



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 09:05 AM JST

PDB ID : 7DKF / pdb_00007dkf
EMDB ID : EMD-30706
Title : Activity optimized supercomplex state4
Authors : Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on : 2020-11-24
Resolution : 8.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

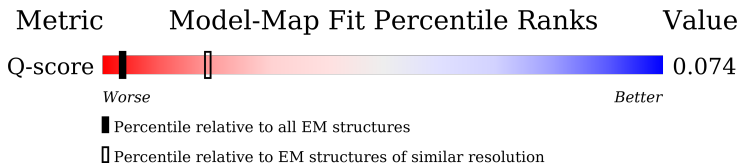
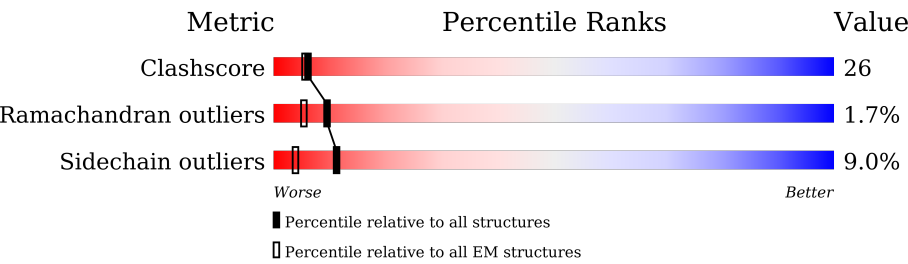
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 8.30 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	280 (7.82 - 8.80)

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

Mol	Chain	Length	Quality of chain
1	A1	480	9% 15% 46% 24% 5% 10%
1	M1	480	23% 16% 48% 23% • 10%
2	B1	453	10% 20% 50% 20% • 8%
2	N1	453	14% 21% 49% 20% • 8%

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Mol	Chain	Length	Quality of chain
3	C1	379	
3	O1	379	
4	D1	325	
4	P1	325	
5	E1	196	
5	Q1	196	
6	F1	111	
6	R1	111	
7	G1	82	
7	S1	82	
8	H1	91	
8	T1	91	
9	I1	78	
9	U1	78	
10	J1	64	
10	V1	64	
11	K1	56	
11	W1	56	
12	22	347	
13	32	115	
14	42	459	
15	52	98	
16	72	175	
17	82	444	
18	92	217	

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Mol	Chain	Length	Quality of chain
19	A2	704	
20	B2	430	
21	C2	228	
22	D2	179	
23	E2	176	
24	F2	75	
25	G2	133	
26	H2	105	
27	I2	96	
28	J2	70	
29	K2	98	
30	L2	83	
31	N2	115	
32	O2	127	
33	P2	112	
34	Q2	171	
35	R2	345	
36	S2	320	
37	T2	140	
38	U2	145	
39	V2	143	
40	M2	88	
40	W2	88	
41	X2	57	
42	Y2	72	

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Mol	Chain	Length	Quality of chain
43	Z2	97	
44	a2	128	
45	b2	143	
46	c2	127	
47	d2	136	
48	f2	178	
49	h2	125	
50	i2	49	
51	j2	120	
52	12	318	
53	62	606	
54	g2	176	
55	e2	158	
56	A3	514	
57	B3	227	
58	C3	261	
59	D3	169	
60	E3	152	
61	F3	129	
62	G3	97	
63	H3	86	
64	I3	74	
65	J3	80	
66	K3	80	
67	L3	63	

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Mol	Chain	Length	Quality of chain
68	M3	70	24% 43% 17% 39%

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
75	SF4	A2	801	-	-	X	-
75	SF4	A2	802	-	-	X	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 105456 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	432	Total	C	N	O	S	0	0
			3356	2098	595	643	20		
1	M1	432	Total	C	N	O	S	0	0
			3356	2098	595	643	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		
2	N1	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
3	O1	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
4	P1	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	75	Total	C	N	O	S	0	0
			566	352	94	118	2		
5	Q1	196	Total	C	N	O	S	0	0
			1518	956	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
6	R1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
7	S1	81	Total	C	N	O	S	0	0
			682	441	128	112	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	64	Total	C	N	O	S	0	0
			524	316	96	107	5		
8	T1	64	Total	C	N	O	S	0	0
			524	316	96	107	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	33	Total	C	N	O	S	0	0
			248	152	51	44	1		
9	U1	33	Total	C	N	O	S	0	0
			248	152	51	44	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J1	62	Total	C	N	O	0	0
			511	335	89	87		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	V1	62	Total	C	N	O	0	0
			511	335	89	87		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K1	22	Total	C	N	O	0	0
			164	109	29	26		
11	W1	22	Total	C	N	O	0	0
			164	109	29	26		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	344	Total	C	N	O	S	0	0
			2582	1707	404	437	34		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	32	93	Total	C	N	O	S	0	0
			719	492	104	120	3		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	42	458	Total	C	N	O	S	1	0
			3447	2293	548	574	32		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	52	96	Total	C	N	O	S	0	0
			697	454	109	124	10		

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	72	172	Total	C	N	O	S	0	0
			1186	798	179	202	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	82	427	Total	C	N	O	S	0	0
			2965	1864	552	534	15		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	92	207	Total	C	N	O	S	0	0
			1535	978	261	286	10		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A2	688	Total	C	N	O	S	0	0
			5183	3254	915	978	36		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B2	385	Total	C	N	O	S	0	0
			3076	1963	530	559	24		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C2	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D2	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E2	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	F2	28	Total	C	N	O	0	0
			183	116	32	35		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G2	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H2	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I2	71	Total	C	N	O	S	0	0
			532	332	99	98	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J2	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	K2	84	Total	C	N	O	0	0
			652	409	125	118		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L2	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N2	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	O2	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	P2	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Q2	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R2	306	Total	C	N	O	S	0	0
			2334	1505	417	409	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S2	319	Total	C	N	O	S	0	0
			2299	1457	395	438	9		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	T2	138	Total	C	N	O	S	0	0
			942	599	165	172	6		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	U2	91	Total	C	N	O	S	0	0
			734	480	123	128	3		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V2	138	Total	C	N	O	S	0	0
			1093	702	189	193	9		

- Molecule 40 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W2	83	Total	C	N	O	S	0	0
			596	386	95	111	4		
40	M2	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X2	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y2	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z2	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	a2	114	Total	C	N	O	S	0	0
			857	550	159	148			

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	b2	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c2	90	Total	C	N	O	S	0	0
			617	391	119	107			

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	d2	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f2	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	h2	91	Total	C	N	O	S	0	0
			721	461	123	135	2		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	i2	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	j2	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

- Molecule 52 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	12	309	Total	C	N	O	S	0	0
			2442	1642	376	401	23		

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	62	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	g2	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	e2	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A3	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B3	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C3	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	D3	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	E3	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	F3	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	G3	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	H3	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	I3	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	J3	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	K3	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

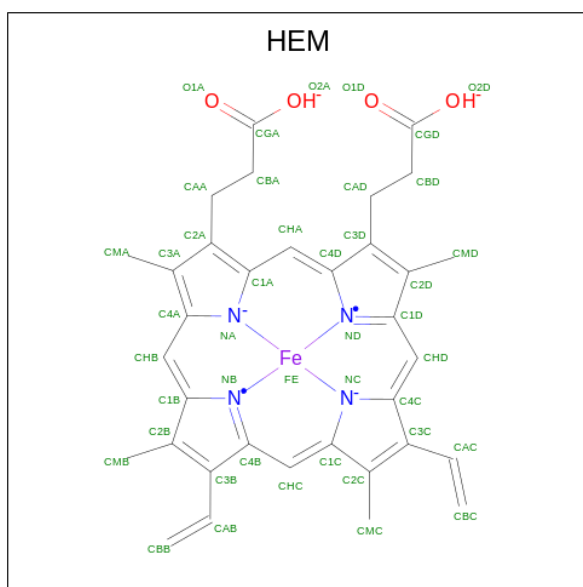
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	L3	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

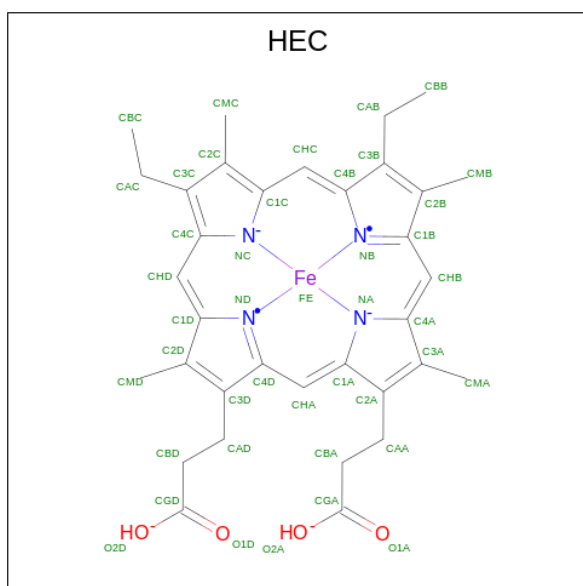
Mol	Chain	Residues	Atoms				AltConf	Trace
68	M3	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 69 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



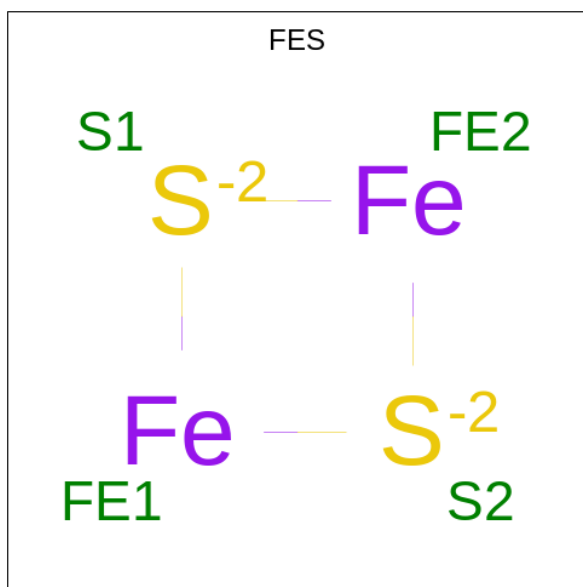
Mol	Chain	Residues	Atoms					AltConf
69	C1	1	Total 43	C 34	Fe 1	N 4	O 4	0
69	C1	1	Total 43	C 34	Fe 1	N 4	O 4	0
69	O1	1	Total 43	C 34	Fe 1	N 4	O 4	0
69	O1	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



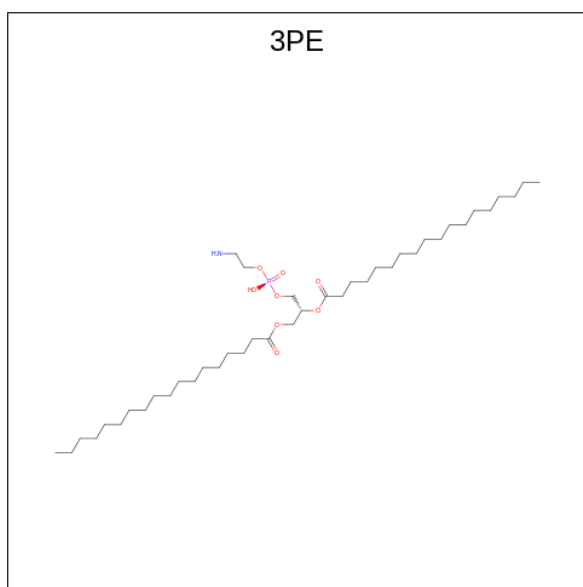
Mol	Chain	Residues	Atoms					AltConf
70	D1	1	Total 43	C 34	Fe 1	N 4	O 4	0
70	P1	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



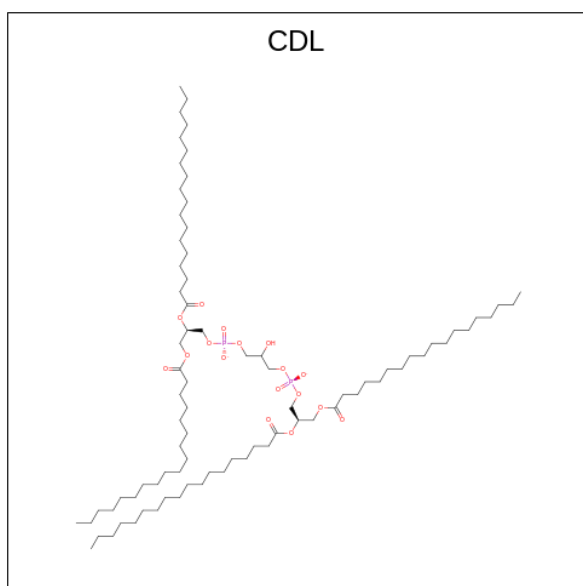
Mol	Chain	Residues	Atoms			AltConf
71	Q1	1	Total	Fe	S	0
			4	2	2	
71	92	1	Total	Fe	S	0
			4	2	2	
71	A2	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



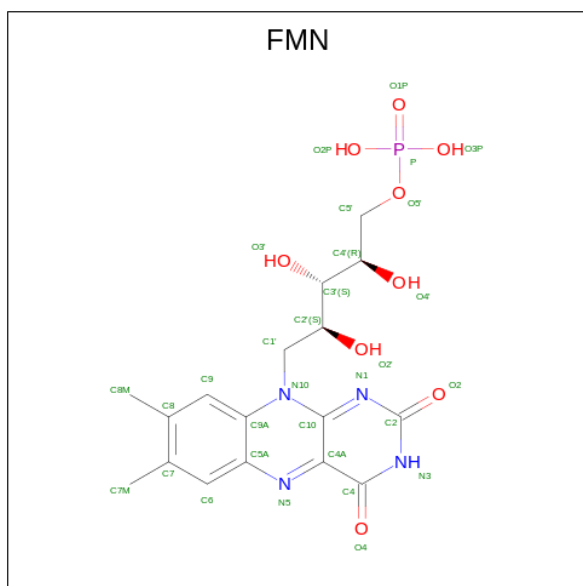
Mol	Chain	Residues	Atoms					AltConf
72	22	1	Total	C	N	O	P	0
			41	31	1	8	1	
72	42	1	Total	C	N	O	P	0
			41	31	1	8	1	
72	B2	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 73 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



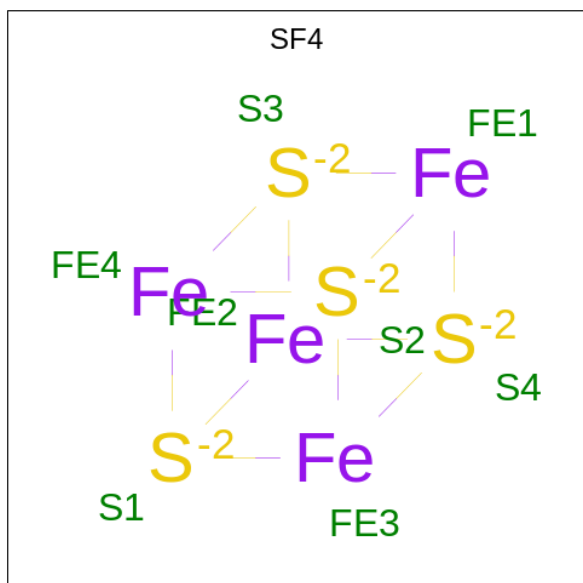
Mol	Chain	Residues	Atoms				AltConf
73	42	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 74 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
74	82	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 75 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

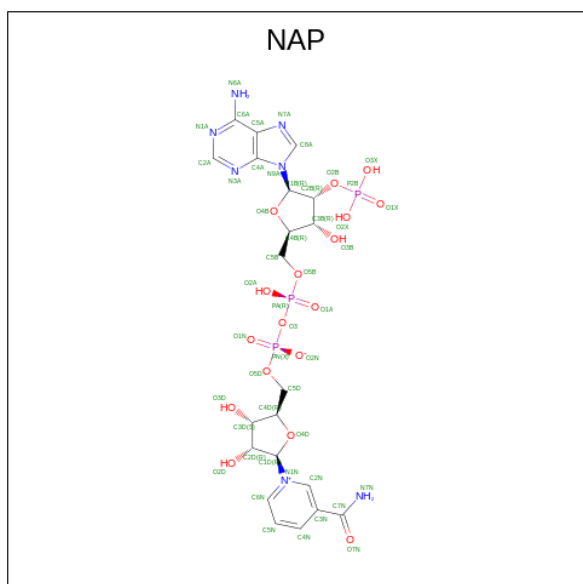


Mol	Chain	Residues	Atoms			AltConf
75	82	1	Total 8	Fe 4	S 4	0
75	A2	1	Total 8	Fe 4	S 4	0
75	A2	1	Total 8	Fe 4	S 4	0
75	D2	1	Total 8	Fe 4	S 4	0
75	E2	1	Total 8	Fe 4	S 4	0
75	E2	1	Total 8	Fe 4	S 4	0

- Molecule 76 is ZINC ION (CCD ID: ZN) (formula: Zn).

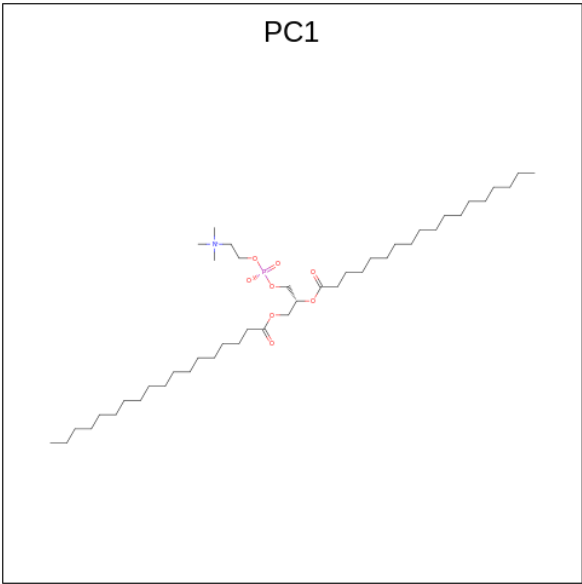
Mol	Chain	Residues	Atoms	AltConf
76	I2	1	Total Zn 1 1	0
76	F3	1	Total Zn 1 1	0

- Molecule 77 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



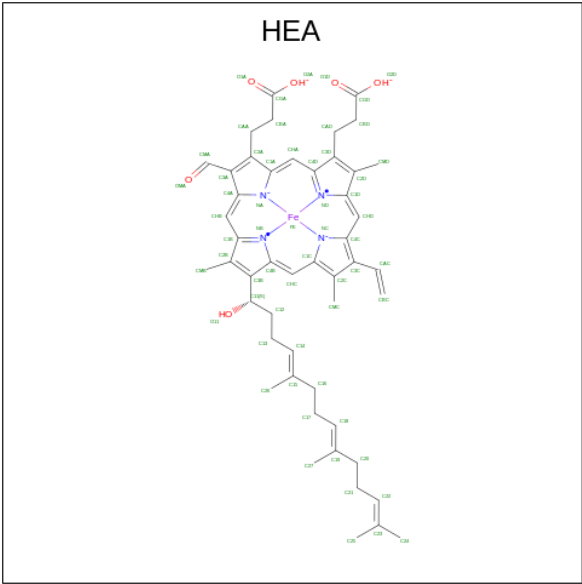
Mol	Chain	Residues	Atoms					AltConf
77	R2	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 78 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
78	S2	1	Total	C	N	O	P	0
			47	37	1	8	1	
78	j2	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
79	A3	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
79	A3	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	A3	1	Total	Cu	0
			1	1	
80	B3	2	Total	Cu	0
			2	2	

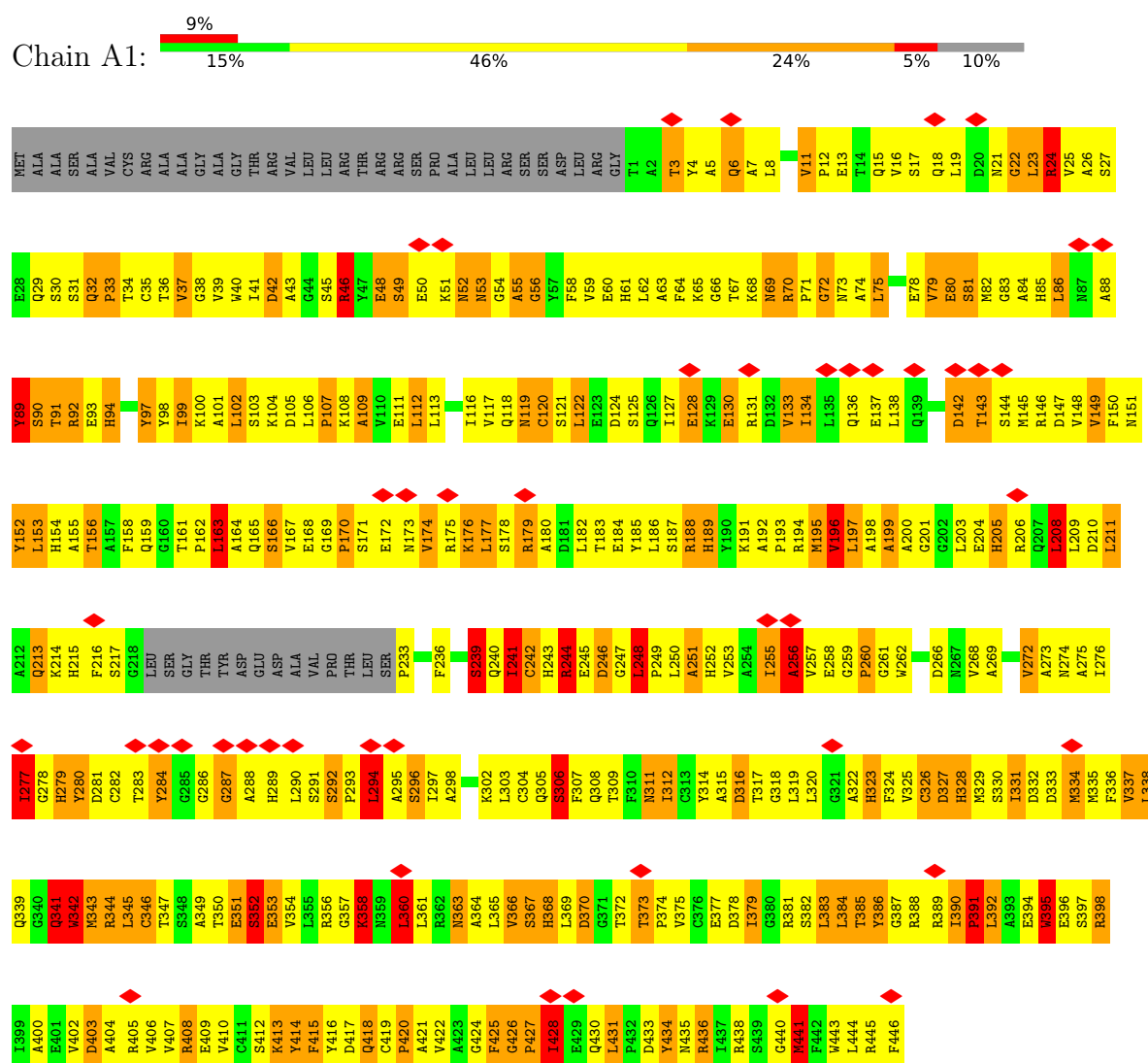
- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	A3	1	Total	Mg	0
			1	1	

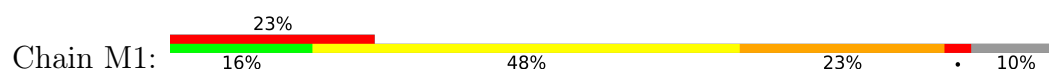
3 Residue-property plots

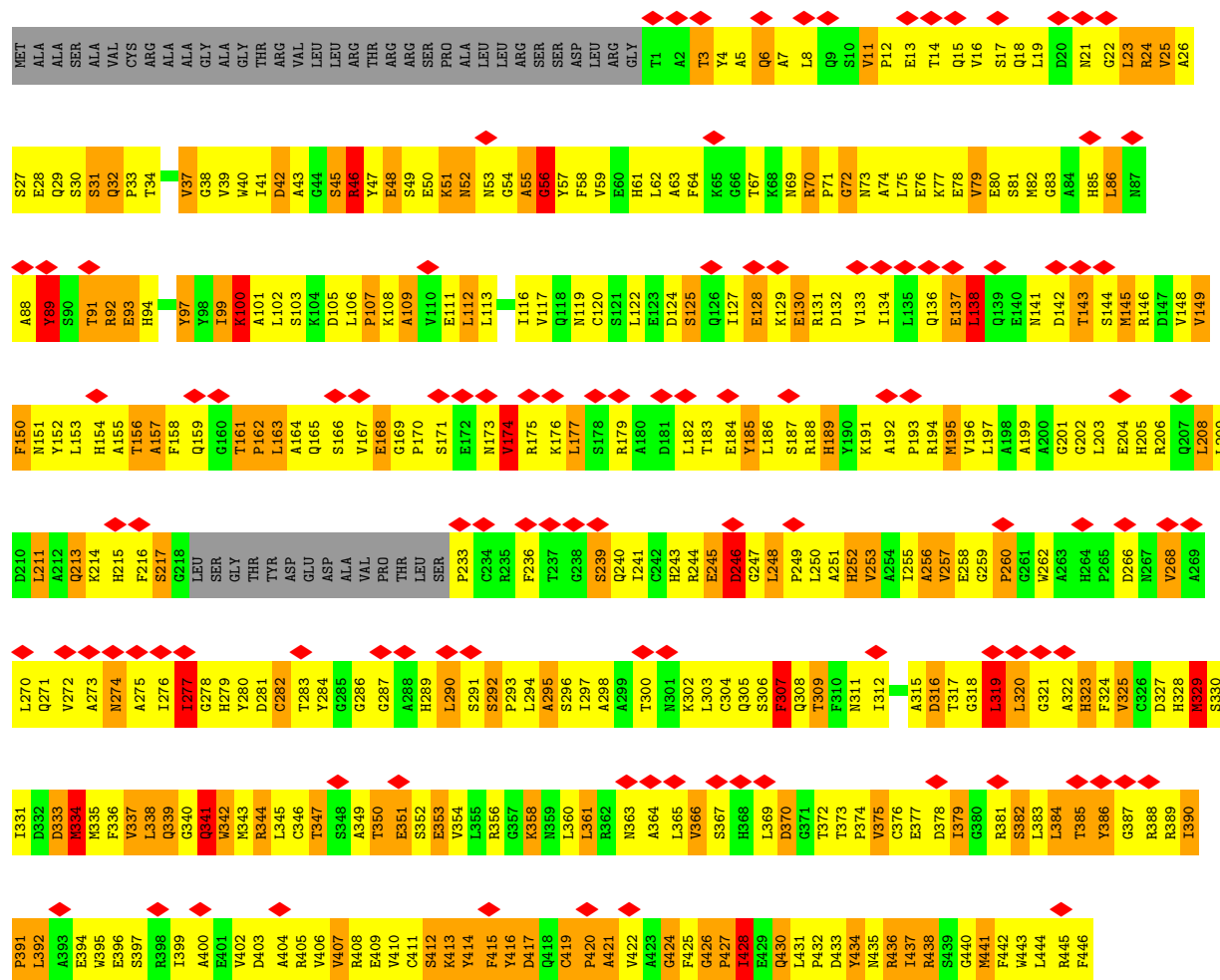
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

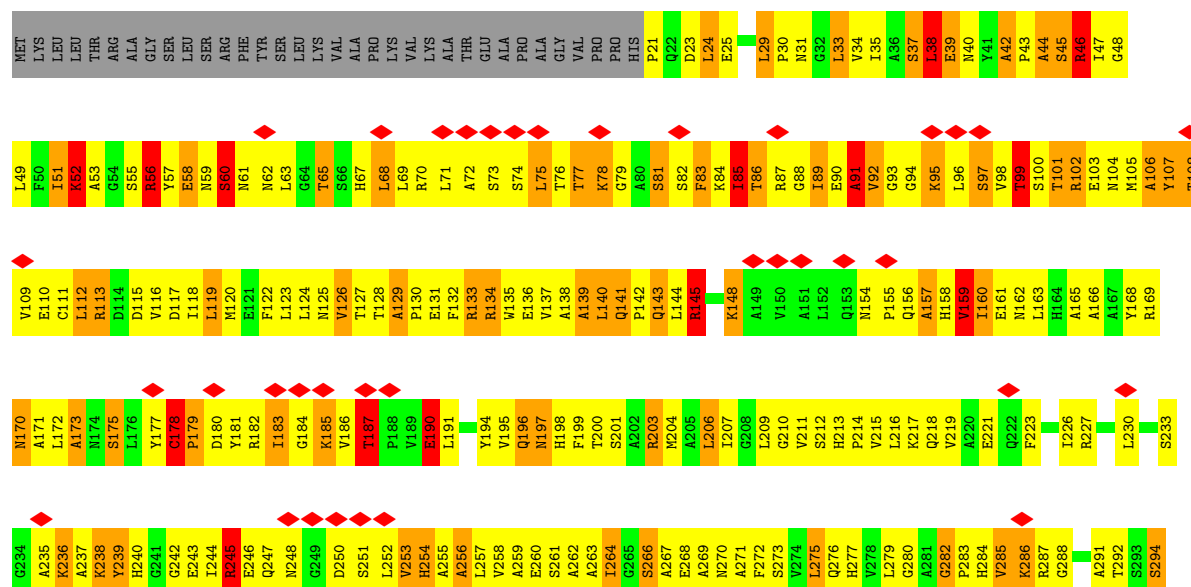
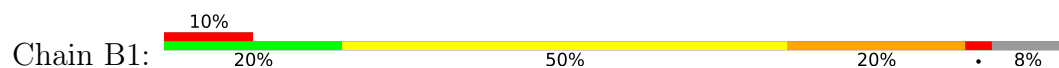


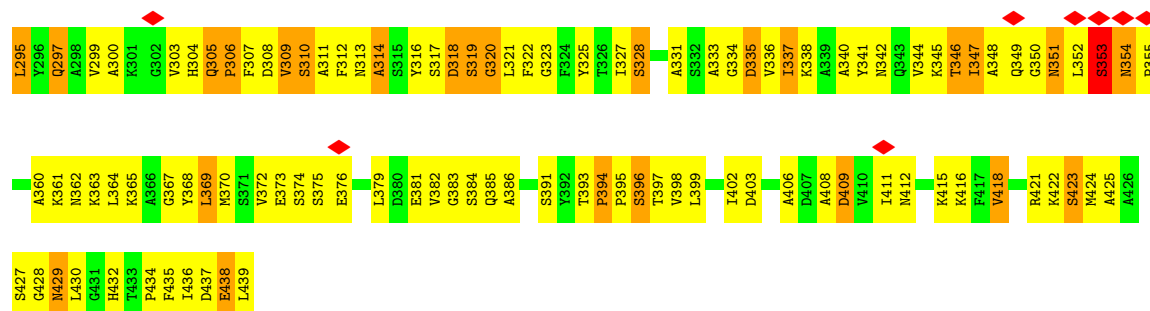
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



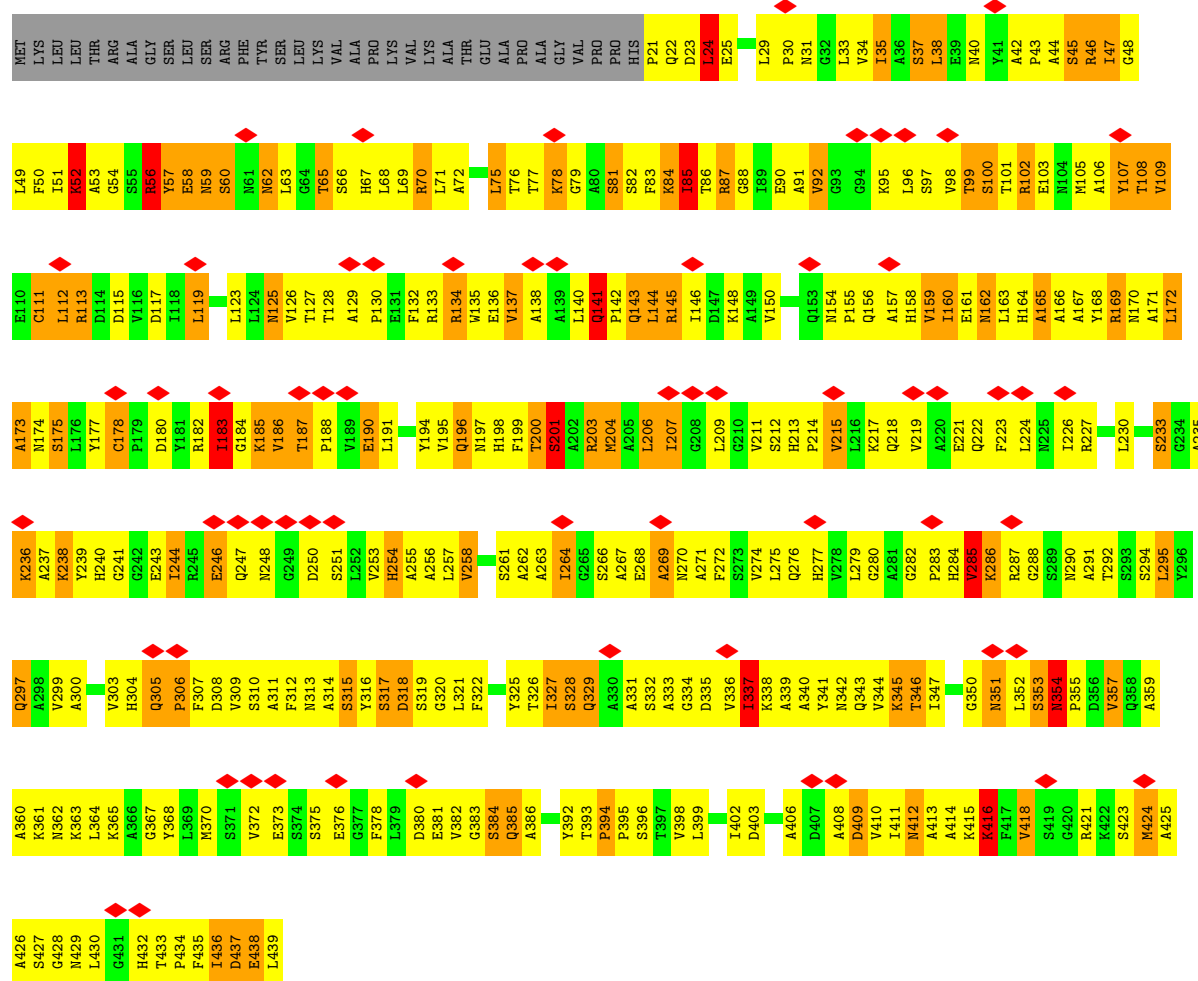
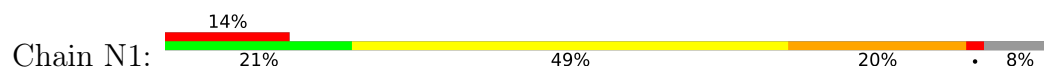


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

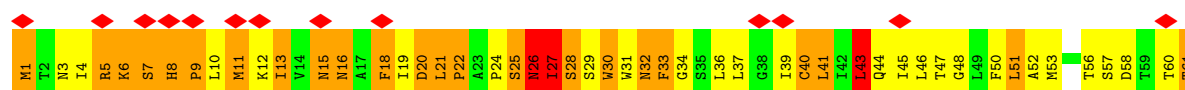
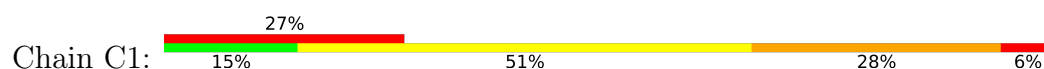


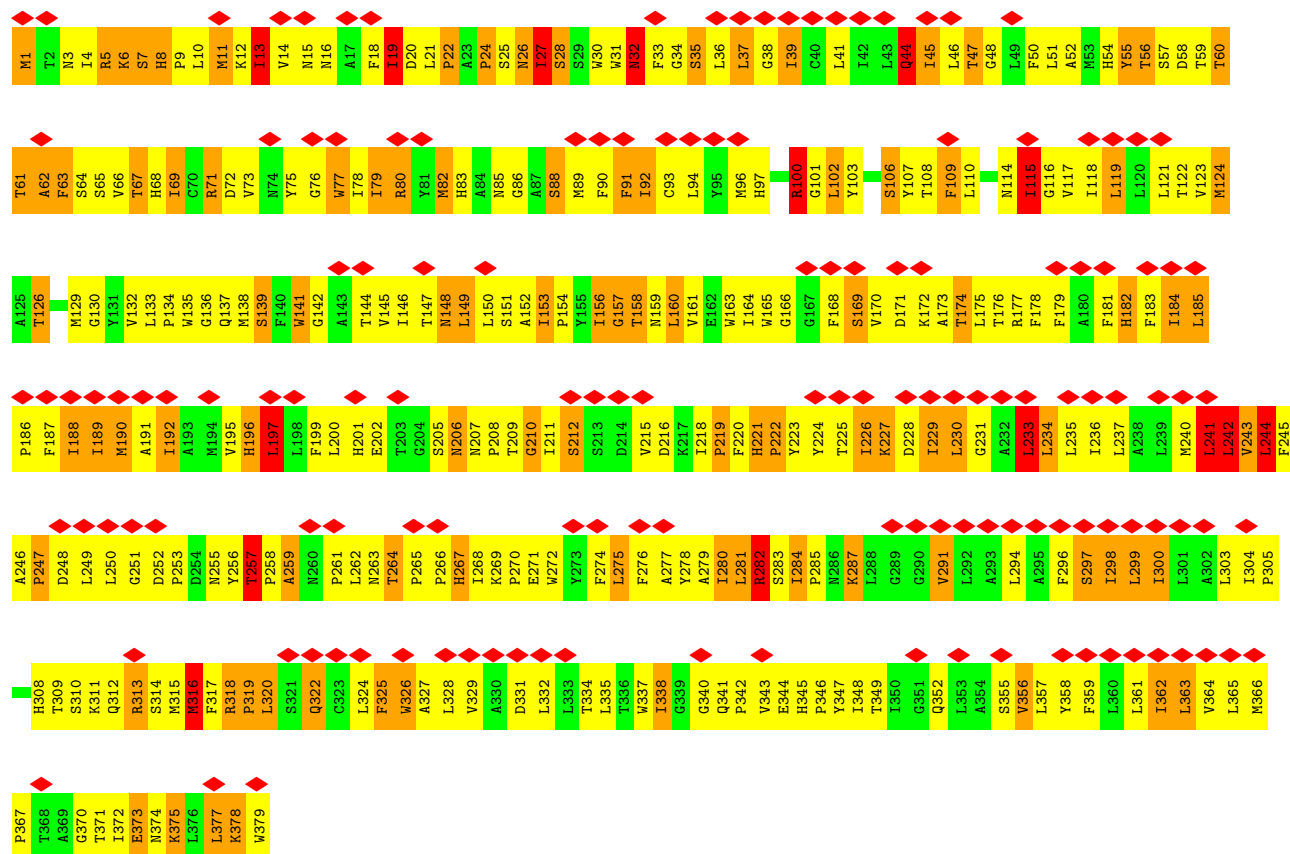
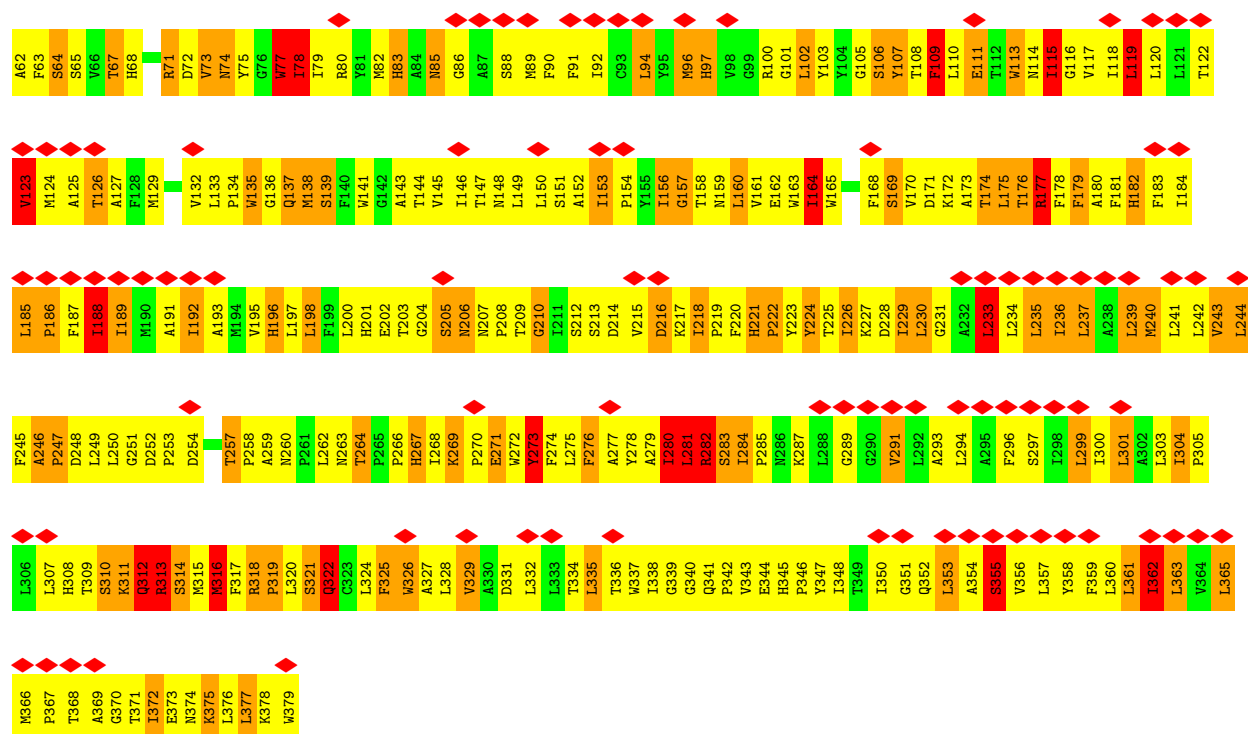


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

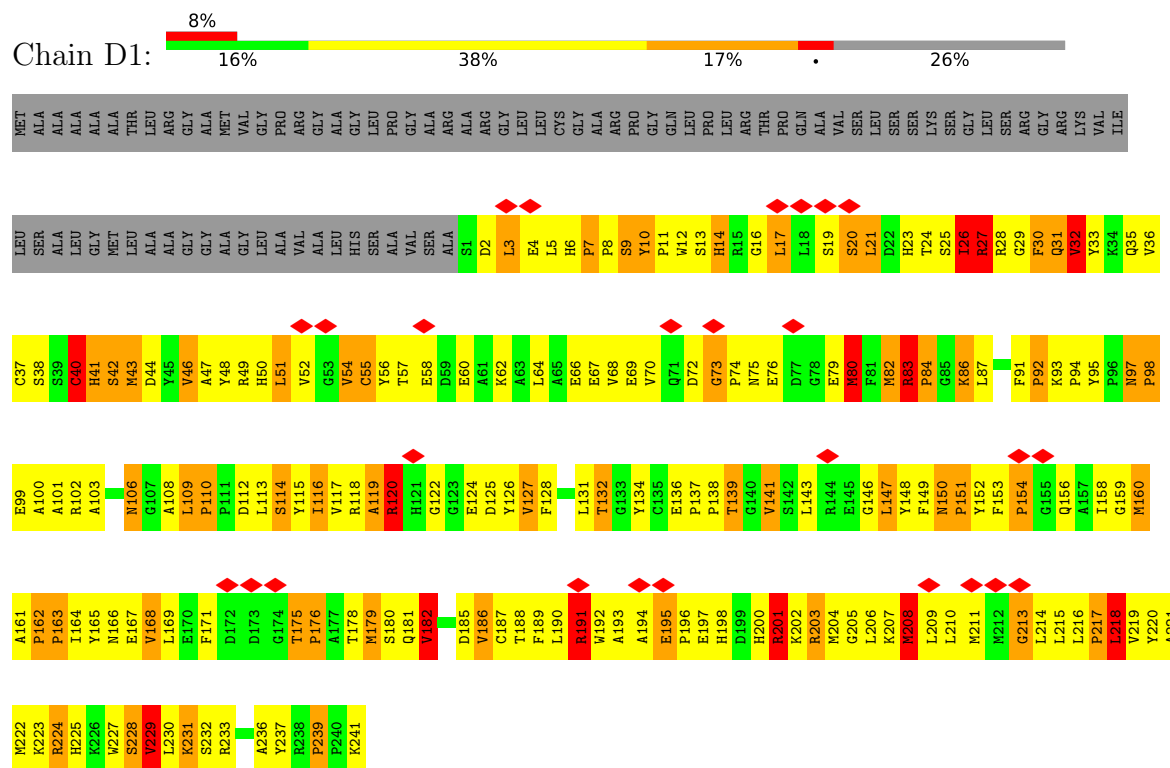


• Molecule 3: Cytochrome b





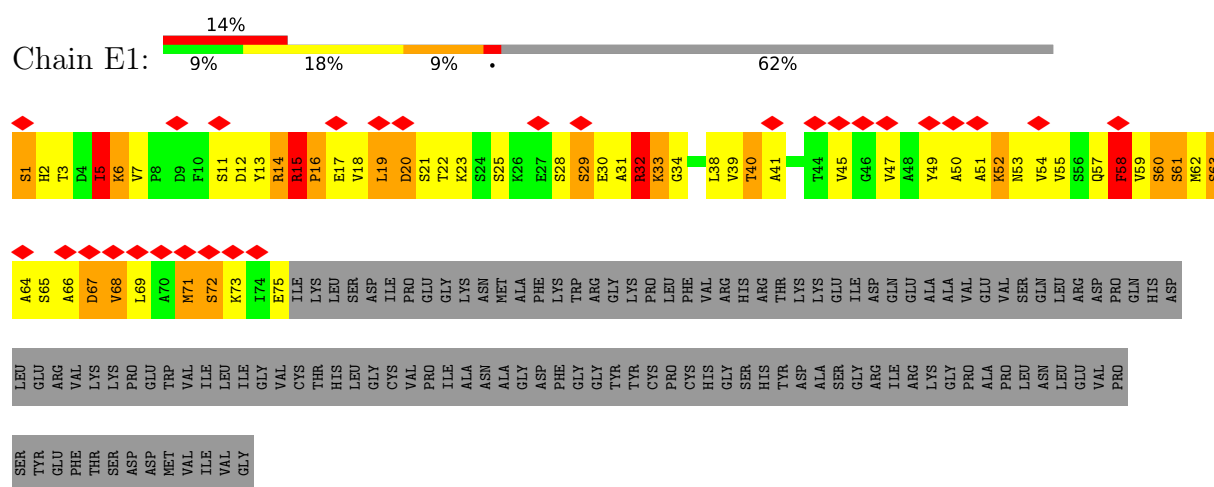
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



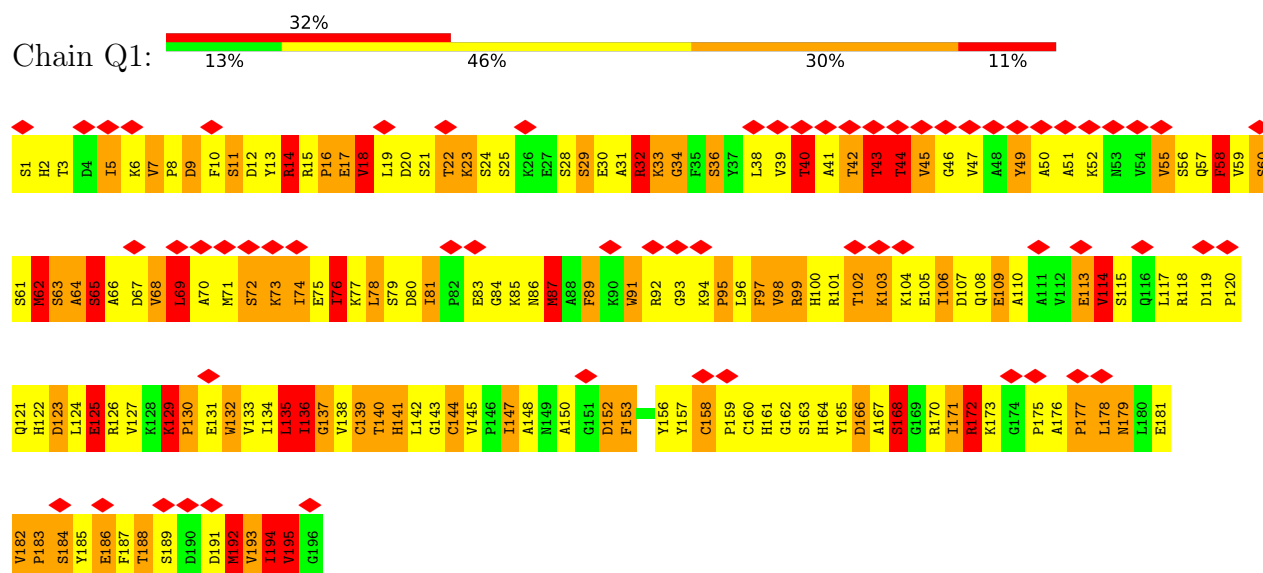
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



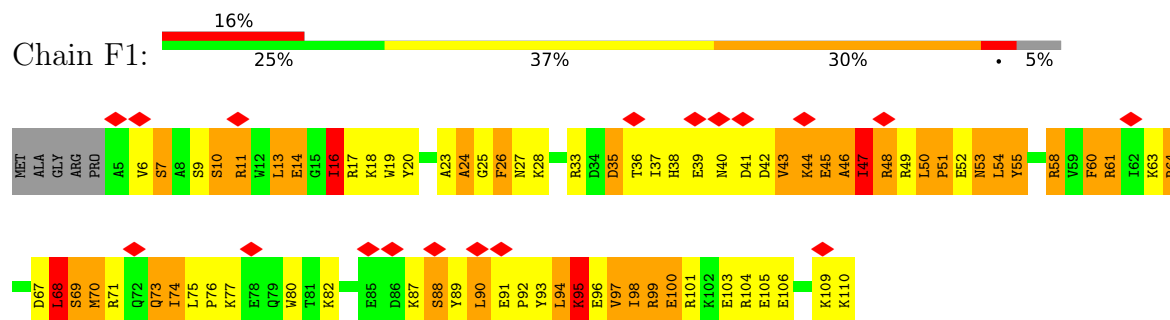
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



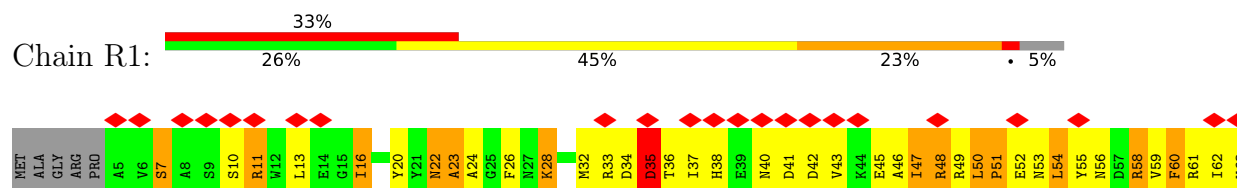
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

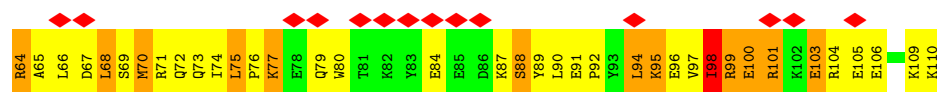


• Molecule 6: Cytochrome b-c1 complex subunit 7

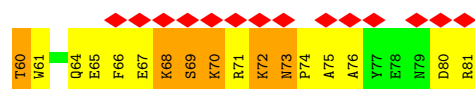
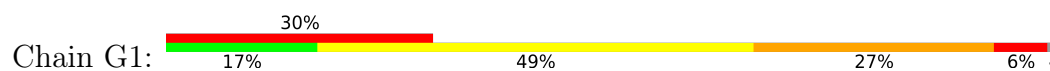


• Molecule 6: Cytochrome b-c1 complex subunit 7

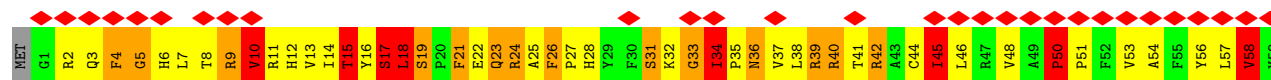
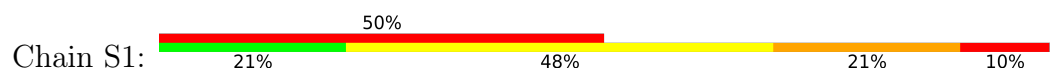




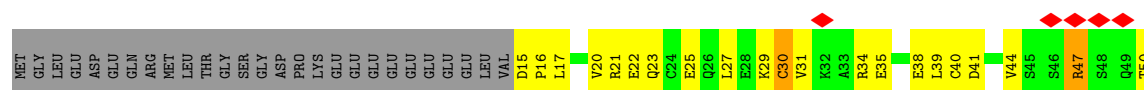
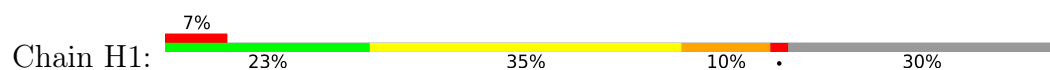
• Molecule 7: Cytochrome b-c1 complex subunit 8



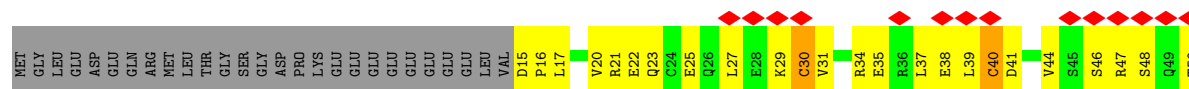
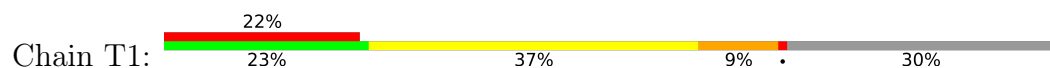
• Molecule 7: Cytochrome b-c1 complex subunit 8



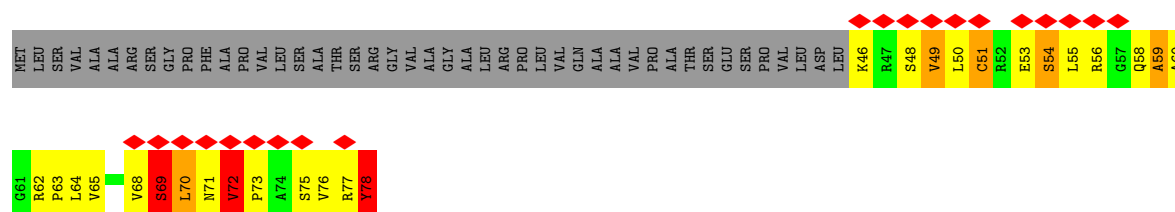
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



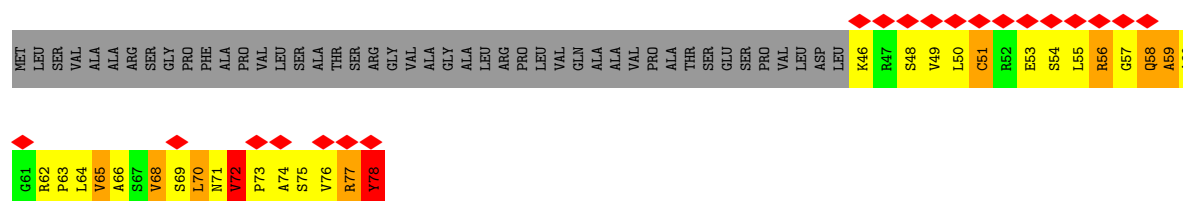
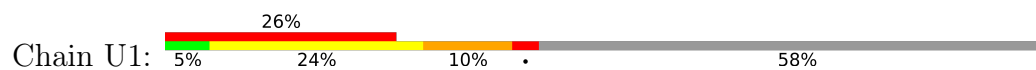
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



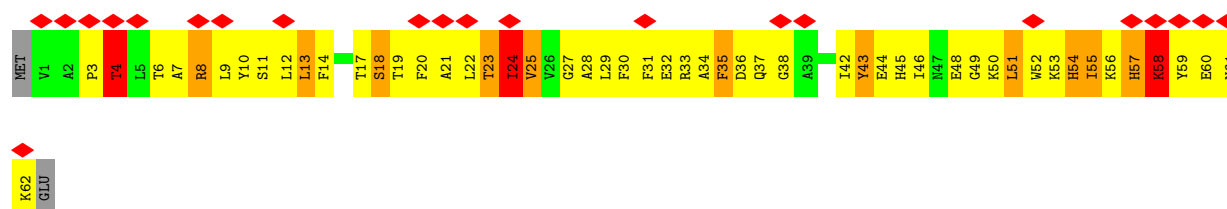
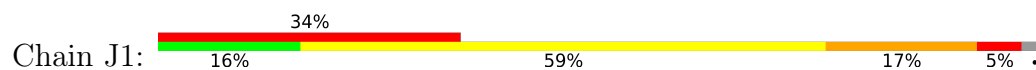
• Molecule 9: Cytochrome b-c1 complex subunit 9



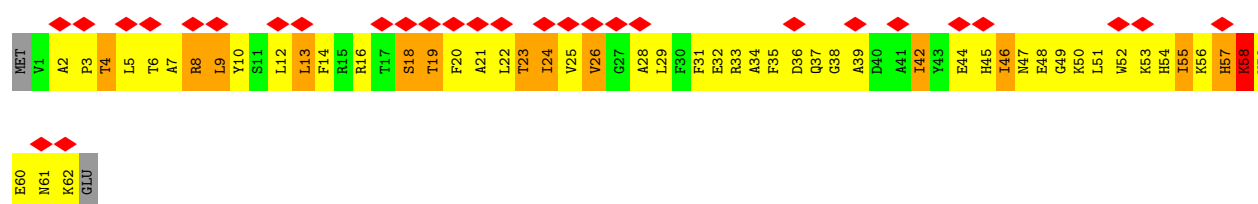
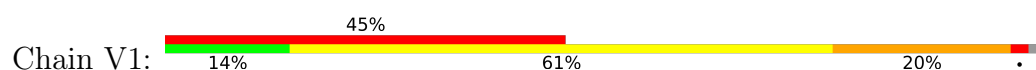
- Molecule 9: Cytochrome b-c1 complex subunit 9



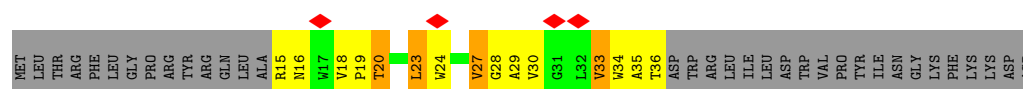
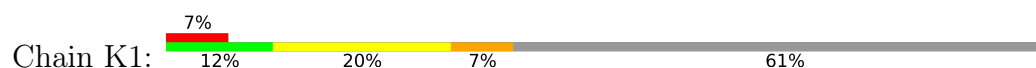
- Molecule 10: Cytochrome b-c1 complex subunit 9



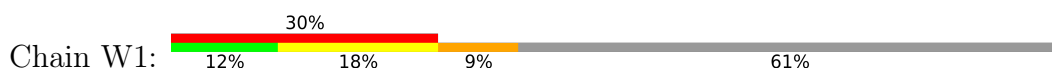
- Molecule 10: Cytochrome b-c1 complex subunit 9



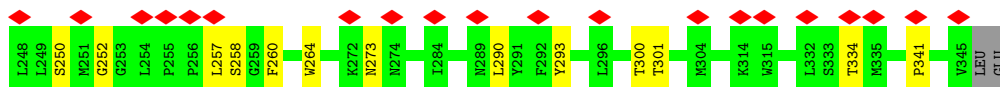
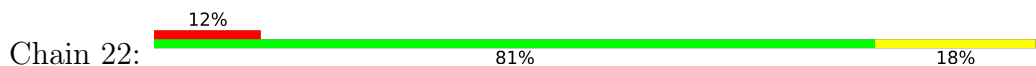
- Molecule 11: Cytochrome b-c1 complex subunit 10



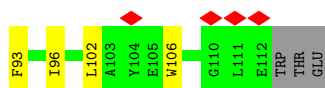
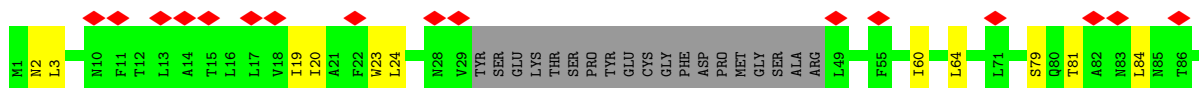
- Molecule 11: Cytochrome b-c1 complex subunit 10



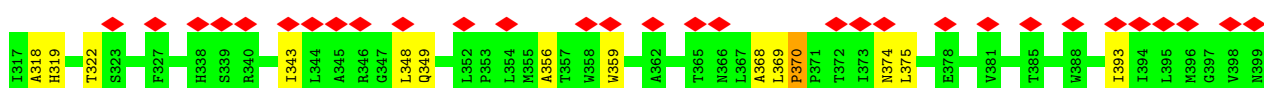
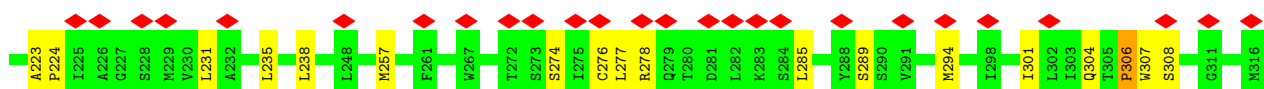
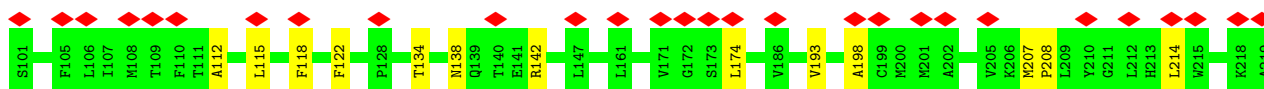
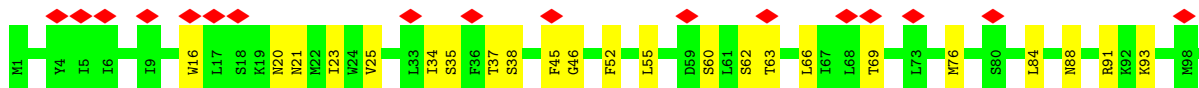
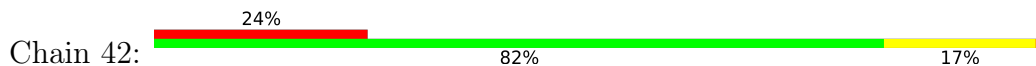
• Molecule 12: NADH-ubiquinone oxidoreductase chain 2

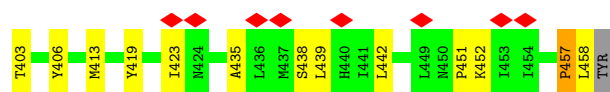


• Molecule 13: NADH-ubiquinone oxidoreductase chain 3

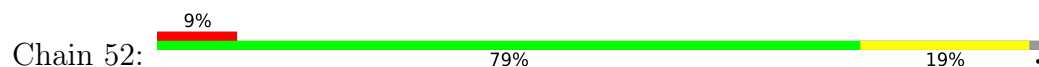


• Molecule 14: NADH-ubiquinone oxidoreductase chain 4

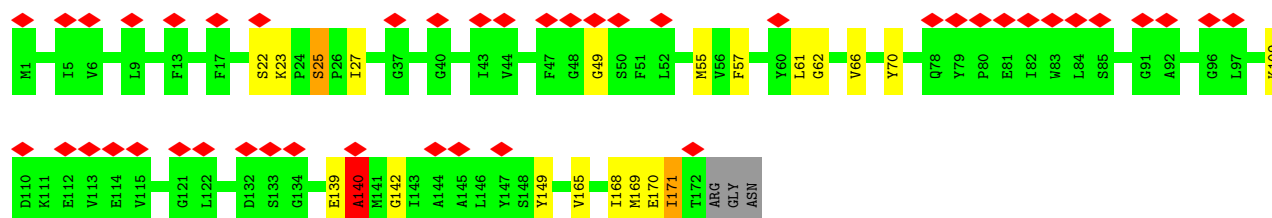
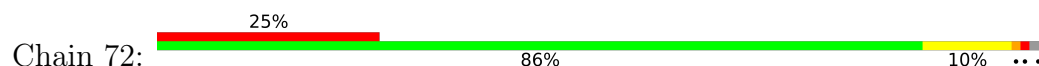




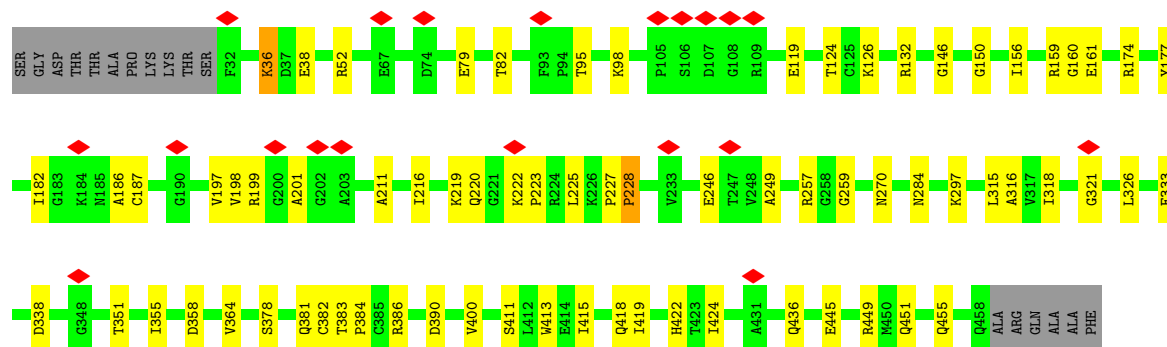
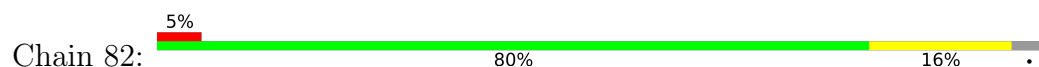
- Molecule 15: NADH-ubiquinone oxidoreductase chain 4L



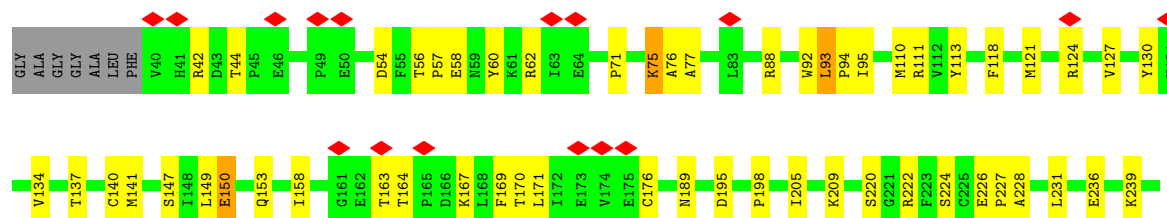
- Molecule 16: NADH-ubiquinone oxidoreductase chain 6

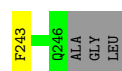


- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



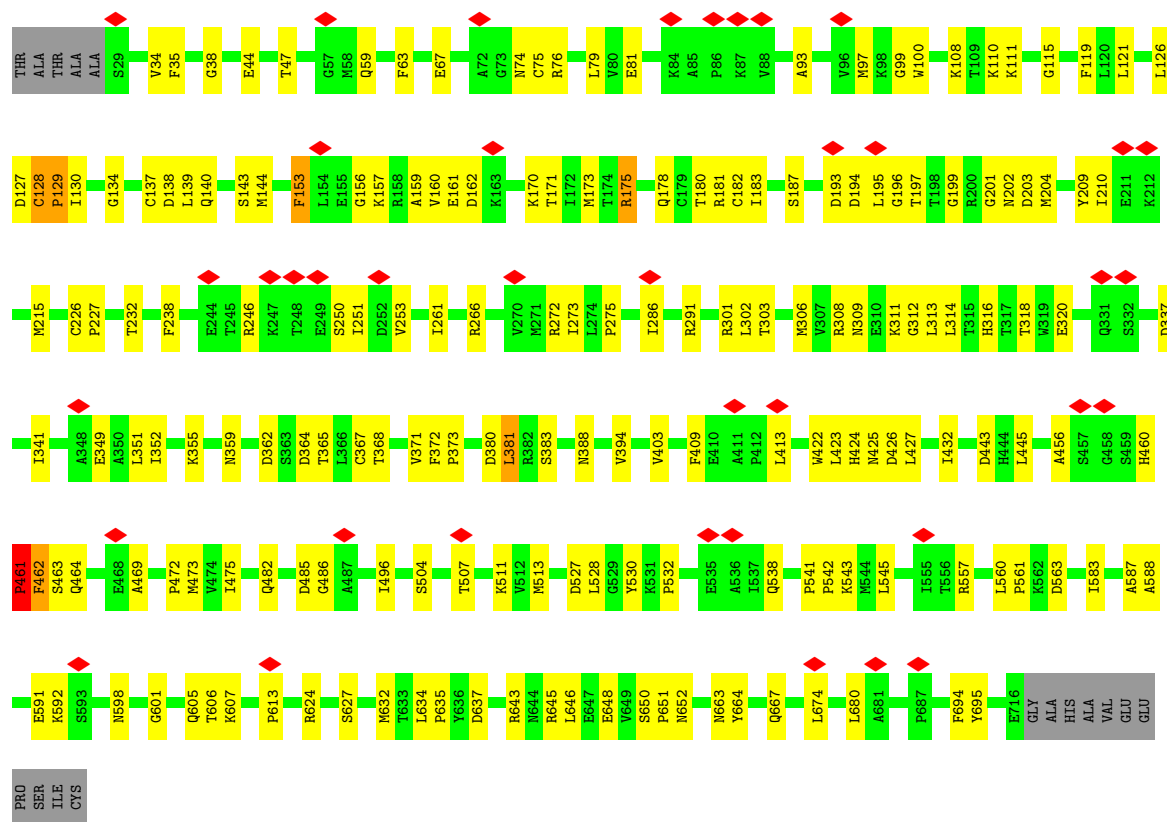
- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





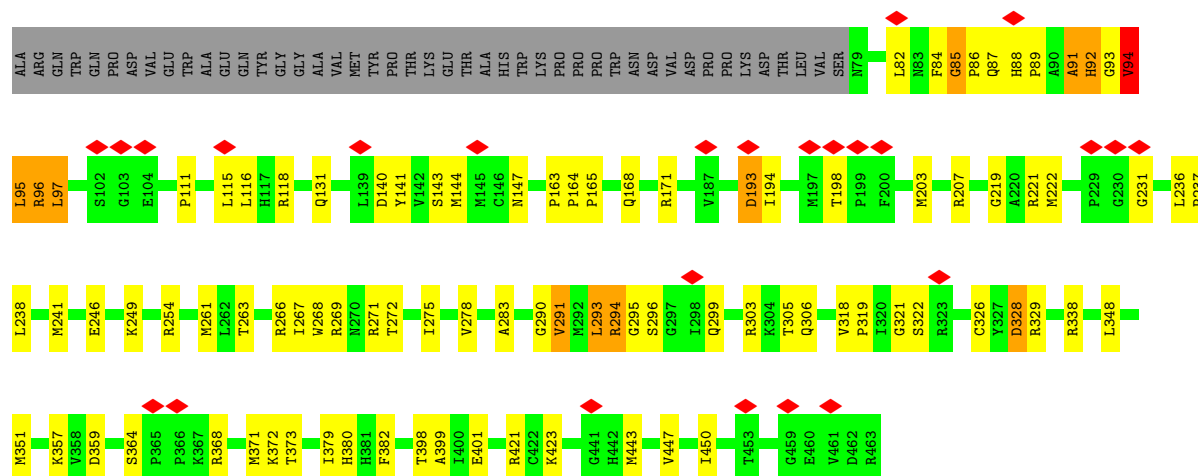
- Molecule 19: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A2: 

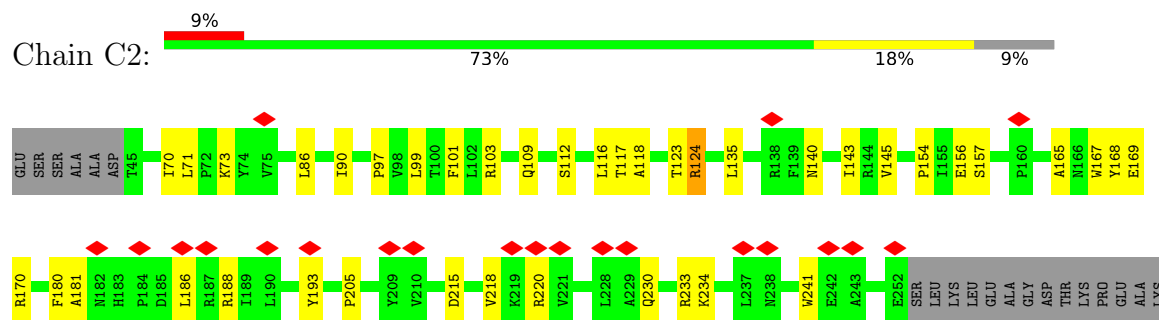


- Molecule 20: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

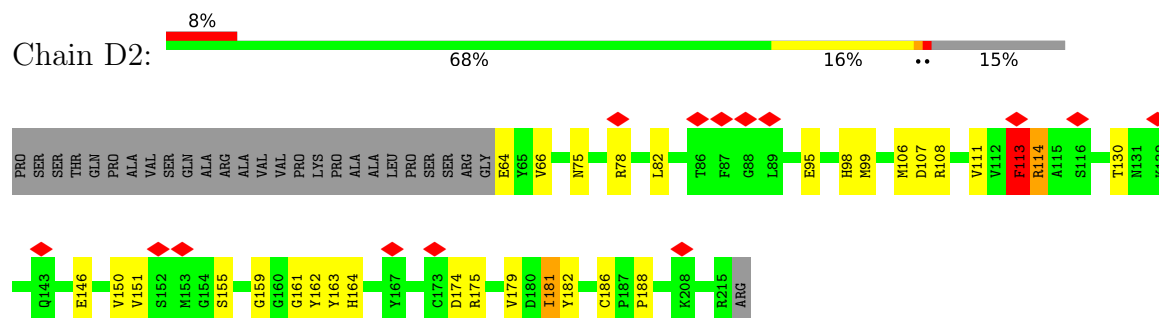
Chain B2: 



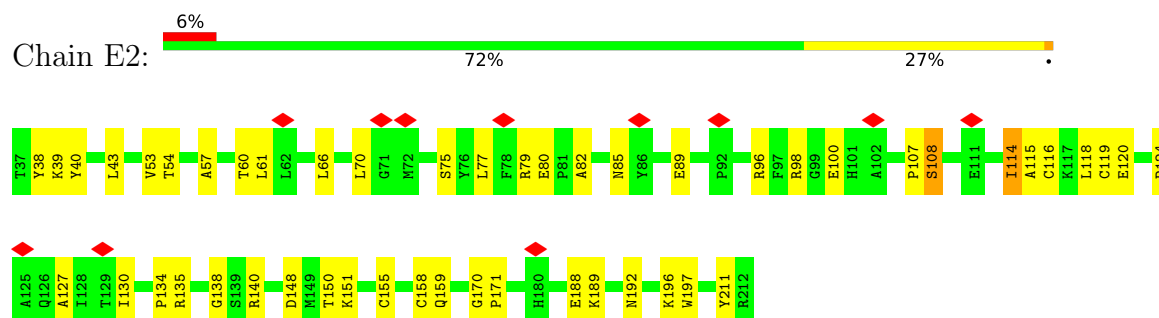
- Molecule 21: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



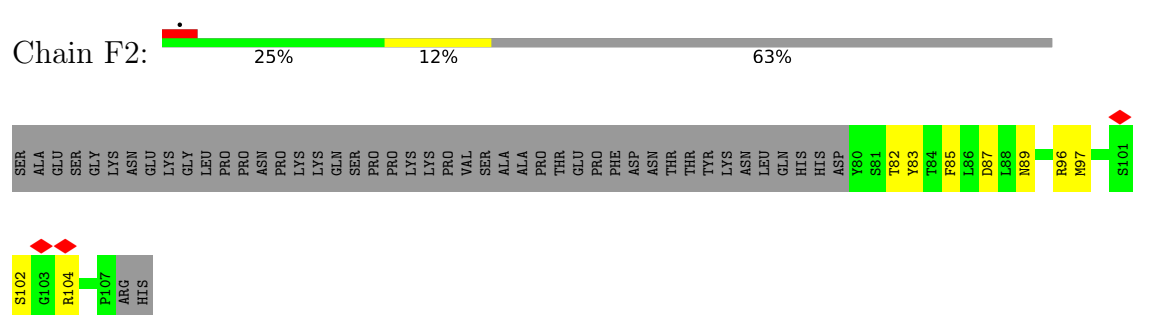
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



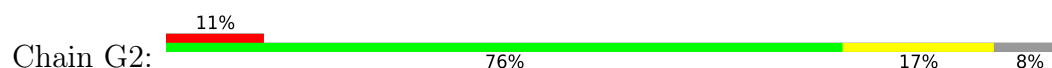
- Molecule 23: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

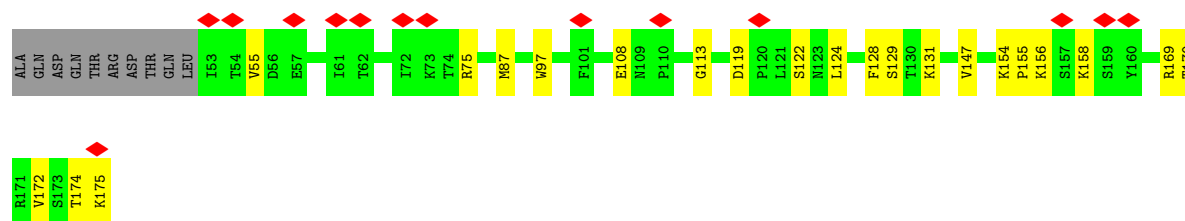


- Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

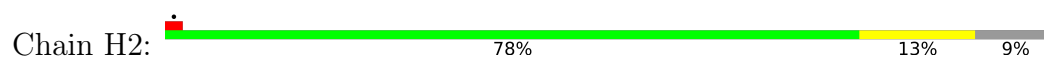


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

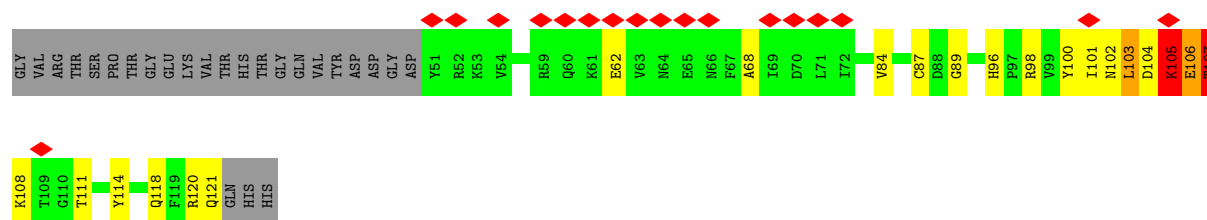




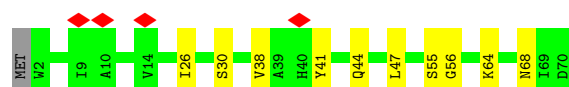
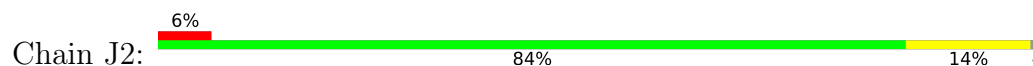
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



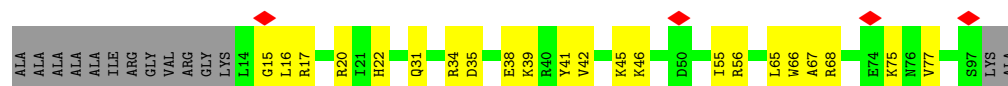
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



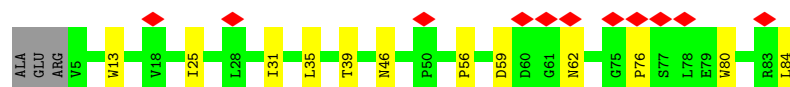
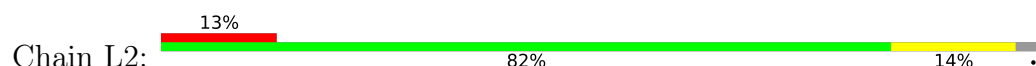
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

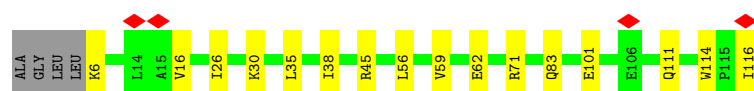


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



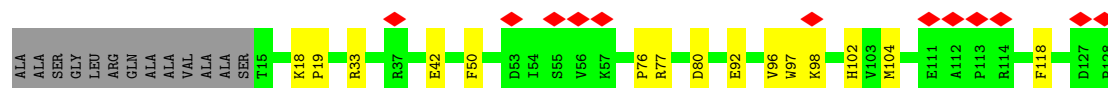
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N2:  83% 14% .



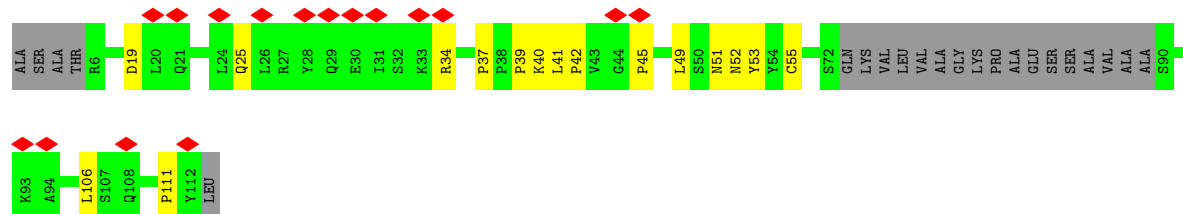
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O2:  9% 78% 12% 10%



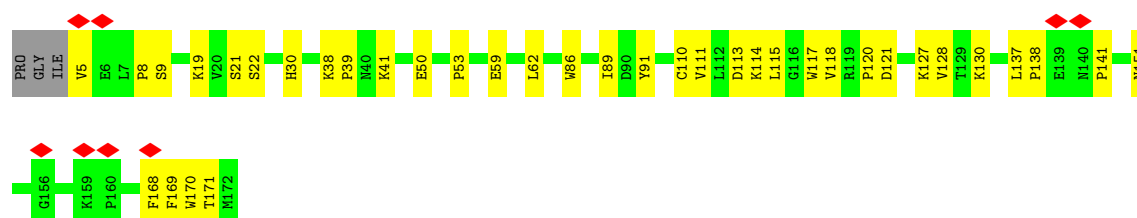
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P2:  14% 66% 14% 20%



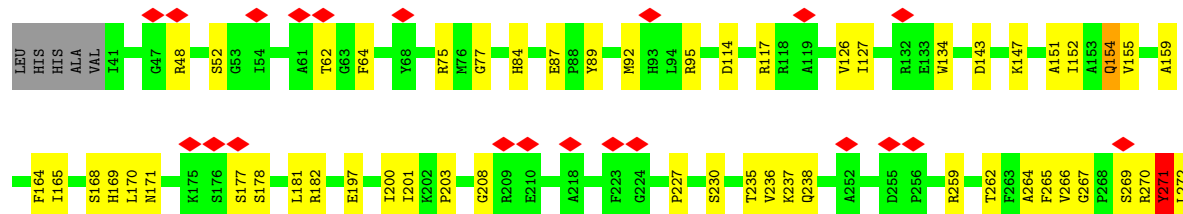
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

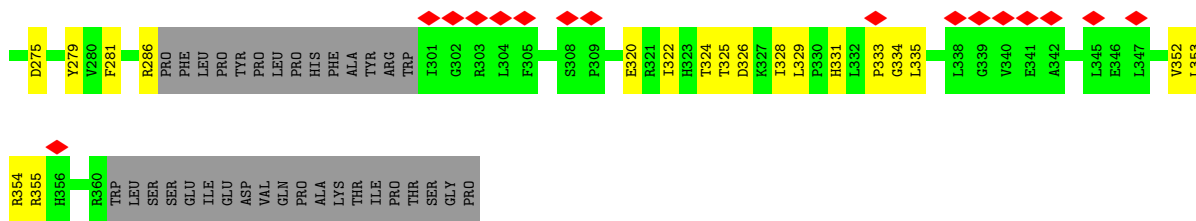
Chain Q2:  5% 77% 22% .



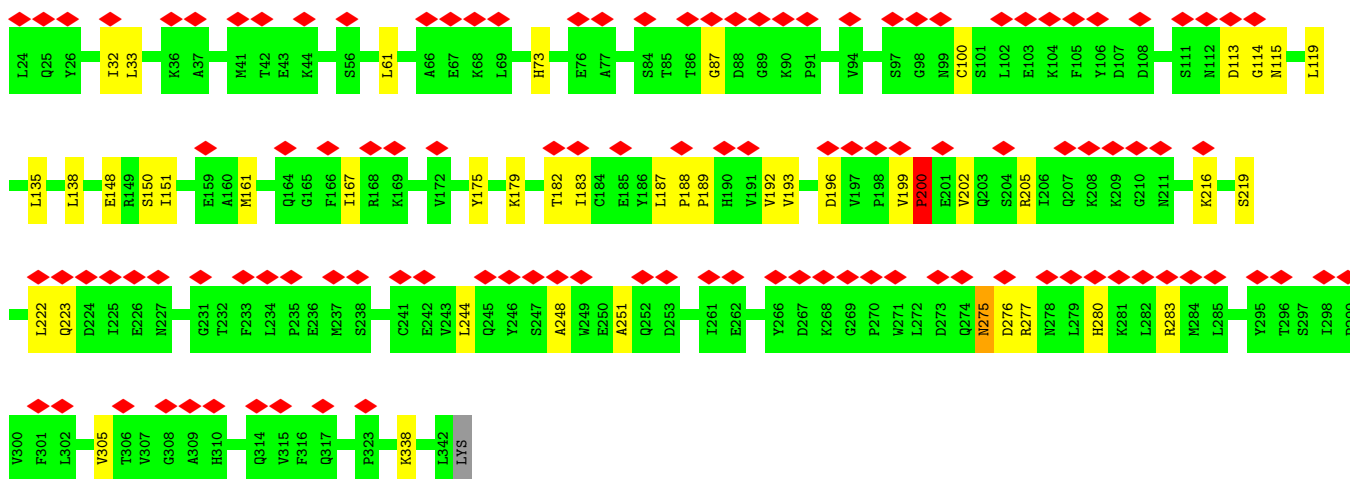
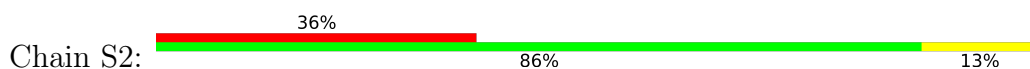
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R2:  11% 68% 21% 11%

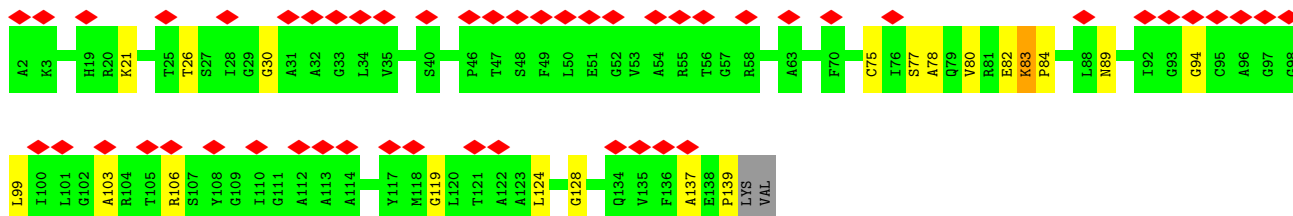
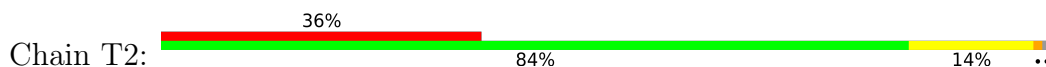




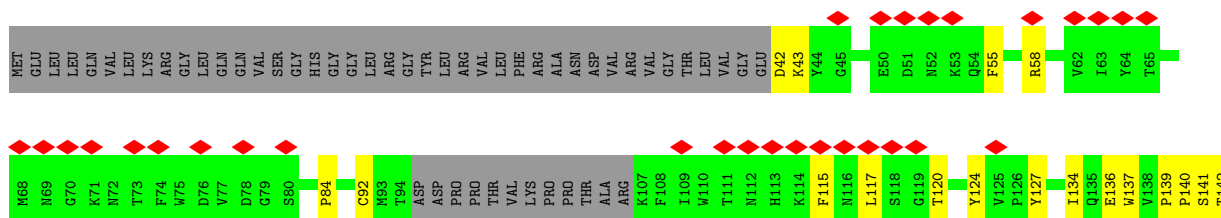
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

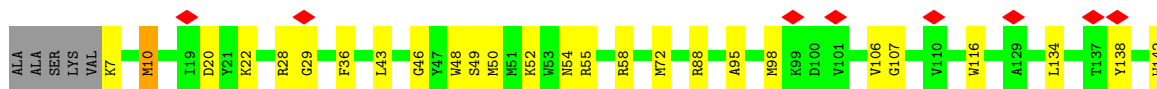
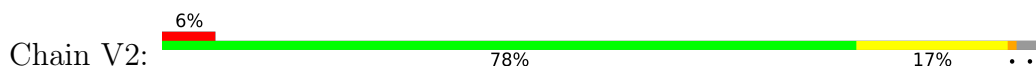


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

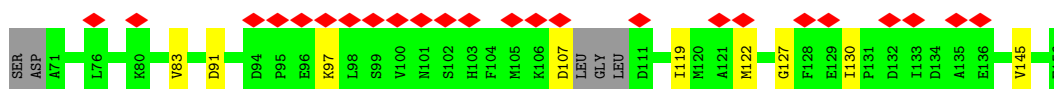
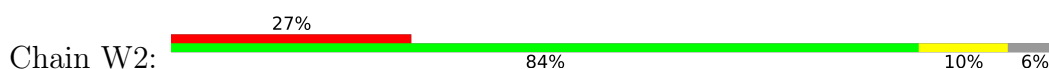




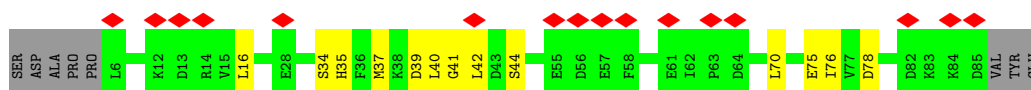
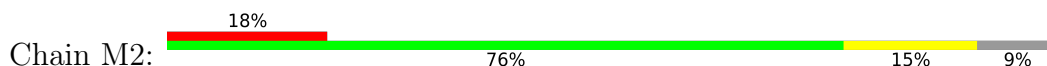
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



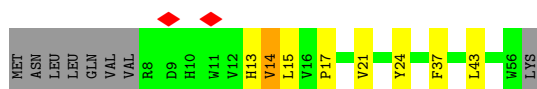
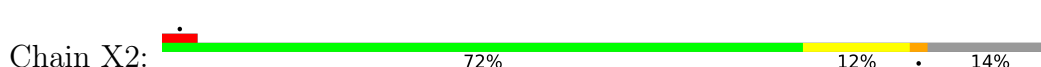
- Molecule 40: Acyl carrier protein, mitochondrial



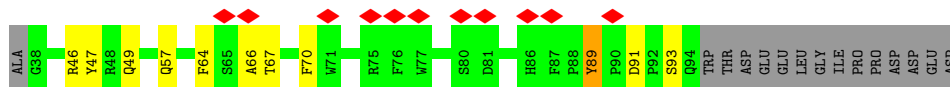
- Molecule 40: Acyl carrier protein, mitochondrial



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

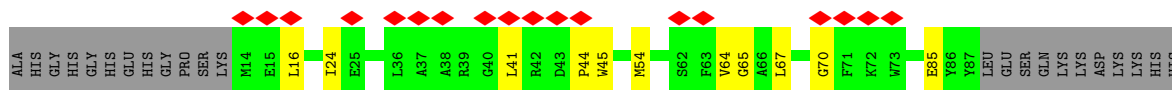


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

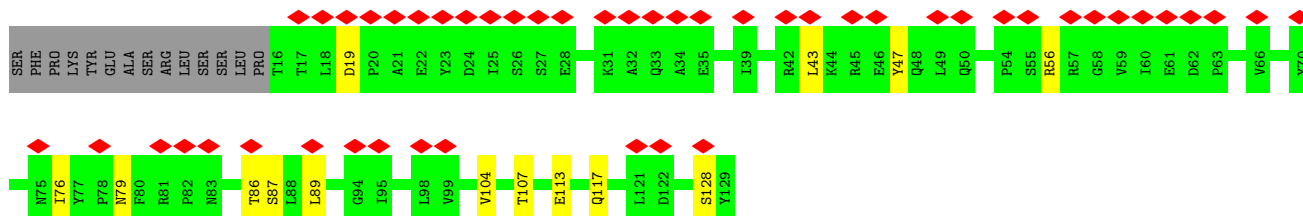
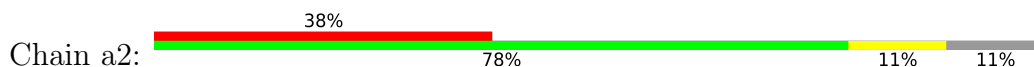


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

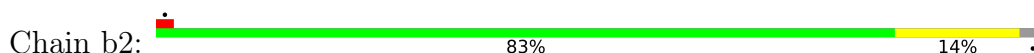




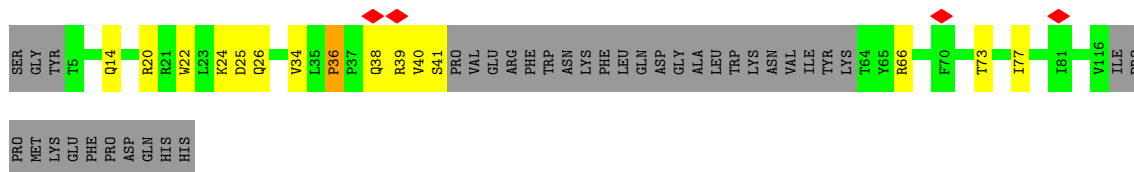
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



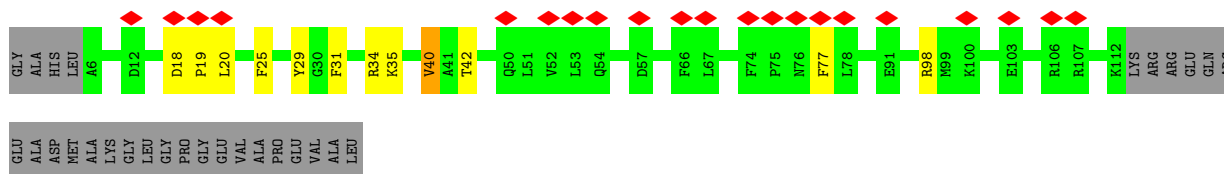
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



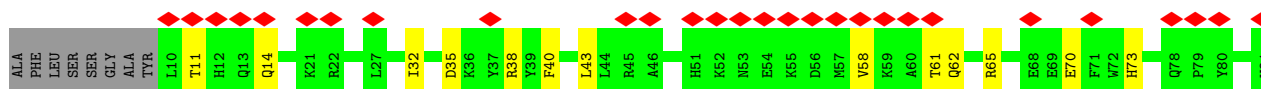
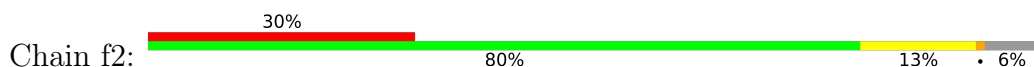
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

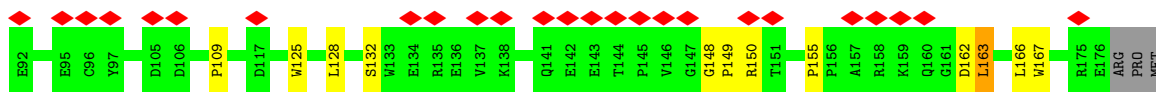


- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

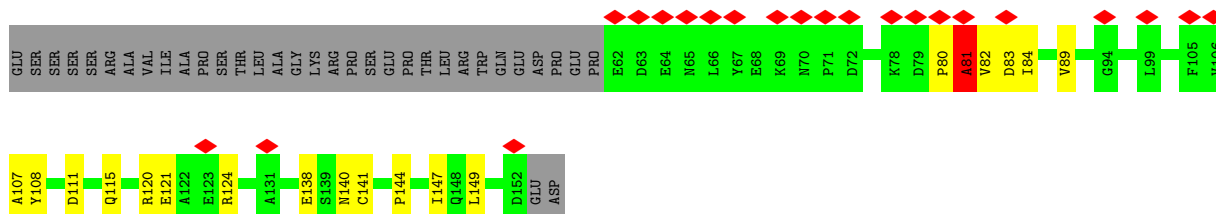


- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

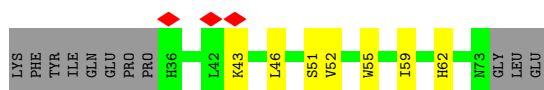




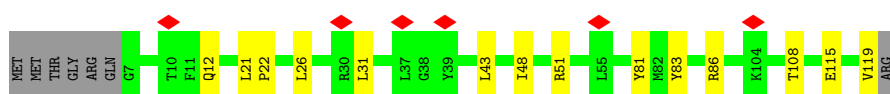
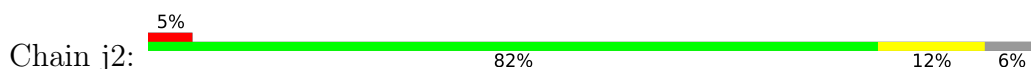
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



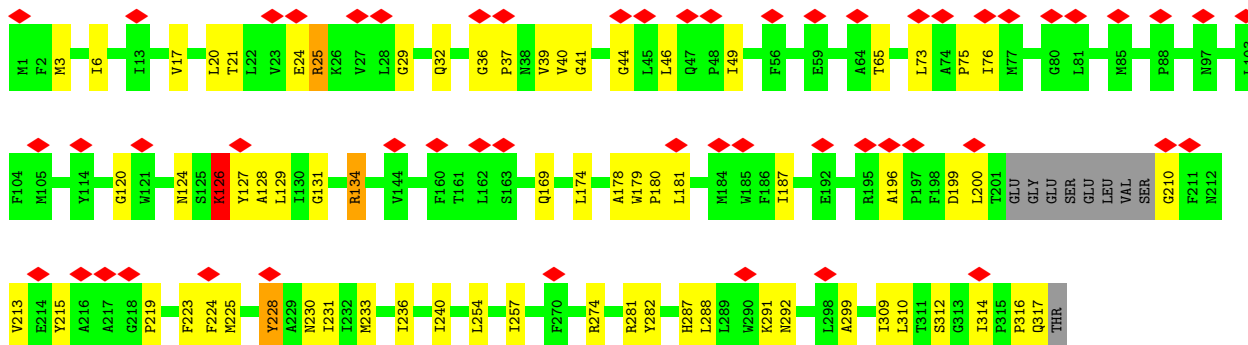
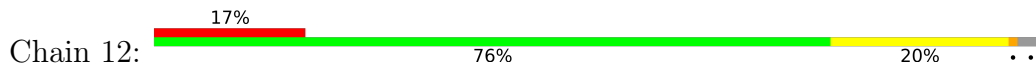
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



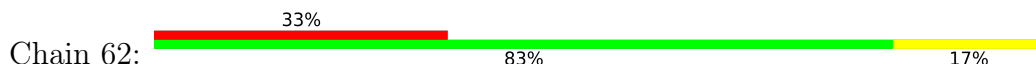
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 subunit C2

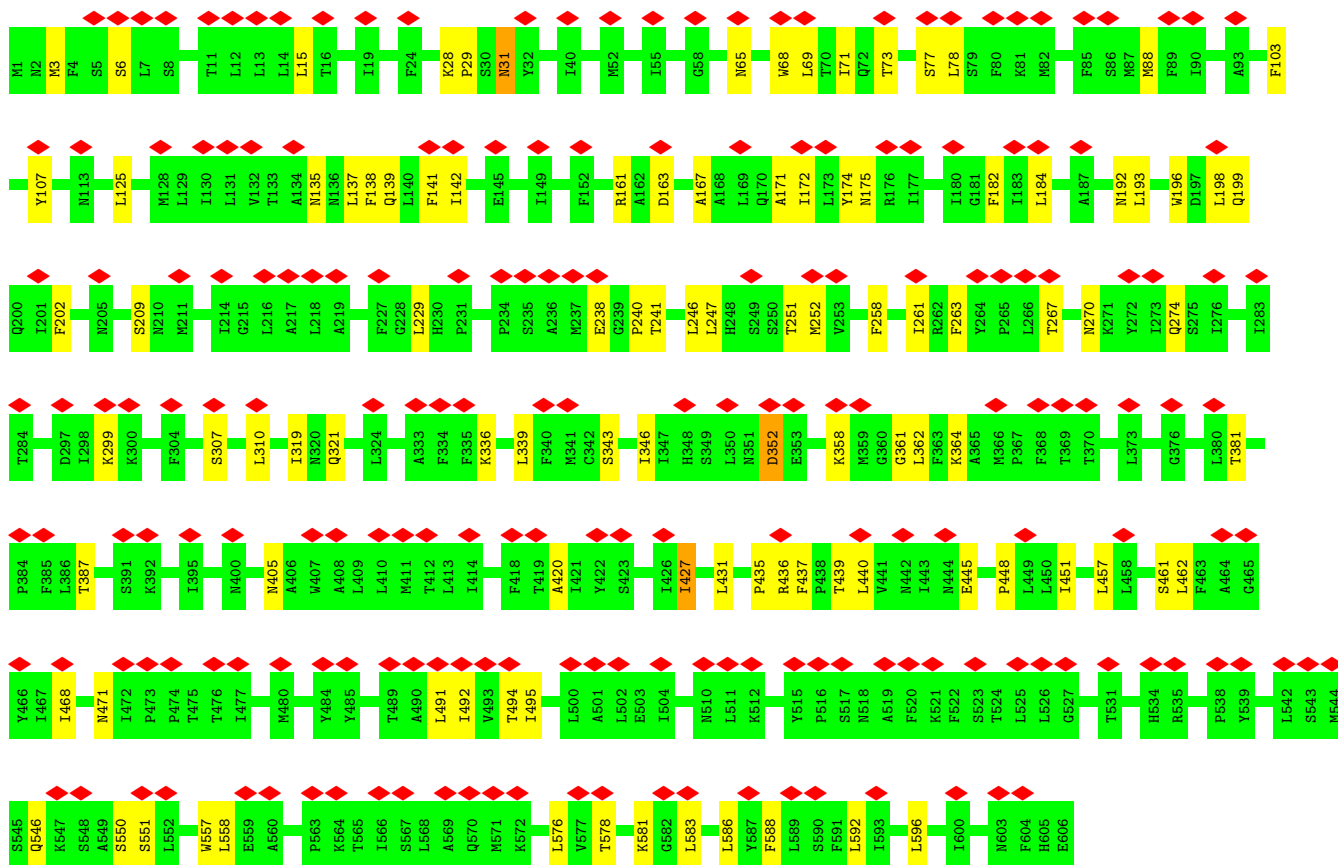


- Molecule 52: NADH-ubiquinone oxidoreductase chain 1

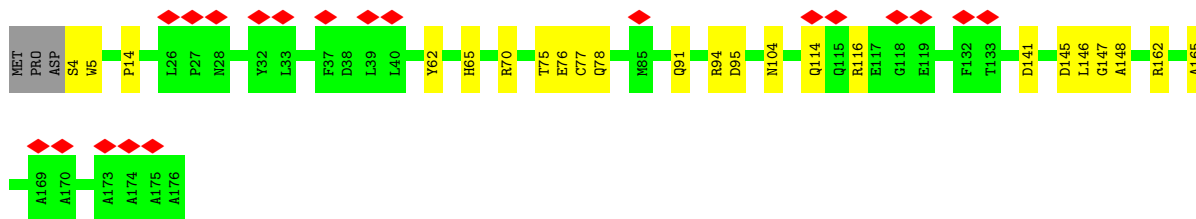
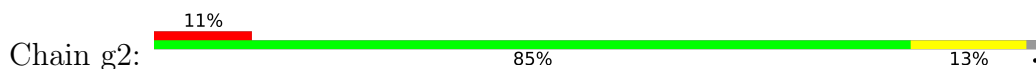


- Molecule 53: NADH-ubiquinone oxidoreductase chain 5

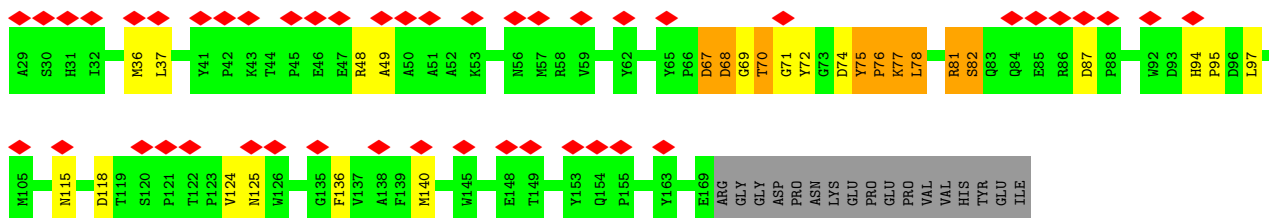
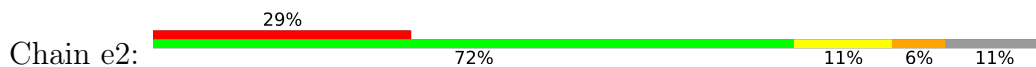




• Molecule 54: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

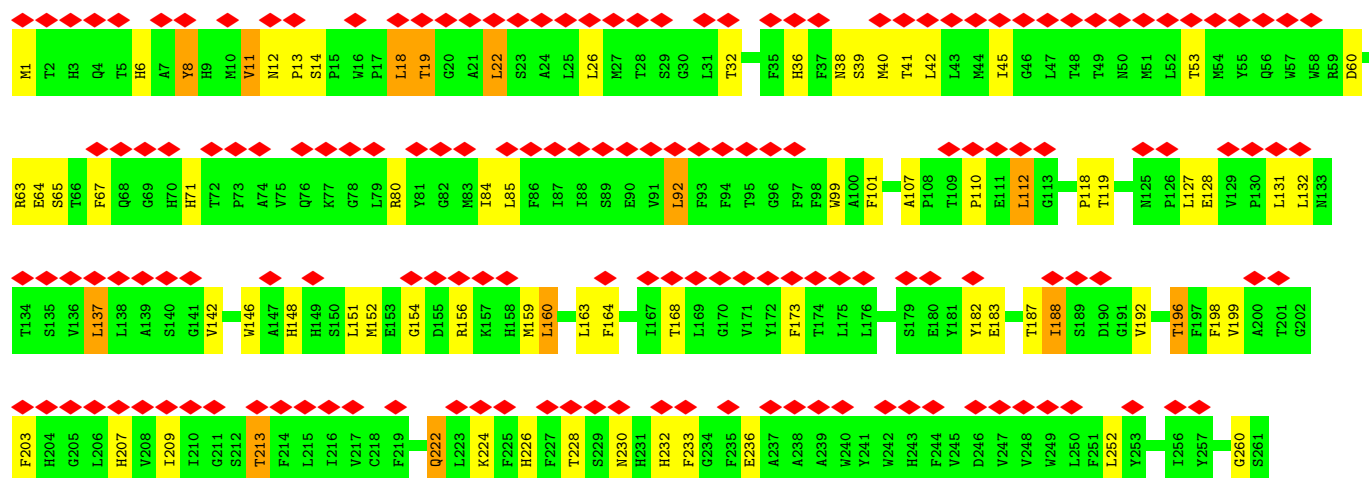


• Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



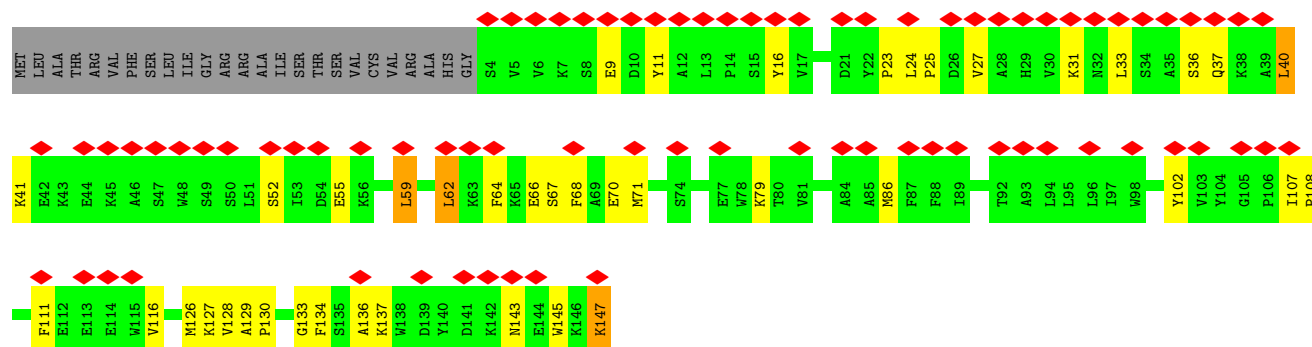
• Molecule 56: Cytochrome c oxidase subunit 1





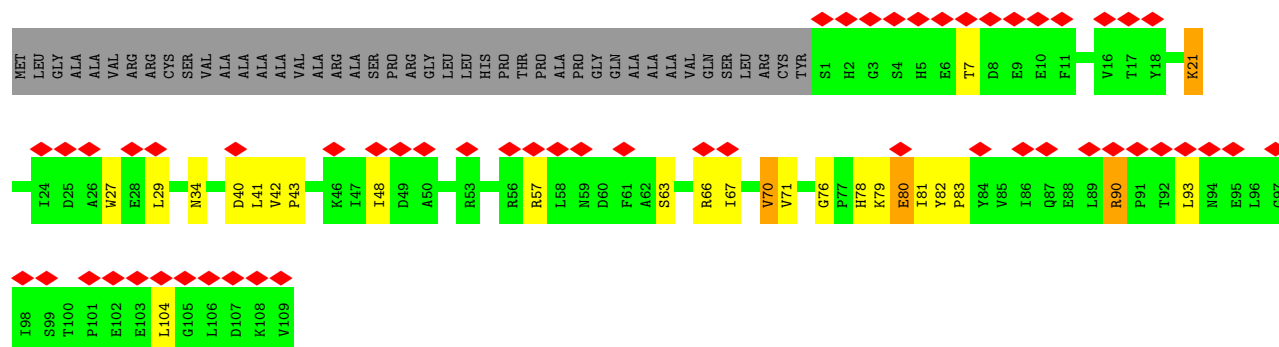
• Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D3: 46% 60% 22% 15%



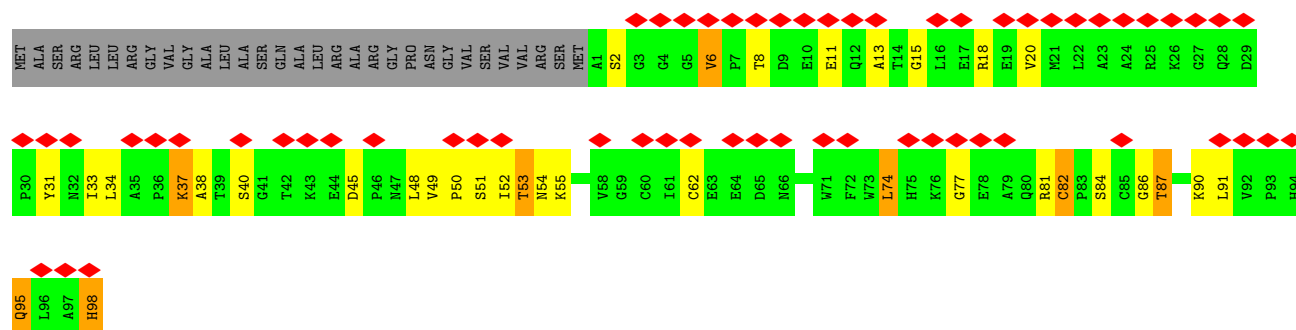
• Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E3: 36% 55% 14% 28%

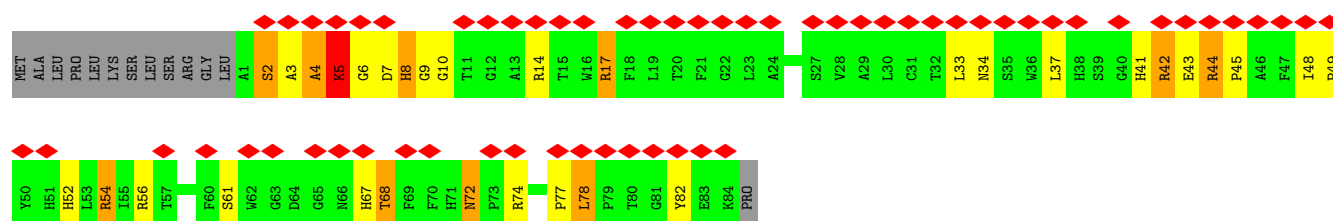


• Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial

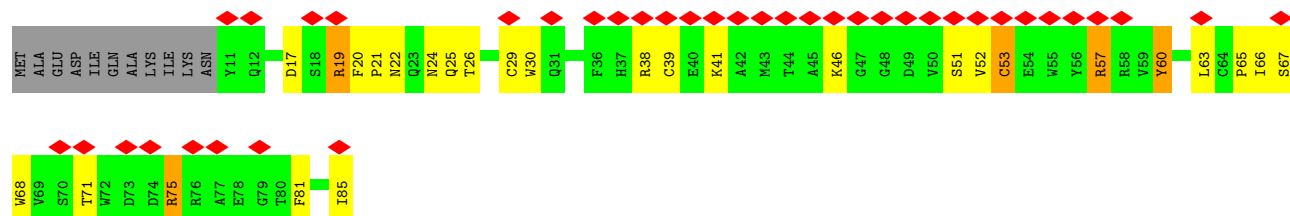
Chain F3: 47% 49% 21% 6% 24%



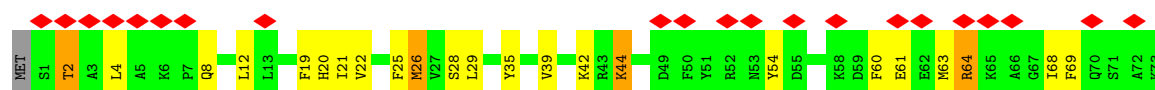
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 63: Cytochrome c oxidase subunit 6B1

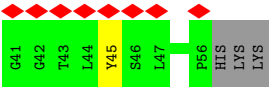


- Molecule 64: Cytochrome c oxidase subunit 6C

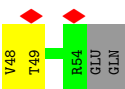
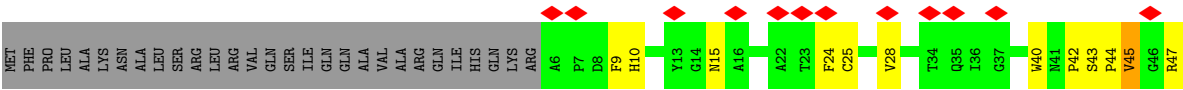


- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial

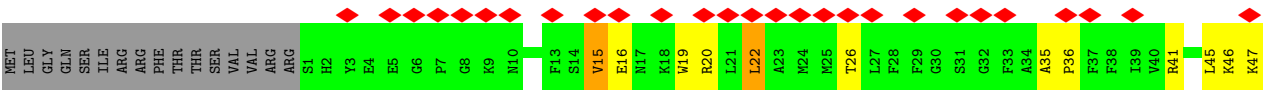
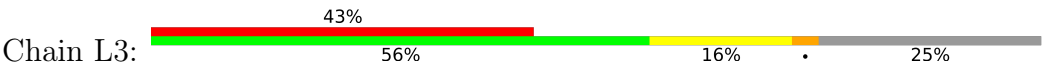




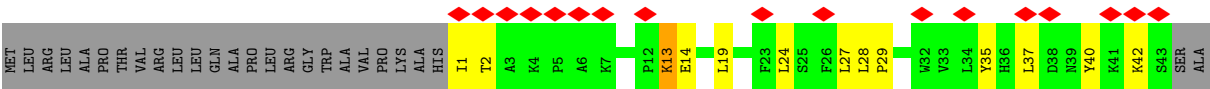
• Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.334	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, FMN, MG, SF4, PC1, FES, CU, HEC, HEA, ZN, NAP, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.78	3/3426 (0.1%)	2.03	135/4644 (2.9%)
1	M1	0.83	4/3426 (0.1%)	2.04	113/4644 (2.4%)
2	B1	0.67	2/3198 (0.1%)	1.89	85/4336 (2.0%)
2	N1	0.65	0/3198	1.81	69/4336 (1.6%)
3	C1	0.92	2/3108 (0.1%)	2.20	137/4252 (3.2%)
3	O1	0.93	6/3108 (0.2%)	2.07	110/4252 (2.6%)
4	D1	0.68	0/1978	1.88	55/2684 (2.0%)
4	P1	0.70	2/1978 (0.1%)	1.83	54/2684 (2.0%)
5	E1	0.76	0/574	2.03	15/775 (1.9%)
5	Q1	0.80	1/1551 (0.1%)	2.16	63/2097 (3.0%)
6	F1	0.74	1/935 (0.1%)	1.83	22/1253 (1.8%)
6	R1	0.73	0/935	1.94	23/1253 (1.8%)
7	G1	0.73	0/704	1.89	25/951 (2.6%)
7	S1	0.74	0/704	1.77	23/951 (2.4%)
8	H1	0.57	0/529	1.61	10/708 (1.4%)
8	T1	0.50	0/529	1.51	4/708 (0.6%)
9	I1	0.61	0/250	1.87	5/335 (1.5%)
9	U1	0.63	0/250	1.85	7/335 (2.1%)
10	J1	0.61	0/524	1.61	8/707 (1.1%)
10	V1	0.63	0/524	1.71	7/707 (1.0%)
11	K1	0.53	0/170	1.37	1/236 (0.4%)
11	W1	0.58	0/170	1.48	1/236 (0.4%)
12	22	0.35	0/2646	0.77	8/3618 (0.2%)
13	32	0.33	0/736	0.91	3/1011 (0.3%)
14	42	0.31	0/3538	0.75	4/4845 (0.1%)
15	52	0.33	0/706	0.75	0/960
16	72	0.29	0/1213	0.75	5/1659 (0.3%)
17	82	0.28	0/3035	0.73	6/4130 (0.1%)
18	92	0.27	0/1572	0.69	0/2150
19	A2	0.33	0/5269	0.71	10/7152 (0.1%)
20	B2	0.40	0/3150	0.77	3/4260 (0.1%)
21	C2	0.33	0/1756	0.69	2/2394 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	D2	0.37	0/1231	0.67	0/1669
23	E2	0.37	0/1418	0.76	3/1922 (0.2%)
24	F2	0.36	0/188	1.31	5/259 (1.9%)
25	G2	0.33	0/1004	0.78	4/1359 (0.3%)
26	H2	0.30	0/800	0.69	0/1076
27	I2	0.27	0/540	0.84	2/725 (0.3%)
28	J2	0.25	0/545	0.54	0/740
29	K2	0.27	0/663	0.67	0/896
30	L2	0.30	0/623	0.80	4/862 (0.5%)
31	N2	0.27	0/882	0.71	0/1203
32	O2	0.26	0/948	0.66	4/1279 (0.3%)
33	P2	0.29	0/719	0.79	1/981 (0.1%)
34	Q2	0.28	0/1381	0.78	2/1869 (0.1%)
35	R2	0.28	0/2392	0.78	5/3248 (0.2%)
36	S2	0.28	0/2348	0.78	6/3198 (0.2%)
37	T2	0.26	0/959	0.70	1/1305 (0.1%)
38	U2	0.29	0/765	0.82	3/1050 (0.3%)
39	V2	0.29	0/1121	0.66	0/1515
40	M2	0.24	0/651	0.79	0/876
40	W2	0.24	0/603	0.73	0/817
41	X2	0.27	0/383	0.86	2/523 (0.4%)
42	Y2	0.27	0/428	0.64	0/592
43	Z2	0.30	0/506	0.90	4/688 (0.6%)
44	a2	0.25	0/878	0.72	4/1195 (0.3%)
45	b2	0.29	0/1058	0.71	0/1434
46	c2	0.32	0/632	0.94	5/871 (0.6%)
47	d2	0.33	0/724	0.69	2/989 (0.2%)
48	f2	0.24	0/1191	0.71	2/1639 (0.1%)
49	h2	0.29	0/743	0.78	0/1013
50	i2	0.20	0/286	0.44	0/392
51	j2	0.28	0/922	0.78	5/1254 (0.4%)
52	l2	0.35	0/2513	0.78	1/3432 (0.0%)
53	62	0.25	0/4892	0.65	2/6660 (0.0%)
54	g2	0.25	0/1380	0.65	0/1872
55	e2	0.40	0/888	1.05	6/1234 (0.5%)
56	A3	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
57	B3	0.77	0/1868	1.12	10/2544 (0.4%)
58	C3	0.74	0/2211	1.01	7/3023 (0.2%)
59	D3	0.67	0/1229	0.96	3/1658 (0.2%)
60	E3	0.64	0/898	1.03	6/1218 (0.5%)
61	F3	0.72	0/765	1.13	4/1038 (0.4%)
62	G3	0.69	0/698	1.09	6/950 (0.6%)
63	H3	0.68	0/648	1.18	5/877 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
64	I3	0.71	0/611	0.94	2/810 (0.2%)
65	J3	0.70	0/451	1.04	3/610 (0.5%)
66	K3	0.75	0/398	1.01	0/546
67	L3	0.77	0/399	0.98	2/534 (0.4%)
68	M3	0.69	0/345	0.98	1/470 (0.2%)
All	All	0.55	28/107280 (0.0%)	1.27	1171/145866 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	13
1	M1	0	3
2	B1	0	9
2	N1	0	6
3	C1	0	14
3	O1	0	6
4	D1	0	5
4	P1	0	4
5	E1	0	1
5	Q1	0	9
6	F1	0	2
7	G1	0	2
7	S1	0	3
8	T1	0	1
9	I1	0	1
9	U1	0	1
10	J1	0	1
11	W1	0	1
12	22	0	2
14	42	0	3
15	52	0	1
16	72	0	3
17	82	0	1
18	92	0	3
19	A2	0	6
20	B2	0	3
22	D2	0	4
23	E2	0	2
33	P2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	Q2	0	2
35	R2	0	2
36	S2	0	1
37	T2	0	1
39	V2	0	3
40	M2	0	1
42	Y2	0	1
45	b2	0	1
48	f2	0	1
49	h2	0	2
52	l2	0	1
53	62	0	2
55	e2	0	4
All	All	0	133

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M1	253	VAL	C-O	11.17	1.36	1.24
3	O1	37	LEU	C-N	-8.10	1.24	1.33
56	A3	61	HIS	CG-CD2	7.61	1.44	1.35
56	A3	378	HIS	ND1-CE1	7.16	1.39	1.32
3	O1	221	HIS	CD2-NE2	-7.09	1.30	1.37
56	A3	378	HIS	CE1-NE2	-6.56	1.25	1.32
4	P1	202	LYS	C-O	6.45	1.31	1.24
3	O1	19	ILE	CA-C	-6.39	1.44	1.52
3	O1	44	GLN	C-N	-6.34	1.26	1.33
56	A3	69	MET	SD-CE	-6.27	1.63	1.79
1	M1	169	GLY	N-CA	-6.18	1.36	1.44
3	O1	185	LEU	CA-CB	-6.11	1.45	1.53
1	A1	153	LEU	N-CA	-6.10	1.39	1.46
3	O1	328	LEU	C-N	5.90	1.41	1.33
1	M1	340	GLY	C-O	-5.81	1.16	1.23
2	B1	148	LYS	C-N	-5.79	1.26	1.33
3	C1	97	HIS	C-O	-5.56	1.17	1.24
1	A1	373	THR	C-O	5.56	1.29	1.24
56	A3	61	HIS	ND1-CE1	5.55	1.38	1.32
5	Q1	55	VAL	C-O	-5.54	1.17	1.24
3	C1	126	THR	N-CA	-5.51	1.39	1.46
56	A3	376	HIS	ND1-CE1	5.49	1.38	1.32
6	F1	68	LEU	C-O	-5.49	1.17	1.24
56	A3	378	HIS	CG-CD2	5.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M1	333	ASP	C-O	-5.31	1.18	1.24
4	P1	228	SER	C-N	-5.22	1.27	1.33
1	A1	104	LYS	CD-CE	5.07	1.67	1.52
2	B1	173	ALA	CA-CB	-5.04	1.44	1.53

All (1171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	253	VAL	O-C-N	-23.38	98.86	123.18
1	M1	253	VAL	CA-C-O	16.98	137.42	120.27
3	C1	196	HIS	CA-CB-CG	16.18	129.98	113.80
3	O1	196	HIS	CA-CB-CG	15.64	129.44	113.80
3	O1	44	GLN	CA-C-N	15.24	139.75	120.70
3	O1	44	GLN	C-N-CA	15.24	139.75	120.70
1	M1	168	GLU	CA-C-N	14.27	144.28	121.87
1	M1	168	GLU	C-N-CA	14.27	144.28	121.87
3	C1	204	GLY	CA-C-N	14.20	142.04	121.02
3	C1	204	GLY	C-N-CA	14.20	142.04	121.02
1	M1	435	ASN	OD1-CG-ND2	13.87	136.47	122.60
1	A1	168	GLU	CA-C-O	13.48	135.33	120.10
6	R1	65	ALA	CA-C-O	12.87	134.16	120.90
55	e2	77	LYS	N-CA-C	-12.71	97.42	111.28
1	A1	419	CYS	CA-CB-SG	12.53	143.22	114.40
6	R1	77	LYS	CG-CD-CE	11.36	137.43	111.30
1	A1	251	ALA	CA-C-O	11.32	132.59	120.36
4	P1	235	LEU	CA-C-O	11.29	133.87	121.11
1	M1	307	PHE	CA-C-O	11.25	135.40	120.21
3	C1	267	HIS	CA-CB-CG	-11.03	102.77	113.80
2	B1	178	CYS	O-C-N	10.81	131.76	121.27
2	B1	177	TYR	O-C-N	10.55	135.75	123.29
8	T1	74	PHE	CA-CB-CG	-10.44	103.36	113.80
56	A3	376	HIS	ND1-CE1-NE2	10.39	118.79	108.40
3	O1	47	THR	O-C-N	-10.29	111.47	122.07
2	B1	70	ARG	NE-CZ-NH2	10.24	128.42	119.20
3	O1	267	HIS	CA-CB-CG	-10.21	103.59	113.80
1	M1	437	ILE	N-CA-C	-10.19	100.78	111.58
1	M1	334	MET	O-C-N	-10.17	110.56	122.15
1	A1	294	LEU	CA-C-N	10.14	134.69	120.29
1	A1	294	LEU	C-N-CA	10.14	134.69	120.29
5	E1	58	PHE	CA-CB-CG	10.06	123.86	113.80
7	G1	13	VAL	CA-C-O	9.95	130.84	120.39
8	H1	74	PHE	CA-CB-CG	-9.92	103.88	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I1	75	SER	N-CA-C	9.90	121.00	107.73
3	C1	196	HIS	CA-C-O	-9.87	110.64	121.00
4	P1	228	SER	CA-C-N	9.86	133.32	120.60
4	P1	228	SER	C-N-CA	9.86	133.32	120.60
55	e2	118	ASP	N-CA-C	9.61	122.42	108.86
3	O1	19	ILE	O-C-N	-9.60	110.57	122.57
1	M1	46	ARG	NE-CZ-NH2	-9.52	110.64	119.20
4	D1	14	HIS	CA-CB-CG	9.49	123.30	113.80
2	B1	245	ARG	NE-CZ-NH2	9.49	127.74	119.20
3	C1	185	LEU	O-C-N	-9.47	112.90	120.38
10	V1	26	VAL	CA-CB-CG1	9.46	126.49	110.40
10	V1	39	ALA	O-C-N	9.45	132.13	122.12
20	B2	193	ASP	N-CA-C	-9.36	101.06	111.07
1	A1	373	THR	CA-C-O	9.24	127.12	118.44
3	C1	41	LEU	N-CA-CB	9.21	123.79	110.16
1	M1	259	GLY	CA-C-N	9.18	129.74	119.92
1	M1	259	GLY	C-N-CA	9.18	129.74	119.92
2	N1	56	ARG	CD-NE-CZ	9.17	137.24	124.40
9	U1	75	SER	N-CA-C	9.07	119.88	107.73
3	C1	115	ILE	CA-C-N	-9.06	109.76	119.99
3	C1	115	ILE	C-N-CA	-9.06	109.76	119.99
2	B1	42	ALA	CA-C-N	9.04	128.68	119.82
2	B1	42	ALA	C-N-CA	9.04	128.68	119.82
5	Q1	7	VAL	CA-C-N	9.04	129.11	119.89
5	Q1	7	VAL	C-N-CA	9.04	129.11	119.89
2	B1	178	CYS	CA-C-O	-9.02	111.28	120.02
3	O1	47	THR	CA-C-O	9.02	130.29	120.82
2	B1	254	HIS	CA-CB-CG	8.98	122.78	113.80
63	H3	52	VAL	N-CA-C	8.94	121.22	108.17
3	O1	221	HIS	N-CA-CB	8.92	118.86	110.39
5	Q1	166	ASP	CA-CB-CG	8.91	121.51	112.60
4	D1	195	GLU	CA-C-N	8.83	129.72	119.47
4	D1	195	GLU	C-N-CA	8.83	129.72	119.47
48	f2	163	LEU	CA-C-N	8.82	148.18	127.00
48	f2	163	LEU	C-N-CA	8.82	148.18	127.00
13	32	3	LEU	CA-C-N	8.82	137.57	121.70
13	32	3	LEU	C-N-CA	8.82	137.57	121.70
63	H3	81	PHE	CA-C-N	8.77	128.42	119.56
63	H3	81	PHE	C-N-CA	8.77	128.42	119.56
4	D1	206	LEU	CB-CA-C	-8.77	96.29	110.84
3	C1	206	ASN	OD1-CG-ND2	8.74	131.34	122.60
1	A1	256	ALA	N-CA-C	8.71	123.26	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V1	14	PHE	CA-CB-CG	8.68	122.48	113.80
1	A1	341	GLN	O-C-N	8.64	131.43	122.09
1	M1	320	LEU	CA-C-O	8.63	130.02	120.70
3	C1	196	HIS	O-C-N	8.63	131.01	122.03
3	C1	43	LEU	O-C-N	-8.61	112.80	122.09
5	Q1	47	VAL	CA-C-O	8.59	129.99	121.05
3	C1	175	LEU	N-CA-CB	8.53	123.44	110.30
5	Q1	192	MET	CA-C-O	8.52	129.27	120.24
2	B1	85	ILE	CB-CA-C	-8.44	101.07	111.88
2	B1	92	VAL	O-C-N	-8.44	114.48	122.16
1	A1	434	TYR	CA-C-O	-8.42	111.53	120.63
5	Q1	183	PRO	CA-C-O	-8.42	110.19	122.31
3	C1	182	HIS	CA-CB-CG	8.40	122.20	113.80
1	A1	292	SER	CA-C-O	8.39	125.53	119.32
6	F1	60	PHE	CA-CB-CG	-8.37	105.43	113.80
3	C1	246	ALA	N-CA-CB	-8.32	101.30	110.71
3	O1	242	LEU	CB-CA-C	-8.28	98.12	110.95
7	G1	13	VAL	O-C-N	-8.27	114.32	123.26
2	B1	369	LEU	CA-C-O	8.25	129.19	120.70
3	O1	182	HIS	CA-CB-CG	8.22	122.02	113.80
6	F1	43	VAL	CA-C-O	8.22	131.05	120.78
2	B1	148	LYS	CA-C-N	8.21	131.11	120.44
2	B1	148	LYS	C-N-CA	8.21	131.11	120.44
3	O1	322	GLN	OE1-CD-NE2	8.21	130.81	122.60
5	Q1	58	PHE	CA-CB-CG	8.18	121.98	113.80
6	F1	64	ARG	CD-NE-CZ	-8.14	113.01	124.40
6	R1	63	LYS	CB-CA-C	8.14	123.66	110.88
5	E1	60	SER	N-CA-C	-8.13	103.36	113.28
67	L3	20	ARG	N-CA-C	-8.12	102.51	111.36
3	C1	216	ASP	CA-CB-CG	8.12	120.72	112.60
1	M1	419	CYS	CA-C-N	8.10	128.15	119.89
1	M1	419	CYS	C-N-CA	8.10	128.15	119.89
56	A3	82	LEU	N-CA-C	8.03	122.35	112.23
6	F1	27	ASN	CA-C-O	8.02	129.49	120.90
1	A1	294	LEU	O-C-N	-8.02	113.62	122.12
2	N1	141	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	A1	341	GLN	CA-C-O	-7.99	112.47	120.70
3	C1	43	LEU	CA-C-O	7.99	128.93	120.70
1	M1	323	HIS	CA-CB-CG	7.99	121.79	113.80
5	Q1	55	VAL	CA-CB-CG1	7.98	123.97	110.40
3	C1	13	ILE	CB-CA-C	-7.96	101.39	112.14
56	A3	378	HIS	ND1-CE1-NE2	7.96	116.36	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P1	202	LYS	CA-C-O	-7.95	112.47	120.82
2	N1	162	ASN	CA-CB-CG	-7.95	104.65	112.60
1	A1	431	LEU	CA-C-N	7.95	129.77	119.84
1	A1	431	LEU	C-N-CA	7.95	129.77	119.84
2	B1	320	GLY	O-C-N	-7.93	117.84	123.95
1	A1	168	GLU	O-C-N	-7.90	112.97	122.22
5	Q1	183	PRO	O-C-N	7.87	132.16	122.71
5	Q1	135	LEU	O-C-N	-7.85	113.58	123.24
3	O1	257	THR	N-CA-CB	7.85	121.47	110.01
4	D1	97	ASN	CA-C-N	7.85	129.65	119.84
4	D1	97	ASN	C-N-CA	7.85	129.65	119.84
4	P1	7	PRO	N-CA-C	7.83	120.26	110.70
5	Q1	7	VAL	O-C-N	7.83	130.02	121.10
3	C1	30	TRP	CA-C-O	7.82	129.07	120.63
2	N1	412	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	M1	325	VAL	O-C-N	-7.81	114.36	123.03
4	D1	120	ARG	NE-CZ-NH2	-7.80	112.18	119.20
3	C1	33	PHE	CG-CD2-CE2	7.75	133.88	120.70
56	A3	56	VAL	N-CA-C	-7.74	103.25	110.53
3	C1	321	SER	CA-C-N	7.72	131.40	120.28
3	C1	321	SER	C-N-CA	7.72	131.40	120.28
1	A1	438	ARG	NE-CZ-NH2	7.72	126.15	119.20
3	O1	82	MET	CA-C-O	7.70	128.59	120.42
3	C1	303	LEU	N-CA-CB	7.68	121.52	110.16
3	C1	195	VAL	CA-C-O	-7.67	112.97	120.95
5	Q1	168	SER	N-CA-C	-7.67	103.93	113.28
7	S1	15	THR	CA-CB-CG2	-7.67	97.47	110.50
56	A3	435	GLY	N-CA-C	7.66	126.08	115.27
2	B1	179	PRO	N-CA-CB	7.65	110.46	103.34
1	M1	392	LEU	N-CA-C	7.64	120.28	111.11
3	C1	185	LEU	CA-C-O	7.63	126.33	119.08
2	N1	145	ARG	O-C-N	7.63	129.93	122.07
5	Q1	56	SER	CA-C-O	7.62	128.82	120.82
1	M1	420	PRO	N-CA-CB	7.62	109.72	103.32
3	C1	123	VAL	CA-C-O	7.59	129.22	120.03
10	V1	39	ALA	CA-C-O	-7.59	112.50	120.55
1	A1	242	CYS	CA-C-O	7.59	128.71	120.43
3	O1	149	LEU	CA-C-O	7.58	128.91	119.05
3	C1	85	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A1	441	MET	CA-CB-CG	-7.55	99.01	114.10
2	B1	56	ARG	CD-NE-CZ	7.54	134.96	124.40
1	A1	323	HIS	CA-CB-CG	7.53	121.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C1	273	TYR	CA-C-N	-7.52	110.31	122.26
3	C1	273	TYR	C-N-CA	-7.52	110.31	122.26
3	O1	242	LEU	N-CA-CB	7.51	120.88	109.98
41	X2	43	LEU	CA-C-N	7.51	135.22	121.70
41	X2	43	LEU	C-N-CA	7.51	135.22	121.70
1	M1	434	TYR	O-C-N	-7.50	114.30	122.09
1	A1	244	ARG	NE-CZ-NH2	7.47	125.92	119.20
6	R1	65	ALA	O-C-N	-7.47	113.96	122.03
3	C1	303	LEU	N-CA-C	7.46	119.50	111.36
7	G1	26	PHE	CA-C-N	7.45	129.15	119.84
7	G1	26	PHE	C-N-CA	7.45	129.15	119.84
3	C1	106	SER	CA-C-O	7.45	128.58	119.79
3	O1	71	ARG	NE-CZ-NH1	-7.43	114.07	121.50
1	M1	275	ALA	N-CA-C	-7.41	103.14	111.07
4	P1	235	LEU	O-C-N	-7.41	113.56	123.19
3	C1	205	SER	O-C-N	-7.41	113.16	123.01
5	Q1	179	ASN	CA-CB-CG	7.40	120.00	112.60
1	M1	442	PHE	CA-CB-CG	7.37	121.17	113.80
56	A3	330	GLY	N-CA-C	7.37	120.44	112.33
3	O1	80	ARG	CD-NE-CZ	-7.37	114.08	124.40
3	C1	221	HIS	CA-CB-CG	-7.36	106.44	113.80
7	G1	13	VAL	CA-C-N	-7.36	110.79	122.64
7	G1	13	VAL	C-N-CA	-7.36	110.79	122.64
68	M3	27	LEU	N-CA-C	7.35	119.38	111.36
4	D1	160	MET	N-CA-C	7.35	120.39	108.41
4	D1	201	ARG	NE-CZ-NH1	-7.35	114.15	121.50
1	A1	364	ALA	O-C-N	7.34	129.90	122.12
3	O1	222	PRO	CA-C-N	7.34	131.90	120.89
3	O1	222	PRO	C-N-CA	7.34	131.90	120.89
3	C1	313	ARG	NE-CZ-NH2	7.31	125.78	119.20
2	B1	92	VAL	CA-C-O	7.30	127.02	119.35
3	C1	195	VAL	O-C-N	7.30	128.95	121.87
3	O1	88	SER	N-CA-C	-7.26	103.30	111.07
1	M1	256	ALA	CB-CA-C	-7.26	93.45	109.56
3	C1	30	TRP	O-C-N	-7.25	114.43	122.12
1	A1	281	ASP	CA-C-N	7.25	130.31	120.38
1	A1	281	ASP	C-N-CA	7.25	130.31	120.38
2	N1	188	PRO	O-C-N	-7.25	112.85	122.64
1	A1	435	ASN	CA-C-O	7.24	128.30	119.97
46	c2	66	ARG	CA-C-N	7.24	134.73	121.70
46	c2	66	ARG	C-N-CA	7.24	134.73	121.70
1	M1	424	GLY	CA-C-O	-7.24	113.59	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N1	385	GLN	CA-C-O	7.23	128.09	120.42
5	Q1	5	ILE	CB-CA-C	-7.23	101.07	111.34
3	C1	113	TRP	O-C-N	-7.22	114.58	122.09
17	82	36	LYS	CA-C-N	7.22	134.69	121.70
17	82	36	LYS	C-N-CA	7.22	134.69	121.70
6	F1	73	GLN	CB-CA-C	7.21	122.37	109.38
5	Q1	72	SER	CA-C-O	-7.21	113.26	121.19
56	A3	376	HIS	CE1-NE2-CD2	-7.21	101.79	109.00
1	A1	419	CYS	N-CA-CB	7.20	119.66	110.23
56	A3	9	SER	N-CA-C	7.19	119.84	110.43
4	D1	215	LEU	CA-C-O	7.18	128.47	119.78
30	L2	62	ASN	CA-C-N	7.16	134.60	121.70
30	L2	62	ASN	C-N-CA	7.16	134.60	121.70
3	C1	106	SER	N-CA-C	-7.16	103.21	112.23
60	E3	42	VAL	N-CA-C	-7.15	99.61	108.05
17	82	228	PRO	CA-C-N	7.15	134.57	121.70
17	82	228	PRO	C-N-CA	7.15	134.57	121.70
4	P1	199	ASP	CA-C-O	-7.15	113.31	120.82
1	M1	417	ASP	CA-C-N	-7.15	109.73	122.74
1	M1	417	ASP	C-N-CA	-7.15	109.73	122.74
3	O1	256	TYR	N-CA-C	-7.13	104.51	112.57
3	O1	37	LEU	CA-C-N	7.12	127.83	120.00
3	O1	37	LEU	C-N-CA	7.12	127.83	120.00
5	Q1	193	VAL	CG1-CB-CG2	7.12	126.47	110.80
1	A1	242	CYS	O-C-N	-7.12	115.23	123.27
3	C1	264	THR	CB-CA-C	-7.11	100.40	109.65
1	A1	343	MET	CA-CB-CG	-7.11	99.88	114.10
1	M1	138	LEU	CA-C-O	-7.11	112.70	121.02
56	A3	332	ILE	N-CA-C	7.10	118.96	109.37
5	E1	14	ARG	CA-C-N	-7.10	113.73	123.96
5	E1	14	ARG	C-N-CA	-7.10	113.73	123.96
60	E3	76	GLY	CA-C-N	7.10	128.33	120.45
60	E3	76	GLY	C-N-CA	7.10	128.33	120.45
4	D1	175	THR	CA-C-O	7.09	125.75	119.59
1	M1	443	TRP	N-CA-C	7.08	121.70	107.41
3	O1	244	LEU	O-C-N	7.07	131.57	122.10
7	S1	21	PHE	CA-CB-CG	-7.07	106.73	113.80
3	O1	231	GLY	CA-C-O	7.06	128.07	120.30
17	82	259	GLY	CA-C-N	7.06	134.41	121.70
17	82	259	GLY	C-N-CA	7.06	134.41	121.70
5	Q1	182	VAL	CA-C-O	-7.04	116.09	120.88
6	R1	60	PHE	CA-CB-CG	-7.04	106.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B1	108	THR	N-CA-C	7.04	119.93	110.35
3	C1	40	CYS	N-CA-C	-7.04	103.36	112.23
2	N1	291	ALA	N-CA-C	-7.04	104.83	113.41
3	O1	196	HIS	CE1-NE2-CD2	-7.03	101.97	109.00
5	Q1	135	LEU	CA-C-N	7.02	133.64	122.33
5	Q1	135	LEU	C-N-CA	7.02	133.64	122.33
6	R1	50	LEU	CA-C-N	7.02	128.62	119.84
6	R1	50	LEU	C-N-CA	7.02	128.62	119.84
43	Z2	85	GLU	CA-C-N	7.00	134.31	121.70
43	Z2	85	GLU	C-N-CA	7.00	134.31	121.70
23	E2	114	ILE	N-CA-C	-7.00	106.48	113.20
1	M1	414	TYR	N-CA-C	6.95	120.99	112.23
1	A1	283	THR	N-CA-C	6.95	121.36	113.02
5	Q1	25	SER	CA-C-O	6.94	127.06	119.15
58	C3	36	HIS	N-CA-C	6.94	122.17	113.43
7	G1	12	HIS	CA-C-N	-6.93	114.06	123.14
7	G1	12	HIS	C-N-CA	-6.93	114.06	123.14
3	C1	201	HIS	CA-CB-CG	-6.93	106.87	113.80
2	B1	97	SER	N-CA-C	6.92	120.95	109.46
4	P1	83	ARG	CA-C-N	6.92	126.95	119.89
4	P1	83	ARG	C-N-CA	6.92	126.95	119.89
6	F1	45	GLU	CA-C-N	-6.91	111.53	120.65
6	F1	45	GLU	C-N-CA	-6.91	111.53	120.65
56	A3	130	PRO	N-CA-C	-6.90	102.28	110.70
2	N1	186	VAL	N-CA-CB	6.89	119.35	111.90
2	N1	187	THR	N-CA-C	6.89	118.75	110.07
3	O1	230	LEU	CA-C-N	6.89	128.97	120.22
3	O1	230	LEU	C-N-CA	6.89	128.97	120.22
1	A1	415	PHE	O-C-N	-6.89	111.80	122.13
6	F1	61	ARG	NE-CZ-NH2	6.87	125.39	119.20
5	Q1	87	MET	CA-C-O	6.87	127.81	120.46
3	O1	284	ILE	CA-C-O	6.86	123.65	119.19
2	B1	70	ARG	NE-CZ-NH1	-6.85	114.65	121.50
5	Q1	14	ARG	NE-CZ-NH1	-6.85	114.65	121.50
4	P1	218	LEU	N-CA-CB	6.85	119.91	109.91
5	E1	61	SER	CA-CB-OG	-6.83	97.44	111.10
24	F2	97	MET	C-N-CD	-6.83	105.58	120.60
24	F2	104	ARG	CA-C-N	6.83	133.99	121.70
24	F2	104	ARG	C-N-CA	6.83	133.99	121.70
2	B1	346	THR	CA-CB-OG1	6.82	119.83	109.60
3	O1	241	LEU	O-C-N	6.82	129.93	122.15
3	C1	135	TRP	CA-C-O	-6.81	113.69	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P1	97	ASN	CA-C-N	6.78	128.32	119.84
4	P1	97	ASN	C-N-CA	6.78	128.32	119.84
19	A2	461	PRO	CA-C-N	6.78	134.49	121.54
19	A2	461	PRO	C-N-CA	6.78	134.49	121.54
1	A1	338	LEU	CA-C-O	6.78	128.11	121.00
2	B1	173	ALA	CA-C-O	6.77	127.99	119.12
2	N1	258	VAL	N-CA-C	6.77	117.29	108.35
3	O1	298	ILE	N-CA-C	6.77	116.89	110.53
10	J1	14	PHE	CA-CB-CG	6.77	120.57	113.80
1	M1	320	LEU	O-C-N	-6.75	114.46	123.23
1	M1	334	MET	N-CA-CB	-6.75	100.17	110.16
5	Q1	34	GLY	N-CA-C	-6.75	104.33	112.49
3	O1	13	ILE	CB-CA-C	-6.74	103.20	112.02
59	D3	133	GLY	N-CA-C	6.74	129.15	113.18
2	N1	141	GLN	CA-C-N	6.73	128.25	119.84
2	N1	141	GLN	C-N-CA	6.73	128.25	119.84
5	Q1	194	ILE	N-CA-CB	-6.73	103.43	111.90
1	A1	436	ARG	O-C-N	6.72	129.35	122.09
56	A3	507	GLU	N-CA-C	-6.72	97.92	109.15
2	B1	102	ARG	NE-CZ-NH2	6.71	125.24	119.20
3	O1	328	LEU	CA-C-N	-6.70	112.12	120.56
3	O1	328	LEU	C-N-CA	-6.70	112.12	120.56
62	G3	5	LYS	N-CA-C	6.70	125.07	110.80
27	I2	107	THR	CA-C-N	-6.70	111.75	122.53
27	I2	107	THR	C-N-CA	-6.70	111.75	122.53
1	A1	259	GLY	CA-C-N	6.69	128.21	119.84
1	A1	259	GLY	C-N-CA	6.69	128.21	119.84
52	I2	200	LEU	N-CA-C	-6.69	104.82	114.12
3	C1	109	PHE	CA-CB-CG	6.69	120.49	113.80
60	E3	81	ILE	N-CA-C	6.69	116.82	110.53
5	Q1	192	MET	N-CA-C	6.68	119.30	108.34
4	D1	7	PRO	N-CA-C	6.68	118.85	110.70
2	N1	173	ALA	CA-C-O	6.65	127.63	119.11
3	C1	143	ALA	N-CA-C	-6.65	104.11	111.36
1	M1	334	MET	CA-C-O	6.65	127.47	120.42
3	O1	222	PRO	CB-CA-C	6.64	122.52	111.56
6	R1	35	ASP	CA-C-O	6.64	127.54	119.31
2	B1	143	GLN	OE1-CD-NE2	-6.64	115.96	122.60
3	C1	218	ILE	O-C-N	6.62	128.65	121.10
5	E1	14	ARG	CD-NE-CZ	-6.62	115.13	124.40
3	C1	186	PRO	O-C-N	-6.61	114.64	122.24
4	D1	32	VAL	N-CA-CB	6.60	117.84	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q1	129	LYS	CA-C-N	6.60	128.09	119.84
5	Q1	129	LYS	C-N-CA	6.60	128.09	119.84
1	M1	268	VAL	N-CA-C	-6.60	106.36	112.96
56	A3	61	HIS	CB-CG-CD2	-6.60	122.62	131.20
3	O1	19	ILE	CA-C-N	6.60	134.33	122.06
3	O1	19	ILE	C-N-CA	6.60	134.33	122.06
1	A1	169	GLY	CA-C-N	6.59	128.08	119.84
1	A1	169	GLY	C-N-CA	6.59	128.08	119.84
2	B1	177	TYR	CA-C-O	-6.58	113.20	120.38
56	A3	506	GLU	N-CA-C	-6.57	104.11	111.28
4	D1	92	PRO	N-CA-CB	6.57	107.63	103.23
3	O1	299	LEU	CA-C-O	6.56	127.43	119.49
9	I1	68	VAL	CB-CA-C	-6.56	101.74	110.98
1	A1	331	ILE	N-CA-C	6.55	117.24	110.36
38	U2	120	THR	CA-C-N	6.55	142.73	127.00
38	U2	120	THR	C-N-CA	6.55	142.73	127.00
2	N1	62	ASN	CA-CB-CG	6.55	119.15	112.60
1	A1	436	ARG	N-CA-CB	6.55	119.57	110.07
2	B1	75	LEU	CA-C-O	-6.54	114.42	121.94
6	R1	79	GLN	N-CA-C	6.54	120.26	112.93
56	A3	74	MET	N-CA-C	6.54	118.07	111.07
1	A1	189	HIS	CA-CB-CG	6.54	120.34	113.80
3	O1	93	CYS	N-CA-CB	6.54	119.84	110.16
5	Q1	24	SER	N-CA-C	6.54	119.71	110.23
8	H1	67	HIS	CA-CB-CG	6.54	120.33	113.80
3	C1	246	ALA	O-C-N	6.53	125.96	121.19
3	O1	244	LEU	CA-C-O	-6.53	111.87	119.64
5	Q1	70	ALA	CA-C-O	6.53	127.34	120.42
44	a2	128	SER	CA-C-N	6.52	133.44	121.70
44	a2	128	SER	C-N-CA	6.52	133.44	121.70
11	K1	35	ALA	N-CA-C	-6.51	104.10	111.07
4	D1	229	VAL	CB-CA-C	-6.51	103.63	111.97
3	C1	312	GLN	O-C-N	-6.51	114.69	122.63
3	C1	322	GLN	OE1-CD-NE2	6.50	129.10	122.60
4	D1	83	ARG	CA-C-N	6.50	126.52	119.89
4	D1	83	ARG	C-N-CA	6.50	126.52	119.89
1	M1	307	PHE	O-C-N	-6.50	115.44	123.44
1	A1	199	ALA	CA-C-N	-6.50	112.39	122.59
1	A1	199	ALA	C-N-CA	-6.50	112.39	122.59
2	B1	187	THR	CA-C-N	6.49	127.95	119.84
2	B1	187	THR	C-N-CA	6.49	127.95	119.84
2	B1	29	LEU	CA-C-N	6.48	126.24	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B1	29	LEU	C-N-CA	6.48	126.24	119.05
3	C1	230	LEU	CA-C-N	6.48	127.31	119.99
3	C1	230	LEU	C-N-CA	6.48	127.31	119.99
2	B1	91	ALA	CA-C-N	6.48	132.34	122.69
2	B1	91	ALA	C-N-CA	6.48	132.34	122.69
5	E1	6	LYS	O-C-N	-6.47	115.37	123.27
56	A3	61	HIS	ND1-CE1-NE2	6.46	114.86	108.40
1	A1	438	ARG	NE-CZ-NH1	-6.46	115.05	121.50
3	C1	224	TYR	N-CA-C	6.45	120.41	112.54
1	A1	435	ASN	OD1-CG-ND2	6.45	129.05	122.60
7	S1	26	PHE	CA-C-N	6.45	127.90	119.84
7	S1	26	PHE	C-N-CA	6.45	127.90	119.84
1	M1	100	LYS	CA-C-O	-6.45	113.40	120.43
3	O1	80	ARG	NE-CZ-NH1	-6.44	115.06	121.50
3	C1	293	ALA	CA-C-N	-6.43	111.16	120.29
3	C1	293	ALA	C-N-CA	-6.43	111.16	120.29
6	R1	36	THR	CA-CB-CG2	6.43	121.43	110.50
1	M1	174	VAL	CA-CB-CG1	6.43	121.33	110.40
1	A1	280	TYR	O-C-N	-6.42	116.07	123.33
5	E1	5	ILE	CB-CA-C	-6.42	102.42	111.21
1	A1	420	PRO	N-CA-CB	6.40	109.41	103.39
3	C1	109	PHE	O-C-N	-6.40	114.07	122.59
5	Q1	29	SER	N-CA-C	6.40	120.81	113.19
7	G1	4	PHE	CA-CB-CG	-6.39	107.41	113.80
2	N1	178	CYS	CA-C-N	6.38	126.14	119.76
2	N1	178	CYS	C-N-CA	6.38	126.14	119.76
2	N1	204	MET	N-CA-C	6.38	120.45	110.17
3	C1	107	TYR	CA-C-N	-6.38	111.64	120.38
3	C1	107	TYR	C-N-CA	-6.38	111.64	120.38
1	A1	436	ARG	CA-C-O	-6.38	114.13	120.70
1	M1	150	PHE	CA-CB-CG	6.38	120.18	113.80
1	A1	147	ASP	CA-C-O	6.37	127.31	120.24
23	E2	75	SER	CA-C-N	6.36	133.14	121.70
23	E2	75	SER	C-N-CA	6.36	133.14	121.70
3	O1	256	TYR	O-C-N	6.35	130.39	122.19
6	F1	14	GLU	CA-C-N	6.34	126.97	120.00
6	F1	14	GLU	C-N-CA	6.34	126.97	120.00
38	U2	120	THR	C-N-CD	-6.34	106.66	120.60
1	A1	11	VAL	CA-C-N	6.33	127.76	119.84
1	A1	11	VAL	C-N-CA	6.33	127.76	119.84
1	M1	239	SER	CA-C-O	-6.33	114.24	121.58
55	e2	70	THR	N-CA-C	6.32	117.35	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	24	ARG	NE-CZ-NH1	-6.32	115.18	121.50
4	D1	168	VAL	CB-CA-C	-6.31	103.78	112.24
1	A1	32	GLN	CA-C-N	6.31	127.73	119.84
1	A1	32	GLN	C-N-CA	6.31	127.73	119.84
1	A1	251	ALA	CA-C-N	-6.31	114.38	122.77
1	A1	251	ALA	C-N-CA	-6.31	114.38	122.77
3	C1	301	LEU	N-CA-C	6.31	118.68	111.11
1	A1	150	PHE	CA-CB-CG	6.31	120.11	113.80
3	O1	325	PHE	O-C-N	6.30	128.58	122.03
2	B1	73	SER	CA-C-O	-6.29	111.52	120.51
2	B1	89	ILE	CA-CB-CG2	6.29	121.18	110.50
36	S2	113	ASP	CA-C-N	6.28	133.01	121.70
36	S2	113	ASP	C-N-CA	6.28	133.01	121.70
2	B1	145	ARG	CA-C-O	-6.28	114.18	120.90
6	R1	24	ALA	CA-C-O	6.28	129.49	120.51
2	N1	254	HIS	CA-C-O	-6.27	113.93	120.70
2	B1	291	ALA	N-CA-C	-6.27	105.76	113.41
56	A3	10	THR	N-CA-C	-6.25	103.84	112.03
12	22	141	VAL	N-CA-C	-6.25	106.87	112.12
5	Q1	123	ASP	CA-CB-CG	-6.25	106.35	112.60
1	M1	319	LEU	N-CA-CB	-6.25	100.74	110.55
3	C1	78	ILE	CA-C-N	-6.24	111.55	120.42
3	C1	78	ILE	C-N-CA	-6.24	111.55	120.42
35	R2	271	TYR	CA-C-N	6.24	133.47	121.54
35	R2	271	TYR	C-N-CA	6.24	133.47	121.54
1	A1	434	TYR	O-C-N	6.23	128.72	122.12
62	G3	2	SER	N-CA-C	6.23	119.51	109.79
1	A1	196	VAL	CA-C-O	-6.22	113.91	120.76
5	Q1	14	ARG	CD-NE-CZ	-6.22	115.69	124.40
4	P1	110	PRO	CA-C-N	6.22	126.17	119.76
4	P1	110	PRO	C-N-CA	6.22	126.17	119.76
7	G1	14	ILE	CA-C-N	6.22	131.95	122.93
7	G1	14	ILE	C-N-CA	6.22	131.95	122.93
1	M1	342	TRP	CA-C-N	6.22	128.93	120.54
1	M1	342	TRP	C-N-CA	6.22	128.93	120.54
60	E3	21	LYS	CA-C-N	6.21	126.40	119.32
60	E3	21	LYS	C-N-CA	6.21	126.40	119.32
1	A1	69	ASN	O-C-N	-6.21	115.58	122.03
2	N1	167	ALA	CA-C-O	6.21	127.11	119.97
1	M1	277	ILE	CA-C-O	-6.20	114.82	121.27
7	S1	58	VAL	N-CA-CB	6.20	117.39	110.51
7	G1	21	PHE	CA-CB-CG	-6.20	107.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	416	TYR	N-CA-C	6.19	118.27	108.67
1	A1	343	MET	CA-C-N	-6.19	111.90	120.38
1	A1	343	MET	C-N-CA	-6.19	111.90	120.38
5	Q1	153	PHE	CA-CB-CG	6.18	119.98	113.80
5	Q1	66	ALA	CA-C-O	6.18	127.22	119.12
1	A1	392	LEU	N-CA-CB	6.18	119.14	109.94
1	M1	161	THR	CA-C-N	6.18	126.64	119.47
1	M1	161	THR	C-N-CA	6.18	126.64	119.47
7	S1	34	ILE	CA-C-N	6.17	125.66	119.24
7	S1	34	ILE	C-N-CA	6.17	125.66	119.24
5	E1	29	SER	N-CA-C	6.17	120.27	112.87
10	J1	8	ARG	CA-C-N	6.17	128.87	120.54
10	J1	8	ARG	C-N-CA	6.17	128.87	120.54
51	j2	22	PRO	CA-C-N	6.16	141.79	127.00
51	j2	22	PRO	C-N-CA	6.16	141.79	127.00
3	C1	231	GLY	CA-C-O	6.15	127.38	121.05
1	M1	142	ASP	N-CA-C	-6.15	105.74	113.18
1	A1	408	ARG	NH1-CZ-NH2	6.14	127.28	119.30
6	R1	98	ILE	CA-C-O	6.13	127.65	121.27
1	A1	440	GLY	CA-C-N	-6.13	112.01	122.56
1	A1	440	GLY	C-N-CA	-6.13	112.01	122.56
4	P1	160	MET	N-CA-C	6.13	118.74	108.02
2	N1	66	SER	N-CA-CB	6.12	118.88	110.01
1	A1	338	LEU	O-C-N	-6.12	115.67	122.03
2	B1	46	ARG	N-CA-C	6.10	118.36	107.80
2	B1	306	PRO	N-CA-CB	6.10	108.18	103.30
3	C1	180	ALA	N-CA-CB	6.10	119.16	110.13
6	R1	58	ARG	NE-CZ-NH2	6.10	124.69	119.20
3	O1	233	LEU	O-C-N	6.09	128.43	122.09
16	72	140	ALA	CA-C-N	6.09	132.67	121.70
16	72	140	ALA	C-N-CA	6.09	132.67	121.70
2	N1	412	ASN	CB-CG-ND2	-6.07	107.29	116.40
7	S1	10	VAL	CA-C-O	-6.07	114.14	120.27
3	C1	13	ILE	CA-CB-CG1	6.07	120.72	110.40
3	O1	196	HIS	ND1-CE1-NE2	6.07	114.47	108.40
1	A1	153	LEU	N-CA-CB	6.07	119.04	109.82
1	A1	418	GLN	CA-C-N	-6.07	113.18	121.61
1	A1	418	GLN	C-N-CA	-6.07	113.18	121.61
36	S2	87	GLY	CA-C-N	6.07	132.62	121.70
36	S2	87	GLY	C-N-CA	6.07	132.62	121.70
3	O1	221	HIS	CB-CA-C	-6.06	104.05	113.57
56	A3	157	SER	N-CA-C	6.06	118.85	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A3	170	ASN	N-CA-C	6.06	120.75	113.23
5	E1	32	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	M1	292	SER	CA-C-N	6.06	127.41	119.84
1	M1	292	SER	C-N-CA	6.06	127.41	119.84
2	N1	87	ARG	O-C-N	6.06	129.31	122.22
3	C1	280	ILE	N-CA-CB	6.04	118.02	110.47
16	72	109	LYS	N-CA-C	-6.04	107.74	114.62
1	A1	277	ILE	CB-CA-C	-6.03	104.00	112.14
1	A1	292	SER	O-C-N	-6.03	115.80	121.35
19	A2	381	LEU	CA-C-N	6.02	133.04	121.54
19	A2	381	LEU	C-N-CA	6.02	133.04	121.54
3	C1	186	PRO	CA-C-O	6.01	130.00	119.84
3	O1	320	LEU	CA-C-N	-6.01	111.17	120.31
3	O1	320	LEU	C-N-CA	-6.01	111.17	120.31
1	M1	205	HIS	CA-CB-CG	-6.01	107.79	113.80
2	N1	85	ILE	O-C-N	6.01	130.08	122.57
2	B1	409	ASP	CA-C-N	6.01	128.64	120.77
2	B1	409	ASP	C-N-CA	6.01	128.64	120.77
2	B1	187	THR	CA-C-O	-6.00	115.20	120.60
56	A3	125	GLY	N-CA-C	-6.00	104.14	112.18
63	H3	63	LEU	N-CA-C	6.00	119.07	111.69
1	M1	54	GLY	O-C-N	6.00	127.67	121.97
2	N1	306	PRO	N-CA-CB	6.00	108.10	103.30
4	D1	86	LYS	N-CA-C	6.00	118.51	110.35
3	C1	19	ILE	CA-C-O	-6.00	113.82	120.96
47	d2	31	PHE	CA-C-N	5.99	141.38	127.00
47	d2	31	PHE	C-N-CA	5.99	141.38	127.00
25	G2	155	PRO	CA-C-N	5.99	132.48	121.70
25	G2	155	PRO	C-N-CA	5.99	132.48	121.70
3	C1	179	PHE	CA-CB-CG	5.98	119.78	113.80
1	M1	274	ASN	OD1-CG-ND2	5.98	128.58	122.60
57	B3	207	MET	CA-C-N	5.98	127.31	119.84
57	B3	207	MET	C-N-CA	5.98	127.31	119.84
57	B3	47	THR	N-CA-C	5.98	119.88	112.59
58	C3	8	TYR	N-CA-C	5.98	118.24	110.53
3	O1	102	LEU	O-C-N	5.98	130.71	122.46
3	C1	143	ALA	CA-C-O	5.97	126.75	120.42
7	S1	50	PRO	N-CA-C	5.97	117.98	110.70
1	M1	438	ARG	CA-CB-CG	-5.97	102.17	114.10
7	S1	4	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A1	425	PHE	N-CA-CB	5.96	121.11	110.79
2	B1	102	ARG	NE-CZ-NH1	-5.96	115.54	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	342	TRP	CH2-CZ2-CE2	5.96	125.25	117.50
1	M1	416	TYR	CA-C-O	-5.96	113.86	120.60
8	H1	55	THR	CA-C-O	5.96	127.08	120.82
33	P2	51	ASN	N-CA-C	-5.96	107.82	114.62
62	G3	44	ARG	CA-C-N	5.96	125.98	119.90
62	G3	44	ARG	C-N-CA	5.96	125.98	119.90
1	A1	166	SER	CA-C-O	5.96	127.83	121.16
5	Q1	80	ASP	CA-CB-CG	-5.95	106.65	112.60
1	A1	440	GLY	N-CA-C	-5.95	107.52	115.32
3	C1	257	THR	CA-C-O	5.94	123.72	119.32
1	A1	284	TYR	O-C-N	-5.93	115.63	122.93
2	B1	145	ARG	O-C-N	5.93	128.26	122.09
3	O1	210	GLY	N-CA-C	-5.93	107.21	114.92
5	Q1	99	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	M1	89	TYR	CA-CB-CG	5.93	124.57	113.90
2	N1	75	LEU	N-CA-CB	5.93	118.92	110.44
1	A1	248	LEU	CA-C-N	5.92	125.80	119.28
1	A1	248	LEU	C-N-CA	5.92	125.80	119.28
2	N1	143	GLN	OE1-CD-NE2	-5.92	116.68	122.60
5	Q1	132	TRP	N-CA-C	5.92	119.46	109.76
12	22	127	GLY	CA-C-N	5.92	132.35	121.70
12	22	127	GLY	C-N-CA	5.92	132.35	121.70
4	D1	110	PRO	CA-C-N	5.91	125.85	119.76
4	D1	110	PRO	C-N-CA	5.91	125.85	119.76
3	C1	22	PRO	CB-CA-C	-5.91	101.80	111.56
10	J1	22	LEU	N-CA-C	-5.91	104.75	111.07
4	P1	138	PRO	N-CD-CG	-5.91	94.33	103.20
56	A3	67	PHE	N-CA-C	5.91	119.68	112.23
3	C1	127	ALA	CA-C-O	5.91	126.76	119.97
44	a2	19	ASP	CA-C-N	5.90	141.17	127.00
44	a2	19	ASP	C-N-CA	5.90	141.17	127.00
56	A3	171	MET	N-CA-C	5.90	120.19	111.87
1	M1	46	ARG	NH1-CZ-NH2	5.90	126.97	119.30
3	C1	71	ARG	NE-CZ-NH1	-5.89	115.61	121.50
4	D1	92	PRO	CB-CA-C	5.89	116.76	111.40
3	C1	91	PHE	CB-CG-CD2	-5.89	110.69	120.70
3	C1	160	LEU	N-CA-C	5.89	118.46	111.33
2	N1	167	ALA	O-C-N	-5.89	115.02	122.27
3	O1	126	THR	O-C-N	5.89	128.14	122.07
56	A3	119	GLU	CB-CA-C	-5.89	109.77	116.54
7	S1	15	THR	CB-CA-C	-5.88	98.94	109.71
57	B3	134	ARG	N-CA-C	5.88	123.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C1	282	ARG	CD-NE-CZ	-5.87	116.18	124.40
3	C1	176	THR	CA-CB-OG1	-5.87	100.79	109.60
3	C1	320	LEU	CA-C-N	-5.87	111.39	120.31
3	C1	320	LEU	C-N-CA	-5.87	111.39	120.31
2	N1	285	VAL	N-CA-C	5.87	116.73	108.17
1	A1	281	ASP	CA-CB-CG	5.85	118.45	112.60
3	C1	177	ARG	CB-CA-C	-5.85	101.95	110.96
2	N1	42	ALA	CA-C-N	5.85	127.15	119.84
2	N1	42	ALA	C-N-CA	5.85	127.15	119.84
2	N1	157	ALA	N-CA-C	5.85	117.33	111.07
5	E1	15	ARG	O-C-N	5.85	126.29	121.32
1	M1	364	ALA	CA-C-O	5.85	126.75	120.55
16	72	139	GLU	CA-C-N	5.85	132.22	121.70
16	72	139	GLU	C-N-CA	5.85	132.22	121.70
3	O1	206	ASN	O-C-N	-5.84	115.78	122.68
3	C1	205	SER	CA-C-O	5.84	127.42	120.70
2	N1	47	ILE	CB-CG1-CD1	5.84	126.07	113.80
2	N1	157	ALA	N-CA-CB	5.84	118.48	110.01
3	O1	227	LYS	O-C-N	5.84	128.08	122.07
3	C1	282	ARG	NE-CZ-NH1	-5.83	115.67	121.50
3	O1	50	PHE	CA-CB-CG	-5.83	107.97	113.80
1	A1	311	ASN	OD1-CG-ND2	5.82	128.42	122.60
2	B1	245	ARG	NE-CZ-NH1	-5.82	115.68	121.50
2	B1	94	GLY	CA-C-O	-5.82	114.31	122.51
2	N1	85	ILE	CA-C-O	-5.81	113.51	120.78
3	O1	280	ILE	CB-CG1-CD1	5.81	126.01	113.80
4	P1	229	VAL	N-CA-CB	5.81	116.96	110.51
2	B1	138	ALA	CA-C-O	-5.81	114.26	120.42
4	D1	182	VAL	N-CA-CB	5.81	119.29	110.58
55	e2	94	HIS	N-CA-C	5.80	122.63	109.81
1	A1	352	SER	CA-CB-OG	5.80	122.69	111.10
4	D1	151	PRO	N-CA-CB	5.79	108.85	103.41
2	N1	167	ALA	CA-C-N	-5.79	112.39	122.64
2	N1	167	ALA	C-N-CA	-5.79	112.39	122.64
14	42	457	PRO	CA-C-N	5.79	132.12	121.70
14	42	457	PRO	C-N-CA	5.79	132.12	121.70
5	Q1	18	VAL	CB-CA-C	-5.78	101.81	111.29
3	O1	201	HIS	CA-C-O	5.77	126.05	119.18
3	C1	189	ILE	CB-CA-C	-5.77	104.48	112.04
19	A2	504	SER	CA-C-N	5.76	132.08	121.70
19	A2	504	SER	C-N-CA	5.76	132.08	121.70
3	C1	75	TYR	N-CA-C	-5.76	106.20	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O1	38	GLY	O-C-N	-5.76	116.60	122.19
58	C3	198	PHE	N-CA-C	5.76	117.56	111.28
6	R1	28	LYS	CA-C-O	5.76	126.59	119.97
1	A1	241	ILE	CA-CB-CG1	-5.75	100.62	110.40
5	Q1	184	SER	CA-C-O	-5.75	114.50	121.05
7	G1	58	VAL	N-CA-CB	5.75	117.65	110.47
4	D1	201	ARG	CA-CB-CG	5.75	125.59	114.10
2	B1	310	SER	N-CA-C	5.74	118.81	109.06
2	B1	157	ALA	N-CA-C	5.73	117.20	111.07
1	M1	339	GLN	O-C-N	5.73	130.21	122.59
1	M1	138	LEU	O-C-N	5.72	129.13	122.20
57	B3	190	GLY	N-CA-C	5.72	117.71	110.38
1	A1	434	TYR	CB-CG-CD1	5.72	129.38	120.80
5	Q1	32	ARG	CB-CA-C	5.72	120.41	110.68
1	M1	56	GLY	O-C-N	-5.72	115.26	122.70
3	O1	63	PHE	O-C-N	5.72	129.12	122.20
1	M1	436	ARG	CA-C-N	-5.71	112.08	121.34
1	M1	436	ARG	C-N-CA	-5.71	112.08	121.34
35	R2	62	THR	N-CA-C	-5.71	107.31	114.56
65	J3	25	GLY	N-CA-C	5.71	118.94	110.60
6	R1	22	ASN	N-CA-C	-5.71	106.15	113.23
3	C1	153	ILE	CA-C-N	5.71	126.97	119.84
3	C1	153	ILE	C-N-CA	5.71	126.97	119.84
3	O1	185	LEU	CA-C-O	-5.71	113.31	118.79
4	P1	50	HIS	N-CA-C	-5.71	106.16	113.23
3	C1	15	ASN	OD1-CG-ND2	5.70	128.30	122.60
2	B1	139	ALA	CA-C-O	5.70	126.81	120.82
1	M1	93	GLU	CA-CB-CG	-5.70	102.70	114.10
3	O1	46	LEU	N-CA-C	-5.70	104.98	111.14
6	F1	24	ALA	CA-C-O	5.70	126.95	120.80
3	O1	256	TYR	CA-C-O	-5.70	112.80	120.15
1	A1	23	LEU	CA-C-N	-5.70	114.86	122.72
1	A1	23	LEU	C-N-CA	-5.70	114.86	122.72
3	C1	97	HIS	CB-CG-ND1	5.70	131.24	122.70
4	D1	203	ARG	CA-C-O	5.70	127.33	121.07
3	O1	22	PRO	N-CA-CB	5.70	108.24	103.17
46	c2	36	PRO	CA-C-N	5.70	140.67	127.00
46	c2	36	PRO	C-N-CA	5.70	140.67	127.00
1	A1	193	PRO	N-CA-CB	5.69	108.86	102.60
1	A1	392	LEU	N-CA-C	5.69	117.94	111.11
2	N1	108	THR	N-CA-C	5.69	118.08	110.35
4	D1	9	SER	N-CA-C	-5.69	101.09	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A3	129	TYR	CB-CA-C	-5.68	100.50	109.42
1	A1	368	HIS	CA-CB-CG	-5.68	108.12	113.80
6	R1	23	ALA	N-CA-C	-5.68	104.78	110.97
9	U1	51	CYS	CA-C-N	5.68	128.46	120.28
9	U1	51	CYS	C-N-CA	5.68	128.46	120.28
4	P1	195	GLU	CA-C-N	5.68	125.53	119.28
4	P1	195	GLU	C-N-CA	5.68	125.53	119.28
2	N1	254	HIS	CA-CB-CG	5.68	119.48	113.80
1	A1	418	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	M1	47	TYR	N-CA-C	-5.68	106.52	113.50
2	B1	102	ARG	CD-NE-CZ	-5.67	116.46	124.40
3	C1	77	TRP	CD2-CE3-CZ3	-5.67	111.22	118.60
59	D3	129	ALA	CA-C-N	5.67	126.93	119.84
59	D3	129	ALA	C-N-CA	5.67	126.93	119.84
2	B1	65	THR	OG1-CB-CG2	5.67	120.64	109.30
2	N1	187	THR	CA-C-N	5.67	126.92	119.84
2	N1	187	THR	C-N-CA	5.67	126.92	119.84
1	M1	32	GLN	CA-C-N	5.66	126.92	119.84
1	M1	32	GLN	C-N-CA	5.66	126.92	119.84
2	B1	61	ASN	OD1-CG-ND2	-5.66	116.94	122.60
3	O1	100	ARG	N-CA-C	-5.65	105.11	112.23
3	C1	22	PRO	N-CA-CB	5.65	109.18	103.25
6	F1	43	VAL	O-C-N	-5.65	115.51	122.57
1	A1	242	CYS	N-CA-C	5.65	118.45	109.24
3	C1	16	ASN	OD1-CG-ND2	-5.64	116.96	122.60
3	C1	96	MET	N-CA-C	-5.64	105.21	111.36
3	C1	191	ALA	N-CA-C	-5.64	105.04	111.07
3	O1	264	THR	CB-CA-C	-5.64	102.32	109.65
1	A1	11	VAL	N-CA-C	5.64	114.26	109.02
1	A1	279	HIS	O-C-N	-5.63	117.17	123.48
3	O1	257	THR	CB-CA-C	-5.63	103.43	109.85
9	U1	56	ARG	CA-C-N	5.63	128.71	121.27
9	U1	56	ARG	C-N-CA	5.63	128.71	121.27
1	M1	428	ILE	O-C-N	-5.63	116.30	122.05
2	N1	201	SER	N-CA-C	5.63	117.11	110.97
4	P1	30	PHE	CA-CB-CG	-5.63	108.17	113.80
1	M1	154	HIS	CA-CB-CG	5.63	119.43	113.80
4	P1	38	SER	CA-C-N	5.62	128.38	120.28
4	P1	38	SER	C-N-CA	5.62	128.38	120.28
2	N1	165	ALA	CA-C-O	5.62	126.28	119.31
1	A1	205	HIS	CA-CB-CG	-5.62	108.19	113.80
1	M1	292	SER	CA-C-O	5.61	124.07	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q1	76	ILE	CA-C-O	-5.61	115.41	121.19
8	H1	63	HIS	CA-CB-CG	-5.61	108.19	113.80
57	B3	104	TRP	N-CA-C	5.61	122.74	110.80
2	N1	45	SER	O-C-N	-5.60	116.63	123.19
3	O1	56	THR	O-C-N	-5.60	116.35	123.24
1	A1	414	TYR	N-CA-C	5.59	120.23	112.90
1	M1	376	CYS	CA-CB-SG	-5.59	101.53	114.40
4	P1	109	LEU	CA-C-N	5.59	126.14	120.38
4	P1	109	LEU	C-N-CA	5.59	126.14	120.38
2	B1	403	ASP	CA-CB-CG	-5.58	107.02	112.60
3	O1	45	ILE	CB-CA-C	-5.58	104.83	111.81
8	H1	54	CYS	CA-C-N	5.58	127.70	120.44
8	H1	54	CYS	C-N-CA	5.58	127.70	120.44
3	C1	111	GLU	CA-C-O	-5.58	114.93	120.90
3	O1	35	SER	CA-C-N	5.57	128.01	120.38
3	O1	35	SER	C-N-CA	5.57	128.01	120.38
3	O1	196	HIS	N-CA-C	-5.57	105.11	111.07
2	B1	197	ASN	N-CA-C	5.57	117.43	111.36
3	O1	126	THR	CA-C-O	-5.56	114.98	120.82
6	R1	99	ARG	CA-C-N	-5.56	112.83	120.28
6	R1	99	ARG	C-N-CA	-5.56	112.83	120.28
3	C1	143	ALA	CA-C-N	-5.56	113.21	120.44
3	C1	143	ALA	C-N-CA	-5.56	113.21	120.44
3	O1	199	PHE	CB-CG-CD2	5.56	130.15	120.70
8	T1	63	HIS	CA-CB-CG	-5.56	108.24	113.80
3	C1	120	LEU	CA-C-O	5.56	126.85	120.90
1	A1	22	GLY	N-CA-C	-5.55	107.12	114.95
4	P1	16	GLY	N-CA-C	5.55	120.15	112.37
7	S1	19	SER	CA-C-N	5.55	125.02	119.24
7	S1	19	SER	C-N-CA	5.55	125.02	119.24
1	A1	360	LEU	N-CA-C	-5.55	105.31	111.36
4	D1	31	GLN	CA-C-O	-5.55	114.96	120.90
3	C1	21	LEU	N-CA-C	5.55	116.69	109.64
1	A1	69	ASN	CA-C-O	5.55	126.83	121.00
3	C1	269	LYS	CA-C-N	5.55	125.86	119.92
3	C1	269	LYS	C-N-CA	5.55	125.86	119.92
1	M1	415	PHE	CA-CB-CG	5.55	119.35	113.80
13	32	20	ILE	N-CA-C	-5.55	106.42	112.80
62	G3	72	ASN	CA-C-N	5.55	125.91	119.47
62	G3	72	ASN	C-N-CA	5.55	125.91	119.47
64	I3	20	HIS	N-CA-C	5.55	118.09	111.71
1	M1	300	THR	CA-CB-OG1	5.54	117.92	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O1	185	LEU	O-C-N	5.54	124.76	120.38
3	C1	182	HIS	N-CA-C	-5.54	105.24	111.28
51	j2	22	PRO	C-N-CD	-5.54	108.41	120.60
61	F3	82	CYS	CA-C-N	5.54	125.37	119.28
61	F3	82	CYS	C-N-CA	5.54	125.37	119.28
2	B1	320	GLY	CA-C-O	5.54	126.51	121.47
3	C1	123	VAL	CA-C-N	-5.54	111.26	120.68
3	C1	123	VAL	C-N-CA	-5.54	111.26	120.68
4	D1	206	LEU	N-CA-CB	5.54	119.13	109.72
5	Q1	47	VAL	N-CA-C	5.54	116.93	110.62
58	C3	188	ILE	CB-CA-C	-5.54	104.67	112.14
1	M1	341	GLN	CA-C-O	-5.53	114.56	120.42
5	Q1	91	TRP	CB-CG-CD2	5.53	134.55	126.80
1	M1	217	SER	N-CA-CB	-5.53	102.52	110.87
7	S1	12	HIS	CA-CB-CG	-5.53	108.27	113.80
4	D1	114	SER	CA-CB-OG	5.53	122.16	111.10
1	M1	189	HIS	CA-CB-CG	5.53	119.33	113.80
5	Q1	40	THR	CA-CB-CG2	5.53	119.89	110.50
3	C1	164	ILE	CA-C-O	-5.52	115.53	121.27
3	C1	205	SER	N-CA-C	5.52	118.18	109.96
1	A1	395	TRP	CD2-CE2-CZ2	5.51	127.92	122.40
5	Q1	29	SER	CA-C-N	5.51	127.67	120.28
5	Q1	29	SER	C-N-CA	5.51	127.67	120.28
3	O1	282	ARG	CD-NE-CZ	-5.51	116.68	124.40
67	L3	16	GLU	N-CA-C	5.51	117.37	111.36
4	D1	40	CYS	CB-CA-C	5.51	116.27	109.16
24	F2	97	MET	CA-C-N	5.51	140.22	127.00
24	F2	97	MET	C-N-CA	5.51	140.22	127.00
3	C1	18	PHE	CA-C-N	5.50	128.61	120.74
3	C1	18	PHE	C-N-CA	5.50	128.61	120.74
2	B1	190	GLU	CA-C-O	-5.50	115.02	120.90
65	J3	2	GLU	N-CA-C	5.50	122.51	110.80
1	A1	46	ARG	NE-CZ-NH2	-5.49	114.25	119.20
7	G1	15	THR	N-CA-C	5.49	118.43	109.59
10	V1	8	ARG	CA-C-N	5.49	127.95	120.54
10	V1	8	ARG	C-N-CA	5.49	127.95	120.54
3	C1	188	ILE	N-CA-CB	5.48	117.59	110.57
43	Z2	41	LEU	CA-C-N	5.48	131.57	121.70
43	Z2	41	LEU	C-N-CA	5.48	131.57	121.70
1	M1	252	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A1	208	LEU	N-CA-C	-5.48	105.00	110.97
6	R1	98	ILE	O-C-N	-5.48	116.46	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N1	329	GLN	CB-CA-C	5.47	119.92	110.45
4	D1	208	MET	CA-CB-CG	5.47	125.04	114.10
1	M1	375	VAL	O-C-N	5.47	127.25	121.89
9	U1	58	GLN	N-CA-C	5.47	118.40	109.59
5	Q1	69	LEU	CA-C-N	5.47	128.06	120.29
5	Q1	69	LEU	C-N-CA	5.47	128.06	120.29
4	D1	182	VAL	CA-CB-CG1	5.46	119.69	110.40
5	E1	49	TYR	N-CA-C	-5.46	104.36	111.02
1	A1	149	VAL	N-CA-CB	5.46	116.94	110.55
2	B1	85	ILE	N-CA-C	5.46	116.09	110.36
3	C1	26	ASN	O-C-N	-5.46	116.57	123.12
2	B1	46	ARG	CB-CA-C	-5.46	102.65	110.62
2	B1	44	ALA	N-CA-C	5.46	117.41	108.52
6	R1	32	MET	N-CA-CB	-5.45	102.06	111.55
55	e2	82	SER	N-CA-C	5.45	122.42	110.80
4	D1	213	GLY	CA-C-O	5.45	125.88	119.45
56	A3	245	ILE	N-CA-C	-5.45	104.24	111.05
19	A2	507	THR	CA-C-N	5.45	131.50	121.70
19	A2	507	THR	C-N-CA	5.45	131.50	121.70
46	c2	36	PRO	C-N-CD	-5.45	108.62	120.60
4	D1	109	LEU	CA-C-N	5.44	125.99	120.38
4	D1	109	LEU	C-N-CA	5.44	125.99	120.38
4	D1	191	ARG	CA-C-O	-5.44	114.66	121.02
7	G1	10	VAL	CA-C-O	5.44	125.64	120.25
3	O1	261	PRO	N-CA-CB	5.44	108.96	103.25
6	R1	16	ILE	N-CA-C	-5.44	105.55	110.82
7	S1	12	HIS	CA-C-N	-5.44	115.87	123.10
7	S1	12	HIS	C-N-CA	-5.44	115.87	123.10
2	B1	309	VAL	N-CA-C	5.43	115.02	108.06
3	C1	195	VAL	CA-C-N	5.43	127.82	120.65
3	C1	195	VAL	C-N-CA	5.43	127.82	120.65
4	P1	48	TYR	CA-C-N	5.43	130.17	122.24
4	P1	48	TYR	C-N-CA	5.43	130.17	122.24
1	A1	373	THR	O-C-N	-5.42	115.47	120.51
1	A1	443	TRP	N-CA-C	5.42	119.20	107.49
5	E1	71	MET	CA-C-O	-5.42	114.68	120.42
1	M1	421	ALA	CB-CA-C	5.42	119.62	110.79
1	A1	142	ASP	CA-C-O	5.42	126.05	119.49
9	I1	51	CYS	N-CA-C	5.42	118.44	109.94
3	O1	32	ASN	CA-CB-CG	-5.42	107.19	112.60
6	F1	76	PRO	N-CA-CB	5.41	108.06	103.35
5	Q1	10	PHE	CA-CB-CG	-5.41	108.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F1	97	VAL	N-CA-CB	-5.41	102.31	111.23
7	G1	18	LEU	O-C-N	-5.41	115.53	122.94
3	C1	74	ASN	N-CA-C	5.41	116.93	109.15
12	22	40	ILE	CA-C-N	5.41	125.62	120.43
12	22	40	ILE	C-N-CA	5.41	125.62	120.43
3	C1	19	ILE	N-CA-C	5.40	116.06	110.82
1	A1	395	TRP	NE1-CE2-CZ2	-5.40	122.00	130.10
34	Q2	141	PRO	CA-C-N	5.39	128.90	120.82
34	Q2	141	PRO	C-N-CA	5.39	128.90	120.82
1	M1	435	ASN	CB-CG-OD1	-5.39	110.03	120.80
3	O1	201	HIS	CA-CB-CG	-5.39	108.41	113.80
5	E1	75	GLU	CA-C-O	-5.38	111.65	120.80
1	M1	390	ILE	N-CA-CB	5.38	118.75	111.21
3	O1	234	LEU	N-CA-C	-5.38	105.49	111.36
1	A1	161	THR	CA-C-N	5.38	125.20	119.28
1	A1	161	THR	C-N-CA	5.38	125.20	119.28
6	F1	90	LEU	O-C-N	5.38	129.54	122.33
7	G1	19	SER	CA-C-N	5.38	125.45	119.32
7	G1	19	SER	C-N-CA	5.38	125.45	119.32
3	C1	239	LEU	CD1-CG-CD2	-5.38	98.97	110.80
2	N1	92	VAL	N-CA-CB	-5.38	105.32	112.26
6	R1	36	THR	CA-C-O	5.38	126.17	119.12
1	A1	94	HIS	CB-CA-C	-5.37	104.06	110.94
1	M1	419	CYS	CA-CB-SG	5.37	126.76	114.40
1	M1	315	ALA	CA-C-O	5.37	126.46	120.82
1	A1	343	MET	O-C-N	-5.37	115.45	122.59
2	B1	89	ILE	O-C-N	-5.37	116.66	121.87
1	A1	428	ILE	CA-CB-CG1	5.37	119.52	110.40
1	M1	415	PHE	CA-C-O	5.36	126.27	119.78
56	A3	305	PHE	N-CA-C	5.36	118.92	112.38
4	P1	84	PRO	N-CA-CB	5.36	107.82	103.32
10	V1	19	THR	CA-CB-OG1	-5.36	101.56	109.60
56	A3	159	LEU	N-CA-C	-5.36	105.52	111.36
4	D1	191	ARG	CA-C-N	5.35	127.71	120.38
4	D1	191	ARG	C-N-CA	5.35	127.71	120.38
4	D1	32	VAL	CB-CA-C	-5.35	105.03	111.88
7	G1	50	PRO	N-CA-CB	5.35	108.27	103.08
3	O1	141	TRP	CA-C-N	5.35	125.88	119.94
3	O1	141	TRP	C-N-CA	5.35	125.88	119.94
2	B1	107	TYR	CA-C-N	5.35	128.83	120.75
2	B1	107	TYR	C-N-CA	5.35	128.83	120.75
10	J1	55	ILE	N-CA-C	5.35	118.95	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	170	PRO	N-CA-CB	5.34	108.86	103.25
2	N1	394	PRO	CA-C-N	5.34	126.52	119.84
2	N1	394	PRO	C-N-CA	5.34	126.52	119.84
3	C1	210	GLY	CA-C-N	5.34	132.09	122.43
3	C1	210	GLY	C-N-CA	5.34	132.09	122.43
9	U1	78	TYR	CA-CB-CG	5.34	123.50	113.90
3	C1	175	LEU	CA-C-O	5.33	126.08	119.79
3	O1	259	ALA	CA-C-O	-5.33	114.68	120.81
3	C1	15	ASN	CA-CB-CG	-5.32	107.28	112.60
3	C1	361	LEU	CA-C-O	-5.32	114.89	120.63
4	P1	209	LEU	O-C-N	-5.32	115.74	122.17
1	A1	436	ARG	CD-NE-CZ	-5.31	116.96	124.40
5	Q1	65	SER	O-C-N	-5.31	116.59	122.86
3	O1	115	ILE	CA-CB-CG1	5.31	119.43	110.40
5	Q1	172	ARG	CA-C-N	5.31	129.78	121.76
5	Q1	172	ARG	C-N-CA	5.31	129.78	121.76
2	B1	60	SER	CA-CB-OG	-5.31	100.49	111.10
4	D1	201	ARG	CD-NE-CZ	-5.31	116.97	124.40
3	O1	199	PHE	CD1-CG-CD2	-5.31	110.64	118.60
2	B1	75	LEU	O-C-N	5.30	129.17	122.65
32	O2	42	GLU	CA-C-N	5.30	124.57	120.33
32	O2	42	GLU	C-N-CA	5.30	124.57	120.33
56	A3	372	TYR	N-CA-C	-5.30	105.40	111.07
1	M1	145	MET	CA-C-N	-5.30	113.12	120.38
1	M1	145	MET	C-N-CA	-5.30	113.12	120.38
1	A1	342	TRP	CD2-CE2-CZ2	5.30	127.70	122.40
2	B1	33	LEU	O-C-N	5.29	129.30	123.16
1	M1	440	GLY	N-CA-C	-5.29	107.75	114.16
1	A1	153	LEU	O-C-N	5.29	127.74	122.08
3	C1	126	THR	N-CA-CB	5.29	118.40	109.78
2	N1	274	VAL	O-C-N	5.29	127.28	121.83
3	O1	106	SER	CA-C-O	5.29	125.88	119.38
1	M1	260	PRO	N-CA-CB	5.29	108.36	103.39
4	D1	239	PRO	CA-C-N	5.28	126.44	119.84
4	D1	239	PRO	C-N-CA	5.28	126.44	119.84
2	B1	133	ARG	NE-CZ-NH1	5.28	126.78	121.50
2	N1	162	ASN	CB-CA-C	5.28	119.51	110.74
1	M1	392	LEU	N-CA-CB	5.28	117.81	109.94
3	O1	45	ILE	O-C-N	5.28	127.38	121.94
3	C1	135	TRP	O-C-N	5.28	128.91	122.58
1	A1	358	LYS	CA-C-N	5.27	127.61	120.38
1	A1	358	LYS	C-N-CA	5.27	127.61	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	247	GLY	O-C-N	-5.27	117.08	122.19
5	Q1	91	TRP	CB-CG-CD1	-5.27	118.99	126.90
1	M1	25	VAL	CA-C-N	-5.27	114.32	122.59
1	M1	25	VAL	C-N-CA	-5.27	114.32	122.59
2	N1	70	ARG	NE-CZ-NH2	-5.27	114.46	119.20
3	C1	260	ASN	CA-CB-CG	5.26	117.86	112.60
3	O1	160	LEU	N-CA-C	5.26	117.43	111.11
1	M1	428	ILE	CA-C-O	5.26	125.40	120.14
5	Q1	136	ILE	N-CA-CB	-5.26	106.22	111.90
5	Q1	182	VAL	O-C-N	5.26	126.01	120.96
2	B1	94	GLY	CA-C-N	5.26	131.41	122.37
2	B1	94	GLY	C-N-CA	5.26	131.41	122.37
2	N1	107	TYR	CA-C-N	5.25	128.68	120.75
2	N1	107	TYR	C-N-CA	5.25	128.68	120.75
7	S1	17	SER	CA-C-O	-5.25	115.30	121.44
1	A1	391	PRO	CA-C-N	5.25	127.63	120.54
1	A1	391	PRO	C-N-CA	5.25	127.63	120.54
3	O1	226	ILE	CA-C-O	5.25	126.42	120.85
4	D1	46	VAL	N-CA-CB	5.25	116.98	111.00
3	C1	356	VAL	O-C-N	-5.25	116.78	121.87
6	F1	99	ARG	O-C-N	-5.25	116.08	122.11
4	D1	46	VAL	CA-C-O	5.24	126.79	120.65
51	j2	115	GLU	CA-C-N	5.24	131.14	121.70
51	j2	115	GLU	C-N-CA	5.24	131.14	121.70
1	M1	162	PRO	CB-CA-C	-5.24	103.51	112.26
2	N1	416	LYS	N-CA-C	5.24	117.74	111.71
5	Q1	39	VAL	N-CA-C	-5.24	105.60	110.53
6	F1	55	TYR	CA-C-O	-5.24	115.00	120.55
4	P1	191	ARG	CD-NE-CZ	-5.24	117.07	124.40
2	B1	353	SER	CA-C-N	5.24	129.84	121.62
2	B1	353	SER	C-N-CA	5.24	129.84	121.62
3	O1	219	PRO	CA-C-O	5.24	126.83	121.23
36	S2	199	VAL	N-CA-C	-5.23	102.80	107.56
8	H1	55	THR	CA-CB-OG1	5.23	117.44	109.60
58	C3	99	TRP	N-CA-C	-5.23	105.48	111.07
1	A1	357	GLY	N-CA-C	-5.22	106.08	112.77
3	C1	355	SER	O-C-N	-5.22	116.58	122.12
56	A3	262	SER	N-CA-C	-5.22	106.59	113.17
3	O1	91	PHE	CA-CB-CG	-5.22	108.58	113.80
4	D1	41	HIS	CA-CB-CG	5.22	119.02	113.80
1	M1	416	TYR	N-CA-CB	5.22	118.29	109.94
1	A1	311	ASN	CA-C-N	-5.21	115.85	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	311	ASN	C-N-CA	-5.21	115.85	122.37
1	A1	167	VAL	N-CA-C	-5.21	105.31	110.62
3	O1	39	ILE	CB-CG1-CD1	5.21	124.74	113.80
1	M1	277	ILE	CB-CA-C	-5.21	105.22	111.88
4	P1	137	PRO	CA-C-N	5.21	126.01	120.13
4	P1	137	PRO	C-N-CA	5.21	126.01	120.13
6	F1	61	ARG	NE-CZ-NH1	-5.21	116.30	121.50
2	N1	138	ALA	N-CA-C	5.21	117.36	111.11
4	P1	85	GLY	CA-C-N	5.21	128.61	120.75
4	P1	85	GLY	C-N-CA	5.21	128.61	120.75
3	C1	196	HIS	N-CA-CB	5.20	117.51	109.91
2	N1	430	LEU	N-CA-C	5.20	119.30	111.81
56	A3	353	LEU	N-CA-C	-5.20	105.69	111.36
1	A1	425	PHE	CA-C-N	5.20	130.03	121.87
1	A1	425	PHE	C-N-CA	5.20	130.03	121.87
3	C1	289	GLY	CA-C-O	-5.20	114.78	120.40
56	A3	6	TRP	N-CA-C	5.20	119.68	113.23
1	A1	403	ASP	CA-C-N	-5.20	112.41	120.31
1	A1	403	ASP	C-N-CA	-5.20	112.41	120.31
8	H1	60	ASP	N-CA-C	-5.20	106.62	113.12
3	C1	233	LEU	CA-C-O	-5.19	115.34	120.90
3	C1	276	PHE	N-CA-CB	5.19	119.27	110.49
3	O1	124	MET	N-CA-C	5.19	116.94	111.28
9	I1	69	SER	CA-C-O	-5.19	114.72	120.33
1	M1	350	THR	CA-C-O	-5.19	115.24	121.11
1	A1	390	ILE	N-CA-CB	5.19	118.47	111.21
4	D1	132	THR	CA-CB-OG1	-5.19	101.82	109.60
2	N1	57	TYR	CA-C-N	-5.19	114.10	122.81
2	N1	57	TYR	C-N-CA	-5.19	114.10	122.81
55	e2	67	ASP	N-CA-C	-5.19	102.66	110.70
2	N1	337	ILE	CA-C-O	-5.19	115.67	121.17
4	P1	175	THR	CA-C-O	5.19	124.10	119.59
63	H3	22	ASN	N-CA-C	5.19	117.75	109.81
2	B1	282	GLY	CA-C-N	5.18	126.32	119.84
2	B1	282	GLY	C-N-CA	5.18	126.32	119.84
4	P1	195	GLU	O-C-N	-5.18	116.60	121.32
6	F1	19	TRP	CA-C-N	5.18	127.54	120.54
6	F1	19	TRP	C-N-CA	5.18	127.54	120.54
1	A1	363	ASN	OD1-CG-ND2	5.18	127.78	122.60
2	B1	83	PHE	CA-CB-CG	-5.17	108.62	113.80
2	B1	394	PRO	N-CA-CB	5.17	108.10	103.08
6	F1	26	PHE	CA-CB-CG	5.17	118.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	329	MET	CA-C-N	-5.17	114.41	122.37
1	M1	329	MET	C-N-CA	-5.17	114.41	122.37
3	C1	230	LEU	CA-C-O	-5.17	115.39	120.82
3	C1	281	LEU	O-C-N	-5.17	116.65	122.03
8	T1	55	THR	CA-CB-OG1	5.17	117.36	109.60
2	B1	173	ALA	O-C-N	-5.17	114.74	122.39
2	N1	246	GLU	N-CA-C	5.17	117.80	107.62
14	42	84	LEU	N-CA-C	-5.16	108.74	114.62
56	A3	401	SER	N-CA-C	5.16	119.71	113.41
3	O1	79	ILE	N-CA-CB	5.16	116.24	110.51
61	F3	38	ALA	N-CA-C	5.16	117.78	110.50
3	O1	60	THR	CB-CA-C	-5.16	102.56	110.81
8	T1	55	THR	CA-C-O	5.15	126.01	120.70
4	P1	195	GLU	CA-C-O	5.15	127.23	120.74
25	G2	55	VAL	CA-C-N	5.15	131.38	121.54
25	G2	55	VAL	C-N-CA	5.15	131.38	121.54
2	N1	169	ARG	N-CA-C	-5.15	106.13	112.72
10	J1	54	HIS	CA-C-N	5.15	128.93	121.52
10	J1	54	HIS	C-N-CA	5.15	128.93	121.52
4	D1	38	SER	CA-C-N	5.15	127.69	120.28
4	D1	38	SER	C-N-CA	5.15	127.69	120.28
58	C3	107	ALA	CA-C-N	5.15	125.95	119.98
58	C3	107	ALA	C-N-CA	5.15	125.95	119.98
3	O1	35	SER	O-C-N	-5.15	115.75	122.59
5	E1	39	VAL	CB-CA-C	-5.14	105.30	111.88
7	S1	36	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	B1	429	ASN	CA-CB-CG	-5.14	107.46	112.60
1	M1	169	GLY	CA-C-N	5.14	125.14	119.90
1	M1	169	GLY	C-N-CA	5.14	125.14	119.90
4	P1	143	LEU	N-CA-C	5.14	116.55	107.61
65	J3	9	GLN	N-CA-C	-5.14	105.57	111.07
7	S1	33	GLY	O-C-N	5.13	127.11	122.18
1	A1	188	ARG	CA-C-N	-5.13	113.70	122.11
1	A1	188	ARG	C-N-CA	-5.13	113.70	122.11
7	G1	9	ARG	NE-CZ-NH1	-5.13	116.37	121.50
4	P1	195	GLU	CB-CG-CD	5.13	121.32	112.60
2	B1	256	ALA	CA-C-O	-5.13	115.31	121.11
1	M1	319	LEU	CA-C-O	5.13	125.96	120.32
12	22	273	ASN	CA-C-N	5.13	131.34	121.54
12	22	273	ASN	C-N-CA	5.13	131.34	121.54
2	N1	66	SER	N-CA-C	-5.12	105.59	111.07
2	N1	165	ALA	O-C-N	-5.12	115.39	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	153	PHE	CA-C-N	5.12	130.91	121.70
19	A2	153	PHE	C-N-CA	5.12	130.91	121.70
3	C1	119	LEU	CA-C-O	5.12	126.70	121.07
7	G1	12	HIS	N-CA-C	5.11	118.45	111.39
1	M1	295	ALA	CA-C-O	5.11	125.97	120.70
5	Q1	44	THR	OG1-CB-CG2	5.11	119.53	109.30
1	A1	306	SER	O-C-N	-5.11	115.79	122.59
4	D1	122	GLY	O-C-N	5.11	128.31	122.33
56	A3	377	PHE	N-CA-C	5.11	119.36	113.18
7	G1	19	SER	CA-C-O	-5.11	116.00	120.60
12	22	129	ILE	N-CA-C	-5.10	106.94	113.22
1	A1	436	ARG	NE-CZ-NH1	-5.10	116.40	121.50
4	P1	33	TYR	CA-C-O	-5.10	115.46	121.07
11	W1	36	THR	CA-C-O	5.10	129.47	120.80
2	B1	314	ALA	CA-C-O	-5.10	115.19	120.70
2	N1	125	ASN	OD1-CG-ND2	5.10	127.70	122.60
2	B1	21	PRO	N-CA-CB	5.10	108.61	103.00
1	M1	100	LYS	N-CA-C	-5.10	100.93	109.24
1	M1	157	ALA	CA-C-O	5.10	125.25	119.18
3	O1	26	ASN	CA-C-O	-5.10	115.54	121.15
9	I1	78	TYR	CA-CB-CG	5.10	123.08	113.90
4	P1	206	LEU	CA-C-N	-5.10	113.17	120.82
4	P1	206	LEU	C-N-CA	-5.10	113.17	120.82
5	Q1	40	THR	O-C-N	-5.10	116.79	122.09
1	A1	326	CYS	N-CA-C	5.09	117.75	109.24
3	O1	275	LEU	CA-C-O	-5.09	115.06	121.02
7	G1	15	THR	CA-C-O	-5.09	115.31	120.71
4	P1	153	PHE	CA-C-N	5.09	126.20	119.84
4	P1	153	PHE	C-N-CA	5.09	126.20	119.84
36	S2	305	VAL	N-CA-C	-5.09	107.79	112.83
2	B1	275	LEU	CB-CA-C	-5.09	102.86	110.90
1	M1	138	LEU	CA-C-N	5.08	127.34	120.38
1	M1	138	LEU	C-N-CA	5.08	127.34	120.38
1	M1	361	LEU	O-C-N	5.08	127.38	122.09
3	O1	221	HIS	CA-C-O	5.08	123.81	119.13
21	C2	124	ARG	CA-C-N	5.08	131.25	121.54
21	C2	124	ARG	C-N-CA	5.08	131.25	121.54
2	N1	59	ASN	OD1-CG-ND2	-5.08	117.52	122.60
4	P1	44	ASP	N-CA-C	5.08	116.90	111.36
8	H1	47	ARG	CA-CB-CG	5.08	124.26	114.10
3	C1	9	PRO	N-CA-CB	5.08	107.72	103.25
8	H1	55	THR	CB-CA-C	-5.08	102.91	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	414	TYR	CA-C-O	-5.08	113.80	119.79
6	R1	34	ASP	CA-CB-CG	-5.08	107.52	112.60
2	B1	170	ASN	N-CA-C	5.07	119.08	112.13
3	O1	197	LEU	N-CA-CB	5.07	117.58	110.12
3	O1	373	GLU	CA-C-O	5.07	126.11	120.63
4	P1	143	LEU	CB-CA-C	-5.07	103.74	110.79
1	A1	119	ASN	CA-CB-CG	-5.07	107.53	112.60
2	B1	266	SER	CA-C-O	-5.07	115.53	121.46
64	I3	2	THR	N-CA-C	5.07	116.12	108.46
2	N1	172	LEU	N-CA-CB	5.07	119.26	110.39
56	A3	70	VAL	N-CA-C	5.07	115.50	110.23
3	C1	325	PHE	CB-CA-C	-5.06	102.90	110.90
2	N1	354	ASN	CA-C-N	5.06	125.09	119.32
2	N1	354	ASN	C-N-CA	5.06	125.09	119.32
4	D1	110	PRO	N-CA-CB	5.06	107.99	103.08
3	O1	197	LEU	N-CA-C	-5.06	105.76	111.28
35	R2	154	GLN	CA-C-N	5.06	128.92	120.62
35	R2	154	GLN	C-N-CA	5.06	128.92	120.62
57	B3	66	THR	N-CA-C	-5.06	107.76	114.04
56	A3	378	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	M1	11	VAL	CA-C-O	5.06	124.42	119.71
1	M1	420	PRO	N-CA-C	5.06	119.16	111.11
32	O2	76	PRO	CA-C-N	5.06	131.21	121.54
32	O2	76	PRO	C-N-CA	5.06	131.21	121.54
4	D1	30	PHE	CA-CB-CG	-5.06	108.74	113.80
10	J1	51	LEU	N-CA-C	5.06	118.06	109.76
2	N1	21	PRO	N-CA-CB	5.06	108.56	103.00
7	S1	5	GLY	CA-C-N	5.06	130.16	122.37
7	S1	5	GLY	C-N-CA	5.06	130.16	122.37
57	B3	165	VAL	CA-C-N	5.06	126.16	119.84
57	B3	165	VAL	C-N-CA	5.06	126.16	119.84
5	Q1	62	MET	CA-C-N	5.05	131.19	121.54
5	Q1	62	MET	C-N-CA	5.05	131.19	121.54
3	O1	358	TYR	N-CA-C	5.05	117.17	111.11
7	G1	34	ILE	CA-C-N	5.05	124.65	119.05
7	G1	34	ILE	C-N-CA	5.05	124.65	119.05
3	C1	102	LEU	N-CA-C	5.04	117.67	111.82
3	O1	227	LYS	CA-C-O	-5.04	115.52	120.82
37	T2	83	LYS	N-CA-C	5.04	120.96	109.81
14	42	370	PRO	N-CA-C	5.04	116.85	110.70
20	B2	293	LEU	CA-C-N	5.04	131.16	121.54
20	B2	293	LEU	C-N-CA	5.04	131.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P1	111	PRO	N-CA-CB	5.04	107.79	103.31
1	A1	89	TYR	CA-CB-CG	5.03	122.96	113.90
3	C1	64	SER	N-CA-C	-5.03	105.69	111.07
4	P1	229	VAL	N-CA-C	-5.03	105.08	110.36
1	A1	163	LEU	CA-C-O	5.03	125.56	119.38
7	S1	73	ASN	CA-C-N	5.03	126.03	120.45
7	S1	73	ASN	C-N-CA	5.03	126.03	120.45
57	B3	12	ALA	N-CA-C	5.03	117.45	109.96
3	C1	143	ALA	O-C-N	-5.03	116.42	122.15
3	O1	185	LEU	CA-CB-CG	5.03	133.89	116.30
56	A3	2	PHE	N-CA-C	-5.03	105.69	111.07
3	C1	361	LEU	O-C-N	5.02	127.44	122.12
3	O1	216	ASP	CA-C-N	-5.02	115.41	122.94
3	O1	216	ASP	C-N-CA	-5.02	115.41	122.94
4	P1	150	ASN	CA-C-N	5.02	124.68	119.56
4	P1	150	ASN	C-N-CA	5.02	124.68	119.56
30	L2	39	THR	CA-C-N	5.02	131.13	121.54
30	L2	39	THR	C-N-CA	5.02	131.13	121.54
4	D1	150	ASN	CA-C-N	5.02	125.09	119.87
4	D1	150	ASN	C-N-CA	5.02	125.09	119.87
4	P1	92	PRO	N-CA-CB	5.02	107.32	103.30
1	M1	23	LEU	CA-C-N	-5.02	115.79	122.72
1	M1	23	LEU	C-N-CA	-5.02	115.79	122.72
1	M1	101	ALA	N-CA-C	5.02	116.15	108.52
3	O1	325	PHE	CG-CD2-CE2	5.02	129.23	120.70
6	F1	47	ILE	CB-CG1-CD1	5.02	124.33	113.80
53	62	405	ASN	CA-C-N	5.02	131.12	121.54
53	62	405	ASN	C-N-CA	5.02	131.12	121.54
2	B1	38	LEU	CB-CA-C	-5.02	104.90	111.82
1	M1	342	TRP	CD2-CE2-CZ2	-5.02	117.38	122.40
3	O1	190	MET	N-CA-CB	5.02	117.49	110.12
3	O1	326	TRP	CA-C-O	-5.01	115.22	120.63
56	A3	378	HIS	N-CA-C	-5.01	106.33	112.90
2	B1	126	VAL	CB-CA-C	-5.01	104.39	112.16
5	Q1	89	PHE	CA-C-N	-5.01	114.33	121.50
5	Q1	89	PHE	C-N-CA	-5.01	114.33	121.50
1	A1	328	HIS	CA-C-O	5.01	125.54	119.38
3	C1	329	VAL	CA-C-O	-5.01	114.52	120.78
4	P1	15	ARG	CA-C-N	5.01	125.66	120.60
4	P1	15	ARG	C-N-CA	5.01	125.66	120.60
61	F3	81	ARG	N-CA-C	5.01	117.61	109.24
4	D1	84	PRO	N-CA-CB	5.01	107.53	103.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M1	430	GLN	CG-CD-NE2	5.01	123.91	116.40
3	O1	54	HIS	CA-C-N	5.00	132.13	122.07
3	O1	54	HIS	C-N-CA	5.00	132.13	122.07

There are no chirality outliers.

All (133) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	12	199	ASP	Peptide
12	22	293	TYR	Peptide
12	22	45	MET	Peptide
14	42	224	PRO	Peptide
14	42	306	PRO	Peptide
14	42	369	LEU	Peptide
15	52	24	SER	Peptide
53	62	29	PRO	Peptide
53	62	352	ASP	Peptide
16	72	140	ALA	Peptide
16	72	170	GLU	Peptide
16	72	25	SER	Peptide
17	82	228	PRO	Peptide
18	92	150	GLU	Peptide
18	92	167	LYS	Peptide
18	92	75	LYS	Peptide
1	A1	118	GLN	Mainchain
1	A1	122	LEU	Mainchain
1	A1	196	VAL	Mainchain
1	A1	210	ASP	Mainchain
1	A1	239	SER	Mainchain
1	A1	242	CYS	Mainchain
1	A1	244	ARG	Mainchain
1	A1	256	ALA	Mainchain
1	A1	294	LEU	Mainchain
1	A1	306	SER	Mainchain
1	A1	345	LEU	Mainchain
1	A1	383	LEU	Mainchain
1	A1	53	ASN	Mainchain
19	A2	128	CYS	Peptide
19	A2	175	ARG	Peptide
19	A2	308	ARG	Peptide
19	A2	309	ASN	Peptide
19	A2	461	PRO	Peptide

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Mol	Chain	Res	Type	Group
19	A2	462	PHE	Peptide
2	B1	106	ALA	Mainchain
2	B1	159	VAL	Mainchain
2	B1	178	CYS	Mainchain
2	B1	239	TYR	Mainchain
2	B1	285	VAL	Mainchain
2	B1	335	ASP	Mainchain
2	B1	353	SER	Mainchain
2	B1	68	LEU	Mainchain
2	B1	99	THR	Mainchain
20	B2	290	GLY	Peptide
20	B2	291	VAL	Peptide
20	B2	328	ASP	Peptide
3	C1	134	PRO	Mainchain
3	C1	164	ILE	Mainchain
3	C1	20	ASP	Mainchain
3	C1	21	LEU	Mainchain
3	C1	222	PRO	Mainchain
3	C1	235	LEU	Mainchain
3	C1	281	LEU	Mainchain
3	C1	322	GLN	Mainchain
3	C1	326	TRP	Mainchain
3	C1	335	LEU	Mainchain
3	C1	355	SER	Mainchain
3	C1	362	ILE	Mainchain
3	C1	77	TRP	Mainchain
3	C1	83	HIS	Mainchain
4	D1	191	ARG	Mainchain
4	D1	217	PRO	Mainchain
4	D1	224	ARG	Mainchain
4	D1	229	VAL	Mainchain
4	D1	54	VAL	Mainchain
22	D2	161	GLY	Peptide
22	D2	162	TYR	Peptide
22	D2	186	CYS	Peptide
22	D2	188	PRO	Peptide
5	E1	20	ASP	Mainchain
23	E2	107	PRO	Peptide
23	E2	108	SER	Peptide
6	F1	16	ILE	Mainchain
6	F1	46	ALA	Mainchain
7	G1	15	THR	Mainchain

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Mol	Chain	Res	Type	Group
7	G1	73	ASN	Mainchain
9	I1	69	SER	Mainchain
10	J1	43	TYR	Mainchain
1	M1	100	LYS	Mainchain
1	M1	141	ASN	Mainchain
1	M1	290	LEU	Mainchain
40	M2	16	LEU	Peptide
2	N1	137	VAL	Mainchain
2	N1	144	LEU	Mainchain
2	N1	200	THR	Mainchain
2	N1	285	VAL	Mainchain
2	N1	290	ASN	Mainchain
2	N1	353	SER	Mainchain
3	O1	148	ASN	Mainchain
3	O1	159	ASN	Mainchain
3	O1	19	ILE	Mainchain
3	O1	355	SER	Mainchain
3	O1	55	TYR	Mainchain
3	O1	77	TRP	Mainchain
4	P1	202	LYS	Mainchain
4	P1	229	VAL	Mainchain
4	P1	24	THR	Mainchain
4	P1	46	VAL	Mainchain
33	P2	52	ASN	Peptide
5	Q1	125	GLU	Mainchain
5	Q1	135	LEU	Mainchain
5	Q1	186	GLU	Mainchain
5	Q1	195	VAL	Mainchain
5	Q1	32	ARG	Mainchain
5	Q1	36	SER	Mainchain
5	Q1	49	TYR	Mainchain
5	Q1	9	ASP	Mainchain
5	Q1	97	PHE	Mainchain
34	Q2	169	PHE	Peptide
34	Q2	91	TYR	Peptide
35	R2	271	TYR	Peptide
35	R2	333	PRO	Peptide
7	S1	17	SER	Mainchain
7	S1	18	LEU	Mainchain
7	S1	34	ILE	Mainchain
36	S2	275	ASN	Peptide
8	T1	40	CYS	Mainchain

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Mol	Chain	Res	Type	Group
37	T2	83	LYS	Peptide
9	U1	72	VAL	Mainchain
39	V2	10	MET	Peptide
39	V2	142	TRP	Peptide
39	V2	72	MET	Peptide
11	W1	24	TRP	Mainchain
42	Y2	89	TYR	Peptide
45	b2	110	TRP	Peptide
55	e2	115	ASN	Mainchain
55	e2	81	ARG	Peptide
55	e2	87	ASP	Peptide
55	e2	97	LEU	Peptide
48	f2	109	PRO	Peptide
49	h2	80	PRO	Peptide
49	h2	81	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	3356	0	3263	486	0
1	M1	3356	0	3263	470	0
2	B1	3141	0	3123	417	0
2	N1	3141	0	3123	423	0
3	C1	3011	0	3077	463	0
3	O1	3011	0	3077	430	0
4	D1	1919	0	1868	309	0
4	P1	1919	0	1868	295	0
5	E1	566	0	564	67	0
5	Q1	1518	0	1499	266	0
6	F1	916	0	911	96	0
6	R1	916	0	911	95	0
7	G1	682	0	679	108	0
7	S1	682	0	679	99	0
8	H1	524	0	504	69	0
8	T1	524	0	504	76	0
9	I1	248	0	265	53	0
9	U1	248	0	265	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J1	511	0	518	73	0
10	V1	511	0	518	78	0
11	K1	164	0	161	29	0
11	W1	164	0	161	28	0
12	22	2582	0	2612	35	0
13	32	719	0	741	9	0
14	42	3447	0	3442	48	0
15	52	697	0	708	14	0
16	72	1186	0	1123	13	0
17	82	2965	0	2595	73	0
18	92	1535	0	1491	62	0
19	A2	5183	0	5174	337	0
20	B2	3076	0	3041	95	0
21	C2	1705	0	1645	29	0
22	D2	1200	0	1195	27	0
23	E2	1388	0	1340	43	0
24	F2	183	0	132	6	0
25	G2	981	0	965	35	0
26	H2	780	0	753	12	0
27	I2	532	0	513	48	0
28	J2	530	0	503	7	0
29	K2	652	0	636	32	0
30	L2	602	0	592	9	0
31	N2	862	0	868	10	0
32	O2	925	0	907	9	0
33	P2	698	0	659	23	0
34	Q2	1345	0	1282	26	0
35	R2	2334	0	2258	51	0
36	S2	2299	0	2028	23	0
37	T2	942	0	890	11	0
38	U2	734	0	628	91	0
39	V2	1093	0	1048	22	0
40	M2	642	0	642	7	0
40	W2	596	0	553	6	0
41	X2	372	0	314	4	0
42	Y2	409	0	318	7	0
43	Z2	493	0	395	6	0
44	a2	857	0	765	11	0
45	b2	1032	0	954	14	0
46	c2	617	0	492	8	0
47	d2	708	0	514	9	0
48	f2	1156	0	892	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	h2	721	0	632	13	0
50	i2	277	0	240	4	0
51	j2	892	0	835	10	0
52	l2	2442	0	2563	72	0
53	62	4765	0	4894	62	0
54	g2	1351	0	1262	18	0
55	e2	864	0	567	26	0
56	A3	4025	0	4003	91	0
57	B3	1822	0	1834	73	0
58	C3	2124	0	2042	51	0
59	D3	1195	0	1183	33	0
60	E3	878	0	868	21	0
61	F3	748	0	728	22	0
62	G3	671	0	645	29	0
63	H3	628	0	582	21	0
64	I3	598	0	612	16	0
65	J3	441	0	439	14	0
66	K3	384	0	366	12	0
67	L3	386	0	388	9	0
68	M3	335	0	352	12	0
69	C1	86	0	60	18	0
69	O1	86	0	60	25	0
70	D1	43	0	30	5	0
70	P1	43	0	30	5	0
71	92	4	0	0	0	0
71	A2	4	0	0	0	0
71	Q1	4	0	0	0	0
72	22	41	0	59	3	0
72	42	41	0	59	1	0
72	B2	51	0	82	1	0
73	42	82	0	114	2	0
74	82	31	0	19	2	0
75	82	8	0	0	0	0
75	A2	16	0	0	12	0
75	D2	8	0	0	0	0
75	E2	16	0	0	0	0
76	F3	1	0	0	0	0
76	I2	1	0	0	1	0
77	R2	48	0	23	3	0
78	S2	47	0	71	0	0
78	j2	39	0	55	1	0
79	A3	120	0	108	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	A3	1	0	0	0	0
80	B3	2	0	0	0	0
81	A3	1	0	0	0	0
All	All	105456	0	102214	5423	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 26.

All (5423) 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)
18:92:42:ARG:NH1	19:A2:199:GLY:HA2	1.33	1.42
19:A2:306:MET:SD	38:U2:139:PRO:HG3	1.60	1.39
52:12:126:LYS:HD3	52:12:127:TYR:N	1.31	1.38
19:A2:227:PRO:HD2	75:A2:802:SF4:S1	1.63	1.37
35:R2:170:LEU:O	35:R2:328:ILE:HD11	1.21	1.36
19:A2:424:HIS:HA	25:G2:170:THR:OG1	1.24	1.33
19:A2:422:TRP:O	25:G2:169:ARG:HD2	1.15	1.31
19:A2:557:ARG:NH2	38:U2:144:TYR:OH	1.64	1.30
35:R2:170:LEU:O	35:R2:328:ILE:CD1	1.78	1.28
19:A2:312:GLY:HA3	38:U2:143:PRO:C	1.57	1.25
77:R2:601:NAP:C1D	77:R2:601:NAP:O4D	1.63	1.24
52:12:75:PRO:HG3	52:12:223:PHE:CZ	1.74	1.22
9:I1:72:VAL:HB	9:I1:73:PRO:HD3	1.20	1.20
19:A2:312:GLY:O	38:U2:141:SER:O	1.61	1.18
7:S1:50:PRO:HB2	7:S1:51:PRO:HD3	1.25	1.17
4:D1:224:ARG:HB2	7:G1:25:ALA:HB1	1.27	1.17
19:A2:314:LEU:CD2	38:U2:140:PRO:HD2	1.74	1.17
7:G1:72:LYS:HB3	7:G1:75:ALA:HB2	1.19	1.16
2:B1:77:THR:HG22	2:B1:130:PRO:HA	1.25	1.15
19:A2:312:GLY:HA3	38:U2:143:PRO:O	0.97	1.15
5:Q1:114:VAL:HA	5:Q1:117:LEU:HD12	1.24	1.14
1:M1:426:GLY:CA	1:M1:428:ILE:HG13	1.78	1.14
11:W1:29:ALA:O	11:W1:33:VAL:HG23	1.46	1.14
55:e2:36:MET:HA	55:e2:77:LYS:CE	1.78	1.13
1:A1:428:ILE:HG22	1:A1:431:LEU:HB2	1.29	1.13
19:A2:312:GLY:CA	38:U2:143:PRO:O	1.94	1.13
1:M1:67:THR:HG23	1:M1:70:ARG:H	1.13	1.13
2:B1:60:SER:HB3	2:N1:429:ASN:HD21	0.96	1.12
4:P1:83:ARG:HB3	4:P1:84:PRO:HD2	1.14	1.12
35:R2:328:ILE:HG22	35:R2:329:LEU:H	1.09	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:428:ILE:HG22	1:M1:431:LEU:HB2	1.19	1.11
19:A2:422:TRP:O	25:G2:169:ARG:CD	1.99	1.11
3:C1:129:MET:HG2	3:C1:178:PHE:HD2	1.03	1.11
4:P1:83:ARG:HB3	4:P1:84:PRO:CD	1.81	1.10
18:92:42:ARG:CZ	19:A2:199:GLY:HA2	1.80	1.10
55:e2:36:MET:HA	55:e2:77:LYS:HE3	1.11	1.10
5:Q1:15:ARG:HB2	5:Q1:16:PRO:HD2	1.19	1.10
19:A2:557:ARG:CZ	38:U2:144:TYR:OH	1.99	1.09
17:82:225:LEU:CD2	19:A2:93:ALA:HB3	1.80	1.09
1:M1:428:ILE:HG21	1:M1:431:LEU:HD22	1.35	1.09
3:C1:77:TRP:CZ3	3:C1:78:ILE:HG23	1.88	1.08
1:M1:403:ASP:HB3	1:M1:406:VAL:HG23	1.34	1.08
36:S2:200:PRO:HG3	36:S2:223:GLN:HE22	1.17	1.08
11:W1:30:VAL:O	11:W1:34:TRP:CD1	2.05	1.08
5:Q1:76:ILE:CG2	5:Q1:194:ILE:HG12	1.84	1.08
19:A2:144:MET:HA	20:B2:380:HIS:NE2	1.68	1.08
4:P1:181:GLN:HG2	8:T1:77:LEU:HD22	1.29	1.07
18:92:124:ARG:NH1	19:A2:209:TYR:OH	1.87	1.07
19:A2:161:GLU:N	27:I2:102:ASN:HD22	1.52	1.07
20:B2:94:VAL:HG12	20:B2:115:LEU:HD22	1.27	1.07
3:O1:26:ASN:HD21	3:O1:207:ASN:HB2	1.15	1.07
3:O1:206:ASN:HB2	3:O1:313:ARG:NH2	1.68	1.07
18:92:95:ILE:HD11	19:A2:210:ILE:CG2	1.84	1.07
3:C1:206:ASN:HB2	3:C1:313:ARG:NH2	1.70	1.07
1:A1:41:ILE:HG13	1:A1:195:MET:HE3	1.36	1.06
9:U1:72:VAL:HB	9:U1:73:PRO:HD3	1.36	1.06
1:A1:67:THR:HG23	1:A1:70:ARG:H	0.94	1.06
19:A2:314:LEU:HD23	38:U2:140:PRO:HD2	1.09	1.06
1:M1:24:ARG:HB2	1:M1:196:VAL:HG22	1.37	1.06
2:N1:200:THR:HG22	2:N1:203:ARG:HD2	1.36	1.06
55:e2:75:TYR:HB3	55:e2:78:LEU:CB	1.83	1.06
1:A1:64:PHE:CE1	1:A1:86:LEU:HG	1.90	1.05
3:C1:310:SER:HA	3:C1:374:ASN:HD21	1.12	1.05
2:N1:305:GLN:HB2	2:N1:306:PRO:HD3	1.34	1.05
3:O1:310:SER:HA	3:O1:374:ASN:HD21	1.21	1.05
9:I1:72:VAL:HB	9:I1:73:PRO:CD	1.86	1.05
5:Q1:96:LEU:HD21	5:Q1:195:VAL:HG21	1.38	1.05
17:82:418:GLN:HE21	19:A2:115:GLY:CA	1.70	1.05
5:Q1:109:GLU:HG2	5:Q1:167:ALA:HB3	1.37	1.04
1:A1:18:GLN:HE21	1:A1:22:GLY:HA2	1.19	1.04
4:D1:181:GLN:HG2	8:H1:77:LEU:HD22	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:426:GLY:CA	1:A1:428:ILE:HG13	1.87	1.04
3:C1:170:VAL:HG13	3:C1:174:THR:HG21	1.34	1.04
7:G1:34:ILE:HB	7:G1:35:PRO:HD3	1.39	1.04
7:S1:72:LYS:HB3	7:S1:75:ALA:HB2	1.39	1.04
3:C1:129:MET:HG2	3:C1:178:PHE:CD2	1.93	1.04
4:D1:83:ARG:HB3	4:D1:84:PRO:CD	1.86	1.04
5:Q1:75:GLU:O	5:Q1:194:ILE:HA	1.57	1.04
2:B1:283:PRO:HG3	9:I1:55:LEU:HD22	1.39	1.03
2:B1:429:ASN:HD21	2:N1:60:SER:HB3	1.15	1.03
20:B2:82:LEU:HD21	52:12:126:LYS:HG3	1.04	1.03
2:B1:24:LEU:H	2:B1:24:LEU:HD12	1.23	1.03
5:Q1:134:ILE:HD11	5:Q1:185:TYR:CD2	1.94	1.03
10:J1:18:SER:HB3	11:K1:23:LEU:HD12	1.42	1.02
52:12:75:PRO:CG	52:12:223:PHE:CZ	2.42	1.02
2:B1:95:LYS:HE3	9:I1:70:LEU:HD22	1.41	1.02
3:C1:202:GLU:OE2	3:O1:10:LEU:HB2	1.59	1.02
47:d2:25:PHE:CD2	47:d2:40:VAL:CB	2.42	1.02
6:R1:28:LYS:HD2	6:R1:74:ILE:HD11	1.42	1.01
19:A2:161:GLU:HB3	27:I2:102:ASN:ND2	1.74	1.01
3:C1:16:ASN:ND2	3:C1:20:ASP:OD2	1.93	1.01
1:M1:428:ILE:HG22	1:M1:431:LEU:CB	1.91	1.01
2:B1:165:ALA:HA	2:B1:173:ALA:HB1	1.39	1.01
4:P1:224:ARG:HB2	7:S1:25:ALA:HB1	1.40	1.01
2:B1:60:SER:CB	2:N1:429:ASN:HD21	1.72	1.01
3:C1:221:HIS:HB3	3:C1:222:PRO:HD3	1.42	1.00
3:O1:174:THR:HG23	3:O1:178:PHE:HE2	1.25	1.00
2:B1:52:LYS:HB2	2:B1:203:ARG:HB3	1.39	1.00
17:82:225:LEU:HD22	19:A2:93:ALA:HB3	1.04	1.00
1:M1:18:GLN:HE21	1:M1:22:GLY:HA2	1.23	1.00
2:N1:166:ALA:HB2	2:N1:244:ILE:HG13	1.39	1.00
52:12:126:LYS:CD	52:12:127:TYR:N	2.24	1.00
19:A2:312:GLY:CA	38:U2:143:PRO:C	2.31	1.00
4:D1:74:PRO:HB2	4:D1:79:GLU:HB2	1.43	1.00
3:C1:100:ARG:HH21	69:C1:402:HEM:HBD1	1.26	1.00
4:D1:83:ARG:HB3	4:D1:84:PRO:HD2	1.00	0.99
4:D1:83:ARG:CB	4:D1:84:PRO:HD2	1.90	0.99
3:C1:206:ASN:HB2	3:C1:313:ARG:HH21	1.24	0.99
1:M1:143:THR:HG21	9:U1:48:SER:H	1.24	0.99
3:C1:264:THR:HG21	5:Q1:144:CYS:HB3	1.44	0.99
3:C1:10:LEU:HB2	3:O1:202:GLU:OE2	1.59	0.99
3:C1:26:ASN:HB2	6:F1:69:SER:OG	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:100:ARG:HH21	69:O1:402:HEM:HBD1	1.23	0.99
17:82:418:GLN:NE2	19:A2:115:GLY:HA2	1.77	0.99
19:A2:613:PRO:CB	38:U2:134:ILE:HG21	1.91	0.99
1:M1:64:PHE:CE1	1:M1:86:LEU:HG	1.98	0.99
9:U1:70:LEU:HD21	9:U1:73:PRO:HD2	1.40	0.99
3:O1:16:ASN:ND2	3:O1:20:ASP:OD2	1.96	0.99
5:Q1:86:ASN:HB2	5:Q1:99:ARG:HD2	1.45	0.99
8:T1:21:ARG:HB3	8:T1:65:ARG:HH21	1.26	0.99
17:82:225:LEU:HD22	19:A2:93:ALA:CB	1.92	0.99
4:D1:118:ARG:HG3	4:D1:194:ALA:HB1	1.44	0.98
1:A1:408:ARG:HH22	11:K1:15:ARG:NE	1.61	0.98
3:C1:179:PHE:HE2	3:O1:179:PHE:HE2	1.05	0.98
20:B2:82:LEU:CD2	52:12:126:LYS:HG3	1.93	0.98
6:F1:51:PRO:HG2	6:F1:54:LEU:HD23	1.44	0.98
52:12:75:PRO:HA	52:12:223:PHE:HE1	1.26	0.98
2:B1:200:THR:HG22	2:B1:203:ARG:HD2	1.44	0.98
2:B1:429:ASN:HD21	2:N1:60:SER:CB	1.74	0.98
17:82:383:THR:HG23	19:A2:75:CYS:HA	1.45	0.98
1:M1:417:ASP:OD2	10:V1:10:TYR:OH	1.82	0.98
4:P1:74:PRO:HB2	4:P1:79:GLU:HB2	1.46	0.98
19:A2:613:PRO:HB3	38:U2:134:ILE:HG21	1.45	0.98
2:N1:111:CYS:HB3	2:N1:119:LEU:HD22	1.46	0.98
20:B2:82:LEU:HD21	52:12:126:LYS:CG	1.93	0.98
1:A1:383:LEU:HD22	1:A1:388:ARG:HA	1.45	0.98
2:B1:24:LEU:HG	2:B1:38:LEU:HD11	1.42	0.98
1:A1:304:CYS:HB3	1:A1:334:MET:SD	2.04	0.97
3:C1:174:THR:HG23	3:C1:178:PHE:CE1	1.98	0.97
3:O1:345:HIS:HB3	3:O1:346:PRO:HD3	1.42	0.97
1:A1:343:MET:HE1	1:A1:416:TYR:CD2	1.98	0.97
55:e2:70:THR:O	55:e2:72:TYR:N	1.96	0.97
70:P1:301:HEC:HHD	70:P1:301:HEC:HBC2	1.45	0.97
1:M1:408:ARG:HH22	11:W1:15:ARG:NE	1.61	0.97
2:N1:24:LEU:HG	2:N1:38:LEU:HD11	1.43	0.97
4:P1:158:ILE:CD1	4:P1:160:MET:HB2	1.94	0.97
18:92:42:ARG:NH1	19:A2:199:GLY:CA	2.27	0.97
1:A1:24:ARG:HB2	1:A1:196:VAL:HG22	1.43	0.97
1:A1:403:ASP:HB3	1:A1:406:VAL:HG23	1.46	0.97
1:M1:392:LEU:HA	1:M1:395:TRP:CD1	1.99	0.97
1:M1:42:ASP:HB3	1:M1:384:LEU:HD22	1.45	0.97
18:92:110:MET:SD	19:A2:194:ASP:O	2.23	0.97
3:O1:77:TRP:CZ3	3:O1:78:ILE:HG23	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:302:LEU:HA	38:U2:137:TRP:CB	1.95	0.96
2:N1:283:PRO:HG3	9:U1:55:LEU:HD22	1.47	0.96
2:B1:67:HIS:HD2	2:B1:144:LEU:HD22	1.27	0.96
1:A1:67:THR:HG23	1:A1:70:ARG:N	1.79	0.96
3:C1:26:ASN:HD21	3:C1:207:ASN:HB2	1.28	0.96
6:F1:50:LEU:HB2	6:F1:55:TYR:HB2	1.45	0.96
27:I2:104:ASP:O	27:I2:105:LYS:HB3	1.63	0.96
3:O1:106:SER:HB3	69:O1:402:HEM:HBD2	1.46	0.96
3:C1:115:ILE:HG21	3:C1:196:HIS:HB2	1.48	0.95
9:I1:70:LEU:HD21	9:I1:73:PRO:HD2	1.48	0.95
7:G1:36:ASN:HA	7:G1:39:ARG:HD3	1.46	0.95
2:B1:60:SER:HB3	2:N1:429:ASN:ND2	1.81	0.95
18:92:42:ARG:HH12	19:A2:199:GLY:HA2	1.23	0.95
19:A2:313:LEU:CD2	38:U2:142:THR:CB	2.43	0.95
17:82:383:THR:CG2	19:A2:75:CYS:HA	1.95	0.95
20:B2:94:VAL:HG12	20:B2:115:LEU:CD2	1.96	0.95
7:S1:31:SER:O	7:S1:35:PRO:HD2	1.65	0.95
2:B1:304:HIS:CD2	2:B1:306:PRO:HD2	2.01	0.95
52:12:75:PRO:HA	52:12:223:PHE:CE1	2.02	0.95
2:B1:305:GLN:HB2	2:B1:306:PRO:HD3	1.46	0.95
2:N1:51:ILE:HG21	2:N1:199:PHE:HA	1.48	0.95
20:B2:97:LEU:H	20:B2:97:LEU:HD12	1.31	0.95
2:B1:159:VAL:HG12	2:B1:160:ILE:HD13	1.48	0.95
3:O1:210:GLY:HA3	3:O1:314:SER:HB2	1.46	0.95
2:N1:77:THR:HG22	2:N1:130:PRO:HA	1.46	0.95
3:O1:174:THR:HG23	3:O1:178:PHE:CE2	2.00	0.95
1:M1:61:HIS:NE2	1:M1:134:ILE:HD11	1.82	0.94
2:B1:51:ILE:HG21	2:B1:199:PHE:HA	1.49	0.94
35:R2:328:ILE:CG2	35:R2:329:LEU:H	1.80	0.94
56:A3:365:ILE:HD12	57:B3:87:MET:HE1	1.48	0.94
3:O1:108:THR:HB	3:O1:313:ARG:HH11	1.31	0.94
4:P1:158:ILE:HD13	4:P1:160:MET:HB2	1.49	0.94
1:M1:21:ASN:HB3	1:M1:217:SER:HB3	1.46	0.94
4:P1:178:THR:HB	4:P1:181:GLN:HG3	1.46	0.94
1:A1:61:HIS:CD2	1:A1:134:ILE:HD11	2.03	0.94
3:C1:240:MET:HA	3:C1:243:VAL:HG12	1.49	0.94
3:C1:310:SER:HB3	3:C1:318:ARG:NH1	1.82	0.94
19:A2:527:ASP:O	29:K2:56:ARG:NH2	2.01	0.94
7:G1:9:ARG:NH2	7:G1:11:ARG:HD2	1.83	0.94
2:N1:248:ASN:HB2	2:N1:428:GLY:HA2	1.46	0.94
3:O1:252:ASP:HB3	3:O1:253:PRO:HD3	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:50:THR:HG22	8:H1:52:GLU:H	1.28	0.94
2:N1:67:HIS:HD2	2:N1:144:LEU:HD22	1.30	0.94
4:D1:165:TYR:O	4:D1:168:VAL:HG23	1.67	0.94
19:A2:674:LEU:HD12	29:K2:46:LYS:HE2	1.49	0.94
3:C1:174:THR:HG23	3:C1:178:PHE:HE1	1.31	0.93
5:Q1:85:LYS:HG2	5:Q1:86:ASN:H	1.33	0.93
2:N1:29:LEU:HB3	2:N1:30:PRO:HD2	1.48	0.93
2:N1:132:PHE:CD2	2:N1:191:LEU:HD13	2.04	0.93
3:O1:135:TRP:HH2	3:O1:170:VAL:HG12	1.32	0.93
9:U1:72:VAL:HB	9:U1:73:PRO:CD	1.98	0.93
62:G3:5:LYS:HZ3	62:G3:6:GLY:H	1.02	0.93
1:A1:133:VAL:HG12	1:A1:134:ILE:HD13	1.48	0.93
1:A1:67:THR:CG2	1:A1:70:ARG:H	1.81	0.93
19:A2:557:ARG:NE	38:U2:144:TYR:OH	2.01	0.93
19:A2:306:MET:SD	38:U2:139:PRO:CG	2.56	0.93
2:N1:316:TYR:OH	9:U1:64:LEU:HD23	1.67	0.93
17:82:418:GLN:HE21	19:A2:115:GLY:HA2	1.30	0.92
1:A1:346:CYS:HB3	1:A1:412:SER:OG	1.68	0.92
1:A1:144:SER:O	1:A1:148:VAL:HG23	1.69	0.92
2:B1:77:THR:HG22	2:B1:130:PRO:CA	1.99	0.92
2:N1:207:ILE:HD11	2:N1:383:GLY:HA2	1.49	0.92
19:A2:161:GLU:OE1	27:I2:102:ASN:ND2	2.00	0.92
56:A3:449:MET:SD	57:B3:5:MET:HE2	2.09	0.92
1:A1:91:THR:HG22	1:A1:93:GLU:H	1.35	0.92
2:B1:111:CYS:HB3	2:B1:119:LEU:HD22	1.49	0.92
2:B1:385:GLN:HG2	9:I1:62:ARG:HH12	1.35	0.92
1:M1:61:HIS:CE1	1:M1:134:ILE:HD11	2.04	0.92
1:A1:417:ASP:OD2	10:J1:10:TYR:OH	1.88	0.91
3:O1:26:ASN:ND2	3:O1:207:ASN:HB2	1.85	0.91
1:M1:91:THR:HG22	1:M1:93:GLU:H	1.32	0.91
1:A1:392:LEU:HA	1:A1:395:TRP:CD1	2.05	0.91
4:D1:74:PRO:HG2	4:D1:82:MET:SD	2.10	0.91
4:P1:23:HIS:HA	4:P1:26:ILE:HD12	1.49	0.91
5:Q1:15:ARG:HH21	5:Q1:32:ARG:HG3	1.35	0.91
5:Q1:109:GLU:CG	5:Q1:167:ALA:HB3	2.01	0.91
2:B1:162:ASN:HD22	2:B1:244:ILE:CG2	1.83	0.91
17:82:381:GLN:O	19:A2:74:ASN:HB2	1.70	0.91
19:A2:424:HIS:CA	25:G2:170:THR:OG1	2.17	0.90
19:A2:266:ARG:NH2	23:E2:130:ILE:O	2.05	0.90
1:A1:69:ASN:O	1:A1:71:PRO:HD3	1.70	0.90
1:A1:143:THR:HG21	9:I1:48:SER:H	1.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:12:75:PRO:CD	52:12:223:PHE:HZ	1.85	0.90
3:C1:34:GLY:O	3:C1:37:LEU:HB2	1.72	0.90
2:B1:29:LEU:HB3	2:B1:30:PRO:HD2	1.54	0.90
19:A2:129:PRO:HD2	27:I2:114:TYR:OH	1.70	0.90
2:B1:342:ASN:O	2:B1:345:LYS:HB2	1.72	0.90
3:C1:252:ASP:HB3	3:C1:253:PRO:HD3	1.52	0.90
3:O1:122:THR:HG22	3:O1:189:ILE:HD11	1.51	0.90
3:O1:206:ASN:HB2	3:O1:313:ARG:HH21	1.28	0.90
5:Q1:15:ARG:NH2	5:Q1:32:ARG:HG3	1.87	0.90
17:82:390:ASP:OD2	19:A2:202:ASN:HB2	1.70	0.89
1:M1:383:LEU:HD22	1:M1:388:ARG:HA	1.54	0.89
3:O1:221:HIS:HB3	3:O1:222:PRO:HD3	1.52	0.89
2:B1:258:VAL:HG11	2:B1:321:LEU:HB3	1.53	0.89
4:D1:178:THR:OG1	4:D1:181:GLN:NE2	2.05	0.89
6:F1:47:ILE:O	6:F1:50:LEU:HG	1.72	0.89
18:92:110:MET:HE2	19:A2:195:LEU:C	1.96	0.89
3:C1:103:TYR:HA	3:C1:315:MET:HE3	1.52	0.89
4:P1:165:TYR:O	4:P1:168:VAL:HG23	1.73	0.89
19:A2:137:CYS:HB3	75:A2:801:SF4:S4	2.12	0.89
19:A2:424:HIS:HA	25:G2:170:THR:HG1	1.32	0.89
52:12:126:LYS:HD3	52:12:127:TYR:H	1.11	0.89
1:A1:236:PHE:CE2	1:A1:258:GLU:HB3	2.07	0.89
4:D1:231:LYS:HD2	6:F1:71:ARG:HG2	1.52	0.89
1:A1:426:GLY:H	1:A1:428:ILE:CG1	1.85	0.89
3:C1:266:PRO:HB3	5:Q1:160:CYS:HA	1.54	0.89
1:M1:236:PHE:CE2	1:M1:258:GLU:HB3	2.07	0.89
7:S1:50:PRO:HB2	7:S1:51:PRO:CD	2.03	0.89
1:M1:158:PHE:CE1	1:M1:317:THR:HG21	2.08	0.89
2:N1:52:LYS:HB2	2:N1:203:ARG:HB3	1.54	0.89
19:A2:302:LEU:CA	38:U2:137:TRP:HB2	2.03	0.89
1:A1:40:TRP:CZ2	1:A1:377:GLU:HA	2.08	0.88
7:S1:9:ARG:NH2	7:S1:11:ARG:HD2	1.87	0.88
1:M1:45:SER:HB3	1:M1:92:ARG:HA	1.53	0.88
2:N1:385:GLN:HG2	9:U1:62:ARG:HH12	1.38	0.88
8:H1:73:LEU:HD23	8:H1:74:PHE:N	1.89	0.88
4:D1:176:PRO:HB2	4:D1:181:GLN:HE22	1.37	0.88
3:O1:361:LEU:HD23	3:O1:365:LEU:HD12	1.54	0.88
20:B2:91:ALA:HB2	20:B2:193:ASP:OD2	1.73	0.88
22:D2:114:ARG:HG3	22:D2:114:ARG:HH21	1.39	0.88
1:A1:408:ARG:NH1	11:K1:15:ARG:HE	1.71	0.88
2:B1:406:ALA:HB3	2:B1:409:ASP:HB2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:182:CYS:N	75:A2:802:SF4:S2	2.47	0.88
18:92:42:ARG:NH2	19:A2:203:ASP:O	2.07	0.88
1:A1:156:THR:HG23	1:A1:239:SER:OG	1.73	0.88
2:N1:123:LEU:O	2:N1:127:THR:HG22	1.74	0.88
4:P1:118:ARG:HG3	4:P1:194:ALA:HB1	1.55	0.88
52:12:25:ARG:HG2	52:12:25:ARG:HH11	1.36	0.88
1:A1:343:MET:HE1	1:A1:416:TYR:HD2	1.33	0.87
1:M1:426:GLY:HA3	1:M1:428:ILE:HG13	1.54	0.87
2:N1:304:HIS:CD2	2:N1:306:PRO:HD2	2.08	0.87
35:R2:328:ILE:HG22	35:R2:329:LEU:N	1.80	0.87
3:C1:179:PHE:CE2	3:O1:179:PHE:HE2	1.92	0.87
3:C1:185:LEU:HB3	3:C1:186:PRO:HD3	1.55	0.87
11:K1:29:ALA:O	11:K1:33:VAL:HG12	1.73	0.87
18:92:95:ILE:CD1	19:A2:210:ILE:CG2	2.53	0.87
58:C3:112:LEU:HG	58:C3:118:PRO:HB3	1.55	0.87
19:A2:313:LEU:HD21	38:U2:142:THR:CB	2.05	0.87
5:E1:15:ARG:HB2	5:E1:16:PRO:HD2	1.57	0.87
1:A1:260:PRO:HD3	1:A1:414:TYR:CE1	2.10	0.87
2:N1:305:GLN:HB2	2:N1:306:PRO:CD	2.05	0.87
3:O1:108:THR:HB	3:O1:313:ARG:NH1	1.89	0.87
2:N1:347:ILE:O	2:N1:411:ILE:HG23	1.75	0.86
5:Q1:15:ARG:HB2	5:Q1:16:PRO:CD	2.02	0.86
3:C1:6:LYS:HE2	3:C1:16:ASN:HD21	1.38	0.86
3:C1:170:VAL:HG13	3:C1:174:THR:CG2	2.04	0.86
3:C1:179:PHE:HE2	3:O1:179:PHE:CE2	1.92	0.86
1:M1:408:ARG:HH12	11:W1:15:ARG:HE	1.20	0.86
3:O1:334:THR:O	3:O1:338:ILE:HD13	1.75	0.86
10:J1:58:LYS:HG2	10:J1:59:TYR:H	1.41	0.86
5:Q1:118:ARG:HH11	5:Q1:171:ILE:CG1	1.88	0.86
5:Q1:60:SER:HA	5:Q1:63:SER:OG	1.75	0.86
17:82:424:ILE:HG12	19:A2:76:ARG:NH2	1.89	0.86
1:M1:408:ARG:NH1	11:W1:15:ARG:HE	1.73	0.86
7:S1:36:ASN:HA	7:S1:39:ARG:HD3	1.57	0.86
35:R2:170:LEU:O	35:R2:328:ILE:HD12	1.73	0.86
2:N1:209:LEU:HD22	2:N1:375:SER:HB2	1.56	0.85
3:C1:10:LEU:HD12	3:C1:13:ILE:HD11	1.55	0.85
1:M1:213:GLN:HB3	1:M1:215:HIS:NE2	1.91	0.85
1:M1:52:ASN:HB2	1:M1:55:ALA:HB2	1.58	0.85
1:A1:213:GLN:HB3	1:A1:215:HIS:NE2	1.91	0.85
9:I1:70:LEU:CD2	9:I1:73:PRO:HD2	2.07	0.85
1:M1:343:MET:HE1	1:M1:416:TYR:CD2	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R1:75:LEU:HD12	6:R1:76:PRO:HD2	1.57	0.85
10:V1:29:LEU:HD13	11:W1:34:TRP:HB3	1.58	0.85
19:A2:67:GLU:O	25:G2:158:LYS:NZ	2.09	0.85
52:12:126:LYS:HD3	52:12:127:TYR:CA	2.07	0.85
18:92:95:ILE:CD1	19:A2:210:ILE:HG22	2.07	0.85
1:A1:46:ARG:HH22	1:A1:316:ASP:CG	1.83	0.85
1:A1:64:PHE:HE1	1:A1:86:LEU:HG	1.36	0.85
18:92:224:SER:OG	18:92:226:GLU:HG2	1.75	0.85
19:A2:227:PRO:CD	75:A2:802:SF4:S1	2.59	0.85
18:92:42:ARG:CZ	19:A2:199:GLY:CA	2.55	0.85
9:I1:72:VAL:CB	9:I1:73:PRO:HD3	2.05	0.85
2:N1:263:ALA:O	2:N1:269:ALA:HB2	1.77	0.85
3:O1:30:TRP:O	3:O1:33:PHE:HD2	1.59	0.85
3:O1:234:LEU:HD23	4:P1:216:LEU:HD21	1.59	0.84
5:Q1:187:PHE:CD2	5:Q1:193:VAL:HB	2.11	0.84
2:B1:286:LYS:HD3	2:B1:287:ARG:NH1	1.92	0.84
7:S1:34:ILE:HB	7:S1:35:PRO:HD3	1.58	0.84
19:A2:312:GLY:C	38:U2:141:SER:O	2.19	0.84
1:A1:21:ASN:HB3	1:A1:217:SER:CB	2.07	0.84
1:A1:408:ARG:HH12	11:K1:15:ARG:HE	1.22	0.84
5:Q1:134:ILE:HD11	5:Q1:185:TYR:CG	2.12	0.84
2:B1:213:HIS:N	2:B1:214:PRO:HD2	1.91	0.84
10:J1:21:ALA:O	10:J1:25:VAL:HG23	1.77	0.84
1:M1:32:GLN:CG	1:M1:33:PRO:HD2	2.08	0.84
2:N1:58:GLU:OE1	2:N1:63:LEU:HA	1.77	0.84
2:N1:126:VAL:O	2:N1:130:PRO:HG3	1.78	0.84
1:A1:61:HIS:NE2	1:A1:134:ILE:HD11	1.91	0.84
1:A1:84:ALA:HB2	1:A1:101:ALA:HB2	1.59	0.84
1:M1:378:ASP:O	1:M1:382:SER:HB2	1.77	0.84
3:O1:245:PHE:CD1	4:P1:17:LEU:HD13	2.11	0.84
2:B1:57:TYR:O	2:B1:233:SER:HB2	1.77	0.84
2:B1:263:ALA:O	2:B1:269:ALA:HB2	1.76	0.84
3:C1:115:ILE:CG2	3:C1:196:HIS:HB2	2.08	0.84
7:G1:73:ASN:N	7:G1:74:PRO:HD2	1.91	0.84
10:J1:18:SER:OG	11:K1:23:LEU:HB2	1.78	0.84
2:B1:198:HIS:HE1	2:B1:233:SER:HB3	1.42	0.84
1:M1:67:THR:HG23	1:M1:70:ARG:N	1.92	0.84
19:A2:159:ALA:HB3	27:I2:84:VAL:CG1	2.08	0.84
1:A1:106:LEU:HD22	1:A1:203:LEU:HD22	1.60	0.84
6:F1:51:PRO:HD3	2:N1:134:ARG:NH1	1.93	0.84
1:A1:308:GLN:O	1:A1:308:GLN:HG3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:163:TRP:CZ2	5:Q1:62:MET:HE2	2.13	0.83
1:M1:40:TRP:CZ2	1:M1:377:GLU:HA	2.13	0.83
6:R1:37:ILE:HG12	6:R1:43:VAL:HG21	1.59	0.83
57:B3:78:LEU:HB2	57:B3:79:PRO:HD3	1.58	0.83
2:N1:341:TYR:HE2	2:N1:345:LYS:HE3	1.41	0.83
5:Q1:114:VAL:HA	5:Q1:117:LEU:CD1	2.06	0.83
56:A3:187:SER:HB2	56:A3:277:MET:HE1	1.60	0.83
1:A1:39:VAL:HG12	1:A1:41:ILE:HD11	1.59	0.83
3:C1:47:THR:HG21	3:C1:83:HIS:HB2	1.61	0.83
1:M1:106:LEU:HD22	1:M1:203:LEU:HD22	1.59	0.83
4:D1:17:LEU:O	4:D1:202:LYS:HD3	1.78	0.83
4:D1:70:VAL:HG23	4:D1:84:PRO:HD3	1.59	0.83
1:A1:426:GLY:HA3	1:A1:428:ILE:HG13	1.59	0.83
3:C1:213:SER:O	3:C1:216:ASP:N	2.10	0.83
1:M1:383:LEU:HA	1:M1:387:GLY:O	1.78	0.83
17:82:424:ILE:CG1	19:A2:76:ARG:HH21	1.92	0.83
2:N1:56:ARG:NH2	2:N1:318:ASP:OD1	2.12	0.82
19:A2:312:GLY:N	38:U2:142:THR:O	2.12	0.82
5:Q1:76:ILE:HG23	5:Q1:194:ILE:HG12	1.60	0.82
1:A1:408:ARG:HH22	11:K1:15:ARG:CZ	1.90	0.82
4:D1:178:THR:HB	4:D1:181:GLN:HG3	1.60	0.82
6:F1:6:VAL:HB	6:F1:10:SER:HB2	1.60	0.82
1:M1:428:ILE:CG2	1:M1:431:LEU:HD22	2.07	0.82
1:A1:145:MET:SD	1:A1:248:LEU:HD12	2.18	0.82
1:M1:408:ARG:HH22	11:W1:15:ARG:CZ	1.91	0.82
2:N1:217:LYS:HZ2	2:N1:221:GLU:CD	1.87	0.82
19:A2:613:PRO:HB2	38:U2:134:ILE:HD13	1.60	0.82
1:A1:241:ILE:HG13	7:G1:16:TYR:CE1	2.15	0.82
7:G1:30:PHE:O	7:G1:34:ILE:HG13	1.78	0.82
4:P1:41:HIS:CD2	4:P1:113:LEU:HD11	2.15	0.82
4:P1:176:PRO:HB2	4:P1:181:GLN:HE22	1.44	0.82
7:S1:72:LYS:CB	7:S1:75:ALA:HB2	2.09	0.82
3:C1:119:LEU:HG	69:C1:402:HEM:CBB	2.09	0.82
4:D1:50:HIS:HB3	4:D1:54:VAL:HB	1.62	0.82
7:G1:50:PRO:HB2	7:G1:51:PRO:HD3	1.61	0.82
19:A2:302:LEU:HA	38:U2:137:TRP:HB2	1.59	0.82
3:O1:297:SER:O	3:O1:300:ILE:HG22	1.79	0.82
7:S1:50:PRO:CB	7:S1:51:PRO:HD3	2.09	0.82
3:O1:234:LEU:CD2	4:P1:216:LEU:HD21	2.08	0.82
19:A2:128:CYS:SG	75:A2:801:SF4:S1	2.78	0.81
2:B1:198:HIS:CE1	2:B1:233:SER:HB3	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:26:ASN:HD21	3:O1:207:ASN:CB	1.90	0.81
1:A1:18:GLN:NE2	1:A1:22:GLY:HA2	1.94	0.81
1:A1:408:ARG:NH2	11:K1:15:ARG:NE	2.28	0.81
3:C1:27:ILE:O	3:C1:27:ILE:HG22	1.79	0.81
4:D1:220:TYR:CE2	7:G1:26:PHE:HE1	1.97	0.81
2:N1:279:LEU:HB3	2:N1:295:LEU:HD22	1.60	0.81
2:N1:331:ALA:HA	2:N1:432:HIS:ND1	1.96	0.81
4:P1:10:TYR:HE1	8:T1:73:LEU:HD21	1.46	0.81
1:A1:379:ILE:HD12	1:A1:390:ILE:HD12	1.62	0.81
1:A1:53:ASN:OD1	1:A1:165:GLN:HB2	1.80	0.81
2:B1:169:ARG:NH2	2:N1:438:GLU:OE2	2.14	0.81
3:O1:218:ILE:CG2	3:O1:223:TYR:CD2	2.63	0.81
19:A2:425:ASN:O	25:G2:169:ARG:NH1	2.13	0.81
3:C1:341:GLN:HB3	3:C1:347:TYR:CD2	2.15	0.81
8:H1:21:ARG:HB3	8:H1:65:ARG:HH21	1.45	0.81
2:B1:42:ALA:HB1	2:B1:43:PRO:HD2	1.62	0.81
5:Q1:99:ARG:HD3	5:Q1:156:TYR:OH	1.80	0.81
44:a2:79:ASN:ND2	55:e2:76:PRO:HD3	1.96	0.81
1:A1:102:LEU:HB2	1:A1:105:ASP:OD2	1.81	0.81
3:C1:266:PRO:HA	5:Q1:160:CYS:SG	2.21	0.81
52:12:75:PRO:N	52:12:223:PHE:HZ	1.79	0.81
62:G3:5:LYS:NZ	62:G3:6:GLY:H	1.78	0.81
1:A1:426:GLY:CA	1:A1:428:ILE:CG1	2.59	0.81
2:B1:248:ASN:HB2	2:B1:428:GLY:HA2	1.63	0.80
9:I1:78:TYR:OXT	9:I1:78:TYR:HD1	1.63	0.80
1:M1:67:THR:HG22	1:M1:70:ARG:HB2	1.61	0.80
3:O1:106:SER:O	3:O1:109:PHE:HD2	1.63	0.80
2:B1:185:LYS:HG3	2:B1:185:LYS:O	1.79	0.80
2:B1:394:PRO:O	2:B1:398:VAL:HG23	1.80	0.80
3:C1:33:PHE:CE1	3:C1:96:MET:HG3	2.16	0.80
5:E1:15:ARG:CB	5:E1:16:PRO:HD2	2.08	0.80
8:T1:50:THR:HG22	8:T1:52:GLU:H	1.47	0.80
17:82:424:ILE:CG1	19:A2:76:ARG:NH2	2.44	0.80
5:Q1:118:ARG:NH1	5:Q1:171:ILE:HG13	1.95	0.80
10:V1:58:LYS:HG2	10:V1:59:TYR:N	1.97	0.80
63:H3:39:CYS:SG	63:H3:53:CYS:HB3	2.22	0.80
1:A1:42:ASP:HB3	1:A1:384:LEU:HD22	1.62	0.80
5:E1:31:ALA:HB2	10:J1:7:ALA:HB2	1.63	0.80
1:M1:182:LEU:O	1:M1:186:LEU:HD12	1.82	0.80
1:M1:445:ARG:O	1:M1:446:PHE:HB2	1.79	0.80
2:N1:200:THR:CG2	2:N1:203:ARG:HD2	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:126:THR:OG1	3:O1:185:LEU:HD23	1.82	0.80
4:P1:10:TYR:HE1	8:T1:73:LEU:CD2	1.94	0.80
4:P1:220:TYR:CE2	7:S1:26:PHE:HE1	1.98	0.80
3:C1:51:LEU:HD11	3:C1:80:ARG:HA	1.63	0.80
69:O1:401:HEM:HBC2	69:O1:401:HEM:HMC1	1.61	0.80
6:R1:33:ARG:NH2	6:R1:91:GLU:OE2	2.14	0.80
2:B1:305:GLN:HB2	2:B1:306:PRO:CD	2.11	0.80
3:C1:5:ARG:O	3:C1:9:PRO:HD2	1.82	0.80
7:G1:72:LYS:CB	7:G1:75:ALA:HB2	2.09	0.80
8:T1:21:ARG:HB3	8:T1:65:ARG:NH2	1.95	0.80
2:B1:207:ILE:HD11	2:B1:383:GLY:HA2	1.62	0.80
5:E1:41:ALA:O	5:E1:45:VAL:HG23	1.81	0.80
1:A1:426:GLY:N	1:A1:428:ILE:CG1	2.45	0.80
3:C1:3:ASN:N	3:C1:8:HIS:NE2	2.30	0.80
2:N1:24:LEU:H	2:N1:24:LEU:HD12	1.47	0.80
3:C1:218:ILE:CG2	3:C1:223:TYR:CD2	2.65	0.79
2:B1:168:TYR:HB2	2:B1:173:ALA:HB2	1.63	0.79
3:O1:185:LEU:HB3	3:O1:186:PRO:HD3	1.61	0.79
52:12:126:LYS:O	52:12:129:LEU:N	2.15	0.79
2:B1:209:LEU:HD22	2:B1:375:SER:HB2	1.64	0.79
3:C1:169:SER:HB2	5:Q1:93:GLY:HA3	1.64	0.79
4:D1:220:TYR:HE2	7:G1:26:PHE:HE1	1.30	0.79
1:M1:260:PRO:HD3	1:M1:414:TYR:CE1	2.18	0.79
4:P1:27:ARG:HH12	10:V1:58:LYS:HG3	1.46	0.79
1:A1:428:ILE:HG22	1:A1:431:LEU:CB	2.12	0.79
2:B1:362:ASN:HA	2:B1:365:LYS:HD3	1.65	0.79
10:J1:58:LYS:HG2	10:J1:59:TYR:N	1.96	0.79
2:N1:68:LEU:HD23	2:N1:186:VAL:CG1	2.12	0.79
3:O1:102:LEU:HD21	3:O1:304:ILE:CD1	2.12	0.79
6:R1:51:PRO:HG2	6:R1:54:LEU:CD2	2.12	0.79
1:A1:155:ALA:HA	1:A1:164:ALA:HB1	1.63	0.79
3:O1:135:TRP:CH2	3:O1:170:VAL:HG12	2.17	0.79
5:Q1:91:TRP:HB3	5:Q1:96:LEU:HB2	1.62	0.79
1:M1:408:ARG:NH2	11:W1:15:ARG:NE	2.30	0.79
2:N1:261:SER:OG	2:N1:320:GLY:HA3	1.83	0.79
4:P1:138:PRO:HG2	8:T1:55:THR:OG1	1.82	0.79
8:T1:73:LEU:HD23	8:T1:74:PHE:N	1.98	0.79
3:C1:111:GLU:O	3:C1:115:ILE:HD13	1.82	0.79
3:C1:264:THR:HG21	5:Q1:144:CYS:CB	2.13	0.79
2:N1:159:VAL:HG12	2:N1:160:ILE:HD13	1.65	0.79
3:O1:246:ALA:HB1	3:O1:249:LEU:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:86:LEU:HD13	1:A1:99:ILE:HG12	1.64	0.79
3:O1:316:MET:HE2	3:O1:317:PHE:CE1	2.17	0.79
63:H3:39:CYS:SG	63:H3:53:CYS:CB	2.70	0.79
4:D1:10:TYR:CZ	4:D1:128:PHE:HE2	2.01	0.79
5:Q1:114:VAL:CA	5:Q1:117:LEU:HD12	2.12	0.79
10:V1:58:LYS:HG2	10:V1:59:TYR:H	1.48	0.79
19:A2:674:LEU:HD12	29:K2:46:LYS:CE	2.13	0.79
3:C1:280:ILE:HD11	3:C1:335:LEU:HD13	1.64	0.78
1:M1:39:VAL:HG12	1:M1:41:ILE:HD11	1.65	0.78
10:V1:3:PRO:HG2	10:V1:8:ARG:HG2	1.63	0.78
19:A2:426:ASP:HA	25:G2:169:ARG:HH12	1.48	0.78
1:M1:262:TRP:CD2	1:M1:385:THR:HG23	2.18	0.78
2:B1:297:GLN:OE1	2:B1:297:GLN:HA	1.82	0.78
2:B1:304:HIS:HD2	2:B1:306:PRO:HD2	1.48	0.78
2:B1:385:GLN:CG	9:I1:62:ARG:HH12	1.96	0.78
4:P1:198:HIS:NE2	4:P1:202:LYS:NZ	2.31	0.78
4:P1:220:TYR:HE2	7:S1:26:PHE:HE1	1.29	0.78
19:A2:302:LEU:HA	38:U2:137:TRP:HB3	1.64	0.78
19:A2:302:LEU:CA	38:U2:137:TRP:CB	2.60	0.78
4:D1:74:PRO:CB	4:D1:79:GLU:HB2	2.13	0.78
7:G1:44:CYS:SG	7:G1:48:VAL:HG21	2.22	0.78
2:N1:309:VAL:HG22	2:N1:326:THR:HA	1.63	0.78
36:S2:200:PRO:CG	36:S2:223:GLN:HE22	1.93	0.78
63:H3:75:ARG:HG2	63:H3:75:ARG:HH11	1.48	0.78
3:C1:51:LEU:HD21	3:C1:79:ILE:HG22	1.63	0.78
3:C1:275:LEU:O	3:C1:276:PHE:C	2.23	0.78
4:D1:3:LEU:HD11	7:G1:71:ARG:HB2	1.64	0.78
4:P1:115:TYR:HD1	4:P1:119:ALA:HB2	1.47	0.78
9:U1:64:LEU:HG	9:U1:65:VAL:HG23	1.65	0.78
47:d2:25:PHE:HD2	47:d2:40:VAL:CB	1.93	0.78
2:B1:438:GLU:OE2	2:N1:169:ARG:NH2	2.16	0.78
3:O1:1:MET:SD	3:O1:7:SER:HB2	2.23	0.78
4:D1:228:SER:HB2	7:G1:23:GLN:NE2	1.98	0.78
7:G1:31:SER:O	7:G1:35:PRO:HD2	1.83	0.78
1:M1:297:ILE:HG22	1:M1:303:LEU:HD12	1.63	0.78
2:B1:347:ILE:O	2:B1:411:ILE:HG23	1.83	0.78
4:P1:10:TYR:CZ	4:P1:128:PHE:HE2	2.01	0.78
1:A1:45:SER:HB3	1:A1:92:ARG:HA	1.66	0.78
2:N1:308:ASP:OD1	2:N1:309:VAL:N	2.17	0.78
3:O1:309:THR:CG2	3:O1:370:GLY:HA3	2.14	0.78
19:A2:557:ARG:HH21	38:U2:144:TYR:HH	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D2:107:ASP:OD2	22:D2:113:PHE:CE1	2.37	0.77
2:N1:286:LYS:HD3	2:N1:287:ARG:NH1	1.98	0.77
1:M1:32:GLN:HG3	1:M1:33:PRO:HD2	1.66	0.77
5:Q1:65:SER:OG	5:Q1:67:ASP:HB3	1.85	0.77
2:N1:297:GLN:OE1	2:N1:297:GLN:HA	1.83	0.77
3:C1:106:SER:O	3:C1:109:PHE:HD1	1.66	0.77
3:C1:108:THR:HB	3:C1:313:ARG:NH1	2.00	0.77
4:D1:14:HIS:HA	4:D1:19:SER:HB3	1.66	0.77
2:N1:341:TYR:CE2	2:N1:345:LYS:HE3	2.19	0.77
1:A1:46:ARG:NH2	1:A1:316:ASP:OD2	2.17	0.77
3:O1:341:GLN:HB3	3:O1:347:TYR:CD2	2.19	0.77
7:S1:9:ARG:HH21	7:S1:11:ARG:HD2	1.44	0.77
1:A1:39:VAL:HG12	1:A1:41:ILE:CD1	2.13	0.77
2:B1:331:ALA:HA	2:B1:432:HIS:ND1	2.00	0.77
3:C1:26:ASN:ND2	3:C1:207:ASN:HB2	1.99	0.77
1:M1:21:ASN:HB3	1:M1:217:SER:CB	2.13	0.77
1:M1:75:LEU:O	1:M1:79:VAL:HG23	1.82	0.77
4:P1:50:HIS:HB3	4:P1:54:VAL:HB	1.64	0.77
1:A1:386:TYR:HD1	1:A1:386:TYR:H	1.32	0.77
1:M1:92:ARG:HD2	1:M1:163:LEU:HD12	1.65	0.77
3:O1:170:VAL:HG13	3:O1:174:THR:HG21	1.66	0.77
6:F1:28:LYS:CD	6:F1:74:ILE:HD11	2.14	0.77
19:A2:159:ALA:HB3	27:I2:84:VAL:HG11	1.65	0.77
20:B2:94:VAL:CG1	20:B2:115:LEU:HD22	2.12	0.77
1:A1:21:ASN:HB3	1:A1:217:SER:OG	1.84	0.76
3:C1:310:SER:HB3	3:C1:318:ARG:HH11	1.47	0.76
3:C1:338:ILE:HD12	3:C1:338:ILE:N	1.99	0.76
4:D1:182:VAL:O	4:D1:186:VAL:HG23	1.84	0.76
1:M1:331:ILE:HD11	1:M1:427:PRO:O	1.85	0.76
3:O1:310:SER:OG	3:O1:318:ARG:NH1	2.18	0.76
2:B1:101:THR:HG23	2:B1:104:ASN:H	1.48	0.76
4:P1:143:LEU:HD22	4:P1:147:LEU:O	1.86	0.76
5:Q1:157:TYR:OH	5:Q1:162:GLY:HA2	1.84	0.76
57:B3:5:MET:HE3	66:K3:42:PRO:HA	1.67	0.76
2:B1:59:ASN:O	2:B1:63:LEU:HG	1.84	0.76
2:N1:29:LEU:HB3	2:N1:30:PRO:CD	2.14	0.76
3:C1:187:PHE:CZ	3:O1:184:ILE:HG13	2.20	0.76
4:D1:229:VAL:HG12	4:D1:233:ARG:HE	1.49	0.76
3:O1:206:ASN:CB	3:O1:313:ARG:HH21	1.99	0.76
4:P1:55:CYS:SG	10:V1:52:TRP:HB2	2.25	0.76
4:P1:178:THR:OG1	4:P1:181:GLN:NE2	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:153:PHE:HE1	5:Q1:173:LYS:HG3	1.50	0.76
27:I2:104:ASP:O	27:I2:105:LYS:CB	2.30	0.76
2:B1:67:HIS:CD2	2:B1:144:LEU:HD22	2.18	0.76
2:B1:148:LYS:HE2	2:B1:180:ASP:OD1	1.85	0.76
1:M1:24:ARG:CB	1:M1:196:VAL:HG22	2.14	0.76
2:N1:200:THR:HG22	2:N1:203:ARG:CD	2.15	0.76
6:R1:73:GLN:NE2	7:S1:32:LYS:NZ	2.33	0.76
1:A1:92:ARG:HD2	1:A1:163:LEU:HD12	1.67	0.76
1:A1:146:ARG:NH2	1:A1:308:GLN:HE22	1.82	0.76
3:C1:210:GLY:HA3	3:C1:314:SER:HB2	1.68	0.76
3:O1:3:ASN:N	3:O1:8:HIS:NE2	2.32	0.76
4:P1:181:GLN:HA	8:T1:77:LEU:HD13	1.67	0.76
18:92:42:ARG:HH12	19:A2:199:GLY:CA	1.96	0.76
3:C1:9:PRO:HG2	3:C1:12:LYS:HB2	1.68	0.76
2:N1:213:HIS:N	2:N1:214:PRO:HD2	2.01	0.76
2:N1:305:GLN:CB	2:N1:306:PRO:HD3	2.15	0.76
1:A1:27:SER:HA	1:A1:199:ALA:O	1.86	0.76
3:C1:47:THR:CG2	3:C1:83:HIS:HB2	2.16	0.76
6:F1:94:LEU:O	6:F1:98:ILE:HG13	1.86	0.76
1:M1:41:ILE:H	1:M1:41:ILE:HD12	1.50	0.76
19:A2:313:LEU:CA	38:U2:142:THR:HA	2.15	0.76
1:M1:102:LEU:HB2	1:M1:105:ASP:OD2	1.85	0.75
2:N1:257:LEU:HD13	2:N1:424:MET:HB2	1.68	0.75
19:A2:313:LEU:HD23	38:U2:142:THR:CA	2.16	0.75
5:E1:55:VAL:O	5:E1:59:VAL:HG23	1.85	0.75
6:R1:28:LYS:CD	6:R1:74:ILE:HD11	2.15	0.75
19:A2:312:GLY:N	38:U2:143:PRO:C	2.45	0.75
19:A2:314:LEU:HD23	38:U2:140:PRO:CD	2.04	0.75
2:B1:141:GLN:HB2	2:B1:142:PRO:HD3	1.68	0.75
4:D1:127:VAL:HG12	4:D1:187:CYS:SG	2.26	0.75
57:B3:59:GLN:H	57:B3:62:GLU:HG3	1.51	0.75
1:A1:249:PRO:O	1:A1:250:LEU:HD23	1.85	0.75
3:C1:310:SER:CB	3:C1:318:ARG:HH11	1.99	0.75
3:O1:47:THR:CG2	3:O1:83:HIS:HB2	2.16	0.75
3:O1:129:MET:HG2	3:O1:178:PHE:HD1	1.49	0.75
10:J1:51:LEU:HD22	10:J1:52:TRP:HZ3	1.50	0.75
9:U1:72:VAL:CB	9:U1:73:PRO:HD3	2.15	0.75
52:12:75:PRO:CA	52:12:223:PHE:CE1	2.69	0.75
2:B1:207:ILE:HD12	2:B1:382:VAL:HG12	1.69	0.75
2:N1:314:ALA:CB	9:U1:64:LEU:HD22	2.17	0.75
3:O1:61:THR:O	3:O1:62:ALA:C	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:177:ARG:O	3:O1:181:PHE:HD2	1.69	0.75
5:Q1:134:ILE:HD11	5:Q1:185:TYR:CE2	2.22	0.75
5:Q1:171:ILE:CD1	5:Q1:176:ALA:HB3	2.17	0.75
6:R1:50:LEU:HB2	6:R1:55:TYR:HB2	1.67	0.75
1:A1:145:MET:HE3	1:A1:252:HIS:CE1	2.21	0.75
2:N1:59:ASN:O	2:N1:63:LEU:HG	1.87	0.75
3:O1:310:SER:CB	3:O1:318:ARG:HH11	2.00	0.75
5:Q1:77:LYS:HG3	5:Q1:89:PHE:CE2	2.22	0.75
7:G1:9:ARG:HH21	7:G1:11:ARG:HD2	1.49	0.75
2:N1:49:LEU:HD11	2:N1:204:MET:SD	2.26	0.75
19:A2:613:PRO:HB2	38:U2:134:ILE:CD1	2.17	0.75
1:A1:236:PHE:HD2	1:A1:258:GLU:HG2	1.52	0.75
1:M1:386:TYR:HD1	1:M1:386:TYR:H	1.33	0.75
58:C3:187:THR:HG21	62:G3:68:THR:HG21	1.68	0.75
3:C1:169:SER:OG	3:C1:170:VAL:N	2.18	0.74
3:C1:345:HIS:HB3	3:C1:346:PRO:CD	2.17	0.74
3:C1:361:LEU:HD23	3:C1:365:LEU:HD12	1.69	0.74
5:Q1:118:ARG:HH11	5:Q1:171:ILE:HG13	1.50	0.74
19:A2:181:ARG:HB3	75:A2:802:SF4:S2	2.27	0.74
19:A2:426:ASP:CA	25:G2:169:ARG:HH12	1.98	0.74
1:A1:72:GLY:O	1:A1:73:ASN:OD1	2.04	0.74
3:C1:126:THR:OG1	3:C1:185:LEU:HD23	1.87	0.74
2:N1:304:HIS:HD2	2:N1:306:PRO:HD2	1.51	0.74
1:A1:316:ASP:OD1	1:A1:316:ASP:N	2.21	0.74
4:D1:5:LEU:HB3	4:D1:152:TYR:CD1	2.22	0.74
1:M1:39:VAL:HG23	1:M1:113:LEU:HD23	1.68	0.74
3:O1:90:PHE:CE1	3:O1:123:VAL:HG21	2.22	0.74
1:M1:18:GLN:NE2	1:M1:22:GLY:HA2	2.01	0.74
5:Q1:118:ARG:HD2	5:Q1:171:ILE:HG12	1.70	0.74
18:92:42:ARG:NH2	19:A2:199:GLY:HA3	2.03	0.74
22:D2:107:ASP:OD2	22:D2:113:PHE:HE1	1.70	0.74
3:C1:206:ASN:ND2	3:C1:207:ASN:H	1.85	0.74
19:A2:426:ASP:HA	25:G2:169:ARG:NH1	2.03	0.74
1:A1:84:ALA:CB	1:A1:101:ALA:HB2	2.18	0.74
3:C1:7:SER:HA	3:C1:13:ILE:HG12	1.69	0.74
4:D1:11:PRO:O	8:H1:74:PHE:CE2	2.41	0.74
1:M1:53:ASN:OD1	1:M1:165:GLN:HB2	1.87	0.74
1:M1:99:ILE:HG13	1:M1:113:LEU:HD13	1.69	0.74
2:N1:68:LEU:HD23	2:N1:186:VAL:HG12	1.69	0.74
19:A2:144:MET:HG2	20:B2:380:HIS:CD2	2.23	0.74
1:A1:75:LEU:O	1:A1:79:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:292:SER:O	1:A1:295:ALA:HB3	1.88	0.74
2:B1:337:ILE:HG21	2:B1:434:PRO:HG2	1.68	0.74
19:A2:161:GLU:CB	27:I2:102:ASN:ND2	2.50	0.74
52:12:17:VAL:HG23	52:12:225:MET:HE1	1.68	0.74
1:A1:236:PHE:CD2	1:A1:258:GLU:HG2	2.22	0.74
1:A1:334:MET:HA	1:A1:334:MET:HE3	1.70	0.74
2:B1:140:LEU:O	2:B1:141:GLN:C	2.30	0.74
3:C1:184:ILE:HG13	3:O1:187:PHE:CZ	2.23	0.74
1:A1:408:ARG:CZ	11:K1:15:ARG:HE	2.01	0.73
8:H1:15:ASP:N	8:H1:16:PRO:HD2	2.03	0.73
2:N1:237:ALA:HB2	2:N1:318:ASP:OD2	1.87	0.73
5:Q1:188:THR:N	5:Q1:192:MET:O	2.21	0.73
2:B1:162:ASN:HD22	2:B1:244:ILE:HG21	1.51	0.73
3:O1:122:THR:CG2	3:O1:189:ILE:HD11	2.17	0.73
3:O1:184:ILE:O	3:O1:188:ILE:HD12	1.88	0.73
5:Q1:121:GLN:O	5:Q1:170:ARG:NH1	2.18	0.73
57:B3:184:LEU:HD11	57:B3:211:LEU:HD21	1.69	0.73
1:A1:236:PHE:HE2	1:A1:258:GLU:HB3	1.50	0.73
1:A1:383:LEU:HA	1:A1:387:GLY:O	1.88	0.73
2:B1:129:ALA:N	2:B1:130:PRO:HD2	2.01	0.73
1:M1:408:ARG:HH12	11:W1:15:ARG:NE	1.85	0.73
5:Q1:55:VAL:O	5:Q1:59:VAL:HG23	1.88	0.73
5:Q1:157:TYR:HE2	5:Q1:159:PRO:HA	1.51	0.73
2:B1:78:LYS:HB3	2:B1:129:ALA:HB1	1.70	0.73
2:B1:347:ILE:H	2:B1:347:ILE:HD12	1.54	0.73
1:M1:426:GLY:CA	1:M1:428:ILE:CG1	2.64	0.73
2:N1:385:GLN:CG	9:U1:62:ARG:HH12	2.00	0.73
3:C1:280:ILE:CD1	3:C1:335:LEU:HD13	2.19	0.73
1:M1:256:ALA:HA	1:M1:320:LEU:O	1.89	0.73
1:M1:363:ASN:OD1	2:N1:112:LEU:HD23	1.88	0.73
2:N1:34:VAL:HG11	2:N1:386:ALA:HB1	1.70	0.73
2:N1:95:LYS:HE3	9:U1:70:LEU:HD22	1.69	0.73
3:O1:361:LEU:CD2	3:O1:365:LEU:HD12	2.18	0.73
17:82:424:ILE:HD11	19:A2:76:ARG:HH21	1.51	0.73
27:I2:106:GLU:O	27:I2:108:LYS:NZ	2.18	0.73
55:e2:36:MET:CA	55:e2:77:LYS:HE3	2.05	0.73
1:A1:274:ASN:HB3	1:A1:309:THR:OG1	1.89	0.73
5:Q1:134:ILE:O	5:Q1:135:LEU:HD23	1.89	0.73
17:82:424:ILE:CD1	19:A2:76:ARG:HH21	2.01	0.73
1:A1:163:LEU:HD12	1:A1:163:LEU:O	1.88	0.73
1:A1:262:TRP:CD2	1:A1:385:THR:HG23	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:328:SER:HB3	2:B1:336:VAL:HG21	1.69	0.73
2:N1:67:HIS:CD2	2:N1:144:LEU:HD22	2.21	0.73
3:O1:147:THR:HG21	3:O1:165:TRP:NE1	2.03	0.73
9:U1:70:LEU:CD2	9:U1:73:PRO:HD2	2.17	0.73
2:B1:182:ARG:NH1	2:B1:185:LYS:HG2	2.03	0.73
3:O1:22:PRO:HG2	7:S1:3:GLN:HB3	1.69	0.73
62:G3:54:ARG:HD3	62:G3:54:ARG:N	2.04	0.73
3:C1:30:TRP:O	3:C1:33:PHE:HD2	1.71	0.73
18:92:44:THR:OG1	19:A2:209:TYR:CE2	2.42	0.73
20:B2:82:LEU:HD11	52:12:126:LYS:CE	2.19	0.73
62:G3:5:LYS:HZ3	62:G3:5:LYS:HB3	1.54	0.73
2:B1:395:PRO:O	2:B1:398:VAL:HB	1.88	0.73
4:D1:41:HIS:CD2	4:D1:113:LEU:HD11	2.24	0.73
2:N1:24:LEU:CG	2:N1:38:LEU:HD11	2.19	0.73
19:A2:238:PHE:O	23:E2:134:PRO:HD3	1.88	0.73
59:D3:23:PRO:O	60:E3:66:ARG:HD3	1.89	0.73
4:D1:224:ARG:CB	7:G1:25:ALA:HB1	2.14	0.72
1:M1:426:GLY:N	1:M1:428:ILE:HG13	2.02	0.72
4:P1:10:TYR:CE1	8:T1:73:LEU:HD21	2.23	0.72
5:Q1:98:VAL:HA	5:Q1:134:ILE:HG22	1.69	0.72
52:12:75:PRO:CD	52:12:223:PHE:CZ	2.67	0.72
1:A1:171:SER:OG	1:A1:172:GLU:N	2.19	0.72
7:S1:15:THR:HG22	7:S1:16:TYR:N	1.97	0.72
11:W1:18:VAL:HB	11:W1:19:PRO:HD3	1.71	0.72
1:A1:408:ARG:HH12	11:K1:15:ARG:NE	1.85	0.72
2:B1:352:LEU:HB3	2:B1:411:ILE:HD11	1.70	0.72
4:D1:27:ARG:HH12	10:J1:58:LYS:HG3	1.55	0.72
1:A1:273:ALA:HA	1:A1:276:ILE:HD12	1.71	0.72
2:B1:279:LEU:CD2	2:B1:295:LEU:HD13	2.19	0.72
6:F1:28:LYS:HB3	6:F1:74:ILE:HD11	1.69	0.72
18:92:110:MET:HG2	19:A2:194:ASP:C	2.14	0.72
19:A2:302:LEU:HB3	38:U2:137:TRP:CB	2.19	0.72
1:M1:335:MET:HE2	1:M1:339:GLN:HG3	1.72	0.72
4:D1:54:VAL:O	4:D1:54:VAL:HG12	1.89	0.72
5:E1:19:LEU:HD12	5:E1:19:LEU:O	1.90	0.72
2:N1:46:ARG:HH12	2:N1:376:GLU:HG3	1.55	0.72
3:C1:297:SER:O	3:C1:300:ILE:HG22	1.90	0.72
5:Q1:121:GLN:HB2	5:Q1:170:ARG:HD3	1.71	0.72
19:A2:314:LEU:O	38:U2:139:PRO:CB	2.38	0.72
2:B1:56:ARG:NH2	2:B1:318:ASP:OD1	2.22	0.72
1:M1:8:LEU:O	1:M1:11:VAL:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:309:THR:HG21	3:O1:370:GLY:HA3	1.70	0.72
4:P1:74:PRO:HG2	4:P1:82:MET:SD	2.30	0.72
3:C1:310:SER:HA	3:C1:374:ASN:ND2	1.97	0.72
4:D1:43:MET:HG2	4:D1:46:VAL:HG23	1.70	0.72
3:O1:51:LEU:HD11	3:O1:80:ARG:HA	1.69	0.72
22:D2:113:PHE:HB2	22:D2:114:ARG:HE	1.54	0.72
55:e2:77:LYS:HG3	55:e2:78:LEU:N	2.02	0.72
1:A1:408:ARG:HH12	11:K1:15:ARG:CG	2.02	0.72
3:C1:252:ASP:HB3	3:C1:253:PRO:CD	2.18	0.72
4:D1:7:PRO:HG3	4:D1:126:TYR:HA	1.71	0.71
4:P1:164:ILE:HD13	4:P1:182:VAL:HG12	1.70	0.71
1:A1:100:LYS:NZ	1:A1:373:THR:OG1	2.18	0.71
1:M1:67:THR:CG2	1:M1:70:ARG:HB2	2.20	0.71
1:M1:262:TRP:CG	1:M1:385:THR:HG23	2.24	0.71
1:M1:329:MET:SD	7:S1:5:GLY:HA3	2.31	0.71
2:N1:277:HIS:NE2	2:N1:364:LEU:HD13	2.05	0.71
2:B1:77:THR:CG2	2:B1:130:PRO:HA	2.13	0.71
6:F1:33:ARG:NH2	6:F1:91:GLU:OE2	2.22	0.71
1:M1:255:ILE:HG13	1:M1:422:VAL:HG22	1.71	0.71
17:82:418:GLN:NE2	19:A2:115:GLY:CA	2.44	0.71
56:A3:176:MET:HE3	56:A3:181:THR:HG22	1.71	0.71
4:D1:10:TYR:HE1	8:H1:73:LEU:CD2	2.03	0.71
2:N1:314:ALA:HB2	9:U1:64:LEU:HD22	1.70	0.71
6:R1:73:GLN:HE21	7:S1:32:LYS:NZ	1.89	0.71
1:A1:41:ILE:H	1:A1:41:ILE:HD12	1.54	0.71
1:A1:286:GLY:O	1:A1:287:GLY:C	2.33	0.71
9:I1:70:LEU:HD12	9:I1:71:ASN:N	2.04	0.71
1:M1:45:SER:OG	1:M1:92:ARG:HG3	1.91	0.71
5:Q1:109:GLU:CD	5:Q1:167:ALA:HB3	2.15	0.71
5:Q1:139:CYS:HB2	5:Q1:165:TYR:HE2	1.54	0.71
19:A2:140:GLN:OE1	75:A2:801:SF4:S4	2.48	0.71
59:D3:147:LYS:HA	59:D3:147:LYS:HE3	1.72	0.71
2:B1:29:LEU:HB3	2:B1:30:PRO:CD	2.20	0.71
37:T2:82:GLU:HG3	37:T2:84:PRO:HD2	1.72	0.71
1:A1:21:ASN:HB3	1:A1:217:SER:HB3	1.72	0.71
2:B1:251:SER:OG	2:B1:252:LEU:N	2.22	0.71
2:B1:300:ALA:HA	2:B1:307:PHE:CZ	2.26	0.71
69:C1:401:HEM:HBC2	69:C1:401:HEM:HMC1	1.73	0.71
6:R1:59:VAL:HG11	7:S1:10:VAL:HG22	1.73	0.71
4:D1:150:ASN:OD1	4:D1:151:PRO:HD2	1.89	0.71
3:O1:237:LEU:HD13	4:P1:212:MET:HG2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:7:PRO:HG3	4:P1:126:TYR:HA	1.73	0.71
2:B1:429:ASN:ND2	2:N1:60:SER:HB3	1.98	0.71
3:C1:100:ARG:NH2	69:C1:402:HEM:HBD1	2.05	0.71
18:92:110:MET:HE2	19:A2:196:GLY:N	2.05	0.71
17:82:381:GLN:C	19:A2:74:ASN:HB2	2.15	0.70
19:A2:427:LEU:N	25:G2:169:ARG:HH12	1.89	0.70
2:B1:162:ASN:ND2	2:B1:244:ILE:HG21	2.06	0.70
2:B1:283:PRO:HG3	9:I1:55:LEU:CD2	2.18	0.70
3:C1:147:THR:HG21	3:C1:165:TRP:NE1	2.06	0.70
2:N1:68:LEU:HD11	2:N1:140:LEU:HD23	1.71	0.70
19:A2:162:ASP:O	27:I2:105:LYS:NZ	2.22	0.70
1:A1:233:PRO:HG2	5:E1:23:LYS:CD	2.20	0.70
2:B1:384:SER:HB2	9:I1:62:ARG:HG2	1.71	0.70
3:C1:110:LEU:HG	3:C1:114:ASN:HD21	1.55	0.70
18:92:42:ARG:NH2	19:A2:199:GLY:CA	2.53	0.70
2:B1:162:ASN:O	2:B1:244:ILE:HD12	1.89	0.70
4:D1:102:ARG:HA	4:D1:108:ALA:O	1.91	0.70
5:E1:15:ARG:HB2	5:E1:16:PRO:CD	2.21	0.70
10:J1:49:GLY:HA2	10:J1:54:HIS:CB	2.20	0.70
2:N1:140:LEU:O	2:N1:141:GLN:C	2.35	0.70
3:O1:5:ARG:O	3:O1:9:PRO:HD2	1.90	0.70
3:O1:47:THR:HG21	3:O1:83:HIS:HB2	1.73	0.70
3:O1:218:ILE:HD13	4:P1:230:LEU:CD1	2.22	0.70
3:O1:280:ILE:HD13	3:O1:335:LEU:HD22	1.72	0.70
19:A2:313:LEU:N	38:U2:142:THR:HA	2.05	0.70
19:A2:314:LEU:O	38:U2:139:PRO:HB2	1.91	0.70
3:C1:156:ILE:HG12	3:C1:157:GLY:H	1.56	0.70
3:C1:174:THR:CG2	3:C1:178:PHE:HE1	2.03	0.70
4:D1:50:HIS:HB3	4:D1:54:VAL:CB	2.22	0.70
4:D1:165:TYR:CZ	4:D1:168:VAL:HG22	2.27	0.70
9:I1:78:TYR:OXT	9:I1:78:TYR:CD1	2.43	0.70
2:N1:352:LEU:HB3	2:N1:411:ILE:HD11	1.73	0.70
1:A1:60:GLU:OE2	1:A1:88:ALA:O	2.09	0.70
1:A1:351:GLU:OE2	1:A1:403:ASP:OD1	2.10	0.70
2:N1:51:ILE:HD13	2:N1:199:PHE:CG	2.26	0.70
4:P1:11:PRO:O	8:T1:74:PHE:CE2	2.45	0.70
5:Q1:95:PRO:HG2	5:Q1:145:VAL:HG22	1.74	0.70
2:B1:237:ALA:HB2	2:B1:318:ASP:OD2	1.92	0.70
1:M1:274:ASN:HB3	1:M1:309:THR:OG1	1.91	0.70
2:N1:182:ARG:NH1	2:N1:185:LYS:HG2	2.06	0.70
2:N1:212:SER:OG	2:N1:215:VAL:HB	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:200:PRO:HG3	36:S2:223:GLN:NE2	2.01	0.70
47:d2:25:PHE:HZ	47:d2:42:THR:O	1.75	0.70
1:A1:298:ALA:HA	1:A1:303:LEU:HB2	1.73	0.70
2:B1:83:PHE:CE2	2:B1:87:ARG:HG3	2.27	0.70
2:B1:277:HIS:NE2	2:B1:364:LEU:HD13	2.07	0.70
1:M1:236:PHE:HE2	1:M1:258:GLU:HB3	1.51	0.70
6:R1:73:GLN:NE2	7:S1:32:LYS:HZ1	1.89	0.70
2:B1:46:ARG:HH12	2:B1:376:GLU:HG3	1.57	0.70
3:C1:18:PHE:O	3:C1:220:PHE:CD2	2.45	0.70
3:O1:27:ILE:HG22	3:O1:27:ILE:O	1.91	0.70
4:P1:74:PRO:CB	4:P1:79:GLU:HB2	2.19	0.70
5:Q1:34:GLY:HA2	10:V1:10:TYR:HD1	1.57	0.70
5:Q1:118:ARG:HH11	5:Q1:171:ILE:HG12	1.55	0.70
5:Q1:171:ILE:HG22	5:Q1:179:ASN:OD1	1.92	0.70
6:R1:96:GLU:O	6:R1:97:VAL:C	2.32	0.70
19:A2:238:PHE:HB3	23:E2:140:ARG:HB3	1.72	0.70
2:B1:166:ALA:HB2	2:B1:244:ILE:HG13	1.74	0.70
3:C1:122:THR:HG22	3:C1:189:ILE:HD11	1.72	0.70
4:D1:51:LEU:HA	4:D1:56:TYR:O	1.91	0.70
5:Q1:185:TYR:HB3	5:Q1:195:VAL:HG13	1.74	0.70
19:A2:422:TRP:C	25:G2:169:ARG:HD2	2.12	0.70
3:C1:26:ASN:HD21	3:C1:207:ASN:CB	2.01	0.69
7:S1:15:THR:CG2	7:S1:16:TYR:N	2.51	0.69
58:C3:156:ARG:HH11	58:C3:156:ARG:HG3	1.56	0.69
2:B1:129:ALA:N	2:B1:130:PRO:CD	2.55	0.69
2:N1:78:LYS:HB3	2:N1:129:ALA:HB1	1.73	0.69
4:D1:82:MET:SD	4:D1:86:LYS:HD2	2.32	0.69
3:O1:225:THR:O	3:O1:229:ILE:HD12	1.92	0.69
4:P1:158:ILE:HD11	4:P1:160:MET:HB2	1.73	0.69
1:A1:162:PRO:O	1:A1:165:GLN:HG2	1.93	0.69
1:A1:379:ILE:HD12	1:A1:390:ILE:CD1	2.22	0.69
4:D1:94:PRO:HB2	4:D1:95:TYR:CD1	2.27	0.69
2:N1:258:VAL:HG11	2:N1:321:LEU:HB3	1.74	0.69
4:P1:10:TYR:CE1	8:T1:73:LEU:CD2	2.75	0.69
5:Q1:158:CYS:SG	5:Q1:158:CYS:O	2.50	0.69
56:A3:11:ASN:HD22	56:A3:14:ASP:H	1.39	0.69
5:E1:13:TYR:O	7:G1:23:GLN:HB3	1.91	0.69
7:G1:34:ILE:CB	7:G1:35:PRO:HD3	2.18	0.69
1:M1:5:ALA:O	1:M1:8:LEU:HB2	1.93	0.69
1:M1:316:ASP:N	1:M1:316:ASP:OD1	2.24	0.69
1:M1:403:ASP:CB	1:M1:406:VAL:HG23	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N1:338:LYS:HG2	2:N1:439:LEU:HD21	1.73	0.69
3:O1:119:LEU:HD23	69:O1:402:HEM:C4B	2.28	0.69
4:P1:97:ASN:OD1	4:P1:98:PRO:HD2	1.93	0.69
4:P1:27:ARG:NH1	10:V1:58:LYS:NZ	2.41	0.69
1:A1:32:GLN:CG	1:A1:33:PRO:HD2	2.22	0.69
2:N1:165:ALA:HA	2:N1:173:ALA:HB1	1.73	0.69
3:O1:156:ILE:HG13	3:O1:157:GLY:H	1.58	0.69
5:Q1:136:ILE:O	5:Q1:136:ILE:HG22	1.93	0.69
20:B2:92:HIS:CE1	20:B2:141:TYR:HE2	2.10	0.69
56:A3:69:MET:HE2	56:A3:70:VAL:HG23	1.74	0.69
1:A1:426:GLY:HA2	1:A1:428:ILE:N	2.08	0.69
2:B1:34:VAL:HG11	2:B1:386:ALA:HB1	1.74	0.69
3:C1:79:ILE:HG12	5:E1:58:PHE:HE1	1.57	0.69
7:G1:73:ASN:N	7:G1:74:PRO:CD	2.55	0.69
1:M1:145:MET:SD	1:M1:248:LEU:HD12	2.32	0.69
1:M1:365:LEU:HD21	1:M1:395:TRP:CD1	2.27	0.69
2:N1:319:SER:OG	2:N1:320:GLY:N	2.26	0.69
3:O1:129:MET:HG2	3:O1:178:PHE:CD1	2.27	0.69
4:P1:220:TYR:CE2	7:S1:26:PHE:CE1	2.81	0.69
5:Q1:68:VAL:HG12	5:Q1:69:LEU:N	2.08	0.69
5:Q1:114:VAL:HG12	5:Q1:115:SER:N	2.08	0.69
19:A2:312:GLY:H	38:U2:143:PRO:C	2.01	0.69
2:B1:247:GLN:HE22	2:B1:429:ASN:ND2	1.91	0.69
3:C1:135:TRP:HH2	3:C1:170:VAL:HG12	1.57	0.69
4:D1:176:PRO:HB2	4:D1:181:GLN:NE2	2.06	0.69
2:N1:47:ILE:HG22	2:N1:48:GLY:N	2.08	0.69
3:O1:103:TYR:O	3:O1:315:MET:HB2	1.93	0.69
19:A2:426:ASP:C	25:G2:169:ARG:HH12	2.00	0.69
1:M1:278:GLY:O	1:M1:309:THR:HG23	1.93	0.69
1:M1:304:CYS:HB3	1:M1:334:MET:SD	2.33	0.69
3:O1:15:ASN:ND2	3:O1:18:PHE:CE2	2.60	0.69
7:S1:2:ARG:HB2	7:S1:6:HIS:HD2	1.58	0.69
55:e2:67:ASP:O	55:e2:68:ASP:C	2.35	0.69
58:C3:12:ASN:HD22	65:J3:20:VAL:H	1.39	0.69
2:B1:308:ASP:OD1	2:B1:309:VAL:N	2.26	0.68
3:C1:132:VAL:HA	3:C1:139:SER:HB3	1.74	0.68
3:C1:177:ARG:NH2	5:Q1:62:MET:O	2.23	0.68
1:M1:343:MET:HE1	1:M1:416:TYR:HD2	1.57	0.68
3:O1:79:ILE:HG12	5:Q1:58:PHE:HE1	1.59	0.68
4:P1:158:ILE:HD13	4:P1:160:MET:CB	2.22	0.68
4:P1:236:ALA:HB3	7:S1:14:ILE:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:83:GLU:HG3	5:Q1:100:HIS:NE2	2.08	0.68
55:e2:75:TYR:CB	55:e2:78:LEU:CB	2.69	0.68
57:B3:13:THR:HB	57:B3:168:LEU:HD23	1.74	0.68
1:A1:244:ARG:HG2	7:G1:10:VAL:HG12	1.74	0.68
4:D1:97:ASN:OD1	4:D1:98:PRO:HD2	1.92	0.68
2:N1:100:SER:HB3	2:N1:105:MET:HG3	1.74	0.68
3:O1:252:ASP:HB3	3:O1:253:PRO:CD	2.23	0.68
1:A1:39:VAL:HG11	1:A1:117:VAL:HG21	1.73	0.68
1:A1:341:GLN:OE1	1:A1:344:ARG:NH1	2.25	0.68
1:M1:245:GLU:OE1	1:M1:248:LEU:HD23	1.92	0.68
1:M1:389:ARG:O	1:M1:390:ILE:HD13	1.94	0.68
2:N1:300:ALA:HA	2:N1:307:PHE:CZ	2.28	0.68
4:P1:102:ARG:HA	4:P1:108:ALA:O	1.92	0.68
5:Q1:121:GLN:HB2	5:Q1:170:ARG:CD	2.24	0.68
8:T1:65:ARG:HG3	8:T1:66:ASP:N	2.09	0.68
1:A1:408:ARG:NH1	11:K1:15:ARG:HG2	2.09	0.68
1:A1:445:ARG:O	1:A1:446:PHE:HB2	1.93	0.68
2:B1:348:ALA:HB1	2:B1:415:LYS:HA	1.76	0.68
3:C1:234:LEU:HD23	4:D1:216:LEU:HD21	1.74	0.68
8:H1:22:GLU:O	8:H1:25:GLU:HG2	1.94	0.68
1:M1:21:ASN:CB	1:M1:217:SER:HB3	2.22	0.68
1:M1:351:GLU:OE2	1:M1:403:ASP:OD1	2.10	0.68
6:R1:75:LEU:HD12	6:R1:76:PRO:CD	2.23	0.68
2:B1:62:ASN:ND2	2:B1:65:THR:OG1	2.26	0.68
4:D1:134:TYR:HE2	4:D1:163:PRO:HG2	1.58	0.68
4:D1:237:TYR:CE2	4:D1:239:PRO:HG3	2.29	0.68
4:P1:211:MET:HE1	10:V1:31:PHE:CZ	2.28	0.68
19:A2:367:CYS:SG	19:A2:368:THR:N	2.66	0.68
55:e2:67:ASP:O	55:e2:69:GLY:N	2.26	0.68
3:C1:245:PHE:CD1	4:D1:17:LEU:HD13	2.27	0.68
6:R1:75:LEU:O	6:R1:80:TRP:NE1	2.27	0.68
2:B1:135:TRP:CD2	6:R1:49:ARG:HD3	2.29	0.68
1:M1:46:ARG:HH22	1:M1:316:ASP:CG	2.02	0.68
5:Q1:76:ILE:HG22	5:Q1:193:VAL:C	2.19	0.68
6:R1:51:PRO:HG2	6:R1:54:LEU:HD22	1.74	0.68
5:E1:18:VAL:HG11	5:E1:32:ARG:NH1	2.09	0.68
1:M1:236:PHE:CD2	1:M1:258:GLU:HG2	2.28	0.68
4:P1:5:LEU:HB3	4:P1:152:TYR:CD1	2.28	0.68
5:Q1:171:ILE:HG23	5:Q1:171:ILE:O	1.94	0.68
7:S1:51:PRO:O	7:S1:54:ALA:HB3	1.94	0.68
10:V1:22:LEU:O	10:V1:26:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:151:ASN:ND2	5:E1:2:HIS:NE2	2.42	0.68
1:A1:350:THR:HB	1:A1:353:GLU:CG	2.24	0.68
1:A1:426:GLY:N	1:A1:428:ILE:HG13	2.06	0.68
3:C1:311:LYS:HD2	3:C1:379:TRP:HB3	1.76	0.68
3:O1:100:ARG:NH2	69:O1:402:HEM:HBD1	2.04	0.68
27:I2:106:GLU:OE1	27:I2:106:GLU:N	2.27	0.68
1:A1:67:THR:HG22	1:A1:70:ARG:HB2	1.76	0.68
1:A1:80:GLU:O	1:A1:83:GLY:N	2.26	0.68
1:A1:365:LEU:HD21	1:A1:395:TRP:CD1	2.29	0.68
3:C1:174:THR:O	3:C1:178:PHE:HD1	1.77	0.68
5:E1:60:SER:HA	5:E1:63:SER:OG	1.94	0.68
1:M1:39:VAL:HG12	1:M1:41:ILE:CD1	2.23	0.68
4:P1:27:ARG:NH1	10:V1:58:LYS:HZ2	1.91	0.68
3:C1:244:LEU:HD23	4:D1:205:GLY:HA2	1.76	0.67
1:M1:4:TYR:CZ	1:M1:8:LEU:HD11	2.28	0.67
2:N1:264:ILE:CG2	2:N1:317:SER:HA	2.23	0.67
60:E3:43:PRO:HB2	60:E3:48:ILE:HD11	1.76	0.67
67:L3:19:TRP:HZ2	68:M3:14:GLU:HG2	1.59	0.67
3:C1:108:THR:HB	3:C1:313:ARG:HH11	1.58	0.67
3:C1:109:PHE:O	3:C1:110:LEU:C	2.36	0.67
1:A1:158:PHE:CE1	1:A1:317:THR:HG21	2.28	0.67
3:C1:22:PRO:HG2	7:G1:3:GLN:HB3	1.76	0.67
1:M1:86:LEU:HD13	1:M1:99:ILE:HG12	1.75	0.67
1:M1:408:ARG:HH12	11:W1:15:ARG:CG	2.07	0.67
3:O1:177:ARG:O	3:O1:181:PHE:CD2	2.47	0.67
3:O1:244:LEU:O	4:P1:201:ARG:HD3	1.95	0.67
3:C1:244:LEU:O	4:D1:201:ARG:HD3	1.95	0.67
5:E1:53:ASN:OD1	5:E1:53:ASN:N	2.27	0.67
6:F1:51:PRO:HD3	2:N1:134:ARG:HH12	1.57	0.67
7:G1:50:PRO:CB	7:G1:51:PRO:HD3	2.24	0.67
17:82:211:ALA:HB2	17:82:223:PRO:HB3	1.76	0.67
63:H3:38:ARG:HG2	63:H3:85:ILE:HG23	1.76	0.67
4:D1:208:MET:HE2	4:D1:208:MET:O	1.95	0.67
5:E1:68:VAL:HG12	5:E1:69:LEU:N	2.10	0.67
9:I1:53:GLU:O	9:I1:55:LEU:HG	1.94	0.67
17:82:422:HIS:ND1	19:A2:79:LEU:HD13	2.10	0.67
20:B2:163:PRO:HG2	20:B2:168:GLN:HE21	1.59	0.67
52:12:120:GLY:O	52:12:128:ALA:O	2.12	0.67
1:A1:408:ARG:NH1	11:K1:15:ARG:CG	2.57	0.67
2:N1:156:GLN:HE22	9:U1:56:ARG:HD3	1.58	0.67
5:Q1:89:PHE:HB2	5:Q1:96:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:313:LEU:CD2	38:U2:142:THR:CA	2.72	0.67
56:A3:151:HIS:O	56:A3:155:VAL:HG23	1.95	0.67
58:C3:154:GLY:HA2	61:F3:6:VAL:HG22	1.75	0.67
1:A1:426:GLY:HA2	1:A1:427:PRO:C	2.19	0.67
2:N1:209:LEU:CD2	2:N1:375:SER:HB2	2.25	0.67
3:O1:244:LEU:HD11	4:P1:204:MET:HE2	1.75	0.67
18:92:224:SER:OG	18:92:226:GLU:CG	2.43	0.67
1:A1:241:ILE:HG13	7:G1:16:TYR:CD1	2.30	0.67
3:C1:234:LEU:CD2	4:D1:216:LEU:HD21	2.24	0.67
3:C1:332:LEU:HD21	3:C1:358:TYR:HE1	1.60	0.67
7:S1:71:ARG:HH21	8:T1:60:ASP:CG	2.02	0.67
19:A2:311:LYS:CB	38:U2:142:THR:O	2.43	0.67
52:12:126:LYS:CD	52:12:127:TYR:H	1.98	0.67
3:O1:22:PRO:CG	7:S1:3:GLN:HB3	2.25	0.67
4:P1:32:VAL:HG11	4:P1:186:VAL:HG22	1.76	0.67
1:A1:53:ASN:OD1	1:A1:170:PRO:HD3	1.95	0.67
1:A1:251:ALA:O	1:A1:325:VAL:HA	1.95	0.67
1:M1:80:GLU:O	1:M1:83:GLY:N	2.28	0.67
9:U1:70:LEU:CD1	9:U1:72:VAL:H	2.08	0.67
1:A1:324:PHE:CD1	1:A1:334:MET:HG2	2.30	0.66
3:C1:56:THR:HG21	3:O1:58:ASP:OD2	1.94	0.66
8:H1:73:LEU:HD21	8:H1:74:PHE:HD1	1.58	0.66
1:M1:27:SER:HA	1:M1:199:ALA:O	1.94	0.66
1:M1:405:ARG:O	1:M1:409:GLU:HG3	1.96	0.66
2:N1:283:PRO:HG3	9:U1:55:LEU:CD2	2.24	0.66
2:N1:394:PRO:O	2:N1:398:VAL:HG23	1.94	0.66
19:A2:313:LEU:CG	38:U2:142:THR:HA	2.24	0.66
1:A1:346:CYS:CB	1:A1:412:SER:OG	2.44	0.66
4:D1:75:ASN:ND2	4:D1:80:MET:O	2.28	0.66
6:F1:42:ASP:OD2	6:F1:101:ARG:NH1	2.28	0.66
4:P1:82:MET:SD	4:P1:86:LYS:HD2	2.35	0.66
19:A2:111:LYS:CE	33:P2:53:TYR:HE2	2.07	0.66
3:C1:169:SER:CB	5:Q1:93:GLY:HA3	2.24	0.66
2:N1:327:ILE:O	2:N1:327:ILE:HG22	1.95	0.66
3:O1:122:THR:HG21	3:O1:189:ILE:HG12	1.78	0.66
4:P1:138:PRO:HB3	8:T1:55:THR:N	2.10	0.66
6:R1:28:LYS:HD2	6:R1:74:ILE:CD1	2.24	0.66
57:B3:186:SER:HB3	57:B3:213:LEU:HD22	1.75	0.66
3:C1:156:ILE:O	3:C1:157:GLY:C	2.39	0.66
4:D1:10:TYR:HE1	8:H1:73:LEU:HD21	1.60	0.66
1:M1:236:PHE:HD2	1:M1:258:GLU:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:408:ARG:CZ	11:W1:15:ARG:HE	2.08	0.66
3:O1:200:LEU:HG	3:O1:200:LEU:O	1.95	0.66
3:O1:267:HIS:NE2	3:O1:269:LYS:HD3	2.10	0.66
17:82:383:THR:HG21	19:A2:75:CYS:HA	1.76	0.66
18:92:137:THR:H	18:92:140:CYS:HB2	1.60	0.66
27:I2:105:LYS:HG3	27:I2:105:LYS:O	1.96	0.66
2:B1:31:ASN:HB3	2:B1:201:SER:HB3	1.78	0.66
2:N1:134:ARG:HG2	2:N1:135:TRP:N	2.11	0.66
2:N1:159:VAL:HG23	2:N1:427:SER:OG	1.95	0.66
3:O1:72:ASP:OD1	4:P1:49:ARG:NH1	2.25	0.66
3:O1:124:MET:HE1	3:O1:298:ILE:HG21	1.77	0.66
3:O1:156:ILE:O	3:O1:157:GLY:C	2.39	0.66
3:O1:359:PHE:O	3:O1:363:LEU:HB2	1.95	0.66
4:P1:26:ILE:HG22	4:P1:54:VAL:HG13	1.78	0.66
58:C3:209:ILE:O	58:C3:213:THR:HG23	1.95	0.66
3:C1:240:MET:HA	3:C1:243:VAL:CG1	2.24	0.66
4:D1:220:TYR:CE2	7:G1:26:PHE:CE1	2.83	0.66
2:N1:129:ALA:N	2:N1:130:PRO:CD	2.58	0.66
2:N1:132:PHE:HB3	2:N1:137:VAL:HG21	1.76	0.66
2:N1:148:LYS:HG3	2:N1:177:TYR:HB3	1.76	0.66
2:N1:180:ASP:O	2:N1:183:ILE:HD12	1.95	0.66
5:Q1:126:ARG:NH2	5:Q1:168:SER:O	2.23	0.66
10:J1:36:ASP:O	10:J1:37:GLN:C	2.35	0.66
1:M1:236:PHE:CD2	1:M1:258:GLU:HB3	2.30	0.66
3:O1:8:HIS:HB3	3:O1:9:PRO:HD3	1.76	0.66
3:O1:26:ASN:ND2	3:O1:208:PRO:HD2	2.11	0.66
3:O1:345:HIS:HB3	3:O1:346:PRO:CD	2.21	0.66
1:A1:236:PHE:CD2	1:A1:258:GLU:HB3	2.31	0.66
1:A1:351:GLU:HA	1:A1:404:ALA:HB2	1.77	0.66
1:M1:91:THR:HG23	1:M1:92:ARG:H	1.60	0.66
1:M1:426:GLY:HA2	1:M1:428:ILE:HG13	1.72	0.66
2:N1:191:LEU:O	2:N1:195:VAL:HG23	1.94	0.66
2:N1:395:PRO:O	2:N1:398:VAL:HB	1.94	0.66
3:O1:32:ASN:O	3:O1:36:LEU:HG	1.95	0.66
3:O1:102:LEU:HD21	3:O1:304:ILE:HD12	1.78	0.66
4:P1:233:ARG:HG3	7:S1:17:SER:HB2	1.77	0.66
5:Q1:1:SER:OG	5:Q1:1:SER:CA	2.44	0.66
8:T1:22:GLU:O	8:T1:25:GLU:HG2	1.94	0.66
19:A2:313:LEU:HD23	38:U2:142:THR:HA	1.76	0.66
1:A1:143:THR:O	1:A1:143:THR:HG23	1.94	0.66
1:A1:331:ILE:HD11	1:A1:427:PRO:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S1:73:ASN:N	7:S1:74:PRO:CD	2.58	0.66
10:V1:35:PHE:O	10:V1:36:ASP:C	2.37	0.66
19:A2:159:ALA:HB3	27:I2:84:VAL:HG12	1.77	0.66
19:A2:303:THR:HG23	38:U2:136:GLU:HA	1.76	0.66
44:a2:79:ASN:CG	55:e2:76:PRO:HG3	2.20	0.66
63:H3:39:CYS:HG	63:H3:53:CYS:HG	0.70	0.66
3:C1:32:ASN:HD21	3:C1:228:ASP:HA	1.61	0.66
5:E1:15:ARG:HH21	5:E1:32:ARG:HB2	1.60	0.66
9:I1:70:LEU:CD1	9:I1:72:VAL:H	2.09	0.66
5:Q1:188:THR:OG1	5:Q1:192:MET:HB2	1.96	0.66
56:A3:298:ASP:HB2	56:A3:301:THR:HG23	1.77	0.66
58:C3:160:LEU:HD13	58:C3:222:GLN:HG2	1.78	0.66
1:A1:262:TRP:CG	1:A1:385:THR:HG23	2.31	0.65
1:M1:161:THR:HB	1:M1:162:PRO:HD2	1.77	0.65
3:O1:44:GLN:OE1	3:O1:83:HIS:ND1	2.30	0.65
4:P1:27:ARG:NH1	10:V1:58:LYS:HG3	2.11	0.65
19:A2:313:LEU:HG	38:U2:142:THR:CB	2.26	0.65
29:K2:20:ARG:HB2	29:K2:66:TRP:HB2	1.77	0.65
1:M1:163:LEU:HD12	1:M1:163:LEU:O	1.95	0.65
3:O1:102:LEU:HD21	3:O1:304:ILE:HD13	1.77	0.65
1:A1:78:GLU:HG2	1:A1:112:LEU:HD21	1.78	0.65
3:C1:243:VAL:HG13	3:C1:244:LEU:HD13	1.77	0.65
1:M1:351:GLU:OE2	1:M1:404:ALA:HB3	1.96	0.65
2:N1:98:VAL:HG22	2:N1:107:TYR:CD2	2.30	0.65
2:N1:247:GLN:HE22	2:N1:429:ASN:ND2	1.95	0.65
2:N1:248:ASN:HB2	2:N1:428:GLY:CA	2.22	0.65
3:O1:122:THR:CG2	3:O1:189:ILE:CD1	2.75	0.65
3:O1:218:ILE:HD13	4:P1:230:LEU:HD11	1.78	0.65
5:Q1:102:THR:O	5:Q1:106:ILE:HG13	1.96	0.65
19:A2:111:LYS:HD2	33:P2:53:TYR:OH	1.96	0.65
1:A1:75:LEU:HD21	1:A1:116:ILE:HG12	1.78	0.65
4:D1:11:PRO:O	8:H1:74:PHE:CZ	2.49	0.65
2:N1:207:ILE:CD1	2:N1:383:GLY:HA2	2.25	0.65
3:O1:310:SER:CB	3:O1:318:ARG:NH1	2.59	0.65
5:Q1:101:ARG:HD3	5:Q1:133:VAL:HG11	1.76	0.65
10:V1:9:LEU:HD12	10:V1:13:LEU:HD12	1.77	0.65
52:12:75:PRO:CA	52:12:223:PHE:CZ	2.79	0.65
57:B3:120:SER:OG	57:B3:138:VAL:HG21	1.97	0.65
4:D1:236:ALA:HB3	7:G1:14:ILE:HB	1.78	0.65
7:G1:2:ARG:HB2	7:G1:6:HIS:HD2	1.59	0.65
10:J1:55:ILE:HG23	10:J1:58:LYS:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R1:42:ASP:OD2	6:R1:101:ARG:NH1	2.30	0.65
58:C3:101:PHE:HZ	58:C3:260:GLY:HA3	1.61	0.65
1:A1:106:LEU:CD2	1:A1:203:LEU:HD13	2.26	0.65
1:A1:426:GLY:N	1:A1:428:ILE:HG12	2.10	0.65
2:B1:56:ARG:NH2	2:B1:172:LEU:HD21	2.12	0.65
2:B1:134:ARG:NH1	6:R1:51:PRO:HD3	2.11	0.65
2:B1:354:ASN:N	2:B1:355:PRO:HD2	2.10	0.65
4:D1:241:LYS:OXT	4:D1:241:LYS:HG2	1.95	0.65
1:M1:45:SER:OG	1:M1:92:ARG:CG	2.44	0.65
1:M1:335:MET:HE1	1:M1:338:LEU:HD23	1.79	0.65
2:N1:156:GLN:NE2	9:U1:56:ARG:HD3	2.12	0.65
2:N1:384:SER:HB2	9:U1:62:ARG:HG2	1.79	0.65
5:Q1:85:LYS:HG2	5:Q1:86:ASN:N	2.11	0.65
1:A1:342:TRP:O	1:A1:343:MET:C	2.38	0.65
5:E1:62:MET:O	3:O1:177:ARG:NH2	2.30	0.65
1:M1:298:ALA:HA	1:M1:303:LEU:HB2	1.77	0.65
3:O1:315:MET:HE2	3:O1:318:ARG:HH21	1.60	0.65
6:R1:73:GLN:HE21	7:S1:32:LYS:HZ1	1.44	0.65
1:A1:198:ALA:O	1:A1:199:ALA:HB2	1.95	0.65
3:C1:174:THR:O	3:C1:178:PHE:CD1	2.50	0.65
3:C1:183:PHE:CE1	3:O1:183:PHE:CD1	2.84	0.65
3:O1:311:LYS:HD2	3:O1:379:TRP:HB3	1.79	0.65
4:P1:50:HIS:HB3	4:P1:54:VAL:CB	2.26	0.65
5:Q1:117:LEU:O	5:Q1:118:ARG:C	2.39	0.65
19:A2:157:LYS:HB2	27:I2:100:TYR:CE2	2.31	0.65
21:C2:123:THR:HG21	25:G2:129:SER:H	1.62	0.65
2:B1:109:VAL:HG22	2:B1:119:LEU:HD23	1.77	0.65
2:B1:279:LEU:HD22	2:B1:295:LEU:HD13	1.76	0.65
4:D1:178:THR:HG23	8:H1:15:ASP:N	2.11	0.65
1:M1:6:GLN:O	1:M1:7:ALA:C	2.39	0.65
4:P1:164:ILE:HD11	4:P1:186:VAL:HG21	1.79	0.65
19:A2:422:TRP:O	25:G2:169:ARG:NH1	2.30	0.65
19:A2:674:LEU:HD12	29:K2:46:LYS:CD	2.26	0.65
1:A1:158:PHE:HB2	1:A1:164:ALA:HB2	1.79	0.65
3:C1:296:PHE:HD1	3:C1:359:PHE:HE1	1.45	0.65
4:D1:138:PRO:HB3	8:H1:55:THR:N	2.12	0.65
6:F1:28:LYS:CB	6:F1:74:ILE:HD11	2.26	0.65
1:M1:38:GLY:HA3	1:M1:40:TRP:HZ3	1.62	0.65
1:M1:91:THR:CG2	1:M1:92:ARG:N	2.60	0.65
1:M1:391:PRO:HB2	1:M1:395:TRP:CZ2	2.32	0.65
2:N1:303:VAL:HG12	2:N1:304:HIS:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N1:436:ILE:HD12	2:N1:437:ASP:OD1	1.96	0.65
56:A3:195:LEU:HD23	56:A3:245:ILE:HD13	1.79	0.65
2:B1:155:PRO:HB2	2:B1:254:HIS:CE1	2.32	0.64
2:B1:333:ALA:O	2:B1:337:ILE:HD12	1.97	0.64
3:C1:78:ILE:HD11	5:E1:57:GLN:NE2	2.12	0.64
3:C1:270:PRO:HB2	3:C1:274:PHE:HB2	1.78	0.64
3:C1:345:HIS:HB3	3:C1:346:PRO:HD3	1.79	0.64
10:J1:12:LEU:HD23	10:J1:13:LEU:HD21	1.79	0.64
4:P1:70:VAL:HG23	4:P1:84:PRO:HD3	1.80	0.64
2:B1:257:LEU:HD13	2:B1:424:MET:HB2	1.77	0.64
4:D1:229:VAL:HG22	7:G1:18:LEU:O	1.97	0.64
4:D1:233:ARG:HG3	7:G1:17:SER:HB2	1.80	0.64
1:M1:426:GLY:N	1:M1:428:ILE:CG1	2.60	0.64
2:N1:71:LEU:HD13	2:N1:143:GLN:HG3	1.78	0.64
4:P1:51:LEU:HA	4:P1:56:TYR:O	1.97	0.64
2:B1:318:ASP:OD1	2:B1:318:ASP:N	2.28	0.64
4:D1:27:ARG:O	4:D1:28:ARG:C	2.41	0.64
1:M1:158:PHE:CZ	1:M1:317:THR:HG21	2.31	0.64
1:M1:279:HIS:HA	1:M1:307:PHE:O	1.97	0.64
2:N1:279:LEU:HD22	2:N1:344:VAL:HG22	1.80	0.64
4:P1:54:VAL:O	4:P1:54:VAL:HG12	1.96	0.64
5:Q1:91:TRP:O	5:Q1:92:ARG:HB2	1.97	0.64
10:V1:51:LEU:HB3	10:V1:52:TRP:CZ3	2.32	0.64
28:J2:47:LEU:HD23	34:Q2:22:SER:HB2	1.80	0.64
1:A1:106:LEU:N	1:A1:107:PRO:HD2	2.11	0.64
2:B1:385:GLN:HG2	9:I1:62:ARG:NH1	2.10	0.64
3:C1:170:VAL:HG12	3:C1:170:VAL:O	1.97	0.64
3:C1:206:ASN:CB	3:C1:313:ARG:HH21	2.05	0.64
4:D1:55:CYS:SG	10:J1:55:ILE:HG22	2.37	0.64
2:N1:133:ARG:HD3	2:N1:135:TRP:CZ2	2.33	0.64
5:Q1:76:ILE:HD12	5:Q1:192:MET:CE	2.28	0.64
19:A2:111:LYS:HE2	33:P2:53:TYR:HE2	1.62	0.64
1:A1:269:ALA:HB3	1:A1:410:VAL:HG11	1.80	0.64
2:B1:128:THR:HG23	2:B1:226:ILE:HD11	1.80	0.64
3:C1:240:MET:O	3:C1:244:LEU:HB2	1.96	0.64
4:D1:178:THR:HG21	8:H1:16:PRO:HG2	1.79	0.64
3:O1:296:PHE:HD1	3:O1:359:PHE:HE1	1.43	0.64
55:e2:70:THR:C	55:e2:72:TYR:H	2.01	0.64
2:B1:253:VAL:HG23	2:B1:427:SER:O	1.96	0.64
3:C1:264:THR:CG2	5:Q1:144:CYS:HB3	2.24	0.64
1:M1:436:ARG:HE	3:O1:222:PRO:HD3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R1:73:GLN:HA	7:S1:39:ARG:HH21	1.61	0.64
17:82:386:ARG:HD2	19:A2:178:GLN:OE1	1.97	0.64
52:12:25:ARG:HG2	52:12:25:ARG:NH1	2.10	0.64
62:G3:5:LYS:HZ3	62:G3:6:GLY:N	1.86	0.64
2:B1:200:THR:CG2	2:B1:203:ARG:HD2	2.23	0.64
1:M1:408:ARG:NH1	11:W1:15:ARG:CG	2.61	0.64
3:O1:172:LYS:O	3:O1:173:ALA:C	2.41	0.64
3:O1:207:ASN:OD1	3:O1:210:GLY:N	2.26	0.64
20:B2:82:LEU:HD11	52:12:126:LYS:HE3	1.80	0.64
49:h2:141:CYS:HA	54:g2:162:ARG:HD3	1.80	0.64
56:A3:172:LYS:HB2	56:A3:172:LYS:NZ	2.12	0.64
1:A1:358:LYS:HD2	1:A1:402:VAL:CG1	2.28	0.64
2:B1:24:LEU:HD12	2:B1:24:LEU:N	2.04	0.64
2:B1:95:LYS:HE3	9:I1:70:LEU:CD2	2.24	0.64
2:B1:347:ILE:HD12	2:B1:347:ILE:N	2.13	0.64
3:C1:338:ILE:N	3:C1:338:ILE:CD1	2.61	0.64
2:N1:352:LEU:HG	2:N1:352:LEU:O	1.96	0.64
5:Q1:63:SER:O	5:Q1:64:ALA:HB2	1.98	0.64
56:A3:84:PRO:HG3	56:A3:92:MET:HE3	1.80	0.64
59:D3:24:LEU:H	60:E3:34:ASN:HD21	1.44	0.64
1:A1:145:MET:SD	1:A1:248:LEU:CD1	2.86	0.64
2:B1:434:PRO:HB3	2:B1:438:GLU:HB3	1.80	0.64
3:C1:47:THR:HG21	3:C1:83:HIS:CB	2.27	0.64
3:C1:309:THR:HG23	3:C1:370:GLY:HA3	1.80	0.64
4:D1:94:PRO:HB2	4:D1:95:TYR:CE1	2.33	0.64
10:J1:34:ALA:O	10:J1:35:PHE:C	2.38	0.64
1:M1:15:GLN:O	1:M1:26:ALA:HA	1.97	0.64
1:M1:199:ALA:HB3	1:M1:208:LEU:HD21	1.79	0.64
3:O1:79:ILE:HG12	5:Q1:58:PHE:CE1	2.33	0.64
5:Q1:15:ARG:CB	5:Q1:16:PRO:HD2	2.06	0.64
6:R1:43:VAL:HG22	6:R1:94:LEU:HD21	1.80	0.64
7:S1:34:ILE:HB	7:S1:35:PRO:CD	2.27	0.64
19:A2:362:ASP:CG	29:K2:17:ARG:HH21	2.06	0.64
1:A1:338:LEU:O	1:A1:339:GLN:C	2.41	0.64
2:B1:319:SER:OG	2:B1:320:GLY:N	2.27	0.64
3:C1:78:ILE:O	3:C1:82:MET:HB2	1.98	0.64
1:M1:408:ARG:NH1	11:W1:15:ARG:HG2	2.13	0.64
3:O1:141:TRP:O	3:O1:145:VAL:HG23	1.98	0.64
5:Q1:118:ARG:HB3	5:Q1:171:ILE:HG23	1.80	0.64
1:A1:385:THR:HG22	1:A1:386:TYR:N	2.12	0.63
3:C1:183:PHE:CD1	3:O1:183:PHE:CE1	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:96:GLU:OE1	6:F1:99:ARG:HD2	1.98	0.63
7:G1:34:ILE:HB	7:G1:35:PRO:CD	2.21	0.63
3:O1:119:LEU:HD13	3:O1:192:ILE:HG22	1.80	0.63
5:Q1:15:ARG:HH21	5:Q1:32:ARG:CG	2.08	0.63
52:12:288:LEU:HA	52:12:292:ASN:HD22	1.63	0.63
53:62:578:THR:HA	53:62:581:LYS:HE2	1.79	0.63
1:A1:64:PHE:CE2	1:A1:88:ALA:HB2	2.33	0.63
1:A1:204:GLU:HG2	1:A1:206:ARG:HB3	1.80	0.63
2:B1:109:VAL:HG22	2:B1:119:LEU:CD2	2.28	0.63
1:M1:426:GLY:CA	1:M1:428:ILE:N	2.61	0.63
3:O1:30:TRP:O	3:O1:33:PHE:CD2	2.47	0.63
6:R1:96:GLU:OE1	6:R1:99:ARG:HD2	1.98	0.63
19:A2:313:LEU:N	38:U2:142:THR:O	2.30	0.63
56:A3:187:SER:CB	56:A3:277:MET:HE1	2.28	0.63
2:B1:384:SER:CB	9:I1:62:ARG:HG2	2.28	0.63
3:C1:44:GLN:OE1	3:C1:83:HIS:ND1	2.30	0.63
1:M1:143:THR:HG23	1:M1:143:THR:O	1.98	0.63
1:M1:385:THR:HG22	1:M1:386:TYR:N	2.13	0.63
4:P1:50:HIS:HB3	4:P1:54:VAL:CG2	2.28	0.63
5:Q1:193:VAL:HG13	5:Q1:193:VAL:O	1.97	0.63
7:S1:25:ALA:C	7:S1:27:PRO:HD3	2.23	0.63
3:C1:78:ILE:HG21	4:D1:204:MET:HE1	1.81	0.63
3:C1:230:LEU:HD12	4:D1:219:VAL:HG12	1.80	0.63
1:M1:352:SER:OG	1:M1:353:GLU:N	2.31	0.63
3:O1:102:LEU:HB3	3:O1:325:PHE:HE1	1.62	0.63
5:Q1:157:TYR:CE2	5:Q1:159:PRO:HA	2.33	0.63
10:V1:51:LEU:HD22	10:V1:52:TRP:HZ3	1.64	0.63
53:62:138:PHE:HB2	53:62:196:TRP:HE1	1.62	0.63
2:B1:338:LYS:HD3	2:B1:439:LEU:HD23	1.81	0.63
3:C1:183:PHE:CD1	3:C1:183:PHE:O	2.52	0.63
3:C1:346:PRO:HG2	7:G1:66:PHE:HD1	1.63	0.63
4:D1:32:VAL:HG21	4:D1:186:VAL:HG22	1.79	0.63
1:M1:72:GLY:O	1:M1:73:ASN:OD1	2.17	0.63
39:V2:58:ARG:HE	52:12:316:PRO:HB3	1.63	0.63
53:62:28:LYS:HE3	53:62:31:ASN:HD21	1.63	0.63
56:A3:273:MET:HG3	56:A3:319:LYS:HZ1	1.63	0.63
1:A1:308:GLN:O	1:A1:308:GLN:CG	2.46	0.63
1:A1:333:ASP:O	1:A1:337:VAL:HG23	1.98	0.63
2:B1:59:ASN:CG	2:B1:60:SER:H	2.07	0.63
3:C1:311:LYS:O	6:F1:38:HIS:HB2	1.98	0.63
4:D1:82:MET:CE	4:D1:86:LYS:HZ2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:138:PRO:O	4:D1:139:THR:C	2.40	0.63
3:O1:137:GLN:OE1	3:O1:259:ALA:HA	1.99	0.63
4:P1:229:VAL:HG12	4:P1:233:ARG:HE	1.63	0.63
2:B1:341:TYR:HE2	2:B1:345:LYS:HE3	1.61	0.63
10:J1:3:PRO:HG2	10:J1:8:ARG:HG2	1.81	0.63
1:M1:155:ALA:HA	1:M1:164:ALA:HB1	1.80	0.63
1:M1:350:THR:HB	1:M1:353:GLU:CG	2.28	0.63
1:M1:404:ALA:O	1:M1:408:ARG:HG3	1.98	0.63
2:N1:257:LEU:HD13	2:N1:424:MET:HE2	1.80	0.63
4:P1:75:ASN:ND2	4:P1:80:MET:O	2.32	0.63
5:Q1:76:ILE:HG22	5:Q1:194:ILE:HG12	1.79	0.63
19:A2:314:LEU:HD22	38:U2:140:PRO:HD2	1.77	0.63
52:12:75:PRO:N	52:12:223:PHE:CZ	2.64	0.63
4:D1:10:TYR:O	4:D1:12:TRP:CD1	2.51	0.63
6:F1:75:LEU:O	6:F1:80:TRP:NE1	2.30	0.63
3:O1:90:PHE:HE1	3:O1:123:VAL:HG21	1.60	0.63
3:O1:115:ILE:CG2	3:O1:196:HIS:HB2	2.27	0.63
3:O1:153:ILE:HG23	3:O1:154:PRO:HD2	1.79	0.63
3:C1:15:ASN:ND2	3:C1:18:PHE:CE1	2.67	0.63
3:C1:296:PHE:CD1	3:C1:359:PHE:HE1	2.17	0.63
7:G1:71:ARG:HH21	8:H1:60:ASP:CG	2.07	0.63
1:M1:151:ASN:ND2	5:Q1:2:HIS:NE2	2.46	0.63
3:O1:28:SER:HB3	3:O1:30:TRP:HD1	1.63	0.63
3:O1:33:PHE:CE1	3:O1:96:MET:HG3	2.34	0.63
3:O1:132:VAL:HA	3:O1:139:SER:HB3	1.81	0.63
19:A2:302:LEU:N	38:U2:137:TRP:HB2	2.13	0.63
67:L3:45:LEU:HD21	68:M3:40:TYR:HA	1.78	0.63
1:A1:38:GLY:HA3	1:A1:40:TRP:HZ3	1.62	0.62
3:C1:119:LEU:HD13	3:C1:192:ILE:HG22	1.80	0.62
1:M1:86:LEU:HB3	2:N1:285:VAL:HG22	1.81	0.62
2:N1:83:PHE:CE2	2:N1:87:ARG:HG3	2.34	0.62
3:O1:207:ASN:HB2	3:O1:208:PRO:HD2	1.80	0.62
49:h2:141:CYS:HB2	49:h2:144:PRO:HG3	1.81	0.62
60:E3:82:TYR:HB3	60:E3:83:PRO:HD3	1.81	0.62
1:A1:370:ASP:OD1	2:B1:375:SER:HB3	1.99	0.62
2:B1:352:LEU:HB3	2:B1:411:ILE:CD1	2.29	0.62
1:M1:45:SER:CB	1:M1:167:VAL:HG22	2.29	0.62
4:P1:50:HIS:O	4:P1:51:LEU:C	2.40	0.62
4:P1:62:LYS:O	4:P1:66:GLU:HG3	1.99	0.62
1:A1:297:ILE:HG22	1:A1:303:LEU:HD12	1.79	0.62
2:B1:111:CYS:CB	2:B1:119:LEU:HD22	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:116:GLY:HA3	69:C1:402:HEM:C3C	2.34	0.62
3:O1:160:LEU:HD11	3:O1:164:ILE:HD11	1.80	0.62
5:Q1:153:PHE:CE1	5:Q1:173:LYS:HG3	2.34	0.62
59:D3:16:TYR:CE1	59:D3:25:PRO:HG3	2.34	0.62
63:H3:57:ARG:HB3	63:H3:57:ARG:HH11	1.64	0.62
1:A1:351:GLU:OE2	1:A1:404:ALA:HB3	2.00	0.62
1:A1:351:GLU:O	1:A1:352:SER:C	2.42	0.62
1:A1:403:ASP:OD1	1:A1:404:ALA:N	2.33	0.62
2:B1:47:ILE:HG22	2:B1:48:GLY:N	2.15	0.62
2:B1:156:GLN:NE2	9:I1:56:ARG:HD3	2.14	0.62
3:C1:119:LEU:HD13	3:C1:192:ILE:CG2	2.29	0.62
3:C1:207:ASN:OD1	3:C1:210:GLY:N	2.32	0.62
4:D1:50:HIS:HB3	4:D1:54:VAL:CG2	2.29	0.62
1:M1:309:THR:HA	1:M1:322:ALA:HA	1.81	0.62
2:N1:154:ASN:O	2:N1:155:PRO:C	2.43	0.62
8:T1:34:ARG:O	8:T1:38:GLU:HG2	1.99	0.62
19:A2:129:PRO:CG	27:I2:114:TYR:HE1	2.12	0.62
34:Q2:50:GLU:HB3	34:Q2:138:PRO:HG3	1.80	0.62
56:A3:92:MET:HE2	56:A3:167:THR:HG21	1.82	0.62
57:B3:122:MET:HB2	57:B3:208:PRO:HD2	1.81	0.62
2:B1:341:TYR:CE2	2:B1:345:LYS:HE3	2.34	0.62
3:C1:27:ILE:O	3:C1:27:ILE:CG2	2.46	0.62
2:N1:37:SER:OG	2:N1:213:HIS:HB2	2.00	0.62
2:N1:56:ARG:NH2	2:N1:172:LEU:HD21	2.14	0.62
2:N1:95:LYS:CE	9:U1:70:LEU:HD22	2.29	0.62
4:P1:127:VAL:HG12	4:P1:187:CYS:SG	2.39	0.62
5:Q1:76:ILE:HG23	5:Q1:194:ILE:CG1	2.29	0.62
5:Q1:78:LEU:HD23	5:Q1:79:SER:H	1.64	0.62
17:82:52:ARG:HH21	17:82:132:ARG:HG3	1.63	0.62
1:A1:43:ALA:CB	1:A1:189:HIS:HB3	2.30	0.62
1:A1:92:ARG:HD2	1:A1:163:LEU:CD1	2.29	0.62
1:A1:158:PHE:CB	1:A1:164:ALA:HB2	2.29	0.62
4:D1:72:ASP:O	4:D1:73:GLY:O	2.18	0.62
6:F1:106:GLU:HA	6:F1:109:LYS:HZ3	1.63	0.62
8:H1:25:GLU:HA	8:H1:30:CYS:SG	2.39	0.62
2:N1:203:ARG:NE	2:N1:230:LEU:HD23	2.15	0.62
2:N1:255:ALA:HB2	2:N1:426:ALA:HB2	1.81	0.62
3:O1:8:HIS:CB	3:O1:9:PRO:HD3	2.29	0.62
4:P1:3:LEU:HD11	7:S1:71:ARG:HB2	1.81	0.62
9:U1:53:GLU:O	9:U1:55:LEU:HG	2.00	0.62
1:A1:6:GLN:O	1:A1:7:ALA:C	2.41	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:91:THR:CG2	1:A1:92:ARG:N	2.62	0.62
1:A1:240:GLN:HG3	1:A1:422:VAL:O	1.98	0.62
1:A1:417:ASP:OD1	1:A1:417:ASP:O	2.17	0.62
2:B1:42:ALA:CB	2:B1:43:PRO:HD2	2.28	0.62
2:B1:187:THR:O	2:B1:190:GLU:HB2	1.99	0.62
3:C1:106:SER:HB3	69:C1:402:HEM:HBD2	1.81	0.62
3:O1:115:ILE:HG21	3:O1:196:HIS:HB2	1.81	0.62
10:V1:51:LEU:HB3	10:V1:52:TRP:CE3	2.35	0.62
11:W1:26:ALA:O	11:W1:30:VAL:HG23	1.99	0.62
19:A2:423:LEU:HD12	25:G2:169:ARG:O	1.98	0.62
27:I2:96:HIS:HB2	27:I2:114:TYR:HB3	1.81	0.62
1:A1:32:GLN:HG3	1:A1:33:PRO:HD2	1.80	0.62
1:A1:61:HIS:NE2	1:A1:134:ILE:CD1	2.62	0.62
1:A1:408:ARG:NH1	11:K1:15:ARG:NE	2.45	0.62
2:B1:58:GLU:OE1	2:B1:63:LEU:HA	2.00	0.62
2:B1:156:GLN:HE22	9:I1:56:ARG:HD3	1.65	0.62
2:B1:163:LEU:HD22	2:B1:256:ALA:CB	2.29	0.62
2:B1:247:GLN:NE2	2:B1:429:ASN:HA	2.14	0.62
5:Q1:103:LYS:HA	5:Q1:106:ILE:HD12	1.82	0.62
2:B1:58:GLU:HB2	2:B1:63:LEU:HD23	1.82	0.62
2:B1:101:THR:OG1	2:B1:102:ARG:N	2.32	0.62
3:C1:329:VAL:HA	3:C1:332:LEU:HD12	1.80	0.62
4:D1:57:THR:HG22	4:D1:58:GLU:H	1.65	0.62
1:M1:53:ASN:OD1	1:M1:170:PRO:HD3	1.99	0.62
1:M1:134:ILE:HG21	1:M1:174:VAL:HG21	1.81	0.62
1:M1:144:SER:O	1:M1:148:VAL:HG23	1.99	0.62
2:N1:195:VAL:HG13	2:N1:199:PHE:CD2	2.34	0.62
2:N1:352:LEU:HB3	2:N1:411:ILE:CD1	2.29	0.62
4:P1:120:ARG:HG2	4:P1:120:ARG:HH11	1.62	0.62
4:P1:231:LYS:HD2	6:R1:71:ARG:HG2	1.81	0.62
5:Q1:187:PHE:CE2	5:Q1:193:VAL:HB	2.34	0.62
17:82:384:PRO:HD3	19:A2:76:ARG:HB2	1.82	0.62
19:A2:111:LYS:HE2	33:P2:53:TYR:CE2	2.35	0.62
19:A2:313:LEU:CG	38:U2:142:THR:CB	2.78	0.62
2:B1:209:LEU:CD2	2:B1:375:SER:HB2	2.30	0.62
2:B1:303:VAL:HG12	2:B1:304:HIS:N	2.14	0.62
3:C1:25:SER:HA	3:C1:218:ILE:CD1	2.29	0.62
3:C1:79:ILE:HG12	5:E1:58:PHE:CE1	2.35	0.62
4:D1:82:MET:HE2	4:D1:86:LYS:HZ2	1.64	0.62
1:M1:162:PRO:O	1:M1:165:GLN:HG2	1.99	0.62
3:O1:7:SER:HA	3:O1:13:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:52:ALA:HB2	69:O1:401:HEM:HMD1	1.81	0.62
4:P1:79:GLU:OE1	4:P1:82:MET:HG3	1.98	0.62
4:P1:176:PRO:HB2	4:P1:181:GLN:NE2	2.14	0.62
6:R1:73:GLN:HE21	7:S1:32:LYS:CE	2.12	0.62
19:A2:140:GLN:HG3	20:B2:379:ILE:HG23	1.81	0.62
20:B2:82:LEU:HD11	52:12:126:LYS:CD	2.30	0.62
1:A1:395:TRP:O	1:A1:396:GLU:C	2.43	0.61
1:A1:433:ASP:HB2	3:C1:219:PRO:HG2	1.82	0.61
3:C1:10:LEU:HD12	3:C1:13:ILE:CD1	2.28	0.61
2:N1:129:ALA:N	2:N1:130:PRO:HD3	2.14	0.61
56:A3:128:VAL:HG22	56:A3:128:VAL:O	1.99	0.61
1:A1:151:ASN:O	1:A1:152:TYR:C	2.43	0.61
1:A1:336:PHE:HE2	1:A1:446:PHE:HD2	1.47	0.61
2:B1:111:CYS:HB3	2:B1:119:LEU:CD2	2.29	0.61
3:C1:207:ASN:ND2	3:C1:209:THR:OG1	2.32	0.61
3:C1:313:ARG:HB3	6:F1:38:HIS:CD2	2.35	0.61
10:J1:51:LEU:HB3	10:J1:52:TRP:CZ3	2.36	0.61
1:M1:373:THR:HB	1:M1:374:PRO:HD3	1.81	0.61
3:O1:304:ILE:N	3:O1:305:PRO:HD2	2.14	0.61
18:92:130:TYR:HA	18:92:189:ASN:HD21	1.65	0.61
19:A2:34:VAL:HG22	19:A2:99:GLY:HA2	1.82	0.61
19:A2:667:GLN:HE22	29:K2:38:GLU:CD	2.07	0.61
57:B3:16:ILE:HD12	57:B3:17:MET:N	2.15	0.61
2:B1:47:ILE:HD12	2:B1:120:MET:SD	2.39	0.61
2:B1:90:GLU:O	2:B1:91:ALA:C	2.44	0.61
2:B1:169:ARG:CZ	2:N1:438:GLU:OE2	2.47	0.61
3:O1:8:HIS:CB	3:O1:9:PRO:CD	2.78	0.61
4:P1:68:VAL:HG12	4:P1:92:PRO:HG2	1.82	0.61
4:P1:83:ARG:CB	4:P1:84:PRO:CD	2.63	0.61
4:P1:138:PRO:HG2	8:T1:55:THR:CB	2.30	0.61
10:V1:55:ILE:HG23	10:V1:58:LYS:HE2	1.82	0.61
22:D2:99:MET:HG2	22:D2:106:MET:HB2	1.83	0.61
61:F3:13:ALA:O	61:F3:18:ARG:HD2	2.00	0.61
1:A1:5:ALA:O	1:A1:8:LEU:HB2	2.00	0.61
1:A1:428:ILE:HG21	1:A1:431:LEU:HD22	1.83	0.61
2:B1:123:LEU:O	2:B1:127:THR:HG22	2.00	0.61
2:B1:162:ASN:ND2	2:B1:244:ILE:CG2	2.61	0.61
3:C1:52:ALA:HB2	69:C1:401:HEM:HMD2	1.83	0.61
3:C1:153:ILE:HG23	3:C1:154:PRO:HD2	1.82	0.61
10:J1:29:LEU:HD13	11:K1:34:TRP:HB3	1.81	0.61
5:Q1:141:HIS:NE2	5:Q1:175:PRO:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S1:54:ALA:O	7:S1:58:VAL:HG23	2.01	0.61
17:82:419:ILE:HD11	19:A2:119:PHE:HE2	1.65	0.61
51:j2:119:VAL:H	54:g2:147:GLY:H	1.47	0.61
58:C3:154:GLY:HA2	61:F3:6:VAL:CG2	2.30	0.61
65:J3:3:ASN:HD22	65:J3:3:ASN:C	2.08	0.61
3:C1:372:ILE:O	3:C1:375:LYS:N	2.32	0.61
1:M1:403:ASP:OD1	1:M1:404:ALA:N	2.33	0.61
2:N1:354:ASN:N	2:N1:355:PRO:HD2	2.16	0.61
3:O1:126:THR:HG21	69:O1:401:HEM:C3B	2.36	0.61
8:T1:15:ASP:HB2	8:T1:16:PRO:HD3	1.83	0.61
19:A2:129:PRO:HG2	27:I2:114:TYR:HE1	1.65	0.61
19:A2:313:LEU:CD2	38:U2:142:THR:HA	2.31	0.61
20:B2:95:LEU:O	20:B2:95:LEU:HD23	2.01	0.61
3:C1:267:HIS:NE2	3:C1:269:LYS:HD3	2.15	0.61
4:D1:204:MET:O	4:D1:205:GLY:C	2.42	0.61
9:I1:62:ARG:HB3	9:I1:63:PRO:HD3	1.83	0.61
1:M1:37:VAL:HG13	1:M1:199:ALA:HB2	1.82	0.61
1:M1:358:LYS:HE3	1:M1:402:VAL:HB	1.82	0.61
3:O1:171:ASP:O	3:O1:172:LYS:C	2.44	0.61
4:P1:27:ARG:HH11	10:V1:58:LYS:NZ	1.98	0.61
4:P1:27:ARG:NH2	4:P1:60:GLU:OE2	2.34	0.61
7:S1:73:ASN:HD22	8:T1:56:GLU:CD	2.08	0.61
19:A2:273:ILE:HD11	19:A2:291:ARG:HA	1.83	0.61
40:M2:70:LEU:HD13	40:M2:76:ILE:HG12	1.82	0.61
1:A1:436:ARG:HE	3:C1:222:PRO:CG	2.12	0.61
2:B1:86:THR:HG23	9:I1:71:ASN:HD21	1.66	0.61
3:C1:146:ILE:O	3:C1:149:LEU:HB3	2.00	0.61
8:H1:40:CYS:HB2	8:H1:57:GLU:HG2	1.83	0.61
2:N1:412:ASN:O	2:N1:415:LYS:HB2	2.01	0.61
14:42:294:MET:SD	14:42:319:HIS:NE2	2.70	0.61
52:12:75:PRO:HG3	52:12:223:PHE:CE2	2.32	0.61
56:A3:92:MET:CE	56:A3:167:THR:HG21	2.31	0.61
58:C3:6:HIS:HD2	58:C3:8:TYR:H	1.49	0.61
2:B1:140:LEU:HD12	2:B1:143:GLN:HB3	1.83	0.61
3:O1:244:LEU:HD23	4:P1:205:GLY:HA2	1.83	0.61
4:P1:13:SER:O	4:P1:19:SER:HB3	1.99	0.61
19:A2:67:GLU:HA	25:G2:158:LYS:HE2	1.81	0.61
47:d2:77:PHE:HA	53:62:471:ASN:HD21	1.65	0.61
56:A3:11:ASN:HD21	56:A3:13:LYS:HB2	1.64	0.61
2:B1:435:PHE:HB2	2:B1:438:GLU:OE1	2.00	0.61
3:C1:315:MET:HA	3:C1:318:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:354:VAL:CG1	1:M1:407:VAL:HG21	2.31	0.61
4:P1:11:PRO:O	8:T1:74:PHE:CZ	2.54	0.61
20:B2:87:GLN:HA	20:B2:87:GLN:OE1	2.01	0.61
58:C3:148:HIS:O	58:C3:152:MET:HG3	2.01	0.61
68:M3:13:LYS:HD3	68:M3:13:LYS:H	1.65	0.61
1:A1:86:LEU:HD13	1:A1:99:ILE:CG1	2.31	0.61
1:A1:244:ARG:CZ	7:G1:10:VAL:HB	2.31	0.61
2:B1:59:ASN:OD1	2:B1:60:SER:N	2.32	0.61
2:B1:434:PRO:HB2	2:B1:439:LEU:HD11	1.81	0.61
3:C1:22:PRO:CG	7:G1:3:GLN:HB3	2.31	0.61
4:D1:10:TYR:CE1	8:H1:73:LEU:CD2	2.84	0.61
5:E1:29:SER:HA	5:E1:32:ARG:HD3	1.81	0.61
1:M1:4:TYR:CE2	1:M1:396:GLU:HG3	2.36	0.61
1:M1:366:VAL:HG12	1:M1:367:SER:N	2.16	0.61
3:O1:129:MET:CG	3:O1:178:PHE:HD1	2.14	0.61
5:Q1:13:TYR:O	7:S1:23:GLN:HB3	2.01	0.61
63:H3:39:CYS:HG	63:H3:53:CYS:CB	2.09	0.61
1:A1:5:ALA:O	1:A1:6:GLN:C	2.43	0.60
1:A1:80:GLU:O	1:A1:82:MET:N	2.34	0.60
2:B1:337:ILE:CG2	2:B1:434:PRO:HG2	2.31	0.60
3:C1:163:TRP:O	3:C1:177:ARG:NH1	2.32	0.60
7:G1:68:LYS:O	7:G1:72:LYS:N	2.34	0.60
1:M1:91:THR:HG23	1:M1:92:ARG:N	2.16	0.60
4:P1:237:TYR:CD2	4:P1:239:PRO:HD3	2.36	0.60
25:G2:75:ARG:NH2	25:G2:119:ASP:OD1	2.34	0.60
1:A1:41:ILE:CG1	1:A1:195:MET:HE3	2.22	0.60
1:A1:236:PHE:HD2	1:A1:258:GLU:CG	2.12	0.60
2:B1:155:PRO:O	2:B1:156:GLN:C	2.43	0.60
7:G1:25:ALA:C	7:G1:27:PRO:HD3	2.26	0.60
5:Q1:188:THR:OG1	5:Q1:189:SER:N	2.33	0.60
19:A2:313:LEU:HG	38:U2:142:THR:CA	2.31	0.60
20:B2:97:LEU:HD12	20:B2:97:LEU:N	2.01	0.60
46:c2:25:ASP:OD2	48:f2:125:TRP:NE1	2.35	0.60
1:A1:182:LEU:O	1:A1:186:LEU:HD12	2.01	0.60
1:A1:413:LYS:HB2	1:A1:414:TYR:CD2	2.37	0.60
2:B1:60:SER:CB	2:N1:429:ASN:ND2	2.53	0.60
2:B1:196:GLN:HG2	2:B1:197:ASN:OD1	2.01	0.60
2:B1:256:ALA:O	2:B1:424:MET:HG3	2.01	0.60
2:B1:299:VAL:O	2:B1:303:VAL:HG23	2.01	0.60
3:C1:18:PHE:O	3:C1:220:PHE:HD2	1.84	0.60
4:D1:165:TYR:CE1	4:D1:168:VAL:HG22	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:106:GLU:HA	6:F1:109:LYS:NZ	2.16	0.60
7:G1:71:ARG:O	8:H1:56:GLU:OE2	2.20	0.60
1:M1:365:LEU:O	1:M1:365:LEU:HG	1.99	0.60
57:B3:226:MET:O	57:B3:227:LEU:HB2	2.02	0.60
1:A1:327:ASP:OD1	1:A1:328:HIS:N	2.32	0.60
3:C1:26:ASN:O	3:C1:27:ILE:HG13	2.01	0.60
3:C1:218:ILE:HG22	3:C1:223:TYR:CD2	2.35	0.60
3:C1:296:PHE:O	3:C1:300:ILE:HB	2.01	0.60
4:D1:27:ARG:NH2	4:D1:60:GLU:OE2	2.33	0.60
6:F1:28:LYS:HD3	6:F1:74:ILE:HD11	1.84	0.60
9:I1:58:GLN:O	9:I1:59:ALA:HB2	2.01	0.60
9:I1:58:GLN:HA	9:I1:78:TYR:CD2	2.36	0.60
9:I1:62:ARG:N	9:I1:63:PRO:HD2	2.17	0.60
2:N1:56:ARG:NE	2:N1:103:GLU:OE1	2.19	0.60
19:A2:302:LEU:HB3	38:U2:137:TRP:CG	2.35	0.60
1:A1:154:HIS:O	1:A1:158:PHE:HB2	2.00	0.60
1:A1:338:LEU:O	1:A1:341:GLN:N	2.35	0.60
3:C1:240:MET:CA	3:C1:243:VAL:HG12	2.28	0.60
4:D1:165:TYR:CE2	4:D1:168:VAL:HG22	2.37	0.60
8:H1:73:LEU:HD21	8:H1:74:PHE:CD1	2.35	0.60
1:M1:39:VAL:HG11	1:M1:117:VAL:HG21	1.81	0.60
1:M1:312:ILE:HB	1:M1:319:LEU:HB2	1.83	0.60
2:N1:34:VAL:HG11	2:N1:386:ALA:CB	2.32	0.60
3:O1:206:ASN:CB	3:O1:313:ARG:NH2	2.55	0.60
3:O1:296:PHE:CD1	3:O1:359:PHE:HE1	2.19	0.60
3:O1:331:ASP:O	3:O1:334:THR:HB	2.00	0.60
4:P1:214:LEU:O	4:P1:218:LEU:HG	2.01	0.60
9:U1:62:ARG:N	9:U1:63:PRO:HD2	2.15	0.60
20:B2:443:MET:SD	52:12:281:ARG:NH1	2.75	0.60
53:62:209:SER:OG	53:62:270:ASN:ND2	2.34	0.60
1:A1:280:TYR:O	1:A1:306:SER:HA	2.00	0.60
1:A1:394:GLU:O	1:A1:395:TRP:C	2.44	0.60
2:B1:200:THR:HG22	2:B1:203:ARG:CD	2.25	0.60
3:C1:72:ASP:OD1	4:D1:49:ARG:NH1	2.28	0.60
4:D1:57:THR:HG22	4:D1:58:GLU:N	2.17	0.60
1:M1:55:ALA:O	1:M1:56:GLY:C	2.43	0.60
2:N1:362:ASN:HA	2:N1:365:LYS:HD3	1.83	0.60
2:N1:385:GLN:HG2	9:U1:62:ARG:NH1	2.13	0.60
3:O1:275:LEU:O	3:O1:276:PHE:C	2.45	0.60
4:P1:32:VAL:HG11	4:P1:186:VAL:CG2	2.31	0.60
5:Q1:29:SER:HA	5:Q1:32:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R1:73:GLN:HG2	7:S1:36:ASN:HD21	1.65	0.60
21:C2:215:ASP:OD2	35:R2:75:ARG:NH2	2.34	0.60
57:B3:59:GLN:HA	57:B3:62:GLU:HB2	1.83	0.60
61:F3:62:CYS:SG	61:F3:84:SER:OG	2.60	0.60
1:A1:373:THR:HB	1:A1:374:PRO:HD3	1.84	0.60
2:B1:98:VAL:HG22	2:B1:107:TYR:CD2	2.37	0.60
3:C1:301:LEU:O	3:C1:304:ILE:HD12	2.02	0.60
1:M1:64:PHE:CE2	1:M1:88:ALA:HB2	2.36	0.60
2:N1:255:ALA:HA	2:N1:425:ALA:O	2.01	0.60
2:N1:352:LEU:HD21	2:N1:357:VAL:HG23	1.82	0.60
3:O1:196:HIS:HE1	69:O1:402:HEM:C1D	2.19	0.60
4:P1:42:SER:O	4:P1:112:ASP:OD1	2.20	0.60
10:V1:13:LEU:O	10:V1:19:THR:OG1	2.17	0.60
20:B2:171:ARG:HH21	20:B2:231:GLY:HA2	1.66	0.60
2:B1:217:LYS:O	2:B1:218:GLN:C	2.45	0.60
4:D1:30:PHE:HD1	4:D1:189:PHE:CE1	2.19	0.60
6:F1:96:GLU:OE2	6:F1:99:ARG:NH1	2.34	0.60
5:Q1:97:PHE:CE1	5:Q1:137:GLY:HA3	2.37	0.60
19:A2:75:CYS:SG	19:A2:76:ARG:N	2.75	0.60
19:A2:143:SER:O	20:B2:380:HIS:NE2	2.35	0.60
36:S2:219:SER:HA	36:S2:222:LEU:HB2	1.83	0.60
45:b2:134:GLU:HA	45:b2:137:MET:HB2	1.82	0.60
4:D1:23:HIS:CD2	10:J1:51:LEU:HA	2.37	0.60
1:M1:146:ARG:NH2	1:M1:308:GLN:HE22	2.00	0.60
3:O1:4:ILE:O	3:O1:4:ILE:HG22	2.00	0.60
3:O1:32:ASN:HD21	3:O1:228:ASP:HA	1.67	0.60
5:Q1:164:HIS:H	5:Q1:173:LYS:HB2	1.67	0.60
55:e2:36:MET:HA	55:e2:77:LYS:HE2	1.78	0.60
58:C3:192:VAL:O	58:C3:196:THR:HB	2.01	0.60
1:M1:91:THR:HG22	1:M1:94:HIS:H	1.67	0.60
1:M1:363:ASN:CG	2:N1:112:LEU:HD23	2.27	0.60
2:N1:269:ALA:O	2:N1:272:PHE:N	2.35	0.60
4:P1:134:TYR:HE2	4:P1:163:PRO:HG2	1.66	0.60
5:Q1:78:LEU:HD23	5:Q1:79:SER:N	2.17	0.60
5:Q1:101:ARG:HD3	5:Q1:133:VAL:CG1	2.31	0.60
7:S1:2:ARG:HB2	7:S1:6:HIS:CD2	2.37	0.60
68:M3:28:LEU:HB2	68:M3:29:PRO:HD3	1.84	0.60
2:B1:258:VAL:CG1	2:B1:321:LEU:HB3	2.29	0.59
3:C1:359:PHE:O	3:C1:363:LEU:HB2	2.02	0.59
4:D1:28:ARG:HD2	4:D1:185:ASP:OD2	2.01	0.59
4:D1:32:VAL:HG11	4:D1:182:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:92:ILE:O	3:O1:96:MET:HG2	2.02	0.59
4:P1:46:VAL:HG12	4:P1:47:ALA:O	2.02	0.59
4:P1:72:ASP:O	4:P1:73:GLY:O	2.20	0.59
5:Q1:121:GLN:HB3	5:Q1:126:ARG:HD3	1.83	0.59
8:T1:37:LEU:HD21	8:T1:58:LEU:HA	1.84	0.59
9:U1:78:TYR:HD1	9:U1:78:TYR:OXT	1.83	0.59
10:V1:9:LEU:HD12	10:V1:13:LEU:CD1	2.32	0.59
10:V1:20:PHE:O	10:V1:23:THR:HB	2.02	0.59
18:92:95:ILE:HD11	19:A2:210:ILE:HG21	1.80	0.59
31:N2:38:ILE:O	31:N2:45:ARG:NH2	2.36	0.59
1:A1:145:MET:HE3	1:A1:252:HIS:HE1	1.67	0.59
2:B1:162:ASN:HB3	2:B1:244:ILE:HG21	1.84	0.59
2:B1:438:GLU:OE2	2:N1:169:ARG:CZ	2.51	0.59
3:C1:312:GLN:HE22	3:C1:317:PHE:HB2	1.67	0.59
4:D1:21:LEU:HD11	4:D1:192:TRP:HB2	1.84	0.59
4:P1:36:VAL:HG23	4:P1:169:LEU:HD11	1.84	0.59
9:U1:62:ARG:HB3	9:U1:63:PRO:HD3	1.84	0.59
9:U1:70:LEU:HD12	9:U1:71:ASN:N	2.16	0.59
19:A2:130:ILE:HG12	27:I2:114:TYR:OH	2.02	0.59
52:12:25:ARG:O	52:12:29:GLY:N	2.34	0.59
57:B3:145:PRO:CG	57:B3:148:MET:HE2	2.33	0.59
58:C3:119:THR:O	62:G3:52:HIS:HE1	1.84	0.59
1:A1:15:GLN:O	1:A1:26:ALA:HA	2.03	0.59
1:A1:317:THR:HG22	1:A1:318:GLY:H	1.67	0.59
1:A1:350:THR:HB	1:A1:353:GLU:HG3	1.84	0.59
3:C1:122:THR:HG23	3:C1:185:LEU:HD11	1.83	0.59
4:D1:164:ILE:HD11	70:D1:301:HEC:HBB2	1.83	0.59
1:M1:184:GLU:O	1:M1:188:ARG:HG3	2.02	0.59
1:M1:426:GLY:HA2	1:M1:428:ILE:N	2.17	0.59
2:N1:261:SER:HG	2:N1:320:GLY:HA3	1.66	0.59
3:O1:78:ILE:O	3:O1:82:MET:HB2	2.02	0.59
5:Q1:118:ARG:NH1	5:Q1:171:ILE:CG1	2.57	0.59
7:S1:71:ARG:O	8:T1:56:GLU:OE2	2.19	0.59
19:A2:583:ILE:HD13	38:U2:137:TRP:CZ3	2.37	0.59
22:D2:114:ARG:HH21	22:D2:114:ARG:CG	2.13	0.59
40:M2:37:MET:HG2	40:M2:42:LEU:H	1.67	0.59
1:A1:32:GLN:HG2	1:A1:33:PRO:CD	2.33	0.59
4:D1:10:TYR:CE1	8:H1:73:LEU:HD21	2.37	0.59
7:G1:73:ASN:HD22	8:H1:56:GLU:CD	2.10	0.59
1:M1:428:ILE:HG22	1:M1:431:LEU:CG	2.32	0.59
3:O1:348:ILE:O	3:O1:352:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:45:VAL:HG23	10:V1:24:ILE:HA	1.83	0.59
5:Q1:101:ARG:HA	5:Q1:105:GLU:OE1	2.02	0.59
8:T1:21:ARG:CB	8:T1:65:ARG:HH21	2.09	0.59
11:W1:30:VAL:O	11:W1:34:TRP:CG	2.56	0.59
18:92:71:PRO:HA	24:F2:102:SER:HB3	1.85	0.59
18:92:149:LEU:HD23	18:92:150:GLU:H	1.67	0.59
18:92:236:GLU:OE1	18:92:239:LYS:NZ	2.35	0.59
19:A2:302:LEU:CB	38:U2:137:TRP:CB	2.79	0.59
60:E3:80:GLU:H	60:E3:80:GLU:CD	2.10	0.59
5:E1:33:LYS:HB3	7:G1:21:PHE:CE2	2.38	0.59
6:F1:96:GLU:O	6:F1:97:VAL:C	2.45	0.59
1:M1:43:ALA:CB	1:M1:189:HIS:HB3	2.32	0.59
1:M1:106:LEU:N	1:M1:107:PRO:HD2	2.18	0.59
1:M1:408:ARG:NH1	11:W1:15:ARG:NE	2.47	0.59
3:O1:242:LEU:HD21	3:O1:250:LEU:HD22	1.83	0.59
5:Q1:118:ARG:HH22	5:Q1:173:LYS:HA	1.66	0.59
7:S1:25:ALA:O	7:S1:27:PRO:HD3	2.02	0.59
52:12:126:LYS:HD3	52:12:126:LYS:C	2.22	0.59
57:B3:179:LEU:HD21	63:H3:65:PRO:HD3	1.85	0.59
63:H3:57:ARG:HG3	63:H3:60:TYR:CE2	2.38	0.59
67:L3:46:LYS:O	67:L3:47:LYS:HB2	2.02	0.59
1:A1:11:VAL:HG13	1:A1:12:PRO:HD2	1.84	0.59
1:A1:64:PHE:HE1	1:A1:86:LEU:CG	2.12	0.59
2:B1:203:ARG:CZ	2:B1:230:LEU:HD23	2.32	0.59
1:M1:239:SER:HB2	7:S1:18:LEU:HD23	1.84	0.59
1:M1:341:GLN:OE1	1:M1:344:ARG:HD3	2.03	0.59
2:N1:76:THR:HG21	2:N1:133:ARG:NH2	2.18	0.59
2:N1:206:LEU:HD13	2:N1:224:LEU:HD11	1.84	0.59
4:P1:139:THR:HB	8:T1:44:VAL:HB	1.83	0.59
5:Q1:104:LYS:HG2	5:Q1:104:LYS:O	2.01	0.59
8:T1:58:LEU:HD11	8:T1:62:LEU:CD1	2.32	0.59
9:U1:58:GLN:HA	9:U1:78:TYR:CD2	2.37	0.59
14:42:60:SER:OG	14:42:63:THR:O	2.19	0.59
15:52:49:LEU:HD21	16:72:49:GLY:H	1.68	0.59
1:A1:233:PRO:HG2	5:E1:23:LYS:HD2	1.84	0.59
3:C1:160:LEU:HD12	3:C1:160:LEU:O	2.03	0.59
3:C1:218:ILE:HG21	3:C1:223:TYR:CD2	2.38	0.59
4:D1:26:ILE:HG22	4:D1:54:VAL:HG13	1.84	0.59
1:M1:233:PRO:HG2	5:Q1:23:LYS:CD	2.32	0.59
1:M1:351:GLU:HA	1:M1:404:ALA:HB2	1.85	0.59
2:N1:203:ARG:CZ	2:N1:230:LEU:HD23	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:40:THR:HG22	10:V1:20:PHE:HZ	1.67	0.59
5:Q1:76:ILE:HA	5:Q1:193:VAL:O	2.03	0.59
6:R1:58:ARG:HG2	6:R1:58:ARG:HH11	1.68	0.59
19:A2:272:ARG:CZ	25:G2:87:MET:HE3	2.33	0.59
23:E2:188:GLU:O	23:E2:192:ASN:ND2	2.36	0.59
32:O2:33:ARG:NH1	40:M2:44:SER:O	2.34	0.59
54:g2:77:CYS:SG	54:g2:78:GLN:N	2.71	0.59
2:B1:132:PHE:HB3	2:B1:137:VAL:HG21	1.85	0.59
3:C1:25:SER:O	3:C1:26:ASN:C	2.45	0.59
3:C1:28:SER:HB3	3:C1:30:TRP:HD1	1.67	0.59
3:C1:115:ILE:CD1	3:C1:115:ILE:N	2.66	0.59
2:N1:264:ILE:HD12	2:N1:315:SER:O	2.03	0.59
3:O1:1:MET:SD	3:O1:4:ILE:HB	2.43	0.59
3:O1:221:HIS:HB3	3:O1:222:PRO:CD	2.29	0.59
52:12:228:TYR:O	52:12:231:ILE:HG22	2.03	0.59
1:A1:62:LEU:O	1:A1:63:ALA:C	2.46	0.59
1:A1:436:ARG:HE	3:C1:222:PRO:HD3	1.68	0.59
3:C1:8:HIS:CB	3:C1:9:PRO:CD	2.81	0.59
3:C1:309:THR:HG21	3:C1:367:PRO:O	2.03	0.59
6:F1:42:ASP:O	6:F1:43:VAL:C	2.43	0.59
1:M1:46:ARG:NH2	1:M1:316:ASP:OD2	2.34	0.59
1:M1:272:VAL:HG21	1:M1:402:VAL:HG21	1.85	0.59
2:N1:69:LEU:HD21	2:N1:199:PHE:CZ	2.37	0.59
19:A2:469:ALA:HB3	19:A2:472:PRO:HG3	1.85	0.59
25:G2:131:LYS:HE3	25:G2:147:VAL:HG11	1.85	0.59
54:g2:91:GLN:NE2	54:g2:95:ASP:OD2	2.36	0.59
4:D1:168:VAL:O	4:D1:169:LEU:HD23	2.01	0.59
7:G1:44:CYS:SG	7:G1:48:VAL:CG2	2.91	0.59
1:M1:308:GLN:HG3	1:M1:308:GLN:O	2.02	0.59
1:M1:397:SER:O	1:M1:400:ALA:HB3	2.03	0.59
2:N1:100:SER:HB3	2:N1:105:MET:CG	2.32	0.59
2:N1:384:SER:CB	9:U1:62:ARG:HG2	2.32	0.59
3:O1:153:ILE:HD12	3:O1:153:ILE:N	2.18	0.59
5:Q1:69:LEU:HG	5:Q1:69:LEU:O	2.02	0.59
14:42:52:PHE:O	45:b2:135:ARG:NH1	2.35	0.59
1:A1:426:GLY:HA2	1:A1:428:ILE:CG1	2.32	0.58
2:B1:247:GLN:HG3	2:B1:248:ASN:N	2.18	0.58
1:M1:236:PHE:HD2	1:M1:258:GLU:CG	2.15	0.58
2:N1:183:ILE:HG22	2:N1:184:GLY:N	2.16	0.58
5:Q1:77:LYS:HG3	5:Q1:89:PHE:HE2	1.68	0.58
1:A1:408:ARG:CZ	11:K1:15:ARG:NE	2.63	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:32:GLN:HG2	1:M1:33:PRO:HD2	1.84	0.58
5:Q1:121:GLN:HG3	5:Q1:179:ASN:HD22	1.67	0.58
10:V1:51:LEU:H	10:V1:54:HIS:HD2	1.49	0.58
14:42:115:LEU:HB2	14:42:174:LEU:HD13	1.85	0.58
19:A2:129:PRO:HD2	27:I2:114:TYR:CZ	2.37	0.58
1:A1:48:GLU:OE1	1:A1:53:ASN:O	2.20	0.58
1:A1:426:GLY:H	1:A1:428:ILE:HG13	1.63	0.58
3:C1:4:ILE:HG22	3:C1:4:ILE:O	2.02	0.58
3:C1:239:LEU:HD12	3:C1:239:LEU:O	2.02	0.58
4:P1:120:ARG:HH11	4:P1:120:ARG:CG	2.16	0.58
10:V1:18:SER:HB3	11:W1:23:LEU:HD12	1.84	0.58
19:A2:161:GLU:N	27:I2:102:ASN:ND2	2.37	0.58
20:B2:92:HIS:O	20:B2:94:VAL:N	2.35	0.58
20:B2:305:THR:HG23	20:B2:306:GLN:HG2	1.85	0.58
27:I2:107:THR:HB	27:I2:121:GLN:O	2.03	0.58
39:V2:50:MET:SD	39:V2:54:ASN:ND2	2.75	0.58
45:b2:119:ARG:NH1	54:g2:62:TYR:O	2.36	0.58
48:f2:11:THR:H	48:f2:14:GLN:HE21	1.51	0.58
1:A1:408:ARG:NH2	11:K1:15:ARG:CZ	2.64	0.58
2:B1:169:ARG:HG2	2:N1:435:PHE:CE1	2.39	0.58
3:C1:332:LEU:HD21	3:C1:358:TYR:CE1	2.38	0.58
6:F1:75:LEU:C	6:F1:80:TRP:HE1	2.12	0.58
2:N1:146:ILE:O	2:N1:150:VAL:HG13	2.03	0.58
1:A1:120:CYS:O	1:A1:122:LEU:HG	2.04	0.58
1:A1:156:THR:OG1	1:A1:241:ILE:HB	2.03	0.58
1:A1:268:VAL:O	1:A1:272:VAL:HG23	2.03	0.58
3:C1:137:GLN:OE1	3:C1:259:ALA:HA	2.02	0.58
4:D1:40:CYS:HB3	4:D1:95:TYR:OH	2.02	0.58
4:D1:43:MET:HG2	4:D1:46:VAL:CG2	2.33	0.58
4:D1:79:GLU:OE1	4:D1:82:MET:HG3	2.03	0.58
3:O1:240:MET:HA	3:O1:243:VAL:HG12	1.86	0.58
19:A2:161:GLU:HB3	27:I2:102:ASN:CG	2.28	0.58
19:A2:313:LEU:HA	38:U2:142:THR:HA	1.85	0.58
21:C2:109:GLN:HE21	31:N2:83:GLN:HE22	1.50	0.58
22:D2:64:GLU:HG2	22:D2:66:VAL:H	1.67	0.58
1:A1:55:ALA:O	1:A1:58:PHE:N	2.35	0.58
2:B1:213:HIS:N	2:B1:214:PRO:CD	2.66	0.58
3:C1:51:LEU:HD21	3:C1:79:ILE:CG2	2.33	0.58
4:D1:224:ARG:O	4:D1:225:HIS:C	2.47	0.58
3:O1:68:HIS:NE2	5:Q1:67:ASP:HB2	2.18	0.58
3:O1:320:LEU:HB2	3:O1:373:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:113:LEU:O	4:P1:114:SER:C	2.46	0.58
7:S1:68:LYS:O	7:S1:72:LYS:N	2.31	0.58
8:T1:73:LEU:O	8:T1:73:LEU:HG	2.02	0.58
10:V1:45:HIS:O	10:V1:48:GLU:HG2	2.02	0.58
12:22:21:MET:HE1	78:j2:201:PC1:H3B1	1.85	0.58
33:P2:40:LYS:O	39:V2:7:LYS:N	2.37	0.58
4:D1:100:ALA:O	4:D1:103:ALA:N	2.37	0.58
5:E1:15:ARG:CB	5:E1:16:PRO:CD	2.79	0.58
3:O1:15:ASN:O	3:O1:18:PHE:HD2	1.87	0.58
3:O1:110:LEU:HG	3:O1:114:ASN:HD21	1.67	0.58
5:Q1:153:PHE:CE1	5:Q1:172:ARG:HB2	2.39	0.58
5:Q1:188:THR:CG2	5:Q1:194:ILE:HG13	2.34	0.58
6:R1:28:LYS:CB	6:R1:74:ILE:HD11	2.34	0.58
10:V1:57:HIS:O	10:V1:58:LYS:C	2.46	0.58
1:A1:36:THR:OG1	1:A1:372:THR:HG22	2.03	0.58
3:C1:67:THR:O	3:C1:71:ARG:HG3	2.04	0.58
5:E1:34:GLY:HA2	10:J1:10:TYR:HD2	1.67	0.58
7:G1:73:ASN:H	7:G1:74:PRO:HD2	1.67	0.58
1:M1:91:THR:CG2	1:M1:93:GLU:H	2.11	0.58
3:O1:377:LEU:O	3:O1:378:LYS:HB3	2.03	0.58
19:A2:311:LYS:HB2	38:U2:142:THR:O	2.04	0.58
2:B1:49:LEU:HD21	2:B1:204:MET:SD	2.44	0.58
2:B1:238:LYS:HE3	2:B1:239:TYR:O	2.04	0.58
3:C1:51:LEU:CD2	3:C1:79:ILE:HG22	2.34	0.58
4:D1:138:PRO:CB	8:H1:55:THR:N	2.66	0.58
7:G1:2:ARG:HB2	7:G1:6:HIS:CD2	2.38	0.58
8:H1:21:ARG:HB3	8:H1:65:ARG:NH2	2.17	0.58
1:M1:233:PRO:HG2	5:Q1:23:LYS:NZ	2.19	0.58
2:N1:299:VAL:HG13	2:N1:303:VAL:HG21	1.86	0.58
3:O1:163:TRP:O	3:O1:177:ARG:NH1	2.34	0.58
3:O1:310:SER:HB3	3:O1:318:ARG:NH1	2.18	0.58
4:P1:26:ILE:O	4:P1:27:ARG:C	2.47	0.58
4:P1:178:THR:CB	4:P1:181:GLN:HG3	2.28	0.58
5:Q1:185:TYR:HA	5:Q1:194:ILE:O	2.04	0.58
8:T1:73:LEU:HD21	8:T1:74:PHE:HD1	1.68	0.58
26:H2:21:GLN:HB3	26:H2:37:GLU:HG3	1.85	0.58
51:j2:108:THR:OG1	54:g2:75:THR:O	2.21	0.58
1:A1:24:ARG:CB	1:A1:196:VAL:HG22	2.25	0.58
1:A1:311:ASN:OD1	1:A1:320:LEU:CD2	2.52	0.58
1:A1:426:GLY:CA	1:A1:428:ILE:N	2.66	0.58
2:B1:68:LEU:HD11	2:B1:140:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:72:ALA:O	2:B1:75:LEU:HG	2.04	0.58
3:C1:377:LEU:HB3	6:F1:33:ARG:HD2	1.85	0.58
2:N1:275:LEU:HD22	2:N1:414:ALA:HB2	1.85	0.58
2:N1:280:GLY:HA2	2:N1:311:ALA:HB3	1.85	0.58
19:A2:226:CYS:SG	75:A2:802:SF4:S3	3.02	0.58
25:G2:154:LYS:HB2	25:G2:156:LYS:HE2	1.85	0.58
3:C1:327:ALA:O	3:C1:331:ASP:N	2.32	0.57
4:D1:3:LEU:HD22	7:G1:70:LYS:NZ	2.19	0.57
4:D1:50:HIS:O	4:D1:54:VAL:N	2.28	0.57
9:I1:58:GLN:HG2	9:I1:78:TYR:CD2	2.38	0.57
10:J1:38:GLY:O	10:J1:42:ILE:HG13	2.04	0.57
1:M1:342:TRP:O	1:M1:345:LEU:HB2	2.04	0.57
2:N1:97:SER:OG	9:U1:70:LEU:HB2	2.04	0.57
5:Q1:114:VAL:O	5:Q1:117:LEU:HB2	2.04	0.57
6:R1:51:PRO:HG2	6:R1:54:LEU:HD23	1.84	0.57
34:Q2:168:PHE:H	34:Q2:170:TRP:HD1	1.52	0.57
3:C1:316:MET:HE2	3:C1:317:PHE:CE1	2.40	0.57
4:D1:178:THR:CB	4:D1:181:GLN:HG3	2.32	0.57
1:M1:64:PHE:HE1	1:M1:86:LEU:HG	1.61	0.57
2:N1:109:VAL:O	2:N1:109:VAL:HG13	2.04	0.57
3:O1:67:THR:O	3:O1:71:ARG:HG3	2.04	0.57
3:O1:240:MET:O	3:O1:244:LEU:HB2	2.04	0.57
7:S1:50:PRO:CB	7:S1:51:PRO:CD	2.70	0.57
8:T1:25:GLU:HA	8:T1:30:CYS:SG	2.44	0.57
19:A2:140:GLN:HB2	75:A2:801:SF4:S4	2.44	0.57
56:A3:404:THR:O	56:A3:480:ARG:NH1	2.37	0.57
57:B3:193:TYR:HE1	59:D3:126:MET:HE1	1.68	0.57
2:B1:99:THR:O	2:B1:106:ALA:N	2.37	0.57
10:J1:32:GLU:CG	10:J1:33:ARG:N	2.67	0.57
1:M1:317:THR:HG22	1:M1:318:GLY:N	2.19	0.57
4:P1:10:TYR:O	4:P1:12:TRP:CD1	2.58	0.57
6:R1:47:ILE:O	6:R1:50:LEU:HG	2.04	0.57
19:A2:302:LEU:CB	38:U2:137:TRP:HB3	2.34	0.57
19:A2:456:ALA:HA	19:A2:496:ILE:HD13	1.86	0.57
2:B1:248:ASN:HB2	2:B1:428:GLY:CA	2.33	0.57
3:C1:221:HIS:CB	3:C1:222:PRO:HD3	2.22	0.57
4:D1:138:PRO:HG2	8:H1:55:THR:OG1	2.04	0.57
5:E1:33:LYS:HA	7:G1:21:PHE:CE2	2.38	0.57
8:H1:35:GLU:O	8:H1:39:LEU:HG	2.04	0.57
8:H1:65:ARG:CG	8:H1:66:ASP:N	2.66	0.57
1:M1:45:SER:HB3	1:M1:167:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:268:VAL:O	1:M1:272:VAL:HG23	2.04	0.57
1:M1:270:LEU:O	1:M1:273:ALA:HB3	2.04	0.57
1:M1:350:THR:HB	1:M1:353:GLU:HG3	1.85	0.57
2:N1:141:GLN:HB2	2:N1:142:PRO:HD3	1.86	0.57
2:N1:264:ILE:HG21	2:N1:317:SER:HA	1.85	0.57
3:O1:309:THR:HG23	3:O1:370:GLY:HA3	1.87	0.57
4:P1:23:HIS:CD2	10:V1:51:LEU:HA	2.38	0.57
13:32:64:LEU:HD13	16:72:165:VAL:HG22	1.85	0.57
18:92:111:ARG:NH1	19:A2:193:ASP:CB	2.68	0.57
19:A2:127:ASP:OD2	19:A2:175:ARG:NH1	2.36	0.57
36:S2:193:VAL:HG22	36:S2:244:LEU:HB3	1.85	0.57
1:A1:106:LEU:HB3	1:A1:107:PRO:HD3	1.85	0.57
3:C1:171:ASP:O	3:C1:172:LYS:C	2.47	0.57
1:M1:270:LEU:O	1:M1:271:GLN:C	2.47	0.57
1:M1:408:ARG:CZ	11:W1:15:ARG:NE	2.67	0.57
3:O1:211:ILE:HG21	6:R1:62:ILE:HD13	1.86	0.57
3:O1:310:SER:HB3	3:O1:318:ARG:HH11	1.70	0.57
10:V1:34:ALA:O	10:V1:35:PHE:C	2.46	0.57
17:82:315:LEU:H	17:82:358:ASP:HA	1.69	0.57
19:A2:161:GLU:CA	27:I2:102:ASN:HD22	2.16	0.57
20:B2:338:ARG:NH1	39:V2:22:LYS:O	2.37	0.57
1:A1:386:TYR:N	1:A1:386:TYR:CD1	2.72	0.57
1:A1:417:ASP:OD1	5:E1:33:LYS:HD2	2.04	0.57
2:B1:52:LYS:HB2	2:B1:203:ARG:CB	2.25	0.57
2:B1:203:ARG:NE	2:B1:230:LEU:HD23	2.20	0.57
3:C1:26:ASN:ND2	3:C1:26:ASN:C	2.63	0.57
3:C1:372:ILE:O	3:C1:373:GLU:C	2.46	0.57
5:E1:29:SER:CB	5:E1:32:ARG:HD3	2.35	0.57
6:F1:39:GLU:HB3	6:F1:44:LYS:HE2	1.87	0.57
8:H1:58:LEU:HD11	8:H1:62:LEU:CD1	2.34	0.57
2:N1:328:SER:HB3	2:N1:336:VAL:HG21	1.86	0.57
4:P1:138:PRO:CB	8:T1:55:THR:N	2.67	0.57
12:22:176:ARG:O	12:22:180:ALA:N	2.37	0.57
16:72:57:PHE:O	16:72:62:GLY:N	2.37	0.57
18:92:95:ILE:HD11	19:A2:210:ILE:HG23	1.79	0.57
19:A2:667:GLN:NE2	29:K2:38:GLU:CD	2.62	0.57
21:C2:230:GLN:HE21	21:C2:233:ARG:HH12	1.53	0.57
37:T2:103:ALA:O	37:T2:106:ARG:NH1	2.37	0.57
52:12:41:GLY:HA3	52:12:44:GLY:H	1.69	0.57
53:62:267:THR:O	53:62:274:GLN:NE2	2.38	0.57
57:B3:193:TYR:CE1	59:D3:126:MET:HE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:K3:43:SER:OG	66:K3:45:VAL:HG12	2.04	0.57
2:B1:134:ARG:HH12	6:R1:51:PRO:HD3	1.69	0.57
3:C1:213:SER:O	3:C1:215:VAL:N	2.36	0.57
1:M1:64:PHE:CE1	1:M1:86:LEU:CG	2.81	0.57
1:M1:354:VAL:HG13	1:M1:407:VAL:HG21	1.86	0.57
2:N1:187:THR:O	2:N1:190:GLU:HB2	2.05	0.57
2:N1:304:HIS:CG	2:N1:305:GLN:H	2.22	0.57
15:52:96:LEU:HD13	53:62:581:LYS:HB3	1.86	0.57
23:E2:66:LEU:HD12	23:E2:70:LEU:HD12	1.87	0.57
26:H2:49:SER:HB3	45:b2:171:TYR:HB2	1.86	0.57
53:62:247:LEU:HD12	53:62:252:MET:HG3	1.87	0.57
55:e2:75:TYR:N	55:e2:75:TYR:CD2	2.72	0.57
67:L3:41:ARG:HG3	68:M3:40:TYR:CE2	2.40	0.57
1:A1:4:TYR:CE2	1:A1:396:GLU:HG3	2.38	0.57
1:A1:143:THR:HG21	9:I1:48:SER:N	2.14	0.57
1:A1:248:LEU:N	1:A1:248:LEU:HD23	2.19	0.57
1:A1:394:GLU:O	1:A1:397:SER:N	2.38	0.57
2:B1:277:HIS:CD2	2:B1:364:LEU:HD13	2.40	0.57
1:M1:240:GLN:HG3	1:M1:422:VAL:O	2.05	0.57
2:N1:79:GLY:CA	2:N1:125:ASN:HD21	2.17	0.57
2:N1:148:LYS:HD2	2:N1:178:CYS:O	2.04	0.57
3:O1:218:ILE:HG23	3:O1:219:PRO:HD2	1.86	0.57
5:Q1:87:MET:HG2	5:Q1:89:PHE:CE1	2.40	0.57
17:82:422:HIS:ND1	19:A2:79:LEU:CD1	2.67	0.57
19:A2:272:ARG:CZ	25:G2:87:MET:CE	2.82	0.57
3:C1:71:ARG:NH2	4:D1:193:ALA:O	2.38	0.57
1:M1:270:LEU:O	1:M1:273:ALA:N	2.38	0.57
3:O1:149:LEU:HD21	3:O1:281:LEU:HD22	1.86	0.57
4:P1:240:PRO:CD	4:P1:241:LYS:H	2.16	0.57
19:A2:422:TRP:CD2	25:G2:169:ARG:HD3	2.40	0.57
20:B2:97:LEU:CB	20:B2:111:PRO:HA	2.35	0.57
20:B2:263:THR:O	20:B2:269:ARG:NH2	2.37	0.57
20:B2:357:LYS:HD3	20:B2:364:SER:HB2	1.87	0.57
22:D2:113:PHE:N	22:D2:113:PHE:CD1	2.73	0.57
3:C1:28:SER:HB3	3:C1:30:TRP:CD1	2.40	0.57
2:N1:59:ASN:CG	2:N1:60:SER:H	2.11	0.57
2:N1:79:GLY:HA3	2:N1:125:ASN:HD21	1.70	0.57
2:N1:206:LEU:HD13	2:N1:224:LEU:CD1	2.34	0.57
2:N1:352:LEU:HD12	2:N1:353:SER:N	2.20	0.57
3:O1:28:SER:HB3	3:O1:30:TRP:CD1	2.38	0.57
3:O1:270:PRO:HB2	3:O1:274:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:161:ALA:HB1	4:P1:162:PRO:HD2	1.86	0.57
5:Q1:20:ASP:O	5:Q1:21:SER:C	2.46	0.57
5:Q1:121:GLN:HG3	5:Q1:179:ASN:ND2	2.20	0.57
6:R1:28:LYS:HB3	6:R1:74:ILE:HD11	1.86	0.57
56:A3:184:PHE:H	56:A3:256:HIS:HE1	1.52	0.57
57:B3:132:GLU:HB3	57:B3:137:GLU:HG3	1.87	0.57
57:B3:145:PRO:HG3	57:B3:148:MET:HE2	1.87	0.57
57:B3:189:PRO:HD2	64:I3:54:TYR:OH	2.05	0.57
3:C1:215:VAL:O	6:F1:63:LYS:NZ	2.37	0.56
8:H1:34:ARG:O	8:H1:38:GLU:HG2	2.05	0.56
1:M1:18:GLN:HG2	1:M1:19:LEU:O	2.04	0.56
1:M1:32:GLN:HG2	1:M1:33:PRO:CD	2.35	0.56
1:M1:134:ILE:HA	1:M1:137:GLU:HG3	1.87	0.56
2:N1:141:GLN:HE22	2:N1:186:VAL:HB	1.70	0.56
2:N1:262:ALA:HB2	2:N1:272:PHE:HE2	1.69	0.56
2:N1:303:VAL:CG1	2:N1:304:HIS:N	2.67	0.56
2:N1:304:HIS:CG	2:N1:305:GLN:N	2.72	0.56
5:Q1:12:ASP:O	7:S1:24:ARG:NH2	2.32	0.56
16:72:57:PHE:HA	16:72:61:LEU:HB3	1.87	0.56
19:A2:121:LEU:HD21	19:A2:139:LEU:HD22	1.87	0.56
19:A2:306:MET:CE	38:U2:139:PRO:HG3	2.32	0.56
1:A1:55:ALA:O	1:A1:56:GLY:C	2.48	0.56
1:A1:86:LEU:HD13	1:A1:99:ILE:CD1	2.35	0.56
1:A1:425:PHE:O	1:A1:426:GLY:O	2.23	0.56
1:A1:436:ARG:HE	3:C1:222:PRO:CD	2.18	0.56
2:B1:160:ILE:HD11	2:B1:325:TYR:CE2	2.40	0.56
1:M1:161:THR:CB	1:M1:162:PRO:HD2	2.34	0.56
3:O1:107:TYR:OH	3:O1:308:HIS:ND1	2.09	0.56
5:Q1:147:ILE:N	5:Q1:157:TYR:O	2.36	0.56
73:42:501:CDL:H312	49:h2:107:ALA:HA	1.86	0.56
19:A2:381:LEU:HD21	19:A2:664:TYR:HB2	1.87	0.56
19:A2:624:ARG:NH1	19:A2:634:LEU:O	2.37	0.56
20:B2:198:THR:HG22	52:12:32:GLN:HE22	1.70	0.56
53:62:174:TYR:HB3	53:62:229:LEU:HD23	1.87	0.56
1:A1:142:ASP:OD1	5:E1:2:HIS:ND1	2.36	0.56
2:B1:237:ALA:HB2	2:B1:318:ASP:CG	2.31	0.56
3:C1:225:THR:O	3:C1:229:ILE:HD12	2.05	0.56
4:D1:115:TYR:HD2	4:D1:119:ALA:HB2	1.69	0.56
4:D1:139:THR:HB	8:H1:44:VAL:HB	1.86	0.56
4:D1:150:ASN:OD1	4:D1:151:PRO:CD	2.53	0.56
4:D1:223:LYS:HZ2	4:D1:227:TRP:CD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:229:VAL:CG1	4:D1:233:ARG:HE	2.18	0.56
6:F1:28:LYS:HD2	6:F1:74:ILE:HD11	1.88	0.56
6:F1:74:ILE:HD13	6:F1:80:TRP:CZ2	2.40	0.56
10:J1:57:HIS:O	10:J1:58:LYS:C	2.46	0.56
10:J1:60:GLU:HG3	10:J1:60:GLU:O	2.06	0.56
1:M1:417:ASP:OD1	5:Q1:33:LYS:HD2	2.05	0.56
2:N1:68:LEU:HD23	2:N1:186:VAL:HG11	1.87	0.56
2:N1:217:LYS:O	2:N1:221:GLU:HG3	2.05	0.56
3:O1:88:SER:HA	3:O1:272:TRP:HZ2	1.70	0.56
3:O1:313:ARG:HB3	6:R1:38:HIS:CD2	2.40	0.56
4:P1:7:PRO:HG3	4:P1:126:TYR:CA	2.36	0.56
4:P1:117:VAL:HG11	4:P1:191:ARG:HH11	1.70	0.56
9:U1:58:GLN:HG2	9:U1:78:TYR:CD2	2.40	0.56
17:82:382:CYS:HB3	17:82:384:PRO:HD2	1.88	0.56
19:A2:140:GLN:HA	20:B2:379:ILE:CG2	2.35	0.56
19:A2:302:LEU:CA	38:U2:137:TRP:HB3	2.32	0.56
20:B2:305:THR:OG1	21:C2:140:ASN:ND2	2.39	0.56
46:c2:14:GLN:NE2	48:f2:155:PRO:O	2.37	0.56
1:A1:309:THR:HA	1:A1:322:ALA:HA	1.86	0.56
1:A1:335:MET:HE2	1:A1:339:GLN:HG3	1.88	0.56
1:A1:354:VAL:HG21	1:A1:404:ALA:HA	1.87	0.56
2:B1:239:TYR:OH	2:B1:421:ARG:O	2.19	0.56
4:D1:181:GLN:HA	8:H1:77:LEU:HD13	1.87	0.56
8:H1:21:ARG:CB	8:H1:65:ARG:HH21	2.18	0.56
1:M1:111:GLU:HG2	1:M1:213:GLN:HE22	1.71	0.56
1:M1:434:TYR:HA	1:M1:437:ILE:HD12	1.87	0.56
3:O1:18:PHE:O	3:O1:220:PHE:CD2	2.58	0.56
3:O1:165:TRP:HA	3:O1:174:THR:OG1	2.04	0.56
6:R1:98:ILE:O	6:R1:99:ARG:C	2.47	0.56
60:E3:78:HIS:ND1	64:I3:12:LEU:HD22	2.21	0.56
62:G3:5:LYS:HD2	62:G3:6:GLY:N	2.21	0.56
63:H3:71:THR:O	63:H3:75:ARG:HD3	2.05	0.56
1:A1:272:VAL:HG13	1:A1:358:LYS:HA	1.88	0.56
3:C1:182:HIS:O	3:C1:186:PRO:HD2	2.06	0.56
4:D1:74:PRO:O	4:D1:79:GLU:N	2.36	0.56
4:D1:113:LEU:O	4:D1:114:SER:C	2.48	0.56
1:M1:349:ALA:HB3	1:M1:408:ARG:CG	2.35	0.56
3:O1:34:GLY:O	3:O1:37:LEU:HB2	2.06	0.56
4:P1:43:MET:HE3	4:P1:91:PHE:CD2	2.41	0.56
4:P1:158:ILE:HG12	4:P1:159:GLY:N	2.19	0.56
20:B2:116:LEU:HD23	20:B2:118:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:47:ILE:CD1	2:B1:120:MET:SD	2.93	0.56
2:B1:89:ILE:O	2:B1:90:GLU:C	2.47	0.56
2:B1:102:ARG:HH12	2:B1:175:SER:HA	1.71	0.56
3:C1:300:ILE:CD1	3:C1:362:ILE:HG21	2.36	0.56
3:C1:337:TRP:O	3:C1:338:ILE:C	2.48	0.56
6:F1:73:GLN:HA	7:G1:39:ARG:HH21	1.71	0.56
10:J1:12:LEU:HD23	10:J1:13:LEU:CD2	2.36	0.56
1:M1:33:PRO:O	1:M1:103:SER:N	2.34	0.56
1:M1:134:ILE:CG2	1:M1:174:VAL:HG21	2.35	0.56
2:N1:294:SER:HB3	2:N1:343:GLN:HE21	1.70	0.56
3:O1:296:PHE:O	3:O1:300:ILE:HB	2.05	0.56
4:P1:182:VAL:O	4:P1:186:VAL:HG23	2.05	0.56
5:Q1:102:THR:OG1	5:Q1:105:GLU:HB2	2.06	0.56
13:32:102:LEU:O	13:32:106:TRP:N	2.38	0.56
17:82:159:ARG:HG2	17:82:161:GLU:H	1.71	0.56
1:A1:278:GLY:O	1:A1:309:THR:HG23	2.05	0.56
2:B1:264:ILE:CG2	2:B1:317:SER:HA	2.36	0.56
2:B1:273:SER:O	2:B1:276:GLN:HB3	2.06	0.56
2:B1:280:GLY:HA2	2:B1:311:ALA:HB3	1.88	0.56
4:D1:21:LEU:CD1	4:D1:192:TRP:HB2	2.36	0.56
4:D1:79:GLU:O	4:D1:80:MET:C	2.49	0.56
1:M1:64:PHE:HA	1:M1:75:LEU:CD2	2.35	0.56
1:M1:334:MET:HE3	1:M1:334:MET:HA	1.86	0.56
3:O1:300:ILE:O	3:O1:300:ILE:HG12	2.05	0.56
3:O1:327:ALA:O	3:O1:331:ASP:N	2.35	0.56
7:S1:31:SER:O	7:S1:35:PRO:CD	2.47	0.56
13:32:81:THR:H	30:L2:46:ASN:HD21	1.53	0.56
14:42:451:PRO:HG2	53:62:69:LEU:HD23	1.88	0.56
17:82:411:SER:HB3	33:P2:49:LEU:HD13	1.86	0.56
17:82:419:ILE:HD11	19:A2:119:PHE:CE2	2.41	0.56
41:X2:37:PHE:HD2	45:b2:137:MET:HB3	1.69	0.56
58:C3:203:PHE:O	58:C3:207:HIS:HD2	1.88	0.56
3:C1:41:LEU:O	3:C1:45:ILE:HG13	2.06	0.56
6:F1:50:LEU:CB	6:F1:55:TYR:HB2	2.29	0.56
2:N1:318:ASP:OD1	2:N1:318:ASP:N	2.39	0.56
3:O1:185:LEU:HB3	3:O1:186:PRO:CD	2.35	0.56
4:P1:21:LEU:HD11	4:P1:192:TRP:HB2	1.88	0.56
4:P1:180:SER:HB3	8:T1:17:LEU:HB2	1.88	0.56
17:82:159:ARG:NH1	18:92:176:CYS:O	2.38	0.56
19:A2:130:ILE:HG12	27:I2:114:TYR:CZ	2.41	0.56
19:A2:313:LEU:HD23	38:U2:142:THR:CB	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:e2:77:LYS:CG	55:e2:78:LEU:N	2.68	0.56
1:A1:106:LEU:HD22	1:A1:203:LEU:CD2	2.31	0.56
1:A1:272:VAL:HG21	1:A1:402:VAL:HG21	1.87	0.56
3:C1:133:LEU:HD21	3:C1:179:PHE:HA	1.88	0.56
3:C1:338:ILE:CD1	3:C1:338:ILE:H	2.19	0.56
5:E1:31:ALA:HB1	10:J1:6:THR:OG1	2.05	0.56
5:E1:45:VAL:HG13	10:J1:28:ALA:N	2.21	0.56
6:F1:91:GLU:HB2	6:F1:92:PRO:HD3	1.86	0.56
2:N1:264:ILE:HB	2:N1:316:TYR:O	2.06	0.56
3:O1:108:THR:CB	3:O1:313:ARG:HH11	2.12	0.56
3:O1:218:ILE:CG2	3:O1:223:TYR:HD2	2.19	0.56
5:Q1:142:LEU:HD12	5:Q1:161:HIS:HE1	1.71	0.56
19:A2:140:GLN:HA	20:B2:379:ILE:HG21	1.87	0.56
1:A1:146:ARG:CZ	1:A1:308:GLN:HE22	2.19	0.56
2:B1:24:LEU:H	2:B1:24:LEU:CD1	2.03	0.56
2:B1:55:SER:OG	2:B1:102:ARG:HG2	2.06	0.56
3:C1:221:HIS:HB3	3:C1:222:PRO:CD	2.27	0.56
3:C1:236:ILE:O	3:C1:237:LEU:C	2.48	0.56
4:D1:228:SER:HB2	7:G1:23:GLN:HE22	1.71	0.56
1:M1:233:PRO:HG2	5:Q1:23:LYS:CE	2.36	0.56
2:N1:264:ILE:HG22	2:N1:317:SER:HA	1.88	0.56
2:N1:308:ASP:OD2	9:U1:55:LEU:HA	2.06	0.56
3:O1:274:PHE:O	3:O1:275:LEU:C	2.47	0.56
5:Q1:76:ILE:O	5:Q1:77:LYS:HG2	2.06	0.56
5:Q1:140:THR:HG21	5:Q1:178:LEU:HB2	1.88	0.56
8:T1:66:ASP:O	8:T1:67:HIS:C	2.49	0.56
18:92:56:THR:HG22	18:92:58:GLU:H	1.70	0.56
19:A2:313:LEU:HG	38:U2:142:THR:HA	1.87	0.56
19:A2:349:GLU:HG2	19:A2:646:LEU:HD11	1.88	0.56
19:A2:588:ALA:O	19:A2:592:LYS:NZ	2.39	0.56
19:A2:645:ARG:NH1	19:A2:648:GLU:OE1	2.39	0.56
19:A2:667:GLN:HB3	29:K2:42:VAL:HB	1.87	0.56
1:A1:25:VAL:HG21	1:A1:209:LEU:HD12	1.87	0.55
3:C1:115:ILE:N	3:C1:115:ILE:HD12	2.21	0.55
3:C1:218:ILE:HG22	3:C1:219:PRO:N	2.20	0.55
4:D1:69:GLU:HA	4:D1:73:GLY:HA2	1.88	0.55
9:I1:53:GLU:O	9:I1:54:SER:C	2.47	0.55
2:N1:435:PHE:HB2	2:N1:438:GLU:OE1	2.05	0.55
3:O1:24:PRO:HG2	3:O1:205:SER:O	2.06	0.55
14:42:193:VAL:HG22	14:42:257:MET:HE1	1.87	0.55
19:A2:111:LYS:HD2	33:P2:53:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:111:LYS:CD	33:P2:53:TYR:CE2	2.89	0.55
19:A2:129:PRO:HB2	27:I2:114:TYR:HE1	1.72	0.55
20:B2:295:GLY:HA2	20:B2:321:GLY:H	1.72	0.55
35:R2:238:GLN:HB3	35:R2:267:GLY:HA3	1.87	0.55
3:C1:72:ASP:HB3	5:E1:67:ASP:H	1.71	0.55
4:D1:27:ARG:NH1	10:J1:58:LYS:HG3	2.18	0.55
4:D1:35:GLN:HB2	4:D1:169:LEU:CD1	2.35	0.55
1:M1:335:MET:CE	1:M1:339:GLN:HG3	2.35	0.55
2:N1:62:ASN:O	2:N1:62:ASN:ND2	2.39	0.55
2:N1:342:ASN:O	2:N1:345:LYS:HB2	2.06	0.55
4:P1:138:PRO:O	4:P1:141:VAL:HB	2.06	0.55
4:P1:139:THR:HG21	8:T1:41:ASP:O	2.06	0.55
5:Q1:139:CYS:HB2	5:Q1:165:TYR:CE2	2.39	0.55
5:Q1:150:ALA:HB3	5:Q1:157:TYR:CB	2.36	0.55
14:42:278:ARG:H	53:62:546:GLN:HE22	1.54	0.55
20:B2:237:PRO:HD3	23:E2:96:ARG:HH22	1.70	0.55
35:R2:84:HIS:HD2	35:R2:87:GLU:H	1.52	0.55
37:T2:78:ALA:HA	37:T2:89:ASN:HD21	1.71	0.55
1:A1:136:GLN:HE21	9:I1:50:LEU:HB3	1.70	0.55
6:F1:101:ARG:HG2	6:F1:105:GLU:OE2	2.06	0.55
3:O1:148:ASN:O	3:O1:151:SER:OG	2.24	0.55
5:Q1:50:ALA:O	5:Q1:51:ALA:C	2.49	0.55
9:U1:62:ARG:H	9:U1:63:PRO:HD2	1.71	0.55
9:U1:70:LEU:HD21	9:U1:73:PRO:CD	2.26	0.55
31:N2:35:LEU:O	31:N2:45:ARG:NH2	2.40	0.55
32:O2:92:GLU:HG3	32:O2:97:TRP:HE3	1.72	0.55
47:d2:25:PHE:CZ	47:d2:42:THR:O	2.57	0.55
52:12:230:ASN:HA	52:12:233:MET:HE2	1.88	0.55
4:D1:50:HIS:O	4:D1:51:LEU:C	2.48	0.55
6:F1:51:PRO:CD	2:N1:134:ARG:NH1	2.68	0.55
1:M1:245:GLU:O	1:M1:247:GLY:N	2.39	0.55
3:O1:109:PHE:O	3:O1:110:LEU:C	2.49	0.55
19:A2:303:THR:CG2	38:U2:136:GLU:HA	2.37	0.55
58:C3:42:LEU:HD13	65:J3:45:TYR:CD2	2.41	0.55
1:A1:33:PRO:O	1:A1:103:SER:N	2.36	0.55
3:C1:135:TRP:HH2	3:C1:170:VAL:O	1.89	0.55
3:C1:137:GLN:HB2	3:C1:257:THR:OG1	2.07	0.55
3:C1:244:LEU:HD11	4:D1:204:MET:CE	2.37	0.55
4:D1:69:GLU:O	4:D1:73:GLY:HA3	2.05	0.55
4:D1:229:VAL:O	4:D1:233:ARG:HG3	2.06	0.55
6:F1:10:SER:OG	6:F1:13:LEU:HD11	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:49:ARG:HD3	2:N1:135:TRP:CD2	2.41	0.55
8:H1:73:LEU:HD23	8:H1:73:LEU:C	2.31	0.55
1:M1:338:LEU:O	1:M1:341:GLN:N	2.38	0.55
1:M1:438:ARG:HH11	1:M1:438:ARG:HG3	1.70	0.55
2:N1:92:VAL:O	2:N1:92:VAL:HG12	2.06	0.55
3:O1:234:LEU:HD21	4:P1:216:LEU:HD21	1.86	0.55
4:P1:7:PRO:CB	4:P1:125:ASP:HB3	2.37	0.55
4:P1:149:PHE:HZ	8:T1:55:THR:HG23	1.71	0.55
6:R1:106:GLU:OE1	6:R1:109:LYS:HE2	2.06	0.55
17:82:156:ILE:HD11	17:82:197:VAL:HG22	1.88	0.55
35:R2:92:MET:HG3	35:R2:95:ARG:HH21	1.71	0.55
1:A1:93:GLU:O	1:A1:94:HIS:ND1	2.40	0.55
3:C1:218:ILE:HG22	3:C1:223:TYR:HD2	1.72	0.55
3:C1:353:LEU:HD23	3:C1:353:LEU:N	2.22	0.55
5:E1:72:SER:O	5:E1:73:LYS:HG2	2.05	0.55
1:M1:334:MET:O	1:M1:335:MET:C	2.48	0.55
2:N1:213:HIS:N	2:N1:214:PRO:CD	2.69	0.55
2:N1:359:ALA:O	2:N1:360:ALA:C	2.50	0.55
3:O1:44:GLN:HE22	3:O1:86:GLY:HA3	1.70	0.55
3:O1:315:MET:HA	3:O1:318:ARG:HG3	1.87	0.55
5:Q1:188:THR:HG21	5:Q1:194:ILE:HD11	1.87	0.55
10:V1:47:ASN:HB3	10:V1:50:LYS:HD2	1.88	0.55
15:52:61:ILE:HG23	16:72:55:MET:HE1	1.89	0.55
19:A2:180:THR:HA	19:A2:183:ILE:HD12	1.89	0.55
19:A2:651:PRO:HD2	29:K2:56:ARG:HB3	1.89	0.55
56:A3:95:PRO:HB2	58:C3:11:VAL:HG13	1.87	0.55
1:A1:30:SER:N	1:A1:201:GLY:O	2.38	0.55
2:B1:100:SER:CB	2:B1:105:MET:HG3	2.37	0.55
2:B1:261:SER:OG	2:B1:262:ALA:N	2.39	0.55
4:D1:164:ILE:HD11	70:D1:301:HEC:CBB	2.37	0.55
10:J1:35:PHE:O	10:J1:36:ASP:C	2.50	0.55
1:M1:331:ILE:CD1	1:M1:427:PRO:O	2.55	0.55
2:N1:168:TYR:HB2	2:N1:173:ALA:HB2	1.88	0.55
3:O1:122:THR:HG22	3:O1:189:ILE:CD1	2.27	0.55
3:O1:206:ASN:ND2	3:O1:207:ASN:H	2.04	0.55
3:O1:210:GLY:CA	3:O1:314:SER:HB2	2.31	0.55
7:S1:33:GLY:O	7:S1:37:VAL:N	2.35	0.55
18:92:88:ARG:NH1	24:F2:82:THR:O	2.39	0.55
19:A2:303:THR:HG21	38:U2:136:GLU:CB	2.37	0.55
19:A2:583:ILE:HD13	38:U2:137:TRP:HZ3	1.71	0.55
20:B2:92:HIS:HE1	20:B2:141:TYR:HE2	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B2:348:LEU:HA	20:B2:351:MET:HE2	1.88	0.55
23:E2:39:LYS:HG3	33:P2:111:PRO:HA	1.88	0.55
1:A1:342:TRP:O	1:A1:345:LEU:N	2.40	0.55
1:A1:385:THR:CG2	1:A1:386:TYR:CD1	2.89	0.55
1:A1:397:SER:O	1:A1:400:ALA:HB3	2.07	0.55
2:B1:86:THR:CG2	9:I1:71:ASN:HD21	2.19	0.55
2:B1:203:ARG:NH2	2:B1:230:LEU:HD23	2.22	0.55
4:D1:178:THR:O	4:D1:179:MET:C	2.50	0.55
4:D1:236:ALA:O	7:G1:14:ILE:N	2.27	0.55
5:E1:15:ARG:NH2	5:E1:32:ARG:HG3	2.22	0.55
1:M1:67:THR:CG2	1:M1:70:ARG:H	2.03	0.55
1:M1:266:ASP:O	1:M1:270:LEU:HG	2.06	0.55
2:N1:33:LEU:O	2:N1:33:LEU:HD23	2.07	0.55
2:N1:155:PRO:HB2	2:N1:254:HIS:CE1	2.41	0.55
2:N1:198:HIS:HE1	2:N1:233:SER:OG	1.89	0.55
3:O1:147:THR:O	3:O1:150:LEU:HB2	2.07	0.55
4:P1:4:GLU:HG3	4:P1:6:HIS:CE1	2.42	0.55
5:Q1:118:ARG:HB3	5:Q1:171:ILE:CG2	2.36	0.55
5:Q1:136:ILE:O	5:Q1:136:ILE:CG2	2.55	0.55
14:42:452:LYS:NZ	49:h2:115:GLN:OE1	2.40	0.55
16:72:66:VAL:O	16:72:70:TYR:N	2.40	0.55
56:A3:407:ASP:O	56:A3:411:LYS:HG3	2.07	0.55
62:G3:5:LYS:HD2	62:G3:5:LYS:C	2.32	0.55
1:A1:112:LEU:O	1:A1:116:ILE:HD12	2.07	0.55
2:B1:161:GLU:OE1	2:B1:175:SER:HB2	2.07	0.55
3:C1:312:GLN:O	3:C1:314:SER:N	2.40	0.55
4:D1:74:PRO:HG2	4:D1:82:MET:HB3	1.89	0.55
4:D1:211:MET:HA	4:D1:211:MET:HE3	1.89	0.55
1:M1:249:PRO:O	1:M1:250:LEU:HD23	2.07	0.55
1:M1:256:ALA:HB3	1:M1:421:ALA:HB3	1.89	0.55
3:O1:244:LEU:HD11	4:P1:204:MET:CE	2.36	0.55
3:O1:371:THR:O	3:O1:372:ILE:C	2.49	0.55
4:P1:42:SER:HB3	4:P1:94:PRO:HD2	1.89	0.55
19:A2:139:LEU:O	20:B2:379:ILE:HD13	2.07	0.55
19:A2:427:LEU:H	25:G2:169:ARG:HH22	1.55	0.55
3:C1:15:ASN:O	3:C1:18:PHE:HD1	1.90	0.55
3:C1:71:ARG:HE	4:D1:196:PRO:HG3	1.72	0.55
3:C1:251:GLY:O	3:C1:252:ASP:C	2.50	0.55
3:C1:310:SER:CB	3:C1:318:ARG:NH1	2.58	0.55
4:D1:219:VAL:HA	4:D1:222:MET:HG3	1.88	0.55
5:E1:12:ASP:O	7:G1:24:ARG:NH2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:112:LEU:O	1:M1:116:ILE:HG13	2.07	0.55
2:N1:155:PRO:O	2:N1:156:GLN:C	2.49	0.55
3:O1:119:LEU:HD13	3:O1:192:ILE:CG2	2.37	0.55
3:O1:132:VAL:HA	3:O1:139:SER:CB	2.36	0.55
5:Q1:187:PHE:HA	5:Q1:193:VAL:HA	1.88	0.55
6:R1:91:GLU:N	6:R1:92:PRO:HD2	2.22	0.55
8:T1:15:ASP:HB2	8:T1:16:PRO:CD	2.37	0.55
12:22:68:MET:HE2	15:52:37:MET:HE2	1.87	0.55
26:H2:51:ARG:NH1	34:Q2:151:ASN:OD1	2.40	0.55
35:R2:203:PRO:HA	35:R2:265:PHE:HB2	1.88	0.55
1:A1:109:ALA:O	1:A1:112:LEU:N	2.40	0.54
3:C1:378:LYS:HD3	6:F1:33:ARG:HH12	1.72	0.54
1:M1:136:GLN:HE21	9:U1:50:LEU:HB3	1.70	0.54
1:M1:394:GLU:O	1:M1:395:TRP:C	2.47	0.54
1:M1:413:LYS:HB2	1:M1:414:TYR:CD2	2.42	0.54
4:P1:94:PRO:HB2	4:P1:95:TYR:CE1	2.42	0.54
8:T1:40:CYS:HB2	8:T1:57:GLU:HG2	1.89	0.54
17:82:174:ARG:NH2	24:F2:87:ASP:O	2.40	0.54
18:92:44:THR:OG1	19:A2:209:TYR:HE2	1.84	0.54
19:A2:303:THR:CG2	38:U2:136:GLU:CB	2.84	0.54
35:R2:354:ARG:O	35:R2:355:ARG:NH2	2.36	0.54
40:W2:91:ASP:H	43:Z2:45:TRP:HB3	1.71	0.54
48:f2:32:ILE:O	53:62:436:ARG:NH2	2.37	0.54
56:A3:69:MET:HE2	56:A3:70:VAL:CG2	2.35	0.54
2:B1:266:SER:O	2:B1:269:ALA:HB3	2.07	0.54
3:C1:192:ILE:HD13	3:C1:192:ILE:N	2.21	0.54
2:N1:408:ALA:O	2:N1:411:ILE:N	2.40	0.54
3:O1:234:LEU:HD21	4:P1:216:LEU:CD2	2.37	0.54
4:P1:50:HIS:HE1	4:P1:91:PHE:HZ	1.54	0.54
70:P1:301:HEC:HBC2	70:P1:301:HEC:CHD	2.26	0.54
9:U1:58:GLN:HG2	9:U1:78:TYR:HD2	1.72	0.54
19:A2:674:LEU:CD1	29:K2:46:LYS:HD2	2.37	0.54
27:I2:106:GLU:O	27:I2:108:LYS:HG3	2.07	0.54
52:12:127:TYR:C	52:12:127:TYR:CD1	2.86	0.54
58:C3:151:LEU:HB2	58:C3:159:MET:HG3	1.89	0.54
1:A1:18:GLN:HG2	1:A1:19:LEU:O	2.07	0.54
1:A1:255:ILE:HG13	1:A1:422:VAL:CG2	2.37	0.54
3:C1:61:THR:O	3:C1:64:SER:N	2.41	0.54
3:C1:68:HIS:NE2	5:E1:67:ASP:HB2	2.22	0.54
3:C1:88:SER:O	3:C1:89:MET:C	2.47	0.54
3:C1:102:LEU:HB3	3:C1:325:PHE:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:106:SER:O	3:C1:109:PHE:CD1	2.54	0.54
3:O1:170:VAL:HG13	3:O1:174:THR:CG2	2.34	0.54
4:P1:128:PHE:HB2	4:P1:187:CYS:SG	2.46	0.54
7:S1:27:PRO:O	7:S1:28:HIS:C	2.48	0.54
10:V1:18:SER:HB3	11:W1:23:LEU:HB2	1.90	0.54
19:A2:137:CYS:SG	19:A2:138:ASP:N	2.80	0.54
55:e2:136:PHE:O	55:e2:140:MET:N	2.40	0.54
58:C3:222:GLN:HE21	58:C3:222:GLN:HA	1.72	0.54
64:I3:63:MET:HB3	64:I3:68:ILE:HD11	1.89	0.54
1:A1:143:THR:O	1:A1:143:THR:CG2	2.56	0.54
1:A1:256:ALA:HA	1:A1:320:LEU:O	2.06	0.54
1:A1:343:MET:O	1:A1:344:ARG:C	2.41	0.54
2:B1:33:LEU:HB2	2:B1:204:MET:O	2.07	0.54
3:C1:25:SER:HA	3:C1:218:ILE:HD12	1.89	0.54
3:C1:88:SER:HA	3:C1:272:TRP:HZ2	1.73	0.54
3:C1:115:ILE:O	3:C1:116:GLY:C	2.46	0.54
4:D1:11:PRO:HB2	8:H1:74:PHE:CG	2.41	0.54
4:D1:131:LEU:CD2	4:D1:163:PRO:HB3	2.38	0.54
5:E1:29:SER:CA	5:E1:32:ARG:HD3	2.37	0.54
6:F1:55:TYR:CD1	6:F1:55:TYR:C	2.86	0.54
10:J1:32:GLU:HG2	10:J1:33:ARG:N	2.22	0.54
10:J1:51:LEU:HB3	10:J1:52:TRP:CE3	2.42	0.54
1:M1:51:LYS:O	1:M1:53:ASN:N	2.38	0.54
1:M1:61:HIS:CB	1:M1:130:GLU:HG3	2.38	0.54
2:N1:372:VAL:O	2:N1:372:VAL:HG12	2.08	0.54
5:Q1:85:LYS:CG	5:Q1:86:ASN:H	2.12	0.54
8:T1:68:CYS:O	8:T1:69:VAL:C	2.51	0.54
17:82:222:LYS:O	25:G2:175:LYS:NZ	2.40	0.54
34:Q2:110:CYS:HA	34:Q2:113:ASP:HB3	1.88	0.54
58:C3:156:ARG:HG3	58:C3:156:ARG:NH1	2.23	0.54
1:A1:111:GLU:HG2	1:A1:213:GLN:HE22	1.73	0.54
1:A1:317:THR:HG22	1:A1:318:GLY:N	2.21	0.54
1:A1:334:MET:HA	1:A1:334:MET:CE	2.37	0.54
3:C1:124:MET:HG2	3:C1:274:PHE:HE1	1.71	0.54
4:D1:51:LEU:HD22	4:D1:58:GLU:HA	1.89	0.54
5:E1:63:SER:O	5:E1:64:ALA:HB2	2.08	0.54
1:M1:106:LEU:O	1:M1:107:PRO:C	2.51	0.54
1:M1:433:ASP:CG	3:O1:223:TYR:HH	2.13	0.54
5:Q1:78:LEU:HD21	5:Q1:132:TRP:CZ2	2.43	0.54
9:U1:53:GLU:O	9:U1:54:SER:C	2.51	0.54
12:22:240:MET:HE1	51:j2:48:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:650:SER:OG	29:K2:56:ARG:HD2	2.08	0.54
20:B2:91:ALA:CB	20:B2:193:ASP:OD2	2.50	0.54
49:h2:138:GLU:OE1	49:h2:140:ASN:ND2	2.41	0.54
40:M2:35:HIS:H	40:M2:39:ASP:HB3	1.72	0.54
61:F3:82:CYS:N	61:F3:86:GLY:O	2.40	0.54
1:A1:236:PHE:CD2	1:A1:258:GLU:CB	2.91	0.54
1:A1:346:CYS:HB3	1:A1:412:SER:HG	1.70	0.54
2:B1:100:SER:HB3	2:B1:105:MET:HG3	1.88	0.54
5:E1:52:LYS:NZ	10:J1:32:GLU:OE1	2.40	0.54
1:M1:22:GLY:O	1:M1:24:ARG:HG2	2.08	0.54
1:M1:241:ILE:HG13	7:S1:16:TYR:CE2	2.43	0.54
1:M1:336:PHE:HE2	1:M1:446:PHE:HD2	1.55	0.54
2:N1:95:LYS:HE3	2:N1:97:SER:OG	2.08	0.54
3:O1:37:LEU:HD11	3:O1:97:HIS:CG	2.43	0.54
3:O1:133:LEU:HB2	3:O1:134:PRO:HD3	1.90	0.54
4:P1:69:GLU:HG3	4:P1:84:PRO:HA	1.89	0.54
17:82:201:ALA:HB1	18:92:121:MET:HB2	1.90	0.54
19:A2:272:ARG:NH1	25:G2:87:MET:HE3	2.23	0.54
19:A2:381:LEU:HB2	29:K2:55:ILE:HD12	1.89	0.54
45:b2:118:SER:OG	49:h2:108:TYR:O	2.25	0.54
1:A1:39:VAL:CG2	1:A1:197:LEU:HD22	2.37	0.54
1:A1:397:SER:OG	1:A1:398:ARG:N	2.41	0.54
1:A1:418:GLN:O	1:A1:420:PRO:HD3	2.08	0.54
2:B1:163:LEU:HD22	2:B1:256:ALA:HB1	1.90	0.54
3:C1:88:SER:HB3	3:C1:250:LEU:CD2	2.38	0.54
3:C1:88:SER:CB	3:C1:250:LEU:HD23	2.37	0.54
6:F1:7:SER:HA	6:F1:11:ARG:HE	1.73	0.54
6:F1:40:ASN:CG	6:F1:41:ASP:H	2.16	0.54
1:M1:324:PHE:CD1	1:M1:334:MET:HG2	2.42	0.54
3:O1:76:GLY:HA2	3:O1:79:ILE:HD12	1.90	0.54
3:O1:169:SER:OG	3:O1:170:VAL:N	2.37	0.54
5:Q1:118:ARG:HH22	5:Q1:173:LYS:CA	2.20	0.54
14:42:403:THR:HA	14:42:406:TYR:HB3	1.90	0.54
19:A2:111:LYS:CD	33:P2:53:TYR:HE2	2.20	0.54
48:f2:150:ARG:HH22	55:e2:95:PRO:HB3	1.73	0.54
53:62:361:GLY:O	53:62:364:LYS:NZ	2.40	0.54
57:B3:203:ASN:HD22	57:B3:206:PHE:HD2	1.55	0.54
59:D3:40:LEU:HD13	59:D3:59:LEU:HD13	1.90	0.54
1:A1:61:HIS:CB	1:A1:130:GLU:HG3	2.37	0.54
1:A1:173:ASN:O	1:A1:177:LEU:HB2	2.07	0.54
2:B1:90:GLU:O	2:B1:92:VAL:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:30:TRP:HA	3:C1:33:PHE:HE2	1.73	0.54
3:C1:58:ASP:OD2	3:O1:56:THR:HG21	2.08	0.54
3:C1:264:THR:O	3:C1:266:PRO:HD3	2.06	0.54
3:C1:348:ILE:O	3:C1:352:GLN:HG3	2.08	0.54
4:D1:4:GLU:HG3	4:D1:6:HIS:CE1	2.43	0.54
1:M1:240:GLN:HA	1:M1:422:VAL:O	2.06	0.54
2:N1:88:GLY:O	2:N1:91:ALA:HB3	2.07	0.54
4:P1:168:VAL:O	4:P1:169:LEU:HD23	2.08	0.54
14:42:319:HIS:HA	14:42:322:THR:HB	1.89	0.54
17:82:220:GLN:HE21	18:92:118:PHE:HB2	1.72	0.54
19:A2:110:LYS:HD2	33:P2:55:CYS:SG	2.48	0.54
48:f2:61:THR:O	48:f2:65:ARG:N	2.40	0.54
1:A1:53:ASN:C	1:A1:53:ASN:HD22	2.16	0.54
1:A1:89:TYR:CD1	1:A1:89:TYR:C	2.85	0.54
1:A1:241:ILE:HG23	1:A1:241:ILE:O	2.07	0.54
4:D1:50:HIS:HE1	4:D1:91:PHE:HZ	1.53	0.54
1:M1:426:GLY:HA3	1:M1:428:ILE:H	1.71	0.54
1:M1:445:ARG:O	1:M1:446:PHE:CB	2.55	0.54
2:N1:255:ALA:HB2	2:N1:426:ALA:CB	2.37	0.54
2:N1:280:GLY:HA2	2:N1:311:ALA:CB	2.38	0.54
3:O1:7:SER:O	3:O1:8:HIS:O	2.26	0.54
3:O1:377:LEU:HB3	6:R1:33:ARG:HD2	1.88	0.54
4:P1:51:LEU:HD22	4:P1:58:GLU:HA	1.90	0.54
4:P1:216:LEU:N	4:P1:217:PRO:HD2	2.22	0.54
5:Q1:109:GLU:HG2	5:Q1:167:ALA:CB	2.25	0.54
8:T1:35:GLU:O	8:T1:39:LEU:HG	2.07	0.54
14:42:289:SER:HB3	14:42:406:TYR:HE2	1.71	0.54
27:I2:106:GLU:HB3	27:I2:108:LYS:NZ	2.23	0.54
30:L2:59:ASP:HB3	34:Q2:130:LYS:HD2	1.90	0.54
34:Q2:9:SER:HA	39:V2:88:ARG:HH12	1.73	0.54
57:B3:165:VAL:HB	57:B3:170:LEU:HD12	1.90	0.54
2:B1:303:VAL:CG1	2:B1:304:HIS:N	2.70	0.54
3:C1:183:PHE:CE1	3:C1:187:PHE:CE2	2.96	0.54
6:F1:35:ASP:OD2	6:F1:61:ARG:HD2	2.07	0.54
8:H1:73:LEU:HG	8:H1:73:LEU:O	2.08	0.54
4:P1:138:PRO:O	4:P1:139:THR:C	2.50	0.54
4:P1:220:TYR:HE2	7:S1:26:PHE:CE1	2.19	0.54
19:A2:302:LEU:HB3	38:U2:137:TRP:HB3	1.90	0.54
23:E2:82:ALA:HB2	33:P2:25:GLN:HE21	1.73	0.54
56:A3:398:PRO:O	56:A3:498:CYS:HB3	2.08	0.54
57:B3:111:THR:HG21	63:H3:66:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:40:TRP:CZ2	1:A1:377:GLU:CA	2.89	0.53
2:B1:62:ASN:ND2	2:B1:62:ASN:O	2.41	0.53
2:B1:340:ALA:O	2:B1:344:VAL:HG23	2.08	0.53
3:C1:309:THR:CG2	3:C1:370:GLY:HA3	2.38	0.53
1:M1:88:ALA:O	2:N1:286:LYS:HE2	2.07	0.53
2:N1:258:VAL:HG12	2:N1:321:LEU:HD22	1.89	0.53
5:Q1:139:CYS:O	5:Q1:143:GLY:HA2	2.08	0.53
6:R1:51:PRO:HG2	6:R1:54:LEU:HB2	1.89	0.53
20:B2:87:GLN:CB	20:B2:89:PRO:HD3	2.32	0.53
61:F3:51:SER:HB2	61:F3:91:LEU:HD11	1.90	0.53
1:A1:252:HIS:CD2	1:A1:325:VAL:CG2	2.92	0.53
2:B1:160:ILE:HD11	2:B1:325:TYR:HE2	1.74	0.53
2:B1:262:ALA:HB2	2:B1:272:PHE:HE2	1.72	0.53
2:B1:304:HIS:CG	2:B1:305:GLN:N	2.76	0.53
2:B1:396:SER:O	2:B1:399:LEU:HB2	2.08	0.53
8:H1:66:ASP:O	8:H1:67:HIS:C	2.50	0.53
1:M1:204:GLU:HG2	1:M1:206:ARG:HB3	1.90	0.53
1:M1:236:PHE:CD2	1:M1:258:GLU:CB	2.91	0.53
2:N1:168:TYR:HD2	2:N1:238:LYS:O	1.92	0.53
3:O1:207:ASN:ND2	3:O1:209:THR:OG1	2.41	0.53
3:O1:265:PRO:O	3:O1:268:ILE:HG13	2.07	0.53
4:P1:11:PRO:HB2	8:T1:74:PHE:CG	2.44	0.53
4:P1:48:TYR:OH	4:P1:68:VAL:HG11	2.08	0.53
5:Q1:32:ARG:HH12	7:S1:22:GLU:CD	2.15	0.53
8:T1:70:ALA:HA	8:T1:73:LEU:HD22	1.89	0.53
19:A2:311:LYS:HB3	38:U2:142:THR:O	2.07	0.53
21:C2:70:ILE:HG13	21:C2:71:LEU:HD12	1.90	0.53
59:D3:108:PRO:HG2	59:D3:111:PHE:CE2	2.42	0.53
2:B1:140:LEU:HD12	2:B1:143:GLN:CB	2.38	0.53
3:C1:1:MET:SD	3:C1:4:ILE:HB	2.48	0.53
3:C1:141:TRP:HB3	3:C1:268:ILE:HD13	1.90	0.53
4:D1:33:TYR:HA	4:D1:37:CYS:HB2	1.89	0.53
5:E1:15:ARG:HH21	5:E1:32:ARG:HG3	1.74	0.53
5:E1:20:ASP:O	5:E1:21:SER:C	2.49	0.53
10:J1:52:TRP:CE3	10:J1:52:TRP:N	2.77	0.53
2:N1:159:VAL:HG12	2:N1:160:ILE:N	2.21	0.53
4:P1:237:TYR:HD1	7:S1:13:VAL:HG22	1.73	0.53
6:R1:7:SER:HA	6:R1:11:ARG:HE	1.73	0.53
52:12:37:PRO:HB2	52:12:44:GLY:HA2	1.90	0.53
6:F1:35:ASP:OD1	6:F1:89:TYR:OH	2.21	0.53
1:M1:152:TYR:O	1:M1:153:LEU:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:218:ILE:HD13	4:P1:230:LEU:HD13	1.91	0.53
3:O1:251:GLY:O	3:O1:252:ASP:C	2.51	0.53
4:P1:106:ASN:C	4:P1:106:ASN:HD22	2.17	0.53
5:Q1:171:ILE:HD12	5:Q1:176:ALA:HB3	1.90	0.53
8:T1:73:LEU:HD21	8:T1:74:PHE:CD1	2.43	0.53
10:V1:49:GLY:HA2	10:V1:54:HIS:CB	2.39	0.53
12:22:224:THR:H	12:22:228:LEU:HD23	1.72	0.53
15:52:17:VAL:HG12	53:62:588:PHE:HB3	1.91	0.53
18:92:111:ARG:NE	25:G2:174:THR:OG1	2.42	0.53
19:A2:129:PRO:HG2	27:I2:114:TYR:CE1	2.43	0.53
59:D3:52:SER:OG	59:D3:55:GLU:HG3	2.08	0.53
61:F3:48:LEU:O	61:F3:50:PRO:HD3	2.08	0.53
1:A1:32:GLN:CG	1:A1:33:PRO:CD	2.86	0.53
1:A1:106:LEU:HD21	1:A1:203:LEU:HD13	1.89	0.53
2:B1:276:GLN:O	2:B1:280:GLY:N	2.40	0.53
3:C1:219:PRO:CB	3:C1:222:PRO:HD2	2.39	0.53
4:D1:149:PHE:HZ	8:H1:55:THR:HG23	1.73	0.53
4:D1:190:LEU:O	4:D1:191:ARG:C	2.52	0.53
4:D1:213:GLY:O	4:D1:217:PRO:HG3	2.07	0.53
6:F1:16:ILE:O	6:F1:17:ARG:C	2.50	0.53
1:M1:25:VAL:HG21	1:M1:209:LEU:CD1	2.39	0.53
1:M1:106:LEU:HD22	1:M1:203:LEU:CD2	2.35	0.53
2:N1:132:PHE:HD2	2:N1:191:LEU:HD13	1.67	0.53
2:N1:285:VAL:HG12	2:N1:288:GLY:HA3	1.91	0.53
3:O1:26:ASN:HD22	3:O1:208:PRO:HD2	1.70	0.53
3:O1:218:ILE:HG23	3:O1:223:TYR:CD2	2.43	0.53
5:Q1:150:ALA:HB3	5:Q1:157:TYR:HB3	1.91	0.53
14:42:118:PHE:O	14:42:122:PHE:N	2.39	0.53
18:92:95:ILE:HD13	19:A2:210:ILE:HG22	1.88	0.53
34:Q2:30:HIS:NE2	34:Q2:120:PRO:O	2.41	0.53
46:c2:34:VAL:HG22	46:c2:36:PRO:HA	1.91	0.53
1:A1:61:HIS:CD2	2:B1:287:ARG:HD3	2.43	0.53
1:A1:134:ILE:HD13	1:A1:134:ILE:N	2.23	0.53
1:A1:134:ILE:HA	1:A1:137:GLU:HG3	1.91	0.53
2:B1:92:VAL:HG12	2:B1:92:VAL:O	2.08	0.53
3:C1:103:TYR:O	3:C1:315:MET:CB	2.57	0.53
7:G1:15:THR:HG22	7:G1:15:THR:O	2.07	0.53
7:G1:64:GLN:O	7:G1:65:GLU:C	2.50	0.53
9:I1:58:GLN:HG2	9:I1:78:TYR:HD2	1.72	0.53
10:J1:45:HIS:O	10:J1:48:GLU:HG2	2.08	0.53
1:M1:53:ASN:HB3	1:M1:170:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:411:CYS:O	1:M1:415:PHE:HD1	1.92	0.53
1:M1:417:ASP:CG	10:V1:10:TYR:OH	2.51	0.53
2:N1:133:ARG:O	2:N1:134:ARG:C	2.49	0.53
2:N1:276:GLN:O	2:N1:280:GLY:N	2.40	0.53
5:Q1:95:PRO:HG2	5:Q1:145:VAL:CG2	2.38	0.53
28:J2:64:LYS:H	34:Q2:21:SER:HB3	1.74	0.53
50:i2:59:ILE:HA	50:i2:62:HIS:HB3	1.90	0.53
57:B3:102:HIS:O	57:B3:104:TRP:N	2.42	0.53
59:D3:67:SER:OG	59:D3:70:GLU:HG3	2.08	0.53
62:G3:8:HIS:O	62:G3:10:GLY:N	2.42	0.53
2:B1:79:GLY:H	2:B1:125:ASN:ND2	2.07	0.53
1:M1:29:GLN:HG3	1:M1:203:LEU:O	2.09	0.53
1:M1:53:ASN:HB3	1:M1:170:PRO:HD2	1.89	0.53
2:N1:25:GLU:O	2:N1:213:HIS:CE1	2.62	0.53
2:N1:217:LYS:O	2:N1:218:GLN:C	2.51	0.53
2:N1:247:GLN:HG3	2:N1:248:ASN:N	2.24	0.53
2:N1:262:ALA:HB3	2:N1:269:ALA:HA	1.91	0.53
3:O1:71:ARG:NH2	4:P1:193:ALA:O	2.42	0.53
3:O1:345:HIS:CB	3:O1:346:PRO:HD3	2.26	0.53
4:P1:219:VAL:HA	4:P1:222:MET:HG3	1.89	0.53
4:P1:237:TYR:CE2	4:P1:239:PRO:HG3	2.44	0.53
19:A2:637:ASP:OD1	32:O2:118:PHE:CE1	2.62	0.53
49:h2:81:ALA:O	49:h2:83:ASP:N	2.42	0.53
56:A3:268:PHE:CZ	57:B3:58:ALA:HA	2.44	0.53
60:E3:41:LEU:HD12	60:E3:41:LEU:O	2.08	0.53
61:F3:55:LYS:HA	61:F3:74:LEU:O	2.08	0.53
1:A1:162:PRO:O	1:A1:165:GLN:NE2	2.38	0.53
2:B1:316:TYR:OH	9:I1:64:LEU:HD23	2.09	0.53
3:O1:219:PRO:HB2	3:O1:222:PRO:HD2	1.89	0.53
3:O1:276:PHE:O	3:O1:277:ALA:C	2.52	0.53
4:P1:3:LEU:HD21	7:S1:71:ARG:HA	1.90	0.53
4:P1:69:GLU:O	4:P1:73:GLY:HA3	2.09	0.53
19:A2:134:GLY:O	20:B2:382:PHE:HE2	1.92	0.53
19:A2:238:PHE:HE2	23:E2:138:GLY:O	1.92	0.53
59:D3:23:PRO:HD2	60:E3:34:ASN:HD22	1.74	0.53
1:A1:34:THR:HB	2:B1:373:GLU:OE1	2.09	0.53
4:D1:138:PRO:HG2	8:H1:55:THR:CB	2.38	0.53
5:E1:2:HIS:O	5:E1:5:ILE:HG12	2.09	0.53
6:F1:25:GLY:O	6:F1:28:LYS:HG3	2.09	0.53
1:M1:106:LEU:HB3	1:M1:107:PRO:HD3	1.90	0.53
2:N1:294:SER:O	2:N1:295:LEU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:120:ARG:HG2	4:P1:120:ARG:NH1	2.24	0.53
5:Q1:45:VAL:CG2	10:V1:24:ILE:HA	2.39	0.53
6:R1:75:LEU:CD1	6:R1:76:PRO:HD2	2.36	0.53
17:82:415:ILE:HD12	19:A2:119:PHE:HE1	1.72	0.53
19:A2:301:ARG:O	38:U2:137:TRP:N	2.41	0.53
54:g2:14:PRO:O	54:g2:116:ARG:NH2	2.42	0.53
57:B3:136:LEU:HB3	57:B3:193:TYR:HD2	1.73	0.53
1:A1:85:HIS:HA	2:B1:284:HIS:O	2.09	0.53
2:B1:300:ALA:HA	2:B1:307:PHE:HZ	1.74	0.53
3:C1:90:PHE:CE1	3:C1:123:VAL:HG21	2.44	0.53
8:H1:65:ARG:HG3	8:H1:66:ASP:N	2.23	0.53
10:J1:52:TRP:HE3	10:J1:52:TRP:H	1.57	0.53
10:J1:56:LYS:HE2	10:J1:60:GLU:OE1	2.09	0.53
1:M1:317:THR:HG22	1:M1:318:GLY:H	1.73	0.53
2:N1:262:ALA:HB2	2:N1:268:GLU:HB3	1.90	0.53
3:O1:106:SER:O	3:O1:109:PHE:CD2	2.54	0.53
3:O1:174:THR:O	3:O1:178:PHE:CD2	2.62	0.53
3:O1:196:HIS:CE1	69:O1:402:HEM:C1D	2.97	0.53
10:V1:4:THR:HG22	10:V1:6:THR:OG1	2.09	0.53
19:A2:473:MET:HE2	19:A2:475:ILE:HD11	1.91	0.53
40:W2:83:VAL:HG21	40:W2:145:VAL:HG22	1.91	0.53
56:A3:11:ASN:ND2	56:A3:14:ASP:H	2.07	0.53
1:A1:11:VAL:CG1	1:A1:12:PRO:HD2	2.39	0.52
1:A1:67:THR:OG1	1:A1:119:ASN:HB2	2.09	0.52
2:B1:132:PHE:CD2	2:B1:191:LEU:HD13	2.43	0.52
2:B1:160:ILE:CD1	2:B1:325:TYR:HE2	2.21	0.52
2:B1:347:ILE:H	2:B1:347:ILE:CD1	2.21	0.52
2:B1:435:PHE:CE1	2:N1:169:ARG:HG2	2.44	0.52
3:C1:80:ARG:O	3:C1:80:ARG:HD3	2.09	0.52
3:C1:103:TYR:HA	3:C1:315:MET:CE	2.32	0.52
4:D1:48:TYR:OH	4:D1:68:VAL:HG11	2.09	0.52
7:G1:25:ALA:O	7:G1:27:PRO:HD3	2.09	0.52
2:N1:277:HIS:CD2	2:N1:364:LEU:HD13	2.43	0.52
2:N1:406:ALA:HB3	2:N1:409:ASP:HB2	1.92	0.52
4:P1:27:ARG:O	4:P1:28:ARG:C	2.52	0.52
4:P1:181:GLN:HG2	8:T1:77:LEU:CD2	2.21	0.52
4:P1:237:TYR:CE2	4:P1:239:PRO:HD3	2.44	0.52
8:T1:58:LEU:HD12	8:T1:58:LEU:O	2.10	0.52
10:V1:36:ASP:O	10:V1:37:GLN:C	2.53	0.52
12:22:164:ILE:HG13	53:62:576:LEU:HD11	1.89	0.52
14:42:439:LEU:H	14:42:442:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:52:93:LEU:HD22	53:62:583:LEU:H	1.73	0.52
21:C2:170:ARG:HG3	21:C2:186:LEU:HD12	1.91	0.52
57:B3:68:LEU:HB3	57:B3:69:PRO:HD3	1.91	0.52
62:G3:2:SER:OG	62:G3:3:ALA:N	2.41	0.52
2:B1:69:LEU:HD21	2:B1:199:PHE:CZ	2.44	0.52
2:B1:141:GLN:OE1	2:B1:183:ILE:O	2.27	0.52
2:B1:268:GLU:O	2:B1:271:ALA:HB3	2.10	0.52
4:D1:82:MET:HE2	4:D1:86:LYS:NZ	2.23	0.52
8:H1:73:LEU:CD2	8:H1:74:PHE:HD1	2.21	0.52
1:M1:64:PHE:HE1	1:M1:86:LEU:CG	2.22	0.52
1:M1:244:ARG:CZ	7:S1:10:VAL:HB	2.38	0.52
1:M1:408:ARG:NH2	11:W1:15:ARG:CZ	2.65	0.52
3:O1:174:THR:O	3:O1:178:PHE:HD2	1.90	0.52
3:O1:200:LEU:HD13	69:O1:402:HEM:HAD2	1.90	0.52
3:O1:275:LEU:O	3:O1:278:TYR:N	2.42	0.52
5:Q1:81:ILE:H	5:Q1:81:ILE:HD12	1.75	0.52
6:R1:96:GLU:OE2	6:R1:99:ARG:NH1	2.43	0.52
12:22:196:TYR:OH	37:T2:137:ALA:O	2.26	0.52
19:A2:313:LEU:CG	38:U2:142:THR:CA	2.86	0.52
36:S2:32:ILE:HG13	36:S2:33:LEU:HD12	1.92	0.52
53:62:241:THR:HG23	53:62:299:LYS:HZ1	1.74	0.52
53:62:427:ILE:HG13	53:62:431:LEU:HD12	1.91	0.52
59:D3:128:VAL:O	59:D3:134:PHE:HB3	2.09	0.52
63:H3:75:ARG:HG2	63:H3:75:ARG:NH1	2.19	0.52
1:A1:53:ASN:CG	1:A1:165:GLN:HB2	2.34	0.52
3:C1:92:ILE:O	3:C1:96:MET:HG2	2.09	0.52
5:E1:31:ALA:O	5:E1:34:GLY:N	2.42	0.52
6:F1:45:GLU:O	6:F1:49:ARG:HG3	2.08	0.52
1:M1:277:ILE:CG2	1:M1:294:LEU:HD12	2.39	0.52
3:O1:304:ILE:N	3:O1:305:PRO:CD	2.72	0.52
4:P1:11:PRO:HG2	8:T1:74:PHE:HB2	1.92	0.52
19:A2:126:LEU:HB2	27:I2:98:ARG:O	2.10	0.52
53:62:550:SER:OG	53:62:551:SER:N	2.42	0.52
56:A3:302:ARG:O	56:A3:306:THR:HG23	2.09	0.52
1:A1:239:SER:OG	1:A1:240:GLN:N	2.39	0.52
1:A1:260:PRO:HD3	1:A1:414:TYR:CD1	2.44	0.52
2:B1:135:TRP:CD1	2:B1:136:GLU:HG3	2.44	0.52
2:B1:191:LEU:O	2:B1:195:VAL:HG23	2.09	0.52
3:C1:103:TYR:O	3:C1:315:MET:HB2	2.10	0.52
3:C1:135:TRP:CH2	3:C1:170:VAL:O	2.62	0.52
3:C1:301:LEU:HA	3:C1:304:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:350:ILE:O	3:C1:351:GLY:C	2.53	0.52
3:C1:368:THR:O	3:C1:371:THR:HB	2.10	0.52
1:M1:25:VAL:HG21	1:M1:209:LEU:HD13	1.91	0.52
1:M1:41:ILE:HD12	1:M1:41:ILE:N	2.24	0.52
1:M1:277:ILE:HB	1:M1:309:THR:HG21	1.91	0.52
2:N1:164:HIS:O	2:N1:173:ALA:HA	2.09	0.52
3:O1:218:ILE:HG21	3:O1:223:TYR:CD2	2.43	0.52
6:R1:75:LEU:C	6:R1:80:TRP:HE1	2.17	0.52
19:A2:157:LYS:HB2	27:I2:100:TYR:HE2	1.71	0.52
20:B2:86:PRO:HG3	20:B2:96:ARG:HB3	1.90	0.52
61:F3:8:THR:OG1	61:F3:11:GLU:HG2	2.10	0.52
2:B1:122:PHE:O	2:B1:123:LEU:C	2.53	0.52
2:B1:308:ASP:OD2	9:I1:55:LEU:HA	2.10	0.52
3:C1:119:LEU:HD23	69:C1:402:HEM:C4B	2.44	0.52
4:D1:68:VAL:HG12	4:D1:92:PRO:HG2	1.91	0.52
4:D1:233:ARG:HG3	7:G1:17:SER:CB	2.40	0.52
5:E1:18:VAL:HG11	5:E1:32:ARG:HH11	1.73	0.52
9:I1:58:GLN:HB3	9:I1:78:TYR:HB2	1.91	0.52
1:M1:111:GLU:HG2	1:M1:213:GLN:NE2	2.25	0.52
1:M1:241:ILE:CD1	7:S1:16:TYR:CE2	2.92	0.52
1:M1:292:SER:O	1:M1:295:ALA:HB3	2.09	0.52
2:N1:304:HIS:CD2	2:N1:305:GLN:N	2.78	0.52
4:P1:146:GLY:O	4:P1:148:TYR:N	2.42	0.52
4:P1:195:GLU:HG3	4:P1:198:HIS:HB2	1.92	0.52
6:R1:73:GLN:HE21	7:S1:32:LYS:HE3	1.74	0.52
8:T1:62:LEU:O	8:T1:65:ARG:HG2	2.09	0.52
8:T1:65:ARG:CG	8:T1:66:ASP:N	2.72	0.52
14:42:23:ILE:HG21	14:42:93:LYS:HE3	1.89	0.52
36:S2:275:ASN:O	36:S2:277:ARG:N	2.41	0.52
1:A1:166:SER:CB	5:E1:3:THR:HG22	2.39	0.52
2:B1:68:LEU:C	2:B1:68:LEU:HD12	2.34	0.52
3:C1:221:HIS:HA	3:C1:225:THR:HG23	1.92	0.52
3:C1:377:LEU:O	3:C1:378:LYS:HB3	2.09	0.52
5:E1:47:VAL:O	5:E1:50:ALA:HB3	2.10	0.52
2:N1:198:HIS:CE1	2:N1:233:SER:HB3	2.45	0.52
2:N1:247:GLN:NE2	2:N1:429:ASN:HA	2.25	0.52
2:N1:275:LEU:HB2	2:N1:410:VAL:HG13	1.92	0.52
3:O1:47:THR:HG22	3:O1:83:HIS:HB2	1.91	0.52
5:Q1:102:THR:H	5:Q1:105:GLU:HB2	1.74	0.52
6:R1:95:LYS:O	6:R1:96:GLU:C	2.53	0.52
12:22:142:LEU:HD23	12:22:145:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D2:114:ARG:HG3	22:D2:114:ARG:NH2	2.15	0.52
23:E2:116:CYS:HA	23:E2:140:ARG:HH22	1.75	0.52
35:R2:264:ALA:H	35:R2:334:GLY:HA3	1.75	0.52
1:A1:37:VAL:HG13	1:A1:199:ALA:CB	2.40	0.52
1:A1:85:HIS:CD2	2:B1:370:MET:HE1	2.45	0.52
1:A1:426:GLY:H	1:A1:428:ILE:CD1	2.22	0.52
3:C1:85:ASN:O	3:C1:86:GLY:C	2.50	0.52
3:C1:183:PHE:CD1	3:C1:183:PHE:C	2.88	0.52
3:C1:183:PHE:CD1	3:O1:183:PHE:CD1	2.97	0.52
4:D1:79:GLU:HB3	4:D1:82:MET:HB2	1.91	0.52
1:M1:426:GLY:HA2	1:M1:428:ILE:CG1	2.37	0.52
3:O1:27:ILE:O	3:O1:27:ILE:CG2	2.58	0.52
3:O1:296:PHE:O	3:O1:297:SER:C	2.52	0.52
4:P1:55:CYS:SG	10:V1:52:TRP:CB	2.97	0.52
4:P1:138:PRO:HB3	8:T1:55:THR:HA	1.90	0.52
19:A2:314:LEU:CD2	38:U2:140:PRO:CD	2.69	0.52
20:B2:299:GLN:HG2	23:E2:38:TYR:HE1	1.75	0.52
57:B3:33:LEU:HD23	64:I3:28:SER:HB2	1.91	0.52
60:E3:63:SER:O	60:E3:67:ILE:HG13	2.10	0.52
2:B1:257:LEU:HD13	2:B1:424:MET:HE2	1.91	0.52
4:D1:10:TYR:HD1	8:H1:74:PHE:CE1	2.28	0.52
4:D1:64:LEU:O	4:D1:68:VAL:HG23	2.09	0.52
4:D1:139:THR:HG21	8:H1:41:ASP:O	2.09	0.52
7:G1:33:GLY:O	7:G1:37:VAL:N	2.36	0.52
1:M1:5:ALA:O	1:M1:6:GLN:C	2.53	0.52
1:M1:151:ASN:O	1:M1:152:TYR:C	2.53	0.52
1:M1:392:LEU:HA	1:M1:395:TRP:NE1	2.25	0.52
2:N1:262:ALA:HB3	2:N1:269:ALA:N	2.24	0.52
3:O1:246:ALA:N	3:O1:247:PRO:CD	2.73	0.52
5:Q1:76:ILE:CG2	5:Q1:194:ILE:CG1	2.74	0.52
12:22:87:MET:HE3	12:22:90:PHE:HE2	1.74	0.52
17:82:390:ASP:OD2	19:A2:202:ASN:CB	2.51	0.52
18:92:62:ARG:NH2	24:F2:83:TYR:OH	2.40	0.52
35:R2:197:GLU:HB2	35:R2:259:ARG:HE	1.75	0.52
52:12:25:ARG:NH1	52:12:25:ARG:CG	2.73	0.52
53:62:258:PHE:HA	53:62:261:ILE:HD12	1.92	0.52
56:A3:225:GLY:HA3	58:C3:112:LEU:HD13	1.92	0.52
57:B3:104:TRP:CG	57:B3:203:ASN:HB2	2.44	0.52
1:A1:19:LEU:HB2	1:A1:23:LEU:HB3	1.92	0.52
1:A1:91:THR:HG23	1:A1:92:ARG:H	1.74	0.52
1:A1:436:ARG:HE	3:C1:222:PRO:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:280:GLY:HA2	2:B1:311:ALA:CB	2.40	0.52
3:C1:300:ILE:HD13	3:C1:362:ILE:HG21	1.92	0.52
4:D1:143:LEU:HD22	4:D1:147:LEU:O	2.09	0.52
5:E1:38:LEU:HD13	10:J1:9:LEU:HD23	1.92	0.52
6:F1:96:GLU:OE1	6:F1:96:GLU:HA	2.09	0.52
1:M1:262:TRP:CE3	1:M1:385:THR:CG2	2.93	0.52
2:N1:51:ILE:CG2	2:N1:199:PHE:HA	2.33	0.52
2:N1:395:PRO:O	2:N1:396:SER:C	2.52	0.52
3:O1:6:LYS:HE2	3:O1:16:ASN:HD21	1.74	0.52
3:O1:245:PHE:CG	4:P1:17:LEU:HD13	2.43	0.52
22:D2:82:LEU:HB2	22:D2:111:VAL:HG22	1.90	0.52
57:B3:100:MET:CE	57:B3:157:GLU:HG3	2.40	0.52
1:A1:326:CYS:SG	1:A1:331:ILE:HA	2.50	0.52
1:A1:433:ASP:CB	3:C1:219:PRO:HG2	2.40	0.52
2:B1:25:GLU:O	2:B1:213:HIS:CE1	2.63	0.52
2:B1:97:SER:OG	9:I1:70:LEU:HB2	2.10	0.52
4:D1:7:PRO:HB2	4:D1:125:ASP:HB3	1.92	0.52
8:H1:15:ASP:N	8:H1:16:PRO:CD	2.73	0.52
1:M1:19:LEU:HD13	1:M1:214:LYS:HG2	1.92	0.52
1:M1:426:GLY:HA3	1:M1:428:ILE:N	2.24	0.52
3:O1:52:ALA:HB2	69:O1:401:HEM:CMD	2.40	0.52
3:O1:200:LEU:HD13	69:O1:402:HEM:CAD	2.40	0.52
4:P1:160:MET:HE3	4:P1:163:PRO:HG3	1.91	0.52
18:92:222:ARG:HD3	18:92:228:ALA:HB2	1.92	0.52
35:R2:127:ILE:HG22	35:R2:165:ILE:HB	1.91	0.52
2:B1:79:GLY:HA3	2:B1:125:ASN:HD21	1.75	0.51
2:B1:279:LEU:HD22	2:B1:344:VAL:HG22	1.91	0.51
2:B1:286:LYS:O	2:B1:287:ARG:HB2	2.09	0.51
4:D1:62:LYS:O	4:D1:66:GLU:HG3	2.10	0.51
6:F1:13:LEU:O	6:F1:16:ILE:N	2.42	0.51
3:O1:170:VAL:HG12	3:O1:170:VAL:O	2.08	0.51
3:O1:200:LEU:CD1	69:O1:402:HEM:HAD2	2.40	0.51
5:Q1:42:THR:O	5:Q1:43:THR:C	2.53	0.51
6:R1:46:ALA:O	6:R1:47:ILE:C	2.53	0.51
7:S1:67:GLU:O	7:S1:71:ARG:HB3	2.10	0.51
8:T1:50:THR:HG22	8:T1:51:GLU:N	2.25	0.51
19:A2:674:LEU:CD1	29:K2:46:LYS:CD	2.88	0.51
20:B2:97:LEU:HB3	20:B2:111:PRO:HB3	1.90	0.51
20:B2:303:ARG:HD3	20:B2:401:GLU:HG2	1.92	0.51
21:C2:124:ARG:NH1	31:N2:111:GLN:O	2.43	0.51
22:D2:159:GLY:O	22:D2:164:HIS:ND1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B3:186:SER:CB	57:B3:213:LEU:HD22	2.40	0.51
1:A1:34:THR:CB	2:B1:373:GLU:OE1	2.59	0.51
1:A1:111:GLU:HG2	1:A1:213:GLN:NE2	2.25	0.51
1:A1:381:ARG:HA	1:A1:384:LEU:HD12	1.91	0.51
4:D1:26:ILE:HG21	4:D1:54:VAL:HG22	1.92	0.51
4:D1:32:VAL:HG11	4:D1:186:VAL:CG2	2.41	0.51
10:J1:49:GLY:HA2	10:J1:54:HIS:HB3	1.92	0.51
10:J1:51:LEU:H	10:J1:54:HIS:HD2	1.57	0.51
1:M1:213:GLN:CB	1:M1:215:HIS:NE2	2.70	0.51
2:N1:258:VAL:CG1	2:N1:321:LEU:HD22	2.40	0.51
3:O1:117:VAL:N	69:O1:402:HEM:HBC2	2.25	0.51
5:Q1:119:ASP:HB3	5:Q1:179:ASN:ND2	2.26	0.51
5:Q1:119:ASP:OD1	5:Q1:120:PRO:HD2	2.09	0.51
19:A2:238:PHE:CE2	23:E2:138:GLY:O	2.63	0.51
20:B2:97:LEU:HB3	20:B2:111:PRO:CB	2.40	0.51
30:L2:76:PRO:HD2	34:Q2:127:LYS:HG2	1.91	0.51
2:B1:178:CYS:SG	2:B1:179:PRO:HD2	2.51	0.51
3:C1:153:ILE:HD12	3:C1:153:ILE:N	2.25	0.51
6:F1:7:SER:O	6:F1:11:ARG:HD2	2.10	0.51
1:M1:134:ILE:HD13	1:M1:137:GLU:HG3	1.91	0.51
4:P1:27:ARG:NH1	10:V1:58:LYS:CE	2.72	0.51
4:P1:82:MET:HE2	4:P1:86:LYS:NZ	2.25	0.51
4:P1:138:PRO:HB3	8:T1:55:THR:CA	2.40	0.51
4:P1:213:GLY:O	4:P1:217:PRO:HG3	2.11	0.51
16:72:165:VAL:O	16:72:169:MET:N	2.42	0.51
19:A2:587:ALA:HB1	19:A2:591:GLU:HB2	1.91	0.51
35:R2:281:PHE:HB3	35:R2:286:ARG:HD3	1.91	0.51
35:R2:329:LEU:HG	35:R2:331:HIS:H	1.76	0.51
51:j2:108:THR:HA	54:g2:78:GLN:HA	1.92	0.51
1:A1:279:HIS:CE1	1:A1:284:TYR:OH	2.63	0.51
2:B1:34:VAL:HG11	2:B1:386:ALA:CB	2.41	0.51
2:B1:412:ASN:O	2:B1:415:LYS:HB2	2.11	0.51
1:M1:46:ARG:NH1	1:M1:316:ASP:OD1	2.40	0.51
1:M1:158:PHE:HE1	1:M1:317:THR:HG21	1.72	0.51
1:M1:428:ILE:CG2	1:M1:431:LEU:CD2	2.85	0.51
2:N1:102:ARG:HH12	2:N1:175:SER:HA	1.75	0.51
2:N1:141:GLN:OE1	2:N1:183:ILE:O	2.29	0.51
3:O1:19:ILE:HG23	3:O1:221:HIS:HB2	1.92	0.51
3:O1:85:ASN:O	3:O1:86:GLY:C	2.53	0.51
3:O1:166:GLY:HA3	3:O1:177:ARG:NH2	2.26	0.51
4:P1:48:TYR:CD2	4:P1:65:ALA:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D2:75:ASN:OD1	22:D2:78:ARG:NH2	2.43	0.51
56:A3:240:HIS:HB3	56:A3:241:PRO:HD3	1.92	0.51
62:G3:42:ARG:HH11	62:G3:42:ARG:HG3	1.74	0.51
1:A1:41:ILE:HD12	1:A1:41:ILE:N	2.24	0.51
1:A1:53:ASN:HB3	1:A1:170:PRO:HD2	1.91	0.51
1:A1:200:ALA:HB2	1:A1:375:VAL:HG12	1.92	0.51
2:B1:162:ASN:HB3	2:B1:244:ILE:CG2	2.40	0.51
2:B1:429:ASN:C	2:B1:429:ASN:HD22	2.19	0.51
3:C1:125:ALA:O	3:C1:126:THR:C	2.53	0.51
3:C1:344:GLU:O	3:C1:348:ILE:HG13	2.11	0.51
2:N1:67:HIS:CE1	2:N1:177:TYR:HD1	2.28	0.51
2:N1:262:ALA:CB	2:N1:268:GLU:HB3	2.41	0.51
2:N1:435:PHE:H	2:N1:438:GLU:HB2	1.74	0.51
3:O1:153:ILE:HD12	3:O1:153:ILE:H	1.74	0.51
4:P1:43:MET:HA	4:P1:112:ASP:OD1	2.10	0.51
14:42:301:ILE:O	14:42:304:GLN:NE2	2.43	0.51
19:A2:199:GLY:HA3	19:A2:204:MET:HA	1.93	0.51
19:A2:380:ASP:OD1	19:A2:380:ASP:N	2.38	0.51
19:A2:557:ARG:HG3	19:A2:560:LEU:HD23	1.91	0.51
36:S2:182:THR:HG23	36:S2:183:ILE:HG13	1.92	0.51
1:A1:39:VAL:CG1	1:A1:41:ILE:HD11	2.35	0.51
1:A1:106:LEU:HB3	1:A1:107:PRO:CD	2.41	0.51
1:A1:211:LEU:O	1:A1:211:LEU:HD12	2.11	0.51
2:B1:148:LYS:HD2	2:B1:178:CYS:O	2.10	0.51
2:B1:261:SER:HB3	2:B1:321:LEU:N	2.25	0.51
3:C1:184:ILE:O	3:C1:188:ILE:HD12	2.10	0.51
3:C1:331:ASP:OD1	3:C1:354:ALA:HB1	2.11	0.51
4:D1:2:ASP:HB3	4:D1:156:GLN:NE2	2.26	0.51
1:M1:106:LEU:HB3	1:M1:107:PRO:CD	2.40	0.51
2:N1:303:VAL:CG1	2:N1:304:HIS:H	2.24	0.51
5:Q1:86:ASN:HD21	5:Q1:97:PHE:HD2	1.54	0.51
14:42:276:CYS:SG	14:42:406:TYR:OH	2.65	0.51
52:12:46:LEU:HG	52:12:49:ILE:HD11	1.91	0.51
52:12:210:GLY:HA2	52:12:213:VAL:HG12	1.91	0.51
57:B3:136:LEU:HB3	57:B3:193:TYR:CD2	2.46	0.51
1:A1:84:ALA:HB2	1:A1:101:ALA:CB	2.37	0.51
1:A1:329:MET:HA	1:A1:430:GLN:OE1	2.10	0.51
2:B1:275:LEU:HD11	2:B1:279:LEU:CD1	2.41	0.51
2:B1:305:GLN:CB	2:B1:306:PRO:HD3	2.31	0.51
2:B1:375:SER:OG	2:B1:376:GLU:N	2.42	0.51
3:C1:177:ARG:O	3:C1:181:PHE:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:240:MET:SD	3:C1:243:VAL:HG11	2.51	0.51
3:C1:277:ALA:O	3:C1:278:TYR:C	2.52	0.51
3:C1:282:ARG:O	3:C1:284:ILE:N	2.43	0.51
4:D1:27:ARG:NH1	10:J1:58:LYS:HE3	2.26	0.51
6:F1:104:ARG:O	6:F1:105:GLU:C	2.53	0.51
7:G1:33:GLY:O	7:G1:37:VAL:HB	2.11	0.51
8:H1:27:LEU:O	8:H1:30:CYS:N	2.38	0.51
8:H1:70:ALA:HA	8:H1:73:LEU:HD22	1.92	0.51
1:M1:131:ARG:O	1:M1:132:ASP:C	2.53	0.51
1:M1:446:PHE:HE2	3:O1:6:LYS:HZ1	1.58	0.51
2:N1:129:ALA:H	2:N1:130:PRO:HD3	1.76	0.51
2:N1:393:THR:HG22	2:N1:394:PRO:O	2.10	0.51
3:O1:196:HIS:CE1	69:O1:402:HEM:ND	2.78	0.51
3:O1:357:LEU:O	3:O1:361:LEU:HG	2.10	0.51
6:R1:37:ILE:HG23	6:R1:37:ILE:O	2.11	0.51
6:R1:49:ARG:NH2	6:R1:100:GLU:OE2	2.37	0.51
19:A2:403:VAL:HG12	19:A2:432:ILE:HB	1.92	0.51
20:B2:140:ASP:OD2	20:B2:143:SER:OG	2.28	0.51
26:H2:21:GLN:O	26:H2:25:GLN:NE2	2.43	0.51
35:R2:171:ASN:HD21	35:R2:324:THR:HB	1.76	0.51
57:B3:1:MET:SD	57:B3:133:LEU:CD1	2.98	0.51
2:B1:85:ILE:O	2:B1:89:ILE:HG13	2.10	0.51
2:B1:350:GLY:HA2	2:B1:411:ILE:HG21	1.92	0.51
3:C1:107:TYR:OH	3:C1:308:HIS:ND1	2.09	0.51
5:E1:15:ARG:HH21	5:E1:32:ARG:CB	2.24	0.51
1:M1:162:PRO:O	1:M1:165:GLN:NE2	2.42	0.51
1:M1:389:ARG:C	1:M1:391:PRO:HD3	2.36	0.51
2:N1:209:LEU:HG	2:N1:209:LEU:O	2.09	0.51
2:N1:261:SER:HB3	2:N1:321:LEU:N	2.26	0.51
3:O1:91:PHE:O	3:O1:92:ILE:C	2.52	0.51
4:P1:220:TYR:O	4:P1:221:ALA:C	2.53	0.51
5:Q1:135:LEU:HD22	5:Q1:182:VAL:HG22	1.92	0.51
5:Q1:191:ASP:OD1	5:Q1:191:ASP:N	2.42	0.51
29:K2:65:LEU:HB3	29:K2:77:VAL:HG23	1.92	0.51
39:V2:48:TRP:O	39:V2:52:LYS:NZ	2.39	0.51
56:A3:250:GLY:O	56:A3:254:ILE:HG12	2.11	0.51
56:A3:347:LEU:HG	56:A3:383:MET:HE3	1.93	0.51
1:A1:426:GLY:H	1:A1:428:ILE:HG12	1.66	0.51
2:B1:88:GLY:O	2:B1:91:ALA:HB3	2.11	0.51
2:B1:112:LEU:O	2:B1:113:ARG:C	2.54	0.51
2:B1:200:THR:OG1	2:B1:201:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:383:GLY:O	2:B1:386:ALA:HB3	2.10	0.51
3:C1:105:GLY:HA2	3:C1:107:TYR:CD1	2.46	0.51
4:D1:42:SER:O	4:D1:112:ASP:OD1	2.29	0.51
4:D1:102:ARG:HG2	4:D1:109:LEU:HB2	1.93	0.51
1:M1:51:LYS:C	1:M1:53:ASN:H	2.19	0.51
1:M1:55:ALA:O	1:M1:58:PHE:N	2.39	0.51
1:M1:82:MET:SD	1:M1:105:ASP:HB3	2.51	0.51
1:M1:124:ASP:O	1:M1:128:GLU:HG2	2.11	0.51
1:M1:279:HIS:ND1	1:M1:284:TYR:OH	2.39	0.51
1:M1:329:MET:HA	1:M1:430:GLN:OE1	2.11	0.51
1:M1:408:ARG:O	1:M1:412:SER:OG	2.28	0.51
3:O1:30:TRP:HA	3:O1:33:PHE:HE2	1.75	0.51
4:P1:79:GLU:O	4:P1:80:MET:C	2.52	0.51
4:P1:79:GLU:HB3	4:P1:82:MET:HB2	1.93	0.51
4:P1:224:ARG:NH2	7:S1:27:PRO:HD2	2.26	0.51
35:R2:168:SER:OG	35:R2:169:HIS:N	2.44	0.51
35:R2:326:ASP:O	35:R2:328:ILE:HG13	2.10	0.51
2:B1:115:ASP:HA	2:B1:118:ILE:HD12	1.92	0.51
4:D1:164:ILE:HG21	4:D1:182:VAL:HG12	1.92	0.51
2:N1:308:ASP:OD2	9:U1:54:SER:O	2.29	0.51
9:U1:58:GLN:HB3	9:U1:78:TYR:HB2	1.92	0.51
12:22:63:GLN:HE21	12:22:114:TRP:HZ2	1.59	0.51
59:D3:40:LEU:HD22	59:D3:59:LEU:HD13	1.92	0.51
1:A1:279:HIS:CE1	1:A1:284:TYR:HH	2.29	0.50
1:A1:378:ASP:O	1:A1:382:SER:HB2	2.11	0.50
2:B1:77:THR:HG22	2:B1:130:PRO:N	2.24	0.50
2:B1:304:HIS:CG	2:B1:305:GLN:H	2.29	0.50
3:C1:100:ARG:NH2	69:C1:402:HEM:O2A	2.44	0.50
3:C1:135:TRP:CH2	3:C1:170:VAL:HG12	2.41	0.50
3:C1:312:GLN:O	3:C1:313:ARG:C	2.53	0.50
3:C1:312:GLN:NE2	3:C1:317:PHE:HB2	2.25	0.50
3:C1:341:GLN:O	3:C1:342:PRO:C	2.52	0.50
3:C1:373:GLU:HB3	6:F1:20:TYR:OH	2.12	0.50
4:D1:120:ARG:HH11	4:D1:120:ARG:CG	2.24	0.50
6:F1:96:GLU:O	6:F1:99:ARG:N	2.44	0.50
7:G1:80:ASP:O	7:G1:81:ARG:HB2	2.10	0.50
1:M1:392:LEU:O	1:M1:392:LEU:HG	2.09	0.50
2:N1:47:ILE:CG2	2:N1:48:GLY:N	2.72	0.50
3:O1:130:GLY:O	69:O1:401:HEM:HAA1	2.11	0.50
3:O1:147:THR:HG21	3:O1:165:TRP:CD1	2.46	0.50
4:P1:14:HIS:HA	4:P1:19:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:24:THR:O	4:P1:25:SER:C	2.54	0.50
5:Q1:45:VAL:HG22	10:V1:28:ALA:N	2.26	0.50
5:Q1:51:ALA:O	5:Q1:55:VAL:HG23	2.11	0.50
9:U1:58:GLN:O	9:U1:59:ALA:HB2	2.11	0.50
9:U1:78:TYR:OXT	9:U1:78:TYR:CD1	2.64	0.50
18:92:54:ASP:OD1	18:92:60:TYR:OH	2.29	0.50
19:A2:126:LEU:HD11	20:B2:373:THR:O	2.11	0.50
31:N2:62:GLU:OE2	31:N2:71:ARG:NH1	2.37	0.50
34:Q2:111:VAL:HG12	34:Q2:117:TRP:HB2	1.93	0.50
47:d2:18:ASP:O	47:d2:20:LEU:N	2.43	0.50
56:A3:75:ILE:O	56:A3:79:GLY:HA3	2.11	0.50
56:A3:377:PHE:HA	56:A3:380:VAL:HG22	1.93	0.50
1:A1:26:ALA:O	1:A1:27:SER:HB3	2.10	0.50
1:A1:236:PHE:HB2	5:E1:25:SER:HB2	1.93	0.50
1:A1:291:SER:HB3	2:B1:87:ARG:HD3	1.93	0.50
2:B1:166:ALA:HB2	2:B1:244:ILE:CD1	2.41	0.50
6:F1:23:ALA:O	6:F1:24:ALA:C	2.52	0.50
1:M1:143:THR:HG21	9:U1:48:SER:N	2.08	0.50
1:M1:256:ALA:CA	1:M1:320:LEU:O	2.59	0.50
3:O1:152:ALA:N	3:O1:287:LYS:NZ	2.59	0.50
5:Q1:51:ALA:O	5:Q1:52:LYS:C	2.54	0.50
11:W1:18:VAL:CB	11:W1:19:PRO:HD3	2.41	0.50
20:B2:203:MET:HE1	20:B2:254:ARG:HB3	1.93	0.50
23:E2:189:LYS:HB2	38:U2:124:TYR:CZ	2.47	0.50
53:62:172:ILE:HA	53:62:175:ASN:HD22	1.76	0.50
1:A1:279:HIS:ND1	1:A1:284:TYR:OH	2.42	0.50
1:A1:331:ILE:CD1	1:A1:427:PRO:O	2.58	0.50
2:B1:352:LEU:HD23	2:B1:411:ILE:HD11	1.92	0.50
4:D1:230:LEU:O	4:D1:233:ARG:HB2	2.12	0.50
7:G1:52:PHE:O	7:G1:53:VAL:C	2.54	0.50
1:M1:294:LEU:CD2	1:M1:337:VAL:HG12	2.41	0.50
1:M1:426:GLY:HA2	1:M1:427:PRO:C	2.36	0.50
2:N1:304:HIS:CD2	2:N1:305:GLN:H	2.30	0.50
3:O1:152:ALA:HB2	3:O1:287:LYS:NZ	2.26	0.50
3:O1:160:LEU:O	3:O1:164:ILE:HD12	2.11	0.50
5:Q1:114:VAL:CG1	5:Q1:115:SER:N	2.73	0.50
10:V1:52:TRP:O	10:V1:53:LYS:C	2.53	0.50
12:22:300:THR:HG23	12:22:301:THR:HG23	1.93	0.50
19:A2:129:PRO:CB	27:I2:114:TYR:HE1	2.24	0.50
52:12:131:GLY:HA2	52:12:134:ARG:HE	1.76	0.50
56:A3:40:GLU:HG2	56:A3:54:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C3:119:THR:O	62:G3:52:HIS:CE1	2.63	0.50
1:A1:64:PHE:HE2	1:A1:88:ALA:HB2	1.75	0.50
1:A1:106:LEU:HD22	1:A1:203:LEU:HD13	1.93	0.50
1:A1:296:SER:O	1:A1:297:ILE:C	2.55	0.50
2:B1:38:LEU:O	2:B1:40:ASN:N	2.45	0.50
3:C1:46:LEU:O	3:C1:50:PHE:HD1	1.94	0.50
3:C1:132:VAL:HA	3:C1:139:SER:CB	2.42	0.50
3:C1:164:ILE:O	3:C1:177:ARG:NH1	2.42	0.50
3:C1:276:PHE:HE2	3:C1:297:SER:OG	1.95	0.50
4:D1:46:VAL:HG12	4:D1:47:ALA:O	2.10	0.50
4:D1:138:PRO:CB	8:H1:55:THR:CA	2.90	0.50
4:D1:161:ALA:O	4:D1:163:PRO:N	2.45	0.50
7:G1:54:ALA:O	7:G1:58:VAL:HG23	2.12	0.50
3:O1:191:ALA:O	3:O1:195:VAL:HG23	2.12	0.50
4:P1:69:GLU:HA	4:P1:73:GLY:HA2	1.93	0.50
4:P1:72:ASP:OD1	4:P1:76:GLU:OE1	2.29	0.50
5:Q1:18:VAL:HG11	5:Q1:32:ARG:NH1	2.27	0.50
10:V1:21:ALA:O	10:V1:22:LEU:C	2.53	0.50
48:f2:70:GLU:H	48:f2:73:HIS:HB3	1.75	0.50
1:A1:64:PHE:HA	1:A1:75:LEU:CD2	2.42	0.50
1:A1:142:ASP:OD2	5:E1:1:SER:HB3	2.11	0.50
3:C1:246:ALA:HB1	3:C1:249:LEU:HB2	1.94	0.50
3:C1:280:ILE:HD13	3:C1:280:ILE:N	2.27	0.50
2:N1:47:ILE:HG22	2:N1:48:GLY:H	1.76	0.50
2:N1:76:THR:HG21	2:N1:133:ARG:CZ	2.42	0.50
2:N1:97:SER:HA	9:U1:70:LEU:HB2	1.94	0.50
3:O1:10:LEU:HD12	3:O1:13:ILE:HD11	1.92	0.50
3:O1:115:ILE:HD13	3:O1:115:ILE:N	2.26	0.50
3:O1:242:LEU:HD21	3:O1:250:LEU:CD2	2.41	0.50
4:P1:10:TYR:HD1	8:T1:74:PHE:CE1	2.29	0.50
4:P1:23:HIS:CD2	10:V1:50:LYS:O	2.65	0.50
10:V1:32:GLU:CG	10:V1:33:ARG:N	2.74	0.50
19:A2:423:LEU:CD1	25:G2:169:ARG:O	2.60	0.50
19:A2:613:PRO:CB	38:U2:134:ILE:HD13	2.38	0.50
21:C2:167:TRP:CD1	21:C2:170:ARG:HH12	2.30	0.50
33:P2:41:LEU:HD12	33:P2:42:PRO:HD2	1.94	0.50
58:C3:18:LEU:HD22	58:C3:22:LEU:HD22	1.92	0.50
2:B1:197:ASN:HB2	2:B1:198:HIS:CD2	2.46	0.50
3:C1:147:THR:O	3:C1:150:LEU:HB2	2.11	0.50
3:C1:163:TRP:CE2	5:Q1:62:MET:HE2	2.46	0.50
4:D1:30:PHE:CE1	4:D1:50:HIS:CE1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:138:PRO:HB3	8:H1:55:THR:HA	1.94	0.50
5:E1:71:MET:O	5:E1:72:SER:C	2.54	0.50
1:M1:53:ASN:CG	1:M1:165:GLN:HB2	2.35	0.50
2:N1:109:VAL:HG22	2:N1:119:LEU:CD2	2.41	0.50
2:N1:198:HIS:HE1	2:N1:233:SER:CB	2.23	0.50
2:N1:340:ALA:O	2:N1:344:VAL:HG23	2.12	0.50
2:N1:350:GLY:HA2	2:N1:411:ILE:HG21	1.93	0.50
4:P1:146:GLY:O	4:P1:148:TYR:CD1	2.65	0.50
6:R1:58:ARG:HG2	6:R1:58:ARG:NH1	2.25	0.50
18:92:111:ARG:HH12	19:A2:193:ASP:HA	1.77	0.50
20:B2:272:THR:HA	20:B2:275:ILE:HD12	1.93	0.50
42:Y2:46:ARG:HA	42:Y2:49:GLN:HE22	1.76	0.50
54:g2:141:ASP:OD1	54:g2:141:ASP:N	2.44	0.50
55:e2:70:THR:C	55:e2:72:TYR:N	2.61	0.50
56:A3:168:ILE:HG21	56:A3:189:MET:HG3	1.94	0.50
56:A3:232:GLN:HB2	56:A3:292:MET:HE3	1.93	0.50
61:F3:37:LYS:HD3	61:F3:37:LYS:N	2.27	0.50
63:H3:60:TYR:C	63:H3:60:TYR:CD1	2.88	0.50
1:A1:48:GLU:HB3	1:A1:52:ASN:O	2.10	0.50
2:B1:429:ASN:ND2	2:N1:60:SER:OG	2.45	0.50
4:D1:72:ASP:OD1	4:D1:76:GLU:OE1	2.30	0.50
9:I1:62:ARG:H	9:I1:63:PRO:HD2	1.76	0.50
10:J1:49:GLY:HA2	10:J1:54:HIS:HB2	1.91	0.50
1:M1:30:SER:N	1:M1:201:GLY:O	2.44	0.50
4:P1:7:PRO:HB2	4:P1:125:ASP:HB3	1.93	0.50
14:42:214:LEU:HD11	53:62:558:LEU:HB3	1.92	0.50
19:A2:238:PHE:CB	23:E2:140:ARG:HB3	2.40	0.50
35:R2:281:PHE:HD1	35:R2:286:ARG:HA	1.75	0.50
53:62:103:PHE:O	53:62:107:TYR:N	2.40	0.50
57:B3:139:ASP:OD1	57:B3:140:ASN:N	2.44	0.50
1:A1:124:ASP:O	1:A1:128:GLU:HG2	2.11	0.50
1:A1:252:HIS:CD2	1:A1:325:VAL:HG22	2.47	0.50
1:A1:272:VAL:O	1:A1:275:ALA:HB3	2.12	0.50
2:B1:170:ASN:CG	2:B1:171:ALA:N	2.70	0.50
2:B1:275:LEU:HD12	2:B1:275:LEU:O	2.12	0.50
3:C1:4:ILE:O	3:C1:5:ARG:C	2.53	0.50
6:F1:51:PRO:CD	2:N1:134:ARG:HH12	2.24	0.50
1:M1:120:CYS:O	1:M1:122:LEU:HG	2.12	0.50
2:N1:130:PRO:HB2	2:N1:132:PHE:CE1	2.46	0.50
2:N1:196:GLN:HG2	2:N1:197:ASN:OD1	2.12	0.50
2:N1:257:LEU:CD1	2:N1:424:MET:HB2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N1:279:LEU:CD2	2:N1:344:VAL:HG22	2.40	0.50
4:P1:30:PHE:HD1	4:P1:189:PHE:CE1	2.29	0.50
4:P1:138:PRO:CB	8:T1:55:THR:CA	2.90	0.50
5:Q1:152:ASP:N	5:Q1:164:HIS:ND1	2.59	0.50
7:S1:64:GLN:O	7:S1:65:GLU:C	2.55	0.50
20:B2:144:MET:HE3	20:B2:222:MET:HB3	1.93	0.50
39:V2:55:ARG:NH2	52:12:312:SER:OG	2.32	0.50
1:A1:113:LEU:HA	1:A1:116:ILE:HD12	1.92	0.50
2:B1:45:SER:HB2	2:B1:210:GLY:HA3	1.93	0.50
2:B1:372:VAL:O	2:B1:372:VAL:HG12	2.11	0.50
3:C1:26:ASN:ND2	3:C1:208:PRO:HD2	2.27	0.50
3:C1:106:SER:CB	69:C1:402:HEM:HBD2	2.41	0.50
4:D1:33:TYR:O	4:D1:37:CYS:HB2	2.12	0.50
4:D1:82:MET:SD	4:D1:86:LYS:NZ	2.82	0.50
9:I1:62:ARG:N	9:I1:63:PRO:CD	2.75	0.50
2:N1:237:ALA:HB2	2:N1:318:ASP:CG	2.37	0.50
3:O1:378:LYS:O	3:O1:378:LYS:HD3	2.11	0.50
4:P1:117:VAL:CG1	4:P1:191:ARG:HH11	2.25	0.50
4:P1:134:TYR:HE2	4:P1:163:PRO:CG	2.25	0.50
4:P1:165:TYR:H	4:P1:168:VAL:CG2	2.24	0.50
5:Q1:34:GLY:CA	10:V1:10:TYR:HD1	2.22	0.50
12:22:245:LEU:HD22	12:22:301:THR:HG21	1.94	0.50
17:82:321:GLY:N	17:82:351:THR:OG1	2.43	0.50
20:B2:326:CYS:HA	20:B2:329:ARG:HG2	1.94	0.50
35:R2:84:HIS:CD2	35:R2:87:GLU:H	2.30	0.50
1:A1:22:GLY:O	1:A1:24:ARG:HG2	2.12	0.49
1:A1:63:ALA:HB2	1:A1:97:TYR:HE2	1.76	0.49
1:A1:335:MET:CE	1:A1:339:GLN:HG3	2.42	0.49
1:A1:395:TRP:O	1:A1:398:ARG:N	2.45	0.49
7:G1:40:ARG:O	7:G1:41:THR:C	2.55	0.49
1:M1:40:TRP:HZ2	1:M1:377:GLU:HB2	1.75	0.49
1:M1:92:ARG:HD2	1:M1:163:LEU:CD1	2.37	0.49
2:N1:185:LYS:HG3	2:N1:185:LYS:O	2.11	0.49
2:N1:206:LEU:CD1	2:N1:224:LEU:HD11	2.41	0.49
3:O1:164:ILE:O	3:O1:177:ARG:NH1	2.44	0.49
3:O1:317:PHE:CD1	6:R1:26:PHE:HB3	2.47	0.49
4:P1:35:GLN:HB2	4:P1:169:LEU:CD1	2.42	0.49
4:P1:138:PRO:HB3	8:T1:54:CYS:C	2.38	0.49
4:P1:232:SER:CB	7:S1:23:GLN:OE1	2.59	0.49
5:Q1:9:ASP:OD1	5:Q1:11:SER:OG	2.30	0.49
5:Q1:119:ASP:HB3	5:Q1:179:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U1:62:ARG:N	9:U1:63:PRO:CD	2.75	0.49
17:82:119:GLU:O	17:82:159:ARG:NH2	2.45	0.49
18:92:227:PRO:HD2	18:92:231:LEU:HA	1.93	0.49
21:C2:188:ARG:NH1	21:C2:193:TYR:O	2.45	0.49
23:E2:188:GLU:OE1	38:U2:127:TYR:OH	2.30	0.49
59:D3:64:PHE:CE1	60:E3:66:ARG:HD2	2.47	0.49
1:A1:158:PHE:O	1:A1:164:ALA:HB2	2.12	0.49
1:A1:408:ARG:HH12	11:K1:15:ARG:CD	2.25	0.49
2:B1:381:GLU:O	2:B1:384:SER:OG	2.24	0.49
3:C1:37:LEU:HD21	3:C1:94:LEU:HD13	1.93	0.49
3:C1:43:LEU:O	3:C1:44:GLN:C	2.51	0.49
3:C1:278:TYR:O	3:C1:279:ALA:C	2.55	0.49
4:D1:138:PRO:O	4:D1:141:VAL:HB	2.12	0.49
1:M1:3:THR:O	1:M1:4:TYR:C	2.54	0.49
3:O1:122:THR:HB	3:O1:189:ILE:HD13	1.95	0.49
10:V1:60:GLU:O	10:V1:60:GLU:HG3	2.11	0.49
49:h2:120:ARG:HH22	54:g2:65:HIS:HA	1.77	0.49
57:B3:186:SER:HB3	57:B3:213:LEU:CD2	2.42	0.49
1:A1:171:SER:O	1:A1:174:VAL:HB	2.13	0.49
1:A1:349:ALA:HB3	1:A1:408:ARG:HG2	1.95	0.49
2:B1:255:ALA:HA	2:B1:425:ALA:O	2.12	0.49
3:C1:338:ILE:HA	3:C1:341:GLN:CG	2.43	0.49
1:M1:307:PHE:HA	1:M1:323:HIS:O	2.12	0.49
3:O1:344:GLU:O	3:O1:348:ILE:HG13	2.11	0.49
4:P1:100:ALA:O	4:P1:103:ALA:N	2.45	0.49
17:82:95:THR:HA	17:82:98:LYS:HG2	1.95	0.49
19:A2:352:ILE:HD11	19:A2:528:LEU:HD22	1.94	0.49
36:S2:189:PRO:HB2	36:S2:192:VAL:HG22	1.94	0.49
56:A3:184:PHE:H	56:A3:256:HIS:CE1	2.29	0.49
1:A1:15:GLN:O	1:A1:205:HIS:CE1	2.66	0.49
1:A1:43:ALA:HB2	1:A1:189:HIS:HB3	1.94	0.49
1:A1:385:THR:HB	1:A1:386:TYR:CD1	2.48	0.49
2:B1:185:LYS:O	2:B1:185:LYS:CG	2.54	0.49
2:B1:352:LEU:HD23	2:B1:411:ILE:CD1	2.43	0.49
3:C1:74:ASN:O	5:E1:61:SER:HA	2.12	0.49
4:D1:237:TYR:HB2	6:F1:60:PHE:CE1	2.47	0.49
9:I1:70:LEU:HG	9:I1:72:VAL:H	1.78	0.49
2:N1:112:LEU:O	2:N1:113:ARG:C	2.54	0.49
3:O1:21:LEU:HD12	3:O1:22:PRO:HD2	1.94	0.49
69:O1:401:HEM:HBC2	69:O1:401:HEM:CMC	2.35	0.49
4:P1:2:ASP:HB3	4:P1:156:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S1:34:ILE:CB	7:S1:35:PRO:HD3	2.32	0.49
7:S1:48:VAL:O	7:S1:51:PRO:HD2	2.12	0.49
7:S1:80:ASP:O	7:S1:81:ARG:HB2	2.11	0.49
19:A2:371:VAL:HB	19:A2:482:GLN:HG3	1.94	0.49
20:B2:97:LEU:CD1	20:B2:97:LEU:C	2.86	0.49
20:B2:143:SER:OG	20:B2:147:ASN:OD1	2.30	0.49
20:B2:266:ARG:HH22	23:E2:60:THR:HA	1.76	0.49
28:J2:26:ILE:O	28:J2:30:SER:N	2.42	0.49
62:G3:42:ARG:NH1	62:G3:74:ARG:HH21	2.10	0.49
1:A1:146:ARG:NH2	1:A1:308:GLN:NE2	2.58	0.49
2:B1:258:VAL:CG1	2:B1:321:LEU:HD22	2.42	0.49
3:C1:269:LYS:CD	3:C1:340:GLY:HA2	2.43	0.49
4:D1:153:PHE:O	4:D1:154:PRO:C	2.54	0.49
5:E1:65:SER:O	5:E1:66:ALA:C	2.55	0.49
8:H1:40:CYS:O	8:H1:44:VAL:HG23	2.12	0.49
1:M1:349:ALA:O	1:M1:408:ARG:NH2	2.45	0.49
2:N1:92:VAL:O	2:N1:92:VAL:CG1	2.60	0.49
2:N1:170:ASN:CG	2:N1:171:ALA:N	2.70	0.49
3:O1:25:SER:HB3	6:R1:70:MET:HE2	1.94	0.49
3:O1:26:ASN:HA	6:R1:70:MET:HA	1.94	0.49
6:R1:10:SER:HA	6:R1:13:LEU:CD1	2.42	0.49
6:R1:40:ASN:CG	6:R1:41:ASP:H	2.20	0.49
14:42:134:THR:O	14:42:142:ARG:NH1	2.44	0.49
18:92:42:ARG:HH22	19:A2:199:GLY:HA3	1.76	0.49
20:B2:86:PRO:HD3	20:B2:96:ARG:HA	1.94	0.49
32:O2:50:PHE:HE1	32:O2:96:VAL:HG12	1.77	0.49
51:j2:26:LEU:HA	51:j2:31:LEU:HD22	1.94	0.49
63:H3:24:ASN:ND2	63:H3:26:THR:H	2.11	0.49
1:A1:43:ALA:HB1	1:A1:189:HIS:HB3	1.94	0.49
3:C1:200:LEU:HD13	69:C1:402:HEM:HAD2	1.93	0.49
4:D1:24:THR:O	4:D1:25:SER:C	2.53	0.49
4:D1:160:MET:HE2	4:D1:163:PRO:HG3	1.95	0.49
1:M1:379:ILE:O	1:M1:383:LEU:HG	2.13	0.49
1:M1:431:LEU:HD12	1:M1:432:PRO:HD2	1.95	0.49
2:N1:255:ALA:CB	2:N1:426:ALA:HB2	2.42	0.49
3:O1:4:ILE:O	3:O1:5:ARG:C	2.55	0.49
3:O1:372:ILE:O	3:O1:375:LYS:N	2.45	0.49
4:P1:168:VAL:HG12	4:P1:169:LEU:CD2	2.42	0.49
4:P1:168:VAL:HG12	4:P1:169:LEU:HD23	1.93	0.49
7:S1:71:ARG:O	7:S1:73:ASN:N	2.46	0.49
19:A2:301:ARG:C	38:U2:137:TRP:HB2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B2:241:MET:HG3	39:V2:10:MET:HB3	1.95	0.49
22:D2:155:SER:OG	23:E2:150:THR:O	2.30	0.49
56:A3:145:LEU:HD21	58:C3:32:THR:HG21	1.93	0.49
1:A1:53:ASN:C	1:A1:53:ASN:ND2	2.69	0.49
2:B1:126:VAL:O	2:B1:126:VAL:HG12	2.11	0.49
2:B1:207:ILE:HG22	2:B1:379:LEU:HD12	1.95	0.49
2:B1:299:VAL:HG13	2:B1:303:VAL:HG21	1.94	0.49
3:C1:103:TYR:OH	3:C1:322:GLN:HG3	2.12	0.49
3:C1:119:LEU:HG	69:C1:402:HEM:HBB2	1.90	0.49
3:C1:122:THR:HG21	3:C1:189:ILE:CG1	2.42	0.49
4:D1:69:GLU:HG3	4:D1:84:PRO:HA	1.94	0.49
4:D1:229:VAL:HG12	4:D1:233:ARG:NE	2.22	0.49
2:N1:24:LEU:HD13	2:N1:392:TYR:CD2	2.48	0.49
2:N1:68:LEU:CD1	2:N1:140:LEU:HD23	2.39	0.49
5:Q1:38:LEU:O	5:Q1:42:THR:OG1	2.30	0.49
5:Q1:42:THR:O	5:Q1:45:VAL:N	2.45	0.49
5:Q1:89:PHE:O	5:Q1:96:LEU:N	2.23	0.49
12:22:78:LEU:HD11	15:52:48:ILE:HD11	1.93	0.49
13:32:93:PHE:HA	13:32:96:ILE:HD12	1.95	0.49
35:R2:178:SER:H	35:R2:181:LEU:HB3	1.78	0.49
56:A3:508:PRO:HG3	58:C3:6:HIS:HB3	1.94	0.49
1:A1:37:VAL:HG13	1:A1:199:ALA:HB2	1.93	0.49
1:A1:37:VAL:CG1	1:A1:199:ALA:HB2	2.43	0.49
1:A1:315:ALA:HB3	1:A1:316:ASP:OD1	2.13	0.49
2:B1:79:GLY:CA	2:B1:125:ASN:HD21	2.26	0.49
2:B1:166:ALA:HB2	2:B1:244:ILE:CG1	2.39	0.49
2:B1:183:ILE:HG22	2:B1:184:GLY:N	2.28	0.49
2:B1:348:ALA:HB3	2:B1:418:VAL:HG21	1.94	0.49
2:B1:381:GLU:OE1	2:B1:381:GLU:HA	2.13	0.49
4:D1:13:SER:O	4:D1:19:SER:HB3	2.11	0.49
4:D1:161:ALA:HB1	4:D1:162:PRO:HD2	1.93	0.49
1:M1:327:ASP:OD1	1:M1:328:HIS:N	2.44	0.49
1:M1:386:TYR:N	1:M1:386:TYR:CD1	2.74	0.49
5:Q1:142:LEU:HD12	5:Q1:161:HIS:CE1	2.46	0.49
8:T1:73:LEU:HD23	8:T1:73:LEU:C	2.37	0.49
14:42:66:LEU:O	14:42:69:THR:OG1	2.28	0.49
15:52:36:MET:O	15:52:39:SER:OG	2.31	0.49
18:92:137:THR:O	18:92:141:MET:N	2.43	0.49
19:A2:312:GLY:N	38:U2:144:TYR:N	2.61	0.49
19:A2:355:LYS:HD2	19:A2:530:TYR:HE1	1.77	0.49
19:A2:674:LEU:CD1	29:K2:46:LYS:HE2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B2:85:GLY:C	20:B2:87:GLN:N	2.70	0.49
39:V2:134:LEU:HG	39:V2:138:TYR:HD2	1.78	0.49
56:A3:87:ILE:O	56:A3:173:PRO:HD3	2.13	0.49
62:G3:44:ARG:HD2	62:G3:74:ARG:O	2.12	0.49
1:A1:286:GLY:O	1:A1:287:GLY:O	2.30	0.49
1:A1:417:ASP:CG	10:J1:10:TYR:OH	2.55	0.49
2:B1:207:ILE:CG2	2:B1:379:LEU:HD12	2.43	0.49
2:B1:429:ASN:ND2	2:N1:60:SER:CB	2.59	0.49
3:C1:88:SER:HB3	3:C1:250:LEU:HD21	1.95	0.49
3:C1:210:GLY:HA3	3:C1:314:SER:CB	2.40	0.49
4:D1:116:ILE:HD11	4:D1:120:ARG:HH11	1.78	0.49
4:D1:139:THR:CG2	8:H1:44:VAL:HB	2.43	0.49
4:D1:237:TYR:CD2	4:D1:239:PRO:HD3	2.48	0.49
6:F1:73:GLN:HG2	7:G1:36:ASN:HD21	1.77	0.49
1:M1:89:TYR:CD1	1:M1:89:TYR:C	2.91	0.49
1:M1:262:TRP:CE3	1:M1:385:THR:HG21	2.48	0.49
1:M1:286:GLY:O	1:M1:287:GLY:C	2.56	0.49
2:N1:254:HIS:O	2:N1:426:ALA:HA	2.13	0.49
3:O1:142:GLY:O	3:O1:146:ILE:HG12	2.12	0.49
3:O1:150:LEU:O	3:O1:153:ILE:HD13	2.13	0.49
3:O1:192:ILE:N	3:O1:192:ILE:HD13	2.28	0.49
3:O1:329:VAL:HA	3:O1:332:LEU:HD12	1.94	0.49
5:Q1:107:ASP:O	5:Q1:108:GLN:C	2.55	0.49
5:Q1:188:THR:HG21	5:Q1:194:ILE:CD1	2.42	0.49
19:A2:246:ARG:HH22	21:C2:234:LYS:H	1.60	0.49
35:R2:329:LEU:HD11	35:R2:331:HIS:HD2	1.77	0.49
39:V2:95:ALA:HB2	39:V2:106:VAL:HG11	1.95	0.49
57:B3:13:THR:HG22	57:B3:13:THR:O	2.11	0.49
1:A1:415:PHE:O	1:A1:441:MET:HE2	2.13	0.49
2:B1:213:HIS:O	2:B1:213:HIS:HD2	1.96	0.49
4:D1:138:PRO:HB3	8:H1:55:THR:CA	2.43	0.49
4:D1:158:ILE:HG13	70:D1:301:HEC:HBD2	1.95	0.49
4:D1:217:PRO:HG2	4:D1:218:LEU:H	1.78	0.49
6:F1:45:GLU:O	6:F1:46:ALA:O	2.31	0.49
1:M1:307:PHE:C	1:M1:307:PHE:CD1	2.91	0.49
1:M1:370:ASP:OD1	2:N1:375:SER:HB3	2.12	0.49
2:N1:227:ARG:HD2	2:N1:227:ARG:N	2.27	0.49
2:N1:267:ALA:O	2:N1:268:GLU:C	2.56	0.49
3:O1:221:HIS:N	3:O1:222:PRO:HD2	2.28	0.49
3:O1:341:GLN:O	3:O1:342:PRO:C	2.55	0.49
4:P1:49:ARG:HG3	4:P1:49:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T1:15:ASP:CB	8:T1:16:PRO:CD	2.91	0.49
18:92:163:THR:HA	18:92:170:THR:HA	1.94	0.49
52:12:73:LEU:HA	52:12:76:ILE:HD12	1.95	0.49
53:62:246:LEU:O	53:62:251:THR:OG1	2.31	0.49
53:62:457:LEU:O	53:62:461:SER:N	2.46	0.49
1:A1:260:PRO:HG3	1:A1:414:TYR:CZ	2.49	0.48
1:A1:347:THR:O	11:K1:16:ASN:ND2	2.43	0.48
1:A1:433:ASP:CG	3:C1:223:TYR:HH	2.14	0.48
2:B1:294:SER:O	2:B1:295:LEU:C	2.55	0.48
2:B1:322:PHE:CD1	2:B1:322:PHE:C	2.90	0.48
3:C1:213:SER:O	3:C1:214:ASP:C	2.56	0.48
4:D1:10:TYR:CZ	4:D1:128:PHE:CE2	2.92	0.48
4:D1:30:PHE:O	4:D1:31:GLN:C	2.53	0.48
4:D1:32:VAL:CB	4:D1:186:VAL:HG22	2.43	0.48
4:D1:134:TYR:HE2	4:D1:163:PRO:CG	2.24	0.48
4:D1:138:PRO:HB3	8:H1:54:CYS:C	2.37	0.48
7:G1:56:TYR:O	7:G1:57:LEU:C	2.56	0.48
7:G1:80:ASP:CG	8:H1:47:ARG:HH22	2.21	0.48
1:M1:243:HIS:CD2	1:M1:425:PHE:CE1	3.01	0.48
1:M1:291:SER:HB3	2:N1:87:ARG:HD3	1.94	0.48
1:M1:436:ARG:HE	3:O1:222:PRO:CD	2.26	0.48
2:N1:72:ALA:HB2	2:N1:140:LEU:CD2	2.43	0.48
2:N1:283:PRO:HG3	9:U1:55:LEU:HB3	1.95	0.48
2:N1:312:PHE:HD1	9:U1:58:GLN:O	1.96	0.48
3:O1:284:ILE:CG2	3:O1:285:PRO:HD2	2.43	0.48
10:V1:61:ASN:O	10:V1:62:LYS:HB2	2.13	0.48
12:22:149:ILE:HD12	12:22:154:ILE:HG21	1.95	0.48
18:92:228:ALA:HA	18:92:231:LEU:HD23	1.94	0.48
19:A2:381:LEU:HB2	29:K2:55:ILE:CD1	2.42	0.48
19:A2:443:ASP:OD1	19:A2:443:ASP:N	2.45	0.48
22:D2:151:VAL:HG22	22:D2:181:ILE:HB	1.95	0.48
27:I2:106:GLU:HB3	27:I2:108:LYS:HZ1	1.78	0.48
37:T2:21:LYS:HG2	37:T2:75:CYS:HB3	1.94	0.48
53:62:381:THR:HA	53:62:420:ALA:HA	1.95	0.48
57:B3:90:ILE:HD12	57:B3:90:ILE:H	1.77	0.48
2:B1:128:THR:C	2:B1:130:PRO:HD2	2.39	0.48
2:B1:141:GLN:OE1	2:B1:141:GLN:HA	2.13	0.48
4:D1:224:ARG:HH21	7:G1:27:PRO:HD2	1.78	0.48
5:E1:32:ARG:HH12	7:G1:22:GLU:CD	2.21	0.48
6:F1:51:PRO:HG3	2:N1:134:ARG:HH12	1.78	0.48
7:G1:34:ILE:O	7:G1:38:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J1:4:THR:HG22	10:J1:6:THR:H	1.77	0.48
1:M1:4:TYR:CE1	2:N1:43:PRO:HB3	2.48	0.48
4:P1:66:GLU:O	4:P1:69:GLU:HG2	2.13	0.48
9:U1:51:CYS:SG	9:U1:53:GLU:HB3	2.52	0.48
19:A2:59:GLN:HB3	21:C2:241:TRP:CZ3	2.49	0.48
19:A2:160:VAL:C	27:I2:102:ASN:HD22	2.19	0.48
31:N2:6:LYS:HE2	31:N2:16:VAL:HG11	1.95	0.48
35:R2:178:SER:H	35:R2:182:ARG:H	1.61	0.48
35:R2:238:GLN:HE22	35:R2:271:TYR:HA	1.77	0.48
35:R2:328:ILE:CG2	35:R2:329:LEU:N	2.49	0.48
56:A3:397:PHE:HB3	56:A3:398:PRO:HD3	1.95	0.48
58:C3:42:LEU:HD13	65:J3:45:TYR:HD2	1.77	0.48
2:B1:198:HIS:HE1	2:B1:233:SER:CB	2.19	0.48
3:C1:357:LEU:O	3:C1:361:LEU:HG	2.13	0.48
4:D1:20:SER:OG	4:D1:21:LEU:N	2.46	0.48
4:D1:102:ARG:HE	4:D1:109:LEU:HB2	1.78	0.48
1:M1:161:THR:HB	1:M1:162:PRO:CD	2.41	0.48
1:M1:349:ALA:HB3	1:M1:408:ARG:HE	1.78	0.48
2:N1:79:GLY:H	2:N1:125:ASN:ND2	2.12	0.48
2:N1:271:ALA:O	2:N1:272:PHE:C	2.57	0.48
3:O1:126:THR:HG21	69:O1:401:HEM:CAB	2.43	0.48
3:O1:218:ILE:HG23	3:O1:223:TYR:CE2	2.48	0.48
4:P1:74:PRO:O	4:P1:79:GLU:N	2.42	0.48
4:P1:178:THR:O	4:P1:179:MET:C	2.55	0.48
10:V1:38:GLY:O	10:V1:42:ILE:HG13	2.14	0.48
19:A2:337:ASP:O	19:A2:543:LYS:N	2.42	0.48
53:62:491:LEU:O	53:62:494:THR:OG1	2.26	0.48
1:A1:433:ASP:O	1:A1:434:TYR:C	2.56	0.48
2:B1:132:PHE:HB3	2:B1:137:VAL:CG2	2.42	0.48
2:B1:187:THR:HG23	2:B1:190:GLU:OE1	2.13	0.48
4:D1:26:ILE:HG22	4:D1:27:ARG:N	2.27	0.48
4:D1:131:LEU:HD22	4:D1:163:PRO:HB3	1.95	0.48
4:D1:165:TYR:H	4:D1:168:VAL:CG2	2.26	0.48
8:H1:62:LEU:O	8:H1:65:ARG:HG2	2.14	0.48
1:M1:62:LEU:HB3	1:M1:122:LEU:HD22	1.94	0.48
1:M1:80:GLU:O	1:M1:82:MET:N	2.46	0.48
1:M1:100:LYS:HD2	1:M1:373:THR:OG1	2.13	0.48
1:M1:280:TYR:O	1:M1:306:SER:HA	2.14	0.48
1:M1:329:MET:CA	1:M1:329:MET:HE3	2.44	0.48
1:M1:385:THR:CG2	1:M1:386:TYR:CD1	2.96	0.48
2:N1:381:GLU:OE1	2:N1:381:GLU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:233:LEU:CD2	4:P1:219:VAL:HG21	2.44	0.48
12:22:122:ILE:HD13	12:22:128:LEU:HD11	1.95	0.48
17:82:381:GLN:O	19:A2:74:ASN:O	2.31	0.48
23:E2:61:LEU:HD23	39:V2:36:PHE:HE1	1.77	0.48
23:E2:80:GLU:O	33:P2:25:GLN:NE2	2.47	0.48
1:A1:239:SER:HB2	7:G1:18:LEU:HD23	1.95	0.48
3:C1:175:LEU:HG	3:C1:175:LEU:O	2.11	0.48
4:D1:3:LEU:HD21	7:G1:71:ARG:HA	1.95	0.48
4:D1:26:ILE:O	4:D1:27:ARG:C	2.56	0.48
4:D1:50:HIS:CE1	4:D1:91:PHE:HZ	2.31	0.48
1:M1:277:ILE:H	1:M1:277:ILE:HG12	1.42	0.48
1:M1:290:LEU:HD13	1:M1:295:ALA:HB1	1.95	0.48
5:Q1:33:LYS:HB2	10:V1:10:TYR:CE1	2.48	0.48
5:Q1:76:ILE:HG22	5:Q1:193:VAL:O	2.12	0.48
19:A2:313:LEU:N	38:U2:142:THR:C	2.70	0.48
23:E2:100:GLU:O	23:E2:170:GLY:N	2.46	0.48
49:h2:121:GLU:OE2	49:h2:124:ARG:NH2	2.46	0.48
64:I3:39:VAL:O	64:I3:42:LYS:HE2	2.14	0.48
65:J3:8:LYS:NZ	65:J3:8:LYS:HB3	2.29	0.48
1:A1:61:HIS:CE1	1:A1:134:ILE:HD11	2.49	0.48
2:B1:130:PRO:HB2	2:B1:132:PHE:CE1	2.48	0.48
2:B1:341:TYR:O	2:B1:342:ASN:C	2.57	0.48
3:C1:218:ILE:CG2	3:C1:223:TYR:CE2	2.97	0.48
4:D1:7:PRO:CB	4:D1:125:ASP:HB3	2.43	0.48
9:I1:60:ALA:HB3	9:I1:63:PRO:O	2.12	0.48
1:M1:329:MET:HA	1:M1:329:MET:HE3	1.95	0.48
1:M1:395:TRP:O	1:M1:396:GLU:C	2.57	0.48
3:O1:248:ASP:CG	4:P1:118:ARG:HH21	2.22	0.48
3:O1:252:ASP:CB	3:O1:253:PRO:HD3	2.34	0.48
4:P1:10:TYR:CE1	8:T1:73:LEU:HD22	2.47	0.48
13:32:19:ILE:HA	13:32:23:TRP:HB2	1.96	0.48
34:Q2:8:PRO:O	39:V2:88:ARG:NH2	2.46	0.48
34:Q2:38:LYS:HG3	34:Q2:39:PRO:HD3	1.95	0.48
1:A1:277:ILE:CG2	1:A1:294:LEU:HD12	2.44	0.48
2:B1:139:ALA:O	2:B1:142:PRO:HD2	2.14	0.48
3:C1:24:PRO:O	3:C1:224:TYR:OH	2.20	0.48
5:E1:72:SER:HB2	3:O1:168:PHE:CE2	2.48	0.48
6:F1:46:ALA:O	6:F1:47:ILE:C	2.56	0.48
7:G1:50:PRO:HB2	7:G1:51:PRO:CD	2.38	0.48
1:M1:33:PRO:O	1:M1:103:SER:HB3	2.14	0.48
1:M1:64:PHE:HA	1:M1:75:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:343:MET:HE1	1:M1:416:TYR:CE2	2.47	0.48
2:N1:128:THR:HG23	2:N1:226:ILE:HD11	1.96	0.48
2:N1:360:ALA:O	2:N1:363:LYS:N	2.46	0.48
5:Q1:96:LEU:CD2	5:Q1:195:VAL:HG21	2.27	0.48
19:A2:318:THR:HG22	19:A2:320:GLU:H	1.79	0.48
19:A2:542:PRO:HG2	19:A2:545:LEU:HD11	1.95	0.48
20:B2:131:GLN:HE21	23:E2:124:PRO:HA	1.77	0.48
22:D2:114:ARG:CG	22:D2:114:ARG:NH2	2.73	0.48
35:R2:147:LYS:O	35:R2:151:ALA:N	2.47	0.48
36:S2:61:LEU:HD22	36:S2:251:ALA:HB2	1.96	0.48
56:A3:11:ASN:ND2	56:A3:13:LYS:HB2	2.28	0.48
56:A3:266:GLU:HB2	56:A3:267:PRO:HD2	1.94	0.48
59:D3:68:PHE:HA	59:D3:71:MET:HG2	1.95	0.48
62:G3:42:ARG:HD2	62:G3:42:ARG:O	2.13	0.48
2:B1:76:THR:HG21	2:B1:133:ARG:NH2	2.29	0.48
2:B1:140:LEU:O	2:B1:142:PRO:N	2.47	0.48
3:C1:108:THR:O	3:C1:110:LEU:N	2.46	0.48
3:C1:297:SER:O	3:C1:300:ILE:CG2	2.62	0.48
3:C1:310:SER:HB3	3:C1:318:ARG:HH12	1.71	0.48
1:M1:406:VAL:O	1:M1:410:VAL:HG23	2.13	0.48
2:N1:132:PHE:CE2	2:N1:191:LEU:HD22	2.49	0.48
2:N1:362:ASN:O	2:N1:363:LYS:C	2.57	0.48
3:O1:51:LEU:HD21	3:O1:79:ILE:HG22	1.95	0.48
3:O1:300:ILE:HD13	3:O1:362:ILE:HG21	1.95	0.48
3:O1:361:LEU:HD23	3:O1:365:LEU:CD1	2.36	0.48
4:P1:137:PRO:HA	4:P1:138:PRO:HD3	1.58	0.48
4:P1:146:GLY:O	4:P1:148:TYR:HD1	1.97	0.48
5:Q1:105:GLU:O	5:Q1:108:GLN:HB3	2.14	0.48
10:V1:32:GLU:HG2	10:V1:33:ARG:N	2.29	0.48
17:82:257:ARG:HA	18:92:243:PHE:HB2	1.96	0.48
19:A2:373:PRO:HG3	19:A2:486:GLY:HA3	1.96	0.48
20:B2:97:LEU:N	20:B2:97:LEU:CD1	2.73	0.48
20:B2:236:LEU:HD11	20:B2:241:MET:HE2	1.96	0.48
21:C2:112:SER:HB2	21:C2:135:LEU:HB3	1.96	0.48
35:R2:170:LEU:HD12	35:R2:328:ILE:HD12	1.95	0.48
56:A3:507:GLU:O	56:A3:508:PRO:O	2.32	0.48
1:A1:39:VAL:HG12	1:A1:41:ILE:HD12	1.95	0.48
1:A1:39:VAL:HG23	1:A1:113:LEU:HD23	1.95	0.48
2:B1:47:ILE:CG2	2:B1:48:GLY:N	2.77	0.48
2:B1:235:ALA:O	2:B1:236:LYS:CB	2.61	0.48
3:C1:147:THR:HG21	3:C1:165:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:215:VAL:O	6:F1:63:LYS:CE	2.62	0.48
4:D1:224:ARG:NH2	7:G1:27:PRO:HD2	2.28	0.48
6:F1:73:GLN:HA	7:G1:39:ARG:NH2	2.28	0.48
1:M1:134:ILE:O	1:M1:137:GLU:N	2.47	0.48
1:M1:335:MET:HE3	1:M1:335:MET:O	2.14	0.48
4:P1:31:GLN:O	4:P1:32:VAL:C	2.56	0.48
4:P1:190:LEU:O	4:P1:191:ARG:C	2.55	0.48
5:Q1:102:THR:O	5:Q1:105:GLU:N	2.46	0.48
5:Q1:188:THR:HG21	5:Q1:194:ILE:HG13	1.96	0.48
17:82:383:THR:HG23	19:A2:74:ASN:O	2.14	0.48
19:A2:226:CYS:SG	75:A2:802:SF4:S1	3.11	0.48
29:K2:67:ALA:O	29:K2:75:LYS:N	2.45	0.48
40:W2:119:ILE:HD12	40:W2:130:ILE:HG21	1.95	0.48
56:A3:197:LEU:O	58:C3:92:LEU:HD22	2.13	0.48
57:B3:4:PRO:HB2	66:K3:43:SER:HA	1.96	0.48
1:A1:84:ALA:HB1	1:A1:100:LYS:O	2.14	0.48
1:A1:106:LEU:O	1:A1:107:PRO:C	2.56	0.48
2:B1:303:VAL:CG1	2:B1:304:HIS:H	2.26	0.48
3:C1:282:ARG:O	3:C1:283:SER:C	2.55	0.48
8:H1:68:CYS:O	8:H1:69:VAL:C	2.55	0.48
1:M1:236:PHE:CD2	1:M1:258:GLU:CG	2.95	0.48
2:N1:24:LEU:HD13	2:N1:392:TYR:HD2	1.78	0.48
2:N1:111:CYS:CB	2:N1:119:LEU:HD22	2.31	0.48
3:O1:47:THR:HG21	3:O1:83:HIS:CB	2.43	0.48
4:P1:153:PHE:O	4:P1:156:GLN:N	2.36	0.48
5:Q1:15:ARG:HH21	5:Q1:32:ARG:CB	2.27	0.48
5:Q1:29:SER:CA	5:Q1:32:ARG:HD3	2.44	0.48
5:Q1:49:TYR:O	5:Q1:50:ALA:C	2.56	0.48
5:Q1:87:MET:HG2	5:Q1:89:PHE:HE1	1.78	0.48
5:Q1:193:VAL:O	5:Q1:193:VAL:CG1	2.61	0.48
7:S1:39:ARG:HA	7:S1:42:ARG:HD2	1.96	0.48
19:A2:129:PRO:HB2	27:I2:114:TYR:CE1	2.48	0.48
56:A3:476:PHE:CD1	67:L3:15:VAL:HG21	2.48	0.48
58:C3:80:ARG:O	58:C3:84:ILE:HG12	2.14	0.48
4:D1:117:VAL:CG1	4:D1:191:ARG:HH11	2.27	0.47
4:D1:232:SER:CB	7:G1:23:GLN:OE1	2.62	0.47
70:D1:301:HEC:HBD1	70:D1:301:HEC:HHA	1.95	0.47
7:G1:67:GLU:O	7:G1:71:ARG:HB3	2.14	0.47
8:H1:15:ASP:HB2	8:H1:16:PRO:CD	2.44	0.47
1:M1:53:ASN:ND2	1:M1:165:GLN:HG3	2.29	0.47
2:N1:194:TYR:O	2:N1:195:VAL:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N1:250:ASP:OD1	2:N1:251:SER:N	2.47	0.47
2:N1:262:ALA:HB3	2:N1:269:ALA:CA	2.44	0.47
3:O1:315:MET:O	3:O1:318:ARG:N	2.40	0.47
5:Q1:127:VAL:CG1	5:Q1:133:VAL:HG23	2.44	0.47
6:R1:7:SER:O	6:R1:11:ARG:HD2	2.13	0.47
17:82:364:VAL:HG12	17:82:400:VAL:HG22	1.95	0.47
20:B2:207:ARG:HD3	22:D2:98:HIS:HE1	1.79	0.47
44:a2:79:ASN:ND2	55:e2:76:PRO:HG3	2.29	0.47
47:d2:25:PHE:HZ	47:d2:42:THR:C	2.21	0.47
48:f2:58:VAL:HG12	48:f2:62:GLN:HG2	1.95	0.47
52:12:169:GLN:HE21	52:12:174:LEU:HD13	1.79	0.47
54:g2:70:ARG:HH22	54:g2:94:ARG:HD2	1.79	0.47
40:M2:34:SER:HB3	40:M2:40:LEU:HD22	1.95	0.47
58:C3:173:PHE:C	58:C3:173:PHE:CD1	2.92	0.47
3:C1:77:TRP:CE3	3:C1:78:ILE:HG23	2.44	0.47
4:D1:36:VAL:HG23	4:D1:169:LEU:HD11	1.96	0.47
5:E1:40:THR:HG22	10:J1:20:PHE:HZ	1.79	0.47
1:M1:24:ARG:CG	1:M1:196:VAL:HG22	2.45	0.47
1:M1:62:LEU:O	1:M1:63:ALA:C	2.57	0.47
1:M1:392:LEU:HA	1:M1:395:TRP:HD1	1.72	0.47
2:N1:346:THR:HG23	2:N1:351:ASN:HB3	1.96	0.47
3:O1:227:LYS:HG2	4:P1:223:LYS:HZ3	1.79	0.47
5:Q1:18:VAL:HG21	7:S1:22:GLU:OE1	2.14	0.47
17:82:220:GLN:OE1	19:A2:197:THR:OG1	2.32	0.47
18:92:42:ARG:HH22	19:A2:199:GLY:CA	2.26	0.47
19:A2:238:PHE:HB3	23:E2:140:ARG:CB	2.42	0.47
19:A2:409:PHE:HD1	19:A2:694:PHE:HB2	1.79	0.47
19:A2:462:PHE:O	19:A2:464:GLN:N	2.39	0.47
34:Q2:5:VAL:N	39:V2:107:GLY:O	2.47	0.47
53:62:202:PHE:HZ	53:62:263:PHE:HA	1.78	0.47
53:62:362:LEU:HB3	53:62:431:LEU:HB3	1.96	0.47
56:A3:115:SER:O	56:A3:121:GLY:HA2	2.14	0.47
57:B3:16:ILE:HD12	57:B3:17:MET:H	1.78	0.47
58:C3:65:SER:HB3	58:C3:71:HIS:CE1	2.48	0.47
1:A1:85:HIS:CE1	2:B1:284:HIS:ND1	2.82	0.47
2:B1:207:ILE:CD1	2:B1:383:GLY:HA2	2.37	0.47
2:B1:242:GLY:H	2:B1:423:SER:HB3	1.80	0.47
3:C1:44:GLN:HE22	3:C1:86:GLY:HA3	1.78	0.47
4:D1:241:LYS:HE3	6:F1:53:ASN:HB3	1.96	0.47
10:J1:13:LEU:O	10:J1:19:THR:OG1	2.16	0.47
3:O1:153:ILE:CG2	3:O1:154:PRO:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:122:HIS:ND1	5:Q1:124:LEU:HB2	2.29	0.47
5:Q1:170:ARG:O	5:Q1:172:ARG:HG2	2.15	0.47
57:B3:22:HIS:CE1	64:I3:44:LYS:HD3	2.49	0.47
57:B3:59:GLN:O	57:B3:62:GLU:HB2	2.13	0.47
1:A1:70:ARG:HB3	1:A1:74:ALA:HB3	1.97	0.47
1:A1:261:GLY:HA2	1:A1:314:TYR:O	2.13	0.47
1:A1:289:HIS:O	1:A1:290:LEU:C	2.55	0.47
1:A1:365:LEU:HG	1:A1:365:LEU:O	2.15	0.47
2:B1:76:THR:HG21	2:B1:133:ARG:CZ	2.44	0.47
2:B1:218:GLN:O	2:B1:221:GLU:HB2	2.15	0.47
3:C1:26:ASN:N	6:F1:70:MET:HB2	2.28	0.47
3:C1:183:PHE:O	3:C1:183:PHE:HD1	1.94	0.47
4:D1:23:HIS:NE2	10:J1:51:LEU:HA	2.29	0.47
4:D1:137:PRO:HA	4:D1:138:PRO:HD3	1.44	0.47
2:N1:24:LEU:HD12	2:N1:24:LEU:N	2.21	0.47
2:N1:84:LYS:O	2:N1:85:ILE:C	2.56	0.47
2:N1:299:VAL:O	2:N1:303:VAL:HG23	2.14	0.47
2:N1:338:LYS:O	2:N1:339:ALA:C	2.58	0.47
3:O1:341:GLN:NE2	3:O1:341:GLN:HA	2.29	0.47
4:P1:131:LEU:HD22	4:P1:163:PRO:HB2	1.96	0.47
5:Q1:122:HIS:HB3	5:Q1:125:GLU:HG3	1.97	0.47
5:Q1:158:CYS:SG	5:Q1:160:CYS:HB2	2.54	0.47
7:S1:56:TYR:HD1	7:S1:57:LEU:HD23	1.78	0.47
10:V1:4:THR:HG22	10:V1:6:THR:H	1.80	0.47
10:V1:52:TRP:CE3	10:V1:52:TRP:N	2.82	0.47
19:A2:238:PHE:CG	23:E2:140:ARG:HB3	2.49	0.47
20:B2:86:PRO:HG3	20:B2:96:ARG:CB	2.44	0.47
34:Q2:110:CYS:O	34:Q2:114:LYS:N	2.42	0.47
44:a2:86:THR:HA	44:a2:89:LEU:HB2	1.96	0.47
52:12:233:MET:HA	52:12:236:ILE:HG22	1.97	0.47
40:M2:37:MET:H	40:M2:41:GLY:H	1.61	0.47
57:B3:83:ILE:O	57:B3:87:MET:HG3	2.14	0.47
1:A1:52:ASN:HB2	1:A1:55:ALA:HB2	1.97	0.47
2:B1:38:LEU:O	2:B1:39:GLU:C	2.56	0.47
3:C1:185:LEU:HB3	3:C1:186:PRO:CD	2.36	0.47
3:C1:284:ILE:CG2	3:C1:285:PRO:HD2	2.44	0.47
3:C1:345:HIS:CB	3:C1:346:PRO:CD	2.85	0.47
1:M1:255:ILE:O	1:M1:321:GLY:HA3	2.14	0.47
1:M1:361:LEU:HG	1:M1:399:ILE:HD11	1.97	0.47
3:O1:107:TYR:HE1	3:O1:305:PRO:HA	1.79	0.47
3:O1:269:LYS:CD	3:O1:340:GLY:HA2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:276:PHE:CG	3:O1:277:ALA:N	2.82	0.47
4:P1:64:LEU:O	4:P1:68:VAL:HG23	2.15	0.47
4:P1:183:ALA:HA	4:P1:186:VAL:HG23	1.97	0.47
5:Q1:118:ARG:HH12	5:Q1:173:LYS:N	2.11	0.47
5:Q1:141:HIS:HA	5:Q1:177:PRO:HD3	1.96	0.47
7:S1:80:ASP:CG	8:T1:47:ARG:HH22	2.21	0.47
23:E2:40:TYR:HB3	23:E2:43:LEU:HD13	1.95	0.47
34:Q2:118:VAL:HG13	34:Q2:120:PRO:HD3	1.96	0.47
35:R2:352:VAL:HG13	35:R2:353:LEU:HD12	1.96	0.47
57:B3:59:GLN:N	57:B3:62:GLU:HG3	2.24	0.47
1:A1:405:ARG:O	1:A1:409:GLU:HG3	2.15	0.47
2:B1:360:ALA:O	2:B1:363:LYS:HB2	2.14	0.47
3:C1:192:ILE:N	3:C1:192:ILE:CD1	2.77	0.47
3:C1:326:TRP:NE1	7:G1:48:VAL:HG22	2.29	0.47
3:C1:361:LEU:CD2	3:C1:365:LEU:HD12	2.42	0.47
4:D1:76:GLU:OE2	4:D1:93:LYS:O	2.33	0.47
7:G1:33:GLY:O	7:G1:34:ILE:C	2.56	0.47
7:G1:44:CYS:O	7:G1:45:ILE:C	2.57	0.47
7:G1:45:ILE:HD12	7:G1:45:ILE:HA	1.67	0.47
11:K1:18:VAL:HB	11:K1:19:PRO:HD3	1.95	0.47
1:M1:34:THR:HB	2:N1:373:GLU:OE1	2.14	0.47
1:M1:251:ALA:O	1:M1:325:VAL:HA	2.14	0.47
1:M1:260:PRO:HG3	1:M1:414:TYR:CZ	2.50	0.47
1:M1:436:ARG:HE	3:O1:222:PRO:HG3	1.79	0.47
2:N1:163:LEU:HD22	2:N1:256:ALA:CB	2.45	0.47
2:N1:197:ASN:HB2	2:N1:198:HIS:CD2	2.49	0.47
3:O1:26:ASN:ND2	3:O1:26:ASN:O	2.48	0.47
3:O1:208:PRO:O	3:O1:314:SER:OG	2.30	0.47
3:O1:221:HIS:N	3:O1:222:PRO:CD	2.77	0.47
4:P1:10:TYR:HD1	8:T1:74:PHE:CD1	2.32	0.47
5:Q1:46:GLY:O	5:Q1:49:TYR:HB3	2.14	0.47
5:Q1:121:GLN:CG	5:Q1:179:ASN:ND2	2.77	0.47
5:Q1:163:SER:HA	5:Q1:173:LYS:O	2.14	0.47
6:R1:103:GLU:O	6:R1:104:ARG:C	2.55	0.47
15:52:79:VAL:O	15:52:83:ASN:N	2.48	0.47
17:82:451:GLN:O	17:82:455:GLN:N	2.44	0.47
19:A2:380:ASP:CG	29:K2:41:TYR:OH	2.58	0.47
21:C2:154:PRO:HG2	32:O2:18:LYS:HE2	1.97	0.47
35:R2:237:LYS:HA	35:R2:325:THR:HG23	1.96	0.47
42:Y2:64:PHE:HA	42:Y2:67:THR:HG22	1.97	0.47
47:d2:29:TYR:H	47:d2:98:ARG:HH12	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B3:63:THR:O	57:B3:66:THR:HG22	2.15	0.47
57:B3:108:TYR:N	57:B3:108:TYR:CD1	2.83	0.47
58:C3:164:PHE:O	58:C3:168:THR:HG23	2.14	0.47
1:A1:64:PHE:HE2	1:A1:88:ALA:CB	2.27	0.47
1:A1:89:TYR:C	1:A1:89:TYR:HD1	2.21	0.47
1:A1:131:ARG:NH2	1:A1:177:LEU:O	2.47	0.47
1:A1:260:PRO:CD	1:A1:414:TYR:CE1	2.92	0.47
1:A1:372:THR:O	1:A1:373:THR:C	2.58	0.47
1:A1:426:GLY:CA	1:A1:427:PRO:C	2.86	0.47
2:B1:52:LYS:CB	2:B1:203:ARG:HB3	2.28	0.47
2:B1:83:PHE:CZ	2:B1:87:ARG:HG3	2.49	0.47
2:B1:207:ILE:HG22	2:B1:379:LEU:CD1	2.44	0.47
2:B1:247:GLN:NE2	2:B1:429:ASN:ND2	2.59	0.47
2:B1:252:LEU:HD11	9:I1:49:VAL:HB	1.95	0.47
3:C1:80:ARG:HD3	3:C1:80:ARG:C	2.39	0.47
3:C1:108:THR:CB	3:C1:313:ARG:HH11	2.27	0.47
4:D1:161:ALA:O	4:D1:163:PRO:HD3	2.14	0.47
4:D1:220:TYR:O	4:D1:221:ALA:C	2.56	0.47
5:E1:33:LYS:HA	7:G1:21:PHE:CD2	2.50	0.47
6:F1:99:ARG:O	6:F1:100:GLU:C	2.57	0.47
8:H1:50:THR:HG22	8:H1:51:GLU:N	2.29	0.47
1:M1:61:HIS:CD2	2:N1:287:ARG:HD3	2.50	0.47
2:N1:56:ARG:HH22	2:N1:318:ASP:CG	2.18	0.47
3:O1:41:LEU:HD23	3:O1:190:MET:HG3	1.96	0.47
3:O1:119:LEU:HD23	69:O1:402:HEM:C3B	2.49	0.47
3:O1:174:THR:CG2	3:O1:178:PHE:HE2	2.12	0.47
3:O1:312:GLN:NE2	3:O1:317:PHE:HB2	2.30	0.47
3:O1:345:HIS:CB	3:O1:346:PRO:CD	2.88	0.47
4:P1:80:MET:H	4:P1:80:MET:HG2	1.49	0.47
4:P1:115:TYR:O	4:P1:119:ALA:N	2.47	0.47
4:P1:220:TYR:CD2	7:S1:26:PHE:CE1	3.02	0.47
6:R1:22:ASN:O	6:R1:23:ALA:C	2.57	0.47
6:R1:45:GLU:O	6:R1:49:ARG:HG3	2.14	0.47
12:22:252:GLY:HA3	12:22:290:LEU:HD13	1.96	0.47
12:22:260:PHE:HE2	12:22:264:TRP:HE3	1.63	0.47
14:42:306:PRO:HA	14:42:308:SER:H	1.80	0.47
14:42:343:ILE:HA	14:42:413:MET:HE2	1.96	0.47
17:82:79:GLU:O	17:82:82:THR:OG1	2.30	0.47
18:92:75:LYS:O	18:92:77:ALA:N	2.45	0.47
19:A2:130:ILE:HG12	27:I2:114:TYR:HH	1.77	0.47
21:C2:73:LYS:NZ	31:N2:101:GLU:OE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I2:62:GLU:HB3	38:U2:124:TYR:HA	1.97	0.47
36:S2:100:CYS:HB3	36:S2:119:LEU:HB2	1.97	0.47
40:W2:97:LYS:HZ3	40:W2:107:ASP:CB	2.27	0.47
40:W2:122:MET:O	40:W2:127:GLY:N	2.43	0.47
52:12:21:THR:O	52:12:25:ARG:HG3	2.14	0.47
52:12:287:HIS:CE1	52:12:291:LYS:HG3	2.49	0.47
53:62:592:LEU:HD23	53:62:596:LEU:HD23	1.97	0.47
59:D3:41:LYS:HD3	59:D3:62:LEU:HD23	1.97	0.47
61:F3:49:VAL:HG21	61:F3:74:LEU:HD12	1.95	0.47
65:J3:16:ASN:ND2	65:J3:16:ASN:H	2.12	0.47
4:D1:32:VAL:CG2	4:D1:186:VAL:HG22	2.44	0.47
8:H1:22:GLU:O	8:H1:23:GLN:C	2.57	0.47
10:J1:32:GLU:HG2	10:J1:33:ARG:H	1.79	0.47
10:J1:51:LEU:O	10:J1:54:HIS:N	2.46	0.47
10:J1:55:ILE:O	10:J1:58:LYS:HD2	2.14	0.47
2:N1:360:ALA:O	2:N1:361:LYS:C	2.58	0.47
3:O1:9:PRO:HB2	3:O1:12:LYS:HB2	1.96	0.47
3:O1:107:TYR:CE1	3:O1:305:PRO:HA	2.50	0.47
3:O1:218:ILE:CD1	4:P1:230:LEU:HD13	2.45	0.47
4:P1:188:THR:O	4:P1:189:PHE:C	2.55	0.47
5:Q1:122:HIS:CE1	5:Q1:124:LEU:HD12	2.50	0.47
5:Q1:141:HIS:HE2	5:Q1:175:PRO:HB2	1.78	0.47
19:A2:97:MET:HB2	19:A2:100:TRP:HE1	1.79	0.47
19:A2:427:LEU:H	25:G2:169:ARG:NH2	2.12	0.47
20:B2:82:LEU:HD11	52:12:126:LYS:CG	2.44	0.47
35:R2:114:ASP:HA	35:R2:117:ARG:HB2	1.95	0.47
37:T2:94:GLY:HA3	37:T2:119:GLY:HA2	1.96	0.47
45:b2:100:GLU:H	45:b2:101:ILE:HA	1.79	0.47
1:A1:36:THR:CB	1:A1:372:THR:HG22	2.45	0.47
1:A1:277:ILE:HG22	1:A1:294:LEU:HD12	1.96	0.47
2:B1:227:ARG:N	2:B1:227:ARG:HD2	2.30	0.47
3:C1:28:SER:CB	3:C1:30:TRP:HD1	2.28	0.47
5:E1:65:SER:OG	5:E1:67:ASP:HB3	2.15	0.47
11:K1:19:PRO:O	11:K1:23:LEU:HG	2.14	0.47
1:M1:32:GLN:CG	1:M1:33:PRO:CD	2.86	0.47
1:M1:276:ILE:O	1:M1:277:ILE:C	2.57	0.47
2:N1:308:ASP:OD1	2:N1:308:ASP:C	2.57	0.47
3:O1:122:THR:CG2	3:O1:189:ILE:HG12	2.44	0.47
5:Q1:76:ILE:HD12	5:Q1:192:MET:HE1	1.97	0.47
7:S1:68:LYS:O	7:S1:69:SER:C	2.58	0.47
10:V1:52:TRP:HE3	10:V1:52:TRP:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:22:120:GLN:HG2	12:22:177:LYS:HE3	1.97	0.47
14:42:435:ALA:O	14:42:438:SER:OG	2.31	0.47
19:A2:261:ILE:HG22	19:A2:286:ILE:HD11	1.97	0.47
19:A2:485:ASP:HB3	19:A2:680:LEU:HG	1.97	0.47
40:M2:75:GLU:HA	40:M2:78:ASP:HB2	1.97	0.47
61:F3:31:TYR:HE1	61:F3:98:HIS:HE1	1.62	0.47
62:G3:67:HIS:CD2	62:G3:78:LEU:HD11	2.50	0.47
2:B1:37:SER:HB3	2:B1:213:HIS:HB2	1.97	0.47
2:B1:216:LEU:O	2:B1:217:LYS:C	2.57	0.47
2:B1:276:GLN:OE1	2:B1:313:ASN:HB3	2.14	0.47
3:C1:26:ASN:HB2	6:F1:69:SER:HG	1.70	0.47
3:C1:105:GLY:HA2	3:C1:107:TYR:CE1	2.50	0.47
3:C1:280:ILE:HD13	3:C1:280:ILE:H	1.80	0.47
3:C1:373:GLU:HA	3:C1:376:LEU:HD12	1.97	0.47
11:K1:30:VAL:HA	11:K1:33:VAL:CG1	2.44	0.47
1:M1:34:THR:CB	2:N1:373:GLU:OE1	2.62	0.47
1:M1:287:GLY:O	1:M1:289:HIS:N	2.48	0.47
3:O1:64:SER:O	3:O1:65:SER:C	2.55	0.47
3:O1:183:PHE:CE1	3:O1:187:PHE:CE2	3.03	0.47
21:C2:156:GLU:HA	21:C2:181:ALA:HB3	1.96	0.47
46:c2:38:GLN:HA	46:c2:39:ARG:HA	1.67	0.47
59:D3:33:LEU:HD22	59:D3:37:GLN:HB3	1.97	0.47
1:A1:312:ILE:HB	1:A1:319:LEU:HB2	1.97	0.46
1:A1:324:PHE:CG	1:A1:334:MET:HG2	2.50	0.46
2:B1:279:LEU:HD23	2:B1:295:LEU:HD13	1.94	0.46
2:B1:308:ASP:OD2	9:I1:54:SER:O	2.32	0.46
4:D1:138:PRO:CB	8:H1:55:THR:HA	2.46	0.46
4:D1:168:VAL:HG12	4:D1:169:LEU:HD23	1.97	0.46
4:D1:220:TYR:CD2	7:G1:26:PHE:CE1	3.03	0.46
6:F1:36:THR:O	6:F1:36:THR:HG22	2.14	0.46
7:G1:36:ASN:O	7:G1:37:VAL:C	2.56	0.46
1:M1:45:SER:OG	1:M1:92:ARG:HG2	2.15	0.46
1:M1:61:HIS:HB3	1:M1:130:GLU:HG3	1.97	0.46
2:N1:68:LEU:HG	2:N1:191:LEU:HD21	1.98	0.46
3:O1:130:GLY:HA3	3:O1:182:HIS:CE1	2.49	0.46
4:P1:233:ARG:HG3	7:S1:17:SER:CB	2.42	0.46
5:Q1:99:ARG:NH1	5:Q1:156:TYR:CZ	2.83	0.46
5:Q1:103:LYS:HA	5:Q1:106:ILE:CD1	2.43	0.46
5:Q1:114:VAL:O	5:Q1:117:LEU:CB	2.63	0.46
6:R1:35:ASP:OD1	6:R1:89:TYR:OH	2.22	0.46
6:R1:73:GLN:HA	7:S1:39:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R1:88:SER:O	6:R1:92:PRO:HD2	2.15	0.46
18:92:57:PRO:HA	18:92:60:TYR:HD2	1.79	0.46
20:B2:322:SER:OG	20:B2:328:ASP:OD2	2.31	0.46
36:S2:161:MET:HG2	36:S2:167:ILE:HB	1.98	0.46
44:a2:79:ASN:ND2	55:e2:76:PRO:CD	2.73	0.46
57:B3:185:MET:SD	57:B3:185:MET:C	2.99	0.46
59:D3:33:LEU:HD13	59:D3:41:LYS:HG3	1.97	0.46
59:D3:108:PRO:HG2	59:D3:111:PHE:CD2	2.50	0.46
2:B1:84:LYS:HG3	2:B1:122:PHE:HZ	1.80	0.46
2:B1:135:TRP:NE1	2:B1:136:GLU:HG3	2.31	0.46
2:B1:159:VAL:HG12	2:B1:160:ILE:N	2.30	0.46
3:C1:15:ASN:ND2	3:C1:18:PHE:HE1	2.12	0.46
3:C1:26:ASN:ND2	3:C1:26:ASN:O	2.48	0.46
3:C1:110:LEU:HG	3:C1:114:ASN:ND2	2.27	0.46
11:K1:33:VAL:HG13	11:K1:34:TRP:CD1	2.50	0.46
1:M1:43:ALA:HB1	1:M1:189:HIS:HB3	1.97	0.46
1:M1:57:TYR:HE2	1:M1:134:ILE:HD12	1.80	0.46
2:N1:262:ALA:HB2	2:N1:272:PHE:CE2	2.49	0.46
3:O1:26:ASN:O	3:O1:27:ILE:HG13	2.14	0.46
4:P1:30:PHE:CE1	4:P1:50:HIS:CE1	3.03	0.46
5:Q1:147:ILE:O	5:Q1:148:ALA:C	2.57	0.46
14:42:88:ASN:HB2	14:42:91:ARG:HE	1.80	0.46
14:42:138:ASN:ND2	14:42:223:ALA:O	2.48	0.46
19:A2:422:TRP:C	25:G2:169:ARG:CD	2.81	0.46
19:A2:427:LEU:N	25:G2:169:ARG:NH1	2.60	0.46
49:h2:147:ILE:HG22	49:h2:149:LEU:H	1.80	0.46
56:A3:240:HIS:NE2	56:A3:244:TYR:CE2	2.81	0.46
59:D3:102:TYR:CD2	68:M3:35:TYR:HE1	2.34	0.46
1:A1:49:SER:N	1:A1:52:ASN:OD1	2.35	0.46
1:A1:60:GLU:OE1	1:A1:90:SER:HB2	2.15	0.46
1:A1:67:THR:CG2	1:A1:70:ARG:HB2	2.43	0.46
2:B1:145:ARG:HG3	2:B1:183:ILE:HD13	1.97	0.46
4:D1:165:TYR:CD1	4:D1:168:VAL:HG22	2.51	0.46
6:F1:95:LYS:O	6:F1:96:GLU:C	2.57	0.46
1:M1:4:TYR:O	1:M1:5:ALA:C	2.56	0.46
1:M1:39:VAL:CG1	1:M1:41:ILE:HD11	2.40	0.46
1:M1:241:ILE:HG13	7:S1:16:TYR:CD2	2.50	0.46
1:M1:253:VAL:O	1:M1:323:HIS:HA	2.16	0.46
2:N1:279:LEU:CD2	2:N1:295:LEU:HD13	2.45	0.46
3:O1:248:ASP:O	3:O1:249:LEU:C	2.58	0.46
3:O1:252:ASP:CB	3:O1:253:PRO:CD	2.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:278:TYR:O	3:O1:281:LEU:N	2.48	0.46
8:T1:73:LEU:CD2	8:T1:74:PHE:HD1	2.28	0.46
18:92:110:MET:HA	18:92:113:TYR:HD2	1.81	0.46
18:92:111:ARG:NH2	19:A2:187:SER:HB2	2.31	0.46
19:A2:312:GLY:H	38:U2:143:PRO:CA	2.28	0.46
19:A2:364:ASP:OD1	19:A2:364:ASP:N	2.48	0.46
26:H2:45:HIS:CE1	45:b2:176:LYS:H	2.32	0.46
29:K2:35:ASP:OD1	29:K2:39:LYS:NZ	2.39	0.46
52:12:127:TYR:C	52:12:127:TYR:HD1	2.23	0.46
53:62:343:SER:HA	53:62:346:ILE:HD12	1.97	0.46
56:A3:172:LYS:HB3	56:A3:176:MET:HE2	1.96	0.46
66:K3:9:PHE:HD1	66:K3:10:HIS:HD2	1.64	0.46
68:M3:1:ILE:HG23	68:M3:1:ILE:O	2.15	0.46
1:A1:120:CYS:HB2	1:A1:122:LEU:HD21	1.96	0.46
3:C1:8:HIS:O	3:C1:9:PRO:C	2.57	0.46
3:C1:40:CYS:HB3	3:C1:90:PHE:HD2	1.81	0.46
3:C1:63:PHE:O	3:C1:67:THR:OG1	2.33	0.46
3:C1:252:ASP:CB	3:C1:253:PRO:CD	2.88	0.46
3:C1:341:GLN:HA	3:C1:341:GLN:NE2	2.31	0.46
3:C1:357:LEU:HG	3:C1:361:LEU:HD11	1.98	0.46
4:D1:93:LYS:O	4:D1:94:PRO:C	2.56	0.46
6:F1:45:GLU:O	6:F1:46:ALA:C	2.56	0.46
1:M1:438:ARG:HG3	1:M1:438:ARG:NH1	2.31	0.46
3:O1:322:GLN:HE21	3:O1:326:TRP:HE1	1.62	0.46
4:P1:241:LYS:NZ	6:R1:53:ASN:HB2	2.31	0.46
5:Q1:43:THR:HG22	5:Q1:44:THR:N	2.30	0.46
5:Q1:133:VAL:HG13	5:Q1:133:VAL:O	2.15	0.46
5:Q1:134:ILE:HD11	5:Q1:185:TYR:CD1	2.48	0.46
14:42:235:LEU:HA	14:42:238:LEU:HG	1.97	0.46
19:A2:111:LYS:CD	33:P2:53:TYR:OH	2.63	0.46
19:A2:394:VAL:HG22	19:A2:473:MET:HE1	1.97	0.46
32:O2:98:LYS:HB3	32:O2:102:HIS:HB2	1.96	0.46
48:f2:40:PHE:HA	48:f2:43:LEU:HB3	1.96	0.46
53:62:139:GLN:HA	53:62:142:ILE:HD12	1.98	0.46
1:A1:91:THR:HG22	1:A1:93:GLU:N	2.18	0.46
2:B1:141:GLN:HE22	2:B1:186:VAL:HB	1.79	0.46
3:C1:310:SER:OG	3:C1:311:LYS:N	2.48	0.46
3:C1:376:LEU:HD13	6:F1:20:TYR:CD2	2.51	0.46
4:D1:153:PHE:O	4:D1:156:GLN:N	2.35	0.46
1:M1:28:GLU:OE1	1:M1:375:VAL:HG11	2.15	0.46
1:M1:70:ARG:HB3	1:M1:74:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:279:HIS:CE1	1:M1:284:TYR:OH	2.68	0.46
2:N1:38:LEU:HD13	2:N1:378:PHE:CE2	2.50	0.46
2:N1:276:GLN:OE1	2:N1:313:ASN:HB3	2.15	0.46
3:O1:102:LEU:HD23	3:O1:102:LEU:HA	1.67	0.46
3:O1:116:GLY:HA3	69:O1:402:HEM:C3C	2.51	0.46
3:O1:236:ILE:O	3:O1:237:LEU:C	2.57	0.46
7:S1:34:ILE:O	7:S1:38:LEU:HG	2.14	0.46
72:22:401:3PE:H2C2	14:42:16:TRP:HE1	1.80	0.46
19:A2:246:ARG:NH2	21:C2:234:LYS:H	2.14	0.46
39:V2:58:ARG:NH2	52:12:314:ILE:O	2.47	0.46
44:a2:43:LEU:O	44:a2:47:TYR:N	2.49	0.46
59:D3:23:PRO:HB3	60:E3:70:VAL:CG2	2.45	0.46
1:A1:184:GLU:O	1:A1:188:ARG:HG3	2.16	0.46
3:C1:152:ALA:CA	3:C1:287:LYS:HZ2	2.29	0.46
7:G1:36:ASN:HA	7:G1:39:ARG:CD	2.32	0.46
2:N1:286:LYS:O	2:N1:287:ARG:HB2	2.14	0.46
3:O1:278:TYR:O	3:O1:279:ALA:C	2.55	0.46
4:P1:240:PRO:CG	4:P1:241:LYS:N	2.79	0.46
5:Q1:94:LYS:HD2	5:Q1:138:VAL:HG21	1.97	0.46
7:S1:40:ARG:O	7:S1:44:CYS:SG	2.71	0.46
10:V1:56:LYS:HE2	10:V1:60:GLU:OE1	2.15	0.46
19:A2:351:LEU:O	19:A2:530:TYR:OH	2.34	0.46
20:B2:293:LEU:O	20:B2:296:SER:N	2.35	0.46
31:N2:114:TRP:O	31:N2:116:ILE:N	2.46	0.46
33:P2:34:ARG:NH2	38:U2:92:CYS:O	2.46	0.46
56:A3:484:THR:HB	68:M3:2:THR:OG1	2.15	0.46
61:F3:98:HIS:ND1	61:F3:98:HIS:N	2.64	0.46
1:A1:61:HIS:HB3	1:A1:130:GLU:HG3	1.97	0.46
1:A1:91:THR:HG22	1:A1:92:ARG:N	2.31	0.46
1:A1:236:PHE:CD2	1:A1:258:GLU:CG	2.92	0.46
2:B1:99:THR:O	2:B1:99:THR:HG22	2.14	0.46
3:C1:30:TRP:HA	3:C1:33:PHE:CE2	2.51	0.46
3:C1:51:LEU:CD2	3:C1:79:ILE:CG2	2.93	0.46
3:C1:246:ALA:N	3:C1:247:PRO:HD3	2.31	0.46
3:C1:334:THR:O	3:C1:337:TRP:HB3	2.15	0.46
4:D1:10:TYR:CE1	4:D1:128:PHE:HE2	2.34	0.46
1:M1:40:TRP:CZ2	1:M1:377:GLU:CA	2.95	0.46
2:N1:269:ALA:O	2:N1:270:ASN:C	2.57	0.46
3:O1:277:ALA:O	3:O1:278:TYR:C	2.57	0.46
4:P1:10:TYR:CZ	4:P1:128:PHE:CE2	2.92	0.46
15:52:17:VAL:HA	15:52:20:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Q2:86:TRP:HA	34:Q2:89:ILE:HG22	1.98	0.46
35:R2:154:GLN:HG3	35:R2:155:VAL:H	1.81	0.46
39:V2:20:ASP:HB2	39:V2:22:LYS:H	1.81	0.46
56:A3:306:THR:HB	56:A3:359:ALA:O	2.15	0.46
64:I3:19:PHE:CD1	64:I3:19:PHE:C	2.94	0.46
1:A1:21:ASN:CB	1:A1:217:SER:HB3	2.45	0.46
1:A1:32:GLN:HG2	1:A1:33:PRO:N	2.30	0.46
1:A1:360:LEU:HD22	2:B1:93:GLY:HA2	1.97	0.46
1:A1:369:LEU:HD21	1:A1:378:ASP:OD2	2.16	0.46
2:B1:113:ARG:O	2:B1:116:VAL:HG23	2.15	0.46
2:B1:182:ARG:NH1	2:B1:185:LYS:CG	2.77	0.46
2:B1:285:VAL:O	2:B1:285:VAL:HG12	2.16	0.46
3:C1:31:TRP:CD2	3:C1:100:ARG:HD2	2.50	0.46
3:C1:328:LEU:O	3:C1:329:VAL:C	2.56	0.46
3:C1:346:PRO:CG	7:G1:66:PHE:HD1	2.28	0.46
3:C1:347:TYR:O	3:C1:348:ILE:C	2.59	0.46
4:D1:10:TYR:CE1	8:H1:73:LEU:HD22	2.51	0.46
4:D1:233:ARG:CG	7:G1:17:SER:CB	2.94	0.46
7:G1:60:THR:O	7:G1:61:TRP:C	2.59	0.46
1:M1:14:THR:HG21	1:M1:390:ILE:HG13	1.98	0.46
1:M1:184:GLU:O	1:M1:185:TYR:C	2.56	0.46
3:O1:61:THR:O	3:O1:64:SER:N	2.48	0.46
3:O1:313:ARG:CB	6:R1:38:HIS:CD2	2.98	0.46
4:P1:23:HIS:NE2	10:V1:51:LEU:HA	2.31	0.46
4:P1:224:ARG:HH21	7:S1:27:PRO:HD2	1.79	0.46
19:A2:157:LYS:HB2	27:I2:100:TYR:CD2	2.51	0.46
19:A2:303:THR:HG23	38:U2:136:GLU:CA	2.46	0.46
20:B2:92:HIS:HE1	20:B2:141:TYR:CE2	2.34	0.46
23:E2:150:THR:OG1	23:E2:151:LYS:N	2.48	0.46
27:I2:106:GLU:N	27:I2:106:GLU:CD	2.73	0.46
40:W2:97:LYS:NZ	40:W2:107:ASP:CB	2.79	0.46
48:f2:128:LEU:O	48:f2:132:SER:OG	2.34	0.46
57:B3:1:MET:SD	57:B3:133:LEU:HD11	2.56	0.46
59:D3:66:GLU:O	60:E3:66:ARG:NH2	2.49	0.46
62:G3:5:LYS:NZ	62:G3:5:LYS:HB3	2.27	0.46
1:A1:51:LYS:O	1:A1:53:ASN:N	2.46	0.46
3:C1:165:TRP:HA	3:C1:174:THR:OG1	2.15	0.46
3:C1:378:LYS:NZ	6:F1:91:GLU:OE1	2.48	0.46
4:D1:195:GLU:HG3	4:D1:195:GLU:O	2.15	0.46
1:M1:11:VAL:CG1	1:M1:12:PRO:HD2	2.46	0.46
1:M1:192:ALA:HA	1:M1:194:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:243:HIS:O	1:M1:425:PHE:HA	2.16	0.46
2:N1:62:ASN:HD21	2:N1:65:THR:CB	2.28	0.46
2:N1:345:LYS:HG2	2:N1:418:VAL:CG1	2.46	0.46
3:O1:373:GLU:O	3:O1:377:LEU:HD12	2.16	0.46
4:P1:33:TYR:O	4:P1:37:CYS:N	2.41	0.46
5:Q1:141:HIS:HB3	5:Q1:142:LEU:H	1.50	0.46
17:82:186:ALA:HA	17:82:187:CYS:HA	1.57	0.46
17:82:422:HIS:O	19:A2:76:ARG:HD2	2.16	0.46
29:K2:31:GLN:HA	29:K2:34:ARG:HE	1.79	0.46
37:T2:99:LEU:O	37:T2:103:ALA:N	2.47	0.46
52:12:21:THR:CG2	52:12:25:ARG:NH2	2.79	0.46
1:A1:192:ALA:HA	1:A1:194:ARG:N	2.31	0.46
1:A1:389:ARG:C	1:A1:391:PRO:HD3	2.41	0.46
2:B1:304:HIS:CD2	2:B1:305:GLN:N	2.84	0.46
3:C1:6:LYS:HG2	3:C1:16:ASN:OD1	2.15	0.46
3:C1:200:LEU:O	3:C1:200:LEU:HG	2.15	0.46
3:C1:345:HIS:N	3:C1:346:PRO:HD2	2.29	0.46
4:D1:23:HIS:O	4:D1:24:THR:C	2.55	0.46
4:D1:98:PRO:O	4:D1:101:ALA:HB3	2.16	0.46
4:D1:116:ILE:HD11	4:D1:120:ARG:HG3	1.97	0.46
4:D1:150:ASN:OD1	4:D1:151:PRO:N	2.49	0.46
6:F1:10:SER:HA	6:F1:13:LEU:CD1	2.45	0.46
7:G1:50:PRO:CB	7:G1:51:PRO:CD	2.92	0.46
1:M1:43:ALA:CB	1:M1:189:HIS:CB	2.94	0.46
1:M1:75:LEU:HD12	1:M1:112:LEU:HD11	1.96	0.46
2:N1:286:LYS:HZ2	2:N1:286:LYS:HG3	1.66	0.46
3:O1:116:GLY:O	3:O1:119:LEU:HB2	2.16	0.46
4:P1:138:PRO:CB	8:T1:55:THR:HA	2.46	0.46
7:S1:73:ASN:N	7:S1:74:PRO:HD2	2.31	0.46
19:A2:583:ILE:CD1	38:U2:137:TRP:CZ3	2.99	0.46
20:B2:91:ALA:HB2	20:B2:193:ASP:CG	2.39	0.46
20:B2:368:ARG:HA	20:B2:371:MET:HG2	1.98	0.46
29:K2:15:GLY:HA2	29:K2:16:LEU:HA	1.58	0.46
49:h2:111:ASP:OD1	49:h2:111:ASP:N	2.47	0.46
56:A3:299:VAL:HA	56:A3:302:ARG:NH1	2.31	0.46
65:J3:11:LEU:O	65:J3:11:LEU:HD23	2.15	0.46
1:A1:39:VAL:CG1	1:A1:195:MET:CE	2.94	0.45
1:A1:46:ARG:NH2	1:A1:316:ASP:CG	2.62	0.45
1:A1:243:HIS:CD2	1:A1:425:PHE:CE2	3.04	0.45
2:B1:264:ILE:HG21	2:B1:317:SER:HA	1.97	0.45
3:C1:26:ASN:HA	6:F1:70:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G1:48:VAL:O	7:G1:51:PRO:HD2	2.16	0.45
10:J1:61:ASN:O	10:J1:62:LYS:HB2	2.15	0.45
1:M1:40:TRP:HZ2	1:M1:377:GLU:CB	2.28	0.45
1:M1:46:ARG:HB3	1:M1:92:ARG:O	2.15	0.45
1:M1:130:GLU:O	1:M1:131:ARG:C	2.57	0.45
1:M1:170:PRO:O	1:M1:171:SER:C	2.55	0.45
1:M1:245:GLU:C	1:M1:247:GLY:H	2.24	0.45
1:M1:252:HIS:O	1:M1:424:GLY:HA2	2.16	0.45
1:M1:441:MET:HE3	1:M1:441:MET:HB3	1.74	0.45
2:N1:352:LEU:HD21	2:N1:357:VAL:CG2	2.46	0.45
3:O1:119:LEU:CD1	3:O1:192:ILE:HG22	2.45	0.45
5:Q1:186:GLU:HG3	5:Q1:186:GLU:O	2.16	0.45
10:V1:4:THR:O	10:V1:5:LEU:C	2.57	0.45
12:22:113:PHE:HA	12:22:116:PRO:HD2	1.97	0.45
16:72:140:ALA:HA	16:72:142:GLY:H	1.80	0.45
19:A2:59:GLN:HB3	21:C2:241:TRP:HZ3	1.79	0.45
19:A2:651:PRO:HD3	29:K2:22:HIS:CE1	2.50	0.45
25:G2:97:TRP:HB2	25:G2:128:PHE:HB2	1.98	0.45
26:H2:28:LYS:HB3	45:b2:184:LYS:HA	1.98	0.45
27:I2:103:LEU:HD13	27:I2:121:GLN:HB3	1.98	0.45
36:S2:196:ASP:HB3	36:S2:248:ALA:H	1.81	0.45
37:T2:139:PRO:HB2	45:b2:161:ARG:HE	1.80	0.45
46:c2:73:THR:HA	46:c2:77:ILE:HD12	1.97	0.45
53:62:137:LEU:HB3	53:62:196:TRP:HD1	1.81	0.45
57:B3:58:ALA:O	57:B3:60:GLU:HG3	2.16	0.45
1:A1:349:ALA:O	1:A1:408:ARG:NH2	2.50	0.45
2:B1:262:ALA:HB3	2:B1:269:ALA:N	2.31	0.45
2:B1:395:PRO:O	2:B1:396:SER:C	2.59	0.45
3:C1:152:ALA:N	3:C1:287:LYS:NZ	2.64	0.45
5:E1:15:ARG:HH21	5:E1:32:ARG:CG	2.29	0.45
10:J1:27:GLY:O	10:J1:28:ALA:C	2.59	0.45
10:J1:57:HIS:O	10:J1:60:GLU:HG2	2.17	0.45
1:M1:53:ASN:CG	1:M1:170:PRO:HD3	2.41	0.45
1:M1:64:PHE:CZ	1:M1:88:ALA:HB2	2.51	0.45
1:M1:262:TRP:CD2	1:M1:385:THR:CG2	2.97	0.45
1:M1:262:TRP:CE3	1:M1:385:THR:HG23	2.52	0.45
1:M1:408:ARG:HH12	11:W1:15:ARG:CD	2.28	0.45
4:P1:50:HIS:O	4:P1:54:VAL:N	2.32	0.45
4:P1:227:TRP:CE3	4:P1:230:LEU:HD12	2.51	0.45
14:42:318:ALA:HB1	14:42:374:ASN:HD22	1.82	0.45
17:82:415:ILE:HG23	19:A2:119:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:92:164:THR:HB	18:92:169:PHE:HB2	1.98	0.45
19:A2:153:PHE:HE2	19:A2:156:GLY:HA3	1.81	0.45
19:A2:613:PRO:HB2	38:U2:134:ILE:HG21	1.91	0.45
23:E2:158:CYS:SG	23:E2:159:GLN:N	2.89	0.45
27:I2:111:THR:HG22	27:I2:118:GLN:HA	1.97	0.45
38:U2:42:ASP:HA	38:U2:43:LYS:HA	1.75	0.45
56:A3:32:ALA:HB3	67:L3:36:PRO:HG2	1.98	0.45
56:A3:147:ILE:HD11	56:A3:209:LEU:HD23	1.98	0.45
56:A3:172:LYS:HB2	56:A3:172:LYS:HZ3	1.81	0.45
56:A3:435:GLY:O	56:A3:437:PRO:HD3	2.15	0.45
1:A1:179:ARG:HG3	1:A1:180:ALA:N	2.31	0.45
2:B1:71:LEU:HD13	2:B1:143:GLN:HG3	1.97	0.45
2:B1:338:LYS:HD3	2:B1:439:LEU:CD2	2.46	0.45
3:C1:61:THR:O	3:C1:64:SER:HB3	2.16	0.45
3:C1:136:GLY:O	3:C1:139:SER:N	2.49	0.45
4:D1:180:SER:HB3	8:H1:17:LEU:HB2	1.98	0.45
7:G1:11:ARG:HB3	7:G1:12:HIS:CD2	2.50	0.45
10:J1:55:ILE:CG2	10:J1:58:LYS:HE2	2.44	0.45
2:N1:35:ILE:HD11	2:N1:213:HIS:CD2	2.50	0.45
3:O1:352:GLN:O	3:O1:356:VAL:HG23	2.17	0.45
4:P1:26:ILE:HG21	4:P1:54:VAL:HG22	1.98	0.45
4:P1:178:THR:HB	4:P1:181:GLN:CG	2.32	0.45
8:T1:40:CYS:O	8:T1:44:VAL:HG23	2.15	0.45
8:T1:65:ARG:O	8:T1:69:VAL:HG23	2.16	0.45
10:V1:55:ILE:CG2	10:V1:58:LYS:HE2	2.45	0.45
14:42:393:ILE:HG21	53:62:184:LEU:HD13	1.98	0.45
17:82:415:ILE:HD12	19:A2:119:PHE:CE1	2.51	0.45
19:A2:181:ARG:N	75:A2:802:SF4:S2	2.89	0.45
19:A2:306:MET:HA	19:A2:316:HIS:HA	1.98	0.45
19:A2:381:LEU:HD12	29:K2:55:ILE:HG21	1.99	0.45
34:Q2:111:VAL:O	34:Q2:117:TRP:N	2.44	0.45
36:S2:114:GLY:HA3	36:S2:115:ASN:HA	1.62	0.45
57:B3:76:ILE:O	57:B3:79:PRO:HD2	2.16	0.45
1:A1:255:ILE:HD12	1:A1:335:MET:CE	2.47	0.45
1:A1:394:GLU:O	1:A1:397:SER:OG	2.26	0.45
2:B1:46:ARG:NH1	2:B1:376:GLU:HG3	2.30	0.45
2:B1:83:PHE:CZ	6:R1:104:ARG:HG2	2.52	0.45
2:B1:161:GLU:CD	2:B1:175:SER:HB2	2.40	0.45
2:B1:201:SER:HG	2:B1:226:ILE:H	1.61	0.45
2:B1:243:GLU:HA	2:B1:424:MET:O	2.17	0.45
2:B1:267:ALA:O	2:B1:268:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:270:ASN:O	2:B1:271:ALA:C	2.59	0.45
2:B1:360:ALA:O	2:B1:361:LYS:C	2.60	0.45
3:C1:26:ASN:HD22	3:C1:208:PRO:HD2	1.82	0.45
3:C1:90:PHE:CE1	3:C1:123:VAL:HG11	2.51	0.45
3:C1:136:GLY:O	3:C1:138:MET:N	2.49	0.45
3:C1:149:LEU:O	3:C1:291:VAL:HG21	2.15	0.45
4:D1:23:HIS:CD2	10:J1:50:LYS:O	2.70	0.45
4:D1:35:GLN:HB2	4:D1:169:LEU:HD11	1.98	0.45
4:D1:74:PRO:CG	4:D1:82:MET:HB3	2.46	0.45
10:J1:52:TRP:N	10:J1:52:TRP:HE3	2.14	0.45
1:M1:125:SER:O	1:M1:129:LYS:HG3	2.16	0.45
1:M1:294:LEU:HD23	1:M1:337:VAL:HG12	1.98	0.45
1:M1:430:GLN:CG	1:M1:430:GLN:O	2.63	0.45
3:O1:10:LEU:O	3:O1:13:ILE:HG13	2.17	0.45
3:O1:24:PRO:O	3:O1:224:TYR:OH	2.22	0.45
3:O1:26:ASN:HB2	6:R1:69:SER:OG	2.17	0.45
3:O1:63:PHE:O	3:O1:67:THR:OG1	2.33	0.45
3:O1:115:ILE:HG22	3:O1:196:HIS:HB2	1.97	0.45
4:P1:228:SER:HB2	7:S1:23:GLN:NE2	2.32	0.45
5:Q1:138:VAL:O	5:Q1:139:CYS:C	2.59	0.45
6:R1:7:SER:O	6:R1:11:ARG:HB2	2.16	0.45
20:B2:97:LEU:HB3	20:B2:111:PRO:HA	1.98	0.45
45:b2:70:LEU:HA	45:b2:73:PHE:HB3	1.97	0.45
53:62:352:ASP:OD1	53:62:352:ASP:N	2.49	0.45
56:A3:158:ILE:O	56:A3:162:ILE:HG13	2.17	0.45
56:A3:240:HIS:O	56:A3:243:VAL:HG22	2.16	0.45
56:A3:273:MET:HG3	56:A3:319:LYS:NZ	2.31	0.45
1:A1:195:MET:HE2	1:A1:195:MET:HB3	1.82	0.45
2:B1:213:HIS:H	2:B1:214:PRO:HD2	1.77	0.45
3:C1:148:ASN:O	3:C1:151:SER:OG	2.26	0.45
4:D1:35:GLN:HA	4:D1:35:GLN:OE1	2.16	0.45
4:D1:168:VAL:HG12	4:D1:169:LEU:CD2	2.47	0.45
7:G1:71:ARG:O	7:G1:73:ASN:N	2.50	0.45
1:M1:246:ASP:HA	1:M1:427:PRO:HD3	1.97	0.45
2:N1:109:VAL:HG22	2:N1:119:LEU:HD23	1.99	0.45
2:N1:141:GLN:CB	2:N1:142:PRO:HD3	2.46	0.45
2:N1:159:VAL:CG1	2:N1:160:ILE:N	2.79	0.45
2:N1:235:ALA:O	2:N1:236:LYS:CB	2.65	0.45
2:N1:258:VAL:HG21	2:N1:312:PHE:HD2	1.82	0.45
2:N1:396:SER:O	2:N1:399:LEU:HB2	2.15	0.45
3:O1:28:SER:CB	3:O1:30:TRP:HD1	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:309:THR:HG23	3:O1:310:SER:N	2.30	0.45
3:O1:338:ILE:HA	3:O1:341:GLN:HG3	1.99	0.45
6:R1:48:ARG:HD3	6:R1:48:ARG:HA	1.51	0.45
6:R1:64:ARG:O	6:R1:68:LEU:HD12	2.16	0.45
6:R1:70:MET:HE3	6:R1:70:MET:HB3	1.65	0.45
12:22:258:SER:HA	12:22:334:THR:HB	1.99	0.45
22:D2:113:PHE:HB2	22:D2:114:ARG:NE	2.28	0.45
46:c2:20:ARG:O	46:c2:24:LYS:N	2.41	0.45
61:F3:40:SER:OG	61:F3:45:ASP:HB3	2.16	0.45
1:A1:332:ASP:O	1:A1:332:ASP:OD1	2.34	0.45
1:A1:341:GLN:OE1	1:A1:344:ARG:HD3	2.16	0.45
4:D1:80:MET:H	4:D1:80:MET:HG2	1.47	0.45
4:D1:165:TYR:CD2	4:D1:168:VAL:HG22	2.52	0.45
1:M1:16:VAL:HG11	1:M1:388:ARG:HB2	1.98	0.45
1:M1:43:ALA:HB2	1:M1:189:HIS:HB3	1.99	0.45
1:M1:241:ILE:HG21	1:M1:241:ILE:HD13	1.64	0.45
1:M1:329:MET:HG3	7:S1:2:ARG:HH11	1.82	0.45
1:M1:333:ASP:O	1:M1:334:MET:C	2.58	0.45
2:N1:53:ALA:HB2	2:N1:198:HIS:HB3	1.99	0.45
3:O1:44:GLN:OE1	3:O1:83:HIS:CE1	2.69	0.45
3:O1:218:ILE:CG2	3:O1:219:PRO:HD2	2.46	0.45
3:O1:347:TYR:O	3:O1:348:ILE:C	2.58	0.45
4:P1:161:ALA:O	4:P1:163:PRO:N	2.49	0.45
4:P1:220:TYR:CD2	7:S1:26:PHE:CZ	3.04	0.45
7:S1:44:CYS:O	7:S1:45:ILE:C	2.59	0.45
11:W1:24:TRP:O	11:W1:25:GLY:C	2.59	0.45
14:42:307:TRP:HE1	53:62:71:ILE:HD12	1.81	0.45
17:82:177:TYR:HD1	17:82:182:ILE:HB	1.82	0.45
18:92:42:ARG:HH12	19:A2:199:GLY:C	2.25	0.45
19:A2:557:ARG:CZ	38:U2:144:TYR:CZ	2.98	0.45
35:R2:52:SER:OG	35:R2:77:GLY:O	2.26	0.45
35:R2:155:VAL:O	35:R2:159:ALA:N	2.49	0.45
57:B3:78:LEU:HB2	57:B3:79:PRO:CD	2.38	0.45
1:A1:64:PHE:CZ	1:A1:88:ALA:HB2	2.51	0.45
1:A1:444:LEU:HA	1:A1:444:LEU:HD12	1.82	0.45
2:B1:56:ARG:HH21	2:B1:103:GLU:CD	2.25	0.45
4:D1:28:ARG:HB2	4:D1:185:ASP:HB3	1.99	0.45
4:D1:221:ALA:O	4:D1:222:MET:C	2.57	0.45
6:F1:43:VAL:O	6:F1:44:LYS:C	2.57	0.45
6:F1:67:ASP:HA	6:F1:70:MET:HE2	1.98	0.45
1:M1:426:GLY:H	1:M1:428:ILE:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N1:239:TYR:HE2	2:N1:421:ARG:HB3	1.81	0.45
2:N1:261:SER:HB3	2:N1:321:LEU:C	2.42	0.45
2:N1:308:ASP:O	2:N1:309:VAL:HG23	2.17	0.45
2:N1:314:ALA:HB1	9:U1:64:LEU:HD22	1.97	0.45
2:N1:338:LYS:O	2:N1:341:TYR:N	2.50	0.45
3:O1:183:PHE:CD1	3:O1:183:PHE:C	2.94	0.45
4:P1:23:HIS:CD2	10:V1:52:TRP:N	2.85	0.45
5:Q1:120:PRO:O	5:Q1:121:GLN:NE2	2.49	0.45
10:V1:52:TRP:CG	10:V1:53:LYS:N	2.84	0.45
13:32:60:ILE:HG21	16:72:168:ILE:HG21	1.97	0.45
14:42:115:LEU:HD12	14:42:174:LEU:HB2	1.98	0.45
14:42:207:MET:HA	14:42:208:PRO:HD3	1.82	0.45
17:82:318:ILE:HD13	17:82:355:ILE:HG13	1.99	0.45
19:A2:381:LEU:HD11	19:A2:664:TYR:HD2	1.81	0.45
34:Q2:121:ASP:N	34:Q2:121:ASP:OD1	2.49	0.45
43:Z2:44:PRO:HA	43:Z2:45:TRP:HA	1.81	0.45
60:E3:78:HIS:CE1	64:I3:12:LEU:HD22	2.52	0.45
1:A1:39:VAL:HG22	1:A1:197:LEU:HD22	1.98	0.45
1:A1:197:LEU:HD11	1:A1:208:LEU:HD11	1.98	0.45
1:A1:255:ILE:HG13	1:A1:422:VAL:HG22	1.98	0.45
1:A1:392:LEU:HA	1:A1:395:TRP:NE1	2.30	0.45
2:B1:160:ILE:HD13	2:B1:160:ILE:N	2.31	0.45
2:B1:262:ALA:HB2	2:B1:268:GLU:HB3	1.98	0.45
3:C1:25:SER:HA	3:C1:218:ILE:HD11	1.98	0.45
3:C1:47:THR:HG23	3:C1:79:ILE:HG23	1.99	0.45
3:C1:182:HIS:O	3:C1:186:PRO:CD	2.64	0.45
4:D1:32:VAL:HG11	4:D1:186:VAL:HG22	1.97	0.45
5:E1:45:VAL:HG13	10:J1:28:ALA:CA	2.46	0.45
1:M1:50:GLU:O	1:M1:173:ASN:ND2	2.49	0.45
1:M1:394:GLU:O	1:M1:397:SER:N	2.49	0.45
1:M1:444:LEU:HD12	1:M1:444:LEU:HA	1.73	0.45
2:N1:50:PHE:CE1	2:N1:207:ILE:HG13	2.52	0.45
2:N1:182:ARG:O	2:N1:185:LYS:HB3	2.17	0.45
3:O1:147:THR:CG2	3:O1:165:TRP:NE1	2.75	0.45
3:O1:316:MET:HE2	3:O1:317:PHE:CZ	2.51	0.45
5:Q1:7:VAL:HG13	5:Q1:8:PRO:HD2	1.98	0.45
5:Q1:131:GLU:HG2	5:Q1:132:TRP:CD1	2.51	0.45
10:V1:23:THR:O	10:V1:24:ILE:C	2.58	0.45
72:22:401:3PE:H292	72:22:401:3PE:H2E1	1.98	0.45
19:A2:81:GLU:HG3	19:A2:108:LYS:HD2	1.99	0.45
35:R2:275:ASP:O	35:R2:279:TYR:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:62:307:SER:HA	53:62:310:LEU:HD12	1.99	0.45
57:B3:41:ILE:O	57:B3:45:MET:HG2	2.16	0.45
57:B3:98:LYS:HB2	57:B3:98:LYS:HE3	1.79	0.45
67:L3:35:ALA:HB3	67:L3:36:PRO:HD3	1.99	0.45
1:A1:46:ARG:NH1	1:A1:316:ASP:OD1	2.50	0.45
1:A1:106:LEU:N	1:A1:107:PRO:CD	2.77	0.45
1:A1:236:PHE:HD2	1:A1:258:GLU:CB	2.28	0.45
1:A1:240:GLN:HE21	1:A1:431:LEU:HD21	1.81	0.45
1:A1:345:LEU:HD23	1:A1:345:LEU:HA	1.68	0.45
2:B1:271:ALA:O	2:B1:272:PHE:C	2.58	0.45
3:C1:53:MET:SD	3:O1:181:PHE:CZ	3.10	0.45
5:E1:7:VAL:HG13	7:G1:16:TYR:CD1	2.51	0.45
1:M1:76:GLU:O	1:M1:77:LYS:C	2.60	0.45
1:M1:272:VAL:HG13	1:M1:358:LYS:HA	1.98	0.45
2:N1:135:TRP:CD1	2:N1:136:GLU:HG3	2.52	0.45
2:N1:159:VAL:CG1	2:N1:160:ILE:HD13	2.40	0.45
2:N1:203:ARG:NH2	2:N1:230:LEU:HD23	2.31	0.45
3:O1:337:TRP:O	3:O1:341:GLN:HG2	2.17	0.45
4:P1:102:ARG:O	4:P1:106:ASN:N	2.49	0.45
7:S1:34:ILE:CB	7:S1:35:PRO:CD	2.91	0.45
9:U1:64:LEU:CG	9:U1:65:VAL:HG23	2.41	0.45
19:A2:181:ARG:CB	75:A2:802:SF4:S2	3.03	0.45
72:B2:501:3PE:H382	52:12:180:PRO:HB3	1.99	0.45
53:62:161:ARG:NH2	53:62:238:GLU:OE1	2.49	0.45
54:g2:4:SER:OG	54:g2:5:TRP:N	2.45	0.45
54:g2:146:LEU:HA	54:g2:147:GLY:HA2	1.67	0.45
56:A3:431:LEU:HD21	56:A3:450:TRP:HB2	1.99	0.45
79:A3:602:HEA:HHC	79:A3:602:HEA:O11	2.17	0.45
58:C3:42:LEU:HD12	58:C3:42:LEU:HA	1.66	0.45
62:G3:3:ALA:O	62:G3:4:ALA:HB2	2.17	0.45
65:J3:2:GLU:CG	65:J3:3:ASN:H	2.30	0.45
1:A1:17:SER:HB2	1:A1:25:VAL:HB	1.99	0.45
1:A1:184:GLU:O	1:A1:185:TYR:C	2.59	0.45
2:B1:29:LEU:HD12	2:B1:33:LEU:HD21	1.98	0.45
2:B1:42:ALA:HB1	2:B1:43:PRO:CD	2.40	0.45
2:B1:124:LEU:HD13	2:B1:223:PHE:CG	2.52	0.45
3:C1:125:ALA:HB3	3:C1:185:LEU:HD21	1.98	0.45
3:C1:153:ILE:HD12	3:C1:153:ILE:H	1.82	0.45
4:D1:228:SER:HB2	7:G1:23:GLN:HE21	1.74	0.45
7:G1:75:ALA:O	7:G1:76:ALA:C	2.60	0.45
1:M1:233:PRO:HG2	5:Q1:23:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:339:GLN:O	1:M1:343:MET:HG2	2.17	0.45
1:M1:426:GLY:CA	1:M1:427:PRO:C	2.90	0.45
2:N1:300:ALA:HA	2:N1:307:PHE:HZ	1.77	0.45
3:O1:137:GLN:HE22	3:O1:263:ASN:HB3	1.80	0.45
4:P1:143:LEU:HD11	4:P1:149:PHE:HB2	1.98	0.45
17:82:413:TRP:HE1	17:82:436:GLN:HG3	1.82	0.45
18:92:110:MET:CG	19:A2:194:ASP:C	2.88	0.45
23:E2:115:ALA:O	23:E2:140:ARG:NH1	2.40	0.45
53:62:171:ALA:O	53:62:175:ASN:ND2	2.50	0.45
61:F3:31:TYR:HE1	61:F3:98:HIS:CE1	2.34	0.45
2:B1:299:VAL:CG1	2:B1:303:VAL:HG21	2.46	0.44
2:B1:346:THR:O	2:B1:349:GLN:N	2.39	0.44
3:C1:113:TRP:O	3:C1:117:VAL:HG23	2.17	0.44
3:C1:177:ARG:HG2	3:C1:181:PHE:HE2	1.82	0.44
3:C1:183:PHE:HZ	3:O1:184:ILE:HB	1.82	0.44
4:D1:25:SER:O	4:D1:26:ILE:C	2.58	0.44
4:D1:197:GLU:O	4:D1:198:HIS:C	2.59	0.44
1:M1:430:GLN:O	1:M1:430:GLN:HG2	2.16	0.44
2:N1:54:GLY:H	2:N1:57:TYR:HD1	1.65	0.44
3:O1:55:TYR:CE2	3:O1:56:THR:O	2.70	0.44
3:O1:90:PHE:CE1	3:O1:123:VAL:HG11	2.52	0.44
3:O1:107:TYR:OH	3:O1:308:HIS:HB2	2.17	0.44
3:O1:185:LEU:N	3:O1:186:PRO:CD	2.80	0.44
3:O1:277:ALA:HB1	3:O1:294:LEU:HD11	1.99	0.44
3:O1:341:GLN:HA	3:O1:341:GLN:HE21	1.82	0.44
4:P1:55:CYS:SG	10:V1:52:TRP:HA	2.57	0.44
4:P1:65:ALA:O	4:P1:69:GLU:OE2	2.35	0.44
4:P1:136:GLU:O	4:P1:137:PRO:C	2.60	0.44
20:B2:382:PHE:HD1	23:E2:118:LEU:HD11	1.81	0.44
21:C2:117:THR:OG1	21:C2:118:ALA:N	2.50	0.44
22:D2:150:VAL:HG12	22:D2:179:VAL:HG13	1.99	0.44
35:R2:64:PHE:HZ	35:R2:208:GLY:HA3	1.82	0.44
36:S2:338:LYS:HZ3	51:j2:51:ARG:HH11	1.64	0.44
39:V2:28:ARG:HA	39:V2:29:GLY:HA3	1.70	0.44
44:a2:104:VAL:O	44:a2:107:THR:OG1	2.31	0.44
51:j2:83:TYR:HD1	51:j2:86:ARG:HH21	1.65	0.44
56:A3:379:TYR:CE2	56:A3:383:MET:HE2	2.52	0.44
57:B3:121:TYR:C	57:B3:138:VAL:HG23	2.42	0.44
58:C3:183:GLU:O	62:G3:42:ARG:NH2	2.50	0.44
2:B1:211:VAL:CG1	2:B1:212:SER:N	2.81	0.44
3:C1:183:PHE:CE1	3:C1:187:PHE:HE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:315:MET:O	3:C1:318:ARG:N	2.35	0.44
3:C1:371:THR:O	3:C1:372:ILE:C	2.61	0.44
4:D1:31:GLN:OE1	4:D1:31:GLN:HA	2.17	0.44
4:D1:67:GLU:O	4:D1:70:VAL:HG12	2.17	0.44
6:F1:58:ARG:HG2	6:F1:58:ARG:HH11	1.82	0.44
9:I1:51:CYS:SG	9:I1:53:GLU:HB3	2.57	0.44
10:J1:4:THR:HG22	10:J1:6:THR:N	2.33	0.44
1:M1:37:VAL:HG13	1:M1:199:ALA:CB	2.45	0.44
2:N1:198:HIS:HE1	2:N1:233:SER:HB3	1.81	0.44
3:O1:48:GLY:HA3	69:O1:401:HEM:C3C	2.52	0.44
3:O1:264:THR:O	3:O1:266:PRO:HD3	2.16	0.44
3:O1:364:VAL:O	3:O1:367:PRO:HG2	2.17	0.44
4:P1:116:ILE:HD12	4:P1:116:ILE:HA	1.74	0.44
5:Q1:171:ILE:O	5:Q1:171:ILE:CG2	2.62	0.44
9:U1:57:GLY:O	9:U1:78:TYR:CE2	2.70	0.44
19:A2:275:PRO:HB3	19:A2:286:ILE:HB	1.99	0.44
23:E2:196:LYS:HD2	23:E2:197:TRP:CZ3	2.52	0.44
36:S2:175:TYR:O	36:S2:179:LYS:N	2.45	0.44
53:G2:199:GLN:O	54:G2:114:GLN:NE2	2.40	0.44
56:A3:131:PRO:HB2	57:B3:159:VAL:HA	2.00	0.44
57:B3:1:MET:SD	57:B3:133:LEU:HD13	2.58	0.44
1:A1:197:LEU:CD1	1:A1:208:LEU:HD11	2.47	0.44
1:A1:252:HIS:NE2	1:A1:325:VAL:HG21	2.32	0.44
2:B1:314:ALA:CB	9:I1:64:LEU:HD22	2.48	0.44
3:C1:26:ASN:CA	6:F1:70:MET:HB2	2.48	0.44
3:C1:271:GLU:OE2	3:C1:273:TYR:OH	2.35	0.44
3:C1:281:LEU:HD12	3:C1:281:LEU:O	2.16	0.44
4:D1:167:GLU:HG2	4:D1:167:GLU:O	2.17	0.44
4:D1:175:THR:HA	4:D1:176:PRO:HD2	1.73	0.44
4:D1:229:VAL:HG12	4:D1:229:VAL:O	2.18	0.44
1:M1:82:MET:HE2	1:M1:82:MET:HB2	1.93	0.44
1:M1:157:ALA:HB2	1:M1:421:ALA:HB1	2.00	0.44
2:N1:81:SER:O	2:N1:84:LYS:N	2.50	0.44
2:N1:275:LEU:O	2:N1:276:GLN:C	2.60	0.44
5:Q1:40:THR:CG2	10:V1:20:PHE:HZ	2.28	0.44
5:Q1:134:ILE:C	5:Q1:135:LEU:HD23	2.42	0.44
6:R1:43:VAL:HG22	6:R1:94:LEU:CD2	2.46	0.44
10:V1:49:GLY:HA2	10:V1:54:HIS:HB3	1.98	0.44
11:W1:23:LEU:N	11:W1:23:LEU:HD23	2.32	0.44
14:42:370:PRO:HA	14:42:375:LEU:HB2	1.99	0.44
17:82:146:GLY:O	17:82:150:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:82:246:GLU:HA	17:82:249:ALA:HB3	1.98	0.44
19:A2:388:ASN:ND2	19:A2:513:MET:O	2.36	0.44
30:L2:56:PRO:HG3	34:Q2:41:LYS:HB3	2.00	0.44
31:N2:56:LEU:HA	31:N2:59:VAL:HB	1.99	0.44
42:Y2:66:ALA:O	42:Y2:70:PHE:N	2.50	0.44
52:12:3:MET:HA	52:12:6:ILE:HD12	2.00	0.44
56:A3:51:ASP:O	56:A3:55:ASN:HB2	2.17	0.44
57:B3:122:MET:HB2	57:B3:208:PRO:CD	2.47	0.44
59:D3:79:LYS:NZ	66:K3:15:ASN:HD21	2.15	0.44
64:I3:21:ILE:HD12	64:I3:21:ILE:HA	1.82	0.44
1:A1:152:TYR:OH	1:A1:243:HIS:CD2	2.70	0.44
2:B1:112:LEU:HD22	2:B1:112:LEU:HA	1.79	0.44
3:C1:243:VAL:O	3:C1:243:VAL:HG22	2.17	0.44
3:C1:310:SER:OG	3:C1:312:GLN:N	2.48	0.44
4:D1:5:LEU:HG	4:D1:152:TYR:CE1	2.51	0.44
5:E1:15:ARG:H	5:E1:15:ARG:HG2	1.66	0.44
10:J1:18:SER:CB	11:K1:23:LEU:HD12	2.30	0.44
2:N1:51:ILE:HD13	2:N1:199:PHE:CD2	2.53	0.44
2:N1:322:PHE:CD1	2:N1:322:PHE:C	2.96	0.44
2:N1:380:ASP:O	2:N1:381:GLU:C	2.61	0.44
4:P1:165:TYR:CZ	4:P1:168:VAL:HG22	2.53	0.44
4:P1:218:LEU:HD23	4:P1:218:LEU:HA	1.73	0.44
6:R1:28:LYS:HB3	6:R1:74:ILE:CD1	2.47	0.44
6:R1:37:ILE:CG1	6:R1:43:VAL:HG21	2.40	0.44
12:22:173:THR:O	12:22:226:THR:OG1	2.27	0.44
19:A2:215:MET:SD	19:A2:695:TYR:OH	2.73	0.44
20:B2:293:LEU:HB3	20:B2:294:ARG:H	1.51	0.44
20:B2:359:ASP:HB2	33:P2:45:PRO:HG2	2.00	0.44
56:A3:195:LEU:CD2	56:A3:245:ILE:HD13	2.45	0.44
56:A3:449:MET:HE3	66:K3:40:TRP:HB3	1.98	0.44
57:B3:60:GLU:CD	57:B3:61:VAL:H	2.25	0.44
61:F3:33:ILE:HG22	61:F3:34:LEU:HD12	1.98	0.44
1:A1:199:ALA:HB3	1:A1:208:LEU:HD21	1.99	0.44
1:A1:349:ALA:HB3	1:A1:408:ARG:CG	2.48	0.44
1:A1:379:ILE:CD1	1:A1:390:ILE:HD12	2.41	0.44
2:B1:154:ASN:O	2:B1:155:PRO:C	2.60	0.44
2:B1:367:GLY:O	2:B1:368:TYR:C	2.59	0.44
3:C1:147:THR:CG2	3:C1:165:TRP:NE1	2.78	0.44
3:C1:338:ILE:HA	3:C1:341:GLN:HG3	1.99	0.44
6:F1:37:ILE:CD1	6:F1:43:VAL:HG22	2.47	0.44
1:M1:8:LEU:HD11	1:M1:396:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:49:SER:N	1:M1:52:ASN:OD1	2.41	0.44
1:M1:349:ALA:O	1:M1:408:ARG:CZ	2.65	0.44
2:N1:140:LEU:O	2:N1:142:PRO:N	2.51	0.44
3:O1:136:GLY:O	3:O1:137:GLN:C	2.60	0.44
3:O1:156:ILE:HG13	3:O1:157:GLY:N	2.29	0.44
4:P1:139:THR:HB	8:T1:54:CYS:SG	2.58	0.44
10:V1:4:THR:CG2	10:V1:6:THR:OG1	2.66	0.44
10:V1:24:ILE:O	10:V1:25:VAL:C	2.61	0.44
10:V1:57:HIS:O	10:V1:60:GLU:HG2	2.18	0.44
12:22:48:HIS:HD2	16:72:171:ILE:HG23	1.83	0.44
14:42:55:LEU:HD22	34:Q2:171:THR:HG22	1.99	0.44
19:A2:111:LYS:HD2	33:P2:53:TYR:CZ	2.52	0.44
22:D2:174:ASP:OD1	22:D2:182:TYR:OH	2.35	0.44
50:i2:52:VAL:HA	50:i2:55:TRP:HB2	2.00	0.44
52:12:254:LEU:HA	52:12:257:ILE:HD12	1.99	0.44
53:62:448:PRO:HA	53:62:451:ILE:HB	2.00	0.44
57:B3:59:GLN:CA	57:B3:62:GLU:HB2	2.46	0.44
59:D3:40:LEU:HD22	59:D3:59:LEU:CD1	2.47	0.44
1:A1:33:PRO:O	1:A1:103:SER:HB3	2.17	0.44
1:A1:51:LYS:C	1:A1:53:ASN:H	2.25	0.44
1:A1:358:LYS:HD2	1:A1:402:VAL:HB	1.98	0.44
1:A1:426:GLY:HA2	1:A1:428:ILE:HG13	1.84	0.44
2:B1:56:ARG:HH22	2:B1:318:ASP:CG	2.22	0.44
2:B1:59:ASN:CG	2:B1:60:SER:N	2.74	0.44
2:B1:264:ILE:HG22	2:B1:317:SER:HA	1.99	0.44
3:C1:11:MET:HE3	3:C1:11:MET:HB3	1.67	0.44
3:C1:156:ILE:HG12	3:C1:157:GLY:N	2.29	0.44
4:D1:233:ARG:CG	7:G1:17:SER:HB3	2.48	0.44
1:M1:324:PHE:CG	1:M1:334:MET:HG2	2.52	0.44
2:N1:161:GLU:O	2:N1:162:ASN:C	2.60	0.44
4:P1:28:ARG:HD2	4:P1:185:ASP:OD2	2.17	0.44
4:P1:161:ALA:O	4:P1:163:PRO:HD3	2.18	0.44
4:P1:237:TYR:HB2	6:R1:60:PHE:CE1	2.53	0.44
5:Q1:186:GLU:O	5:Q1:186:GLU:CG	2.66	0.44
9:U1:72:VAL:CB	9:U1:73:PRO:CD	2.76	0.44
72:22:401:3PE:H281	51:j2:43:LEU:HD13	2.00	0.44
19:A2:422:TRP:HA	19:A2:427:LEU:HB3	1.99	0.44
20:B2:221:ARG:NH1	22:D2:95:GLU:OE2	2.51	0.44
22:D2:175:ARG:HG2	35:R2:48:ARG:HH21	1.83	0.44
25:G2:108:GLU:HG2	25:G2:113:GLY:HA2	1.99	0.44
26:H2:9:ARG:NH2	51:j2:12:GLN:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Q2:59:GLU:HA	34:Q2:62:LEU:HD13	2.00	0.44
77:R2:601:NAP:O4D	77:R2:601:NAP:C2N	2.65	0.44
49:h2:81:ALA:HA	49:h2:84:ILE:HD12	1.99	0.44
50:i2:51:SER:O	50:i2:55:TRP:N	2.46	0.44
60:E3:70:VAL:HG12	60:E3:71:VAL:N	2.31	0.44
1:A1:32:GLN:HE22	2:B1:373:GLU:HA	1.83	0.44
1:A1:385:THR:HG22	1:A1:386:TYR:CD1	2.52	0.44
2:B1:24:LEU:HG	2:B1:38:LEU:CD1	2.31	0.44
2:B1:55:SER:HG	2:B1:102:ARG:HG2	1.83	0.44
2:B1:211:VAL:HG12	2:B1:212:SER:N	2.32	0.44
3:C1:103:TYR:CE1	3:C1:322:GLN:HG3	2.53	0.44
3:C1:276:PHE:CE2	3:C1:297:SER:OG	2.68	0.44
8:H1:69:VAL:O	8:H1:73:LEU:HB3	2.18	0.44
1:M1:245:GLU:C	1:M1:247:GLY:N	2.76	0.44
3:O1:30:TRP:HA	3:O1:33:PHE:CE2	2.52	0.44
4:P1:27:ARG:NH1	10:V1:58:LYS:HE3	2.33	0.44
4:P1:50:HIS:CE1	4:P1:91:PHE:HZ	2.33	0.44
4:P1:131:LEU:CD2	4:P1:163:PRO:HB3	2.48	0.44
5:Q1:99:ARG:NH1	5:Q1:148:ALA:HB1	2.32	0.44
14:42:16:TRP:HA	14:42:93:LYS:HD3	1.99	0.44
14:42:25:VAL:HG23	49:h2:89:VAL:HG11	1.99	0.44
15:52:51:SER:HA	26:H2:32:ARG:HE	1.83	0.44
17:82:219:LYS:NZ	25:G2:172:VAL:O	2.42	0.44
17:82:383:THR:CG2	19:A2:75:CYS:CA	2.82	0.44
52:12:39:VAL:HG13	52:12:40:VAL:HG13	1.99	0.44
53:62:135:ASN:HA	53:62:198:LEU:HD12	1.99	0.44
1:A1:277:ILE:HB	1:A1:309:THR:HG21	2.00	0.44
2:B1:135:TRP:CE2	6:R1:49:ARG:HD3	2.53	0.44
3:C1:233:LEU:HD12	3:C1:233:LEU:HA	1.80	0.44
4:D1:7:PRO:HG3	4:D1:126:TYR:CA	2.43	0.44
4:D1:10:TYR:HD1	8:H1:74:PHE:CD1	2.36	0.44
4:D1:178:THR:HB	4:D1:181:GLN:CG	2.42	0.44
5:E1:15:ARG:O	5:E1:16:PRO:C	2.61	0.44
6:F1:106:GLU:OE1	6:F1:109:LYS:HE2	2.17	0.44
1:M1:287:GLY:O	1:M1:290:LEU:HG	2.18	0.44
2:N1:433:THR:HA	2:N1:434:PRO:HD2	1.58	0.44
4:P1:26:ILE:CG2	4:P1:54:VAL:HG13	2.46	0.44
4:P1:34:LYS:O	4:P1:34:LYS:HG2	2.18	0.44
5:Q1:81:ILE:HD11	5:Q1:132:TRP:HH2	1.82	0.44
5:Q1:136:ILE:O	5:Q1:138:VAL:N	2.49	0.44
35:R2:143:ASP:O	35:R2:147:LYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:62:73:THR:O	54:g2:104:ASN:ND2	2.49	0.44
57:B3:162:SER:HB2	57:B3:198:GLU:HB2	1.99	0.44
1:A1:198:ALA:O	1:A1:199:ALA:CB	2.63	0.44
1:A1:293:PRO:HA	1:A1:296:SER:OG	2.17	0.44
2:B1:181:TYR:CD1	2:B1:181:TYR:C	2.96	0.44
2:B1:258:VAL:HG11	2:B1:321:LEU:HD22	2.00	0.44
2:B1:275:LEU:HD11	2:B1:279:LEU:HD12	1.99	0.44
2:B1:334:GLY:O	2:B1:335:ASP:C	2.59	0.44
3:C1:357:LEU:HD12	3:C1:361:LEU:HG	2.00	0.44
4:D1:120:ARG:HH11	4:D1:120:ARG:HG2	1.82	0.44
7:G1:26:PHE:N	7:G1:27:PRO:HD3	2.33	0.44
1:M1:385:THR:HB	1:M1:386:TYR:CD1	2.53	0.44
2:N1:160:ILE:HD11	2:N1:325:TYR:CE2	2.53	0.44
3:O1:88:SER:O	3:O1:89:MET:C	2.61	0.44
3:O1:160:LEU:O	3:O1:160:LEU:HD12	2.18	0.44
3:O1:197:LEU:HD12	3:O1:197:LEU:HA	1.77	0.44
4:P1:35:GLN:OE1	4:P1:35:GLN:HA	2.18	0.44
4:P1:68:VAL:CG1	4:P1:92:PRO:HG2	2.47	0.44
5:Q1:171:ILE:HB	5:Q1:178:LEU:O	2.17	0.44
7:S1:26:PHE:N	7:S1:27:PRO:HD3	2.32	0.44
10:V1:51:LEU:O	10:V1:52:TRP:C	2.61	0.44
17:82:124:THR:HG22	17:82:126:LYS:H	1.83	0.44
17:82:445:GLU:O	17:82:449:ARG:NH1	2.51	0.44
19:A2:634:LEU:HA	19:A2:635:PRO:HD3	1.81	0.44
35:R2:235:THR:HA	35:R2:236:VAL:HA	1.57	0.44
35:R2:269:SER:HA	35:R2:270:ARG:HA	1.64	0.44
44:a2:113:GLU:O	44:a2:117:GLN:N	2.46	0.44
53:62:319:ILE:HG22	53:62:321:GLN:HG2	1.99	0.44
2:B1:262:ALA:CB	2:B1:268:GLU:HB3	2.48	0.43
2:B1:285:VAL:HG12	2:B1:288:GLY:HA3	1.98	0.43
3:C1:242:LEU:HD21	3:C1:250:LEU:HD22	1.99	0.43
3:C1:254:ASP:HB3	4:D1:119:ALA:O	2.18	0.43
3:C1:294:LEU:O	3:C1:297:SER:HB3	2.17	0.43
69:C1:401:HEM:CMB	69:C1:401:HEM:HBB2	2.48	0.43
4:D1:72:ASP:OD2	4:D1:92:PRO:HB2	2.18	0.43
4:D1:131:LEU:HD13	4:D1:164:ILE:CD1	2.48	0.43
4:D1:161:ALA:O	4:D1:163:PRO:CD	2.66	0.43
1:M1:85:HIS:HA	2:N1:284:HIS:O	2.18	0.43
1:M1:152:TYR:OH	1:M1:243:HIS:CD2	2.71	0.43
2:N1:62:ASN:ND2	2:N1:65:THR:CB	2.81	0.43
3:O1:101:GLY:O	3:O1:107:TYR:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:327:ALA:HA	7:S1:51:PRO:HB3	1.99	0.43
4:P1:102:ARG:HE	4:P1:109:LEU:HB2	1.83	0.43
4:P1:210:LEU:O	4:P1:211:MET:C	2.60	0.43
8:T1:58:LEU:CD1	8:T1:62:LEU:HG	2.48	0.43
14:42:76:MET:HG2	14:42:231:LEU:HD12	1.99	0.43
17:82:284:ASN:HD22	18:92:228:ALA:HB3	1.83	0.43
19:A2:250:SER:OG	19:A2:251:ILE:N	2.51	0.43
27:I2:89:GLY:H	27:I2:96:HIS:CE1	2.35	0.43
42:Y2:47:TYR:HD2	43:Z2:16:LEU:HD12	1.82	0.43
58:C3:19:THR:CG2	58:C3:53:THR:OG1	2.66	0.43
1:A1:16:VAL:HG11	1:A1:388:ARG:HB2	1.99	0.43
2:B1:257:LEU:HD22	2:B1:424:MET:HE2	2.00	0.43
3:C1:8:HIS:HB2	3:C1:9:PRO:HD2	2.00	0.43
3:C1:245:PHE:CE1	4:D1:17:LEU:HB3	2.53	0.43
5:E1:33:LYS:HA	7:G1:21:PHE:HE2	1.82	0.43
7:G1:27:PRO:O	7:G1:28:HIS:C	2.62	0.43
9:I1:64:LEU:HG	9:I1:65:VAL:HG23	1.99	0.43
1:M1:64:PHE:HE1	1:M1:86:LEU:CD1	2.31	0.43
1:M1:252:HIS:CD2	1:M1:325:VAL:HG22	2.53	0.43
2:N1:53:ALA:O	2:N1:105:MET:HB2	2.17	0.43
2:N1:83:PHE:CZ	2:N1:87:ARG:HG3	2.53	0.43
2:N1:99:THR:O	2:N1:106:ALA:N	2.51	0.43
2:N1:109:VAL:O	2:N1:109:VAL:CG1	2.66	0.43
2:N1:129:ALA:O	2:N1:130:PRO:C	2.58	0.43
2:N1:206:LEU:C	2:N1:207:ILE:HG12	2.43	0.43
3:O1:31:TRP:CD2	3:O1:100:ARG:HD2	2.53	0.43
3:O1:282:ARG:O	3:O1:283:SER:C	2.59	0.43
3:O1:316:MET:HE2	3:O1:317:PHE:HE1	1.77	0.43
4:P1:12:TRP:O	4:P1:13:SER:C	2.61	0.43
5:Q1:150:ALA:CB	5:Q1:157:TYR:HB2	2.48	0.43
5:Q1:153:PHE:HE1	5:Q1:173:LYS:CG	2.25	0.43
5:Q1:185:TYR:HB3	5:Q1:195:VAL:HA	2.00	0.43
19:A2:35:PHE:HB3	19:A2:38:GLY:HA2	2.00	0.43
19:A2:380:ASP:OD2	29:K2:45:LYS:HE3	2.18	0.43
52:12:75:PRO:CB	52:12:223:PHE:CE1	3.02	0.43
58:C3:63:ARG:HA	58:C3:67:PHE:CD2	2.53	0.43
65:J3:3:ASN:ND2	65:J3:5:VAL:HG13	2.33	0.43
67:L3:22:LEU:HD23	67:L3:22:LEU:HA	1.83	0.43
1:A1:347:THR:HA	11:K1:16:ASN:HD22	1.84	0.43
3:C1:7:SER:O	3:C1:8:HIS:O	2.36	0.43
3:C1:107:TYR:CE2	3:C1:305:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:170:VAL:CG1	3:C1:174:THR:CG2	2.89	0.43
4:D1:138:PRO:CG	8:H1:55:THR:HA	2.48	0.43
1:M1:64:PHE:CD1	1:M1:86:LEU:HG	2.51	0.43
1:M1:211:LEU:HD12	1:M1:211:LEU:O	2.18	0.43
2:N1:222:GLN:HB3	2:N1:223:PHE:CD2	2.53	0.43
3:O1:56:THR:HG22	3:O1:57:SER:N	2.34	0.43
5:Q1:29:SER:OG	5:Q1:32:ARG:HD3	2.17	0.43
14:42:368:ALA:HB1	14:42:374:ASN:HB2	1.99	0.43
45:b2:68:LEU:H	45:b2:71:LEU:HD13	1.82	0.43
52:12:20:LEU:O	52:12:24:GLU:N	2.49	0.43
58:C3:60:ASP:O	58:C3:64:GLU:HG3	2.19	0.43
1:A1:7:ALA:O	1:A1:8:LEU:C	2.60	0.43
1:A1:21:ASN:CB	1:A1:217:SER:CB	2.89	0.43
2:B1:346:THR:O	2:B1:347:ILE:C	2.60	0.43
3:C1:32:ASN:O	3:C1:36:LEU:HG	2.18	0.43
3:C1:192:ILE:HD13	3:C1:192:ILE:H	1.82	0.43
3:C1:206:ASN:ND2	3:C1:207:ASN:N	2.60	0.43
3:C1:269:LYS:HA	3:C1:270:PRO:HD3	1.81	0.43
1:M1:19:LEU:HB2	1:M1:23:LEU:HB3	2.00	0.43
1:M1:75:LEU:HD21	1:M1:116:ILE:HG12	2.00	0.43
1:M1:292:SER:O	1:M1:295:ALA:N	2.52	0.43
1:M1:381:ARG:HA	1:M1:384:LEU:HD12	1.99	0.43
2:N1:182:ARG:NH1	2:N1:185:LYS:CG	2.79	0.43
3:O1:25:SER:HB2	3:O1:26:ASN:H	1.30	0.43
3:O1:183:PHE:CD1	3:O1:183:PHE:O	2.72	0.43
3:O1:227:LYS:CG	4:P1:223:LYS:NZ	2.82	0.43
3:O1:280:ILE:HD13	3:O1:335:LEU:CD2	2.44	0.43
4:P1:82:MET:HE2	4:P1:86:LYS:HZ3	1.82	0.43
4:P1:204:MET:O	4:P1:205:GLY:C	2.60	0.43
5:Q1:121:GLN:O	5:Q1:170:ARG:HD3	2.18	0.43
5:Q1:122:HIS:O	5:Q1:123:ASP:C	2.62	0.43
7:S1:68:LYS:HD3	7:S1:72:LYS:HE3	2.01	0.43
12:22:146:PHE:HE1	12:22:195:PRO:HA	1.82	0.43
14:42:198:ALA:HB2	72:42:502:3PE:H271	2.00	0.43
17:82:378:SER:OG	19:A2:201:GLY:HA2	2.18	0.43
74:82:501:FMN:H9	74:82:501:FMN:H1'1	1.68	0.43
20:B2:85:GLY:C	20:B2:87:GLN:H	2.26	0.43
20:B2:97:LEU:C	20:B2:97:LEU:HD13	2.43	0.43
20:B2:118:ARG:HD3	22:D2:163:TYR:CZ	2.54	0.43
21:C2:157:SER:HB3	21:C2:180:PHE:HB3	2.01	0.43
23:E2:197:TRP:HB3	38:U2:84:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R2:177:SER:HA	35:R2:178:SER:HA	1.68	0.43
50:i2:43:LYS:HA	50:i2:46:LEU:HD12	1.99	0.43
52:12:178:ALA:HB1	52:12:181:LEU:HB2	2.00	0.43
58:C3:19:THR:HG22	58:C3:53:THR:OG1	2.18	0.43
1:A1:154:HIS:HE1	1:A1:314:TYR:OH	2.02	0.43
2:B1:262:ALA:HB2	2:B1:272:PHE:CE2	2.53	0.43
3:C1:226:ILE:O	3:C1:227:LYS:C	2.61	0.43
6:F1:70:MET:HE2	6:F1:70:MET:HB3	1.60	0.43
1:M1:106:LEU:HA	1:M1:109:ALA:HB3	2.01	0.43
1:M1:158:PHE:O	1:M1:164:ALA:HB2	2.18	0.43
2:N1:47:ILE:CG2	2:N1:48:GLY:H	2.31	0.43
2:N1:162:ASN:ND2	2:N1:244:ILE:HG21	2.33	0.43
2:N1:204:MET:HE1	2:N1:224:LEU:HB3	2.00	0.43
3:O1:276:PHE:HE2	3:O1:297:SER:OG	2.00	0.43
3:O1:373:GLU:HB3	6:R1:20:TYR:OH	2.18	0.43
4:P1:28:ARG:O	4:P1:29:GLY:C	2.61	0.43
4:P1:131:LEU:HD22	4:P1:163:PRO:CB	2.48	0.43
5:Q1:122:HIS:HB3	5:Q1:125:GLU:CG	2.48	0.43
17:82:177:TYR:O	24:F2:96:ARG:NH1	2.52	0.43
28:J2:68:ASN:ND2	34:Q2:19:LYS:O	2.51	0.43
36:S2:73:HIS:NE2	36:S2:148:GLU:OE2	2.41	0.43
41:X2:21:VAL:HA	41:X2:24:TYR:HB3	1.99	0.43
43:Z2:65:GLY:O	43:Z2:70:GLY:N	2.48	0.43
44:a2:87:SER:O	53:62:557:TRP:NE1	2.52	0.43
56:A3:353:LEU:HD12	56:A3:353:LEU:HA	1.91	0.43
1:A1:428:ILE:CG2	1:A1:431:LEU:HD22	2.47	0.43
2:B1:245:ARG:HH11	2:B1:245:ARG:HD3	1.53	0.43
2:B1:259:ALA:O	2:B1:260:GLU:C	2.61	0.43
3:C1:34:GLY:O	3:C1:37:LEU:CB	2.57	0.43
3:C1:89:MET:O	3:C1:90:PHE:C	2.62	0.43
3:C1:122:THR:CG2	3:C1:189:ILE:CG1	2.96	0.43
4:D1:220:TYR:CD2	7:G1:26:PHE:CZ	3.06	0.43
10:J1:31:PHE:CD1	10:J1:31:PHE:C	2.96	0.43
1:M1:4:TYR:CD1	2:N1:43:PRO:HB3	2.53	0.43
1:M1:134:ILE:HA	1:M1:134:ILE:HD13	1.53	0.43
1:M1:145:MET:CE	1:M1:248:LEU:HD12	2.48	0.43
1:M1:153:LEU:CD2	1:M1:319:LEU:HD13	2.48	0.43
1:M1:271:GLN:O	1:M1:272:VAL:C	2.59	0.43
1:M1:366:VAL:HG11	2:N1:44:ALA:HB2	1.99	0.43
2:N1:207:ILE:CD1	2:N1:383:GLY:CA	2.93	0.43
3:O1:207:ASN:OD1	3:O1:207:ASN:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O1:319:PRO:O	3:O1:320:LEU:C	2.61	0.43
4:P1:7:PRO:HB3	4:P1:125:ASP:HB3	2.01	0.43
4:P1:165:TYR:CE1	4:P1:168:VAL:HA	2.54	0.43
4:P1:229:VAL:HG12	4:P1:233:ARG:NE	2.32	0.43
5:Q1:122:HIS:ND1	5:Q1:124:LEU:N	2.57	0.43
10:V1:44:GLU:O	10:V1:45:HIS:C	2.62	0.43
14:42:34:ILE:O	14:42:37:THR:OG1	2.33	0.43
17:82:418:GLN:HE21	19:A2:115:GLY:C	2.21	0.43
19:A2:560:LEU:HD12	19:A2:561:PRO:HD2	1.99	0.43
20:B2:267:ILE:O	20:B2:271:ARG:N	2.49	0.43
36:S2:280:HIS:O	36:S2:283:ARG:N	2.51	0.43
54:g2:162:ARG:HA	54:g2:165:ALA:HB3	2.00	0.43
57:B3:63:THR:HA	57:B3:66:THR:HG22	2.00	0.43
58:C3:40:MET:O	58:C3:41:THR:C	2.62	0.43
60:E3:27:TRP:CH2	61:F3:86:GLY:HA2	2.54	0.43
62:G3:42:ARG:HG3	62:G3:42:ARG:NH1	2.32	0.43
64:I3:21:ILE:O	64:I3:25:PHE:HD2	2.02	0.43
64:I3:68:ILE:HG13	64:I3:69:PHE:N	2.33	0.43
65:J3:30:ILE:HG13	65:J3:31:LEU:N	2.33	0.43
66:K3:44:PRO:HA	66:K3:47:ARG:NH1	2.34	0.43
2:B1:348:ALA:CB	2:B1:418:VAL:HG21	2.49	0.43
3:C1:92:ILE:HG12	3:C1:272:TRP:CH2	2.54	0.43
3:C1:109:PHE:HE2	3:C1:203:THR:HG1	1.58	0.43
3:C1:200:LEU:HD13	69:C1:402:HEM:CAD	2.49	0.43
3:C1:342:PRO:HG2	7:G1:66:PHE:CZ	2.53	0.43
10:J1:52:TRP:CG	10:J1:53:LYS:N	2.86	0.43
1:M1:64:PHE:HE2	1:M1:88:ALA:HB2	1.81	0.43
2:N1:283:PRO:HG3	9:U1:55:LEU:CG	2.49	0.43
2:N1:332:SER:O	2:N1:333:ALA:C	2.60	0.43
2:N1:334:GLY:O	2:N1:335:ASP:C	2.60	0.43
2:N1:357:VAL:O	2:N1:360:ALA:HB3	2.18	0.43
3:O1:257:THR:O	3:O1:258:PRO:C	2.62	0.43
4:P1:91:PHE:HA	4:P1:92:PRO:HD3	1.60	0.43
4:P1:195:GLU:HA	4:P1:196:PRO:HD2	1.73	0.43
5:Q1:14:ARG:HA	7:S1:23:GLN:HA	2.01	0.43
5:Q1:141:HIS:CE1	5:Q1:175:PRO:HG2	2.54	0.43
9:U1:70:LEU:CD2	9:U1:73:PRO:CD	2.92	0.43
19:A2:650:SER:OG	19:A2:652:ASN:OD1	2.30	0.43
20:B2:238:LEU:HD23	39:V2:10:MET:HE1	1.99	0.43
20:B2:278:VAL:HG12	20:B2:283:ALA:HB2	2.00	0.43
27:I2:105:LYS:HB3	27:I2:105:LYS:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:12:65:THR:OG1	52:12:124:ASN:ND2	2.49	0.43
53:62:15:LEU:HD21	53:62:125:LEU:HD22	1.99	0.43
56:A3:513:LEU:HD12	56:A3:513:LEU:HA	1.65	0.43
57:B3:52:HIS:CD2	60:E3:40:ASP:HB2	2.54	0.43
58:C3:148:HIS:CE1	58:C3:152:MET:HE3	2.54	0.43
63:H3:57:ARG:HB3	63:H3:57:ARG:NH1	2.31	0.43
1:A1:19:LEU:HD22	1:A1:214:LYS:NZ	2.34	0.43
2:B1:110:GLU:O	2:B1:111:CYS:HB3	2.18	0.43
2:B1:122:PHE:O	2:B1:126:VAL:HG23	2.18	0.43
2:B1:369:LEU:O	2:B1:370:MET:C	2.61	0.43
3:C1:9:PRO:CG	3:C1:12:LYS:HB2	2.45	0.43
3:C1:37:LEU:CD1	3:C1:97:HIS:CD2	3.02	0.43
3:C1:71:ARG:HB3	4:D1:49:ARG:HH22	1.84	0.43
3:C1:107:TYR:HE2	3:C1:305:PRO:HA	1.83	0.43
3:C1:196:HIS:HE1	69:C1:402:HEM:C1D	2.37	0.43
3:C1:218:ILE:CG2	3:C1:219:PRO:N	2.82	0.43
4:D1:41:HIS:CD2	70:D1:301:HEC:NB	2.84	0.43
6:F1:49:ARG:NH2	6:F1:100:GLU:OE2	2.47	0.43
2:N1:47:ILE:HB	2:N1:109:VAL:CG1	2.49	0.43
2:N1:363:LYS:O	2:N1:364:LEU:C	2.61	0.43
2:N1:372:VAL:O	2:N1:372:VAL:CG1	2.67	0.43
3:O1:119:LEU:CD1	3:O1:192:ILE:CG2	2.97	0.43
3:O1:338:ILE:HA	3:O1:341:GLN:CG	2.49	0.43
4:P1:150:ASN:OD1	4:P1:151:PRO:HD2	2.19	0.43
4:P1:220:TYR:O	4:P1:223:LYS:N	2.52	0.43
6:R1:94:LEU:O	6:R1:98:ILE:HG13	2.19	0.43
16:72:25:SER:O	16:72:27:ILE:N	2.47	0.43
19:A2:162:ASP:O	27:I2:105:LYS:CE	2.66	0.43
19:A2:251:ILE:HB	19:A2:606:THR:HG22	2.01	0.43
19:A2:313:LEU:N	38:U2:142:THR:CA	2.78	0.43
20:B2:398:THR:OG1	20:B2:399:ALA:N	2.52	0.43
42:Y2:57:GLN:HE22	53:62:445:GLU:HB3	1.83	0.43
58:C3:41:THR:O	58:C3:45:ILE:HG13	2.18	0.43
1:A1:86:LEU:HD12	1:A1:98:TYR:O	2.19	0.43
1:A1:86:LEU:CD1	1:A1:99:ILE:HG12	2.44	0.43
1:A1:152:TYR:O	1:A1:153:LEU:C	2.57	0.43
3:C1:336:THR:O	3:C1:336:THR:HG22	2.18	0.43
7:G1:36:ASN:OD1	7:G1:39:ARG:NE	2.52	0.43
8:H1:15:ASP:HB2	8:H1:16:PRO:HD3	2.01	0.43
1:M1:73:ASN:O	1:M1:77:LYS:CD	2.66	0.43
1:M1:281:ASP:HB3	1:M1:284:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:349:ALA:HB3	1:M1:408:ARG:NE	2.34	0.43
2:N1:67:HIS:HD2	2:N1:144:LEU:CD2	2.16	0.43
3:O1:7:SER:O	3:O1:8:HIS:C	2.61	0.43
3:O1:103:TYR:CE1	3:O1:322:GLN:HG3	2.53	0.43
3:O1:230:LEU:O	3:O1:230:LEU:HG	2.17	0.43
4:P1:5:LEU:HG	4:P1:152:TYR:CE1	2.54	0.43
5:Q1:20:ASP:O	5:Q1:22:THR:N	2.52	0.43
5:Q1:182:VAL:C	5:Q1:183:PRO:O	2.57	0.43
6:R1:101:ARG:HG2	6:R1:105:GLU:OE2	2.19	0.43
12:22:200:MET:HG2	12:22:341:PRO:HB3	2.01	0.43
18:92:153:GLN:HG3	18:92:158:ILE:HG13	2.00	0.43
19:A2:144:MET:HG2	20:B2:380:HIS:HD2	1.80	0.43
23:E2:170:GLY:HA2	23:E2:171:PRO:HD3	1.78	0.43
48:f2:35:ASP:HA	48:f2:38:ARG:HB3	2.01	0.43
56:A3:70:VAL:HG11	56:A3:246:LEU:HD22	2.00	0.43
58:C3:110:PRO:HB3	63:H3:30:TRP:CD2	2.54	0.43
62:G3:5:LYS:CD	62:G3:6:GLY:N	2.81	0.43
67:L3:41:ARG:HD2	68:M3:40:TYR:CZ	2.54	0.43
1:A1:3:THR:O	1:A1:4:TYR:C	2.62	0.43
1:A1:136:GLN:HE21	9:I1:50:LEU:HG	1.84	0.43
1:A1:255:ILE:HD12	1:A1:335:MET:HE1	2.01	0.43
1:A1:343:MET:H	1:A1:343:MET:HG2	1.34	0.43
2:B1:295:LEU:O	2:B1:299:VAL:HG23	2.19	0.43
3:C1:307:LEU:O	3:C1:308:HIS:C	2.62	0.43
3:C1:368:THR:O	3:C1:369:ALA:C	2.62	0.43
4:D1:21:LEU:CD1	4:D1:26:ILE:HD11	2.49	0.43
1:M1:19:LEU:CD1	1:M1:214:LYS:HG2	2.48	0.43
1:M1:213:GLN:CB	1:M1:215:HIS:CD2	3.02	0.43
2:N1:70:ARG:HD2	9:U1:69:SER:HB3	2.01	0.43
6:R1:87:LYS:HE2	6:R1:89:TYR:HB3	2.01	0.43
8:T1:22:GLU:O	8:T1:23:GLN:C	2.60	0.43
19:A2:140:GLN:HE22	20:B2:382:PHE:HE2	1.66	0.43
21:C2:165:ALA:HB1	21:C2:169:GLU:HG3	2.00	0.43
54:g2:76:GLU:HA	54:g2:77:CYS:HA	1.74	0.43
57:B3:3:TYR:CD1	57:B3:3:TYR:N	2.87	0.43
61:F3:53:THR:HG22	61:F3:54:ASN:OD1	2.19	0.43
65:J3:36:MET:O	65:J3:40:LEU:HG	2.18	0.43
1:A1:80:GLU:C	1:A1:82:MET:N	2.77	0.42
1:A1:260:PRO:HG3	1:A1:414:TYR:OH	2.19	0.42
1:A1:343:MET:CE	1:A1:416:TYR:HD2	2.17	0.42
3:C1:157:GLY:O	3:C1:160:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:316:MET:HG2	3:C1:317:PHE:CD1	2.54	0.42
4:D1:3:LEU:HD22	7:G1:70:LYS:HZ3	1.81	0.42
4:D1:10:TYR:CE1	4:D1:128:PHE:CE2	3.07	0.42
4:D1:116:ILE:CD1	4:D1:120:ARG:HG3	2.49	0.42
4:D1:209:LEU:O	4:D1:210:LEU:C	2.62	0.42
7:G1:44:CYS:O	7:G1:47:ARG:N	2.47	0.42
11:K1:20:THR:HG23	11:K1:24:TRP:CD1	2.54	0.42
1:M1:56:GLY:O	1:M1:57:TYR:C	2.59	0.42
1:M1:283:THR:OG1	9:U1:74:ALA:HB3	2.19	0.42
2:N1:24:LEU:H	2:N1:24:LEU:CD1	2.18	0.42
2:N1:211:VAL:HG12	2:N1:212:SER:N	2.34	0.42
2:N1:367:GLY:O	2:N1:368:TYR:C	2.61	0.42
3:O1:211:ILE:HG22	3:O1:212:SER:N	2.34	0.42
4:P1:94:PRO:HB2	4:P1:95:TYR:CD1	2.54	0.42
12:22:63:GLN:HA	12:22:66:ALA:HB3	2.01	0.42
12:22:257:LEU:HD23	12:22:257:LEU:HA	1.89	0.42
17:82:160:GLY:HA2	17:82:199:ARG:HD2	2.00	0.42
19:A2:605:GLN:HG3	19:A2:607:LYS:HZ2	1.84	0.42
21:C2:86:LEU:HB2	21:C2:143:ILE:HG13	2.01	0.42
21:C2:99:LEU:O	21:C2:103:ARG:N	2.52	0.42
26:H2:96:PRO:HA	26:H2:97:HIS:HA	1.65	0.42
36:S2:150:SER:OG	36:S2:151:ILE:N	2.51	0.42
41:X2:14:VAL:HA	41:X2:17:PRO:HD2	2.01	0.42
53:62:68:TRP:H	53:62:77:SER:HA	1.84	0.42
64:I3:61:GLU:OE1	64:I3:64:ARG:NH1	2.51	0.42
65:J3:11:LEU:HD23	65:J3:11:LEU:C	2.44	0.42
1:A1:29:GLN:HA	1:A1:201:GLY:O	2.18	0.42
1:A1:248:LEU:HA	1:A1:249:PRO:HD3	1.59	0.42
1:A1:311:ASN:CG	1:A1:320:LEU:CD2	2.91	0.42
2:B1:79:GLY:H	2:B1:125:ASN:HD22	1.67	0.42
2:B1:286:LYS:HD3	2:B1:287:ARG:HH12	1.81	0.42
3:C1:90:PHE:CZ	3:C1:123:VAL:HG21	2.54	0.42
4:D1:214:LEU:O	4:D1:218:LEU:HG	2.19	0.42
6:F1:87:LYS:HG3	6:F1:89:TYR:HB3	2.01	0.42
6:F1:103:GLU:O	6:F1:104:ARG:C	2.62	0.42
7:G1:39:ARG:HA	7:G1:42:ARG:HD2	2.00	0.42
1:M1:38:GLY:HA3	1:M1:40:TRP:CZ3	2.49	0.42
1:M1:277:ILE:HG22	1:M1:294:LEU:HD12	1.99	0.42
2:N1:163:LEU:HD22	2:N1:256:ALA:HB1	2.01	0.42
2:N1:264:ILE:HB	2:N1:316:TYR:C	2.44	0.42
4:P1:139:THR:CB	8:T1:44:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:29:SER:CB	5:Q1:32:ARG:HD3	2.49	0.42
12:22:80:PHE:HB3	26:H2:64:ARG:HH12	1.82	0.42
23:E2:119:CYS:SG	23:E2:120:GLU:N	2.92	0.42
52:12:196:ALA:HB2	52:12:274:ARG:HH21	1.83	0.42
53:62:88:MET:HE1	53:62:468:ILE:HD13	2.00	0.42
55:e2:77:LYS:CG	55:e2:78:LEU:H	2.32	0.42
56:A3:106:PRO:HB2	56:A3:107:PRO:HD3	2.01	0.42
62:G3:5:LYS:NZ	62:G3:6:GLY:N	2.54	0.42
64:I3:26:MET:N	64:I3:26:MET:SD	2.91	0.42
1:A1:297:ILE:H	1:A1:297:ILE:HG12	1.63	0.42
1:A1:311:ASN:OD1	1:A1:320:LEU:HD23	2.18	0.42
1:A1:328:HIS:NE2	1:A1:329:MET:HG2	2.35	0.42
2:B1:295:LEU:HD12	2:B1:295:LEU:HA	1.88	0.42
3:C1:235:LEU:HG	3:C1:236:ILE:N	2.32	0.42
3:C1:257:THR:O	3:C1:258:PRO:C	2.61	0.42
1:M1:63:ALA:HB2	1:M1:97:TYR:HE2	1.84	0.42
1:M1:85:HIS:CD2	2:N1:370:MET:HE1	2.54	0.42
2:N1:279:LEU:HD23	2:N1:295:LEU:HD13	2.00	0.42
3:O1:44:GLN:OE1	3:O1:44:GLN:HA	2.19	0.42
3:O1:146:ILE:O	3:O1:147:THR:C	2.62	0.42
5:Q1:40:THR:HG22	10:V1:20:PHE:CZ	2.51	0.42
5:Q1:102:THR:H	5:Q1:105:GLU:CB	2.32	0.42
18:92:92:TRP:HB3	18:92:127:VAL:HG22	2.00	0.42
19:A2:674:LEU:CD1	29:K2:46:LYS:CE	2.90	0.42
22:D2:108:ARG:HD3	52:12:36:GLY:HA2	2.01	0.42
34:Q2:30:HIS:CD2	34:Q2:120:PRO:HG2	2.55	0.42
34:Q2:137:LEU:HD12	34:Q2:138:PRO:HD2	2.01	0.42
46:c2:40:VAL:HA	46:c2:41:SER:HA	1.63	0.42
56:A3:474:GLU:HG3	56:A3:475:ALA:N	2.34	0.42
57:B3:162:SER:HB3	57:B3:197:SER:C	2.44	0.42
58:C3:80:ARG:HG2	58:C3:233:PHE:CE1	2.54	0.42
59:D3:37:GLN:O	59:D3:41:LYS:HG2	2.18	0.42
60:E3:43:PRO:HB2	60:E3:48:ILE:CD1	2.48	0.42
1:A1:61:HIS:HB2	1:A1:130:GLU:HG3	2.00	0.42
1:A1:80:GLU:O	1:A1:81:SER:C	2.63	0.42
1:A1:381:ARG:O	1:A1:382:SER:C	2.62	0.42
3:C1:78:ILE:HG21	3:C1:78:ILE:HD13	1.80	0.42
3:C1:235:LEU:HD12	3:C1:235:LEU:O	2.19	0.42
3:C1:239:LEU:O	3:C1:243:VAL:HB	2.19	0.42
4:D1:43:MET:HA	4:D1:112:ASP:OD1	2.20	0.42
6:F1:48:ARG:HD3	6:F1:48:ARG:HA	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:88:SER:O	6:F1:92:PRO:HD3	2.18	0.42
10:J1:24:ILE:O	10:J1:25:VAL:C	2.62	0.42
1:M1:59:VAL:CG2	1:M1:186:LEU:HD11	2.50	0.42
2:N1:59:ASN:OD1	2:N1:60:SER:N	2.43	0.42
2:N1:90:GLU:O	2:N1:91:ALA:C	2.62	0.42
3:O1:183:PHE:CE1	3:O1:187:PHE:HE2	2.37	0.42
3:O1:192:ILE:N	3:O1:192:ILE:CD1	2.82	0.42
3:O1:235:LEU:O	3:O1:235:LEU:HD12	2.19	0.42
3:O1:366:MET:N	3:O1:367:PRO:HD2	2.33	0.42
4:P1:116:ILE:O	4:P1:117:VAL:C	2.60	0.42
4:P1:149:PHE:CZ	8:T1:55:THR:HG23	2.53	0.42
4:P1:192:TRP:CE3	4:P1:193:ALA:N	2.88	0.42
5:Q1:114:VAL:HG13	5:Q1:120:PRO:HB3	2.01	0.42
5:Q1:134:ILE:HD13	5:Q1:134:ILE:HG21	1.76	0.42
5:Q1:172:ARG:HE	5:Q1:172:ARG:HB3	1.67	0.42
6:R1:71:ARG:O	6:R1:72:GLN:HB2	2.19	0.42
8:T1:67:HIS:O	8:T1:68:CYS:C	2.63	0.42
14:42:62:SER:HB2	14:42:457:PRO:HD3	2.00	0.42
18:92:195:ASP:OD2	18:92:220:SER:OG	2.34	0.42
19:A2:111:LYS:CE	33:P2:53:TYR:CE2	2.93	0.42
20:B2:116:LEU:HA	22:D2:130:THR:HG21	2.02	0.42
20:B2:193:ASP:O	20:B2:194:ILE:C	2.61	0.42
35:R2:200:ILE:O	35:R2:262:THR:OG1	2.30	0.42
36:S2:187:LEU:HD13	36:S2:277:ARG:HB2	2.01	0.42
48:f2:166:LEU:HA	48:f2:167:TRP:HA	1.64	0.42
53:62:492:ILE:HA	53:62:495:ILE:HD12	2.02	0.42
56:A3:377:PHE:CD2	79:A3:602:HEA:HAD1	2.53	0.42
57:B3:5:MET:CE	66:K3:42:PRO:HA	2.45	0.42
1:A1:151:ASN:O	1:A1:154:HIS:N	2.53	0.42
1:A1:277:ILE:O	1:A1:292:SER:OG	2.30	0.42
2:B1:83:PHE:CE1	6:R1:104:ARG:HG2	2.54	0.42
2:B1:92:VAL:O	2:B1:92:VAL:CG1	2.68	0.42
2:B1:92:VAL:HG11	2:B1:115:ASP:HB3	2.02	0.42
2:B1:206:LEU:HA	2:B1:206:LEU:HD12	1.85	0.42
3:C1:248:ASP:CG	4:D1:118:ARG:HH21	2.28	0.42
3:C1:372:ILE:HD13	3:C1:372:ILE:HG21	1.84	0.42
4:D1:116:ILE:CD1	4:D1:120:ARG:HH11	2.32	0.42
4:D1:158:ILE:CG1	4:D1:159:GLY:N	2.82	0.42
5:E1:51:ALA:O	5:E1:52:LYS:C	2.62	0.42
6:F1:64:ARG:O	6:F1:68:LEU:HD12	2.20	0.42
10:J1:43:TYR:O	10:J1:43:TYR:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:149:VAL:CG1	1:M1:150:PHE:N	2.81	0.42
1:M1:195:MET:HE3	1:M1:195:MET:HB3	1.61	0.42
1:M1:334:MET:HA	1:M1:334:MET:CE	2.49	0.42
2:N1:72:ALA:HB1	2:N1:75:LEU:CD1	2.49	0.42
2:N1:99:THR:OG1	9:U1:68:VAL:HG13	2.19	0.42
2:N1:102:ARG:NH1	2:N1:174:ASN:O	2.53	0.42
2:N1:312:PHE:CD1	9:U1:58:GLN:O	2.73	0.42
3:O1:170:VAL:O	3:O1:170:VAL:CG1	2.68	0.42
3:O1:218:ILE:HG22	3:O1:223:TYR:HD2	1.85	0.42
4:P1:23:HIS:O	4:P1:26:ILE:HB	2.20	0.42
4:P1:178:THR:HG23	8:T1:15:ASP:N	2.34	0.42
4:P1:233:ARG:O	4:P1:234:LYS:HE2	2.19	0.42
5:Q1:62:MET:HE3	5:Q1:62:MET:HB3	1.79	0.42
5:Q1:97:PHE:CD1	5:Q1:137:GLY:HA3	2.54	0.42
6:R1:73:GLN:HG2	7:S1:36:ASN:ND2	2.34	0.42
6:R1:84:GLU:H	6:R1:84:GLU:CD	2.28	0.42
17:82:316:ALA:HB1	17:82:326:LEU:HD22	2.02	0.42
19:A2:380:ASP:HB2	29:K2:41:TYR:OH	2.20	0.42
23:E2:38:TYR:HB2	33:P2:106:LEU:HA	2.00	0.42
30:L2:25:ILE:HB	52:12:299:ALA:HB1	2.00	0.42
36:S2:202:VAL:HA	36:S2:205:ARG:HB2	2.01	0.42
46:c2:22:TRP:O	46:c2:26:GLN:N	2.52	0.42
53:62:358:LYS:HB3	53:62:437:PHE:HA	2.02	0.42
60:E3:90:ARG:HD3	60:E3:90:ARG:HA	1.77	0.42
66:K3:9:PHE:CD1	66:K3:9:PHE:C	2.97	0.42
1:A1:54:GLY:O	1:A1:55:ALA:O	2.37	0.42
1:A1:56:GLY:O	1:A1:59:VAL:HB	2.19	0.42
1:A1:213:GLN:HB3	1:A1:215:HIS:CD2	2.53	0.42
1:A1:436:ARG:NE	3:C1:222:PRO:HG3	2.33	0.42
2:B1:158:HIS:ND1	2:B1:246:GLU:OE1	2.52	0.42
3:C1:3:ASN:HA	3:C1:8:HIS:CD2	2.55	0.42
3:C1:126:THR:HG21	69:C1:401:HEM:C3B	2.54	0.42
4:D1:50:HIS:HB3	4:D1:54:VAL:HG21	2.01	0.42
10:J1:49:GLY:H	10:J1:54:HIS:CD2	2.37	0.42
1:M1:28:GLU:OE1	1:M1:375:VAL:CG1	2.68	0.42
1:M1:168:GLU:H	1:M1:168:GLU:HG3	1.66	0.42
2:N1:29:LEU:HG	2:N1:33:LEU:CD2	2.50	0.42
2:N1:213:HIS:HD2	2:N1:213:HIS:O	2.02	0.42
3:O1:244:LEU:O	4:P1:201:ARG:HG2	2.20	0.42
4:P1:43:MET:HE3	4:P1:91:PHE:CE2	2.54	0.42
4:P1:139:THR:CG2	8:T1:44:VAL:HB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q1:129:LYS:HA	5:Q1:130:PRO:HD2	1.85	0.42
19:A2:63:PHE:O	19:A2:181:ARG:NH2	2.51	0.42
19:A2:359:ASN:HD21	29:K2:17:ARG:HG2	1.85	0.42
20:B2:447:VAL:HA	20:B2:450:ILE:HD12	2.02	0.42
23:E2:53:VAL:O	23:E2:57:ALA:N	2.53	0.42
27:I2:108:LYS:HA	27:I2:120:ARG:HA	2.01	0.42
32:O2:77:ARG:HA	32:O2:80:ASP:HB3	2.01	0.42
53:62:163:ASP:O	53:62:167:ALA:N	2.51	0.42
56:A3:311:ILE:HG21	56:A3:311:ILE:HD13	1.75	0.42
58:C3:137:LEU:HA	58:C3:137:LEU:HD12	1.69	0.42
58:C3:154:GLY:CA	61:F3:6:VAL:HG22	2.47	0.42
63:H3:57:ARG:HA	63:H3:60:TYR:CD2	2.55	0.42
3:C1:30:TRP:O	3:C1:33:PHE:CD2	2.62	0.42
3:C1:36:LEU:HD22	3:C1:235:LEU:HB2	2.02	0.42
3:C1:73:VAL:O	3:C1:73:VAL:HG12	2.19	0.42
4:D1:237:TYR:HE2	4:D1:239:PRO:HG3	1.80	0.42
6:F1:10:SER:HA	6:F1:13:LEU:HG	2.01	0.42
1:M1:88:ALA:O	2:N1:286:LYS:HD2	2.20	0.42
1:M1:100:LYS:HG2	2:N1:370:MET:SD	2.59	0.42
2:N1:34:VAL:O	2:N1:35:ILE:HG22	2.19	0.42
2:N1:156:GLN:OE1	9:U1:58:GLN:NE2	2.39	0.42
2:N1:201:SER:OG	2:N1:226:ILE:N	2.51	0.42
2:N1:304:HIS:HD2	2:N1:306:PRO:CD	2.28	0.42
3:O1:126:THR:CG2	69:O1:401:HEM:C3B	3.01	0.42
7:S1:71:ARG:NH2	8:T1:60:ASP:OD1	2.38	0.42
19:A2:359:ASN:ND2	29:K2:68:ARG:HH22	2.17	0.42
21:C2:116:LEU:HD23	21:C2:168:TYR:HB3	2.02	0.42
23:E2:79:ARG:NH2	33:P2:19:ASP:OD2	2.50	0.42
28:J2:55:SER:OG	28:J2:56:GLY:N	2.52	0.42
53:62:336:LYS:HA	53:62:339:LEU:HB3	2.01	0.42
53:62:583:LEU:HD23	53:62:586:LEU:HD13	2.02	0.42
79:A3:601:HEA:HHC	79:A3:601:HEA:H122	2.02	0.42
1:A1:5:ALA:O	1:A1:6:GLN:O	2.38	0.42
1:A1:106:LEU:HA	1:A1:106:LEU:HD12	1.74	0.42
1:A1:255:ILE:CD1	1:A1:335:MET:HE1	2.49	0.42
1:A1:257:VAL:N	1:A1:320:LEU:O	2.48	0.42
1:A1:262:TRP:CE3	1:A1:385:THR:CG2	3.02	0.42
1:A1:280:TYR:CD1	1:A1:280:TYR:C	2.98	0.42
1:A1:366:VAL:HG11	2:B1:44:ALA:HB2	2.01	0.42
2:B1:57:TYR:HB3	2:B1:198:HIS:CE1	2.55	0.42
2:B1:72:ALA:HB2	2:B1:140:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:162:ASN:CB	2:B1:244:ILE:HG21	2.50	0.42
2:B1:239:TYR:OH	2:B1:423:SER:OG	2.37	0.42
3:C1:177:ARG:O	3:C1:181:PHE:CD2	2.72	0.42
3:C1:313:ARG:HH11	3:C1:313:ARG:HD2	1.59	0.42
4:D1:7:PRO:HB2	4:D1:125:ASP:CB	2.49	0.42
4:D1:69:GLU:O	4:D1:73:GLY:CA	2.67	0.42
4:D1:171:PHE:HZ	4:D1:182:VAL:HG22	1.85	0.42
4:D1:187:CYS:O	4:D1:188:THR:C	2.60	0.42
4:D1:211:MET:HA	4:D1:211:MET:CE	2.49	0.42
4:D1:237:TYR:HD1	7:G1:13:VAL:HG22	1.85	0.42
1:M1:67:THR:OG1	1:M1:119:ASN:HB2	2.20	0.42
1:M1:329:MET:HA	1:M1:329:MET:CE	2.50	0.42
2:N1:31:ASN:HB3	2:N1:201:SER:CB	2.50	0.42
2:N1:294:SER:O	2:N1:297:GLN:N	2.53	0.42
3:O1:234:LEU:O	3:O1:237:LEU:HB3	2.19	0.42
3:O1:314:SER:OG	3:O1:316:MET:HB3	2.19	0.42
4:P1:58:GLU:O	4:P1:62:LYS:HB2	2.19	0.42
4:P1:206:LEU:O	4:P1:207:LYS:C	2.61	0.42
4:P1:240:PRO:CG	4:P1:241:LYS:H	2.33	0.42
6:R1:67:ASP:HA	6:R1:70:MET:HE3	2.01	0.42
17:82:297:LYS:N	17:82:333:GLU:O	2.45	0.42
19:A2:34:VAL:HG13	19:A2:100:TRP:H	1.84	0.42
19:A2:140:GLN:NE2	20:B2:382:PHE:CD2	2.88	0.42
19:A2:583:ILE:CD1	38:U2:137:TRP:HZ3	2.31	0.42
23:E2:211:TYR:CZ	33:P2:39:PRO:HG3	2.55	0.42
29:K2:55:ILE:O	29:K2:56:ARG:NH1	2.43	0.42
35:R2:266:VAL:HG23	35:R2:335:LEU:HB3	2.02	0.42
36:S2:187:LEU:HA	36:S2:188:PRO:HD3	1.84	0.42
43:Z2:24:ILE:HG23	43:Z2:54:MET:HE1	2.02	0.42
53:62:439:THR:OG1	53:62:440:LEU:N	2.42	0.42
56:A3:247:ILE:HB	79:A3:602:HEA:HBC1	2.01	0.42
1:A1:38:GLY:HA3	1:A1:40:TRP:CZ3	2.50	0.42
1:A1:64:PHE:CE1	1:A1:86:LEU:CG	2.81	0.42
1:A1:361:LEU:HD12	1:A1:361:LEU:O	2.19	0.42
2:B1:81:SER:O	2:B1:82:SER:C	2.62	0.42
2:B1:129:ALA:O	2:B1:130:PRO:C	2.62	0.42
2:B1:312:PHE:N	2:B1:323:GLY:O	2.47	0.42
3:C1:172:LYS:O	3:C1:173:ALA:C	2.60	0.42
4:D1:8:PRO:O	4:D1:125:ASP:CG	2.63	0.42
4:D1:57:THR:CG2	4:D1:58:GLU:N	2.83	0.42
4:D1:223:LYS:NZ	4:D1:227:TRP:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:94:LEU:O	6:F1:94:LEU:HD12	2.20	0.42
10:J1:3:PRO:O	10:J1:4:THR:C	2.63	0.42
1:M1:158:PHE:HB2	1:M1:164:ALA:HB2	2.02	0.42
1:M1:213:GLN:HB2	1:M1:215:HIS:CD2	2.55	0.42
1:M1:345:LEU:HA	1:M1:345:LEU:HD23	1.69	0.42
1:M1:420:PRO:HG3	1:M1:441:MET:SD	2.60	0.42
1:M1:428:ILE:CG2	1:M1:431:LEU:CG	2.97	0.42
3:O1:14:VAL:O	3:O1:14:VAL:HG12	2.20	0.42
3:O1:41:LEU:HD12	69:O1:401:HEM:HBB1	2.00	0.42
5:Q1:13:TYR:O	7:S1:24:ARG:HG3	2.20	0.42
12:22:7:ILE:O	12:22:11:LEU:N	2.53	0.42
15:52:32:CYS:O	15:52:36:MET:N	2.53	0.42
74:82:501:FMN:O4'	74:82:501:FMN:O2'	2.34	0.42
19:A2:511:LYS:HD3	19:A2:663:ASN:HB3	2.02	0.42
19:A2:613:PRO:CG	38:U2:134:ILE:HG21	2.46	0.42
52:12:75:PRO:CB	52:12:223:PHE:CZ	2.99	0.42
52:12:126:LYS:CD	52:12:126:LYS:C	2.89	0.42
56:A3:356:ILE:HD13	56:A3:356:ILE:HA	1.90	0.42
59:D3:126:MET:HG3	59:D3:128:VAL:HG23	2.00	0.42
60:E3:93:LEU:HD23	60:E3:93:LEU:HA	1.88	0.42
1:A1:43:ALA:CB	1:A1:189:HIS:CB	2.97	0.42
2:B1:283:PRO:CG	9:I1:55:LEU:HD13	2.50	0.42
3:C1:53:MET:SD	3:O1:181:PHE:HZ	2.43	0.42
3:C1:159:ASN:O	3:C1:162:GLU:HB2	2.20	0.42
3:C1:184:ILE:O	3:C1:184:ILE:HG12	2.19	0.42
3:C1:317:PHE:CD1	6:F1:26:PHE:HB3	2.55	0.42
3:C1:365:LEU:O	3:C1:366:MET:C	2.61	0.42
3:C1:373:GLU:O	3:C1:377:LEU:HD12	2.19	0.42
4:D1:44:ASP:OD1	4:D1:93:LYS:HE3	2.20	0.42
4:D1:57:THR:CG2	4:D1:58:GLU:H	2.32	0.42
4:D1:146:GLY:O	4:D1:148:TYR:CD1	2.73	0.42
4:D1:162:PRO:O	4:D1:163:PRO:C	2.63	0.42
11:K1:20:THR:HG23	11:K1:24:TRP:HD1	1.83	0.42
1:M1:152:TYR:CE2	1:M1:243:HIS:HD2	2.38	0.42
2:N1:81:SER:O	2:N1:82:SER:C	2.63	0.42
2:N1:343:GLN:O	2:N1:343:GLN:HG3	2.20	0.42
3:O1:233:LEU:HD12	3:O1:233:LEU:HA	1.74	0.42
4:P1:115:TYR:O	4:P1:116:ILE:C	2.60	0.42
9:U1:66:ALA:O	9:U1:77:ARG:HG3	2.20	0.42
11:W1:20:THR:HG23	11:W1:24:TRP:HD1	1.85	0.42
35:R2:320:GLU:O	35:R2:324:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:135:LEU:HA	36:S2:138:LEU:HD13	2.02	0.42
45:b2:96:ALA:HA	45:b2:97:GLU:HA	1.67	0.42
55:e2:75:TYR:H	55:e2:75:TYR:HD2	1.68	0.42
58:C3:224:LYS:NZ	58:C3:226:HIS:HE2	2.18	0.42
59:D3:86:MET:O	66:K3:25:CYS:HB2	2.20	0.42
61:F3:86:GLY:O	61:F3:87:THR:O	2.37	0.42
64:I3:35:TYR:O	64:I3:39:VAL:HB	2.19	0.42
68:M3:19:LEU:HD23	68:M3:19:LEU:C	2.45	0.42
1:A1:253:VAL:O	1:A1:323:HIS:HA	2.20	0.41
1:A1:292:SER:O	1:A1:293:PRO:C	2.63	0.41
2:B1:168:TYR:CB	2:B1:173:ALA:HB2	2.44	0.41
2:B1:282:GLY:HA2	2:B1:283:PRO:HD2	1.77	0.41
3:C1:234:LEU:HD21	4:D1:216:LEU:HD21	2.01	0.41
4:D1:29:GLY:HA2	4:D1:32:VAL:HG23	2.02	0.41
4:D1:150:ASN:OD1	4:D1:150:ASN:C	2.59	0.41
10:J1:20:PHE:O	10:J1:23:THR:HB	2.20	0.41
1:M1:69:ASN:C	1:M1:71:PRO:HD3	2.45	0.41
1:M1:78:GLU:HG2	1:M1:112:LEU:HD21	2.01	0.41
1:M1:91:THR:HG22	1:M1:94:HIS:N	2.33	0.41
1:M1:137:GLU:O	1:M1:138:LEU:C	2.63	0.41
2:N1:180:ASP:HA	2:N1:183:ILE:HD12	2.02	0.41
2:N1:243:GLU:HA	2:N1:424:MET:O	2.20	0.41
3:O1:15:ASN:ND2	3:O1:18:PHE:CD2	2.88	0.41
3:O1:123:VAL:O	3:O1:123:VAL:CG1	2.65	0.41
4:P1:10:TYR:CE1	4:P1:128:PHE:HE2	2.36	0.41
4:P1:25:SER:O	4:P1:26:ILE:C	2.61	0.41
4:P1:164:ILE:CD1	4:P1:186:VAL:HG21	2.50	0.41
4:P1:206:LEU:HG	4:P1:210:LEU:HD11	2.02	0.41
10:V1:31:PHE:CD2	10:V1:31:PHE:C	2.98	0.41
14:42:45:PHE:HA	14:42:46:GLY:HA3	1.68	0.41
20:B2:194:ILE:HD13	20:B2:268:TRP:HE1	1.85	0.41
37:T2:77:SER:HA	37:T2:80:VAL:HG22	2.02	0.41
56:A3:314:ILE:HB	56:A3:315:PRO:CD	2.51	0.41
57:B3:100:MET:HE3	57:B3:157:GLU:HG3	2.02	0.41
58:C3:252:LEU:HD23	58:C3:252:LEU:HA	1.90	0.41
1:A1:33:PRO:O	1:A1:103:SER:CB	2.67	0.41
1:A1:46:ARG:NH2	1:A1:316:ASP:OD1	2.52	0.41
2:B1:342:ASN:O	2:B1:345:LYS:N	2.52	0.41
3:C1:101:GLY:HA2	3:C1:106:SER:HB2	2.02	0.41
3:C1:198:LEU:HD22	3:O1:11:MET:HG2	2.02	0.41
3:C1:264:THR:HG21	5:Q1:144:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:106:ASN:C	4:D1:106:ASN:HD22	2.28	0.41
4:D1:204:MET:O	4:D1:207:LYS:N	2.53	0.41
2:N1:135:TRP:NE1	2:N1:136:GLU:HG3	2.35	0.41
3:O1:211:ILE:CG2	6:R1:62:ILE:HD13	2.50	0.41
3:O1:378:LYS:CD	6:R1:33:ARG:HH12	2.32	0.41
5:Q1:109:GLU:OE2	5:Q1:166:ASP:CG	2.63	0.41
5:Q1:109:GLU:OE2	5:Q1:166:ASP:OD2	2.37	0.41
7:S1:33:GLY:O	7:S1:37:VAL:HB	2.19	0.41
17:82:383:THR:HG23	19:A2:75:CYS:CA	2.32	0.41
18:92:134:VAL:HG23	18:92:171:LEU:HD11	2.01	0.41
19:A2:598:ASN:OD1	19:A2:601:GLY:N	2.53	0.41
21:C2:230:GLN:HE21	21:C2:233:ARG:NH1	2.16	0.41
22:D2:114:ARG:HD2	22:D2:114:ARG:O	2.20	0.41
35:R2:154:GLN:HG3	35:R2:155:VAL:HG23	2.02	0.41
48:f2:162:ASP:HA	48:f2:163:LEU:HA	1.79	0.41
56:A3:354:THR:HG21	56:A3:376:HIS:HA	2.03	0.41
58:C3:146:TRP:CE2	62:G3:17:ARG:HB2	2.56	0.41
58:C3:146:TRP:NE1	62:G3:17:ARG:HB2	2.35	0.41
62:G3:77:PRO:HA	62:G3:82:TYR:HA	2.02	0.41
1:A1:136:GLN:NE2	9:I1:50:LEU:HG	2.35	0.41
2:B1:24:LEU:CG	2:B1:38:LEU:HD11	2.31	0.41
2:B1:134:ARG:HG2	2:B1:135:TRP:N	2.35	0.41
2:B1:154:ASN:O	2:B1:157:ALA:N	2.54	0.41
4:D1:161:ALA:O	4:D1:162:PRO:C	2.63	0.41
1:M1:347:THR:HA	11:W1:16:ASN:HD22	1.85	0.41
1:M1:426:GLY:H	1:M1:428:ILE:HG13	1.83	0.41
2:N1:56:ARG:HH21	2:N1:103:GLU:CD	2.29	0.41
2:N1:200:THR:OG1	2:N1:201:SER:N	2.53	0.41
2:N1:255:ALA:HA	2:N1:426:ALA:HA	2.02	0.41
2:N1:264:ILE:HD12	2:N1:315:SER:OG	2.20	0.41
2:N1:285:VAL:HG12	2:N1:285:VAL:O	2.20	0.41
2:N1:309:VAL:CG2	2:N1:326:THR:HG22	2.50	0.41
3:O1:10:LEU:HD12	3:O1:13:ILE:CD1	2.50	0.41
3:O1:122:THR:HB	3:O1:189:ILE:CD1	2.49	0.41
3:O1:156:ILE:O	3:O1:158:THR:N	2.54	0.41
4:P1:139:THR:O	8:T1:44:VAL:HG11	2.20	0.41
5:Q1:75:GLU:O	5:Q1:194:ILE:CA	2.47	0.41
5:Q1:150:ALA:CB	5:Q1:157:TYR:CB	2.98	0.41
5:Q1:181:GLU:HG2	5:Q1:182:VAL:N	2.35	0.41
5:Q1:184:SER:O	5:Q1:195:VAL:HA	2.20	0.41
8:T1:15:ASP:CB	8:T1:16:PRO:HD3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T1:65:ARG:HH11	8:T1:65:ARG:HD2	1.65	0.41
12:22:106:LEU:HD13	12:22:139:MET:HE2	2.02	0.41
12:22:108:MET:HE1	12:22:191:THR:HG21	2.02	0.41
12:22:216:PHE:HA	12:22:219:PHE:HB2	2.02	0.41
19:A2:613:PRO:HB2	38:U2:134:ILE:HD12	2.01	0.41
20:B2:238:LEU:HD13	33:P2:37:PRO:HD2	2.02	0.41
22:D2:150:VAL:HB	22:D2:179:VAL:HA	2.02	0.41
23:E2:98:ARG:NH2	23:E2:155:CYS:O	2.53	0.41
28:J2:38:VAL:O	28:J2:44:GLN:NE2	2.53	0.41
56:A3:461:SER:O	56:A3:465:VAL:HG13	2.21	0.41
1:A1:53:ASN:CG	1:A1:170:PRO:HD3	2.45	0.41
1:A1:66:GLY:O	1:A1:121:SER:N	2.50	0.41
2:B1:55:SER:OG	2:B1:102:ARG:HA	2.20	0.41
2:B1:160:ILE:HA	2:B1:160:ILE:HD12	1.73	0.41
2:B1:279:LEU:CD2	2:B1:344:VAL:HG22	2.50	0.41
3:C1:61:THR:O	3:C1:62:ALA:C	2.63	0.41
3:C1:280:ILE:HA	3:C1:355:SER:OG	2.20	0.41
3:C1:319:PRO:O	3:C1:322:GLN:N	2.52	0.41
4:D1:7:PRO:CG	4:D1:126:TYR:HA	2.47	0.41
4:D1:165:TYR:O	4:D1:166:ASN:C	2.61	0.41
4:D1:208:MET:HE2	4:D1:208:MET:C	2.44	0.41
8:H1:15:ASP:CB	8:H1:16:PRO:CD	2.97	0.41
1:M1:31:SER:N	1:M1:202:GLY:HA2	2.35	0.41
1:M1:34:THR:OG1	2:N1:373:GLU:OE1	2.37	0.41
1:M1:156:THR:OG1	1:M1:241:ILE:HB	2.21	0.41
1:M1:166:SER:HB2	5:Q1:3:THR:HG22	2.02	0.41
1:M1:236:PHE:HD2	1:M1:258:GLU:CB	2.29	0.41
1:M1:369:LEU:HD21	1:M1:378:ASP:OD2	2.20	0.41
1:M1:385:THR:HG22	1:M1:386:TYR:CD1	2.55	0.41
2:N1:95:LYS:HG3	9:U1:70:LEU:HD13	2.02	0.41
2:N1:168:TYR:CZ	2:N1:172:LEU:HD12	2.56	0.41
2:N1:435:PHE:N	2:N1:438:GLU:HB2	2.35	0.41
3:O1:26:ASN:ND2	3:O1:26:ASN:C	2.78	0.41
3:O1:26:ASN:O	3:O1:26:ASN:CG	2.63	0.41
3:O1:45:ILE:CD1	3:O1:190:MET:HE2	2.51	0.41
3:O1:47:THR:HG23	3:O1:79:ILE:HG23	2.01	0.41
3:O1:58:ASP:O	3:O1:59:THR:C	2.60	0.41
3:O1:115:ILE:N	3:O1:115:ILE:CD1	2.83	0.41
3:O1:219:PRO:HB2	3:O1:222:PRO:CD	2.50	0.41
3:O1:282:ARG:NH1	3:O1:343:VAL:HG22	2.36	0.41
4:P1:174:GLY:O	4:P1:175:THR:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P1:230:LEU:O	4:P1:233:ARG:HB2	2.19	0.41
4:P1:240:PRO:HG2	4:P1:241:LYS:N	2.34	0.41
5:Q1:41:ALA:HA	10:V1:24:ILE:HD11	2.03	0.41
5:Q1:107:ASP:O	5:Q1:110:ALA:N	2.51	0.41
5:Q1:119:ASP:OD1	5:Q1:120:PRO:CD	2.67	0.41
5:Q1:177:PRO:HB2	5:Q1:178:LEU:HG	2.03	0.41
6:R1:74:ILE:HG23	6:R1:75:LEU:O	2.21	0.41
15:52:7:ASN:HA	15:52:8:ILE:HA	1.72	0.41
20:B2:318:VAL:HA	20:B2:319:PRO:HD3	1.94	0.41
24:F2:85:PHE:O	24:F2:89:ASN:N	2.44	0.41
39:V2:143:TYR:HD1	39:V2:143:TYR:HA	1.73	0.41
60:E3:21:LYS:O	60:E3:57:ARG:NH1	2.53	0.41
65:J3:12:PHE:O	65:J3:23:LYS:HE2	2.21	0.41
1:A1:134:ILE:O	1:A1:137:GLU:N	2.53	0.41
1:A1:143:THR:CG2	9:I1:48:SER:H	2.18	0.41
1:A1:280:TYR:HB3	1:A1:307:PHE:CD2	2.55	0.41
1:A1:291:SER:OG	2:B1:90:GLU:OE1	2.26	0.41
1:A1:426:GLY:H	1:A1:428:ILE:HD11	1.83	0.41
2:B1:283:PRO:HG3	9:I1:55:LEU:CG	2.50	0.41
3:C1:360:LEU:HA	3:C1:360:LEU:HD12	1.82	0.41
4:D1:91:PHE:N	4:D1:91:PHE:CD1	2.89	0.41
4:D1:165:TYR:CE1	4:D1:168:VAL:HA	2.56	0.41
6:F1:51:PRO:O	6:F1:52:GLU:C	2.63	0.41
1:M1:43:ALA:HB1	1:M1:189:HIS:CB	2.50	0.41
2:N1:182:ARG:O	2:N1:185:LYS:N	2.54	0.41
2:N1:333:ALA:O	2:N1:337:ILE:HD12	2.20	0.41
3:O1:277:ALA:HB1	3:O1:294:LEU:CD1	2.50	0.41
3:O1:282:ARG:CZ	3:O1:343:VAL:HG22	2.49	0.41
3:O1:337:TRP:NE1	3:O1:341:GLN:OE1	2.54	0.41
4:P1:102:ARG:HG2	4:P1:109:LEU:HB2	2.02	0.41
4:P1:165:TYR:CE2	4:P1:168:VAL:HG22	2.55	0.41
4:P1:211:MET:O	4:P1:212:MET:C	2.62	0.41
70:P1:301:HEC:CHD	70:P1:301:HEC:CBC	2.95	0.41
5:Q1:33:LYS:HA	7:S1:21:PHE:CE1	2.55	0.41
6:R1:74:ILE:H	7:S1:39:ARG:NH2	2.19	0.41
17:82:418:GLN:HE21	19:A2:115:GLY:HA3	1.70	0.41
18:92:147:SER:HB2	18:92:198:PRO:HG3	2.01	0.41
19:A2:627:SER:OG	19:A2:632:MET:O	2.31	0.41
23:E2:85:ASN:O	23:E2:89:GLU:N	2.42	0.41
23:E2:114:ILE:HD12	23:E2:114:ILE:HA	1.97	0.41
31:N2:26:ILE:O	31:N2:30:LYS:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:V2:43:LEU:HB2	52:12:179:TRP:HE1	1.86	0.41
42:Y2:89:TYR:O	42:Y2:91:ASP:N	2.53	0.41
47:d2:34:ARG:HA	47:d2:35:LYS:HA	1.70	0.41
56:A3:198:SER:HB2	56:A3:238:PHE:HA	2.03	0.41
56:A3:264:LYS:NZ	57:B3:56:MET:HE2	2.35	0.41
58:C3:182:TYR:O	62:G3:72:ASN:HB2	2.21	0.41
59:D3:130:PRO:O	59:D3:136:ALA:HB2	2.20	0.41
63:H3:24:ASN:HD22	63:H3:25:GLN:N	2.18	0.41
1:A1:260:PRO:HG3	1:A1:414:TYR:CE1	2.55	0.41
1:A1:314:TYR:HB2	1:A1:317:THR:O	2.20	0.41
2:B1:68:LEU:HB2	2:B1:144:LEU:HD21	2.02	0.41
2:B1:68:LEU:O	2:B1:71:LEU:N	2.50	0.41
2:B1:170:ASN:OD1	2:B1:171:ALA:N	2.52	0.41
2:B1:397:THR:O	2:B1:398:VAL:C	2.63	0.41
3:C1:163:TRP:CD1	5:Q1:63:SER:HA	2.55	0.41
6:F1:28:LYS:HB3	6:F1:74:ILE:CD1	2.44	0.41
10:J1:29:LEU:HD12	10:J1:32:GLU:OE2	2.21	0.41
11:K1:24:TRP:CE3	11:K1:24:TRP:HA	2.56	0.41
1:M1:61:HIS:HB2	1:M1:130:GLU:HG3	2.02	0.41
1:M1:64:PHE:HE2	1:M1:88:ALA:CB	2.34	0.41
2:N1:33:LEU:HB2	2:N1:204:MET:O	2.20	0.41
2:N1:49:LEU:HD21	2:N1:204:MET:SD	2.60	0.41
2:N1:160:ILE:CD1	2:N1:325:TYR:HE2	2.33	0.41
2:N1:309:VAL:CG1	2:N1:310:SER:N	2.82	0.41
2:N1:436:ILE:H	2:N1:436:ILE:HG13	1.41	0.41
3:O1:11:MET:O	3:O1:14:VAL:HB	2.21	0.41
3:O1:196:HIS:HE1	69:O1:402:HEM:CHD	2.32	0.41
3:O1:211:ILE:CG2	3:O1:212:SER:N	2.83	0.41
3:O1:276:PHE:CE2	3:O1:297:SER:OG	2.74	0.41
3:O1:284:ILE:HG23	3:O1:285:PRO:HD2	2.02	0.41
4:P1:120:ARG:HD2	70:P1:301:HEC:CGA	2.50	0.41
4:P1:138:PRO:CG	8:T1:55:THR:HA	2.50	0.41
5:Q1:31:ALA:HB2	10:V1:7:ALA:HB2	2.03	0.41
6:R1:35:ASP:OD2	6:R1:61:ARG:HD2	2.20	0.41
10:V1:52:TRP:N	10:V1:52:TRP:HE3	2.18	0.41
17:82:36:LYS:HB2	17:82:38:GLU:HG3	2.01	0.41
19:A2:613:PRO:HG3	38:U2:134:ILE:CG2	2.51	0.41
23:E2:54:THR:HG22	30:L2:13:TRP:HH2	1.85	0.41
27:I2:87:CYS:O	27:I2:96:HIS:NE2	2.53	0.41
28:J2:41:TYR:OH	52:12:317:GLN:NE2	2.39	0.41
51:j2:21:LEU:HD11	51:j2:81:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B3:146:MET:SD	57:B3:189:PRO:HB3	2.60	0.41
58:C3:6:HIS:CD2	58:C3:8:TYR:HB2	2.55	0.41
59:D3:11:TYR:CD1	59:D3:11:TYR:C	2.99	0.41
1:A1:4:TYR:O	1:A1:5:ALA:C	2.63	0.41
1:A1:433:ASP:O	1:A1:436:ARG:N	2.52	0.41
2:B1:211:VAL:HG11	2:B1:216:LEU:HD13	2.02	0.41
2:B1:250:ASP:OD1	2:B1:251:SER:N	2.54	0.41
3:C1:122:THR:HG21	3:C1:189:ILE:HG12	2.03	0.41
4:D1:55:CYS:SG	10:J1:52:TRP:HB2	2.60	0.41
6:F1:68:LEU:HD11	6:F1:75:LEU:HD13	2.01	0.41
7:G1:31:SER:O	7:G1:35:PRO:CD	2.62	0.41
8:H1:59:LEU:HD23	8:H1:59:LEU:HA	1.76	0.41
8:H1:61:PHE:O	8:H1:62:LEU:C	2.64	0.41
1:M1:48:GLU:HB3	1:M1:52:ASN:O	2.21	0.41
1:M1:257:VAL:O	1:M1:320:LEU:HB2	2.21	0.41
1:M1:282:CYS:SG	1:M1:305:GLN:CD	3.03	0.41
1:M1:426:GLY:H	1:M1:428:ILE:CG1	2.30	0.41
2:N1:47:ILE:HB	2:N1:109:VAL:HG12	2.02	0.41
2:N1:346:THR:O	2:N1:347:ILE:C	2.62	0.41
3:O1:88:SER:HA	3:O1:272:TRP:CZ2	2.53	0.41
3:O1:133:LEU:HA	3:O1:175:LEU:HD11	2.01	0.41
3:O1:149:LEU:O	3:O1:291:VAL:HG21	2.21	0.41
3:O1:184:ILE:O	3:O1:184:ILE:HG12	2.20	0.41
4:P1:48:TYR:OH	4:P1:68:VAL:HG21	2.21	0.41
4:P1:153:PHE:O	4:P1:154:PRO:C	2.64	0.41
4:P1:224:ARG:O	4:P1:225:HIS:C	2.62	0.41
5:Q1:87:MET:O	5:Q1:89:PHE:HD1	2.04	0.41
5:Q1:185:TYR:HD2	5:Q1:193:VAL:HG21	1.84	0.41
6:R1:55:TYR:CD1	6:R1:55:TYR:C	2.99	0.41
11:W1:24:TRP:HA	11:W1:24:TRP:CE3	2.55	0.41
12:22:190:MET:HB2	12:22:201:THR:HG23	2.02	0.41
13:32:84:LEU:HD21	52:12:309:ILE:HD13	2.03	0.41
16:72:140:ALA:HA	16:72:142:GLY:N	2.36	0.41
18:92:93:LEU:HA	18:92:94:PRO:HD3	1.94	0.41
19:A2:44:GLU:HB3	19:A2:47:THR:HG23	2.03	0.41
23:E2:135:ARG:NH1	27:I2:68:ALA:O	2.54	0.41
35:R2:126:VAL:HG13	35:R2:164:PHE:HD1	1.86	0.41
35:R2:227:PRO:HG2	35:R2:230:SER:HA	2.02	0.41
56:A3:23:GLY:HA3	56:A3:73:ILE:HG13	2.03	0.41
56:A3:462:LEU:O	56:A3:466:MET:HG3	2.20	0.41
56:A3:501:PRO:O	56:A3:502:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B3:193:TYR:CD1	57:B3:193:TYR:N	2.88	0.41
1:A1:8:LEU:HD23	1:A1:8:LEU:HA	1.94	0.41
1:A1:29:GLN:HG3	1:A1:203:LEU:O	2.21	0.41
1:A1:97:TYR:CD1	1:A1:97:TYR:N	2.88	0.41
1:A1:244:ARG:NH1	7:G1:10:VAL:HG21	2.35	0.41
1:A1:292:SER:HA	1:A1:293:PRO:HD2	1.88	0.41
1:A1:385:THR:HB	1:A1:386:TYR:HD1	1.83	0.41
3:C1:200:LEU:CD1	69:C1:402:HEM:HAD2	2.51	0.41
3:C1:257:THR:OG1	3:C1:257:THR:O	2.38	0.41
3:C1:300:ILE:HD11	3:C1:362:ILE:CG2	2.50	0.41
4:D1:5:LEU:HG	4:D1:152:TYR:HE1	1.86	0.41
6:F1:91:GLU:O	6:F1:92:PRO:C	2.62	0.41
7:G1:68:LYS:O	7:G1:69:SER:C	2.64	0.41
5:Q1:76:ILE:O	5:Q1:77:LYS:CG	2.68	0.41
6:R1:52:GLU:HG3	6:R1:56:ASN:ND2	2.36	0.41
6:R1:62:ILE:O	6:R1:66:LEU:HG	2.21	0.41
9:U1:62:ARG:HB3	9:U1:63:PRO:CD	2.51	0.41
14:42:423:ILE:HD12	44:a2:56:ARG:HB3	2.03	0.41
73:42:501:CDL:H742	73:42:501:CDL:H712	1.80	0.41
34:Q2:53:PRO:HD2	39:V2:116:TRP:CD1	2.56	0.41
35:R2:201:ILE:HD12	35:R2:201:ILE:HA	1.95	0.41
48:f2:148:GLY:HA3	48:f2:149:PRO:HD3	1.87	0.41
52:12:126:LYS:CD	52:12:127:TYR:CA	2.91	0.41
52:12:215:TYR:HD1	52:12:219:PRO:HB2	1.86	0.41
53:62:3:MET:HA	53:62:6:SER:HB2	2.02	0.41
56:A3:276:ALA:O	56:A3:280:ILE:HG13	2.21	0.41
59:D3:79:LYS:HZ3	66:K3:15:ASN:HD21	1.68	0.41
1:A1:46:ARG:NE	1:A1:163:LEU:HD22	2.36	0.41
1:A1:64:PHE:HA	1:A1:75:LEU:HD22	2.02	0.41
1:A1:136:GLN:HE21	9:I1:50:LEU:CB	2.34	0.41
1:A1:252:HIS:O	1:A1:424:GLY:HA2	2.20	0.41
1:A1:282:CYS:SG	1:A1:305:GLN:CD	3.04	0.41
1:A1:297:ILE:HG22	1:A1:303:LEU:CD1	2.49	0.41
2:B1:68:LEU:HD12	2:B1:68:LEU:O	2.21	0.41
2:B1:71:LEU:HA	2:B1:71:LEU:HD23	1.72	0.41
2:B1:159:VAL:CG1	2:B1:160:ILE:N	2.84	0.41
2:B1:312:PHE:HB3	2:B1:323:GLY:O	2.20	0.41
3:C1:1:MET:HG3	3:C1:4:ILE:HB	2.03	0.41
3:C1:8:HIS:CB	3:C1:9:PRO:HD2	2.51	0.41
3:C1:115:ILE:HG21	3:C1:196:HIS:CB	2.33	0.41
3:C1:168:PHE:CE2	5:Q1:72:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:275:LEU:O	3:C1:276:PHE:O	2.39	0.41
4:D1:207:LYS:HB3	10:J1:35:PHE:HE2	1.85	0.41
5:E1:20:ASP:O	5:E1:22:THR:N	2.54	0.41
6:F1:13:LEU:O	6:F1:14:GLU:C	2.64	0.41
6:F1:98:ILE:O	6:F1:99:ARG:C	2.64	0.41
7:G1:3:GLN:OE1	7:G1:3:GLN:HA	2.20	0.41
8:H1:65:ARG:HG2	8:H1:66:ASP:OD2	2.21	0.41
10:J1:29:LEU:O	10:J1:30:PHE:C	2.64	0.41
1:M1:32:GLN:HG2	1:M1:33:PRO:N	2.36	0.41
1:M1:97:TYR:CD1	1:M1:97:TYR:N	2.88	0.41
1:M1:136:GLN:HE21	9:U1:50:LEU:HG	1.84	0.41
1:M1:166:SER:CB	5:Q1:3:THR:HG22	2.51	0.41
1:M1:244:ARG:NH1	7:S1:10:VAL:HB	2.36	0.41
1:M1:248:LEU:HA	1:M1:249:PRO:HD3	1.78	0.41
1:M1:289:HIS:O	2:N1:87:ARG:NE	2.54	0.41
2:N1:223:PHE:O	2:N1:224:LEU:HD23	2.21	0.41
2:N1:396:SER:HA	2:N1:399:LEU:HD12	2.02	0.41
2:N1:413:ALA:O	2:N1:416:LYS:HB2	2.21	0.41
3:O1:47:THR:O	3:O1:48:GLY:C	2.64	0.41
3:O1:207:ASN:O	3:O1:208:PRO:C	2.62	0.41
3:O1:241:LEU:HD12	3:O1:241:LEU:HA	1.81	0.41
3:O1:303:LEU:HD23	3:O1:303:LEU:HA	1.85	0.41
4:P1:21:LEU:CD1	4:P1:192:TRP:HB2	2.50	0.41
4:P1:34:LYS:O	4:P1:38:SER:HB3	2.21	0.41
5:Q1:16:PRO:O	5:Q1:17:GLU:C	2.63	0.41
5:Q1:73:LYS:O	5:Q1:74:ILE:HD13	2.20	0.41
5:Q1:113:GLU:O	5:Q1:114:VAL:C	2.63	0.41
6:R1:51:PRO:O	6:R1:52:GLU:C	2.62	0.41
7:S1:36:ASN:OD1	7:S1:39:ARG:NE	2.53	0.41
7:S1:61:TRP:O	7:S1:62:GLY:C	2.64	0.41
9:U1:60:ALA:HB3	9:U1:63:PRO:O	2.21	0.41
13:32:79:SER:O	30:L2:46:ASN:ND2	2.50	0.41
16:72:22:SER:OG	16:72:23:LYS:N	2.54	0.41
19:A2:171:THR:HG23	19:A2:173:MET:HE2	2.03	0.41
19:A2:643:ARG:HA	19:A2:646:LEU:HB2	2.03	0.41
20:B2:246:GLU:HA	20:B2:249:LYS:HE3	2.02	0.41
23:E2:127:ALA:HB1	23:E2:148:ASP:H	1.86	0.41
29:K2:67:ALA:N	29:K2:75:LYS:O	2.54	0.41
30:L2:31:ILE:HG22	30:L2:35:LEU:HD11	2.03	0.41
32:O2:18:LYS:HA	32:O2:19:PRO:HD3	1.93	0.41
44:a2:79:ASN:HD22	55:e2:76:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:12:236:ILE:HD12	52:12:236:ILE:HA	1.97	0.41
53:62:65:ASN:HB2	53:62:78:LEU:HD11	2.01	0.41
53:62:364:LYS:HD3	53:62:435:PRO:HB3	2.01	0.41
58:C3:233:PHE:HA	58:C3:236:GLU:HG3	2.03	0.41
59:D3:102:TYR:HD2	68:M3:35:TYR:HE1	1.68	0.41
59:D3:127:LYS:O	59:D3:130:PRO:HD3	2.20	0.41
60:E3:104:LEU:HA	60:E3:104:LEU:HD23	1.87	0.41
63:H3:20:PHE:N	63:H3:21:PRO:HD3	2.35	0.41
1:A1:62:LEU:HB3	1:A1:122:LEU:HD22	2.02	0.41
1:A1:133:VAL:O	1:A1:134:ILE:C	2.63	0.41
2:B1:51:ILE:CG2	2:B1:199:PHE:HA	2.34	0.41
2:B1:134:ARG:HE	2:B1:134:ARG:HB3	1.54	0.41
3:C1:244:LEU:HD11	4:D1:204:MET:HE3	2.03	0.41
3:C1:263:ASN:OD1	3:C1:264:THR:N	2.54	0.41
3:C1:299:LEU:HD22	3:C1:299:LEU:HA	1.79	0.41
4:D1:16:GLY:O	4:D1:17:LEU:C	2.64	0.41
10:J1:49:GLY:N	10:J1:54:HIS:CD2	2.89	0.41
1:M1:71:PRO:O	1:M1:72:GLY:C	2.64	0.41
1:M1:333:ASP:O	1:M1:337:VAL:HG23	2.21	0.41
2:N1:24:LEU:CD2	2:N1:38:LEU:HD11	2.51	0.41
2:N1:241:GLY:HA2	2:N1:423:SER:HB3	2.03	0.41
2:N1:345:LYS:HG2	2:N1:418:VAL:HG11	2.03	0.41
3:O1:246:ALA:N	3:O1:247:PRO:HD3	2.36	0.41
3:O1:363:LEU:HD12	3:O1:363:LEU:HA	1.85	0.41
4:P1:6:HIS:HA	4:P1:7:PRO:HD3	1.87	0.41
4:P1:167:GLU:O	4:P1:167:GLU:HG2	2.20	0.41
5:Q1:115:SER:C	5:Q1:117:LEU:H	2.28	0.41
8:T1:37:LEU:HD21	8:T1:58:LEU:CA	2.49	0.41
13:32:2:ASN:OD1	13:32:2:ASN:N	2.52	0.41
19:A2:557:ARG:NE	38:U2:144:TYR:CZ	2.85	0.41
20:B2:326:CYS:SG	20:B2:329:ARG:NH1	2.94	0.41
21:C2:97:PRO:O	21:C2:101:PHE:N	2.50	0.41
22:D2:146:GLU:O	35:R2:89:TYR:OH	2.35	0.41
77:R2:601:NAP:H3B	77:R2:601:NAP:PA	2.61	0.41
38:U2:55:PHE:HB3	38:U2:58:ARG:HG3	2.03	0.41
52:12:75:PRO:HG3	52:12:223:PHE:CE1	2.45	0.41
55:e2:37:LEU:O	55:e2:76:PRO:CB	2.69	0.41
56:A3:168:ILE:CG2	56:A3:189:MET:HG3	2.51	0.41
63:H3:65:PRO:HG2	63:H3:68:TRP:CG	2.55	0.41
1:A1:43:ALA:HB1	1:A1:189:HIS:CB	2.51	0.40
1:A1:256:ALA:HB3	1:A1:421:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:266:ASP:OD1	1:A1:266:ASP:N	2.54	0.40
1:A1:367:SER:O	1:A1:368:HIS:C	2.63	0.40
1:A1:392:LEU:HA	1:A1:395:TRP:HD1	1.76	0.40
2:B1:122:PHE:HD1	2:B1:122:PHE:HA	1.69	0.40
2:B1:133:ARG:O	2:B1:134:ARG:C	2.64	0.40
3:C1:40:CYS:CB	3:C1:90:PHE:HD2	2.34	0.40
3:C1:213:SER:C	3:C1:215:VAL:N	2.79	0.40
3:C1:226:ILE:HD13	3:C1:226:ILE:N	2.35	0.40
3:C1:301:LEU:HA	3:C1:304:ILE:CD1	2.51	0.40
4:D1:56:TYR:HD1	4:D1:60:GLU:CD	2.29	0.40
7:G1:18:LEU:HD23	7:G1:18:LEU:HA	1.94	0.40
1:M1:131:ARG:NH2	1:M1:177:LEU:O	2.54	0.40
1:M1:297:ILE:HG22	1:M1:303:LEU:CD1	2.43	0.40
2:N1:22:GLN:OE1	2:N1:22:GLN:HA	2.21	0.40
2:N1:54:GLY:HA3	2:N1:102:ARG:O	2.20	0.40
2:N1:286:LYS:HD3	2:N1:287:ARG:HH12	1.80	0.40
3:O1:51:LEU:HD12	69:O1:401:HEM:O1D	2.21	0.40
3:O1:63:PHE:CD1	3:O1:63:PHE:C	2.98	0.40
3:O1:300:ILE:CD1	3:O1:362:ILE:HG21	2.50	0.40
4:P1:224:ARG:HH21	7:S1:27:PRO:CD	2.34	0.40
5:Q1:15:ARG:HH21	5:Q1:32:ARG:HB2	1.85	0.40
5:Q1:76:ILE:O	5:Q1:77:LYS:HE2	2.21	0.40
8:T1:27:LEU:O	8:T1:30:CYS:N	2.48	0.40
10:V1:23:THR:HG22	10:V1:24:ILE:N	2.36	0.40
12:22:76:ILE:HG21	12:22:91:ASN:HD22	1.86	0.40
19:A2:372:PHE:HB3	19:A2:532:PRO:HB2	2.02	0.40
20:B2:421:ARG:HH21	20:B2:423:LYS:HB2	1.86	0.40
21:C2:90:ILE:HD12	21:C2:145:VAL:HG13	2.03	0.40
26:H2:82:GLN:HE21	39:V2:98:MET:HB2	1.87	0.40
38:U2:115:PHE:HB3	38:U2:117:LEU:HG	2.02	0.40
42:Y2:91:ASP:O	42:Y2:93:SER:N	2.54	0.40
43:Z2:64:VAL:HA	43:Z2:67:LEU:HG	2.02	0.40
56:A3:440:TYR:CG	57:B3:205:SER:HB3	2.57	0.40
62:G3:44:ARG:HA	62:G3:45:PRO:HD2	1.76	0.40
1:A1:53:ASN:O	1:A1:53:ASN:ND2	2.53	0.40
1:A1:176:LYS:O	1:A1:177:LEU:C	2.64	0.40
1:A1:358:LYS:HD2	1:A1:402:VAL:HG12	2.03	0.40
1:A1:363:ASN:OD1	2:B1:112:LEU:HD23	2.21	0.40
2:B1:53:ALA:HB2	2:B1:198:HIS:HB3	2.03	0.40
2:B1:163:LEU:HA	2:B1:163:LEU:HD12	1.78	0.40
3:C1:34:GLY:O	3:C1:37:LEU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:133:LEU:HA	3:C1:175:LEU:HD11	2.04	0.40
3:C1:145:VAL:O	3:C1:145:VAL:HG12	2.20	0.40
3:C1:317:PHE:O	6:F1:24:ALA:CB	2.70	0.40
4:D1:241:LYS:OXT	4:D1:241:LYS:CG	2.62	0.40
7:G1:40:ARG:O	7:G1:43:ALA:N	2.52	0.40
9:I1:70:LEU:CG	9:I1:72:VAL:H	2.34	0.40
1:M1:4:TYR:HE2	1:M1:396:GLU:HG3	1.85	0.40
1:M1:17:SER:HB2	1:M1:25:VAL:HB	2.03	0.40
1:M1:42:ASP:O	1:M1:42:ASP:CG	2.63	0.40
1:M1:146:ARG:CZ	1:M1:308:GLN:HE22	2.34	0.40
1:M1:311:ASN:CG	1:M1:320:LEU:CD2	2.95	0.40
1:M1:372:THR:O	1:M1:373:THR:C	2.62	0.40
2:N1:38:LEU:O	2:N1:40:ASN:N	2.54	0.40
2:N1:57:TYR:O	2:N1:233:SER:HB2	2.21	0.40
2:N1:59:ASN:CG	2:N1:60:SER:N	2.77	0.40
2:N1:102:ARG:NH1	2:N1:175:SER:HA	2.37	0.40
2:N1:158:HIS:ND1	2:N1:246:GLU:OE1	2.54	0.40
2:N1:237:ALA:O	2:N1:238:LYS:HB2	2.20	0.40
3:O1:115:ILE:O	3:O1:116:GLY:C	2.64	0.40
4:P1:7:PRO:HB3	4:P1:125:ASP:C	2.46	0.40
4:P1:153:PHE:HA	4:P1:154:PRO:HD2	1.88	0.40
4:P1:206:LEU:O	4:P1:210:LEU:HD12	2.22	0.40
5:Q1:109:GLU:OE2	5:Q1:166:ASP:HB2	2.21	0.40
6:R1:43:VAL:O	6:R1:47:ILE:HG13	2.22	0.40
7:S1:50:PRO:O	7:S1:53:VAL:HB	2.21	0.40
14:42:285:LEU:O	14:42:406:TYR:OH	2.32	0.40
14:42:356:ALA:HA	14:42:359:TRP:HD1	1.87	0.40
19:A2:312:GLY:H	38:U2:144:TYR:N	2.19	0.40
20:B2:261:MET:HA	23:E2:70:LEU:HD21	2.03	0.40
21:C2:220:ARG:NH2	32:O2:104:MET:O	2.55	0.40
37:T2:124:LEU:O	37:T2:128:GLY:N	2.55	0.40
39:V2:46:GLY:O	39:V2:49:SER:OG	2.30	0.40
41:X2:13:HIS:O	41:X2:15:LEU:N	2.54	0.40
53:62:387:THR:HG22	53:62:462:LEU:HA	2.03	0.40
55:e2:48:ARG:HA	55:e2:49:ALA:HA	1.59	0.40
56:A3:34:SER:HB3	56:A3:61:HIS:CE1	2.57	0.40
56:A3:442:ASP:OD2	57:B3:134:ARG:NH2	2.54	0.40
57:B3:164:ALA:HB2	57:B3:171:LYS:HD3	2.03	0.40
58:C3:228:THR:O	58:C3:232:HIS:HD2	2.04	0.40
64:I3:29:LEU:HD23	64:I3:29:LEU:HA	1.85	0.40
68:M3:37:LEU:HD23	68:M3:37:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:303:VAL:HG12	2:B1:304:HIS:H	1.86	0.40
2:B1:353:SER:C	2:B1:355:PRO:HD2	2.47	0.40
3:C1:48:GLY:HA3	69:C1:401:HEM:C3C	2.56	0.40
4:D1:27:ARG:CZ	10:J1:58:LYS:HE3	2.52	0.40
4:D1:82:MET:SD	4:D1:86:LYS:CD	3.08	0.40
4:D1:99:GLU:H	4:D1:99:GLU:HG2	1.73	0.40
4:D1:125:ASP:O	4:D1:126:TYR:C	2.64	0.40
4:D1:220:TYR:HD2	7:G1:26:PHE:CZ	2.40	0.40
6:F1:93:TYR:O	6:F1:97:VAL:HG23	2.22	0.40
10:J1:34:ALA:O	10:J1:35:PHE:O	2.39	0.40
10:J1:44:GLU:O	10:J1:45:HIS:C	2.63	0.40
2:N1:282:GLY:HA2	2:N1:283:PRO:HD2	1.78	0.40
3:O1:75:TYR:CG	5:Q1:57:GLN:HG2	2.56	0.40
3:O1:121:LEU:HA	3:O1:124:MET:SD	2.62	0.40
4:P1:216:LEU:N	4:P1:217:PRO:CD	2.85	0.40
5:Q1:122:HIS:HE1	5:Q1:124:LEU:HD12	1.85	0.40
12:22:250:SER:HB2	12:22:257:LEU:HD13	2.03	0.40
14:42:274:SER:HA	14:42:277:LEU:HD13	2.03	0.40
17:82:198:VAL:HG11	17:82:216:ILE:HD11	2.03	0.40
18:92:205:ILE:HG22	18:92:209:LYS:HE2	2.03	0.40
20:B2:164:PRO:HA	20:B2:165:PRO:HD3	1.93	0.40
37:T2:26:THR:O	37:T2:30:GLY:N	2.52	0.40
53:62:192:ASN:HB2	53:62:193:LEU:HD12	2.03	0.40
54:g2:145:ASP:O	54:g2:148:ALA:N	2.54	0.40
55:e2:124:VAL:HG22	55:e2:125:ASN:H	1.87	0.40
56:A3:398:PRO:HB3	56:A3:482:VAL:HG21	2.03	0.40
56:A3:498:CYS:HA	56:A3:499:PRO:HA	1.78	0.40
59:D3:137:LYS:O	59:D3:145:TRP:HE3	2.03	0.40
61:F3:49:VAL:O	61:F3:91:LEU:HD12	2.21	0.40
61:F3:77:GLY:O	61:F3:90:LYS:NZ	2.54	0.40
62:G3:42:ARG:NH1	62:G3:74:ARG:NH2	2.68	0.40
1:A1:8:LEU:HD11	1:A1:396:GLU:HG3	2.02	0.40
1:A1:24:ARG:HH11	1:A1:24:ARG:HD2	1.57	0.40
2:B1:141:GLN:CB	2:B1:142:PRO:HD3	2.41	0.40
2:B1:156:GLN:O	2:B1:157:ALA:C	2.63	0.40
2:B1:194:TYR:O	2:B1:195:VAL:C	2.64	0.40
2:B1:346:THR:HG23	2:B1:351:ASN:HB3	2.03	0.40
2:B1:408:ALA:O	2:B1:411:ILE:N	2.54	0.40
3:C1:170:VAL:O	3:C1:170:VAL:CG1	2.68	0.40
3:C1:274:PHE:O	3:C1:275:LEU:C	2.62	0.40
3:C1:341:GLN:OE1	3:C1:347:TYR:CZ	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:35:GLN:HB2	4:D1:169:LEU:HD13	2.02	0.40
4:D1:95:TYR:CD1	4:D1:95:TYR:N	2.90	0.40
4:D1:146:GLY:O	4:D1:148:TYR:HD1	2.04	0.40
4:D1:165:TYR:HD1	4:D1:166:ASN:O	2.04	0.40
8:H1:50:THR:CG2	8:H1:51:GLU:N	2.83	0.40
1:M1:85:HIS:CE1	2:N1:284:HIS:ND1	2.90	0.40
1:M1:349:ALA:O	1:M1:408:ARG:NE	2.54	0.40
2:N1:92:VAL:HG11	2:N1:115:ASP:CB	2.51	0.40
2:N1:257:LEU:HD13	2:N1:424:MET:CB	2.45	0.40
2:N1:276:GLN:OE1	9:U1:59:ALA:HB1	2.21	0.40
3:O1:25:SER:HA	3:O1:218:ILE:HD12	2.02	0.40
3:O1:156:ILE:H	3:O1:156:ILE:HG12	1.63	0.40
4:P1:43:MET:HG2	4:P1:114:SER:N	2.37	0.40
6:R1:99:ARG:O	6:R1:100:GLU:C	2.63	0.40
10:V1:2:ALA:HB1	10:V1:3:PRO:HD2	2.03	0.40
14:42:457:PRO:HG2	14:42:458:LEU:HA	2.04	0.40
19:A2:170:LYS:HB3	19:A2:232:THR:HG23	2.02	0.40
19:A2:312:GLY:CA	38:U2:144:TYR:N	2.82	0.40
19:A2:445:LEU:HD21	19:A2:460:HIS:HD2	1.87	0.40
29:K2:31:GLN:HB3	29:K2:34:ARG:HH21	1.86	0.40
35:R2:322:ILE:H	35:R2:322:ILE:HG13	1.72	0.40
45:b2:166:GLY:HA2	45:b2:167:PRO:HD3	1.86	0.40
53:62:141:PHE:HB2	53:62:182:PHE:HE2	1.86	0.40
57:B3:86:MET:HE3	57:B3:86:MET:HB2	1.80	0.40
66:K3:24:PHE:CE1	66:K3:28:VAL:HG21	2.56	0.40
1:A1:50:GLU:O	1:A1:173:ASN:ND2	2.55	0.40
1:A1:213:GLN:CB	1:A1:215:HIS:CD2	3.05	0.40
2:B1:213:HIS:O	2:B1:213:HIS:CD2	2.74	0.40
3:C1:68:HIS:NE2	5:E1:67:ASP:CB	2.85	0.40
3:C1:192:ILE:O	3:C1:193:ALA:C	2.62	0.40
4:D1:136:GLU:O	4:D1:137:PRO:C	2.62	0.40
4:D1:200:HIS:O	4:D1:203:ARG:HB3	2.20	0.40
5:E1:53:ASN:O	5:E1:54:VAL:C	2.65	0.40
11:K1:27:VAL:HG12	11:K1:28:GLY:N	2.37	0.40
1:M1:241:ILE:HD11	7:S1:16:TYR:CE2	2.55	0.40
2:N1:207:ILE:HD12	2:N1:382:VAL:HG12	2.04	0.40
3:O1:66:VAL:O	3:O1:69:ILE:HB	2.21	0.40
3:O1:227:LYS:HG3	4:P1:223:LYS:NZ	2.36	0.40
3:O1:297:SER:O	3:O1:300:ILE:CG2	2.62	0.40
4:P1:14:HIS:HA	4:P1:19:SER:CB	2.51	0.40
4:P1:175:THR:HA	4:P1:176:PRO:HD2	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:P1:301:HEC:HHD	70:P1:301:HEC:CBC	2.30	0.40
5:Q1:83:GLU:HA	5:Q1:100:HIS:CG	2.57	0.40
6:R1:91:GLU:O	6:R1:95:LYS:HG3	2.21	0.40
9:U1:70:LEU:HD11	9:U1:72:VAL:H	1.85	0.40
10:V1:42:ILE:O	10:V1:46:ILE:HG12	2.22	0.40
12:22:45:MET:HE1	12:22:53:THR:HA	2.02	0.40
14:42:35:SER:O	14:42:38:SER:OG	2.35	0.40
14:42:348:LEU:HG	14:42:349:GLN:H	1.87	0.40
15:52:26:LEU:HB3	15:52:88:ASP:HB2	2.04	0.40
17:82:270:ASN:HD21	17:82:338:ASP:HA	1.86	0.40
19:A2:413:LEU:HD23	19:A2:413:LEU:HA	1.92	0.40
21:C2:205:PRO:HA	25:G2:124:LEU:HD21	2.03	0.40
26:H2:15:ASP:OD1	26:H2:15:ASP:N	2.52	0.40
27:I2:87:CYS:HB3	76:I2:300:ZN:ZN	1.52	0.40
30:L2:80:TRP:O	30:L2:84:LEU:N	2.54	0.40
53:62:107:TYR:HE2	53:62:240:PRO:HB3	1.87	0.40
56:A3:240:HIS:O	56:A3:241:PRO:C	2.64	0.40
56:A3:373:VAL:O	56:A3:377:PHE:CD2	2.75	0.40
56:A3:430:PHE:O	56:A3:431:LEU:C	2.64	0.40
57:B3:215:PRO:HD3	64:I3:60:PHE:CD1	2.57	0.40
63:H3:17:ASP:OD1	63:H3:19:ARG:HG2	2.22	0.40
65:J3:5:VAL:O	65:J3:9:GLN:HG3	2.21	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	A1	428/480 (89%)	348 (81%)	57 (13%)	23 (5%)	1	15
1	M1	428/480 (89%)	360 (84%)	50 (12%)	18 (4%)	2	17
2	B1	417/453 (92%)	341 (82%)	67 (16%)	9 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N1	417/453 (92%)	344 (82%)	62 (15%)	11 (3%)	4	25
3	C1	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	2	20
3	O1	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3	23
4	D1	239/325 (74%)	188 (79%)	36 (15%)	15 (6%)	1	13
4	P1	239/325 (74%)	195 (82%)	32 (13%)	12 (5%)	1	16
5	E1	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	4	25
5	Q1	194/196 (99%)	149 (77%)	34 (18%)	11 (6%)	1	14
6	F1	104/111 (94%)	89 (86%)	12 (12%)	3 (3%)	3	23
6	R1	104/111 (94%)	86 (83%)	16 (15%)	2 (2%)	6	32
7	G1	79/82 (96%)	63 (80%)	13 (16%)	3 (4%)	2	19
7	S1	79/82 (96%)	60 (76%)	16 (20%)	3 (4%)	2	19
8	H1	62/91 (68%)	52 (84%)	10 (16%)	0	100	100
8	T1	62/91 (68%)	51 (82%)	10 (16%)	1 (2%)	7	38
9	I1	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	12
9	U1	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	7
10	J1	60/64 (94%)	41 (68%)	13 (22%)	6 (10%)	0	7
10	V1	60/64 (94%)	45 (75%)	11 (18%)	4 (7%)	1	12
11	K1	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
11	W1	20/56 (36%)	17 (85%)	3 (15%)	0	100	100
12	22	342/347 (99%)	295 (86%)	47 (14%)	0	100	100
13	32	89/115 (77%)	74 (83%)	14 (16%)	1 (1%)	11	46
14	42	457/459 (100%)	383 (84%)	70 (15%)	4 (1%)	14	51
15	52	94/98 (96%)	82 (87%)	12 (13%)	0	100	100
16	72	170/175 (97%)	140 (82%)	28 (16%)	2 (1%)	10	44
17	82	425/444 (96%)	346 (81%)	78 (18%)	1 (0%)	43	78
18	92	205/217 (94%)	169 (82%)	35 (17%)	1 (0%)	24	63
19	A2	686/704 (97%)	572 (83%)	107 (16%)	7 (1%)	12	49
20	B2	383/430 (89%)	334 (87%)	40 (10%)	9 (2%)	5	28
21	C2	206/228 (90%)	177 (86%)	29 (14%)	0	100	100
22	D2	150/179 (84%)	130 (87%)	19 (13%)	1 (1%)	18	56
23	E2	174/176 (99%)	158 (91%)	15 (9%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	F2	26/75 (35%)	19 (73%)	7 (27%)	0	100	100
25	G2	121/133 (91%)	100 (83%)	20 (16%)	1 (1%)	16	54
26	H2	94/105 (90%)	73 (78%)	21 (22%)	0	100	100
27	I2	69/96 (72%)	53 (77%)	14 (20%)	2 (3%)	3	23
28	J2	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
29	K2	82/98 (84%)	63 (77%)	19 (23%)	0	100	100
30	L2	78/83 (94%)	66 (85%)	12 (15%)	0	100	100
31	N2	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
32	O2	112/127 (88%)	97 (87%)	15 (13%)	0	100	100
33	P2	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
34	Q2	166/171 (97%)	126 (76%)	40 (24%)	0	100	100
35	R2	302/345 (88%)	241 (80%)	59 (20%)	2 (1%)	18	56
36	S2	317/320 (99%)	246 (78%)	69 (22%)	2 (1%)	21	59
37	T2	136/140 (97%)	116 (85%)	20 (15%)	0	100	100
38	U2	87/145 (60%)	63 (72%)	24 (28%)	0	100	100
39	V2	136/143 (95%)	121 (89%)	14 (10%)	1 (1%)	18	56
40	M2	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
40	W2	79/88 (90%)	68 (86%)	11 (14%)	0	100	100
41	X2	47/57 (82%)	38 (81%)	8 (17%)	1 (2%)	5	30
42	Y2	55/72 (76%)	46 (84%)	9 (16%)	0	100	100
43	Z2	72/97 (74%)	57 (79%)	15 (21%)	0	100	100
44	a2	112/128 (88%)	95 (85%)	17 (15%)	0	100	100
45	b2	137/143 (96%)	113 (82%)	24 (18%)	0	100	100
46	c2	86/127 (68%)	68 (79%)	18 (21%)	0	100	100
47	d2	105/136 (77%)	82 (78%)	21 (20%)	2 (2%)	6	32
48	f2	165/178 (93%)	135 (82%)	30 (18%)	0	100	100
49	h2	89/125 (71%)	62 (70%)	25 (28%)	2 (2%)	5	29
50	i2	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
51	j2	111/120 (92%)	92 (83%)	19 (17%)	0	100	100
52	12	305/318 (96%)	269 (88%)	34 (11%)	2 (1%)	18	56
53	62	604/606 (100%)	536 (89%)	67 (11%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	g2	171/176 (97%)	139 (81%)	32 (19%)	0	100	100
55	e2	139/158 (88%)	82 (59%)	50 (36%)	7 (5%)	1	16
56	A3	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
57	B3	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
58	C3	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	D3	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	E3	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	F3	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
62	G3	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	13
63	H3	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	40
64	I3	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	J3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	20
66	K3	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	L3	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	M3	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13415/15148 (89%)	11221 (84%)	1971 (15%)	223 (2%)	9	36

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	327	ASP
1	A1	426	GLY
1	A1	427	PRO
2	B1	141	GLN
2	B1	183	ILE
2	B1	305	GLN
3	C1	8	HIS
3	C1	27	ILE
3	C1	109	PHE
4	D1	51	LEU
4	D1	73	GLY
4	D1	98	PRO
9	I1	72	VAL
1	M1	55	ALA
1	M1	427	PRO
2	N1	141	GLN
2	N1	183	ILE

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Mol	Chain	Res	Type
2	N1	351	ASN
3	O1	8	HIS
3	O1	27	ILE
3	O1	157	GLY
4	P1	51	LEU
4	P1	73	GLY
5	Q1	114	VAL
5	Q1	141	HIS
9	U1	72	VAL
10	V1	58	LYS
19	A2	463	SER
20	B2	88	HIS
20	B2	294	ARG
27	I2	105	LYS
36	S2	200	PRO
36	S2	276	ASP
47	d2	40	VAL
49	h2	81	ALA
49	h2	82	VAL
52	l2	126	LYS
55	e2	68	ASP
55	e2	71	GLY
55	e2	81	ARG
55	e2	82	SER
56	A3	328	HIS
56	A3	508	PRO
61	F3	2	SER
61	F3	87	THR
61	F3	95	GLN
62	G3	4	ALA
62	G3	9	GLY
63	H3	46	LYS
65	J3	2	GLU
1	A1	55	ALA
1	A1	56	GLY
1	A1	72	GLY
1	A1	80	GLU
1	A1	81	SER
1	A1	287	GLY
1	A1	288	ALA
1	A1	342	TRP
2	B1	236	LYS

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Mol	Chain	Res	Type
2	B1	351	ASN
3	C1	28	SER
3	C1	137	GLN
3	C1	157	GLY
3	C1	313	ARG
4	D1	154	PRO
7	G1	68	LYS
9	I1	59	ALA
10	J1	58	LYS
11	K1	33	VAL
1	M1	52	ASN
1	M1	72	GLY
1	M1	246	ASP
1	M1	282	CYS
1	M1	385	THR
2	N1	236	LYS
5	Q1	137	GLY
9	U1	59	ALA
10	V1	23	THR
10	V1	24	ILE
16	72	171	ILE
20	B2	84	PHE
20	B2	91	ALA
20	B2	93	GLY
20	B2	94	VAL
22	D2	113	PHE
27	I2	107	THR
41	X2	14	VAL
52	12	282	TYR
55	e2	74	ASP
55	e2	76	PRO
62	G3	5	LYS
1	A1	52	ASN
1	A1	352	SER
1	A1	385	THR
1	A1	395	TRP
2	B1	91	ALA
3	C1	283	SER
3	C1	319	PRO
4	D1	27	ARG
4	D1	119	ALA
4	D1	162	PRO

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Mol	Chain	Res	Type
4	D1	218	LEU
5	E1	16	PRO
5	E1	72	SER
10	J1	23	THR
10	J1	35	PHE
1	M1	81	SER
1	M1	107	PRO
1	M1	426	GLY
2	N1	24	LEU
2	N1	305	GLN
3	O1	28	SER
3	O1	62	ALA
3	O1	316	MET
3	O1	319	PRO
4	P1	80	MET
4	P1	162	PRO
5	Q1	64	ALA
5	Q1	177	PRO
7	S1	68	LYS
10	V1	57	HIS
14	42	20	ASN
14	42	21	ASN
14	42	419	TYR
16	72	149	TYR
19	A2	365	THR
19	A2	383	SER
20	B2	85	GLY
25	G2	122	SER
35	R2	134	TRP
35	R2	272	LEU
57	B3	104	TRP
62	G3	61	SER
1	A1	107	PRO
1	A1	246	ASP
1	A1	391	PRO
3	C1	236	ILE
3	C1	365	LEU
4	D1	80	MET
6	F1	95	LYS
10	J1	4	THR
10	J1	57	HIS
1	M1	6	GLN

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Mol	Chain	Res	Type
1	M1	109	ALA
2	N1	269	ALA
2	N1	409	ASP
3	O1	24	PRO
3	O1	109	PHE
5	Q1	130	PRO
6	R1	95	LYS
17	82	227	PRO
18	92	76	ALA
19	A2	563	ASP
39	V2	143	TYR
47	d2	19	PRO
56	A3	51	ASP
1	A1	6	GLN
1	A1	152	TYR
2	B1	39	GLU
3	C1	316	MET
4	D1	147	LEU
7	G1	72	LYS
1	M1	338	LEU
1	M1	391	PRO
3	O1	247	PRO
3	O1	255	ASN
4	P1	83	ARG
4	P1	98	PRO
4	P1	110	PRO
4	P1	147	LEU
4	P1	154	PRO
5	Q1	16	PRO
5	Q1	43	THR
5	Q1	69	LEU
5	Q1	188	THR
7	S1	50	PRO
14	42	112	ALA
19	A2	541	PRO
20	B2	291	VAL
23	E2	108	SER
57	B3	103	GLN
65	J3	3	ASN
1	A1	33	PRO
1	A1	109	ALA
2	B1	52	LYS

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Mol	Chain	Res	Type
4	D1	110	PRO
4	D1	163	PRO
4	D1	176	PRO
7	G1	45	ILE
1	M1	185	TYR
2	N1	52	LYS
4	P1	176	PRO
53	62	31	ASN
56	A3	91	ASP
57	B3	158	ASP
62	G3	49	PRO
2	B1	129	ALA
6	F1	51	PRO
1	M1	56	GLY
1	M1	293	PRO
20	B2	219	GLY
3	C1	339	GLY
4	D1	83	ARG
2	N1	85	ILE
2	N1	109	VAL
5	Q1	84	GLY
8	T1	69	VAL
10	J1	24	ILE
4	P1	123	GLY
6	R1	51	PRO
7	S1	45	ILE
13	32	24	LEU
61	F3	15	GLY
1	A1	260	PRO
4	D1	26	ILE
4	P1	163	PRO
9	U1	65	VAL
19	A2	461	PRO
3	C1	372	ILE
6	F1	47	ILE
19	A2	129	PRO
55	e2	78	LEU
1	M1	193	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	358/394 (91%)	269 (75%)	89 (25%)	0	4
1	M1	358/394 (91%)	276 (77%)	82 (23%)	1	6
2	B1	328/355 (92%)	254 (77%)	74 (23%)	1	6
2	N1	328/355 (92%)	254 (77%)	74 (23%)	1	6
3	C1	327/327 (100%)	251 (77%)	76 (23%)	1	5
3	O1	327/327 (100%)	259 (79%)	68 (21%)	1	6
4	D1	206/257 (80%)	172 (84%)	34 (16%)	2	10
4	P1	206/257 (80%)	170 (82%)	36 (18%)	2	9
5	E1	65/168 (39%)	47 (72%)	18 (28%)	0	3
5	Q1	167/168 (99%)	110 (66%)	57 (34%)	0	1
6	F1	96/99 (97%)	68 (71%)	28 (29%)	0	2
6	R1	96/99 (97%)	76 (79%)	20 (21%)	1	6
7	G1	71/72 (99%)	53 (75%)	18 (25%)	0	3
7	S1	71/72 (99%)	51 (72%)	20 (28%)	0	3
8	H1	61/85 (72%)	50 (82%)	11 (18%)	2	9
8	T1	61/85 (72%)	50 (82%)	11 (18%)	2	9
9	I1	27/60 (45%)	18 (67%)	9 (33%)	0	2
9	U1	27/60 (45%)	19 (70%)	8 (30%)	0	2
10	J1	52/54 (96%)	43 (83%)	9 (17%)	2	9
10	V1	52/54 (96%)	42 (81%)	10 (19%)	1	8
11	K1	15/46 (33%)	11 (73%)	4 (27%)	0	3
11	W1	15/46 (33%)	10 (67%)	5 (33%)	0	2
12	22	274/316 (87%)	274 (100%)	0	100	100
13	32	75/101 (74%)	75 (100%)	0	100	100
14	42	351/413 (85%)	351 (100%)	0	100	100
15	52	75/86 (87%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	72	104/142 (73%)	104 (100%)	0	100	100
17	82	236/353 (67%)	236 (100%)	0	100	100
18	92	160/183 (87%)	159 (99%)	1 (1%)	78	83
19	A2	551/588 (94%)	548 (100%)	3 (0%)	81	83
20	B2	330/371 (89%)	324 (98%)	6 (2%)	51	68
21	C2	183/204 (90%)	182 (100%)	1 (0%)	81	83
22	D2	126/150 (84%)	123 (98%)	3 (2%)	43	64
23	E2	145/151 (96%)	144 (99%)	1 (1%)	76	81
24	F2	13/69 (19%)	13 (100%)	0	100	100
25	G2	105/119 (88%)	105 (100%)	0	100	100
26	H2	80/95 (84%)	80 (100%)	0	100	100
27	I2	53/79 (67%)	49 (92%)	4 (8%)	12	33
28	J2	50/59 (85%)	50 (100%)	0	100	100
29	K2	66/81 (82%)	66 (100%)	0	100	100
30	L2	63/71 (89%)	63 (100%)	0	100	100
31	N2	88/101 (87%)	88 (100%)	0	100	100
32	O2	95/113 (84%)	95 (100%)	0	100	100
33	P2	72/96 (75%)	72 (100%)	0	100	100
34	Q2	142/154 (92%)	140 (99%)	2 (1%)	59	72
35	R2	230/298 (77%)	229 (100%)	1 (0%)	84	84
36	S2	205/283 (72%)	203 (99%)	2 (1%)	68	78
37	T2	79/101 (78%)	79 (100%)	0	100	100
38	U2	71/131 (54%)	71 (100%)	0	100	100
39	V2	107/120 (89%)	107 (100%)	0	100	100
40	M2	73/81 (90%)	73 (100%)	0	100	100
40	W2	55/81 (68%)	55 (100%)	0	100	100
41	X2	32/54 (59%)	32 (100%)	0	100	100
42	Y2	29/62 (47%)	29 (100%)	0	100	100
43	Z2	28/75 (37%)	28 (100%)	0	100	100
44	a2	70/114 (61%)	69 (99%)	1 (1%)	59	72
45	b2	85/124 (68%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	c2	45/121 (37%)	45 (100%)	0	100	100
47	d2	42/119 (35%)	42 (100%)	0	100	100
48	f2	80/160 (50%)	80 (100%)	0	100	100
49	h2	70/112 (62%)	70 (100%)	0	100	100
50	i2	23/45 (51%)	23 (100%)	0	100	100
51	j2	88/106 (83%)	88 (100%)	0	100	100
52	12	267/275 (97%)	259 (97%)	8 (3%)	36	57
53	62	523/534 (98%)	522 (100%)	1 (0%)	87	87
54	g2	130/157 (83%)	130 (100%)	0	100	100
55	e2	44/141 (31%)	43 (98%)	1 (2%)	44	64
56	A3	427/427 (100%)	387 (91%)	40 (9%)	8	26
57	B3	211/211 (100%)	191 (90%)	20 (10%)	8	25
58	C3	226/226 (100%)	199 (88%)	27 (12%)	5	18
59	D3	128/148 (86%)	117 (91%)	11 (9%)	10	29
60	E3	95/123 (77%)	89 (94%)	6 (6%)	16	37
61	F3	81/103 (79%)	73 (90%)	8 (10%)	7	24
62	G3	68/79 (86%)	52 (76%)	16 (24%)	1	5
63	H3	67/76 (88%)	58 (87%)	9 (13%)	4	14
64	I3	58/59 (98%)	51 (88%)	7 (12%)	5	17
65	J3	47/68 (69%)	41 (87%)	6 (13%)	4	15
66	K3	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	L3	40/55 (73%)	37 (92%)	3 (8%)	12	33
68	M3	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10651/12921 (82%)	9696 (91%)	955 (9%)	11	27

All (955) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	3	THR
1	A1	13	GLU
1	A1	24	ARG
1	A1	31	SER
1	A1	35	CYS
1	A1	37	VAL

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Mol	Chain	Res	Type
1	A1	42	ASP
1	A1	46	ARG
1	A1	48	GLU
1	A1	49	SER
1	A1	65	LYS
1	A1	68	LYS
1	A1	70	ARG
1	A1	75	LEU
1	A1	79	VAL
1	A1	86	LEU
1	A1	89	TYR
1	A1	90	SER
1	A1	91	THR
1	A1	92	ARG
1	A1	97	TYR
1	A1	99	ILE
1	A1	102	LEU
1	A1	108	LYS
1	A1	112	LEU
1	A1	120	CYS
1	A1	125	SER
1	A1	127	ILE
1	A1	128	GLU
1	A1	130	GLU
1	A1	133	VAL
1	A1	134	ILE
1	A1	138	LEU
1	A1	143	THR
1	A1	149	VAL
1	A1	156	THR
1	A1	159	GLN
1	A1	163	LEU
1	A1	174	VAL
1	A1	175	ARG
1	A1	176	LYS
1	A1	177	LEU
1	A1	178	SER
1	A1	179	ARG
1	A1	183	THR
1	A1	187	SER
1	A1	191	LYS
1	A1	195	MET

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Mol	Chain	Res	Type
1	A1	196	VAL
1	A1	197	LEU
1	A1	208	LEU
1	A1	211	LEU
1	A1	213	GLN
1	A1	216	PHE
1	A1	239	SER
1	A1	241	ILE
1	A1	245	GLU
1	A1	246	ASP
1	A1	248	LEU
1	A1	255	ILE
1	A1	272	VAL
1	A1	277	ILE
1	A1	296	SER
1	A1	302	LYS
1	A1	312	ILE
1	A1	316	ASP
1	A1	330	SER
1	A1	334	MET
1	A1	337	VAL
1	A1	341	GLN
1	A1	344	ARG
1	A1	346	CYS
1	A1	351	GLU
1	A1	352	SER
1	A1	353	GLU
1	A1	356	ARG
1	A1	358	LYS
1	A1	360	LEU
1	A1	366	VAL
1	A1	367	SER
1	A1	370	ASP
1	A1	379	ILE
1	A1	384	LEU
1	A1	386	TYR
1	A1	398	ARG
1	A1	407	VAL
1	A1	413	LYS
1	A1	428	ILE
1	A1	441	MET
2	B1	23	ASP

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Mol	Chain	Res	Type
2	B1	24	LEU
2	B1	35	ILE
2	B1	37	SER
2	B1	38	LEU
2	B1	45	SER
2	B1	46	ARG
2	B1	51	ILE
2	B1	52	LYS
2	B1	56	ARG
2	B1	58	GLU
2	B1	60	SER
2	B1	74	SER
2	B1	77	THR
2	B1	78	LYS
2	B1	81	SER
2	B1	85	ILE
2	B1	86	THR
2	B1	95	LYS
2	B1	96	LEU
2	B1	99	THR
2	B1	101	THR
2	B1	108	THR
2	B1	112	LEU
2	B1	113	ARG
2	B1	117	ASP
2	B1	119	LEU
2	B1	131	GLU
2	B1	134	ARG
2	B1	140	LEU
2	B1	145	ARG
2	B1	159	VAL
2	B1	160	ILE
2	B1	175	SER
2	B1	185	LYS
2	B1	187	THR
2	B1	190	GLU
2	B1	196	GLN
2	B1	203	ARG
2	B1	206	LEU
2	B1	215	VAL
2	B1	219	VAL
2	B1	238	LYS

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Mol	Chain	Res	Type
2	B1	240	HIS
2	B1	245	ARG
2	B1	253	VAL
2	B1	264	ILE
2	B1	286	LYS
2	B1	292	THR
2	B1	294	SER
2	B1	295	LEU
2	B1	297	GLN
2	B1	310	SER
2	B1	318	ASP
2	B1	319	SER
2	B1	327	ILE
2	B1	328	SER
2	B1	337	ILE
2	B1	347	ILE
2	B1	353	SER
2	B1	354	ASN
2	B1	374	SER
2	B1	391	SER
2	B1	393	THR
2	B1	396	SER
2	B1	402	ILE
2	B1	416	LYS
2	B1	418	VAL
2	B1	422	LYS
2	B1	423	SER
2	B1	430	LEU
2	B1	436	ILE
2	B1	437	ASP
2	B1	438	GLU
3	C1	1	MET
3	C1	5	ARG
3	C1	6	LYS
3	C1	7	SER
3	C1	11	MET
3	C1	25	SER
3	C1	26	ASN
3	C1	27	ILE
3	C1	29	SER
3	C1	32	ASN
3	C1	39	ILE

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Mol	Chain	Res	Type
3	C1	43	LEU
3	C1	51	LEU
3	C1	57	SER
3	C1	60	THR
3	C1	61	THR
3	C1	65	SER
3	C1	67	THR
3	C1	73	VAL
3	C1	78	ILE
3	C1	94	LEU
3	C1	115	ILE
3	C1	118	ILE
3	C1	119	LEU
3	C1	123	VAL
3	C1	138	MET
3	C1	139	SER
3	C1	144	THR
3	C1	156	ILE
3	C1	158	THR
3	C1	161	VAL
3	C1	169	SER
3	C1	174	THR
3	C1	176	THR
3	C1	177	ARG
3	C1	188	ILE
3	C1	192	ILE
3	C1	197	LEU
3	C1	198	LEU
3	C1	205	SER
3	C1	212	SER
3	C1	217	LYS
3	C1	226	ILE
3	C1	229	ILE
3	C1	233	LEU
3	C1	237	LEU
3	C1	240	MET
3	C1	241	LEU
3	C1	243	VAL
3	C1	244	LEU
3	C1	247	PRO
3	C1	262	LEU
3	C1	271	GLU

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Mol	Chain	Res	Type
3	C1	273	TYR
3	C1	280	ILE
3	C1	281	LEU
3	C1	282	ARG
3	C1	284	ILE
3	C1	291	VAL
3	C1	299	LEU
3	C1	304	ILE
3	C1	310	SER
3	C1	311	LYS
3	C1	312	GLN
3	C1	313	ARG
3	C1	314	SER
3	C1	316	MET
3	C1	318	ARG
3	C1	321	SER
3	C1	324	LEU
3	C1	343	VAL
3	C1	353	LEU
3	C1	362	ILE
3	C1	363	LEU
3	C1	375	LYS
3	C1	377	LEU
4	D1	3	LEU
4	D1	9	SER
4	D1	10	TYR
4	D1	17	LEU
4	D1	20	SER
4	D1	21	LEU
4	D1	26	ILE
4	D1	27	ARG
4	D1	32	VAL
4	D1	40	CYS
4	D1	42	SER
4	D1	43	MET
4	D1	52	VAL
4	D1	55	CYS
4	D1	80	MET
4	D1	82	MET
4	D1	83	ARG
4	D1	87	LEU
4	D1	106	ASN

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Mol	Chain	Res	Type
4	D1	116	ILE
4	D1	120	ARG
4	D1	124	GLU
4	D1	127	VAL
4	D1	132	THR
4	D1	139	THR
4	D1	141	VAL
4	D1	179	MET
4	D1	182	VAL
4	D1	186	VAL
4	D1	201	ARG
4	D1	208	MET
4	D1	218	LEU
4	D1	228	SER
4	D1	231	LYS
5	E1	1	SER
5	E1	5	ILE
5	E1	6	LYS
5	E1	11	SER
5	E1	14	ARG
5	E1	15	ARG
5	E1	17	GLU
5	E1	19	LEU
5	E1	28	SER
5	E1	30	GLU
5	E1	32	ARG
5	E1	33	LYS
5	E1	40	THR
5	E1	52	LYS
5	E1	58	PHE
5	E1	63	SER
5	E1	67	ASP
5	E1	68	VAL
6	F1	7	SER
6	F1	9	SER
6	F1	10	SER
6	F1	11	ARG
6	F1	13	LEU
6	F1	16	ILE
6	F1	18	LYS
6	F1	35	ASP
6	F1	44	LYS

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Mol	Chain	Res	Type
6	F1	47	ILE
6	F1	48	ARG
6	F1	50	LEU
6	F1	53	ASN
6	F1	54	LEU
6	F1	58	ARG
6	F1	68	LEU
6	F1	69	SER
6	F1	70	MET
6	F1	74	ILE
6	F1	77	LYS
6	F1	82	LYS
6	F1	88	SER
6	F1	90	LEU
6	F1	94	LEU
6	F1	95	LYS
6	F1	98	ILE
6	F1	100	GLU
6	F1	110	LYS
7	G1	4	PHE
7	G1	8	THR
7	G1	9	ARG
7	G1	10	VAL
7	G1	15	THR
7	G1	19	SER
7	G1	23	GLN
7	G1	24	ARG
7	G1	39	ARG
7	G1	40	ARG
7	G1	41	THR
7	G1	42	ARG
7	G1	45	ILE
7	G1	46	LEU
7	G1	58	VAL
7	G1	60	THR
7	G1	69	SER
7	G1	70	LYS
8	H1	20	VAL
8	H1	29	LYS
8	H1	30	CYS
8	H1	31	VAL
8	H1	54	CYS

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Mol	Chain	Res	Type
8	H1	57	GLU
8	H1	58	LEU
8	H1	59	LEU
8	H1	73	LEU
8	H1	74	PHE
8	H1	76	SER
9	I1	46	LYS
9	I1	49	VAL
9	I1	54	SER
9	I1	69	SER
9	I1	70	LEU
9	I1	72	VAL
9	I1	76	VAL
9	I1	77	ARG
9	I1	78	TYR
10	J1	4	THR
10	J1	11	SER
10	J1	13	LEU
10	J1	17	THR
10	J1	18	SER
10	J1	24	ILE
10	J1	25	VAL
10	J1	46	ILE
10	J1	58	LYS
11	K1	20	THR
11	K1	23	LEU
11	K1	27	VAL
11	K1	36	THR
1	M1	3	THR
1	M1	13	GLU
1	M1	24	ARG
1	M1	31	SER
1	M1	37	VAL
1	M1	42	ASP
1	M1	45	SER
1	M1	46	ARG
1	M1	48	GLU
1	M1	51	LYS
1	M1	70	ARG
1	M1	79	VAL
1	M1	86	LEU
1	M1	89	TYR

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Mol	Chain	Res	Type
1	M1	91	THR
1	M1	92	ARG
1	M1	97	TYR
1	M1	99	ILE
1	M1	108	LYS
1	M1	112	LEU
1	M1	125	SER
1	M1	127	ILE
1	M1	128	GLU
1	M1	130	GLU
1	M1	133	VAL
1	M1	137	GLU
1	M1	138	LEU
1	M1	143	THR
1	M1	149	VAL
1	M1	156	THR
1	M1	159	GLN
1	M1	163	LEU
1	M1	174	VAL
1	M1	175	ARG
1	M1	176	LYS
1	M1	177	LEU
1	M1	179	ARG
1	M1	183	THR
1	M1	187	SER
1	M1	191	LYS
1	M1	195	MET
1	M1	197	LEU
1	M1	208	LEU
1	M1	211	LEU
1	M1	213	GLN
1	M1	216	PHE
1	M1	245	GLU
1	M1	246	ASP
1	M1	248	LEU
1	M1	257	VAL
1	M1	277	ILE
1	M1	296	SER
1	M1	302	LYS
1	M1	307	PHE
1	M1	309	THR
1	M1	316	ASP

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Mol	Chain	Res	Type
1	M1	319	LEU
1	M1	329	MET
1	M1	330	SER
1	M1	334	MET
1	M1	337	VAL
1	M1	341	GLN
1	M1	344	ARG
1	M1	346	CYS
1	M1	347	THR
1	M1	351	GLU
1	M1	353	GLU
1	M1	356	ARG
1	M1	358	LYS
1	M1	360	LEU
1	M1	366	VAL
1	M1	370	ASP
1	M1	379	ILE
1	M1	382	SER
1	M1	384	LEU
1	M1	386	TYR
1	M1	407	VAL
1	M1	412	SER
1	M1	413	LYS
1	M1	419	CYS
1	M1	428	ILE
1	M1	441	MET
2	N1	23	ASP
2	N1	24	LEU
2	N1	35	ILE
2	N1	37	SER
2	N1	38	LEU
2	N1	45	SER
2	N1	46	ARG
2	N1	52	LYS
2	N1	56	ARG
2	N1	58	GLU
2	N1	60	SER
2	N1	65	THR
2	N1	78	LYS
2	N1	81	SER
2	N1	84	LYS
2	N1	85	ILE

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Mol	Chain	Res	Type
2	N1	86	THR
2	N1	96	LEU
2	N1	99	THR
2	N1	100	SER
2	N1	101	THR
2	N1	102	ARG
2	N1	108	THR
2	N1	111	CYS
2	N1	112	LEU
2	N1	113	ARG
2	N1	117	ASP
2	N1	119	LEU
2	N1	134	ARG
2	N1	145	ARG
2	N1	159	VAL
2	N1	160	ILE
2	N1	175	SER
2	N1	183	ILE
2	N1	185	LYS
2	N1	190	GLU
2	N1	196	GLN
2	N1	201	SER
2	N1	203	ARG
2	N1	206	LEU
2	N1	207	ILE
2	N1	215	VAL
2	N1	219	VAL
2	N1	233	SER
2	N1	238	LYS
2	N1	240	HIS
2	N1	244	ILE
2	N1	253	VAL
2	N1	264	ILE
2	N1	266	SER
2	N1	286	LYS
2	N1	292	THR
2	N1	295	LEU
2	N1	297	GLN
2	N1	315	SER
2	N1	317	SER
2	N1	318	ASP
2	N1	327	ILE

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Mol	Chain	Res	Type
2	N1	328	SER
2	N1	329	GLN
2	N1	337	ILE
2	N1	345	LYS
2	N1	346	THR
2	N1	354	ASN
2	N1	357	VAL
2	N1	384	SER
2	N1	402	ILE
2	N1	403	ASP
2	N1	416	LYS
2	N1	418	VAL
2	N1	424	MET
2	N1	436	ILE
2	N1	437	ASP
2	N1	438	GLU
3	O1	1	MET
3	O1	5	ARG
3	O1	6	LYS
3	O1	7	SER
3	O1	11	MET
3	O1	13	ILE
3	O1	27	ILE
3	O1	32	ASN
3	O1	35	SER
3	O1	39	ILE
3	O1	44	GLN
3	O1	60	THR
3	O1	61	THR
3	O1	67	THR
3	O1	69	ILE
3	O1	73	VAL
3	O1	92	ILE
3	O1	94	LEU
3	O1	100	ARG
3	O1	115	ILE
3	O1	118	ILE
3	O1	119	LEU
3	O1	138	MET
3	O1	139	SER
3	O1	144	THR
3	O1	153	ILE

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Mol	Chain	Res	Type
3	O1	156	ILE
3	O1	158	THR
3	O1	161	VAL
3	O1	169	SER
3	O1	174	THR
3	O1	176	THR
3	O1	184	ILE
3	O1	188	ILE
3	O1	189	ILE
3	O1	192	ILE
3	O1	197	LEU
3	O1	212	SER
3	O1	215	VAL
3	O1	226	ILE
3	O1	229	ILE
3	O1	233	LEU
3	O1	241	LEU
3	O1	242	LEU
3	O1	243	VAL
3	O1	244	LEU
3	O1	257	THR
3	O1	262	LEU
3	O1	271	GLU
3	O1	281	LEU
3	O1	282	ARG
3	O1	287	LYS
3	O1	291	VAL
3	O1	297	SER
3	O1	299	LEU
3	O1	300	ILE
3	O1	313	ARG
3	O1	316	MET
3	O1	318	ARG
3	O1	324	LEU
3	O1	338	ILE
3	O1	349	THR
3	O1	356	VAL
3	O1	362	ILE
3	O1	363	LEU
3	O1	375	LYS
3	O1	377	LEU
3	O1	378	LYS

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Mol	Chain	Res	Type
4	P1	3	LEU
4	P1	10	TYR
4	P1	13	SER
4	P1	17	LEU
4	P1	20	SER
4	P1	21	LEU
4	P1	38	SER
4	P1	39	SER
4	P1	40	CYS
4	P1	42	SER
4	P1	43	MET
4	P1	52	VAL
4	P1	55	CYS
4	P1	80	MET
4	P1	82	MET
4	P1	83	ARG
4	P1	88	SER
4	P1	106	ASN
4	P1	120	ARG
4	P1	124	GLU
4	P1	127	VAL
4	P1	132	THR
4	P1	139	THR
4	P1	141	VAL
4	P1	158	ILE
4	P1	160	MET
4	P1	179	MET
4	P1	180	SER
4	P1	182	VAL
4	P1	186	VAL
4	P1	201	ARG
4	P1	208	MET
4	P1	210	LEU
4	P1	223	LYS
4	P1	226	LYS
4	P1	231	LYS
5	Q1	5	ILE
5	Q1	6	LYS
5	Q1	11	SER
5	Q1	14	ARG
5	Q1	17	GLU
5	Q1	18	VAL

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Mol	Chain	Res	Type
5	Q1	19	LEU
5	Q1	22	THR
5	Q1	23	LYS
5	Q1	28	SER
5	Q1	30	GLU
5	Q1	32	ARG
5	Q1	33	LYS
5	Q1	36	SER
5	Q1	40	THR
5	Q1	42	THR
5	Q1	43	THR
5	Q1	44	THR
5	Q1	45	VAL
5	Q1	58	PHE
5	Q1	60	SER
5	Q1	61	SER
5	Q1	62	MET
5	Q1	63	SER
5	Q1	65	SER
5	Q1	68	VAL
5	Q1	71	MET
5	Q1	73	LYS
5	Q1	74	ILE
5	Q1	76	ILE
5	Q1	78	LEU
5	Q1	81	ILE
5	Q1	87	MET
5	Q1	95	PRO
5	Q1	98	VAL
5	Q1	102	THR
5	Q1	103	LYS
5	Q1	106	ILE
5	Q1	109	GLU
5	Q1	113	GLU
5	Q1	114	VAL
5	Q1	125	GLU
5	Q1	129	LYS
5	Q1	136	ILE
5	Q1	139	CYS
5	Q1	140	THR
5	Q1	144	CYS
5	Q1	147	ILE

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Mol	Chain	Res	Type
5	Q1	152	ASP
5	Q1	158	CYS
5	Q1	168	SER
5	Q1	171	ILE
5	Q1	172	ARG
5	Q1	178	LEU
5	Q1	192	MET
5	Q1	194	ILE
5	Q1	195	VAL
6	R1	7	SER
6	R1	11	ARG
6	R1	16	ILE
6	R1	35	ASP
6	R1	47	ILE
6	R1	48	ARG
6	R1	54	LEU
6	R1	64	ARG
6	R1	68	LEU
6	R1	70	MET
6	R1	75	LEU
6	R1	77	LYS
6	R1	88	SER
6	R1	90	LEU
6	R1	94	LEU
6	R1	98	ILE
6	R1	100	GLU
6	R1	101	ARG
6	R1	103	GLU
6	R1	110	LYS
7	S1	4	PHE
7	S1	7	LEU
7	S1	8	THR
7	S1	9	ARG
7	S1	10	VAL
7	S1	15	THR
7	S1	18	LEU
7	S1	19	SER
7	S1	23	GLN
7	S1	24	ARG
7	S1	31	SER
7	S1	39	ARG
7	S1	40	ARG

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Mol	Chain	Res	Type
7	S1	41	THR
7	S1	42	ARG
7	S1	45	ILE
7	S1	46	LEU
7	S1	58	VAL
7	S1	69	SER
7	S1	70	LYS
8	T1	20	VAL
8	T1	29	LYS
8	T1	30	CYS
8	T1	31	VAL
8	T1	46	SER
8	T1	48	SER
8	T1	54	CYS
8	T1	57	GLU
8	T1	58	LEU
8	T1	73	LEU
8	T1	74	PHE
9	U1	46	LYS
9	U1	49	VAL
9	U1	68	VAL
9	U1	70	LEU
9	U1	72	VAL
9	U1	76	VAL
9	U1	77	ARG
9	U1	78	TYR
10	V1	4	THR
10	V1	9	LEU
10	V1	12	LEU
10	V1	13	LEU
10	V1	16	ARG
10	V1	18	SER
10	V1	42	ILE
10	V1	46	ILE
10	V1	55	ILE
10	V1	58	LYS
11	W1	20	THR
11	W1	23	LEU
11	W1	27	VAL
11	W1	33	VAL
11	W1	36	THR
18	92	93	LEU

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Mol	Chain	Res	Type
19	A2	253	VAL
19	A2	341	ILE
19	A2	538	GLN
20	B2	92	HIS
20	B2	94	VAL
20	B2	95	LEU
20	B2	96	ARG
20	B2	97	LEU
20	B2	372	LYS
21	C2	218	VAL
22	D2	113	PHE
22	D2	114	ARG
22	D2	181	ILE
23	E2	77	LEU
27	I2	101	ILE
27	I2	103	LEU
27	I2	105	LYS
27	I2	106	GLU
34	Q2	115	LEU
34	Q2	128	VAL
35	R2	152	ILE
36	S2	200	PRO
36	S2	216	LYS
44	a2	76	ILE
52	12	25	ARG
52	12	126	LYS
52	12	134	ARG
52	12	187	ILE
52	12	224	PHE
52	12	228	TYR
52	12	240	ILE
52	12	310	LEU
53	62	427	ILE
55	e2	75	TYR
56	A3	18	LEU
56	A3	35	LEU
56	A3	92	MET
56	A3	96	ARG
56	A3	105	LEU
56	A3	115	SER
56	A3	136	LEU
56	A3	138	HIS

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Mol	Chain	Res	Type
56	A3	150	LEU
56	A3	158	ILE
56	A3	159	LEU
56	A3	187	SER
56	A3	188	VAL
56	A3	189	MET
56	A3	194	LEU
56	A3	199	LEU
56	A3	213	ARG
56	A3	241	PRO
56	A3	273	MET
56	A3	295	VAL
56	A3	301	THR
56	A3	306	THR
56	A3	318	VAL
56	A3	324	LEU
56	A3	347	LEU
56	A3	353	LEU
56	A3	354	THR
56	A3	365	ILE
56	A3	369	ASP
56	A3	373	VAL
56	A3	383	MET
56	A3	417	MET
56	A3	444	PRO
56	A3	465	VAL
56	A3	467	LEU
56	A3	474	GLU
56	A3	492	LEU
56	A3	508	PRO
56	A3	509	THR
56	A3	512	ASN
57	B3	7	LEU
57	B3	16	ILE
57	B3	31	VAL
57	B3	33	LEU
57	B3	52	HIS
57	B3	60	GLU
57	B3	63	THR
57	B3	67	ILE
57	B3	88	ASP
57	B3	92	ASN

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Mol	Chain	Res	Type
57	B3	125	THR
57	B3	130	PRO
57	B3	134	ARG
57	B3	142	VAL
57	B3	147	GLU
57	B3	170	LEU
57	B3	171	LYS
57	B3	185	MET
57	B3	205	SER
57	B3	216	LEU
58	C3	1	MET
58	C3	11	VAL
58	C3	13	PRO
58	C3	14	SER
58	C3	18	LEU
58	C3	19	THR
58	C3	22	LEU
58	C3	26	LEU
58	C3	38	ASN
58	C3	39	SER
58	C3	85	LEU
58	C3	92	LEU
58	C3	112	LEU
58	C3	127	LEU
58	C3	128	GLU
58	C3	131	LEU
58	C3	132	LEU
58	C3	137	LEU
58	C3	142	VAL
58	C3	160	LEU
58	C3	163	LEU
58	C3	188	ILE
58	C3	196	THR
58	C3	199	VAL
58	C3	213	THR
58	C3	222	GLN
58	C3	230	ASN
59	D3	9	GLU
59	D3	27	VAL
59	D3	31	LYS
59	D3	36	SER
59	D3	40	LEU

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Mol	Chain	Res	Type
59	D3	59	LEU
59	D3	62	LEU
59	D3	107	ILE
59	D3	116	VAL
59	D3	143	ASN
59	D3	147	LYS
60	E3	7	THR
60	E3	29	LEU
60	E3	70	VAL
60	E3	79	LYS
60	E3	80	GLU
60	E3	90	ARG
61	F3	6	VAL
61	F3	20	VAL
61	F3	37	LYS
61	F3	52	ILE
61	F3	53	THR
61	F3	74	LEU
61	F3	95	GLN
61	F3	98	HIS
62	G3	5	LYS
62	G3	7	ASP
62	G3	8	HIS
62	G3	14	ARG
62	G3	17	ARG
62	G3	33	LEU
62	G3	34	ASN
62	G3	37	LEU
62	G3	41	HIS
62	G3	42	ARG
62	G3	43	GLU
62	G3	48	ILE
62	G3	54	ARG
62	G3	56	ARG
62	G3	68	THR
62	G3	78	LEU
63	H3	19	ARG
63	H3	29	CYS
63	H3	41	LYS
63	H3	51	SER
63	H3	53	CYS
63	H3	57	ARG

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Mol	Chain	Res	Type
63	H3	60	TYR
63	H3	67	SER
63	H3	75	ARG
64	I3	2	THR
64	I3	4	LEU
64	I3	8	GLN
64	I3	22	VAL
64	I3	26	MET
64	I3	44	LYS
64	I3	64	ARG
65	J3	2	GLU
65	J3	5	VAL
65	J3	8	LYS
65	J3	16	ASN
65	J3	23	LYS
65	J3	27	THR
66	K3	45	VAL
66	K3	48	VAL
66	K3	49	THR
67	L3	15	VAL
67	L3	22	LEU
67	L3	26	THR
68	M3	13	LYS
68	M3	24	LEU
68	M3	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	18	GLN
1	A1	21	ASN
1	A1	32	GLN
1	A1	73	ASN
1	A1	85	HIS
1	A1	136	GLN
1	A1	151	ASN
1	A1	154	HIS
1	A1	189	HIS
1	A1	240	GLN
1	A1	243	HIS
1	A1	252	HIS
1	A1	289	HIS

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Mol	Chain	Res	Type
1	A1	308	GLN
1	A1	435	ASN
2	B1	62	ASN
2	B1	67	HIS
2	B1	125	ASN
2	B1	162	ASN
2	B1	164	HIS
2	B1	198	HIS
2	B1	247	GLN
2	B1	304	HIS
2	B1	429	ASN
3	C1	15	ASN
3	C1	26	ASN
3	C1	32	ASN
3	C1	114	ASN
3	C1	206	ASN
3	C1	312	GLN
3	C1	374	ASN
4	D1	6	HIS
4	D1	50	HIS
4	D1	75	ASN
4	D1	106	ASN
4	D1	181	GLN
5	E1	57	GLN
6	F1	38	HIS
7	G1	6	HIS
7	G1	36	ASN
9	I1	71	ASN
10	J1	54	HIS
1	M1	18	GLN
1	M1	32	GLN
1	M1	85	HIS
1	M1	136	GLN
1	M1	151	ASN
1	M1	154	HIS
1	M1	159	GLN
1	M1	173	ASN
1	M1	189	HIS
1	M1	213	GLN
1	M1	240	GLN
1	M1	243	HIS
1	M1	308	GLN

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Mol	Chain	Res	Type
1	M1	323	HIS
1	M1	339	GLN
1	M1	435	ASN
2	N1	62	ASN
2	N1	67	HIS
2	N1	125	ASN
2	N1	141	GLN
2	N1	198	HIS
2	N1	247	GLN
2	N1	304	HIS
2	N1	429	ASN
3	O1	15	ASN
3	O1	26	ASN
3	O1	32	ASN
3	O1	54	HIS
3	O1	114	ASN
3	O1	206	ASN
3	O1	374	ASN
4	P1	6	HIS
4	P1	50	HIS
4	P1	75	ASN
4	P1	106	ASN
4	P1	181	GLN
4	P1	225	HIS
5	Q1	53	ASN
5	Q1	121	GLN
6	R1	38	HIS
6	R1	73	GLN
7	S1	6	HIS
10	V1	54	HIS
12	22	48	HIS
12	22	120	GLN
12	22	186	HIS
13	32	80	GLN
14	42	26	ASN
14	42	83	HIS
14	42	338	HIS
14	42	366	ASN
14	42	374	ASN
15	52	7	ASN
16	72	46	ASN
17	82	220	GLN

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Mol	Chain	Res	Type
17	82	346	GLN
17	82	418	GLN
17	82	441	HIS
19	A2	140	GLN
19	A2	142	GLN
19	A2	221	ASN
19	A2	359	ASN
19	A2	424	HIS
19	A2	571	HIS
19	A2	572	HIS
19	A2	666	GLN
20	B2	92	HIS
20	B2	131	GLN
20	B2	168	GLN
20	B2	182	ASN
20	B2	250	ASN
20	B2	431	HIS
21	C2	84	ASN
21	C2	140	ASN
21	C2	230	GLN
22	D2	98	HIS
26	H2	27	HIS
26	H2	45	HIS
26	H2	97	HIS
27	I2	102	ASN
29	K2	22	HIS
29	K2	86	GLN
31	N2	83	GLN
33	P2	25	GLN
34	Q2	103	GLN
35	R2	43	HIS
35	R2	79	GLN
35	R2	84	HIS
35	R2	169	HIS
35	R2	171	ASN
35	R2	251	ASN
35	R2	331	HIS
36	S2	211	ASN
36	S2	223	GLN
36	S2	252	GLN
38	U2	59	HIS
38	U2	91	HIS

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Mol	Chain	Res	Type
41	X2	10	HIS
41	X2	13	HIS
42	Y2	57	GLN
44	a2	33	GLN
44	a2	79	ASN
44	a2	126	ASN
45	b2	141	GLN
45	b2	181	HIS
46	c2	14	GLN
46	c2	89	HIS
48	f2	12	HIS
48	f2	14	GLN
51	j2	59	HIS
52	12	32	GLN
52	12	47	GLN
52	12	169	GLN
52	12	235	ASN
52	12	292	ASN
52	12	317	GLN
53	62	31	ASN
53	62	175	ASN
53	62	270	ASN
53	62	295	GLN
53	62	296	ASN
53	62	332	HIS
53	62	471	ASN
53	62	546	GLN
54	g2	55	GLN
54	g2	161	GLN
40	M2	33	ASN
56	A3	4	ASN
56	A3	11	ASN
56	A3	12	HIS
56	A3	55	ASN
56	A3	99	ASN
56	A3	170	ASN
56	A3	256	HIS
56	A3	360	ASN
56	A3	368	HIS
56	A3	413	HIS
56	A3	503	HIS
56	A3	512	ASN

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Mol	Chain	Res	Type
57	B3	52	HIS
57	B3	102	HIS
57	B3	103	GLN
57	B3	195	GLN
57	B3	203	ASN
58	C3	3	HIS
58	C3	6	HIS
58	C3	12	ASN
58	C3	133	ASN
58	C3	148	HIS
58	C3	158	HIS
58	C3	204	HIS
58	C3	207	HIS
58	C3	222	GLN
58	C3	232	HIS
59	D3	32	ASN
59	D3	109	HIS
60	E3	34	ASN
61	F3	66	ASN
62	G3	51	HIS
62	G3	52	HIS
63	H3	23	GLN
63	H3	24	ASN
63	H3	25	GLN
63	H3	28	ASN
63	H3	32	ASN
63	H3	37	HIS
65	J3	3	ASN
65	J3	16	ASN
65	J3	21	HIS
66	K3	10	HIS
66	K3	15	ASN
66	K3	35	GLN
66	K3	41	ASN
67	L3	42	HIS
68	M3	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 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	$\# Z > 2$
78	PC1	S2	401	-	46,46,53	0.99	4 (8%)	52,54,61	1.03	2 (3%)
72	3PE	42	502	-	40,40,50	0.94	3 (7%)	43,45,55	1.20	2 (4%)
75	SF4	D2	301	-	0,12,12	-	-	-	-	-
75	SF4	E2	302	23	0,12,12	-	-	-	-	-
77	NAP	R2	601	-	49,52,52	4.40	22 (44%)	69,80,80	1.87	18 (26%)
70	HEC	D1	301	4	50,50,50	1.28	3 (6%)	68,82,82	1.14	5 (7%)
75	SF4	82	502	-	0,12,12	-	-	-	-	-
78	PC1	j2	201	-	38,38,53	1.08	4 (10%)	44,46,61	1.03	2 (4%)
75	SF4	A2	801	19	0,12,12	-	-	-	-	-
75	SF4	E2	301	23	0,12,12	-	-	-	-	-
79	HEA	A3	601	56	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
69	HEM	O1	402	3	50,50,50	1.35	7 (14%)	66,82,82	1.76	15 (22%)
69	HEM	C1	402	3	50,50,50	1.26	6 (12%)	66,82,82	1.85	18 (27%)
69	HEM	C1	401	3	50,50,50	1.30	6 (12%)	66,82,82	1.54	10 (15%)
74	FMN	82	501	-	33,33,33	1.05	2 (6%)	48,50,50	1.42	10 (20%)
71	FES	92	301	18	0,4,4	-	-	-	-	-
70	HEC	P1	301	4	50,50,50	1.31	5 (10%)	68,82,82	1.04	4 (5%)
75	SF4	A2	802	19	0,12,12	-	-	-	-	-
79	HEA	A3	602	56	66,67,67	1.22	7 (10%)	78,103,103	1.37	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	3PE	22	401	-	40,40,50	0.94	3 (7%)	43,45,55	1.13	2 (4%)
69	HEM	O1	401	3	50,50,50	1.40	7 (14%)	66,82,82	1.92	18 (27%)
71	FES	A2	803	19	0,4,4	-	-	-	-	-
72	3PE	B2	501	20	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
73	CDL	42	501	-	81,81,99	0.96	6 (7%)	87,93,111	1.10	5 (5%)
71	FES	Q1	201	5	0,4,4	-	-	-	-	-

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
78	PC1	S2	401	-	-	20/50/50/57	-
72	3PE	42	502	-	-	25/44/44/54	-
75	SF4	D2	301	-	-	-	0/6/5/5
75	SF4	E2	302	23	-	-	0/6/5/5
77	NAP	R2	601	-	-	17/35/67/67	0/5/5/5
70	HEC	D1	301	4	-	8/14/54/54	-
75	SF4	82	502	-	-	-	0/6/5/5
78	PC1	j2	201	-	-	21/42/42/57	-
75	SF4	A2	801	19	-	-	0/6/5/5
75	SF4	E2	301	23	-	-	0/6/5/5
79	HEA	A3	601	56	-	9/36/76/76	-
69	HEM	O1	402	3	-	4/14/54/54	-
69	HEM	C1	402	3	-	6/14/54/54	-
69	HEM	C1	401	3	-	4/14/54/54	-
74	FMN	82	501	-	-	7/18/18/18	0/3/3/3
71	FES	92	301	18	-	-	0/1/1/1
70	HEC	P1	301	4	-	8/14/54/54	-
75	SF4	A2	802	19	-	-	0/6/5/5
79	HEA	A3	602	56	-	7/36/76/76	-
72	3PE	22	401	-	-	20/44/44/54	-
69	HEM	O1	401	3	-	6/14/54/54	-
71	FES	A2	803	19	-	-	0/1/1/1
72	3PE	B2	501	20	-	26/54/54/54	-
73	CDL	42	501	-	-	42/92/92/110	-
71	FES	Q1	201	5	-	-	0/1/1/1

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	R2	601	NAP	O4D-C1D	16.06	1.63	1.41
77	R2	601	NAP	C2D-C1D	-14.73	1.31	1.53
77	R2	601	NAP	C2B-C1B	-9.08	1.29	1.53
77	R2	601	NAP	O4B-C1B	8.42	1.62	1.42
77	R2	601	NAP	C7N-N7N	7.23	1.46	1.33
77	R2	601	NAP	O4D-C4D	-6.60	1.30	1.45
77	R2	601	NAP	O4B-C4B	-5.76	1.32	1.45
77	R2	601	NAP	C3N-C7N	5.38	1.58	1.50
77	R2	601	NAP	C6A-N6A	4.31	1.44	1.34
77	R2	601	NAP	C5A-N7A	-4.24	1.31	1.39
77	R2	601	NAP	O3D-C3D	-4.20	1.33	1.43
79	A3	602	HEA	CMA-C3A	-3.74	1.37	1.45
70	D1	301	HEC	CBB-CAB	-3.53	1.35	1.51
77	R2	601	NAP	O2D-C2D	3.52	1.51	1.43
70	P1	301	HEC	CBC-CAC	-3.50	1.35	1.51
70	D1	301	HEC	CBC-CAC	-3.39	1.36	1.51
77	R2	601	NAP	O7N-C7N	-3.38	1.17	1.24
69	C1	401	HEM	CAB-C3B	3.37	1.56	1.47
69	O1	402	HEM	FE-NA	3.35	2.06	1.95
70	P1	301	HEC	CBB-CAB	-3.34	1.36	1.51
69	O1	401	HEM	CAB-C3B	3.29	1.56	1.47
69	O1	402	HEM	FE-NC	3.28	2.06	1.95
74	82	501	FMN	C4A-N5	3.27	1.37	1.30
69	C1	401	HEM	FE-NB	3.16	2.04	1.94
69	C1	401	HEM	C3B-C2B	-3.09	1.31	1.37
69	O1	401	HEM	FE-NB	3.09	2.04	1.94
69	C1	402	HEM	CHB-C4A	-3.08	1.32	1.39
79	A3	602	HEA	FE-NA	2.89	2.04	1.95
69	O1	401	HEM	C1B-C2B	2.83	1.50	1.44
77	R2	601	NAP	O3B-C3B	-2.76	1.36	1.43
72	B2	501	3PE	O21-C2	-2.72	1.39	1.46
79	A3	601	HEA	C1A-C2A	-2.71	1.40	1.45
79	A3	601	HEA	CMA-C3A	-2.69	1.39	1.45
79	A3	602	HEA	C1D-C2D	2.68	1.49	1.44
73	42	501	CDL	OA6-CA4	-2.65	1.40	1.46
77	R2	601	NAP	PA-O5B	2.64	1.70	1.59
69	O1	402	HEM	CAC-C3C	2.64	1.54	1.47
77	R2	601	NAP	C4A-N9A	-2.64	1.31	1.37
79	A3	602	HEA	C1D-ND	-2.62	1.35	1.40
79	A3	602	HEA	C3A-C2A	-2.62	1.31	1.36
78	j2	201	PC1	O21-C2	-2.57	1.40	1.46
73	42	501	CDL	OB6-CB5	2.57	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	R2	601	NAP	P2B-O2B	2.55	1.64	1.59
69	O1	401	HEM	CAC-C3C	2.53	1.54	1.47
78	S2	401	PC1	O21-C2	-2.49	1.40	1.46
69	C1	401	HEM	FE-ND	2.49	2.02	1.94
77	R2	601	NAP	C8A-N9A	-2.47	1.33	1.37
72	42	502	3PE	O21-C21	2.46	1.41	1.34
73	42	501	CDL	OA8-CA7	2.44	1.40	1.33
72	22	401	3PE	O31-C31	2.44	1.40	1.33
72	22	401	3PE	O21-C21	2.44	1.41	1.34
78	S2	401	PC1	O31-C31	2.42	1.40	1.33
69	O1	402	HEM	FE-NB	2.40	2.02	1.94
70	P1	301	HEC	FE-ND	2.39	2.02	1.94
73	42	501	CDL	OB8-CB7	2.36	1.40	1.33
69	C1	401	HEM	CAC-C3C	2.36	1.53	1.47
69	O1	402	HEM	C1A-NA	2.35	1.44	1.39
79	A3	601	HEA	C3A-C4A	-2.32	1.42	1.46
69	C1	402	HEM	FE-ND	2.30	2.02	1.94
72	B2	501	3PE	O31-C3	-2.29	1.39	1.45
79	A3	602	HEA	CMD-C2D	2.29	1.55	1.50
72	42	502	3PE	O31-C3	-2.28	1.40	1.45
69	O1	401	HEM	C3D-C2D	-2.28	1.31	1.36
72	B2	501	3PE	O31-C31	2.27	1.40	1.33
72	B2	501	3PE	O21-C21	2.26	1.40	1.34
72	42	502	3PE	O31-C31	2.26	1.39	1.33
77	R2	601	NAP	PN-O5D	2.26	1.68	1.59
78	j2	201	PC1	O31-C31	2.25	1.39	1.33
77	R2	601	NAP	C5A-C4A	-2.25	1.34	1.39
73	42	501	CDL	OB8-CB6	-2.23	1.40	1.45
69	C1	402	HEM	FE-NC	2.23	2.02	1.95
69	O1	401	HEM	C2A-C3A	-2.22	1.32	1.38
74	82	501	FMN	C10-N1	2.22	1.37	1.33
69	O1	402	HEM	CAB-C3B	2.20	1.53	1.47
78	j2	201	PC1	O31-C3	-2.17	1.40	1.45
69	C1	401	HEM	C2A-C3A	-2.17	1.33	1.38
69	C1	402	HEM	FE-NB	2.17	2.01	1.94
70	P1	301	HEC	CAB-C3B	2.14	1.56	1.51
69	O1	402	HEM	C2A-C3A	-2.13	1.33	1.38
70	P1	301	HEC	C3C-C2C	-2.12	1.33	1.38
69	O1	401	HEM	FE-NA	2.11	2.02	1.95
77	R2	601	NAP	C4N-C3N	-2.10	1.35	1.39
78	j2	201	PC1	O21-C21	2.09	1.40	1.34
78	S2	401	PC1	O21-C21	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	C1	402	HEM	CAB-C3B	2.08	1.53	1.47
79	A3	602	HEA	FE-NC	2.05	2.02	1.95
69	C1	402	HEM	C1C-C2C	2.03	1.49	1.45
70	D1	301	HEC	FE-ND	2.02	2.01	1.94
73	42	501	CDL	OA8-CA6	-2.02	1.40	1.45
78	S2	401	PC1	O31-C3	-2.02	1.40	1.45
77	R2	601	NAP	O2B-C2B	2.01	1.51	1.44
72	22	401	3PE	O31-C3	-2.01	1.40	1.45

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	R2	601	NAP	N3A-C2A-N1A	-5.76	119.60	128.60
69	O1	401	HEM	C3B-C2B-C1B	-5.51	102.40	106.49
77	R2	601	NAP	C5A-C4A-N3A	-4.97	120.26	126.75
69	O1	402	HEM	C3B-C2B-C1B	4.94	110.15	106.49
69	O1	401	HEM	CMA-C3A-C4A	-4.91	117.90	125.37
77	R2	601	NAP	N6A-C6A-N1A	-4.81	107.81	118.35
69	C1	401	HEM	CBD-CAD-C3D	4.74	125.78	112.63
69	C1	402	HEM	CAA-CBA-CGA	4.73	123.78	113.60
77	R2	601	NAP	N9A-C8A-N7A	-4.43	107.85	113.91
69	O1	401	HEM	C4B-C3B-C2B	4.36	110.57	107.11
72	22	401	3PE	O21-C21-C22	4.35	120.88	111.50
72	42	502	3PE	O21-C21-C22	4.23	120.63	111.50
78	S2	401	PC1	O21-C21-C22	4.18	120.51	111.50
73	42	501	CDL	OA6-CA5-C11	4.17	120.50	111.50
69	O1	402	HEM	C2A-C1A-NA	-4.17	105.48	110.15
69	O1	402	HEM	CHC-C4B-NB	4.09	128.86	124.42
69	C1	401	HEM	O1D-CGD-CBD	-3.99	110.25	123.08
79	A3	601	HEA	C17-C18-C19	-3.97	118.10	127.66
72	B2	501	3PE	O21-C21-C22	3.92	119.95	111.50
69	C1	401	HEM	CBB-CAB-C3B	-3.90	108.20	127.62
69	O1	402	HEM	CHA-C1A-C2A	3.88	133.83	125.36
77	R2	601	NAP	C5A-C6A-N6A	3.87	131.86	123.43
69	O1	402	HEM	CHB-C1B-NB	-3.79	119.71	124.37
73	42	501	CDL	OB6-CB5-C51	3.75	119.58	111.50
69	C1	402	HEM	C4D-ND-C1D	3.70	108.89	105.07
69	O1	401	HEM	C2B-C1B-NB	3.61	114.12	109.84
74	82	501	FMN	C4-N3-C2	-3.58	119.04	125.64
69	O1	401	HEM	O1D-CGD-CBD	-3.57	111.60	123.08
69	O1	401	HEM	O2D-CGD-O1D	3.57	132.19	123.30
77	R2	601	NAP	C2A-N3A-C4A	3.54	120.12	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	O1	401	HEM	CHB-C1B-NB	-3.51	120.04	124.37
69	C1	402	HEM	C4C-NC-C1C	-3.50	101.92	105.35
69	C1	402	HEM	C3C-C2C-C1C	-3.46	103.77	107.08
78	j2	201	PC1	O21-C21-C22	3.45	120.41	110.80
69	C1	402	HEM	CMA-C3A-C4A	-3.42	120.16	125.37
69	C1	402	HEM	CHD-C1D-ND	3.34	128.05	124.42
77	R2	601	NAP	PN-O3-PA	-3.31	121.46	132.83
69	C1	402	HEM	CAD-CBD-CGD	3.31	120.72	113.60
79	A3	602	HEA	CHA-C1A-NA	-3.26	120.91	124.44
69	O1	401	HEM	CMA-C3A-C2A	3.25	132.64	125.61
79	A3	601	HEA	C13-C14-C15	-3.18	120.00	127.66
77	R2	601	NAP	C5A-N7A-C8A	3.11	107.93	103.51
74	82	501	FMN	O4-C4-C4A	-3.11	118.35	126.60
69	O1	402	HEM	O1D-CGD-CBD	-3.04	113.31	123.08
69	C1	402	HEM	O2A-CGA-CBA	3.01	123.70	114.03
74	82	501	FMN	C4A-C10-N1	-2.99	117.79	124.73
69	C1	401	HEM	O2A-CGA-O1A	2.91	130.56	123.30
69	C1	402	HEM	O2A-CGA-O1A	-2.91	116.06	123.30
69	C1	402	HEM	C4A-CHB-C1B	2.91	133.23	126.34
74	82	501	FMN	C4A-C4-N3	2.90	120.54	113.19
69	C1	402	HEM	CHC-C1C-NC	-2.88	121.32	124.44
69	O1	401	HEM	C1B-NB-C4B	-2.84	102.14	105.07
79	A3	601	HEA	C1B-C2B-C3B	2.83	110.18	106.80
69	C1	402	HEM	CHB-C1B-NB	-2.82	120.90	124.37
69	O1	401	HEM	CMD-C2D-C1D	-2.80	120.77	125.04
69	C1	401	HEM	CMB-C2B-C1B	-2.80	120.77	125.04
69	C1	402	HEM	C4A-NA-C1A	2.80	108.09	105.35
69	C1	402	HEM	CMA-C3A-C2A	2.79	131.63	125.61
69	O1	402	HEM	CAA-C2A-C1A	-2.70	119.57	124.89
74	82	501	FMN	C5'-C4'-C3'	-2.68	107.02	112.20
70	P1	301	HEC	O1D-CGD-CBD	-2.65	114.58	123.08
79	A3	602	HEA	C4A-C3A-C2A	2.64	108.92	106.75
77	R2	601	NAP	N3A-C4A-N9A	2.62	131.39	127.08
69	O1	401	HEM	CAB-C3B-C2B	-2.61	120.02	128.60
79	A3	602	HEA	CMD-C2D-C1D	2.60	129.00	125.04
73	42	501	CDL	OA8-CA7-C31	2.59	120.02	111.91
73	42	501	CDL	OB8-CB7-C71	2.58	119.99	111.91
69	C1	402	HEM	CBD-CAD-C3D	2.57	119.77	112.63
72	B2	501	3PE	O31-C31-C32	2.55	119.92	111.91
77	R2	601	NAP	C4A-N9A-C1B	-2.55	120.51	126.59
72	22	401	3PE	O31-C31-C32	2.53	119.84	111.91
70	D1	301	HEC	O1A-CGA-CBA	-2.53	114.97	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	401	PC1	O31-C31-C32	2.52	119.81	111.91
70	D1	301	HEC	O2D-CGD-O1D	2.51	129.55	123.30
74	82	501	FMN	C5A-C9A-N10	2.49	120.53	117.95
79	A3	601	HEA	C3C-C4C-NC	2.49	111.78	110.25
78	j2	201	PC1	O31-C31-C32	2.48	119.68	111.91
69	O1	402	HEM	C4B-C3B-C2B	-2.47	105.15	107.11
69	C1	402	HEM	CAA-C2A-C1A	-2.47	120.03	124.89
69	O1	401	HEM	CBD-CAD-C3D	2.46	119.47	112.63
69	C1	401	HEM	O2D-CGD-CBD	2.46	121.92	114.03
69	O1	401	HEM	CMB-C2B-C3B	2.45	134.29	128.30
79	A3	602	HEA	C1D-C2D-C3D	-2.44	104.39	106.96
69	O1	401	HEM	CHA-C4D-ND	-2.44	121.37	124.37
69	C1	401	HEM	C4B-C3B-C2B	2.41	109.03	107.11
74	82	501	FMN	C10-N1-C2	2.41	121.73	116.90
79	A3	601	HEA	C17-C16-C15	-2.41	105.05	112.98
72	42	502	3PE	O31-C31-C32	2.41	119.47	111.91
70	P1	301	HEC	CAD-CBD-CGD	2.39	118.75	113.60
79	A3	602	HEA	CAA-C2A-C1A	2.39	129.39	124.89
77	R2	601	NAP	C6N-N1N-C2N	-2.38	119.80	121.97
69	O1	402	HEM	CMB-C2B-C3B	-2.38	122.47	128.30
69	C1	401	HEM	CMA-C3A-C4A	-2.38	121.74	125.37
69	O1	402	HEM	C4A-NA-C1A	2.38	107.67	105.35
79	A3	601	HEA	C20-C19-C18	2.37	125.91	121.12
77	R2	601	NAP	C3D-C2D-C1D	2.36	104.53	100.98
74	82	501	FMN	C4-C4A-C10	2.36	120.75	116.79
79	A3	601	HEA	CAD-C3D-C4D	2.35	128.76	124.66
79	A3	602	HEA	C25-C23-C24	2.34	119.78	114.60
79	A3	602	HEA	CMB-C2B-C3B	-2.33	125.91	130.34
79	A3	601	HEA	C16-C17-C18	-2.32	104.24	111.88
69	C1	402	HEM	C3D-C4D-ND	-2.32	107.58	110.17
79	A3	602	HEA	C13-C14-C15	-2.31	122.10	127.66
70	D1	301	HEC	CAD-C3D-C2D	2.29	132.14	127.88
70	D1	301	HEC	O1D-CGD-CBD	-2.26	115.81	123.08
69	O1	401	HEM	CAA-CBA-CGA	2.25	118.44	113.60
69	C1	401	HEM	CHC-C1C-NC	2.23	126.85	124.44
69	O1	402	HEM	CMD-C2D-C1D	-2.23	121.65	125.04
69	O1	402	HEM	O2D-CGD-CBD	2.21	121.13	114.03
79	A3	602	HEA	C26-C15-C16	2.21	118.99	115.27
69	C1	402	HEM	C2A-C1A-NA	-2.21	107.68	110.15
77	R2	601	NAP	C5A-C4A-N9A	2.20	108.34	105.78
69	O1	401	HEM	C4A-C3A-C2A	2.19	109.40	106.83
77	R2	601	NAP	C3N-C7N-N7N	2.19	120.38	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	R2	601	NAP	C4A-C5A-N7A	-2.18	107.97	110.62
79	A3	601	HEA	C12-C13-C14	-2.17	106.51	112.23
70	D1	301	HEC	CAD-C3D-C4D	-2.16	120.89	124.66
70	P1	301	HEC	CAC-C3C-C4C	-2.15	121.93	124.92
74	82	501	FMN	C4A-C10-N10	2.14	119.61	116.48
79	A3	601	HEA	C4B-C3B-C2B	-2.14	103.75	107.41
69	O1	401	HEM	C3C-C2C-C1C	2.12	109.09	107.08
69	O1	402	HEM	CMC-C2C-C1C	-2.11	120.99	124.71
69	O1	402	HEM	CHA-C1A-NA	-2.10	119.98	123.85
77	R2	601	NAP	C4B-O4B-C1B	-2.10	104.85	109.47
74	82	501	FMN	C9A-C5A-N5	-2.09	120.16	122.43
79	A3	602	HEA	C3C-C4C-NC	2.09	111.53	110.25
79	A3	601	HEA	C27-C19-C18	-2.06	118.40	123.68
79	A3	602	HEA	CBD-CAD-C3D	2.06	118.34	112.63
69	O1	401	HEM	O1A-CGA-CBA	-2.06	116.48	123.08
69	O1	402	HEM	CAA-CBA-CGA	2.05	118.01	113.60
73	42	501	CDL	CA4-OA6-CA5	-2.02	112.82	117.79
79	A3	602	HEA	C3A-C2A-C1A	-2.01	105.15	107.08
69	C1	401	HEM	CMA-C3A-C2A	2.01	129.96	125.61
77	R2	601	NAP	C2N-C3N-C4N	2.01	120.54	118.26
77	R2	601	NAP	C4A-N9A-C8A	2.01	107.91	105.73
70	P1	301	HEC	O1A-CGA-CBA	-2.00	116.64	123.08

There are no chirality outliers.

All (230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	O1	401	HEM	C2B-C3B-CAB-CBB
72	22	401	3PE	C1-O11-P-O14
72	22	401	3PE	C22-C21-O21-C2
72	42	502	3PE	C11-O13-P-O12
72	42	502	3PE	C11-O13-P-O14
72	42	502	3PE	C2-C1-O11-P
72	42	502	3PE	O13-C11-C12-N
72	42	502	3PE	C22-C21-O21-C2
72	B2	501	3PE	C1-O11-P-O13
72	B2	501	3PE	O11-C1-C2-O21
72	B2	501	3PE	O22-C21-O21-C2
72	B2	501	3PE	C22-C21-O21-C2
73	42	501	CDL	CA2-OA2-PA1-OA4
73	42	501	CDL	OA6-CA4-CA6-OA8
73	42	501	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
73	42	501	CDL	C11-CA5-OA6-CA4
74	82	501	FMN	N10-C1'-C2'-O2'
74	82	501	FMN	N10-C1'-C2'-C3'
74	82	501	FMN	C5'-O5'-P-O2P
74	82	501	FMN	C5'-O5'-P-O3P
77	R2	601	NAP	C5B-O5B-PA-O1A
77	R2	601	NAP	C5B-O5B-PA-O2A
77	R2	601	NAP	C1B-C2B-O2B-P2B
77	R2	601	NAP	C2B-O2B-P2B-O3X
77	R2	601	NAP	PA-O3-PN-O5D
77	R2	601	NAP	C5D-O5D-PN-O3
77	R2	601	NAP	C5D-O5D-PN-O2N
77	R2	601	NAP	C2D-C1D-N1N-C2N
77	R2	601	NAP	C2D-C1D-N1N-C6N
78	j2	201	PC1	C11-O13-P-O12
78	j2	201	PC1	C11-O13-P-O14
78	j2	201	PC1	C11-O13-P-O11
78	j2	201	PC1	O22-C21-O21-C2
79	A3	601	HEA	C2A-C3A-CMA-OMA
79	A3	601	HEA	C4A-C3A-CMA-OMA
79	A3	601	HEA	C12-C11-C3B-C2B
79	A3	602	HEA	C2A-C3A-CMA-OMA
79	A3	602	HEA	C4A-C3A-CMA-OMA
72	42	502	3PE	O32-C31-O31-C3
72	22	401	3PE	O22-C21-O21-C2
72	42	502	3PE	O22-C21-O21-C2
72	42	502	3PE	C32-C31-O31-C3
78	j2	201	PC1	C22-C21-O21-C2
70	D1	301	HEC	C2B-C3B-CAB-CBB
70	P1	301	HEC	C2C-C3C-CAC-CBC
73	42	501	CDL	C71-CB7-OB8-CB6
78	S2	401	PC1	O22-C21-O21-C2
73	42	501	CDL	OB9-CB7-OB8-CB6
70	D1	301	HEC	C4B-C3B-CAB-CBB
78	S2	401	PC1	C22-C21-O21-C2
77	R2	601	NAP	O4B-C4B-C5B-O5B
77	R2	601	NAP	O4D-C4D-C5D-O5D
79	A3	601	HEA	C15-C16-C17-C18
73	42	501	CDL	C31-CA7-OA8-CA6
70	P1	301	HEC	C4C-C3C-CAC-CBC
73	42	501	CDL	CB5-C51-C52-C53
72	B2	501	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
73	42	501	CDL	CA5-C11-C12-C13
73	42	501	CDL	OA9-CA7-OA8-CA6
72	42	502	3PE	C1-O11-P-O13
72	42	502	3PE	C11-O13-P-O11
73	42	501	CDL	CA2-OA2-PA1-OA5
73	42	501	CDL	CB2-OB2-PB2-OB5
78	S2	401	PC1	C11-O13-P-O11
73	42	501	CDL	C51-CB5-OB6-CB4
72	22	401	3PE	C2C-C2D-C2E-C2F
73	42	501	CDL	C78-C79-C80-C81
73	42	501	CDL	OB7-CB5-OB6-CB4
72	22	401	3PE	C21-C22-C23-C24
72	B2	501	3PE	C23-C24-C25-C26
73	42	501	CDL	C1-CA2-OA2-PA1
73	42	501	CDL	C13-C14-C15-C16
73	42	501	CDL	CA7-C31-C32-C33
78	S2	401	PC1	C25-C26-C27-C28
72	42	502	3PE	C28-C29-C2A-C2B
72	B2	501	3PE	C37-C38-C39-C3A
73	42	501	CDL	C73-C74-C75-C76
78	S2	401	PC1	C33-C34-C35-C36
73	42	501	CDL	C72-C73-C74-C75
72	22	401	3PE	C32-C33-C34-C35
73	42	501	CDL	C77-C78-C79-C80
73	42	501	CDL	C74-C75-C76-C77
70	D1	301	HEC	C2C-C3C-CAC-CBC
72	22	401	3PE	C32-C31-O31-C3
72	B2	501	3PE	C31-C32-C33-C34
72	42	502	3PE	C34-C35-C36-C37
72	B2	501	3PE	C2E-C2F-C2G-C2H
73	42	501	CDL	C75-C76-C77-C78
69	O1	401	HEM	C4B-C3B-CAB-CBB
72	22	401	3PE	O32-C31-O31-C3
73	42	501	CDL	C83-C84-C85-C86
78	S2	401	PC1	O11-C1-C2-C3
72	42	502	3PE	C23-C24-C25-C26
72	B2	501	3PE	C35-C36-C37-C38
72	22	401	3PE	C1-C2-C3-O31
78	j2	201	PC1	C1-C2-C3-O31
70	P1	301	HEC	C1A-C2A-CAA-CBA
73	42	501	CDL	C80-C81-C82-C83
72	B2	501	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
72	B2	501	3PE	C3C-C3D-C3E-C3F
72	22	401	3PE	C28-C29-C2A-C2B
72	B2	501	3PE	C27-C28-C29-C2A
72	22	401	3PE	C3-C2-O21-C21
73	42	501	CDL	C51-C52-C53-C54
78	j2	201	PC1	C34-C35-C36-C37
74	82	501	FMN	C5'-O5'-P-O1P
73	42	501	CDL	OA5-CA3-CA4-OA6
70	D1	301	HEC	C4C-C3C-CAC-CBC
77	R2	601	NAP	PN-O3-PA-O1A
78	j2	201	PC1	C32-C31-O31-C3
72	42	502	3PE	C24-C25-C26-C27
72	42	502	3PE	C26-C27-C28-C29
72	22	401	3PE	O11-C1-C2-C3
72	B2	501	3PE	O11-C1-C2-C3
73	42	501	CDL	OB5-CB3-CB4-CB6
72	42	502	3PE	C29-C2A-C2B-C2C
78	S2	401	PC1	C21-C22-C23-C24
78	S2	401	PC1	C32-C31-O31-C3
72	22	401	3PE	C22-C23-C24-C25
73	42	501	CDL	CA3-CA4-CA6-OA8
72	22	401	3PE	C2A-C2B-C2C-C2D
70	P1	301	HEC	C3A-C2A-CAA-CBA
72	22	401	3PE	C25-C26-C27-C28
78	S2	401	PC1	C3B-C3C-C3D-C3E
78	S2	401	PC1	C32-C33-C34-C35
72	B2	501	3PE	C2-C1-O11-P
73	42	501	CDL	CA4-CA3-OA5-PA1
77	R2	601	NAP	PN-O3-PA-O5B
77	R2	601	NAP	C3B-C4B-C5B-O5B
69	C1	402	HEM	C2B-C3B-CAB-CBB
72	42	502	3PE	C3-C2-O21-C21
73	42	501	CDL	CB3-CB4-OB6-CB5
73	42	501	CDL	OB5-CB3-CB4-OB6
78	S2	401	PC1	O11-C1-C2-O21
78	S2	401	PC1	O32-C31-O31-C3
78	j2	201	PC1	O32-C31-O31-C3
78	j2	201	PC1	O21-C2-C3-O31
70	D1	301	HEC	C1A-C2A-CAA-CBA
72	B2	501	3PE	C32-C31-O31-C3
72	22	401	3PE	C1-O11-P-O13
72	22	401	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
72	42	502	3PE	C1-O11-P-O12
72	42	502	3PE	C1-O11-P-O14
73	42	501	CDL	CB2-OB2-PB2-OB4
78	S2	401	PC1	C11-O13-P-O12
78	S2	401	PC1	C1-O11-P-O12
73	42	501	CDL	OA5-CA3-CA4-CA6
72	42	502	3PE	C12-C11-O13-P
74	82	501	FMN	C1'-C2'-C3'-O3'
72	22	401	3PE	O11-C1-C2-O21
72	42	502	3PE	C27-C28-C29-C2A
78	S2	401	PC1	O13-C11-C12-N
78	j2	201	PC1	O13-C11-C12-N
72	22	401	3PE	O21-C2-C3-O31
72	42	502	3PE	O21-C2-C3-O31
74	82	501	FMN	O2'-C2'-C3'-C4'
72	B2	501	3PE	O32-C31-O31-C3
73	42	501	CDL	C52-C53-C54-C55
72	B2	501	3PE	C24-C25-C26-C27
78	j2	201	PC1	O11-C1-C2-O21
70	D1	301	HEC	C3A-C2A-CAA-CBA
78	j2	201	PC1	C1-O11-P-O13
73	42	501	CDL	CB4-CB3-OB5-PB2
77	R2	601	NAP	C4B-C5B-O5B-PA
73	42	501	CDL	C14-C15-C16-C17
72	22	401	3PE	C26-C27-C28-C29
78	S2	401	PC1	C2-C1-O11-P
69	O1	401	HEM	CAD-CBD-CGD-O2D
69	O1	402	HEM	CAA-CBA-CGA-O1A
77	R2	601	NAP	C3D-C4D-C5D-O5D
69	C1	402	HEM	CAA-CBA-CGA-O2A
69	O1	401	HEM	CAD-CBD-CGD-O1D
79	A3	601	HEA	CAD-CBD-CGD-O1D
69	C1	401	HEM	CAD-CBD-CGD-O2D
69	C1	402	HEM	CAA-CBA-CGA-O1A
70	D1	301	HEC	CAA-CBA-CGA-O1A
70	P1	301	HEC	CAA-CBA-CGA-O1A
69	C1	401	HEM	CAD-CBD-CGD-O1D
72	B2	501	3PE	C2D-C2E-C2F-C2G
79	A3	602	HEA	CAD-CBD-CGD-O1D
73	42	501	CDL	C58-C59-C60-C61
70	P1	301	HEC	C2A-CAA-CBA-CGA
69	C1	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
70	D1	301	HEC	CAA-CBA-CGA-O2A
79	A3	602	HEA	CAD-CBD-CGD-O2D
72	B2	501	3PE	C32-C33-C34-C35
69	O1	402	HEM	CAA-CBA-CGA-O2A
72	42	502	3PE	C2E-C2F-C2G-C2H
73	42	501	CDL	CA2-C1-CB2-OB2
70	P1	301	HEC	CAA-CBA-CGA-O2A
79	A3	601	HEA	CAA-CBA-CGA-O1A
69	O1	401	HEM	CAA-CBA-CGA-O2A
69	O1	402	HEM	CAD-CBD-CGD-O2D
72	42	502	3PE	C1-C2-C3-O31
79	A3	601	HEA	CAD-CBD-CGD-O2D
69	C1	402	HEM	CAD-CBD-CGD-O2D
72	B2	501	3PE	C38-C39-C3A-C3B
72	B2	501	3PE	C26-C27-C28-C29
78	j2	201	PC1	O21-C21-C22-C23
72	B2	501	3PE	C25-C26-C27-C28
69	O1	402	HEM	CAD-CBD-CGD-O1D
69	C1	401	HEM	CAA-CBA-CGA-O2A
69	O1	401	HEM	CAA-CBA-CGA-O1A
73	42	501	CDL	C71-C72-C73-C74
72	B2	501	3PE	C1-C2-C3-O31
69	C1	402	HEM	C4B-C3B-CAB-CBB
79	A3	602	HEA	CAA-CBA-CGA-O2A
69	C1	401	HEM	CAA-CBA-CGA-O1A
72	B2	501	3PE	O21-C2-C3-O31
78	j2	201	PC1	O22-C21-C22-C23
78	S2	401	PC1	C23-C24-C25-C26
78	S2	401	PC1	C26-C27-C28-C29
79	A3	602	HEA	CAA-CBA-CGA-O1A
77	R2	601	NAP	C5B-O5B-PA-O3
72	B2	501	3PE	C3B-C3C-C3D-C3E
72	42	502	3PE	C2B-C2C-C2D-C2E
79	A3	601	HEA	CAA-CBA-CGA-O2A
73	42	501	CDL	C76-C77-C78-C79
70	P1	301	HEC	CAD-CBD-CGD-O2D
73	42	501	CDL	CB2-OB2-PB2-OB3
78	S2	401	PC1	C11-O13-P-O14
78	j2	201	PC1	C1-O11-P-O14
78	j2	201	PC1	O11-C1-C2-C3
78	S2	401	PC1	O21-C21-C22-C23
78	j2	201	PC1	O31-C31-C32-C33

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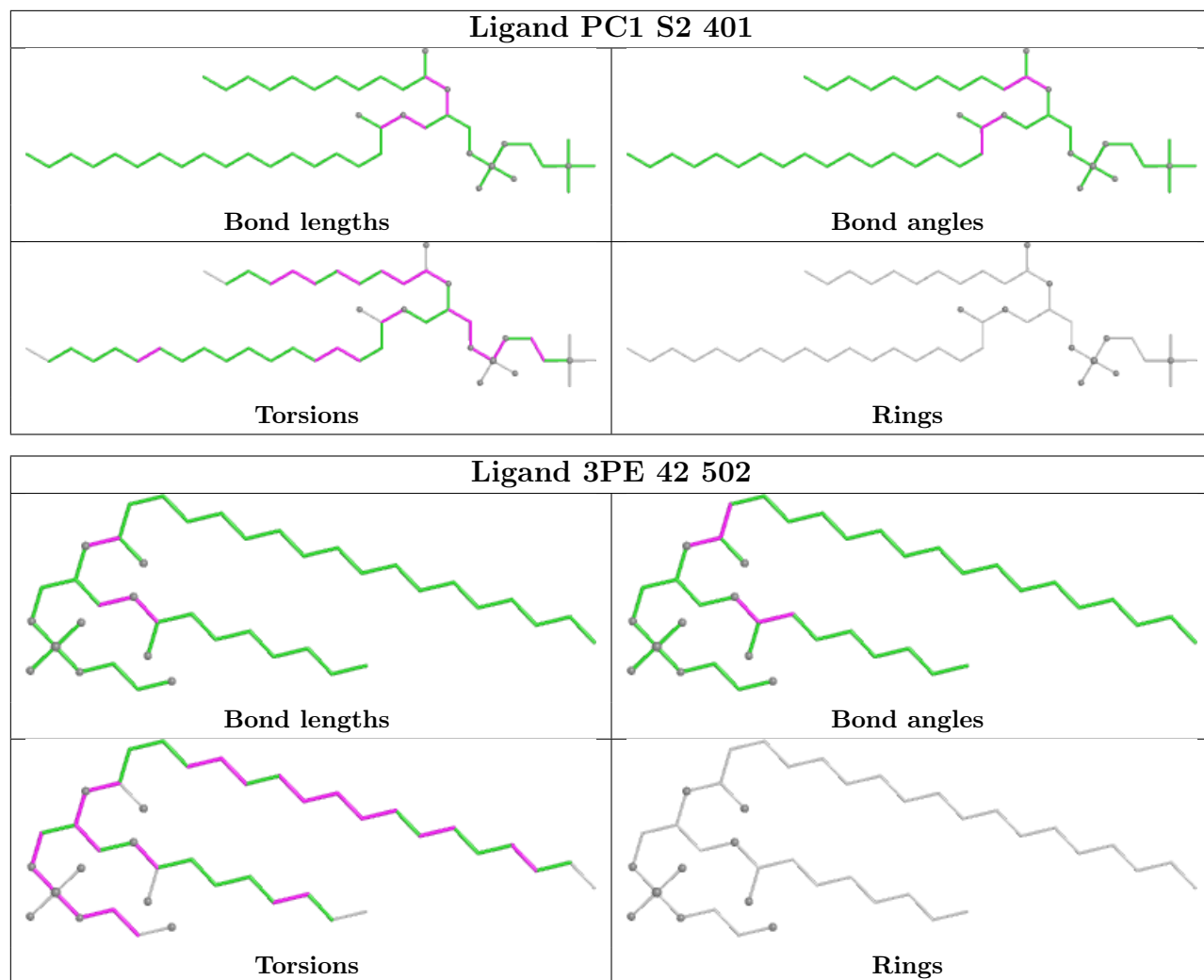
Mol	Chain	Res	Type	Atoms
78	j2	201	PC1	C12-C11-O13-P
79	A3	602	HEA	C26-C15-C16-C17
79	A3	601	HEA	O11-C11-C3B-C2B
78	j2	201	PC1	O32-C31-C32-C33
78	j2	201	PC1	C3A-C3B-C3C-C3D

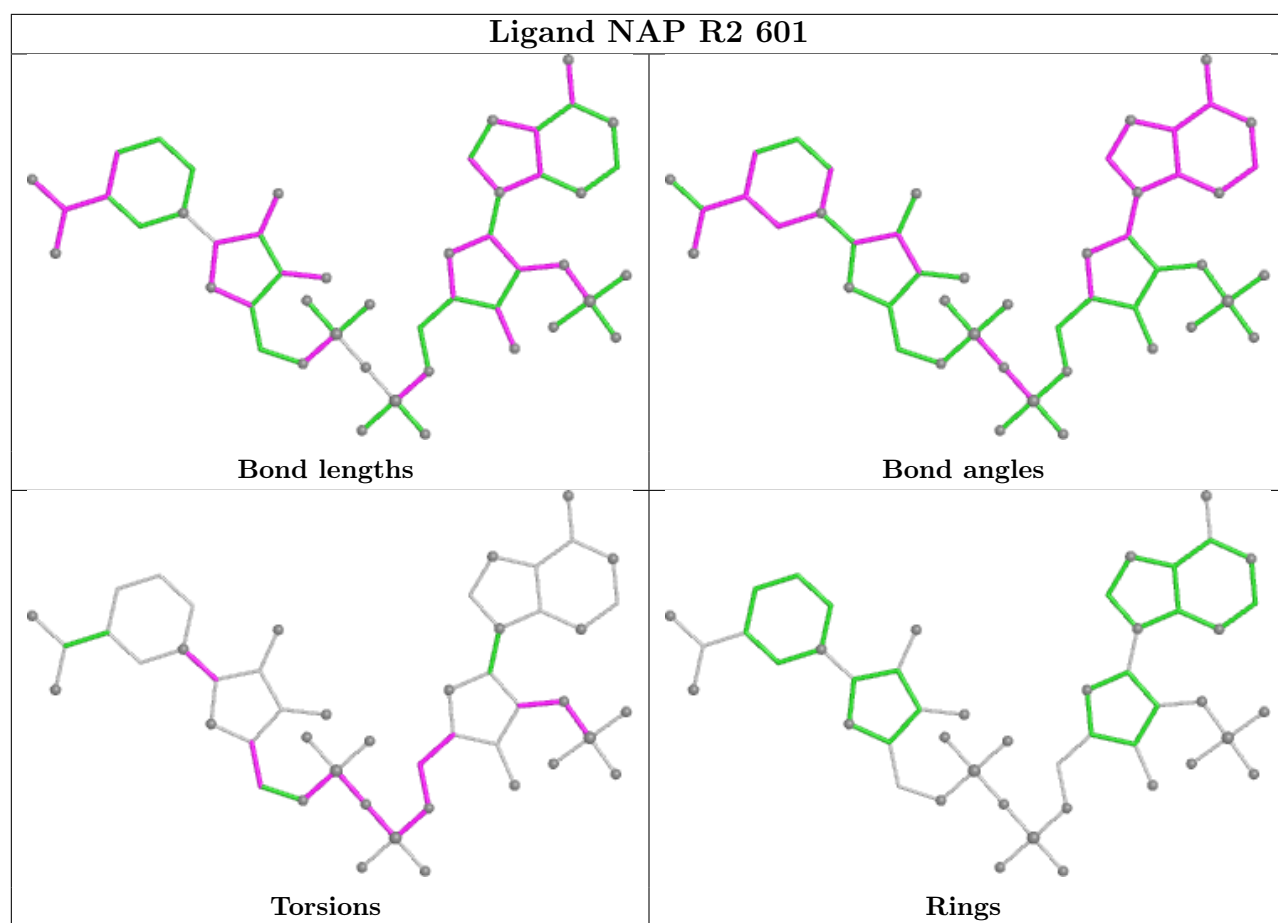
There are no ring outliers.

17 monomers are involved in 82 short contacts:

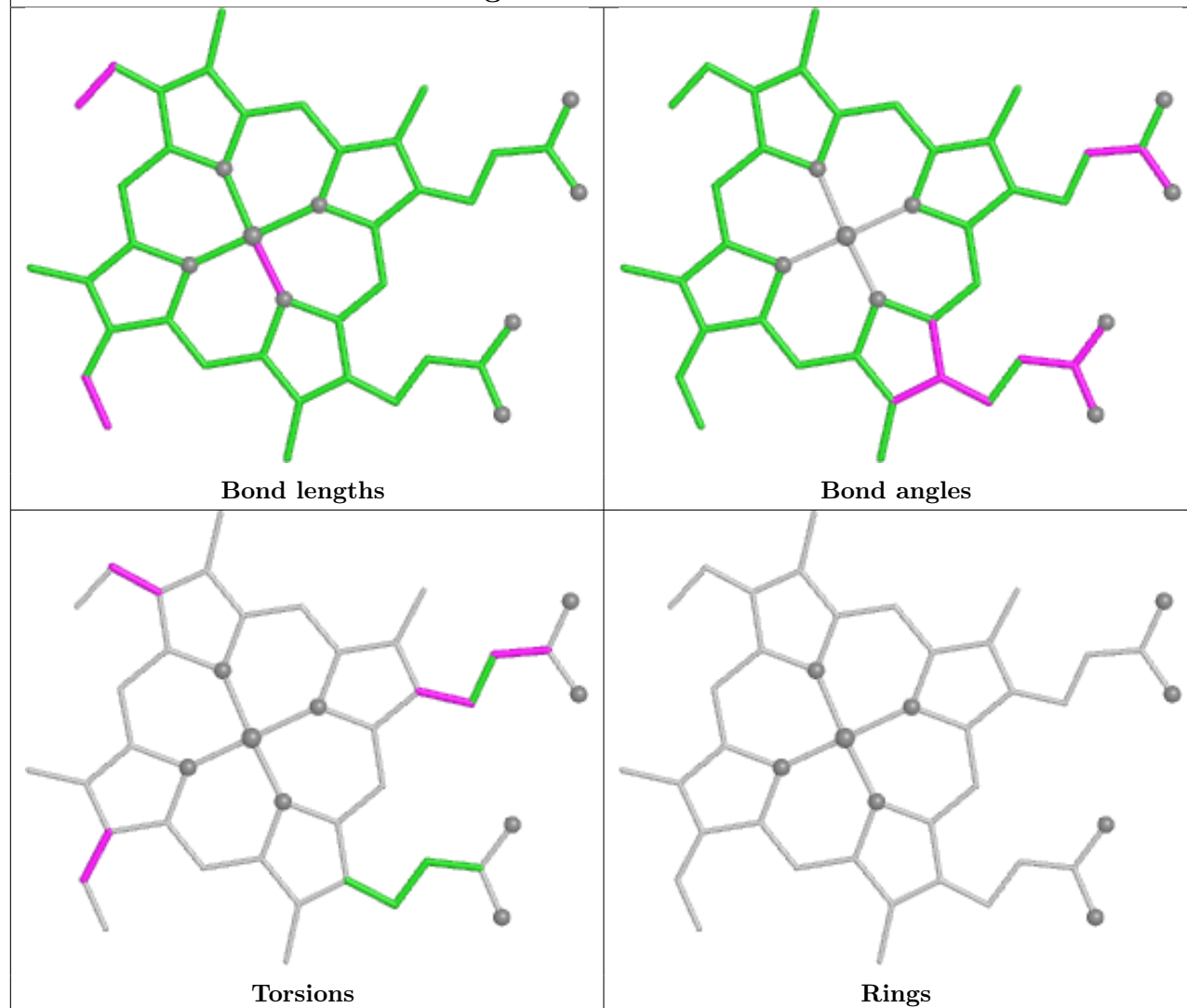
Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	42	502	3PE	1	0
77	R2	601	NAP	3	0
70	D1	301	HEC	5	0
78	j2	201	PC1	1	0
75	A2	801	SF4	4	0
79	A3	601	HEA	1	0
69	O1	402	HEM	14	0
69	C1	402	HEM	13	0
69	C1	401	HEM	5	0
74	82	501	FMN	2	0
70	P1	301	HEC	5	0
75	A2	802	SF4	8	0
79	A3	602	HEA	3	0
72	22	401	3PE	3	0
69	O1	401	HEM	11	0
72	B2	501	3PE	1	0
73	42	501	CDL	2	0

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



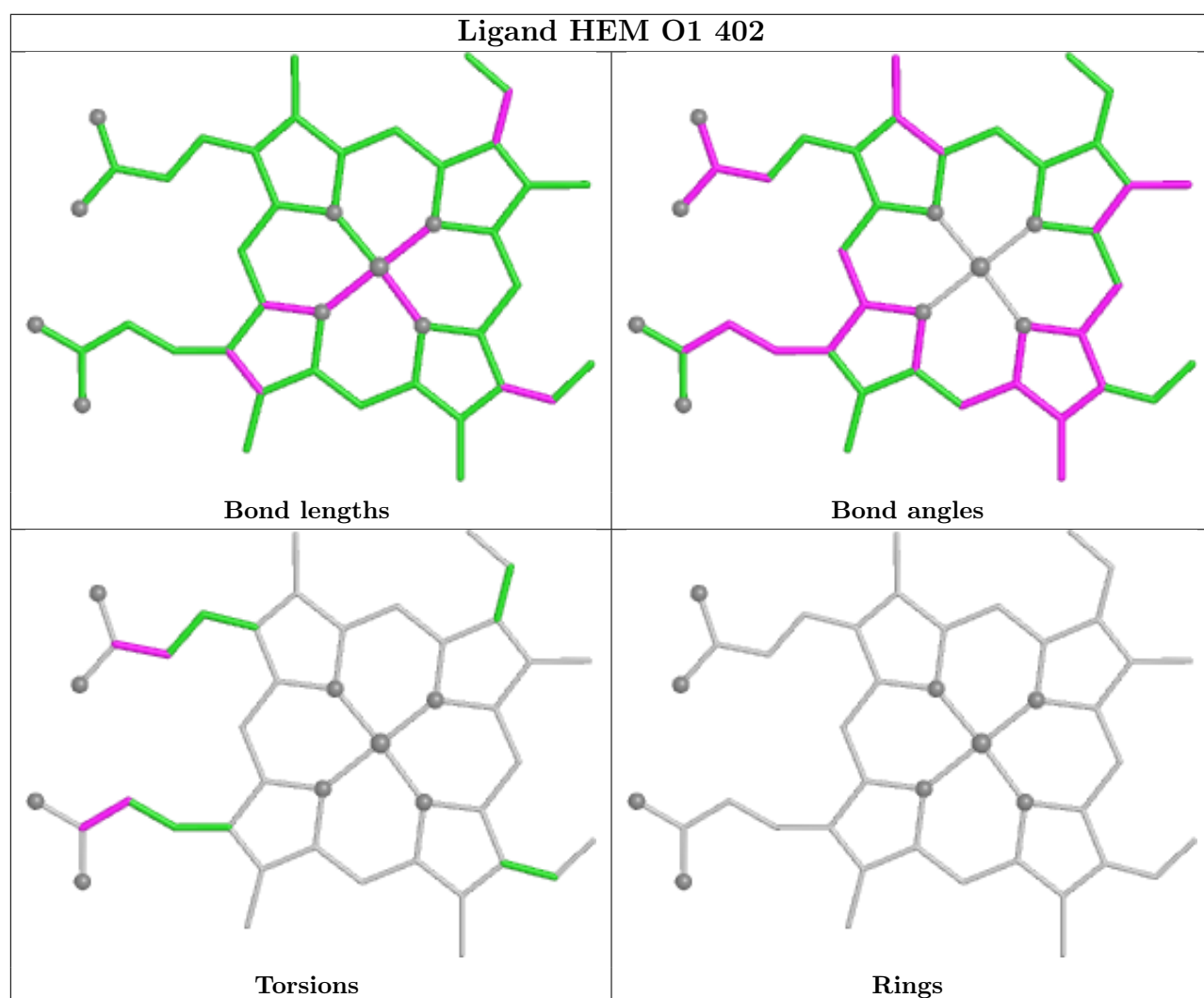
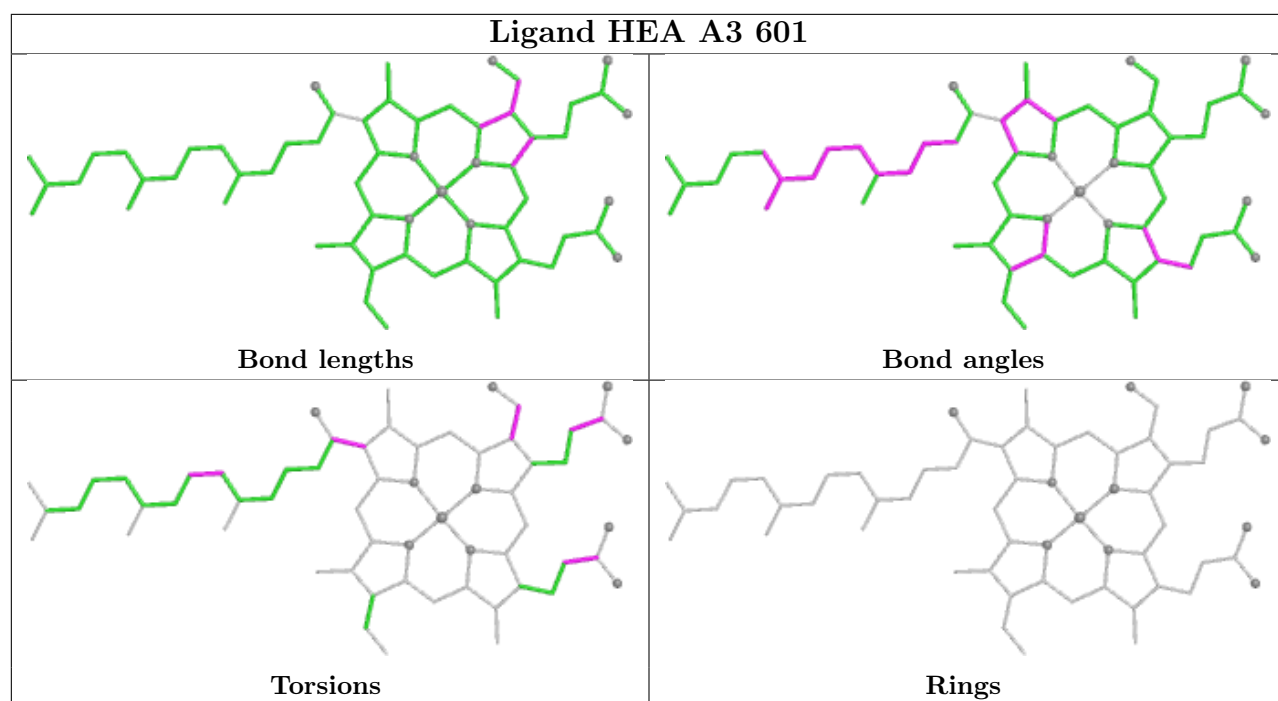


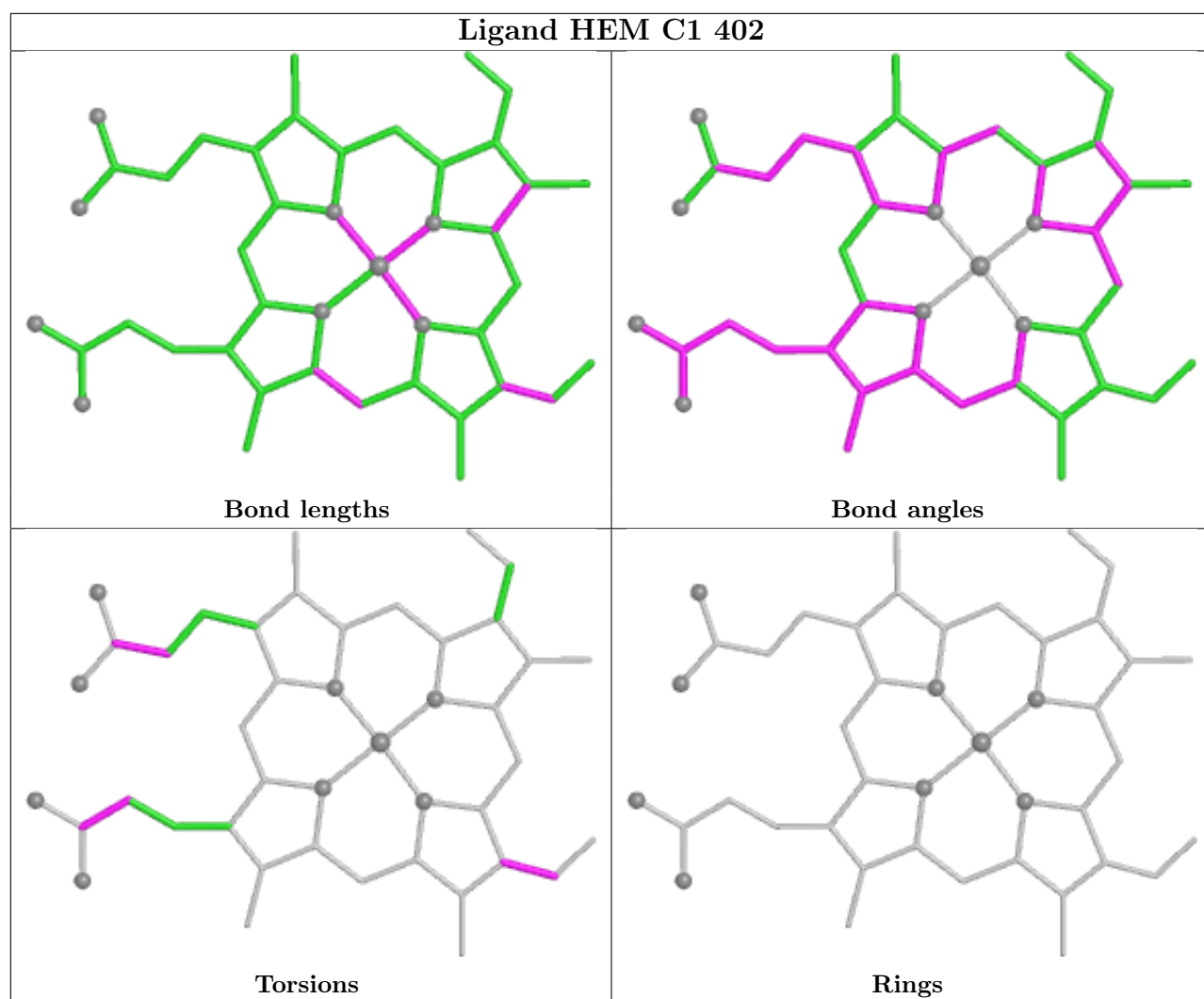
Ligand HEC D1 301

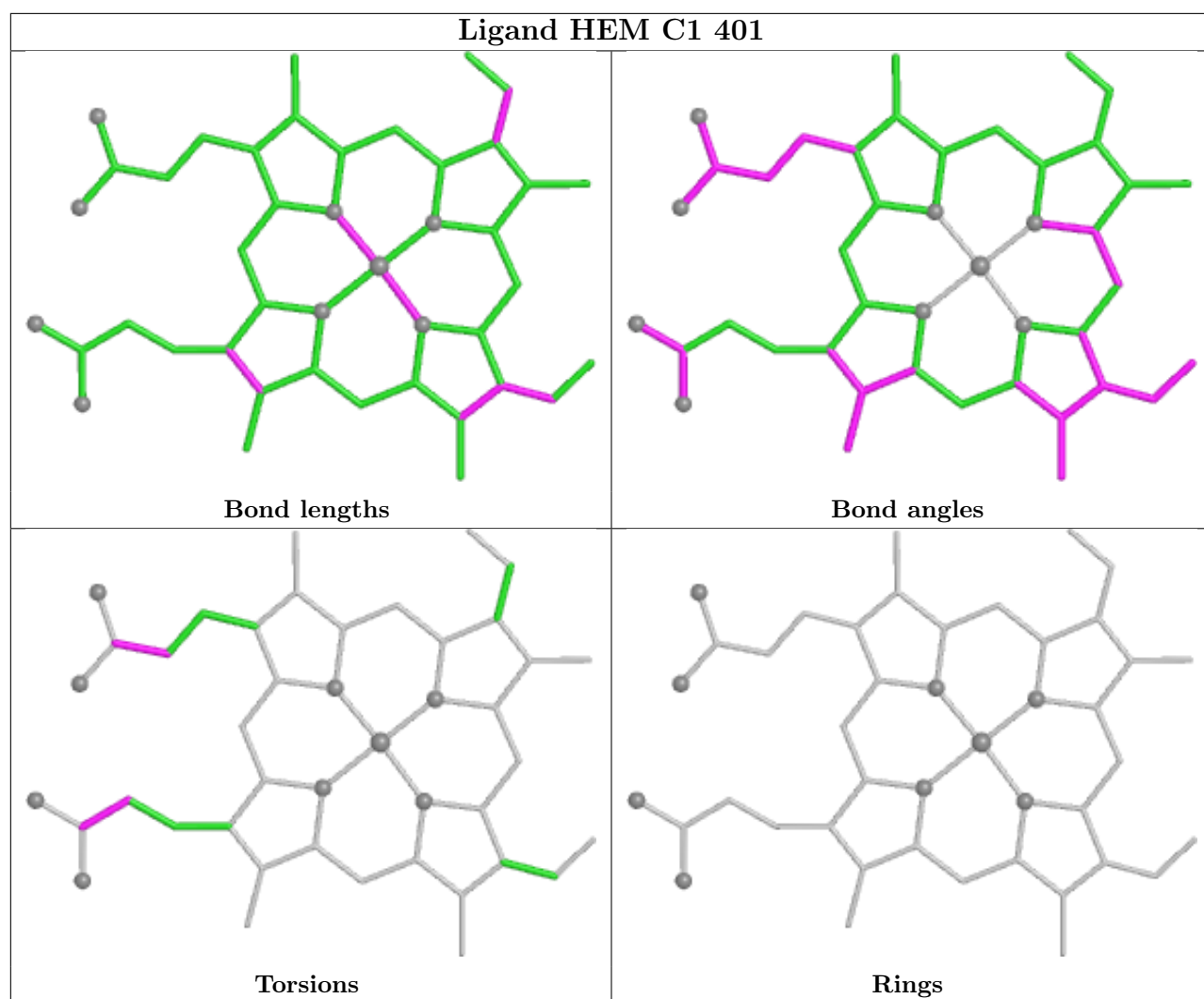


Ligand PC1 j2 201

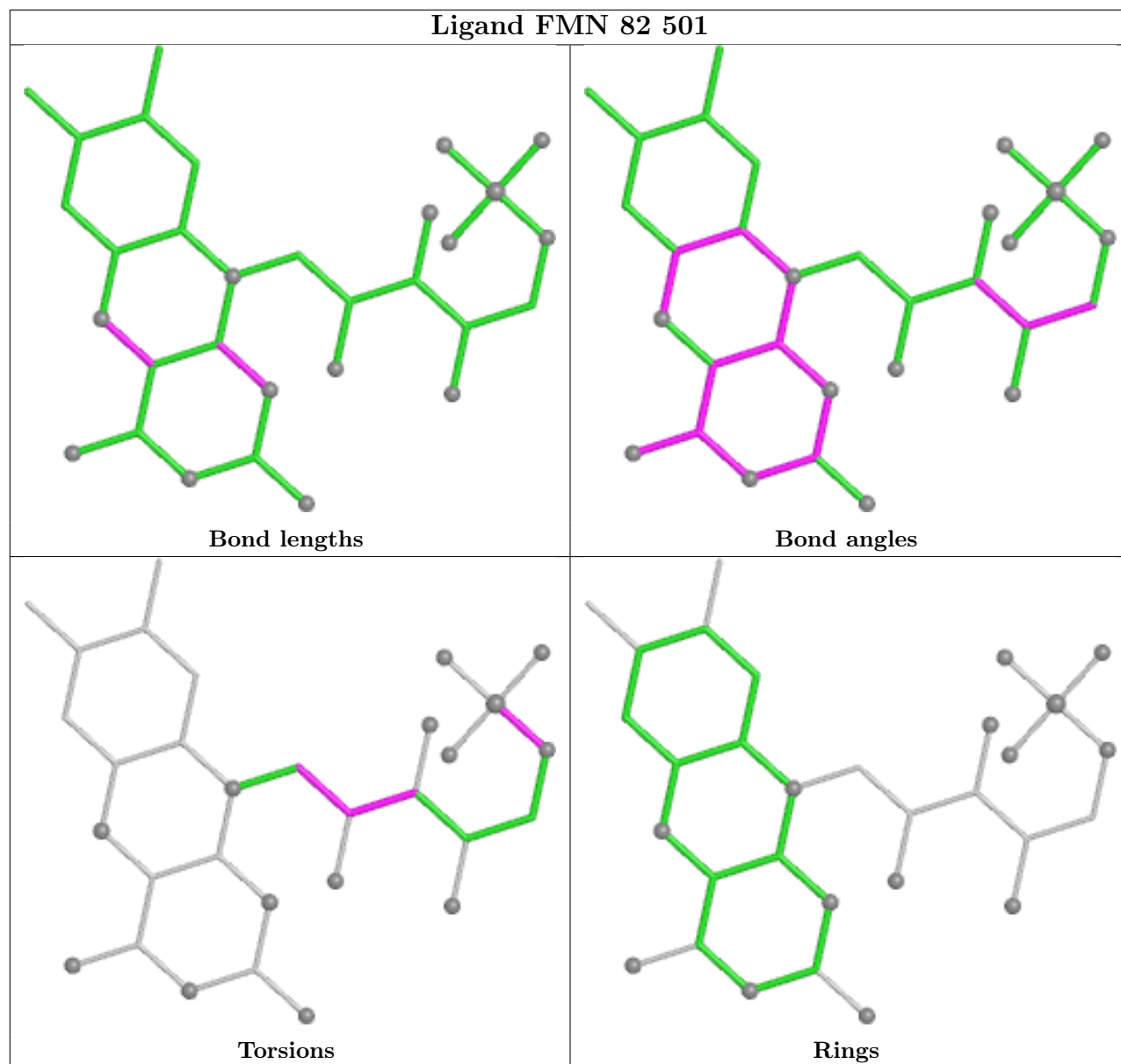




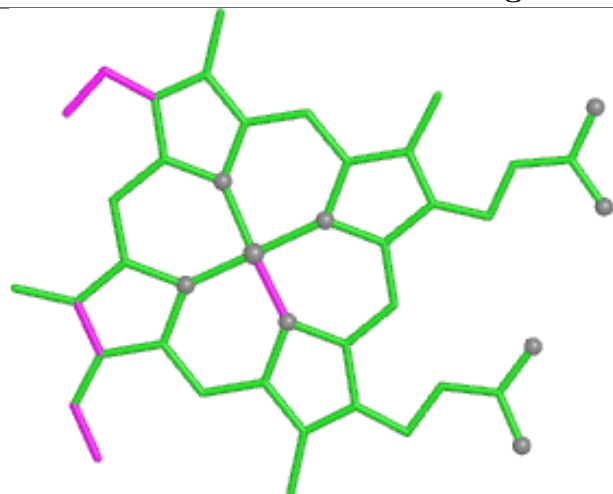




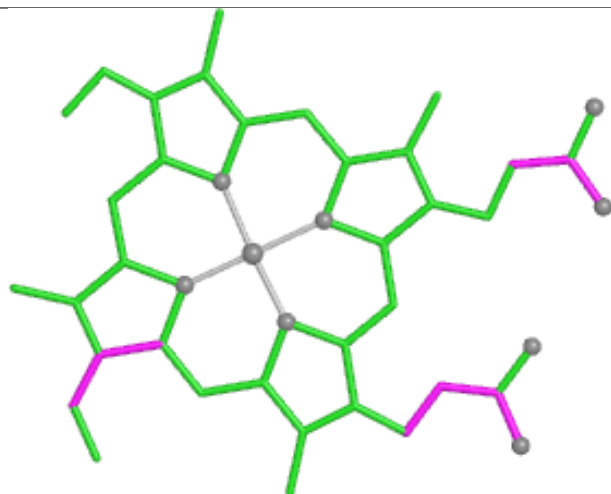
Ligand FMN 82 501



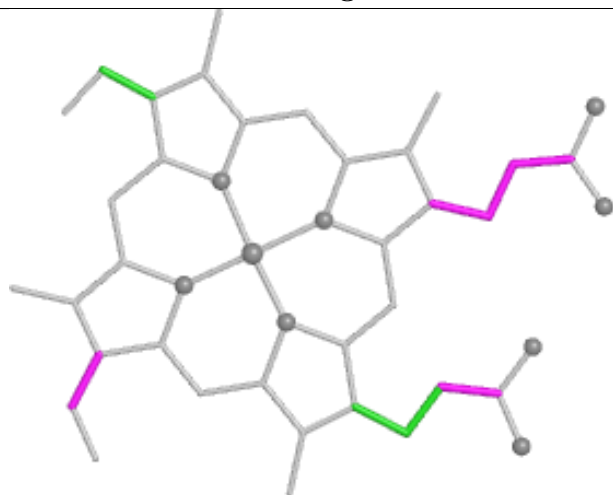
Ligand HEC P1 301



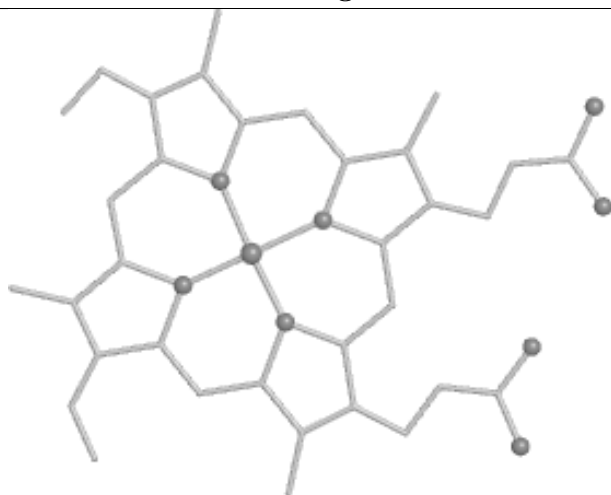
Bond lengths



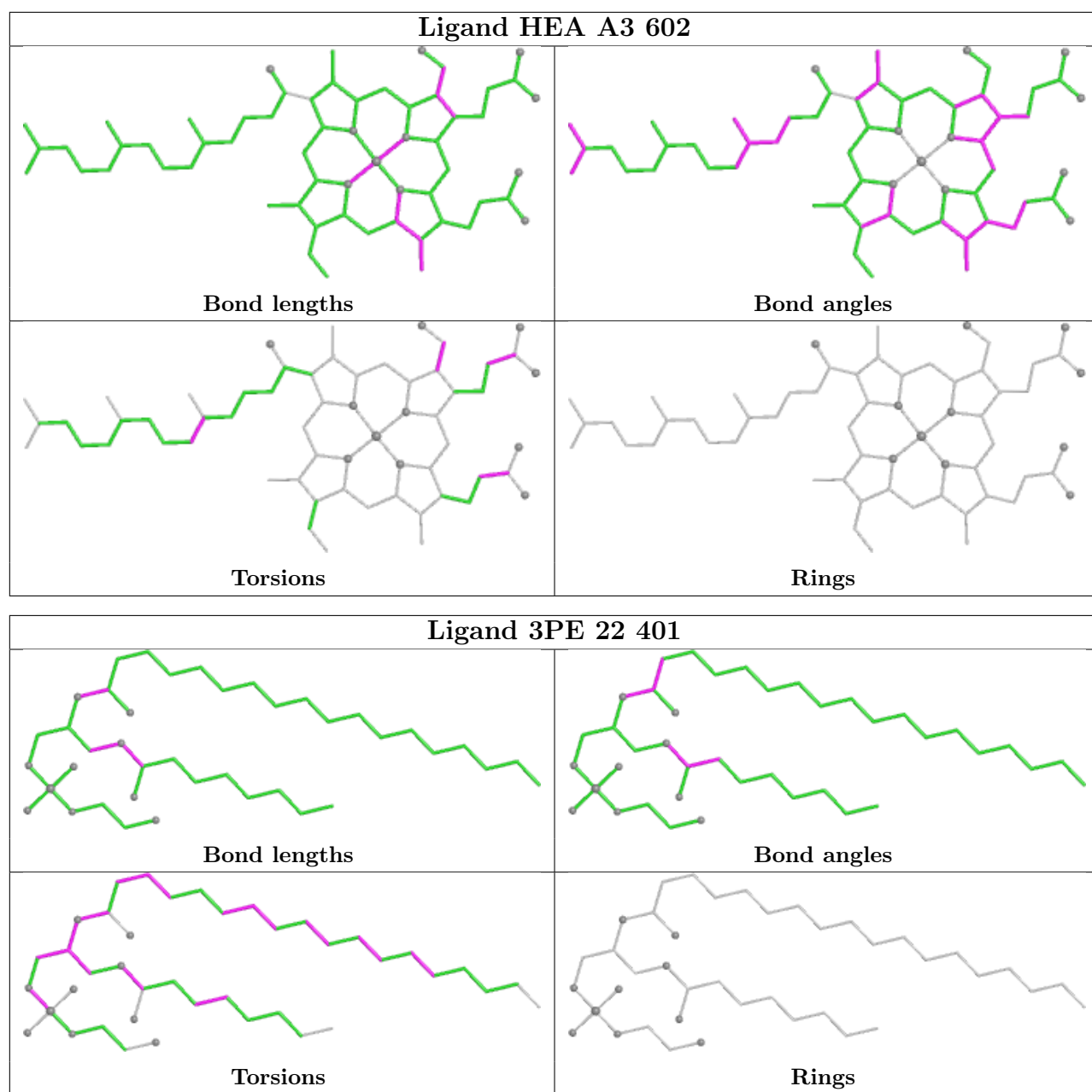
Bond angles



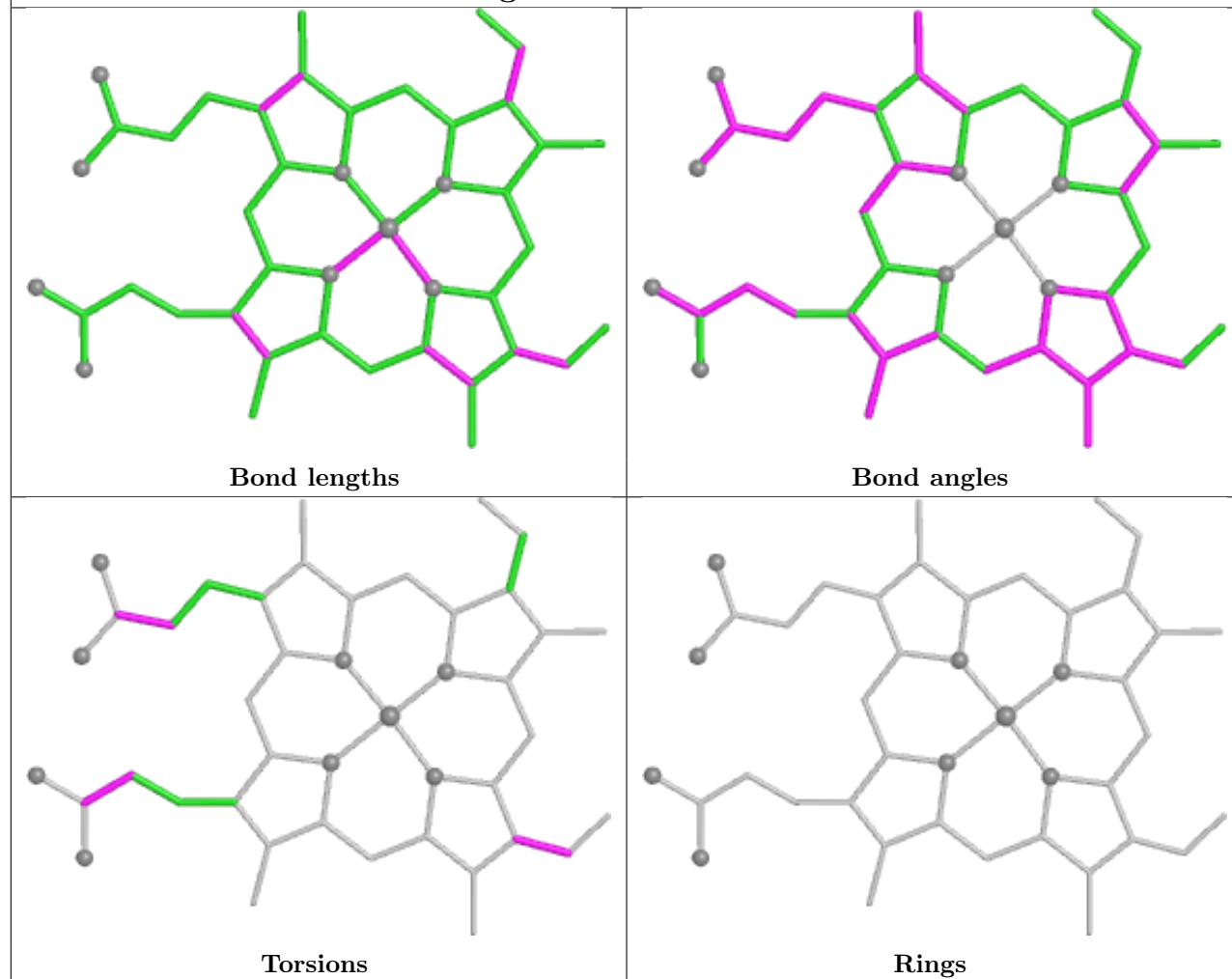
Torsions



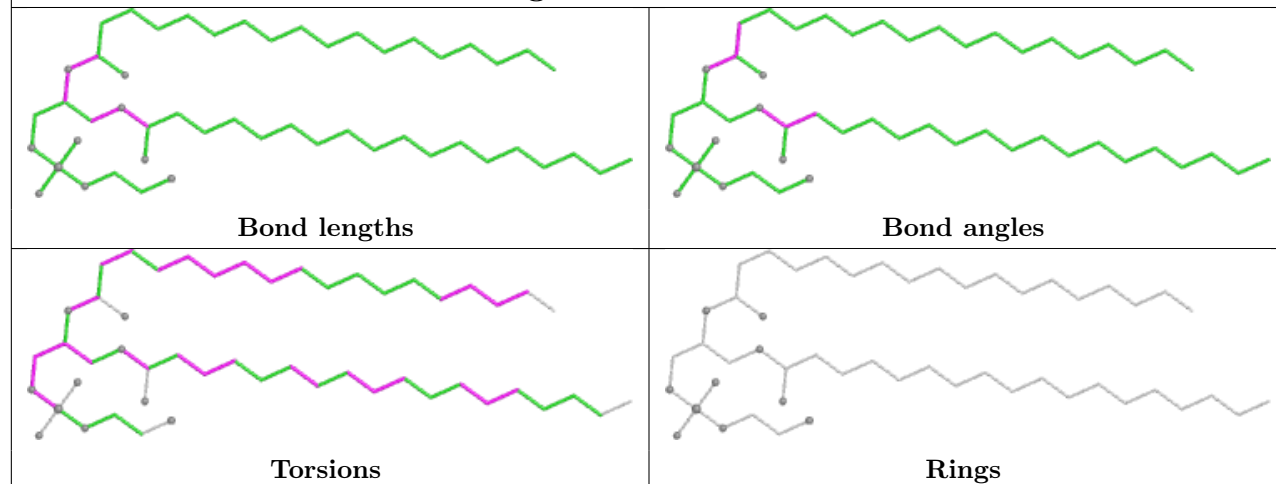
Rings

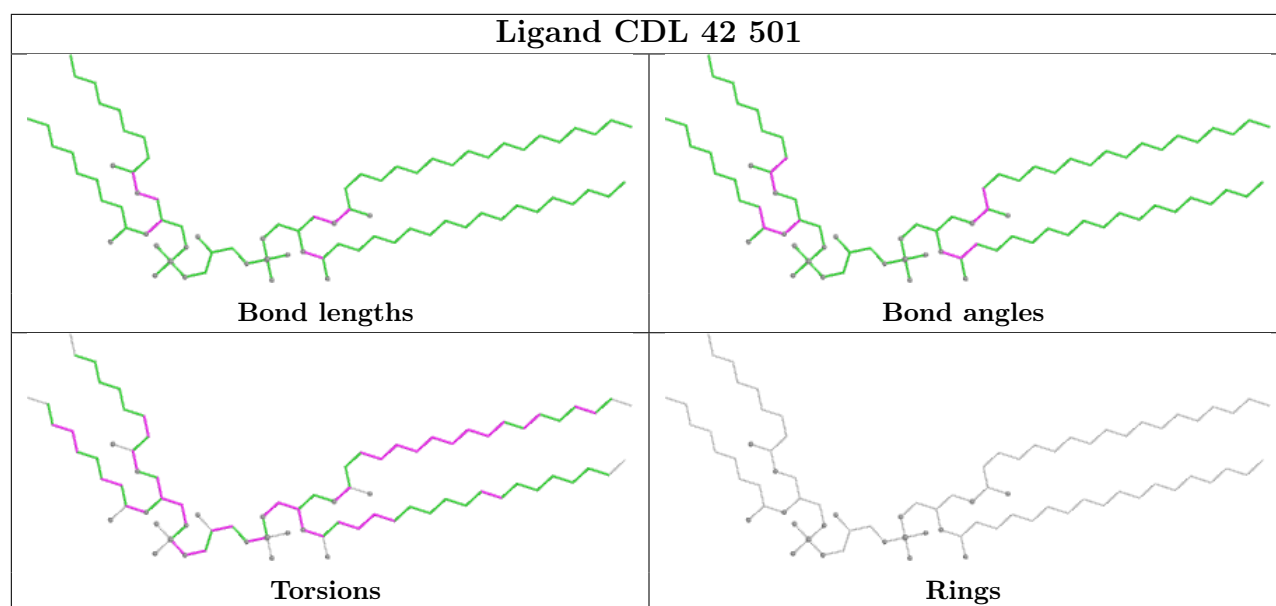


Ligand HEM O1 401



Ligand 3PE B2 501





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.

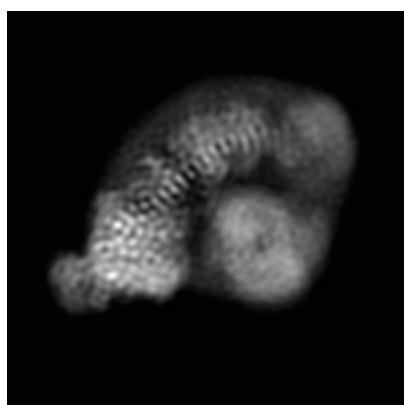
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30706. These allow visual inspection of the internal detail of the map and identification of artifacts.

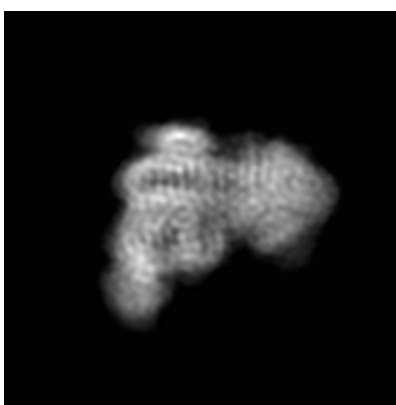
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

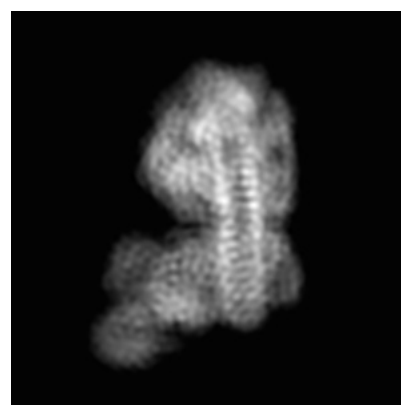
6.1.1 Primary map



X



Y

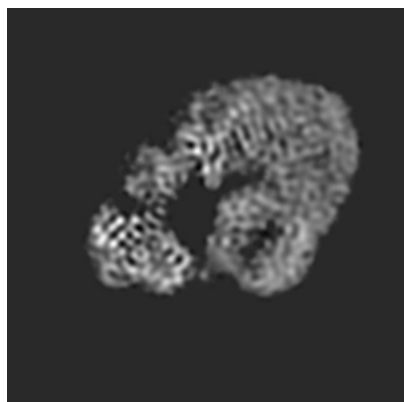


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

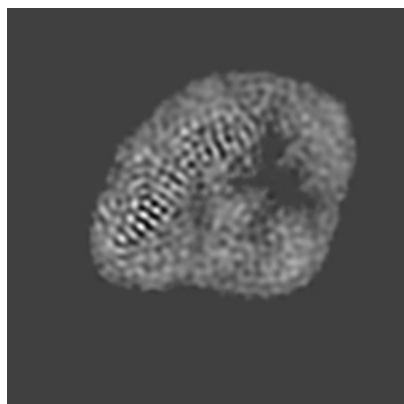


Z Index: 140

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

6.3 Largest variance slices [i](#)

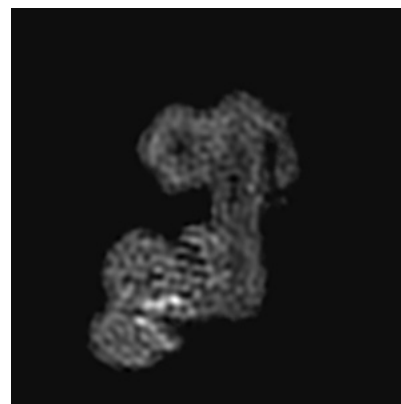
6.3.1 Primary map



X Index: 149



Y Index: 79



Z Index: 95

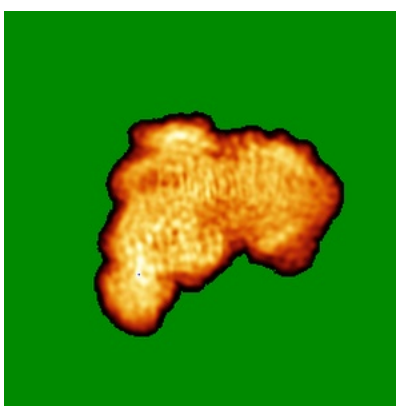
The images above show the largest variance slices of the map in three orthogonal directions.

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

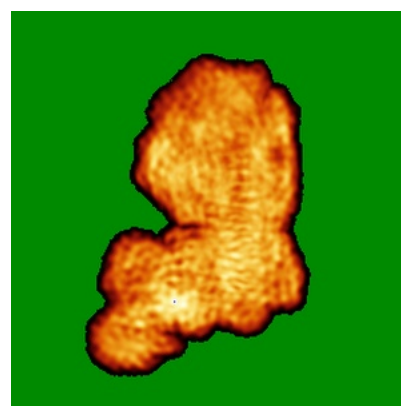
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

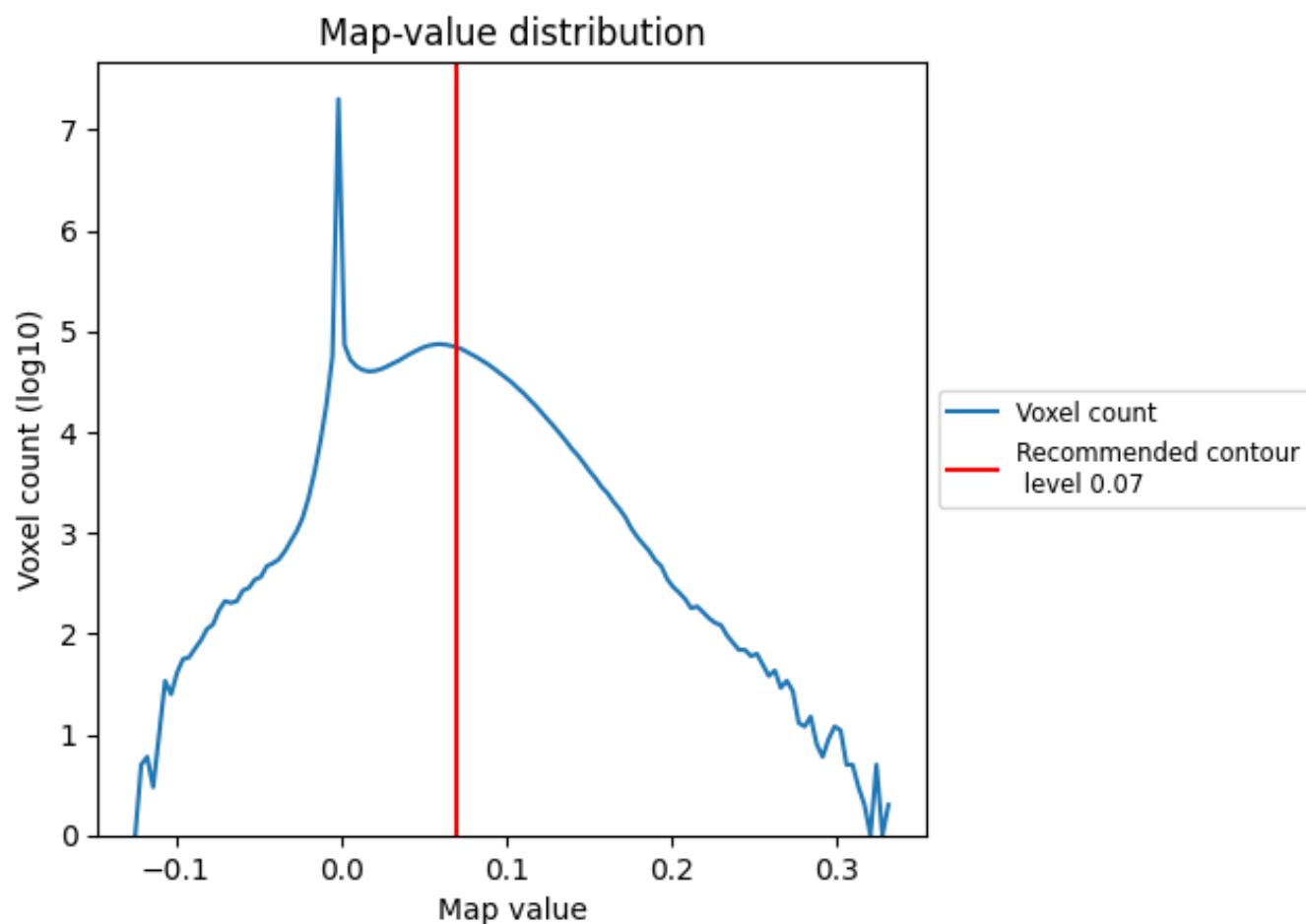
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

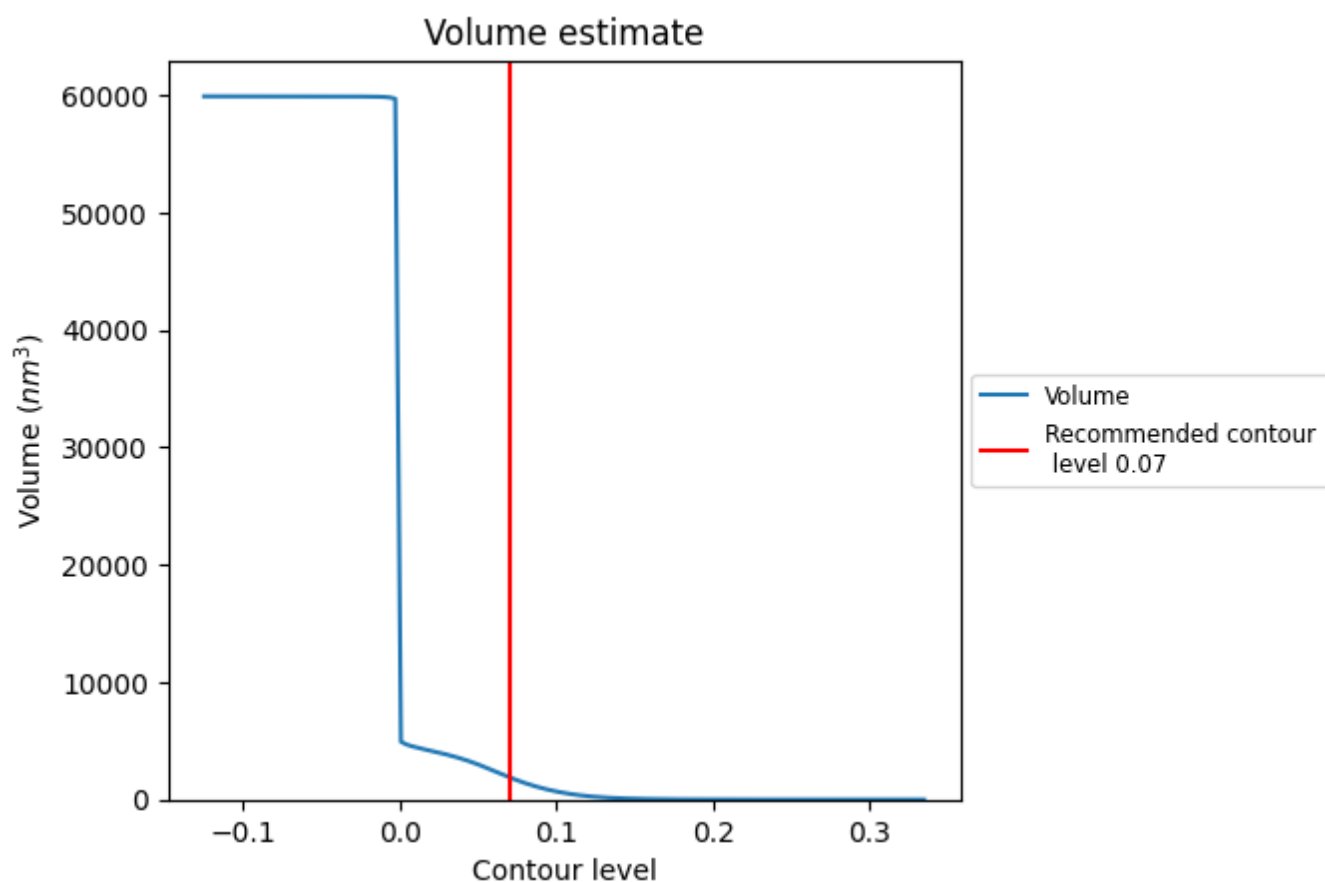
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

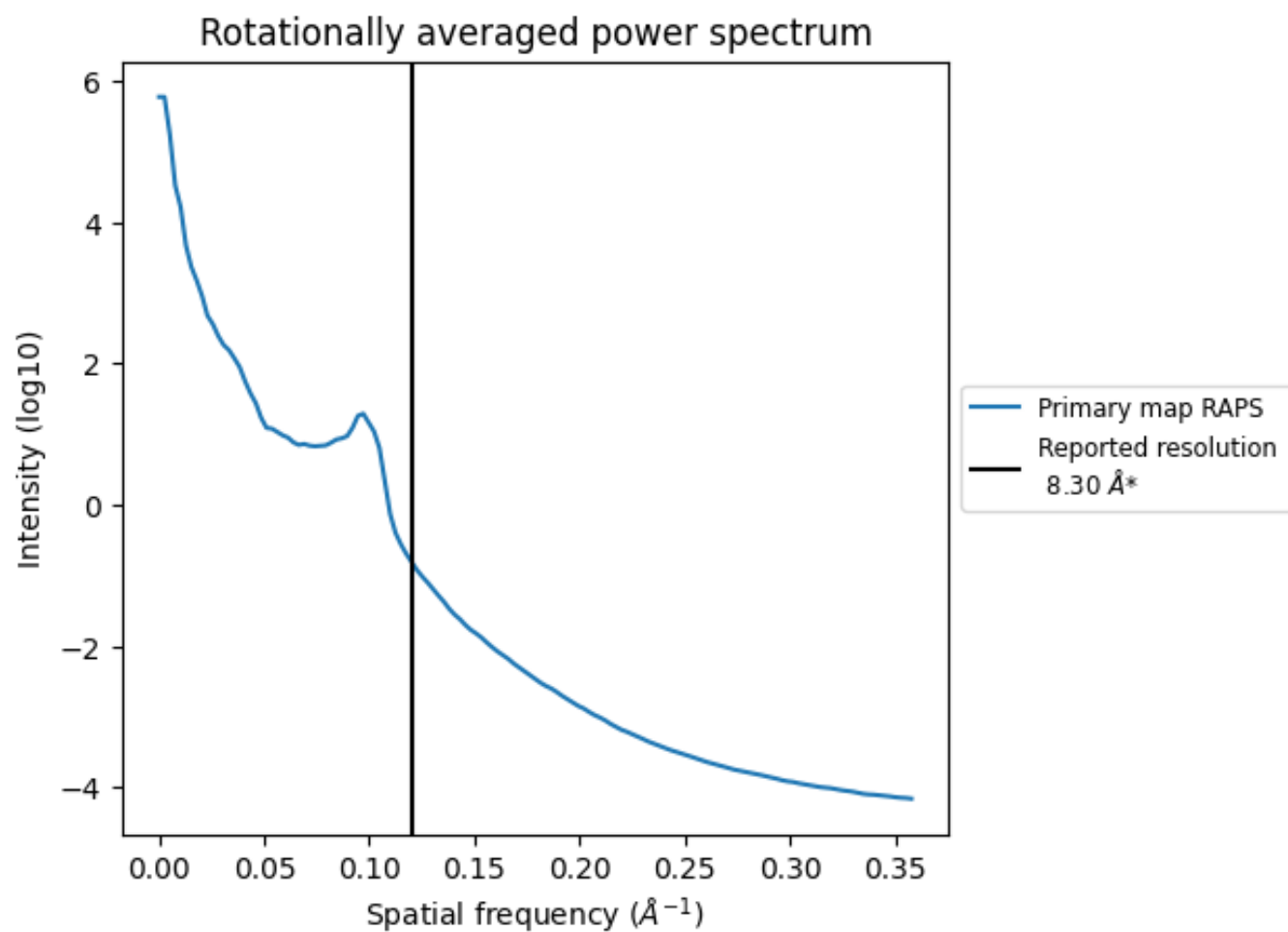
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1904 nm³; this corresponds to an approximate mass of 1720 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.120 Å⁻¹

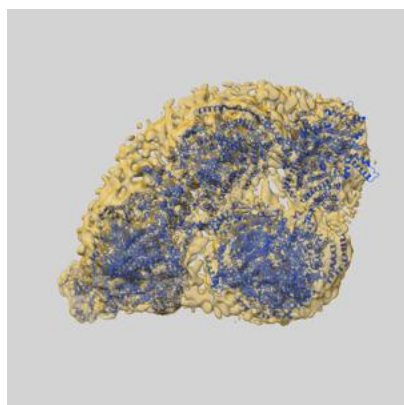
8 Fourier-Shell correlation

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

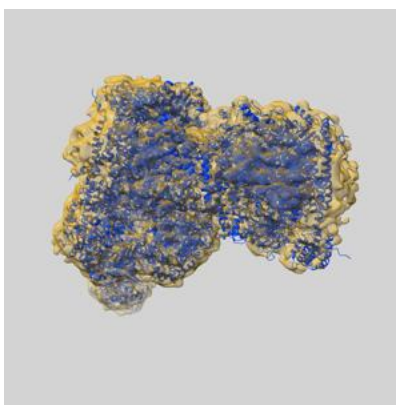
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30706 and PDB model 7DKF. Per-residue inclusion information can be found in section [3](#) on page [25](#).

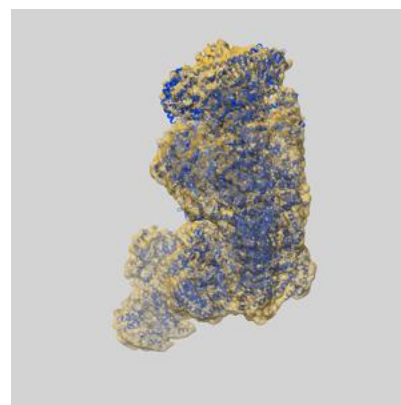
9.1 Map-model overlay [i](#)



X



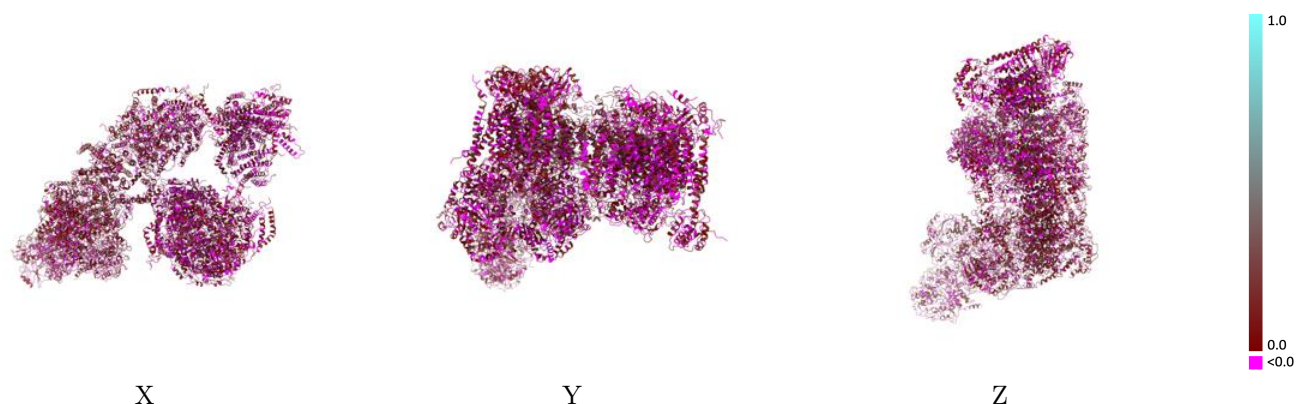
Y



Z

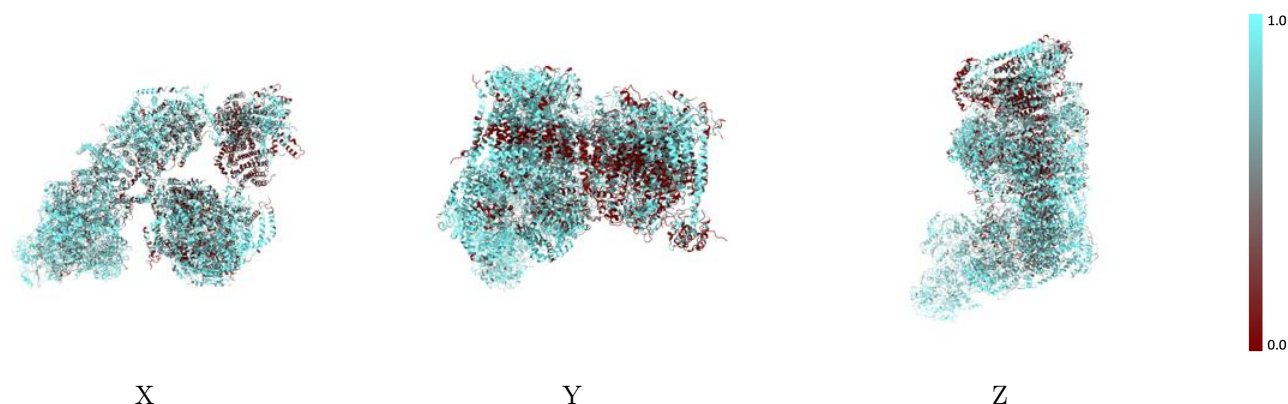
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



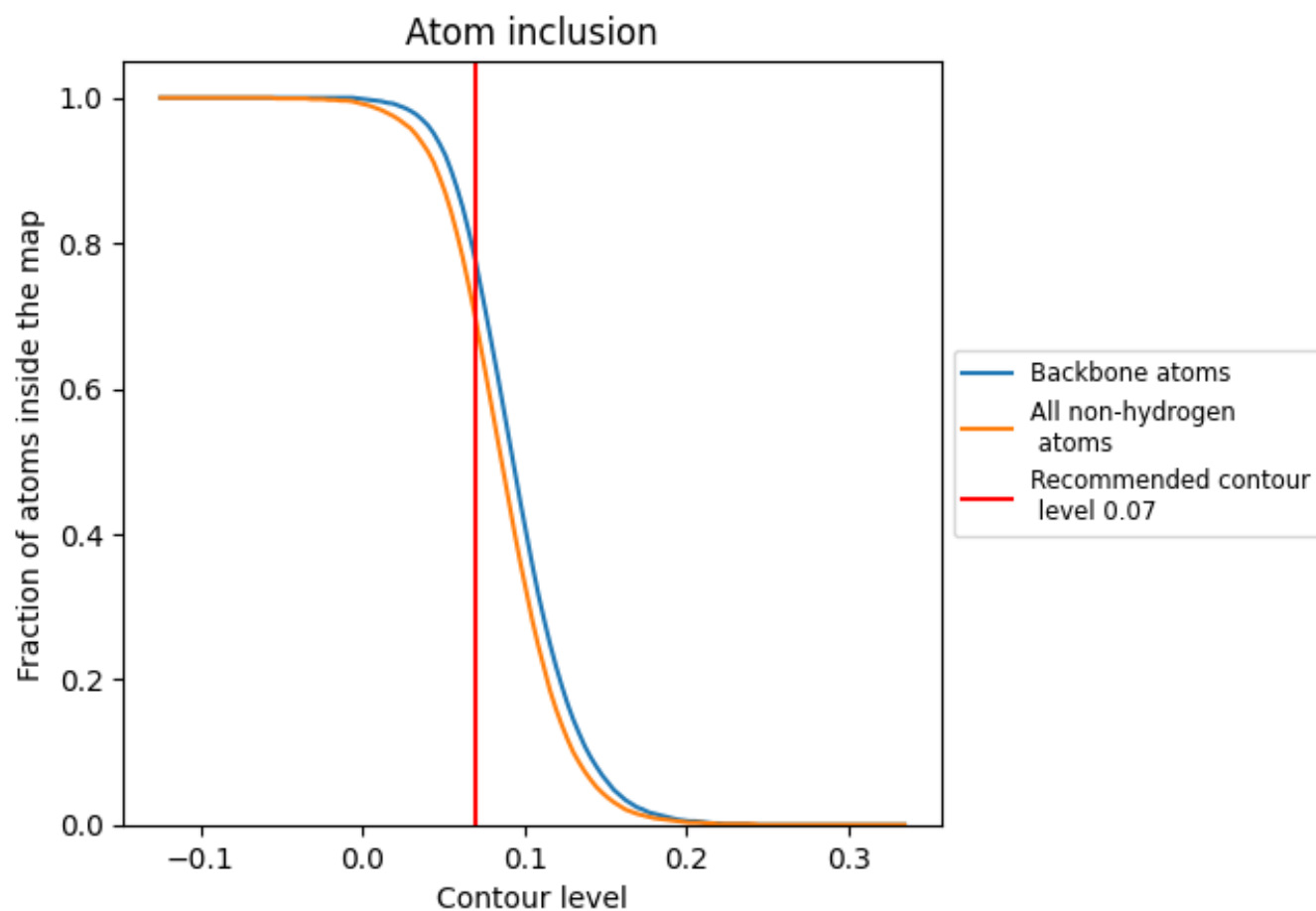
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.0740
12	 0.6860	 0.0940
22	 0.6830	 0.1120
32	 0.6530	 0.1220
42	 0.6360	 0.0960
52	 0.7230	 0.1370
62	 0.5780	 0.0660
72	 0.6180	 0.1000
82	 0.9020	 0.0870
92	 0.8570	 0.0660
A1	 0.8310	 0.0620
A2	 0.8730	 0.0890
A3	 0.4940	 0.0340
B1	 0.8390	 0.0590
B2	 0.7920	 0.0930
B3	 0.6750	 0.0240
C1	 0.6440	 0.0780
C2	 0.7840	 0.0880
C3	 0.3640	 0.0330
D1	 0.8390	 0.0660
D2	 0.7750	 0.0850
D3	 0.4080	 0.0180
E1	 0.6030	 0.0280
E2	 0.8570	 0.0840
E3	 0.4270	 0.0480
F1	 0.7560	 0.0750
F2	 0.8600	 0.1250
F3	 0.3470	 0.0430
G1	 0.6280	 0.0510
G2	 0.7500	 0.0850
G3	 0.2610	 0.0210
H1	 0.8150	 0.0760
H2	 0.8520	 0.1200
H3	 0.4570	 0.0170
I1	 0.3710	 -0.0560



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Chain	Atom inclusion	Q-score
I2	 0.6500	 0.0530
I3	 0.6620	 0.0800
J1	 0.6190	 0.0260
J2	 0.8410	 0.1030
J3	 0.2490	 0.0540
K1	 0.6160	 0.0770
K2	 0.9020	 0.1150
K3	 0.5650	 0.0470
L2	 0.7600	 0.1050
L3	 0.4180	 0.0440
M1	 0.6890	 0.0380
M2	 0.6580	 0.1210
M3	 0.4820	 0.1140
N1	 0.7870	 0.0460
N2	 0.8970	 0.1390
O1	 0.5690	 0.0530
O2	 0.7560	 0.1220
P1	 0.7400	 0.0410
P2	 0.7500	 0.1080
Q1	 0.6350	 0.0400
Q2	 0.8640	 0.1250
R1	 0.5960	 0.0680
R2	 0.7930	 0.0950
S1	 0.4540	 0.0610
S2	 0.5560	 0.1020
T1	 0.6370	 0.0660
T2	 0.5780	 0.1090
U1	 0.3420	 -0.0100
U2	 0.5780	 0.0750
V1	 0.4770	 0.0600
V2	 0.8740	 0.1340
W1	 0.3020	 0.0720
W2	 0.6500	 0.0430
X2	 0.8470	 0.1100
Y2	 0.7370	 0.0930
Z2	 0.6530	 0.0540
a2	 0.5460	 0.0940
b2	 0.8980	 0.1150
c2	 0.8810	 0.1120
d2	 0.7520	 0.0280
e2	 0.6240	 0.0750
f2	 0.6410	 0.0690

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Chain	Atom inclusion	Q-score
g2	 0.8340	 0.0960
h2	 0.7420	 0.1060
i2	 0.8430	 0.1620
j2	 0.8470	 0.1310