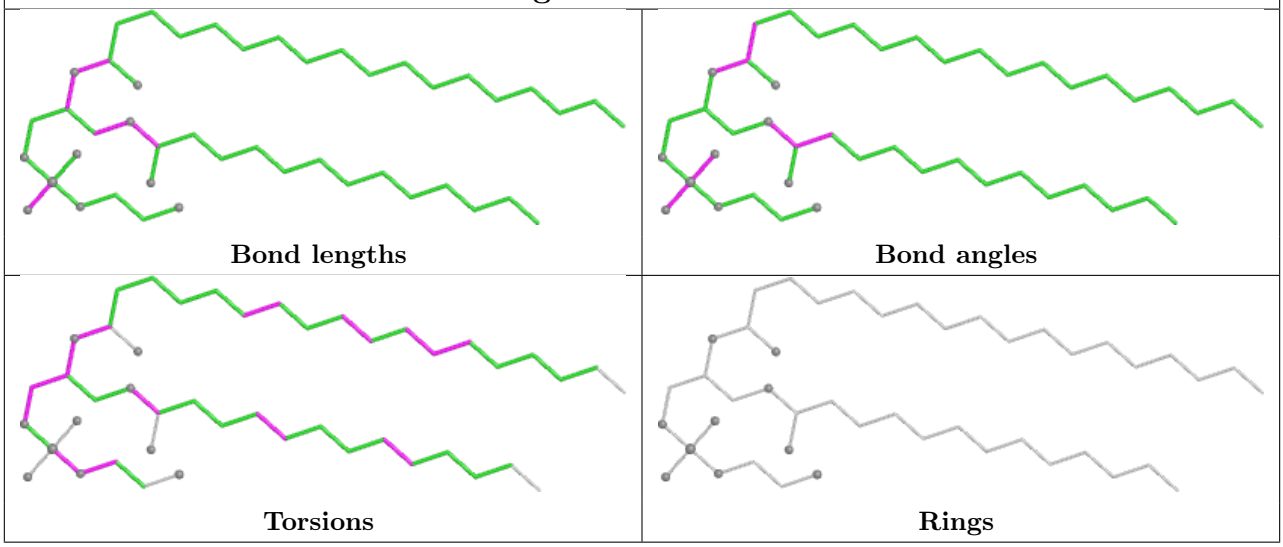
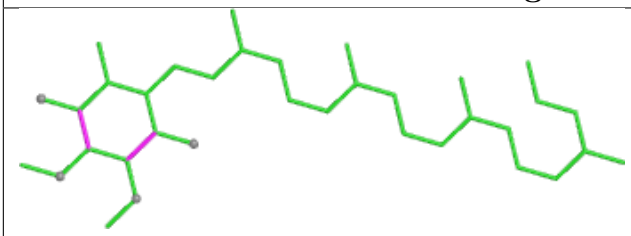
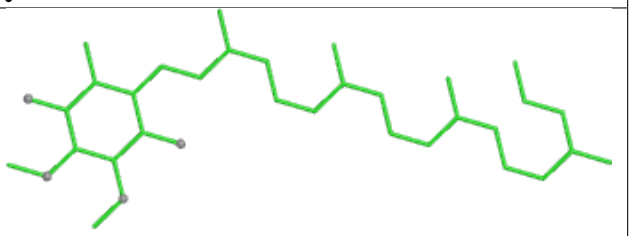


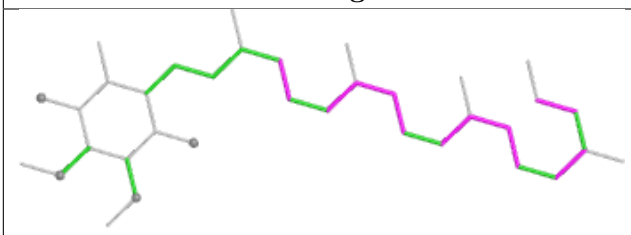
Ligand UQ9 H 400



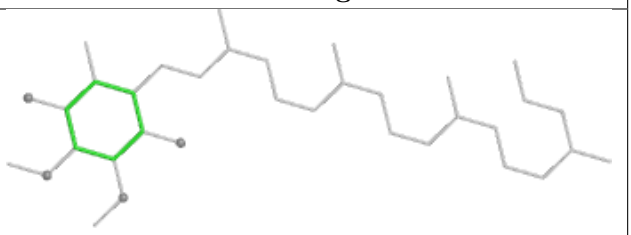
Bond lengths



Bond angles

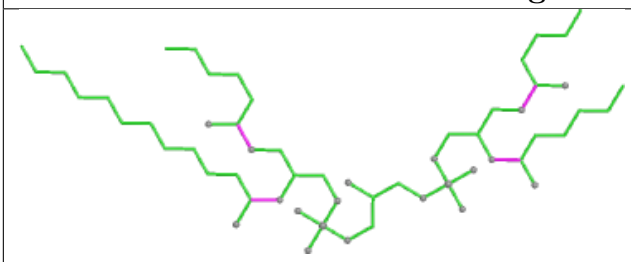


Torsions



Rings

Ligand CDL a 101



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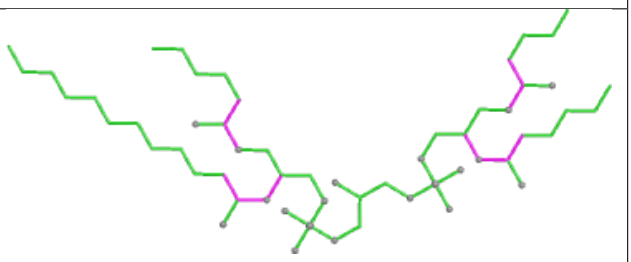
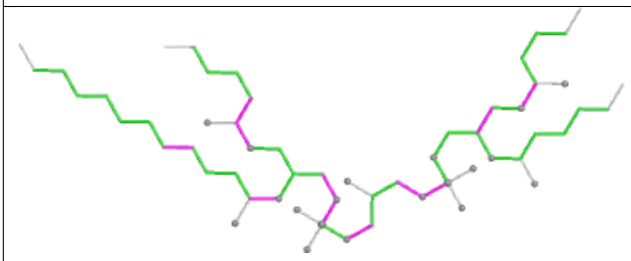


Bond angles



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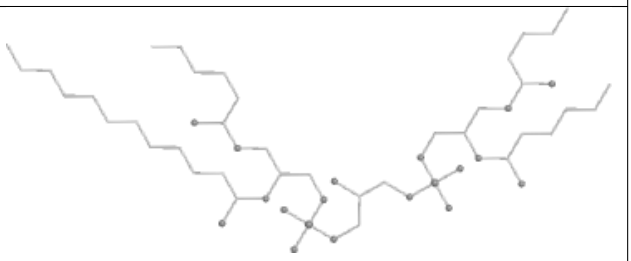
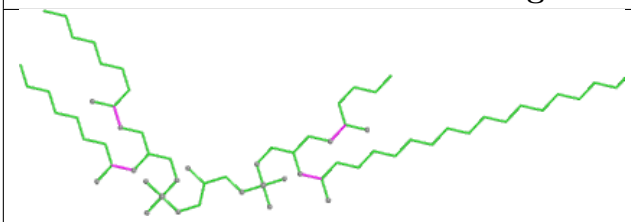


Rings

Ligand CDL d 201



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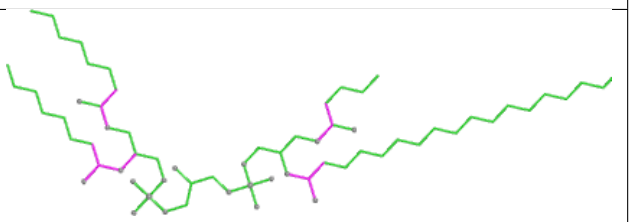
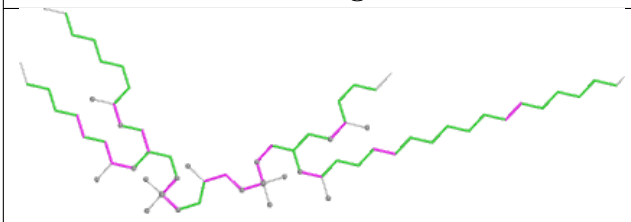


Bond angles



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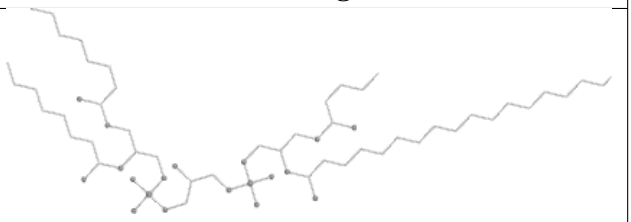
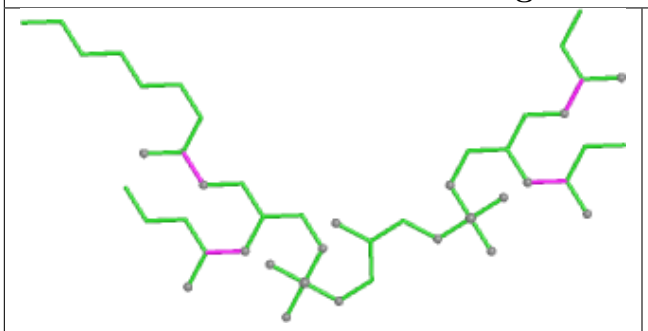


Rings

Ligand CDL Aa 501



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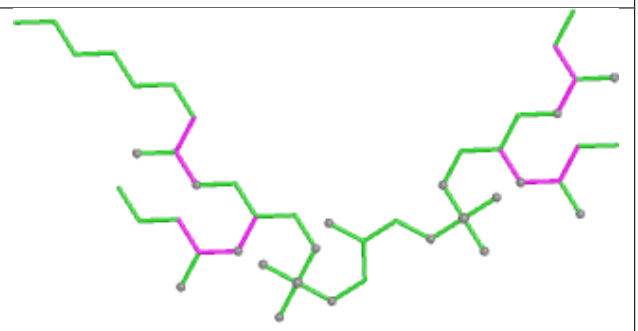

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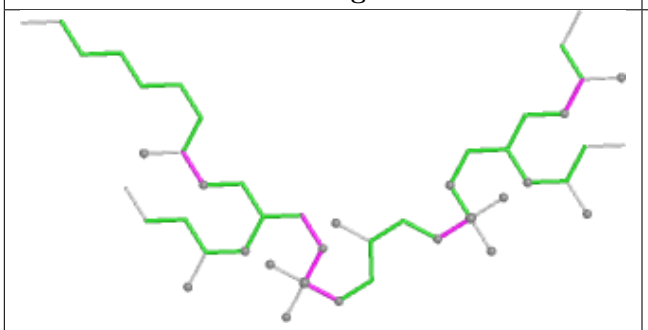

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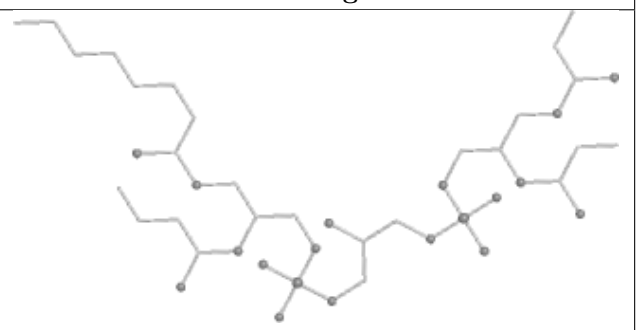
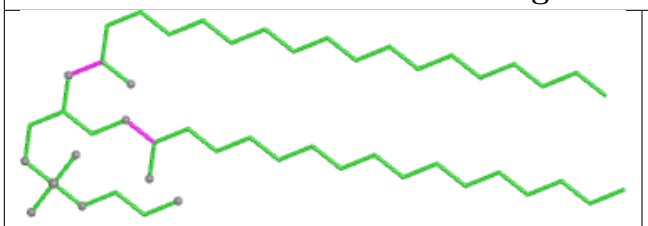


Rings

Ligand 3PE L 701



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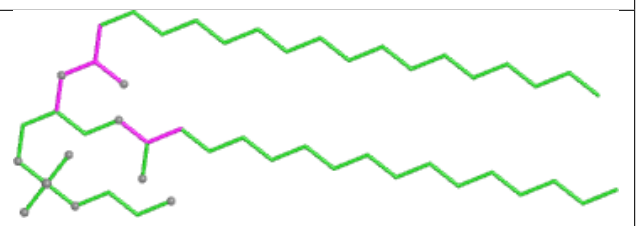
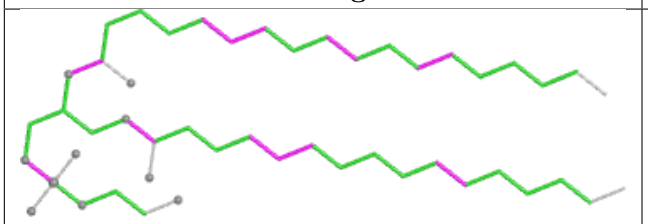


Bond angles



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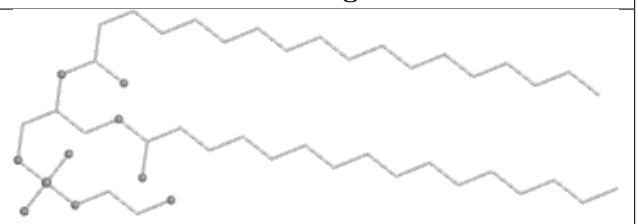
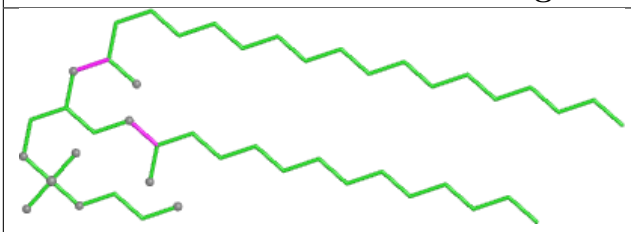
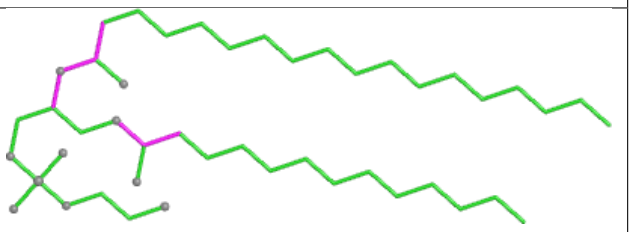
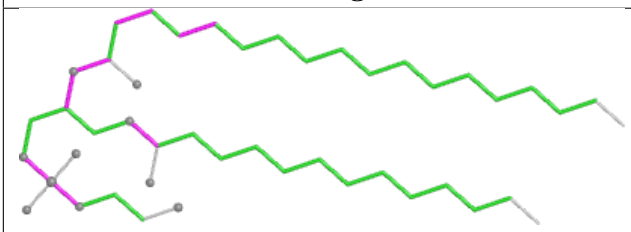
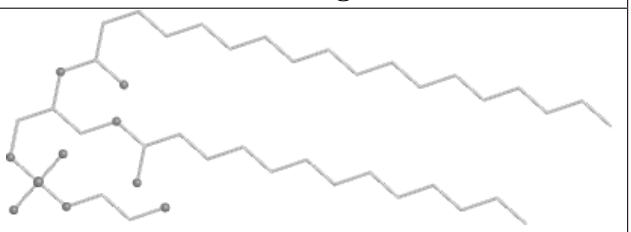


Rings

Ligand 3PE I 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

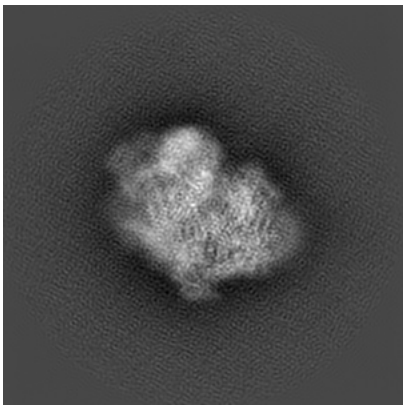
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35336. These allow visual inspection of the internal detail of the map and identification of artifacts.

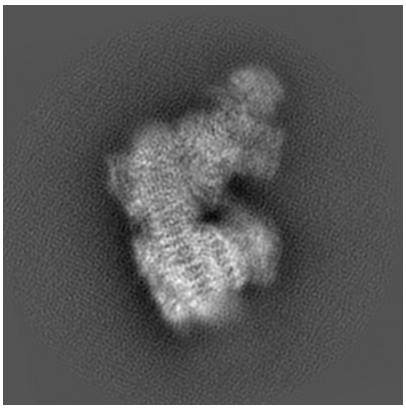
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

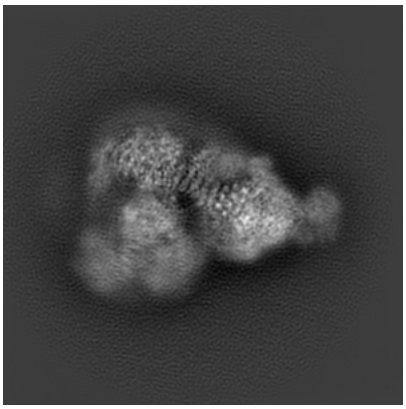
6.1.1 Primary map



X

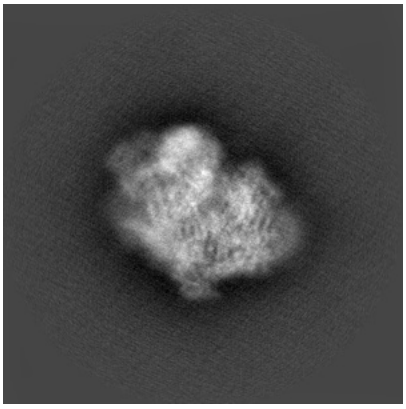


Y

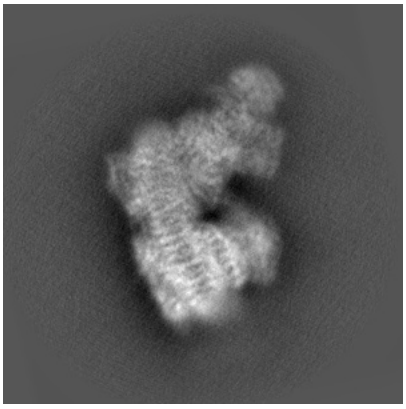


Z

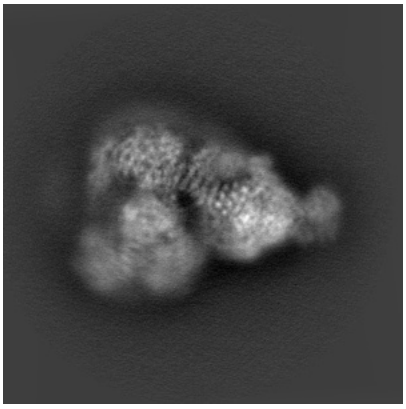
6.1.2 Raw map



X



Y

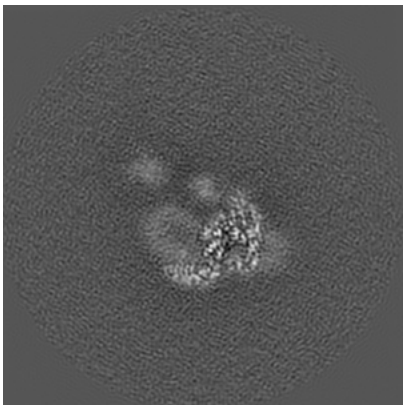


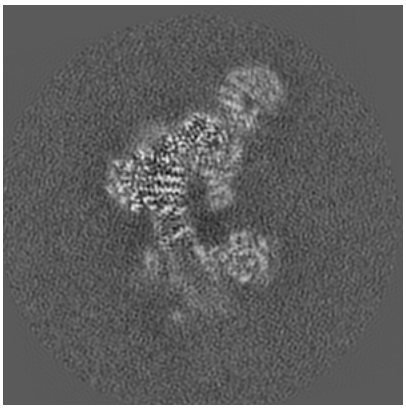
Z

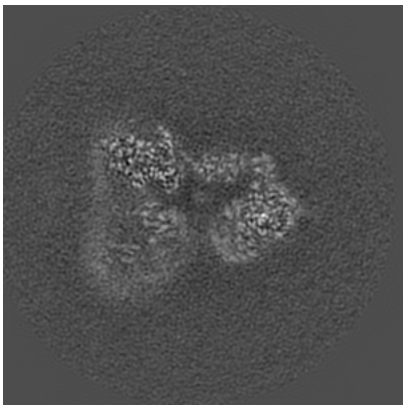
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

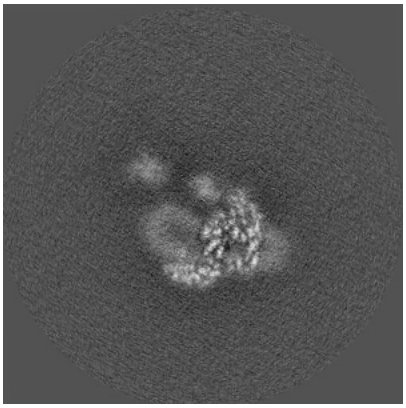
6.2.1 Primary map

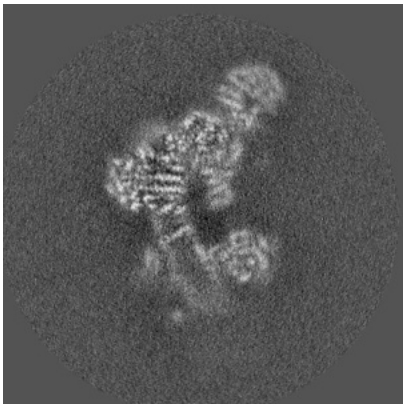

X Index: 192

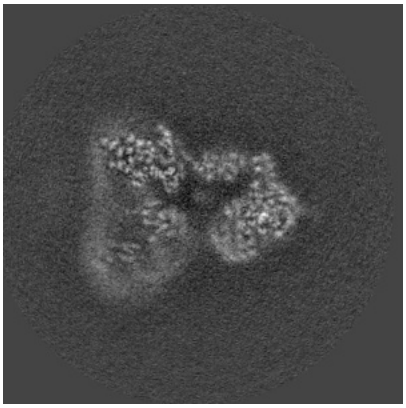

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

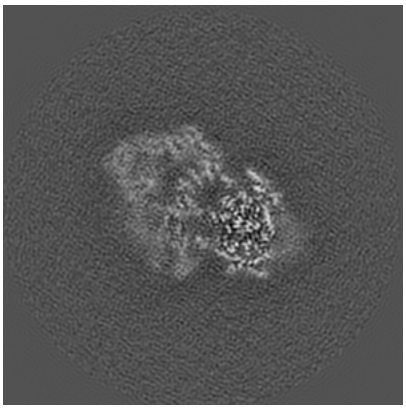

Y Index: 192

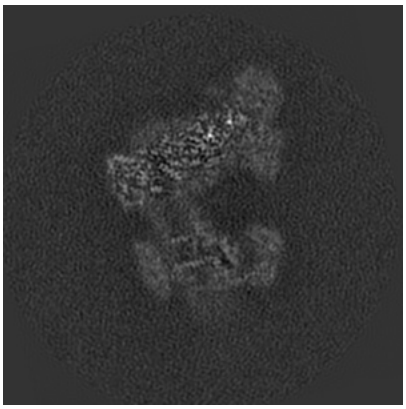

Z Index: 192

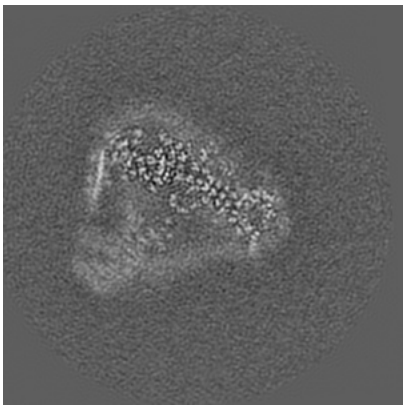
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

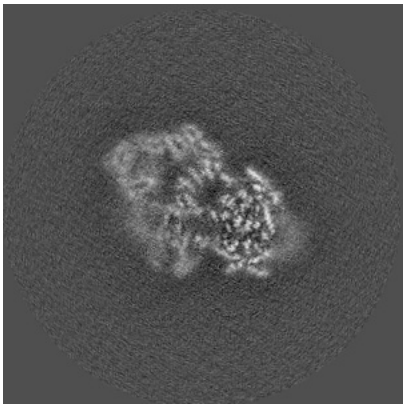
6.3.1 Primary map

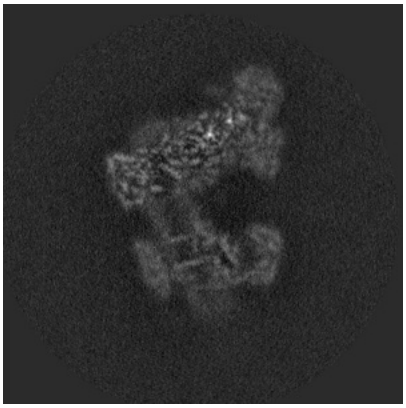

X Index: 154

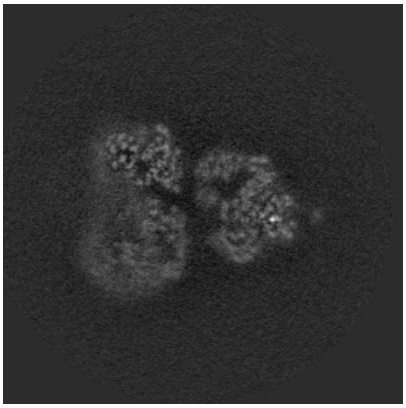

Y Index: 177


Z Index: 167

6.3.2 Raw map


X Index: 154

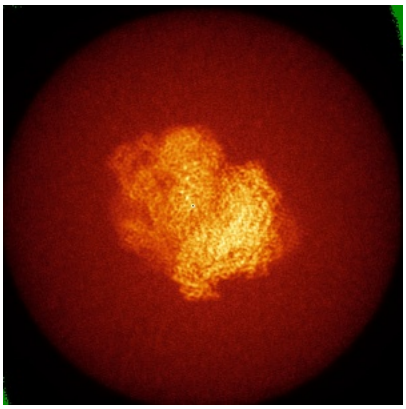

Y Index: 177


Z Index: 198

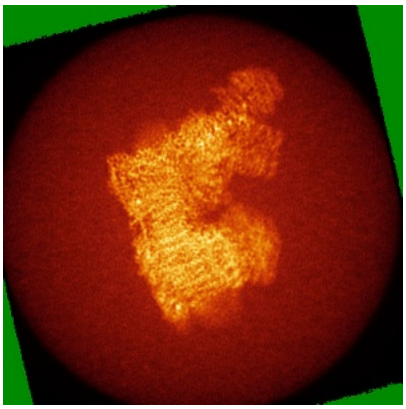
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

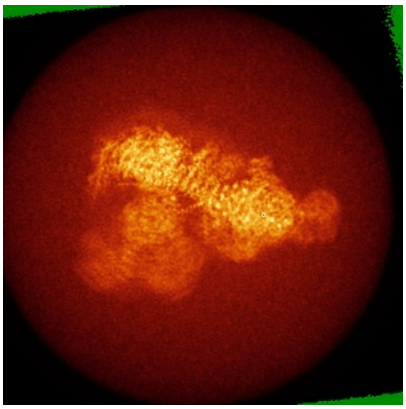
6.4.1 Primary map



X

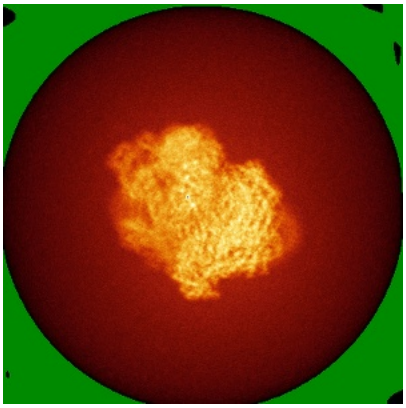


Y

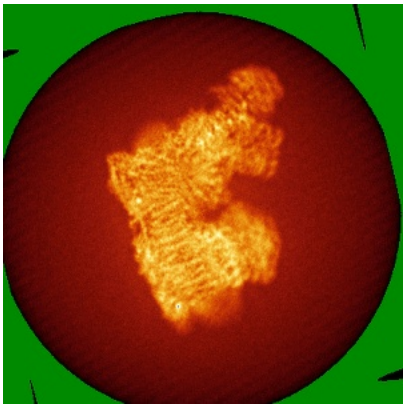


Z

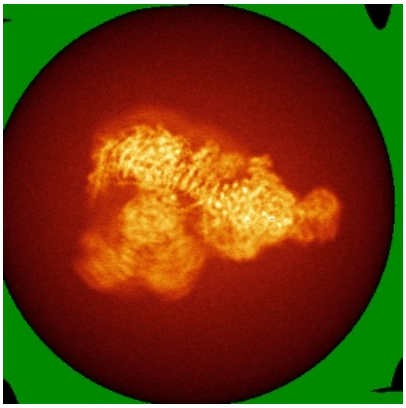
6.4.2 Raw map



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.

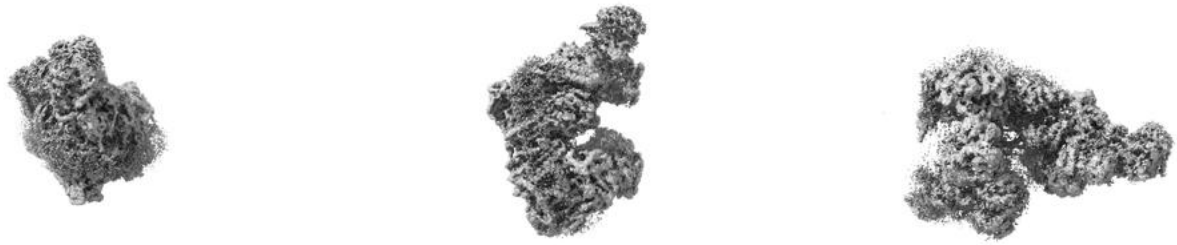
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map



X Y Z

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.

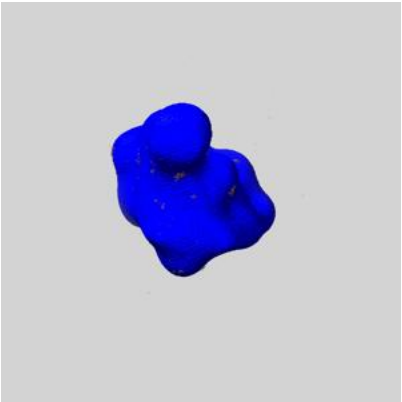
6.6 Mask visualisation (i)

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

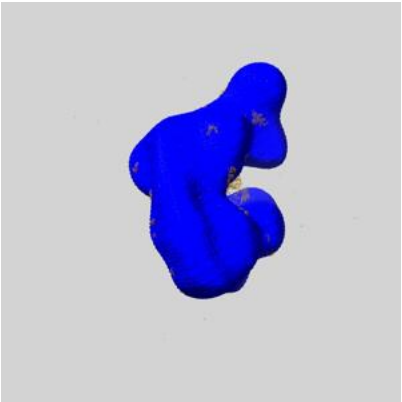
A mask typically either:

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

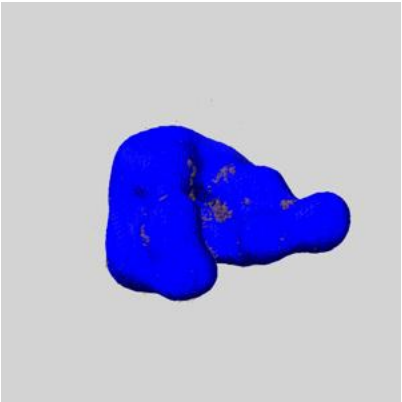
6.6.1 emd_35336_msk_1.map (i)



X



Y

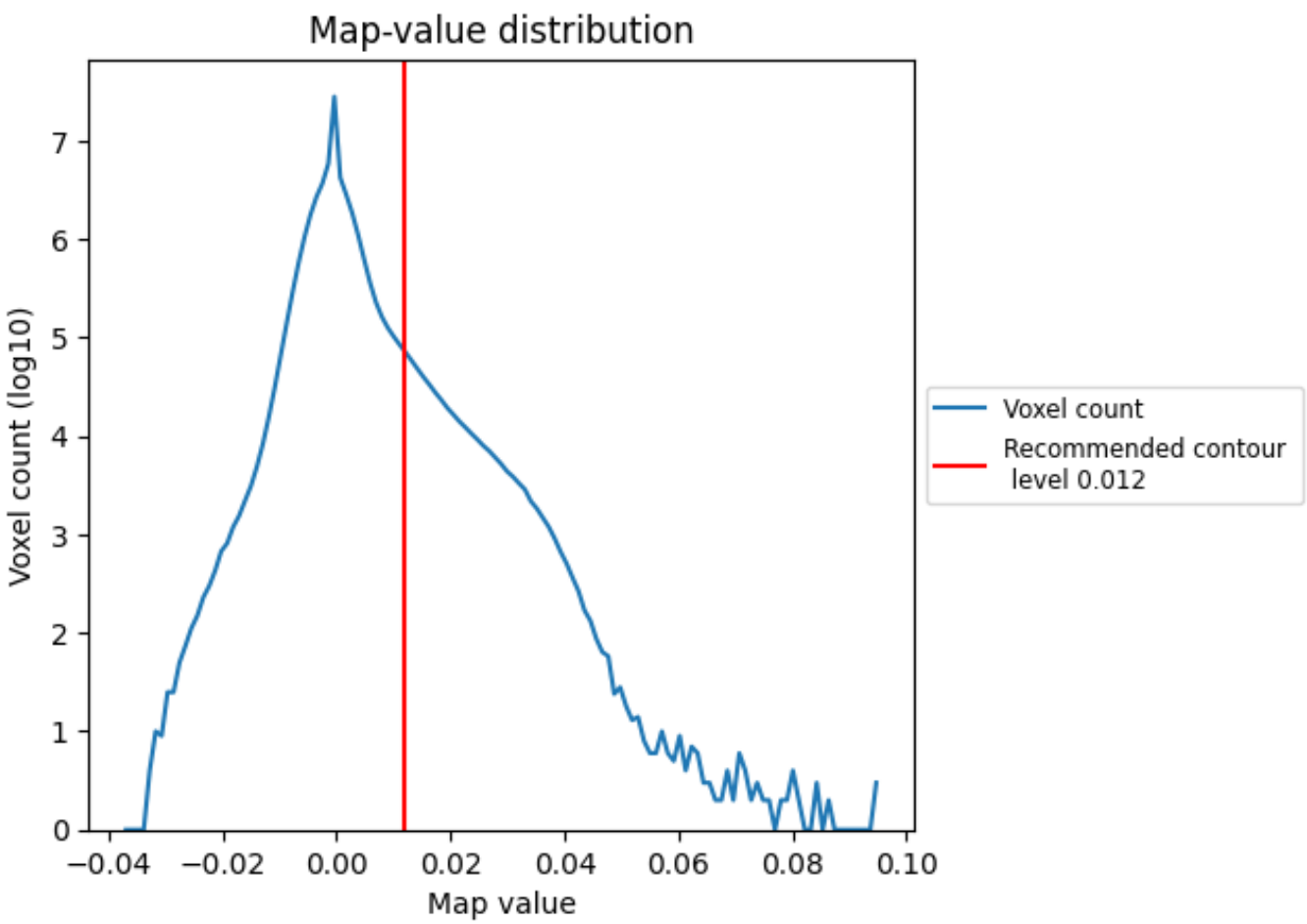


Z

7 Map analysis (i)

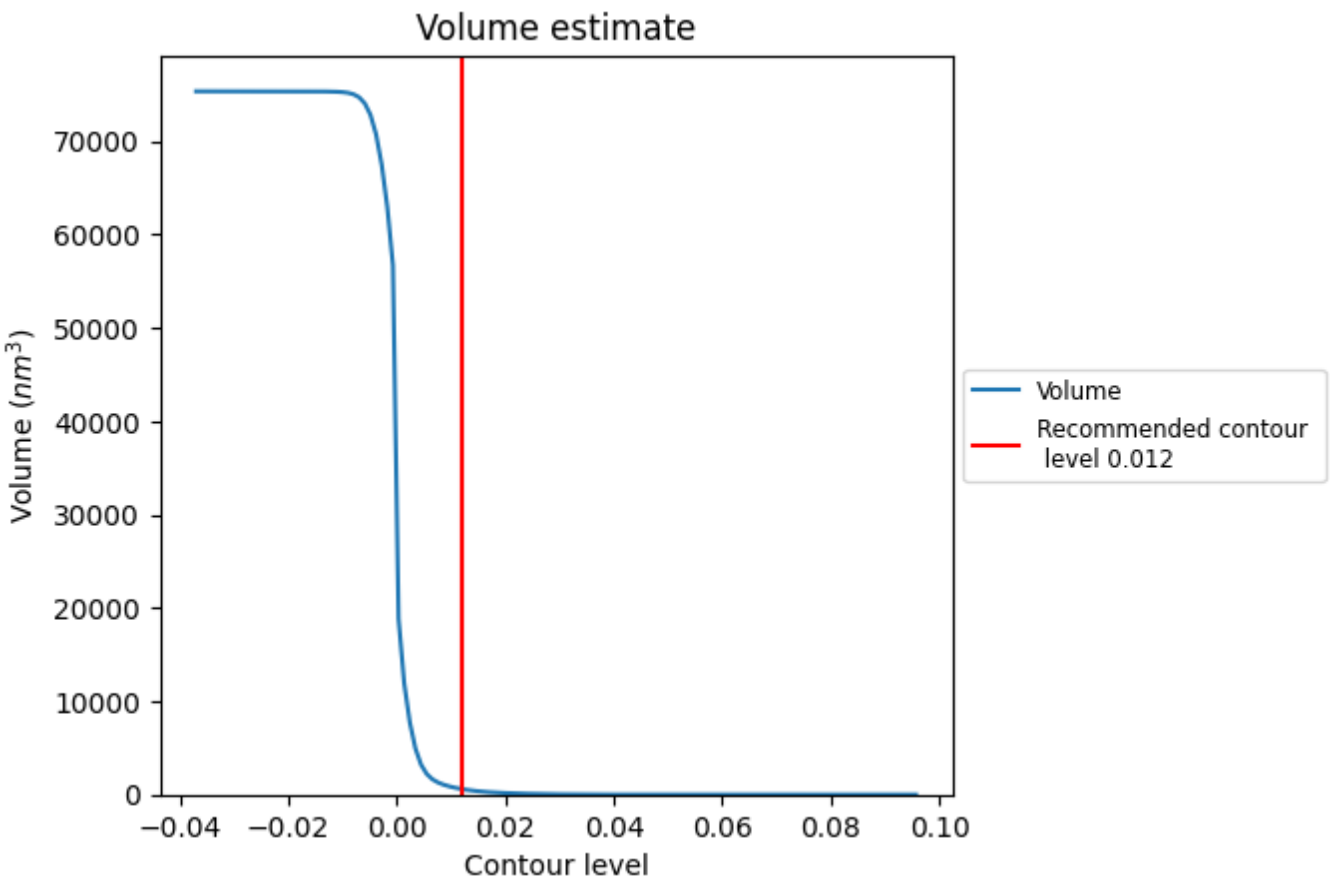
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

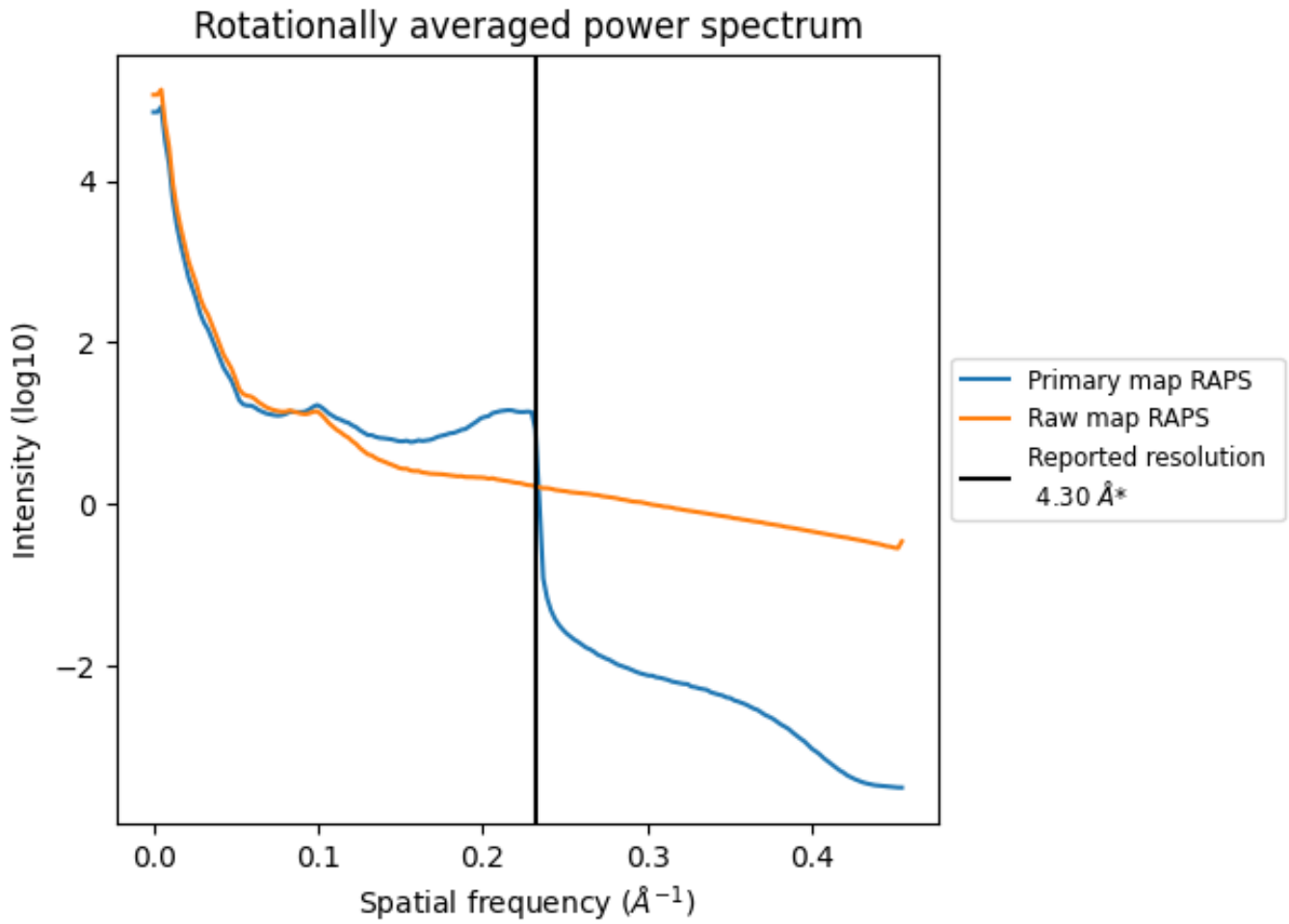
7.2 Volume estimate (i)



The volume at the recommended contour level is 593 nm^3; this corresponds to an approximate mass of 535 kDa.

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

7.3 Rotationally averaged power spectrum (i)

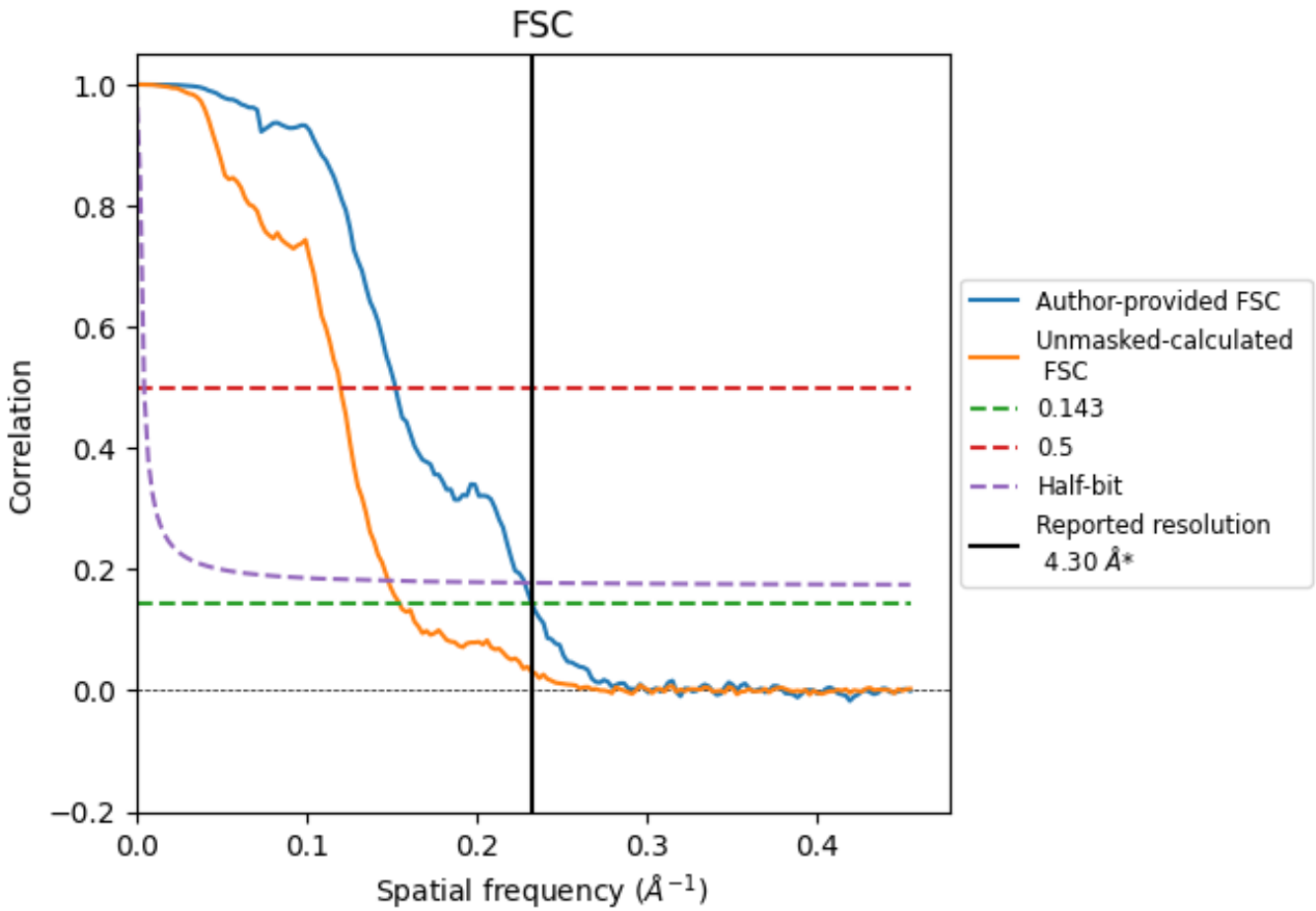


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

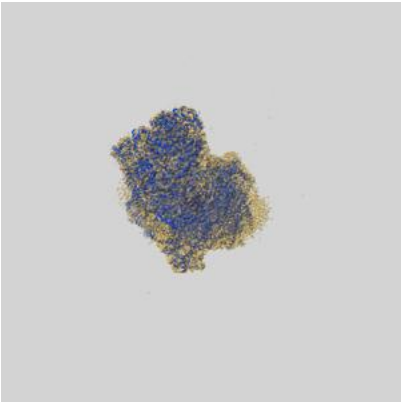
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.30	6.57	4.39
Unmasked-calculated*	6.47	8.34	6.76

*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 6.47 differs from the reported value 4.3 by more than 10 %

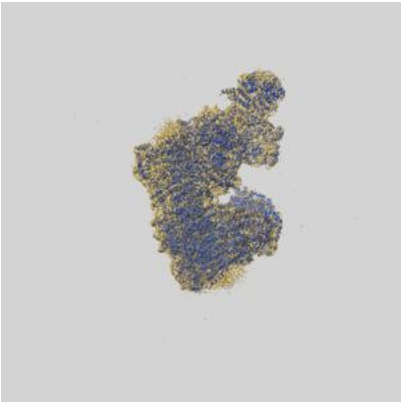
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35336 and PDB model 8IB9. Per-residue inclusion information can be found in section 3 on page 26.

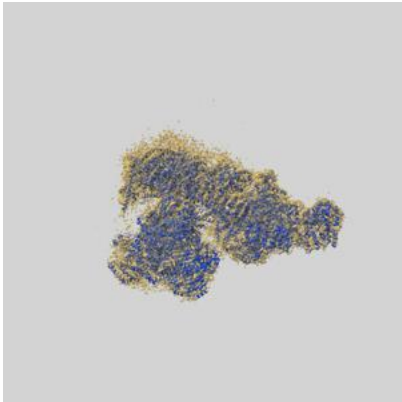
9.1 Map-model overlay (i)



X



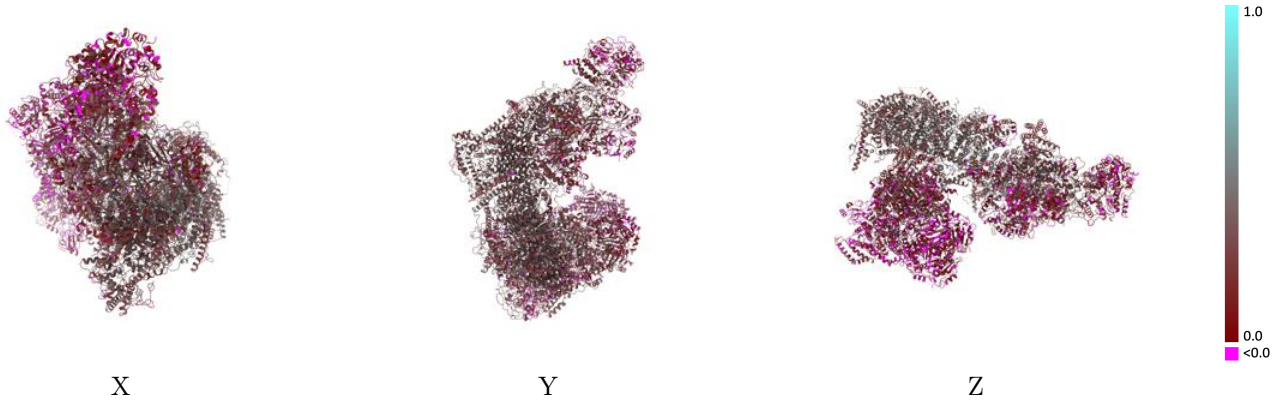
Y



Z

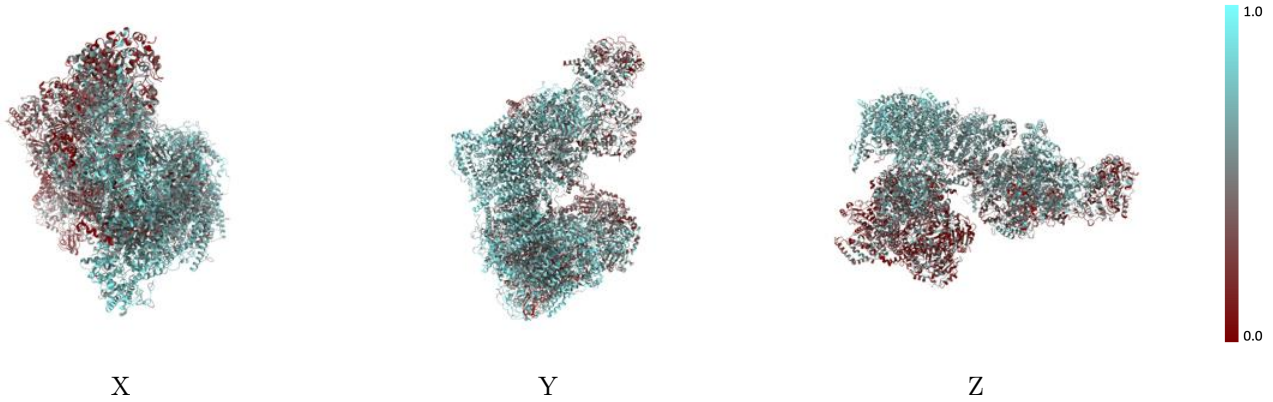
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



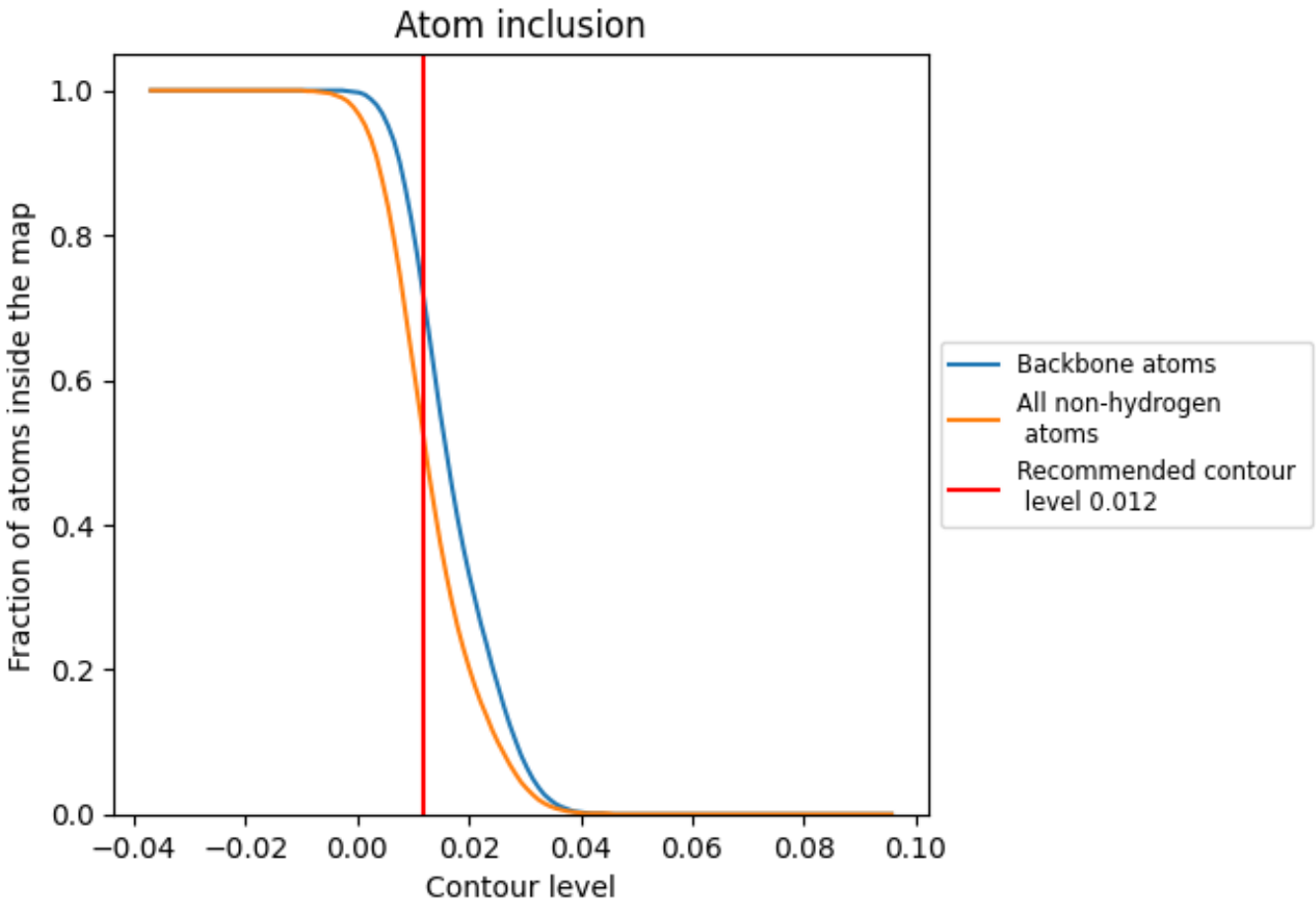
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.5140	0.2380
A	0.5960	0.3270
AA	0.3290	0.1030
AB	0.2800	0.0900
AC	0.2780	0.1230
AD	0.3430	0.0940
AE	0.0840	0.0530
AF	0.3680	0.1070
AG	0.2370	0.0720
AH	0.3380	0.0940
AI	0.1240	0.0610
AJ	0.0640	0.0090
AK	0.1170	0.0500
Aa	0.5520	0.2310
Ab	0.4690	0.1540
Ac	0.4130	0.2080
Ad	0.4000	0.1620
Ae	0.1310	0.0920
Af	0.4420	0.2140
Ag	0.4580	0.2400
Ah	0.4290	0.1560
Aj	0.2020	0.1590
Ak	0.1080	0.0950
B	0.6790	0.3330
C	0.6230	0.2680
D	0.6690	0.3310
E	0.3600	0.1540
F	0.4060	0.1480
G	0.4830	0.1870
H	0.6610	0.3420
I	0.6850	0.3280
J	0.5890	0.3280
K	0.6280	0.3540
L	0.6350	0.3430
M	0.6780	0.3790

Continued on next page...

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Chain	Atom inclusion	Q-score
N	0.6860	0.3750
O	0.5860	0.2720
P	0.4300	0.1700
Q	0.4520	0.2360
R	0.2640	0.1660
S	0.3870	0.0920
T	0.3070	0.1080
U	0.7020	0.3260
V	0.5970	0.2090
W	0.5010	0.1940
X	0.7410	0.3300
Y	0.6210	0.3320
Z	0.7270	0.3200
a	0.6720	0.3210
b	0.6520	0.2910
c	0.6350	0.2860
d	0.6950	0.3610
e	0.7320	0.3330
f	0.6430	0.2960
g	0.6770	0.3440
h	0.6950	0.3330
i	0.6980	0.3340
j	0.6830	0.3100
k	0.7330	0.3390
l	0.7130	0.3600
m	0.6280	0.3340
n	0.7510	0.3480
o	0.6680	0.2740
p	0.7220	0.3290
q	0.2190	0.2020
r	0.3220	0.1890
s	0.1130	0.0810