



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:55 AM UTC

PDB ID : 7DGQ / pdb_00007dgq
EMDB ID : EMD-30673
Title : Activity optimized supercomplex state1
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 : 2020-11-12
Resolution : 5.00 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:

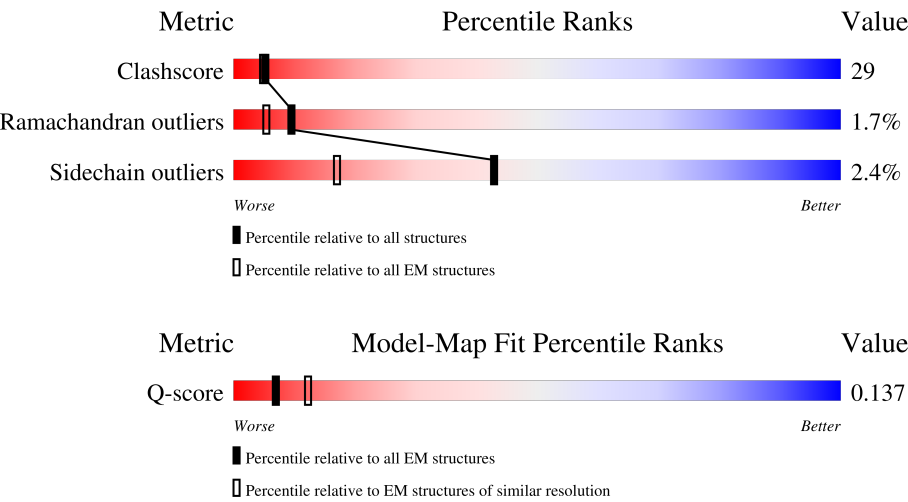
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 5.00 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	1057 (4.50 - 5.50)

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	3	115	
2	1	318	
3	9	217	
4	7	175	

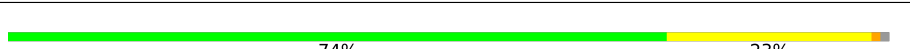
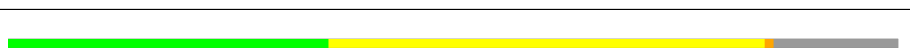
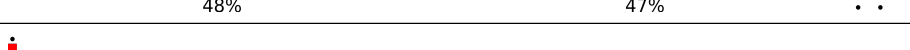
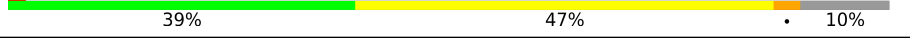
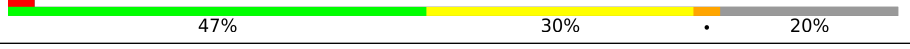
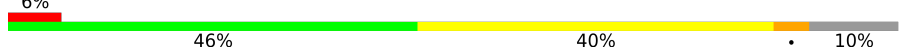
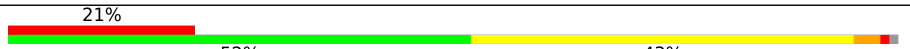
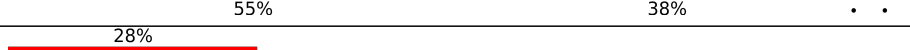
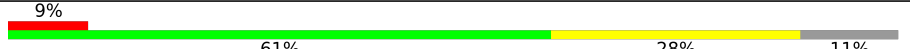
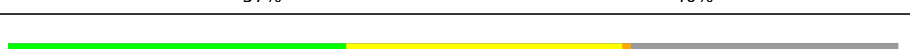
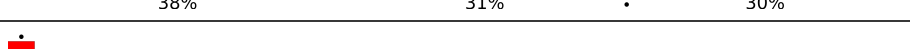
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Mol	Chain	Length	Quality of chain
5	4	459	
6	5	98	
7	6	606	
8	2	347	
9	8	444	
10	C3	514	
11	C1	227	
12	A9	261	
13	A7	169	
14	B4	152	
15	A5	129	
16	A6	97	
17	C0	86	
18	C2	74	
19	B2	80	
20	B3	80	
21	A0	63	
22	A8	70	
23	A	704	
24	B	430	
25	C	228	
26	D	179	
27	E	176	
28	F	75	
29	G	133	

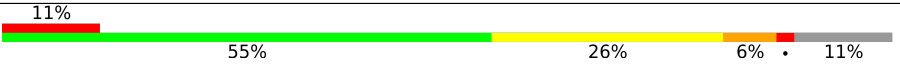
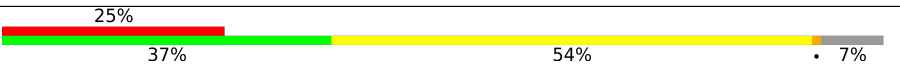
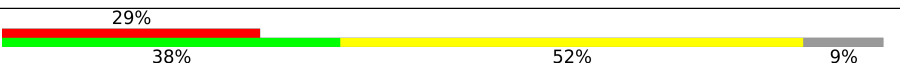
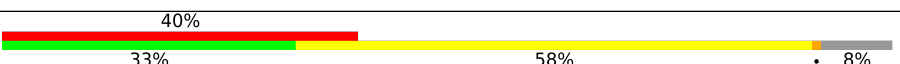
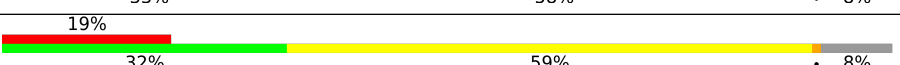
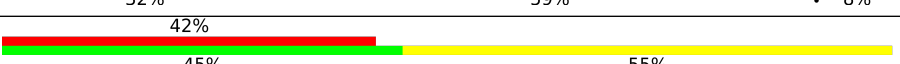
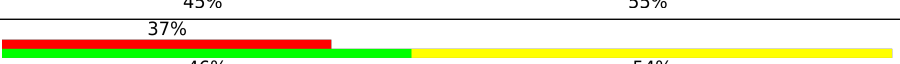
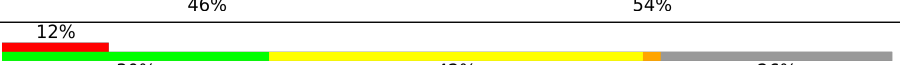
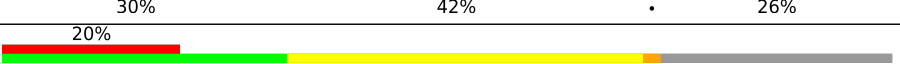
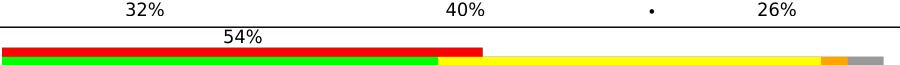
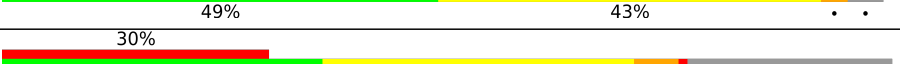
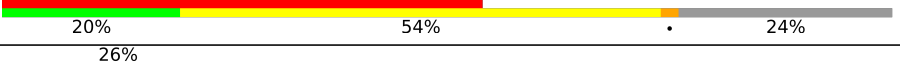
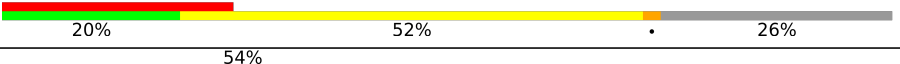
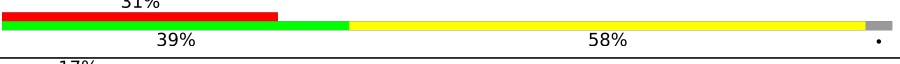
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Mol	Chain	Length	Quality of chain
30	H	105	
31	I	96	
32	J	70	
33	K	98	
34	L	83	
35	N	115	
36	O	127	
37	P	112	
38	Q	171	
39	R	345	
40	S	320	
41	T	140	
42	U	145	
43	V	143	
44	M	86	
44	W	86	
45	X	57	
46	Y	72	
47	Z	98	
48	a	128	
49	b	143	
50	c	128	
51	d	117	
52	f	178	
53	h	125	

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Mol	Chain	Length	Quality of chain
54	i	49	
55	j	120	
56	g	176	
57	e	158	
58	k	480	
58	w	480	
59	l	453	
59	x	453	
60	m	379	
60	y	379	
61	o	325	
61	z	325	
62	A1	196	
62	p	196	
63	A2	111	
63	q	111	
64	A3	82	
64	r	82	
65	B7	91	
65	s	91	
66	A4	56	
66	t	56	
67	B6	64	
67	u	64	
68	B5	78	

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Mol	Chain	Length	Quality of chain
68	v	78	

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
71	FES	A	803	-	-	X	-
73	FMN	8	501	-	-	X	-
74	SF4	A	801	-	-	X	-
74	SF4	A	802	-	-	X	-
82	UQ2	A2	201	-	-	X	-

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 107321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	112	Total	C	N	O	S	0	0
			882	596	128	151	7		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	318	Total	C	N	O	S	0	0
			2503	1678	385	417	23		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9	207	Total	C	N	O	S	0	0
			1579	1006	269	294	10		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	172	Total	C	N	O	S	0	0
			1235	835	181	211	8		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	458	Total	C	N	O	S	1	0
			3577	2382	561	599	35		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	96	Total	C	N	O	S	0	0
			712	464	110	125	13		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	606	Total	C	N	O	S	0	0
			4766	3172	732	820	42		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	344	Total	C	N	O	S	0	0
			2681	1779	413	449	40		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	427	Total	C	N	O	S	0	0
			3065	1927	563	559	16		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C3	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C1	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A9	261	Total	C	N	O	S	0	0
			2125	1421	338	353	13		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A7	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B4	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A5	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C0	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C2	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B2	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B3	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A0	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A8	43	Total	C	N	O		0	0
			335	223	53	59			

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	688	Total	C	N	O	S	0	0
			5218	3273	920	988	37		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	430	Total	C	N	O	S	0	0
			3422	2185	588	624	25		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	C	208	Total	C	N	O	S	0	0
			1726	1114	297	312	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	152	Total	C	N	O	S	0	0
			1206	772	212	208	14		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	176	Total	C	N	O	S	0	0
			1401	880	243	267	11		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F	28	Total	C	N	O	S	0	0
			186	118	32	35	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	123	Total	C	N	O	S	0	0
			985	622	178	182	3		

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

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	71	Total	C	N	O	S	0	0
			535	333	99	100	3		

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

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	84	Total	C	N	O		0	0
			656	412	126	118			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	90	Total	C	N	O	S	0	0
			702	445	129	126	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	309	Total	C	N	O	S	0	0
			2349	1514	420	412	3		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	138	Total	C	N	O	S	0	0
			923	584	162	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	138	Total	C	N	O	S	0	0
			1087	699	186	193	9		

- Molecule 44 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	86	Total	C	N	O	S	0	0
			616	400	98	114	4		
44	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

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

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d	107	Total	C	N	O	S	0	0
			710	447	134	125	4		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	h	84	Total	C	N	O	S	0	0
			658	423	115	118	2		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	i	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	k	446	Total	C	N	O	S	0	0
			3454	2159	608	667	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	436	Total	C	N	O	S	0	0
			3385	2117	599	649	20		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	l	419	Total	C	N	O	S	0	0
			3135	1969	553	606	7		
59	x	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 60 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	m	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
60	y	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 61 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	o	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
61	z	241	Total	C	N	O	S	0	0
			1906	1216	329	347	14		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	p	151	Total	C	N	O	S	0	0
			938	572	170	194	2		
62	A1	188	Total	C	N	O	S	0	0
			1117	679	207	229	2		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	q	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
63	A2	106	Total	C	N	O	S	0	0
			907	574	166	165	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	r	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
64	A3	81	Total	C	N	O	S	0	0
			676	438	125	112	1		

- Molecule 65 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	s	67	Total	C	N	O	S	0	0
			548	332	99	112	5		
65	B7	69	Total	C	N	O	S	0	0
			566	342	101	118	5		

- Molecule 66 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	t	33	Total	C	N	O	0	0
			262	174	46	42		
66	A4	39	Total	C	N	O	0	0
			318	212	56	50		

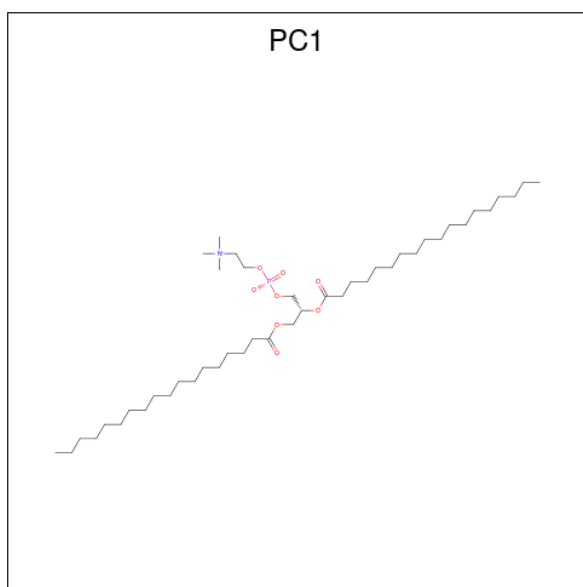
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	u	62	Total	C	N	O	0	0
			511	335	89	87		
67	B6	62	Total	C	N	O	0	0
			511	335	89	87		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

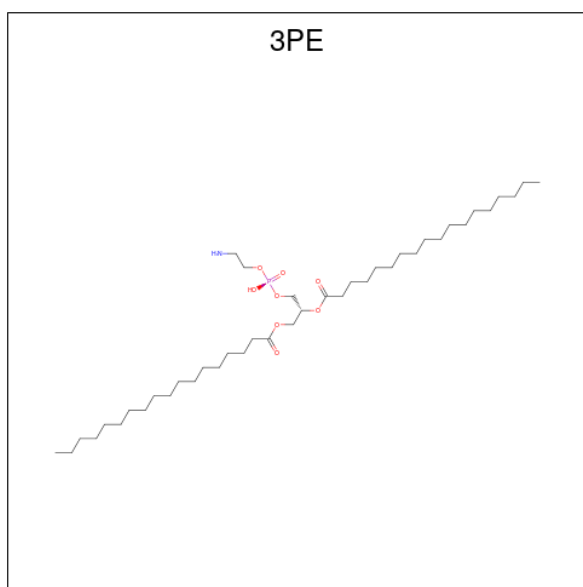
Mol	Chain	Residues	Atoms				AltConf	Trace
68	v	18	Total	C	N	O	0	0
			114	70	22	22		
68	B5	22	Total	C	N	O	0	0
			148	91	30	27		

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



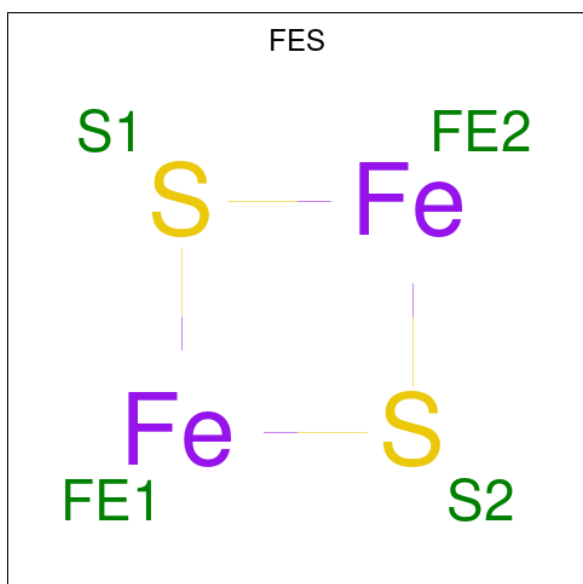
Mol	Chain	Residues	Atoms					AltConf
69	3	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 70 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



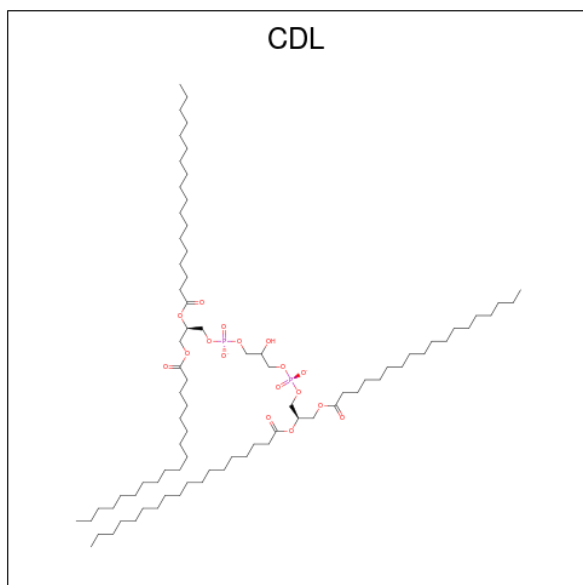
Mol	Chain	Residues	Atoms					AltConf
70	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
70	j	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



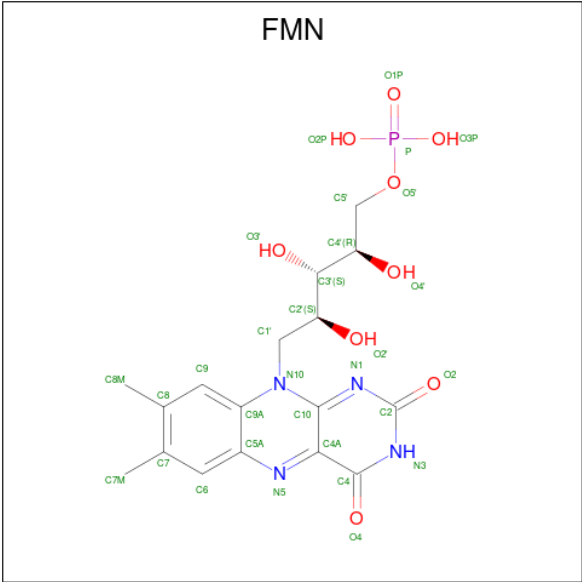
Mol	Chain	Residues	Atoms			AltConf
71	9	1	Total	Fe	S	0
			4	2	2	
71	A	1	Total	Fe	S	0
			4	2	2	
71	m	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



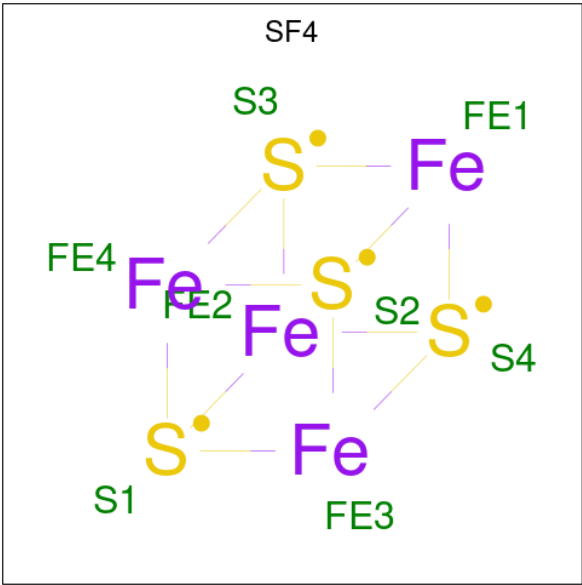
Mol	Chain	Residues	Atoms				AltConf
72	6	1	Total	C	O	P	0
			64	45	17	2	
72	J	1	Total	C	O	P	0
			58	39	17	2	
72	b	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 73 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
73	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
74	8	1	Total	Fe	S	0
			8	4	4	
74	A	1	Total	Fe	S	0
			8	4	4	
74	A	1	Total	Fe	S	0
			8	4	4	

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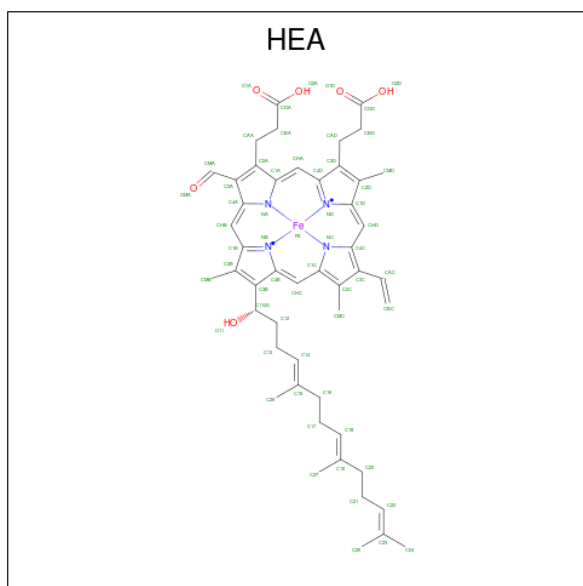
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Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 75 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	C3	1	Total	Cu	0
			1	1	
75	C1	2	Total	Cu	0
			2	2	

- Molecule 76 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
76	C3	1	Total 60	C 49	Fe 1	N 4	O 6	0
76	C3	1	Total 60	C 49	Fe 1	N 4	O 6	0

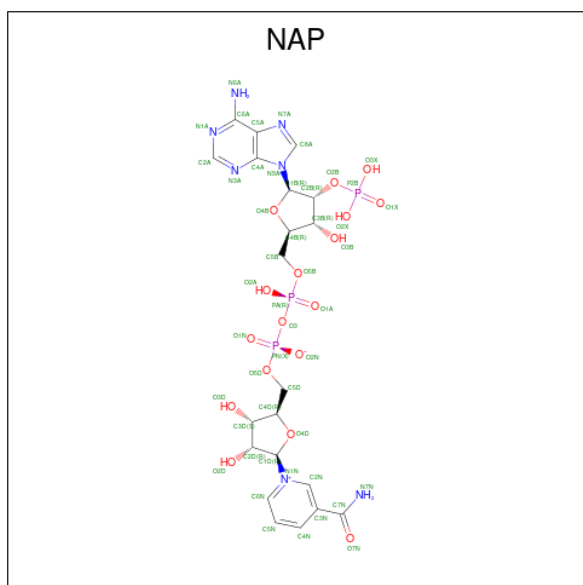
- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	C1	1	Total 1	Mg 1	0

- Molecule 78 is ZINC ION (CCD ID: ZN) (formula: Zn).

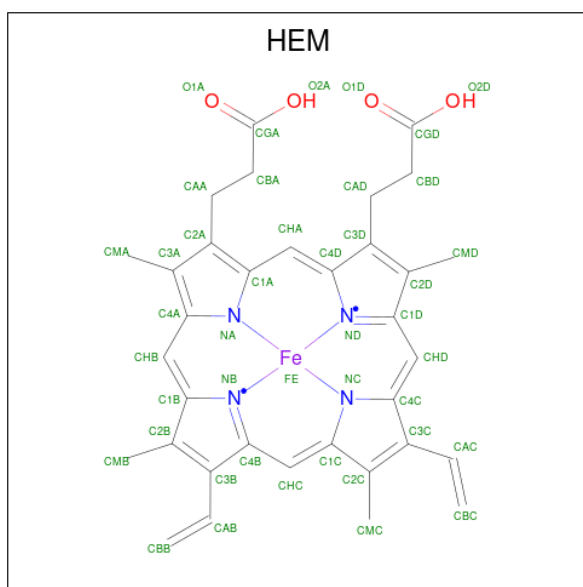
Mol	Chain	Residues	Atoms	AltConf
78	A5	1	Total Zn 1 1	0
78	I	1	Total Zn 1 1	0

- Molecule 79 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



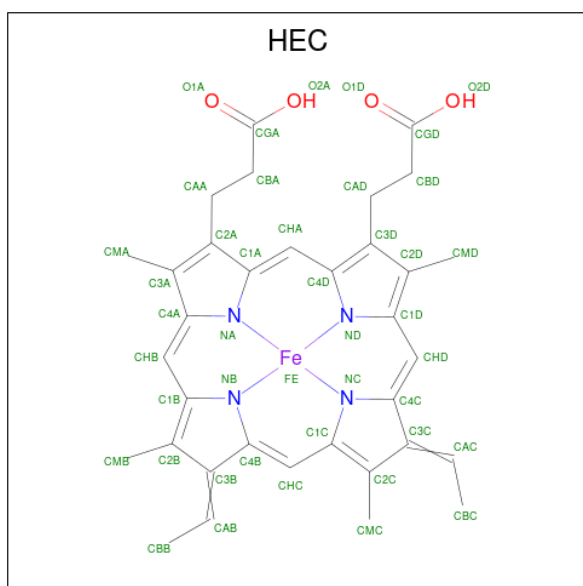
Mol	Chain	Residues	Atoms					AltConf
79	R	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



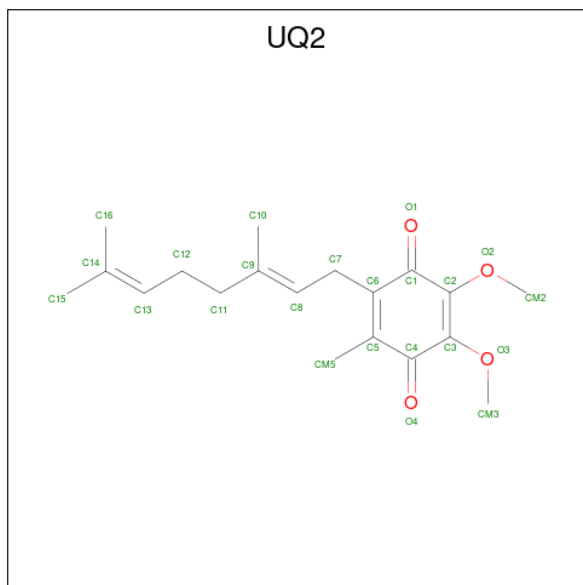
Mol	Chain	Residues	Atoms					AltConf
80	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	y	1	Total 43	C 34	Fe 1	N 4	O 4	0
80	y	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
81	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	z	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).

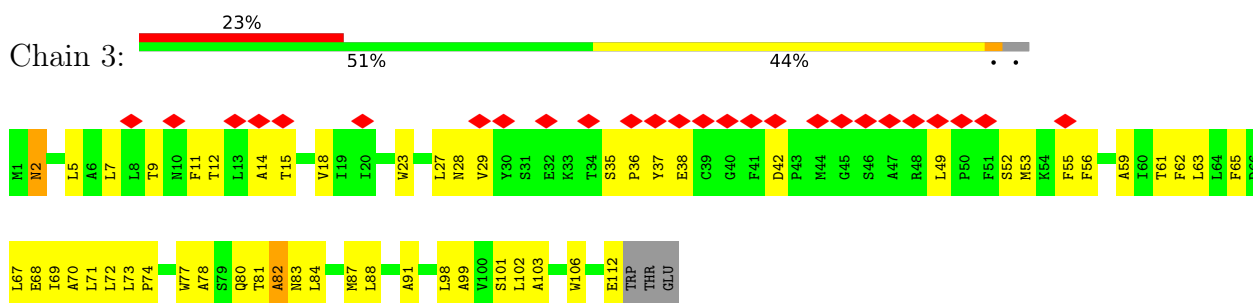


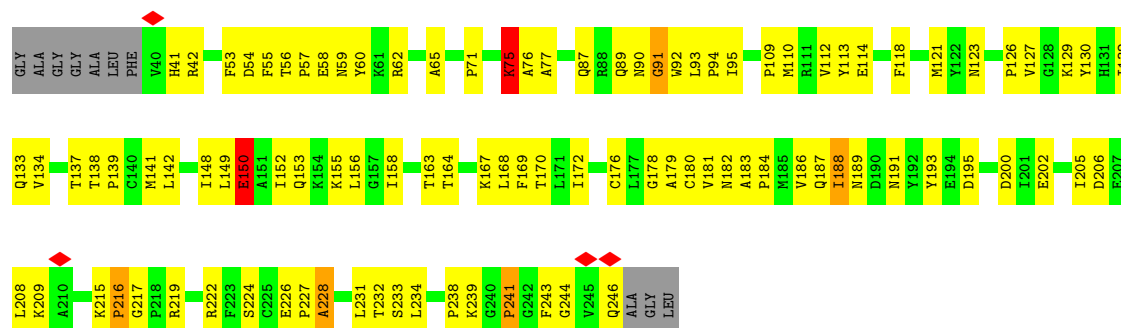
Mol	Chain	Residues	Atoms			AltConf
82	A2	1	Total	C	O	0
			23	19	4	

3 Residue-property plots

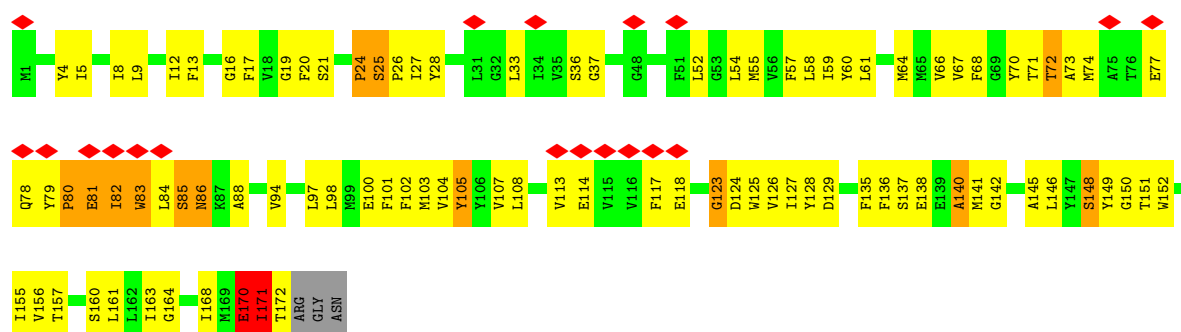
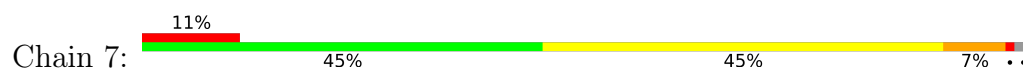
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

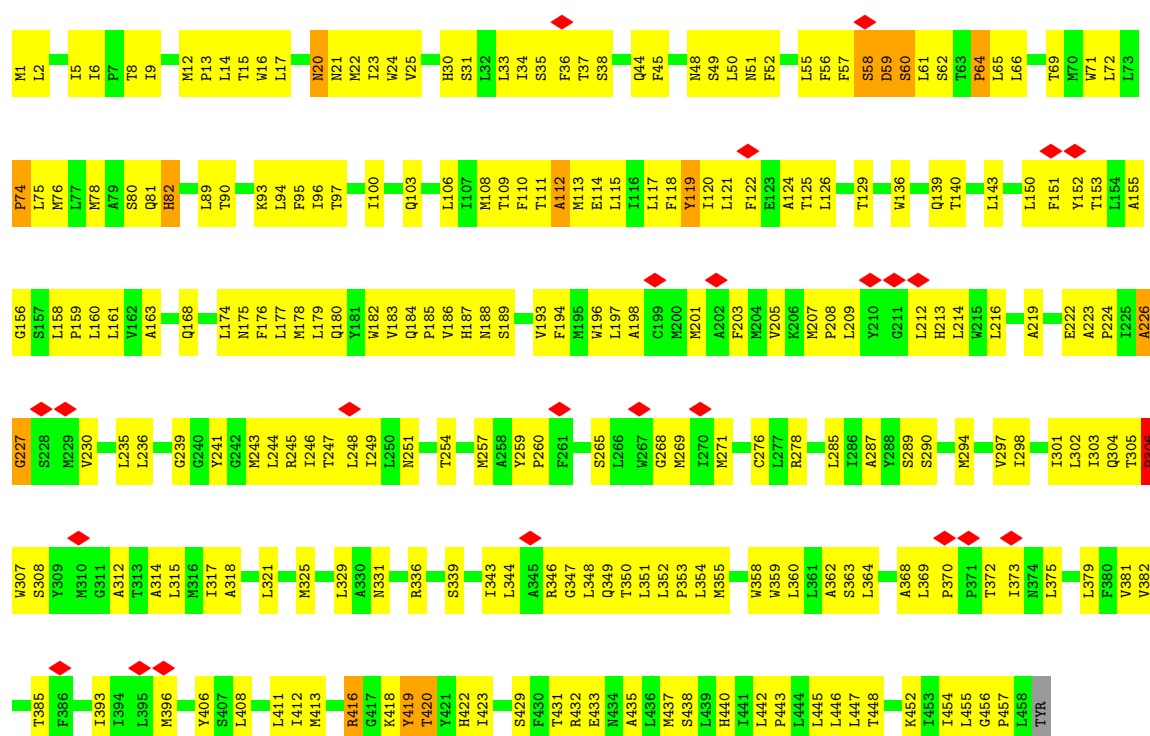




• Molecule 4: NADH-ubiquinone oxidoreductase chain 6



• Molecule 5: NADH-ubiquinone oxidoreductase chain 4



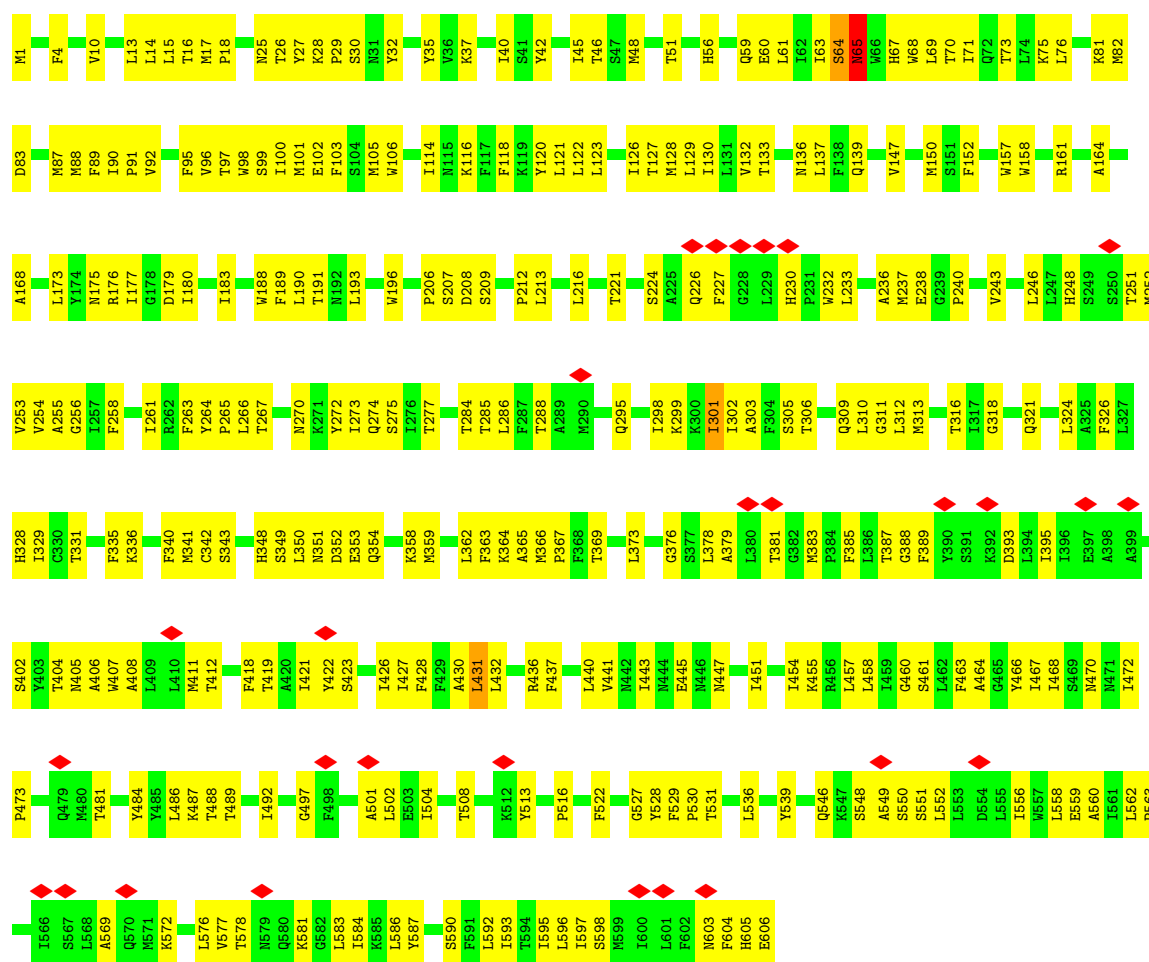
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5:  46% 45% 7%



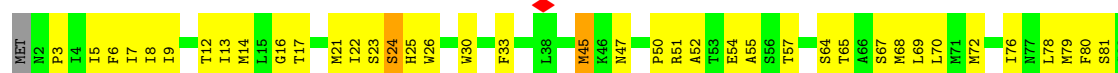
• Molecule 7: NADH-ubiquinone oxidoreductase chain 5

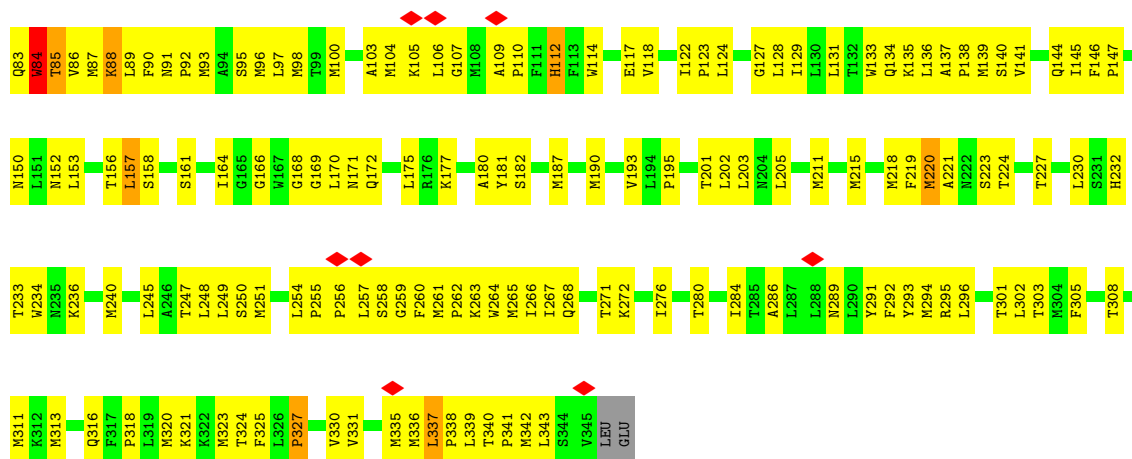
Chain 6:  5% 52% 48%



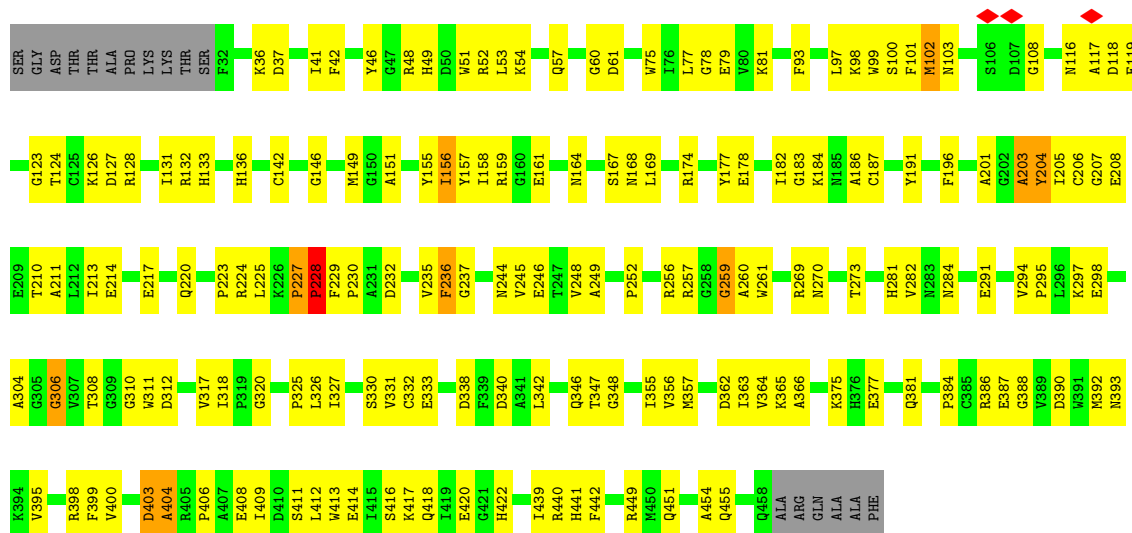
• Molecule 8: NADH-ubiquinone oxidoreductase chain 2

Chain 2:  45% 51%

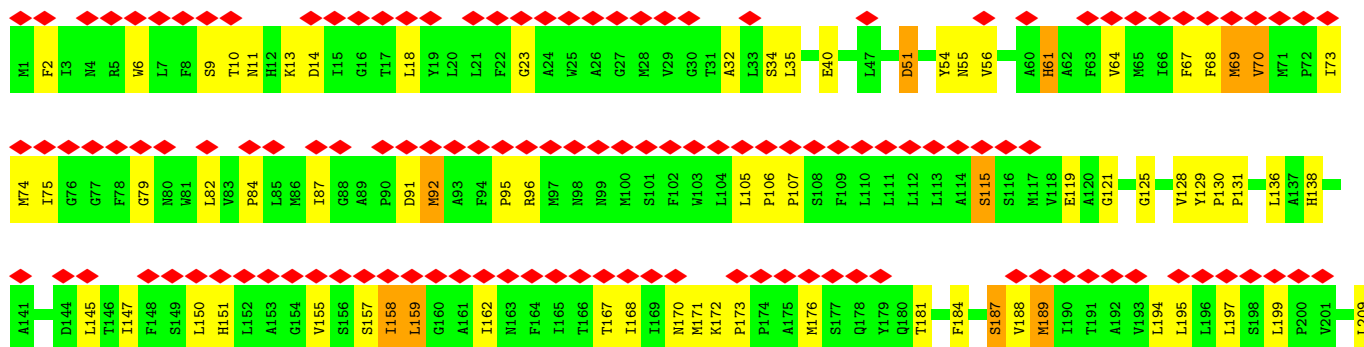
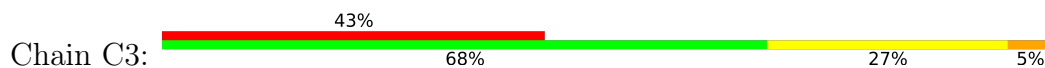


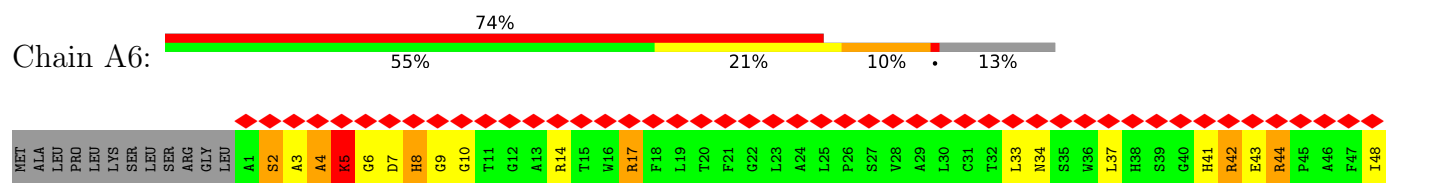
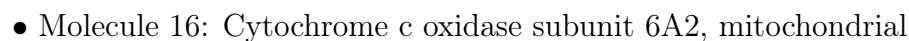
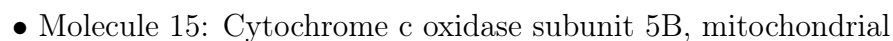
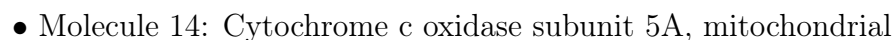


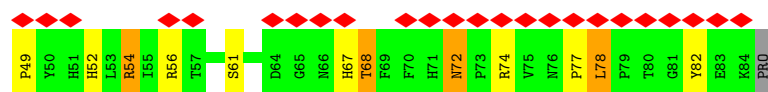
• Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



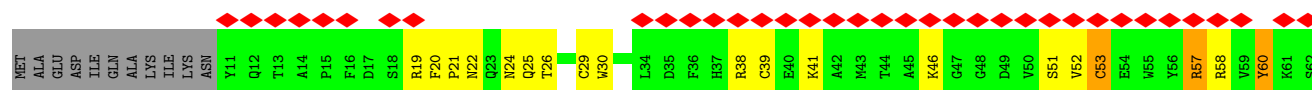
• Molecule 10: Cytochrome c oxidase subunit 1



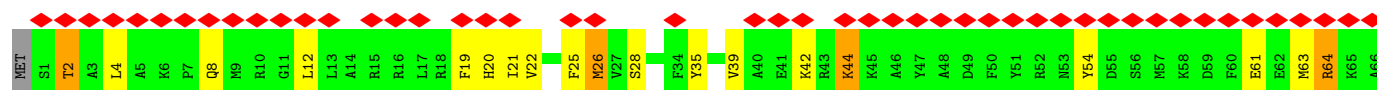
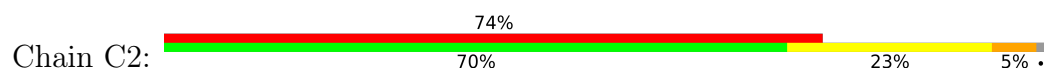




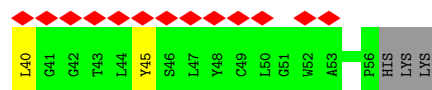
- Molecule 17: Cytochrome c oxidase subunit 6B1



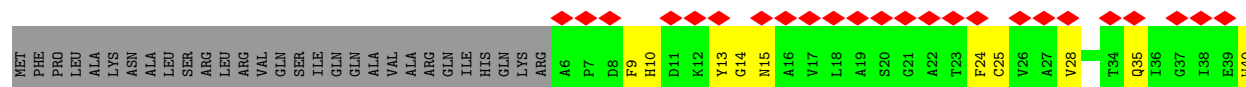
- Molecule 18: Cytochrome c oxidase subunit 6C



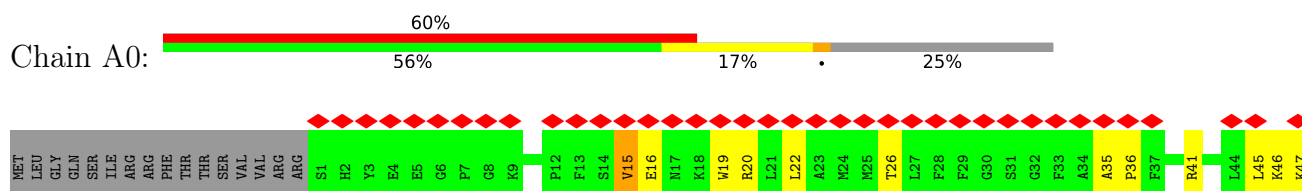
- Molecule 19: Cytochrome c oxidase subunit 7A1, mitochondrial



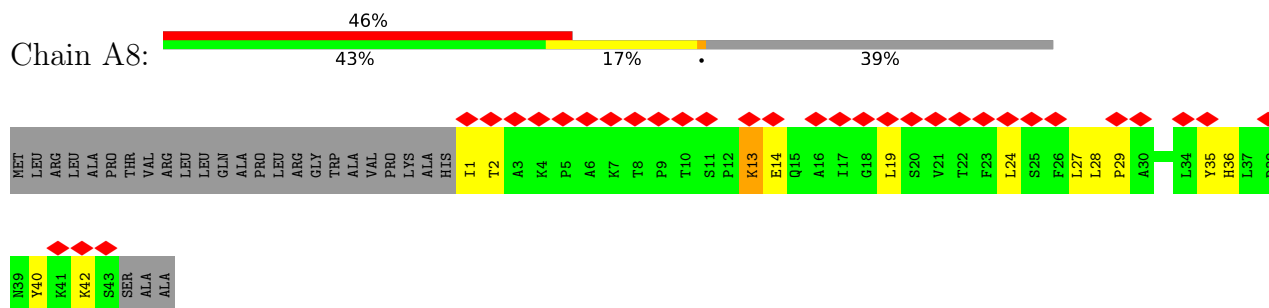
- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial



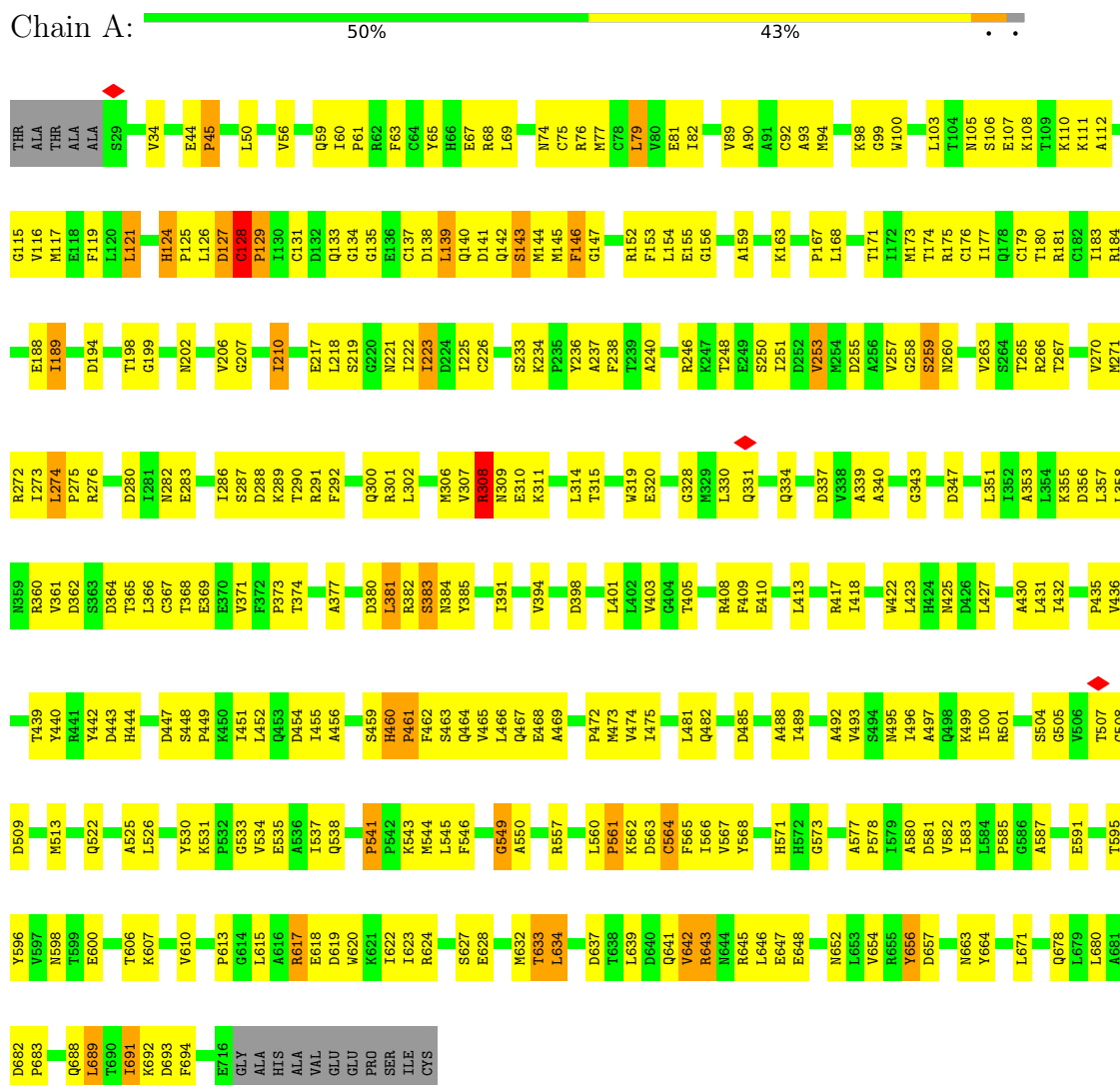
- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial



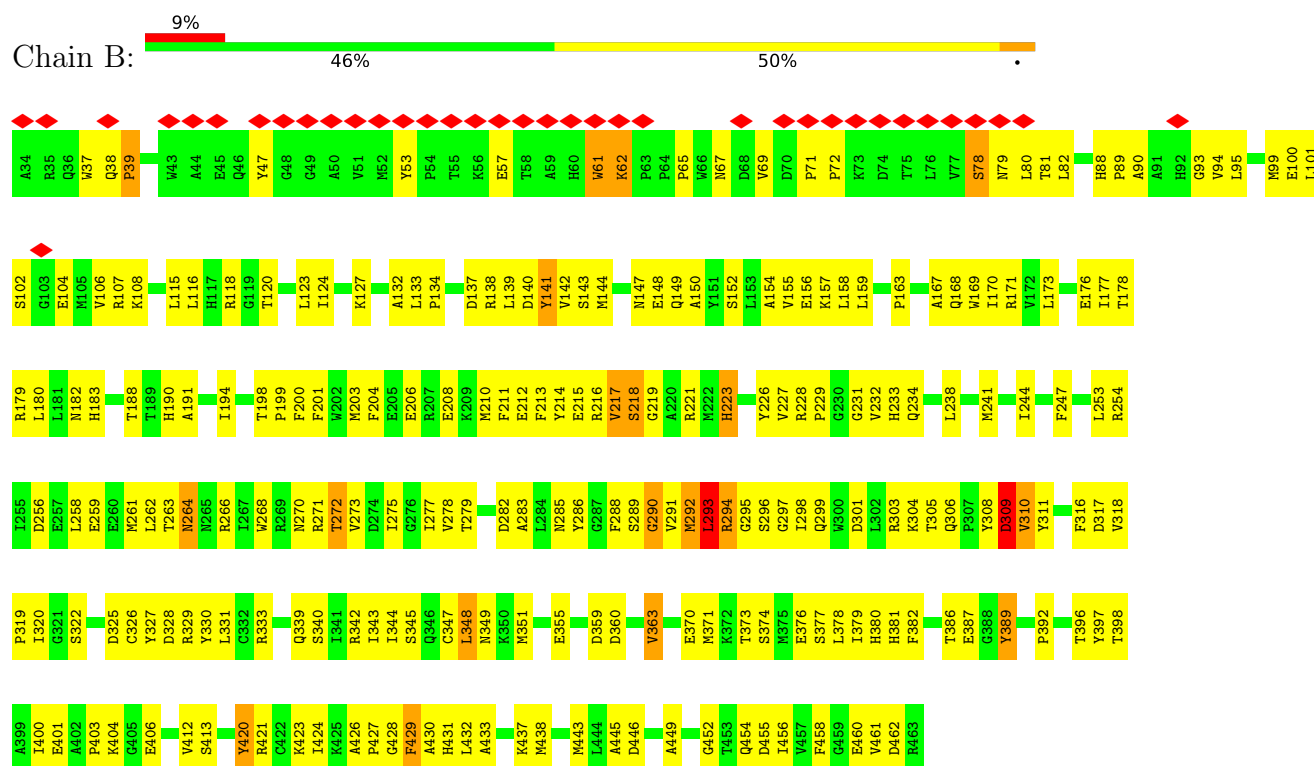
- Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial



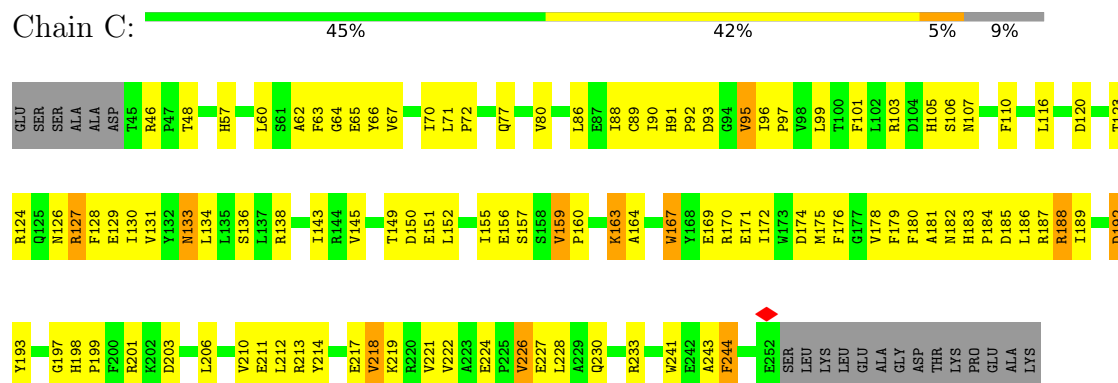
- Molecule 23: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



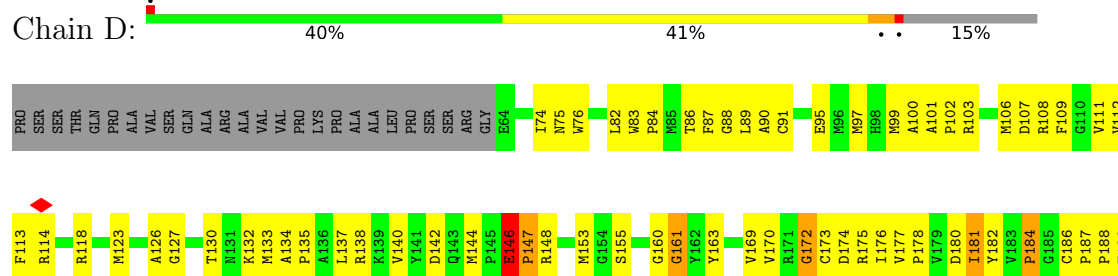
• Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

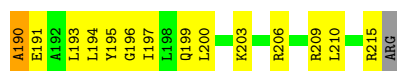


• Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



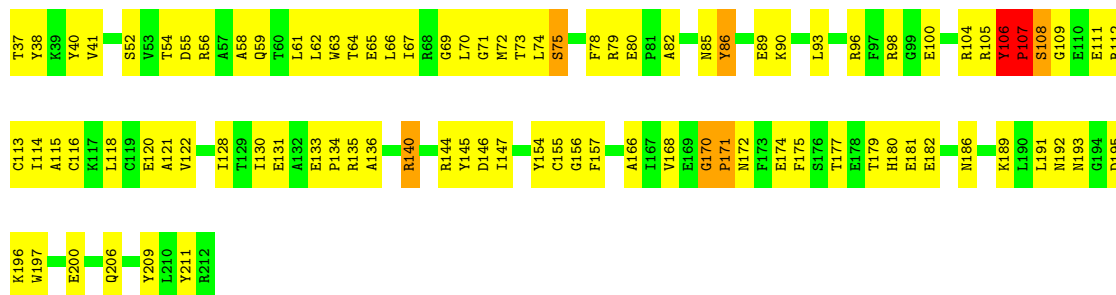
• Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





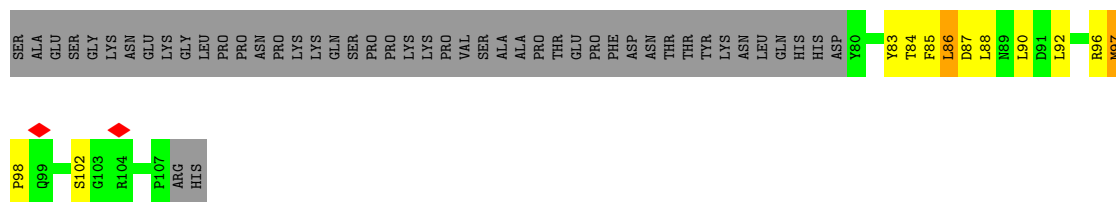
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E: 48% 48%



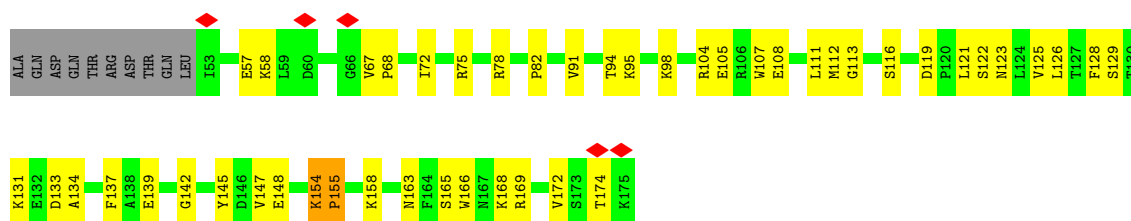
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F: 21% 13% 63%



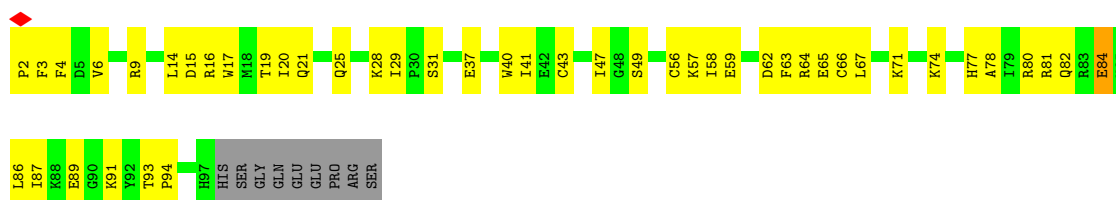
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G: 57% 34% 8%

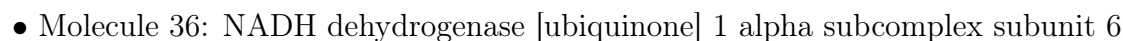
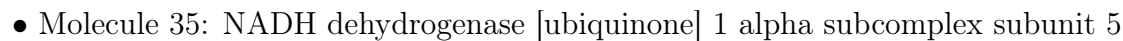
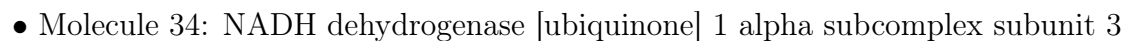
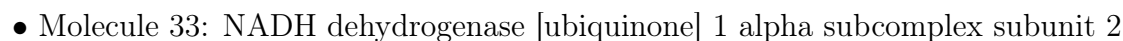
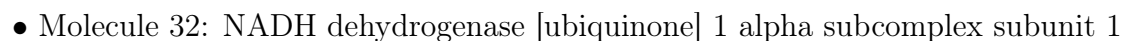


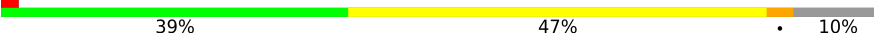
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

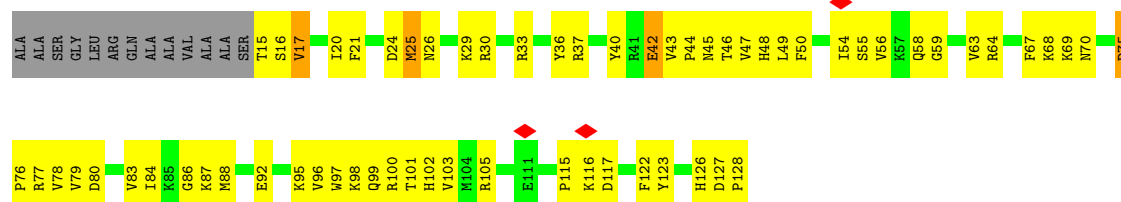
Chain H: 48% 43% 9%



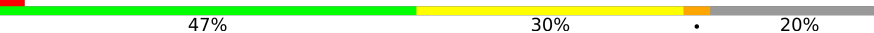
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



Chain O: 



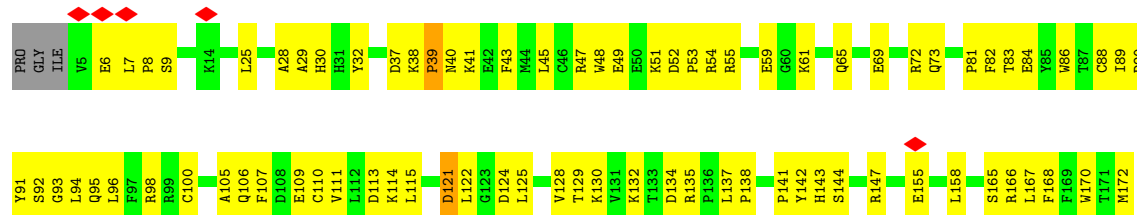
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P: 



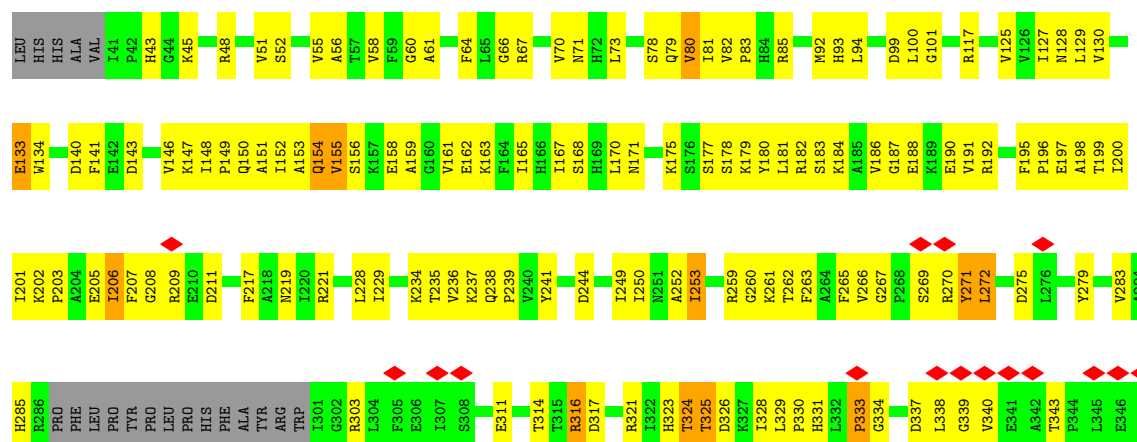
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

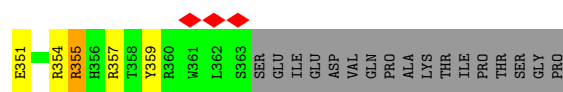
Chain Q: 



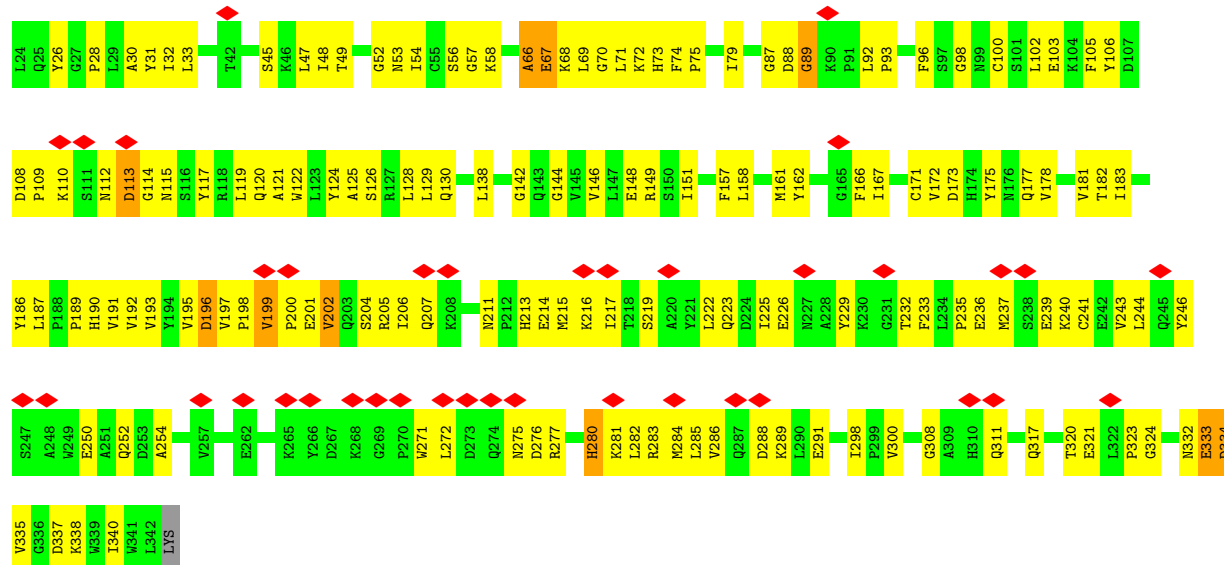
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R: 

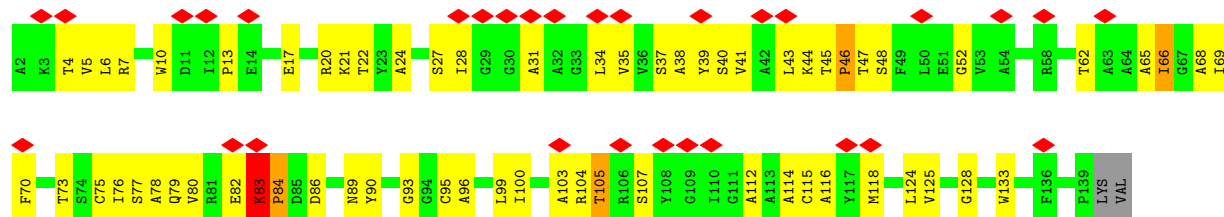




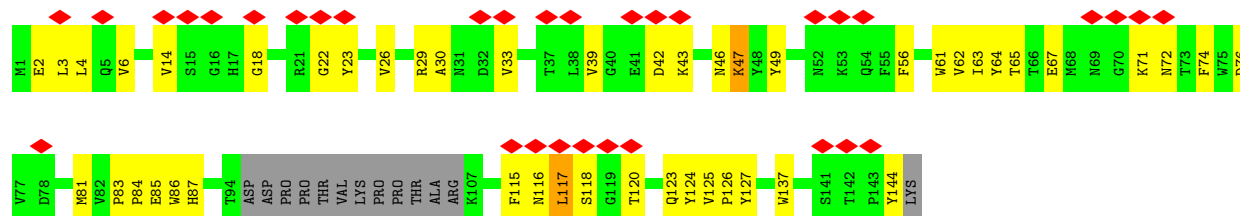
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

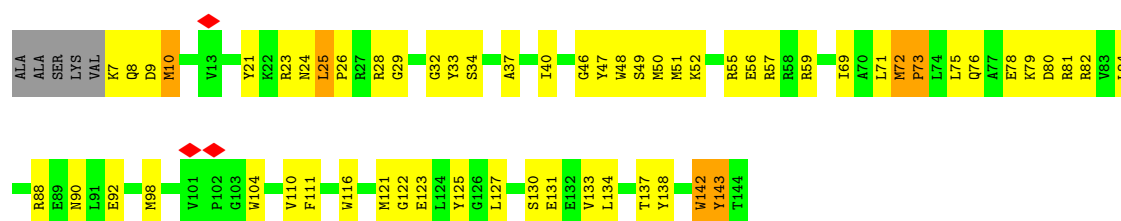


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain V: 



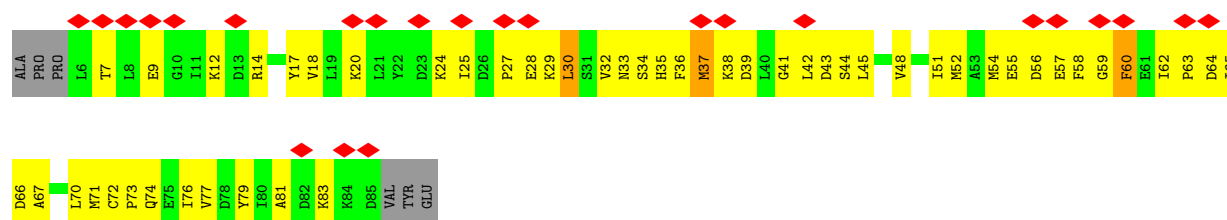
- Molecule 44: Acyl carrier protein, mitochondrial

Chain W: 



- Molecule 44: Acyl carrier protein, mitochondrial

Chain M: 



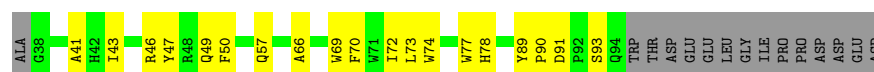
- Molecule 45: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain X: 



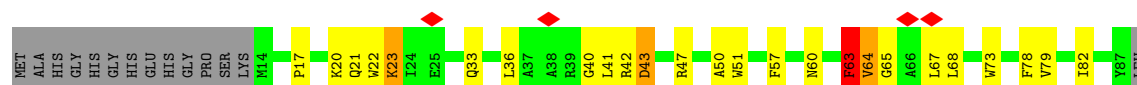
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 



GLU
SER
PHE
GLN
LYS
LYS
ASP
LYS
LYS
HIS

- Molecule 48: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain a: 9% 61% 28% 11%

SER PHE PRO LYS TYR GLU ALA SER ARG LEU SER LEU PRO T16 E22 I25 S26 S27 E28 T29 R30 L37 R40 L43 E46 Y47 Q50 Y51 Y52 D53 P54 S55 R56 R57 G58 V59 A64 W68 T69 Y70 N75 I76 N79 F80 T84 K85 T86

G90 A91 L92 F93 G94 I95 L98 F105 D108 R109 D110 L121 D122 N126 I127 S128 Y129

- Molecule 49: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain b: 57% 40% 3%

SER GLY ASP HIS K52 K53 G61 K65 R66 F67 L68 K69 L70 L76 G79 A83 T87 V91 F92 I93 A96 E97 E100 I101 W110 E111 Y112 R119 W120 I121 A122 G128 P129 E130 K131 N132 Y133 E134 R135 T136 M137 A138 I139 E143 A144 E145

K146 L149 R150 L151 K152 E153 R157 R158 L159 M160 R161 A162 R163 G164 D165 G166 P167 W168 I174 K184 A185 T186 P187 D188 N189

- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain c: 38% 31% 30%

NET SER GLY TYR T5 P6 E7 R11 L12 Q13 Q14 L15 R16 E17 L18 R19 R20 R21 K24 L28 S29 P30 R31 E32 P33 V34 V35 L36 P36 P37 Q38 R39 V40 S41 PRO VAL GLU ARG PHE TRP ASN LYS PHE LEU GLN ASP GLY ALA LEU TRP LYS ASN VAL ILE TYR T64

Y65 R66 H67 S68 A71 V75 L76 P78 H83 R87 Y88 H89 T92 K93 P94 R95 T96 R103 I104 F105 P106 G107 V116 ILE PRO PRO MET LYS GLU PHE PRO ASP GLN HIS HIS

- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

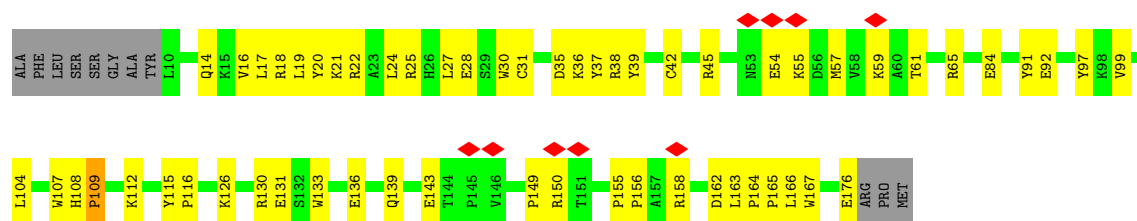
Chain d: 65% 24% 9%

GLY ALA HIS LEU A6 Y9 L10 A13 D18 P19 L20 F25 F31 P32 E33 R34 K35 E36 K39 V40 A41 T42 Q43 K46 Q50 R56 L63 F66 K70 F74 P75 N76 F77 L78 H82 E83 D86 W87 D88 H92 Y96 R104

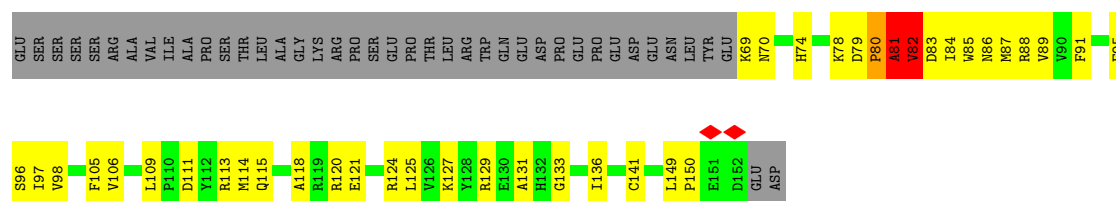
K112 LYS ARG ARG GLU GLN ARG

- Molecule 52: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

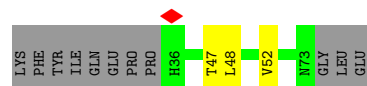
Chain f: 5% 61% 32% 6%



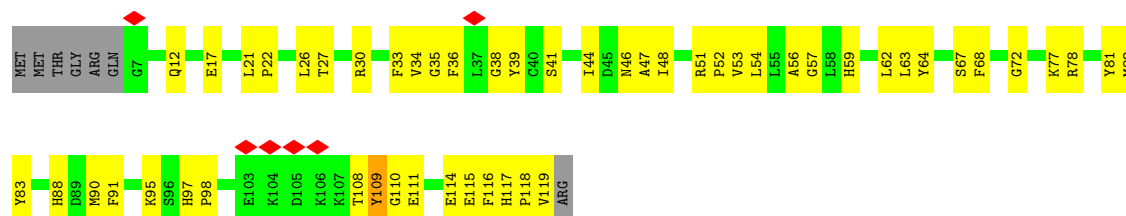
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



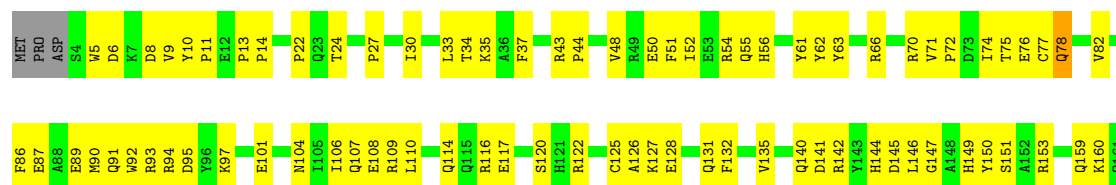
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2

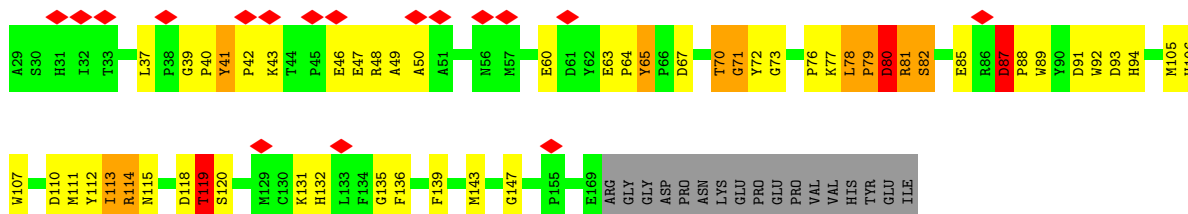


- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

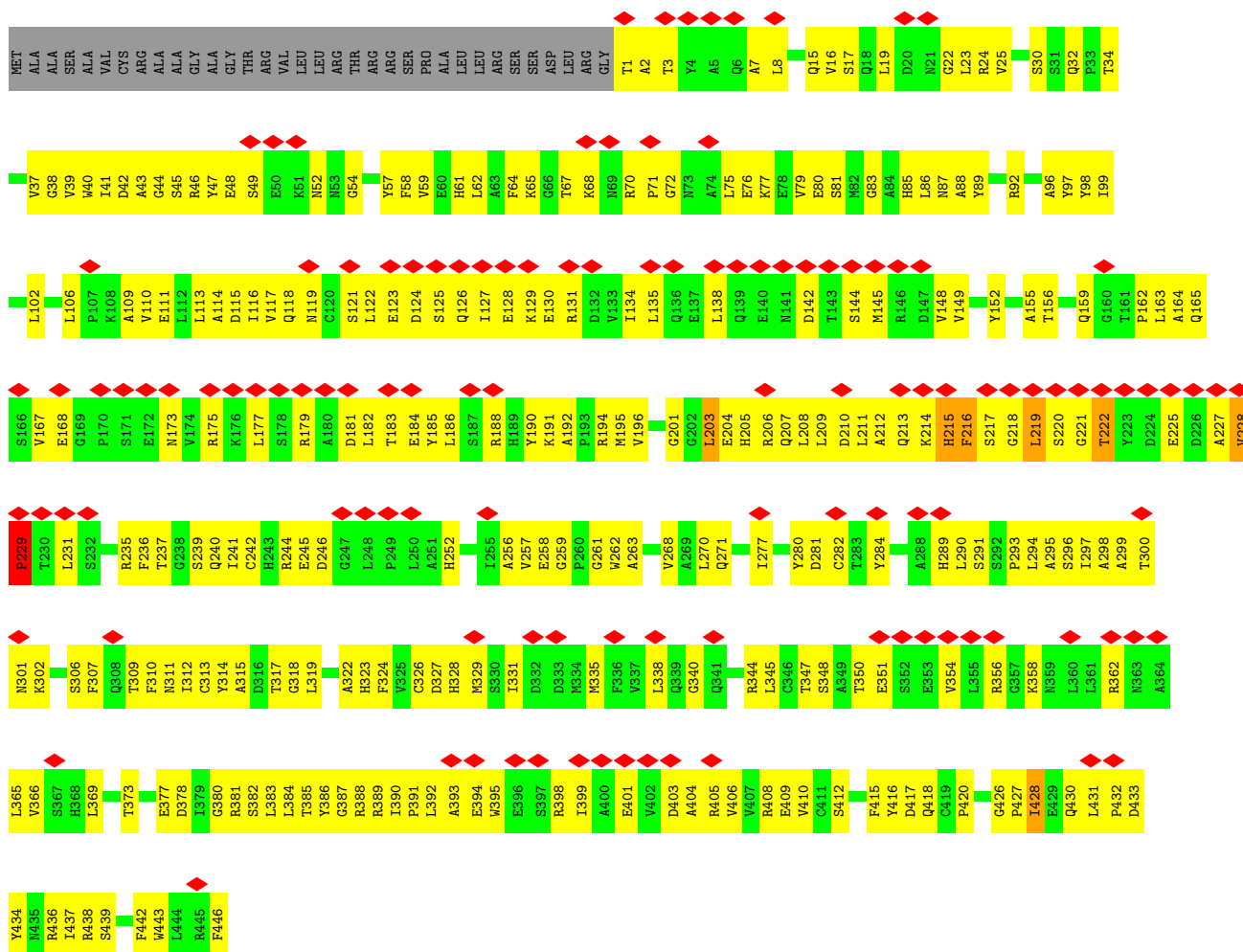




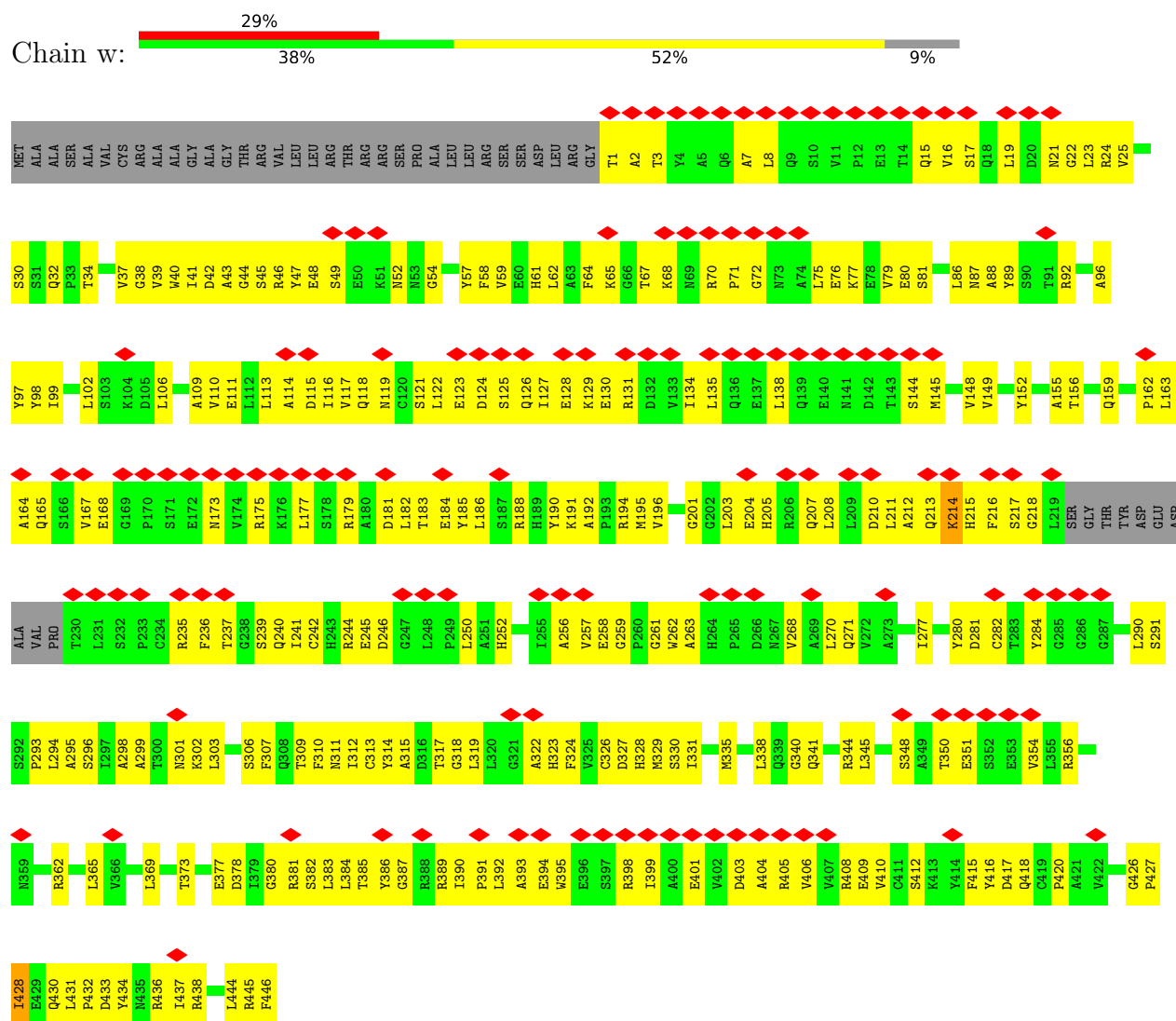
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial

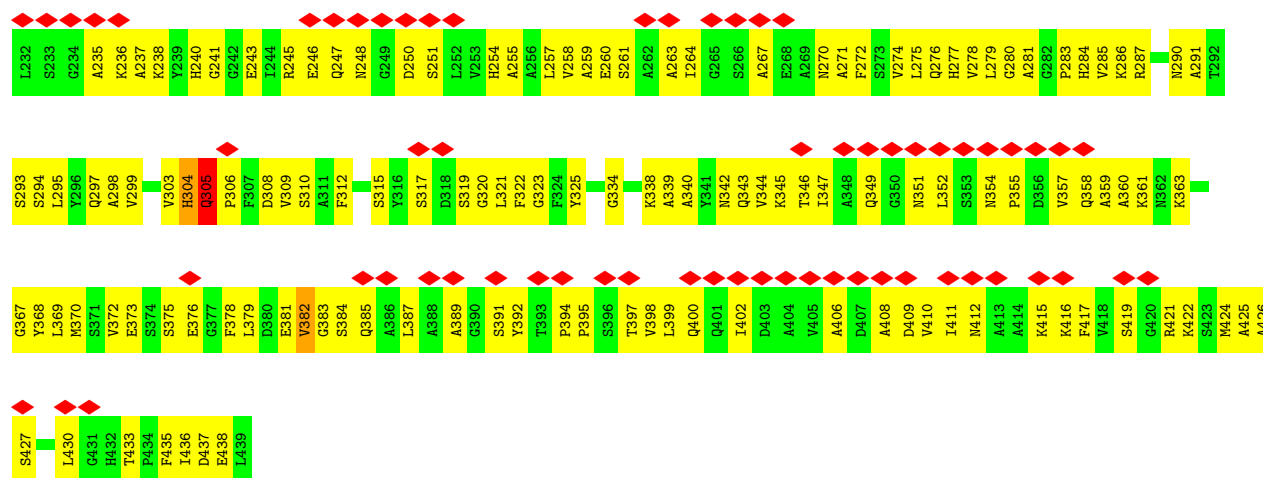


- Molecule 58: Cytochrome b-c1 complex subunit 1, mitochondrial

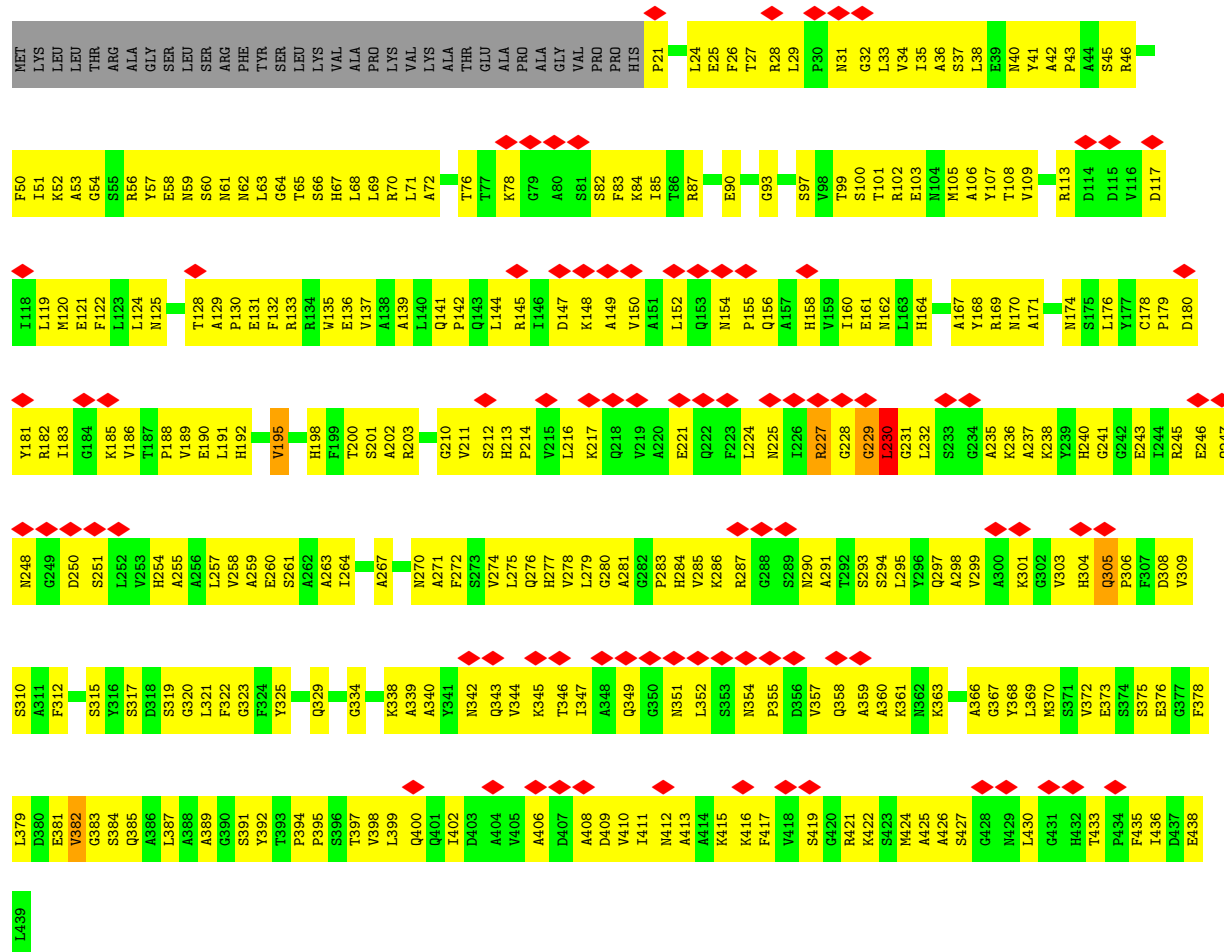


- Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

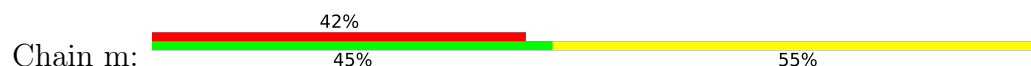


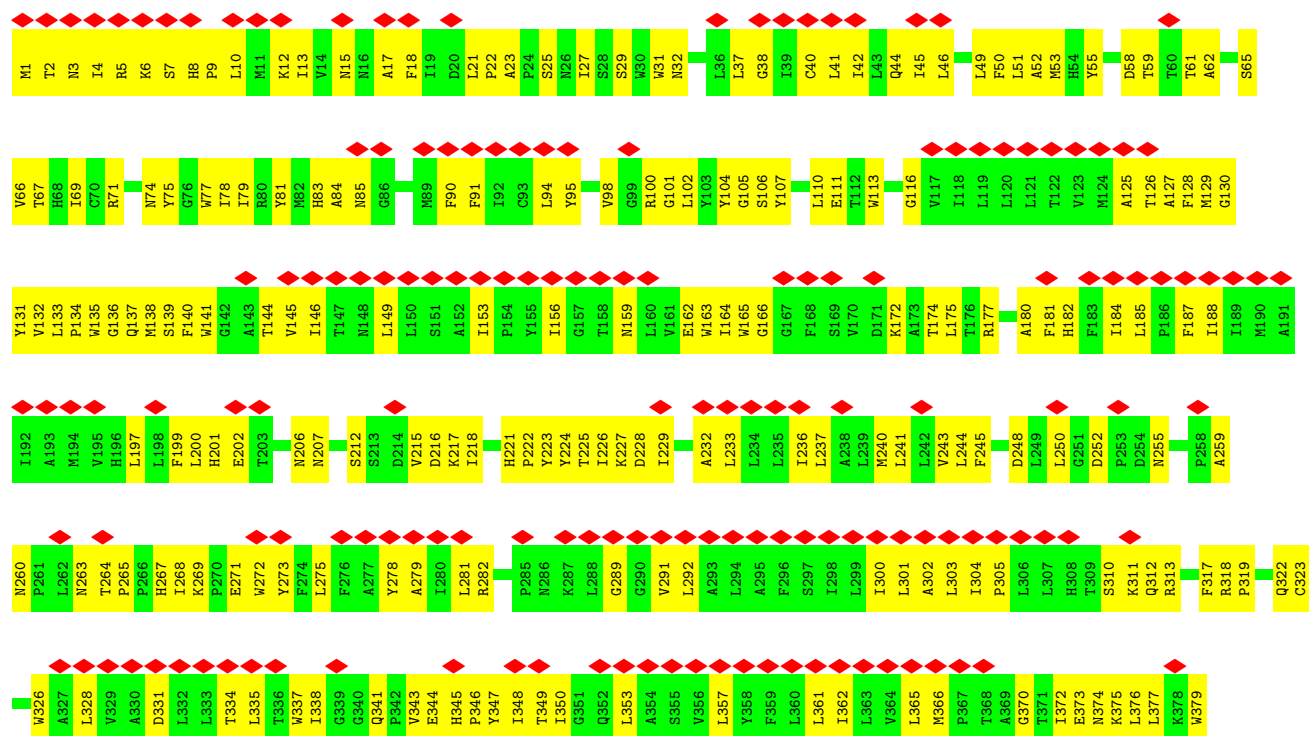


• Molecule 59: Cytochrome b-c1 complex subunit 2, mitochondrial

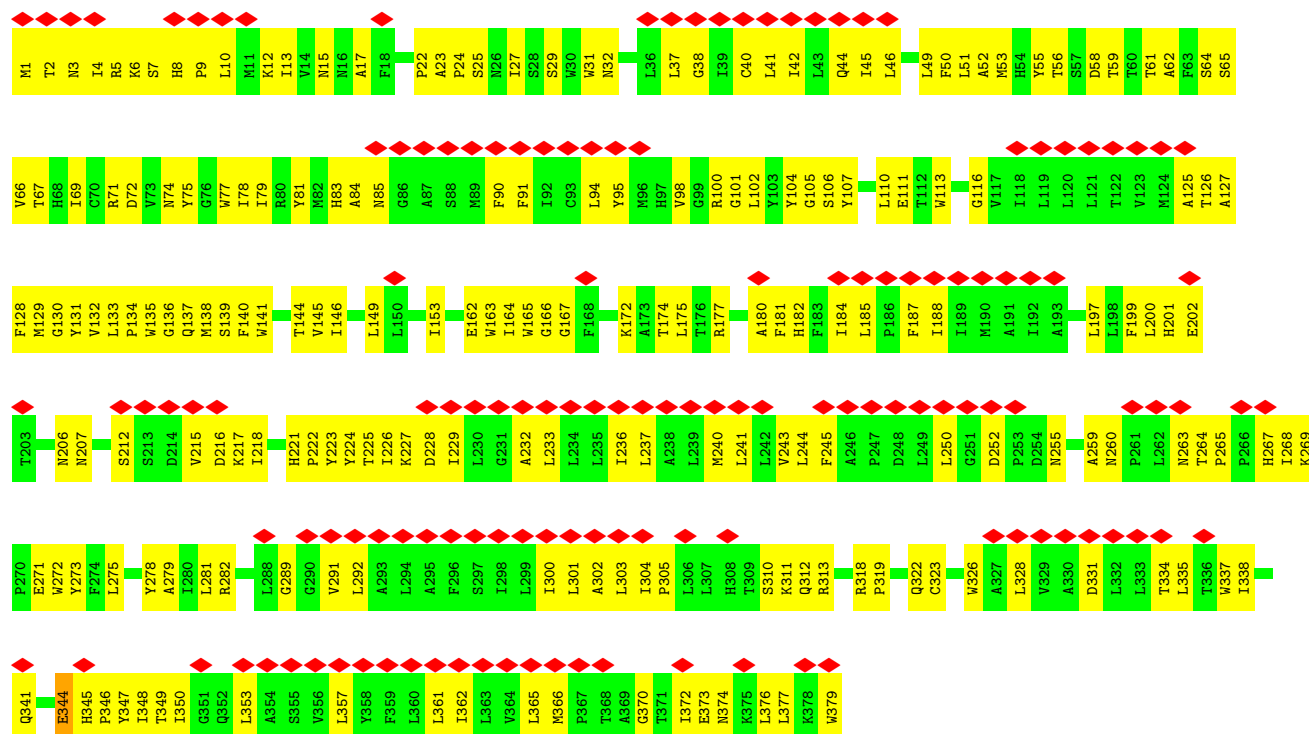


• Molecule 60: Cytochrome b

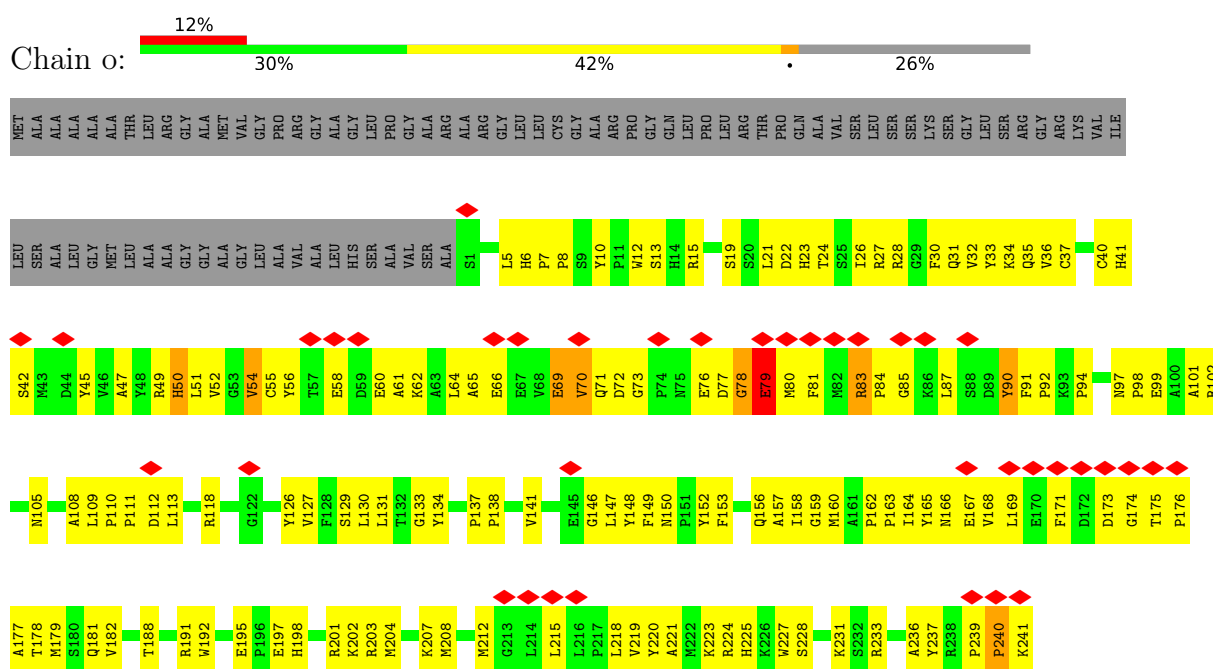




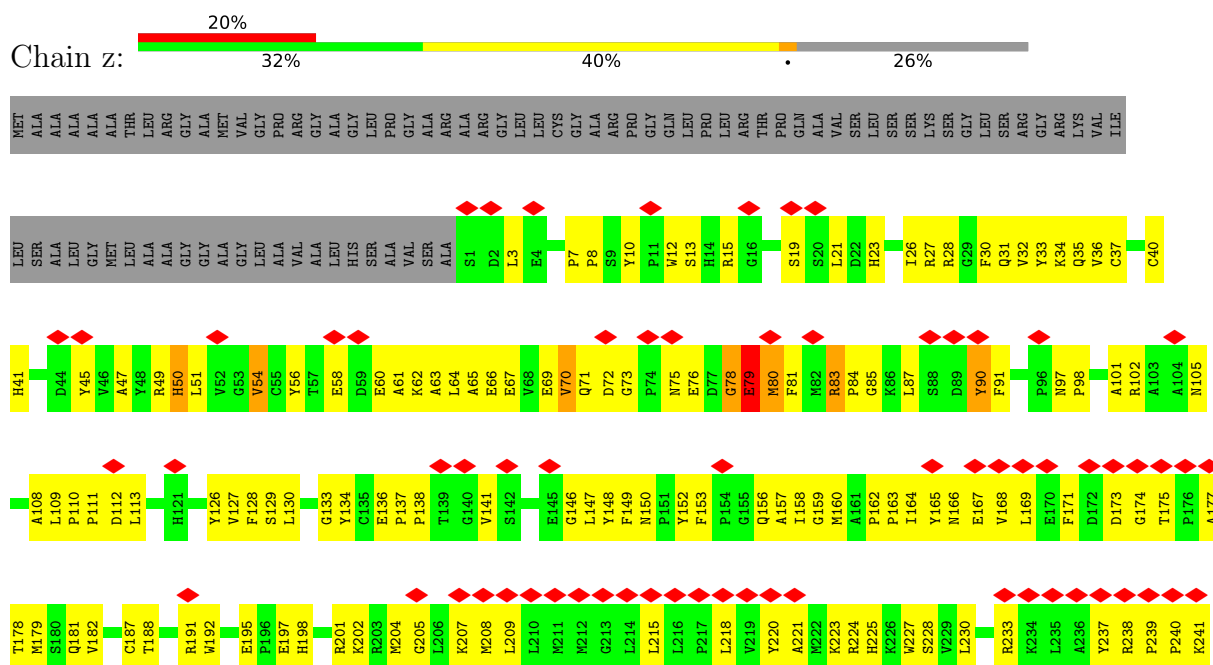
• Molecule 60: Cytochrome b



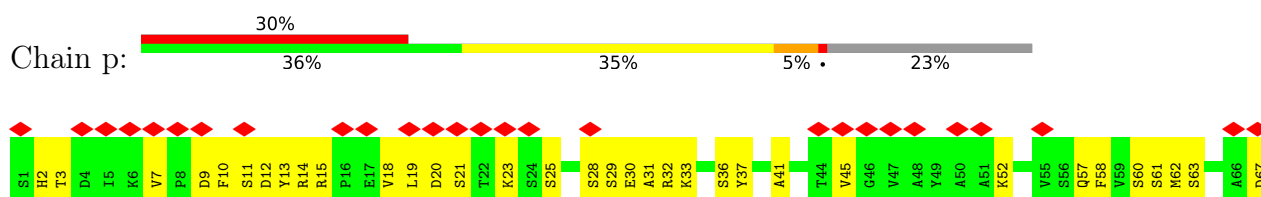
• Molecule 61: Cytochrome c1, heme protein, mitochondrial

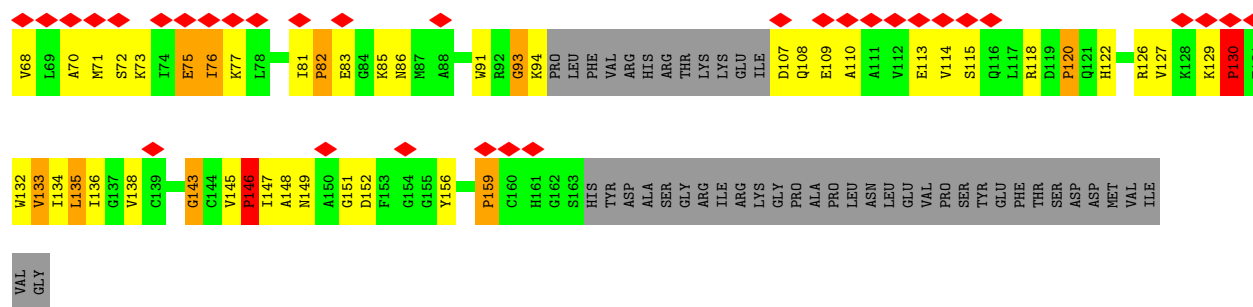


- Molecule 61: Cytochrome c1, heme protein, mitochondrial

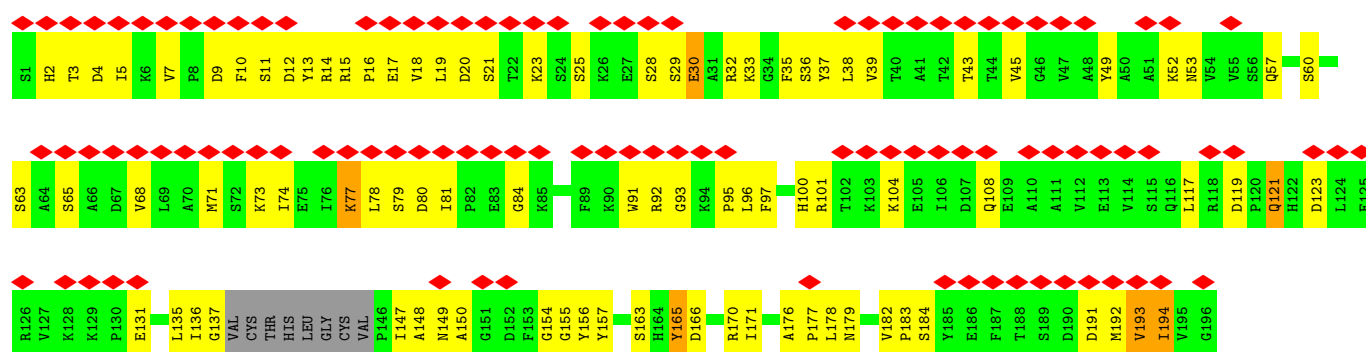


- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial

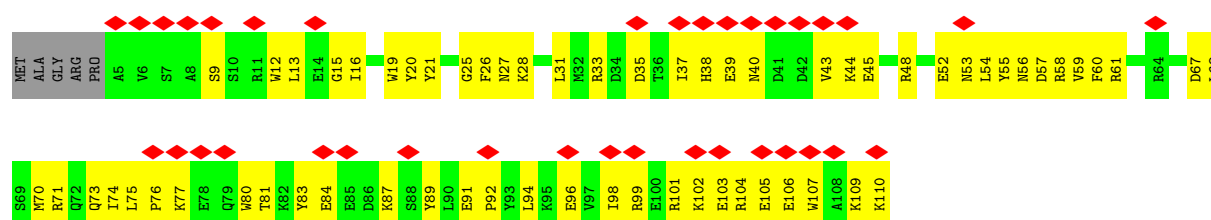




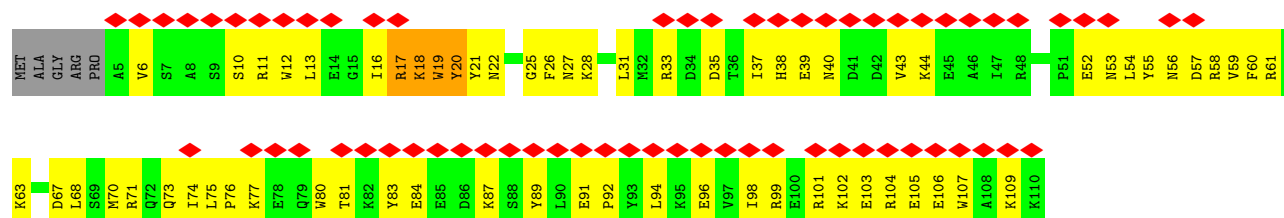
- Molecule 62: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 63: Cytochrome b-c1 complex subunit 7

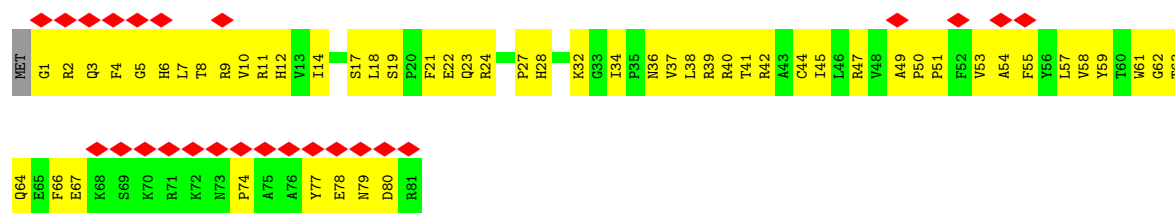


- Molecule 63: Cytochrome b-c1 complex subunit 7

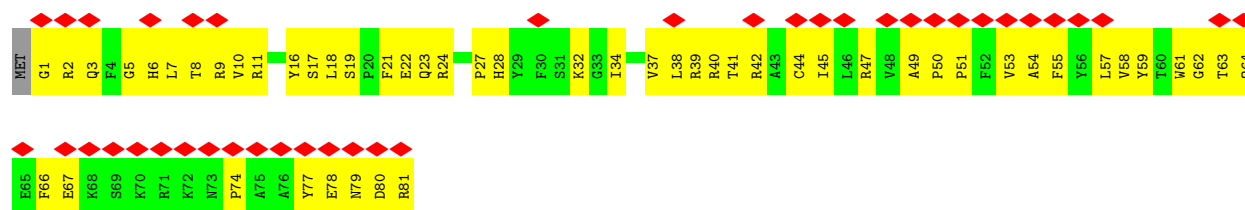


- Molecule 64: Cytochrome b-c1 complex subunit 8

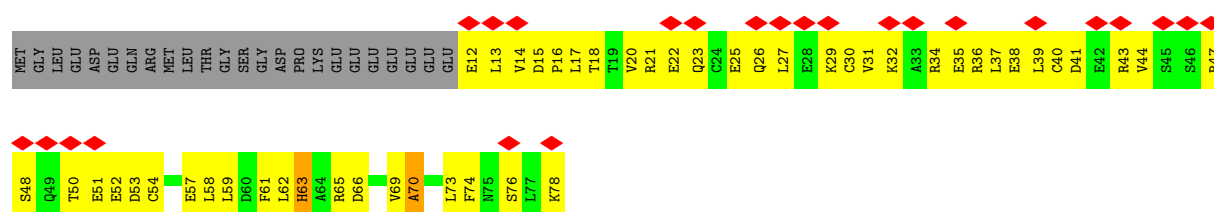
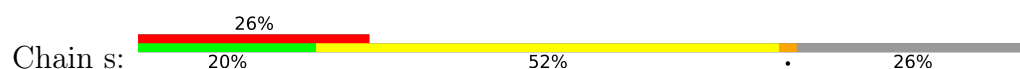




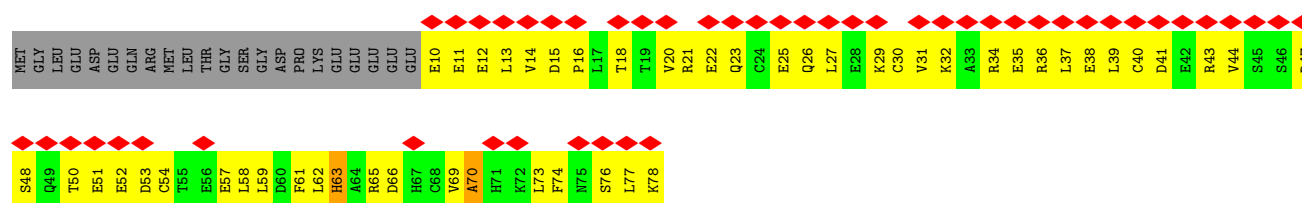
• Molecule 64: Cytochrome b-c1 complex subunit 8



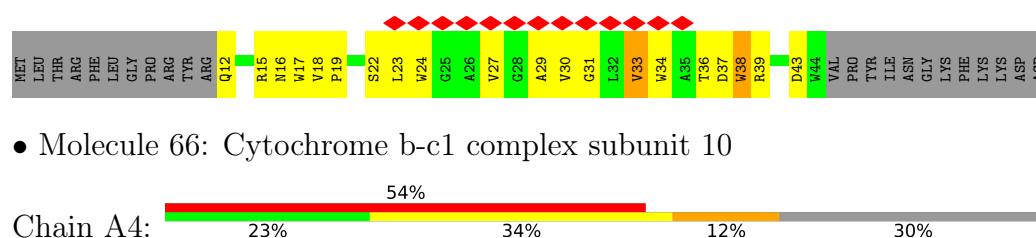
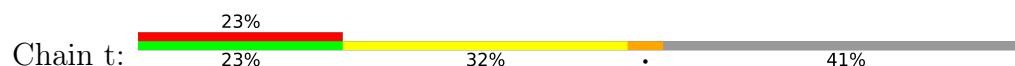
• Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial



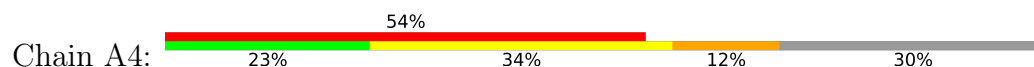
• Molecule 65: Cytochrome b-c1 complex subunit 6, mitochondrial

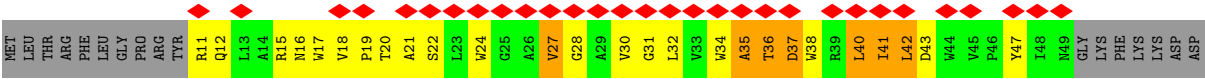


• Molecule 66: Cytochrome b-c1 complex subunit 10

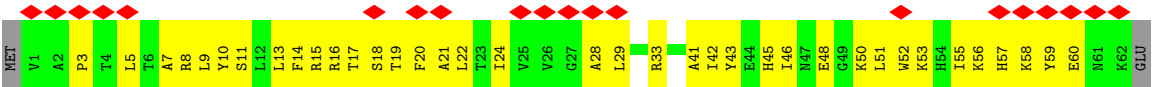


• Molecule 66: Cytochrome b-c1 complex subunit 10

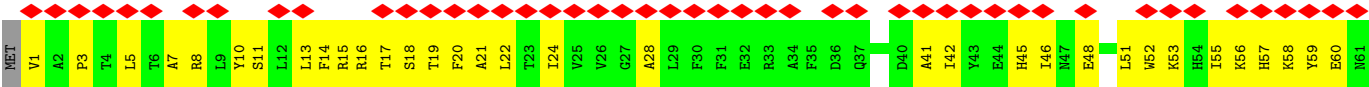
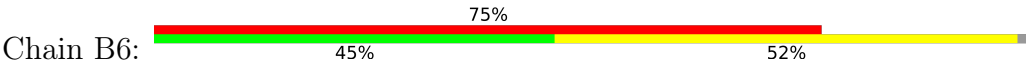




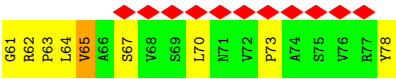
• Molecule 67: Cytochrome b-c1 complex subunit 9



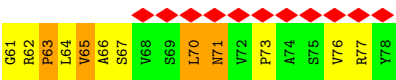
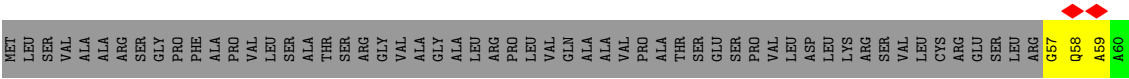
• Molecule 67: Cytochrome b-c1 complex subunit 9



• Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 68: Cytochrome b-c1 complex subunit Rieske, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48729	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	0.398	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.019	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: MG, NAP, 3PE, SF4, CDL, ZN, HEA, CU, HEM, HEC, UQ2, PC1, FMN, FES

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	3	0.54	0/905	0.82	2/1237 (0.2%)
2	1	0.71	1/2575 (0.0%)	1.05	15/3518 (0.4%)
3	9	0.43	0/1618	0.69	0/2207
4	7	0.56	0/1267	0.88	2/1731 (0.1%)
5	4	0.65	1/3674 (0.0%)	0.88	6/5020 (0.1%)
6	5	0.67	0/721	1.04	5/977 (0.5%)
7	6	0.44	0/4893	0.74	2/6661 (0.0%)
8	2	0.74	1/2749 (0.0%)	0.97	5/3744 (0.1%)
9	8	0.46	0/3136	0.80	12/4258 (0.3%)
10	C3	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
11	C1	0.77	0/1868	1.12	10/2544 (0.4%)
12	A9	0.74	0/2212	1.02	7/3025 (0.2%)
13	A7	0.67	0/1229	0.96	3/1658 (0.2%)
14	B4	0.64	0/898	1.02	6/1218 (0.5%)
15	A5	0.72	0/765	1.13	3/1038 (0.3%)
16	A6	0.69	0/698	1.10	6/950 (0.6%)
17	C0	0.68	0/648	1.17	5/877 (0.6%)
18	C2	0.71	0/611	0.94	2/810 (0.2%)
19	B2	0.70	0/451	1.04	3/610 (0.5%)
20	B3	0.75	0/398	1.01	1/546 (0.2%)
21	A0	0.77	0/399	0.98	2/534 (0.4%)
22	A8	0.68	0/345	0.99	1/470 (0.2%)
23	A	0.69	2/5304 (0.0%)	0.95	8/7193 (0.1%)
24	B	0.85	0/3512	1.06	12/4763 (0.3%)
25	C	0.74	0/1777	0.95	3/2420 (0.1%)
26	D	0.93	2/1237 (0.2%)	1.06	1/1676 (0.1%)
27	E	0.88	0/1431	1.11	8/1938 (0.4%)
28	F	0.40	0/191	1.08	2/262 (0.8%)
29	G	0.72	0/1008	0.97	3/1363 (0.2%)
30	H	0.54	0/800	0.80	0/1076
31	I	0.53	0/543	0.99	3/729 (0.4%)
32	J	0.56	0/545	0.68	0/740

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.42	0/667	0.70	0/900
34	L	0.43	0/623	0.75	0/862
35	N	0.48	0/882	0.88	2/1203 (0.2%)
36	O	0.50	0/948	0.83	3/1279 (0.2%)
37	P	0.49	0/723	0.81	1/985 (0.1%)
38	Q	0.44	0/1381	0.82	2/1869 (0.1%)
39	R	0.51	0/2407	0.86	6/3269 (0.2%)
40	S	0.35	0/2348	0.79	5/3198 (0.2%)
41	T	0.45	0/938	0.75	0/1278
42	U	0.39	0/1053	0.85	3/1439 (0.2%)
43	V	0.53	1/1115 (0.1%)	0.79	1/1508 (0.1%)
44	M	0.42	0/651	0.77	0/876
44	W	0.32	0/624	0.73	1/847 (0.1%)
45	X	0.36	0/383	0.71	0/523
46	Y	0.35	0/428	0.72	0/592
47	Z	0.35	0/506	0.85	2/688 (0.3%)
48	a	0.44	0/878	0.71	0/1195
49	b	0.51	0/1058	0.78	0/1434
50	c	0.38	0/632	1.01	3/871 (0.3%)
51	d	0.44	1/726 (0.1%)	0.70	2/992 (0.2%)
52	f	0.32	0/1191	0.73	2/1639 (0.1%)
53	h	0.44	0/679	0.82	1/926 (0.1%)
54	i	0.34	0/286	0.56	0/392
55	j	0.50	0/922	0.85	4/1254 (0.3%)
56	g	0.43	1/1380 (0.1%)	0.77	3/1872 (0.2%)
57	e	0.47	0/888	1.03	9/1234 (0.7%)
58	k	0.44	0/3527	0.67	4/4787 (0.1%)
58	w	0.43	0/3455	0.63	0/4685
59	l	0.41	0/3192	0.62	5/4329 (0.1%)
59	x	0.40	0/3198	0.64	3/4336 (0.1%)
60	m	0.53	0/3108	0.61	0/4252
60	y	0.53	0/3108	0.62	0/4252
61	o	0.49	1/1978 (0.1%)	0.71	4/2684 (0.1%)
61	z	0.51	2/1965 (0.1%)	0.71	5/2669 (0.2%)
62	A1	0.38	0/1124	0.82	2/1538 (0.1%)
62	p	0.44	0/945	1.09	10/1288 (0.8%)
63	A2	0.46	0/926	0.65	0/1243
63	q	0.47	0/935	0.61	0/1253
64	A3	0.43	0/698	0.69	0/944
64	r	0.43	0/704	0.69	0/951
65	B7	0.38	0/571	0.71	0/765
65	s	0.38	0/553	0.67	0/741
66	A4	0.43	0/330	0.81	1/457 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
66	t	0.33	0/272	0.59	1/377 (0.3%)
67	B6	0.36	0/524	0.55	0/707
67	u	0.36	0/524	0.54	0/707
68	B5	0.51	0/149	1.27	0/203
68	v	0.43	0/114	1.43	2/156 (1.3%)
All	All	0.58	20/108789 (0.0%)	0.86	261/147930 (0.2%)

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	3	0	2
2	1	0	3
3	9	0	6
4	7	0	6
5	4	0	9
6	5	0	4
7	6	0	5
8	2	0	10
9	8	0	8
23	A	0	16
24	B	0	4
26	D	0	6
27	E	0	5
30	H	0	2
31	I	0	1
33	K	0	1
34	L	0	1
35	N	0	1
36	O	0	1
37	P	0	3
38	Q	0	2
39	R	0	8
40	S	0	4
41	T	0	2
42	U	0	3
43	V	0	3
44	M	0	3
44	W	0	2
47	Z	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	a	0	1
49	b	0	4
51	d	0	1
52	f	0	3
53	h	0	3
55	j	0	4
56	g	0	2
57	e	0	7
58	k	0	6
58	w	0	2
59	l	0	4
59	x	0	3
60	y	0	1
61	o	0	6
61	z	0	6
62	A1	0	8
62	p	0	5
68	B5	0	4
All	All	0	193

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	161	LEU	CA-C	-9.73	1.38	1.52
51	d	74	PHE	C-N	8.08	1.52	1.33
10	C3	61	HIS	CG-CD2	7.56	1.44	1.35
10	C3	378	HIS	ND1-CE1	7.07	1.39	1.32
23	A	240	ALA	C-N	6.90	1.52	1.33
61	z	70	VAL	CA-C	-6.67	1.47	1.52
10	C3	378	HIS	CE1-NE2	-6.54	1.26	1.32
10	C3	69	MET	SD-CE	-6.28	1.63	1.79
26	D	88	GLY	C-N	-5.90	1.25	1.33
43	V	25	LEU	C-N	-5.70	1.20	1.33
2	1	37	PRO	C-N	-5.62	1.25	1.33
10	C3	376	HIS	ND1-CE1	5.58	1.38	1.32
26	D	190	ALA	C-N	-5.55	1.25	1.33
10	C3	61	HIS	ND1-CE1	5.54	1.38	1.32
10	C3	378	HIS	CG-CD2	5.46	1.41	1.35
61	o	90	TYR	C-N	-5.35	1.23	1.33
56	g	27	PRO	C-N	5.29	1.43	1.33
8	2	157	LEU	C-N	-5.29	1.27	1.33
61	z	90	TYR	C-N	-5.28	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	93	ALA	CA-CB	-5.21	1.46	1.53

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	128	CYS	CA-C-N	-13.74	102.66	119.84
23	A	128	CYS	C-N-CA	-13.74	102.66	119.84
59	x	230	LEU	N-CA-C	12.23	128.22	110.24
9	8	227	PRO	CA-C-N	-10.53	108.02	118.97
9	8	227	PRO	C-N-CA	-10.53	108.02	118.97
10	C3	376	HIS	ND1-CE1-NE2	10.33	118.73	108.40
24	B	420	TYR	N-CA-C	-9.92	94.38	108.07
2	1	176	LEU	CA-C-N	9.82	132.11	119.84
2	1	176	LEU	C-N-CA	9.82	132.11	119.84
26	D	172	GLY	N-CA-C	9.49	126.32	114.37
4	7	80	PRO	CA-N-CD	-8.98	99.42	112.00
17	C0	52	VAL	N-CA-C	8.96	121.26	108.17
2	1	315	PRO	CA-C-N	8.96	131.04	119.84
2	1	315	PRO	C-N-CA	8.96	131.04	119.84
6	5	12	PHE	CA-C-N	-8.87	108.86	122.16
6	5	12	PHE	C-N-CA	-8.87	108.86	122.16
17	C0	81	PHE	CA-C-N	8.74	128.38	119.56
17	C0	81	PHE	C-N-CA	8.74	128.38	119.56
35	N	62	GLU	CA-C-N	8.55	128.69	120.31
35	N	62	GLU	C-N-CA	8.55	128.69	120.31
62	p	146	PRO	N-CA-CB	8.49	111.94	102.60
68	v	62	ARG	CA-C-N	8.44	128.05	118.85
68	v	62	ARG	C-N-CA	8.44	128.05	118.85
24	B	309	ASP	N-CA-C	-8.38	94.42	108.75
6	5	14	VAL	N-CA-C	-8.21	104.49	113.43
2	1	158	GLY	N-CA-C	8.13	126.13	114.67
21	A0	20	ARG	N-CA-C	-8.10	102.53	111.36
10	C3	378	HIS	ND1-CE1-NE2	8.09	116.49	108.40
10	C3	82	LEU	N-CA-C	8.01	122.32	112.23
27	E	140	ARG	CG-CD-NE	7.99	129.57	112.00
50	c	36	PRO	CA-C-N	7.91	145.99	127.00
50	c	36	PRO	C-N-CA	7.91	145.99	127.00
10	C3	56	VAL	N-CA-C	-7.81	103.19	110.53
24	B	292	MET	CA-C-N	7.76	136.36	121.54
24	B	292	MET	C-N-CA	7.76	136.36	121.54
50	c	36	PRO	C-N-CD	-7.74	103.57	120.60
58	k	215	HIS	CA-C-N	7.67	135.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	k	215	HIS	C-N-CA	7.67	135.50	121.70
24	B	293	LEU	N-CA-C	-7.59	94.64	110.80
10	C3	435	GLY	N-CA-C	7.57	125.95	115.27
47	Z	43	ASP	CA-C-N	7.53	127.99	119.93
47	Z	43	ASP	C-N-CA	7.53	127.99	119.93
62	p	159	PRO	N-CA-CB	7.53	110.88	102.60
4	7	123	GLY	N-CA-C	7.52	122.58	113.79
22	A8	27	LEU	N-CA-C	7.43	119.45	111.36
10	C3	330	GLY	N-CA-C	7.41	120.49	112.33
62	p	82	PRO	N-CA-CB	7.25	110.87	103.25
10	C3	376	HIS	CE1-NE2-CD2	-7.23	101.77	109.00
10	C3	332	ILE	N-CA-C	7.15	119.02	109.37
14	B4	76	GLY	CA-C-N	7.14	128.38	120.45
14	B4	76	GLY	C-N-CA	7.14	128.38	120.45
10	C3	9	SER	N-CA-C	7.14	119.78	110.43
14	B4	42	VAL	N-CA-C	-7.11	99.66	108.05
27	E	156	GLY	N-CA-C	-7.07	105.05	115.72
61	o	79	GLU	N-CA-C	7.04	125.80	110.80
10	C3	130	PRO	N-CA-C	-6.93	102.25	110.70
57	e	119	THR	N-CA-C	6.88	125.44	110.80
12	A9	36	HIS	N-CA-C	6.86	122.07	113.43
55	j	22	PRO	N-CA-C	6.83	119.04	110.70
2	1	265	LEU	N-CA-C	-6.81	101.14	111.56
52	f	108	HIS	CA-C-N	6.78	128.31	119.84
52	f	108	HIS	C-N-CA	6.78	128.31	119.84
13	A7	133	GLY	N-CA-C	6.75	129.18	113.18
10	C3	507	GLU	N-CA-C	-6.73	97.92	109.15
16	A6	5	LYS	N-CA-C	6.71	125.09	110.80
36	O	17	VAL	CA-C-N	-6.69	111.70	120.67
36	O	17	VAL	C-N-CA	-6.69	111.70	120.67
2	1	237	PHE	N-CA-C	-6.67	102.99	112.13
5	4	416	ARG	CA-C-N	-6.63	115.01	120.98
5	4	416	ARG	C-N-CA	-6.63	115.01	120.98
14	B4	81	ILE	N-CA-C	6.59	116.73	110.53
40	S	308	GLY	N-CA-C	6.58	121.06	112.25
10	C3	61	HIS	CB-CG-CD2	-6.54	122.70	131.20
9	8	404	ALA	CA-C-N	6.53	131.31	120.86
9	8	404	ALA	C-N-CA	6.53	131.31	120.86
27	E	140	ARG	CB-CG-CD	-6.53	96.28	111.30
57	e	85	GLU	CA-C-N	6.52	134.00	121.54
57	e	85	GLU	C-N-CA	6.52	134.00	121.54
59	x	229	GLY	CA-C-N	6.51	130.37	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	229	GLY	C-N-CA	6.51	130.37	121.05
10	C3	506	GLU	N-CA-C	-6.49	104.20	111.28
10	C3	74	MET	N-CA-C	6.49	118.02	111.07
10	C3	61	HIS	ND1-CE1-NE2	6.47	114.87	108.40
2	1	41	GLY	N-CA-C	6.45	125.50	112.34
62	p	120	PRO	N-CA-CB	6.44	110.02	103.25
27	E	122	VAL	CB-CA-C	-6.33	100.74	111.37
31	I	108	LYS	CA-C-N	6.29	133.56	121.54
31	I	108	LYS	C-N-CA	6.29	133.56	121.54
16	A6	2	SER	N-CA-C	6.26	119.56	109.79
10	C3	10	THR	N-CA-C	-6.25	103.84	112.03
61	z	54	VAL	N-CA-C	-6.23	106.43	112.29
24	B	217	VAL	CA-C-N	-6.22	113.39	121.79
24	B	217	VAL	C-N-CA	-6.22	113.39	121.79
27	E	140	ARG	CA-CB-CG	6.22	126.54	114.10
61	o	54	VAL	N-CA-C	-6.21	106.45	112.29
8	2	308	THR	CA-C-N	-6.21	111.98	121.66
8	2	308	THR	C-N-CA	-6.21	111.98	121.66
59	l	305	GLN	CA-C-N	-6.18	112.73	120.51
59	l	305	GLN	C-N-CA	-6.18	112.73	120.51
2	1	253	GLU	CA-C-N	-6.17	108.97	121.18
2	1	253	GLU	C-N-CA	-6.17	108.97	121.18
62	p	130	PRO	N-CA-CB	6.17	109.73	103.25
14	B4	21	LYS	CA-C-N	6.12	126.30	119.32
14	B4	21	LYS	C-N-CA	6.12	126.30	119.32
10	C3	157	SER	N-CA-C	6.08	118.87	111.82
24	B	218	SER	CA-C-N	-6.06	109.53	121.41
24	B	218	SER	C-N-CA	-6.06	109.53	121.41
10	C3	170	ASN	N-CA-C	6.05	120.73	113.23
11	C1	47	THR	N-CA-C	6.04	119.96	112.59
17	C0	63	LEU	N-CA-C	6.03	119.11	111.69
23	A	309	ASN	N-CA-C	6.02	118.78	110.35
12	A9	8	TYR	N-CA-C	6.00	118.27	110.53
11	C1	207	MET	CA-C-N	5.99	127.33	119.84
11	C1	207	MET	C-N-CA	5.99	127.33	119.84
24	B	363	VAL	CA-C-N	-5.98	105.03	122.38
24	B	363	VAL	C-N-CA	-5.98	105.03	122.38
31	I	106	GLU	N-CA-C	-5.96	98.10	110.80
10	C3	125	GLY	N-CA-C	-5.96	104.19	112.18
62	p	133	VAL	CA-C-N	5.96	132.43	121.70
62	p	133	VAL	C-N-CA	5.96	132.43	121.70
16	A6	44	ARG	CA-C-N	5.96	125.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A6	44	ARG	C-N-CA	5.96	125.98	119.90
10	C3	171	MET	N-CA-C	5.94	120.25	111.87
10	C3	67	PHE	N-CA-C	5.94	119.72	112.23
40	S	89	GLY	CA-C-N	-5.94	109.66	120.94
40	S	89	GLY	C-N-CA	-5.94	109.66	120.94
11	C1	134	ARG	N-CA-C	5.91	123.38	110.80
7	6	431	LEU	CA-C-N	-5.90	113.08	122.17
7	6	431	LEU	C-N-CA	-5.90	113.08	122.17
10	C3	119	GLU	CB-CA-C	-5.89	109.77	116.54
23	A	461	PRO	CA-C-N	5.88	132.76	121.54
23	A	461	PRO	C-N-CA	5.88	132.76	121.54
61	z	90	TYR	CA-C-N	-5.87	108.56	122.31
61	z	90	TYR	C-N-CA	-5.87	108.56	122.31
25	C	93	ASP	CA-C-N	-5.86	115.70	120.98
25	C	93	ASP	C-N-CA	-5.86	115.70	120.98
11	C1	190	GLY	N-CA-C	5.84	117.86	110.38
61	o	90	TYR	CA-C-N	-5.82	108.69	122.31
61	o	90	TYR	C-N-CA	-5.82	108.69	122.31
39	R	80	VAL	CA-C-N	-5.81	115.11	122.43
39	R	80	VAL	C-N-CA	-5.81	115.11	122.43
42	U	120	THR	C-N-CD	-5.81	107.82	120.60
59	l	305	GLN	N-CA-C	5.79	122.61	109.81
42	U	120	THR	CA-C-N	5.78	140.88	127.00
42	U	120	THR	C-N-CA	5.78	140.88	127.00
19	B2	25	GLY	N-CA-C	5.75	119.00	110.60
58	k	203	LEU	CA-C-N	-5.74	110.58	121.54
58	k	203	LEU	C-N-CA	-5.74	110.58	121.54
12	A9	198	PHE	N-CA-C	5.73	117.52	111.28
55	j	22	PRO	CA-C-N	5.72	140.74	127.00
55	j	22	PRO	C-N-CA	5.72	140.74	127.00
40	S	113	ASP	N-CA-C	5.71	117.31	111.14
13	A7	129	ALA	CA-C-N	5.70	126.96	119.84
13	A7	129	ALA	C-N-CA	5.70	126.96	119.84
9	8	228	PRO	CA-C-O	-5.67	111.81	120.03
10	C3	129	TYR	CB-CA-C	-5.66	100.53	109.42
59	l	230	LEU	CA-C-N	5.65	130.89	122.30
59	l	230	LEU	C-N-CA	5.65	130.89	122.30
56	g	27	PRO	CA-C-N	-5.64	109.10	122.31
56	g	27	PRO	C-N-CA	-5.64	109.10	122.31
39	R	175	LYS	CA-C-N	-5.63	113.05	122.17
39	R	175	LYS	C-N-CA	-5.63	113.05	122.17
40	S	196	ASP	N-CA-C	-5.62	101.96	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C1	104	TRP	N-CA-C	5.61	122.76	110.80
61	z	79	GLU	CA-C-N	5.60	132.23	121.54
61	z	79	GLU	C-N-CA	5.60	132.23	121.54
18	C2	20	HIS	N-CA-C	5.58	118.13	111.71
57	e	82	SER	N-CA-C	5.57	122.65	110.80
57	e	80	ASP	CA-C-N	5.56	132.16	121.54
57	e	80	ASP	C-N-CA	5.56	132.16	121.54
5	4	59	ASP	CA-C-N	-5.56	110.92	121.54
5	4	59	ASP	C-N-CA	-5.56	110.92	121.54
23	A	139	LEU	CA-CB-CG	-5.56	96.84	116.30
27	E	86	TYR	CA-CB-CG	-5.55	103.90	113.90
15	A5	82	CYS	CA-C-N	5.53	125.37	119.28
15	A5	82	CYS	C-N-CA	5.53	125.37	119.28
27	E	154	TYR	CA-CB-CG	-5.53	103.95	113.90
21	A0	16	GLU	N-CA-C	5.52	117.38	111.36
12	A9	188	ILE	CB-CA-C	-5.52	104.69	112.14
16	A6	72	ASN	CA-C-N	5.52	125.88	119.47
16	A6	72	ASN	C-N-CA	5.52	125.88	119.47
19	B2	2	GLU	N-CA-C	5.50	122.52	110.80
39	R	133	GLU	CA-C-N	5.50	129.50	121.31
39	R	133	GLU	C-N-CA	5.50	129.50	121.31
10	C3	159	LEU	N-CA-C	-5.48	105.38	111.36
10	C3	245	ILE	N-CA-C	-5.47	104.22	111.05
8	2	85	THR	CB-CA-C	-5.46	108.68	115.89
2	1	252	PRO	N-CA-C	-5.45	105.68	113.47
62	A1	77	LYS	CA-C-N	5.43	131.48	121.70
62	A1	77	LYS	C-N-CA	5.43	131.48	121.70
8	2	157	LEU	CA-C-N	-5.40	113.29	120.63
8	2	157	LEU	C-N-CA	-5.40	113.29	120.63
27	E	170	GLY	C-N-CD	-5.39	102.91	125.00
10	C3	305	PHE	N-CA-C	5.37	118.93	112.38
23	A	121	LEU	CA-CB-CG	-5.33	97.66	116.30
9	8	36	LYS	CA-C-N	5.32	131.27	121.70
9	8	36	LYS	C-N-CA	5.32	131.27	121.70
57	e	87	ASP	CA-C-N	-5.31	114.33	119.90
57	e	87	ASP	C-N-CA	-5.31	114.33	119.90
10	C3	372	TYR	N-CA-C	-5.28	105.42	111.07
2	1	68	ALA	N-CA-C	5.27	117.77	111.71
1	3	2	ASN	CA-C-N	-5.26	113.29	120.44
1	3	2	ASN	C-N-CA	-5.26	113.29	120.44
5	4	119	TYR	CA-CB-CG	-5.25	104.44	113.90
37	P	57	ARG	N-CA-C	-5.25	102.13	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	259	GLY	N-CA-C	-5.25	104.54	112.84
9	8	108	GLY	CA-C-N	-5.24	111.19	122.67
9	8	108	GLY	C-N-CA	-5.24	111.19	122.67
9	8	259	GLY	CA-C-N	5.24	131.12	121.70
9	8	259	GLY	C-N-CA	5.24	131.12	121.70
29	G	155	PRO	CA-C-O	-5.24	112.44	120.03
5	4	227	GLY	N-CA-C	-5.23	106.85	114.90
29	G	154	LYS	CA-C-N	-5.21	113.55	118.97
29	G	154	LYS	C-N-CA	-5.21	113.55	118.97
55	j	22	PRO	C-N-CD	-5.21	109.13	120.60
62	p	75	GLU	N-CA-C	5.21	117.96	111.24
25	C	159	VAL	CB-CA-C	-5.21	108.83	114.35
19	B2	9	GLN	N-CA-C	-5.20	105.51	111.07
10	C3	377	PHE	N-CA-C	5.20	119.47	113.18
24	B	428	GLY	N-CA-C	-5.19	107.83	114.37
43	V	10	MET	N-CA-C	5.19	119.23	112.17
12	A9	99	TRP	N-CA-C	-5.19	105.52	111.07
2	1	236	ILE	N-CA-C	-5.18	107.42	112.29
10	C3	6	TRP	N-CA-C	5.18	119.65	113.23
10	C3	262	SER	N-CA-C	-5.18	106.64	113.17
15	A5	38	ALA	N-CA-C	5.17	117.78	110.50
38	Q	147	ARG	CA-C-N	5.15	139.35	127.00
38	Q	147	ARG	C-N-CA	5.15	139.35	127.00
17	C0	22	ASN	N-CA-C	5.14	117.68	109.81
10	C3	353	LEU	N-CA-C	-5.13	105.77	111.36
18	C2	2	THR	N-CA-C	5.13	116.21	108.46
12	A9	107	ALA	CA-C-N	5.13	125.93	119.98
12	A9	107	ALA	C-N-CA	5.13	125.93	119.98
10	C3	401	SER	N-CA-C	5.12	119.65	113.41
51	d	31	PHE	CA-C-N	5.11	139.26	127.00
51	d	31	PHE	C-N-CA	5.11	139.26	127.00
2	1	204	GLU	CA-C-N	5.11	129.15	120.88
2	1	204	GLU	C-N-CA	5.11	129.15	120.88
23	A	308	ARG	N-CA-C	5.10	119.56	113.23
62	p	75	GLU	CA-C-N	5.10	130.88	121.70
62	p	75	GLU	C-N-CA	5.10	130.88	121.70
44	W	106	LYS	N-CA-C	-5.08	105.83	112.23
10	C3	2	PHE	N-CA-C	-5.08	105.64	111.07
11	C1	165	VAL	CA-C-N	5.07	126.18	119.84
11	C1	165	VAL	C-N-CA	5.07	126.18	119.84
28	F	97	MET	CA-C-N	5.07	125.51	120.14
28	F	97	MET	C-N-CA	5.07	125.51	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	A4	37	ASP	CB-CA-C	-5.06	109.76	115.79
6	5	90	VAL	CA-C-N	5.06	131.21	121.54
6	5	90	VAL	C-N-CA	5.06	131.21	121.54
10	C3	378	HIS	CB-CG-CD2	-5.06	124.62	131.20
10	C3	70	VAL	N-CA-C	5.05	115.48	110.23
10	C3	378	HIS	N-CA-C	-5.05	106.28	112.90
11	C1	66	THR	N-CA-C	-5.05	107.78	114.04
36	O	75	ASP	N-CA-C	5.05	116.41	108.23
56	g	76	GLU	N-CA-C	-5.04	103.39	110.50
66	t	33	VAL	N-CA-C	-5.03	105.49	110.62
53	h	82	VAL	N-CA-C	5.02	119.79	109.34
11	C1	12	ALA	N-CA-C	5.02	117.44	109.96
57	e	113	ILE	N-CA-C	-5.02	107.86	112.83
20	B3	35	GLN	N-CA-C	5.00	119.14	113.19

There are no chirality outliers.

All (193) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	125	SER	Peptide
2	1	195	ARG	Peptide
2	1	66	SER	Mainchain
8	2	106	LEU	Peptide
8	2	112	HIS	Peptide
8	2	147	PRO	Peptide
8	2	193	VAL	Peptide
8	2	220	MET	Peptide
8	2	24	SER	Peptide
8	2	327	PRO	Peptide
8	2	336	MET	Peptide
8	2	337	LEU	Peptide
8	2	45	MET	Peptide
1	3	42	ASP	Peptide
1	3	69	ILE	Peptide
5	4	20	ASN	Peptide
5	4	226	ALA	Peptide
5	4	306	PRO	Peptide
5	4	419	TYR	Peptide
5	4	48	ASN	Peptide
5	4	56	PHE	Peptide
5	4	60	SER	Peptide
5	4	64	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	4	74	PRO	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
6	5	93	LEU	Peptide
7	6	30	SER	Peptide
7	6	351	ASN	Peptide
7	6	522	PHE	Peptide
7	6	64	SER	Peptide
7	6	65	ASN	Peptide
4	7	137	SER	Peptide
4	7	170	GLU	Peptide
4	7	24	PRO	Peptide
4	7	25	SER	Peptide
4	7	26	PRO	Peptide
4	7	72	THR	Peptide
9	8	102	MET	Peptide
9	8	203	ALA	Peptide
9	8	204	TYR	Peptide
9	8	208	GLU	Peptide
9	8	228	PRO	Peptide
9	8	260	ALA	Peptide
9	8	306	GLY	Peptide
9	8	404	ALA	Peptide
3	9	109	PRO	Peptide
3	9	150	GLU	Peptide
3	9	167	LYS	Peptide
3	9	228	ALA	Peptide
3	9	75	LYS	Peptide
3	9	91	GLY	Peptide
23	A	124	HIS	Peptide
23	A	127	ASP	Peptide
23	A	128	CYS	Peptide
23	A	143	SER	Peptide
23	A	147	GLY	Peptide
23	A	236	TYR	Peptide
23	A	253	VAL	Peptide
23	A	259	SER	Peptide
23	A	274	LEU	Peptide
23	A	308	ARG	Peptide
23	A	460	HIS	Peptide
23	A	549	GLY	Peptide

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Mol	Chain	Res	Type	Group
23	A	564	CYS	Peptide
23	A	689	LEU	Peptide
23	A	691	ILE	Peptide
23	A	98	LYS	Peptide
62	A1	119	ASP	Peptide
62	A1	121	GLN	Peptide
62	A1	123	ASP	Peptide
62	A1	163	SER	Peptide
62	A1	165	TYR	Peptide
62	A1	177	PRO	Peptide
62	A1	184	SER	Peptide
62	A1	193	VAL	Peptide
24	B	219	GLY	Peptide
24	B	272	THR	Peptide
24	B	290	GLY	Peptide
24	B	309	ASP	Peptide
68	B5	58	GLN	Peptide
68	B5	61	GLY	Peptide
68	B5	63	PRO	Peptide
68	B5	71	ASN	Peptide
26	D	113	PHE	Peptide
26	D	126	ALA	Peptide
26	D	161	GLY	Peptide
26	D	184	PRO	Peptide
26	D	186	CYS	Peptide
26	D	188	PRO	Peptide
27	E	106	TYR	Peptide
27	E	107	PRO	Peptide
27	E	108	SER	Peptide
27	E	75	SER	Peptide
27	E	85	ASN	Peptide
30	H	84	GLU	Peptide
30	H	94	PRO	Peptide
31	I	69	ILE	Peptide
33	K	40	ARG	Peptide
34	L	40	LYS	Peptide
44	M	24	LYS	Peptide
44	M	37	MET	Peptide
44	M	63	PRO	Peptide
35	N	17	CYS	Peptide
36	O	42	GLU	Peptide
37	P	109	ASP	Peptide

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Mol	Chain	Res	Type	Group
37	P	44	GLY	Peptide
37	P	62	GLU	Peptide
38	Q	39	PRO	Peptide
38	Q	91	TYR	Peptide
39	R	154	GLN	Peptide
39	R	221	ARG	Peptide
39	R	253	ILE	Peptide
39	R	271	TYR	Peptide
39	R	324	THR	Peptide
39	R	333	PRO	Peptide
39	R	355	ARG	Peptide
39	R	78	SER	Peptide
40	S	311	GLN	Peptide
40	S	337	ASP	Peptide
40	S	66	ALA	Peptide
40	S	67	GLU	Peptide
41	T	105	THR	Peptide
41	T	83	LYS	Peptide
42	U	117	LEU	Peptide
42	U	118	SER	Peptide
42	U	47	LYS	Peptide
43	V	142	TRP	Peptide
43	V	24	ASN	Peptide
43	V	72	MET	Peptide
44	W	128	PHE	Peptide
44	W	154	VAL	Peptide
47	Z	23	LYS	Peptide
47	Z	63	PHE	Peptide
48	a	26	SER	Peptide
49	b	110	TRP	Peptide
49	b	129	PRO	Peptide
49	b	132	ASN	Peptide
49	b	134	GLU	Peptide
51	d	18	ASP	Peptide
57	e	107	TRP	Peptide
57	e	60	GLU	Peptide
57	e	65	TYR	Peptide
57	e	79	PRO	Peptide
57	e	80	ASP	Peptide
57	e	81	ARG	Peptide
57	e	87	ASP	Peptide
52	f	109	PRO	Peptide

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Mol	Chain	Res	Type	Group
52	f	131	GLU	Peptide
52	f	150	ARG	Peptide
56	g	160	LYS	Peptide
56	g	78	GLN	Peptide
53	h	133	GLY	Peptide
53	h	80	PRO	Peptide
53	h	81	ALA	Peptide
55	j	109	TYR	Peptide
55	j	110	GLY	Peptide
55	j	21	LEU	Peptide
55	j	54	LEU	Peptide
58	k	212	ALA	Peptide
58	k	216	PHE	Peptide
58	k	222	THR	Peptide
58	k	228	VAL	Peptide
58	k	229	PRO	Peptide
58	k	428	ILE	Peptide
59	l	227	ARG	Peptide
59	l	229	GLY	Mainchain
59	l	231	GLY	Peptide
59	l	304	HIS	Peptide
61	o	240	PRO	Peptide
61	o	50	HIS	Peptide
61	o	69	GLU	Mainchain
61	o	78	GLY	Peptide
61	o	79	GLU	Peptide
61	o	83	ARG	Peptide
62	p	133	VAL	Peptide
62	p	135	LEU	Peptide
62	p	143	GLY	Peptide
62	p	76	ILE	Peptide
62	p	77	LYS	Peptide
58	w	212	ALA	Peptide
58	w	428	ILE	Peptide
59	x	227	ARG	Peptide
59	x	229	GLY	Mainchain
59	x	230	LEU	Peptide
60	y	344	GLU	Peptide
61	z	240	PRO	Peptide
61	z	50	HIS	Peptide
61	z	69	GLU	Peptide,Mainchain
61	z	78	GLY	Peptide

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Mol	Chain	Res	Type	Group
61	z	83	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	882	0	915	69	0
2	1	2503	0	2617	290	0
3	9	1579	0	1558	103	0
4	7	1235	0	1182	109	0
5	4	3577	0	3674	238	0
6	5	712	0	742	64	0
7	6	4766	0	4897	231	0
8	2	2681	0	2823	191	0
9	8	3065	0	2801	167	0
10	C3	4025	0	4003	89	0
11	C1	1822	0	1834	74	0
12	A9	2125	0	2046	52	0
13	A7	1195	0	1183	34	0
14	B4	878	0	868	20	0
15	A5	748	0	728	26	0
16	A6	671	0	645	28	0
17	C0	628	0	582	22	0
18	C2	598	0	612	15	0
19	B2	441	0	439	15	0
20	B3	384	0	366	13	0
21	A0	386	0	388	8	0
22	A8	335	0	352	13	0
23	A	5218	0	5232	308	0
24	B	3422	0	3345	252	0
25	C	1726	0	1677	108	0
26	D	1206	0	1204	86	0
27	E	1401	0	1353	108	0
28	F	186	0	139	15	0
29	G	985	0	976	53	0
30	H	780	0	753	65	0
31	I	535	0	514	41	0
32	J	530	0	503	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	K	656	0	647	34	0
34	L	602	0	592	43	0
35	N	862	0	868	41	0
36	O	925	0	907	53	0
37	P	702	0	670	42	0
38	Q	1345	0	1282	78	0
39	R	2349	0	2264	135	0
40	S	2299	0	2027	135	0
41	T	923	0	865	50	0
42	U	1019	0	900	50	0
43	V	1087	0	1037	69	0
44	M	642	0	642	54	0
44	W	616	0	579	27	0
45	X	372	0	314	14	0
46	Y	409	0	318	17	0
47	Z	493	0	395	27	0
48	a	857	0	765	34	0
49	b	1032	0	954	55	0
50	c	617	0	492	34	0
51	d	710	0	521	24	0
52	f	1156	0	892	49	0
53	h	658	0	584	43	0
54	i	277	0	240	2	0
55	j	892	0	835	50	0
56	g	1351	0	1262	79	0
57	e	864	0	567	39	0
58	k	3454	0	3350	279	0
58	w	3385	0	3296	253	0
59	l	3135	0	3112	263	0
59	x	3141	0	3123	282	0
60	m	3011	0	3077	217	0
60	y	3011	0	3077	204	0
61	o	1919	0	1870	180	0
61	z	1906	0	1841	153	0
62	A1	1117	0	808	75	0
62	p	938	0	733	74	0
63	A2	907	0	893	114	0
63	q	916	0	911	70	0
64	A3	676	0	668	54	0
64	r	682	0	679	64	0
65	B7	566	0	542	55	0
65	s	548	0	530	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	A4	318	0	314	54	0
66	t	262	0	250	38	0
67	B6	511	0	518	38	0
67	u	511	0	518	52	0
68	B5	148	0	154	22	0
68	v	114	0	107	10	0
69	2	46	0	66	8	0
69	3	47	0	71	8	0
69	Q	46	0	66	4	0
69	S	47	0	71	5	0
69	j	39	0	55	3	0
70	1	51	0	82	5	0
70	2	41	0	59	5	0
70	4	41	0	59	1	0
70	B	51	0	82	9	0
70	j	46	0	69	3	0
71	9	4	0	0	0	0
71	A	4	0	0	2	0
71	m	4	0	0	0	0
72	6	64	0	72	12	0
72	J	58	0	60	6	0
72	b	82	0	114	4	0
73	8	31	0	19	10	0
74	8	8	0	0	0	0
74	A	16	0	0	6	0
74	D	8	0	0	1	0
74	E	16	0	0	1	0
75	C1	2	0	0	0	0
75	C3	1	0	0	0	0
76	C3	120	0	108	4	0
77	C1	1	0	0	0	0
78	A5	1	0	0	0	0
78	I	1	0	0	0	0
79	R	48	0	23	4	0
80	m	86	0	60	20	0
80	y	86	0	60	19	0
81	o	43	0	32	9	0
81	z	43	0	32	9	0
82	A2	23	0	26	24	0
All	All	107321	0	104027	6050	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 29.

All (6050) 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)
1:3:84:LEU:HD21	2:1:309:ILE:CD1	1.22	1.60
2:1:172:MET:HE1	2:1:176:LEU:CD1	0.98	1.45
2:1:172:MET:CE	2:1:176:LEU:HD12	0.89	1.35
23:A:355:LYS:HD2	23:A:530:TYR:CE1	1.61	1.35
2:1:79:LEU:CD1	2:1:222:LEU:HD22	1.55	1.34
1:3:84:LEU:CD2	2:1:309:ILE:CD1	2.06	1.33
31:I:109:THR:CB	31:I:119:PHE:O	1.77	1.33
66:A4:37:ASP:CG	66:A4:38:TRP:H	1.34	1.31
2:1:176:LEU:HB2	2:1:177:PRO:CD	1.61	1.31
63:A2:11:ARG:HG3	82:A2:201:UQ2:O4	1.31	1.28
63:A2:17:ARG:CD	82:A2:201:UQ2:H2M2	1.61	1.28
66:A4:40:LEU:O	66:A4:41:ILE:HG12	1.12	1.27
2:1:233:MET:HA	2:1:236:ILE:CG2	1.67	1.25
31:I:109:THR:CB	31:I:120:ARG:HA	1.67	1.25
63:A2:16:ILE:HD13	63:A2:19:TRP:CZ3	1.71	1.24
63:A2:16:ILE:HG21	63:A2:19:TRP:CZ3	1.73	1.24
40:S:196:ASP:OD1	40:S:246:TYR:CB	1.85	1.23
64:A3:37:VAL:O	64:A3:41:THR:HG23	1.37	1.23
63:A2:16:ILE:CG2	63:A2:19:TRP:CE3	2.22	1.22
1:3:84:LEU:CD2	2:1:309:ILE:HD11	1.65	1.22
24:B:61:TRP:CD1	24:B:62:LYS:O	1.93	1.20
2:1:71:PHE:CZ	2:1:215:TYR:CE1	1.93	1.19
40:S:196:ASP:OD1	40:S:246:TYR:HB3	1.39	1.18
1:3:88:LEU:HD11	2:1:309:ILE:HG21	1.20	1.16
4:7:78:GLN:O	4:7:80:PRO:HD3	1.47	1.15
66:A4:40:LEU:O	66:A4:41:ILE:CG1	1.94	1.14
2:1:176:LEU:HB2	2:1:177:PRO:HD2	1.26	1.14
2:1:72:ILE:HG22	2:1:76:ILE:HD11	1.23	1.13
40:S:199:VAL:CB	40:S:200:PRO:CD	2.27	1.12
31:I:109:THR:CB	31:I:120:ARG:CA	2.28	1.12
1:3:84:LEU:CD2	2:1:309:ILE:HD13	1.75	1.12
3:9:224:SER:OG	3:9:226:GLU:OE2	1.65	1.12
2:1:176:LEU:CB	2:1:177:PRO:CD	2.25	1.11
2:1:172:MET:HE2	2:1:176:LEU:HD12	1.25	1.11
23:A:310:GLU:OE2	23:A:311:LYS:NZ	1.85	1.09
39:R:328:ILE:HG22	39:R:329:LEU:H	1.03	1.09
63:A2:17:ARG:HD3	82:A2:201:UQ2:CM2	1.82	1.09
2:1:79:LEU:HD12	2:1:222:LEU:HD22	1.27	1.09
23:A:355:LYS:CD	23:A:530:TYR:HE1	1.64	1.09
2:1:245:THR:OG1	2:1:255:TYR:CE1	2.04	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:61:TRP:CD1	24:B:62:LYS:N	2.21	1.08
41:T:48:SER:CB	41:T:52:GLY:N	2.16	1.08
1:3:49:LEU:HD23	2:1:126:LYS:NZ	1.68	1.08
23:A:127:ASP:OD2	23:A:175:ARG:NH1	1.86	1.08
60:m:156:ILE:HG22	66:A4:38:TRP:HE1	1.17	1.08
41:T:48:SER:CB	41:T:52:GLY:H	1.67	1.08
63:A2:17:ARG:HD2	82:A2:201:UQ2:H2M2	1.27	1.07
63:A2:16:ILE:CG2	63:A2:19:TRP:CZ3	2.36	1.07
1:3:49:LEU:CD2	2:1:129:LEU:HD21	1.84	1.06
2:1:172:MET:HE1	2:1:176:LEU:HD11	1.35	1.05
2:1:232:ILE:O	2:1:236:ILE:HG22	1.56	1.05
1:3:49:LEU:HD21	2:1:129:LEU:CD2	1.84	1.05
66:A4:40:LEU:HG	66:A4:41:ILE:N	1.59	1.05
56:g:91:GLN:NE2	56:g:95:ASP:OD2	1.90	1.04
2:1:79:LEU:HD11	2:1:222:LEU:HD22	1.37	1.03
63:A2:17:ARG:HD3	82:A2:201:UQ2:H2M2	1.33	1.03
61:o:7:PRO:HG2	61:o:126:TYR:HA	1.40	1.03
2:1:176:LEU:HB2	2:1:177:PRO:HD3	1.38	1.02
66:t:36:THR:CG2	66:t:38:TRP:CD1	2.43	1.02
61:z:7:PRO:HG2	61:z:126:TYR:HA	1.40	1.02
23:A:355:LYS:HB2	23:A:530:TYR:OH	1.60	1.02
66:A4:40:LEU:CG	66:A4:41:ILE:H	1.71	1.02
39:R:328:ILE:CG2	39:R:329:LEU:H	1.72	1.01
60:m:156:ILE:HG22	66:A4:38:TRP:NE1	1.74	1.01
63:A2:16:ILE:HG21	63:A2:19:TRP:CE3	1.89	1.01
40:S:196:ASP:OD1	40:S:246:TYR:HB2	1.59	1.01
5:4:278:ARG:H	7:6:546:GLN:HE22	1.07	1.01
8:2:85:THR:HG22	30:H:19:THR:CG2	1.91	1.01
2:1:176:LEU:CB	2:1:177:PRO:HD3	1.88	1.00
66:A4:40:LEU:CG	66:A4:41:ILE:N	2.23	1.00
58:k:213:GLN:HG3	58:k:214:LYS:HG3	1.42	1.00
58:k:215:HIS:HB2	58:k:216:PHE:HB2	1.42	0.99
61:z:239:PRO:HB2	61:z:241:LYS:HB3	1.44	0.99
66:A4:37:ASP:CG	66:A4:38:TRP:N	2.09	0.99
2:1:72:ILE:CG2	2:1:76:ILE:HD11	1.91	0.98
2:1:157:SER:OG	2:1:168:THR:HG21	1.60	0.98
63:A2:16:ILE:CD1	63:A2:19:TRP:CZ3	2.46	0.98
23:A:355:LYS:HD2	23:A:530:TYR:HE1	0.82	0.98
61:o:239:PRO:HB2	61:o:241:LYS:HB3	1.44	0.98
39:R:170:LEU:O	39:R:328:ILE:HD12	1.62	0.98
63:A2:10:SER:O	82:A2:201:UQ2:CM5	2.11	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:75:CYS:SG	23:A:76:ARG:N	2.37	0.98
26:D:99:MET:HG2	26:D:106:MET:HB2	1.46	0.98
66:A4:40:LEU:HG	66:A4:41:ILE:H	0.85	0.97
4:7:28:TYR:CE2	4:7:83:TRP:HD1	1.83	0.97
29:G:57:GLU:OE2	36:O:16:SER:OG	1.82	0.97
4:7:28:TYR:CE2	4:7:83:TRP:CD1	2.51	0.97
1:3:49:LEU:HD21	2:1:129:LEU:HD21	0.98	0.96
59:l:59:ASN:H	59:l:62:ASN:HB3	1.26	0.96
2:1:172:MET:CE	2:1:176:LEU:CD1	1.81	0.96
63:A2:17:ARG:CD	82:A2:201:UQ2:CM2	2.42	0.96
24:B:266:ARG:NH1	70:B:501:3PE:O22	1.99	0.95
2:1:316:PRO:HG2	43:V:57:ARG:HE	1.28	0.95
39:R:328:ILE:HG22	39:R:329:LEU:N	1.76	0.95
40:S:199:VAL:CB	40:S:200:PRO:HD3	1.92	0.95
59:x:59:ASN:H	59:x:62:ASN:HB3	1.27	0.95
2:1:233:MET:HA	2:1:236:ILE:HG23	1.48	0.95
27:E:171:PRO:HB2	27:E:200:GLU:OE2	1.67	0.95
63:A2:16:ILE:HG21	63:A2:19:TRP:HZ3	1.31	0.95
2:1:79:LEU:CD1	2:1:222:LEU:CD2	2.44	0.95
2:1:71:PHE:HZ	2:1:215:TYR:CE1	1.81	0.95
52:f:136:GLU:OE2	52:f:164:PRO:CB	2.14	0.95
63:A2:16:ILE:HG23	63:A2:19:TRP:CE3	2.01	0.95
66:t:36:THR:CG2	66:t:38:TRP:HD1	1.77	0.94
2:1:232:ILE:O	2:1:236:ILE:CG2	2.15	0.94
24:B:61:TRP:NE1	24:B:62:LYS:O	1.99	0.94
2:1:72:ILE:HG22	2:1:76:ILE:CD1	1.98	0.94
2:1:79:LEU:HD11	2:1:222:LEU:CD2	1.97	0.94
10:C3:365:ILE:HD12	11:C1:87:MET:HE1	1.48	0.94
31:I:108:LYS:HA	31:I:108:LYS:NZ	1.83	0.94
66:t:34:TRP:O	66:t:37:ASP:OD1	1.85	0.94
31:I:105:LYS:C	31:I:106:GLU:HG3	1.90	0.93
31:I:108:LYS:HA	31:I:108:LYS:HZ2	1.33	0.93
58:k:436:ARG:HH21	60:m:221:HIS:HB3	1.34	0.93
23:A:367:CYS:SG	23:A:368:THR:N	2.39	0.93
66:t:36:THR:HG22	66:t:38:TRP:CD1	2.04	0.93
10:C3:449:MET:SD	11:C1:5:MET:HE2	2.09	0.92
7:6:366:MET:HE3	7:6:369:THR:HG21	1.52	0.92
57:e:70:THR:O	57:e:72:TYR:N	2.02	0.92
4:7:80:PRO:HD2	4:7:81:GLU:H	1.34	0.92
53:h:84:ILE:HG22	53:h:88:ARG:HH12	1.33	0.92
63:A2:19:TRP:O	63:A2:21:TYR:N	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:t:30:VAL:O	66:t:33:VAL:CG2	2.18	0.92
57:e:114:ARG:N	57:e:114:ARG:HD3	1.85	0.92
60:y:244:LEU:O	61:z:201:ARG:NH1	2.03	0.92
63:A2:16:ILE:HD13	63:A2:19:TRP:CH2	2.04	0.92
2:1:203:GLY:H	2:1:210:GLY:H	1.12	0.91
2:1:267:THR:O	2:1:269:SER:N	2.04	0.90
41:T:65:ALA:O	41:T:66:ILE:HG13	1.70	0.90
40:S:48:ILE:HD13	40:S:191:VAL:HB	1.50	0.90
24:B:120:THR:OG1	24:B:462:ASP:OD2	1.90	0.90
41:T:65:ALA:O	41:T:66:ILE:CG1	2.20	0.90
2:1:172:MET:HE1	2:1:176:LEU:CG	2.02	0.90
53:h:120:ARG:HH22	56:g:66:ARG:H	1.20	0.90
60:m:45:ILE:HA	80:m:401:HEM:HMC3	1.54	0.90
40:S:237:MET:HA	40:S:243:VAL:HG11	1.54	0.89
60:m:74:ASN:ND2	62:p:60:SER:O	2.06	0.89
60:y:45:ILE:HA	80:y:401:HEM:HMC3	1.53	0.89
40:S:73:HIS:NE2	40:S:148:GLU:OE2	2.05	0.89
60:m:312:GLN:HE21	60:m:318:ARG:HG3	1.36	0.89
66:t:19:PRO:O	66:t:22:SER:OG	1.90	0.89
63:A2:16:ILE:CD1	63:A2:19:TRP:HZ3	1.85	0.89
66:t:36:THR:HG22	66:t:38:TRP:HD1	1.38	0.89
12:A9:112:LEU:HG	12:A9:118:PRO:HB3	1.55	0.89
31:I:109:THR:CB	31:I:120:ARG:CB	2.50	0.89
60:m:244:LEU:O	61:o:201:ARG:NH1	2.07	0.88
67:B6:52:TRP:HB2	67:B6:56:LYS:HB2	1.55	0.88
2:1:71:PHE:CZ	2:1:215:TYR:CD1	2.62	0.88
31:I:108:LYS:HA	31:I:108:LYS:CE	2.04	0.88
66:t:36:THR:HG21	66:t:38:TRP:CD1	2.08	0.88
2:1:172:MET:CE	2:1:176:LEU:CG	2.51	0.88
59:l:78:LYS:HB3	59:l:129:ALA:HB1	1.54	0.88
16:A6:5:LYS:HZ3	16:A6:6:GLY:H	0.94	0.88
63:A2:19:TRP:CD1	63:A2:22:ASN:HD22	1.92	0.87
2:1:245:THR:OG1	2:1:255:TYR:HE1	1.52	0.87
59:x:78:LYS:HB3	59:x:129:ALA:HB1	1.54	0.87
63:A2:73:GLN:HA	64:A3:39:ARG:HH22	1.37	0.87
67:u:52:TRP:HB2	67:u:56:LYS:HB2	1.55	0.87
41:T:77:SER:HA	41:T:80:VAL:HG22	1.56	0.87
61:o:176:PRO:HB2	65:s:13:LEU:HD21	1.55	0.87
57:e:70:THR:C	57:e:72:TYR:H	1.82	0.87
58:k:301:ASN:ND2	60:m:2:THR:OG1	2.08	0.87
64:A3:37:VAL:O	64:A3:41:THR:CG2	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:192:ALA:H	58:w:218:GLY:HA3	1.40	0.87
59:x:315:SER:HA	59:x:320:GLY:HA3	1.56	0.87
59:x:101:THR:HG23	59:x:103:GLU:H	1.39	0.86
6:5:37:MET:HE2	8:2:68:MET:HE2	1.55	0.86
8:2:104:MET:O	8:2:114:TRP:HZ3	1.57	0.86
35:N:106:GLU:OE2	37:P:71:SER:OG	1.92	0.86
2:1:41:GLY:HA3	2:1:44:GLY:H	1.40	0.86
23:A:343:GLY:H	23:A:549:GLY:HA2	1.41	0.86
58:k:348:SER:OG	66:t:17:TRP:NE1	2.08	0.86
60:y:312:GLN:HE21	60:y:318:ARG:HG3	1.36	0.86
9:8:327:ILE:HG21	9:8:332:CYS:HB2	1.57	0.86
24:B:61:TRP:CD1	24:B:62:LYS:H	1.90	0.86
39:R:314:THR:HG22	39:R:316:ARG:HB2	1.55	0.86
26:D:191:GLU:OE2	27:E:86:TYR:OH	1.94	0.86
39:R:61:ALA:HA	39:R:66:GLY:HA3	1.58	0.86
59:l:101:THR:HG23	59:l:103:GLU:H	1.39	0.86
60:y:377:LEU:HD12	63:A2:20:TYR:HE2	1.40	0.86
8:2:51:ARG:NH2	24:B:61:TRP:CH2	2.44	0.86
23:A:618:GLU:OE2	23:A:620:TRP:NE1	2.09	0.85
40:S:275:ASN:O	40:S:277:ARG:N	2.07	0.85
53:h:79:ASP:N	53:h:83:ASP:OD2	2.09	0.85
59:l:315:SER:HA	59:l:320:GLY:HA3	1.56	0.85
63:A2:18:LYS:O	63:A2:19:TRP:O	1.94	0.85
2:1:233:MET:CA	2:1:236:ILE:CG2	2.53	0.85
60:m:156:ILE:CG2	66:A4:38:TRP:HE1	1.88	0.85
61:o:41:HIS:NE2	81:o:301:HEC:ND	2.25	0.85
11:C1:78:LEU:HB2	11:C1:79:PRO:HD3	1.58	0.85
61:z:41:HIS:NE2	81:z:301:HEC:ND	2.25	0.85
5:4:139:GLN:N	5:4:222:GLU:OE2	2.08	0.85
44:M:7:THR:HG22	44:M:9:GLU:H	1.42	0.85
58:w:313:CYS:HA	58:w:318:GLY:HA2	1.59	0.85
66:A4:19:PRO:O	66:A4:22:SER:OG	1.93	0.85
59:l:438:GLU:OE2	59:x:169:ARG:NH2	2.09	0.84
63:A2:17:ARG:HD2	82:A2:201:UQ2:O1	1.77	0.84
1:3:81:THR:H	34:L:46:ASN:HD21	1.17	0.84
2:1:316:PRO:CG	43:V:57:ARG:HE	1.89	0.84
58:k:216:PHE:H	58:k:219:LEU:H	1.26	0.84
58:k:313:CYS:HA	58:k:318:GLY:HA2	1.59	0.84
49:b:160:MET:HB3	49:b:161:ARG:HA	1.58	0.84
66:A4:15:ARG:HG3	66:A4:16:ASN:H	1.42	0.84
58:w:412:SER:O	67:B6:15:ARG:NH2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:462:PHE:O	23:A:465:VAL:N	2.11	0.84
27:E:192:ASN:ND2	31:I:62:GLU:OE2	2.10	0.84
3:9:75:LYS:O	3:9:77:ALA:N	2.11	0.84
24:B:179:ARG:NH2	24:B:401:GLU:O	2.10	0.84
24:B:293:LEU:O	24:B:295:GLY:N	2.11	0.84
41:T:41:VAL:HG23	41:T:46:PRO:CB	2.07	0.84
66:t:30:VAL:O	66:t:33:VAL:HG23	1.77	0.84
23:A:462:PHE:O	23:A:464:GLN:N	2.11	0.83
63:A2:87:LYS:HE3	63:A2:89:TYR:HB3	1.60	0.83
25:C:66:TYR:OH	25:C:107:ASN:ND2	2.11	0.83
57:e:119:THR:OG1	57:e:120:SER:N	2.10	0.83
10:C3:187:SER:HB2	10:C3:277:MET:HE1	1.60	0.83
4:7:84:LEU:O	4:7:85:SER:O	1.96	0.83
52:f:163:LEU:N	52:f:164:PRO:HA	1.94	0.83
23:A:391:ILE:HG12	23:A:600:GLU:OE2	1.78	0.83
23:A:501:ARG:HA	23:A:505:GLY:HA3	1.61	0.83
27:E:197:TRP:HB3	42:U:84:PRO:HB3	1.60	0.83
63:q:87:LYS:HE3	63:q:89:TYR:HB3	1.60	0.83
5:4:1:MET:HG2	5:4:2:LEU:H	1.41	0.83
25:C:150:ASP:OD1	25:C:151:GLU:N	2.12	0.83
56:g:11:PRO:HD2	56:g:109:ARG:HH12	1.43	0.83
51:d:76:ASN:ND2	51:d:78:LEU:O	2.12	0.82
66:A4:41:ILE:O	66:A4:42:LEU:O	1.95	0.82
24:B:61:TRP:HD1	24:B:62:LYS:O	1.57	0.82
58:w:122:LEU:HB3	58:w:179:ARG:HD2	1.61	0.82
4:7:4:TYR:HE1	4:7:123:GLY:HA2	1.44	0.82
8:2:87:MET:HE2	8:2:90:PHE:HZ	1.43	0.82
58:k:122:LEU:HB3	58:k:179:ARG:HD2	1.61	0.82
60:y:127:ALA:HA	80:y:401:HEM:HHB	1.62	0.82
64:A3:19:SER:HB3	64:A3:22:GLU:HG2	1.60	0.82
1:3:84:LEU:HD22	2:1:309:ILE:HD13	1.62	0.82
25:C:127:ARG:HE	25:C:128:PHE:HE1	1.28	0.82
27:E:105:ARG:NH1	27:E:195:ASP:OD2	2.12	0.82
58:k:131:ARG:NH2	58:k:177:LEU:O	2.13	0.82
64:r:19:SER:HB3	64:r:22:GLU:HG2	1.59	0.81
1:3:49:LEU:HD23	2:1:126:LYS:HZ3	1.39	0.81
5:4:64:PRO:O	5:4:66:LEU:N	2.13	0.81
23:A:238:PHE:CD2	27:E:140:ARG:HD3	2.15	0.81
53:h:121:GLU:OE2	53:h:124:ARG:NH2	2.13	0.81
55:j:119:VAL:HB	56:g:147:GLY:HA3	1.61	0.81
58:k:220:SER:HB2	58:k:222:THR:HG22	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:o:51:LEU:HD22	61:o:58:GLU:HA	1.63	0.81
3:9:188:ILE:HD12	3:9:189:ASN:H	1.42	0.81
8:2:135:LYS:HD2	8:2:187:MET:HE3	1.60	0.81
60:m:127:ALA:HA	80:m:401:HEM:HHB	1.62	0.81
58:w:131:ARG:NH2	58:w:177:LEU:O	2.13	0.81
61:z:51:LEU:HD22	61:z:58:GLU:HA	1.63	0.81
23:A:124:HIS:NE2	74:A:801:SF4:S3	2.53	0.81
73:8:501:FMN:N1	73:8:501:FMN:O3'	2.13	0.81
58:k:240:GLN:NE2	58:k:242:CYS:SG	2.53	0.81
4:7:80:PRO:HD2	4:7:81:GLU:N	1.95	0.81
24:B:61:TRP:HD1	24:B:62:LYS:H	1.26	0.81
58:w:240:GLN:NE2	58:w:242:CYS:SG	2.53	0.81
66:A4:41:ILE:O	66:A4:42:LEU:C	2.24	0.81
3:9:118:PHE:HB2	9:8:220:GLN:HE21	1.46	0.81
58:w:203:LEU:HA	58:w:207:GLN:HE21	1.45	0.81
40:S:158:LEU:HA	40:S:161:MET:HB3	1.63	0.81
41:T:65:ALA:O	41:T:66:ILE:CB	2.27	0.81
59:l:122:PHE:HA	59:l:125:ASN:HD22	1.45	0.81
58:w:362:ARG:HE	58:w:399:ILE:HG21	1.46	0.81
2:1:8:MET:O	2:1:12:PRO:HG2	1.82	0.80
38:Q:90:ASP:O	38:Q:92:SER:OG	2.00	0.80
3:9:149:LEU:HD23	3:9:150:GLU:H	1.46	0.80
3:9:188:ILE:HD11	3:9:191:ASN:HB2	1.63	0.80
16:A6:5:LYS:NZ	16:A6:6:GLY:H	1.78	0.80
23:A:469:ALA:HB3	23:A:472:PRO:HG3	1.63	0.80
4:7:28:TYR:CZ	4:7:83:TRP:HD1	1.99	0.80
17:C0:39:CYS:SG	17:C0:53:CYS:HB3	2.22	0.80
40:S:109:PRO:HB2	40:S:112:ASN:HB3	1.61	0.80
24:B:426:ALA:HB3	24:B:460:GLU:OE2	1.80	0.80
59:x:160:ILE:HG21	68:B5:64:LEU:HD11	1.63	0.80
31:I:109:THR:CB	31:I:119:PHE:C	2.53	0.80
41:T:62:THR:CG2	41:T:104:ARG:HD3	2.12	0.80
67:B6:53:LYS:O	67:B6:57:HIS:NE2	2.15	0.80
26:D:107:ASP:OD1	26:D:108:ARG:N	2.15	0.80
39:R:171:ASN:HD21	39:R:324:THR:HB	1.45	0.80
4:7:100:GLU:O	4:7:104:VAL:N	2.14	0.80
53:h:81:ALA:O	53:h:83:ASP:N	2.14	0.80
58:k:203:LEU:HA	58:k:207:GLN:HE21	1.45	0.80
59:x:122:PHE:HA	59:x:125:ASN:HD22	1.45	0.80
36:O:99:GLN:O	36:O:101:THR:N	2.15	0.79
4:7:33:LEU:HD11	6:5:31:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:370:PRO:HA	5:4:375:LEU:HD12	1.64	0.79
60:y:74:ASN:ND2	62:A1:60:SER:O	2.13	0.79
63:A2:16:ILE:CG2	63:A2:19:TRP:HE3	1.87	0.79
9:8:398:ARG:HG3	9:8:403:ASP:HB3	1.63	0.79
16:A6:5:LYS:HZ3	16:A6:6:GLY:N	1.77	0.79
40:S:199:VAL:CB	40:S:200:PRO:HD2	2.11	0.79
61:o:23:HIS:CD2	67:u:55:ILE:HD12	2.17	0.79
61:z:41:HIS:NE2	81:z:301:HEC:NA	2.31	0.79
23:A:545:LEU:HB2	23:A:566:ILE:HG22	1.65	0.79
39:R:209:ARG:NH1	39:R:351:GLU:OE2	2.15	0.79
62:p:58:PHE:O	62:p:61:SER:OG	1.99	0.79
67:u:53:LYS:O	67:u:57:HIS:NE2	2.15	0.79
24:B:143:SER:HB3	24:B:182:ASN:HD21	1.48	0.79
58:k:329:MET:HE2	64:r:2:ARG:HE	1.48	0.79
8:2:144:GLN:HE21	30:H:3:PHE:HB2	1.47	0.79
17:C0:39:CYS:SG	17:C0:53:CYS:CB	2.70	0.79
36:O:42:GLU:OE2	36:O:45:ASN:HB3	1.83	0.79
62:p:14:ARG:HA	64:r:23:GLN:HA	1.64	0.79
40:S:92:LEU:HD13	40:S:96:PHE:HB2	1.64	0.79
58:k:362:ARG:HE	58:k:399:ILE:HG21	1.46	0.79
61:o:147:LEU:HB3	61:o:157:ALA:HB1	1.64	0.79
2:1:35:LYS:O	26:D:108:ARG:HD3	1.83	0.79
61:o:41:HIS:NE2	81:o:301:HEC:NA	2.31	0.79
66:A4:37:ASP:OD1	66:A4:38:TRP:N	2.12	0.79
2:1:233:MET:HA	2:1:236:ILE:HG22	1.64	0.79
59:x:276:GLN:O	59:x:280:GLY:N	2.15	0.79
23:A:144:MET:HG2	24:B:380:HIS:HD2	1.47	0.78
62:A1:78:LEU:N	62:A1:191:ASP:O	2.15	0.78
66:A4:40:LEU:C	66:A4:41:ILE:HG12	2.07	0.78
5:4:60:SER:O	5:4:62:SER:N	2.16	0.78
23:A:308:ARG:NH1	23:A:308:ARG:O	2.15	0.78
52:f:162:ASP:C	52:f:164:PRO:HA	2.09	0.78
53:h:141:CYS:HA	56:g:162:ARG:HH11	1.48	0.78
60:m:361:LEU:HA	60:m:365:LEU:HD12	1.66	0.78
25:C:99:LEU:O	25:C:103:ARG:N	2.16	0.78
59:x:61:ASN:O	59:x:182:ARG:NH1	2.17	0.78
23:A:382:ARG:O	23:A:384:ASN:N	2.14	0.78
59:l:61:ASN:O	59:l:182:ARG:NH1	2.17	0.78
59:x:385:GLN:O	59:x:389:ALA:N	2.16	0.78
60:y:361:LEU:HA	60:y:365:LEU:HD12	1.66	0.78
38:Q:38:LYS:HG3	38:Q:39:PRO:HD3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S:239:GLU:HG2	40:S:240:LYS:H	1.48	0.78
58:k:245:GLU:HA	64:r:11:ARG:HA	1.65	0.78
66:t:30:VAL:O	66:t:33:VAL:HG22	1.84	0.78
63:A2:19:TRP:HD1	63:A2:22:ASN:HD22	1.27	0.78
59:x:24:LEU:HG	59:x:38:LEU:HD11	1.66	0.78
23:A:355:LYS:CB	23:A:530:TYR:OH	2.32	0.78
27:E:98:ARG:NH1	27:E:155:CYS:O	2.17	0.78
6:5:36:MET:O	6:5:39:SER:OG	2.01	0.78
27:E:52:SER:O	27:E:55:ASP:N	2.16	0.78
38:Q:6:GLU:OE2	38:Q:55:ARG:NH2	2.16	0.78
38:Q:110:CYS:O	38:Q:114:LYS:N	2.15	0.78
52:f:104:LEU:HA	52:f:107:TRP:HE1	1.49	0.78
58:k:378:ASP:OD1	58:k:382:SER:OG	2.01	0.78
59:l:276:GLN:O	59:l:280:GLY:N	2.15	0.78
61:z:147:LEU:HB3	61:z:157:ALA:HB1	1.64	0.78
60:y:1:MET:SD	60:y:7:SER:OG	2.40	0.78
58:k:87:ASN:OD1	58:k:88:ALA:N	2.17	0.77
58:k:417:ASP:O	62:p:33:LYS:NZ	2.17	0.77
66:A4:43:ASP:OD1	66:A4:47:TYR:N	2.16	0.77
2:1:261:ILE:O	2:1:261:ILE:HG22	1.83	0.77
40:S:197:VAL:HG12	40:S:199:VAL:H	1.49	0.77
47:Z:43:ASP:O	52:f:38:ARG:NH2	2.18	0.77
59:l:385:GLN:O	59:l:389:ALA:N	2.16	0.77
59:x:281:ALA:HB1	59:x:290:ASN:HD22	1.49	0.77
60:y:133:LEU:HD11	60:y:182:HIS:CD2	2.19	0.77
7:6:576:LEU:HD11	8:2:164:ILE:HG13	1.66	0.77
41:T:75:CYS:HA	41:T:78:ALA:HB3	1.65	0.77
58:w:87:ASN:OD1	58:w:88:ALA:N	2.17	0.77
17:C0:75:ARG:HG2	17:C0:75:ARG:HH11	1.48	0.77
23:A:382:ARG:O	23:A:385:TYR:N	2.17	0.77
23:A:501:ARG:NH2	23:A:509:ASP:OD1	2.17	0.77
35:N:19:THR:HB	35:N:22:GLU:OE2	1.84	0.77
60:m:1:MET:SD	60:m:7:SER:OG	2.40	0.77
60:m:5:ARG:HA	60:m:8:HIS:CD2	2.20	0.77
58:w:378:ASP:OD1	58:w:382:SER:OG	2.01	0.77
58:k:216:PHE:N	58:k:219:LEU:H	1.82	0.77
59:l:24:LEU:HG	59:l:38:LEU:HD11	1.66	0.77
62:A1:79:SER:O	62:A1:81:ILE:N	2.16	0.77
68:B5:64:LEU:HG	68:B5:65:VAL:HG22	1.65	0.77
6:5:26:LEU:HD23	6:5:78:LEU:HD13	1.67	0.77
33:K:41:TYR:HE1	33:K:53:ILE:HG21	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:c:15:LEU:HA	50:c:18:LEU:HB2	1.67	0.77
60:m:133:LEU:HD11	60:m:182:HIS:CD2	2.19	0.77
63:A2:73:GLN:HA	64:A3:39:ARG:NH2	1.98	0.77
5:4:44:GLN:HG2	5:4:45:PHE:H	1.49	0.77
25:C:211:GLU:OE2	26:D:175:ARG:NH1	2.17	0.77
58:w:412:SER:C	67:B6:15:ARG:HH22	1.92	0.77
60:y:72:ASP:OD1	61:z:49:ARG:NH1	2.18	0.77
5:4:355:MET:HA	5:4:358:TRP:HD1	1.49	0.77
9:8:119:GLU:O	9:8:159:ARG:NH2	2.18	0.77
51:d:88:ASP:O	51:d:92:HIS:N	2.18	0.77
5:4:143:LEU:HD21	8:2:302:LEU:HD21	1.64	0.77
59:l:281:ALA:HB1	59:l:290:ASN:HD22	1.49	0.77
60:y:5:ARG:HA	60:y:8:HIS:CD2	2.20	0.77
63:A2:87:LYS:HG3	63:A2:89:TYR:HD2	1.50	0.77
9:8:196:PHE:CE1	28:F:97:MET:HE3	2.20	0.76
55:j:35:GLY:O	55:j:39:TYR:N	2.18	0.76
39:R:133:GLU:HG3	39:R:134:TRP:H	1.49	0.76
58:k:142:ASP:OD1	62:p:2:HIS:ND1	2.17	0.76
61:o:10:TYR:OH	61:o:129:SER:OG	2.03	0.76
25:C:213:ARG:NH1	25:C:224:GLU:OE2	2.18	0.76
60:y:282:ARG:NH1	60:y:341:GLN:O	2.18	0.76
41:T:99:LEU:O	41:T:103:ALA:N	2.17	0.76
58:w:294:LEU:HB3	58:w:307:PHE:HZ	1.49	0.76
64:A3:42:ARG:HA	64:A3:45:ILE:HG22	1.67	0.76
8:2:339:LEU:HD13	8:2:343:LEU:HD13	1.66	0.76
27:E:79:ARG:NH2	37:P:19:ASP:OD2	2.16	0.76
58:k:294:LEU:HB3	58:k:307:PHE:HZ	1.49	0.76
60:m:52:ALA:HA	60:m:55:TYR:HB3	1.66	0.76
60:m:282:ARG:NH1	60:m:341:GLN:O	2.18	0.76
58:w:118:GLN:NE2	58:w:217:SER:O	2.18	0.76
2:1:199:ASP:OD2	2:1:279:ARG:NH2	2.19	0.76
9:8:259:GLY:HA3	9:8:261:TRP:H	1.49	0.76
24:B:134:PRO:O	24:B:137:ASP:N	2.19	0.76
39:R:237:LYS:O	39:R:239:PRO:HD3	1.86	0.76
40:S:219:SER:O	40:S:223:GLN:N	2.19	0.76
61:z:204:MET:HA	61:z:207:LYS:HB3	1.67	0.76
2:1:173:TRP:O	2:1:175:ILE:N	2.19	0.76
11:C1:5:MET:HE3	20:B3:42:PRO:HA	1.67	0.76
27:E:59:GLN:HA	27:E:64:THR:HG22	1.66	0.76
51:d:40:VAL:HG12	51:d:41:ALA:N	1.99	0.76
1:3:49:LEU:HD23	2:1:126:LYS:HZ2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:28:TYR:CD2	4:7:83:TRP:CD1	2.73	0.76
9:8:364:VAL:HG12	9:8:400:VAL:HG22	1.68	0.76
2:1:301:CYS:O	2:1:305:VAL:HG23	1.85	0.76
23:A:144:MET:HG2	24:B:380:HIS:CD2	2.21	0.76
61:o:32:VAL:O	61:o:36:VAL:N	2.16	0.76
68:B5:70:LEU:HD12	68:B5:71:ASN:H	1.48	0.76
60:y:52:ALA:HA	60:y:55:TYR:HB3	1.66	0.75
25:C:120:ASP:OD2	25:C:201:ARG:HA	1.87	0.75
56:g:77:CYS:SG	56:g:78:GLN:N	2.55	0.75
62:p:28:SER:O	62:p:32:ARG:N	2.18	0.75
59:x:82:SER:HA	59:x:85:ILE:HD12	1.69	0.75
61:z:133:GLY:O	61:z:150:ASN:ND2	2.19	0.75
23:A:334:GLN:NE2	23:A:361:VAL:O	2.19	0.75
63:q:87:LYS:HG3	63:q:89:TYR:HD2	1.50	0.75
59:x:63:LEU:O	59:x:182:ARG:NE	2.20	0.75
5:4:25:VAL:HG23	53:h:89:VAL:HG11	1.67	0.75
12:A9:187:THR:HG21	16:A6:68:THR:HG21	1.68	0.75
39:R:55:VAL:HG12	39:R:56:ALA:H	1.51	0.75
56:g:52:ILE:HA	56:g:55:GLN:HB3	1.67	0.75
58:w:65:LYS:HD3	58:w:126:GLN:HB3	1.67	0.75
1:3:81:THR:O	34:L:46:ASN:ND2	2.20	0.75
3:9:176:CYS:O	9:8:159:ARG:NH1	2.20	0.75
27:E:69:GLY:O	27:E:73:THR:N	2.19	0.75
40:S:226:GLU:HA	40:S:229:TYR:HD2	1.51	0.75
59:l:82:SER:HA	59:l:85:ILE:HD12	1.69	0.75
59:l:200:THR:HG23	59:l:203:ARG:H	1.52	0.75
61:o:133:GLY:O	61:o:150:ASN:ND2	2.19	0.75
61:o:204:MET:HA	61:o:207:LYS:HB3	1.67	0.75
58:w:184:GLU:OE1	58:w:188:ARG:NH2	2.19	0.75
2:1:311:THR:O	43:V:55:ARG:NH2	2.20	0.75
9:8:295:PRO:HG2	9:8:298:GLU:HG2	1.69	0.75
26:D:91:CYS:HB2	74:D:301:SF4:S2	2.26	0.75
58:k:65:LYS:HD3	58:k:126:GLN:HB3	1.67	0.75
67:u:57:HIS:ND1	67:u:60:GLU:OE2	2.20	0.75
8:2:85:THR:HG22	30:H:19:THR:HG21	1.67	0.75
8:2:316:GLN:HB3	8:2:318:PRO:HD3	1.67	0.75
23:A:307:VAL:HG22	23:A:308:ARG:H	1.52	0.75
24:B:458:PHE:C	24:B:460:GLU:H	1.95	0.75
58:k:184:GLU:OE1	58:k:188:ARG:NH2	2.19	0.75
61:z:12:TRP:HB2	61:z:15:ARG:HB2	1.68	0.75
2:1:171:GLN:HE21	2:1:171:GLN:N	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:J:38:VAL:O	32:J:44:GLN:NE2	2.19	0.75
44:W:156:GLU:OE2	50:c:24:LYS:HA	1.86	0.75
67:B6:57:HIS:ND1	67:B6:60:GLU:OE2	2.20	0.75
3:9:90:ASN:ND2	3:9:92:TRP:O	2.21	0.74
3:9:148:ILE:HD12	3:9:184:PRO:HB2	1.69	0.74
11:C1:184:LEU:HD11	11:C1:211:LEU:HD21	1.69	0.74
30:H:84:GLU:OE2	43:V:127:LEU:HD11	1.87	0.74
59:x:200:THR:HG23	59:x:203:ARG:H	1.51	0.74
8:2:338:PRO:O	55:j:83:TYR:OH	2.03	0.74
30:H:15:ASP:O	30:H:17:TRP:N	2.20	0.74
61:z:158:ILE:HG12	61:z:160:MET:H	1.52	0.74
4:7:81:GLU:HG2	39:R:357:ARG:HH22	1.50	0.74
47:Z:64:VAL:HG12	47:Z:68:LEU:HG	1.69	0.74
52:f:126:LYS:O	52:f:130:ARG:N	2.21	0.74
44:M:17:TYR:OH	44:M:57:GLU:OE2	2.03	0.74
61:o:158:ILE:HG12	61:o:160:MET:H	1.52	0.74
8:2:25:HIS:HB2	30:H:15:ASP:OD2	1.86	0.74
8:2:30:TRP:CZ3	8:2:67:SER:HB3	2.22	0.74
39:R:168:SER:HB2	39:R:188:GLU:OE2	1.86	0.74
59:l:247:GLN:HE22	59:l:430:LEU:H	1.35	0.74
61:o:80:MET:HG3	61:o:81:PHE:H	1.52	0.74
64:r:42:ARG:HA	64:r:45:ILE:HG22	1.67	0.74
3:9:183:ALA:HB3	3:9:195:ASP:HA	1.68	0.74
8:2:109:ALA:O	8:2:112:HIS:NE2	2.20	0.74
39:R:203:PRO:HA	39:R:265:PHE:HB2	1.70	0.74
55:j:30:ARG:O	55:j:34:VAL:N	2.14	0.74
63:A2:52:GLU:HA	63:A2:55:TYR:HB3	1.69	0.74
5:4:75:LEU:HD21	5:4:440:HIS:CE1	2.21	0.74
59:l:63:LEU:O	59:l:182:ARG:NE	2.20	0.74
2:1:146:LEU:HD11	2:1:185:TRP:CZ3	2.21	0.74
23:A:259:SER:O	23:A:260:ASN:ND2	2.20	0.74
36:O:50:PHE:HE1	36:O:96:VAL:HG12	1.51	0.74
61:o:12:TRP:HB2	61:o:15:ARG:HB2	1.68	0.74
57:e:113:ILE:C	57:e:114:ARG:HD3	2.13	0.74
58:k:159:GLN:O	58:k:235:ARG:NH2	2.21	0.74
59:l:437:ASP:OD2	59:x:240:HIS:NE2	2.16	0.74
58:w:62:LEU:HD23	58:w:65:LYS:HZ3	1.52	0.74
7:6:88:MET:HE2	7:6:468:ILE:HG12	1.68	0.74
24:B:95:LEU:HD23	24:B:458:PHE:CZ	2.23	0.74
46:Y:46:ARG:HA	46:Y:49:GLN:HE22	1.52	0.74
58:k:436:ARG:NH2	60:m:221:HIS:HB3	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:z:32:VAL:O	61:z:36:VAL:N	2.16	0.74
8:2:51:ARG:NH2	24:B:61:TRP:HH2	1.83	0.73
60:y:377:LEU:CD1	63:A2:20:TYR:HE2	1.99	0.73
35:N:36:GLY:O	35:N:45:ARG:NH2	2.20	0.73
39:R:154:GLN:O	39:R:156:SER:N	2.20	0.73
55:j:115:GLU:HB3	55:j:117:HIS:ND1	2.02	0.73
2:1:317:GLN:NE2	2:1:317:GLN:HA	2.03	0.73
11:C1:59:GLN:H	11:C1:62:GLU:HG3	1.51	0.73
23:A:34:VAL:HG22	23:A:99:GLY:HA2	1.70	0.73
27:E:37:THR:HB	37:P:107:SER:HB2	1.69	0.73
41:T:78:ALA:HA	41:T:89:ASN:HD21	1.53	0.73
9:8:317:VAL:HG23	9:8:356:VAL:HG12	1.71	0.73
32:J:55:SER:HB2	32:J:62:VAL:HG23	1.68	0.73
61:z:10:TYR:OH	61:z:129:SER:OG	2.03	0.73
2:1:176:LEU:HB3	2:1:177:PRO:HD3	1.70	0.73
3:9:200:ASP:OD2	3:9:219:ARG:HD3	1.87	0.73
9:8:98:LYS:NZ	73:8:501:FMN:O2P	2.19	0.73
23:A:627:SER:OG	23:A:632:MET:O	2.06	0.73
38:Q:110:CYS:HA	38:Q:113:ASP:HB3	1.69	0.73
63:q:52:GLU:HA	63:q:55:TYR:HB3	1.69	0.73
58:w:329:MET:HE2	64:A3:2:ARG:HE	1.54	0.73
62:A1:101:ARG:N	62:A1:131:GLU:O	2.19	0.73
69:3:200:PC1:H121	34:L:16:GLU:HG2	1.69	0.73
2:1:171:GLN:HE21	2:1:171:GLN:H	1.36	0.73
16:A6:54:ARG:HD3	16:A6:54:ARG:N	2.04	0.73
34:L:67:PRO:HA	38:Q:130:LYS:HE3	1.70	0.73
8:2:153:LEU:O	8:2:156:THR:N	2.21	0.73
26:D:146:GLU:O	26:D:148:ARG:N	2.21	0.73
58:k:65:LYS:HE2	58:k:130:GLU:HB2	1.70	0.73
58:w:159:GLN:O	58:w:235:ARG:NH2	2.21	0.73
59:x:148:LYS:NZ	59:x:178:CYS:O	2.18	0.73
37:P:109:ASP:H	37:P:111:PRO:HD3	1.53	0.73
39:R:182:ARG:O	39:R:183:SER:OG	2.07	0.73
1:3:53:MET:O	1:3:56:PHE:N	2.22	0.73
2:1:222:LEU:O	2:1:226:ALA:N	2.21	0.73
5:4:208:PRO:HB3	5:4:213:HIS:HB3	1.71	0.73
5:4:278:ARG:H	7:6:546:GLN:NE2	1.84	0.73
8:2:51:ARG:CZ	24:B:61:TRP:HH2	2.02	0.73
13:A7:23:PRO:O	14:B4:66:ARG:HD3	1.89	0.73
31:I:66:ASN:OD1	31:I:67:PHE:N	2.22	0.73
72:J:101:CDL:H122	42:U:2:GLU:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:c:7:GLU:OE2	52:f:155:PRO:HG3	1.88	0.73
58:k:62:LEU:HD23	58:k:65:LYS:HZ3	1.52	0.73
58:w:19:LEU:HD12	58:w:23:LEU:HD23	1.70	0.73
59:x:133:ARG:HD3	59:x:135:TRP:CZ2	2.24	0.73
25:C:123:THR:HG21	29:G:129:SER:H	1.54	0.72
59:l:133:ARG:HD3	59:l:135:TRP:CZ2	2.24	0.72
66:A4:18:VAL:HB	66:A4:19:PRO:HD3	1.71	0.72
30:H:2:PRO:HB2	69:j:201:PC1:H131	1.71	0.72
59:l:148:LYS:NZ	59:l:178:CYS:O	2.18	0.72
63:q:16:ILE:HA	63:q:19:TRP:HB3	1.70	0.72
23:A:217:GLU:OE2	23:A:408:ARG:NE	2.21	0.72
58:w:438:ARG:HH22	62:A1:37:TYR:HH	1.35	0.72
60:y:310:SER:HA	60:y:374:ASN:HD21	1.54	0.72
61:z:167:GLU:HA	61:z:177:ALA:HB3	1.70	0.72
5:4:69:THR:HG22	5:4:235:LEU:HD11	1.71	0.72
5:4:244:LEU:HD21	5:4:301:ILE:HD12	1.69	0.72
10:C3:176:MET:HE3	10:C3:181:THR:HG22	1.71	0.72
36:O:46:THR:O	36:O:49:LEU:N	2.22	0.72
43:V:48:TRP:O	43:V:52:LYS:NZ	2.22	0.72
2:1:237:PHE:CD1	2:1:240:ILE:HD11	2.24	0.72
27:E:105:ARG:HD3	27:E:109:GLY:HA3	1.70	0.72
58:k:34:THR:HG22	58:k:102:LEU:HD23	1.71	0.72
61:o:236:ALA:HB3	64:r:14:ILE:HB	1.71	0.72
61:z:159:GLY:N	81:z:301:HEC:O1D	2.22	0.72
2:1:169:GLN:O	2:1:170:GLU:O	2.07	0.72
13:A7:147:LYS:HA	13:A7:147:LYS:HE3	1.72	0.72
23:A:69:LEU:O	29:G:158:LYS:NZ	2.21	0.72
62:p:149:ASN:N	62:p:152:ASP:O	2.14	0.72
2:1:172:MET:O	2:1:173:TRP:C	2.29	0.72
26:D:215:ARG:HD2	39:R:85:ARG:HD2	1.69	0.72
58:k:2:ALA:O	59:l:113:ARG:NE	2.22	0.72
63:A2:103:GLU:O	63:A2:107:TRP:N	2.19	0.72
66:A4:40:LEU:O	66:A4:41:ILE:CB	2.38	0.72
2:1:172:MET:SD	2:1:176:LEU:HD12	2.25	0.72
24:B:241:MET:HG3	43:V:10:MET:HB3	1.69	0.72
40:S:67:GLU:HA	40:S:70:GLY:H	1.55	0.72
57:e:70:THR:C	57:e:72:TYR:N	2.43	0.72
58:k:327:ASP:OD1	58:k:328:HIS:N	2.23	0.72
60:m:185:LEU:HD12	60:m:188:ILE:HD12	1.71	0.72
24:B:259:GLU:OE2	43:V:23:ARG:NH2	2.22	0.71
63:q:73:GLN:HA	64:r:39:ARG:HH22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:324:THR:HG22	55:j:48:ILE:HD12	1.72	0.71
25:C:157:SER:HB2	25:C:159:VAL:HG23	1.72	0.71
39:R:275:ASP:O	39:R:279:TYR:N	2.19	0.71
44:W:105:MET:HA	44:W:108:LEU:HB2	1.70	0.71
6:5:24:SER:HB3	6:5:89:TYR:HA	1.72	0.71
60:m:310:SER:HA	60:m:374:ASN:HD21	1.54	0.71
58:w:211:LEU:HA	58:w:213:GLN:HB2	1.72	0.71
5:4:118:PHE:O	5:4:122:PHE:N	2.24	0.71
40:S:31:TYR:OH	40:S:285:LEU:O	2.06	0.71
58:k:19:LEU:HD12	58:k:23:LEU:HD23	1.70	0.71
59:l:102:ARG:NH1	59:l:174:ASN:O	2.23	0.71
61:o:21:LEU:HD22	61:o:188:THR:HG23	1.72	0.71
61:o:167:GLU:HA	61:o:177:ALA:HB3	1.70	0.71
63:q:16:ILE:O	63:q:20:TYR:N	2.14	0.71
66:t:34:TRP:C	66:t:37:ASP:OD1	2.34	0.71
58:w:65:LYS:HE2	58:w:130:GLU:HB2	1.70	0.71
58:w:327:ASP:OD1	58:w:328:HIS:N	2.23	0.71
59:x:247:GLN:HE22	59:x:430:LEU:H	1.35	0.71
63:A2:57:ASP:HB3	63:A2:61:ARG:HH12	1.55	0.71
12:A9:12:ASN:HD22	19:B2:20:VAL:H	1.39	0.71
59:l:257:LEU:HD11	59:l:422:LYS:HB3	1.71	0.71
37:P:27:ARG:HA	42:U:56:PHE:HB3	1.73	0.71
58:w:34:THR:HG22	58:w:102:LEU:HD23	1.70	0.71
58:w:403:ASP:OD1	58:w:404:ALA:N	2.24	0.71
66:A4:40:LEU:CD1	66:A4:41:ILE:N	2.53	0.71
3:9:130:TYR:HA	3:9:189:ASN:HD21	1.53	0.71
58:w:438:ARG:NH2	62:A1:37:TYR:OH	2.22	0.71
58:k:403:ASP:OD1	58:k:404:ALA:N	2.24	0.71
63:q:57:ASP:HB3	63:q:61:ARG:HH12	1.55	0.71
59:x:257:LEU:HD11	59:x:422:LYS:HB3	1.71	0.71
60:y:185:LEU:HD12	60:y:188:ILE:HD12	1.72	0.71
7:6:157:TRP:HD1	7:6:158:TRP:CD1	2.08	0.71
8:2:14:MET:HA	8:2:17:THR:HG22	1.73	0.71
24:B:141:TYR:OH	24:B:458:PHE:O	2.08	0.71
29:G:75:ARG:NH2	29:G:119:ASP:OD1	2.24	0.71
79:R:601:NAP:O2X	79:R:601:NAP:H1B	1.87	0.71
60:y:370:GLY:O	60:y:374:ASN:N	2.19	0.71
61:z:21:LEU:HD22	61:z:188:THR:HG23	1.72	0.71
7:6:432:LEU:O	47:Z:60:ASN:ND2	2.23	0.70
23:A:217:GLU:OE1	23:A:217:GLU:N	2.20	0.70
24:B:139:LEU:HD21	24:B:424:ILE:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:299:GLN:HG2	27:E:38:TYR:CE1	2.26	0.70
36:O:20:ILE:HB	36:O:80:ASP:OD2	1.91	0.70
53:h:149:LEU:HD22	56:g:166:GLU:HB3	1.73	0.70
60:m:370:GLY:O	60:m:374:ASN:N	2.19	0.70
25:C:149:THR:HB	25:C:155:ILE:HD11	1.72	0.70
62:p:126:ARG:O	62:p:130:PRO:N	2.25	0.70
3:9:228:ALA:HA	3:9:231:LEU:HD23	1.72	0.70
4:7:80:PRO:CD	4:7:81:GLU:H	2.04	0.70
4:7:107:VAL:HG13	4:7:108:LEU:H	1.56	0.70
37:P:29:GLN:HG3	37:P:30:GLU:H	1.56	0.70
61:o:70:VAL:HA	61:o:83:ARG:H	1.55	0.70
63:q:75:LEU:HD12	63:q:76:PRO:HD2	1.72	0.70
60:y:319:PRO:O	60:y:323:CYS:N	2.21	0.70
4:7:170:GLU:O	4:7:172:THR:N	2.24	0.70
7:6:237:MET:HB3	7:6:299:LYS:HD3	1.73	0.70
60:m:228:ASP:O	60:m:232:ALA:N	2.19	0.70
63:A2:10:SER:O	82:A2:201:UQ2:H5M2	1.88	0.70
9:8:98:LYS:HG3	9:8:99:TRP:CD1	2.26	0.70
12:A9:156:ARG:HG3	12:A9:156:ARG:HH11	1.56	0.70
59:x:102:ARG:NH1	59:x:174:ASN:O	2.23	0.70
3:9:56:THR:HG22	3:9:58:GLU:H	1.57	0.70
26:D:195:TYR:OH	42:U:116:ASN:ND2	2.23	0.70
48:a:43:LEU:O	48:a:47:TYR:N	2.17	0.70
63:A2:75:LEU:HD12	63:A2:76:PRO:HD2	1.72	0.70
2:1:237:PHE:O	2:1:238:THR:C	2.33	0.70
23:A:111:LYS:HA	37:P:53:TYR:OH	1.92	0.70
24:B:301:ASP:OD2	24:B:318:VAL:HG21	1.92	0.70
41:T:4:THR:O	41:T:7:ARG:N	2.25	0.70
41:T:62:THR:HG23	41:T:104:ARG:HD3	1.74	0.70
63:q:53:ASN:OD1	63:q:54:LEU:N	2.23	0.70
58:w:37:VAL:O	58:w:99:ILE:N	2.24	0.70
59:x:272:PHE:HA	59:x:275:LEU:HB3	1.72	0.70
63:A2:11:ARG:HA	82:A2:201:UQ2:H5M1	1.72	0.70
4:7:140:ALA:O	4:7:142:GLY:N	2.24	0.70
24:B:289:SER:OG	24:B:406:GLU:N	2.24	0.70
41:T:65:ALA:O	41:T:66:ILE:HB	1.89	0.70
42:U:124:TYR:CE2	42:U:126:PRO:HG3	2.27	0.70
44:W:79:ILE:HG12	44:W:145:VAL:HG13	1.74	0.70
58:k:37:VAL:O	58:k:99:ILE:N	2.24	0.70
61:o:99:GLU:HB3	61:z:76:GLU:HG3	1.73	0.70
5:4:20:ASN:O	5:4:22:MET:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:196:PHE:CD1	28:F:97:MET:HE3	2.26	0.70
60:m:379:TRP:HA	63:q:33:ARG:NH1	2.07	0.70
65:B7:44:VAL:O	65:B7:48:SER:N	2.24	0.70
2:1:232:ILE:C	2:1:236:ILE:HG22	2.16	0.70
9:8:93:PHE:CE2	9:8:98:LYS:HB3	2.27	0.70
24:B:378:LEU:O	24:B:381:HIS:N	2.24	0.70
58:k:433:ASP:OD2	60:m:223:TYR:OH	2.10	0.70
59:x:59:ASN:OD1	59:x:60:SER:N	2.24	0.70
8:2:104:MET:O	8:2:114:TRP:CZ3	2.44	0.69
38:Q:109:GLU:HG3	38:Q:110:CYS:H	1.56	0.69
47:Z:63:PHE:O	47:Z:65:GLY:N	2.24	0.69
57:e:111:MET:HG2	57:e:112:TYR:H	1.56	0.69
67:u:56:LYS:HG2	67:u:60:GLU:HB3	1.74	0.69
10:C3:69:MET:HE2	10:C3:70:VAL:HG23	1.74	0.69
23:A:112:ALA:O	23:A:115:GLY:N	2.23	0.69
38:Q:124:ASP:OD1	38:Q:125:LEU:N	2.25	0.69
39:R:168:SER:OG	39:R:202:LYS:NZ	2.20	0.69
57:e:65:TYR:O	57:e:67:ASP:N	2.24	0.69
58:k:348:SER:HG	66:t:17:TRP:HE1	1.39	0.69
59:x:97:SER:HA	68:B5:70:LEU:HD22	1.73	0.69
2:1:8:MET:O	2:1:8:MET:HG3	1.92	0.69
5:4:207:MET:HG3	5:4:298:ILE:HD11	1.74	0.69
8:2:261:MET:HE2	8:2:337:LEU:HD12	1.72	0.69
9:8:142:CYS:O	9:8:146:GLY:N	2.15	0.69
10:C3:11:ASN:HD22	10:C3:14:ASP:H	1.39	0.69
41:T:62:THR:CG2	41:T:104:ARG:CD	2.71	0.69
58:w:362:ARG:HG2	58:w:399:ILE:HD13	1.74	0.69
63:A2:53:ASN:OD1	63:A2:54:LEU:N	2.23	0.69
25:C:175:MET:O	25:C:198:HIS:HB3	1.92	0.69
39:R:207:PHE:HA	39:R:211:ASP:OD2	1.92	0.69
44:M:25:ILE:HD12	44:M:42:LEU:HG	1.73	0.69
59:l:158:HIS:CE1	59:l:162:ASN:HD21	2.10	0.69
2:1:172:MET:O	2:1:172:MET:HE3	1.93	0.69
25:C:218:VAL:HG13	25:C:219:LYS:H	1.57	0.69
43:V:121:MET:HE3	43:V:137:THR:HG22	1.75	0.69
58:k:281:ASP:OD1	58:k:282:CYS:N	2.26	0.69
59:l:272:PHE:HA	59:l:275:LEU:HB3	1.72	0.69
61:o:69:GLU:HG2	61:o:84:PRO:HB3	1.72	0.69
65:s:44:VAL:O	65:s:48:SER:N	2.24	0.69
53:h:82:VAL:O	53:h:86:ASN:N	2.24	0.69
58:k:239:SER:HA	64:r:18:LEU:HA	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C1:13:THR:HB	11:C1:168:LEU:HD23	1.73	0.69
58:k:32:GLN:NE2	59:l:373:GLU:OE1	2.26	0.69
59:x:40:ASN:OD1	59:x:41:TYR:N	2.25	0.69
1:3:84:LEU:HD21	2:1:309:ILE:HD11	0.70	0.69
4:7:13:PHE:O	4:7:16:GLY:N	2.26	0.69
23:A:181:ARG:HA	23:A:184:ARG:HH21	1.58	0.69
23:A:319:TRP:HE1	36:O:122:PHE:HE2	1.40	0.69
24:B:278:VAL:HG23	24:B:438:MET:HG3	1.73	0.69
37:P:40:LYS:O	43:V:7:LYS:N	2.26	0.69
38:Q:38:LYS:CG	38:Q:39:PRO:HD3	2.23	0.69
40:S:162:TYR:HD1	40:S:172:VAL:HG21	1.58	0.69
51:d:83:GLU:O	51:d:87:TRP:N	2.26	0.69
58:k:362:ARG:HG2	58:k:399:ILE:HD13	1.74	0.69
59:l:182:ARG:HD2	59:l:185:LYS:HD3	1.74	0.69
62:p:12:ASP:O	64:r:24:ARG:NH2	2.25	0.69
58:w:281:ASP:OD1	58:w:282:CYS:N	2.26	0.69
59:x:158:HIS:CE1	59:x:162:ASN:HD21	2.10	0.69
59:x:182:ARG:HD2	59:x:185:LYS:HD3	1.74	0.69
59:x:305:GLN:NE2	59:x:329:GLN:OE1	2.26	0.69
59:l:40:ASN:OD1	59:l:41:TYR:N	2.25	0.69
60:m:319:PRO:O	60:m:323:CYS:N	2.21	0.69
60:y:377:LEU:HD12	63:A2:20:TYR:CE2	2.26	0.69
62:A1:52:LYS:HB2	66:A4:34:TRP:CH2	2.28	0.69
2:1:77:MET:C	2:1:79:LEU:H	2.01	0.69
5:4:64:PRO:C	5:4:66:LEU:H	2.01	0.69
23:A:168:LEU:O	23:A:234:LYS:HB2	1.93	0.69
24:B:150:ALA:HB2	24:B:400:ILE:HD13	1.75	0.69
63:A2:77:LYS:HA	63:A2:80:TRP:CE2	2.28	0.69
17:C0:39:CYS:HG	17:C0:53:CYS:CB	2.05	0.68
24:B:188:THR:O	24:B:191:ALA:N	2.26	0.68
59:l:59:ASN:OD1	59:l:60:SER:N	2.24	0.68
60:y:240:MET:HB3	61:z:208:MET:HE1	1.74	0.68
5:4:188:ASN:OD1	5:4:189:SER:N	2.26	0.68
5:4:346:ARG:HD3	5:4:413:MET:HE3	1.75	0.68
23:A:355:LYS:HB2	23:A:530:TYR:CZ	2.28	0.68
23:A:504:SER:H	23:A:505:GLY:HA2	1.59	0.68
30:H:41:ILE:HG12	49:b:174:ILE:HG21	1.74	0.68
39:R:150:GLN:HA	39:R:153:ALA:HB3	1.75	0.68
44:M:60:PHE:HE1	44:M:83:LYS:HG2	1.56	0.68
58:k:252:HIS:HD2	58:k:323:HIS:CE1	2.11	0.68
60:m:137:GLN:HE21	60:m:141:TRP:CD1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:204:GLU:HB3	58:w:207:GLN:HG2	1.76	0.68
3:9:179:ALA:HB1	3:9:181:VAL:HG22	1.75	0.68
67:B6:56:LYS:HG2	67:B6:60:GLU:HB3	1.74	0.68
23:A:464:GLN:O	23:A:468:GLU:N	2.26	0.68
42:U:115:PHE:HB2	42:U:117:LEU:HG	1.75	0.68
58:k:436:ARG:HH21	60:m:222:PRO:HD3	1.57	0.68
60:y:228:ASP:O	60:y:232:ALA:N	2.19	0.68
3:9:191:ASN:OD1	9:8:164:ASN:ND2	2.21	0.68
14:B4:43:PRO:HB2	14:B4:48:ILE:HD11	1.76	0.68
39:R:197:GLU:HB3	39:R:259:ARG:HB2	1.75	0.68
44:M:70:LEU:HD13	44:M:76:ILE:HG12	1.75	0.68
58:k:111:GLU:HG2	58:k:215:HIS:NE2	2.08	0.68
58:w:252:HIS:HD2	58:w:323:HIS:CE1	2.11	0.68
60:y:345:HIS:HA	60:y:348:ILE:HD12	1.73	0.68
2:1:77:MET:O	2:1:80:GLY:N	2.21	0.68
60:m:345:HIS:HA	60:m:348:ILE:HD12	1.74	0.68
60:y:137:GLN:HE21	60:y:141:TRP:CD1	2.12	0.68
40:S:193:VAL:HG22	40:S:244:LEU:HB3	1.75	0.68
45:X:13:HIS:O	45:X:15:LEU:N	2.26	0.68
56:g:43:ARG:HB2	56:g:44:PRO:HD3	1.75	0.68
9:8:131:ILE:HG23	9:8:169:LEU:HD21	1.75	0.68
39:R:208:GLY:N	39:R:211:ASP:OD2	2.25	0.68
59:x:375:SER:O	59:x:379:LEU:N	2.22	0.68
61:z:105:ASN:HB3	61:z:108:ALA:HB3	1.75	0.68
8:2:84:TRP:CD1	8:2:84:TRP:H	2.11	0.68
58:k:217:SER:N	58:k:218:GLY:HA3	2.08	0.68
61:o:10:TYR:HH	61:o:129:SER:HG	1.35	0.68
21:A0:19:TRP:HZ2	22:A8:14:GLU:HG2	1.59	0.68
58:k:314:TYR:N	58:k:317:THR:O	2.27	0.68
60:m:145:VAL:O	60:m:149:LEU:N	2.25	0.68
60:y:111:GLU:N	60:y:111:GLU:OE1	2.25	0.68
58:k:426:GLY:HA2	58:k:428:ILE:HG13	1.76	0.67
8:2:250:SER:HB2	8:2:257:LEU:HD13	1.76	0.67
23:A:61:PRO:HG3	23:A:146:PHE:CE2	2.29	0.67
63:q:15:GLY:O	63:q:19:TRP:N	2.22	0.67
58:w:111:GLU:HG2	58:w:215:HIS:NE2	2.08	0.67
62:A1:91:TRP:C	62:A1:93:GLY:H	2.01	0.67
63:A2:101:ARG:HB3	63:A2:104:ARG:HH21	1.58	0.67
68:B5:65:VAL:O	68:B5:77:ARG:NE	2.25	0.67
7:6:224:SER:HB3	7:6:256:GLY:HA3	1.76	0.67
23:A:643:ARG:NH1	23:A:656:TYR:OH	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:187:ARG:HG2	36:O:88:MET:HE1	1.76	0.67
59:l:109:VAL:HG22	59:l:119:LEU:HD21	1.77	0.67
7:6:605:HIS:HE1	8:2:93:MET:SD	2.18	0.67
10:C3:151:HIS:O	10:C3:155:VAL:HG23	1.95	0.67
23:A:382:ARG:HG3	23:A:383:SER:H	1.59	0.67
23:A:535:GLU:O	23:A:538:GLN:N	2.27	0.67
24:B:106:VAL:HG23	24:B:107:ARG:H	1.59	0.67
35:N:88:LEU:HD11	35:N:92:ARG:HH21	1.59	0.67
52:f:156:PRO:HG2	52:f:158:ARG:H	1.60	0.67
56:g:89:GLU:O	56:g:93:ARG:N	2.25	0.67
60:m:240:MET:HB3	61:o:208:MET:HE1	1.76	0.67
38:Q:9:SER:HA	43:V:88:ARG:HH12	1.60	0.67
58:k:159:GLN:HG3	58:k:235:ARG:HH21	1.60	0.67
63:q:77:LYS:HA	63:q:80:TRP:CE2	2.29	0.67
63:q:101:ARG:HB3	63:q:104:ARG:HH21	1.58	0.67
1:3:98:LEU:HD22	2:1:298:LEU:HD21	1.77	0.67
2:1:276:SER:HB3	27:E:70:LEU:HD13	1.77	0.67
11:C1:186:SER:HB3	11:C1:213:LEU:HD22	1.76	0.67
39:R:143:ASP:O	39:R:147:LYS:N	2.27	0.67
59:l:375:SER:O	59:l:379:LEU:N	2.22	0.67
61:o:101:ALA:O	61:o:105:ASN:ND2	2.28	0.67
67:u:58:LYS:HG3	67:u:59:TYR:H	1.59	0.67
12:A9:154:GLY:HA2	15:A5:6:VAL:HG22	1.75	0.67
41:T:82:GLU:HG3	41:T:84:PRO:HD2	1.77	0.67
48:a:108:ASP:C	48:a:110:ASP:H	2.01	0.67
56:g:50:GLU:OE2	56:g:54:ARG:NE	2.21	0.67
62:p:13:TYR:HD1	64:r:27:PRO:HG2	1.60	0.67
61:z:101:ALA:O	61:z:105:ASN:ND2	2.28	0.67
2:1:233:MET:CA	2:1:236:ILE:HG22	2.23	0.67
4:7:136:PHE:N	4:7:138:GLU:O	2.27	0.67
10:C3:298:ASP:HB2	10:C3:301:THR:HG23	1.77	0.67
30:H:65:GLU:OE2	30:H:71:LYS:HB2	1.94	0.67
67:u:55:ILE:HG23	67:u:58:LYS:HE3	1.76	0.67
61:z:148:TYR:N	61:z:158:ILE:O	2.27	0.67
63:A2:35:ASP:OD1	63:A2:89:TYR:OH	2.13	0.67
2:1:176:LEU:CB	2:1:177:PRO:HD2	2.08	0.67
8:2:227:THR:HA	8:2:230:LEU:HD13	1.76	0.67
25:C:62:ALA:O	25:C:65:GLU:N	2.25	0.67
31:I:108:LYS:HZ2	31:I:108:LYS:CA	2.06	0.67
58:k:17:SER:OG	58:k:205:HIS:NE2	2.28	0.67
61:o:105:ASN:HB3	61:o:108:ALA:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:p:91:TRP:C	62:p:93:GLY:H	2.03	0.67
63:q:35:ASP:OD1	63:q:89:TYR:OH	2.13	0.67
23:A:382:ARG:HH22	23:A:652:ASN:HD21	1.43	0.67
24:B:293:LEU:O	24:B:296:SER:N	2.24	0.67
58:w:159:GLN:HG3	58:w:235:ARG:HH21	1.60	0.67
58:w:436:ARG:HH21	60:y:221:HIS:HB3	1.59	0.67
2:1:75:PRO:C	2:1:77:MET:H	2.03	0.66
2:1:77:MET:C	2:1:79:LEU:N	2.53	0.66
23:A:624:ARG:NH2	23:A:628:GLU:OE2	2.28	0.66
24:B:272:THR:HA	24:B:275:ILE:HD12	1.74	0.66
25:C:110:PHE:CD1	25:C:136:SER:HB3	2.30	0.66
52:f:42:CYS:HA	52:f:45:ARG:HB3	1.76	0.66
60:m:111:GLU:OE1	60:m:111:GLU:N	2.25	0.66
61:o:33:TYR:CD1	61:o:37:CYS:HB2	2.30	0.66
58:w:17:SER:OG	58:w:205:HIS:NE2	2.28	0.66
67:B6:58:LYS:HG3	67:B6:59:TYR:H	1.60	0.66
9:8:177:TYR:OH	28:F:96:ARG:O	2.06	0.66
31:I:105:LYS:C	31:I:106:GLU:CG	2.68	0.66
38:Q:45:LEU:HB3	38:Q:135:ARG:HH22	1.60	0.66
52:f:163:LEU:N	52:f:164:PRO:CA	2.58	0.66
59:x:438:GLU:OE1	59:x:438:GLU:N	2.26	0.66
62:A1:95:PRO:O	62:A1:137:GLY:N	2.28	0.66
66:A4:30:VAL:O	66:A4:34:TRP:N	2.21	0.66
6:5:12:PHE:HB2	6:5:39:SER:HB2	1.76	0.66
23:A:347:ASP:OD1	23:A:347:ASP:N	2.25	0.66
24:B:95:LEU:HD23	24:B:458:PHE:HZ	1.57	0.66
39:R:51:VAL:HG23	39:R:52:SER:H	1.59	0.66
41:T:78:ALA:HA	41:T:89:ASN:ND2	2.10	0.66
44:M:62:ILE:HG23	44:M:66:ASP:HB2	1.77	0.66
59:x:109:VAL:HG22	59:x:119:LEU:HD21	1.77	0.66
59:x:171:ALA:HB2	59:x:235:ALA:HB1	1.76	0.66
60:y:59:THR:OG1	60:y:172:LYS:HG2	1.96	0.66
61:z:33:TYR:CD1	61:z:37:CYS:HB2	2.30	0.66
2:1:26:LYS:HD3	2:1:36:GLY:HA3	1.76	0.66
2:1:190:LEU:HD11	2:1:197:PRO:HD2	1.77	0.66
7:6:68:TRP:CD1	7:6:69:LEU:HG	2.30	0.66
12:A9:209:ILE:O	12:A9:213:THR:HG23	1.95	0.66
29:G:108:GLU:OE2	29:G:113:GLY:HA2	1.95	0.66
44:M:60:PHE:CE1	44:M:83:LYS:HG2	2.30	0.66
61:o:23:HIS:NE2	67:u:51:LEU:HA	2.10	0.66
58:w:8:LEU:HD22	58:w:393:ALA:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:314:TYR:N	58:w:317:THR:O	2.27	0.66
59:x:213:HIS:O	59:x:217:LYS:N	2.23	0.66
60:y:32:ASN:HD21	60:y:227:LYS:HE2	1.61	0.66
67:B6:51:LEU:O	67:B6:55:ILE:N	2.20	0.66
24:B:94:VAL:HG21	26:D:89:LEU:HG	1.78	0.66
24:B:386:THR:OG1	24:B:387:GLU:N	2.27	0.66
39:R:208:GLY:H	39:R:211:ASP:CG	2.04	0.66
63:q:103:GLU:O	63:q:107:TRP:N	2.19	0.66
25:C:88:ILE:HD11	25:C:143:ILE:HD11	1.76	0.66
63:q:77:LYS:HA	63:q:80:TRP:CD2	2.31	0.66
58:w:426:GLY:HA2	58:w:428:ILE:HG13	1.76	0.66
59:x:26:PHE:HA	59:x:36:ALA:HA	1.78	0.66
2:1:74:ALA:O	2:1:77:MET:HB2	1.95	0.66
8:2:87:MET:HE2	8:2:90:PHE:CZ	2.29	0.66
10:C3:273:MET:HG3	10:C3:319:LYS:HZ1	1.60	0.66
33:K:16:LEU:HD23	33:K:94:VAL:HG12	1.78	0.66
41:T:6:LEU:HB3	41:T:10:TRP:CD1	2.31	0.66
58:k:124:ASP:HA	58:k:127:ILE:HB	1.78	0.66
59:l:28:ARG:HH21	59:l:32:GLY:HA2	1.60	0.66
59:l:171:ALA:HB2	59:l:235:ALA:HB1	1.76	0.66
59:l:438:GLU:N	59:l:438:GLU:OE1	2.26	0.66
59:x:58:GLU:OE2	59:x:66:SER:N	2.29	0.66
5:4:76:MET:O	5:4:80:SER:N	2.27	0.66
8:2:137:ALA:O	8:2:140:SER:OG	2.13	0.66
9:8:269:ARG:HG2	9:8:340:ASP:OD2	1.96	0.66
38:Q:45:LEU:O	38:Q:135:ARG:NH2	2.29	0.66
41:T:62:THR:HG23	41:T:104:ARG:CD	2.26	0.66
46:Y:93:SER:O	51:d:104:ARG:NH1	2.28	0.66
4:7:66:VAL:O	4:7:70:TYR:N	2.29	0.66
58:k:19:LEU:HD13	58:k:217:SER:HA	1.77	0.66
58:k:404:ALA:HB1	58:k:408:ARG:HH12	1.60	0.66
59:l:26:PHE:HA	59:l:36:ALA:HA	1.78	0.66
60:m:32:ASN:HD21	60:m:227:LYS:HE2	1.61	0.66
58:w:124:ASP:HA	58:w:127:ILE:HB	1.78	0.66
59:x:339:ALA:O	59:x:343:GLN:N	2.25	0.66
2:1:169:GLN:HG2	2:1:174:LEU:HB2	1.77	0.66
7:6:310:LEU:HA	7:6:313:MET:HE3	1.78	0.66
24:B:203:MET:HE1	24:B:254:ARG:HB3	1.78	0.66
34:L:63:MET:HE2	38:Q:130:LYS:HD2	1.78	0.66
53:h:84:ILE:HG22	53:h:88:ARG:NH1	2.09	0.66
66:t:12:GLN:NE2	63:A2:109:LYS:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:B6:55:ILE:HG23	67:B6:58:LYS:HE3	1.76	0.66
29:G:107:TRP:HD1	29:G:108:GLU:O	1.78	0.65
40:S:190:HIS:HA	40:S:241:CYS:HB3	1.77	0.65
62:p:14:ARG:O	64:r:24:ARG:NE	2.28	0.65
58:w:17:SER:HG	58:w:205:HIS:CE1	2.14	0.65
8:2:22:ILE:HD11	30:H:4:PHE:HB2	1.79	0.65
27:E:106:TYR:CE1	27:E:112:ARG:HG3	2.31	0.65
35:N:38:ILE:O	35:N:45:ARG:NH2	2.29	0.65
40:S:182:THR:HG23	40:S:183:ILE:HG13	1.77	0.65
58:k:110:VAL:O	58:k:114:ALA:N	2.26	0.65
61:o:79:GLU:O	61:o:80:MET:HG2	1.96	0.65
58:w:38:GLY:HA2	58:w:98:TYR:HA	1.79	0.65
58:w:408:ARG:HE	66:A4:15:ARG:NH2	1.94	0.65
63:A2:77:LYS:HA	63:A2:80:TRP:CD2	2.31	0.65
2:1:237:PHE:O	2:1:240:ILE:HG13	1.96	0.65
2:1:266:LEU:O	2:1:269:SER:HB2	1.95	0.65
8:2:87:MET:O	8:2:88:LYS:C	2.37	0.65
24:B:241:MET:HE3	24:B:351:MET:HE1	1.79	0.65
40:S:226:GLU:HA	40:S:229:TYR:CD2	2.30	0.65
41:T:27:SER:O	41:T:31:ALA:N	2.28	0.65
61:o:198:HIS:O	61:o:201:ARG:HG2	1.97	0.65
59:x:267:ALA:O	59:x:271:ALA:N	2.29	0.65
61:z:19:SER:O	61:z:202:LYS:NZ	2.29	0.65
1:3:112:GLU:OE2	2:1:290:TRP:NE1	2.29	0.65
5:4:1:MET:HB2	5:4:52:PHE:CZ	2.31	0.65
12:A9:101:PHE:HZ	12:A9:260:GLY:HA3	1.61	0.65
21:A0:45:LEU:HD21	22:A8:40:TYR:HA	1.78	0.65
23:A:355:LYS:CD	23:A:530:TYR:CE1	2.52	0.65
25:C:70:ILE:HD11	25:C:101:PHE:CZ	2.31	0.65
59:l:58:GLU:OE2	59:l:66:SER:N	2.29	0.65
60:m:164:ILE:O	60:m:177:ARG:NH1	2.30	0.65
61:o:237:TYR:HB2	63:q:60:PHE:CD1	2.31	0.65
66:t:43:ASP:O	67:u:33:ARG:NH1	2.29	0.65
59:x:21:PRO:HD3	59:x:41:TYR:HD2	1.61	0.65
3:9:222:ARG:HD2	3:9:226:GLU:HB2	1.77	0.65
9:8:325:PRO:HD2	9:8:347:THR:HG21	1.78	0.65
23:A:320:GLU:OE1	36:O:123:TYR:OH	2.10	0.65
23:A:628:GLU:HA	23:A:633:THR:HG22	1.78	0.65
52:f:35:ASP:OD1	52:f:36:LYS:N	2.29	0.65
58:k:38:GLY:HA2	58:k:98:TYR:HA	1.79	0.65
59:x:25:GLU:O	59:x:37:SER:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:200:ASP:OD2	3:9:219:ARG:NH1	2.30	0.65
3:9:224:SER:OG	3:9:226:GLU:CD	2.40	0.65
11:C1:120:SER:OG	11:C1:138:VAL:HG21	1.97	0.65
17:C0:38:ARG:HG2	17:C0:85:ILE:HG23	1.76	0.65
23:A:255:ASP:N	23:A:255:ASP:OD1	2.28	0.65
59:l:83:PHE:CZ	63:A2:104:ARG:HG2	2.32	0.65
61:o:148:TYR:N	61:o:158:ILE:O	2.27	0.65
59:x:105:MET:SD	59:x:107:TYR:OH	2.50	0.65
62:A1:96:LEU:HA	62:A1:136:ILE:HA	1.79	0.65
3:9:228:ALA:O	9:8:284:ASN:ND2	2.30	0.65
40:S:237:MET:HG3	40:S:243:VAL:HG21	1.78	0.65
59:l:21:PRO:HD3	59:l:41:TYR:HD2	1.61	0.65
61:z:198:HIS:O	61:z:201:ARG:HG2	1.97	0.65
2:1:74:ALA:HB3	2:1:75:PRO:HD3	1.79	0.65
2:1:311:THR:O	2:1:312:SER:OG	2.15	0.65
8:2:80:PHE:HB3	30:H:64:ARG:HH12	1.61	0.65
23:A:155:GLU:OE1	23:A:155:GLU:N	2.28	0.65
40:S:162:TYR:CD1	40:S:172:VAL:HG21	2.30	0.65
40:S:286:VAL:O	40:S:289:LYS:N	2.29	0.65
59:l:339:ALA:O	59:l:343:GLN:N	2.25	0.65
60:m:71:ARG:NH1	61:o:45:TYR:O	2.30	0.65
61:o:19:SER:O	61:o:202:LYS:NZ	2.30	0.65
62:A1:12:ASP:O	64:A3:24:ARG:NH2	2.29	0.65
62:A1:155:GLY:HA3	62:A1:166:ASP:C	2.22	0.65
63:A2:17:ARG:HD3	82:A2:201:UQ2:H2M1	1.77	0.65
10:C3:195:LEU:HD23	10:C3:245:ILE:HD13	1.79	0.65
17:C0:39:CYS:HG	17:C0:53:CYS:HG	0.73	0.65
39:R:203:PRO:HB3	39:R:265:PHE:HD2	1.60	0.65
45:X:37:PHE:HD2	49:b:137:MET:HB3	1.61	0.65
56:g:52:ILE:O	56:g:56:HIS:N	2.28	0.65
5:4:304:GLN:O	5:4:305:THR:OG1	2.15	0.65
9:8:177:TYR:HD1	9:8:182:ILE:HB	1.60	0.65
12:A9:160:LEU:HD13	12:A9:222:GLN:HG2	1.78	0.65
26:D:182:TYR:CE2	27:E:180:HIS:HB2	2.32	0.65
27:E:104:ARG:HH12	27:E:112:ARG:NH2	1.95	0.65
27:E:128:ILE:HD13	27:E:147:ILE:HG12	1.77	0.65
33:K:62:GLN:O	33:K:64:LYS:N	2.30	0.65
59:l:267:ALA:O	59:l:271:ALA:N	2.29	0.65
62:A1:77:LYS:CB	62:A1:78:LEU:HA	2.27	0.65
24:B:396:THR:OG1	24:B:397:TYR:N	2.29	0.64
60:m:59:THR:OG1	60:m:172:LYS:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:o:159:GLY:N	81:o:301:HEC:O1D	2.22	0.64
59:x:227:ARG:HB3	59:x:228:GLY:HA3	1.78	0.64
60:y:164:ILE:O	60:y:177:ARG:NH1	2.30	0.64
63:A2:16:ILE:HD12	63:A2:19:TRP:HZ3	1.62	0.64
66:A4:15:ARG:CG	66:A4:16:ASN:H	2.10	0.64
5:4:71:TRP:O	5:4:74:PRO:HD2	1.97	0.64
5:4:382:VAL:HG22	5:4:396:MET:HE3	1.79	0.64
6:5:9:MET:O	6:5:12:PHE:N	2.30	0.64
6:5:97:GLN:N	8:2:117:GLU:OE2	2.30	0.64
23:A:259:SER:OG	23:A:260:ASN:N	2.30	0.64
24:B:322:SER:OG	24:B:328:ASP:OD2	2.13	0.64
40:S:275:ASN:C	40:S:277:ARG:H	2.04	0.64
57:e:47:GLU:O	57:e:50:ALA:N	2.25	0.64
60:m:289:GLY:HA2	60:m:292:LEU:HD12	1.79	0.64
60:y:138:MET:HB2	60:y:255:ASN:HD22	1.63	0.64
60:y:145:VAL:O	60:y:149:LEU:N	2.25	0.64
60:y:215:VAL:HG12	64:A3:8:THR:HG21	1.78	0.64
60:y:289:GLY:HA2	60:y:292:LEU:HD12	1.79	0.64
62:A1:79:SER:C	62:A1:81:ILE:H	2.05	0.64
65:B7:10:GLU:N	65:B7:11:GLU:HA	2.12	0.64
9:8:342:LEU:HB3	9:8:348:GLY:HA2	1.79	0.64
10:C3:172:LYS:HB2	10:C3:172:LYS:NZ	2.12	0.64
13:A7:24:LEU:H	14:B4:34:ASN:HD21	1.44	0.64
25:C:106:SER:HB2	35:N:51:ILE:HD12	1.79	0.64
33:K:32:GLY:O	33:K:36:PHE:N	2.28	0.64
33:K:45:LYS:NZ	33:K:51:LEU:O	2.30	0.64
47:Z:36:LEU:O	47:Z:40:GLY:N	2.29	0.64
57:e:70:THR:HG22	57:e:71:GLY:H	1.61	0.64
61:o:61:ALA:O	61:o:65:ALA:N	2.24	0.64
3:9:152:ILE:O	3:9:156:LEU:N	2.30	0.64
4:7:80:PRO:O	4:7:81:GLU:HG3	1.96	0.64
5:4:62:SER:OG	5:4:455:LEU:O	2.15	0.64
5:4:175:ASN:ND2	38:Q:168:PHE:O	2.30	0.64
7:6:81:LYS:N	7:6:133:THR:O	2.30	0.64
23:A:624:ARG:NH1	23:A:634:LEU:O	2.30	0.64
59:l:263:ALA:HA	59:l:319:SER:HA	1.79	0.64
5:4:372:THR:HA	5:4:448:THR:HG21	1.80	0.64
9:8:78:GLY:HA2	9:8:81:LYS:HG2	1.80	0.64
23:A:163:LYS:HE3	23:A:207:GLY:HA3	1.79	0.64
33:K:55:ILE:O	33:K:56:ARG:NH1	2.29	0.64
40:S:121:ALA:O	40:S:125:ALA:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:f:133:TRP:O	52:f:136:GLU:N	2.30	0.64
59:l:25:GLU:O	59:l:37:SER:N	2.27	0.64
58:w:404:ALA:HB1	58:w:408:ARG:HH12	1.60	0.64
2:1:233:MET:HA	2:1:236:ILE:HG21	1.77	0.64
4:7:136:PHE:O	4:7:138:GLU:N	2.31	0.64
23:A:76:ARG:NH1	23:A:90:ALA:HB2	2.12	0.64
58:k:8:LEU:HD22	58:k:393:ALA:HA	1.77	0.64
60:m:138:MET:HB2	60:m:255:ASN:HD22	1.63	0.64
61:z:237:TYR:OH	63:A2:57:ASP:OD1	2.12	0.64
1:3:12:THR:HA	1:3:15:THR:HG22	1.80	0.64
2:1:153:VAL:HA	2:1:156:MET:HE2	1.80	0.64
4:7:80:PRO:CD	4:7:81:GLU:N	2.60	0.64
58:k:403:ASP:HB3	58:k:406:VAL:HG23	1.80	0.64
59:l:31:ASN:ND2	59:l:225:ASN:OD1	2.31	0.64
59:l:213:HIS:O	59:l:217:LYS:N	2.23	0.64
60:m:226:ILE:HA	60:m:229:ILE:HD12	1.80	0.64
66:t:34:TRP:HA	66:t:37:ASP:OD1	1.98	0.64
59:x:28:ARG:HH21	59:x:32:GLY:HA2	1.60	0.64
61:z:23:HIS:HA	61:z:26:ILE:HD12	1.80	0.64
5:4:243:MET:O	5:4:247:THR:HG22	1.98	0.64
7:6:378:LEU:O	7:6:381:THR:OG1	2.15	0.64
24:B:61:TRP:CD1	24:B:62:LYS:C	2.73	0.64
24:B:278:VAL:HG12	24:B:283:ALA:HB2	1.78	0.64
60:m:312:GLN:NE2	60:m:318:ARG:HG3	2.12	0.64
61:o:237:TYR:HB2	63:q:60:PHE:CE1	2.32	0.64
58:w:348:SER:OG	66:A4:17:TRP:NE1	2.29	0.64
60:y:226:ILE:HA	60:y:229:ILE:HD12	1.80	0.64
61:z:61:ALA:O	61:z:65:ALA:N	2.24	0.64
2:1:316:PRO:CG	43:V:57:ARG:NE	2.59	0.64
5:4:276:CYS:SG	5:4:285:LEU:HD12	2.38	0.64
7:6:1:MET:HG2	7:6:59:GLN:HE22	1.61	0.64
23:A:568:TYR:HB3	23:A:583:ILE:HG22	1.80	0.64
24:B:67:ASN:HB2	40:S:181:VAL:HG13	1.80	0.64
27:E:118:LEU:O	27:E:121:ALA:N	2.30	0.64
41:T:69:ILE:HD13	41:T:100:ILE:HD11	1.80	0.64
43:V:72:MET:HE2	43:V:75:LEU:HD23	1.79	0.64
59:l:52:LYS:HD2	59:l:203:ARG:HG2	1.80	0.64
59:l:70:ARG:NH1	68:v:67:SER:OG	2.30	0.64
58:w:80:GLU:HG2	59:x:284:HIS:HB2	1.80	0.64
62:A1:11:SER:O	62:A1:14:ARG:N	2.30	0.64
62:A1:84:GLY:N	62:A1:100:HIS:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:529:PHE:HB3	7:6:530:PRO:HD3	1.80	0.64
23:A:137:CYS:SG	23:A:138:ASP:N	2.70	0.64
30:H:82:GLN:NE2	43:V:98:MET:O	2.31	0.64
56:g:11:PRO:HD2	56:g:109:ARG:NH1	2.11	0.64
58:k:347:THR:O	66:t:16:ASN:ND2	2.30	0.64
60:m:344:GLU:HG2	60:m:346:PRO:HD2	1.80	0.64
59:x:31:ASN:ND2	59:x:225:ASN:OD1	2.31	0.64
59:x:66:SER:HA	59:x:69:LEU:HB3	1.79	0.64
62:A1:136:ILE:N	62:A1:182:VAL:O	2.31	0.64
2:1:31:MET:HB3	27:E:74:LEU:HD11	1.79	0.63
4:7:17:PHE:CE2	6:5:11:ALA:HB1	2.33	0.63
6:5:92:ASN:ND2	8:2:54:GLU:OE2	2.31	0.63
26:D:176:ILE:HG22	26:D:177:VAL:HG13	1.80	0.63
39:R:203:PRO:HG2	79:R:601:NAP:H72N	1.62	0.63
60:m:71:ARG:HH12	61:o:45:TYR:HB3	1.61	0.63
61:o:23:HIS:HD2	67:u:55:ILE:HD12	1.62	0.63
58:w:110:VAL:O	58:w:114:ALA:N	2.26	0.63
58:w:403:ASP:HB3	58:w:406:VAL:HG23	1.80	0.63
59:x:325:TYR:HB3	68:B5:57:GLY:N	2.13	0.63
67:B6:18:SER:O	67:B6:22:LEU:N	2.30	0.63
7:6:341:MET:HE3	7:6:454:ILE:HD13	1.80	0.63
40:S:206:ILE:HD11	40:S:214:GLU:HB3	1.80	0.63
58:k:438:ARG:NH2	62:p:37:TYR:OH	2.32	0.63
59:l:105:MET:SD	59:l:107:TYR:OH	2.50	0.63
59:l:117:ASP:HA	59:l:120:MET:HE2	1.81	0.63
61:o:23:HIS:HA	61:o:26:ILE:HD12	1.80	0.63
59:x:117:ASP:HA	59:x:120:MET:HE2	1.81	0.63
60:y:31:TRP:HA	60:y:100:ARG:HH11	1.63	0.63
63:A2:16:ILE:O	63:A2:17:ARG:C	2.42	0.63
3:9:228:ALA:HB3	9:8:284:ASN:HD22	1.63	0.63
5:4:354:LEU:HA	72:6:701:CDL:HA22	1.79	0.63
9:8:395:VAL:HG23	9:8:398:ARG:NH1	2.13	0.63
9:8:420:GLU:H	9:8:422:HIS:HD2	1.44	0.63
26:D:146:GLU:CB	26:D:147:PRO:CD	2.76	0.63
26:D:169:VAL:HG12	26:D:170:VAL:O	1.98	0.63
40:S:213:HIS:HA	40:S:215:MET:HE2	1.80	0.63
58:k:86:LEU:N	59:l:284:HIS:O	2.31	0.63
59:l:66:SER:HA	59:l:69:LEU:HB3	1.79	0.63
59:l:312:PHE:N	59:l:323:GLY:O	2.28	0.63
62:p:31:ALA:HB2	67:u:7:ALA:HB2	1.79	0.63
65:s:57:GLU:OE1	65:s:57:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:y:67:THR:O	60:y:71:ARG:HG2	1.98	0.63
8:2:13:ILE:O	8:2:16:GLY:N	2.30	0.63
23:A:59:GLN:HE21	29:G:91:VAL:HG22	1.63	0.63
26:D:178:PRO:HB2	39:R:92:MET:HG2	1.79	0.63
60:m:67:THR:O	60:m:71:ARG:HG2	1.98	0.63
63:q:75:LEU:O	63:q:80:TRP:NE1	2.32	0.63
7:6:457:LEU:O	7:6:461:SER:N	2.32	0.63
27:E:115:ALA:O	27:E:140:ARG:NH1	2.32	0.63
46:Y:89:TYR:O	46:Y:91:ASP:N	2.30	0.63
60:m:31:TRP:HA	60:m:100:ARG:HH11	1.63	0.63
62:p:13:TYR:O	64:r:24:ARG:N	2.30	0.63
7:6:4:PHE:HD2	7:6:61:LEU:HD12	1.64	0.63
8:2:52:ALA:HB2	8:2:123:PRO:HD2	1.81	0.63
9:8:98:LYS:HE3	9:8:99:TRP:HE1	1.63	0.63
23:A:340:ALA:HB2	23:A:546:PHE:HD2	1.63	0.63
29:G:68:PRO:HG2	29:G:72:ILE:HD11	1.80	0.63
61:o:61:ALA:HA	61:o:64:LEU:HB3	1.80	0.63
62:p:20:ASP:OD1	62:p:21:SER:N	2.31	0.63
62:p:71:MET:HG3	62:p:72:SER:H	1.61	0.63
59:x:52:LYS:HD2	59:x:203:ARG:HG2	1.80	0.63
59:x:263:ALA:HA	59:x:319:SER:HA	1.80	0.63
62:A1:78:LEU:H	62:A1:192:MET:HA	1.62	0.63
66:A4:40:LEU:C	66:A4:40:LEU:HD12	2.23	0.63
7:6:335:PHE:CE2	7:6:383:MET:HE1	2.33	0.63
10:C3:187:SER:CB	10:C3:277:MET:HE1	2.28	0.63
25:C:174:ASP:OD2	25:C:189:ILE:N	2.30	0.63
29:G:121:LEU:O	29:G:123:ASN:N	2.28	0.63
40:S:47:LEU:HD12	40:S:48:ILE:H	1.64	0.63
8:2:80:PHE:O	8:2:81:SER:OG	2.12	0.63
11:C1:122:MET:HB2	11:C1:208:PRO:HD2	1.81	0.63
13:A7:16:TYR:CE1	13:A7:25:PRO:HG3	2.34	0.63
25:C:171:GLU:OE1	25:C:172:ILE:N	2.31	0.63
57:e:63:GLU:O	57:e:65:TYR:N	2.27	0.63
61:o:165:TYR:HA	61:o:179:MET:HE2	1.81	0.63
58:w:152:TYR:HB3	58:w:241:ILE:HD13	1.81	0.63
59:x:258:VAL:HG22	59:x:323:GLY:HA3	1.80	0.63
61:z:73:GLY:HA2	61:z:79:GLU:HG3	1.81	0.63
2:1:237:PHE:CE1	2:1:240:ILE:HD11	2.34	0.63
24:B:206:GLU:OE2	24:B:247:PHE:HZ	1.81	0.63
27:E:131:GLU:OE1	27:E:144:ARG:NH1	2.31	0.63
41:T:24:ALA:O	41:T:27:SER:OG	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:k:235:ARG:NH1	62:p:14:ARG:HH12	1.96	0.63
61:o:13:SER:O	61:o:19:SER:HB3	1.99	0.63
58:w:213:GLN:OE1	58:w:214:LYS:NZ	2.25	0.63
60:y:212:SER:OG	63:A2:39:GLU:OE2	2.12	0.63
60:y:312:GLN:NE2	60:y:318:ARG:HG3	2.12	0.63
61:z:61:ALA:HA	61:z:64:LEU:HB3	1.81	0.63
61:z:70:VAL:HG23	61:z:81:PHE:O	1.99	0.63
63:A2:26:PHE:HB2	63:A2:31:LEU:HD12	1.81	0.63
23:A:639:LEU:O	23:A:642:VAL:N	2.28	0.62
26:D:193:LEU:O	26:D:196:GLY:N	2.28	0.62
30:H:56:CYS:O	30:H:58:ILE:N	2.31	0.62
49:b:121:ILE:HD11	53:h:105:PHE:CE1	2.34	0.62
58:k:46:ARG:HA	58:k:162:PRO:HB2	1.80	0.62
59:l:305:GLN:HB3	59:l:306:PRO:HD3	1.80	0.62
59:l:308:ASP:OD1	59:l:309:VAL:N	2.32	0.62
61:o:69:GLU:OE1	61:o:69:GLU:N	2.31	0.62
67:u:18:SER:O	67:u:22:LEU:N	2.30	0.62
61:z:173:ASP:OD2	61:z:175:THR:OG1	2.14	0.62
65:B7:57:GLU:OE1	65:B7:57:GLU:N	2.31	0.62
2:1:261:ILE:O	2:1:261:ILE:CG2	2.47	0.62
4:7:78:GLN:O	4:7:80:PRO:CD	2.38	0.62
4:7:84:LEU:O	4:7:84:LEU:HD23	1.98	0.62
5:4:308:SER:O	5:4:312:ALA:N	2.30	0.62
23:A:380:ASP:OD2	33:K:41:TYR:OH	2.17	0.62
59:x:133:ARG:HD2	59:x:136:GLU:CD	2.24	0.62
5:4:287:ALA:O	5:4:290:SER:OG	2.16	0.62
9:8:346:GLN:OE1	9:8:441:HIS:NE2	2.32	0.62
10:C3:11:ASN:HD21	10:C3:13:LYS:HB2	1.64	0.62
10:C3:84:PRO:HG3	10:C3:92:MET:HE3	1.80	0.62
17:C0:57:ARG:HB3	17:C0:57:ARG:HH11	1.64	0.62
25:C:192:ASP:OD1	25:C:193:TYR:N	2.26	0.62
30:H:84:GLU:HA	30:H:87:ILE:HG13	1.81	0.62
30:H:84:GLU:HG3	30:H:87:ILE:HD11	1.81	0.62
58:k:152:TYR:HB3	58:k:241:ILE:HD13	1.81	0.62
62:p:75:GLU:HG2	62:p:76:ILE:HA	1.80	0.62
63:A2:75:LEU:O	63:A2:80:TRP:NE1	2.32	0.62
1:3:7:LEU:HD21	70:1:401:3PE:H391	1.79	0.62
5:4:219:ALA:O	5:4:223:ALA:HB2	1.99	0.62
10:C3:92:MET:HE2	10:C3:167:THR:HG21	1.82	0.62
27:E:72:MET:O	27:E:75:SER:N	2.32	0.62
27:E:82:ALA:HB2	37:P:25:GLN:HE21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:I:62:GLU:HB3	42:U:124:TYR:HD1	1.64	0.62
58:w:46:ARG:HA	58:w:162:PRO:HB2	1.80	0.62
60:y:377:LEU:CD1	63:A2:20:TYR:CE2	2.82	0.62
61:z:83:ARG:O	61:z:85:GLY:N	2.33	0.62
3:9:54:ASP:OD1	3:9:55:PHE:N	2.33	0.62
7:6:137:LEU:HB3	7:6:196:TRP:HB2	1.81	0.62
9:8:246:GLU:HA	9:8:249:ALA:HB3	1.81	0.62
24:B:308:TYR:OH	24:B:401:GLU:N	2.23	0.62
36:O:42:GLU:CD	36:O:45:ASN:HB3	2.23	0.62
59:l:245:ARG:HH21	59:l:433:THR:HB	1.65	0.62
60:m:237:LEU:HA	60:m:240:MET:HB2	1.81	0.62
61:o:83:ARG:O	61:o:85:GLY:N	2.33	0.62
63:q:26:PHE:HB2	63:q:31:LEU:HD12	1.81	0.62
80:y:401:HEM:CGD	80:y:401:HEM:HHA	2.30	0.62
63:A2:16:ILE:HG23	63:A2:19:TRP:CZ3	2.22	0.62
67:B6:52:TRP:HA	67:B6:55:ILE:HB	1.82	0.62
9:8:60:GLY:O	9:8:256:ARG:NH1	2.33	0.62
39:R:186:VAL:O	39:R:190:GLU:N	2.31	0.62
60:m:74:ASN:HB2	62:p:61:SER:HA	1.81	0.62
80:m:401:HEM:CGD	80:m:401:HEM:HHA	2.30	0.62
59:x:308:ASP:OD1	59:x:309:VAL:N	2.32	0.62
82:A2:201:UQ2:CM5	82:A2:201:UQ2:H8	2.29	0.62
9:8:318:ILE:HB	9:8:355:ILE:HG13	1.82	0.62
23:A:418:ILE:O	23:A:422:TRP:N	2.30	0.62
24:B:370:GLU:OE2	24:B:374:SER:OG	2.16	0.62
39:R:178:SER:H	39:R:181:LEU:HB3	1.63	0.62
45:X:55:THR:HG21	49:b:131:LYS:HD2	1.82	0.62
57:e:89:TRP:CD1	57:e:89:TRP:H	2.15	0.62
58:k:135:LEU:HD23	58:k:138:LEU:HD12	1.82	0.62
67:u:52:TRP:HA	67:u:55:ILE:HB	1.82	0.62
66:A4:40:LEU:HD12	66:A4:41:ILE:N	2.14	0.62
23:A:163:LYS:CE	23:A:207:GLY:HA3	2.29	0.62
50:c:83:HIS:CE1	50:c:87:LYS:HB2	2.35	0.62
56:g:89:GLU:O	56:g:92:TRP:N	2.33	0.62
61:o:129:SER:HB3	61:o:152:TYR:CZ	2.35	0.62
2:1:260:THR:O	2:1:264:LEU:HB3	1.98	0.62
6:5:94:ASN:OD1	6:5:95:LEU:N	2.32	0.62
8:2:109:ALA:O	8:2:112:HIS:CD2	2.53	0.62
30:H:62:ASP:OD1	30:H:63:PHE:N	2.32	0.62
31:I:111:THR:HG21	31:I:118:GLN:HA	1.82	0.62
39:R:61:ALA:H	39:R:129:LEU:HD11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Z:41:LEU:H	47:Z:42:ARG:HA	1.64	0.62
59:l:133:ARG:HD2	59:l:136:GLU:CD	2.24	0.62
59:l:399:LEU:HD23	59:l:402:ILE:HD12	1.81	0.62
80:y:402:HEM:HBB2	80:y:402:HEM:HMB1	1.82	0.62
61:z:165:TYR:HA	61:z:179:MET:HE2	1.81	0.62
63:A2:101:ARG:HA	63:A2:104:ARG:HE	1.65	0.62
26:D:155:SER:O	26:D:155:SER:OG	2.15	0.62
27:E:181:GLU:OE2	39:R:101:GLY:HA2	1.99	0.62
59:l:259:ALA:HB3	59:l:417:PHE:HA	1.81	0.62
8:2:50:PRO:HB2	24:B:72:PRO:HG2	1.81	0.61
11:C1:16:ILE:HD12	11:C1:17:MET:N	2.15	0.61
24:B:303:ARG:HD2	24:B:311:TYR:OH	2.00	0.61
40:S:120:GLN:O	40:S:124:TYR:N	2.29	0.61
59:l:258:VAL:HG22	59:l:323:GLY:HA3	1.80	0.61
67:u:51:LEU:O	67:u:55:ILE:N	2.20	0.61
58:w:203:LEU:HA	58:w:207:GLN:NE2	2.15	0.61
59:x:312:PHE:N	59:x:323:GLY:O	2.28	0.61
60:y:177:ARG:HB3	60:y:181:PHE:HE2	1.64	0.61
7:6:120:TYR:OH	72:6:701:CDL:OB6	2.19	0.61
10:C3:128:VAL:O	10:C3:128:VAL:HG22	1.99	0.61
25:C:213:ARG:HE	39:R:48:ARG:NH1	1.97	0.61
36:O:50:PHE:HE2	36:O:103:VAL:HG21	1.65	0.61
38:Q:47:ARG:CZ	38:Q:53:PRO:HB3	2.30	0.61
56:g:151:SER:C	56:g:153:ARG:H	2.09	0.61
59:l:59:ASN:N	59:l:62:ASN:HB3	2.08	0.61
60:m:162:GLU:O	60:m:166:GLY:N	2.32	0.61
80:m:402:HEM:HMB1	80:m:402:HEM:HBB2	1.82	0.61
62:p:75:GLU:OE1	62:p:75:GLU:N	2.33	0.61
60:y:237:LEU:HA	60:y:240:MET:HB2	1.81	0.61
61:z:13:SER:O	61:z:19:SER:HB3	1.99	0.61
61:z:129:SER:HB3	61:z:152:TYR:CZ	2.35	0.61
2:1:266:LEU:O	2:1:266:LEU:HD12	2.01	0.61
23:A:153:PHE:HE2	23:A:156:GLY:HA3	1.64	0.61
40:S:280:HIS:O	40:S:282:LEU:N	2.34	0.61
58:k:203:LEU:HA	58:k:207:GLN:NE2	2.15	0.61
59:l:200:THR:OG1	59:l:228:GLY:N	2.30	0.61
59:l:360:ALA:HA	59:l:363:LYS:HD2	1.81	0.61
60:m:71:ARG:HH21	61:o:49:ARG:NH2	1.98	0.61
59:x:21:PRO:HD2	59:x:40:ASN:HA	1.81	0.61
59:x:245:ARG:HH21	59:x:433:THR:HB	1.64	0.61
59:x:399:LEU:HD23	59:x:402:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:57:PHE:O	5:4:111:THR:HG23	2.01	0.61
8:2:69:LEU:HD23	8:2:97:LEU:HD11	1.81	0.61
12:A9:148:HIS:O	12:A9:152:MET:HG3	2.01	0.61
23:A:251:ILE:HB	23:A:606:THR:HG22	1.82	0.61
25:C:90:ILE:HG22	25:C:91:HIS:O	2.00	0.61
31:I:63:VAL:HG22	31:I:64:ASN:H	1.64	0.61
52:f:133:TRP:HA	52:f:136:GLU:HB3	1.81	0.61
59:l:399:LEU:HA	59:l:402:ILE:HD12	1.81	0.61
58:w:135:LEU:HD23	58:w:138:LEU:HD12	1.82	0.61
60:y:102:LEU:O	60:y:105:GLY:N	2.29	0.61
66:A4:11:ARG:N	66:A4:12:GLN:HA	2.16	0.61
7:6:418:PHE:HA	7:6:421:ILE:HG12	1.81	0.61
19:B2:3:ASN:C	19:B2:3:ASN:HD22	2.08	0.61
22:A8:13:LYS:H	22:A8:13:LYS:HD3	1.65	0.61
23:A:111:LYS:HD3	37:P:53:TYR:OH	2.00	0.61
36:O:98:LYS:HB3	36:O:102:HIS:HB2	1.81	0.61
41:T:112:ALA:O	41:T:116:ALA:N	2.32	0.61
58:k:215:HIS:HB2	58:k:216:PHE:CB	2.27	0.61
58:k:280:TYR:HA	58:k:284:TYR:HE2	1.66	0.61
63:q:101:ARG:HA	63:q:104:ARG:HE	1.65	0.61
61:z:178:THR:O	61:z:182:VAL:N	2.29	0.61
1:3:68:GLU:O	1:3:72:LEU:N	2.31	0.61
2:1:153:VAL:O	2:1:156:MET:N	2.32	0.61
2:1:312:SER:OG	43:V:55:ARG:NH1	2.32	0.61
3:9:92:TRP:CD1	3:9:126:PRO:HA	2.36	0.61
26:D:95:GLU:OE1	26:D:190:ALA:HB2	2.01	0.61
26:D:182:TYR:HE2	27:E:180:HIS:HB2	1.64	0.61
36:O:76:PRO:O	36:O:77:ARG:HG2	2.01	0.61
40:S:236:GLU:HA	40:S:239:GLU:HB2	1.82	0.61
55:j:44:ILE:O	55:j:47:ALA:N	2.32	0.61
44:M:12:LYS:HZ2	44:M:77:VAL:HG21	1.65	0.61
60:m:177:ARG:HB3	60:m:181:PHE:HE2	1.64	0.61
58:w:280:TYR:HA	58:w:284:TYR:HE2	1.65	0.61
59:x:56:ARG:NE	59:x:103:GLU:OE1	2.34	0.61
59:x:399:LEU:HA	59:x:402:ILE:HD12	1.81	0.61
1:3:73:LEU:HB3	1:3:74:PRO:HD3	1.83	0.61
2:1:203:GLY:N	2:1:210:GLY:H	1.93	0.61
2:1:235:ASN:N	2:1:235:ASN:OD1	2.32	0.61
2:1:311:THR:O	2:1:311:THR:HG22	2.01	0.61
7:6:123:LEU:HA	7:6:126:ILE:HD12	1.82	0.61
8:2:109:ALA:HB3	8:2:110:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:119:VAL:H	56:g:147:GLY:H	1.49	0.61
58:k:75:LEU:HD11	58:k:116:ILE:HD11	1.83	0.61
65:B7:53:ASP:OD1	65:B7:54:CYS:N	2.34	0.61
2:1:233:MET:O	2:1:236:ILE:HG23	2.01	0.61
4:7:125:TRP:CD1	43:V:138:TYR:HH	2.19	0.61
9:8:395:VAL:HG23	9:8:398:ARG:HH11	1.66	0.61
24:B:80:LEU:HD22	24:B:82:LEU:HG	1.83	0.61
35:N:81:ILE:O	35:N:85:GLU:N	2.32	0.61
58:k:262:TRP:N	58:k:314:TYR:O	2.34	0.61
59:l:21:PRO:HD2	59:l:40:ASN:HA	1.81	0.61
62:p:71:MET:O	62:p:72:SER:OG	2.15	0.61
58:w:259:GLY:N	58:w:318:GLY:O	2.33	0.61
58:w:262:TRP:N	58:w:314:TYR:O	2.34	0.61
58:w:416:TYR:HB3	67:B6:15:ARG:HH21	1.64	0.61
59:x:113:ARG:HH12	59:x:211:VAL:HA	1.66	0.61
59:x:360:ALA:HA	59:x:363:LYS:HD2	1.81	0.61
7:6:82:MET:HB3	7:6:87:MET:HE2	1.81	0.61
8:2:150:ASN:N	8:2:150:ASN:OD1	2.30	0.61
15:A5:13:ALA:O	15:A5:18:ARG:HD2	2.00	0.61
23:A:615:LEU:O	23:A:617:ARG:NH1	2.33	0.61
24:B:61:TRP:CG	24:B:62:LYS:N	2.69	0.61
24:B:264:ASN:OD1	24:B:264:ASN:N	2.26	0.61
56:g:125:CYS:O	56:g:127:LYS:N	2.34	0.61
57:e:78:LEU:O	57:e:80:ASP:N	2.34	0.61
2:1:172:MET:HE2	2:1:176:LEU:HB2	1.81	0.61
7:6:298:ILE:HD13	7:6:354:GLN:HA	1.83	0.61
9:8:211:ALA:HB2	9:8:223:PRO:HB3	1.83	0.61
9:8:384:PRO:HG2	9:8:422:HIS:O	2.01	0.61
23:A:59:GLN:HE21	29:G:91:VAL:CG2	2.13	0.61
24:B:286:TYR:HA	25:C:164:ALA:HB2	1.83	0.61
24:B:355:GLU:OE1	24:B:355:GLU:N	2.22	0.61
39:R:234:LYS:O	39:R:271:TYR:OH	2.17	0.61
65:s:53:ASP:OD1	65:s:54:CYS:N	2.34	0.61
5:4:254:THR:HG21	5:4:257:MET:HE3	1.83	0.60
7:6:152:PHE:HD1	7:6:168:ALA:HB1	1.64	0.60
10:C3:92:MET:CE	10:C3:167:THR:HG21	2.31	0.60
36:O:99:GLN:C	36:O:101:THR:H	2.07	0.60
50:c:89:HIS:O	50:c:92:THR:N	2.30	0.60
58:k:312:ILE:O	58:k:319:LEU:N	2.34	0.60
60:m:91:PHE:O	60:m:94:LEU:N	2.33	0.60
60:y:162:GLU:O	60:y:166:GLY:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:196:TRP:CD1	5:4:251:ASN:HD22	2.19	0.60
12:A9:154:GLY:HA2	15:A5:6:VAL:CG2	2.30	0.60
24:B:170:ILE:O	24:B:173:LEU:N	2.34	0.60
39:R:85:ARG:HH21	79:R:601:NAP:C6A	2.13	0.60
55:j:51:ARG:HB3	55:j:53:VAL:H	1.66	0.60
60:y:71:ARG:HH12	61:z:45:TYR:HB3	1.65	0.60
8:2:249:LEU:HD21	8:2:254:LEU:HD12	1.82	0.60
9:8:362:ASP:HB3	9:8:365:LYS:HB3	1.83	0.60
23:A:382:ARG:HG3	23:A:383:SER:N	2.14	0.60
36:O:21:PHE:N	36:O:80:ASP:OD2	2.34	0.60
49:b:166:GLY:O	49:b:168:TRP:N	2.32	0.60
59:l:137:VAL:HG21	59:l:188:PRO:HG3	1.83	0.60
60:m:132:VAL:HA	60:m:139:SER:HB2	1.84	0.60
61:o:175:THR:OG1	65:s:78:LYS:NZ	2.34	0.60
58:w:239:SER:HA	64:A3:18:LEU:HA	1.83	0.60
58:w:312:ILE:O	58:w:319:LEU:N	2.35	0.60
60:y:91:PHE:O	60:y:94:LEU:N	2.33	0.60
2:1:63:PRO:HG3	2:1:214:GLU:OE2	2.01	0.60
2:1:267:THR:C	2:1:269:SER:N	2.59	0.60
27:E:40:TYR:HE2	37:P:106:LEU:HD11	1.67	0.60
29:G:75:ARG:HH22	29:G:119:ASP:CG	2.08	0.60
58:k:152:TYR:HD1	58:k:241:ILE:HD11	1.66	0.60
58:k:268:VAL:HA	58:k:271:GLN:HG2	1.83	0.60
59:l:250:ASP:OD1	59:l:251:SER:N	2.34	0.60
61:o:173:ASP:OD2	61:o:175:THR:OG1	2.13	0.60
58:w:192:ALA:N	58:w:218:GLY:HA3	2.15	0.60
5:4:193:VAL:HG22	5:4:257:MET:HE1	1.83	0.60
14:B4:82:TYR:HB3	14:B4:83:PRO:HD3	1.81	0.60
44:M:12:LYS:HD3	44:M:77:VAL:HG11	1.83	0.60
58:k:434:TYR:CE2	58:k:438:ARG:HB2	2.36	0.60
61:o:28:ARG:NH2	61:o:173:ASP:OD2	2.34	0.60
58:w:39:VAL:N	58:w:97:TYR:O	2.33	0.60
58:w:75:LEU:HD11	58:w:116:ILE:HD11	1.83	0.60
59:x:259:ALA:HB3	59:x:417:PHE:HA	1.81	0.60
2:1:174:LEU:O	2:1:174:LEU:HD22	2.01	0.60
51:d:33:GLU:O	51:d:36:GLU:N	2.35	0.60
59:l:169:ARG:NH2	59:x:438:GLU:OE2	2.34	0.60
60:m:212:SER:OG	63:q:39:GLU:OE2	2.14	0.60
59:x:250:ASP:OD1	59:x:251:SER:N	2.34	0.60
60:y:4:ILE:HG22	60:y:6:LYS:H	1.67	0.60
3:9:123:ASN:HD22	3:9:127:VAL:HG11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:423:ILE:HB	48:a:57:ARG:HA	1.81	0.60
5:4:447:LEU:HD13	5:4:454:ILE:HD11	1.83	0.60
72:6:701:CDL:HB31	72:6:701:CDL:OA3	2.01	0.60
8:2:3:PRO:HG3	40:S:31:TYR:CE2	2.37	0.60
12:A9:6:HIS:HD2	12:A9:8:TYR:H	1.49	0.60
12:A9:119:THR:O	16:A6:52:HIS:HE1	1.85	0.60
12:A9:192:VAL:O	12:A9:196:THR:HB	2.01	0.60
24:B:204:PHE:HE2	26:D:97:MET:HE2	1.66	0.60
24:B:342:ARG:NH2	43:V:21:TYR:OH	2.32	0.60
30:H:15:ASP:OD1	30:H:15:ASP:N	2.26	0.60
39:R:238:GLN:HE22	39:R:271:TYR:HA	1.66	0.60
60:y:132:VAL:HA	60:y:139:SER:HB2	1.83	0.60
61:z:3:LEU:HB2	65:B7:59:LEU:HD13	1.81	0.60
14:B4:80:GLU:CD	14:B4:80:GLU:H	2.10	0.60
23:A:92:CYS:SG	71:A:803:FES:S2	2.99	0.60
24:B:212:GLU:O	24:B:215:GLU:N	2.34	0.60
42:U:29:ARG:HH12	42:U:63:ILE:HG12	1.66	0.60
50:c:15:LEU:O	50:c:19:ARG:N	2.33	0.60
59:l:299:VAL:HG13	59:l:303:VAL:HG21	1.84	0.60
66:A4:35:ALA:O	66:A4:36:THR:HG23	2.02	0.60
2:1:101:GLY:O	2:1:104:PHE:N	2.28	0.60
2:1:169:GLN:NE2	2:1:174:LEU:HB2	2.16	0.60
23:A:105:ASN:OD1	23:A:110:LYS:HE2	2.02	0.60
25:C:123:THR:HG23	29:G:133:ASP:OD2	2.01	0.60
25:C:128:PHE:HD2	25:C:178:VAL:HG23	1.66	0.60
25:C:228:LEU:O	29:G:116:SER:HB2	2.02	0.60
29:G:139:GLU:OE2	29:G:145:TYR:HE2	1.84	0.60
52:f:164:PRO:O	52:f:166:LEU:N	2.34	0.60
53:h:78:LYS:H	53:h:83:ASP:CG	2.10	0.60
56:g:33:LEU:O	56:g:37:PHE:N	2.35	0.60
58:k:259:GLY:N	58:k:318:GLY:O	2.33	0.60
60:m:71:ARG:HH21	61:o:49:ARG:HH21	1.49	0.60
60:m:71:ARG:NH2	61:o:45:TYR:O	2.34	0.60
60:m:102:LEU:O	60:m:105:GLY:N	2.29	0.60
60:m:271:GLU:OE2	60:m:273:TYR:OH	2.19	0.60
58:w:2:ALA:O	59:x:113:ARG:NE	2.29	0.60
61:z:28:ARG:NH2	61:z:173:ASP:OD2	2.34	0.60
24:B:326:CYS:O	24:B:329:ARG:N	2.33	0.60
39:R:117:ARG:NE	39:R:155:VAL:HG21	2.17	0.60
39:R:133:GLU:HG3	39:R:134:TRP:N	2.16	0.60
39:R:234:LYS:HB3	39:R:323:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:k:297:ILE:HD12	60:m:2:THR:HG21	1.84	0.60
59:l:56:ARG:NE	59:l:103:GLU:OE1	2.34	0.60
60:m:374:ASN:HA	60:m:379:TRP:CD1	2.37	0.60
80:m:402:HEM:HBC2	80:m:402:HEM:HMC2	1.84	0.60
61:o:50:HIS:HE1	61:o:91:PHE:HZ	1.50	0.60
64:r:74:PRO:HA	64:r:77:TYR:O	2.02	0.60
80:y:402:HEM:HMC2	80:y:402:HEM:HBC2	1.84	0.60
62:A1:78:LEU:N	62:A1:192:MET:HA	2.16	0.60
66:A4:41:ILE:O	66:A4:41:ILE:HG22	2.01	0.60
2:1:119:SER:HB2	2:1:211:PHE:HE1	1.66	0.59
5:4:35:SER:O	5:4:38:SER:OG	2.12	0.59
6:5:87:THR:HB	6:5:89:TYR:CD2	2.37	0.59
23:A:565:PHE:HB2	23:A:581:ASP:CB	2.31	0.59
23:A:618:GLU:OE2	23:A:620:TRP:CD1	2.54	0.59
26:D:197:ILE:O	26:D:200:LEU:N	2.35	0.59
43:V:78:GLU:O	43:V:82:ARG:HG2	2.02	0.59
58:k:395:TRP:HA	58:k:398:ARG:HD2	1.84	0.59
59:x:299:VAL:HG13	59:x:303:VAL:HG21	1.84	0.59
62:A1:150:ALA:N	62:A1:155:GLY:O	2.31	0.59
8:2:260:PHE:CE2	8:2:264:TRP:HB2	2.37	0.59
8:2:340:THR:OG1	8:2:341:PRO:HD3	2.01	0.59
11:C1:59:GLN:HA	11:C1:62:GLU:HB2	1.83	0.59
23:A:260:ASN:H	23:A:282:ASN:ND2	2.00	0.59
25:C:233:ARG:NH2	27:E:120:GLU:OE2	2.33	0.59
50:c:103:ARG:HG3	51:d:50:GLN:H	1.67	0.59
59:l:97:SER:HB2	59:l:108:THR:HB	1.84	0.59
60:m:4:ILE:HG22	60:m:6:LYS:H	1.67	0.59
63:q:40:ASN:H	63:q:43:VAL:HB	1.66	0.59
59:x:59:ASN:N	59:x:62:ASN:HB3	2.08	0.59
59:x:97:SER:HB2	59:x:108:THR:HB	1.84	0.59
60:y:62:ALA:O	60:y:65:SER:OG	2.20	0.59
60:y:137:GLN:HA	60:y:259:ALA:HA	1.82	0.59
60:y:377:LEU:HB2	60:y:379:TRP:CD1	2.37	0.59
63:A2:87:LYS:HG3	63:A2:89:TYR:CD2	2.36	0.59
1:3:59:ALA:HB1	4:7:67:VAL:HG22	1.83	0.59
8:2:267:ILE:O	8:2:271:THR:HG22	2.02	0.59
8:2:338:PRO:HB3	38:Q:167:LEU:HD22	1.83	0.59
9:8:204:TYR:HB3	9:8:377:GLU:HG2	1.84	0.59
25:C:71:LEU:N	25:C:72:PRO:HD3	2.17	0.59
29:G:128:PHE:HD2	29:G:134:ALA:HA	1.68	0.59
33:K:41:TYR:CE1	33:K:53:ILE:HG21	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:U:14:VAL:HG22	42:U:23:TYR:CE1	2.38	0.59
60:m:137:GLN:HA	60:m:259:ALA:HA	1.82	0.59
60:m:302:ALA:O	60:m:305:PRO:HD2	2.02	0.59
67:u:16:ARG:O	67:u:19:THR:OG1	2.20	0.59
58:w:395:TRP:HA	58:w:398:ARG:HD2	1.84	0.59
59:x:137:VAL:HG21	59:x:188:PRO:HG3	1.84	0.59
60:y:374:ASN:HA	60:y:379:TRP:CD1	2.37	0.59
5:4:34:ILE:O	5:4:37:THR:OG1	2.14	0.59
7:6:576:LEU:HD22	8:2:168:GLY:HA2	1.82	0.59
8:2:337:LEU:HB2	8:2:339:LEU:HG	1.84	0.59
23:A:153:PHE:HB3	23:A:154:LEU:HA	1.84	0.59
25:C:167:TRP:O	25:C:170:ARG:N	2.34	0.59
26:D:75:ASN:ND2	26:D:206:ARG:O	2.35	0.59
55:j:46:ASN:HA	55:j:51:ARG:HE	1.66	0.59
60:m:237:LEU:HD11	61:o:212:MET:SD	2.42	0.59
59:x:54:GLY:H	59:x:57:TYR:HD2	1.50	0.59
62:A1:13:TYR:CD1	64:A3:27:PRO:HG2	2.38	0.59
2:1:8:MET:O	2:1:12:PRO:CG	2.50	0.59
5:4:185:PRO:HD3	55:j:114:GLU:OE2	2.01	0.59
5:4:347:GLY:HA2	5:4:416:ARG:O	2.01	0.59
5:4:353:PRO:HB2	72:6:701:CDL:HB22	1.84	0.59
25:C:77:GLN:HB3	25:C:89:CYS:HB2	1.84	0.59
27:E:100:GLU:OE2	27:E:193:ASN:ND2	2.34	0.59
40:S:48:ILE:HD12	40:S:49:THR:H	1.68	0.59
59:x:198:HIS:CE1	59:x:232:LEU:HD12	2.38	0.59
59:x:245:ARG:HG2	59:x:426:ALA:HB3	1.84	0.59
62:A1:15:ARG:HB3	64:A3:24:ARG:HG3	1.83	0.59
6:5:96:LEU:HD11	7:6:581:LYS:HB3	1.84	0.59
22:A8:28:LEU:HB2	22:A8:29:PRO:HD3	1.84	0.59
25:C:128:PHE:CE2	25:C:176:PHE:HB3	2.38	0.59
40:S:157:PHE:O	40:S:161:MET:N	2.34	0.59
40:S:161:MET:HG3	40:S:166:PHE:CE1	2.38	0.59
43:V:50:MET:C	43:V:52:LYS:H	2.09	0.59
60:m:377:LEU:HB2	60:m:379:TRP:CD1	2.38	0.59
62:p:75:GLU:HG2	62:p:76:ILE:C	2.27	0.59
58:w:152:TYR:HD1	58:w:241:ILE:HD11	1.66	0.59
58:w:183:THR:HA	58:w:186:LEU:HD12	1.84	0.59
60:y:71:ARG:NH1	61:z:45:TYR:HB3	2.18	0.59
1:3:77:TRP:CD1	2:1:318:THR:C	2.81	0.59
2:1:70:MET:HE1	2:1:118:TRP:CD1	2.38	0.59
5:4:442:LEU:HB2	5:4:443:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:73:LEU:O	6:5:76:SER:N	2.29	0.59
7:6:402:SER:OG	7:6:404:THR:HG23	2.02	0.59
8:2:26:TRP:CD1	8:2:85:THR:O	2.55	0.59
24:B:263:THR:OG1	24:B:264:ASN:OD1	2.20	0.59
35:N:42:ALA:HB2	35:N:100:TRP:HB3	1.85	0.59
36:O:26:ASN:O	36:O:30:ARG:N	2.36	0.59
59:l:113:ARG:HH12	59:l:211:VAL:HA	1.66	0.59
68:v:70:LEU:HD13	68:v:73:PRO:HD2	1.85	0.59
63:A2:40:ASN:H	63:A2:43:VAL:HB	1.66	0.59
2:1:53:ILE:O	2:1:53:ILE:HG22	2.03	0.59
6:5:8:ILE:HG13	6:5:8:ILE:O	2.01	0.59
8:2:144:GLN:NE2	30:H:3:PHE:HB2	2.15	0.59
11:C1:145:PRO:CG	11:C1:148:MET:HE2	2.33	0.59
15:A5:62:CYS:SG	15:A5:84:SER:OG	2.60	0.59
23:A:146:PHE:N	23:A:146:PHE:CD1	2.70	0.59
25:C:183:HIS:ND1	25:C:185:ASP:O	2.36	0.59
59:l:245:ARG:HG2	59:l:426:ALA:HB3	1.84	0.59
61:o:165:TYR:CZ	61:o:168:VAL:HA	2.38	0.59
58:w:434:TYR:CE2	58:w:438:ARG:HB2	2.37	0.59
60:y:302:ALA:O	60:y:305:PRO:HD2	2.03	0.59
61:z:80:MET:O	61:z:81:PHE:HB2	2.01	0.59
2:1:71:PHE:HZ	2:1:215:TYR:CD1	2.12	0.59
6:5:96:LEU:HB3	24:B:61:TRP:HE3	1.67	0.59
72:6:701:CDL:H712	72:6:701:CDL:H331	1.85	0.59
9:8:411:SER:O	9:8:414:GLU:N	2.35	0.59
11:C1:226:MET:O	11:C1:227:LEU:HB2	2.02	0.59
23:A:423:LEU:C	23:A:425:ASN:H	2.09	0.59
34:L:69:HIS:NE2	34:L:71:GLN:HB2	2.18	0.59
60:y:71:ARG:NH1	61:z:45:TYR:O	2.36	0.59
5:4:186:VAL:HB	5:4:251:ASN:OD1	2.03	0.59
7:6:67:HIS:ND1	7:6:67:HIS:O	2.36	0.59
8:2:321:LYS:HD2	69:2:402:PC1:H242	1.85	0.59
23:A:577:ALA:HB3	23:A:578:PRO:HD3	1.85	0.59
23:A:691:ILE:O	23:A:693:ASP:N	2.35	0.59
35:N:114:TRP:O	35:N:116:ILE:N	2.35	0.59
38:Q:93:GLY:O	38:Q:95:GLN:N	2.35	0.59
60:m:62:ALA:O	60:m:65:SER:OG	2.20	0.59
60:m:248:ASP:OD1	61:o:118:ARG:NH2	2.36	0.59
58:w:145:MET:HE3	58:w:252:HIS:HE1	1.68	0.59
58:w:445:ARG:HG3	66:A4:24:TRP:HZ2	1.67	0.59
60:y:328:LEU:HD22	60:y:366:MET:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A2:19:TRP:HD1	63:A2:22:ASN:ND2	1.98	0.59
64:A3:74:PRO:HA	64:A3:77:TYR:O	2.02	0.59
11:C1:179:LEU:HD21	17:C0:65:PRO:HD3	1.85	0.58
11:C1:193:TYR:HE1	13:A7:126:MET:HE1	1.68	0.58
20:B3:43:SER:OG	20:B3:45:VAL:HG12	2.04	0.58
23:A:250:SER:OG	23:A:251:ILE:N	2.34	0.58
29:G:94:THR:HG22	29:G:95:LYS:H	1.68	0.58
58:k:329:MET:HE1	64:r:5:GLY:HA3	1.84	0.58
59:l:66:SER:O	59:l:70:ARG:N	2.30	0.58
60:y:271:GLU:OE2	60:y:273:TYR:OH	2.19	0.58
61:z:165:TYR:CZ	61:z:168:VAL:HA	2.38	0.58
64:A3:62:GLY:O	64:A3:66:PHE:N	2.29	0.58
66:A4:31:GLY:O	66:A4:35:ALA:N	2.36	0.58
1:3:28:ASN:OD1	1:3:29:VAL:N	2.34	0.58
4:7:101:PHE:O	4:7:105:TYR:N	2.33	0.58
7:6:578:THR:O	7:6:581:LYS:HG2	2.04	0.58
39:R:200:ILE:O	39:R:262:THR:OG1	2.16	0.58
47:Z:47:ARG:HA	47:Z:50:ALA:HB3	1.84	0.58
51:d:25:PHE:CE1	51:d:43:GLN:HB3	2.38	0.58
62:p:30:GLU:HG3	67:u:7:ALA:HA	1.84	0.58
58:w:268:VAL:HA	58:w:271:GLN:HG2	1.83	0.58
59:x:66:SER:O	59:x:70:ARG:N	2.30	0.58
2:1:233:MET:CA	2:1:236:ILE:HG23	2.25	0.58
9:8:54:LYS:HA	9:8:136:HIS:CE1	2.38	0.58
9:8:284:ASN:OD1	9:8:304:ALA:N	2.33	0.58
38:Q:43:PHE:HD1	38:Q:59:GLU:HB2	1.69	0.58
40:S:120:GLN:NE2	40:S:161:MET:SD	2.77	0.58
44:M:34:SER:O	44:M:72:CYS:HA	2.03	0.58
61:o:178:THR:O	61:o:182:VAL:N	2.29	0.58
65:B7:13:LEU:C	65:B7:15:ASP:H	2.11	0.58
2:1:310:LEU:HD11	34:L:32:LEU:HB3	1.85	0.58
3:9:191:ASN:HB3	3:9:216:PRO:HB3	1.86	0.58
4:7:25:SER:O	4:7:27:ILE:N	2.37	0.58
8:2:133:TRP:O	8:2:136:LEU:N	2.34	0.58
23:A:238:PHE:CG	27:E:140:ARG:HD3	2.38	0.58
26:D:99:MET:SD	26:D:193:LEU:HD22	2.42	0.58
36:O:92:GLU:HG3	36:O:97:TRP:HE3	1.68	0.58
40:S:320:THR:O	40:S:324:GLY:HA3	2.03	0.58
50:c:95:TYR:OH	56:g:11:PRO:O	2.20	0.58
56:g:140:GLN:O	56:g:144:HIS:HB3	2.04	0.58
44:M:41:GLY:O	44:M:42:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:y:275:LEU:O	60:y:279:ALA:N	2.34	0.58
3:9:163:THR:HG22	3:9:170:THR:HB	1.86	0.58
7:6:562:LEU:HB3	7:6:563:PRO:HD3	1.84	0.58
8:2:311:MET:HE1	40:S:98:GLY:H	1.68	0.58
17:C0:57:ARG:HG3	17:C0:60:TYR:CE2	2.38	0.58
59:l:54:GLY:H	59:l:57:TYR:HD2	1.50	0.58
61:o:72:ASP:OD1	61:o:73:GLY:N	2.36	0.58
58:w:3:THR:O	58:w:7:ALA:N	2.29	0.58
67:B6:21:ALA:HA	67:B6:24:ILE:HD12	1.85	0.58
2:1:172:MET:HE2	2:1:176:LEU:CD1	2.01	0.58
2:1:307:LEU:HD23	43:V:47:TYR:CE1	2.39	0.58
7:6:89:PHE:HB2	7:6:326:PHE:HZ	1.68	0.58
10:C3:404:THR:O	10:C3:480:ARG:NH1	2.37	0.58
16:A6:5:LYS:HZ3	16:A6:5:LYS:HB3	1.68	0.58
25:C:217:GLU:HB2	39:R:71:ASN:ND2	2.19	0.58
38:Q:83:THR:HA	38:Q:86:TRP:NE1	2.19	0.58
59:l:412:ASN:HA	59:l:415:LYS:HD3	1.85	0.58
2:1:76:ILE:O	2:1:76:ILE:HG22	2.03	0.58
2:1:77:MET:O	2:1:79:LEU:N	2.36	0.58
9:8:49:HIS:ND1	9:8:49:HIS:O	2.36	0.58
24:B:141:TYR:HH	24:B:458:PHE:C	2.11	0.58
33:K:25:GLN:NE2	33:K:57:GLU:OE2	2.36	0.58
39:R:250:ILE:HA	39:R:253:ILE:HB	1.85	0.58
47:Z:63:PHE:CE2	47:Z:64:VAL:HG23	2.38	0.58
44:M:37:MET:HA	44:M:41:GLY:HA2	1.85	0.58
62:p:73:LYS:HD3	62:p:94:LYS:HA	1.86	0.58
66:t:30:VAL:C	66:t:33:VAL:HG22	2.28	0.58
67:B6:16:ARG:O	67:B6:19:THR:OG1	2.20	0.58
5:4:198:ALA:HB2	70:4:501:3PE:H271	1.85	0.58
21:A0:46:LYS:O	21:A0:47:LYS:HB2	2.03	0.58
29:G:58:LYS:H	36:O:15:THR:N	2.02	0.58
40:S:88:ASP:N	40:S:89:GLY:HA3	2.19	0.58
44:M:37:MET:HG2	44:M:41:GLY:HA2	1.86	0.58
58:k:183:THR:HA	58:k:186:LEU:HD12	1.84	0.58
59:l:279:LEU:HD13	59:l:295:LEU:HD13	1.86	0.58
60:m:71:ARG:NH1	61:o:45:TYR:HB3	2.19	0.58
60:m:77:TRP:CD1	60:m:77:TRP:H	2.21	0.58
67:u:21:ALA:HA	67:u:24:ILE:HD12	1.85	0.58
63:A2:10:SER:C	82:A2:201:UQ2:H5M1	2.29	0.58
5:4:325:MET:HE3	5:4:362:ALA:HB2	1.84	0.58
8:2:51:ARG:NH1	24:B:61:TRP:HH2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:466:LEU:HB3	23:A:500:ILE:HD11	1.86	0.58
24:B:238:LEU:HD23	43:V:10:MET:HE1	1.84	0.58
25:C:95:VAL:H	25:C:97:PRO:HD2	1.67	0.58
30:H:15:ASP:C	30:H:17:TRP:H	2.10	0.58
38:Q:109:GLU:HG3	38:Q:110:CYS:N	2.19	0.58
39:R:154:GLN:HG3	39:R:155:VAL:H	1.68	0.58
43:V:46:GLY:O	43:V:49:SER:OG	2.17	0.58
43:V:72:MET:HG3	43:V:72:MET:O	2.03	0.58
56:g:128:GLU:O	56:g:132:PHE:N	2.28	0.58
44:M:28:GLU:HA	44:M:30:LEU:HD13	1.85	0.58
58:k:390:ILE:O	58:k:392:LEU:N	2.37	0.58
59:l:197:ASN:O	59:l:230:LEU:HB3	2.03	0.58
61:z:50:HIS:HE1	61:z:91:PHE:HZ	1.49	0.58
2:1:310:LEU:HD23	2:1:310:LEU:O	2.03	0.58
7:6:274:GLN:O	7:6:277:THR:OG1	2.22	0.58
7:6:497:GLY:O	7:6:501:ALA:N	2.37	0.58
7:6:583:LEU:HB3	7:6:586:LEU:HD13	1.86	0.58
11:C1:193:TYR:CE1	13:A7:126:MET:HE1	2.39	0.58
23:A:371:VAL:HB	23:A:482:GLN:HG3	1.84	0.58
24:B:215:GLU:OE2	27:E:93:LEU:HA	2.03	0.58
27:E:179:THR:OG1	42:U:123:GLN:NE2	2.37	0.58
49:b:143:GLU:O	49:b:146:LYS:N	2.28	0.58
59:l:415:LYS:O	59:l:419:SER:N	2.37	0.58
61:o:7:PRO:CG	61:o:126:TYR:HA	2.25	0.58
59:x:279:LEU:HD13	59:x:295:LEU:HD13	1.86	0.58
8:2:169:GLY:O	8:2:172:GLN:N	2.35	0.57
9:8:207:GLY:HA2	73:8:501:FMN:C5A	2.33	0.57
10:C3:184:PHE:H	10:C3:256:HIS:HE1	1.52	0.57
23:A:452:LEU:O	23:A:455:ILE:HG22	2.04	0.57
40:S:100:CYS:HB3	40:S:119:LEU:HB2	1.86	0.57
58:k:145:MET:HE3	58:k:252:HIS:HE1	1.68	0.57
60:m:328:LEU:HD22	60:m:366:MET:HE1	1.85	0.57
64:r:53:VAL:HG12	64:r:57:LEU:HD11	1.86	0.57
59:x:25:GLU:OE2	59:x:213:HIS:ND1	2.37	0.57
64:A3:55:PHE:O	64:A3:59:TYR:N	2.25	0.57
8:2:91:ASN:OD1	8:2:92:PRO:HD2	2.04	0.57
8:2:234:TRP:NE1	8:2:303:THR:HG1	2.02	0.57
36:O:88:MET:HE3	36:O:92:GLU:OE2	2.03	0.57
39:R:329:LEU:HD12	39:R:330:PRO:HD2	1.86	0.57
59:l:25:GLU:OE2	59:l:213:HIS:ND1	2.38	0.57
60:m:184:ILE:O	60:m:187:PHE:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:m:402:HEM:O2A	80:m:402:HEM:HHA	2.05	0.57
61:o:31:GLN:O	61:o:35:GLN:HG2	2.05	0.57
62:p:75:GLU:HG2	62:p:76:ILE:CA	2.35	0.57
64:r:62:GLY:O	64:r:66:PHE:N	2.30	0.57
59:x:179:PRO:O	59:x:182:ARG:HB3	2.04	0.57
60:y:225:THR:O	60:y:229:ILE:HG13	2.03	0.57
62:A1:45:VAL:HG22	67:B6:28:ALA:HB2	1.86	0.57
1:3:49:LEU:CD2	2:1:129:LEU:CD2	2.62	0.57
5:4:336:ARG:HH22	5:4:429:SER:HA	1.68	0.57
7:6:40:ILE:HG22	7:6:98:TRP:HD1	1.69	0.57
9:8:151:ALA:O	9:8:191:TYR:OH	2.21	0.57
12:A9:203:PHE:O	12:A9:207:HIS:HD2	1.88	0.57
41:T:48:SER:CB	41:T:52:GLY:CA	2.81	0.57
43:V:90:ASN:ND2	43:V:123:GLU:O	2.37	0.57
56:g:142:ARG:O	56:g:162:ARG:NH2	2.37	0.57
58:k:257:VAL:HG12	58:k:420:PRO:HA	1.87	0.57
59:l:179:PRO:O	59:l:182:ARG:HB3	2.04	0.57
60:m:265:PRO:HG2	60:m:268:ILE:HG12	1.86	0.57
64:r:38:LEU:O	64:r:41:THR:OG1	2.21	0.57
7:6:313:MET:O	7:6:316:THR:OG1	2.21	0.57
23:A:656:TYR:O	23:A:657:ASP:OD1	2.21	0.57
24:B:273:VAL:O	24:B:275:ILE:HG13	2.05	0.57
58:k:39:VAL:N	58:k:97:TYR:O	2.33	0.57
58:k:114:ALA:HB1	58:k:216:PHE:CD2	2.40	0.57
60:y:184:ILE:O	60:y:187:PHE:HD2	1.87	0.57
60:y:311:LYS:O	63:A2:38:HIS:N	2.23	0.57
80:y:402:HEM:O2A	80:y:402:HEM:HHA	2.05	0.57
61:z:224:ARG:O	61:z:228:SER:N	2.35	0.57
63:A2:19:TRP:C	63:A2:21:TYR:N	2.62	0.57
65:B7:40:CYS:O	65:B7:44:VAL:HG23	2.05	0.57
5:4:36:PHE:HZ	53:h:97:ILE:HG13	1.69	0.57
7:6:305:SER:OG	7:6:336:LYS:NZ	2.22	0.57
27:E:37:THR:CB	37:P:107:SER:HB2	2.34	0.57
56:g:13:PRO:O	56:g:116:ARG:NH2	2.37	0.57
58:k:77:LYS:O	58:k:81:SER:OG	2.22	0.57
61:o:224:ARG:O	61:o:228:SER:N	2.35	0.57
58:w:184:GLU:O	58:w:188:ARG:N	2.35	0.57
58:w:257:VAL:HG12	58:w:420:PRO:HA	1.86	0.57
58:w:390:ILE:O	58:w:392:LEU:N	2.37	0.57
59:x:148:LYS:NZ	59:x:180:ASP:OD1	2.35	0.57
60:y:77:TRP:CD1	60:y:77:TRP:H	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:z:112:ASP:OD1	61:z:113:LEU:N	2.37	0.57
65:B7:38:GLU:HA	65:B7:41:ASP:HB3	1.86	0.57
3:9:138:THR:HB	3:9:139:PRO:HD3	1.86	0.57
11:C1:145:PRO:HG3	11:C1:148:MET:HE2	1.87	0.57
24:B:154:ALA:HB2	24:B:398:THR:HG21	1.86	0.57
26:D:137:LEU:O	26:D:140:VAL:N	2.37	0.57
26:D:155:SER:O	26:D:161:GLY:N	2.36	0.57
34:L:62:ASN:HA	34:L:63:MET:HB3	1.86	0.57
43:V:51:MET:HG3	43:V:55:ARG:HH21	1.70	0.57
44:W:80:LYS:HE2	44:W:142:GLN:HE22	1.68	0.57
55:j:26:LEU:O	55:j:27:THR:HG22	2.05	0.57
57:e:70:THR:HG22	57:e:71:GLY:N	2.19	0.57
60:m:216:ASP:O	60:m:217:LYS:HD2	2.05	0.57
60:m:275:LEU:O	60:m:279:ALA:N	2.34	0.57
61:o:225:HIS:O	61:o:228:SER:OG	2.20	0.57
59:x:412:ASN:HA	59:x:415:LYS:HD3	1.85	0.57
64:A3:53:VAL:HG12	64:A3:57:LEU:HD11	1.86	0.57
5:4:140:THR:HB	24:B:38:GLN:HB3	1.86	0.57
7:6:25:ASN:O	7:6:26:THR:OG1	2.20	0.57
23:A:44:GLU:HG2	23:A:45:PRO:HD2	1.86	0.57
23:A:218:LEU:HD21	23:A:413:LEU:HD21	1.87	0.57
36:O:44:PRO:O	36:O:47:VAL:HG12	2.05	0.57
56:g:70:ARG:HH22	56:g:94:ARG:HD2	1.67	0.57
59:l:152:LEU:HD22	59:l:158:HIS:HB2	1.86	0.57
65:s:13:LEU:C	65:s:15:ASP:H	2.11	0.57
66:t:30:VAL:HA	66:t:33:VAL:CG2	2.35	0.57
58:w:49:SER:H	58:w:52:ASN:HB2	1.70	0.57
62:A1:12:ASP:O	64:A3:27:PRO:HB3	2.05	0.57
3:9:41:HIS:NE2	31:I:104:ASP:OD2	2.37	0.57
4:7:84:LEU:O	4:7:85:SER:C	2.48	0.57
5:4:160:LEU:O	5:4:163:ALA:N	2.37	0.57
8:2:280:THR:O	8:2:284:ILE:N	2.33	0.57
17:C0:75:ARG:HG2	17:C0:75:ARG:NH1	2.19	0.57
21:A0:41:ARG:HG3	22:A8:40:TYR:CE2	2.40	0.57
24:B:282:ASP:HA	24:B:285:ASN:HB3	1.86	0.57
24:B:378:LEU:O	24:B:382:PHE:N	2.33	0.57
24:B:389:TYR:N	24:B:389:TYR:CD1	2.69	0.57
40:S:71:LEU:HG	40:S:144:GLY:HA3	1.87	0.57
59:l:148:LYS:NZ	59:l:180:ASP:OD1	2.35	0.57
59:l:213:HIS:CD2	59:l:217:LYS:HB2	2.40	0.57
58:w:32:GLN:NE2	59:x:373:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:152:LEU:HD22	59:x:158:HIS:HB2	1.86	0.57
60:y:216:ASP:O	60:y:217:LYS:HD2	2.05	0.57
2:1:277:TYR:OH	27:E:66:LEU:O	2.23	0.57
3:9:121:MET:HB2	9:8:201:ALA:HB1	1.87	0.57
7:6:48:MET:O	7:6:51:THR:OG1	2.23	0.57
8:2:79:MET:O	30:H:67:LEU:HD21	2.04	0.57
8:2:112:HIS:O	8:2:112:HIS:CG	2.57	0.57
25:C:149:THR:OG1	25:C:150:ASP:N	2.38	0.57
26:D:172:GLY:O	26:D:174:ASP:N	2.38	0.57
34:L:79:GLU:OE1	34:L:79:GLU:N	2.37	0.57
38:Q:37:ASP:HA	38:Q:40:ASN:OD1	2.05	0.57
40:S:202:VAL:HA	40:S:205:ARG:HB2	1.87	0.57
48:a:76:ILE:O	48:a:80:PHE:N	2.38	0.57
56:g:163:MET:O	56:g:167:ARG:N	2.32	0.57
64:r:53:VAL:O	64:r:57:LEU:HG	2.04	0.57
65:s:40:CYS:O	65:s:44:VAL:HG23	2.05	0.57
61:z:31:GLN:O	61:z:35:GLN:HG2	2.05	0.57
8:2:181:TYR:O	8:2:182:SER:OG	2.21	0.57
9:8:441:HIS:O	9:8:442:PHE:HD1	1.87	0.57
24:B:223:HIS:CE1	26:D:91:CYS:HB3	2.40	0.57
33:K:40:ARG:HB3	33:K:44:LEU:HB2	1.87	0.57
48:a:79:ASN:ND2	57:e:73:GLY:O	2.34	0.57
56:g:9:VAL:O	56:g:109:ARG:NH2	2.37	0.57
58:k:438:ARG:HH21	64:r:21:PHE:HE2	1.53	0.57
59:l:113:ARG:NH1	59:l:210:GLY:O	2.38	0.57
59:l:260:GLU:HG2	59:l:261:SER:O	2.05	0.57
60:m:225:THR:O	60:m:229:ILE:HG13	2.04	0.57
59:x:213:HIS:CD2	59:x:217:LYS:HB2	2.40	0.57
62:A1:13:TYR:HD1	64:A3:27:PRO:HG2	1.70	0.57
1:3:38:GLU:OE1	2:1:64:ALA:N	2.35	0.56
1:3:98:LEU:O	1:3:101:SER:OG	2.20	0.56
9:8:281:HIS:HD2	9:8:357:MET:HA	1.69	0.56
24:B:226:TYR:CE2	24:B:232:VAL:HG13	2.40	0.56
38:Q:158:LEU:HD22	55:j:17:GLU:OE2	2.05	0.56
58:k:148:VAL:HG12	58:k:152:TYR:HE2	1.70	0.56
58:k:213:GLN:CG	58:k:214:LYS:HG3	2.28	0.56
58:k:220:SER:HA	58:k:221:GLY:C	2.30	0.56
58:k:309:THR:HG22	58:k:322:ALA:HB2	1.87	0.56
59:l:169:ARG:HD3	59:l:238:LYS:HD3	1.87	0.56
58:w:262:TRP:HD1	58:w:315:ALA:HA	1.70	0.56
59:x:56:ARG:HB2	59:x:171:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:113:ARG:NH1	59:x:210:GLY:O	2.38	0.56
59:x:415:LYS:O	59:x:419:SER:N	2.37	0.56
60:y:350:ILE:HA	60:y:353:LEU:HD12	1.87	0.56
61:z:7:PRO:CG	61:z:126:TYR:HA	2.25	0.56
62:A1:71:MET:HA	62:A1:74:ILE:HD11	1.86	0.56
62:A1:165:TYR:HA	62:A1:170:ARG:O	2.05	0.56
64:A3:53:VAL:O	64:A3:57:LEU:HG	2.04	0.56
7:6:285:THR:O	7:6:288:THR:OG1	2.22	0.56
7:6:312:LEU:HD11	7:6:395:ILE:HG21	1.87	0.56
7:6:359:MET:HB3	7:6:430:ALA:HA	1.87	0.56
23:A:339:ALA:HB2	23:A:365:THR:HG23	1.87	0.56
26:D:86:THR:O	26:D:87:PHE:HD1	1.88	0.56
39:R:155:VAL:HG12	39:R:159:ALA:HB2	1.86	0.56
39:R:171:ASN:ND2	39:R:324:THR:HB	2.19	0.56
52:f:35:ASP:O	52:f:39:TYR:N	2.31	0.56
59:l:56:ARG:HB2	59:l:171:ALA:HB1	1.87	0.56
60:m:350:ILE:HA	60:m:353:LEU:HD12	1.87	0.56
65:s:29:LYS:HA	65:s:32:LYS:HB3	1.87	0.56
59:x:260:GLU:HG2	59:x:261:SER:O	2.05	0.56
65:B7:18:THR:HA	65:B7:21:ARG:HD2	1.87	0.56
68:B5:59:ALA:HB1	68:B5:62:ARG:O	2.04	0.56
2:1:153:VAL:HA	2:1:156:MET:CE	2.35	0.56
6:5:17:VAL:HA	6:5:20:LEU:HB3	1.86	0.56
10:C3:69:MET:HE2	10:C3:70:VAL:CG2	2.36	0.56
11:C1:189:PRO:HD2	18:C2:54:TYR:OH	2.05	0.56
14:B4:78:HIS:ND1	18:C2:12:LEU:HD22	2.21	0.56
24:B:134:PRO:HB3	24:B:138:ARG:NH1	2.20	0.56
25:C:88:ILE:HG22	25:C:90:ILE:HG13	1.88	0.56
27:E:80:GLU:O	37:P:25:GLN:NE2	2.38	0.56
29:G:165:SER:HB3	29:G:168:LYS:HB2	1.86	0.56
37:P:36:GLN:HB2	37:P:37:PRO:HD3	1.87	0.56
37:P:108:GLN:OE1	37:P:108:GLN:N	2.35	0.56
38:Q:49:GLU:OE2	38:Q:138:PRO:HD2	2.05	0.56
40:S:197:VAL:HG11	40:S:226:GLU:OE2	2.06	0.56
40:S:321:GLU:C	40:S:324:GLY:H	2.13	0.56
52:f:16:VAL:O	52:f:20:TYR:N	2.33	0.56
58:k:229:PRO:O	58:k:231:LEU:HG	2.04	0.56
58:k:412:SER:O	67:u:15:ARG:NH2	2.38	0.56
60:m:138:MET:HB2	60:m:255:ASN:ND2	2.21	0.56
61:o:112:ASP:OD1	61:o:113:LEU:N	2.37	0.56
63:q:87:LYS:HG3	63:q:89:TYR:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:s:12:GLU:HG2	65:s:13:LEU:H	1.70	0.56
59:x:169:ARG:HD3	59:x:238:LYS:HD3	1.87	0.56
60:y:265:PRO:HG2	60:y:268:ILE:HG12	1.87	0.56
60:y:379:TRP:HA	63:A:2:33:ARG:NH1	2.20	0.56
65:B:7:66:ASP:HA	65:B:7:69:VAL:HB	1.86	0.56
5:4:111:THR:O	5:4:113:MET:N	2.35	0.56
5:4:455:LEU:HD23	5:4:456:GLY:O	2.05	0.56
23:A:422:TRP:CZ2	29:G:169:ARG:HD3	2.40	0.56
23:A:431:LEU:HD23	23:A:432:ILE:N	2.21	0.56
39:R:266:VAL:HG12	39:R:267:GLY:O	2.05	0.56
44:W:94:ASP:OD1	44:W:97:LYS:HB2	2.05	0.56
46:Y:46:ARG:HA	46:Y:49:GLN:NE2	2.18	0.56
44:M:37:MET:HG2	44:M:42:LEU:H	1.69	0.56
5:4:150:LEU:C	5:4:152:TYR:H	2.14	0.56
8:2:87:MET:O	8:2:88:LYS:O	2.24	0.56
8:2:127:GLY:HA3	8:2:129:ILE:H	1.71	0.56
24:B:308:TYR:HH	24:B:401:GLU:H	1.51	0.56
38:Q:53:PRO:HD2	43:V:116:TRP:HD1	1.70	0.56
38:Q:141:PRO:HG2	38:Q:144:SER:HB3	1.88	0.56
39:R:81:ILE:O	39:R:83:PRO:HD3	2.06	0.56
42:U:71:LYS:NZ	42:U:76:ASP:OD2	2.37	0.56
56:g:162:ARG:HA	56:g:165:ALA:HB3	1.88	0.56
58:k:42:ASP:HB3	58:k:384:LEU:HD23	1.88	0.56
58:k:191:LYS:O	58:k:194:ARG:HB2	2.05	0.56
64:r:55:PHE:O	64:r:59:TYR:N	2.25	0.56
59:x:275:LEU:HB2	59:x:410:VAL:HG13	1.87	0.56
59:x:279:LEU:HD22	59:x:295:LEU:HB2	1.86	0.56
6:5:59:MET:SD	8:2:84:TRP:HH2	2.28	0.56
9:8:164:ASN:O	9:8:167:SER:OG	2.18	0.56
23:A:266:ARG:HG3	23:A:267:THR:HG23	1.88	0.56
24:B:301:ASP:O	24:B:301:ASP:OD1	2.23	0.56
25:C:128:PHE:CD2	25:C:178:VAL:HG23	2.40	0.56
35:N:93:LYS:O	35:N:96:GLN:N	2.33	0.56
39:R:180:TYR:N	39:R:317:ASP:OD2	2.38	0.56
58:k:49:SER:H	58:k:52:ASN:HB2	1.70	0.56
61:o:81:PHE:CE1	61:o:84:PRO:HA	2.40	0.56
58:w:42:ASP:HB3	58:w:384:LEU:HD23	1.88	0.56
58:w:309:THR:HG22	58:w:322:ALA:HB2	1.87	0.56
2:1:70:MET:HE1	2:1:118:TRP:CG	2.40	0.56
2:1:272:TRP:CH2	27:E:71:GLY:HA2	2.41	0.56
6:5:37:MET:O	6:5:38:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:64:LEU:O	6:5:67:ALA:N	2.39	0.56
8:2:233:THR:HG23	8:2:234:TRP:CD1	2.41	0.56
9:8:237:GLY:HA3	29:G:166:TRP:HE3	1.71	0.56
11:C1:132:GLU:HB3	11:C1:137:GLU:HG3	1.87	0.56
23:A:301:ARG:HE	23:A:613:PRO:HG3	1.70	0.56
25:C:197:GLY:HA2	29:G:67:VAL:HG13	1.88	0.56
27:E:172:ASN:HB2	27:E:197:TRP:CZ2	2.41	0.56
31:I:62:GLU:HB3	42:U:124:TYR:CD1	2.40	0.56
40:S:280:HIS:O	40:S:283:ARG:N	2.39	0.56
43:V:79:LYS:O	43:V:82:ARG:N	2.39	0.56
44:M:35:HIS:HA	44:M:71:MET:O	2.06	0.56
59:l:58:GLU:OE1	59:l:64:GLY:N	2.37	0.56
60:m:146:ILE:O	60:m:149:LEU:HB3	2.06	0.56
62:p:107:ASP:HA	62:p:108:GLN:C	2.30	0.56
66:t:30:VAL:HA	66:t:33:VAL:HG22	1.87	0.56
67:u:17:THR:HA	67:u:20:PHE:HB3	1.88	0.56
59:x:368:TYR:CZ	59:x:372:VAL:HG21	2.41	0.56
60:y:77:TRP:CZ3	60:y:78:ILE:HG22	2.40	0.56
62:A1:9:ASP:OD1	62:A1:10:PHE:N	2.39	0.56
2:1:39:VAL:HG13	2:1:40:VAL:HG13	1.88	0.56
3:9:87:GLN:O	3:9:91:GLY:N	2.37	0.56
5:4:115:LEU:HB2	5:4:174:LEU:HD13	1.87	0.56
7:6:42:TYR:O	7:6:46:THR:OG1	2.18	0.56
23:A:61:PRO:HG3	23:A:146:PHE:CD2	2.40	0.56
59:l:368:TYR:CZ	59:l:372:VAL:HG21	2.41	0.56
63:q:73:GLN:HA	64:r:39:ARG:NH2	2.20	0.56
65:s:38:GLU:HA	65:s:41:ASP:HB3	1.86	0.56
59:x:58:GLU:OE1	59:x:64:GLY:N	2.37	0.56
62:A1:9:ASP:OD2	62:A1:11:SER:HB3	2.06	0.56
2:1:184:MET:HE3	70:B:501:3PE:H352	1.88	0.56
3:9:227:PRO:O	9:8:284:ASN:ND2	2.39	0.56
5:4:119:TYR:HA	5:4:122:PHE:HB3	1.86	0.56
7:6:587:TYR:O	7:6:590:SER:N	2.37	0.56
17:C0:71:THR:O	17:C0:75:ARG:HD3	2.05	0.56
23:A:250:SER:O	23:A:251:ILE:HD13	2.06	0.56
23:A:374:THR:OG1	23:A:377:ALA:O	2.23	0.56
70:B:501:3PE:H232	27:E:63:TRP:HE1	1.71	0.56
35:N:51:ILE:HD11	35:N:87:GLU:OE2	2.05	0.56
39:R:238:GLN:NE2	39:R:270:ARG:O	2.36	0.56
39:R:244:ASP:OD2	39:R:343:THR:HG23	2.05	0.56
40:S:79:ILE:O	40:S:122:TRP:NE1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:b:92:PHE:HB2	49:b:93:ILE:HD12	1.87	0.56
56:g:114:GLN:O	56:g:117:GLU:N	2.32	0.56
65:s:15:ASP:OD1	65:s:18:THR:N	2.37	0.56
65:s:66:ASP:HA	65:s:69:VAL:HB	1.87	0.56
58:w:191:LYS:O	58:w:194:ARG:HB2	2.05	0.56
59:x:201:SER:OG	59:x:224:LEU:O	2.23	0.56
60:y:146:ILE:O	60:y:149:LEU:HB3	2.06	0.56
2:1:203:GLY:H	2:1:210:GLY:N	1.94	0.56
8:2:134:GLN:N	8:2:134:GLN:OE1	2.35	0.56
8:2:305:PHE:HZ	40:S:317:GLN:HG2	1.70	0.56
24:B:124:ILE:HG22	24:B:124:ILE:O	2.06	0.56
24:B:238:LEU:HA	43:V:10:MET:HE1	1.88	0.56
40:S:219:SER:HA	40:S:222:LEU:HB2	1.88	0.56
41:T:70:PHE:HE2	41:T:90:TYR:HH	1.54	0.56
43:V:131:GLU:O	43:V:134:LEU:N	2.39	0.56
48:a:54:PRO:HD3	52:f:133:TRP:CE2	2.39	0.56
52:f:104:LEU:CA	52:f:107:TRP:HE1	2.18	0.56
59:l:310:SER:HG	68:v:61:GLY:N	2.04	0.56
64:r:79:ASN:HB3	65:s:52:GLU:HB2	1.88	0.56
66:t:43:ASP:HB3	67:u:33:ARG:HH22	1.71	0.56
58:w:245:GLU:HA	64:A3:11:ARG:HA	1.87	0.56
58:w:314:TYR:HB2	58:w:317:THR:HB	1.87	0.56
67:B6:17:THR:HA	67:B6:20:PHE:HB3	1.88	0.56
5:4:364:LEU:HD21	5:4:369:LEU:HD12	1.88	0.55
7:6:152:PHE:CD1	7:6:168:ALA:HB1	2.41	0.55
7:6:428:PHE:O	7:6:432:LEU:HB3	2.06	0.55
72:6:701:CDL:H721	72:6:701:CDL:H542	1.87	0.55
8:2:85:THR:CG2	30:H:19:THR:CG2	2.75	0.55
11:C1:111:THR:HG21	17:C0:66:ILE:HD11	1.88	0.55
27:E:52:SER:OG	27:E:56:ARG:NH1	2.39	0.55
27:E:118:LEU:C	27:E:120:GLU:N	2.62	0.55
34:L:22:SER:O	34:L:26:ALA:N	2.39	0.55
40:S:138:LEU:O	40:S:142:GLY:N	2.40	0.55
53:h:95:PHE:O	53:h:96:SER:OG	2.20	0.55
58:k:210:ASP:OD1	58:k:211:LEU:N	2.39	0.55
58:k:262:TRP:HD1	58:k:315:ALA:HA	1.70	0.55
60:m:77:TRP:CZ3	60:m:78:ILE:HG22	2.40	0.55
58:w:21:ASN:ND2	58:w:217:SER:H	2.04	0.55
59:x:100:SER:HA	59:x:105:MET:HA	1.88	0.55
62:A1:104:LYS:O	62:A1:108:GLN:N	2.36	0.55
65:B7:15:ASP:OD1	65:B7:18:THR:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:B7:44:VAL:HG12	65:B7:48:SER:HB2	1.88	0.55
2:1:138:GLN:OE1	2:1:285:LEU:HD21	2.06	0.55
2:1:169:GLN:HE21	2:1:174:LEU:CB	2.19	0.55
5:4:385:THR:HG21	5:4:396:MET:HE1	1.88	0.55
7:6:101:MET:HB3	7:6:118:PHE:HE1	1.71	0.55
7:6:373:LEU:HD12	7:6:431:LEU:HD11	1.88	0.55
9:8:409:ILE:HG23	9:8:439:ILE:HD12	1.87	0.55
12:A9:42:LEU:HD13	19:B2:45:TYR:CD2	2.41	0.55
16:A6:5:LYS:HD2	16:A6:6:GLY:N	2.21	0.55
23:A:180:THR:HG23	23:A:183:ILE:HD12	1.87	0.55
50:c:28:LEU:HG	50:c:30:PRO:HD2	1.88	0.55
59:l:201:SER:OG	59:l:224:LEU:O	2.23	0.55
61:o:33:TYR:HD1	61:o:37:CYS:HB2	1.71	0.55
64:r:80:ASP:HB2	65:s:47:ARG:NH1	2.21	0.55
66:t:34:TRP:CA	66:t:37:ASP:OD1	2.55	0.55
63:A2:18:LYS:O	63:A2:19:TRP:C	2.49	0.55
63:A2:33:ARG:NH2	63:A2:91:GLU:OE2	2.29	0.55
65:B7:29:LYS:HA	65:B7:32:LYS:HB3	1.87	0.55
2:1:236:ILE:O	2:1:236:ILE:HD12	2.06	0.55
3:9:222:ARG:NE	3:9:226:GLU:O	2.40	0.55
7:6:97:THR:HA	7:6:100:ILE:HG22	1.87	0.55
8:2:51:ARG:O	8:2:55:ALA:N	2.39	0.55
23:A:422:TRP:CH2	29:G:169:ARG:HD3	2.42	0.55
24:B:141:TYR:CD1	24:B:141:TYR:N	2.67	0.55
24:B:182:ASN:HD22	24:B:403:PRO:HB2	1.71	0.55
24:B:430:ALA:O	24:B:433:ALA:N	2.39	0.55
35:N:86:ASN:O	35:N:89:SER:N	2.39	0.55
36:O:48:HIS:ND1	39:R:359:TYR:OH	2.35	0.55
39:R:155:VAL:O	39:R:159:ALA:N	2.24	0.55
49:b:67:PHE:O	49:b:68:LEU:HB2	2.06	0.55
52:f:84:GLU:HA	52:f:91:TYR:HA	1.88	0.55
58:w:17:SER:HB2	58:w:25:VAL:HB	1.88	0.55
58:w:77:LYS:O	58:w:81:SER:OG	2.22	0.55
63:A2:10:SER:C	82:A2:201:UQ2:CM5	2.79	0.55
4:7:82:ILE:HG22	4:7:83:TRP:N	2.20	0.55
10:C3:95:PRO:HB2	12:A9:11:VAL:HG13	1.87	0.55
10:C3:407:ASP:O	10:C3:411:LYS:HG3	2.07	0.55
58:k:314:TYR:HB2	58:k:317:THR:HB	1.87	0.55
59:l:100:SER:HA	59:l:105:MET:HA	1.88	0.55
59:l:279:LEU:HD22	59:l:295:LEU:HB2	1.86	0.55
58:w:335:MET:O	58:w:338:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:55:PHE:HB2	3:9:60:TYR:CZ	2.41	0.55
5:4:51:ASN:HD21	49:b:136:THR:HG22	1.71	0.55
5:4:248:LEU:HD11	56:g:151:SER:HA	1.87	0.55
6:5:20:LEU:HD21	8:2:65:THR:HG21	1.89	0.55
7:6:37:LYS:HD2	7:6:102:GLU:HG3	1.87	0.55
23:A:394:VAL:HG11	23:A:418:ILE:HD13	1.89	0.55
40:S:282:LEU:CB	40:S:288:ASP:H	2.19	0.55
53:h:141:CYS:HA	56:g:162:ARG:HD3	1.88	0.55
58:k:186:LEU:HD23	58:k:190:TYR:HE2	1.72	0.55
59:l:28:ARG:HH21	59:l:32:GLY:CA	2.19	0.55
58:w:391:PRO:HG2	58:w:398:ARG:HH22	1.71	0.55
64:A3:39:ARG:HG3	64:A3:40:ARG:N	2.22	0.55
4:7:28:TYR:CZ	4:7:83:TRP:CD1	2.86	0.55
7:6:376:GLY:O	7:6:379:ALA:N	2.39	0.55
7:6:407:TRP:O	7:6:411:MET:N	2.31	0.55
52:f:17:LEU:O	52:f:21:LYS:N	2.35	0.55
57:e:46:GLU:O	57:e:50:ALA:HB2	2.06	0.55
58:k:17:SER:HB2	58:k:25:VAL:HB	1.88	0.55
61:o:134:TYR:CE1	61:o:162:PRO:HG3	2.41	0.55
64:r:39:ARG:HG3	64:r:40:ARG:N	2.22	0.55
60:y:138:MET:HB2	60:y:255:ASN:ND2	2.20	0.55
61:z:30:PHE:CE2	61:z:34:LYS:HD2	2.42	0.55
2:1:29:GLY:HA2	26:D:108:ARG:HH21	1.70	0.55
3:9:59:ASN:OD1	28:F:83:TYR:OH	2.24	0.55
3:9:155:LYS:HZ1	3:9:205:ILE:HG21	1.71	0.55
7:6:132:VAL:HG23	7:6:133:THR:HG23	1.88	0.55
23:A:367:CYS:SG	23:A:533:GLY:N	2.80	0.55
24:B:61:TRP:CD1	24:B:62:LYS:CA	2.90	0.55
24:B:81:THR:HA	24:B:100:GLU:OE2	2.07	0.55
24:B:147:ASN:O	24:B:148:GLU:HB2	2.06	0.55
24:B:460:GLU:CD	24:B:460:GLU:C	2.75	0.55
25:C:171:GLU:OE1	25:C:172:ILE:HG13	2.07	0.55
25:C:213:ARG:HH11	25:C:224:GLU:CD	2.15	0.55
33:K:23:LEU:HA	33:K:63:PRO:HB3	1.89	0.55
40:S:333:GLU:C	40:S:335:VAL:H	2.15	0.55
61:o:52:VAL:HG22	67:u:56:LYS:HZ1	1.71	0.55
62:p:18:VAL:HG11	62:p:32:ARG:NH1	2.21	0.55
64:r:63:THR:O	64:r:67:GLU:HG3	2.06	0.55
67:u:10:TYR:HA	67:u:14:PHE:HB2	1.87	0.55
58:w:148:VAL:HG12	58:w:152:TYR:HE2	1.70	0.55
59:x:65:THR:O	59:x:69:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:65:THR:HG23	59:x:191:LEU:HD23	1.88	0.55
60:y:101:GLY:HA2	60:y:106:SER:HB2	1.88	0.55
61:z:134:TYR:CE1	61:z:162:PRO:HG3	2.41	0.55
63:A2:11:ARG:HA	82:A2:201:UQ2:CM5	2.37	0.55
3:9:123:ASN:HD22	3:9:127:VAL:CG1	2.20	0.55
6:5:20:LEU:O	6:5:29:SER:HB2	2.07	0.55
8:2:247:THR:O	8:2:250:SER:N	2.40	0.55
70:2:401:3PE:H2A1	70:2:401:3PE:H371	1.89	0.55
23:A:221:ASN:OD1	23:A:291:ARG:NH2	2.40	0.55
23:A:587:ALA:HB1	23:A:591:GLU:HB2	1.89	0.55
34:L:53:TYR:HD1	43:V:69:ILE:HG23	1.71	0.55
35:N:88:LEU:O	35:N:91:ALA:N	2.40	0.55
40:S:332:ASN:C	40:S:334:ASP:H	2.14	0.55
55:j:62:LEU:HG	55:j:63:LEU:H	1.72	0.55
58:k:15:GLN:HG3	58:k:205:HIS:HB2	1.89	0.55
58:k:335:MET:O	58:k:338:LEU:N	2.40	0.55
59:l:246:GLU:O	59:l:427:SER:HA	2.07	0.55
60:m:101:GLY:HA2	60:m:106:SER:HB2	1.88	0.55
61:o:30:PHE:CE2	61:o:34:LYS:HD2	2.42	0.55
61:o:156:GLN:HE22	65:s:59:LEU:HD11	1.71	0.55
65:s:18:THR:HA	65:s:21:ARG:HD2	1.87	0.55
58:w:210:ASP:OD1	58:w:211:LEU:N	2.39	0.55
59:x:246:GLU:O	59:x:427:SER:HA	2.07	0.55
59:x:305:GLN:OE1	59:x:305:GLN:N	2.39	0.55
61:z:138:PRO:HG3	65:B7:58:LEU:HD22	1.88	0.55
1:3:77:TRP:CD1	2:1:318:THR:O	2.60	0.55
2:1:196:ALA:O	2:1:199:ASP:HB2	2.06	0.55
2:1:310:LEU:HD12	34:L:33:PRO:HA	1.89	0.55
7:6:114:ILE:HD11	7:6:118:PHE:HE2	1.71	0.55
8:2:311:MET:HB3	8:2:313:MET:HE3	1.89	0.55
24:B:272:THR:O	24:B:273:VAL:HG13	2.06	0.55
33:K:41:TYR:HE1	33:K:53:ILE:CG2	2.18	0.55
57:e:41:TYR:O	57:e:43:LYS:N	2.39	0.55
58:k:289:HIS:O	59:l:87:ARG:NE	2.39	0.55
59:l:28:ARG:HD2	59:l:34:VAL:HG22	1.87	0.55
59:l:65:THR:HG23	59:l:191:LEU:HD23	1.88	0.55
60:m:267:HIS:NE2	60:m:269:LYS:HD3	2.22	0.55
58:w:64:PHE:HA	58:w:75:LEU:HD23	1.88	0.55
3:9:239:LYS:HE2	9:8:42:PHE:HB2	1.89	0.55
5:4:359:TRP:HB3	5:4:411:LEU:HD22	1.89	0.55
6:5:79:VAL:O	6:5:83:ASN:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:260:ASN:H	23:A:282:ASN:HD22	1.54	0.55
24:B:168:GLN:O	24:B:171:ARG:N	2.40	0.55
35:N:107:PRO:O	35:N:109:ALA:N	2.34	0.55
41:T:86:ASP:O	41:T:89:ASN:N	2.40	0.55
62:p:68:VAL:HG11	60:y:167:GLY:HA2	1.88	0.55
58:w:298:ALA:O	58:w:302:LYS:HA	2.07	0.55
61:z:33:TYR:HD1	61:z:37:CYS:HB2	1.71	0.55
61:z:165:TYR:CE1	61:z:168:VAL:HA	2.42	0.55
2:1:84:THR:O	2:1:87:ILE:HG13	2.07	0.54
2:1:159:SER:HB3	2:1:317:GLN:CG	2.38	0.54
5:4:1:MET:HG2	5:4:2:LEU:N	2.17	0.54
18:C2:63:MET:HB3	18:C2:68:ILE:HD11	1.89	0.54
23:A:63:PHE:O	23:A:181:ARG:NH2	2.22	0.54
23:A:456:ALA:O	23:A:499:LYS:NZ	2.40	0.54
24:B:61:TRP:O	24:B:62:LYS:HB2	2.07	0.54
53:h:120:ARG:NH2	56:g:66:ARG:H	1.96	0.54
58:k:436:ARG:HE	60:m:222:PRO:HG3	1.71	0.54
60:m:311:LYS:HD2	60:m:379:TRP:HB3	1.89	0.54
61:o:23:HIS:HB3	61:o:54:VAL:HA	1.88	0.54
59:x:28:ARG:HD2	59:x:34:VAL:HG22	1.87	0.54
60:y:311:LYS:HD2	60:y:379:TRP:HB3	1.89	0.54
64:A3:63:THR:O	64:A3:67:GLU:HG3	2.06	0.54
2:1:237:PHE:O	2:1:240:ILE:N	2.36	0.54
2:1:266:LEU:HD12	2:1:266:LEU:C	2.33	0.54
2:1:312:SER:HG	43:V:55:ARG:HH22	1.54	0.54
3:9:155:LYS:HE2	3:9:205:ILE:HD13	1.89	0.54
5:4:214:LEU:HD11	7:6:558:LEU:HB3	1.89	0.54
7:6:157:TRP:CD1	7:6:158:TRP:CD1	2.94	0.54
7:6:546:GLN:O	7:6:550:SER:N	2.40	0.54
8:2:335:MET:SD	69:Q:201:PC1:H2D1	2.47	0.54
9:8:210:THR:HG22	9:8:224:ARG:HB2	1.89	0.54
12:A9:151:LEU:HB2	12:A9:159:MET:HG3	1.89	0.54
25:C:227:GLU:OE2	29:G:107:TRP:CH2	2.60	0.54
31:I:87:CYS:O	31:I:96:HIS:NE2	2.40	0.54
58:k:184:GLU:O	58:k:188:ARG:HG3	2.08	0.54
58:k:298:ALA:O	58:k:302:LYS:HA	2.07	0.54
58:k:391:PRO:HG2	58:k:398:ARG:HH22	1.71	0.54
59:l:283:PRO:HA	59:l:290:ASN:HD21	1.72	0.54
61:o:165:TYR:CE1	61:o:168:VAL:HA	2.42	0.54
63:q:98:ILE:O	63:q:102:LYS:HG2	2.08	0.54
58:w:244:ARG:CZ	64:A3:10:VAL:HB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:A2:201:UQ2:H2M2	82:A2:201:UQ2:O1	2.07	0.54
67:B6:10:TYR:HA	67:B6:14:PHE:HB2	1.88	0.54
2:1:253:GLU:CG	2:1:254:LEU:N	2.71	0.54
8:2:24:SER:O	8:2:85:THR:HA	2.07	0.54
9:8:159:ARG:HG2	9:8:161:GLU:H	1.71	0.54
23:A:146:PHE:N	23:A:146:PHE:HD1	2.04	0.54
41:T:22:THR:OG1	41:T:68:ALA:O	2.18	0.54
41:T:124:LEU:O	41:T:128:GLY:N	2.38	0.54
44:W:115:GLN:HE21	44:W:135:ALA:C	2.15	0.54
59:l:51:ILE:HG22	59:l:53:ALA:H	1.72	0.54
61:o:80:MET:CG	61:o:81:PHE:H	2.19	0.54
61:o:138:PRO:O	61:o:141:VAL:HG12	2.07	0.54
58:w:15:GLN:HG3	58:w:205:HIS:HB2	1.89	0.54
58:w:184:GLU:O	58:w:188:ARG:HG3	2.08	0.54
58:w:186:LEU:HD23	58:w:190:TYR:HE2	1.72	0.54
60:y:75:TYR:HB3	60:y:78:ILE:HG12	1.88	0.54
61:z:215:LEU:HD22	62:A1:43:THR:HG23	1.90	0.54
63:A2:12:TRP:C	63:A2:12:TRP:CD1	2.86	0.54
2:1:284:GLN:O	2:1:288:LEU:HD23	2.08	0.54
4:7:33:LEU:O	4:7:36:SER:N	2.40	0.54
7:6:255:ALA:HA	7:6:258:PHE:HB3	1.89	0.54
9:8:413:TRP:O	9:8:416:SER:OG	2.23	0.54
25:C:179:PHE:CE1	36:O:84:ILE:HG21	2.43	0.54
37:P:19:ASP:C	37:P:21:GLN:H	2.16	0.54
58:k:3:THR:O	58:k:7:ALA:N	2.29	0.54
58:k:64:PHE:HA	58:k:75:LEU:HD23	1.88	0.54
58:k:68:LYS:HB3	58:k:119:ASN:HB3	1.89	0.54
59:l:203:ARG:NH1	59:l:231:GLY:HA2	2.22	0.54
59:l:275:LEU:HB2	59:l:410:VAL:HG13	1.88	0.54
63:q:58:ARG:HA	63:q:61:ARG:NH2	2.23	0.54
64:r:54:ALA:HA	64:r:57:LEU:HD12	1.90	0.54
67:u:10:TYR:CE1	67:u:15:ARG:HA	2.42	0.54
58:w:426:GLY:HA2	58:w:428:ILE:H	1.72	0.54
59:x:43:PRO:HA	59:x:113:ARG:HB2	1.88	0.54
59:x:200:THR:OG1	59:x:228:GLY:N	2.30	0.54
59:x:283:PRO:HA	59:x:290:ASN:HD21	1.73	0.54
59:x:294:SER:O	59:x:298:ALA:N	2.30	0.54
60:y:372:ILE:O	60:y:376:LEU:HG	2.08	0.54
61:z:138:PRO:O	61:z:141:VAL:HG12	2.07	0.54
67:B6:10:TYR:CE1	67:B6:15:ARG:HA	2.42	0.54
2:1:146:LEU:HD11	2:1:185:TRP:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:227:GLY:HA2	5:4:230:VAL:HB	1.89	0.54
7:6:408:ALA:HA	7:6:411:MET:HB3	1.87	0.54
9:8:103:ASN:HD22	9:8:149:MET:HE1	1.73	0.54
16:A6:5:LYS:HD2	16:A6:5:LYS:C	2.32	0.54
23:A:138:ASP:O	23:A:139:LEU:HD23	2.07	0.54
30:H:9:ARG:NH2	55:j:12:GLN:OE1	2.40	0.54
31:I:108:LYS:HA	31:I:108:LYS:HE3	1.84	0.54
59:l:43:PRO:HA	59:l:113:ARG:HB2	1.88	0.54
60:m:22:PRO:HG2	64:r:3:GLN:HB3	1.89	0.54
63:q:25:GLY:O	63:q:28:LYS:N	2.38	0.54
67:u:52:TRP:O	67:u:56:LYS:N	2.39	0.54
59:x:28:ARG:HH21	59:x:32:GLY:CA	2.19	0.54
59:x:135:TRP:CD1	59:x:136:GLU:HG3	2.43	0.54
59:x:305:GLN:HG2	59:x:306:PRO:HD2	1.88	0.54
61:z:23:HIS:CD2	67:B6:55:ILE:HD12	2.43	0.54
65:B7:12:GLU:O	65:B7:13:LEU:HB2	2.07	0.54
5:4:179:LEU:O	5:4:180:GLN:NE2	2.41	0.54
7:6:598:SER:O	7:6:604:PHE:HD2	1.91	0.54
8:2:265:MET:HE2	8:2:341:PRO:HG2	1.90	0.54
9:8:98:LYS:HG3	9:8:99:TRP:HD1	1.72	0.54
23:A:127:ASP:O	23:A:128:CYS:HB2	2.07	0.54
27:E:155:CYS:HB2	27:E:157:PHE:H	1.73	0.54
38:Q:28:ALA:O	38:Q:30:HIS:N	2.41	0.54
38:Q:39:PRO:O	38:Q:43:PHE:N	2.41	0.54
38:Q:47:ARG:NE	38:Q:53:PRO:HB3	2.22	0.54
40:S:124:TYR:OH	40:S:182:THR:HG21	2.08	0.54
48:a:51:TYR:HD1	48:a:56:ARG:HH12	1.55	0.54
49:b:93:ILE:HG23	56:g:61:TYR:CE2	2.43	0.54
52:f:14:GLN:HB2	52:f:17:LEU:HD12	1.90	0.54
57:e:37:LEU:H	57:e:77:LYS:HD3	1.72	0.54
44:M:14:ARG:HA	44:M:17:TYR:CE2	2.42	0.54
59:l:245:ARG:NH2	59:l:430:LEU:HB3	2.22	0.54
60:m:75:TYR:HB3	60:m:78:ILE:HG12	1.88	0.54
60:m:163:TRP:CD1	62:A1:63:SER:HG	2.25	0.54
61:o:223:LYS:O	61:o:227:TRP:HD1	1.91	0.54
65:s:44:VAL:HG12	65:s:48:SER:HB2	1.88	0.54
2:1:264:LEU:HG	2:1:264:LEU:O	2.07	0.54
2:1:303:TRP:HE3	34:L:29:ALA:HB2	1.72	0.54
3:9:55:PHE:HA	3:9:89:GLN:HE22	1.73	0.54
7:6:176:ARG:O	7:6:179:ASP:HB3	2.08	0.54
7:6:191:THR:O	48:a:126:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:175:LEU:HG	8:2:224:THR:O	2.08	0.54
24:B:163:PRO:HB2	24:B:167:ALA:HB3	1.90	0.54
24:B:279:THR:OG1	35:N:12:VAL:HG12	2.07	0.54
25:C:227:GLU:HG2	39:R:48:ARG:O	2.07	0.54
38:Q:105:ALA:O	38:Q:109:GLU:N	2.41	0.54
38:Q:132:LYS:HE3	38:Q:134:ASP:OD1	2.08	0.54
58:k:252:HIS:CD2	58:k:323:HIS:CE1	2.95	0.54
61:o:150:ASN:O	61:o:156:GLN:HA	2.08	0.54
58:w:67:THR:HG22	58:w:70:ARG:HB2	1.90	0.54
58:w:135:LEU:HA	58:w:138:LEU:HD12	1.89	0.54
61:z:150:ASN:O	61:z:156:GLN:HA	2.08	0.54
61:z:221:ALA:O	61:z:225:HIS:N	2.34	0.54
63:A2:25:GLY:O	63:A2:28:LYS:N	2.38	0.54
63:A2:58:ARG:HA	63:A2:61:ARG:NH2	2.23	0.54
64:A3:54:ALA:HA	64:A3:57:LEU:HD12	1.90	0.54
67:B6:52:TRP:O	67:B6:56:LYS:N	2.38	0.54
7:6:603:ASN:O	7:6:606:GLU:N	2.27	0.54
14:B4:41:LEU:O	14:B4:41:LEU:HD12	2.08	0.54
15:A5:48:LEU:O	15:A5:50:PRO:HD3	2.08	0.54
23:A:126:LEU:HD21	24:B:373:THR:O	2.08	0.54
23:A:355:LYS:CA	23:A:530:TYR:OH	2.56	0.54
24:B:190:HIS:ND1	24:B:452:GLY:HA3	2.23	0.54
24:B:305:THR:HG23	24:B:306:GLN:HG2	1.90	0.54
26:D:99:MET:HE3	26:D:106:MET:HG2	1.89	0.54
26:D:191:GLU:OE2	27:E:86:TYR:CZ	2.60	0.54
40:S:173:ASP:O	40:S:177:GLN:N	2.32	0.54
48:a:22:GLU:OE1	48:a:22:GLU:N	2.41	0.54
58:k:163:LEU:HD21	58:k:314:TYR:CD2	2.43	0.54
58:k:431:LEU:HD12	58:k:432:PRO:HD2	1.90	0.54
60:m:215:VAL:HG12	64:r:8:THR:HG21	1.90	0.54
61:o:52:VAL:HG22	67:u:56:LYS:NZ	2.23	0.54
62:p:73:LYS:HD3	62:p:94:LYS:CA	2.38	0.54
58:w:7:ALA:HB1	59:x:43:PRO:HD3	1.88	0.54
60:y:233:LEU:HD12	60:y:236:ILE:HG13	1.90	0.54
60:y:377:LEU:HB3	63:A2:33:ARG:HD2	1.90	0.54
61:z:3:LEU:HB2	65:B7:59:LEU:CD1	2.38	0.54
63:A2:10:SER:O	82:A2:201:UQ2:H5M1	2.04	0.54
7:6:487:LYS:HG3	7:6:488:THR:H	1.73	0.54
7:6:504:ILE:O	7:6:508:THR:N	2.41	0.54
8:2:9:ILE:O	8:2:12:THR:HG22	2.07	0.54
8:2:95:SER:O	8:2:98:MET:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A7:67:SER:OG	13:A7:70:GLU:HG3	2.08	0.54
26:D:146:GLU:HB3	26:D:147:PRO:CD	2.38	0.54
27:E:128:ILE:CD1	27:E:147:ILE:HG12	2.38	0.54
34:L:36:SER:O	34:L:39:THR:HG22	2.08	0.54
40:S:52:GLY:H	40:S:195:VAL:HB	1.73	0.54
40:S:190:HIS:HB2	40:S:277:ARG:NE	2.23	0.54
53:h:85:TRP:HA	53:h:88:ARG:HH11	1.72	0.54
58:k:215:HIS:C	58:k:219:LEU:H	2.16	0.54
60:m:372:ILE:O	60:m:376:LEU:HG	2.08	0.54
58:w:381:ARG:O	58:w:385:THR:N	2.41	0.54
59:x:334:GLY:O	59:x:338:LYS:N	2.26	0.54
2:1:105:MET:O	2:1:109:SER:N	2.33	0.54
2:1:190:LEU:HD12	2:1:195:ARG:HB2	1.89	0.54
2:1:232:ILE:O	2:1:236:ILE:HG21	2.04	0.54
3:9:129:LYS:H	3:9:168:LEU:HA	1.73	0.54
3:9:224:SER:OG	3:9:226:GLU:HG2	2.08	0.54
5:4:52:PHE:HZ	5:4:58:SER:HG	1.51	0.54
7:6:206:PRO:HD2	7:6:266:LEU:HD13	1.89	0.54
12:A9:222:GLN:HA	12:A9:222:GLN:HE21	1.72	0.54
13:A7:52:SER:OG	13:A7:55:GLU:HG3	2.08	0.54
24:B:294:ARG:HH21	24:B:301:ASP:HB3	1.73	0.54
30:H:62:ASP:O	30:H:66:CYS:N	2.41	0.54
41:T:95:CYS:HA	41:T:115:CYS:HA	1.89	0.54
44:W:81:ASP:O	44:W:85:TYR:N	2.40	0.54
58:k:416:TYR:O	58:k:418:GLN:NE2	2.37	0.54
59:l:155:PRO:HB2	59:l:254:HIS:CE1	2.43	0.54
59:l:243:GLU:HB2	59:l:424:MET:HB3	1.90	0.54
61:o:69:GLU:HB2	61:o:84:PRO:HD3	1.90	0.54
61:o:147:LEU:HD22	61:o:157:ALA:O	2.08	0.54
63:q:9:SER:HA	63:q:12:TRP:HB3	1.90	0.54
58:w:416:TYR:O	58:w:418:GLN:NE2	2.37	0.54
59:x:155:PRO:HB2	59:x:254:HIS:CE1	2.43	0.54
60:y:29:SER:HA	60:y:32:ASN:HD22	1.72	0.54
60:y:300:ILE:HG13	60:y:303:LEU:HD12	1.90	0.54
61:z:171:PHE:HE2	61:z:177:ALA:HA	1.73	0.54
2:1:143:GLU:OE1	2:1:143:GLU:N	2.41	0.53
3:9:118:PHE:HB2	9:8:220:GLN:NE2	2.19	0.53
7:6:161:ARG:O	7:6:164:ALA:N	2.39	0.53
8:2:294:MET:O	8:2:295:ARG:HB3	2.08	0.53
15:A5:82:CYS:N	15:A5:86:GLY:O	2.41	0.53
23:A:152:ARG:HG3	23:A:152:ARG:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:473:MET:HE2	23:A:475:ILE:HD11	1.89	0.53
24:B:203:MET:O	24:B:206:GLU:N	2.35	0.53
27:E:114:ILE:O	27:E:114:ILE:HG13	2.08	0.53
27:E:171:PRO:CB	27:E:200:GLU:OE2	2.49	0.53
45:X:19:GLY:O	45:X:22:PHE:HB3	2.08	0.53
55:j:68:PHE:O	55:j:72:GLY:N	2.30	0.53
44:M:29:LYS:HE2	44:M:39:ASP:OD1	2.08	0.53
59:l:135:TRP:CD1	59:l:136:GLU:HG3	2.43	0.53
66:t:36:THR:HG21	66:t:38:TRP:HD1	1.51	0.53
58:w:68:LYS:HB3	58:w:119:ASN:HB3	1.89	0.53
59:x:124:LEU:O	59:x:128:THR:N	2.32	0.53
63:A2:98:ILE:O	63:A2:102:LYS:HG2	2.08	0.53
66:A4:35:ALA:O	66:A4:36:THR:CG2	2.57	0.53
2:1:153:VAL:HG23	2:1:154:LEU:HD12	1.90	0.53
4:7:71:THR:O	4:7:72:THR:OG1	2.19	0.53
9:8:207:GLY:HA2	73:8:501:FMN:C6	2.38	0.53
11:C1:203:ASN:HD22	11:C1:206:PHE:HD2	1.55	0.53
24:B:217:VAL:HG13	24:B:218:SER:H	1.73	0.53
39:R:55:VAL:HG12	39:R:56:ALA:N	2.21	0.53
39:R:317:ASP:O	39:R:321:ARG:N	2.41	0.53
40:S:291:GLU:OE1	40:S:291:GLU:N	2.40	0.53
49:b:76:LEU:O	49:b:79:GLY:N	2.41	0.53
52:f:61:THR:O	52:f:65:ARG:N	2.36	0.53
55:j:64:TYR:O	55:j:67:SER:N	2.39	0.53
58:k:67:THR:HG22	58:k:70:ARG:HB2	1.90	0.53
58:k:184:GLU:O	58:k:188:ARG:N	2.35	0.53
60:m:300:ILE:HG13	60:m:303:LEU:HD12	1.90	0.53
61:o:197:GLU:OE1	61:o:197:GLU:N	2.34	0.53
66:t:30:VAL:CA	66:t:33:VAL:HG22	2.39	0.53
58:w:67:THR:HA	58:w:121:SER:H	1.72	0.53
58:w:186:LEU:HA	58:w:190:TYR:CD2	2.43	0.53
58:w:431:LEU:HD12	58:w:432:PRO:HD2	1.90	0.53
59:x:203:ARG:NH1	59:x:231:GLY:HA2	2.23	0.53
61:z:147:LEU:HD22	61:z:157:ALA:O	2.08	0.53
1:3:68:GLU:HA	1:3:71:LEU:HB2	1.90	0.53
2:1:126:LYS:HD3	2:1:129:LEU:HD23	1.90	0.53
3:9:238:PRO:HG3	9:8:60:GLY:HA2	1.90	0.53
3:9:238:PRO:HG2	3:9:241:PRO:HG3	1.89	0.53
5:4:348:LEU:O	5:4:349:GLN:HB3	2.07	0.53
8:2:5:ILE:O	8:2:8:ILE:N	2.40	0.53
8:2:84:TRP:H	8:2:84:TRP:HD1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:234:TRP:NE1	8:2:303:THR:OG1	2.40	0.53
13:A7:108:PRO:HG2	13:A7:111:PHE:CE2	2.42	0.53
25:C:90:ILE:HD12	25:C:145:VAL:HG13	1.91	0.53
44:W:123:GLU:HB2	44:W:130:ILE:HD12	1.90	0.53
50:c:71:ALA:O	50:c:75:VAL:HG12	2.08	0.53
55:j:78:ARG:O	55:j:81:TYR:HB3	2.08	0.53
58:k:389:ARG:C	58:k:391:PRO:HD3	2.34	0.53
60:m:345:HIS:CE1	60:m:346:PRO:HD3	2.43	0.53
63:q:28:LYS:HG2	63:q:80:TRP:CE3	2.44	0.53
58:w:163:LEU:HD21	58:w:314:TYR:CD2	2.43	0.53
59:x:29:LEU:HD12	59:x:33:LEU:HG	1.90	0.53
59:x:51:ILE:HG22	59:x:53:ALA:H	1.72	0.53
61:z:23:HIS:HB3	61:z:54:VAL:HA	1.88	0.53
64:A3:79:ASN:HB3	65:B7:52:GLU:HB2	1.90	0.53
1:3:88:LEU:HD21	2:1:309:ILE:HD12	1.90	0.53
3:9:62:ARG:O	3:9:65:ALA:N	2.42	0.53
7:6:60:GLU:CD	7:6:83:ASP:HA	2.34	0.53
8:2:112:HIS:O	8:2:112:HIS:ND1	2.41	0.53
8:2:190:MET:HB2	8:2:201:THR:HG23	1.90	0.53
9:8:398:ARG:HG3	9:8:403:ASP:OD2	2.08	0.53
12:A9:156:ARG:HG3	12:A9:156:ARG:NH1	2.22	0.53
13:A7:40:LEU:HD13	13:A7:59:LEU:HD13	1.90	0.53
24:B:286:TYR:OH	24:B:437:LYS:HD2	2.08	0.53
24:B:404:LYS:HE2	24:B:455:ASP:OD2	2.09	0.53
27:E:135:ARG:HG2	27:E:136:ALA:H	1.74	0.53
58:k:135:LEU:HA	58:k:138:LEU:HD12	1.89	0.53
58:k:181:ASP:HA	58:k:184:GLU:CD	2.33	0.53
59:l:102:ARG:NH2	59:l:161:GLU:OE1	2.42	0.53
58:w:181:ASP:HA	58:w:184:GLU:CD	2.33	0.53
58:w:252:HIS:CD2	58:w:323:HIS:CE1	2.95	0.53
60:y:345:HIS:CE1	60:y:346:PRO:HD3	2.43	0.53
64:A3:64:GLN:HA	64:A3:67:GLU:OE1	2.08	0.53
1:3:2:ASN:HB2	2:1:2:PHE:CE2	2.44	0.53
11:C1:68:LEU:HB3	11:C1:69:PRO:HD3	1.91	0.53
15:A5:55:LYS:HA	15:A5:74:LEU:O	2.08	0.53
23:A:560:LEU:HD12	23:A:561:PRO:HD2	1.90	0.53
24:B:294:ARG:HH21	24:B:301:ASP:CB	2.21	0.53
26:D:106:MET:HE3	26:D:111:VAL:HB	1.91	0.53
27:E:86:TYR:OH	27:E:90:LYS:NZ	2.42	0.53
34:L:19:LEU:O	34:L:22:SER:OG	2.13	0.53
50:c:5:THR:HG22	50:c:7:GLU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:79:ASP:H	53:h:83:ASP:CG	2.17	0.53
54:i:47:THR:OG1	55:j:59:HIS:HB2	2.07	0.53
44:M:51:ILE:HD12	44:M:70:LEU:HD12	1.91	0.53
58:k:183:THR:HA	58:k:186:LEU:HB2	1.91	0.53
58:k:227:ALA:O	58:k:228:VAL:HG23	2.09	0.53
58:w:183:THR:HA	58:w:186:LEU:HB2	1.91	0.53
59:x:227:ARG:HB3	59:x:228:GLY:CA	2.38	0.53
59:x:243:GLU:HB2	59:x:424:MET:HB3	1.90	0.53
60:y:267:HIS:NE2	60:y:269:LYS:HD3	2.22	0.53
60:y:313:ARG:HB2	63:A2:38:HIS:HD2	1.73	0.53
62:A1:135:LEU:HA	62:A1:183:PRO:N	2.24	0.53
63:A2:28:LYS:HG2	63:A2:80:TRP:CE3	2.44	0.53
65:B7:37:LEU:O	65:B7:41:ASP:N	2.28	0.53
3:9:95:ILE:HD11	23:A:210:ILE:HG22	1.89	0.53
8:2:80:PHE:HB3	30:H:64:ARG:NH1	2.23	0.53
9:8:93:PHE:HE2	9:8:98:LYS:HB3	1.73	0.53
11:C1:136:LEU:HB3	11:C1:193:TYR:HD2	1.73	0.53
16:A6:2:SER:OG	16:A6:3:ALA:N	2.41	0.53
23:A:355:LYS:CG	23:A:530:TYR:HE1	2.18	0.53
24:B:421:ARG:HH21	24:B:423:LYS:HB2	1.73	0.53
30:H:56:CYS:C	30:H:58:ILE:H	2.17	0.53
58:k:215:HIS:H	58:k:216:PHE:C	2.15	0.53
61:o:69:GLU:OE1	61:o:84:PRO:HD3	2.09	0.53
58:w:389:ARG:C	58:w:391:PRO:HD3	2.34	0.53
59:x:102:ARG:NH2	59:x:161:GLU:OE1	2.42	0.53
59:x:245:ARG:NH2	59:x:430:LEU:HB3	2.22	0.53
5:4:359:TRP:HB3	5:4:411:LEU:CD2	2.38	0.53
6:5:90:VAL:HG22	7:6:584:ILE:HG23	1.91	0.53
7:6:177:ILE:O	7:6:180:ILE:N	2.37	0.53
7:6:484:TYR:HA	7:6:487:LYS:HD3	1.91	0.53
24:B:198:THR:OG1	24:B:199:PRO:HD3	2.08	0.53
25:C:129:GLU:O	25:C:130:ILE:HD13	2.09	0.53
34:L:59:ASP:HB3	38:Q:130:LYS:HB2	1.90	0.53
56:g:14:PRO:O	56:g:116:ARG:NH2	2.41	0.53
58:k:67:THR:HA	58:k:121:SER:H	1.72	0.53
58:k:426:GLY:HA2	58:k:428:ILE:H	1.72	0.53
59:l:29:LEU:HD12	59:l:33:LEU:HG	1.90	0.53
59:l:334:GLY:O	59:l:338:LYS:N	2.26	0.53
60:m:29:SER:HA	60:m:32:ASN:HD22	1.72	0.53
60:m:159:ASN:ND2	66:A4:38:TRP:HH2	2.06	0.53
60:m:163:TRP:CD1	62:A1:63:SER:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:m:233:LEU:HD12	60:m:236:ILE:HG13	1.90	0.53
60:y:250:LEU:C	60:y:252:ASP:H	2.16	0.53
2:1:1:MET:O	2:1:4:ILE:HG22	2.09	0.53
4:7:4:TYR:CE1	4:7:123:GLY:HA2	2.35	0.53
4:7:82:ILE:CG2	4:7:83:TRP:N	2.72	0.53
7:6:305:SER:O	7:6:309:GLN:HG2	2.09	0.53
7:6:335:PHE:HE2	7:6:383:MET:HE1	1.74	0.53
8:2:118:VAL:O	8:2:122:ILE:HG13	2.08	0.53
10:C3:268:PHE:CZ	11:C1:58:ALA:HA	2.44	0.53
11:C1:165:VAL:HB	11:C1:170:LEU:HD12	1.90	0.53
15:A5:51:SER:HB2	15:A5:91:LEU:HD11	1.90	0.53
58:k:86:LEU:HB3	59:l:285:VAL:HG22	1.90	0.53
58:k:381:ARG:O	58:k:385:THR:N	2.41	0.53
60:m:349:THR:O	60:m:353:LEU:HG	2.08	0.53
61:o:166:ASN:HA	61:o:179:MET:H	1.74	0.53
61:o:241:LYS:NZ	63:q:56:ASN:HB2	2.23	0.53
64:r:64:GLN:HA	64:r:67:GLU:OE1	2.08	0.53
61:z:223:LYS:O	61:z:227:TRP:HD1	1.91	0.53
2:1:8:MET:O	2:1:12:PRO:CD	2.57	0.53
5:4:93:LYS:O	5:4:97:THR:HG23	2.09	0.53
5:4:168:GLN:HE21	49:b:150:ARG:NH1	2.07	0.53
8:2:127:GLY:CA	8:2:129:ILE:H	2.22	0.53
11:C1:33:LEU:HD23	18:C2:28:SER:HB2	1.91	0.53
13:A7:128:VAL:O	13:A7:134:PHE:HB3	2.09	0.53
23:A:307:VAL:O	23:A:314:LEU:HD12	2.09	0.53
40:S:32:ILE:HG13	40:S:33:LEU:HD12	1.91	0.53
49:b:119:ARG:NH1	56:g:62:TYR:O	2.41	0.53
61:o:160:MET:HB2	81:o:301:HEC:C4D	2.39	0.53
2:1:100:LEU:HD11	4:7:54:LEU:HD12	1.90	0.53
3:9:130:TYR:CZ	3:9:208:LEU:HD11	2.43	0.53
4:7:170:GLU:O	4:7:172:THR:OG1	2.26	0.53
5:4:126:LEU:HD21	5:4:153:THR:HG21	1.91	0.53
5:4:278:ARG:HB2	7:6:546:GLN:NE2	2.24	0.53
9:8:93:PHE:CZ	9:8:98:LYS:HB3	2.43	0.53
9:8:375:LYS:HD3	9:8:393:ASN:HD22	1.74	0.53
13:A7:23:PRO:HD2	14:B4:34:ASN:HD22	1.74	0.53
16:A6:42:ARG:HH11	16:A6:42:ARG:HG3	1.75	0.53
23:A:566:ILE:HD11	23:A:580:ALA:HA	1.90	0.53
31:I:108:LYS:CE	31:I:108:LYS:CA	2.85	0.53
36:O:43:VAL:HG11	36:O:59:GLY:HA3	1.89	0.53
38:Q:110:CYS:HB2	38:Q:114:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:155:VAL:HA	39:R:158:GLU:HB3	1.90	0.53
45:X:30:ASN:OD1	45:X:31:ASP:N	2.41	0.53
49:b:93:ILE:HG23	56:g:61:TYR:HE2	1.74	0.53
52:f:97:TYR:C	52:f:99:VAL:H	2.17	0.53
44:M:59:GLY:O	44:M:60:PHE:HB2	2.10	0.53
59:l:99:THR:HG23	68:v:67:SER:O	2.09	0.53
60:m:116:GLY:HA3	80:m:402:HEM:C3C	2.44	0.53
61:o:21:LEU:O	67:u:50:LYS:HB3	2.08	0.53
62:p:2:HIS:NE2	62:p:3:THR:HG23	2.23	0.53
65:s:12:GLU:HG2	65:s:13:LEU:N	2.24	0.53
67:u:41:ALA:O	67:u:45:HIS:N	2.26	0.53
2:1:162:LEU:HD23	2:1:240:ILE:HD13	1.91	0.52
2:1:283:ASP:O	2:1:285:LEU:N	2.42	0.52
3:9:222:ARG:HH22	9:8:284:ASN:HB2	1.74	0.52
5:4:57:PHE:C	5:4:111:THR:HG23	2.34	0.52
5:4:209:LEU:HD22	5:4:265:SER:HB3	1.90	0.52
7:6:592:LEU:HA	7:6:595:ILE:HG22	1.89	0.52
8:2:64:SER:OG	8:2:65:THR:N	2.42	0.52
8:2:127:GLY:HA2	8:2:128:LEU:HB2	1.91	0.52
9:8:297:LYS:NZ	9:8:310:GLY:O	2.41	0.52
10:C3:398:PRO:O	10:C3:498:CYS:HB3	2.08	0.52
11:C1:102:HIS:O	11:C1:104:TRP:N	2.42	0.52
23:A:238:PHE:CD2	27:E:140:ARG:HB3	2.44	0.52
23:A:464:GLN:HA	23:A:467:GLN:HB3	1.90	0.52
70:B:501:3PE:H392	27:E:61:LEU:HD11	1.91	0.52
25:C:213:ARG:HD3	25:C:224:GLU:OE1	2.09	0.52
49:b:153:GLU:OE2	55:j:90:MET:SD	2.67	0.52
44:M:66:ASP:OD2	44:M:79:TYR:OH	2.20	0.52
60:m:372:ILE:O	60:m:376:LEU:N	2.42	0.52
58:w:444:LEU:HD22	58:w:446:PHE:CZ	2.44	0.52
60:y:40:CYS:HB2	60:y:90:PHE:HD1	1.74	0.52
60:y:372:ILE:O	60:y:376:LEU:N	2.43	0.52
61:z:197:GLU:OE1	61:z:197:GLU:N	2.34	0.52
61:z:237:TYR:HB2	63:A2:60:PHE:CE1	2.44	0.52
63:A2:40:ASN:O	63:A2:43:VAL:HB	2.09	0.52
65:B7:20:VAL:HG12	65:B7:69:VAL:HG13	1.92	0.52
2:1:78:ALA:O	2:1:226:ALA:HB1	2.08	0.52
2:1:143:GLU:O	2:1:146:LEU:N	2.37	0.52
4:7:94:VAL:O	4:7:97:LEU:N	2.42	0.52
24:B:272:THR:HG22	24:B:327:TYR:HB2	1.91	0.52
34:L:65:ASP:HB3	34:L:74:GLN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:k:216:PHE:N	58:k:218:GLY:HA3	2.23	0.52
58:w:294:LEU:HB3	58:w:307:PHE:CZ	2.39	0.52
60:y:244:LEU:HD21	61:z:205:GLY:HA2	1.92	0.52
61:z:160:MET:HB2	81:z:301:HEC:C4D	2.39	0.52
5:4:58:SER:O	5:4:111:THR:OG1	2.16	0.52
7:6:232:TRP:CE3	7:6:233:LEU:HD12	2.44	0.52
8:2:166:GLY:O	8:2:292:PHE:HZ	1.93	0.52
23:A:183:ILE:HD11	23:A:206:VAL:HG13	1.90	0.52
25:C:199:PRO:O	25:C:201:ARG:N	2.43	0.52
39:R:55:VAL:HG13	39:R:79:GLN:HB3	1.92	0.52
49:b:163:ARG:HB3	49:b:165:ASP:HB2	1.90	0.52
58:k:186:LEU:HA	58:k:190:TYR:CD2	2.44	0.52
61:z:72:ASP:OD1	61:z:73:GLY:N	2.42	0.52
64:A3:8:THR:HG22	64:A3:9:ARG:H	1.75	0.52
66:A4:35:ALA:C	66:A4:36:THR:HG23	2.34	0.52
8:2:21:MET:HG2	8:2:140:SER:HB2	1.90	0.52
8:2:22:ILE:CD1	30:H:4:PHE:HB2	2.39	0.52
16:A6:8:HIS:O	16:A6:10:GLY:N	2.42	0.52
23:A:307:VAL:N	23:A:315:THR:O	2.42	0.52
24:B:171:ARG:HH21	24:B:231:GLY:HA2	1.74	0.52
26:D:90:ALA:HB3	26:D:127:GLY:HA2	1.91	0.52
39:R:67:ARG:HH11	39:R:93:HIS:CD2	2.27	0.52
46:Y:73:LEU:HD22	46:Y:74:TRP:CD1	2.45	0.52
51:d:40:VAL:HG12	51:d:41:ALA:H	1.73	0.52
61:o:165:TYR:HA	61:o:179:MET:CE	2.40	0.52
63:q:33:ARG:NH2	63:q:91:GLU:OE2	2.29	0.52
63:q:40:ASN:O	63:q:43:VAL:HB	2.09	0.52
58:w:351:GLU:O	58:w:354:VAL:HB	2.09	0.52
61:z:165:TYR:CD2	61:z:168:VAL:HG22	2.45	0.52
2:1:46:LEU:HG	2:1:49:ILE:HD11	1.91	0.52
5:4:95[B]:PHE:CZ	5:4:136:TRP:CD1	2.97	0.52
5:4:106:LEU:HD13	5:4:235:LEU:HD22	1.91	0.52
9:8:174:ARG:NH2	28:F:87:ASP:O	2.43	0.52
9:8:392:MET:O	9:8:395:VAL:HG12	2.09	0.52
10:C3:302:ARG:O	10:C3:306:THR:HG23	2.09	0.52
23:A:143:SER:O	23:A:143:SER:OG	2.19	0.52
24:B:61:TRP:CD1	24:B:61:TRP:C	2.88	0.52
24:B:261:MET:HE1	27:E:70:LEU:HD11	1.91	0.52
45:X:10:HIS:HB3	45:X:13:HIS:HD2	1.74	0.52
52:f:31:CYS:SG	52:f:37:TYR:HB2	2.50	0.52
52:f:163:LEU:CB	52:f:166:LEU:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:119:VAL:N	56:g:147:GLY:H	2.07	0.52
59:l:355:PRO:HA	59:l:358:GLN:HB3	1.92	0.52
58:w:159:GLN:HG3	58:w:235:ARG:NH2	2.24	0.52
59:x:247:GLN:HE22	59:x:430:LEU:N	2.06	0.52
60:y:131:TYR:O	60:y:134:PRO:HD2	2.10	0.52
60:y:349:THR:O	60:y:353:LEU:HG	2.09	0.52
67:B6:41:ALA:O	67:B6:45:HIS:N	2.26	0.52
4:7:17:PHE:HE2	6:5:11:ALA:HB1	1.71	0.52
5:4:2:LEU:HB3	5:4:6:ILE:HD12	1.91	0.52
5:4:194:PHE:O	5:4:198:ALA:N	2.40	0.52
5:4:223:ALA:HB1	5:4:224:PRO:HD2	1.92	0.52
5:4:431:THR:O	5:4:435:ALA:N	2.41	0.52
8:2:215:MET:HE2	8:2:215:MET:HA	1.92	0.52
9:8:48:ARG:HG3	9:8:133:HIS:CD2	2.44	0.52
11:C1:104:TRP:CG	11:C1:203:ASN:HB2	2.44	0.52
23:A:121:LEU:HD13	24:B:376:GLU:OE2	2.09	0.52
30:H:15:ASP:O	30:H:17:TRP:CD1	2.63	0.52
39:R:148:ILE:HB	39:R:149:PRO:HD3	1.91	0.52
41:T:65:ALA:C	41:T:66:ILE:HG13	2.35	0.52
50:c:66:ARG:HA	50:c:67:HIS:C	2.35	0.52
60:m:131:TYR:O	60:m:134:PRO:HD2	2.10	0.52
61:o:165:TYR:CD2	61:o:168:VAL:HG22	2.45	0.52
62:p:143:GLY:O	62:p:146:PRO:N	2.43	0.52
58:w:185:TYR:HA	58:w:188:ARG:HD2	1.92	0.52
59:x:45:SER:HB2	59:x:113:ARG:HA	1.92	0.52
60:y:116:GLY:HA3	80:y:402:HEM:C3C	2.44	0.52
61:z:238:ARG:HH21	62:A1:5:ILE:HG22	1.75	0.52
63:A2:28:LYS:HB3	63:A2:74:ILE:HD11	1.90	0.52
1:3:78:ALA:HB2	4:7:145:ALA:HB1	1.91	0.52
4:7:72:THR:HG23	6:5:27:MET:HE2	1.92	0.52
5:4:226:ALA:HA	5:4:331:ASN:ND2	2.24	0.52
5:4:257:MET:O	5:4:260:PRO:HD2	2.09	0.52
8:2:85:THR:HG22	30:H:19:THR:HG23	1.87	0.52
9:8:75:TRP:O	9:8:79:GLU:HB2	2.09	0.52
9:8:97:LEU:HD23	9:8:101:PHE:HB2	1.91	0.52
10:C3:11:ASN:ND2	10:C3:14:ASP:H	2.07	0.52
23:A:435:PRO:HG3	23:A:444:HIS:CG	2.45	0.52
24:B:322:SER:O	35:N:12:VAL:HG21	2.09	0.52
24:B:371:MET:HA	24:B:377:SER:OG	2.10	0.52
25:C:70:ILE:HG13	25:C:71:LEU:HD12	1.91	0.52
27:E:100:GLU:O	27:E:170:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:G:131:LYS:HZ1	29:G:147:VAL:HG11	1.73	0.52
40:S:333:GLU:O	40:S:335:VAL:N	2.40	0.52
53:h:97:ILE:HG23	53:h:98:VAL:HG23	1.92	0.52
58:k:80:GLU:HG2	59:l:284:HIS:HB2	1.92	0.52
58:k:245:GLU:H	58:k:426:GLY:HA3	1.75	0.52
59:l:69:LEU:HD12	59:l:72:ALA:HB3	1.90	0.52
59:l:247:GLN:HG3	59:x:181:TYR:OH	2.09	0.52
63:q:28:LYS:HB3	63:q:74:ILE:HD11	1.90	0.52
63:q:38:HIS:ND1	63:q:39:GLU:O	2.43	0.52
59:x:69:LEU:HD12	59:x:72:ALA:HB3	1.90	0.52
61:z:47:ALA:HB2	61:z:90:TYR:HE1	1.75	0.52
61:z:225:HIS:O	61:z:228:SER:OG	2.20	0.52
68:B5:70:LEU:HD12	68:B5:71:ASN:O	2.09	0.52
5:4:49:SER:HB2	5:4:60:SER:CB	2.40	0.52
5:4:297:VAL:O	5:4:301:ILE:HG12	2.10	0.52
5:4:381:VAL:O	5:4:385:THR:HG22	2.10	0.52
7:6:569:ALA:O	7:6:572:LYS:N	2.43	0.52
13:A7:40:LEU:HD22	13:A7:59:LEU:HD13	1.91	0.52
30:H:71:LYS:O	30:H:74:LYS:N	2.39	0.52
33:K:23:LEU:O	33:K:58:CYS:HA	2.10	0.52
43:V:32:GLY:O	43:V:33:TYR:HB3	2.09	0.52
55:j:33:PHE:O	55:j:36:PHE:HB3	2.10	0.52
60:m:40:CYS:HB2	60:m:90:PHE:HD1	1.74	0.52
61:o:71:GLN:OE1	61:o:71:GLN:N	2.42	0.52
61:o:171:PHE:HE2	61:o:177:ALA:HA	1.73	0.52
58:w:245:GLU:H	58:w:426:GLY:HA3	1.75	0.52
59:x:121:GLU:O	59:x:125:ASN:ND2	2.43	0.52
59:x:355:PRO:HA	59:x:358:GLN:HB3	1.92	0.52
60:y:105:GLY:HA2	60:y:107:TYR:CE2	2.44	0.52
61:z:166:ASN:HA	61:z:179:MET:H	1.74	0.52
62:A1:2:HIS:CG	62:A1:3:THR:H	2.27	0.52
4:7:17:PHE:O	4:7:19:GLY:N	2.43	0.52
4:7:107:VAL:HG23	4:7:117:PHE:HB3	1.92	0.52
7:6:270:ASN:HB2	7:6:273:ILE:HD12	1.92	0.52
8:2:271:THR:O	8:2:272:LYS:HB3	2.09	0.52
9:8:386:ARG:C	9:8:388:GLY:H	2.18	0.52
17:C0:60:TYR:CD1	17:C0:60:TYR:C	2.88	0.52
25:C:63:PHE:CD2	37:P:97:PRO:HG3	2.44	0.52
38:Q:40:ASN:OD1	38:Q:41:LYS:N	2.41	0.52
39:R:125:VAL:HG21	39:R:253:ILE:HD11	1.91	0.52
40:S:92:LEU:HB2	40:S:93:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Z:63:PHE:CG	47:Z:64:VAL:N	2.78	0.52
50:c:77:ILE:HB	50:c:78:PRO:HD3	1.91	0.52
57:e:136:PHE:O	57:e:139:PHE:N	2.41	0.52
59:l:241:GLY:H	59:l:421:ARG:CZ	2.23	0.52
59:l:294:SER:O	59:l:298:ALA:N	2.30	0.52
66:t:29:ALA:O	66:t:33:VAL:HG22	2.10	0.52
61:z:165:TYR:HA	61:z:179:MET:CE	2.40	0.52
65:B7:22:GLU:HA	65:B7:25:GLU:HG2	1.91	0.52
67:B6:3:PRO:HB2	67:B6:7:ALA:HB3	1.92	0.52
2:1:73:LEU:C	2:1:76:ILE:HD12	2.20	0.52
5:4:1:MET:HB2	5:4:52:PHE:CE1	2.45	0.52
5:4:205:VAL:HA	5:4:212:LEU:HD13	1.92	0.52
7:6:328:HIS:O	7:6:331:THR:OG1	2.28	0.52
7:6:358:LYS:HA	7:6:436:ARG:HG3	1.91	0.52
8:2:218:MET:SD	8:2:323:MET:HE2	2.49	0.52
12:A9:119:THR:O	16:A6:52:HIS:CE1	2.63	0.52
15:A5:8:THR:OG1	15:A5:11:GLU:HG2	2.09	0.52
23:A:310:GLU:HG2	23:A:311:LYS:HG3	1.91	0.52
23:A:443:ASP:N	23:A:443:ASP:OD1	2.43	0.52
23:A:507:THR:CB	23:A:508:GLY:HA3	2.40	0.52
25:C:123:THR:HG22	25:C:123:THR:O	2.10	0.52
38:Q:172:MET:O	55:j:30:ARG:NH1	2.42	0.52
51:d:46:MET:HE2	51:d:56:ARG:HA	1.91	0.52
58:k:216:PHE:H	58:k:219:LEU:N	2.01	0.52
58:k:351:GLU:O	58:k:354:VAL:HB	2.09	0.52
59:l:281:ALA:HB2	59:l:293:SER:OG	2.10	0.52
60:m:5:ARG:HA	60:m:8:HIS:NE2	2.24	0.52
60:m:140:PHE:HD2	60:m:141:TRP:CD1	2.29	0.52
61:o:228:SER:HB2	64:r:23:GLN:HE21	1.73	0.52
59:x:241:GLY:H	59:x:421:ARG:CZ	2.23	0.52
59:x:279:LEU:HB3	59:x:295:LEU:HB2	1.92	0.52
61:z:73:GLY:HA3	61:z:81:PHE:HA	1.91	0.52
62:A1:148:ALA:HA	62:A1:156:TYR:HA	1.91	0.52
63:A2:38:HIS:ND1	63:A2:39:GLU:O	2.43	0.52
2:1:272:TRP:HH2	27:E:71:GLY:HA2	1.75	0.51
3:9:180:CYS:HB2	9:8:123:GLY:HA2	1.92	0.51
4:7:84:LEU:HD23	4:7:84:LEU:C	2.35	0.51
5:4:55:LEU:HA	5:4:113:MET:HG2	1.92	0.51
7:6:385:PHE:O	7:6:466:TYR:OH	2.27	0.51
8:2:250:SER:O	8:2:259:GLY:HA3	2.09	0.51
9:8:37:ASP:CB	9:8:294:VAL:HB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:398:ASP:O	23:A:427:LEU:HD12	2.10	0.51
38:Q:142:TYR:HD1	38:Q:143:HIS:CD2	2.28	0.51
38:Q:166:ARG:NH1	49:b:149:LEU:HB3	2.25	0.51
40:S:117:TYR:HE1	40:S:175:TYR:HD2	1.57	0.51
48:a:47:TYR:O	48:a:51:TYR:N	2.38	0.51
56:g:5:TRP:HD1	56:g:6:ASP:O	1.93	0.51
58:k:24:ARG:HD2	58:k:196:VAL:HG22	1.92	0.51
58:k:159:GLN:HG3	58:k:235:ARG:NH2	2.24	0.51
59:l:45:SER:HB2	59:l:113:ARG:HA	1.92	0.51
59:l:279:LEU:HB3	59:l:295:LEU:HB2	1.92	0.51
66:t:23:LEU:O	66:t:27:VAL:N	2.37	0.51
58:w:24:ARG:HD2	58:w:196:VAL:HG22	1.93	0.51
59:x:228:GLY:C	59:x:230:LEU:H	2.17	0.51
4:7:86:ASN:OD1	4:7:88:ALA:HB3	2.11	0.51
5:4:176:PHE:HE2	49:b:143:GLU:HB2	1.74	0.51
5:4:178:MET:HE1	49:b:136:THR:HB	1.90	0.51
7:6:61:LEU:H	7:6:82:MET:HB2	1.74	0.51
8:2:103:ALA:O	8:2:107:GLY:HA2	2.10	0.51
23:A:139:LEU:HD11	23:A:177:ILE:HG21	1.91	0.51
24:B:80:LEU:HD23	24:B:81:THR:N	2.25	0.51
24:B:244:ILE:HG22	24:B:348:LEU:HD11	1.93	0.51
24:B:256:ASP:O	24:B:256:ASP:OD1	2.27	0.51
25:C:243:ALA:HB1	37:P:61:ARG:HH21	1.76	0.51
35:N:49:GLU:O	35:N:52:THR:OG1	2.22	0.51
36:O:64:ARG:O	36:O:68:LYS:HE2	2.09	0.51
52:f:54:GLU:OE1	52:f:59:LYS:NZ	2.43	0.51
53:h:113:ARG:O	53:h:115:GLN:N	2.43	0.51
56:g:22:PRO:O	56:g:24:THR:N	2.44	0.51
58:k:185:TYR:HA	58:k:188:ARG:HD2	1.92	0.51
59:l:247:GLN:HE22	59:l:430:LEU:N	2.06	0.51
60:m:328:LEU:HA	60:m:361:LEU:HD13	1.92	0.51
63:q:57:ASP:HB3	63:q:61:ARG:NH1	2.25	0.51
59:x:24:LEU:HD22	59:x:392:TYR:CG	2.46	0.51
59:x:76:THR:HA	59:x:82:SER:HB2	1.93	0.51
59:x:259:ALA:HB2	59:x:422:LYS:HG2	1.93	0.51
1:3:7:LEU:HD21	70:1:401:3PE:H3B1	1.92	0.51
5:4:24:TRP:CG	5:4:81:GLN:HE22	2.28	0.51
5:4:336:ARG:NH2	5:4:433:GLU:HG3	2.25	0.51
9:8:53:LEU:C	9:8:136:HIS:HE2	2.19	0.51
11:C1:1:MET:SD	11:C1:133:LEU:CD1	2.99	0.51
23:A:167:PRO:O	23:A:168:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:127:LYS:HB2	24:B:132:ALA:HB2	1.91	0.51
26:D:146:GLU:HB3	26:D:147:PRO:HD3	1.92	0.51
44:M:33:ASN:OD1	44:M:74:GLN:NE2	2.43	0.51
59:l:169:ARG:HG3	59:l:240:HIS:HB3	1.91	0.51
61:o:141:VAL:HB	65:s:53:ASP:OD2	2.10	0.51
67:u:3:PRO:HB2	67:u:7:ALA:HB3	1.92	0.51
58:w:307:PHE:HB3	58:w:324:PHE:CB	2.41	0.51
60:y:2:THR:HG22	60:y:3:ASN:HD22	1.75	0.51
60:y:328:LEU:HA	60:y:361:LEU:HD13	1.92	0.51
61:z:40:CYS:HB3	61:z:110:PRO:HG2	1.91	0.51
1:3:81:THR:N	34:L:46:ASN:HD21	1.99	0.51
2:1:78:ALA:O	2:1:226:ALA:CB	2.58	0.51
2:1:230:ASN:HA	2:1:233:MET:HE2	1.92	0.51
2:1:278:PRO:CB	24:B:194:ILE:HG22	2.40	0.51
7:6:1:MET:HG2	7:6:59:GLN:NE2	2.25	0.51
7:6:221:THR:HG22	7:6:226:GLN:HG3	1.91	0.51
7:6:264:TYR:CE1	7:6:265:PRO:HG3	2.45	0.51
9:8:207:GLY:HA2	73:8:501:FMN:C9A	2.41	0.51
11:C1:100:MET:CE	11:C1:157:GLU:HG3	2.40	0.51
11:C1:139:ASP:OD1	11:C1:140:ASN:N	2.44	0.51
24:B:316:PHE:HA	24:B:342:ARG:HH11	1.76	0.51
25:C:77:GLN:HG3	37:P:70:MET:CB	2.40	0.51
25:C:133:ASN:C	25:C:134:LEU:HD12	2.35	0.51
25:C:227:GLU:OE2	29:G:107:TRP:HH2	1.93	0.51
31:I:85:ILE:HG21	31:I:119:PHE:HZ	1.76	0.51
34:L:70:PRO:HD3	38:Q:37:ASP:OD2	2.11	0.51
39:R:128:ASN:HD21	39:R:130:VAL:HG12	1.75	0.51
41:T:39:TYR:HB3	41:T:43:LEU:HD12	1.92	0.51
50:c:83:HIS:HE1	50:c:87:LYS:HE2	1.75	0.51
65:s:20:VAL:HG12	65:s:69:VAL:HG13	1.91	0.51
67:u:55:ILE:O	67:u:58:LYS:HG2	2.11	0.51
61:z:153:PHE:HB3	61:z:156:GLN:HA	1.92	0.51
62:A1:20:ASP:OD1	62:A1:21:SER:N	2.43	0.51
1:3:80:GLN:HG3	2:1:317:GLN:O	2.10	0.51
5:4:94:LEU:O	5:4:97:THR:N	2.44	0.51
5:4:180:GLN:HG3	5:4:249:ILE:HD12	1.92	0.51
5:4:336:ARG:NH1	5:4:352:LEU:HD21	2.26	0.51
6:5:46:LEU:O	6:5:49:LEU:N	2.43	0.51
10:C3:240:HIS:HB3	10:C3:241:PRO:HD3	1.92	0.51
14:B4:63:SER:O	14:B4:67:ILE:HG13	2.10	0.51
24:B:149:GLN:O	24:B:149:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:203:ASP:OD2	29:G:137:PHE:HZ	1.93	0.51
40:S:66:ALA:O	40:S:71:LEU:N	2.27	0.51
40:S:102:LEU:HD23	40:S:105:PHE:HE2	1.76	0.51
44:M:20:LYS:HB2	44:M:30:LEU:HD11	1.92	0.51
58:k:162:PRO:O	58:k:165:GLN:HG2	2.11	0.51
60:m:278:TYR:CD1	60:m:281:LEU:HD23	2.46	0.51
61:o:102:ARG:HA	61:o:108:ALA:O	2.10	0.51
68:v:63:PRO:N	68:v:64:LEU:HA	2.25	0.51
64:A3:79:ASN:CB	65:B7:52:GLU:HB2	2.41	0.51
2:1:237:PHE:O	2:1:239:ALA:N	2.43	0.51
8:2:263:LYS:O	8:2:266:ILE:HG22	2.10	0.51
28:F:83:TYR:O	28:F:84:THR:OG1	2.27	0.51
31:I:79:GLN:HA	31:I:120:ARG:O	2.09	0.51
35:N:44:TYR:CE1	35:N:94:MET:HE3	2.45	0.51
38:Q:53:PRO:HD2	43:V:116:TRP:CD1	2.45	0.51
40:S:189:PRO:HB2	40:S:192:VAL:HG22	1.93	0.51
40:S:190:HIS:HE1	40:S:271:TRP:O	1.94	0.51
41:T:79:GLN:HA	41:T:83:LYS:HD3	1.93	0.51
43:V:56:GLU:HA	43:V:59:ARG:NH1	2.25	0.51
47:Z:20:LYS:HA	47:Z:23:LYS:HE2	1.92	0.51
52:f:176:GLU:OE1	52:f:176:GLU:N	2.44	0.51
58:k:89:TYR:CZ	58:k:96:ALA:HB3	2.45	0.51
59:l:52:LYS:HB2	59:l:203:ARG:HE	1.76	0.51
59:l:132:PHE:CB	59:l:188:PRO:HB3	2.41	0.51
60:m:244:LEU:HD11	61:o:201:ARG:O	2.10	0.51
65:s:22:GLU:HA	65:s:25:GLU:HG2	1.91	0.51
58:w:291:SER:HB2	58:w:356:ARG:NH1	2.26	0.51
58:w:391:PRO:HG2	58:w:398:ARG:NH2	2.26	0.51
60:y:140:PHE:HD2	60:y:141:TRP:CD1	2.28	0.51
61:z:31:GLN:O	61:z:35:GLN:N	2.42	0.51
2:1:178:ALA:O	2:1:179:TRP:C	2.52	0.51
3:9:149:LEU:CD2	3:9:150:GLU:H	2.22	0.51
7:6:233:LEU:HG	7:6:248:HIS:HE1	1.75	0.51
10:C3:232:GLN:HB2	10:C3:292:MET:HE3	1.93	0.51
24:B:102:SER:HB3	24:B:107:ARG:HH11	1.76	0.51
25:C:169:GLU:OE1	25:C:183:HIS:CD2	2.63	0.51
33:K:59:SER:C	33:K:61:VAL:H	2.18	0.51
39:R:154:GLN:HG3	39:R:155:VAL:HG23	1.93	0.51
58:k:110:VAL:HA	58:k:113:LEU:HB3	1.93	0.51
58:k:213:GLN:HB3	58:k:214:LYS:HZ3	1.76	0.51
59:l:76:THR:HA	59:l:82:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:259:ALA:HB2	59:l:422:LYS:HG2	1.93	0.51
61:o:77:ASP:O	61:o:79:GLU:HG3	2.11	0.51
61:o:153:PHE:HB3	61:o:156:GLN:HA	1.91	0.51
59:x:132:PHE:HB3	59:x:188:PRO:HB3	1.93	0.51
59:x:258:VAL:HA	59:x:417:PHE:HE1	1.76	0.51
60:y:5:ARG:HA	60:y:8:HIS:NE2	2.24	0.51
62:A1:2:HIS:CD2	62:A1:3:THR:H	2.28	0.51
66:A4:43:ASP:CG	66:A4:47:TYR:H	2.17	0.51
67:B6:55:ILE:O	67:B6:58:LYS:HG2	2.11	0.51
3:9:137:THR:HG22	3:9:138:THR:H	1.75	0.51
4:7:68:PHE:CZ	6:5:31:LEU:HD13	2.46	0.51
5:4:385:THR:CG2	5:4:396:MET:HE1	2.41	0.51
8:2:23:SER:O	30:H:3:PHE:HE1	1.94	0.51
8:2:84:TRP:CD1	8:2:84:TRP:N	2.77	0.51
73:8:501:FMN:O4'	73:8:501:FMN:O2'	2.22	0.51
10:C3:377:PHE:HA	10:C3:380:VAL:HG22	1.93	0.51
11:C1:186:SER:CB	11:C1:213:LEU:HD22	2.40	0.51
23:A:280:ASP:O	23:A:417:ARG:NH2	2.40	0.51
24:B:270:ASN:HB2	70:B:501:3PE:HN1	1.76	0.51
25:C:169:GLU:HB3	25:C:180:PHE:HD2	1.75	0.51
30:H:47:ILE:HG22	30:H:49:SER:H	1.76	0.51
56:g:120:SER:C	56:g:122:ARG:H	2.17	0.51
58:k:391:PRO:HG2	58:k:398:ARG:NH2	2.26	0.51
59:l:121:GLU:O	59:l:125:ASN:ND2	2.43	0.51
62:p:85:LYS:HA	62:p:86:ASN:C	2.36	0.51
62:p:127:VAL:CB	62:p:132:TRP:H	2.24	0.51
58:w:162:PRO:O	58:w:165:GLN:HG2	2.11	0.51
58:w:329:MET:HE1	64:A3:5:GLY:HA3	1.92	0.51
59:x:169:ARG:HG3	59:x:240:HIS:HB3	1.91	0.51
59:x:281:ALA:HB2	59:x:293:SER:OG	2.10	0.51
60:y:165:TRP:O	60:y:174:THR:OG1	2.24	0.51
3:9:110:MET:HG2	23:A:194:ASP:O	2.11	0.51
10:C3:347:LEU:HG	10:C3:383:MET:HE3	1.93	0.51
12:A9:18:LEU:HD22	12:A9:22:LEU:HD22	1.92	0.51
23:A:306:MET:HB2	23:A:583:ILE:HD11	1.91	0.51
29:G:112:MET:HE1	42:U:126:PRO:HB2	1.93	0.51
39:R:238:GLN:HB3	39:R:267:GLY:HA3	1.92	0.51
44:W:104:PHE:HB2	44:W:139:MET:O	2.11	0.51
55:j:115:GLU:HB2	55:j:116:PHE:HA	1.92	0.51
58:k:412:SER:C	67:u:15:ARG:HH22	2.19	0.51
60:m:250:LEU:C	60:m:252:ASP:H	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:o:191:ARG:O	61:o:195:GLU:HG2	2.10	0.51
58:w:89:TYR:CZ	58:w:96:ALA:HB3	2.45	0.51
60:y:337:TRP:O	60:y:341:GLN:HG2	2.11	0.51
62:A1:36:SER:O	62:A1:39:VAL:N	2.44	0.51
63:A2:57:ASP:HB3	63:A2:61:ARG:NH1	2.26	0.51
5:4:89:LEU:HD12	5:4:90:THR:N	2.26	0.51
6:5:89:TYR:HB3	6:5:91:GLN:HG2	1.93	0.51
7:6:161:ARG:HD3	7:6:164:ALA:HB2	1.92	0.51
23:A:328:GLY:O	23:A:331:GLN:N	2.44	0.51
24:B:176:GLU:HG3	24:B:176:GLU:O	2.11	0.51
30:H:37:GLU:O	30:H:40:TRP:N	2.44	0.51
48:a:128:SER:HA	48:a:129:TYR:HB3	1.93	0.51
58:k:76:GLU:O	58:k:79:VAL:N	2.44	0.51
58:k:181:ASP:O	58:k:184:GLU:HB2	2.11	0.51
59:l:124:LEU:O	59:l:128:THR:N	2.32	0.51
59:l:271:ALA:O	59:l:275:LEU:N	2.37	0.51
60:m:105:GLY:HA2	60:m:107:TYR:CE2	2.45	0.51
60:m:159:ASN:ND2	66:A4:38:TRP:CH2	2.79	0.51
63:q:105:GLU:O	63:q:109:LYS:NZ	2.42	0.51
58:w:76:GLU:O	58:w:79:VAL:N	2.44	0.51
59:x:132:PHE:CB	59:x:188:PRO:HB3	2.40	0.51
2:1:283:ASP:C	2:1:285:LEU:H	2.18	0.50
4:7:168:ILE:O	4:7:172:THR:OG1	2.28	0.50
5:4:196:TRP:CD1	5:4:251:ASN:ND2	2.78	0.50
5:4:349:GLN:NE2	5:4:349:GLN:O	2.44	0.50
7:6:137:LEU:CB	7:6:196:TRP:HB2	2.41	0.50
7:6:387:THR:OG1	7:6:388:GLY:N	2.44	0.50
9:8:213:ILE:HD11	9:8:236:PHE:HB2	1.93	0.50
9:8:273:THR:HA	9:8:291:GLU:HA	1.93	0.50
10:C3:75:ILE:O	10:C3:79:GLY:HA3	2.11	0.50
36:O:75:ASP:O	36:O:79:VAL:HG23	2.11	0.50
49:b:53:ARG:HG2	50:c:29:SER:CB	2.41	0.50
56:g:159:GLN:O	56:g:163:MET:HG2	2.11	0.50
59:l:258:VAL:HA	59:l:417:PHE:HE1	1.76	0.50
60:m:8:HIS:HB2	60:m:9:PRO:HD3	1.93	0.50
60:m:337:TRP:O	60:m:341:GLN:HG2	2.11	0.50
59:x:78:LYS:N	59:x:129:ALA:O	2.37	0.50
59:x:392:TYR:OH	59:x:394:PRO:HA	2.11	0.50
61:z:102:ARG:HA	61:z:108:ALA:O	2.10	0.50
61:z:191:ARG:O	61:z:195:GLU:HG2	2.10	0.50
3:9:153:GLN:OE1	3:9:153:GLN:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:83:TRP:C	4:7:83:TRP:HE3	2.18	0.50
5:4:431:THR:HG21	53:h:91:PHE:HZ	1.75	0.50
10:C3:184:PHE:H	10:C3:256:HIS:CE1	2.29	0.50
23:A:173:MET:SD	23:A:176:CYS:SG	3.09	0.50
42:U:49:TYR:HD2	42:U:61:TRP:CH2	2.29	0.50
54:i:48:LEU:O	54:i:52:VAL:HG23	2.11	0.50
59:l:145:ARG:O	59:l:149:ALA:N	2.36	0.50
59:l:392:TYR:OH	59:l:394:PRO:HA	2.11	0.50
60:m:222:PRO:HB2	60:m:223:TYR:CE1	2.47	0.50
61:o:40:CYS:HB3	61:o:110:PRO:HG2	1.91	0.50
64:r:8:THR:HG22	64:r:9:ARG:H	1.75	0.50
62:A1:97:PHE:N	62:A1:135:LEU:O	2.44	0.50
6:5:59:MET:SD	8:2:84:TRP:CH2	3.04	0.50
7:6:75:LYS:HE2	56:g:108:GLU:OE2	2.11	0.50
7:6:419:THR:HA	7:6:422:TYR:CD2	2.47	0.50
7:6:472:ILE:HG12	7:6:473:PRO:O	2.10	0.50
7:6:528:TYR:O	7:6:531:THR:OG1	2.29	0.50
8:2:86:VAL:O	8:2:86:VAL:HG12	2.11	0.50
9:8:330:SER:OG	9:8:331:VAL:N	2.43	0.50
9:8:363:ILE:H	9:8:363:ILE:HD12	1.76	0.50
11:C1:59:GLN:N	11:C1:62:GLU:HG3	2.24	0.50
23:A:223:ILE:HD12	23:A:233:SER:HB2	1.93	0.50
24:B:344:ILE:O	24:B:348:LEU:HG	2.12	0.50
30:H:2:PRO:HG2	30:H:4:PHE:CE1	2.46	0.50
50:c:66:ARG:HA	50:c:68:SER:N	2.26	0.50
44:M:32:VAL:O	44:M:74:GLN:N	2.44	0.50
58:k:7:ALA:HB1	59:l:43:PRO:HD3	1.92	0.50
58:k:307:PHE:HB3	58:k:324:PHE:CB	2.41	0.50
58:k:426:GLY:HA2	58:k:428:ILE:N	2.27	0.50
59:l:65:THR:O	59:l:69:LEU:N	2.22	0.50
59:l:78:LYS:N	59:l:129:ALA:O	2.37	0.50
59:l:257:LEU:HD21	59:l:422:LYS:HD2	1.94	0.50
60:m:140:PHE:O	60:m:144:THR:OG1	2.14	0.50
61:o:35:GLN:HG3	61:o:169:LEU:HD13	1.93	0.50
61:o:47:ALA:HB2	61:o:90:TYR:HE1	1.75	0.50
58:w:110:VAL:HA	58:w:113:LEU:HB3	1.93	0.50
59:x:52:LYS:HB2	59:x:203:ARG:HE	1.76	0.50
59:x:145:ARG:O	59:x:149:ALA:N	2.36	0.50
60:y:222:PRO:HB2	60:y:223:TYR:CE1	2.47	0.50
64:A3:58:VAL:HA	64:A3:61:TRP:HB3	1.93	0.50
1:3:35:SER:OG	25:C:219:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:157:THR:HG22	6:5:66:PHE:HE2	1.75	0.50
5:4:278:ARG:N	7:6:546:GLN:HE22	1.92	0.50
6:5:19:LEU:HA	6:5:22:TYR:O	2.11	0.50
10:C3:145:LEU:HD21	12:A9:32:THR:HG21	1.94	0.50
23:A:355:LYS:HD2	23:A:530:TYR:CD1	2.36	0.50
23:A:481:LEU:HA	23:A:489:ILE:HD11	1.93	0.50
29:G:105:GLU:OE1	29:G:105:GLU:N	2.36	0.50
31:I:80:VAL:HG13	31:I:82:SER:H	1.75	0.50
36:O:83:VAL:O	36:O:86:GLY:N	2.44	0.50
58:k:291:SER:HB2	58:k:356:ARG:NH1	2.25	0.50
60:m:17:ALA:HB1	60:m:201:HIS:CE1	2.47	0.50
59:x:271:ALA:O	59:x:275:LEU:N	2.37	0.50
60:y:129:MET:O	60:y:132:VAL:N	2.43	0.50
60:y:278:TYR:CD1	60:y:281:LEU:HD23	2.46	0.50
5:4:203:PHE:HE2	5:4:246:ILE:HD12	1.76	0.50
9:8:177:TYR:HE2	28:F:96:ARG:HB3	1.77	0.50
10:C3:225:GLY:HA3	12:A9:112:LEU:HD13	1.92	0.50
53:h:150:PRO:HG2	55:j:111:GLU:O	2.10	0.50
58:k:383:LEU:HA	58:k:387:GLY:C	2.37	0.50
58:k:403:ASP:H	58:k:406:VAL:HB	1.77	0.50
59:l:24:LEU:HD22	59:l:392:TYR:CG	2.46	0.50
60:m:300:ILE:O	60:m:304:ILE:HG13	2.12	0.50
61:o:138:PRO:HB2	65:s:53:ASP:OD1	2.12	0.50
61:o:221:ALA:O	61:o:225:HIS:N	2.34	0.50
61:z:35:GLN:HG3	61:z:169:LEU:HD13	1.93	0.50
61:z:165:TYR:H	61:z:168:VAL:CG2	2.25	0.50
61:z:181:GLN:HE21	65:B7:78:LYS:HB2	1.76	0.50
3:9:179:ALA:HB2	9:8:128:ARG:HH21	1.77	0.50
4:7:52:LEU:HD11	6:5:60:PRO:HB2	1.93	0.50
5:4:16:TRP:CD1	5:4:17:LEU:N	2.80	0.50
8:2:169:GLY:O	8:2:171:ASN:N	2.45	0.50
9:8:42:PHE:HE2	9:8:261:TRP:CE2	2.30	0.50
9:8:117:ALA:HB3	9:8:158:ILE:HG12	1.93	0.50
13:A7:64:PHE:CE1	14:B4:66:ARG:HD2	2.47	0.50
15:A5:37:LYS:N	15:A5:37:LYS:HD3	2.27	0.50
24:B:355:GLU:HG3	37:P:45:PRO:HG3	1.93	0.50
72:J:101:CDL:H512	42:U:6:VAL:HG13	1.92	0.50
56:g:71:VAL:N	56:g:72:PRO:HD2	2.27	0.50
59:l:240:HIS:CE1	59:l:421:ARG:HH22	2.30	0.50
60:m:310:SER:HA	60:m:374:ASN:ND2	2.23	0.50
60:m:362:ILE:HA	60:m:366:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:280:TYR:CE1	58:w:299:ALA:HB2	2.46	0.50
58:w:403:ASP:H	58:w:406:VAL:HB	1.76	0.50
59:x:286:LYS:HG2	59:x:287:ARG:HG3	1.94	0.50
59:x:304:HIS:CD2	59:x:305:GLN:HB3	2.47	0.50
62:A1:35:PHE:O	62:A1:39:VAL:HG23	2.11	0.50
5:4:196:TRP:HD1	5:4:251:ASN:HD22	1.59	0.50
7:6:63:ILE:HD13	7:6:65:ASN:ND2	2.27	0.50
8:2:161:SER:HA	8:2:164:ILE:HG22	1.94	0.50
9:8:318:ILE:HG13	9:8:326:LEU:HD23	1.93	0.50
10:C3:250:GLY:O	10:C3:254:ILE:HG12	2.11	0.50
11:C1:136:LEU:HB3	11:C1:193:TYR:CD2	2.46	0.50
23:A:289:LYS:HB2	23:A:694:PHE:CZ	2.47	0.50
24:B:253:LEU:HD23	24:B:254:ARG:HH12	1.76	0.50
24:B:299:GLN:HG2	27:E:38:TYR:HE1	1.75	0.50
36:O:101:THR:O	36:O:105:ARG:HG3	2.10	0.50
39:R:252:ALA:HB2	39:R:338:LEU:HD11	1.93	0.50
47:Z:21:GLN:HB3	47:Z:22:TRP:CE3	2.46	0.50
57:e:131:LYS:O	57:e:135:GLY:N	2.45	0.50
59:l:139:ALA:O	59:l:142:PRO:HD2	2.12	0.50
61:o:31:GLN:O	61:o:35:GLN:N	2.42	0.50
64:r:80:ASP:HA	65:s:47:ARG:HD3	1.93	0.50
58:w:181:ASP:O	58:w:184:GLU:HB2	2.11	0.50
59:x:304:HIS:CD2	59:x:305:GLN:H	2.30	0.50
59:x:310:SER:HB3	68:B5:57:GLY:N	2.26	0.50
60:y:8:HIS:HB2	60:y:9:PRO:HD3	1.93	0.50
60:y:362:ILE:HA	60:y:366:MET:SD	2.52	0.50
2:1:136:VAL:O	2:1:139:THR:OG1	2.28	0.50
3:9:137:THR:O	3:9:141:MET:N	2.44	0.50
4:7:78:GLN:C	4:7:80:PRO:HD3	2.32	0.50
8:2:258:SER:OG	8:2:330:VAL:O	2.29	0.50
10:C3:508:PRO:HG3	12:A9:6:HIS:HB3	1.94	0.50
23:A:423:LEU:O	23:A:425:ASN:N	2.44	0.50
26:D:146:GLU:CB	26:D:147:PRO:HD3	2.42	0.50
27:E:172:ASN:ND2	27:E:197:TRP:CZ3	2.75	0.50
29:G:131:LYS:NZ	29:G:147:VAL:HG11	2.26	0.50
39:R:192:ARG:HH21	39:R:200:ILE:HG22	1.77	0.50
42:U:85:GLU:OE1	42:U:86:TRP:HD1	1.94	0.50
56:g:30:ILE:O	56:g:34:THR:HG22	2.12	0.50
58:k:215:HIS:O	58:k:219:LEU:N	2.44	0.50
58:k:280:TYR:CE1	58:k:299:ALA:HB2	2.46	0.50
60:m:2:THR:HG22	60:m:3:ASN:HD22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:o:165:TYR:H	61:o:168:VAL:CG2	2.25	0.50
63:q:9:SER:O	63:q:13:LEU:HG	2.12	0.50
2:1:296:LEU:O	2:1:299:ALA:N	2.45	0.50
7:6:10:VAL:O	7:6:14:LEU:HD13	2.12	0.50
7:6:175:ASN:O	7:6:179:ASP:N	2.45	0.50
7:6:353:GLU:O	7:6:354:GLN:HG2	2.12	0.50
9:8:244:ASN:O	9:8:248:VAL:HG22	2.11	0.50
9:8:270:ASN:HD21	9:8:338:ASP:CB	2.25	0.50
23:A:81:GLU:HG3	23:A:108:LYS:HB3	1.94	0.50
24:B:234:GLN:HE22	27:E:96:ARG:CD	2.24	0.50
30:H:65:GLU:OE2	43:V:110:VAL:HG12	2.12	0.50
31:I:109:THR:CB	31:I:120:ARG:N	2.74	0.50
34:L:32:LEU:N	34:L:33:PRO:HD2	2.27	0.50
34:L:53:TYR:CD1	43:V:69:ILE:HG23	2.47	0.50
49:b:167:PRO:O	49:b:168:TRP:HD1	1.95	0.50
59:l:286:LYS:HG2	59:l:287:ARG:HG3	1.94	0.50
60:m:25:SER:OG	60:m:216:ASP:OD2	2.28	0.50
61:o:240:PRO:HD3	64:r:12:HIS:CG	2.47	0.50
62:p:91:TRP:O	62:p:93:GLY:N	2.45	0.50
64:r:58:VAL:HA	64:r:61:TRP:HB3	1.93	0.50
59:x:182:ARG:CD	59:x:185:LYS:HD3	2.42	0.50
59:x:257:LEU:HD21	59:x:422:LYS:HD2	1.94	0.50
60:y:172:LYS:O	60:y:175:LEU:HB3	2.12	0.50
60:y:300:ILE:O	60:y:304:ILE:HG13	2.12	0.50
67:B6:58:LYS:HG3	67:B6:59:TYR:N	2.25	0.50
2:1:288:LEU:O	2:1:292:ASN:HB2	2.12	0.49
3:9:132:ILE:HG22	3:9:170:THR:O	2.12	0.49
5:4:82:HIS:CE1	5:4:432:ARG:HH12	2.29	0.49
5:4:305:THR:OG1	5:4:305:THR:O	2.29	0.49
11:C1:186:SER:HB3	11:C1:213:LEU:CD2	2.42	0.49
16:A6:5:LYS:NZ	16:A6:5:LYS:HB3	2.27	0.49
23:A:567:VAL:HG13	23:A:582:VAL:O	2.12	0.49
39:R:329:LEU:HD11	39:R:331:HIS:CD2	2.47	0.49
39:R:354:ARG:O	39:R:355:ARG:NH2	2.37	0.49
43:V:76:GLN:HE22	49:b:187:PRO:HG2	1.75	0.49
49:b:66:ARG:HG2	53:h:74:HIS:CE1	2.47	0.49
58:k:213:GLN:HB3	58:k:214:LYS:NZ	2.27	0.49
59:l:248:ASN:ND2	59:l:427:SER:HB3	2.27	0.49
60:m:221:HIS:O	60:m:225:THR:OG1	2.27	0.49
61:o:240:PRO:HD3	64:r:12:HIS:ND1	2.27	0.49
62:p:29:SER:HA	62:p:32:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:q:9:SER:O	63:q:13:LEU:N	2.45	0.49
58:w:41:ILE:HG22	58:w:43:ALA:H	1.77	0.49
58:w:259:GLY:O	58:w:318:GLY:N	2.45	0.49
58:w:383:LEU:HA	58:w:387:GLY:C	2.37	0.49
62:A1:30:GLU:HG3	67:B6:7:ALA:HA	1.94	0.49
65:B7:36:ARG:HA	65:B7:39:LEU:HD12	1.94	0.49
66:A4:20:THR:HG22	66:A4:24:TRP:HE1	1.76	0.49
3:9:164:THR:HG22	3:9:169:PHE:H	1.77	0.49
5:4:15:THR:OG1	5:4:16:TRP:N	2.45	0.49
5:4:112:ALA:O	5:4:114:GLU:HG2	2.11	0.49
5:4:241:TYR:O	5:4:244:LEU:N	2.24	0.49
6:5:97:GLN:OE1	7:6:577:VAL:HG13	2.12	0.49
7:6:56:HIS:HB2	51:d:74:PHE:CE1	2.47	0.49
9:8:281:HIS:CD2	9:8:357:MET:HA	2.47	0.49
9:8:386:ARG:O	9:8:388:GLY:N	2.45	0.49
24:B:320:ILE:O	27:E:41:VAL:HG22	2.13	0.49
35:N:62:GLU:OE2	35:N:71:ARG:NH1	2.46	0.49
58:k:262:TRP:O	58:k:386:TYR:OH	2.30	0.49
59:l:132:PHE:HB3	59:l:188:PRO:HB3	1.93	0.49
62:p:109:GLU:N	62:p:110:ALA:HB3	2.27	0.49
59:x:240:HIS:CE1	59:x:421:ARG:HH22	2.30	0.49
62:A1:29:SER:O	62:A1:33:LYS:N	2.32	0.49
2:1:172:MET:HE2	2:1:176:LEU:CB	2.42	0.49
8:2:321:LYS:HE3	69:2:402:PC1:H221	1.93	0.49
9:8:51:TRP:CH2	9:8:57:GLN:HA	2.47	0.49
9:8:306:GLY:O	9:8:308:THR:N	2.46	0.49
9:8:398:ARG:HG3	9:8:403:ASP:CB	2.39	0.49
11:C1:16:ILE:HD12	11:C1:17:MET:H	1.77	0.49
26:D:86:THR:H	26:D:114:ARG:HH21	1.59	0.49
26:D:189:THR:C	26:D:191:GLU:H	2.19	0.49
29:G:165:SER:CB	29:G:168:LYS:HB2	2.43	0.49
38:Q:7:LEU:O	43:V:88:ARG:NH2	2.45	0.49
39:R:147:LYS:O	39:R:151:ALA:N	2.38	0.49
48:a:37:LEU:HA	48:a:40:ARG:HG2	1.94	0.49
56:g:145:ASP:O	56:g:149:HIS:N	2.45	0.49
59:l:97:SER:HA	68:v:70:LEU:HB3	1.93	0.49
62:p:13:TYR:CD1	64:r:27:PRO:HG2	2.45	0.49
63:q:84:GLU:OE1	63:q:84:GLU:N	2.38	0.49
62:A1:53:ASN:O	62:A1:57:GLN:N	2.31	0.49
2:1:210:GLY:O	2:1:212:ASN:N	2.45	0.49
6:5:6:MET:O	6:5:7:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:101:MET:HE2	7:6:121:LEU:HD22	1.94	0.49
7:6:342:CYS:SG	7:6:369:THR:OG1	2.66	0.49
8:2:45:MET:O	8:2:47:ASN:N	2.46	0.49
8:2:114:TRP:CD1	8:2:114:TRP:C	2.90	0.49
11:C1:13:THR:O	11:C1:13:THR:HG22	2.12	0.49
12:A9:42:LEU:HD13	19:B2:45:TYR:HD2	1.77	0.49
16:A6:42:ARG:HD2	16:A6:42:ARG:O	2.12	0.49
16:A6:44:ARG:HD2	16:A6:74:ARG:O	2.12	0.49
26:D:203:LYS:HG2	26:D:203:LYS:O	2.13	0.49
29:G:82:PRO:HG3	29:G:98:LYS:NZ	2.28	0.49
32:J:2:TRP:HE3	32:J:3:PHE:CD1	2.30	0.49
39:R:178:SER:O	39:R:181:LEU:N	2.45	0.49
46:Y:69:TRP:O	46:Y:72:ILE:HG22	2.13	0.49
58:k:259:GLY:O	58:k:318:GLY:N	2.45	0.49
60:m:172:LYS:O	60:m:175:LEU:HB3	2.12	0.49
65:s:36:ARG:HA	65:s:39:LEU:HD12	1.94	0.49
58:w:57:TYR:CZ	58:w:168:GLU:HG2	2.47	0.49
58:w:281:ASP:OD2	68:B5:73:PRO:HB3	2.13	0.49
58:w:415:PHE:O	58:w:418:GLN:HG2	2.12	0.49
60:y:17:ALA:HB1	60:y:201:HIS:CE1	2.47	0.49
63:A2:106:GLU:HA	63:A2:109:LYS:HG2	1.93	0.49
82:A2:201:UQ2:H5M2	82:A2:201:UQ2:H8	1.94	0.49
2:1:101:GLY:O	2:1:104:PHE:HB3	2.13	0.49
7:6:147:VAL:HB	7:6:252:MET:SD	2.52	0.49
7:6:286:LEU:HD22	7:6:411:MET:SD	2.52	0.49
7:6:548:SER:HA	7:6:552:LEU:HD13	1.94	0.49
8:2:30:TRP:HZ3	8:2:67:SER:HB3	1.73	0.49
23:A:573:GLY:HA2	23:A:577:ALA:HB2	1.94	0.49
27:E:118:LEU:O	27:E:120:GLU:N	2.45	0.49
32:J:3:PHE:CE2	72:J:101:CDL:HB22	2.47	0.49
38:Q:8:PRO:O	43:V:88:ARG:NH2	2.46	0.49
38:Q:88:CYS:SG	38:Q:89:ILE:N	2.86	0.49
39:R:143:ASP:C	39:R:146:VAL:H	2.18	0.49
39:R:179:LYS:HB3	39:R:317:ASP:OD1	2.12	0.49
55:j:108:THR:OG1	56:g:75:THR:O	2.28	0.49
55:j:109:TYR:O	56:g:75:THR:OG1	2.29	0.49
57:e:70:THR:CG2	57:e:71:GLY:H	2.22	0.49
58:k:106:LEU:HD12	58:k:109:ALA:HB3	1.95	0.49
59:l:170:ASN:OD1	59:l:170:ASN:N	2.34	0.49
60:m:71:ARG:HE	61:o:49:ARG:NH2	2.11	0.49
60:m:182:HIS:NE2	80:m:401:HEM:ND	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:p:29:SER:OG	62:p:32:ARG:NH2	2.46	0.49
58:w:106:LEU:HD12	58:w:109:ALA:HB3	1.95	0.49
58:w:262:TRP:O	58:w:386:TYR:OH	2.30	0.49
58:w:426:GLY:HA2	58:w:428:ILE:N	2.27	0.49
59:x:40:ASN:CG	59:x:42:ALA:H	2.21	0.49
60:y:182:HIS:NE2	80:y:401:HEM:ND	2.60	0.49
60:y:244:LEU:HD21	61:z:205:GLY:CA	2.43	0.49
61:z:178:THR:HB	61:z:181:GLN:HB2	1.94	0.49
63:A2:68:LEU:HD23	63:A2:71:ARG:NH2	2.27	0.49
5:4:294:MET:O	5:4:297:VAL:HG22	2.13	0.49
7:6:13:LEU:O	7:6:16:THR:OG1	2.30	0.49
9:8:362:ASP:OD1	9:8:449:ARG:NH2	2.46	0.49
10:C3:87:ILE:O	10:C3:173:PRO:HD3	2.13	0.49
23:A:103:LEU:HD21	23:A:106:SER:HB3	1.93	0.49
23:A:276:ARG:HG2	23:A:276:ARG:O	2.11	0.49
24:B:241:MET:CE	24:B:351:MET:HE1	2.42	0.49
24:B:309:ASP:O	24:B:310:VAL:C	2.54	0.49
33:K:14:LEU:N	33:K:70:ALA:H	2.10	0.49
40:S:204:SER:HA	40:S:207:GLN:HB3	1.94	0.49
43:V:125:TYR:CD2	43:V:133:VAL:HG22	2.47	0.49
49:b:87:THR:O	49:b:91:VAL:HG23	2.12	0.49
44:M:35:HIS:HB2	44:M:39:ASP:HB2	1.93	0.49
58:k:134:ILE:O	58:k:138:LEU:N	2.39	0.49
58:k:205:HIS:O	58:k:208:LEU:HB3	2.12	0.49
60:m:163:TRP:CE3	60:m:164:ILE:HG13	2.48	0.49
60:y:310:SER:HA	60:y:374:ASN:ND2	2.23	0.49
61:z:41:HIS:CD2	81:z:301:HEC:NB	2.80	0.49
65:B7:73:LEU:HA	65:B7:76:SER:HB2	1.95	0.49
2:1:53:ILE:O	2:1:53:ILE:CG2	2.60	0.49
2:1:188:SER:O	2:1:191:ALA:N	2.45	0.49
10:C3:40:GLU:HG2	10:C3:54:TYR:CD1	2.47	0.49
11:C1:90:ILE:H	11:C1:90:ILE:HD12	1.77	0.49
23:A:356:ASP:OD2	23:A:645:ARG:NE	2.44	0.49
25:C:230:GLN:NE2	25:C:233:ARG:NH1	2.61	0.49
27:E:172:ASN:ND2	27:E:197:TRP:CE3	2.81	0.49
29:G:94:THR:HG22	29:G:95:LYS:N	2.28	0.49
34:L:39:THR:O	34:L:40:LYS:HB3	2.11	0.49
40:S:113:ASP:N	40:S:114:GLY:HA2	2.27	0.49
40:S:117:TYR:HB2	40:S:167:ILE:CD1	2.43	0.49
41:T:40:SER:O	41:T:44:LYS:HB3	2.12	0.49
59:l:186:VAL:HA	59:l:190:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:248:ASN:HD22	59:l:427:SER:HB3	1.78	0.49
60:m:10:LEU:HD12	60:m:13:ILE:HD12	1.95	0.49
61:o:41:HIS:CD2	81:o:301:HEC:NB	2.80	0.49
61:o:171:PHE:O	61:o:174:GLY:N	2.46	0.49
62:p:126:ARG:HA	62:p:135:LEU:HA	1.95	0.49
63:q:102:LYS:HD2	63:q:105:GLU:OE1	2.13	0.49
67:u:58:LYS:HG3	67:u:59:TYR:N	2.25	0.49
60:y:140:PHE:O	60:y:144:THR:OG1	2.14	0.49
1:3:5:LEU:O	1:3:9:THR:OG1	2.28	0.49
5:4:50:LEU:HD21	5:4:52:PHE:HD2	1.77	0.49
7:6:102:GLU:O	7:6:105:MET:HB3	2.13	0.49
23:A:76:ARG:O	23:A:116:VAL:HG21	2.12	0.49
23:A:373:PRO:HD2	23:A:481:LEU:HG	1.95	0.49
24:B:446:ASP:O	24:B:449:ALA:N	2.44	0.49
44:M:18:VAL:HG21	44:M:54:MET:SD	2.52	0.49
59:l:395:PRO:O	59:l:399:LEU:HG	2.13	0.49
60:m:129:MET:O	60:m:132:VAL:N	2.43	0.49
65:s:37:LEU:O	65:s:41:ASP:N	2.28	0.49
65:s:73:LEU:HA	65:s:76:SER:HB2	1.95	0.49
58:w:191:LYS:HA	58:w:218:GLY:HA3	1.94	0.49
58:w:205:HIS:O	58:w:208:LEU:HB3	2.12	0.49
59:x:29:LEU:HD13	59:x:221:GLU:HG2	1.95	0.49
59:x:56:ARG:HA	59:x:174:ASN:HD22	1.77	0.49
59:x:248:ASN:ND2	59:x:427:SER:HB3	2.27	0.49
59:x:248:ASN:HD22	59:x:427:SER:HB3	1.78	0.49
60:y:22:PRO:HG2	64:A3:3:GLN:HB3	1.94	0.49
60:y:130:GLY:HA3	80:y:401:HEM:C4A	2.48	0.49
61:z:105:ASN:HB2	61:z:108:ALA:O	2.13	0.49
63:A2:105:GLU:O	63:A2:109:LYS:NZ	2.42	0.49
5:4:12:MET:HG2	5:4:16:TRP:CH2	2.48	0.49
5:4:214:LEU:HD11	7:6:558:LEU:HD13	1.95	0.49
5:4:329:LEU:HD23	5:4:437:MET:HE3	1.93	0.49
6:5:24:SER:CB	6:5:89:TYR:HA	2.42	0.49
6:5:26:LEU:O	6:5:29:SER:OG	2.25	0.49
7:6:272:TYR:O	7:6:275:SER:OG	2.24	0.49
24:B:320:ILE:HD11	27:E:38:TYR:CD1	2.47	0.49
25:C:185:ASP:OD1	25:C:186:LEU:N	2.45	0.49
26:D:86:THR:H	26:D:114:ARG:NH2	2.11	0.49
26:D:101:ALA:HB1	26:D:102:PRO:HD2	1.94	0.49
27:E:191:LEU:O	27:E:195:ASP:N	2.45	0.49
34:L:8:PHE:HD2	34:L:9:LEU:HD12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:a:54:PRO:HD3	52:f:133:TRP:NE1	2.27	0.49
56:g:90:MET:HB3	56:g:94:ARG:HH12	1.77	0.49
58:k:57:TYR:CZ	58:k:168:GLU:HG2	2.47	0.49
58:k:159:GLN:OE1	62:p:7:VAL:HG11	2.12	0.49
59:l:56:ARG:HA	59:l:174:ASN:HD22	1.77	0.49
61:o:178:THR:HB	61:o:181:GLN:HB2	1.94	0.49
63:q:68:LEU:HD23	63:q:71:ARG:NH2	2.27	0.49
59:x:186:VAL:HA	59:x:190:GLU:OE1	2.12	0.49
60:y:95:TYR:O	60:y:98:VAL:HB	2.13	0.49
60:y:113:TRP:HE1	60:y:302:ALA:HA	1.78	0.49
62:A1:18:VAL:HG11	62:A1:32:ARG:HH11	1.78	0.49
1:3:35:SER:HB2	1:3:37:TYR:HD2	1.78	0.49
2:1:75:PRO:C	2:1:77:MET:N	2.69	0.49
2:1:105:MET:O	2:1:108:MET:N	2.46	0.49
2:1:248:ASN:C	2:1:250:HIS:H	2.20	0.49
3:9:77:ALA:HB3	9:8:217:GLU:O	2.13	0.49
4:7:135:PHE:HB2	32:J:41:TYR:HB3	1.93	0.49
5:4:62:SER:HB2	53:h:113:ARG:HH22	1.78	0.49
6:5:15:SER:O	6:5:20:LEU:HB2	2.13	0.49
7:6:353:GLU:OE2	7:6:358:LYS:HB2	2.12	0.49
7:6:454:ILE:HG22	7:6:458:LEU:HD23	1.94	0.49
10:C3:266:GLU:HB2	10:C3:267:PRO:HD2	1.95	0.49
23:A:287:SER:OG	23:A:288:ASP:N	2.45	0.49
24:B:301:ASP:OD1	24:B:301:ASP:C	2.56	0.49
30:H:78:ALA:HB1	43:V:104:TRP:HH2	1.77	0.49
33:K:20:ARG:HG2	33:K:54:LEU:HB2	1.95	0.49
41:T:96:ALA:HA	41:T:99:LEU:HD12	1.95	0.49
42:U:46:ASN:HD21	42:U:83:PRO:HD3	1.78	0.49
58:k:415:PHE:O	58:k:418:GLN:HG2	2.12	0.49
59:l:133:ARG:HD3	59:l:135:TRP:HZ2	1.75	0.49
64:r:51:PRO:O	64:r:54:ALA:N	2.46	0.49
58:w:125:SER:O	58:w:129:LYS:HG3	2.13	0.49
60:y:84:ALA:HB2	80:y:401:HEM:O2A	2.13	0.49
2:1:171:GLN:H	2:1:171:GLN:NE2	2.08	0.48
5:4:66:LEU:O	5:4:69:THR:OG1	2.28	0.48
7:6:451:ILE:HG22	7:6:455:LYS:HD2	1.94	0.48
12:A9:65:SER:HB3	12:A9:71:HIS:CE1	2.48	0.48
13:A7:68:PHE:HA	13:A7:71:MET:HG2	1.95	0.48
16:A6:42:ARG:NH1	16:A6:74:ARG:HH21	2.10	0.48
26:D:173:CYS:O	26:D:173:CYS:SG	2.71	0.48
27:E:111:GLU:OE2	31:I:68:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:25:MET:HB3	36:O:29:LYS:NZ	2.28	0.48
39:R:329:LEU:HD11	39:R:331:HIS:HD2	1.78	0.48
55:j:91:PHE:O	55:j:95:LYS:N	2.38	0.48
58:k:244:ARG:CZ	64:r:10:VAL:HB	2.43	0.48
59:l:29:LEU:HD13	59:l:221:GLU:HG2	1.95	0.48
59:l:133:ARG:HB3	59:l:135:TRP:CZ2	2.48	0.48
60:m:27:ILE:HD12	60:m:224:TYR:CZ	2.48	0.48
60:m:130:GLY:HA3	80:m:401:HEM:C4A	2.48	0.48
58:w:49:SER:N	58:w:52:ASN:HB2	2.29	0.48
58:w:115:ASP:OD1	58:w:119:ASN:HB2	2.14	0.48
59:x:346:THR:HG22	59:x:351:ASN:HD22	1.78	0.48
60:y:83:HIS:HE1	80:y:401:HEM:CHC	2.26	0.48
60:y:163:TRP:CE3	60:y:164:ILE:HG13	2.48	0.48
3:9:114:GLU:OE2	9:8:220:GLN:OE1	2.31	0.48
3:9:233:SER:HB3	9:8:41:ILE:HD13	1.94	0.48
5:4:187:HIS:CG	5:4:188:ASN:H	2.31	0.48
5:4:227:GLY:CA	5:4:230:VAL:HB	2.43	0.48
5:4:360:LEU:HD22	72:6:701:CDL:H532	1.95	0.48
7:6:550:SER:OG	7:6:551:SER:N	2.44	0.48
8:2:339:LEU:O	8:2:343:LEU:N	2.44	0.48
10:C3:168:ILE:HG21	10:C3:189:MET:HG3	1.94	0.48
24:B:223:HIS:NE2	26:D:91:CYS:SG	2.82	0.48
26:D:193:LEU:HD23	26:D:193:LEU:C	2.39	0.48
36:O:37:ARG:HA	36:O:40:TYR:HB3	1.95	0.48
45:X:38:ARG:HA	45:X:56:TRP:CZ3	2.48	0.48
58:k:382:SER:O	58:k:386:TYR:N	2.46	0.48
58:k:398:ARG:HA	58:k:401:GLU:HG2	1.94	0.48
59:l:37:SER:HB3	59:l:216:LEU:HD23	1.94	0.48
61:o:164:ILE:HG22	61:o:179:MET:HG3	1.94	0.48
63:q:106:GLU:HA	63:q:109:LYS:HG2	1.94	0.48
58:w:382:SER:O	58:w:386:TYR:N	2.46	0.48
59:x:37:SER:HB3	59:x:216:LEU:HD23	1.94	0.48
59:x:139:ALA:O	59:x:142:PRO:HD2	2.12	0.48
59:x:395:PRO:O	59:x:399:LEU:HG	2.13	0.48
60:y:241:LEU:HD12	60:y:245:PHE:HD2	1.79	0.48
62:A1:15:ARG:HH21	62:A1:32:ARG:CG	2.26	0.48
2:1:11:ILE:HB	2:1:12:PRO:HD3	1.95	0.48
4:7:140:ALA:C	4:7:142:GLY:N	2.72	0.48
6:5:17:VAL:HA	6:5:20:LEU:CB	2.43	0.48
9:8:228:PRO:HB2	9:8:229:PHE:CB	2.42	0.48
9:8:244:ASN:CG	9:8:245:VAL:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:J:3:PHE:HA	32:J:6:LEU:HD13	1.95	0.48
32:J:48:MET:O	32:J:51:ASP:N	2.45	0.48
44:W:78:GLY:O	44:W:82:ARG:N	2.36	0.48
44:W:89:LEU:HD21	47:Z:47:ARG:H	1.79	0.48
56:g:159:GLN:O	56:g:163:MET:N	2.45	0.48
57:e:40:PRO:CB	57:e:67:ASP:CB	2.92	0.48
58:k:237:THR:HG22	58:k:239:SER:HB3	1.94	0.48
60:m:241:LEU:HD12	60:m:245:PHE:HD2	1.79	0.48
60:m:346:PRO:O	60:m:350:ILE:HG13	2.14	0.48
61:o:105:ASN:HB2	61:o:108:ALA:O	2.13	0.48
59:x:133:ARG:HD3	59:x:135:TRP:HZ2	1.75	0.48
59:x:398:VAL:O	59:x:402:ILE:N	2.34	0.48
61:z:171:PHE:O	61:z:174:GLY:N	2.46	0.48
63:A2:16:ILE:CD1	63:A2:19:TRP:CH2	2.87	0.48
63:A2:102:LYS:HD2	63:A2:105:GLU:OE1	2.13	0.48
2:1:253:GLU:HG2	2:1:254:LEU:N	2.29	0.48
2:1:256:THR:HA	2:1:259:PHE:HB3	1.96	0.48
2:1:316:PRO:HG3	43:V:57:ARG:NE	2.28	0.48
3:9:168:LEU:HD12	3:9:169:PHE:CG	2.48	0.48
4:7:107:VAL:HG13	4:7:108:LEU:N	2.25	0.48
9:8:98:LYS:HA	9:8:101:PHE:CB	2.43	0.48
10:C3:115:SER:O	10:C3:121:GLY:HA2	2.14	0.48
11:C1:59:GLN:O	11:C1:62:GLU:HB2	2.13	0.48
23:A:385:TYR:CZ	23:A:526:LEU:HD22	2.49	0.48
24:B:177:ILE:HG23	24:B:210:MET:HE3	1.96	0.48
24:B:360:ASP:OD1	24:B:360:ASP:N	2.45	0.48
69:S:401:PC1:O14	69:S:401:PC1:H342	2.13	0.48
47:Z:41:LEU:N	47:Z:42:ARG:HA	2.26	0.48
49:b:66:ARG:HH12	49:b:70:LEU:HD11	1.78	0.48
56:g:8:ASP:HA	56:g:11:PRO:HG3	1.95	0.48
56:g:107:GLN:O	56:g:110:LEU:HB3	2.12	0.48
58:k:214:LYS:HA	58:k:217:SER:OG	2.13	0.48
59:l:182:ARG:CD	59:l:185:LYS:HD3	2.42	0.48
60:m:75:TYR:CE2	62:p:57:GLN:HA	2.48	0.48
63:q:67:ASP:O	63:q:70:MET:HB3	2.14	0.48
58:w:291:SER:OG	59:x:90:GLU:OE1	2.24	0.48
59:x:133:ARG:HB3	59:x:135:TRP:CZ2	2.48	0.48
60:y:27:ILE:HD12	60:y:224:TYR:CZ	2.48	0.48
60:y:182:HIS:HE1	80:y:401:HEM:CHB	2.26	0.48
61:z:164:ILE:HG22	61:z:179:MET:HG3	1.94	0.48
63:A2:67:ASP:O	63:A2:70:MET:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:5:ASN:HD21	32:J:23:THR:HG23	1.78	0.48
2:1:169:GLN:O	2:1:170:GLU:C	2.55	0.48
3:9:206:ASP:HA	3:9:209:LYS:HE2	1.95	0.48
4:7:125:TRP:HB3	4:7:128:TYR:CB	2.43	0.48
6:5:38:LEU:HA	6:5:41:PHE:HB3	1.95	0.48
7:6:362:LEU:HA	7:6:431:LEU:HD22	1.96	0.48
72:6:701:CDL:H561	72:6:701:CDL:H742	1.95	0.48
9:8:204:TYR:HB3	9:8:377:GLU:CG	2.43	0.48
10:C3:197:LEU:O	12:A9:92:LEU:HD22	2.13	0.48
25:C:126:ASN:HB3	25:C:149:THR:O	2.13	0.48
26:D:155:SER:OG	26:D:161:GLY:HA2	2.14	0.48
27:E:54:THR:HG22	34:L:13:TRP:HH2	1.78	0.48
39:R:143:ASP:O	39:R:146:VAL:N	2.43	0.48
39:R:178:SER:O	39:R:182:ARG:N	2.30	0.48
47:Z:79:VAL:O	47:Z:82:ILE:N	2.42	0.48
49:b:112:TYR:O	56:g:63:TYR:HB2	2.13	0.48
49:b:128:GLY:O	49:b:130:GLU:N	2.46	0.48
58:k:49:SER:N	58:k:52:ASN:HB2	2.29	0.48
58:k:294:LEU:HB3	58:k:307:PHE:CZ	2.39	0.48
59:l:369:LEU:HD11	59:l:399:LEU:HD11	1.95	0.48
60:m:81:TYR:HB3	60:m:85:ASN:OD1	2.14	0.48
60:m:83:HIS:HE1	80:m:401:HEM:CHC	2.26	0.48
58:w:433:ASP:OD2	60:y:223:TYR:OH	2.30	0.48
59:x:397:THR:HA	59:x:400:GLN:OE1	2.13	0.48
61:z:228:SER:HB2	64:A3:23:GLN:HE21	1.79	0.48
1:3:7:LEU:HD11	1:3:11:PHE:HE2	1.78	0.48
2:1:169:GLN:HE21	2:1:174:LEU:HB2	1.74	0.48
9:8:99:TRP:CD1	9:8:99:TRP:N	2.79	0.48
11:C1:22:HIS:CE1	18:C2:44:LYS:HD3	2.49	0.48
19:B2:16:ASN:ND2	19:B2:16:ASN:H	2.12	0.48
23:A:270:VAL:C	23:A:271:MET:HE2	2.39	0.48
23:A:308:ARG:HH22	42:U:144:TYR:HE1	1.61	0.48
27:E:166:ALA:O	27:E:168:VAL:HG23	2.14	0.48
29:G:163:ASN:HB3	29:G:172:VAL:HG22	1.94	0.48
58:k:41:ILE:HG22	58:k:43:ALA:H	1.77	0.48
58:k:125:SER:O	58:k:129:LYS:HG3	2.13	0.48
58:k:389:ARG:O	58:k:390:ILE:HD13	2.13	0.48
59:l:397:THR:HA	59:l:400:GLN:OE1	2.13	0.48
1:3:106:TRP:HZ2	69:3:200:PC1:H111	1.79	0.48
7:6:298:ILE:O	7:6:302:ILE:HG12	2.14	0.48
8:2:219:PHE:O	8:2:223:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:2:402:PC1:H131	40:S:28:PRO:HG3	1.95	0.48
23:A:403:VAL:HG12	23:A:432:ILE:HD12	1.96	0.48
23:A:413:LEU:HD23	23:A:413:LEU:HA	1.64	0.48
24:B:88:HIS:HB2	24:B:89:PRO:HD3	1.95	0.48
24:B:229:PRO:HG2	24:B:389:TYR:OH	2.12	0.48
48:a:68:TRP:CZ3	57:e:110:ASP:HA	2.48	0.48
48:a:108:ASP:C	48:a:110:ASP:N	2.69	0.48
51:d:63:LEU:HD22	51:d:87:TRP:HE1	1.78	0.48
60:m:45:ILE:HA	80:m:401:HEM:CMC	2.36	0.48
58:w:252:HIS:CD2	58:w:323:HIS:HE1	2.30	0.48
59:x:378:PHE:HA	59:x:381:GLU:HB3	1.96	0.48
60:y:10:LEU:HD12	60:y:13:ILE:HD12	1.95	0.48
61:z:175:THR:OG1	65:B7:78:LYS:NZ	2.46	0.48
68:B5:66:ALA:HB2	68:B5:77:ARG:CZ	2.43	0.48
2:1:185:TRP:NE1	2:1:238:THR:OG1	2.46	0.48
2:1:276:SER:OG	27:E:70:LEU:HD22	2.14	0.48
4:7:73:ALA:C	4:7:74:MET:HE2	2.38	0.48
5:4:193:VAL:O	5:4:197:LEU:N	2.44	0.48
7:6:116:LYS:HZ3	72:6:701:CDL:PA1	2.36	0.48
7:6:349:SER:OG	7:6:443:ILE:HA	2.14	0.48
9:8:362:ASP:O	9:8:366:ALA:N	2.46	0.48
10:C3:476:PHE:CD1	21:A0:15:VAL:HG21	2.49	0.48
15:A5:31:TYR:HE1	15:A5:98:HIS:HE1	1.62	0.48
23:A:522:GLN:O	23:A:525:ALA:N	2.47	0.48
23:A:643:ARG:O	23:A:647:GLU:N	2.47	0.48
23:A:688:GLN:O	23:A:689:LEU:HD12	2.14	0.48
24:B:359:ASP:HB3	25:C:48:THR:HG21	1.94	0.48
27:E:146:ASP:OD1	27:E:186:ASN:HA	2.13	0.48
27:E:189:LYS:NZ	27:E:193:ASN:HB2	2.28	0.48
28:F:86:LEU:O	28:F:90:LEU:N	2.25	0.48
31:I:80:VAL:HG11	31:I:85:ILE:HD11	1.95	0.48
36:O:83:VAL:O	36:O:87:LYS:N	2.39	0.48
38:Q:47:ARG:NH2	49:b:187:PRO:HB2	2.28	0.48
39:R:235:THR:HA	39:R:236:VAL:HA	1.66	0.48
39:R:333:PRO:HB3	39:R:337:ASP:OD2	2.14	0.48
48:a:22:GLU:H	48:a:22:GLU:CD	2.22	0.48
48:a:27:SER:HA	48:a:28:GLU:HA	1.69	0.48
44:M:35:HIS:HB3	44:M:38:LYS:NZ	2.28	0.48
58:k:256:ALA:HB2	58:k:310:PHE:HZ	1.79	0.48
58:k:405:ARG:HB3	58:k:409:GLU:OE2	2.14	0.48
59:l:40:ASN:CG	59:l:42:ALA:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:191:LEU:O	59:l:195:VAL:HG23	2.14	0.48
60:m:95:TYR:O	60:m:98:VAL:HB	2.13	0.48
60:m:182:HIS:HE1	80:m:401:HEM:CHB	2.26	0.48
60:m:370:GLY:HA2	60:m:373:GLU:HB2	1.96	0.48
58:w:326:CYS:SG	58:w:331:ILE:HA	2.54	0.48
59:x:191:LEU:O	59:x:195:VAL:HG23	2.14	0.48
60:y:81:TYR:HB3	60:y:85:ASN:OD1	2.14	0.48
60:y:346:PRO:O	60:y:350:ILE:HG13	2.13	0.48
63:A2:91:GLU:N	63:A2:92:PRO:HD2	2.29	0.48
64:A3:51:PRO:O	64:A3:54:ALA:N	2.46	0.48
65:B7:12:GLU:OE1	65:B7:12:GLU:N	2.46	0.48
2:1:173:TRP:C	2:1:175:ILE:H	2.19	0.48
70:1:401:3PE:O32	4:7:54:LEU:HD21	2.13	0.48
4:7:55:MET:O	4:7:58:LEU:N	2.47	0.48
5:4:57:PHE:CE2	5:4:113:MET:HA	2.49	0.48
6:5:77:LEU:HD23	8:2:57:THR:HB	1.96	0.48
11:C1:83:ILE:O	11:C1:87:MET:HG3	2.14	0.48
12:A9:80:ARG:O	12:A9:84:ILE:HG12	2.14	0.48
23:A:380:ASP:C	23:A:382:ARG:H	2.20	0.48
24:B:217:VAL:HG13	24:B:218:SER:N	2.28	0.48
25:C:101:PHE:HE1	25:C:105:HIS:CD2	2.32	0.48
38:Q:81:PRO:HA	38:Q:84:GLU:OE2	2.14	0.48
58:k:252:HIS:CD2	58:k:323:HIS:HE1	2.30	0.48
58:k:326:CYS:SG	58:k:331:ILE:HA	2.54	0.48
59:l:346:THR:HG22	59:l:351:ASN:HD22	1.78	0.48
59:l:378:PHE:HA	59:l:381:GLU:HB3	1.96	0.48
60:m:278:TYR:HD1	60:m:281:LEU:HD23	1.78	0.48
61:o:12:TRP:HA	65:s:74:PHE:CZ	2.48	0.48
61:o:28:ARG:O	61:o:31:GLN:N	2.47	0.48
66:t:34:TRP:HD1	67:u:29:LEU:HD13	1.79	0.48
66:t:43:ASP:CB	67:u:33:ARG:HH22	2.27	0.48
58:w:45:SER:HB2	58:w:165:GLN:HE21	1.78	0.48
60:y:370:GLY:HA2	60:y:373:GLU:HB2	1.96	0.48
2:1:312:SER:OG	43:V:55:ARG:NH2	2.47	0.48
5:4:14:LEU:O	5:4:14:LEU:HD23	2.14	0.48
5:4:110:PHE:CD1	5:4:241:TYR:CE2	3.02	0.48
5:4:289:SER:HB3	5:4:406:TYR:OH	2.14	0.48
7:6:303:ALA:O	7:6:306:THR:HG22	2.14	0.48
7:6:364:LYS:O	7:6:366:MET:HG2	2.14	0.48
12:A9:173:PHE:CD1	12:A9:173:PHE:C	2.92	0.48
17:C0:24:ASN:ND2	17:C0:26:THR:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:643:ARG:HA	23:A:646:LEU:HB2	1.95	0.48
24:B:65:PRO:HG2	24:B:71:PRO:HD3	1.95	0.48
24:B:152:SER:HG	24:B:228:ARG:C	2.18	0.48
24:B:458:PHE:C	24:B:460:GLU:N	2.63	0.48
25:C:66:TYR:OH	37:P:95:VAL:O	2.27	0.48
36:O:54:ILE:HB	36:O:58:GLN:OE1	2.14	0.48
45:X:20:PHE:O	45:X:23:GLY:N	2.47	0.48
48:a:121:LEU:HD12	48:a:122:ASP:N	2.28	0.48
49:b:67:PHE:CG	49:b:68:LEU:N	2.81	0.48
58:k:45:SER:HB2	58:k:165:GLN:HE21	1.78	0.48
59:l:304:HIS:CD2	59:l:305:GLN:HG3	2.49	0.48
61:o:51:LEU:HD13	61:o:58:GLU:HB2	1.95	0.48
62:p:11:SER:HB2	62:p:19:LEU:HD11	1.96	0.48
62:p:109:GLU:HA	62:p:110:ALA:C	2.39	0.48
65:s:44:VAL:HG22	65:s:52:GLU:HG2	1.96	0.48
58:w:215:HIS:O	58:w:216:PHE:HB2	2.12	0.48
58:w:389:ARG:O	58:w:390:ILE:HD13	2.13	0.48
58:w:398:ARG:HA	58:w:401:GLU:HG2	1.95	0.48
1:3:106:TRP:CZ2	69:3:200:PC1:H111	2.49	0.47
7:6:114:ILE:HD11	7:6:118:PHE:CE2	2.48	0.47
7:6:437:PHE:CD1	7:6:441:VAL:HG21	2.49	0.47
7:6:463:PHE:O	7:6:467:ILE:HG12	2.14	0.47
7:6:470:ASN:ND2	51:d:77:PHE:HB3	2.29	0.47
23:A:449:PRO:HD3	23:A:682:ASP:O	2.14	0.47
23:A:504:SER:N	23:A:505:GLY:HA2	2.23	0.47
24:B:137:ASP:HB2	24:B:148:GLU:OE2	2.14	0.47
33:K:14:LEU:HG	33:K:17:ARG:NH2	2.29	0.47
39:R:228:LEU:HA	39:R:229:ILE:HA	1.53	0.47
40:S:232:THR:O	40:S:235:PRO:HD2	2.13	0.47
58:k:217:SER:N	58:k:218:GLY:CA	2.76	0.47
59:l:98:VAL:H	68:v:70:LEU:HB3	1.79	0.47
60:m:71:ARG:HE	61:o:49:ARG:HH22	1.62	0.47
60:m:84:ALA:HB2	80:m:401:HEM:O2A	2.13	0.47
60:m:165:TRP:O	60:m:174:THR:OG1	2.24	0.47
63:q:110:LYS:HE3	66:A4:11:ARG:HB3	1.96	0.47
67:u:17:THR:O	67:u:21:ALA:N	2.42	0.47
59:x:202:ALA:HB3	59:x:230:LEU:HD22	1.95	0.47
62:A1:73:LYS:HD2	62:A1:194:ILE:HA	1.95	0.47
2:1:37:PRO:HD3	26:D:108:ARG:HG2	1.96	0.47
2:1:169:GLN:NE2	2:1:174:LEU:CB	2.77	0.47
2:1:237:PHE:HD1	2:1:240:ILE:HD11	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:156:VAL:O	4:7:160:SER:N	2.41	0.47
5:4:158:LEU:HB2	5:4:159:PRO:HD3	1.97	0.47
6:5:17:VAL:C	6:5:20:LEU:H	2.22	0.47
7:6:306:THR:HB	7:6:336:LYS:HE3	1.95	0.47
9:8:101:PHE:CG	9:8:102:MET:N	2.83	0.47
23:A:140:GLN:HG3	24:B:379:ILE:CG2	2.44	0.47
23:A:154:LEU:HD12	23:A:155:GLU:HB3	1.96	0.47
23:A:663:ASN:CG	23:A:664:TYR:H	2.21	0.47
24:B:178:THR:HG22	24:B:214:TYR:OH	2.14	0.47
25:C:150:ASP:CG	25:C:151:GLU:H	2.17	0.47
27:E:105:ARG:HD3	27:E:109:GLY:CA	2.41	0.47
35:N:40:LYS:HB2	35:N:45:ARG:NH1	2.29	0.47
39:R:355:ARG:O	39:R:357:ARG:N	2.47	0.47
40:S:158:LEU:O	40:S:162:TYR:N	2.37	0.47
42:U:47:LYS:O	42:U:86:TRP:HH2	1.97	0.47
56:g:34:THR:HG23	56:g:35:LYS:HD2	1.96	0.47
58:k:115:ASP:OD1	58:k:119:ASN:HB2	2.14	0.47
59:l:198:HIS:HA	59:l:230:LEU:O	2.13	0.47
63:q:25:GLY:HA2	63:q:28:LYS:NZ	2.29	0.47
63:q:52:GLU:O	63:q:56:ASN:N	2.42	0.47
64:r:1:GLY:O	64:r:3:GLN:NE2	2.47	0.47
58:w:280:TYR:CG	58:w:281:ASP:N	2.81	0.47
58:w:405:ARG:HB3	58:w:409:GLU:CD	2.40	0.47
58:w:405:ARG:HB3	58:w:409:GLU:OE2	2.14	0.47
59:x:369:LEU:HD11	59:x:399:LEU:HD11	1.95	0.47
61:z:23:HIS:O	61:z:27:ARG:HG3	2.15	0.47
63:A2:25:GLY:HA2	63:A2:28:LYS:NZ	2.29	0.47
3:9:54:ASP:OD1	3:9:60:TYR:OH	2.33	0.47
7:6:335:PHE:CZ	7:6:383:MET:HE1	2.48	0.47
7:6:481:THR:HG22	51:d:92:HIS:CD2	2.49	0.47
8:2:112:HIS:HE2	8:2:164:ILE:HD13	1.79	0.47
10:C3:397:PHE:HB3	10:C3:398:PRO:HD3	1.95	0.47
23:A:50:LEU:HD12	23:A:60:ILE:HD11	1.95	0.47
23:A:124:HIS:CD2	74:A:801:SF4:S3	3.07	0.47
23:A:168:LEU:HD13	23:A:292:PHE:HE2	1.79	0.47
24:B:123:LEU:CD1	25:C:206:LEU:HD21	2.45	0.47
26:D:180:ASP:HB3	26:D:181:ILE:HD12	1.96	0.47
27:E:189:LYS:HZ2	27:E:193:ASN:HB2	1.79	0.47
34:L:59:ASP:HB2	34:L:63:MET:HE3	1.95	0.47
40:S:26:TYR:O	40:S:30:ALA:HB3	2.14	0.47
46:Y:47:TYR:N	46:Y:49:GLN:OE1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:f:163:LEU:H	52:f:166:LEU:HB2	1.79	0.47
55:j:118:PRO:HB2	56:g:147:GLY:N	2.29	0.47
44:M:77:VAL:O	44:M:81:ALA:N	2.45	0.47
58:k:1:THR:OG1	58:k:2:ALA:N	2.47	0.47
60:m:31:TRP:CE2	60:m:100:ARG:HD2	2.49	0.47
60:m:250:LEU:HD11	60:m:272:TRP:CD1	2.49	0.47
60:m:311:LYS:O	63:q:38:HIS:N	2.24	0.47
61:o:23:HIS:O	61:o:27:ARG:HG3	2.15	0.47
58:w:1:THR:OG1	58:w:2:ALA:N	2.47	0.47
58:w:59:VAL:HA	58:w:62:LEU:HD12	1.96	0.47
61:z:129:SER:HB3	61:z:152:TYR:OH	2.15	0.47
61:z:233:ARG:HD3	64:A3:17:SER:HB3	1.96	0.47
5:4:80:SER:HA	5:4:226:ALA:HB2	1.96	0.47
5:4:429:SER:HA	5:4:433:GLU:HG3	1.95	0.47
7:6:68:TRP:CD1	7:6:69:LEU:H	2.31	0.47
7:6:246:LEU:O	7:6:251:THR:OG1	2.31	0.47
72:6:701:CDL:H111	49:b:68:LEU:HD23	1.97	0.47
9:8:103:ASN:ND2	9:8:149:MET:HE1	2.29	0.47
11:C1:4:PRO:HB2	20:B3:43:SER:HA	1.96	0.47
23:A:74:ASN:OD1	23:A:74:ASN:N	2.35	0.47
23:A:179:CYS:SG	74:A:802:SF4:S1	3.11	0.47
24:B:106:VAL:HG23	24:B:107:ARG:N	2.28	0.47
32:J:3:PHE:HE2	72:J:101:CDL:HB22	1.80	0.47
60:m:182:HIS:HE1	80:m:401:HEM:C1B	2.32	0.47
61:o:129:SER:HB3	61:o:152:TYR:OH	2.15	0.47
59:x:21:PRO:HD3	59:x:41:TYR:CD2	2.47	0.47
60:y:278:TYR:HD1	60:y:281:LEU:HD23	1.79	0.47
61:z:51:LEU:HD13	61:z:58:GLU:HB2	1.95	0.47
61:z:149:PHE:HA	61:z:156:GLN:O	2.15	0.47
4:7:152:TRP:HA	4:7:155:ILE:HG22	1.96	0.47
6:5:12:PHE:CG	6:5:12:PHE:O	2.67	0.47
7:6:4:PHE:CD2	7:6:61:LEU:HD12	2.48	0.47
7:6:556:ILE:HD11	48:a:76:ILE:HD12	1.96	0.47
8:2:137:ALA:HB3	8:2:138:PRO:HD3	1.97	0.47
9:8:61:ASP:HA	9:8:256:ARG:HH12	1.79	0.47
9:8:330:SER:O	9:8:332:CYS:N	2.48	0.47
23:A:257:VAL:HG23	23:A:258:GLY:O	2.15	0.47
23:A:454:ASP:HB2	23:A:460:HIS:CE1	2.49	0.47
24:B:263:THR:OG1	24:B:264:ASN:N	2.47	0.47
26:D:83:TRP:CD1	26:D:112:VAL:HG12	2.49	0.47
30:H:43:CYS:HB2	30:H:59:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:J:16:LEU:C	32:J:19:PRO:HD2	2.39	0.47
38:Q:121:ASP:CG	38:Q:122:LEU:H	2.22	0.47
39:R:64:PHE:CZ	39:R:208:GLY:HA3	2.49	0.47
42:U:26:VAL:O	42:U:29:ARG:HG2	2.14	0.47
58:k:191:LYS:NZ	58:k:225:GLU:O	2.48	0.47
58:k:280:TYR:CG	58:k:281:ASP:N	2.81	0.47
60:m:12:LYS:O	60:m:15:ASN:HB3	2.15	0.47
60:m:58:ASP:HB2	60:m:61:THR:HB	1.95	0.47
60:m:75:TYR:HE2	62:p:57:GLN:HA	1.79	0.47
58:w:111:GLU:HG2	58:w:215:HIS:CE1	2.48	0.47
59:x:357:VAL:O	59:x:361:LYS:N	2.31	0.47
61:z:7:PRO:HG3	61:z:152:TYR:CE1	2.50	0.47
61:z:28:ARG:O	61:z:31:GLN:N	2.47	0.47
7:6:285:THR:HG22	7:6:311:GLY:HA3	1.96	0.47
8:2:218:MET:HE1	8:2:240:MET:SD	2.53	0.47
9:8:97:LEU:O	9:8:101:PHE:N	2.48	0.47
10:C3:11:ASN:ND2	10:C3:13:LYS:HB2	2.28	0.47
15:A5:49:VAL:HG21	15:A5:74:LEU:HD12	1.95	0.47
16:A6:67:HIS:CD2	16:A6:78:LEU:HD11	2.50	0.47
24:B:288:PHE:CD2	24:B:292:MET:HE3	2.50	0.47
25:C:123:THR:HG21	29:G:129:SER:N	2.26	0.47
33:K:39:LYS:HG3	33:K:84:ALA:HB1	1.96	0.47
36:O:24:ASP:O	36:O:26:ASN:N	2.47	0.47
38:Q:111:VAL:HG13	38:Q:115:LEU:HD11	1.95	0.47
41:T:114:ALA:O	41:T:118:MET:HB3	2.14	0.47
45:X:43:LEU:HA	45:X:44:TYR:C	2.39	0.47
48:a:68:TRP:CH2	57:e:110:ASP:HA	2.49	0.47
50:c:75:VAL:O	50:c:78:PRO:HD2	2.14	0.47
51:d:63:LEU:HD13	51:d:87:TRP:NE1	2.30	0.47
55:j:36:PHE:O	55:j:39:TYR:N	2.47	0.47
69:j:201:PC1:O32	69:j:201:PC1:H132	2.15	0.47
57:e:132:HIS:C	57:e:135:GLY:H	2.23	0.47
58:k:351:GLU:HG2	58:k:404:ALA:HB2	1.97	0.47
58:k:365:LEU:O	58:k:369:LEU:HG	2.15	0.47
60:m:113:TRP:HE1	60:m:302:ALA:HA	1.78	0.47
61:o:31:GLN:O	61:o:34:LYS:HB3	2.15	0.47
62:p:10:PHE:CB	64:r:18:LEU:HD11	2.45	0.47
58:w:86:LEU:N	59:x:284:HIS:O	2.45	0.47
59:x:298:ALA:HA	59:x:301:LYS:HE3	1.96	0.47
60:y:271:GLU:CD	60:y:273:TYR:HH	2.23	0.47
65:B7:35:GLU:O	65:B7:39:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:29:VAL:HB	39:R:303:ARG:CB	2.45	0.47
1:3:52:SER:O	1:3:55:PHE:HB2	2.14	0.47
2:1:205:SER:H	2:1:279:ARG:NH1	2.13	0.47
3:9:224:SER:OG	3:9:226:GLU:CG	2.62	0.47
4:7:12:ILE:O	4:7:16:GLY:N	2.48	0.47
6:5:93:LEU:HD12	6:5:94:ASN:HA	1.96	0.47
7:6:128:MET:HE2	7:6:251:THR:HA	1.97	0.47
7:6:556:ILE:O	7:6:560:ALA:N	2.45	0.47
9:8:53:LEU:O	9:8:136:HIS:NE2	2.45	0.47
13:A7:33:LEU:HD22	13:A7:37:GLN:HB3	1.97	0.47
18:C2:39:VAL:O	18:C2:42:LYS:HE2	2.14	0.47
19:B2:8:LYS:NZ	19:B2:8:LYS:HB3	2.28	0.47
23:A:217:GLU:C	23:A:219:SER:H	2.22	0.47
23:A:259:SER:HA	23:A:282:ASN:HD21	1.80	0.47
23:A:671:LEU:HD12	33:K:42:VAL:HA	1.96	0.47
24:B:421:ARG:NH2	24:B:423:LYS:HD3	2.29	0.47
25:C:91:HIS:CG	25:C:92:PRO:HD2	2.49	0.47
25:C:123:THR:HA	29:G:133:ASP:OD2	2.14	0.47
29:G:104:ARG:NH1	36:O:127:ASP:O	2.48	0.47
29:G:112:MET:CE	42:U:126:PRO:HB2	2.44	0.47
30:H:65:GLU:HG2	43:V:111:PHE:HE1	1.80	0.47
35:N:59:VAL:O	35:N:61:ALA:HA	2.14	0.47
36:O:115:PRO:C	36:O:117:ASP:H	2.23	0.47
38:Q:83:THR:HA	38:Q:86:TRP:HE1	1.80	0.47
39:R:328:ILE:CG2	39:R:329:LEU:N	2.44	0.47
40:S:187:LEU:HD13	40:S:277:ARG:HB2	1.96	0.47
42:U:3:LEU:HD12	42:U:4:LEU:N	2.30	0.47
47:Z:64:VAL:O	47:Z:67:LEU:N	2.47	0.47
44:M:62:ILE:HG21	44:M:67:ALA:HB2	1.96	0.47
58:k:57:TYR:CE2	58:k:168:GLU:HG2	2.50	0.47
59:l:26:PHE:CE1	59:l:391:SER:HA	2.49	0.47
59:l:334:GLY:O	59:l:338:LYS:HG3	2.15	0.47
59:l:435:PHE:H	59:l:438:GLU:CD	2.23	0.47
61:o:171:PHE:CE2	61:o:177:ALA:HA	2.50	0.47
66:t:18:VAL:HB	66:t:19:PRO:HD3	1.97	0.47
58:w:65:LYS:O	58:w:72:GLY:HA2	2.14	0.47
58:w:237:THR:HG22	58:w:239:SER:HB3	1.94	0.47
59:x:270:ASN:O	59:x:274:VAL:N	2.43	0.47
60:y:12:LYS:O	60:y:15:ASN:HB3	2.15	0.47
60:y:31:TRP:CE2	60:y:100:ARG:HD2	2.49	0.47
60:y:45:ILE:HA	80:y:401:HEM:CMC	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:y:127:ALA:O	60:y:131:TYR:N	2.42	0.47
60:y:137:GLN:NE2	60:y:260:ASN:H	2.13	0.47
61:z:31:GLN:O	61:z:34:LYS:HB3	2.15	0.47
61:z:171:PHE:CE2	61:z:177:ALA:HA	2.50	0.47
82:A2:201:UQ2:CM5	82:A2:201:UQ2:C8	2.92	0.47
64:A3:80:ASP:HA	65:B7:47:ARG:HD3	1.96	0.47
65:B7:44:VAL:HG22	65:B7:52:GLU:HG2	1.96	0.47
3:9:164:THR:N	3:9:169:PHE:O	2.29	0.47
5:4:31:SER:OG	5:4:74:PRO:HB3	2.15	0.47
5:4:95[B]:PHE:CE2	5:4:136:TRP:CD1	3.03	0.47
5:4:114:GLU:HB3	5:4:175:ASN:O	2.15	0.47
5:4:214:LEU:HD23	7:6:559:GLU:OE1	2.14	0.47
5:4:393:ILE:HD11	7:6:183:ILE:HD12	1.95	0.47
6:5:7:ASN:HA	6:5:8:ILE:HA	1.68	0.47
7:6:445:GLU:HB2	46:Y:57:GLN:NE2	2.30	0.47
7:6:536:LEU:O	7:6:539:TYR:N	2.47	0.47
10:C3:172:LYS:HB3	10:C3:176:MET:HE2	1.96	0.47
13:A7:33:LEU:HD13	13:A7:41:LYS:HG3	1.97	0.47
22:A8:1:ILE:HG23	22:A8:1:ILE:O	2.15	0.47
23:A:343:GLY:HA3	23:A:369:GLU:H	1.79	0.47
23:A:366:LEU:O	23:A:531:LYS:HG2	2.14	0.47
23:A:439:THR:HG1	23:A:440:TYR:HD2	1.63	0.47
24:B:169:TRP:HE3	24:B:347:CYS:HG	1.54	0.47
24:B:238:LEU:HD21	43:V:8:GLN:HB3	1.95	0.47
34:L:27:GLY:O	34:L:28:LEU:HB3	2.15	0.47
35:N:35:LEU:CD2	35:N:45:ARG:HG3	2.45	0.47
38:Q:81:PRO:HB2	38:Q:107:PHE:HA	1.97	0.47
39:R:167:ILE:HA	39:R:201:ILE:HG22	1.96	0.47
39:R:271:TYR:OH	39:R:325:THR:HG21	2.15	0.47
40:S:175:TYR:HA	40:S:178:VAL:HB	1.96	0.47
42:U:18:GLY:HA3	42:U:22:GLY:HA3	1.97	0.47
51:d:18:ASP:O	51:d:20:LEU:N	2.47	0.47
58:k:67:THR:OG1	58:k:119:ASN:O	2.33	0.47
58:k:261:GLY:HA2	58:k:317:THR:O	2.15	0.47
58:k:416:TYR:HB3	67:u:15:ARG:HH21	1.80	0.47
59:l:357:VAL:O	59:l:361:LYS:N	2.31	0.47
60:m:38:GLY:O	60:m:42:ILE:HG12	2.15	0.47
62:p:25:SER:O	62:p:29:SER:OG	2.25	0.47
58:w:365:LEU:O	58:w:369:LEU:HG	2.15	0.47
58:w:403:ASP:O	58:w:406:VAL:HB	2.15	0.47
59:x:50:PHE:CE2	59:x:383:GLY:HA3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:69:LEU:O	59:x:72:ALA:N	2.38	0.47
59:x:164:HIS:NE2	68:B5:64:LEU:HD22	2.30	0.47
59:x:334:GLY:O	59:x:338:LYS:HG3	2.15	0.47
2:1:118:TRP:O	2:1:122:ALA:N	2.42	0.47
2:1:171:GLN:NE2	2:1:171:GLN:C	2.72	0.47
2:1:311:THR:C	2:1:312:SER:HG	2.21	0.47
8:2:14:MET:HE2	8:2:133:TRP:CZ2	2.49	0.47
8:2:87:MET:CE	8:2:90:PHE:HZ	2.23	0.47
8:2:122:ILE:HG22	8:2:124:LEU:H	1.78	0.47
10:C3:507:GLU:O	10:C3:508:PRO:O	2.32	0.47
12:A9:164:PHE:O	12:A9:168:THR:HG23	2.14	0.47
38:Q:155:GLU:O	55:j:88:HIS:NE2	2.48	0.47
44:W:113:LEU:CB	52:f:45:ARG:HH21	2.27	0.47
44:W:140:CYS:HB3	44:W:143:GLU:CB	2.43	0.47
53:h:86:ASN:HA	53:h:89:VAL:HG12	1.96	0.47
58:k:403:ASP:O	58:k:406:VAL:HB	2.15	0.47
59:l:50:PHE:CE2	59:l:383:GLY:HA3	2.50	0.47
59:l:141:GLN:HB2	59:l:142:PRO:HD3	1.97	0.47
60:m:156:ILE:CG2	66:A4:38:TRP:NE1	2.59	0.47
61:o:7:PRO:HG3	61:o:152:TYR:CE1	2.50	0.47
62:p:41:ALA:HB2	67:u:20:PHE:CE1	2.49	0.47
58:w:67:THR:OG1	58:w:119:ASN:O	2.33	0.47
58:w:211:LEU:CA	58:w:213:GLN:HB2	2.44	0.47
58:w:280:TYR:HB2	58:w:295:ALA:HA	1.97	0.47
58:w:351:GLU:HG2	58:w:404:ALA:HB2	1.97	0.47
60:y:58:ASP:HB2	60:y:61:THR:HB	1.96	0.47
60:y:182:HIS:HE1	80:y:401:HEM:C1B	2.32	0.47
60:y:250:LEU:HD11	60:y:272:TRP:CD1	2.49	0.47
2:1:36:GLY:C	26:D:108:ARG:HB3	2.40	0.47
4:7:151:THR:O	4:7:155:ILE:HG22	2.14	0.47
5:4:139:GLN:H	5:4:222:GLU:CD	2.14	0.47
6:5:37:MET:HE3	6:5:67:ALA:HB2	1.96	0.47
6:5:96:LEU:HB3	24:B:61:TRP:CE3	2.48	0.47
8:2:33:PHE:CD1	8:2:105:LYS:HE3	2.51	0.47
8:2:255:PRO:N	8:2:256:PRO:HD2	2.30	0.47
23:A:357:LEU:HD23	23:A:358:LEU:HD12	1.97	0.47
24:B:179:ARG:O	24:B:183:HIS:CD2	2.68	0.47
24:B:297:GLY:O	24:B:298:ILE:C	2.58	0.47
27:E:116:CYS:SG	74:E:302:SF4:S2	3.13	0.47
27:E:197:TRP:O	27:E:197:TRP:CD1	2.67	0.47
39:R:163:LYS:O	39:R:165:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:T:44:LYS:HD2	41:T:45:THR:H	1.80	0.47
41:T:128:GLY:HA2	41:T:133:TRP:CE3	2.50	0.47
56:g:141:ASP:N	56:g:141:ASP:OD1	2.40	0.47
58:k:195:MET:HE1	58:k:216:PHE:HE1	1.80	0.47
58:k:405:ARG:HB3	58:k:409:GLU:CD	2.40	0.47
59:l:132:PHE:HE2	59:l:192:HIS:HA	1.80	0.47
62:p:10:PHE:HB2	64:r:18:LEU:HD11	1.96	0.47
63:q:91:GLU:N	63:q:92:PRO:HD2	2.29	0.47
65:s:35:GLU:O	65:s:39:LEU:HG	2.14	0.47
58:w:21:ASN:HD21	58:w:217:SER:H	1.62	0.47
58:w:57:TYR:CE2	58:w:168:GLU:HG2	2.50	0.47
58:w:340:GLY:O	58:w:344:ARG:HG2	2.15	0.47
58:w:438:ARG:HH21	64:A3:21:PHE:HE2	1.61	0.47
59:x:132:PHE:HE2	59:x:192:HIS:HA	1.80	0.47
59:x:304:HIS:CG	59:x:305:GLN:H	2.32	0.47
60:y:38:GLY:O	60:y:42:ILE:HG12	2.15	0.47
61:z:23:HIS:HD2	67:B6:55:ILE:HD12	1.80	0.47
61:z:204:MET:O	61:z:208:MET:N	2.30	0.47
1:3:49:LEU:CD2	2:1:126:LYS:HZ3	2.19	0.46
1:3:88:LEU:CG	2:1:309:ILE:HD12	2.45	0.46
2:1:99:ASN:O	2:1:161:THR:HB	2.15	0.46
2:1:178:ALA:C	2:1:180:PRO:HD2	2.40	0.46
4:7:125:TRP:CE3	4:7:125:TRP:HA	2.50	0.46
5:4:208:PRO:HB3	5:4:213:HIS:CB	2.42	0.46
6:5:88:ASP:N	6:5:88:ASP:OD1	2.48	0.46
7:6:15:LEU:C	7:6:18:PRO:HD2	2.40	0.46
7:6:96:VAL:O	7:6:99:SER:N	2.47	0.46
8:2:5:ILE:HG13	8:2:6:PHE:N	2.30	0.46
8:2:33:PHE:CE1	8:2:105:LYS:HE3	2.51	0.46
70:2:401:3PE:H331	70:2:401:3PE:H362	1.55	0.46
9:8:116:ASN:HD22	73:8:501:FMN:C2	2.28	0.46
9:8:418:GLN:HE21	23:A:115:GLY:CA	2.27	0.46
10:C3:484:THR:HB	22:A8:2:THR:OG1	2.15	0.46
11:C1:63:THR:O	11:C1:66:THR:HG22	2.15	0.46
13:A7:108:PRO:HG2	13:A7:111:PHE:CD2	2.50	0.46
23:A:77:MET:HG3	23:A:77:MET:O	2.15	0.46
23:A:129:PRO:HD2	31:I:114:TYR:OH	2.16	0.46
23:A:381:LEU:HD21	23:A:664:TYR:O	2.15	0.46
24:B:431:HIS:HB3	24:B:454:GLN:HB3	1.97	0.46
25:C:211:GLU:HB2	25:C:226:VAL:HG23	1.97	0.46
31:I:85:ILE:HG22	31:I:86:SER:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S:196:ASP:OD2	40:S:250:GLU:C	2.58	0.46
50:c:12:LEU:O	50:c:16:ARG:HG2	2.15	0.46
58:k:280:TYR:HB2	58:k:295:ALA:HA	1.97	0.46
59:l:270:ASN:O	59:l:274:VAL:N	2.43	0.46
60:m:163:TRP:HE3	60:m:164:ILE:HG13	1.79	0.46
62:p:91:TRP:C	62:p:93:GLY:N	2.70	0.46
67:u:52:TRP:HA	67:u:56:LYS:H	1.80	0.46
58:w:246:ASP:H	64:A3:11:ARG:HG2	1.80	0.46
58:w:256:ALA:HB2	58:w:310:PHE:HZ	1.79	0.46
59:x:303:VAL:HG12	59:x:304:HIS:N	2.29	0.46
60:y:163:TRP:HE3	60:y:164:ILE:HG13	1.79	0.46
82:A2:201:UQ2:H3M3	82:A2:201:UQ2:O2	2.15	0.46
3:9:153:GLN:HG3	3:9:158:ILE:O	2.15	0.46
3:9:179:ALA:HB2	9:8:128:ARG:NH2	2.29	0.46
5:4:368:ALA:HB1	5:4:375:LEU:HG	1.97	0.46
69:2:402:PC1:H241	69:2:402:PC1:H321	1.95	0.46
9:8:346:GLN:NE2	9:8:440:ARG:HD3	2.30	0.46
9:8:420:GLU:H	9:8:422:HIS:CD2	2.30	0.46
10:C3:172:LYS:HB2	10:C3:172:LYS:HZ3	1.79	0.46
10:C3:306:THR:HB	10:C3:359:ALA:O	2.15	0.46
23:A:131:CYS:O	23:A:134:GLY:N	2.48	0.46
24:B:420:TYR:O	24:B:421:ARG:C	2.58	0.46
26:D:82:LEU:O	26:D:83:TRP:HD1	1.98	0.46
26:D:181:ILE:HD13	26:D:200:LEU:HD13	1.96	0.46
31:I:105:LYS:O	31:I:106:GLU:HG3	2.13	0.46
36:O:126:HIS:C	36:O:128:PRO:HD3	2.40	0.46
38:Q:81:PRO:O	38:Q:84:GLU:HG2	2.15	0.46
39:R:205:GLU:O	39:R:239:PRO:HA	2.14	0.46
40:S:102:LEU:HD23	40:S:105:PHE:CE2	2.50	0.46
40:S:161:MET:O	40:S:167:ILE:HG22	2.15	0.46
47:Z:79:VAL:C	47:Z:82:ILE:H	2.23	0.46
56:g:125:CYS:HB3	56:g:128:GLU:OE1	2.16	0.46
58:k:59:VAL:HA	58:k:62:LEU:HD12	1.96	0.46
61:o:41:HIS:CE1	61:o:111:PRO:HD2	2.50	0.46
61:o:50:HIS:HE1	61:o:91:PHE:CZ	2.33	0.46
61:z:8:PRO:HD2	61:z:10:TYR:OH	2.15	0.46
62:A1:176:ALA:O	62:A1:178:LEU:N	2.48	0.46
63:A2:11:ARG:CA	82:A2:201:UQ2:H5M1	2.44	0.46
2:1:172:MET:CE	2:1:176:LEU:CB	2.93	0.46
5:4:329:LEU:HD13	5:4:359:TRP:CE3	2.51	0.46
8:2:30:TRP:CH2	8:2:67:SER:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A7:23:PRO:HB3	14:B4:70:VAL:CG2	2.45	0.46
23:A:75:CYS:SG	71:A:803:FES:S2	3.02	0.46
23:A:401:LEU:O	23:A:474:VAL:HA	2.14	0.46
23:A:405:THR:OG1	23:A:410:GLU:OE2	2.30	0.46
23:A:430:ALA:HB2	23:A:462:PHE:HZ	1.79	0.46
27:E:78:PHE:HB2	37:P:12:ARG:HG2	1.97	0.46
27:E:172:ASN:OD1	42:U:87:HIS:ND1	2.48	0.46
27:E:177:THR:HG21	27:E:182:GLU:OE2	2.15	0.46
34:L:66:VAL:HG22	38:Q:129:THR:HA	1.98	0.46
39:R:171:ASN:OD1	39:R:326:ASP:HB3	2.14	0.46
69:S:401:PC1:O14	69:S:401:PC1:H321	2.16	0.46
51:d:34:ARG:HA	51:d:35:LYS:HA	1.54	0.46
58:k:340:GLY:O	58:k:344:ARG:HG2	2.15	0.46
61:o:149:PHE:HA	61:o:156:GLN:O	2.15	0.46
59:x:276:GLN:HG3	59:x:277:HIS:N	2.30	0.46
61:z:28:ARG:HB3	61:z:171:PHE:CD1	2.51	0.46
65:B7:11:GLU:N	65:B7:12:GLU:OE1	2.49	0.46
4:7:80:PRO:O	4:7:81:GLU:CG	2.64	0.46
7:6:73:THR:O	56:g:104:ASN:ND2	2.44	0.46
8:2:26:TRP:HH2	8:2:145:ILE:HD11	1.81	0.46
13:A7:41:LYS:HD3	13:A7:62:LEU:HD23	1.97	0.46
13:A7:102:TYR:CD2	22:A8:35:TYR:HE1	2.33	0.46
23:A:246:ARG:HB2	23:A:265:THR:HG23	1.97	0.46
23:A:259:SER:CA	23:A:282:ASN:HD21	2.29	0.46
23:A:351:LEU:HD23	23:A:351:LEU:HA	1.51	0.46
25:C:95:VAL:N	25:C:97:PRO:HD2	2.29	0.46
26:D:134:ALA:HB3	26:D:135:PRO:HD3	1.98	0.46
31:I:93:ALA:O	31:I:94:LEU:HD12	2.16	0.46
35:N:42:ALA:HB2	35:N:100:TRP:CB	2.45	0.46
40:S:117:TYR:HE1	40:S:175:TYR:CD2	2.33	0.46
40:S:124:TYR:CE1	40:S:151:ILE:HD11	2.50	0.46
58:k:65:LYS:O	58:k:72:GLY:HA2	2.14	0.46
58:k:111:GLU:HG2	58:k:215:HIS:CE1	2.48	0.46
58:k:436:ARG:HE	60:m:222:PRO:CG	2.28	0.46
61:o:73:GLY:O	61:o:79:GLU:HG2	2.15	0.46
61:o:163:PRO:HG2	81:o:301:HEC:HBB2	1.98	0.46
58:w:134:ILE:O	58:w:138:LEU:N	2.38	0.46
59:x:26:PHE:CE1	59:x:391:SER:HA	2.50	0.46
59:x:435:PHE:H	59:x:438:GLU:CD	2.23	0.46
60:y:66:VAL:HA	60:y:69:ILE:HD12	1.97	0.46
62:A1:117:LEU:HA	62:A1:179:ASN:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A2:96:GLU:HA	63:A2:99:ARG:NH1	2.31	0.46
64:A3:1:GLY:O	64:A3:3:GLN:NE2	2.47	0.46
5:4:111:THR:C	5:4:113:MET:H	2.21	0.46
5:4:419:TYR:CD1	5:4:420:THR:HA	2.50	0.46
7:6:321:GLN:OE1	7:6:324:LEU:HD12	2.14	0.46
8:2:110:PRO:HD2	8:2:157:LEU:CD2	2.46	0.46
11:C1:1:MET:SD	11:C1:133:LEU:HD11	2.56	0.46
11:C1:108:TYR:N	11:C1:108:TYR:CD1	2.83	0.46
16:A6:78:LEU:HD12	16:A6:78:LEU:HA	1.75	0.46
23:A:226:CYS:SG	74:A:802:SF4:S3	3.14	0.46
23:A:495:ASN:O	23:A:499:LYS:N	2.33	0.46
24:B:261:MET:HE3	24:B:261:MET:HB3	1.64	0.46
25:C:95:VAL:HG13	25:C:96:ILE:H	1.80	0.46
36:O:45:ASN:OD1	36:O:48:HIS:NE2	2.48	0.46
38:Q:93:GLY:C	38:Q:95:GLN:H	2.22	0.46
41:T:73:THR:HB	41:T:93:GLY:HA2	1.97	0.46
43:V:48:TRP:CZ2	43:V:52:LYS:HE3	2.51	0.46
55:j:17:GLU:OE1	55:j:81:TYR:HE1	1.99	0.46
58:k:45:SER:O	58:k:48:GLU:N	2.49	0.46
58:k:309:THR:HA	58:k:322:ALA:HA	1.97	0.46
58:k:366:VAL:HG11	59:l:43:PRO:HG2	1.97	0.46
59:l:21:PRO:HD3	59:l:41:TYR:CD2	2.47	0.46
62:p:62:MET:HE2	62:p:62:MET:HB3	1.78	0.46
58:w:213:GLN:O	58:w:214:LYS:C	2.59	0.46
58:w:236:PHE:HB3	58:w:258:GLU:CD	2.41	0.46
58:w:281:ASP:HB3	58:w:284:TYR:CE1	2.50	0.46
58:w:309:THR:HA	58:w:322:ALA:HA	1.97	0.46
61:z:41:HIS:CE1	61:z:111:PRO:HD2	2.50	0.46
62:A1:13:TYR:O	64:A3:24:ARG:N	2.46	0.46
1:3:49:LEU:HD21	2:1:129:LEU:CG	2.44	0.46
8:2:67:SER:O	8:2:70:LEU:HB3	2.15	0.46
8:2:109:ALA:CB	8:2:110:PRO:HD3	2.46	0.46
8:2:169:GLY:CA	8:2:292:PHE:HE1	2.28	0.46
9:8:118:ASP:HB3	9:8:206:CYS:CB	2.46	0.46
23:A:116:VAL:O	23:A:119:PHE:N	2.37	0.46
26:D:191:GLU:C	26:D:193:LEU:N	2.72	0.46
27:E:38:TYR:CE1	37:P:104:TRP:HB2	2.50	0.46
30:H:77:HIS:ND1	30:H:77:HIS:O	2.48	0.46
37:P:33:LYS:O	37:P:34:ARG:HD3	2.15	0.46
40:S:335:VAL:HB	55:j:52:PRO:HG3	1.98	0.46
42:U:42:ASP:HA	42:U:43:LYS:HA	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:63:LEU:HD22	70:j:202:3PE:O14	2.16	0.46
56:g:48:VAL:O	56:g:51:PHE:HB3	2.16	0.46
58:k:144:SER:O	58:k:148:VAL:HG23	2.15	0.46
59:l:303:VAL:HG12	59:l:304:HIS:N	2.29	0.46
59:l:376:GLU:O	59:l:379:LEU:HB3	2.15	0.46
60:m:66:VAL:HA	60:m:69:ILE:HD12	1.97	0.46
60:m:127:ALA:O	60:m:131:TYR:N	2.42	0.46
61:o:28:ARG:HB3	61:o:171:PHE:CD1	2.51	0.46
61:o:220:TYR:CE2	61:o:224:ARG:HD2	2.51	0.46
64:r:2:ARG:NH2	64:r:6:HIS:HE1	2.13	0.46
58:w:261:GLY:HA2	58:w:317:THR:O	2.15	0.46
59:x:170:ASN:OD1	59:x:170:ASN:N	2.34	0.46
62:A1:16:PRO:HA	62:A1:19:LEU:HB3	1.97	0.46
63:A2:28:LYS:HG2	63:A2:80:TRP:CD2	2.50	0.46
1:3:18:VAL:HG11	2:1:72:ILE:HG23	1.98	0.46
1:3:68:GLU:H	1:3:68:GLU:HG2	1.57	0.46
2:1:71:PHE:C	2:1:72:ILE:HG13	2.40	0.46
4:7:150:GLY:HA2	30:H:17:TRP:CZ2	2.50	0.46
5:4:64:PRO:C	5:4:66:LEU:N	2.71	0.46
5:4:208:PRO:HG2	5:4:216:LEU:HD22	1.98	0.46
5:4:422:HIS:ND1	48:a:59:VAL:HG12	2.30	0.46
6:5:15:SER:O	6:5:16:LEU:C	2.58	0.46
70:2:401:3PE:H232	70:2:401:3PE:H262	1.62	0.46
9:8:210:THR:CG2	9:8:224:ARG:HB2	2.46	0.46
11:C1:58:ALA:O	11:C1:60:GLU:HG3	2.16	0.46
23:A:272:ARG:HH12	23:A:274:LEU:HD11	1.80	0.46
23:A:562:LYS:O	23:A:564:CYS:N	2.49	0.46
29:G:139:GLU:O	29:G:142:GLY:N	2.49	0.46
36:O:63:VAL:O	36:O:67:PHE:HD2	1.99	0.46
39:R:43:HIS:HB2	39:R:51:VAL:CG2	2.45	0.46
48:a:90:GLY:O	48:a:94:GLY:N	2.45	0.46
58:k:244:ARG:NE	64:r:10:VAL:HB	2.31	0.46
60:m:41:LEU:O	60:m:44:GLN:HB2	2.15	0.46
60:m:46:LEU:O	60:m:49:LEU:HB3	2.16	0.46
60:m:137:GLN:NE2	60:m:260:ASN:H	2.13	0.46
60:m:241:LEU:HD12	60:m:245:PHE:CD2	2.51	0.46
61:o:66:GLU:HA	61:o:84:PRO:HD2	1.98	0.46
63:q:28:LYS:HG2	63:q:80:TRP:CD2	2.50	0.46
64:r:28:HIS:HB2	64:r:32:LYS:HE2	1.98	0.46
58:w:144:SER:O	58:w:148:VAL:HG23	2.15	0.46
59:x:376:GLU:O	59:x:379:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:z:136:GLU:O	61:z:137:PRO:C	2.59	0.46
2:1:32:GLN:HB3	24:B:201:PHE:HB3	1.97	0.46
2:1:61:LEU:HD11	26:D:118:ARG:HD2	1.98	0.46
4:7:100:GLU:HA	4:7:103:MET:HB3	1.97	0.46
5:4:248:LEU:HD11	56:g:151:SER:CA	2.44	0.46
7:6:89:PHE:O	7:6:92:VAL:N	2.48	0.46
7:6:408:ALA:O	7:6:412:THR:N	2.37	0.46
7:6:489:THR:HA	7:6:492:ILE:HD12	1.96	0.46
8:2:335:MET:SD	69:Q:201:PC1:H282	2.56	0.46
9:8:52:ARG:HH22	9:8:168:ASN:ND2	2.14	0.46
9:8:93:PHE:HE2	9:8:98:LYS:HD3	1.79	0.46
10:C3:365:ILE:HD12	11:C1:87:MET:CE	2.34	0.46
10:C3:449:MET:HE3	20:B3:40:TRP:HB3	1.98	0.46
18:C2:21:ILE:HD12	18:C2:21:ILE:HA	1.82	0.46
19:B2:11:LEU:HD23	19:B2:11:LEU:O	2.15	0.46
23:A:61:PRO:HG3	23:A:146:PHE:HE2	1.76	0.46
23:A:248:THR:O	23:A:248:THR:OG1	2.28	0.46
24:B:292:MET:HG3	24:B:329:ARG:HE	1.81	0.46
27:E:89:GLU:HG2	42:U:61:TRP:HB3	1.97	0.46
27:E:172:ASN:OD1	42:U:87:HIS:CE1	2.69	0.46
30:H:65:GLU:OE2	30:H:71:LYS:HD3	2.15	0.46
35:N:80:VAL:O	35:N:83:GLN:HB2	2.15	0.46
35:N:106:GLU:HG3	35:N:107:PRO:HD2	1.96	0.46
36:O:33:ARG:HH22	44:M:44:SER:HB2	1.81	0.46
36:O:55:SER:OG	36:O:58:GLN:HG3	2.15	0.46
38:Q:89:ILE:N	38:Q:100:CYS:SG	2.88	0.46
40:S:45:SER:O	40:S:144:GLY:HA2	2.15	0.46
40:S:298:ILE:O	40:S:300:VAL:N	2.44	0.46
58:k:44:GLY:H	58:k:47:TYR:HD2	1.63	0.46
58:k:245:GLU:HG2	64:r:11:ARG:HB3	1.97	0.46
59:l:78:LYS:HE3	59:l:129:ALA:HA	1.98	0.46
59:l:276:GLN:HG3	59:l:277:HIS:N	2.30	0.46
59:l:354:ASN:N	59:l:355:PRO:HD2	2.31	0.46
60:m:272:TRP:CE2	60:m:273:TYR:HD2	2.34	0.46
58:w:44:GLY:H	58:w:47:TYR:HD2	1.63	0.46
58:w:149:VAL:HA	58:w:152:TYR:HD2	1.81	0.46
59:x:27:THR:HB	59:x:35:ILE:HG13	1.96	0.46
59:x:141:GLN:HB2	59:x:142:PRO:HD3	1.97	0.46
60:y:241:LEU:HD12	60:y:245:PHE:CD2	2.51	0.46
61:z:163:PRO:HG2	81:z:301:HEC:HBB2	1.98	0.46
65:B7:13:LEU:O	65:B7:15:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:B7:16:PRO:HB3	65:B7:76:SER:HB3	1.98	0.46
2:1:107:ALA:O	2:1:111:LEU:HD13	2.16	0.46
3:9:187:GLN:HG3	3:9:191:ASN:O	2.15	0.46
5:4:1:MET:CG	5:4:2:LEU:H	2.18	0.46
6:5:54:THR:HG21	30:H:29:ILE:HD11	1.97	0.46
7:6:101:MET:HE2	7:6:121:LEU:CD2	2.46	0.46
7:6:405:ASN:OD1	57:e:143:MET:HA	2.15	0.46
8:2:325:PHE:HE1	55:j:68:PHE:CE1	2.33	0.46
17:C0:58:ARG:HD2	17:C0:58:ARG:HA	1.74	0.46
23:A:409:PHE:CD1	23:A:694:PHE:HB2	2.51	0.46
24:B:262:LEU:O	24:B:263:THR:C	2.59	0.46
24:B:271:ARG:HD2	24:B:271:ARG:HA	1.75	0.46
27:E:106:TYR:CE1	27:E:112:ARG:NH1	2.83	0.46
38:Q:28:ALA:C	38:Q:30:HIS:H	2.24	0.46
49:b:159:LEU:HD12	49:b:161:ARG:HB2	1.96	0.46
50:c:105:PHE:O	50:c:107:GLY:N	2.40	0.46
58:k:149:VAL:HA	58:k:152:TYR:HD2	1.81	0.46
58:k:195:MET:HE1	58:k:216:PHE:CE1	2.50	0.46
58:k:436:ARG:NH2	60:m:222:PRO:HD3	2.29	0.46
60:m:263:ASN:OD1	60:m:264:THR:N	2.49	0.46
61:o:51:LEU:O	61:o:56:TYR:N	2.48	0.46
61:o:66:GLU:HA	61:o:84:PRO:CD	2.45	0.46
58:w:43:ALA:HA	58:w:47:TYR:CD2	2.51	0.46
59:x:243:GLU:OE1	59:x:436:ILE:HG23	2.16	0.46
61:z:66:GLU:HA	61:z:84:PRO:CD	2.45	0.46
63:A2:10:SER:O	82:A2:201:UQ2:H5M3	2.10	0.46
67:B6:52:TRP:HA	67:B6:56:LYS:H	1.80	0.46
2:1:73:LEU:HA	2:1:76:ILE:HD13	1.24	0.46
2:1:101:GLY:O	2:1:102:VAL:C	2.59	0.46
3:9:118:PHE:CB	9:8:220:GLN:HE21	2.22	0.46
4:7:157:THR:HG22	6:5:66:PHE:CE2	2.50	0.46
5:4:187:HIS:CD2	5:4:188:ASN:H	2.34	0.46
7:6:596:LEU:HD12	7:6:597:ILE:N	2.31	0.46
23:A:217:GLU:O	23:A:218:LEU:HB2	2.17	0.46
23:A:222:ILE:O	23:A:225:ILE:N	2.37	0.46
23:A:253:VAL:HG23	23:A:253:VAL:O	2.15	0.46
23:A:382:ARG:CG	23:A:383:SER:H	2.26	0.46
23:A:607:LYS:HE2	29:G:78:ARG:CZ	2.46	0.46
24:B:101:LEU:HA	24:B:106:VAL:O	2.16	0.46
26:D:106:MET:SD	26:D:194:LEU:HD21	2.56	0.46
27:E:54:THR:O	27:E:58:ALA:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:70:GLU:C	35:N:72:LEU:H	2.24	0.46
39:R:196:PRO:HG2	39:R:197:GLU:OE1	2.16	0.46
40:S:73:HIS:CD2	40:S:74:PHE:N	2.84	0.46
58:k:210:ASP:O	58:k:213:GLN:HB2	2.16	0.46
58:k:386:TYR:HB3	58:k:389:ARG:HD2	1.97	0.46
61:o:102:ARG:NH2	61:o:109:LEU:HD22	2.31	0.46
62:p:15:ARG:HB3	64:r:24:ARG:CG	2.46	0.46
65:s:16:PRO:HB3	65:s:76:SER:HB3	1.98	0.46
59:x:381:GLU:HA	59:x:384:SER:OG	2.16	0.46
60:y:46:LEU:O	60:y:49:LEU:HB3	2.16	0.46
60:y:263:ASN:OD1	60:y:264:THR:N	2.49	0.46
61:z:51:LEU:O	61:z:56:TYR:N	2.48	0.46
4:7:124:ASP:OD1	43:V:133:VAL:HG11	2.16	0.45
5:4:112:ALA:O	5:4:114:GLU:N	2.49	0.45
5:4:180:GLN:O	5:4:183:VAL:HG23	2.16	0.45
8:2:291:TYR:O	8:2:291:TYR:CG	2.69	0.45
9:8:390:ASP:OD2	23:A:202:ASN:HB2	2.16	0.45
11:C1:59:GLN:CA	11:C1:62:GLU:HB2	2.46	0.45
15:A5:31:TYR:HE1	15:A5:98:HIS:CE1	2.34	0.45
15:A5:98:HIS:ND1	15:A5:98:HIS:N	2.64	0.45
24:B:163:PRO:HB2	24:B:167:ALA:CB	2.45	0.45
31:I:59:ARG:HG3	42:U:125:VAL:HG21	1.98	0.45
33:K:28:PRO:HA	33:K:34:ARG:NH2	2.30	0.45
39:R:333:PRO:HB2	39:R:334:GLY:HA2	1.98	0.45
48:a:51:TYR:HA	48:a:56:ARG:NH1	2.30	0.45
52:f:136:GLU:O	52:f:139:GLN:HG2	2.16	0.45
53:h:106:VAL:HA	53:h:109:LEU:CB	2.46	0.45
59:l:52:LYS:HB2	59:l:203:ARG:HH21	1.82	0.45
59:l:69:LEU:O	59:l:72:ALA:N	2.38	0.45
61:o:8:PRO:HD2	61:o:10:TYR:OH	2.15	0.45
62:p:118:ARG:H	62:p:122:HIS:CB	2.29	0.45
63:q:107:TRP:HZ3	59:x:87:ARG:HH11	1.63	0.45
59:x:78:LYS:HE3	59:x:129:ALA:HA	1.98	0.45
60:y:71:ARG:HH21	61:z:49:ARG:HH21	1.64	0.45
60:y:313:ARG:HB2	63:A2:38:HIS:CD2	2.51	0.45
61:z:66:GLU:HA	61:z:84:PRO:HD2	1.98	0.45
2:1:6:ILE:O	2:1:8:MET:N	2.49	0.45
2:1:278:PRO:HB3	24:B:194:ILE:HG22	1.99	0.45
5:4:112:ALA:C	5:4:114:GLU:H	2.24	0.45
5:4:317:ILE:HD11	5:4:454:ILE:HG23	1.98	0.45
7:6:1:MET:HA	7:6:4:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:40:ILE:HD11	7:6:101:MET:CE	2.47	0.45
7:6:264:TYR:HA	7:6:267:THR:HG22	1.97	0.45
8:2:268:GLN:NE2	8:2:272:LYS:HE2	2.31	0.45
9:8:52:ARG:HH12	9:8:168:ASN:ND2	2.14	0.45
9:8:177:TYR:CE2	28:F:96:ARG:HB3	2.51	0.45
9:8:362:ASP:CG	9:8:449:ARG:HH22	2.25	0.45
9:8:416:SER:O	9:8:420:GLU:OE2	2.33	0.45
10:C3:299:VAL:HA	10:C3:302:ARG:NH1	2.31	0.45
10:C3:435:GLY:O	10:C3:437:PRO:HD3	2.16	0.45
23:A:272:ARG:NH1	23:A:274:LEU:HD21	2.31	0.45
24:B:378:LEU:O	24:B:380:HIS:N	2.50	0.45
27:E:65:GLU:O	27:E:66:LEU:HB3	2.16	0.45
27:E:111:GLU:O	27:E:113:CYS:N	2.49	0.45
38:Q:155:GLU:O	55:j:88:HIS:CE1	2.69	0.45
40:S:126:SER:O	40:S:129:LEU:N	2.50	0.45
43:V:80:ASP:OD1	43:V:81:ARG:N	2.49	0.45
48:a:64:ALA:HB2	57:e:106:HIS:CB	2.46	0.45
49:b:145:GLU:OE1	49:b:145:GLU:N	2.49	0.45
44:M:64:ASP:C	44:M:66:ASP:H	2.23	0.45
58:k:15:GLN:HB3	58:k:205:HIS:ND1	2.32	0.45
58:k:236:PHE:HB3	58:k:258:GLU:CD	2.41	0.45
59:l:342:ASN:HA	59:l:345:LYS:HD2	1.98	0.45
59:l:381:GLU:HA	59:l:384:SER:OG	2.16	0.45
60:m:29:SER:HA	60:m:32:ASN:ND2	2.31	0.45
61:o:203:ARG:NE	67:u:43:TYR:CE2	2.84	0.45
63:q:96:GLU:HA	63:q:99:ARG:NH1	2.31	0.45
65:s:13:LEU:O	65:s:15:ASP:N	2.49	0.45
65:s:23:GLN:O	65:s:26:GLN:HB3	2.16	0.45
58:w:128:GLU:OE2	58:w:131:ARG:NH1	2.49	0.45
59:x:52:LYS:HB2	59:x:203:ARG:HH21	1.81	0.45
59:x:276:GLN:HG3	59:x:277:HIS:H	1.81	0.45
60:y:8:HIS:HB2	60:y:9:PRO:CD	2.47	0.45
60:y:344:GLU:C	60:y:346:PRO:HD2	2.41	0.45
61:z:102:ARG:NH2	61:z:109:LEU:HD22	2.31	0.45
2:1:172:MET:CE	2:1:176:LEU:HB2	2.47	0.45
4:7:83:TRP:C	4:7:85:SER:H	2.23	0.45
5:4:2:LEU:HD23	5:4:6:ILE:HD11	1.97	0.45
5:4:177:LEU:HD21	5:4:245:ARG:HB3	1.98	0.45
7:6:127:THR:O	7:6:130:ILE:HG22	2.16	0.45
7:6:190:LEU:HD11	7:6:196:TRP:CE3	2.51	0.45
7:6:316:THR:O	7:6:321:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:548:SER:O	7:6:552:LEU:HB3	2.15	0.45
8:2:72:MET:O	8:2:76:ILE:HG12	2.16	0.45
9:8:230:PRO:O	9:8:232:ASP:N	2.49	0.45
10:C3:240:HIS:O	10:C3:243:VAL:HG22	2.16	0.45
11:C1:185:MET:SD	11:C1:185:MET:C	2.99	0.45
13:A7:66:GLU:O	14:B4:66:ARG:NH2	2.49	0.45
21:A0:35:ALA:HB3	21:A0:36:PRO:HD3	1.99	0.45
23:A:163:LYS:HZ1	23:A:207:GLY:HA3	1.80	0.45
23:A:355:LYS:HB2	23:A:530:TYR:CE1	2.50	0.45
23:A:485:ASP:HB3	23:A:680:LEU:HG	1.98	0.45
24:B:213:PHE:O	24:B:217:VAL:HG12	2.16	0.45
24:B:317:ASP:O	24:B:319:PRO:HD3	2.16	0.45
24:B:431:HIS:HB3	24:B:454:GLN:HG2	1.98	0.45
25:C:169:GLU:OE1	25:C:183:HIS:HD2	2.00	0.45
29:G:147:VAL:HG12	29:G:148:GLU:O	2.16	0.45
33:K:35:ASP:OD1	33:K:39:LYS:NZ	2.34	0.45
33:K:92:GLU:HA	33:K:95:LEU:HB3	1.98	0.45
37:P:40:LYS:HB3	43:V:7:LYS:N	2.32	0.45
46:Y:77:TRP:HA	46:Y:78:HIS:HA	1.50	0.45
49:b:61:GLY:O	49:b:65:LYS:HG2	2.16	0.45
72:b:201:CDL:H161	72:b:201:CDL:H561	1.98	0.45
58:k:43:ALA:HA	58:k:47:TYR:CD2	2.51	0.45
58:k:395:TRP:O	58:k:399:ILE:HG13	2.17	0.45
60:m:104:TYR:O	60:m:313:ARG:HG2	2.17	0.45
63:q:37:ILE:HG12	63:q:38:HIS:O	2.16	0.45
67:u:8:ARG:O	67:u:11:SER:OG	2.28	0.45
58:w:45:SER:O	58:w:48:GLU:N	2.49	0.45
58:w:156:THR:HG22	58:w:239:SER:OG	2.16	0.45
59:x:200:THR:HG21	59:x:230:LEU:HD22	1.98	0.45
61:z:127:VAL:HA	61:z:130:LEU:HB3	1.98	0.45
64:A3:2:ARG:NH2	64:A3:6:HIS:HE1	2.13	0.45
9:8:295:PRO:HD2	9:8:298:GLU:OE2	2.16	0.45
10:C3:32:ALA:HB3	21:A0:36:PRO:HG2	1.98	0.45
19:B2:2:GLU:CG	19:B2:3:ASN:H	2.30	0.45
24:B:208:GLU:O	24:B:210:MET:N	2.49	0.45
24:B:208:GLU:O	24:B:211:PHE:N	2.49	0.45
29:G:121:LEU:C	29:G:123:ASN:H	2.19	0.45
30:H:82:GLN:HE21	43:V:98:MET:H	1.64	0.45
34:L:19:LEU:HD12	34:L:20:VAL:N	2.32	0.45
35:N:77:ILE:O	35:N:80:VAL:N	2.48	0.45
39:R:195:PHE:O	39:R:195:PHE:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:136:ILE:HD11	56:g:106:ILE:HD11	1.99	0.45
55:j:118:PRO:HB2	56:g:146:LEU:O	2.17	0.45
59:l:135:TRP:NE1	59:l:136:GLU:HG3	2.32	0.45
61:o:40:CYS:HB3	61:o:110:PRO:CG	2.46	0.45
62:p:11:SER:HA	62:p:14:ARG:CD	2.47	0.45
62:p:20:ASP:HB3	62:p:23:LYS:HG2	1.98	0.45
66:t:31:GLY:HA2	66:t:34:TRP:HB3	1.98	0.45
58:w:163:LEU:HD21	58:w:314:TYR:CE2	2.52	0.45
59:x:97:SER:CA	68:B5:70:LEU:HD22	2.46	0.45
59:x:354:ASN:N	59:x:355:PRO:HD2	2.31	0.45
60:y:41:LEU:O	60:y:44:GLN:HB2	2.15	0.45
61:z:153:PHE:HD2	61:z:156:GLN:N	2.15	0.45
62:A1:2:HIS:C	62:A1:4:ASP:H	2.24	0.45
62:A1:7:VAL:HG23	64:A3:16:TYR:CD2	2.51	0.45
63:A2:52:GLU:O	63:A2:56:ASN:N	2.42	0.45
65:B7:23:GLN:O	65:B7:26:GLN:HB3	2.16	0.45
2:1:80:GLY:O	2:1:83:LEU:N	2.50	0.45
2:1:146:LEU:HD12	2:1:146:LEU:HA	1.63	0.45
3:9:134:VAL:HG11	3:9:149:LEU:HD12	1.99	0.45
3:9:215:LYS:O	3:9:217:GLY:N	2.49	0.45
4:7:17:PHE:HD1	4:7:20:PHE:CE2	2.35	0.45
5:4:431:THR:HG21	53:h:91:PHE:CZ	2.50	0.45
7:6:484:TYR:C	7:6:486:LEU:H	2.24	0.45
10:C3:495:LEU:HA	10:C3:495:LEU:HD23	1.68	0.45
11:C1:41:ILE:O	11:C1:45:MET:HG2	2.16	0.45
24:B:115:LEU:HD23	26:D:133:MET:SD	2.57	0.45
24:B:331:LEU:HA	24:B:331:LEU:HD23	1.56	0.45
33:K:15:GLY:HA3	33:K:16:LEU:HA	1.76	0.45
34:L:36:SER:HA	34:L:37:PRO:HD3	1.82	0.45
40:S:53:ASN:N	40:S:56:SER:OG	2.39	0.45
40:S:191:VAL:O	40:S:191:VAL:HG12	2.15	0.45
41:T:28:ILE:O	41:T:31:ALA:N	2.49	0.45
46:Y:73:LEU:HG	47:Z:78:PHE:CD1	2.52	0.45
58:k:246:ASP:H	64:r:11:ARG:HG2	1.81	0.45
58:k:290:LEU:O	59:l:87:ARG:NH2	2.46	0.45
59:l:46:ARG:HD3	59:l:379:LEU:HD22	1.98	0.45
61:o:47:ALA:HB3	61:o:49:ARG:HG2	1.98	0.45
65:s:59:LEU:O	65:s:63:HIS:N	2.47	0.45
58:w:15:GLN:HB3	58:w:205:HIS:ND1	2.32	0.45
58:w:293:PRO:O	58:w:296:SER:OG	2.24	0.45
58:w:395:TRP:O	58:w:399:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:135:TRP:NE1	59:x:136:GLU:HG3	2.32	0.45
60:y:29:SER:HA	60:y:32:ASN:ND2	2.31	0.45
61:z:63:ALA:O	61:z:67:GLU:HG2	2.15	0.45
62:A1:30:GLU:OE2	67:B6:10:TYR:HD2	2.00	0.45
63:A2:55:TYR:O	63:A2:59:VAL:HG23	2.17	0.45
64:A3:34:ILE:O	64:A3:38:LEU:HG	2.16	0.45
67:B6:17:THR:O	67:B6:21:ALA:N	2.42	0.45
2:1:33:LEU:CD2	37:P:24:LEU:HD22	2.46	0.45
2:1:178:ALA:O	2:1:181:LEU:N	2.49	0.45
4:7:77:GLU:H	4:7:77:GLU:CD	2.23	0.45
4:7:160:SER:O	4:7:163:ILE:HG22	2.17	0.45
6:5:57:SER:O	6:5:60:PRO:HD2	2.17	0.45
11:C1:76:ILE:O	11:C1:79:PRO:HD2	2.16	0.45
25:C:217:GLU:HB2	39:R:71:ASN:HD21	1.80	0.45
52:f:104:LEU:C	52:f:107:TRP:HE1	2.24	0.45
70:j:202:3PE:H2H2	70:j:202:3PE:H2E1	1.79	0.45
58:k:128:GLU:OE2	58:k:131:ARG:NH1	2.49	0.45
58:k:155:ALA:HA	58:k:164:ALA:HB1	1.99	0.45
58:k:156:THR:HG22	58:k:239:SER:OG	2.16	0.45
59:l:27:THR:HB	59:l:35:ILE:HG13	1.96	0.45
59:l:291:ALA:HA	59:l:297:GLN:NE2	2.32	0.45
59:l:345:LYS:O	59:l:349:GLN:HG3	2.17	0.45
60:m:125:ALA:O	60:m:128:PHE:HB3	2.17	0.45
61:o:127:VAL:HA	61:o:130:LEU:HB3	1.98	0.45
61:o:138:PRO:HG3	65:s:58:LEU:HD22	1.99	0.45
61:o:239:PRO:HB2	61:o:241:LYS:CB	2.32	0.45
63:q:104:ARG:HG2	59:x:83:PHE:CZ	2.51	0.45
68:v:65:VAL:HA	68:v:78:TYR:HA	1.98	0.45
58:w:434:TYR:O	58:w:437:ILE:N	2.49	0.45
60:y:272:TRP:CE2	60:y:273:TYR:HD2	2.34	0.45
61:z:220:TYR:CE2	61:z:224:ARG:HD2	2.51	0.45
64:A3:8:THR:HG22	64:A3:9:ARG:N	2.31	0.45
64:A3:38:LEU:O	64:A3:41:THR:OG1	2.22	0.45
4:7:80:PRO:C	4:7:81:GLU:HG3	2.42	0.45
4:7:98:LEU:O	4:7:102:PHE:N	2.39	0.45
5:4:315:LEU:HA	5:4:315:LEU:HD23	1.78	0.45
7:6:68:TRP:CD1	7:6:76:LEU:HD11	2.51	0.45
8:2:152:ASN:O	8:2:156:THR:OG1	2.29	0.45
11:C1:60:GLU:CD	11:C1:61:VAL:H	2.24	0.45
16:A6:42:ARG:HG3	16:A6:42:ARG:NH1	2.32	0.45
24:B:173:LEU:HD11	24:B:244:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:160:GLY:O	26:D:161:GLY:C	2.60	0.45
72:J:101:CDL:H161	37:P:7:PHE:CG	2.52	0.45
79:R:601:NAP:H8A	79:R:601:NAP:H2B	1.88	0.45
40:S:167:ILE:HD11	40:S:171:CYS:HB2	1.98	0.45
40:S:236:GLU:HA	40:S:239:GLU:CB	2.46	0.45
52:f:28:GLU:HA	52:f:31:CYS:SG	2.56	0.45
56:g:174:ALA:HA	56:g:175:ALA:HA	1.68	0.45
44:M:35:HIS:HB3	44:M:38:LYS:HZ3	1.81	0.45
58:k:281:ASP:HB3	58:k:284:TYR:CE1	2.51	0.45
58:k:405:ARG:HG2	58:k:408:ARG:HH21	1.82	0.45
59:l:90:GLU:O	59:l:93:GLY:N	2.49	0.45
60:m:23:ALA:HB3	60:m:224:TYR:HE2	1.82	0.45
60:m:223:TYR:O	60:m:226:ILE:N	2.49	0.45
60:m:319:PRO:HB3	64:r:47:ARG:CZ	2.47	0.45
61:o:52:VAL:HG13	67:u:56:LYS:HD2	1.99	0.45
59:x:90:GLU:O	59:x:93:GLY:N	2.49	0.45
59:x:168:TYR:HE2	59:x:321:LEU:HD11	1.82	0.45
59:x:258:VAL:HG13	59:x:322:PHE:O	2.17	0.45
59:x:342:ASN:HA	59:x:345:LYS:HD2	1.98	0.45
61:z:40:CYS:HB3	61:z:110:PRO:CG	2.46	0.45
62:A1:15:ARG:HH21	62:A1:32:ARG:HG2	1.81	0.45
65:B7:65:ARG:O	65:B7:69:VAL:HG23	2.17	0.45
1:3:9:THR:O	1:3:12:THR:HG22	2.17	0.45
3:9:71:PRO:HB3	28:F:102:SER:HB3	1.99	0.45
4:7:83:TRP:C	4:7:85:SER:N	2.73	0.45
5:4:5:ILE:HA	5:4:8:THR:HG22	1.99	0.45
5:4:96:ILE:O	5:4:100:ILE:HG13	2.17	0.45
11:C1:98:LYS:HB2	11:C1:98:LYS:HE3	1.80	0.45
23:A:175:ARG:O	23:A:176:CYS:C	2.59	0.45
23:A:360:ARG:HB3	23:A:632:MET:SD	2.57	0.45
70:B:501:3PE:H341	27:E:61:LEU:HD12	1.99	0.45
25:C:57:HIS:CE1	25:C:80:VAL:HG11	2.51	0.45
25:C:70:ILE:HG13	25:C:71:LEU:CD1	2.47	0.45
25:C:167:TRP:O	25:C:169:GLU:N	2.50	0.45
26:D:107:ASP:C	26:D:109:PHE:H	2.25	0.45
28:F:92:LEU:O	28:F:96:ARG:HB2	2.17	0.45
30:H:28:LYS:HB3	49:b:184:LYS:HA	1.99	0.45
40:S:53:ASN:H	40:S:56:SER:HG	1.63	0.45
40:S:72:LYS:HE3	40:S:74:PHE:CE1	2.51	0.45
42:U:64:TYR:HE1	42:U:81:MET:HB2	1.81	0.45
43:V:71:LEU:C	43:V:73:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Y:70:PHE:O	46:Y:73:LEU:HB2	2.16	0.45
44:M:56:ASP:OD1	44:M:56:ASP:N	2.48	0.45
58:k:434:TYR:O	58:k:437:ILE:N	2.49	0.45
59:l:315:SER:HA	59:l:320:GLY:CA	2.39	0.45
60:m:78:ILE:HG13	60:m:79:ILE:N	2.32	0.45
61:o:91:PHE:HA	61:o:92:PRO:HD3	1.89	0.45
61:o:215:LEU:HA	61:o:218:LEU:HD12	1.99	0.45
65:s:65:ARG:O	65:s:69:VAL:HG23	2.17	0.45
66:t:16:ASN:C	66:t:18:VAL:H	2.25	0.45
67:u:57:HIS:HA	67:u:60:GLU:CD	2.42	0.45
59:x:37:SER:C	59:x:38:LEU:HD12	2.42	0.45
59:x:46:ARG:HD3	59:x:379:LEU:HD22	1.98	0.45
59:x:291:ALA:HA	59:x:297:GLN:NE2	2.32	0.45
60:y:272:TRP:O	60:y:275:LEU:N	2.38	0.45
5:4:62:SER:HB3	5:4:457:PRO:HD3	1.99	0.45
7:6:295:GLN:O	7:6:301:ILE:HD11	2.17	0.45
9:8:177:TYR:CD1	9:8:182:ILE:HB	2.46	0.45
9:8:183:GLY:HA2	9:8:184:LYS:HA	1.62	0.45
9:8:207:GLY:HA2	73:8:501:FMN:C7	2.47	0.45
10:C3:158:ILE:O	10:C3:162:ILE:HG13	2.17	0.45
23:A:360:ARG:HD2	23:A:632:MET:SD	2.57	0.45
24:B:258:LEU:HD23	24:B:258:LEU:HA	1.78	0.45
24:B:272:THR:HG23	24:B:326:CYS:HB2	1.98	0.45
25:C:67:VAL:O	25:C:67:VAL:HG12	2.16	0.45
27:E:37:THR:N	37:P:104:TRP:HD1	2.14	0.45
27:E:74:LEU:HA	27:E:74:LEU:HD12	1.61	0.45
30:H:82:GLN:HE21	43:V:98:MET:HB2	1.80	0.45
39:R:201:ILE:HG23	39:R:203:PRO:HD3	1.98	0.45
48:a:108:ASP:O	48:a:109:ARG:HB3	2.17	0.45
49:b:96:ALA:HA	49:b:97:GLU:HA	1.66	0.45
58:k:443:TRP:CD2	58:k:446:PHE:OXT	2.70	0.45
59:l:37:SER:C	59:l:38:LEU:HD12	2.42	0.45
59:l:276:GLN:HG3	59:l:277:HIS:H	1.81	0.45
59:l:408:ALA:HA	59:l:411:ILE:HB	1.99	0.45
61:o:153:PHE:HD2	61:o:156:GLN:N	2.15	0.45
62:p:71:MET:HG3	62:p:72:SER:N	2.31	0.45
63:q:35:ASP:OD1	63:q:58:ARG:NE	2.50	0.45
63:q:40:ASN:O	63:q:44:LYS:HG2	2.17	0.45
63:q:55:TYR:O	63:q:59:VAL:HG23	2.17	0.45
60:y:223:TYR:O	60:y:226:ILE:N	2.49	0.45
60:y:377:LEU:HD23	63:A2:33:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A2:37:ILE:HG12	63:A2:38:HIS:O	2.16	0.45
64:A3:28:HIS:HB2	64:A3:32:LYS:HE2	1.98	0.45
65:B7:27:LEU:O	65:B7:30:CYS:HB2	2.17	0.45
1:3:23:TRP:CZ2	1:3:27:LEU:HD22	2.52	0.45
1:3:99:ALA:HB1	69:3:200:PC1:H291	1.99	0.45
2:1:184:MET:HE2	2:1:293:PHE:CD1	2.51	0.45
2:1:283:ASP:OD2	24:B:443:MET:SD	2.75	0.45
3:9:238:PRO:HG2	3:9:241:PRO:CG	2.47	0.45
5:4:52:PHE:HZ	5:4:58:SER:OG	2.00	0.45
5:4:62:SER:HB3	5:4:457:PRO:CD	2.47	0.45
7:6:460:GLY:O	7:6:464:ALA:HB2	2.17	0.45
76:C3:603:HEA:O11	76:C3:603:HEA:HHC	2.17	0.45
14:B4:78:HIS:CE1	18:C2:12:LEU:HD22	2.52	0.45
15:A5:33:ILE:HG22	15:A5:34:LEU:HD12	1.98	0.45
15:A5:40:SER:OG	15:A5:45:ASP:HB3	2.16	0.45
24:B:94:VAL:CG2	26:D:89:LEU:HG	2.45	0.45
26:D:172:GLY:C	26:D:174:ASP:H	2.24	0.45
26:D:195:TYR:O	26:D:195:TYR:CG	2.69	0.45
27:E:196:LYS:HD2	27:E:197:TRP:CZ3	2.52	0.45
35:N:24:LEU:O	35:N:27:LEU:N	2.49	0.45
40:S:67:GLU:HA	40:S:68:LYS:C	2.42	0.45
50:c:83:HIS:HE1	50:c:87:LYS:HB2	1.80	0.45
51:d:25:PHE:HE1	51:d:43:GLN:HB3	1.82	0.45
53:h:113:ARG:O	53:h:114:MET:C	2.60	0.45
57:e:39:GLY:HA3	57:e:40:PRO:HA	1.64	0.45
44:M:64:ASP:CG	44:M:65:ILE:H	2.25	0.45
59:l:243:GLU:OE1	59:l:436:ILE:HG23	2.16	0.45
61:o:148:TYR:O	61:o:158:ILE:HG22	2.17	0.45
64:r:8:THR:HG22	64:r:9:ARG:N	2.32	0.45
59:x:378:PHE:O	59:x:382:VAL:HG23	2.17	0.45
60:y:104:TYR:O	60:y:313:ARG:HG2	2.17	0.45
60:y:125:ALA:O	60:y:128:PHE:HB3	2.17	0.45
60:y:345:HIS:ND1	60:y:346:PRO:HD3	2.32	0.45
61:z:62:LYS:HA	61:z:87:LEU:HD11	1.98	0.45
65:B7:44:VAL:HG22	65:B7:52:GLU:CD	2.42	0.45
67:B6:8:ARG:O	67:B6:11:SER:OG	2.28	0.45
1:3:11:PHE:CE2	70:1:401:3PE:H3C2	2.51	0.44
2:1:19:PHE:CG	32:J:11:VAL:HG11	2.52	0.44
4:7:126:VAL:HG13	43:V:122:GLY:HA3	1.99	0.44
5:4:143:LEU:HA	5:4:143:LEU:HD23	1.69	0.44
5:4:151:PHE:O	5:4:155:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:189:PHE:O	7:6:193:LEU:N	2.49	0.44
7:6:362:LEU:HD12	7:6:363:PHE:HB2	1.98	0.44
11:C1:121:TYR:C	11:C1:138:VAL:HG23	2.42	0.44
12:A9:42:LEU:HD12	12:A9:42:LEU:HA	1.66	0.44
16:A6:3:ALA:O	16:A6:4:ALA:HB2	2.17	0.44
23:A:117:MET:SD	23:A:143:SER:HB2	2.56	0.44
24:B:80:LEU:HD23	24:B:81:THR:H	1.81	0.44
31:I:111:THR:HG22	31:I:119:PHE:HB3	1.98	0.44
36:O:95:LYS:HB2	36:O:95:LYS:HE3	1.72	0.44
38:Q:106:GLN:OE1	38:Q:106:GLN:N	2.42	0.44
39:R:70:VAL:HG13	39:R:80:VAL:HG11	1.97	0.44
40:S:128:LEU:HD11	40:S:186:TYR:OH	2.17	0.44
40:S:158:LEU:HA	40:S:161:MET:HE2	1.98	0.44
44:W:85:TYR:CE2	47:Z:51:TRP:HZ3	2.35	0.44
53:h:69:LYS:O	53:h:70:ASN:ND2	2.50	0.44
44:M:44:SER:O	44:M:48:VAL:HG23	2.17	0.44
44:M:57:GLU:C	44:M:59:GLY:H	2.25	0.44
60:m:206:ASN:CG	60:m:207:ASN:H	2.25	0.44
58:w:386:TYR:HB3	58:w:389:ARG:HD2	1.97	0.44
59:x:240:HIS:CD2	59:x:421:ARG:HH22	2.36	0.44
59:x:408:ALA:HA	59:x:411:ILE:HB	1.99	0.44
60:y:23:ALA:HB3	60:y:224:TYR:HE2	1.82	0.44
60:y:78:ILE:HG13	60:y:79:ILE:N	2.32	0.44
60:y:347:TYR:HA	60:y:350:ILE:HD12	1.99	0.44
61:z:148:TYR:O	61:z:158:ILE:HG22	2.18	0.44
61:z:166:ASN:HA	61:z:179:MET:N	2.32	0.44
63:A2:16:ILE:HG22	63:A2:19:TRP:HE3	1.78	0.44
63:A2:28:LYS:CB	63:A2:74:ILE:HD11	2.47	0.44
63:A2:40:ASN:O	63:A2:44:LYS:HG2	2.17	0.44
3:9:155:LYS:NZ	3:9:205:ILE:HG21	2.31	0.44
4:7:113:VAL:HA	4:7:114:GLU:HA	1.62	0.44
7:6:230:HIS:O	7:6:232:TRP:N	2.49	0.44
7:6:353:GLU:CD	7:6:358:LYS:HB2	2.43	0.44
7:6:353:GLU:OE1	7:6:358:LYS:HB2	2.17	0.44
8:2:84:TRP:HB2	8:2:85:THR:H	1.59	0.44
9:8:326:LEU:HD11	9:8:363:ILE:HG21	1.98	0.44
23:A:639:LEU:HD21	23:A:643:ARG:NE	2.32	0.44
70:B:501:3PE:H3D1	43:V:40:ILE:HD11	1.99	0.44
35:N:56:LEU:HD12	35:N:59:VAL:HB	1.98	0.44
36:O:25:MET:HB3	36:O:29:LYS:HZ1	1.82	0.44
37:P:52:ASN:HB3	37:P:57:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:43:HIS:H	39:R:51:VAL:HG23	1.82	0.44
39:R:339:GLY:HA3	39:R:340:VAL:HA	1.65	0.44
42:U:29:ARG:NH2	42:U:61:TRP:HZ3	2.14	0.44
46:Y:47:TYR:O	47:Z:51:TRP:NE1	2.50	0.44
49:b:100:GLU:CB	49:b:101:ILE:HA	2.47	0.44
59:l:200:THR:HG1	59:l:228:GLY:H	1.60	0.44
64:r:34:ILE:O	64:r:38:LEU:HG	2.16	0.44
65:s:36:ARG:HA	65:s:39:LEU:HB2	1.98	0.44
59:x:70:ARG:NH1	68:B5:67:SER:HB3	2.33	0.44
59:x:345:LYS:O	59:x:349:GLN:HG3	2.17	0.44
63:A2:35:ASP:OD1	63:A2:58:ARG:NE	2.50	0.44
1:3:106:TRP:HH2	69:3:200:PC1:O11	2.01	0.44
69:3:200:PC1:H341	34:L:23:PHE:HD2	1.82	0.44
2:1:63:PRO:HG3	2:1:214:GLU:CD	2.43	0.44
3:9:183:ALA:HB1	3:9:184:PRO:HD2	2.00	0.44
5:4:2:LEU:HA	5:4:5:ILE:HG12	1.98	0.44
7:6:207:SER:OG	7:6:208:ASP:N	2.50	0.44
7:6:264:TYR:CD2	7:6:265:PRO:HD3	2.52	0.44
9:8:178:GLU:HG2	28:F:96:ARG:NH1	2.33	0.44
11:C1:1:MET:SD	11:C1:133:LEU:HD13	2.58	0.44
11:C1:122:MET:HB2	11:C1:208:PRO:CD	2.47	0.44
19:B2:30:ILE:HG13	19:B2:31:LEU:N	2.32	0.44
23:A:330:LEU:HA	23:A:544:MET:HE1	2.00	0.44
24:B:340:SER:O	24:B:343:ILE:N	2.50	0.44
24:B:427:PRO:HB3	24:B:431:HIS:ND1	2.33	0.44
36:O:47:VAL:HG11	36:O:56:VAL:HG22	1.98	0.44
39:R:92:MET:C	39:R:94:LEU:N	2.76	0.44
39:R:203:PRO:HB3	39:R:265:PHE:CD2	2.47	0.44
43:V:23:ARG:HH12	43:V:25:LEU:H	1.66	0.44
44:M:12:LYS:NZ	44:M:77:VAL:HG21	2.33	0.44
44:M:64:ASP:OD1	44:M:65:ILE:N	2.45	0.44
59:l:258:VAL:HG13	59:l:322:PHE:O	2.17	0.44
60:m:347:TYR:HA	60:m:350:ILE:HB	1.99	0.44
61:o:47:ALA:HB2	61:o:90:TYR:CE1	2.52	0.44
63:q:28:LYS:CB	63:q:74:ILE:HD11	2.47	0.44
59:x:167:ALA:O	59:x:240:HIS:N	2.51	0.44
59:x:228:GLY:O	59:x:230:LEU:N	2.50	0.44
60:y:206:ASN:CG	60:y:207:ASN:H	2.25	0.44
61:z:47:ALA:HB3	61:z:49:ARG:HG2	1.98	0.44
61:z:113:LEU:HD11	81:z:301:HEC:HHB	1.99	0.44
65:B7:36:ARG:HA	65:B7:39:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:A4:15:ARG:O	66:A4:17:TRP:N	2.51	0.44
1:3:87:MET:O	1:3:91:ALA:N	2.25	0.44
3:9:87:GLN:NE2	3:9:123:ASN:OD1	2.50	0.44
7:6:27:TYR:HD1	7:6:28:LYS:O	1.99	0.44
7:6:441:VAL:HG12	7:6:443:ILE:HG23	2.00	0.44
8:2:67:SER:O	8:2:70:LEU:N	2.51	0.44
8:2:84:TRP:HD1	30:H:19:THR:O	2.00	0.44
8:2:234:TRP:HE1	8:2:303:THR:CB	2.29	0.44
8:2:335:MET:O	38:Q:170:TRP:HH2	1.99	0.44
9:8:186:ALA:HA	9:8:187:CYS:HA	1.41	0.44
9:8:399:PHE:HE2	9:8:412:LEU:HD13	1.83	0.44
23:A:171:THR:HG23	23:A:173:MET:HE2	1.99	0.44
23:A:286:ILE:HG23	23:A:287:SER:O	2.18	0.44
24:B:221:ARG:HD3	24:B:221:ARG:HA	1.60	0.44
24:B:379:ILE:HD13	24:B:379:ILE:HG21	1.69	0.44
25:C:210:VAL:HG23	25:C:210:VAL:O	2.17	0.44
25:C:214:TYR:OH	26:D:138:ARG:NH2	2.32	0.44
27:E:106:TYR:C	27:E:107:PRO:O	2.59	0.44
30:H:91:LYS:HB3	30:H:93:THR:HG23	1.98	0.44
34:L:78:LEU:HD11	38:Q:122:LEU:HB3	2.00	0.44
40:S:68:LYS:HB3	40:S:69:LEU:HD12	1.99	0.44
49:b:133:TYR:CE1	56:g:86:PHE:HE2	2.35	0.44
52:f:166:LEU:HA	52:f:167:TRP:HA	1.47	0.44
44:M:14:ARG:HA	44:M:17:TYR:HE2	1.82	0.44
58:k:206:ARG:O	58:k:209:LEU:N	2.49	0.44
59:l:247:GLN:OE1	59:l:430:LEU:HB2	2.17	0.44
60:m:347:TYR:HA	60:m:350:ILE:HD12	2.00	0.44
61:o:62:LYS:HA	61:o:87:LEU:HD11	1.98	0.44
61:o:191:ARG:NH2	61:o:195:GLU:OE1	2.51	0.44
58:w:394:GLU:HG2	58:w:398:ARG:HG3	2.00	0.44
58:w:395:TRP:O	58:w:398:ARG:HB2	2.18	0.44
61:z:75:ASN:ND2	61:z:79:GLU:OE1	2.50	0.44
61:z:191:ARG:NE	61:z:195:GLU:OE2	2.50	0.44
2:1:71:PHE:O	2:1:72:ILE:HG13	2.17	0.44
5:4:268:GLY:HA2	5:4:271:MET:HB3	1.99	0.44
7:6:177:ILE:O	7:6:180:ILE:HG22	2.17	0.44
7:6:340:PHE:O	7:6:343:SER:N	2.51	0.44
8:2:3:PRO:HG3	40:S:31:TYR:CD2	2.53	0.44
9:8:46:TYR:HE2	9:8:51:TRP:HE1	1.65	0.44
9:8:128:ARG:O	9:8:132:ARG:HB2	2.18	0.44
73:8:501:FMN:H1'1	73:8:501:FMN:H9	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C3:379:TYR:CE2	10:C3:383:MET:HE2	2.53	0.44
13:A7:79:LYS:NZ	20:B3:15:ASN:HD21	2.15	0.44
14:B4:70:VAL:HG12	14:B4:71:VAL:N	2.31	0.44
20:B3:9:PHE:HD1	20:B3:10:HIS:HD2	1.63	0.44
23:A:76:ARG:HD3	23:A:76:ARG:HA	1.71	0.44
23:A:126:LEU:HD12	23:A:126:LEU:N	2.32	0.44
23:A:140:GLN:HG3	24:B:379:ILE:HG23	1.98	0.44
23:A:382:ARG:HH22	23:A:652:ASN:ND2	2.13	0.44
23:A:591:GLU:HG3	23:A:610:VAL:O	2.18	0.44
25:C:179:PHE:CE1	36:O:84:ILE:HD13	2.53	0.44
27:E:133:GLU:CG	27:E:134:PRO:HD2	2.47	0.44
27:E:211:TYR:CZ	37:P:39:PRO:HG3	2.53	0.44
30:H:2:PRO:HG2	30:H:4:PHE:HE1	1.83	0.44
38:Q:28:ALA:C	38:Q:30:HIS:N	2.76	0.44
39:R:199:THR:OG1	39:R:259:ARG:HA	2.17	0.44
41:T:62:THR:HG21	41:T:104:ARG:HD3	1.95	0.44
51:d:25:PHE:CE2	51:d:41:ALA:O	2.70	0.44
52:f:55:LYS:CB	52:f:59:LYS:HB3	2.48	0.44
55:j:118:PRO:HB2	56:g:146:LEU:C	2.43	0.44
58:k:373:THR:O	58:k:377:GLU:N	2.50	0.44
59:l:312:PHE:HA	68:v:61:GLY:HA3	1.97	0.44
59:l:352:LEU:HD21	59:l:354:ASN:HD21	1.82	0.44
59:l:378:PHE:O	59:l:382:VAL:HG23	2.17	0.44
60:m:83:HIS:HE1	80:m:401:HEM:C1C	2.35	0.44
61:o:24:THR:OG1	67:u:58:LYS:NZ	2.37	0.44
61:o:76:GLU:C	61:o:78:GLY:H	2.26	0.44
61:o:113:LEU:HD11	81:o:301:HEC:HHB	1.99	0.44
61:o:191:ARG:NE	61:o:195:GLU:OE2	2.50	0.44
60:y:50:PHE:O	60:y:53:MET:HB2	2.17	0.44
60:y:347:TYR:HA	60:y:350:ILE:HB	1.99	0.44
2:1:1:MET:HB2	2:1:4:ILE:HG22	2.00	0.44
2:1:248:ASN:O	2:1:250:HIS:N	2.49	0.44
8:2:78:LEU:HD23	8:2:78:LEU:O	2.18	0.44
10:C3:51:ASP:O	10:C3:55:ASN:HB2	2.17	0.44
10:C3:70:VAL:HG11	10:C3:246:LEU:HD22	2.00	0.44
19:B2:3:ASN:ND2	19:B2:5:VAL:HG13	2.33	0.44
24:B:152:SER:OG	24:B:228:ARG:O	2.22	0.44
24:B:266:ARG:HE	24:B:266:ARG:HB2	1.52	0.44
24:B:404:LYS:CE	24:B:455:ASP:OD2	2.66	0.44
24:B:429:PHE:HD1	24:B:429:PHE:HA	1.59	0.44
35:N:114:TRP:C	35:N:116:ILE:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Q:109:GLU:CG	38:Q:110:CYS:H	2.29	0.44
46:Y:41:ALA:O	46:Y:43:ILE:N	2.51	0.44
50:c:95:TYR:CE2	56:g:10:TYR:HB3	2.52	0.44
56:g:82:VAL:O	56:g:86:PHE:N	2.51	0.44
57:e:88:PRO:HD2	57:e:114:ARG:HG3	1.99	0.44
58:k:163:LEU:HD21	58:k:314:TYR:CE2	2.52	0.44
58:k:394:GLU:HG2	58:k:398:ARG:HG3	2.00	0.44
59:l:338:LYS:O	59:l:342:ASN:N	2.26	0.44
60:m:8:HIS:HB2	60:m:9:PRO:CD	2.47	0.44
62:p:45:VAL:HG13	67:u:28:ALA:HB2	1.99	0.44
58:w:290:LEU:O	59:x:87:ARG:NH2	2.41	0.44
58:w:319:LEU:HA	58:w:319:LEU:HD23	1.71	0.44
59:x:325:TYR:H	68:B5:57:GLY:N	2.16	0.44
61:z:21:LEU:HD13	61:z:192:TRP:HB2	1.99	0.44
61:z:191:ARG:NH2	61:z:195:GLU:OE1	2.51	0.44
61:z:215:LEU:HA	61:z:218:LEU:HD12	1.99	0.44
63:A2:84:GLU:OE1	63:A2:84:GLU:N	2.38	0.44
65:B7:10:GLU:OE1	65:B7:12:GLU:N	2.50	0.44
65:B7:59:LEU:O	65:B7:63:HIS:N	2.48	0.44
67:B6:57:HIS:HA	67:B6:60:GLU:CD	2.42	0.44
5:4:314:ALA:O	5:4:318:ALA:HB2	2.17	0.44
5:4:317:ILE:HD11	5:4:454:ILE:CG2	2.47	0.44
6:5:49:LEU:HA	6:5:49:LEU:HD12	1.68	0.44
7:6:606:GLU:N	7:6:606:GLU:OE1	2.50	0.44
8:2:112:HIS:CD2	8:2:112:HIS:H	2.36	0.44
8:2:245:LEU:HD22	8:2:301:THR:HG21	2.00	0.44
9:8:48:ARG:HG3	9:8:133:HIS:NE2	2.33	0.44
9:8:52:ARG:HH12	9:8:168:ASN:HD21	1.66	0.44
17:C0:57:ARG:HB3	17:C0:57:ARG:NH1	2.31	0.44
24:B:293:LEU:O	24:B:294:ARG:C	2.59	0.44
24:B:421:ARG:HH21	24:B:423:LYS:HD3	1.83	0.44
37:P:19:ASP:O	37:P:21:GLN:N	2.51	0.44
38:Q:69:GLU:O	38:Q:73:GLN:N	2.42	0.44
40:S:75:PRO:O	40:S:130:GLN:NE2	2.50	0.44
40:S:100:CYS:CB	40:S:119:LEU:HB2	2.48	0.44
40:S:235:PRO:O	40:S:239:GLU:N	2.51	0.44
53:h:125:LEU:HG	53:h:129:ARG:HH12	1.82	0.44
44:M:36:PHE:N	44:M:39:ASP:HB3	2.33	0.44
44:M:52:MET:HA	44:M:55:GLU:OE1	2.18	0.44
58:k:296:SER:O	58:k:300:THR:OG1	2.27	0.44
60:m:6:LYS:O	60:m:12:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:m:331:ASP:OD1	60:m:357:LEU:HD23	2.18	0.44
62:p:18:VAL:HG11	62:p:32:ARG:HH11	1.80	0.44
62:p:60:SER:HA	62:p:63:SER:OG	2.16	0.44
62:p:145:VAL:HA	62:p:156:TYR:CB	2.48	0.44
63:q:27:ASN:OD1	63:q:81:THR:HB	2.18	0.44
65:s:44:VAL:HG22	65:s:52:GLU:CD	2.42	0.44
59:x:261:SER:H	59:x:321:LEU:HA	1.83	0.44
60:y:331:ASP:OD1	60:y:357:LEU:HD23	2.18	0.44
61:z:76:GLU:C	61:z:78:GLY:H	2.26	0.44
2:1:107:ALA:C	2:1:108:MET:HE2	2.43	0.44
2:1:200:LEU:HD12	2:1:206:GLU:HG2	2.00	0.44
2:1:278:PRO:HB2	24:B:194:ILE:HG22	2.00	0.44
4:7:136:PHE:C	4:7:138:GLU:N	2.75	0.44
4:7:152:TRP:CD1	30:H:14:LEU:HB3	2.53	0.44
5:4:30:HIS:O	5:4:33:LEU:N	2.51	0.44
5:4:379:LEU:HD23	5:4:379:LEU:HA	1.84	0.44
7:6:350:LEU:O	7:6:350:LEU:HD23	2.18	0.44
7:6:593:ILE:HD13	41:T:38:ALA:HB1	1.99	0.44
8:2:320:MET:O	8:2:321:LYS:C	2.60	0.44
69:2:402:PC1:H292	69:2:402:PC1:H261	1.60	0.44
9:8:203:ALA:HB1	9:8:205:ILE:H	1.81	0.44
10:C3:147:ILE:HD11	10:C3:209:LEU:HD23	1.98	0.44
12:A9:137:LEU:HD12	12:A9:137:LEU:HA	1.69	0.44
18:C2:19:PHE:C	18:C2:19:PHE:CD1	2.94	0.44
18:C2:42:LYS:HE2	18:C2:42:LYS:HB3	1.83	0.44
23:A:308:ARG:NH2	42:U:144:TYR:HE1	2.16	0.44
23:A:643:ARG:HG2	23:A:646:LEU:HD12	1.99	0.44
39:R:60:GLY:HA3	39:R:129:LEU:HD11	1.99	0.44
39:R:156:SER:O	39:R:161:VAL:HG22	2.17	0.44
39:R:238:GLN:NE2	39:R:271:TYR:HA	2.33	0.44
39:R:249:ILE:O	39:R:252:ALA:N	2.51	0.44
44:W:109:GLY:HA2	44:W:110:LEU:HA	1.75	0.44
44:W:136:GLU:OE1	44:W:136:GLU:N	2.49	0.44
45:X:34:LEU:HD22	49:b:139:ILE:HG22	1.99	0.44
50:c:36:PRO:HG2	50:c:37:PRO:O	2.18	0.44
59:l:167:ALA:O	59:l:240:HIS:N	2.51	0.44
60:m:51:LEU:HD11	60:m:83:HIS:CG	2.53	0.44
60:m:335:LEU:HA	60:m:338:ILE:HB	2.00	0.44
65:s:27:LEU:O	65:s:30:CYS:HB2	2.17	0.44
58:w:155:ALA:HA	58:w:164:ALA:HB1	1.99	0.44
58:w:263:ALA:HA	58:w:386:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:43:PRO:O	59:x:113:ARG:N	2.51	0.44
59:x:247:GLN:OE1	59:x:430:LEU:HB2	2.18	0.44
60:y:51:LEU:HD11	60:y:83:HIS:CG	2.53	0.44
63:A2:102:LYS:HA	63:A2:105:GLU:OE1	2.18	0.44
2:1:150:LEU:O	2:1:154:LEU:HD13	2.18	0.44
2:1:210:GLY:C	2:1:212:ASN:H	2.26	0.44
4:7:125:TRP:HH2	6:5:4:VAL:HG23	1.83	0.44
5:4:108:MET:HB3	5:4:121:LEU:HD13	1.99	0.44
5:4:121:LEU:HA	5:4:124:ALA:CB	2.48	0.44
9:8:318:ILE:HG22	9:8:320:GLY:O	2.18	0.44
9:8:451:GLN:HA	9:8:454:ALA:HB3	1.99	0.44
9:8:451:GLN:O	9:8:455:GLN:HG2	2.18	0.44
12:A9:223:LEU:HA	12:A9:223:LEU:HD23	1.79	0.44
19:B2:36:MET:O	19:B2:40:LEU:HG	2.18	0.44
23:A:63:PHE:HB2	23:A:75:CYS:HB2	2.00	0.44
23:A:81:GLU:HG3	23:A:108:LYS:HD3	2.00	0.44
23:A:619:ASP:O	23:A:622:ILE:HG22	2.17	0.44
24:B:363:VAL:O	24:B:363:VAL:HG12	2.18	0.44
33:K:59:SER:O	33:K:61:VAL:N	2.51	0.44
33:K:94:VAL:O	33:K:97:SER:OG	2.27	0.44
38:Q:132:LYS:HE3	38:Q:134:ASP:CG	2.42	0.44
40:S:206:ILE:HD11	40:S:214:GLU:CB	2.47	0.44
45:X:38:ARG:HA	45:X:56:TRP:HZ3	1.83	0.44
46:Y:66:ALA:HB2	47:Z:73:TRP:CD2	2.53	0.44
48:a:47:TYR:O	48:a:50:GLN:HB3	2.17	0.44
50:c:32:GLU:C	50:c:34:VAL:H	2.26	0.44
52:f:57:MET:O	52:f:59:LYS:N	2.51	0.44
53:h:149:LEU:HD21	56:g:167:ARG:HA	1.99	0.44
55:j:118:PRO:HB2	56:g:147:GLY:H	1.82	0.44
58:k:118:GLN:HE22	58:k:221:GLY:N	2.16	0.44
59:l:171:ALA:HB3	59:l:237:ALA:HB2	2.00	0.44
60:m:345:HIS:ND1	60:m:346:PRO:HD3	2.32	0.44
65:s:44:VAL:HG22	65:s:52:GLU:CG	2.48	0.44
59:x:352:LEU:HD21	59:x:354:ASN:HD21	1.82	0.44
60:y:6:LYS:O	60:y:12:LYS:HB2	2.18	0.44
60:y:77:TRP:CZ3	61:z:201:ARG:HB2	2.53	0.44
60:y:335:LEU:HA	60:y:338:ILE:HB	1.99	0.44
63:A2:16:ILE:O	63:A2:18:LYS:N	2.51	0.44
65:B7:44:VAL:O	65:B7:47:ARG:N	2.51	0.44
2:1:149:ILE:HD11	2:1:185:TRP:HE3	1.83	0.43
2:1:221:ALA:O	2:1:225:MET:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:158:SER:O	8:2:161:SER:HB3	2.18	0.43
8:2:169:GLY:C	8:2:171:ASN:N	2.75	0.43
9:8:98:LYS:O	9:8:101:PHE:HB3	2.18	0.43
12:A9:19:THR:CG2	12:A9:53:THR:OG1	2.66	0.43
12:A9:19:THR:HG22	12:A9:53:THR:OG1	2.18	0.43
12:A9:60:ASP:O	12:A9:64:GLU:HG3	2.18	0.43
18:C2:68:ILE:HG13	18:C2:69:PHE:N	2.33	0.43
24:B:412:VAL:HG12	24:B:413:SER:N	2.33	0.43
34:L:67:PRO:HA	38:Q:130:LYS:CE	2.46	0.43
39:R:154:GLN:HG3	39:R:155:VAL:N	2.33	0.43
39:R:271:TYR:O	39:R:272:LEU:HB2	2.18	0.43
40:S:49:THR:HG22	40:S:192:VAL:HG22	1.99	0.43
41:T:17:GLU:O	41:T:20:ARG:HG2	2.17	0.43
44:W:106:LYS:H	44:W:106:LYS:HG2	1.44	0.43
55:j:77:LYS:HB2	55:j:77:LYS:HE3	1.77	0.43
57:e:92:TRP:O	57:e:94:HIS:HB2	2.18	0.43
44:M:29:LYS:HE2	44:M:39:ASP:CG	2.43	0.43
58:k:311:ASN:HA	58:k:319:LEU:O	2.18	0.43
59:l:43:PRO:O	59:l:113:ARG:N	2.51	0.43
60:m:37:LEU:HA	60:m:37:LEU:HD23	1.79	0.43
61:o:21:LEU:HD13	61:o:192:TRP:HB2	1.99	0.43
63:q:102:LYS:HA	63:q:105:GLU:OE1	2.18	0.43
65:s:17:LEU:O	65:s:21:ARG:N	2.39	0.43
65:s:44:VAL:O	65:s:47:ARG:N	2.51	0.43
58:w:270:LEU:HD23	58:w:270:LEU:HA	1.85	0.43
59:x:160:ILE:HG22	59:x:164:HIS:HE1	1.83	0.43
59:x:409:ASP:O	59:x:413:ALA:N	2.42	0.43
62:A1:65:SER:HB3	62:A1:68:VAL:HG23	2.00	0.43
63:A2:27:ASN:OD1	63:A2:81:THR:HB	2.18	0.43
82:A2:201:UQ2:H101	82:A2:201:UQ2:H121	1.56	0.43
65:B7:66:ASP:O	65:B7:70:ALA:N	2.51	0.43
2:1:106:LEU:HA	2:1:106:LEU:HD23	1.75	0.43
3:9:53:PHE:HE2	3:9:55:PHE:CE1	2.36	0.43
3:9:155:LYS:HD3	3:9:202:GLU:OE1	2.17	0.43
4:7:13:PHE:C	4:7:16:GLY:H	2.21	0.43
4:7:60:TYR:O	4:7:64:MET:HB3	2.18	0.43
5:4:298:ILE:O	5:4:302:LEU:HD13	2.18	0.43
5:4:393:ILE:HD11	7:6:183:ILE:CD1	2.48	0.43
7:6:161:ARG:NH1	7:6:238:GLU:O	2.51	0.43
9:8:406:PRO:C	9:8:408:GLU:H	2.26	0.43
10:C3:431:LEU:HD21	10:C3:450:TRP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A9:41:THR:O	12:A9:45:ILE:HG13	2.18	0.43
12:A9:183:GLU:O	16:A6:42:ARG:NH2	2.50	0.43
18:C2:61:GLU:OE1	18:C2:64:ARG:NH1	2.51	0.43
19:B2:11:LEU:HD23	19:B2:11:LEU:C	2.44	0.43
23:A:273:ILE:HD11	23:A:290:THR:O	2.18	0.43
25:C:96:ILE:HB	25:C:97:PRO:HD3	2.00	0.43
27:E:104:ARG:HD2	27:E:168:VAL:HG21	2.00	0.43
34:L:27:GLY:C	34:L:29:ALA:H	2.26	0.43
36:O:103:VAL:O	36:O:105:ARG:N	2.51	0.43
38:Q:172:MET:C	69:Q:201:PC1:H11	2.43	0.43
41:T:69:ILE:HG21	41:T:100:ILE:CD1	2.48	0.43
42:U:81:MET:HG2	42:U:115:PHE:HE1	1.83	0.43
44:W:128:PHE:O	44:W:130:ILE:N	2.37	0.43
50:c:94:PRO:HB2	56:g:10:TYR:CD1	2.52	0.43
58:k:86:LEU:HD23	59:l:285:VAL:HG22	1.99	0.43
59:l:160:ILE:HG22	59:l:164:HIS:HE1	1.83	0.43
59:l:240:HIS:CD2	59:l:421:ARG:HH22	2.36	0.43
60:m:50:PHE:O	60:m:53:MET:HB2	2.17	0.43
60:m:344:GLU:HG3	60:m:345:HIS:H	1.83	0.43
60:m:373:GLU:HA	60:m:376:LEU:HD12	2.00	0.43
61:o:146:GLY:O	61:o:159:GLY:HA2	2.19	0.43
58:w:213:GLN:CD	58:w:214:LYS:HZ1	2.20	0.43
58:w:294:LEU:HD13	58:w:307:PHE:CZ	2.53	0.43
60:y:83:HIS:HE1	80:y:401:HEM:C1C	2.35	0.43
61:z:56:TYR:HD1	61:z:60:GLU:CD	2.26	0.43
65:B7:44:VAL:HG22	65:B7:52:GLU:CG	2.48	0.43
66:A4:16:ASN:HA	66:A4:19:PRO:HD2	1.99	0.43
66:A4:32:LEU:HD12	66:A4:35:ALA:HB3	2.00	0.43
67:B6:45:HIS:HA	67:B6:48:GLU:OE2	2.18	0.43
2:1:205:SER:H	2:1:279:ARG:HH12	1.65	0.43
7:6:136:ASN:O	7:6:139:GLN:N	2.51	0.43
9:8:103:ASN:ND2	9:8:232:ASP:OD2	2.51	0.43
11:C1:162:SER:HB2	11:C1:198:GLU:HB2	1.99	0.43
13:A7:40:LEU:HD22	13:A7:59:LEU:CD1	2.47	0.43
13:A7:126:MET:HG3	13:A7:128:VAL:HG23	2.00	0.43
23:A:79:LEU:HD12	23:A:112:ALA:HB1	1.99	0.43
24:B:180:LEU:HD23	24:B:180:LEU:HA	1.66	0.43
24:B:371:MET:HB2	24:B:371:MET:HE3	1.74	0.43
30:H:71:LYS:HE3	30:H:71:LYS:HB3	1.77	0.43
31:I:105:LYS:O	31:I:106:GLU:CG	2.65	0.43
33:K:48:ASN:C	33:K:50:ASP:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:143:ASP:O	39:R:147:LYS:HG2	2.18	0.43
45:X:14:VAL:C	45:X:17:PRO:HD2	2.42	0.43
49:b:153:GLU:O	49:b:157:ARG:N	2.48	0.43
50:c:8:GLU:OE1	50:c:8:GLU:N	2.38	0.43
52:f:24:LEU:O	52:f:27:LEU:HB3	2.19	0.43
52:f:139:GLN:O	52:f:143:GLU:N	2.43	0.43
58:k:117:VAL:HG11	58:k:195:MET:HE3	2.00	0.43
58:k:294:LEU:HD13	58:k:307:PHE:CZ	2.53	0.43
59:l:58:GLU:HA	59:l:62:ASN:HD22	1.83	0.43
60:m:22:PRO:CG	64:r:3:GLN:HB3	2.48	0.43
65:s:66:ASP:O	65:s:70:ALA:N	2.51	0.43
67:u:45:HIS:HA	67:u:48:GLU:OE2	2.19	0.43
58:w:405:ARG:HG2	58:w:408:ARG:HH21	1.82	0.43
59:x:58:GLU:HA	59:x:62:ASN:HD22	1.83	0.43
59:x:363:LYS:O	59:x:367:GLY:N	2.30	0.43
60:y:334:THR:O	60:y:338:ILE:HG12	2.18	0.43
65:B7:31:VAL:O	65:B7:35:GLU:HG3	2.19	0.43
2:1:79:LEU:HD11	2:1:222:LEU:HD23	1.91	0.43
4:7:57:PHE:CD1	4:7:61:LEU:HD22	2.54	0.43
4:7:161:LEU:O	4:7:164:GLY:N	2.45	0.43
5:4:23:ILE:HG13	5:4:24:TRP:N	2.33	0.43
5:4:72:LEU:O	5:4:76:MET:HE3	2.18	0.43
5:4:339:SER:OG	5:4:344:LEU:HD23	2.17	0.43
6:5:89:TYR:O	6:5:91:GLN:N	2.51	0.43
7:6:95:PHE:O	7:6:98:TRP:HB3	2.19	0.43
12:A9:63:ARG:HA	12:A9:67:PHE:CD2	2.53	0.43
18:C2:26:MET:N	18:C2:26:MET:SD	2.91	0.43
24:B:65:PRO:HB2	24:B:69:VAL:HA	2.00	0.43
70:B:501:3PE:H232	27:E:63:TRP:NE1	2.33	0.43
37:P:108:GLN:HG2	37:P:108:GLN:O	2.19	0.43
40:S:87:GLY:HA3	40:S:88:ASP:C	2.43	0.43
44:W:144:ILE:O	44:W:148:ILE:HG12	2.19	0.43
53:h:115:GLN:O	53:h:118:ALA:N	2.51	0.43
59:l:52:LYS:HE3	59:l:203:ARG:HA	1.99	0.43
60:m:133:LEU:HD12	80:m:401:HEM:C4D	2.54	0.43
60:m:245:PHE:C	61:o:201:ARG:HH12	2.26	0.43
60:m:271:GLU:O	60:m:275:LEU:HG	2.18	0.43
58:w:192:ALA:H	58:w:218:GLY:CA	2.22	0.43
61:z:71:GLN:HG3	61:z:72:ASP:CG	2.43	0.43
61:z:146:GLY:O	61:z:159:GLY:HA2	2.19	0.43
62:A1:14:ARG:O	64:A3:24:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:A1:91:TRP:C	62:A1:93:GLY:N	2.67	0.43
2:1:47:GLN:HB3	2:1:48:PRO:HD3	2.00	0.43
2:1:283:ASP:C	2:1:285:LEU:N	2.73	0.43
3:9:57:PRO:HA	3:9:60:TYR:HD2	1.83	0.43
5:4:156:GLY:C	5:4:159:PRO:HD2	2.43	0.43
5:4:182:TRP:O	5:4:182:TRP:CD1	2.72	0.43
7:6:70:THR:HG21	53:h:115:GLN:HE22	1.84	0.43
72:6:701:CDL:H731	72:6:701:CDL:H762	1.83	0.43
8:2:211:MET:HE1	8:2:259:GLY:HA2	1.99	0.43
8:2:321:LYS:HG3	69:2:402:PC1:H251	2.01	0.43
8:2:323:MET:HE1	8:2:327:PRO:HG3	2.01	0.43
9:8:203:ALA:CB	9:8:205:ILE:HD12	2.48	0.43
10:C3:131:PRO:HB2	11:C1:159:VAL:HA	2.00	0.43
10:C3:498:CYS:HA	10:C3:499:PRO:HA	1.78	0.43
23:A:302:LEU:HG	23:A:571:HIS:O	2.19	0.43
23:A:356:ASP:CG	23:A:645:ARG:HH21	2.26	0.43
23:A:380:ASP:OD1	23:A:380:ASP:N	2.49	0.43
23:A:488:ALA:O	23:A:492:ALA:N	2.47	0.43
23:A:557:ARG:CZ	42:U:144:TYR:OH	2.66	0.43
24:B:141:TYR:O	24:B:144:MET:HE2	2.18	0.43
29:G:58:LYS:HB3	29:G:58:LYS:HE2	1.81	0.43
34:L:66:VAL:HG21	38:Q:128:VAL:O	2.19	0.43
38:Q:96:LEU:HD23	38:Q:98:ARG:HG2	2.00	0.43
42:U:124:TYR:O	42:U:125:VAL:C	2.62	0.43
55:j:67:SER:HB2	70:j:202:3PE:H352	2.00	0.43
58:k:22:GLY:C	58:k:192:ALA:HB1	2.43	0.43
58:k:263:ALA:HA	58:k:386:TYR:CE1	2.53	0.43
58:k:270:LEU:HA	58:k:270:LEU:HD23	1.85	0.43
58:k:395:TRP:O	58:k:398:ARG:HB2	2.17	0.43
59:l:29:LEU:HD22	59:l:221:GLU:OE2	2.18	0.43
59:l:183:ILE:C	59:l:185:LYS:H	2.26	0.43
59:l:416:LYS:O	59:l:419:SER:N	2.52	0.43
60:m:6:LYS:O	60:m:13:ILE:HG13	2.18	0.43
62:p:20:ASP:OD2	62:p:23:LYS:HG2	2.18	0.43
58:w:22:GLY:C	58:w:192:ALA:HB1	2.43	0.43
59:x:171:ALA:HB3	59:x:237:ALA:HB2	2.00	0.43
59:x:416:LYS:O	59:x:419:SER:N	2.52	0.43
60:y:6:LYS:O	60:y:13:ILE:HG13	2.18	0.43
60:y:373:GLU:HA	60:y:376:LEU:HD12	2.00	0.43
62:A1:149:ASN:HA	62:A1:154:GLY:O	2.17	0.43
63:A2:11:ARG:CG	82:A2:201:UQ2:O4	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:126:LYS:HA	2:1:129:LEU:HB3	2.00	0.43
5:4:25:VAL:HG11	53:h:82:VAL:HG11	2.01	0.43
7:6:90:ILE:HB	7:6:91:PRO:HD3	2.00	0.43
7:6:254:VAL:O	7:6:258:PHE:N	2.50	0.43
8:2:146:PHE:HE1	8:2:195:PRO:HA	1.84	0.43
8:2:221:ALA:HB3	8:2:236:LYS:NZ	2.34	0.43
8:2:248:LEU:HD13	8:2:296:LEU:HD23	2.01	0.43
10:C3:106:PRO:HB2	10:C3:107:PRO:HD3	2.01	0.43
11:C1:3:TYR:CD1	11:C1:3:TYR:N	2.87	0.43
16:A6:5:LYS:CD	16:A6:6:GLY:N	2.81	0.43
20:B3:44:PRO:HA	20:B3:47:ARG:NH1	2.34	0.43
23:A:234:LYS:O	23:A:237:ALA:HB2	2.18	0.43
23:A:364:ASP:CG	23:A:365:THR:H	2.26	0.43
24:B:106:VAL:C	24:B:108:LYS:H	2.25	0.43
27:E:197:TRP:HB3	42:U:84:PRO:CB	2.41	0.43
69:Q:201:PC1:H362	69:Q:201:PC1:H391	1.78	0.43
40:S:71:LEU:HD23	40:S:146:VAL:HG13	2.01	0.43
51:d:82:HIS:O	51:d:86:ASP:N	2.34	0.43
58:k:213:GLN:O	58:k:217:SER:OG	2.17	0.43
58:k:406:VAL:O	58:k:410:VAL:HG23	2.19	0.43
59:l:71:LEU:HD12	59:l:144:LEU:HD23	2.01	0.43
61:o:41:HIS:NE2	81:o:301:HEC:C1D	2.82	0.43
64:r:39:ARG:HG3	64:r:40:ARG:H	1.82	0.43
66:t:34:TRP:CD1	67:u:29:LEU:HD13	2.54	0.43
58:w:106:LEU:CD2	58:w:203:LEU:HD21	2.48	0.43
58:w:173:ASN:O	58:w:177:LEU:N	2.52	0.43
59:x:133:ARG:O	59:x:136:GLU:N	2.51	0.43
59:x:189:VAL:O	59:x:192:HIS:N	2.51	0.43
60:y:244:LEU:HD11	61:z:201:ARG:O	2.18	0.43
61:z:3:LEU:HD12	65:B7:59:LEU:HB2	1.99	0.43
65:B7:10:GLU:OE1	65:B7:13:LEU:N	2.51	0.43
2:1:32:GLN:O	2:1:33:LEU:HB2	2.18	0.43
2:1:171:GLN:N	2:1:171:GLN:NE2	2.60	0.43
2:1:233:MET:HE2	2:1:233:MET:HB3	1.75	0.43
2:1:265:LEU:HD22	2:1:265:LEU:HA	1.55	0.43
2:1:316:PRO:HG3	43:V:57:ARG:HG2	2.01	0.43
3:9:54:ASP:O	3:9:89:GLN:NE2	2.51	0.43
3:9:244:GLY:O	3:9:246:GLN:HG3	2.19	0.43
10:C3:195:LEU:CD2	10:C3:245:ILE:HD13	2.45	0.43
12:A9:40:MET:O	12:A9:41:THR:C	2.62	0.43
23:A:145:MET:C	23:A:146:PHE:HD1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:230:GLN:NE2	25:C:233:ARG:HH12	2.16	0.43
27:E:206:GLN:HA	27:E:209:TYR:CD2	2.54	0.43
30:H:15:ASP:C	30:H:17:TRP:N	2.75	0.43
30:H:80:ARG:HG2	30:H:81:ARG:HH12	1.82	0.43
33:K:25:GLN:HG2	33:K:57:GLU:OE2	2.18	0.43
37:P:52:ASN:HB3	37:P:57:ARG:NH1	2.34	0.43
39:R:179:LYS:HB3	39:R:317:ASP:CG	2.44	0.43
42:U:65:THR:O	42:U:74:PHE:HD1	2.02	0.43
44:W:104:PHE:O	44:W:107:ASP:C	2.62	0.43
47:Z:33:GLN:HA	47:Z:36:LEU:HG	2.00	0.43
49:b:151:LEU:HD23	49:b:151:LEU:HA	1.75	0.43
58:k:109:ALA:O	58:k:113:LEU:N	2.41	0.43
58:k:350:THR:O	58:k:354:VAL:HG23	2.19	0.43
59:l:68:LEU:HD23	59:l:191:LEU:HD21	2.01	0.43
59:l:168:TYR:HE2	59:l:321:LEU:HD11	1.83	0.43
64:r:44:CYS:O	64:r:47:ARG:N	2.49	0.43
64:r:59:TYR:O	64:r:63:THR:OG1	2.14	0.43
66:t:24:TRP:O	66:t:27:VAL:HB	2.19	0.43
58:w:86:LEU:HD13	58:w:99:ILE:HG12	2.00	0.43
58:w:406:VAL:O	58:w:410:VAL:HG23	2.19	0.43
59:x:154:ASN:HD21	68:B5:76:VAL:HG21	1.83	0.43
60:y:271:GLU:O	60:y:275:LEU:HG	2.18	0.43
61:z:76:GLU:O	61:z:78:GLY:N	2.50	0.43
66:A4:15:ARG:CZ	66:A4:16:ASN:HD21	2.32	0.43
2:1:234:MET:O	2:1:237:PHE:HB3	2.19	0.43
3:9:188:ILE:H	3:9:188:ILE:HG13	1.63	0.43
4:7:152:TRP:CD2	30:H:14:LEU:HD22	2.53	0.43
5:4:2:LEU:HB3	5:4:6:ILE:CD1	2.48	0.43
5:4:51:ASN:ND2	49:b:136:THR:HG22	2.34	0.43
5:4:109:THR:HG22	5:4:110:PHE:N	2.33	0.43
12:A9:80:ARG:HG2	12:A9:233:PHE:CE1	2.54	0.43
13:A7:37:GLN:O	13:A7:41:LYS:HG2	2.18	0.43
23:A:259:SER:HA	23:A:282:ASN:ND2	2.33	0.43
24:B:102:SER:C	24:B:104:GLU:H	2.25	0.43
24:B:203:MET:HE2	24:B:203:MET:HA	2.00	0.43
24:B:381:HIS:O	24:B:381:HIS:CG	2.71	0.43
27:E:106:TYR:HE1	27:E:112:ARG:HG3	1.83	0.43
39:R:198:ALA:H	39:R:260:GLY:H	1.67	0.43
40:S:52:GLY:O	40:S:149:ARG:NH2	2.52	0.43
40:S:282:LEU:O	40:S:284:MET:N	2.52	0.43
41:T:82:GLU:CG	41:T:84:PRO:HD2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:U:39:VAL:HG12	42:U:49:TYR:HE1	1.84	0.43
42:U:64:TYR:CE1	42:U:81:MET:HB2	2.54	0.43
46:Y:50:PHE:CD1	47:Z:57:PHE:HE1	2.36	0.43
56:g:87:GLU:O	56:g:90:MET:N	2.51	0.43
56:g:97:LYS:HE3	56:g:97:LYS:HB3	1.89	0.43
58:k:54:GLY:O	58:k:57:TYR:HB3	2.18	0.43
59:l:255:ALA:HA	59:l:425:ALA:O	2.18	0.43
59:l:261:SER:H	59:l:321:LEU:HA	1.83	0.43
60:m:25:SER:HA	60:m:218:ILE:CD1	2.49	0.43
60:m:126:THR:OG1	60:m:185:LEU:HD23	2.19	0.43
60:m:334:THR:O	60:m:338:ILE:HG12	2.18	0.43
61:o:56:TYR:HD1	61:o:60:GLU:CD	2.27	0.43
61:o:166:ASN:HA	61:o:179:MET:N	2.32	0.43
58:w:207:GLN:O	58:w:211:LEU:HG	2.18	0.43
58:w:311:ASN:HA	58:w:319:LEU:O	2.18	0.43
58:w:417:ASP:CG	62:A1:37:TYR:HH	2.23	0.43
59:x:71:LEU:HD12	59:x:144:LEU:HD23	2.01	0.43
59:x:367:GLY:HA2	59:x:370:MET:HE3	2.00	0.43
61:z:47:ALA:HB2	61:z:90:TYR:CE1	2.52	0.43
62:A1:25:SER:HB3	62:A1:32:ARG:NH1	2.34	0.43
67:B6:13:LEU:O	67:B6:19:THR:OG1	2.36	0.43
2:1:96:ILE:HG21	2:1:98:MET:HE3	2.01	0.43
2:1:282:TYR:O	2:1:285:LEU:HB3	2.18	0.43
7:6:173:LEU:O	7:6:177:ILE:HD12	2.18	0.43
7:6:237:MET:HE1	7:6:248:HIS:CD2	2.54	0.43
7:6:310:LEU:HD23	7:6:313:MET:CE	2.49	0.43
7:6:389:PHE:O	7:6:393:ASP:HB3	2.19	0.43
8:2:131:LEU:HA	8:2:131:LEU:HD23	1.57	0.43
70:2:401:3PE:H2C1	70:2:401:3PE:H2F2	1.86	0.43
9:8:249:ALA:O	9:8:252:PRO:HD2	2.19	0.43
10:C3:474:GLU:HG3	10:C3:475:ALA:N	2.34	0.43
12:A9:110:PRO:HB3	17:C0:30:TRP:CD2	2.54	0.43
23:A:355:LYS:HA	23:A:530:TYR:OH	2.19	0.43
24:B:90:ALA:HB1	24:B:93:GLY:O	2.19	0.43
39:R:134:TRP:CZ2	39:R:311:GLU:HG3	2.54	0.43
39:R:217:PHE:C	39:R:219:ASN:H	2.26	0.43
40:S:338:LYS:HE2	55:j:51:ARG:HD2	2.01	0.43
42:U:26:VAL:HG13	42:U:33:VAL:HG23	2.01	0.43
50:c:32:GLU:O	50:c:34:VAL:N	2.51	0.43
50:c:83:HIS:CE1	50:c:87:LYS:HE2	2.53	0.43
53:h:79:ASP:O	53:h:83:ASP:OD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:e:63:GLU:C	57:e:65:TYR:H	2.22	0.43
58:k:277:ILE:HD11	58:k:345:LEU:HD11	2.01	0.43
59:l:367:GLY:HA2	59:l:370:MET:HE3	2.00	0.43
60:m:58:ASP:OD2	60:y:56:THR:HG21	2.19	0.43
60:m:129:MET:O	60:m:133:LEU:HG	2.19	0.43
60:m:322:GLN:O	60:m:326:TRP:HD1	2.02	0.43
62:p:83:GLU:HA	62:p:138:VAL:HA	1.99	0.43
58:w:301:ASN:ND2	60:y:2:THR:OG1	2.50	0.43
60:y:25:SER:HA	60:y:218:ILE:CD1	2.49	0.43
60:y:133:LEU:HD12	80:y:401:HEM:C4D	2.54	0.43
62:A1:14:ARG:HH21	62:A1:18:VAL:HG23	1.83	0.43
63:A2:17:ARG:O	63:A2:19:TRP:N	2.52	0.43
64:A3:39:ARG:HG3	64:A3:40:ARG:H	1.82	0.43
1:3:11:PHE:O	1:3:14:ALA:N	2.52	0.43
1:3:88:LEU:CD1	2:1:309:ILE:HG21	2.15	0.43
2:1:98:MET:SD	70:1:401:3PE:H32	2.59	0.43
2:1:303:TRP:CE2	2:1:307:LEU:HD21	2.53	0.43
3:9:188:ILE:CD1	3:9:189:ASN:H	2.23	0.43
4:7:17:PHE:HD1	4:7:20:PHE:HE2	1.67	0.43
4:7:125:TRP:CH2	6:5:4:VAL:HG23	2.53	0.43
5:4:59:ASP:OD2	5:4:64:PRO:HA	2.19	0.43
72:6:701:CDL:H311	72:6:701:CDL:HA61	1.84	0.43
8:2:144:GLN:C	8:2:146:PHE:H	2.27	0.43
23:A:159:ALA:O	31:I:102:ASN:HB2	2.19	0.43
23:A:300:GLN:HE21	42:U:137:TRP:CD1	2.37	0.43
23:A:657:ASP:OD1	23:A:657:ASP:O	2.36	0.43
24:B:78:SER:O	24:B:79:ASN:ND2	2.52	0.43
25:C:174:ASP:OD2	25:C:189:ILE:O	2.36	0.43
26:D:123:MET:HE3	26:D:123:MET:HB2	1.93	0.43
34:L:58:ARG:NH1	38:Q:137:LEU:HD13	2.34	0.43
38:Q:25:LEU:O	38:Q:29:ALA:HB2	2.19	0.43
39:R:207:PHE:CZ	39:R:241:TYR:HB2	2.54	0.43
41:T:69:ILE:HG21	41:T:100:ILE:HD13	2.01	0.43
42:U:83:PRO:O	42:U:85:GLU:N	2.45	0.43
43:V:84:LEU:HA	43:V:84:LEU:HD23	1.76	0.43
52:f:25:ARG:O	52:f:28:GLU:HG2	2.19	0.43
52:f:109:PRO:HA	52:f:112:LYS:H	1.84	0.43
57:e:89:TRP:CD1	57:e:89:TRP:N	2.86	0.43
58:k:58:PHE:O	58:k:62:LEU:HG	2.19	0.43
58:k:173:ASN:O	58:k:177:LEU:N	2.52	0.43
58:k:293:PRO:O	58:k:296:SER:OG	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:m:136:GLY:N	60:m:139:SER:OG	2.52	0.43
60:m:350:ILE:O	60:m:353:LEU:HB2	2.19	0.43
61:o:241:LYS:HZ3	63:q:56:ASN:HB2	1.84	0.43
65:s:31:VAL:O	65:s:35:GLU:HG3	2.19	0.43
65:s:37:LEU:HD11	65:s:61:PHE:CG	2.54	0.43
66:t:23:LEU:O	66:t:27:VAL:HG23	2.18	0.43
58:w:109:ALA:O	58:w:113:LEU:N	2.41	0.43
59:x:29:LEU:HD22	59:x:221:GLU:OE2	2.18	0.43
59:x:52:LYS:HE3	59:x:203:ARG:HA	1.99	0.43
59:x:68:LEU:HD23	59:x:191:LEU:HD21	2.01	0.43
59:x:133:ARG:HB3	59:x:135:TRP:CE2	2.54	0.43
59:x:183:ILE:C	59:x:185:LYS:H	2.26	0.43
60:y:40:CYS:CB	60:y:90:PHE:HD1	2.32	0.43
60:y:126:THR:OG1	60:y:185:LEU:HD23	2.19	0.43
62:A1:101:ARG:H	62:A1:131:GLU:C	2.21	0.43
64:A3:44:CYS:O	64:A3:47:ARG:N	2.49	0.43
65:B7:22:GLU:HA	65:B7:25:GLU:OE2	2.18	0.43
66:A4:15:ARG:CG	66:A4:16:ASN:N	2.81	0.43
4:7:140:ALA:C	4:7:142:GLY:H	2.26	0.42
5:4:12:MET:HB3	5:4:13:PRO:HD3	2.01	0.42
5:4:143:LEU:CD2	8:2:302:LEU:HD21	2.41	0.42
5:4:184:GLN:OE1	5:4:184:GLN:N	2.52	0.42
5:4:350:THR:OG1	5:4:351:LEU:HG	2.19	0.42
7:6:597:ILE:HD11	41:T:35:VAL:HG22	2.01	0.42
8:2:47:ASN:HD21	8:2:123:PRO:HB2	1.83	0.42
8:2:96:MET:O	8:2:100:MET:HG2	2.19	0.42
9:8:155:TYR:CE1	9:8:196:PHE:HD2	2.36	0.42
12:A9:148:HIS:CE1	12:A9:152:MET:HE3	2.54	0.42
19:B2:31:LEU:HA	19:B2:31:LEU:HD23	1.82	0.42
23:A:455:ILE:HB	23:A:460:HIS:NE2	2.34	0.42
24:B:169:TRP:HE3	24:B:347:CYS:SG	2.42	0.42
24:B:406:GLU:O	24:B:427:PRO:HD3	2.19	0.42
26:D:76:TRP:O	26:D:76:TRP:CG	2.72	0.42
27:E:118:LEU:C	27:E:120:GLU:H	2.27	0.42
30:H:6:VAL:HG21	69:j:201:PC1:H3H2	2.00	0.42
30:H:86:LEU:O	30:H:89:GLU:N	2.48	0.42
38:Q:52:ASP:HA	43:V:116:TRP:HB3	2.00	0.42
48:a:70:TYR:O	48:a:75:ASN:ND2	2.52	0.42
55:j:51:ARG:HG2	55:j:56:ALA:HB2	2.01	0.42
44:M:25:ILE:HB	44:M:42:LEU:HD11	2.01	0.42
58:k:86:LEU:HD13	58:k:99:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:303:VAL:CG1	59:l:304:HIS:H	2.32	0.42
61:o:65:ALA:O	61:o:69:GLU:OE1	2.37	0.42
65:s:22:GLU:HA	65:s:25:GLU:OE2	2.19	0.42
65:s:31:VAL:HA	65:s:34:ARG:HB3	2.00	0.42
58:w:58:PHE:CE2	58:w:62:LEU:HD11	2.53	0.42
60:y:350:ILE:O	60:y:353:LEU:HB2	2.19	0.42
65:B7:15:ASP:OD2	65:B7:18:THR:HG23	2.19	0.42
68:B5:66:ALA:HB2	68:B5:77:ARG:NE	2.33	0.42
2:l:312:SER:HA	34:L:42:SER:HB2	2.00	0.42
4:7:5:ILE:HA	4:7:8:ILE:HG22	2.02	0.42
7:6:106:TRP:CD1	7:6:447:ASN:HD21	2.37	0.42
8:2:51:ARG:HG3	24:B:69:VAL:HG21	2.00	0.42
8:2:260:PHE:HE2	8:2:264:TRP:CE3	2.37	0.42
9:8:127:ASP:O	9:8:128:ARG:HB3	2.19	0.42
9:8:325:PRO:HD2	9:8:347:THR:CG2	2.48	0.42
10:C3:377:PHE:CD2	76:C3:603:HEA:HAD1	2.53	0.42
11:C1:63:THR:HA	11:C1:66:THR:HG22	2.00	0.42
11:C1:148:MET:HE3	11:C1:148:MET:HB3	1.78	0.42
14:B4:27:TRP:CH2	15:A5:86:GLY:HA2	2.54	0.42
23:A:128:CYS:N	74:A:801:SF4:S1	2.93	0.42
24:B:155:VAL:O	24:B:156:GLU:C	2.61	0.42
24:B:304:LYS:HE2	24:B:304:LYS:HB3	1.77	0.42
26:D:209:ARG:HG2	26:D:210:LEU:N	2.35	0.42
30:H:14:LEU:HA	30:H:14:LEU:HD23	1.76	0.42
36:O:69:LYS:HE3	36:O:70:ASN:OD1	2.20	0.42
39:R:206:ILE:H	39:R:206:ILE:HG13	1.54	0.42
40:S:114:GLY:HA3	40:S:115:ASN:HA	1.59	0.42
40:S:211:ASN:HB3	40:S:214:GLU:HB2	2.01	0.42
43:V:88:ARG:O	43:V:92:GLU:N	2.48	0.42
43:V:142:TRP:C	43:V:143:TYR:CD2	2.98	0.42
44:W:81:ASP:OD2	47:Z:17:PRO:HG2	2.20	0.42
44:W:106:LYS:HE2	44:W:106:LYS:HB3	1.40	0.42
44:W:123:GLU:CD	44:W:127:GLY:HA2	2.44	0.42
47:Z:64:VAL:HA	47:Z:67:LEU:HG	2.01	0.42
49:b:67:PHE:C	49:b:69:LYS:H	2.26	0.42
58:k:92:ARG:HG2	58:k:167:VAL:HG22	2.00	0.42
58:k:121:SER:HB2	58:k:123:GLU:OE2	2.19	0.42
60:m:180:ALA:O	60:m:184:ILE:HG22	2.20	0.42
62:p:108:GLN:CB	62:p:113:GLU:H	2.32	0.42
64:r:74:PRO:O	64:r:78:GLU:HG2	2.19	0.42
67:u:13:LEU:O	67:u:19:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:86:LEU:HB3	59:x:285:VAL:HG22	2.01	0.42
58:w:117:VAL:HG11	58:w:195:MET:HE3	2.00	0.42
60:y:136:GLY:N	60:y:139:SER:OG	2.52	0.42
60:y:300:ILE:HA	60:y:303:LEU:HG	2.01	0.42
60:y:322:GLN:O	60:y:326:TRP:HD1	2.02	0.42
62:A1:17:GLU:OE1	62:A1:28:SER:HB3	2.19	0.42
62:A1:121:GLN:CB	62:A1:170:ARG:HA	2.49	0.42
63:A2:91:GLU:HA	63:A2:94:LEU:HB3	2.01	0.42
2:1:159:SER:HB3	2:1:317:GLN:HG3	2.01	0.42
5:4:62:SER:HB3	5:4:457:PRO:HG3	2.00	0.42
5:4:440:HIS:C	5:4:443:PRO:HD2	2.44	0.42
9:8:54:LYS:HA	9:8:136:HIS:NE2	2.34	0.42
11:C1:52:HIS:CD2	14:B4:40:ASP:HB2	2.54	0.42
11:C1:78:LEU:HB2	11:C1:79:PRO:CD	2.38	0.42
18:C2:21:ILE:O	18:C2:25:PHE:HD2	2.02	0.42
23:A:81:GLU:CG	23:A:108:LYS:HD3	2.48	0.42
23:A:337:ASP:O	23:A:543:LYS:N	2.52	0.42
23:A:607:LYS:HE2	29:G:78:ARG:NE	2.34	0.42
27:E:206:GLN:HA	27:E:209:TYR:HD2	1.84	0.42
32:J:55:SER:OG	32:J:56:GLY:N	2.52	0.42
33:K:83:SER:N	33:K:86:GLN:OE1	2.47	0.42
35:N:107:PRO:C	35:N:109:ALA:H	2.26	0.42
36:O:76:PRO:C	36:O:78:VAL:H	2.27	0.42
39:R:73:LEU:HA	39:R:73:LEU:HD23	1.74	0.42
40:S:117:TYR:HB2	40:S:167:ILE:HD11	2.01	0.42
40:S:124:TYR:CZ	40:S:151:ILE:HD11	2.55	0.42
52:f:92:GLU:OE1	52:f:92:GLU:N	2.52	0.42
55:j:97:HIS:N	55:j:98:PRO:HD3	2.34	0.42
58:k:106:LEU:CD2	58:k:203:LEU:HD21	2.48	0.42
59:l:45:SER:CB	59:l:113:ARG:HA	2.50	0.42
59:l:87:ARG:HH11	63:A2:107:TRP:HZ3	1.67	0.42
59:l:189:VAL:O	59:l:192:HIS:N	2.51	0.42
62:p:28:SER:O	62:p:31:ALA:N	2.52	0.42
64:r:37:VAL:O	64:r:41:THR:HG23	2.19	0.42
65:s:73:LEU:HD12	65:s:74:PHE:N	2.35	0.42
58:w:54:GLY:O	58:w:57:TYR:HB3	2.18	0.42
58:w:373:THR:O	58:w:377:GLU:N	2.50	0.42
59:x:21:PRO:HG2	59:x:40:ASN:C	2.45	0.42
59:x:99:THR:O	59:x:106:ALA:N	2.36	0.42
59:x:303:VAL:CG1	59:x:304:HIS:H	2.32	0.42
61:z:36:VAL:HG12	81:z:301:HEC:HHC	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:A1:23:LYS:HA	62:A1:23:LYS:HD2	1.87	0.42
65:B7:43:ARG:NE	65:B7:52:GLU:OE2	2.52	0.42
2:1:34:ARG:CZ	26:D:108:ARG:NH1	2.82	0.42
2:1:140:ILE:HA	2:1:143:GLU:OE1	2.20	0.42
2:1:216:ALA:O	2:1:220:PHE:HB3	2.20	0.42
2:1:303:TRP:CH2	2:1:307:LEU:HD11	2.54	0.42
4:7:81:GLU:O	4:7:82:ILE:HB	2.18	0.42
7:6:366:MET:N	7:6:367:PRO:HD3	2.35	0.42
7:6:437:PHE:CE1	7:6:441:VAL:HG21	2.54	0.42
8:2:89:LEU:O	8:2:91:ASN:N	2.52	0.42
10:C3:240:HIS:NE2	10:C3:244:TYR:CE2	2.81	0.42
15:A5:53:THR:HG22	15:A5:54:ASN:OD1	2.19	0.42
21:A0:41:ARG:HD2	22:A8:40:TYR:CZ	2.54	0.42
23:A:89:VAL:HB	23:A:94:MET:SD	2.60	0.42
23:A:353:ALA:HB1	23:A:623:ILE:HG21	2.01	0.42
23:A:541:PRO:CB	23:A:561:PRO:HG3	2.50	0.42
25:C:138:ARG:O	37:P:101:ILE:HG13	2.19	0.42
25:C:183:HIS:O	25:C:184:PRO:C	2.61	0.42
30:H:82:GLN:HE21	43:V:98:MET:N	2.18	0.42
34:L:16:GLU:OE1	34:L:16:GLU:N	2.53	0.42
39:R:197:GLU:HG2	39:R:259:ARG:HE	1.84	0.42
40:S:56:SER:OG	40:S:57:GLY:N	2.52	0.42
40:S:108:ASP:O	40:S:110:LYS:N	2.51	0.42
41:T:6:LEU:HB3	41:T:10:TRP:HD1	1.82	0.42
43:V:9:ASP:C	43:V:10:MET:HE2	2.44	0.42
59:l:21:PRO:HG2	59:l:40:ASN:C	2.45	0.42
59:l:133:ARG:HB3	59:l:135:TRP:CE2	2.54	0.42
59:l:133:ARG:O	59:l:136:GLU:N	2.51	0.42
59:l:167:ALA:HA	59:l:241:GLY:HA2	2.02	0.42
59:l:254:HIS:ND1	59:l:325:TYR:OH	2.53	0.42
59:l:305:GLN:CB	59:l:306:PRO:HD3	2.45	0.42
60:m:300:ILE:HA	60:m:303:LEU:HG	2.01	0.42
62:p:67:ASP:O	62:p:70:ALA:N	2.52	0.42
58:w:30:SER:N	58:w:201:GLY:O	2.48	0.42
59:x:50:PHE:HB3	59:x:387:LEU:HD11	2.01	0.42
59:x:167:ALA:HA	59:x:241:GLY:HA2	2.01	0.42
59:x:168:TYR:CE2	59:x:321:LEU:HD11	2.54	0.42
59:x:254:HIS:ND1	59:x:325:TYR:OH	2.53	0.42
60:y:216:ASP:CG	63:A2:63:LYS:HE3	2.44	0.42
63:A2:99:ARG:CZ	63:A2:99:ARG:HB2	2.50	0.42
65:B7:31:VAL:HA	65:B7:34:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:B7:37:LEU:HD11	65:B7:61:PHE:CG	2.54	0.42
4:7:9:LEU:HD23	4:7:9:LEU:HA	1.82	0.42
4:7:145:ALA:O	4:7:146:LEU:HD23	2.19	0.42
5:4:89:LEU:HD13	5:4:93:LYS:NZ	2.35	0.42
5:4:363:SER:HB3	5:4:411:LEU:HD11	2.01	0.42
7:6:440:LEU:HB2	44:W:82:ARG:HH22	1.83	0.42
7:6:527:GLY:C	7:6:529:PHE:H	2.27	0.42
7:6:576:LEU:HD23	7:6:576:LEU:O	2.20	0.42
10:C3:247:ILE:HB	76:C3:603:HEA:HBC1	2.01	0.42
11:C1:162:SER:HB3	11:C1:197:SER:C	2.44	0.42
13:A7:102:TYR:HD2	22:A8:35:TYR:HE1	1.68	0.42
20:B3:9:PHE:CD1	20:B3:9:PHE:C	2.97	0.42
23:A:82:ILE:HD11	23:A:100:TRP:HB3	2.00	0.42
23:A:385:TYR:O	23:A:385:TYR:CG	2.72	0.42
23:A:385:TYR:CE1	23:A:526:LEU:HD13	2.55	0.42
23:A:436:VAL:O	23:A:442:TYR:OH	2.34	0.42
24:B:71:PRO:N	24:B:72:PRO:HD3	2.35	0.42
25:C:188:ARG:HD3	25:C:192:ASP:O	2.19	0.42
26:D:86:THR:C	26:D:87:PHE:HD1	2.27	0.42
26:D:90:ALA:O	26:D:91:CYS:C	2.61	0.42
27:E:100:GLU:CD	27:E:193:ASN:HD21	2.27	0.42
35:N:6:LYS:O	35:N:16:VAL:HG21	2.19	0.42
35:N:38:ILE:HG22	35:N:39:PRO:O	2.19	0.42
48:a:76:ILE:O	48:a:79:ASN:N	2.52	0.42
55:j:34:VAL:HG11	55:j:72:GLY:HA3	2.01	0.42
58:k:58:PHE:CE2	58:k:62:LEU:HD11	2.53	0.42
58:k:149:VAL:HA	58:k:152:TYR:CD2	2.54	0.42
59:l:50:PHE:HB3	59:l:387:LEU:HD11	2.00	0.42
59:l:363:LYS:O	59:l:367:GLY:N	2.30	0.42
80:m:402:HEM:HBB2	80:m:402:HEM:CMB	2.49	0.42
64:r:74:PRO:HB3	64:r:79:ASN:ND2	2.35	0.42
58:w:121:SER:HB2	58:w:123:GLU:OE2	2.19	0.42
58:w:235:ARG:NH1	62:A1:14:ARG:HH12	2.16	0.42
59:x:255:ALA:HA	59:x:425:ALA:O	2.18	0.42
60:y:129:MET:O	60:y:133:LEU:HG	2.19	0.42
67:B6:5:LEU:HD23	67:B6:8:ARG:HD2	2.01	0.42
2:1:169:GLN:CG	2:1:174:LEU:HB2	2.47	0.42
3:9:149:LEU:HD23	3:9:150:GLU:N	2.24	0.42
4:7:100:GLU:O	4:7:103:MET:HB3	2.19	0.42
4:7:127:ILE:O	4:7:129:ASP:N	2.52	0.42
5:4:188:ASN:O	5:4:189:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:214:LEU:HD21	7:6:558:LEU:HB3	2.02	0.42
8:2:150:ASN:O	8:2:152:ASN:N	2.51	0.42
23:A:448:SER:OG	23:A:451:ILE:HG12	2.20	0.42
24:B:65:PRO:HD2	24:B:69:VAL:HG12	2.00	0.42
24:B:182:ASN:OD1	24:B:182:ASN:N	2.48	0.42
24:B:397:TYR:CD2	24:B:398:THR:N	2.88	0.42
25:C:110:PHE:CG	25:C:136:SER:HB3	2.53	0.42
25:C:156:GLU:N	25:C:156:GLU:OE1	2.53	0.42
26:D:175:ARG:HE	26:D:175:ARG:HB2	1.51	0.42
27:E:135:ARG:HG2	27:E:136:ALA:N	2.33	0.42
33:K:26:ARG:O	33:K:27:SER:OG	2.21	0.42
36:O:42:GLU:OE1	36:O:45:ASN:HB3	2.19	0.42
37:P:110:GLU:O	37:P:112:TYR:N	2.53	0.42
38:Q:158:LEU:HB2	55:j:17:GLU:OE2	2.19	0.42
39:R:45:LYS:HA	39:R:45:LYS:HD3	1.83	0.42
41:T:4:THR:O	41:T:5:VAL:C	2.63	0.42
43:V:130:SER:OG	43:V:131:GLU:N	2.53	0.42
44:W:108:LEU:O	44:W:109:GLY:C	2.63	0.42
49:b:83:ALA:HB1	72:b:201:CDL:H792	2.02	0.42
57:e:91:ASP:O	57:e:92:TRP:C	2.62	0.42
44:M:12:LYS:HA	44:M:12:LYS:HD2	1.84	0.42
44:M:32:VAL:C	44:M:73:PRO:HG2	2.44	0.42
58:k:83:GLY:HA3	59:l:363:LYS:HA	2.01	0.42
58:k:207:GLN:O	58:k:211:LEU:HG	2.18	0.42
60:m:40:CYS:CB	60:m:90:PHE:HD1	2.32	0.42
61:o:36:VAL:HG12	81:o:301:HEC:HHC	2.02	0.42
61:o:220:TYR:O	61:o:223:LYS:HB3	2.20	0.42
58:w:92:ARG:HG2	58:w:167:VAL:HG22	2.00	0.42
59:x:45:SER:CB	59:x:113:ARG:HA	2.50	0.42
59:x:245:ARG:HA	59:x:426:ALA:O	2.20	0.42
60:y:301:LEU:HA	60:y:304:ILE:HD12	2.01	0.42
60:y:377:LEU:HD11	63:A2:20:TYR:CE2	2.54	0.42
61:z:50:HIS:HE1	61:z:91:PHE:CZ	2.33	0.42
64:A3:74:PRO:O	64:A3:78:GLU:HG2	2.19	0.42
66:A4:27:VAL:O	66:A4:30:VAL:HB	2.20	0.42
2:1:70:MET:HE2	2:1:70:MET:HB3	1.77	0.42
4:7:19:GLY:O	4:7:24:PRO:HG3	2.20	0.42
4:7:152:TRP:HA	4:7:155:ILE:CG2	2.50	0.42
5:4:51:ASN:OD1	49:b:136:THR:HG22	2.20	0.42
5:4:119:TYR:O	5:4:122:PHE:N	2.53	0.42
5:4:303:ILE:HG22	5:4:304:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:321:LEU:HD23	5:4:321:LEU:HA	1.79	0.42
5:4:347:GLY:HA3	5:4:418:LYS:CB	2.50	0.42
7:6:513:TYR:CD1	52:f:36:LYS:HE3	2.55	0.42
8:2:150:ASN:C	8:2:152:ASN:H	2.28	0.42
9:8:225:LEU:O	9:8:228:PRO:HD3	2.19	0.42
9:8:413:TRP:CZ3	9:8:417:LYS:HG3	2.55	0.42
10:C3:298:ASP:HB2	10:C3:301:THR:CG2	2.49	0.42
10:C3:462:LEU:O	10:C3:466:MET:HG3	2.20	0.42
17:C0:57:ARG:HA	17:C0:60:TYR:CD2	2.55	0.42
23:A:246:ARG:HB2	23:A:265:THR:CG2	2.50	0.42
24:B:268:TRP:HZ3	24:B:327:TYR:HE1	1.67	0.42
25:C:171:GLU:O	25:C:174:ASP:N	2.51	0.42
27:E:170:GLY:HA2	27:E:171:PRO:HD3	1.64	0.42
29:G:128:PHE:CD2	29:G:134:ALA:HA	2.52	0.42
31:I:71:LEU:HD23	31:I:71:LEU:O	2.19	0.42
34:L:38:TYR:O	34:L:41:TYR:HB2	2.19	0.42
39:R:127:ILE:HG22	39:R:165:ILE:HD12	2.02	0.42
39:R:182:ARG:C	39:R:184:LYS:H	2.26	0.42
39:R:261:LYS:HG2	39:R:263:PHE:HE1	1.84	0.42
39:R:283:VAL:O	39:R:285:HIS:ND1	2.33	0.42
40:S:53:ASN:O	40:S:149:ARG:NH2	2.53	0.42
41:T:34:LEU:O	41:T:37:SER:OG	2.26	0.42
42:U:67:GLU:HA	42:U:71:LYS:HB3	2.02	0.42
47:Z:63:PHE:CZ	47:Z:64:VAL:HG23	2.54	0.42
50:c:38:GLN:HA	50:c:39:ARG:HA	1.90	0.42
52:f:18:ARG:O	52:f:22:ARG:NE	2.52	0.42
53:h:82:VAL:O	53:h:83:ASP:C	2.62	0.42
56:g:6:ASP:HB2	56:g:9:VAL:HB	2.02	0.42
59:l:236:LYS:C	59:l:238:LYS:H	2.28	0.42
60:m:199:PHE:O	60:m:202:GLU:HB2	2.19	0.42
63:q:91:GLU:HA	63:q:94:LEU:HB3	2.01	0.42
58:w:58:PHE:O	58:w:62:LEU:HG	2.19	0.42
58:w:131:ARG:NE	58:w:175:ARG:HA	2.35	0.42
58:w:149:VAL:HA	58:w:152:TYR:CD2	2.54	0.42
58:w:204:GLU:HG2	58:w:205:HIS:N	2.34	0.42
59:x:52:LYS:NZ	59:x:203:ARG:HG2	2.34	0.42
60:y:180:ALA:O	60:y:184:ILE:HG22	2.20	0.42
60:y:199:PHE:O	60:y:202:GLU:HB2	2.19	0.42
65:B7:62:LEU:HD23	65:B7:65:ARG:HD3	2.02	0.42
1:3:67:LEU:HD23	1:3:67:LEU:HA	1.76	0.42
1:3:70:ALA:CB	4:7:59:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:123:ASN:OD1	3:9:123:ASN:N	2.50	0.42
4:7:135:PHE:O	4:7:135:PHE:CG	2.72	0.42
5:4:113:MET:O	5:4:113:MET:HG3	2.20	0.42
5:4:239:GLY:C	5:4:241:TYR:H	2.27	0.42
5:4:408:LEU:O	5:4:412:ILE:HG22	2.20	0.42
6:5:37:MET:HG3	6:5:67:ALA:HB1	2.01	0.42
7:6:17:MET:HB3	7:6:18:PRO:HD3	2.01	0.42
7:6:206:PRO:HD2	7:6:266:LEU:CD1	2.50	0.42
7:6:359:MET:CB	7:6:430:ALA:HA	2.49	0.42
9:8:77:LEU:HD23	9:8:100:SER:HA	2.02	0.42
12:A9:146:TRP:NE1	16:A6:17:ARG:HB2	2.35	0.42
24:B:142:VAL:HG12	24:B:182:ASN:OD1	2.20	0.42
26:D:153:MET:HE1	26:D:193:LEU:HD11	2.01	0.42
34:L:61:GLY:O	34:L:63:MET:HB3	2.19	0.42
40:S:167:ILE:HD12	40:S:167:ILE:HA	1.82	0.42
42:U:62:VAL:HG22	42:U:63:ILE:N	2.34	0.42
44:W:119:ILE:HB	44:W:130:ILE:HD13	2.01	0.42
51:d:92:HIS:CE1	51:d:96:VAL:HG21	2.55	0.42
58:k:57:TYR:CE2	58:k:61:HIS:HE1	2.38	0.42
58:k:89:TYR:CE2	58:k:96:ALA:HB3	2.54	0.42
58:k:204:GLU:OE1	58:k:204:GLU:N	2.53	0.42
59:l:406:ALA:O	59:l:409:ASP:HB3	2.19	0.42
60:m:221:HIS:HB3	60:m:222:PRO:HD3	2.02	0.42
61:o:97:ASN:OD1	61:o:98:PRO:HD2	2.20	0.42
63:q:107:TRP:CH2	59:x:87:ARG:HB3	2.55	0.42
67:u:5:LEU:HD23	67:u:8:ARG:HD2	2.01	0.42
58:w:350:THR:O	58:w:354:VAL:HG23	2.19	0.42
60:y:221:HIS:HB3	60:y:222:PRO:HD3	2.01	0.42
60:y:236:ILE:O	60:y:240:MET:HG2	2.20	0.42
61:z:97:ASN:OD1	61:z:98:PRO:HD2	2.20	0.42
61:z:220:TYR:O	61:z:223:LYS:HB3	2.20	0.42
62:A1:35:PHE:O	62:A1:38:LEU:HB3	2.20	0.42
62:A1:147:ILE:O	62:A1:156:TYR:HA	2.20	0.42
2:1:6:ILE:C	2:1:8:MET:H	2.27	0.42
2:1:6:ILE:C	2:1:8:MET:N	2.78	0.42
2:1:28:LEU:O	2:1:32:GLN:HG2	2.20	0.42
2:1:290:TRP:O	2:1:295:PRO:HD3	2.19	0.42
3:9:181:VAL:HG23	3:9:182:ASN:OD1	2.19	0.42
3:9:183:ALA:CB	3:9:195:ASP:HA	2.43	0.42
3:9:222:ARG:NH2	9:8:284:ASN:HB2	2.35	0.42
3:9:238:PRO:HD3	9:8:60:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:151:PHE:C	5:4:155:ALA:HB2	2.45	0.42
5:4:382:VAL:HA	5:4:385:THR:HG22	2.01	0.42
7:6:106:TRP:CH2	7:6:348:HIS:ND1	2.85	0.42
8:2:21:MET:HG2	8:2:140:SER:CB	2.49	0.42
8:2:169:GLY:O	8:2:170:LEU:C	2.63	0.42
17:C0:84:LYS:HD2	17:C0:84:LYS:HA	1.82	0.42
23:A:302:LEU:HD11	23:A:585:PRO:HA	2.01	0.42
23:A:334:GLN:HE22	23:A:361:VAL:HG22	1.84	0.42
24:B:118:ARG:HD3	26:D:163:TYR:CE2	2.54	0.42
24:B:157:LYS:O	24:B:159:LEU:N	2.53	0.42
24:B:262:LEU:HD23	24:B:262:LEU:HA	1.72	0.42
25:C:120:ASP:OD1	25:C:120:ASP:N	2.49	0.42
25:C:212:LEU:HD21	25:C:221:VAL:CG1	2.50	0.42
30:H:80:ARG:HG2	30:H:81:ARG:NH1	2.35	0.42
31:I:85:ILE:HG22	31:I:86:SER:H	1.83	0.42
33:K:16:LEU:HA	33:K:69:TYR:HB3	2.01	0.42
34:L:40:LYS:HB3	34:L:40:LYS:HE3	1.76	0.42
35:N:35:LEU:HD21	35:N:45:ARG:HG3	2.00	0.42
35:N:103:LEU:HD23	35:N:104:VAL:N	2.35	0.42
38:Q:51:LYS:NZ	49:b:189:ASN:HD21	2.17	0.42
39:R:187:GLY:HA2	39:R:191:VAL:HG23	2.01	0.42
39:R:191:VAL:HG12	39:R:195:PHE:CE2	2.55	0.42
40:S:53:ASN:CG	40:S:54:ILE:H	2.27	0.42
40:S:103:GLU:HA	40:S:106:TYR:CD2	2.54	0.42
40:S:109:PRO:HB2	40:S:112:ASN:CB	2.40	0.42
40:S:196:ASP:OD2	40:S:250:GLU:HA	2.20	0.42
40:S:252:GLN:C	40:S:254:ALA:H	2.28	0.42
42:U:71:LYS:HG3	42:U:72:ASN:O	2.20	0.42
42:U:83:PRO:C	42:U:85:GLU:H	2.27	0.42
42:U:125:VAL:HG23	42:U:125:VAL:O	2.20	0.42
43:V:34:SER:O	43:V:37:ALA:HB3	2.20	0.42
49:b:128:GLY:C	49:b:130:GLU:H	2.27	0.42
44:M:57:GLU:O	44:M:58:PHE:HB3	2.20	0.42
44:M:60:PHE:HE2	44:M:62:ILE:HG13	1.85	0.42
58:k:59:VAL:CG2	58:k:182:LEU:HD22	2.50	0.42
58:k:404:ALA:HB1	58:k:408:ARG:NH1	2.32	0.42
59:l:67:HIS:ND1	59:l:70:ARG:NH2	2.68	0.42
59:l:213:HIS:CE1	59:l:217:LYS:HD2	2.55	0.42
60:m:236:ILE:O	60:m:240:MET:HG2	2.20	0.42
61:o:79:GLU:HB3	61:o:80:MET:O	2.19	0.42
63:q:31:LEU:HD23	63:q:31:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:w:37:VAL:HG21	58:w:106:LEU:HD13	2.01	0.42
58:w:89:TYR:CE2	58:w:96:ALA:HB3	2.54	0.42
59:x:67:HIS:ND1	59:x:70:ARG:NH2	2.68	0.42
59:x:264:ILE:HG22	59:x:317:SER:HA	2.02	0.42
60:y:135:TRP:O	60:y:135:TRP:CG	2.73	0.42
2:1:171:GLN:NE2	2:1:171:GLN:CA	2.83	0.42
2:1:184:MET:HE2	2:1:293:PHE:HD1	1.83	0.42
2:1:236:ILE:CD1	2:1:259:PHE:CE2	3.03	0.42
2:1:311:THR:HG22	43:V:51:MET:HG3	2.02	0.42
3:9:112:VAL:O	3:9:113:TYR:C	2.62	0.42
7:6:64:SER:OG	50:c:96:THR:HA	2.19	0.42
7:6:516:PRO:HB3	52:f:30:TRP:CD1	2.55	0.42
70:2:401:3PE:H371	70:2:401:3PE:C2A	2.50	0.42
10:C3:311:ILE:HG21	10:C3:311:ILE:HD13	1.75	0.42
12:A9:146:TRP:CE2	16:A6:17:ARG:HB2	2.55	0.42
16:A6:42:ARG:NH1	16:A6:74:ARG:NH2	2.68	0.42
18:C2:35:TYR:O	18:C2:39:VAL:HB	2.19	0.42
20:B3:13:TYR:O	20:B3:14:GLY:C	2.63	0.42
23:A:125:PRO:HG3	23:A:174:THR:CG2	2.50	0.42
23:A:133:GLN:O	23:A:135:GLY:N	2.53	0.42
23:A:275:PRO:HB3	23:A:286:ILE:HB	2.01	0.42
23:A:310:GLU:HG2	23:A:311:LYS:N	2.34	0.42
23:A:381:LEU:HG	23:A:664:TYR:HB3	2.02	0.42
23:A:691:ILE:HG23	23:A:692:LYS:N	2.34	0.42
24:B:78:SER:O	24:B:79:ASN:CG	2.63	0.42
24:B:228:ARG:NH2	24:B:233:HIS:HD2	2.18	0.42
24:B:378:LEU:HD12	24:B:378:LEU:N	2.35	0.42
25:C:86:LEU:HB2	25:C:143:ILE:HG13	2.01	0.42
27:E:107:PRO:O	27:E:108:SER:C	2.63	0.42
29:G:154:LYS:HB3	29:G:155:PRO:CD	2.49	0.42
31:I:55:ARG:NH1	42:U:127:TYR:HA	2.34	0.42
39:R:171:ASN:O	39:R:181:LEU:HD21	2.18	0.42
48:a:53:ASP:OD1	48:a:53:ASP:N	2.50	0.42
51:d:63:LEU:HD12	51:d:66:PHE:HB3	2.01	0.42
51:d:66:PHE:O	51:d:70:LYS:HG2	2.19	0.42
53:h:127:LYS:O	53:h:131:ALA:N	2.53	0.42
55:j:56:ALA:O	55:j:57:GLY:C	2.61	0.42
57:e:48:ARG:HA	57:e:49:ALA:HA	1.46	0.42
59:l:52:LYS:NZ	59:l:203:ARG:HG2	2.34	0.42
59:l:245:ARG:HA	59:l:426:ALA:O	2.20	0.42
61:o:70:VAL:CA	61:o:83:ARG:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:o:233:ARG:HD3	64:r:17:SER:HB3	2.02	0.42
62:p:33:LYS:O	62:p:36:SER:N	2.52	0.42
63:q:28:LYS:HA	63:q:80:TRP:CG	2.55	0.42
58:w:57:TYR:CE2	58:w:61:HIS:HE1	2.38	0.42
58:w:428:ILE:O	58:w:430:GLN:N	2.53	0.42
59:x:213:HIS:CE1	59:x:217:LYS:HD2	2.55	0.42
59:x:347:ILE:HA	59:x:351:ASN:HB3	2.01	0.42
2:1:37:PRO:HA	26:D:108:ARG:O	2.19	0.41
2:1:61:LEU:HD21	26:D:118:ARG:HD2	2.01	0.41
3:9:133:GLN:O	3:9:186:VAL:HG23	2.19	0.41
4:7:54:LEU:HD23	4:7:54:LEU:HA	1.85	0.41
4:7:148:SER:O	4:7:150:GLY:N	2.53	0.41
5:4:80:SER:HA	5:4:226:ALA:CB	2.50	0.41
5:4:160:LEU:HD23	5:4:160:LEU:HA	1.88	0.41
8:2:286:ALA:O	8:2:289:ASN:HB3	2.20	0.41
8:2:342:MET:O	55:j:82:MET:HG2	2.20	0.41
9:8:156:ILE:HD12	9:8:157:TYR:N	2.35	0.41
9:8:204:TYR:O	9:8:207:GLY:N	2.38	0.41
9:8:214:GLU:O	9:8:217:GLU:HB3	2.20	0.41
10:C3:314:ILE:HB	10:C3:315:PRO:CD	2.50	0.41
13:A7:130:PRO:O	13:A7:136:ALA:HB2	2.20	0.41
23:A:50:LEU:CG	23:A:60:ILE:HD11	2.50	0.41
23:A:94:MET:HE3	23:A:94:MET:HB2	1.92	0.41
23:A:253:VAL:HG11	23:A:596:TYR:CG	2.55	0.41
23:A:431:LEU:HD23	23:A:432:ILE:C	2.45	0.41
24:B:286:TYR:HE1	25:C:163:LYS:HB3	1.85	0.41
24:B:461:VAL:O	24:B:461:VAL:HG12	2.20	0.41
38:Q:69:GLU:HA	38:Q:72:ARG:HB3	2.01	0.41
39:R:177:SER:HA	39:R:178:SER:HA	1.85	0.41
40:S:272:LEU:HB3	40:S:275:ASN:CB	2.50	0.41
50:c:18:LEU:O	50:c:21:ARG:HB3	2.19	0.41
52:f:19:LEU:HA	52:f:22:ARG:NH2	2.35	0.41
55:j:38:GLY:HA2	55:j:41:SER:HB3	2.02	0.41
57:e:92:TRP:O	57:e:93:ASP:C	2.63	0.41
58:k:186:LEU:HD23	58:k:190:TYR:CE2	2.54	0.41
58:k:280:TYR:HA	58:k:284:TYR:CE2	2.51	0.41
59:l:156:GLN:O	59:l:160:ILE:HG12	2.19	0.41
64:r:49:ALA:O	64:r:50:PRO:C	2.63	0.41
58:w:16:VAL:O	58:w:205:HIS:NE2	2.52	0.41
59:x:200:THR:CG2	59:x:203:ARG:H	2.27	0.41
59:x:406:ALA:O	59:x:409:ASP:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A2:13:LEU:HD13	63:A2:13:LEU:HA	1.83	0.41
63:A2:28:LYS:HA	63:A2:80:TRP:CG	2.55	0.41
2:1:159:SER:HB3	2:1:317:GLN:HG2	2.01	0.41
2:1:169:GLN:HE21	2:1:174:LEU:HD12	1.84	0.41
3:9:42:ARG:NH1	23:A:199:GLY:HA2	2.35	0.41
5:4:6:ILE:HA	5:4:9:ILE:HG22	2.02	0.41
5:4:82:HIS:CE1	5:4:432:ARG:NH1	2.88	0.41
5:4:125:THR:O	5:4:126:LEU:HB2	2.20	0.41
7:6:122:LEU:HD12	7:6:122:LEU:HA	1.83	0.41
7:6:406:ALA:HB2	57:e:147:GLY:HA2	2.01	0.41
9:8:346:GLN:CD	9:8:440:ARG:HD3	2.45	0.41
10:C3:501:PRO:O	10:C3:502:TYR:C	2.63	0.41
23:A:121:LEU:HD23	23:A:121:LEU:HA	1.62	0.41
23:A:534:VAL:O	23:A:534:VAL:HG13	2.19	0.41
23:A:607:LYS:HE2	29:G:78:ARG:NH2	2.35	0.41
24:B:228:ARG:CZ	24:B:233:HIS:HD2	2.33	0.41
24:B:289:SER:C	24:B:290:GLY:O	2.63	0.41
25:C:155:ILE:HD13	25:C:155:ILE:HG21	1.84	0.41
30:H:21:GLN:HE21	30:H:31:SER:CB	2.34	0.41
35:N:94:MET:SD	35:N:99:PRO:HG2	2.59	0.41
40:S:47:LEU:HD12	40:S:48:ILE:N	2.34	0.41
40:S:191:VAL:O	40:S:193:VAL:HG23	2.21	0.41
44:W:103:HIS:C	44:W:105:MET:H	2.28	0.41
49:b:121:ILE:HG23	49:b:122:ALA:N	2.35	0.41
53:h:141:CYS:SG	56:g:162:ARG:HB3	2.60	0.41
57:e:37:LEU:H	57:e:77:LYS:CD	2.33	0.41
58:k:317:THR:HG22	58:k:318:GLY:N	2.35	0.41
59:l:78:LYS:HB2	59:l:131:GLU:HG3	2.02	0.41
61:o:27:ARG:O	61:o:31:GLN:HG2	2.20	0.41
58:w:281:ASP:HA	58:w:306:SER:CB	2.50	0.41
58:w:317:THR:HG22	58:w:318:GLY:N	2.35	0.41
59:x:78:LYS:HB2	59:x:131:GLU:HG3	2.02	0.41
59:x:370:MET:O	59:x:373:GLU:HG2	2.20	0.41
60:y:133:LEU:HB2	60:y:134:PRO:HD3	2.03	0.41
61:z:27:ARG:O	61:z:31:GLN:HG2	2.21	0.41
61:z:207:LYS:HD3	62:A1:49:TYR:OH	2.20	0.41
66:A4:21:ALA:HA	66:A4:24:TRP:HD1	1.85	0.41
1:3:77:TRP:NE1	2:1:318:THR:O	2.53	0.41
2:1:71:PHE:CZ	2:1:215:TYR:HE1	2.04	0.41
2:1:79:LEU:HD23	2:1:79:LEU:HA	1.80	0.41
2:1:108:MET:HE1	2:1:111:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:233:MET:C	2:1:236:ILE:HG23	2.44	0.41
5:4:246:ILE:O	5:4:248:LEU:N	2.54	0.41
6:5:89:TYR:CD1	6:5:91:GLN:NE2	2.88	0.41
7:6:385:PHE:HB3	46:Y:72:ILE:HD12	2.01	0.41
8:2:230:LEU:C	8:2:232:HIS:H	2.27	0.41
8:2:276:ILE:O	8:2:276:ILE:HG22	2.20	0.41
69:2:402:PC1:H362	69:2:402:PC1:H391	1.64	0.41
10:C3:430:PHE:O	10:C3:431:LEU:C	2.64	0.41
17:C0:65:PRO:HG2	17:C0:68:TRP:CG	2.55	0.41
23:A:82:ILE:HD12	23:A:82:ILE:HA	1.93	0.41
23:A:259:SER:CB	23:A:282:ASN:HD21	2.33	0.41
23:A:454:ASP:HB3	23:A:459:SER:OG	2.20	0.41
24:B:317:ASP:OD1	24:B:317:ASP:N	2.52	0.41
24:B:330:TYR:O	24:B:333:ARG:N	2.49	0.41
24:B:456:ILE:HA	24:B:456:ILE:HD13	1.70	0.41
26:D:137:LEU:O	26:D:138:ARG:C	2.64	0.41
37:P:19:ASP:OD1	37:P:19:ASP:N	2.53	0.41
40:S:225:ILE:HG13	40:S:226:GLU:N	2.34	0.41
41:T:13:PRO:CG	41:T:21:LYS:HD3	2.50	0.41
49:b:160:MET:CB	49:b:161:ARG:HA	2.33	0.41
72:b:201:CDL:H151	72:b:201:CDL:H122	1.48	0.41
44:M:43:ASP:OD1	44:M:44:SER:N	2.54	0.41
58:k:131:ARG:HE	58:k:175:ARG:HA	1.85	0.41
60:m:133:LEU:HB2	60:m:134:PRO:HD3	2.03	0.41
60:m:310:SER:OG	60:m:318:ARG:NH1	2.53	0.41
67:u:52:TRP:C	67:u:56:LYS:H	2.26	0.41
59:x:52:LYS:HD2	59:x:203:ARG:CG	2.50	0.41
59:x:156:GLN:O	59:x:160:ILE:HG12	2.19	0.41
59:x:182:ARG:HH11	59:x:185:LYS:CD	2.34	0.41
59:x:303:VAL:HG12	59:x:304:HIS:H	1.85	0.41
59:x:340:ALA:O	59:x:344:VAL:HG23	2.21	0.41
62:A1:150:ALA:HB3	62:A1:157:TYR:H	1.85	0.41
65:B7:73:LEU:HD12	65:B7:74:PHE:N	2.35	0.41
1:3:62:PHE:O	1:3:63:LEU:C	2.63	0.41
3:9:137:THR:HG22	3:9:138:THR:N	2.35	0.41
4:7:71:THR:C	4:7:73:ALA:H	2.28	0.41
5:4:60:SER:C	5:4:62:SER:H	2.21	0.41
5:4:74:PRO:O	5:4:78:MET:HE2	2.20	0.41
5:4:89:LEU:HD12	5:4:90:THR:HG23	2.02	0.41
5:4:95[B]:PHE:CE2	5:4:136:TRP:HD1	2.38	0.41
5:4:112:ALA:C	5:4:114:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:196:TRP:HB2	5:4:251:ASN:ND2	2.35	0.41
5:4:269:MET:HE1	5:4:396:MET:HB2	2.03	0.41
7:6:28:LYS:HD2	7:6:29:PRO:HD2	2.03	0.41
7:6:233:LEU:O	7:6:236:ALA:N	2.45	0.41
14:B4:79:LYS:HE2	14:B4:79:LYS:HB2	1.92	0.41
15:A5:86:GLY:O	15:A5:87:THR:O	2.37	0.41
23:A:111:LYS:HD3	37:P:53:TYR:CZ	2.55	0.41
23:A:117:MET:SD	23:A:142:GLN:HB2	2.60	0.41
23:A:380:ASP:O	23:A:382:ARG:N	2.46	0.41
23:A:435:PRO:HG3	23:A:444:HIS:ND1	2.35	0.41
24:B:100:GLU:HB2	24:B:108:LYS:HD3	2.03	0.41
24:B:382:PHE:O	24:B:382:PHE:CG	2.73	0.41
24:B:392:PRO:HA	25:C:244:PHE:CE2	2.55	0.41
26:D:82:LEU:C	26:D:84:PRO:HD3	2.45	0.41
27:E:130:ILE:HG12	27:E:145:TYR:CD1	2.55	0.41
28:F:85:PHE:O	28:F:88:LEU:HB2	2.20	0.41
29:G:98:LYS:HD3	29:G:125:VAL:HG21	2.02	0.41
34:L:45:ILE:HD12	34:L:81:LEU:HD22	2.00	0.41
36:O:44:PRO:O	36:O:47:VAL:N	2.53	0.41
39:R:125:VAL:HA	39:R:162:GLU:O	2.21	0.41
39:R:128:ASN:ND2	39:R:130:VAL:HG12	2.35	0.41
40:S:215:MET:O	40:S:217:ILE:N	2.53	0.41
46:Y:73:LEU:HD11	47:Z:78:PHE:O	2.19	0.41
53:h:87:MET:O	53:h:91:PHE:HD2	2.04	0.41
56:g:101:GLU:O	56:g:104:ASN:N	2.53	0.41
58:k:428:ILE:O	58:k:430:GLN:N	2.53	0.41
59:l:398:VAL:O	59:l:402:ILE:HG13	2.21	0.41
61:o:219:VAL:O	61:o:223:LYS:N	2.34	0.41
65:s:62:LEU:HD23	65:s:65:ARG:HD3	2.02	0.41
58:w:32:GLN:HG2	58:w:34:THR:H	1.85	0.41
60:y:245:PHE:CZ	61:z:209:LEU:HD11	2.55	0.41
61:z:41:HIS:NE2	81:z:301:HEC:C1D	2.82	0.41
62:A1:91:TRP:O	62:A1:93:GLY:N	2.53	0.41
2:1:117:LEU:HD12	2:1:136:VAL:HG21	2.03	0.41
2:1:187:ILE:HD11	27:E:63:TRP:CH2	2.56	0.41
7:6:126:ILE:O	7:6:129:LEU:HB3	2.21	0.41
7:6:213:LEU:HD13	7:6:273:ILE:HD13	2.03	0.41
7:6:329:ILE:H	7:6:329:ILE:HD12	1.84	0.41
8:2:177:LYS:O	8:2:180:ALA:N	2.53	0.41
8:2:337:LEU:HD12	8:2:337:LEU:O	2.20	0.41
69:2:402:PC1:H2B2	69:2:402:PC1:H281	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C3:264:LYS:NZ	11:C1:56:MET:HE2	2.36	0.41
11:C1:146:MET:SD	11:C1:189:PRO:HB3	2.60	0.41
19:B2:5:VAL:O	19:B2:9:GLN:HG3	2.21	0.41
23:A:121:LEU:CD1	24:B:376:GLU:OE2	2.68	0.41
23:A:145:MET:SD	25:C:241:TRP:HB2	2.60	0.41
24:B:133:LEU:O	24:B:134:PRO:C	2.64	0.41
25:C:167:TRP:NE1	25:C:170:ARG:HH12	2.18	0.41
25:C:192:ASP:CG	25:C:193:TYR:N	2.79	0.41
26:D:191:GLU:OE2	27:E:86:TYR:CE1	2.73	0.41
31:I:80:VAL:HG13	31:I:81:GLY:N	2.36	0.41
72:J:101:CDL:H571	72:J:101:CDL:H541	1.66	0.41
33:K:42:VAL:O	33:K:46:LYS:HB2	2.20	0.41
36:O:75:ASP:OD2	36:O:76:PRO:O	2.39	0.41
56:g:5:TRP:CD1	56:g:10:TYR:HB2	2.55	0.41
58:k:16:VAL:O	58:k:205:HIS:NE2	2.52	0.41
58:k:40:TRP:CZ2	58:k:377:GLU:HA	2.56	0.41
58:k:131:ARG:NE	58:k:175:ARG:HA	2.35	0.41
58:k:281:ASP:HA	58:k:306:SER:CB	2.50	0.41
59:l:264:ILE:HG22	59:l:317:SER:HA	2.02	0.41
59:l:346:THR:HA	59:l:349:GLN:OE1	2.20	0.41
60:m:71:ARG:CZ	61:o:45:TYR:O	2.69	0.41
60:m:301:LEU:HA	60:m:304:ILE:HD12	2.02	0.41
60:m:375:LYS:HE3	60:m:375:LYS:HB3	1.80	0.41
61:o:137:PRO:HB3	61:o:141:VAL:HG13	2.03	0.41
62:p:52:LYS:HD2	66:t:34:TRP:CZ2	2.56	0.41
63:q:21:TYR:CG	63:q:83:TYR:HD1	2.39	0.41
64:r:2:ARG:NH2	64:r:6:HIS:CE1	2.88	0.41
64:r:79:ASN:CB	65:s:52:GLU:HB2	2.49	0.41
66:t:16:ASN:O	66:t:17:TRP:HB2	2.20	0.41
66:t:24:TRP:HA	66:t:27:VAL:HB	2.02	0.41
58:w:39:VAL:O	58:w:96:ALA:HA	2.21	0.41
58:w:408:ARG:HE	66:A4:15:ARG:HH21	1.67	0.41
59:x:325:TYR:HB3	68:B5:57:GLY:CA	2.50	0.41
60:y:49:LEU:O	60:y:52:ALA:N	2.54	0.41
80:y:402:HEM:HBB2	80:y:402:HEM:CMB	2.49	0.41
61:z:230:LEU:HA	61:z:230:LEU:HD23	1.88	0.41
63:A2:21:TYR:CG	63:A2:83:TYR:HD1	2.39	0.41
1:3:88:LEU:CD2	2:1:309:ILE:HD12	2.51	0.41
3:9:133:GLN:HB2	3:9:187:GLN:HB3	2.03	0.41
3:9:138:THR:O	3:9:142:LEU:HG	2.21	0.41
4:7:21:SER:OG	6:5:14:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:171:ILE:H	4:7:171:ILE:HG13	1.60	0.41
5:4:129:THR:HG21	5:4:236:LEU:HD11	2.02	0.41
5:4:178:MET:HE3	5:4:178:MET:HB2	1.96	0.41
7:6:481:THR:HG22	51:d:92:HIS:HD2	1.86	0.41
8:2:203:LEU:HD23	8:2:203:LEU:C	2.46	0.41
8:2:220:MET:HE3	8:2:220:MET:HB3	1.86	0.41
8:2:251:MET:HE3	8:2:293:TYR:OH	2.21	0.41
8:2:257:LEU:HD22	8:2:331:VAL:HG13	2.02	0.41
9:8:297:LYS:HB2	9:8:333:GLU:HB2	2.03	0.41
10:C3:240:HIS:O	10:C3:241:PRO:C	2.64	0.41
76:C3:602:HEA:HH C	76:C3:602:HEA:H122	2.02	0.41
11:C1:164:ALA:HB2	11:C1:171:LYS:HD3	2.03	0.41
12:A9:154:GLY:CA	15:A5:6:VAL:HG22	2.48	0.41
15:A5:16:LEU:O	15:A5:20:VAL:HG13	2.21	0.41
15:A5:77:GLY:O	15:A5:90:LYS:NZ	2.54	0.41
17:C0:20:PHE:N	17:C0:21:PRO:HD3	2.35	0.41
23:A:141:ASP:HB3	25:C:241:TRP:CD1	2.55	0.41
23:A:226:CYS:SG	74:A:802:SF4:S1	3.18	0.41
23:A:362:ASP:HB2	33:K:71:PHE:HD1	1.85	0.41
70:B:501:3PE:H381	70:B:501:3PE:H351	1.61	0.41
29:G:139:GLU:OE2	29:G:145:TYR:CE2	2.71	0.41
35:N:86:ASN:OD1	35:N:86:ASN:N	2.46	0.41
36:O:37:ARG:HH21	44:M:48:VAL:HG13	1.85	0.41
37:P:45:PRO:O	37:P:46:SER:OG	2.23	0.41
42:U:62:VAL:HG23	42:U:86:TRP:HZ3	1.85	0.41
48:a:84:THR:OG1	48:a:86:THR:HG22	2.20	0.41
49:b:161:ARG:HA	49:b:161:ARG:HD2	1.80	0.41
57:e:47:GLU:CB	57:e:64:PRO:HG2	2.50	0.41
58:k:30:SER:N	58:k:201:GLY:O	2.48	0.41
58:k:37:VAL:HG21	58:k:106:LEU:HD13	2.01	0.41
58:k:39:VAL:O	58:k:96:ALA:HA	2.21	0.41
59:l:52:LYS:HD2	59:l:203:ARG:CG	2.49	0.41
60:m:135:TRP:O	60:m:135:TRP:CG	2.73	0.41
61:o:204:MET:O	61:o:208:MET:N	2.30	0.41
59:x:198:HIS:NE2	59:x:232:LEU:HD12	2.36	0.41
59:x:236:LYS:C	59:x:238:LYS:H	2.28	0.41
59:x:312:PHE:HB2	68:B5:57:GLY:HA2	2.02	0.41
59:x:315:SER:HA	59:x:320:GLY:CA	2.39	0.41
59:x:398:VAL:O	59:x:402:ILE:HG13	2.21	0.41
60:y:4:ILE:HD13	60:y:4:ILE:HA	1.90	0.41
60:y:100:ARG:NH2	80:y:402:HEM:HBD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:y:310:SER:OG	60:y:318:ARG:NH1	2.54	0.41
60:y:373:GLU:HA	60:y:376:LEU:HB2	2.03	0.41
64:A3:2:ARG:NH2	64:A3:6:HIS:CE1	2.88	0.41
65:B7:43:ARG:HD2	65:B7:47:ARG:NH1	2.36	0.41
1:3:61:THR:O	1:3:65:PHE:HD2	2.03	0.41
2:1:281:ARG:HG3	24:B:445:ALA:HB3	2.02	0.41
3:9:133:GLN:HG3	3:9:172:ILE:HD11	2.02	0.41
3:9:243:PHE:HD2	9:8:257:ARG:HB2	1.85	0.41
5:4:271:MET:HE3	7:6:549:ALA:CB	2.51	0.41
5:4:373:ILE:HD12	5:4:373:ILE:H	1.86	0.41
7:6:75:LYS:HB3	7:6:75:LYS:HE3	1.74	0.41
7:6:251:THR:O	7:6:253:VAL:N	2.48	0.41
8:2:52:ALA:HB2	8:2:123:PRO:CD	2.49	0.41
9:8:228:PRO:HB2	9:8:229:PHE:O	2.21	0.41
10:C3:168:ILE:CG2	10:C3:189:MET:HG3	2.51	0.41
15:A5:6:VAL:HA	15:A5:7:PRO:HD3	1.91	0.41
15:A5:10:GLU:HG2	15:A5:25:ARG:HH22	1.86	0.41
17:C0:24:ASN:HD22	17:C0:25:GLN:N	2.18	0.41
23:A:79:LEU:HA	23:A:79:LEU:HD23	1.86	0.41
23:A:125:PRO:O	23:A:127:ASP:N	2.52	0.41
23:A:154:LEU:H	23:A:154:LEU:HG	1.66	0.41
23:A:447:ASP:O	23:A:448:SER:HB3	2.20	0.41
23:A:454:ASP:HB2	23:A:460:HIS:HE1	1.86	0.41
24:B:53:TYR:CB	24:B:57:GLU:HG3	2.51	0.41
24:B:79:ASN:ND2	24:B:102:SER:HA	2.35	0.41
24:B:81:THR:O	24:B:82:LEU:C	2.64	0.41
24:B:140:ASP:OD1	24:B:140:ASP:N	2.50	0.41
24:B:182:ASN:ND2	24:B:403:PRO:HG2	2.36	0.41
25:C:46:ARG:CZ	25:C:46:ARG:HB2	2.50	0.41
26:D:197:ILE:C	26:D:199:GLN:N	2.76	0.41
27:E:192:ASN:O	27:E:195:ASP:N	2.54	0.41
27:E:192:ASN:O	27:E:196:LYS:N	2.53	0.41
30:H:78:ALA:HB1	43:V:104:TRP:CH2	2.55	0.41
35:N:114:TRP:HB3	35:N:115:PRO:HD3	2.02	0.41
38:Q:48:TRP:HH2	49:b:186:THR:H	1.68	0.41
38:Q:82:PHE:HD1	38:Q:107:PHE:CE1	2.39	0.41
39:R:217:PHE:CD1	39:R:217:PHE:N	2.88	0.41
40:S:198:PRO:HB2	40:S:201:GLU:HB3	2.02	0.41
40:S:333:GLU:C	40:S:335:VAL:N	2.79	0.41
49:b:133:TYR:OH	56:g:87:GLU:HG2	2.21	0.41
53:h:111:ASP:N	53:h:111:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:M:35:HIS:H	44:M:39:ASP:CG	2.28	0.41
58:k:307:PHE:HB3	58:k:324:PHE:HB3	2.02	0.41
58:k:405:ARG:HH21	66:t:15:ARG:NH2	2.19	0.41
59:l:168:TYR:CE2	59:l:321:LEU:HD11	2.55	0.41
59:l:340:ALA:O	59:l:344:VAL:HG23	2.21	0.41
59:l:342:ASN:O	59:l:345:LYS:HB2	2.20	0.41
59:l:370:MET:O	59:l:373:GLU:HG2	2.20	0.41
61:o:55:CYS:SG	67:u:52:TRP:HB3	2.60	0.41
61:o:80:MET:CG	61:o:81:PHE:N	2.83	0.41
62:p:9:ASP:OD1	62:p:10:PHE:N	2.53	0.41
64:r:36:ASN:O	64:r:40:ARG:HG2	2.19	0.41
65:s:50:THR:HG22	65:s:51:GLU:H	1.84	0.41
58:w:15:GLN:HB3	58:w:205:HIS:CG	2.56	0.41
58:w:436:ARG:HD3	58:w:436:ARG:HA	1.88	0.41
59:x:338:LYS:O	59:x:342:ASN:N	2.26	0.41
59:x:397:THR:O	59:x:400:GLN:HB2	2.21	0.41
60:y:110:LEU:O	60:y:113:TRP:HB3	2.20	0.41
60:y:133:LEU:HB2	80:y:401:HEM:O2D	2.21	0.41
60:y:185:LEU:HD12	60:y:185:LEU:HA	1.87	0.41
64:A3:74:PRO:HB3	64:A3:79:ASN:ND2	2.34	0.41
3:9:92:TRP:CZ3	3:9:94:PRO:HG3	2.55	0.41
4:7:148:SER:O	4:7:149:TYR:C	2.64	0.41
5:4:121:LEU:HA	5:4:124:ALA:HB2	2.02	0.41
6:5:62:ILE:O	6:5:62:ILE:HG22	2.21	0.41
8:2:218:MET:HE3	8:2:218:MET:HB3	1.93	0.41
10:C3:23:GLY:HA3	10:C3:73:ILE:HG13	2.03	0.41
12:A9:6:HIS:CD2	12:A9:8:TYR:HB2	2.55	0.41
13:A7:86:MET:O	20:B3:25:CYS:HB2	2.20	0.41
19:B2:12:PHE:O	19:B2:23:LYS:HE2	2.21	0.41
22:A8:13:LYS:HD3	22:A8:13:LYS:N	2.35	0.41
22:A8:19:LEU:HD23	22:A8:19:LEU:C	2.45	0.41
23:A:198:THR:O	23:A:198:THR:OG1	2.37	0.41
24:B:308:TYR:OH	24:B:400:ILE:HB	2.20	0.41
25:C:181:ALA:O	25:C:182:ASN:C	2.62	0.41
27:E:37:THR:N	37:P:104:TRP:CD1	2.89	0.41
27:E:135:ARG:NH1	31:I:68:ALA:O	2.54	0.41
33:K:65:LEU:HD12	33:K:66:TRP:H	1.86	0.41
35:N:47:TYR:HE1	37:P:92:LYS:CB	2.33	0.41
38:Q:142:TYR:CD1	38:Q:143:HIS:N	2.89	0.41
55:j:51:ARG:HA	55:j:51:ARG:HD3	1.88	0.41
56:g:125:CYS:C	56:g:127:LYS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:k:15:GLN:HB3	58:k:205:HIS:CG	2.56	0.41
59:l:97:SER:HA	68:v:70:LEU:CB	2.50	0.41
60:m:100:ARG:NH2	80:m:402:HEM:HBD1	2.36	0.41
60:m:110:LEU:O	60:m:113:TRP:HB3	2.21	0.41
63:q:99:ARG:CZ	63:q:99:ARG:HB2	2.50	0.41
64:r:3:GLN:O	64:r:7:LEU:HG	2.21	0.41
65:s:43:ARG:NE	65:s:52:GLU:OE2	2.52	0.41
58:w:59:VAL:CG2	58:w:182:LEU:HD22	2.50	0.41
58:w:277:ILE:HD11	58:w:345:LEU:HD11	2.01	0.41
58:w:380:GLY:O	58:w:384:LEU:HD13	2.21	0.41
65:B7:50:THR:HG22	65:B7:51:GLU:H	1.84	0.41
66:A4:16:ASN:O	66:A4:19:PRO:HD2	2.21	0.41
1:3:35:SER:HA	1:3:36:PRO:HD3	1.84	0.41
1:3:82:ALA:O	1:3:83:ASN:C	2.62	0.41
1:3:102:LEU:O	1:3:103:ALA:C	2.64	0.41
2:1:174:LEU:HA	2:1:174:LEU:HD23	1.87	0.41
3:9:134:VAL:HG11	3:9:149:LEU:HB2	2.03	0.41
3:9:193:TYR:CD1	3:9:216:PRO:HA	2.56	0.41
4:7:152:TRP:CG	30:H:14:LEU:HD22	2.55	0.41
5:4:150:LEU:O	5:4:152:TYR:N	2.54	0.41
5:4:187:HIS:CG	5:4:188:ASN:N	2.89	0.41
5:4:343:ILE:O	5:4:346:ARG:HG3	2.21	0.41
5:4:445:LEU:HD12	5:4:446:LEU:N	2.35	0.41
5:4:452:LYS:HD2	5:4:455:LEU:HD13	2.02	0.41
8:2:84:TRP:CD1	30:H:19:THR:O	2.74	0.41
9:8:210:THR:HG22	9:8:210:THR:O	2.20	0.41
10:C3:337:ALA:HB2	10:C3:394:VAL:HG23	2.03	0.41
11:C1:100:MET:HE3	11:C1:157:GLU:HG3	2.01	0.41
12:A9:160:LEU:HD12	12:A9:160:LEU:HA	1.94	0.41
12:A9:224:LYS:NZ	12:A9:226:HIS:HE2	2.18	0.41
13:A7:24:LEU:HA	13:A7:25:PRO:HD2	1.93	0.41
13:A7:127:LYS:O	13:A7:130:PRO:HD3	2.20	0.41
16:A6:77:PRO:HA	16:A6:82:TYR:HA	2.02	0.41
22:A8:35:TYR:HD2	22:A8:36:HIS:CE1	2.39	0.41
23:A:50:LEU:HD23	23:A:50:LEU:O	2.21	0.41
23:A:107:GLU:O	23:A:111:LYS:HG2	2.21	0.41
23:A:139:LEU:HD23	23:A:139:LEU:HA	1.33	0.41
23:A:408:ARG:HD3	23:A:409:PHE:CE2	2.56	0.41
23:A:493:VAL:O	23:A:496:ILE:HG22	2.20	0.41
23:A:591:GLU:OE1	23:A:591:GLU:N	2.54	0.41
24:B:71:PRO:CD	24:B:72:PRO:HD3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:221:ARG:HG3	26:D:95:GLU:OE2	2.20	0.41
24:B:438:MET:HE3	24:B:438:MET:HB2	1.96	0.41
25:C:62:ALA:O	25:C:64:GLY:N	2.54	0.41
25:C:127:ARG:HB3	25:C:128:PHE:CD1	2.56	0.41
26:D:97:MET:O	26:D:100:ALA:N	2.50	0.41
26:D:142:ASP:O	26:D:144:MET:N	2.54	0.41
29:G:111:LEU:HD13	39:R:100:LEU:HD23	2.02	0.41
29:G:126:LEU:HA	29:G:126:LEU:HD23	1.82	0.41
32:J:41:TYR:O	32:J:44:GLN:N	2.53	0.41
34:L:31:ILE:C	34:L:33:PRO:HD2	2.46	0.41
36:O:101:THR:O	36:O:101:THR:HG22	2.20	0.41
40:S:103:GLU:HA	40:S:106:TYR:HD2	1.85	0.41
42:U:123:GLN:O	42:U:124:TYR:HB3	2.21	0.41
45:X:23:GLY:O	45:X:26:LEU:N	2.53	0.41
52:f:166:LEU:HD12	52:f:167:TRP:HB3	2.03	0.41
53:h:82:VAL:HA	53:h:85:TRP:HD1	1.86	0.41
56:g:131:GLN:O	56:g:135:VAL:HG23	2.21	0.41
44:M:72:CYS:SG	44:M:74:GLN:HB2	2.61	0.41
58:k:319:LEU:HD23	58:k:319:LEU:HA	1.71	0.41
58:k:380:GLY:O	58:k:384:LEU:HD13	2.21	0.41
59:l:168:TYR:CZ	59:l:172:LEU:HD12	2.56	0.41
59:l:303:VAL:HG12	59:l:304:HIS:H	1.85	0.41
59:l:347:ILE:HA	59:l:351:ASN:HB3	2.01	0.41
60:m:18:PHE:O	60:m:21:LEU:N	2.46	0.41
60:m:22:PRO:HG3	64:r:4:PHE:CE2	2.56	0.41
60:m:373:GLU:HA	60:m:376:LEU:HB2	2.03	0.41
61:o:22:ASP:OD1	61:o:23:HIS:N	2.54	0.41
61:o:41:HIS:HB3	61:o:113:LEU:HG	2.03	0.41
61:o:42:SER:HB3	61:o:94:PRO:HD2	2.03	0.41
61:o:231:LYS:HA	63:q:70:MET:HE3	2.03	0.41
62:p:147:ILE:HA	62:p:148:ALA:C	2.45	0.41
62:p:147:ILE:N	62:p:148:ALA:HB3	2.36	0.41
62:p:151:GLY:N	62:p:152:ASP:HA	2.35	0.41
65:s:43:ARG:HD2	65:s:47:ARG:NH1	2.36	0.41
58:w:15:GLN:HE21	58:w:205:HIS:CB	2.34	0.41
58:w:40:TRP:CZ2	58:w:377:GLU:HA	2.56	0.41
58:w:416:TYR:HB3	67:B6:15:ARG:NH2	2.33	0.41
59:x:46:ARG:HH12	59:x:376:GLU:HG3	1.86	0.41
59:x:102:ARG:HG2	59:x:176:LEU:HD21	2.03	0.41
59:x:152:LEU:HA	59:x:152:LEU:HD23	1.81	0.41
59:x:154:ASN:ND2	68:B5:76:VAL:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:x:342:ASN:O	59:x:345:LYS:HB2	2.20	0.41
59:x:346:THR:HA	59:x:349:GLN:OE1	2.20	0.41
59:x:366:ALA:HB1	59:x:370:MET:HE2	2.03	0.41
61:z:62:LYS:HE2	61:z:62:LYS:HB2	1.90	0.41
62:A1:11:SER:O	62:A1:12:ASP:C	2.63	0.41
63:A2:33:ARG:HH22	63:A2:91:GLU:CD	2.24	0.41
67:B6:52:TRP:C	67:B6:56:LYS:H	2.26	0.41
2:1:220:PHE:O	2:1:220:PHE:CG	2.74	0.41
4:7:86:ASN:OD1	4:7:88:ALA:CB	2.68	0.41
5:4:14:LEU:HD21	5:4:30:HIS:CD2	2.56	0.41
5:4:435:ALA:O	5:4:438:SER:OG	2.28	0.41
6:5:17:VAL:O	6:5:20:LEU:N	2.54	0.41
6:5:89:TYR:C	6:5:91:GLN:H	2.28	0.41
6:5:96:LEU:HD23	24:B:61:TRP:HB2	2.02	0.41
7:6:103:PHE:CD1	7:6:341:MET:HG3	2.56	0.41
7:6:227:PHE:H	7:6:284:THR:HG22	1.85	0.41
7:6:240:PRO:HD2	7:6:243:VAL:HG21	2.02	0.41
8:2:141:VAL:O	8:2:144:GLN:N	2.53	0.41
8:2:202:LEU:O	8:2:205:LEU:N	2.52	0.41
8:2:261:MET:HE2	8:2:337:LEU:CD1	2.48	0.41
8:2:266:ILE:HD13	8:2:266:ILE:HG21	1.82	0.41
11:C1:5:MET:CE	20:B3:42:PRO:HA	2.45	0.41
12:A9:188:ILE:H	12:A9:188:ILE:HG13	1.62	0.41
23:A:139:LEU:HD11	23:A:177:ILE:CG2	2.50	0.41
23:A:497:ALA:CB	23:A:513:MET:HB2	2.50	0.41
23:A:543:LYS:HG3	23:A:544:MET:N	2.36	0.41
24:B:339:GLN:O	24:B:342:ARG:HB3	2.20	0.41
25:C:124:ARG:C	25:C:126:ASN:H	2.29	0.41
26:D:146:GLU:O	26:D:148:ARG:HG2	2.21	0.41
27:E:174:GLU:O	27:E:175:PHE:CG	2.74	0.41
28:F:96:ARG:O	28:F:98:PRO:HD3	2.21	0.41
35:N:27:LEU:O	35:N:31:ILE:N	2.46	0.41
38:Q:61:LYS:O	38:Q:65:GLN:HB2	2.21	0.41
39:R:168:SER:HB3	39:R:201:ILE:O	2.21	0.41
39:R:191:VAL:HG12	39:R:195:PHE:CZ	2.56	0.41
40:S:102:LEU:HA	40:S:105:PHE:HE2	1.85	0.41
40:S:233:PHE:O	40:S:233:PHE:CG	2.74	0.41
44:M:64:ASP:C	44:M:66:ASP:N	2.78	0.41
58:k:46:ARG:NE	58:k:231:LEU:HD22	2.35	0.41
59:l:182:ARG:HH11	59:l:185:LYS:CD	2.34	0.41
59:l:359:ALA:O	59:l:363:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:397:THR:O	59:l:400:GLN:HB2	2.21	0.41
60:m:197:LEU:O	60:m:200:LEU:HB3	2.21	0.41
60:m:272:TRP:CD1	60:m:272:TRP:H	2.39	0.41
61:o:5:LEU:HD12	61:o:6:HIS:H	1.85	0.41
61:o:131:LEU:HD23	61:o:131:LEU:HA	1.92	0.41
61:o:165:TYR:CE2	61:o:168:VAL:HG22	2.56	0.41
65:s:15:ASP:OD2	65:s:18:THR:HG23	2.20	0.41
58:w:148:VAL:CG1	58:w:152:TYR:HE2	2.33	0.41
59:x:295:LEU:HD21	59:x:309:VAL:HG12	2.03	0.41
59:x:325:TYR:H	68:B5:57:GLY:CA	2.34	0.41
62:A1:166:ASP:CB	62:A1:170:ARG:H	2.34	0.41
66:A4:28:GLY:O	66:A4:32:LEU:N	2.43	0.41
1:3:88:LEU:HD11	2:1:309:ILE:CD1	2.51	0.40
1:3:106:TRP:HZ2	69:3:200:PC1:H143	1.86	0.40
4:7:33:LEU:O	4:7:37:GLY:N	2.45	0.40
5:4:114:GLU:OE2	5:4:117:LEU:HG	2.21	0.40
5:4:197:LEU:HD11	5:4:201:MET:HE2	2.02	0.40
5:4:306:PRO:HD3	56:g:150:TYR:N	2.36	0.40
6:5:62:ILE:HD12	6:5:62:ILE:HG23	1.87	0.40
7:6:150:MET:HE2	7:6:150:MET:HA	2.02	0.40
7:6:216:LEU:HD13	7:6:263:PHE:CE2	2.56	0.40
7:6:261:ILE:HD13	7:6:326:PHE:HB2	2.01	0.40
8:2:14:MET:HB3	8:2:133:TRP:CH2	2.55	0.40
9:8:124:THR:C	9:8:126:LYS:H	2.29	0.40
14:B4:21:LYS:O	14:B4:57:ARG:NH1	2.53	0.40
14:B4:93:LEU:HD23	14:B4:93:LEU:HA	1.88	0.40
23:A:168:LEU:HD22	23:A:292:PHE:CE2	2.56	0.40
23:A:189:ILE:H	23:A:189:ILE:HG13	1.64	0.40
23:A:223:ILE:H	23:A:223:ILE:HG12	1.52	0.40
24:B:99:MET:HE3	24:B:99:MET:HB2	1.88	0.40
24:B:292:MET:HE2	24:B:431:HIS:CD2	2.56	0.40
27:E:133:GLU:HG3	27:E:134:PRO:HD2	2.02	0.40
39:R:150:GLN:O	39:R:154:GLN:N	2.54	0.40
43:V:76:GLN:O	43:V:79:LYS:N	2.54	0.40
48:a:105:PHE:O	48:a:108:ASP:N	2.54	0.40
72:b:201:CDL:H831	72:b:201:CDL:H802	1.79	0.40
50:c:17:GLU:O	50:c:21:ARG:HB2	2.21	0.40
50:c:40:VAL:HA	50:c:41:SER:HA	1.90	0.40
56:g:120:SER:C	56:g:122:ARG:N	2.78	0.40
58:k:358:LYS:HB2	58:k:358:LYS:HE3	1.83	0.40
59:l:33:LEU:HB3	59:l:201:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:l:99:THR:O	59:l:106:ALA:N	2.36	0.40
59:l:128:THR:C	59:l:130:PRO:HD3	2.46	0.40
60:m:49:LEU:O	60:m:52:ALA:N	2.54	0.40
60:m:137:GLN:NE2	60:m:141:TRP:CD1	2.86	0.40
60:m:365:LEU:H	60:m:365:LEU:HG	1.65	0.40
62:p:9:ASP:OD1	62:p:11:SER:N	2.28	0.40
67:u:5:LEU:O	67:u:9:LEU:N	2.48	0.40
67:u:42:ILE:O	67:u:46:ILE:HG13	2.21	0.40
58:w:186:LEU:HD23	58:w:190:TYR:CE2	2.54	0.40
59:x:33:LEU:HB3	59:x:201:SER:O	2.21	0.40
59:x:128:THR:C	59:x:130:PRO:HD3	2.46	0.40
59:x:303:VAL:CG1	59:x:304:HIS:N	2.84	0.40
60:y:64:SER:O	60:y:67:THR:HB	2.22	0.40
61:z:41:HIS:HB3	61:z:113:LEU:HG	2.03	0.40
61:z:128:PHE:HD1	61:z:187:CYS:SG	2.45	0.40
69:3:200:PC1:H142	34:L:19:LEU:HD23	2.03	0.40
2:1:36:GLY:HA2	26:D:108:ARG:HD3	2.03	0.40
2:1:236:ILE:O	2:1:236:ILE:CD1	2.69	0.40
3:9:178:GLY:N	9:8:119:GLU:OE2	2.54	0.40
5:4:375:LEU:HD23	5:4:375:LEU:HA	1.83	0.40
7:6:45:ILE:HD12	7:6:45:ILE:HA	1.97	0.40
7:6:224:SER:O	7:6:310:LEU:HD13	2.21	0.40
7:6:502:LEU:HD22	47:Z:63:PHE:CG	2.56	0.40
8:2:127:GLY:HA2	8:2:128:LEU:CB	2.51	0.40
8:2:139:MET:HE3	8:2:190:MET:SD	2.60	0.40
8:2:150:ASN:HD21	8:2:153:LEU:HD22	1.86	0.40
9:8:207:GLY:HA2	73:8:501:FMN:C9	2.52	0.40
10:C3:34:SER:HB3	10:C3:61:HIS:CE1	2.57	0.40
10:C3:398:PRO:HB3	10:C3:482:VAL:HG21	2.03	0.40
10:C3:440:TYR:CG	11:C1:205:SER:HB3	2.56	0.40
10:C3:442:ASP:OD2	11:C1:134:ARG:NH2	2.54	0.40
11:C1:168:LEU:HD13	11:C1:184:LEU:HG	2.03	0.40
13:A7:11:TYR:CD1	13:A7:11:TYR:C	2.99	0.40
23:A:364:ASP:N	23:A:364:ASP:OD1	2.49	0.40
24:B:37:TRP:CD1	24:B:39:PRO:HD3	2.55	0.40
24:B:157:LYS:O	24:B:158:LEU:C	2.64	0.40
24:B:277:ILE:HG12	24:B:325:ASP:HB3	2.03	0.40
24:B:316:PHE:HA	24:B:342:ARG:NH1	2.36	0.40
24:B:443:MET:HE2	24:B:443:MET:HB3	1.90	0.40
25:C:60:LEU:O	25:C:86:LEU:HD21	2.21	0.40
28:F:96:ARG:C	28:F:98:PRO:HD3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:36:TYR:CD1	44:M:45:LEU:HD11	2.56	0.40
38:Q:9:SER:HA	43:V:88:ARG:NH1	2.31	0.40
39:R:82:VAL:HG13	39:R:82:VAL:O	2.22	0.40
39:R:140:ASP:O	39:R:141:PHE:HB3	2.20	0.40
69:S:401:PC1:H132	69:S:401:PC1:H111	1.56	0.40
43:V:28:ARG:HA	43:V:29:GLY:HA3	1.76	0.40
52:f:115:TYR:N	52:f:116:PRO:HD3	2.35	0.40
58:k:85:HIS:CE1	59:l:284:HIS:ND1	2.88	0.40
59:l:147:ASP:O	59:l:150:VAL:HG22	2.22	0.40
59:l:295:LEU:HD21	59:l:309:VAL:HG12	2.03	0.40
60:m:133:LEU:HB2	80:m:401:HEM:O2D	2.21	0.40
62:p:9:ASP:OD2	62:p:11:SER:OG	2.24	0.40
62:p:75:GLU:HG2	62:p:76:ILE:O	2.22	0.40
67:u:52:TRP:CA	67:u:56:LYS:H	2.34	0.40
59:x:147:ASP:O	59:x:150:VAL:HG22	2.21	0.40
59:x:214:PRO:HA	59:x:217:LYS:HB3	2.03	0.40
60:y:25:SER:OG	60:y:216:ASP:OD2	2.28	0.40
60:y:149:LEU:HD11	60:y:291:VAL:HG22	2.04	0.40
60:y:240:MET:HA	60:y:243:VAL:HG12	2.04	0.40
64:A3:49:ALA:O	64:A3:50:PRO:C	2.63	0.40
64:A3:63:THR:HG22	64:A3:67:GLU:OE2	2.21	0.40
67:B6:52:TRP:CA	67:B6:56:LYS:H	2.34	0.40
2:1:36:GLY:O	2:1:37:PRO:C	2.63	0.40
4:7:118:GLU:O	30:H:74:LYS:NZ	2.48	0.40
5:4:100:ILE:O	5:4:103:GLN:N	2.54	0.40
5:4:115:LEU:HD23	5:4:115:LEU:HA	1.68	0.40
5:4:120:ILE:O	5:4:124:ALA:HB2	2.22	0.40
7:6:188:TRP:CD2	7:6:212:PRO:HB3	2.56	0.40
8:2:261:MET:N	8:2:262:PRO:HD2	2.36	0.40
9:8:149:MET:HE3	9:8:149:MET:HB3	1.80	0.40
9:8:311:TRP:CG	9:8:312:ASP:N	2.90	0.40
9:8:386:ARG:C	9:8:388:GLY:N	2.80	0.40
11:C1:193:TYR:CD1	11:C1:193:TYR:N	2.88	0.40
12:A9:182:TYR:O	16:A6:72:ASN:HB2	2.21	0.40
12:A9:228:THR:O	12:A9:232:HIS:HD2	2.04	0.40
20:B3:24:PHE:CE1	20:B3:28:VAL:HG21	2.56	0.40
23:A:126:LEU:HD13	31:I:98:ARG:O	2.21	0.40
23:A:482:GLN:HG2	23:A:482:GLN:O	2.21	0.40
23:A:682:ASP:OD1	23:A:683:PRO:HD2	2.21	0.40
24:B:200:PHE:CE1	24:B:204:PHE:CE2	3.10	0.40
26:D:132:LYS:HB3	26:D:132:LYS:HE2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:17:VAL:O	36:O:77:ARG:NH1	2.54	0.40
37:P:29:GLN:CG	37:P:30:GLU:H	2.31	0.40
38:Q:52:ASP:O	38:Q:54:ARG:N	2.42	0.40
69:S:401:PC1:H372	69:S:401:PC1:H341	1.67	0.40
42:U:29:ARG:HG3	42:U:30:ALA:N	2.37	0.40
49:b:66:ARG:HG2	53:h:74:HIS:NE2	2.37	0.40
49:b:131:LYS:O	49:b:135:ARG:HB3	2.20	0.40
50:c:11:ARG:C	50:c:13:GLN:H	2.29	0.40
50:c:11:ARG:HB2	52:f:155:PRO:CB	2.51	0.40
58:k:2:ALA:HB2	59:l:40:ASN:O	2.21	0.40
58:k:439:SER:HA	58:k:442:PHE:CE2	2.56	0.40
60:m:317:PHE:O	60:m:319:PRO:HD3	2.21	0.40
63:q:45:GLU:OE1	63:q:48:ARG:HG3	2.21	0.40
65:s:12:GLU:O	65:s:13:LEU:HB2	2.21	0.40
58:w:303:LEU:O	58:w:330:SER:OG	2.34	0.40
59:x:259:ALA:HB2	59:x:422:LYS:CG	2.51	0.40
60:y:24:PRO:O	60:y:224:TYR:OH	2.37	0.40
61:z:7:PRO:HA	61:z:8:PRO:HD3	1.90	0.40
61:z:239:PRO:HB2	61:z:241:LYS:CB	2.32	0.40
63:A2:19:TRP:CD1	63:A2:22:ASN:ND2	2.72	0.40
68:B5:65:VAL:C	68:B5:77:ARG:HB3	2.45	0.40
1:3:29:VAL:O	1:3:29:VAL:HG12	2.22	0.40
3:9:114:GLU:OE2	29:G:174:THR:HG23	2.22	0.40
5:4:259:TYR:N	5:4:260:PRO:HD2	2.37	0.40
5:4:306:PRO:O	5:4:307:TRP:HB2	2.22	0.40
7:6:32:TYR:O	7:6:35:TYR:HB3	2.22	0.40
7:6:68:TRP:CD1	7:6:69:LEU:N	2.90	0.40
7:6:209:SER:OG	7:6:273:ILE:HD11	2.22	0.40
10:C3:64:VAL:HA	10:C3:68:PHE:HD2	1.87	0.40
10:C3:273:MET:HG3	10:C3:319:LYS:NZ	2.30	0.40
13:A7:79:LYS:HZ3	20:B3:15:ASN:HD21	1.68	0.40
13:A7:137:LYS:O	13:A7:145:TRP:HE3	2.03	0.40
23:A:119:PHE:HD1	23:A:119:PHE:HA	1.76	0.40
23:A:550:ALA:HB3	23:A:568:TYR:HE1	1.85	0.40
24:B:116:LEU:HD11	26:D:89:LEU:HD23	2.03	0.40
26:D:130:THR:H	26:D:130:THR:HG23	1.65	0.40
29:G:131:LYS:C	29:G:134:ALA:H	2.29	0.40
30:H:20:ILE:HD13	30:H:20:ILE:HG21	1.91	0.40
30:H:86:LEU:O	30:H:87:ILE:C	2.65	0.40
30:H:89:GLU:N	30:H:89:GLU:OE1	2.54	0.40
38:Q:165:SER:O	38:Q:166:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:58:VAL:HG12	39:R:61:ALA:HB2	2.03	0.40
40:S:282:LEU:C	40:S:284:MET:H	2.29	0.40
48:a:43:LEU:O	48:a:46:GLU:N	2.54	0.40
48:a:53:ASP:HA	52:f:133:TRP:CZ2	2.56	0.40
58:k:58:PHE:CD2	58:k:62:LEU:HD11	2.57	0.40
58:k:388:ARG:O	58:k:390:ILE:HG12	2.21	0.40
59:l:102:ARG:HG2	59:l:176:LEU:HD21	2.03	0.40
59:l:200:THR:CG2	59:l:203:ARG:H	2.27	0.40
59:l:214:PRO:HA	59:l:217:LYS:HB3	2.03	0.40
58:w:250:LEU:HD23	58:w:250:LEU:HA	1.89	0.40
58:w:408:ARG:NE	66:A4:15:ARG:CZ	2.85	0.40
58:w:408:ARG:NE	66:A4:15:ARG:NH2	2.65	0.40
59:x:212:SER:HB2	59:x:214:PRO:HD2	2.03	0.40
59:x:359:ALA:O	59:x:363:LYS:HG3	2.21	0.40
60:y:37:LEU:HA	60:y:37:LEU:HD23	1.79	0.40
60:y:245:PHE:HZ	61:z:209:LEU:HD11	1.86	0.40
60:y:272:TRP:CD1	60:y:272:TRP:H	2.39	0.40
64:A3:3:GLN:O	64:A3:7:LEU:HG	2.20	0.40
66:A4:32:LEU:O	66:A4:35:ALA:HB3	2.21	0.40
67:B6:42:ILE:O	67:B6:46:ILE:HG13	2.22	0.40
2:1:264:LEU:O	2:1:264:LEU:CG	2.70	0.40
5:4:440:HIS:O	5:4:443:PRO:HD2	2.21	0.40
7:6:264:TYR:CG	7:6:265:PRO:HD3	2.56	0.40
7:6:277:THR:OG1	7:6:318:GLY:HA2	2.21	0.40
7:6:302:ILE:HD12	7:6:302:ILE:HG23	1.88	0.40
7:6:365:ALA:C	7:6:367:PRO:HD3	2.47	0.40
7:6:423:SER:O	7:6:426:ILE:HG13	2.22	0.40
8:2:83:GLN:NE2	49:b:174:ILE:HD13	2.36	0.40
8:2:255:PRO:HA	8:2:260:PHE:CG	2.57	0.40
10:C3:354:THR:HG21	10:C3:376:HIS:HA	2.03	0.40
14:B4:79:LYS:H	14:B4:79:LYS:HD3	1.87	0.40
15:A5:19:GLU:HB3	15:A5:98:HIS:CE1	2.57	0.40
15:A5:30:PRO:HG2	15:A5:31:TYR:CD1	2.57	0.40
24:B:147:ASN:C	24:B:149:GLN:H	2.30	0.40
24:B:404:LYS:HE2	24:B:404:LYS:HB3	1.80	0.40
25:C:63:PHE:CG	37:P:97:PRO:HG3	2.56	0.40
26:D:95:GLU:HG3	26:D:187:PRO:CB	2.52	0.40
29:G:129:SER:OG	35:N:116:ILE:HG22	2.21	0.40
33:K:40:ARG:HG3	33:K:88:THR:HG23	2.03	0.40
39:R:269:SER:HA	39:R:270:ARG:HA	1.52	0.40
40:S:187:LEU:HD12	40:S:187:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:S:401:PC1:H292	69:S:401:PC1:H232	2.04	0.40
43:V:71:LEU:O	43:V:72:MET:HB3	2.21	0.40
45:X:14:VAL:O	45:X:17:PRO:HD2	2.22	0.40
48:a:68:TRP:HH2	57:e:110:ASP:OD1	2.04	0.40
44:M:70:LEU:HD22	44:M:76:ILE:HG12	2.04	0.40
58:k:15:GLN:HE21	58:k:205:HIS:CB	2.34	0.40
58:k:32:GLN:HG2	58:k:34:THR:H	1.85	0.40
59:l:201:SER:HA	59:l:204:MET:HE3	2.03	0.40
59:l:293:SER:O	59:l:297:GLN:HG2	2.21	0.40
60:m:149:LEU:HD11	60:m:291:VAL:HG22	2.04	0.40
60:m:172:LYS:O	60:m:175:LEU:N	2.54	0.40
60:m:240:MET:HA	60:m:243:VAL:HG12	2.04	0.40
80:m:401:HEM:HMB1	80:m:401:HEM:HBB2	2.04	0.40
61:o:62:LYS:HB2	61:o:62:LYS:HE2	1.90	0.40
61:o:165:TYR:O	61:o:168:VAL:HG23	2.21	0.40
63:q:103:GLU:OE2	59:x:84:LYS:HB2	2.22	0.40
58:w:87:ASN:OD1	59:x:286:LYS:HE2	2.22	0.40
58:w:125:SER:HB3	58:w:129:LYS:NZ	2.37	0.40
58:w:131:ARG:HE	58:w:175:ARG:HA	1.86	0.40
58:w:277:ILE:HD12	58:w:341:GLN:HB3	2.02	0.40
59:x:128:THR:O	59:x:130:PRO:HD3	2.21	0.40
60:y:197:LEU:O	60:y:200:LEU:HB3	2.22	0.40
61:z:230:LEU:O	61:z:233:ARG:HG2	2.21	0.40
65:B7:73:LEU:O	65:B7:77:LEU:HG	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	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	14 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	316/318 (99%)	254 (80%)	49 (16%)	13 (4%)	2	17
3	9	205/217 (94%)	167 (82%)	31 (15%)	7 (3%)	3	20
4	7	170/175 (97%)	133 (78%)	27 (16%)	10 (6%)	1	13
5	4	457/459 (100%)	392 (86%)	57 (12%)	8 (2%)	6	32
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	6	604/606 (100%)	519 (86%)	82 (14%)	3 (0%)	24	63
8	2	342/347 (99%)	284 (83%)	56 (16%)	2 (1%)	21	58
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	7	36
10	C3	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
11	C1	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	40
12	A9	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
13	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
14	B4	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
15	A5	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
16	A6	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	12
17	C0	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	38
18	C2	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
19	B2	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	19
20	B3	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
21	A0	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
22	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
23	A	686/704 (97%)	560 (82%)	112 (16%)	14 (2%)	6	30
24	B	428/430 (100%)	344 (80%)	77 (18%)	7 (2%)	7	36
25	C	206/228 (90%)	172 (84%)	32 (16%)	2 (1%)	12	47
26	D	150/179 (84%)	122 (81%)	24 (16%)	4 (3%)	4	24
27	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	7	34
28	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	2	18
29	G	121/133 (91%)	102 (84%)	18 (15%)	1 (1%)	16	53
30	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	3	20
31	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	17
32	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	K	82/98 (84%)	66 (80%)	15 (18%)	1 (1%)	10	42
34	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
35	N	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
36	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	4	24
37	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
38	Q	166/171 (97%)	115 (69%)	48 (29%)	3 (2%)	6	32
39	R	305/345 (88%)	240 (79%)	60 (20%)	5 (2%)	7	36
40	S	317/320 (99%)	239 (75%)	67 (21%)	11 (4%)	3	20
41	T	136/140 (97%)	115 (85%)	12 (9%)	9 (7%)	1	11
42	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
43	V	136/143 (95%)	111 (82%)	22 (16%)	3 (2%)	5	28
44	M	78/86 (91%)	56 (72%)	19 (24%)	3 (4%)	2	18
44	W	84/86 (98%)	68 (81%)	15 (18%)	1 (1%)	10	42
45	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
46	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	6	32
47	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	4	24
48	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
49	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	18	55
50	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
51	d	105/117 (90%)	89 (85%)	13 (12%)	3 (3%)	3	23
52	f	165/178 (93%)	129 (78%)	34 (21%)	2 (1%)	10	42
53	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	2	19
54	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
55	j	111/120 (92%)	96 (86%)	15 (14%)	0	100	100
56	g	171/176 (97%)	142 (83%)	27 (16%)	2 (1%)	10	42
57	e	139/158 (88%)	80 (58%)	47 (34%)	12 (9%)	0	8
58	k	444/480 (92%)	405 (91%)	35 (8%)	4 (1%)	14	50
58	w	432/480 (90%)	400 (93%)	29 (7%)	3 (1%)	18	55
59	l	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	12	47
59	x	417/453 (92%)	384 (92%)	29 (7%)	4 (1%)	12	47
60	m	377/379 (100%)	341 (90%)	35 (9%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	y	377/379 (100%)	341 (90%)	36 (10%)	0	100	100
61	o	239/325 (74%)	204 (85%)	34 (14%)	1 (0%)	30	67
61	z	239/325 (74%)	205 (86%)	32 (13%)	2 (1%)	16	53
62	A1	184/196 (94%)	137 (74%)	41 (22%)	6 (3%)	3	20
62	p	147/196 (75%)	100 (68%)	35 (24%)	12 (8%)	0	9
63	A2	104/111 (94%)	91 (88%)	8 (8%)	5 (5%)	2	16
63	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
64	A3	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
64	r	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
65	B7	67/91 (74%)	57 (85%)	7 (10%)	3 (4%)	2	16
65	s	65/91 (71%)	55 (85%)	7 (11%)	3 (5%)	2	16
66	A4	37/56 (66%)	23 (62%)	8 (22%)	6 (16%)	0	3
66	t	31/56 (55%)	24 (77%)	7 (23%)	0	100	100
67	B6	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
67	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
68	B5	20/78 (26%)	10 (50%)	8 (40%)	2 (10%)	0	7
68	v	16/78 (20%)	8 (50%)	7 (44%)	1 (6%)	1	12
All	All	13628/15127 (90%)	11521 (84%)	1873 (14%)	234 (2%)	9	34

All (234) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	170	GLU
2	1	174	LEU
2	1	268	MET
4	7	79	TYR
4	7	82	ILE
4	7	85	SER
4	7	141	MET
4	7	171	ILE
8	2	84	TRP
10	C3	328	HIS
10	C3	508	PRO
15	A5	2	SER
15	A5	87	THR
15	A5	95	GLN

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Mol	Chain	Res	Type
16	A6	4	ALA
16	A6	9	GLY
17	C0	46	LYS
19	B2	2	GLU
23	A	383	SER
23	A	461	PRO
23	A	463	SER
24	B	294	ARG
26	D	146	GLU
31	I	106	GLU
31	I	109	THR
40	S	199	VAL
40	S	202	VAL
40	S	276	ASP
41	T	46	PRO
41	T	66	ILE
43	V	143	TYR
47	Z	63	PHE
47	Z	64	VAL
53	h	81	ALA
53	h	82	VAL
57	e	41	TYR
57	e	81	ARG
57	e	82	SER
57	e	115	ASN
62	p	82	PRO
62	p	120	PRO
62	p	129	LYS
62	p	146	PRO
62	p	159	PRO
65	s	14	VAL
61	z	79	GLU
61	z	80	MET
63	A2	17	ARG
63	A2	18	LYS
63	A2	19	TRP
63	A2	20	TYR
65	B7	14	VAL
66	A4	40	LEU
66	A4	41	ILE
66	A4	42	LEU
2	1	76	ILE

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Mol	Chain	Res	Type
2	1	78	ALA
2	1	173	TRP
2	1	176	LEU
2	1	282	TYR
3	9	75	LYS
3	9	76	ALA
5	4	21	ASN
5	4	420	THR
8	2	88	LYS
16	A6	5	LYS
23	A	189	ILE
24	B	310	VAL
26	D	147	PRO
26	D	184	PRO
30	H	16	ARG
36	O	100	ARG
39	R	155	VAL
39	R	272	LEU
40	S	58	LYS
45	X	14	VAL
57	e	71	GLY
62	p	130	PRO
68	v	65	VAL
58	w	214	LYS
62	A1	80	ASP
62	A1	92	ARG
68	B5	65	VAL
1	3	82	ALA
2	1	177	PRO
4	7	140	ALA
4	7	148	SER
4	7	170	GLU
5	4	61	LEU
5	4	65	LEU
7	6	352	ASP
9	8	235	VAL
9	8	403	ASP
11	C1	104	TRP
16	A6	61	SER
23	A	129	PRO
23	A	283	GLU
23	A	541	PRO

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Mol	Chain	Res	Type
24	B	291	VAL
24	B	293	LEU
33	K	52	PRO
38	Q	94	LEU
38	Q	121	ASP
39	R	99	ASP
40	S	280	HIS
40	S	333	GLU
41	T	47	THR
44	W	129	GLU
56	g	74	ILE
56	g	126	ALA
57	e	70	THR
59	l	305	GLN
62	p	81	ILE
2	1	71	PHE
4	7	81	GLU
10	C3	51	ASP
24	B	62	LYS
25	C	127	ARG
26	D	103	ARG
27	E	106	TYR
27	E	107	PRO
29	G	122	SER
30	H	57	LYS
31	I	108	LYS
36	O	25	MET
39	R	325	THR
40	S	216	LYS
40	S	281	LYS
41	T	105	THR
51	d	19	PRO
51	d	39	MET
52	f	165	PRO
57	e	42	PRO
57	e	76	PRO
44	M	30	LEU
44	M	60	PHE
58	k	219	LEU
58	k	427	PRO
62	p	115	SER
62	p	134	ILE

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Mol	Chain	Res	Type
58	w	427	PRO
66	A4	36	THR
2	1	316	PRO
3	9	150	GLU
3	9	232	THR
3	9	234	LEU
5	4	58	SER
5	4	112	ALA
9	8	282	VAL
9	8	381	GLN
11	C1	103	GLN
19	B2	3	ASN
23	A	188	GLU
23	A	563	ASP
24	B	78	SER
27	E	171	PRO
38	Q	32	TYR
39	R	316	ARG
40	S	334	ASP
41	T	107	SER
45	X	13	HIS
49	b	111	GLU
57	e	79	PRO
65	s	63	HIS
62	A1	30	GLU
62	A1	171	ILE
65	B7	63	HIS
4	7	105	TYR
5	4	82	HIS
7	6	65	ASN
9	8	227	PRO
9	8	236	PHE
9	8	387	GLU
10	C3	91	ASP
11	C1	158	ASP
16	A6	49	PRO
23	A	128	CYS
28	F	86	LEU
32	J	55	SER
36	O	116	LYS
52	f	149	PRO
57	e	105	MET

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Mol	Chain	Res	Type
58	k	229	PRO
59	l	195	VAL
59	l	278	VAL
61	o	70	VAL
62	p	136	ILE
65	s	70	ALA
59	x	195	VAL
59	x	278	VAL
65	B7	70	ALA
66	A4	35	ALA
7	6	71	ILE
23	A	561	PRO
24	B	39	PRO
32	J	57	VAL
43	V	26	PRO
51	d	40	VAL
62	A1	194	ILE
66	A4	27	VAL
2	1	249	PRO
41	T	83	LYS
41	T	84	PRO
43	V	73	PRO
53	h	80	PRO
59	l	382	VAL
59	x	305	GLN
59	x	382	VAL
2	1	208	VAL
15	A5	15	GLY
23	A	45	PRO
23	A	210	ILE
41	T	76	ILE
41	T	125	VAL
46	Y	90	PRO
3	9	241	PRO
5	4	306	PRO
23	A	263	VAL
25	C	218	VAL
30	H	25	GLN
58	k	71	PRO
62	p	93	GLY
62	p	114	VAL
58	w	71	PRO

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Mol	Chain	Res	Type
62	A1	193	VAL
63	A2	6	VAL
3	9	216	PRO
40	S	340	ILE
57	e	78	LEU
57	e	87	ASP
44	M	27	PRO
60	m	343	VAL
68	B5	63	PRO
40	S	323	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	3	96/101 (95%)	96 (100%)	0	100	100
2	1	274/275 (100%)	257 (94%)	17 (6%)	16	38
3	9	170/183 (93%)	168 (99%)	2 (1%)	63	74
4	7	115/142 (81%)	112 (97%)	3 (3%)	40	61
5	4	389/413 (94%)	389 (100%)	0	100	100
6	5	80/86 (93%)	80 (100%)	0	100	100
7	6	524/534 (98%)	522 (100%)	2 (0%)	84	83
8	2	304/316 (96%)	302 (99%)	2 (1%)	76	80
9	8	270/353 (76%)	269 (100%)	1 (0%)	84	83
10	C3	427/427 (100%)	387 (91%)	40 (9%)	8	26
11	C1	211/211 (100%)	191 (90%)	20 (10%)	8	26
12	A9	226/226 (100%)	199 (88%)	27 (12%)	5	19
13	A7	128/148 (86%)	117 (91%)	11 (9%)	10	29
14	B4	95/123 (77%)	89 (94%)	6 (6%)	16	38
15	A5	81/103 (79%)	73 (90%)	8 (10%)	7	24
16	A6	68/79 (86%)	52 (76%)	16 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C0	67/76 (88%)	58 (87%)	9 (13%)	4	15
18	C2	58/59 (98%)	51 (88%)	7 (12%)	5	18
19	B2	47/68 (69%)	41 (87%)	6 (13%)	4	17
20	B3	39/66 (59%)	36 (92%)	3 (8%)	12	32
21	A0	40/55 (73%)	37 (92%)	3 (8%)	12	33
22	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
23	A	560/588 (95%)	538 (96%)	22 (4%)	28	50
24	B	363/371 (98%)	350 (96%)	13 (4%)	31	52
25	C	188/204 (92%)	175 (93%)	13 (7%)	14	36
26	D	127/150 (85%)	124 (98%)	3 (2%)	43	63
27	E	148/151 (98%)	146 (99%)	2 (1%)	59	72
28	F	14/69 (20%)	14 (100%)	0	100	100
29	G	106/119 (89%)	106 (100%)	0	100	100
30	H	80/95 (84%)	80 (100%)	0	100	100
31	I	54/79 (68%)	50 (93%)	4 (7%)	13	34
32	J	50/59 (85%)	49 (98%)	1 (2%)	48	66
33	K	67/81 (83%)	67 (100%)	0	100	100
34	L	63/71 (89%)	63 (100%)	0	100	100
35	N	88/101 (87%)	88 (100%)	0	100	100
36	O	95/113 (84%)	95 (100%)	0	100	100
37	P	73/96 (76%)	72 (99%)	1 (1%)	59	72
38	Q	142/154 (92%)	142 (100%)	0	100	100
39	R	230/298 (77%)	228 (99%)	2 (1%)	70	77
40	S	205/283 (72%)	205 (100%)	0	100	100
41	T	76/101 (75%)	76 (100%)	0	100	100
42	U	95/131 (72%)	95 (100%)	0	100	100
43	V	106/120 (88%)	106 (100%)	0	100	100
44	M	73/79 (92%)	73 (100%)	0	100	100
44	W	57/79 (72%)	55 (96%)	2 (4%)	32	53
45	X	32/54 (59%)	32 (100%)	0	100	100
46	Y	29/62 (47%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Z	28/76 (37%)	28 (100%)	0	100	100
48	a	70/114 (61%)	70 (100%)	0	100	100
49	b	85/124 (68%)	85 (100%)	0	100	100
50	c	45/122 (37%)	45 (100%)	0	100	100
51	d	43/107 (40%)	43 (100%)	0	100	100
52	f	80/160 (50%)	80 (100%)	0	100	100
53	h	63/112 (56%)	63 (100%)	0	100	100
54	i	23/45 (51%)	23 (100%)	0	100	100
55	j	88/106 (83%)	88 (100%)	0	100	100
56	g	130/157 (83%)	130 (100%)	0	100	100
57	e	44/141 (31%)	41 (93%)	3 (7%)	14	36
58	k	369/394 (94%)	369 (100%)	0	100	100
58	w	362/394 (92%)	362 (100%)	0	100	100
59	l	327/355 (92%)	327 (100%)	0	100	100
59	x	328/355 (92%)	328 (100%)	0	100	100
60	m	327/327 (100%)	326 (100%)	1 (0%)	86	84
60	y	327/327 (100%)	326 (100%)	1 (0%)	86	84
61	o	206/257 (80%)	206 (100%)	0	100	100
61	z	202/257 (79%)	202 (100%)	0	100	100
62	A1	64/168 (38%)	64 (100%)	0	100	100
62	p	65/168 (39%)	65 (100%)	0	100	100
63	A2	93/99 (94%)	93 (100%)	0	100	100
63	q	96/99 (97%)	96 (100%)	0	100	100
64	A3	70/72 (97%)	69 (99%)	1 (1%)	59	72
64	r	71/72 (99%)	71 (100%)	0	100	100
65	B7	66/85 (78%)	66 (100%)	0	100	100
65	s	64/85 (75%)	64 (100%)	0	100	100
66	A4	31/46 (67%)	31 (100%)	0	100	100
66	t	24/46 (52%)	22 (92%)	2 (8%)	10	30
67	B6	52/54 (96%)	51 (98%)	1 (2%)	50	66
67	u	52/54 (96%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	B5	15/60 (25%)	14 (93%)	1 (7%)	15	37
68	v	11/60 (18%)	11 (100%)	0	100	100
All	All	10788/12907 (84%)	10529 (98%)	259 (2%)	43	63

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	70	MET
2	1	71	PHE
2	1	77	MET
2	1	156	MET
2	1	157	SER
2	1	171	GLN
2	1	172	MET
2	1	174	LEU
2	1	235	ASN
2	1	236	ILE
2	1	250	HIS
2	1	251	MET
2	1	265	LEU
2	1	266	LEU
2	1	309	ILE
2	1	317	GLN
2	1	318	THR
3	9	93	LEU
3	9	188	ILE
4	7	83	TRP
4	7	86	ASN
4	7	171	ILE
7	6	301	ILE
7	6	427	ILE
8	2	7	ILE
8	2	84	TRP
9	8	156	ILE
10	C3	18	LEU
10	C3	35	LEU
10	C3	92	MET
10	C3	96	ARG
10	C3	105	LEU
10	C3	115	SER
10	C3	136	LEU

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Mol	Chain	Res	Type
10	C3	138	HIS
10	C3	150	LEU
10	C3	158	ILE
10	C3	159	LEU
10	C3	187	SER
10	C3	188	VAL
10	C3	189	MET
10	C3	194	LEU
10	C3	199	LEU
10	C3	213	ARG
10	C3	241	PRO
10	C3	273	MET
10	C3	295	VAL
10	C3	301	THR
10	C3	306	THR
10	C3	318	VAL
10	C3	324	LEU
10	C3	347	LEU
10	C3	353	LEU
10	C3	354	THR
10	C3	365	ILE
10	C3	369	ASP
10	C3	373	VAL
10	C3	383	MET
10	C3	417	MET
10	C3	444	PRO
10	C3	465	VAL
10	C3	467	LEU
10	C3	474	GLU
10	C3	492	LEU
10	C3	508	PRO
10	C3	509	THR
10	C3	512	ASN
11	C1	7	LEU
11	C1	16	ILE
11	C1	31	VAL
11	C1	33	LEU
11	C1	52	HIS
11	C1	60	GLU
11	C1	63	THR
11	C1	67	ILE
11	C1	88	ASP

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Mol	Chain	Res	Type
11	C1	92	ASN
11	C1	125	THR
11	C1	130	PRO
11	C1	134	ARG
11	C1	142	VAL
11	C1	147	GLU
11	C1	170	LEU
11	C1	171	LYS
11	C1	185	MET
11	C1	205	SER
11	C1	216	LEU
12	A9	1	MET
12	A9	11	VAL
12	A9	13	PRO
12	A9	14	SER
12	A9	18	LEU
12	A9	19	THR
12	A9	22	LEU
12	A9	26	LEU
12	A9	38	ASN
12	A9	39	SER
12	A9	85	LEU
12	A9	92	LEU
12	A9	112	LEU
12	A9	127	LEU
12	A9	128	GLU
12	A9	131	LEU
12	A9	132	LEU
12	A9	137	LEU
12	A9	142	VAL
12	A9	160	LEU
12	A9	163	LEU
12	A9	188	ILE
12	A9	196	THR
12	A9	199	VAL
12	A9	213	THR
12	A9	222	GLN
12	A9	230	ASN
13	A7	9	GLU
13	A7	27	VAL
13	A7	31	LYS
13	A7	36	SER

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Mol	Chain	Res	Type
13	A7	40	LEU
13	A7	59	LEU
13	A7	62	LEU
13	A7	107	ILE
13	A7	116	VAL
13	A7	143	ASN
13	A7	147	LYS
14	B4	7	THR
14	B4	29	LEU
14	B4	70	VAL
14	B4	79	LYS
14	B4	80	GLU
14	B4	90	ARG
15	A5	6	VAL
15	A5	20	VAL
15	A5	37	LYS
15	A5	52	ILE
15	A5	53	THR
15	A5	74	LEU
15	A5	95	GLN
15	A5	98	HIS
16	A6	5	LYS
16	A6	7	ASP
16	A6	8	HIS
16	A6	14	ARG
16	A6	17	ARG
16	A6	33	LEU
16	A6	34	ASN
16	A6	37	LEU
16	A6	41	HIS
16	A6	42	ARG
16	A6	43	GLU
16	A6	48	ILE
16	A6	54	ARG
16	A6	56	ARG
16	A6	68	THR
16	A6	78	LEU
17	C0	19	ARG
17	C0	29	CYS
17	C0	41	LYS
17	C0	51	SER
17	C0	53	CYS

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Mol	Chain	Res	Type
17	C0	57	ARG
17	C0	60	TYR
17	C0	67	SER
17	C0	75	ARG
18	C2	2	THR
18	C2	4	LEU
18	C2	8	GLN
18	C2	22	VAL
18	C2	26	MET
18	C2	44	LYS
18	C2	64	ARG
19	B2	2	GLU
19	B2	5	VAL
19	B2	8	LYS
19	B2	16	ASN
19	B2	23	LYS
19	B2	27	THR
20	B3	45	VAL
20	B3	48	VAL
20	B3	49	THR
21	A0	15	VAL
21	A0	22	LEU
21	A0	26	THR
22	A8	13	LYS
22	A8	24	LEU
22	A8	42	LYS
23	A	56	VAL
23	A	65	TYR
23	A	67	GLU
23	A	68	ARG
23	A	79	LEU
23	A	146	PHE
23	A	223	ILE
23	A	381	LEU
23	A	537	ILE
23	A	595	THR
23	A	598	ASN
23	A	617	ARG
23	A	633	THR
23	A	634	LEU
23	A	637	ASP
23	A	641	GLN

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Mol	Chain	Res	Type
23	A	642	VAL
23	A	643	ARG
23	A	648	GLU
23	A	654	VAL
23	A	656	TYR
23	A	678	GLN
24	B	47	TYR
24	B	61	TRP
24	B	141	TYR
24	B	216	ARG
24	B	223	HIS
24	B	227	VAL
24	B	264	ASN
24	B	345	SER
24	B	348	LEU
24	B	349	ASN
24	B	389	TYR
24	B	429	PHE
24	B	432	LEU
25	C	95	VAL
25	C	116	LEU
25	C	131	VAL
25	C	133	ASN
25	C	152	LEU
25	C	160	PRO
25	C	163	LYS
25	C	167	TRP
25	C	188	ARG
25	C	192	ASP
25	C	222	VAL
25	C	226	VAL
25	C	244	PHE
26	D	74	ILE
26	D	146	GLU
26	D	181	ILE
27	E	62	LEU
27	E	67	ILE
31	I	101	ILE
31	I	103	LEU
31	I	106	GLU
31	I	108	LYS
32	J	18	ILE

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Mol	Chain	Res	Type
37	P	106	LEU
39	R	152	ILE
39	R	206	ILE
44	W	106	LYS
44	W	108	LEU
57	e	114	ARG
57	e	118	ASP
57	e	119	THR
60	m	153	ILE
66	t	38	TRP
66	t	39	ARG
60	y	153	ILE
64	A3	81	ARG
67	B6	1	VAL
68	B5	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	5	ASN
2	1	47	GLN
2	1	169	GLN
2	1	171	GLN
2	1	230	ASN
2	1	287	HIS
2	1	317	GLN
3	9	87	GLN
5	4	30	HIS
5	4	44	GLN
5	4	81	GLN
5	4	168	GLN
5	4	251	ASN
5	4	304	GLN
5	4	366	ASN
5	4	390	ASN
5	4	440	HIS
6	5	7	ASN
6	5	97	GLN
7	6	59	GLN
7	6	113	ASN
7	6	296	ASN
7	6	332	HIS

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Mol	Chain	Res	Type
7	6	447	ASN
7	6	471	ASN
7	6	546	GLN
7	6	605	HIS
8	2	36	ASN
8	2	48	HIS
8	2	49	ASN
8	2	120	GLN
8	2	268	GLN
9	8	103	ASN
9	8	116	ASN
9	8	168	ASN
9	8	220	GLN
9	8	281	HIS
9	8	376	HIS
9	8	393	ASN
9	8	418	GLN
9	8	422	HIS
10	C3	4	ASN
10	C3	11	ASN
10	C3	12	HIS
10	C3	55	ASN
10	C3	99	ASN
10	C3	170	ASN
10	C3	178	GLN
10	C3	256	HIS
10	C3	360	ASN
10	C3	368	HIS
10	C3	413	HIS
10	C3	503	HIS
10	C3	512	ASN
11	C1	52	HIS
11	C1	92	ASN
11	C1	102	HIS
11	C1	103	GLN
11	C1	195	GLN
11	C1	203	ASN
12	A9	3	HIS
12	A9	6	HIS
12	A9	12	ASN
12	A9	133	ASN
12	A9	148	HIS

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Mol	Chain	Res	Type
12	A9	158	HIS
12	A9	207	HIS
12	A9	222	GLN
12	A9	232	HIS
13	A7	32	ASN
13	A7	109	HIS
14	B4	34	ASN
15	A5	66	ASN
16	A6	51	HIS
16	A6	52	HIS
17	C0	23	GLN
17	C0	24	ASN
17	C0	25	GLN
17	C0	28	ASN
17	C0	31	GLN
17	C0	32	ASN
17	C0	37	HIS
19	B2	3	ASN
19	B2	16	ASN
20	B3	10	HIS
20	B3	15	ASN
20	B3	35	GLN
20	B3	41	ASN
22	A8	39	ASN
23	A	59	GLN
23	A	140	GLN
23	A	142	GLN
23	A	282	ASN
23	A	359	ASN
23	A	424	HIS
23	A	460	HIS
23	A	572	HIS
24	B	46	GLN
24	B	79	ASN
24	B	182	ASN
24	B	183	HIS
24	B	234	GLN
24	B	285	ASN
24	B	346	GLN
24	B	349	ASN
24	B	381	HIS
25	C	126	ASN

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Mol	Chain	Res	Type
25	C	230	GLN
26	D	75	ASN
26	D	164	HIS
27	E	172	ASN
27	E	186	ASN
27	E	204	ASN
30	H	21	GLN
30	H	45	HIS
30	H	82	GLN
32	J	27	HIS
33	K	22	HIS
33	K	48	ASN
34	L	46	ASN
34	L	62	ASN
36	O	102	HIS
37	P	52	ASN
38	Q	143	HIS
39	R	323	HIS
39	R	331	HIS
40	S	120	GLN
40	S	164	GLN
40	S	190	HIS
40	S	211	ASN
42	U	13	GLN
42	U	123	GLN
43	V	76	GLN
44	W	115	GLN
45	X	13	HIS
50	c	26	GLN
50	c	74	HIS
50	c	83	HIS
50	c	89	HIS
51	d	92	HIS
52	f	62	GLN
53	h	70	ASN
53	h	74	HIS
53	h	86	ASN
53	h	115	GLN
54	i	62	HIS
55	j	79	GLN
55	j	97	HIS
56	g	55	GLN

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Mol	Chain	Res	Type
56	g	144	HIS
57	e	94	HIS
57	e	160	GLN
44	M	35	HIS
44	M	74	GLN
58	k	15	GLN
58	k	32	GLN
58	k	165	GLN
58	k	207	GLN
58	k	252	HIS
58	k	289	HIS
58	k	301	ASN
58	k	323	HIS
58	k	368	HIS
59	l	31	ASN
59	l	125	ASN
59	l	141	GLN
59	l	158	HIS
59	l	162	ASN
59	l	174	ASN
59	l	247	GLN
59	l	277	HIS
59	l	290	ASN
59	l	297	GLN
59	l	304	HIS
59	l	354	ASN
60	m	3	ASN
60	m	32	ASN
60	m	159	ASN
60	m	255	ASN
60	m	312	GLN
60	m	341	GLN
61	o	50	HIS
61	o	156	GLN
62	p	53	ASN
64	r	3	GLN
64	r	6	HIS
64	r	12	HIS
64	r	23	GLN
64	r	79	ASN
58	w	15	GLN
58	w	165	GLN

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Mol	Chain	Res	Type
58	w	207	GLN
58	w	252	HIS
58	w	323	HIS
58	w	368	HIS
59	x	31	ASN
59	x	125	ASN
59	x	141	GLN
59	x	162	ASN
59	x	174	ASN
59	x	247	GLN
59	x	290	ASN
59	x	297	GLN
59	x	304	HIS
59	x	354	ASN
59	x	358	GLN
59	x	362	ASN
60	y	3	ASN
60	y	32	ASN
60	y	255	ASN
60	y	312	GLN
60	y	341	GLN
61	z	50	HIS
61	z	71	GLN
61	z	75	ASN
61	z	181	GLN
62	A1	57	GLN
64	A3	3	GLN
64	A3	23	GLN
64	A3	79	ASN
66	A4	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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
74	SF4	8	502	-	0,12,12	-	-	-		
74	SF4	E	302	27	0,12,12	-	-	-		
71	FES	9	301	-	0,4,4	-	-	-		
74	SF4	E	301	27	0,12,12	-	-	-		
71	FES	m	403	-	0,4,4	-	-	-		
70	3PE	1	401	-	50,50,50	0.88	3 (6%)	53,55,55	1.14	2 (3%)
70	3PE	2	401	-	40,40,50	0.95	3 (7%)	43,45,55	1.09	2 (4%)
74	SF4	A	802	-	0,12,12	-	-	-		
70	3PE	4	501	-	40,40,50	0.91	3 (7%)	43,45,55	1.38	3 (6%)
81	HEC	z	301	61	46,50,50	1.96	6 (13%)	58,82,82	2.38	11 (18%)
72	CDL	b	201	-	81,81,99	0.98	8 (9%)	87,93,111	1.16	4 (4%)
76	HEA	C3	602	10	67,67,67	1.21	4 (5%)	81,103,103	1.34	10 (12%)
80	HEM	m	401	60	50,50,50	1.83	16 (32%)	67,82,82	1.36	8 (11%)
82	UQ2	A2	201	-	23,23,23	1.86	2 (8%)	30,31,31	1.48	6 (20%)
73	FMN	8	501	-	33,33,33	1.20	2 (6%)	48,50,50	1.68	13 (27%)
71	FES	A	803	23	0,4,4	-	-	-		
80	HEM	m	402	60	50,50,50	1.77	17 (34%)	67,82,82	1.27	8 (11%)
69	PC1	3	200	-	46,46,53	1.00	3 (6%)	52,54,61	1.09	2 (3%)
69	PC1	j	201	-	38,38,53	1.17	6 (15%)	44,46,61	1.02	2 (4%)
69	PC1	2	402	-	45,45,53	1.03	4 (8%)	51,53,61	1.00	2 (3%)
72	CDL	J	101	-	57,57,99	1.18	7 (12%)	63,69,111	1.20	5 (7%)
81	HEC	o	301	61	46,50,50	1.95	6 (13%)	58,82,82	2.38	11 (18%)
70	3PE	j	202	-	45,45,50	0.91	3 (6%)	48,50,55	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	HEM	y	401	60	50,50,50	1.83	16 (32%)	67,82,82	1.36	8 (11%)
80	HEM	y	402	60	50,50,50	1.77	18 (36%)	67,82,82	1.27	8 (11%)
74	SF4	D	301	26	0,12,12	-	-	-	-	-
74	SF4	A	801	23	0,12,12	-	-	-	-	-
70	3PE	B	501	-	50,50,50	0.88	2 (4%)	53,55,55	1.34	4 (7%)
72	CDL	6	701	-	63,63,99	1.09	8 (12%)	69,75,111	1.27	4 (5%)
76	HEA	C3	603	10	67,67,67	1.19	7 (10%)	81,103,103	1.34	12 (14%)
69	PC1	S	401	-	46,46,53	1.04	5 (10%)	52,54,61	1.09	2 (3%)
69	PC1	Q	201	-	45,45,53	1.08	3 (6%)	51,53,61	1.14	2 (3%)
79	NAP	R	601	-	50,52,52	4.21	22 (44%)	71,80,80	1.97	18 (25%)

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
74	SF4	8	502	-	-	-	0/6/5/5
74	SF4	E	302	27	-	-	0/6/5/5
71	FES	9	301	-	-	-	0/1/1/1
74	SF4	E	301	27	-	-	0/6/5/5
71	FES	m	403	-	-	-	0/1/1/1
70	3PE	1	401	-	-	14/54/54/54	-
70	3PE	2	401	-	-	24/44/44/54	-
74	SF4	A	802	-	-	-	0/6/5/5
70	3PE	4	501	-	-	23/44/44/54	-
81	HEC	z	301	61	-	5/14/54/54	-
72	CDL	b	201	-	-	39/92/92/110	-
76	HEA	C3	602	10	-	7/36/76/76	-
80	HEM	m	401	60	-	3/14/54/54	-
82	UQ2	A2	201	-	-	7/15/39/39	0/1/1/1
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
71	FES	A	803	23	-	-	0/1/1/1
80	HEM	m	402	60	-	1/14/54/54	-
69	PC1	3	200	-	-	23/50/50/57	-
69	PC1	j	201	-	-	21/42/42/57	-
69	PC1	2	402	-	-	29/49/49/57	-
72	CDL	J	101	-	-	23/68/68/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	HEC	o	301	61	-	5/14/54/54	-
70	3PE	j	202	-	-	21/49/49/54	-
80	HEM	y	401	60	-	3/14/54/54	-
80	HEM	y	402	60	-	1/14/54/54	-
74	SF4	D	301	26	-	-	0/6/5/5
74	SF4	A	801	23	-	-	0/6/5/5
70	3PE	B	501	-	-	28/54/54/54	-
72	CDL	6	701	-	-	33/74/74/110	-
76	HEA	C3	603	10	-	7/36/76/76	-
69	PC1	S	401	-	-	26/50/50/57	-
69	PC1	Q	201	-	-	23/49/49/57	-
79	NAP	R	601	-	-	16/35/67/67	0/5/5/5

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	R	601	NAP	O4D-C1D	16.46	1.62	1.40
79	R	601	NAP	C2B-C1B	-10.09	1.28	1.53
79	R	601	NAP	O4B-C1B	8.64	1.62	1.42
79	R	601	NAP	PN-O3	8.41	1.68	1.59
82	A2	201	UQ2	C6-C5	7.78	1.49	1.35
79	R	601	NAP	C7N-N7N	7.20	1.46	1.33
79	R	601	NAP	O4D-C4D	-7.11	1.29	1.45
79	R	601	NAP	O4B-C4B	-6.16	1.31	1.45
81	z	301	HEC	CAB-C3B	5.69	1.53	1.35
81	z	301	HEC	CAC-C3C	5.66	1.53	1.35
81	o	301	HEC	CAB-C3B	5.65	1.53	1.35
81	o	301	HEC	CAC-C3C	5.64	1.53	1.35
81	o	301	HEC	C3D-C2D	5.11	1.52	1.38
81	z	301	HEC	C3D-C2D	5.07	1.52	1.38
80	m	401	HEM	FE-NB	-5.06	1.79	1.94
79	R	601	NAP	PA-O3	5.00	1.64	1.59
80	y	401	HEM	FE-NB	-4.99	1.79	1.94
79	R	601	NAP	C3N-C7N	4.74	1.57	1.50
79	R	601	NAP	C5A-N7A	-4.45	1.31	1.39
80	m	402	HEM	FE-NB	-4.18	1.82	1.94
80	y	402	HEM	FE-NB	-4.18	1.82	1.94
79	R	601	NAP	O3D-C3D	-4.17	1.32	1.43
76	C3	602	HEA	C11-C3B	-4.10	1.46	1.51
79	R	601	NAP	C6A-N6A	3.83	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	R	601	NAP	O7N-C7N	-3.77	1.17	1.24
76	C3	603	HEA	CMA-C3A	-3.57	1.37	1.45
82	A2	201	UQ2	C3-C2	3.55	1.49	1.36
79	R	601	NAP	O2D-C2D	3.43	1.51	1.43
79	R	601	NAP	C5A-C4A	-3.35	1.33	1.39
80	y	402	HEM	C2A-C3A	-3.26	1.30	1.38
80	m	402	HEM	C2A-C3A	-3.26	1.30	1.38
79	R	601	NAP	C4A-N9A	-3.26	1.30	1.37
80	m	401	HEM	FE-NC	-3.18	1.84	1.95
69	Q	201	PC1	O21-C2	-3.17	1.39	1.46
80	y	401	HEM	FE-NC	-3.17	1.84	1.95
70	B	501	3PE	O21-C2	-3.08	1.39	1.46
80	m	401	HEM	C2A-C3A	-3.03	1.31	1.38
80	y	401	HEM	C2A-C3A	-3.01	1.31	1.38
70	1	401	3PE	O21-C2	-2.99	1.39	1.46
76	C3	603	HEA	FE-NA	2.95	2.04	1.95
72	6	701	CDL	OA6-CA4	-2.94	1.39	1.46
79	R	601	NAP	C4N-C3N	-2.92	1.35	1.39
72	J	101	CDL	OB6-CB4	-2.88	1.39	1.46
79	R	601	NAP	C8A-N9A	-2.86	1.32	1.37
72	b	201	CDL	OA6-CA4	-2.85	1.39	1.46
70	j	202	3PE	O21-C2	-2.84	1.39	1.46
72	J	101	CDL	OA6-CA4	-2.82	1.40	1.46
80	y	402	HEM	CHB-C4A	-2.80	1.33	1.39
80	m	402	HEM	CHB-C4A	-2.80	1.33	1.39
70	2	401	3PE	O21-C2	-2.78	1.40	1.46
79	R	601	NAP	O3B-C3B	-2.78	1.36	1.43
80	y	402	HEM	C3D-C2D	-2.75	1.30	1.36
80	y	401	HEM	C1B-NB	-2.73	1.35	1.40
80	m	402	HEM	C3D-C2D	-2.72	1.30	1.36
76	C3	602	HEA	C1A-C2A	-2.71	1.40	1.45
72	b	201	CDL	OB8-CB7	2.71	1.41	1.33
69	3	200	PC1	O21-C2	-2.67	1.40	1.46
81	z	301	HEC	C3C-C2C	-2.67	1.32	1.41
69	S	401	PC1	O21-C2	-2.65	1.40	1.46
81	o	301	HEC	C3C-C2C	-2.63	1.32	1.41
80	m	401	HEM	C1B-NB	-2.61	1.35	1.40
76	C3	602	HEA	CMA-C3A	-2.61	1.39	1.45
70	B	501	3PE	O31-C3	-2.61	1.39	1.45
72	J	101	CDL	OA8-CA7	2.60	1.40	1.33
70	4	501	3PE	O31-C3	-2.59	1.39	1.45
80	m	402	HEM	C3B-C2B	-2.58	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	y	401	HEM	C3D-C2D	-2.57	1.31	1.36
69	Q	201	PC1	O31-C3	-2.57	1.39	1.45
79	R	601	NAP	PA-O5B	2.57	1.69	1.59
80	y	401	HEM	FE-NA	-2.57	1.86	1.95
80	m	401	HEM	C3D-C2D	-2.57	1.31	1.36
80	m	401	HEM	FE-NA	-2.56	1.86	1.95
72	b	201	CDL	OB6-CB5	2.55	1.41	1.34
80	y	402	HEM	C3B-C2B	-2.55	1.32	1.37
76	C3	603	HEA	C1D-ND	-2.54	1.35	1.40
69	2	402	PC1	O21-C21	2.52	1.41	1.34
76	C3	603	HEA	C1D-C2D	2.50	1.49	1.44
72	6	701	CDL	OA8-CA6	-2.48	1.39	1.45
73	8	501	FMN	C4A-N5	2.48	1.36	1.30
80	m	401	HEM	CHA-C1A	-2.47	1.33	1.39
81	z	301	HEC	C3B-C2B	-2.47	1.32	1.41
72	6	701	CDL	OB8-CB6	-2.47	1.39	1.45
80	m	401	HEM	CAB-C3B	2.47	1.54	1.47
69	2	402	PC1	O31-C31	2.46	1.40	1.33
76	C3	603	HEA	C3A-C2A	-2.46	1.31	1.37
81	o	301	HEC	C3B-C2B	-2.46	1.32	1.41
69	S	401	PC1	O31-C31	2.46	1.40	1.33
72	b	201	CDL	OA8-CA7	2.46	1.40	1.33
69	j	201	PC1	O31-C31	2.45	1.40	1.33
80	y	401	HEM	CAB-C3B	2.45	1.53	1.47
76	C3	603	HEA	CMD-C2D	2.44	1.55	1.50
80	m	401	HEM	C3C-C2C	-2.43	1.32	1.37
72	6	701	CDL	OB6-CB5	2.43	1.41	1.34
80	y	401	HEM	CHA-C1A	-2.42	1.34	1.39
80	y	401	HEM	C3C-C2C	-2.42	1.32	1.37
69	j	201	PC1	O21-C2	-2.40	1.41	1.46
80	m	402	HEM	C3C-C2C	-2.40	1.32	1.37
79	R	601	NAP	C5N-C4N	-2.40	1.34	1.38
80	y	402	HEM	CHB-C1B	-2.39	1.33	1.38
70	2	401	3PE	O31-C31	2.38	1.40	1.33
80	m	402	HEM	CAB-C3B	2.38	1.53	1.47
76	C3	602	HEA	C3A-C4A	-2.38	1.41	1.46
80	m	402	HEM	CHB-C1B	-2.38	1.33	1.38
69	3	200	PC1	O31-C3	-2.36	1.39	1.45
80	y	402	HEM	CAB-C3B	2.36	1.53	1.47
80	y	402	HEM	C3C-C2C	-2.36	1.32	1.37
80	m	402	HEM	C1B-NB	-2.34	1.36	1.40
80	y	402	HEM	C1B-NB	-2.33	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	j	201	PC1	O21-C21	2.33	1.40	1.34
80	m	402	HEM	CHA-C1A	-2.32	1.34	1.39
80	y	402	HEM	CHA-C1A	-2.31	1.34	1.39
70	1	401	3PE	O31-C31	2.30	1.40	1.33
70	j	202	3PE	O31-C31	2.29	1.40	1.33
72	J	101	CDL	OB8-CB7	2.29	1.40	1.33
80	m	401	HEM	CHB-C4A	-2.28	1.34	1.39
81	o	301	HEC	C2A-C3A	-2.28	1.31	1.36
80	y	401	HEM	CHB-C4A	-2.27	1.34	1.39
80	y	402	HEM	CAC-C3C	2.27	1.53	1.47
70	1	401	3PE	O31-C3	-2.26	1.40	1.45
80	m	402	HEM	CHD-C1D	-2.26	1.34	1.39
80	m	402	HEM	CAC-C3C	2.26	1.53	1.47
81	z	301	HEC	C2A-C3A	-2.26	1.31	1.36
80	y	402	HEM	CHD-C1D	-2.25	1.34	1.39
69	j	201	PC1	C12-N	-2.25	1.44	1.51
80	y	402	HEM	CHA-C4D	-2.25	1.34	1.38
72	J	101	CDL	OB8-CB6	-2.24	1.40	1.45
80	m	402	HEM	CHA-C4D	-2.23	1.34	1.38
69	S	401	PC1	O31-C3	-2.22	1.40	1.45
69	j	201	PC1	O31-C3	-2.19	1.40	1.45
80	y	401	HEM	CHC-C4B	-2.19	1.34	1.39
73	8	501	FMN	C4A-C10	-2.19	1.37	1.44
80	y	401	HEM	CHA-C4D	-2.18	1.34	1.38
80	m	401	HEM	C3B-C2B	-2.18	1.32	1.37
70	4	501	3PE	O21-C21	2.18	1.40	1.34
80	m	401	HEM	CHC-C4B	-2.18	1.34	1.39
72	J	101	CDL	OA6-CA5	2.18	1.40	1.34
72	J	101	CDL	OB6-CB5	2.17	1.40	1.34
80	m	401	HEM	CHA-C4D	-2.17	1.34	1.38
70	4	501	3PE	O21-C2	-2.16	1.41	1.46
69	Q	201	PC1	O31-C31	2.15	1.39	1.33
80	m	402	HEM	C3C-C4C	-2.15	1.42	1.46
72	b	201	CDL	OA8-CA6	-2.15	1.40	1.45
72	6	701	CDL	OA8-CA7	2.14	1.39	1.33
79	R	601	NAP	P2B-O2B	2.14	1.63	1.59
80	y	401	HEM	C3B-C2B	-2.14	1.32	1.37
70	2	401	3PE	O31-C3	-2.14	1.40	1.45
80	y	402	HEM	C3C-C4C	-2.14	1.42	1.46
70	j	202	3PE	O31-C3	-2.12	1.40	1.45
72	6	701	CDL	OB6-CB4	-2.12	1.41	1.46
69	3	200	PC1	O21-C21	2.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	b	201	CDL	OB6-CB4	-2.11	1.41	1.46
80	m	402	HEM	CHC-C1C	-2.11	1.34	1.38
80	y	402	HEM	CHD-C4C	-2.11	1.34	1.38
69	S	401	PC1	O21-C21	2.11	1.40	1.34
80	m	401	HEM	CAC-C3C	2.10	1.53	1.47
80	y	402	HEM	C4D-ND	-2.10	1.36	1.40
80	y	401	HEM	CAC-C3C	2.10	1.53	1.47
69	2	402	PC1	O21-C2	-2.10	1.41	1.46
76	C3	603	HEA	FE-NC	2.09	2.02	1.95
80	m	402	HEM	C4D-ND	-2.08	1.36	1.40
72	b	201	CDL	OA6-CA5	2.08	1.40	1.34
69	j	201	PC1	C13-N	-2.08	1.44	1.50
80	y	401	HEM	CHB-C1B	-2.06	1.34	1.38
80	m	401	HEM	CHB-C1B	-2.05	1.34	1.38
80	m	402	HEM	CHD-C4C	-2.05	1.34	1.38
80	y	401	HEM	C3C-C4C	-2.04	1.42	1.46
80	y	402	HEM	CHC-C1C	-2.04	1.34	1.38
69	2	402	PC1	O31-C3	-2.04	1.40	1.45
72	6	701	CDL	OA6-CA5	2.03	1.40	1.34
80	m	401	HEM	C3C-C4C	-2.03	1.42	1.46
72	b	201	CDL	OB8-CB6	-2.03	1.40	1.45
69	S	401	PC1	C12-N	-2.02	1.45	1.51
72	6	701	CDL	OB8-CB7	2.00	1.39	1.33
80	y	402	HEM	CHC-C4B	-2.00	1.34	1.39

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	z	301	HEC	CBC-CAC-C3C	-10.95	105.55	127.43
81	o	301	HEC	CBC-CAC-C3C	-10.93	105.58	127.43
81	z	301	HEC	CBB-CAB-C3B	-10.54	106.38	127.43
81	o	301	HEC	CBB-CAB-C3B	-10.52	106.41	127.43
79	R	601	NAP	N3A-C2A-N1A	-6.56	118.65	128.58
79	R	601	NAP	N6A-C6A-N1A	-5.47	106.19	118.38
70	B	501	3PE	O21-C21-C22	5.41	123.18	111.48
80	m	401	HEM	C1C-CHC-C4B	-5.30	114.75	126.02
80	y	401	HEM	C1C-CHC-C4B	-5.27	114.81	126.02
70	4	501	3PE	O21-C21-C22	5.10	122.51	111.48
79	R	601	NAP	N9A-C8A-N7A	-4.81	107.12	113.94
79	R	601	NAP	C5A-C4A-N3A	-4.75	120.17	126.72
72	6	701	CDL	OB6-CB5-C51	4.62	121.47	111.48
72	J	101	CDL	OA6-CA5-C11	4.43	121.06	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	8	501	FMN	C4-N3-C2	-4.17	118.23	125.64
76	C3	602	HEA	C17-C18-C19	-4.17	118.09	127.62
69	S	401	PC1	O21-C21-C22	4.14	120.44	111.48
72	b	201	CDL	OA6-CA5-C11	4.12	120.39	111.48
72	6	701	CDL	OA6-CA5-C11	4.09	120.34	111.48
69	Q	201	PC1	O21-C21-C22	4.04	120.21	111.48
70	2	401	3PE	O21-C21-C22	3.83	119.76	111.48
79	R	601	NAP	C2A-N3A-C4A	3.81	121.14	111.83
72	b	201	CDL	OB6-CB5-C51	3.81	119.72	111.48
79	R	601	NAP	C2B-C1B-N9A	-3.74	107.60	113.75
69	3	200	PC1	O21-C21-C22	3.73	119.56	111.48
79	R	601	NAP	C4D-O4D-C1D	-3.68	106.55	109.92
82	A2	201	UQ2	C7-C8-C9	-3.68	120.49	126.83
70	j	202	3PE	O21-C21-C22	3.62	119.31	111.48
79	R	601	NAP	C5A-C6A-N6A	3.51	131.97	123.29
73	8	501	FMN	C5A-C9A-N10	3.49	121.12	117.97
70	1	401	3PE	O21-C21-C22	3.48	119.00	111.48
72	J	101	CDL	OB6-CB5-C51	3.46	118.96	111.48
69	2	402	PC1	O21-C21-C22	3.43	118.91	111.48
80	y	401	HEM	C4A-CHB-C1B	-3.40	118.26	126.25
80	m	401	HEM	C4A-CHB-C1B	-3.39	118.27	126.25
70	B	501	3PE	O31-C31-C32	3.39	122.17	111.83
76	C3	602	HEA	C13-C14-C15	-3.33	120.00	127.62
80	m	401	HEM	CAD-C3D-C4D	3.31	130.46	124.70
80	y	401	HEM	CAD-C3D-C4D	3.29	130.44	124.70
72	b	201	CDL	OB8-CB7-C71	3.17	121.51	111.83
76	C3	603	HEA	CHA-C1A-NA	-3.13	121.04	124.45
73	8	501	FMN	C4A-C10-N10	3.12	120.95	116.48
70	1	401	3PE	O31-C31-C32	3.10	121.30	111.83
73	8	501	FMN	O4-C4-C4A	-3.02	118.57	126.53
81	z	301	HEC	CHD-C4C-NC	3.00	127.72	124.45
72	b	201	CDL	OA8-CA7-C31	2.99	120.96	111.83
69	Q	201	PC1	O31-C31-C32	2.99	120.94	111.83
72	J	101	CDL	OA8-CA7-C31	2.97	120.89	111.83
79	R	601	NAP	C4A-N9A-C1B	-2.95	119.74	126.63
81	o	301	HEC	CHD-C4C-NC	2.95	127.66	124.45
73	8	501	FMN	C4'-C3'-C2'	-2.92	108.72	113.57
72	6	701	CDL	OA8-CA7-C31	2.91	120.71	111.83
76	C3	602	HEA	C1B-C2B-C3B	2.91	110.16	106.80
69	j	201	PC1	O31-C31-C32	2.89	120.64	111.83
79	R	601	NAP	C5A-N7A-C8A	2.88	107.98	103.45
82	A2	201	UQ2	C7-C6-C5	-2.87	119.97	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	8	501	FMN	C4A-C10-N1	-2.85	117.61	124.59
73	8	501	FMN	C4A-C4-N3	2.82	120.44	113.25
69	S	401	PC1	O31-C31-C32	2.82	120.44	111.83
81	z	301	HEC	CAA-CBA-CGA	-2.82	106.20	113.67
80	m	402	HEM	C4A-CHB-C1B	-2.81	119.63	126.25
72	6	701	CDL	OB8-CB7-C71	2.81	120.41	111.83
72	J	101	CDL	OB8-CB7-C71	2.81	120.41	111.83
81	o	301	HEC	CAA-CBA-CGA	-2.80	106.24	113.67
80	y	402	HEM	C4A-CHB-C1B	-2.79	119.68	126.25
81	z	301	HEC	C4D-ND-C1D	2.79	110.37	105.82
82	A2	201	UQ2	C10-C9-C11	2.79	120.06	115.23
80	m	401	HEM	CAD-C3D-C2D	-2.78	122.66	127.87
80	y	401	HEM	CAD-C3D-C2D	-2.78	122.66	127.87
81	o	301	HEC	C1C-CHC-C4B	-2.77	116.11	124.66
80	y	401	HEM	C1A-CHA-C4D	-2.76	119.76	126.25
81	z	301	HEC	C1C-CHC-C4B	-2.76	116.16	124.66
80	m	401	HEM	C1A-CHA-C4D	-2.75	119.78	126.25
81	o	301	HEC	C4D-ND-C1D	2.73	110.28	105.82
70	2	401	3PE	O31-C31-C32	2.73	120.15	111.83
69	2	402	PC1	O31-C31-C32	2.73	120.14	111.83
70	j	202	3PE	O31-C31-C32	2.72	120.12	111.83
82	A2	201	UQ2	CM5-C5-C6	-2.70	120.00	124.45
80	y	401	HEM	CAD-CBD-CGD	-2.60	106.78	113.67
79	R	601	NAP	C4A-N9A-C8A	2.59	108.46	105.74
80	m	401	HEM	CAD-CBD-CGD	-2.59	106.81	113.67
80	y	402	HEM	C4C-CHD-C1D	-2.58	120.54	126.02
80	m	402	HEM	C4C-CHD-C1D	-2.55	120.60	126.02
76	C3	603	HEA	C4A-C3A-C2A	2.55	109.02	106.81
80	y	402	HEM	CHC-C4B-NB	2.53	127.15	124.42
79	R	601	NAP	N3A-C4A-N9A	2.53	131.48	127.17
73	8	501	FMN	C4-C4A-C10	2.53	121.28	116.93
69	j	201	PC1	O21-C21-C22	2.53	120.21	110.93
76	C3	603	HEA	CMD-C2D-C1D	2.51	128.96	125.03
73	8	501	FMN	C2'-C1'-N10	2.51	122.07	110.20
80	m	401	HEM	C4C-CHD-C1D	-2.50	120.70	126.02
81	o	301	HEC	C4D-CHA-C1A	-2.49	116.97	124.66
80	m	402	HEM	CHC-C4B-NB	2.49	127.10	124.42
81	z	301	HEC	C4D-CHA-C1A	-2.49	116.99	124.66
73	8	501	FMN	O2'-C2'-C3'	-2.48	103.44	109.25
76	C3	602	HEA	C3C-C4C-NC	2.47	111.88	109.80
80	y	402	HEM	CHD-C4C-NC	2.46	127.14	124.45
80	y	401	HEM	C4C-CHD-C1D	-2.46	120.79	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	C3	602	HEA	C17-C16-C15	-2.45	105.06	113.19
76	C3	603	HEA	C12-C11-C3B	2.44	115.93	112.12
80	m	402	HEM	CHD-C4C-NC	2.44	127.11	124.45
76	C3	603	HEA	C1D-C2D-C3D	-2.43	104.42	106.98
70	4	501	3PE	C23-C22-C21	-2.42	104.81	113.69
76	C3	603	HEA	C13-C14-C15	-2.41	122.10	127.62
80	m	402	HEM	CHB-C1B-NB	2.36	127.29	124.37
82	A2	201	UQ2	C16-C14-C15	2.35	119.99	114.59
80	y	402	HEM	CHB-C1B-NB	2.34	127.27	124.37
79	R	601	NAP	C5A-C4A-N9A	2.33	108.34	105.81
76	C3	602	HEA	CAD-C3D-C4D	2.30	128.71	124.70
76	C3	603	HEA	CMB-C2B-C3B	-2.30	125.83	130.28
72	J	101	CDL	CA4-OA6-CA5	-2.28	112.33	117.80
76	C3	603	HEA	CAA-C2A-C1A	2.26	129.44	124.85
70	B	501	3PE	O31-C31-O32	-2.26	117.98	123.63
70	B	501	3PE	C23-C22-C21	-2.25	105.43	113.69
80	y	402	HEM	CBA-CAA-C2A	-2.25	106.33	112.53
79	R	601	NAP	C2N-C3N-C4N	2.24	120.87	118.26
80	m	402	HEM	CBA-CAA-C2A	-2.24	106.35	112.53
76	C3	602	HEA	C4B-C3B-C2B	-2.23	103.69	107.44
76	C3	603	HEA	C25-C23-C24	2.21	119.69	114.59
81	o	301	HEC	C1B-CHB-C4A	-2.20	117.88	124.66
73	8	501	FMN	C9A-N10-C10	-2.19	117.41	120.75
81	z	301	HEC	C1B-CHB-C4A	-2.18	117.93	124.66
81	o	301	HEC	CHA-C1A-C2A	2.17	128.29	124.86
79	R	601	NAP	C4A-C5A-N7A	-2.17	108.10	110.58
80	m	402	HEM	C1C-CHC-C4B	-2.17	121.42	126.02
76	C3	602	HEA	C12-C13-C14	-2.17	106.47	112.16
79	R	601	NAP	O4B-C1B-N9A	2.16	112.25	108.09
80	y	402	HEM	C1C-CHC-C4B	-2.16	121.42	126.02
76	C3	603	HEA	C26-C15-C16	2.16	118.98	115.23
80	m	401	HEM	CAA-CBA-CGA	-2.16	107.93	113.67
73	8	501	FMN	C10-N1-C2	2.16	121.53	116.85
81	o	301	HEC	CBD-CAD-C3D	-2.16	106.56	112.53
81	z	301	HEC	CBD-CAD-C3D	-2.16	106.56	112.53
82	A2	201	UQ2	C12-C13-C14	-2.16	120.45	127.64
80	y	401	HEM	CAA-CBA-CGA	-2.16	107.94	113.67
81	z	301	HEC	CHA-C1A-C2A	2.13	128.24	124.86
80	m	402	HEM	CAA-CBA-CGA	-2.12	108.03	113.67
69	3	200	PC1	O31-C31-C32	2.12	118.30	111.83
79	R	601	NAP	C1B-N9A-C8A	2.12	131.80	127.09
76	C3	602	HEA	C20-C19-C18	2.12	125.92	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	o	301	HEC	CAD-CBD-CGD	-2.12	108.05	113.67
80	y	402	HEM	CAA-CBA-CGA	-2.12	108.06	113.67
73	8	501	FMN	C6-C5A-C9A	2.11	121.94	119.05
79	R	601	NAP	O3B-C3B-C2B	-2.11	105.29	111.19
81	z	301	HEC	CAD-CBD-CGD	-2.10	108.09	113.67
76	C3	603	HEA	CBD-CAD-C3D	2.10	118.35	112.53
76	C3	603	HEA	C3A-C2A-C1A	-2.08	105.08	107.05
76	C3	602	HEA	C27-C19-C18	-2.06	118.34	123.63
70	4	501	3PE	O31-C31-C32	2.04	118.04	111.83

There are no chirality outliers.

All (391) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	3	200	PC1	C22-C21-O21-C2
69	2	402	PC1	C11-O13-P-O12
69	2	402	PC1	C1-O11-P-O12
69	2	402	PC1	C1-O11-P-O14
69	2	402	PC1	C1-O11-P-O13
69	Q	201	PC1	C11-O13-P-O12
69	Q	201	PC1	C11-O13-P-O11
69	Q	201	PC1	C1-O11-P-O12
69	Q	201	PC1	C1-O11-P-O13
69	Q	201	PC1	O13-C11-C12-N
69	Q	201	PC1	C22-C21-O21-C2
69	S	401	PC1	C11-O13-P-O12
69	S	401	PC1	C11-O13-P-O14
69	S	401	PC1	O13-C11-C12-N
69	j	201	PC1	C11-O13-P-O12
69	j	201	PC1	C1-O11-P-O12
69	j	201	PC1	C1-O11-P-O13
69	j	201	PC1	O13-C11-C12-N
69	j	201	PC1	O22-C21-O21-C2
69	j	201	PC1	C22-C21-O21-C2
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	C22-C21-O21-C2
70	2	401	3PE	C11-O13-P-O11
70	2	401	3PE	C11-O13-P-O12
70	2	401	3PE	C11-O13-P-O14
70	2	401	3PE	O13-C11-C12-N
70	2	401	3PE	C22-C21-O21-C2
70	B	501	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
70	B	501	3PE	C1-O11-P-O14
70	B	501	3PE	O22-C21-O21-C2
70	B	501	3PE	C22-C21-O21-C2
70	j	202	3PE	C11-O13-P-O11
70	j	202	3PE	C11-O13-P-O12
70	j	202	3PE	C11-O13-P-O14
70	j	202	3PE	O13-C11-C12-N
72	6	701	CDL	CA3-OA5-PA1-OA2
72	6	701	CDL	CA3-OA5-PA1-OA4
72	6	701	CDL	CB2-OB2-PB2-OB3
72	6	701	CDL	CB2-OB2-PB2-OB4
72	6	701	CDL	CB2-OB2-PB2-OB5
72	6	701	CDL	CB3-OB5-PB2-OB2
72	6	701	CDL	CB3-OB5-PB2-OB3
72	J	101	CDL	CA2-OA2-PA1-OA3
72	J	101	CDL	CA2-OA2-PA1-OA5
72	J	101	CDL	C11-CA5-OA6-CA4
72	J	101	CDL	CB2-OB2-PB2-OB3
72	J	101	CDL	CB2-OB2-PB2-OB4
72	J	101	CDL	CB2-OB2-PB2-OB5
72	J	101	CDL	OB5-CB3-CB4-OB6
72	b	201	CDL	CA2-OA2-PA1-OA3
72	b	201	CDL	CA2-OA2-PA1-OA5
72	b	201	CDL	CB2-OB2-PB2-OB5
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	O4'-C4'-C5'-O5'
73	8	501	FMN	C5'-O5'-P-O1P
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P
76	C3	602	HEA	C2A-C3A-CMA-OMA
76	C3	602	HEA	C4A-C3A-CMA-OMA
76	C3	603	HEA	C2A-C3A-CMA-OMA
76	C3	603	HEA	C4A-C3A-CMA-OMA
79	R	601	NAP	C5B-O5B-PA-O2A
79	R	601	NAP	C5B-O5B-PA-O3
79	R	601	NAP	C1B-C2B-O2B-P2B
79	R	601	NAP	C5D-O5D-PN-O3
79	R	601	NAP	C5D-O5D-PN-O1N
79	R	601	NAP	C5D-O5D-PN-O2N
79	R	601	NAP	C2D-C1D-N1N-C2N
79	R	601	NAP	C2D-C1D-N1N-C6N
81	o	301	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
81	z	301	HEC	C2B-C3B-CAB-CBB
70	j	202	3PE	O32-C31-O31-C3
72	6	701	CDL	OA9-CA7-OA8-CA6
72	b	201	CDL	OA9-CA7-OA8-CA6
70	j	202	3PE	C32-C31-O31-C3
72	6	701	CDL	C31-CA7-OA8-CA6
72	b	201	CDL	OB9-CB7-OB8-CB6
69	3	200	PC1	O22-C21-O21-C2
69	2	402	PC1	O22-C21-O21-C2
69	Q	201	PC1	O22-C21-O21-C2
70	2	401	3PE	O22-C21-O21-C2
72	J	101	CDL	OA7-CA5-OA6-CA4
72	b	201	CDL	C31-CA7-OA8-CA6
72	J	101	CDL	OA9-CA7-OA8-CA6
72	J	101	CDL	C71-CB7-OB8-CB6
72	b	201	CDL	C71-CB7-OB8-CB6
72	J	101	CDL	OB9-CB7-OB8-CB6
80	m	401	HEM	C4D-C3D-CAD-CBD
80	y	401	HEM	C4D-C3D-CAD-CBD
70	4	501	3PE	O22-C21-O21-C2
70	2	401	3PE	C32-C31-O31-C3
69	2	402	PC1	C22-C21-O21-C2
72	J	101	CDL	C31-CA7-OA8-CA6
76	C3	602	HEA	C15-C16-C17-C18
70	4	501	3PE	C2-C1-O11-P
70	2	401	3PE	O32-C31-O31-C3
69	3	200	PC1	C32-C31-O31-C3
69	Q	201	PC1	C32-C31-O31-C3
69	j	201	PC1	C32-C31-O31-C3
69	2	402	PC1	C36-C37-C38-C39
69	2	402	PC1	C26-C27-C28-C29
82	A2	201	UQ2	C12-C11-C9-C10
82	A2	201	UQ2	C12-C11-C9-C8
80	m	401	HEM	C2D-C3D-CAD-CBD
80	y	401	HEM	C2D-C3D-CAD-CBD
69	S	401	PC1	C23-C24-C25-C26
69	j	201	PC1	O32-C31-O31-C3
69	2	402	PC1	C21-C22-C23-C24
69	2	402	PC1	C32-C33-C34-C35
79	R	601	NAP	O4D-C4D-C5D-O5D
69	3	200	PC1	C34-C35-C36-C37
72	b	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
69	S	401	PC1	C3B-C3C-C3D-C3E
69	3	200	PC1	C21-C22-C23-C24
69	Q	201	PC1	C21-C22-C23-C24
70	4	501	3PE	C31-C32-C33-C34
70	j	202	3PE	C31-C32-C33-C34
69	Q	201	PC1	O32-C31-O31-C3
69	3	200	PC1	O32-C31-O31-C3
72	J	101	CDL	CA7-C31-C32-C33
70	4	501	3PE	C2B-C2C-C2D-C2E
70	1	401	3PE	C21-C22-C23-C24
72	6	701	CDL	OB7-CB5-OB6-CB4
69	S	401	PC1	C22-C21-O21-C2
72	6	701	CDL	C51-CB5-OB6-CB4
72	b	201	CDL	O1-C1-CA2-OA2
69	Q	201	PC1	C24-C25-C26-C27
72	6	701	CDL	C32-C33-C34-C35
70	2	401	3PE	C33-C34-C35-C36
70	4	501	3PE	C27-C28-C29-C2A
69	S	401	PC1	O22-C21-O21-C2
69	S	401	PC1	C32-C31-O31-C3
70	4	501	3PE	C32-C31-O31-C3
69	S	401	PC1	C34-C35-C36-C37
70	4	501	3PE	C2E-C2F-C2G-C2H
70	B	501	3PE	C2B-C2C-C2D-C2E
70	2	401	3PE	C21-C22-C23-C24
69	Q	201	PC1	C26-C27-C28-C29
70	B	501	3PE	C2A-C2B-C2C-C2D
72	b	201	CDL	C60-C61-C62-C63
69	3	200	PC1	C3C-C3D-C3E-C3F
69	S	401	PC1	C24-C25-C26-C27
70	2	401	3PE	C27-C28-C29-C2A
69	j	201	PC1	C35-C36-C37-C38
69	j	201	PC1	C3B-C3C-C3D-C3E
69	3	200	PC1	C3B-C3C-C3D-C3E
69	2	402	PC1	C2C-C2D-C2E-C2F
72	J	101	CDL	C14-C15-C16-C17
69	j	201	PC1	C3D-C3E-C3F-C3G
72	b	201	CDL	C11-C12-C13-C14
69	S	401	PC1	C37-C38-C39-C3A
69	j	201	PC1	C33-C34-C35-C36
70	B	501	3PE	C39-C3A-C3B-C3C
72	b	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
72	b	201	CDL	C81-C82-C83-C84
70	1	401	3PE	C2B-C2C-C2D-C2E
70	B	501	3PE	C35-C36-C37-C38
69	2	402	PC1	C28-C29-C2A-C2B
69	S	401	PC1	O32-C31-O31-C3
72	6	701	CDL	C11-CA5-OA6-CA4
70	2	401	3PE	C32-C33-C34-C35
70	B	501	3PE	C37-C38-C39-C3A
69	j	201	PC1	C31-C32-C33-C34
70	4	501	3PE	O32-C31-O31-C3
70	4	501	3PE	C23-C24-C25-C26
70	j	202	3PE	C35-C36-C37-C38
72	b	201	CDL	CA5-C11-C12-C13
70	B	501	3PE	C2D-C2E-C2F-C2G
69	3	200	PC1	C32-C33-C34-C35
72	J	101	CDL	C15-C16-C17-C18
70	j	202	3PE	C28-C29-C2A-C2B
70	j	202	3PE	C22-C21-O21-C2
70	j	202	3PE	C22-C23-C24-C25
69	3	200	PC1	C22-C23-C24-C25
70	1	401	3PE	C24-C25-C26-C27
70	4	501	3PE	C2A-C2B-C2C-C2D
70	4	501	3PE	C2C-C2D-C2E-C2F
69	3	200	PC1	C11-C12-N-C13
69	3	200	PC1	C11-C12-N-C14
69	3	200	PC1	C11-C12-N-C15
69	2	402	PC1	C22-C23-C24-C25
70	j	202	3PE	O22-C21-O21-C2
69	3	200	PC1	O11-C1-C2-O21
70	B	501	3PE	O11-C1-C2-O21
72	b	201	CDL	C51-CB5-OB6-CB4
69	S	401	PC1	C35-C36-C37-C38
70	4	501	3PE	C21-C22-C23-C24
69	3	200	PC1	C3A-C3B-C3C-C3D
70	B	501	3PE	C28-C29-C2A-C2B
70	1	401	3PE	C23-C24-C25-C26
69	2	402	PC1	C23-C24-C25-C26
69	Q	201	PC1	C33-C34-C35-C36
69	Q	201	PC1	C27-C28-C29-C2A
72	J	101	CDL	CB5-C51-C52-C53
70	2	401	3PE	C23-C24-C25-C26
72	6	701	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
69	Q	201	PC1	C1-C2-C3-O31
70	1	401	3PE	C1-C2-C3-O31
72	b	201	CDL	C76-C77-C78-C79
72	6	701	CDL	C31-C32-C33-C34
70	B	501	3PE	C23-C24-C25-C26
82	A2	201	UQ2	C3-C2-O2-CM2
70	2	401	3PE	C25-C26-C27-C28
72	b	201	CDL	C31-C32-C33-C34
70	2	401	3PE	C3-C2-O21-C21
69	2	402	PC1	C25-C26-C27-C28
70	j	202	3PE	C2D-C2E-C2F-C2G
70	1	401	3PE	C35-C36-C37-C38
79	R	601	NAP	C2B-C1B-N9A-C8A
72	6	701	CDL	C34-C35-C36-C37
70	B	501	3PE	C3B-C3C-C3D-C3E
69	2	402	PC1	C24-C25-C26-C27
69	Q	201	PC1	C2A-C2B-C2C-C2D
70	j	202	3PE	C36-C37-C38-C39
70	j	202	3PE	C3A-C3B-C3C-C3D
70	1	401	3PE	O21-C2-C3-O31
72	b	201	CDL	OB6-CB4-CB6-OB8
70	j	202	3PE	C34-C35-C36-C37
70	4	501	3PE	C35-C36-C37-C38
70	4	501	3PE	C33-C34-C35-C36
80	m	401	HEM	C3D-CAD-CBD-CGD
80	y	401	HEM	C3D-CAD-CBD-CGD
72	6	701	CDL	C72-C73-C74-C75
72	J	101	CDL	C51-C52-C53-C54
69	3	200	PC1	O11-C1-C2-C3
70	B	501	3PE	O11-C1-C2-C3
72	J	101	CDL	OB5-CB3-CB4-CB6
70	2	401	3PE	C2F-C2G-C2H-C2I
72	b	201	CDL	OB7-CB5-OB6-CB4
69	2	402	PC1	C39-C3A-C3B-C3C
72	b	201	CDL	C59-C60-C61-C62
69	3	200	PC1	C1-C2-C3-O31
70	2	401	3PE	C1-C2-C3-O31
70	B	501	3PE	C38-C39-C3A-C3B
70	1	401	3PE	C27-C28-C29-C2A
72	J	101	CDL	OA5-CA3-CA4-OA6
72	b	201	CDL	C57-C58-C59-C60
80	m	402	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
80	y	402	HEM	C2A-CAA-CBA-CGA
69	S	401	PC1	C3C-C3D-C3E-C3F
69	3	200	PC1	O21-C2-C3-O31
69	S	401	PC1	O21-C2-C3-O31
70	2	401	3PE	O21-C2-C3-O31
72	b	201	CDL	OA6-CA4-CA6-OA8
79	R	601	NAP	C3D-C4D-C5D-O5D
70	B	501	3PE	C3C-C3D-C3E-C3F
70	1	401	3PE	C34-C35-C36-C37
70	1	401	3PE	C3E-C3F-C3G-C3H
79	R	601	NAP	PN-O3-PA-O5B
70	1	401	3PE	C28-C29-C2A-C2B
72	6	701	CDL	C51-C52-C53-C54
72	6	701	CDL	CA5-C11-C12-C13
69	3	200	PC1	O31-C31-C32-C33
72	b	201	CDL	C11-CA5-OA6-CA4
69	S	401	PC1	O11-C1-C2-C3
70	2	401	3PE	O11-C1-C2-C3
73	8	501	FMN	C1'-C2'-C3'-O3'
69	2	402	PC1	C37-C38-C39-C3A
69	2	402	PC1	C32-C31-O31-C3
72	b	201	CDL	OA7-CA5-OA6-CA4
70	1	401	3PE	C33-C34-C35-C36
70	4	501	3PE	C1-C2-O21-C21
69	Q	201	PC1	C2B-C2C-C2D-C2E
69	S	401	PC1	O11-C1-C2-O21
69	j	201	PC1	O11-C1-C2-O21
69	j	201	PC1	C12-C11-O13-P
70	2	401	3PE	C12-C11-O13-P
82	A2	201	UQ2	C1-C6-C7-C8
70	j	202	3PE	O21-C2-C3-O31
70	B	501	3PE	C3A-C3B-C3C-C3D
72	6	701	CDL	C71-C72-C73-C74
70	4	501	3PE	C24-C25-C26-C27
70	1	401	3PE	C38-C39-C3A-C3B
69	3	200	PC1	O13-C11-C12-N
69	2	402	PC1	O13-C11-C12-N
72	b	201	CDL	C34-C35-C36-C37
72	b	201	CDL	OB5-CB3-CB4-CB6
70	j	202	3PE	C2E-C2F-C2G-C2H
81	o	301	HEC	C4B-C3B-CAB-CBB
81	o	301	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
81	z	301	HEC	C4B-C3B-CAB-CBB
81	z	301	HEC	C4C-C3C-CAC-CBC
70	2	401	3PE	O11-C1-C2-O21
69	2	402	PC1	C38-C39-C3A-C3B
69	2	402	PC1	O32-C31-O31-C3
69	Q	201	PC1	O21-C2-C3-O31
69	3	200	PC1	C26-C27-C28-C29
69	S	401	PC1	C1-C2-C3-O31
72	b	201	CDL	CB3-CB4-CB6-OB8
70	B	501	3PE	C24-C25-C26-C27
69	S	401	PC1	C32-C33-C34-C35
69	2	402	PC1	C11-O13-P-O11
69	Q	201	PC1	C11-O13-P-O14
69	Q	201	PC1	C1-O11-P-O14
69	S	401	PC1	C11-O13-P-O11
69	j	201	PC1	C11-O13-P-O14
69	j	201	PC1	C11-O13-P-O11
70	4	501	3PE	C1-O11-P-O12
70	4	501	3PE	C1-O11-P-O13
70	4	501	3PE	C1-O11-P-O14
70	B	501	3PE	C1-O11-P-O12
72	6	701	CDL	CA2-OA2-PA1-OA3
72	6	701	CDL	CA3-OA5-PA1-OA3
72	J	101	CDL	CA3-OA5-PA1-OA4
72	b	201	CDL	CA2-OA2-PA1-OA4
72	b	201	CDL	CB2-OB2-PB2-OB3
73	8	501	FMN	C2'-C1'-N10-C10
79	R	601	NAP	C5B-O5B-PA-O1A
81	o	301	HEC	C2C-C3C-CAC-CBC
81	z	301	HEC	C2C-C3C-CAC-CBC
70	2	401	3PE	C26-C27-C28-C29
72	6	701	CDL	C1-CA2-OA2-PA1
72	b	201	CDL	C63-C64-C65-C66
70	B	501	3PE	C2C-C2D-C2E-C2F
72	J	101	CDL	OA5-CA3-CA4-CA6
72	b	201	CDL	C77-C78-C79-C80
70	B	501	3PE	C29-C2A-C2B-C2C
70	j	202	3PE	O21-C21-C22-C23
79	R	601	NAP	C2B-C1B-N9A-C4A
82	A2	201	UQ2	C5-C6-C7-C8
69	j	201	PC1	C38-C39-C3A-C3B
69	Q	201	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
69	j	201	PC1	C3F-C3G-C3H-C3I
72	6	701	CDL	OA6-CA4-CA6-OA8
73	8	501	FMN	C3'-C4'-C5'-O5'
72	b	201	CDL	CA2-C1-CB2-OB2
69	2	402	PC1	C1-C2-O21-C21
72	6	701	CDL	CB3-CB4-OB6-CB5
72	b	201	CDL	CB3-CB4-OB6-CB5
76	C3	603	HEA	CAD-CBD-CGD-O1D
69	2	402	PC1	C31-C32-C33-C34
70	B	501	3PE	C31-C32-C33-C34
76	C3	602	HEA	CAD-CBD-CGD-O1D
69	j	201	PC1	O11-C1-C2-C3
72	b	201	CDL	C71-C72-C73-C74
76	C3	603	HEA	CAD-CBD-CGD-O2D
69	Q	201	PC1	C38-C39-C3A-C3B
70	B	501	3PE	C26-C27-C28-C29
72	6	701	CDL	CA4-CA3-OA5-PA1
76	C3	602	HEA	CAD-CBD-CGD-O2D
82	A2	201	UQ2	C4-C3-O3-CM3
72	J	101	CDL	CA2-C1-CB2-OB2
72	b	201	CDL	CB2-C1-CA2-OA2
70	4	501	3PE	C22-C23-C24-C25
69	S	401	PC1	C28-C29-C2A-C2B
72	6	701	CDL	O1-C1-CB2-OB2
69	2	402	PC1	C29-C2A-C2B-C2C
70	B	501	3PE	C32-C33-C34-C35
69	3	200	PC1	O32-C31-C32-C33
76	C3	602	HEA	CAA-CBA-CGA-O1A
72	b	201	CDL	OB5-CB3-CB4-OB6
70	j	202	3PE	C21-C22-C23-C24
76	C3	603	HEA	CAA-CBA-CGA-O2A
72	6	701	CDL	C15-C16-C17-C18
72	6	701	CDL	C72-C71-CB7-OB8
69	S	401	PC1	C21-C22-C23-C24
70	2	401	3PE	O31-C31-C32-C33
69	2	402	PC1	C2D-C2E-C2F-C2G
76	C3	603	HEA	CAA-CBA-CGA-O1A
82	A2	201	UQ2	C9-C11-C12-C13
72	b	201	CDL	C12-C11-CA5-OA6
70	1	401	3PE	C3C-C3D-C3E-C3F
79	R	601	NAP	C2B-O2B-P2B-O3X
72	b	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
76	C3	603	HEA	C26-C15-C16-C17
69	2	402	PC1	O31-C31-C32-C33
70	B	501	3PE	O31-C31-C32-C33
72	6	701	CDL	CA7-C31-C32-C33
73	8	501	FMN	N10-C1'-C2'-O2'
69	S	401	PC1	C1-C2-O21-C21
69	S	401	PC1	C27-C28-C29-C2A
70	B	501	3PE	C25-C26-C27-C28
81	o	301	HEC	CAA-CBA-CGA-O1A
81	z	301	HEC	CAA-CBA-CGA-O1A
79	R	601	NAP	O4B-C1B-N9A-C8A
69	S	401	PC1	C33-C34-C35-C36
72	J	101	CDL	C55-C56-C57-C58
69	j	201	PC1	C36-C37-C38-C39
69	3	200	PC1	C38-C39-C3A-C3B
70	2	401	3PE	O32-C31-C32-C33
69	S	401	PC1	O31-C31-C32-C33
69	2	402	PC1	O32-C31-C32-C33
72	b	201	CDL	C12-C11-CA5-OA7
70	4	501	3PE	C26-C27-C28-C29
76	C3	602	HEA	CAA-CBA-CGA-O2A
72	6	701	CDL	C72-C71-CB7-OB9
70	j	202	3PE	C1-C2-C3-O31
72	6	701	CDL	CA3-CA4-CA6-OA8
69	Q	201	PC1	O31-C31-C32-C33
72	6	701	CDL	C74-C75-C76-C77
70	B	501	3PE	O32-C31-C32-C33

There are no ring outliers.

29 monomers are involved in 182 short contacts:

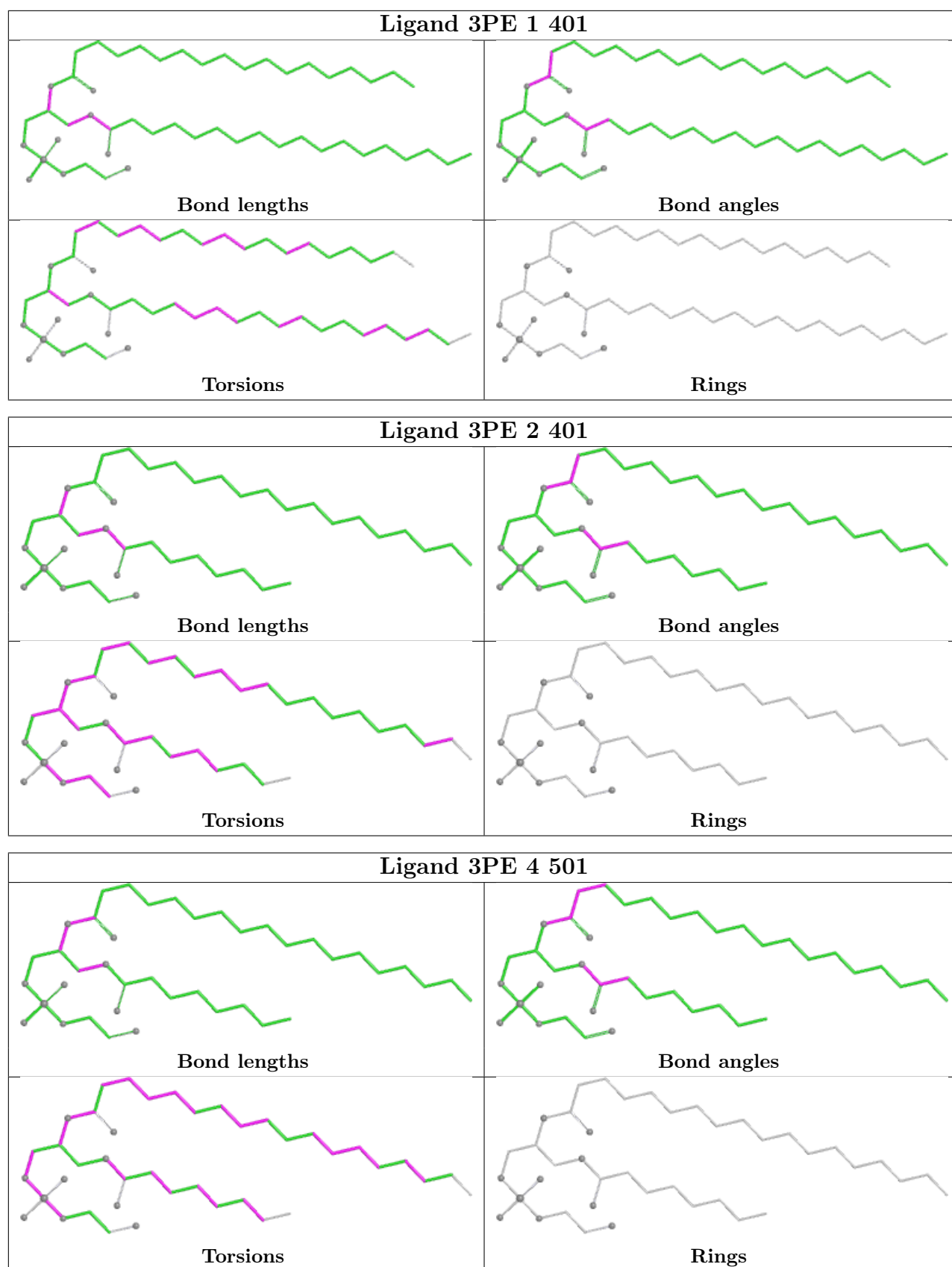
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	E	302	SF4	1	0
70	1	401	3PE	5	0
70	2	401	3PE	5	0
74	A	802	SF4	3	0
70	4	501	3PE	1	0
81	z	301	HEC	9	0
72	b	201	CDL	4	0
76	C3	602	HEA	1	0
80	m	401	HEM	14	0
82	A2	201	UQ2	24	0

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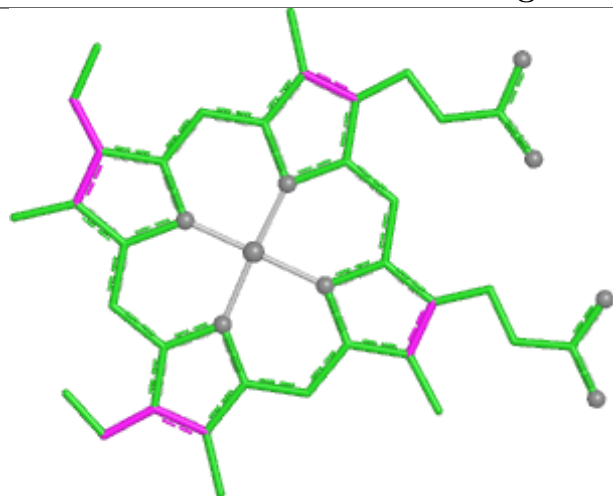
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	8	501	FMN	10	0
71	A	803	FES	2	0
80	m	402	HEM	6	0
69	3	200	PC1	8	0
69	j	201	PC1	3	0
69	2	402	PC1	8	0
72	J	101	CDL	6	0
81	o	301	HEC	9	0
70	j	202	3PE	3	0
80	y	401	HEM	13	0
80	y	402	HEM	6	0
74	D	301	SF4	1	0
74	A	801	SF4	3	0
70	B	501	3PE	9	0
72	6	701	CDL	12	0
76	C3	603	HEA	3	0
69	S	401	PC1	5	0
69	Q	201	PC1	4	0
79	R	601	NAP	4	0

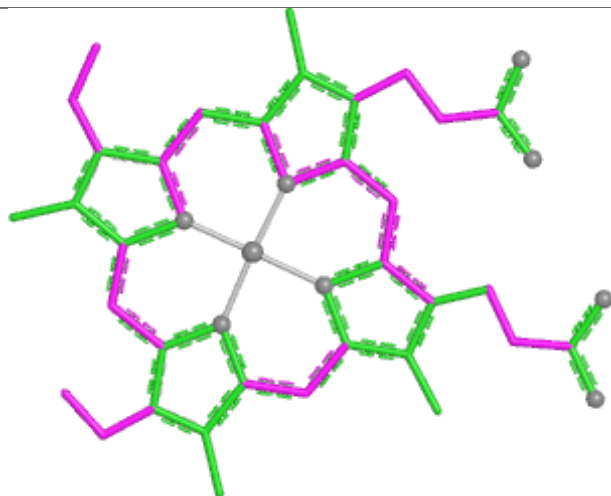
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



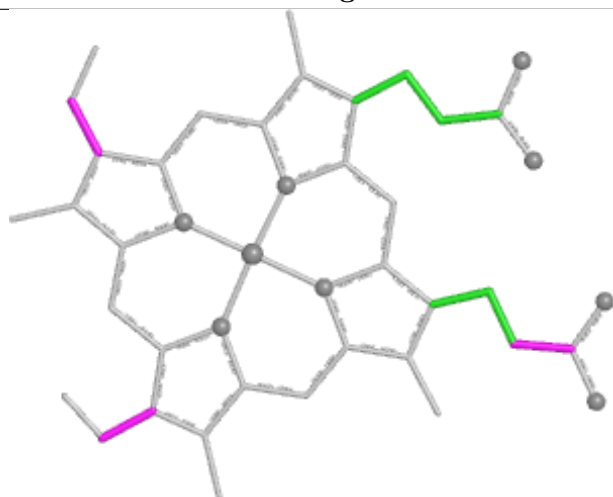
Ligand HEC z 301



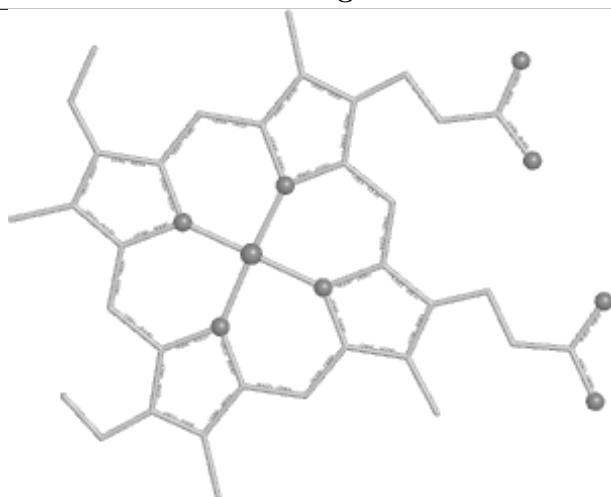
Bond lengths



Bond angles

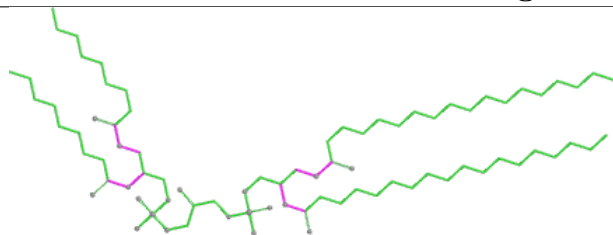


Torsions

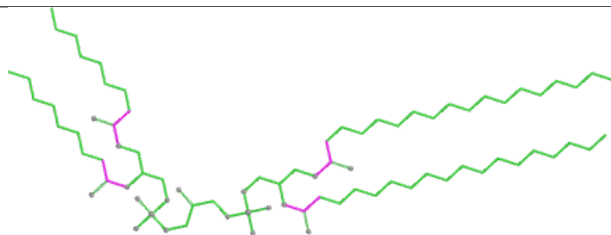


Rings

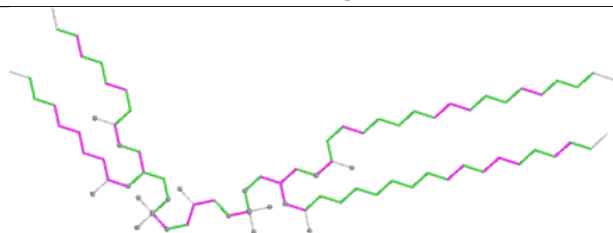
Ligand CDL b 201



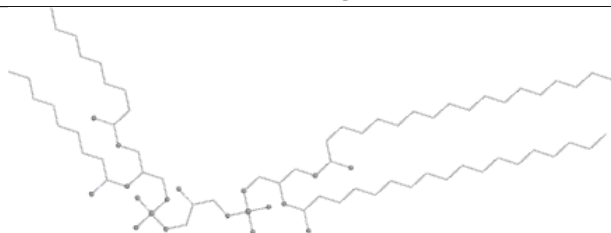
Bond lengths



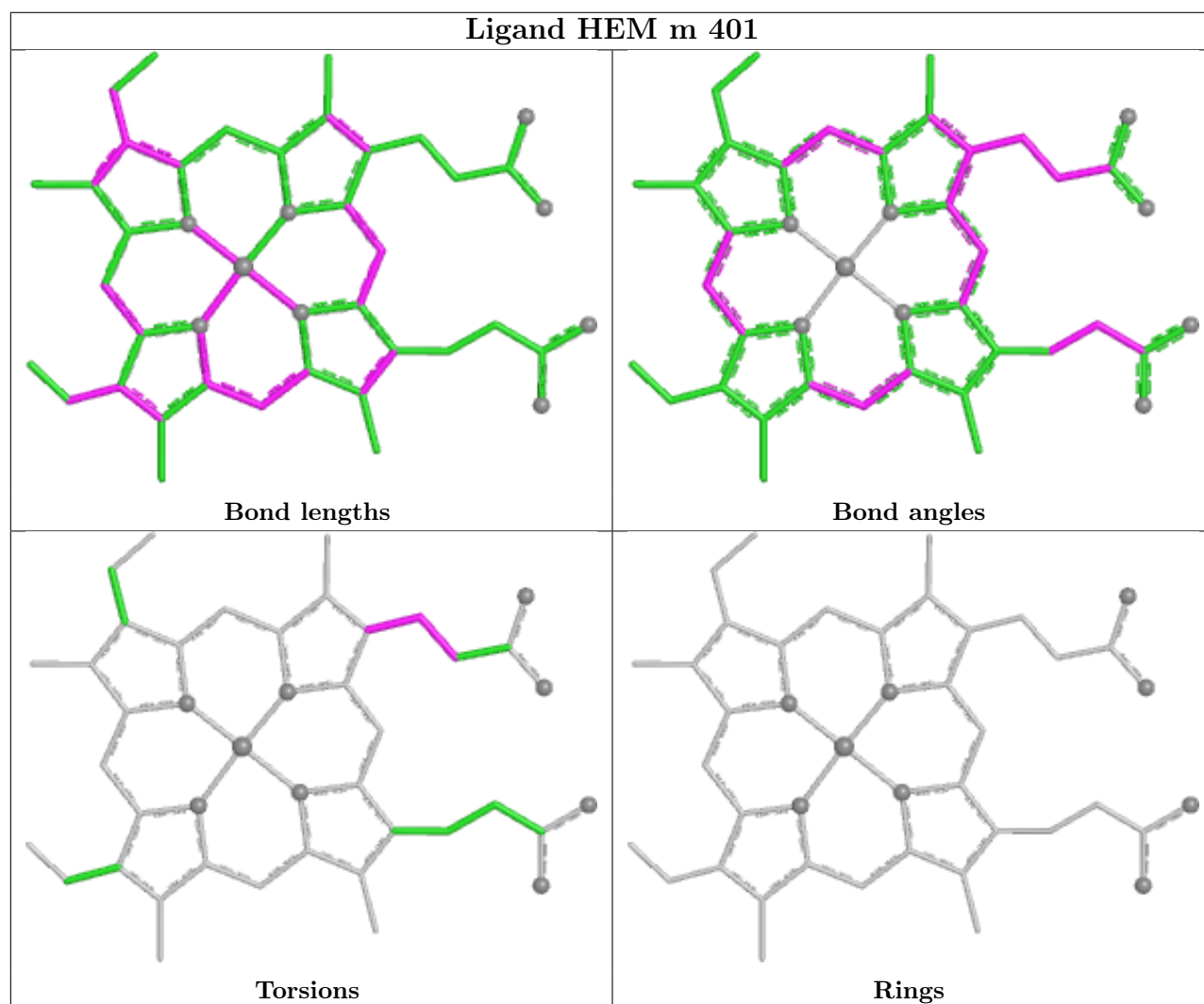
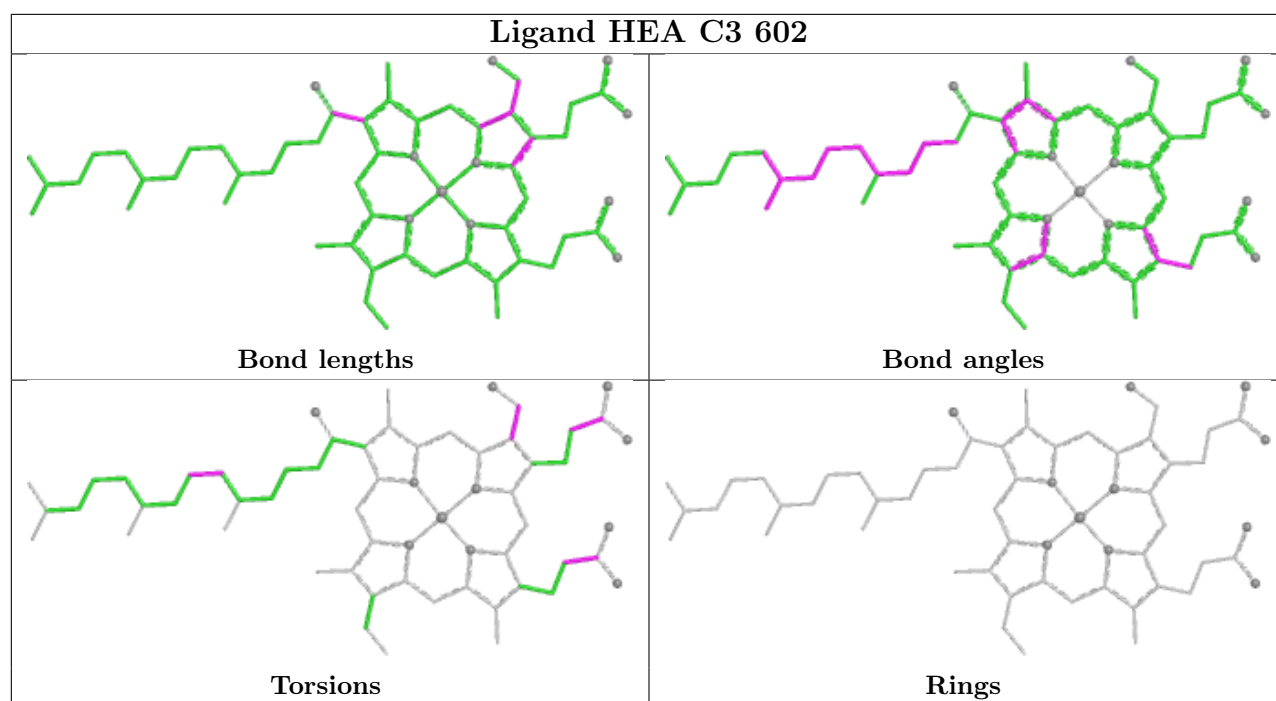
Bond angles

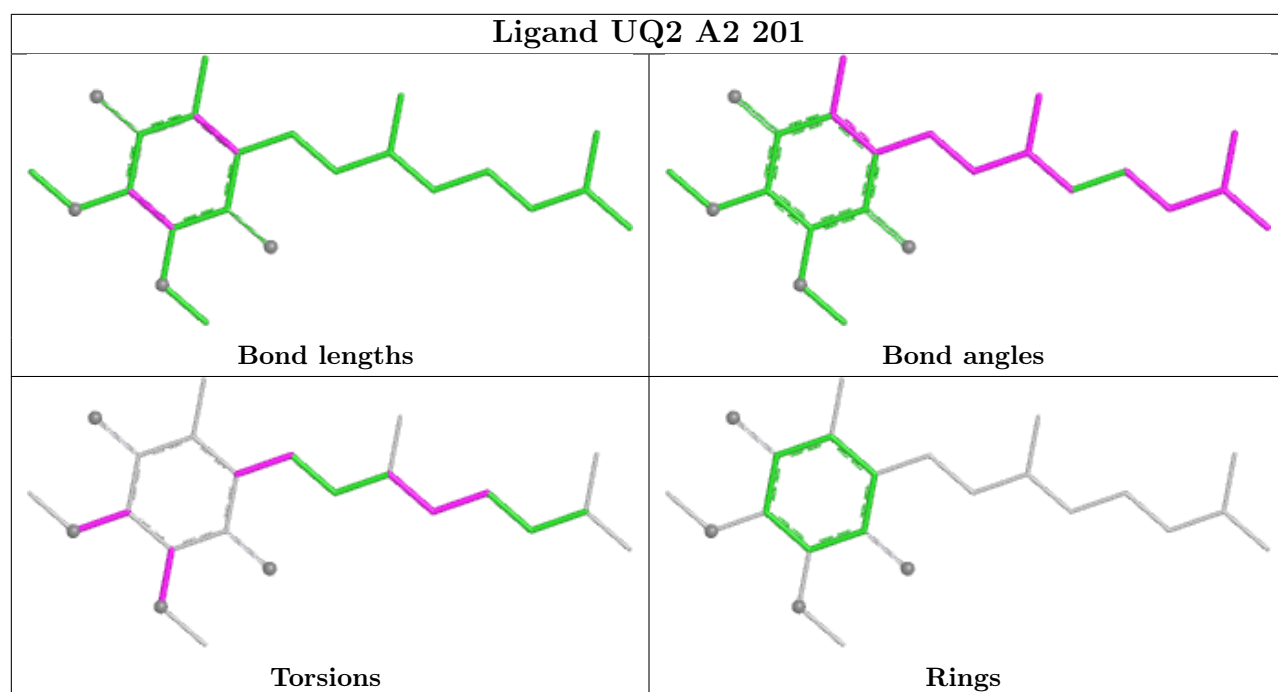


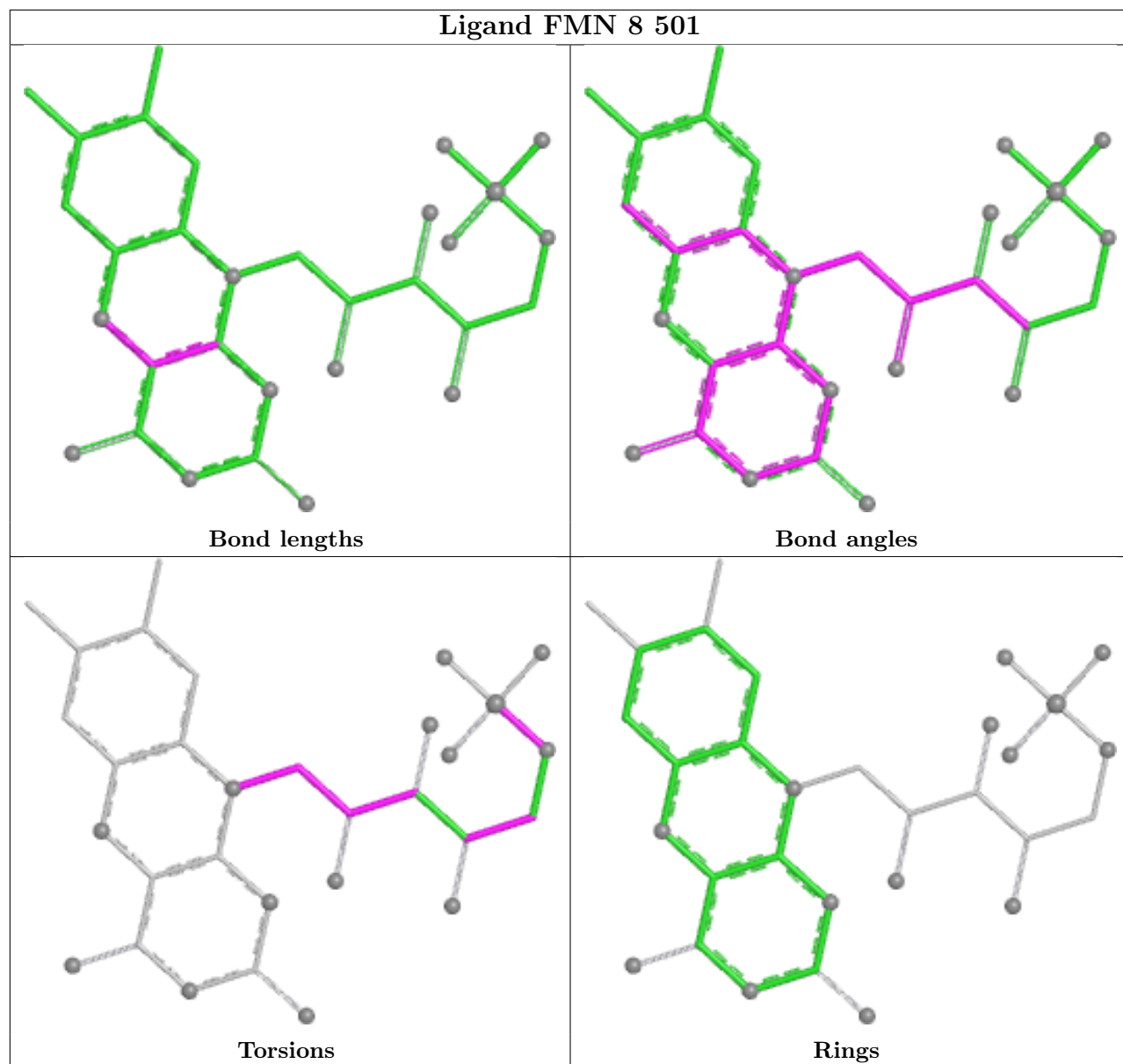
Torsions

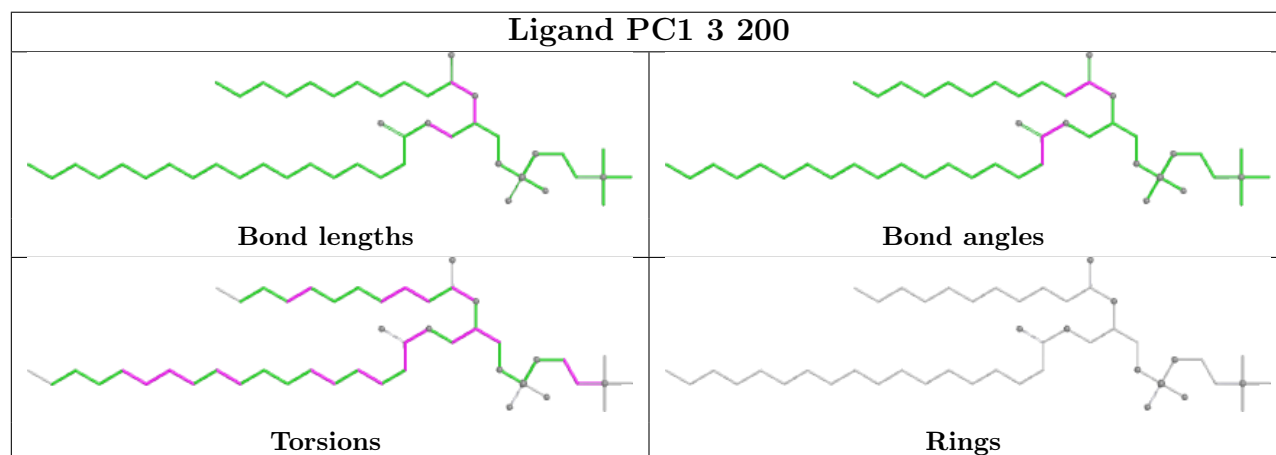
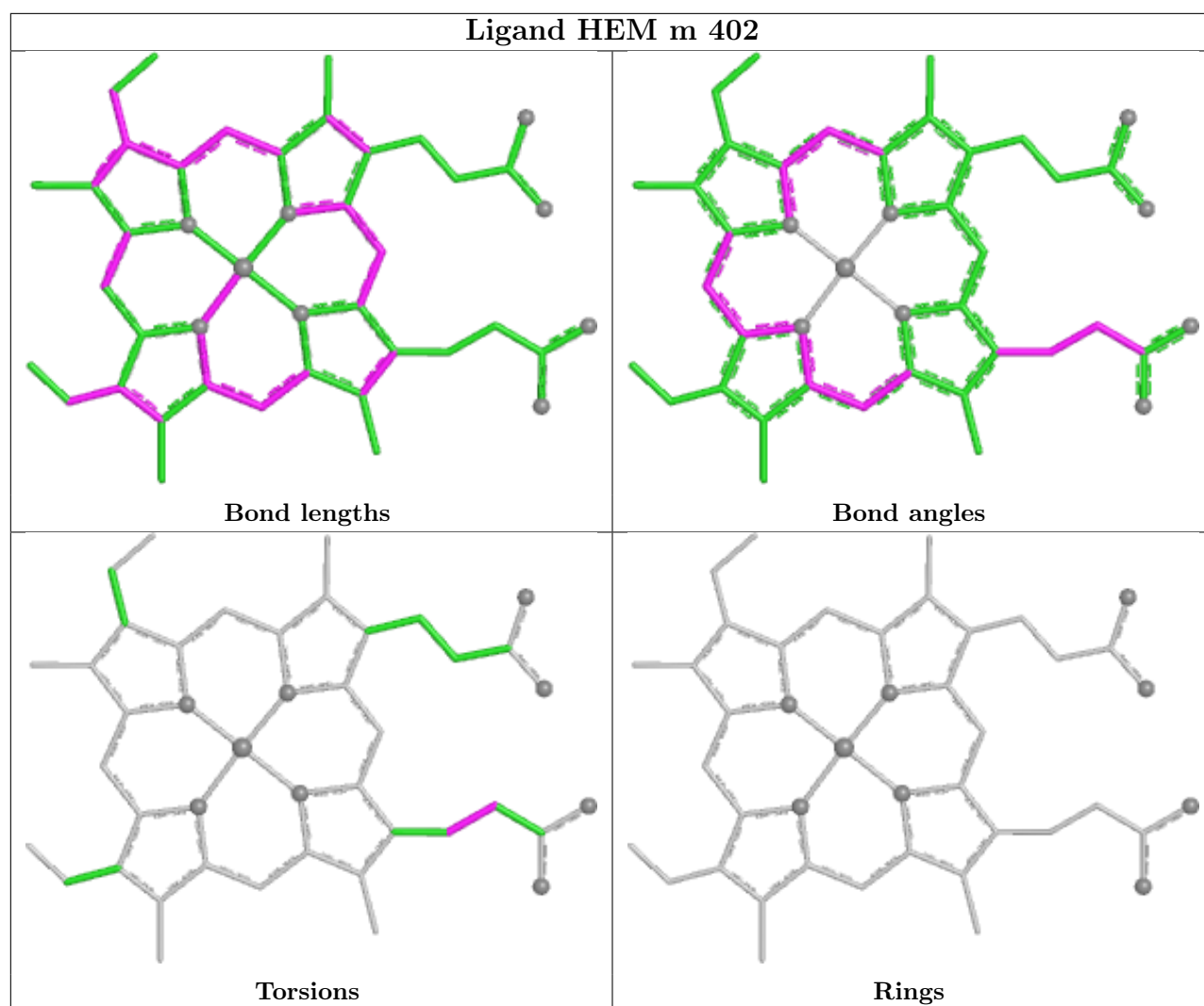


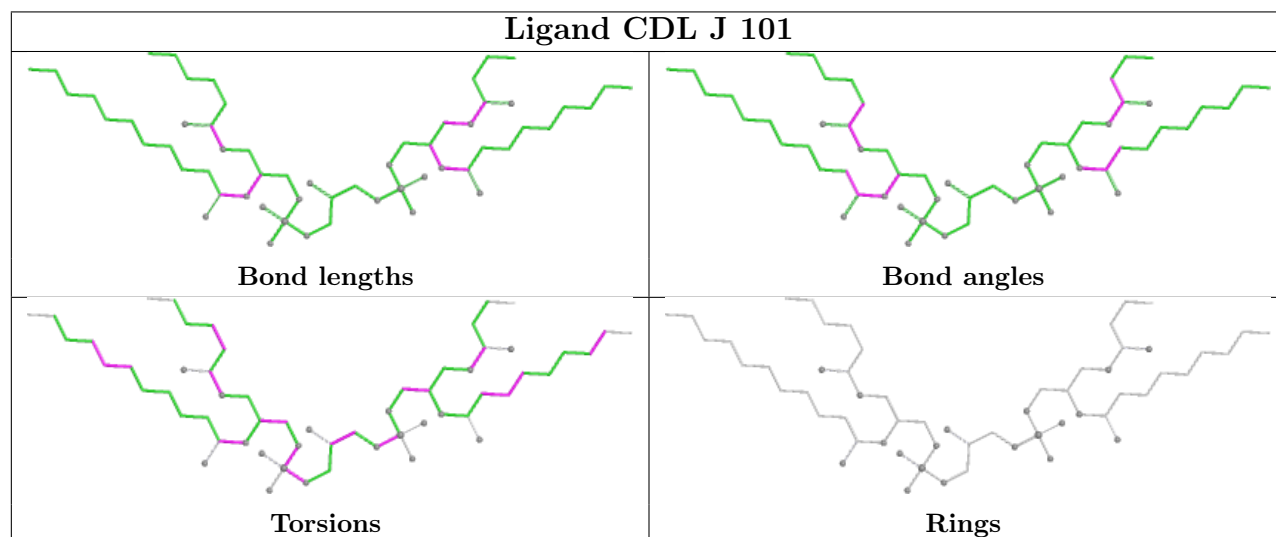
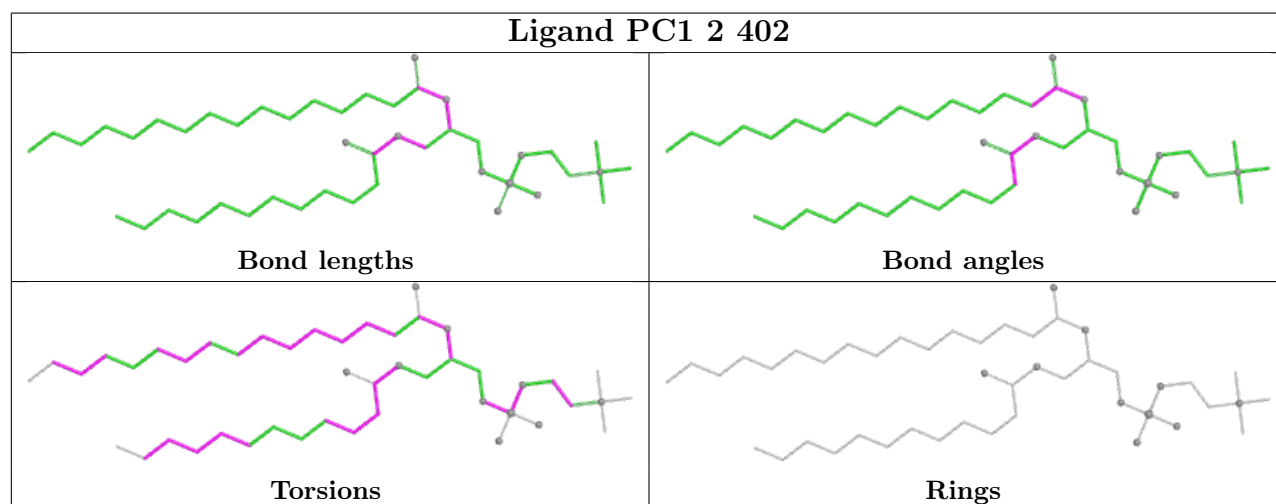
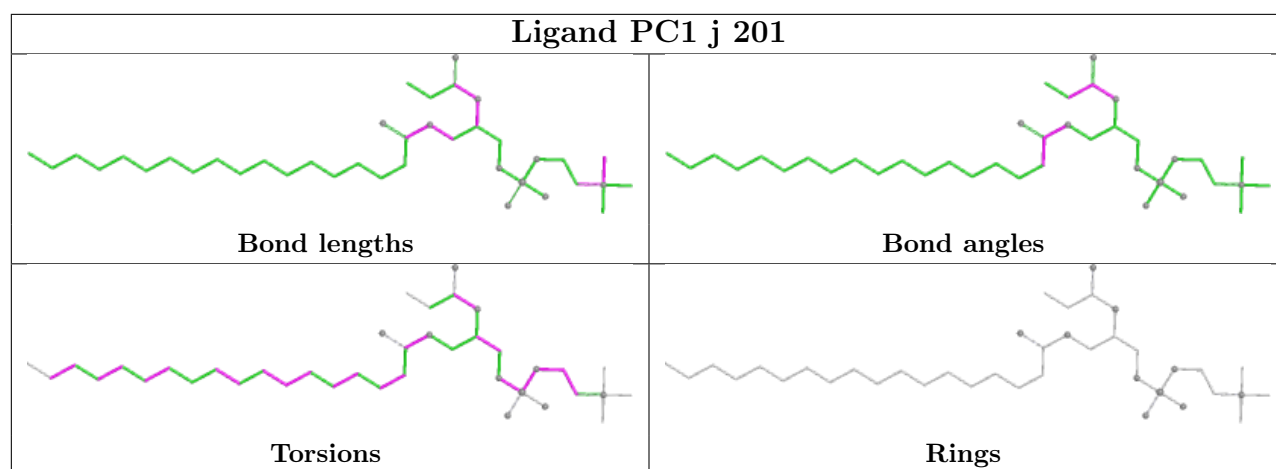
Rings



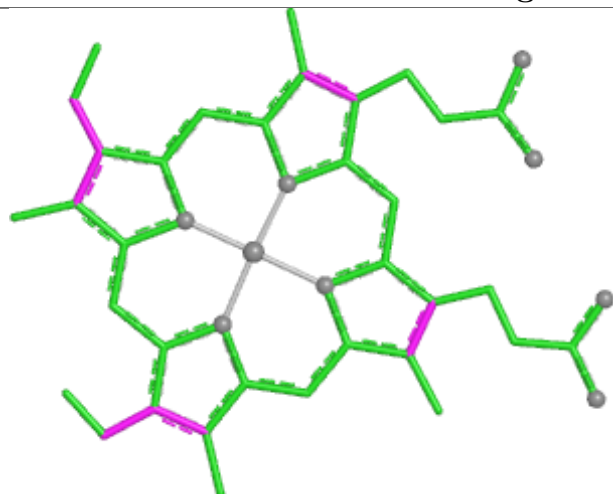




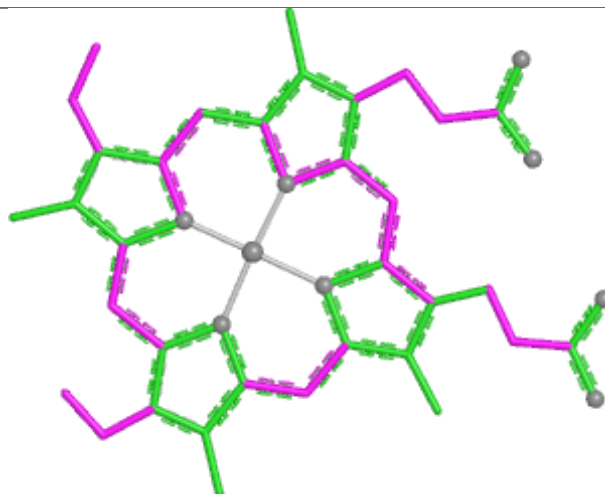




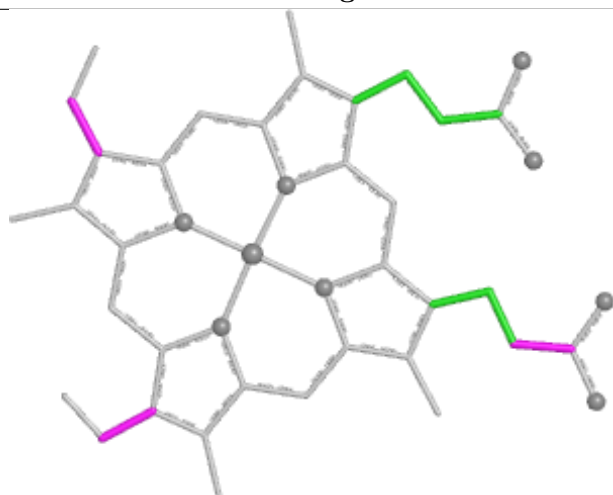
Ligand HEC o 301



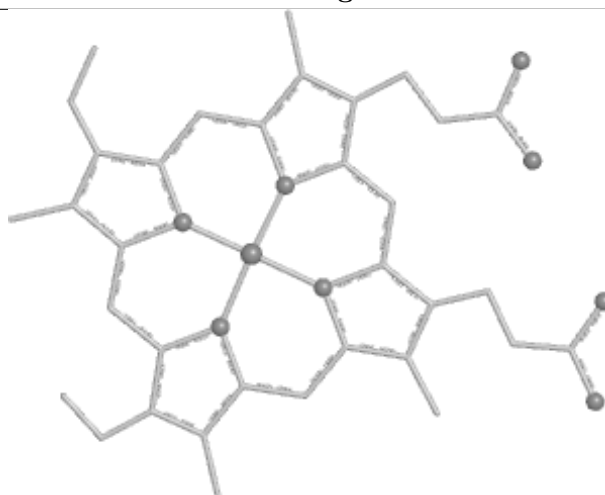
Bond lengths



Bond angles

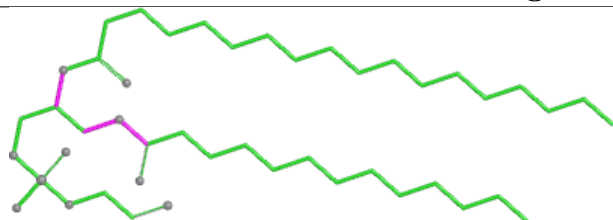


Torsions

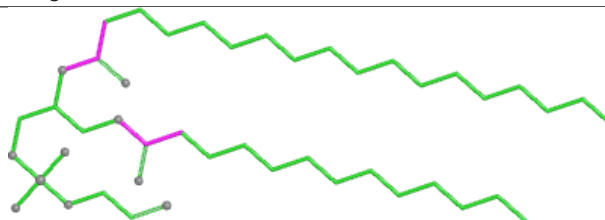


Rings

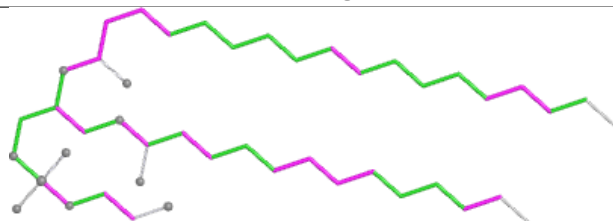
Ligand 3PE j 202



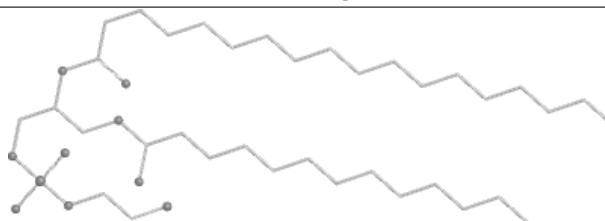
Bond lengths



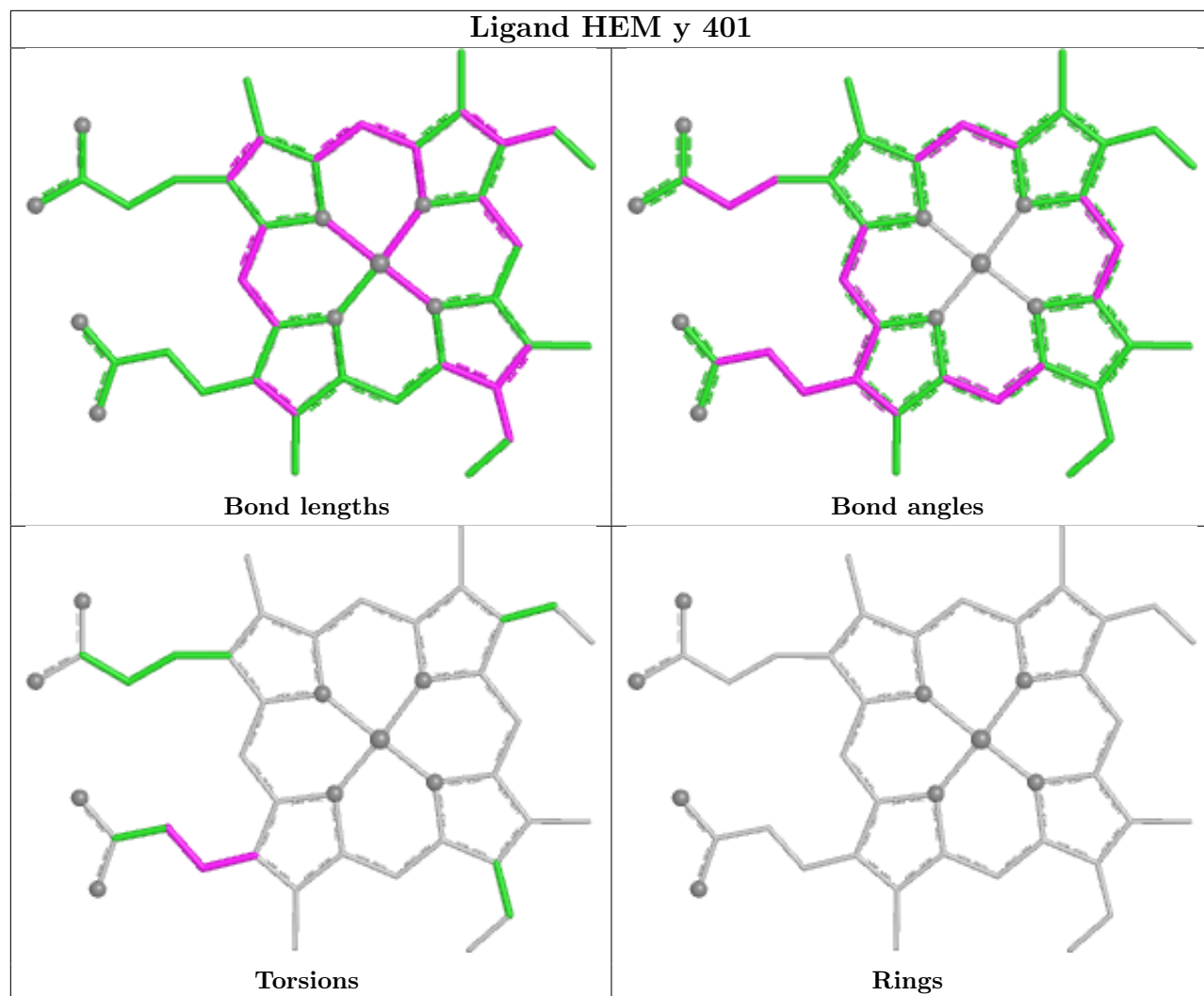
Bond angles

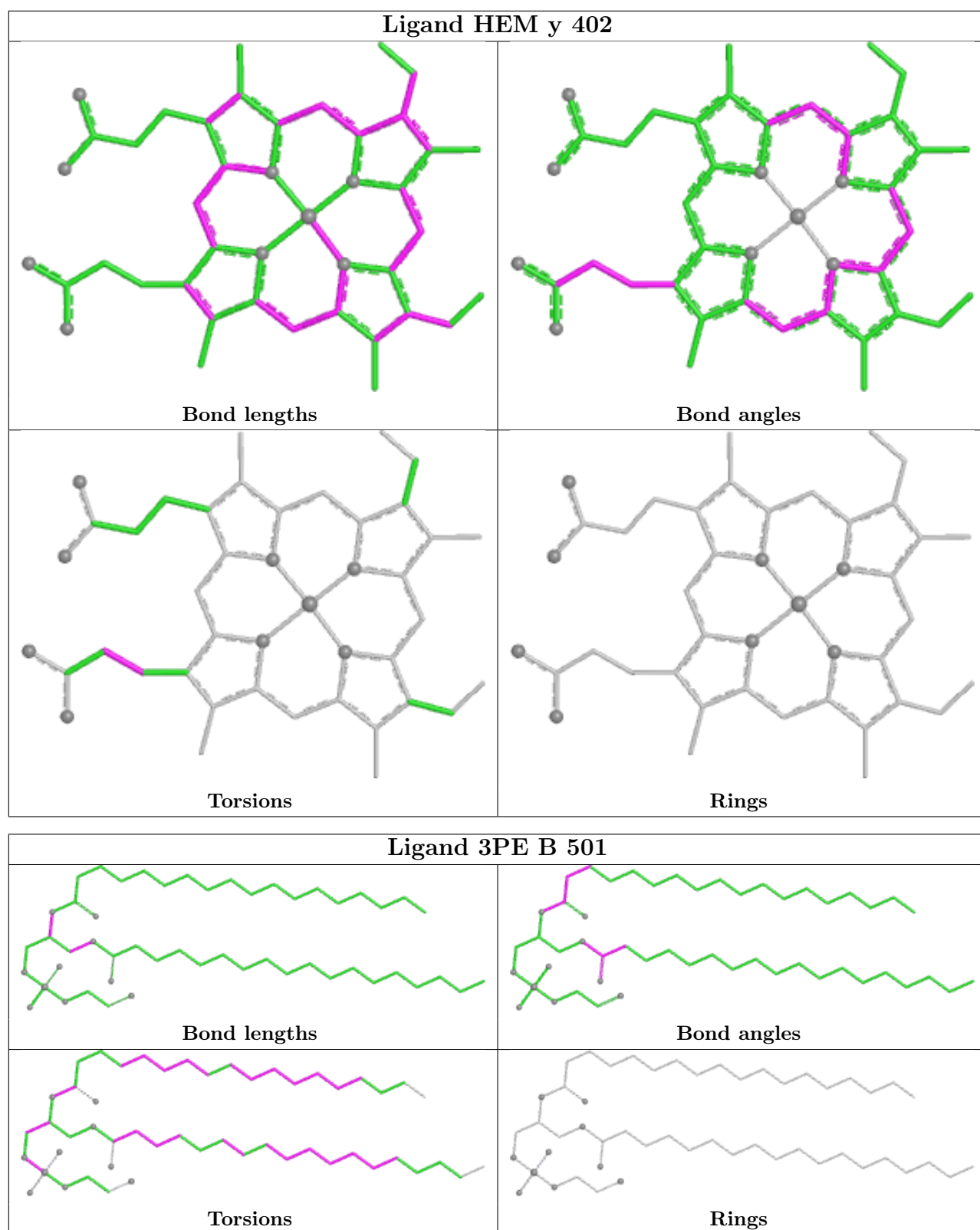


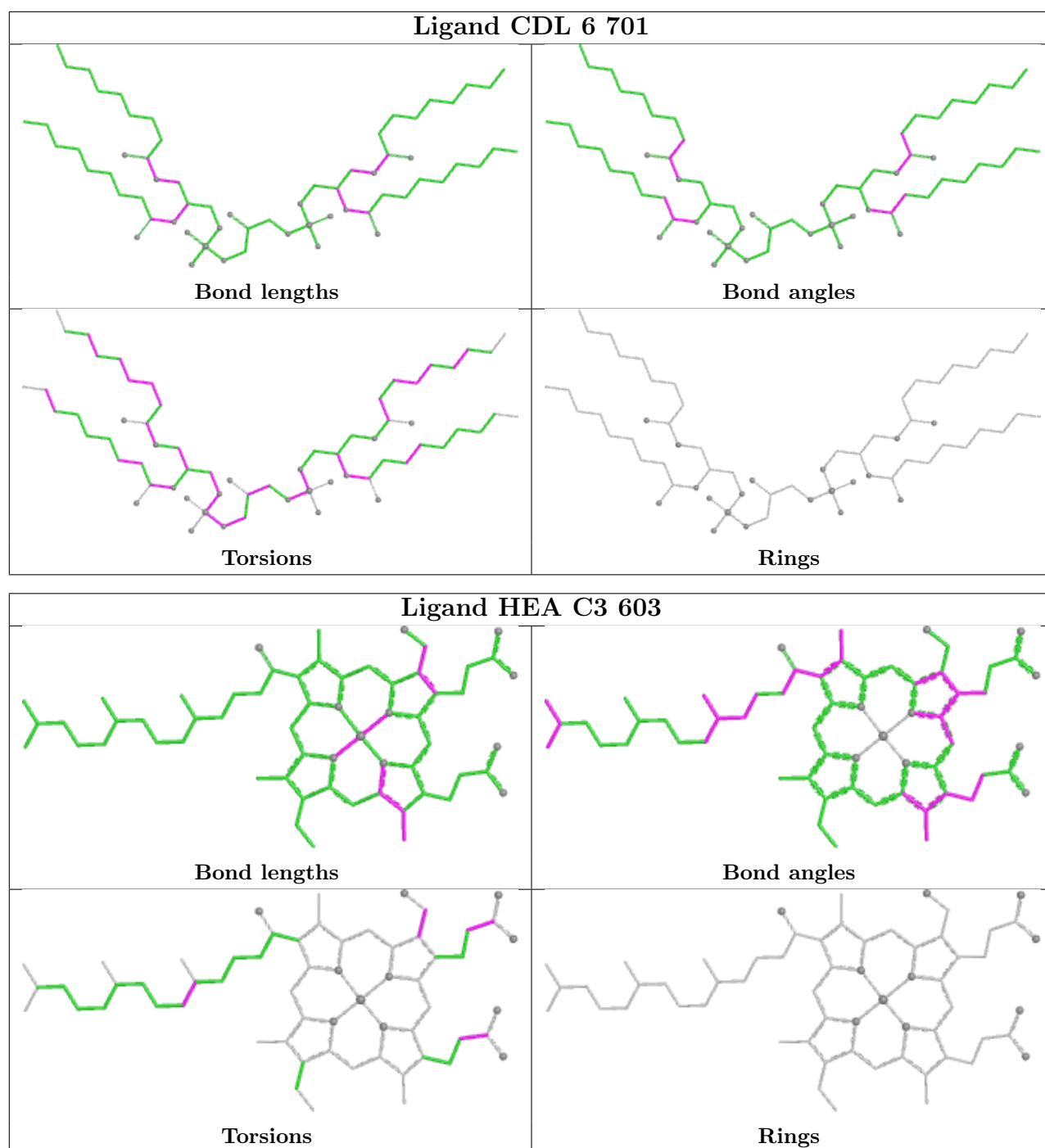
Torsions

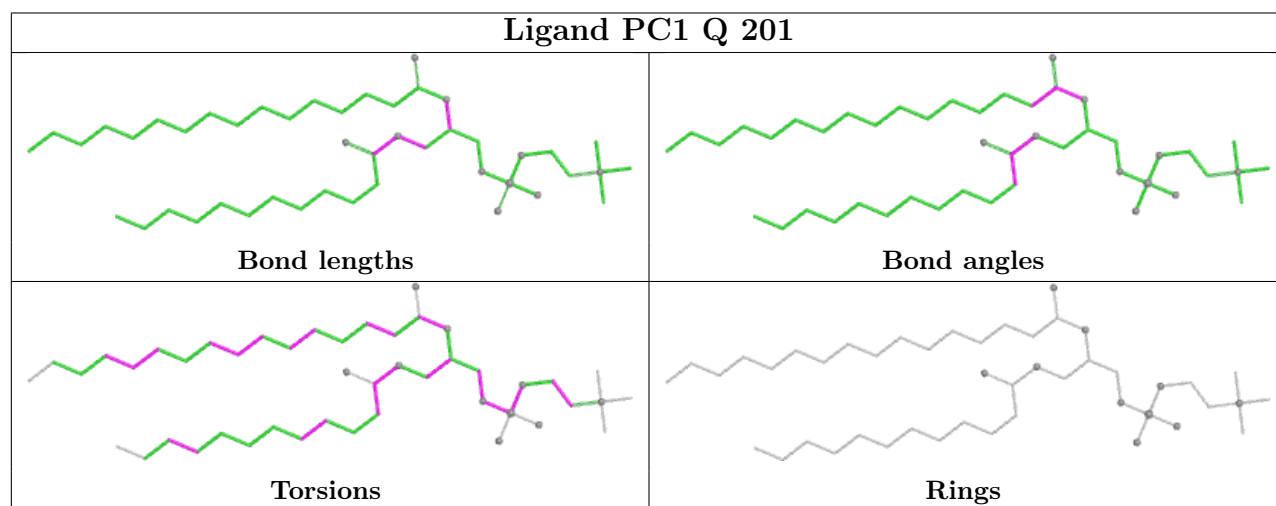
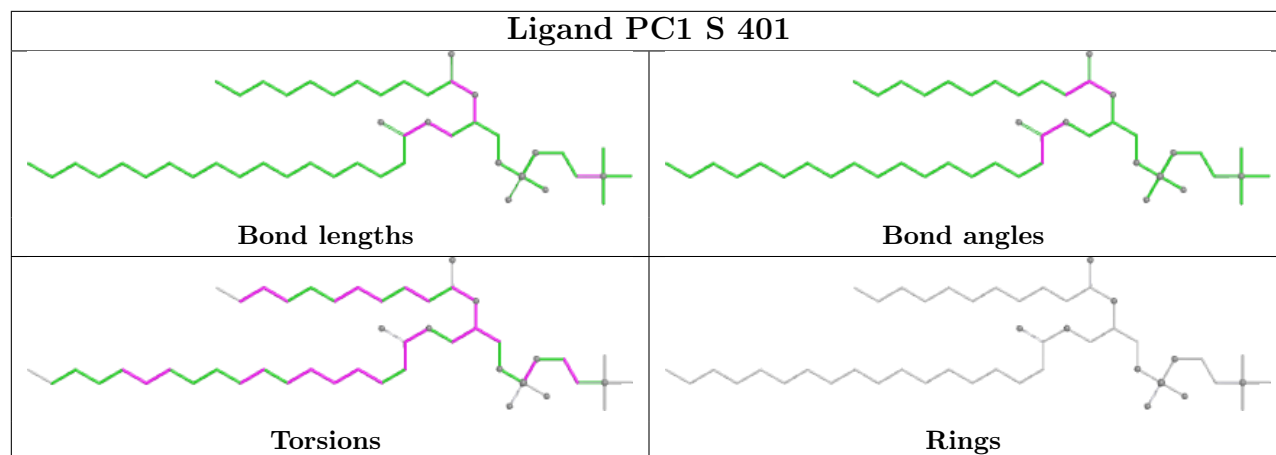


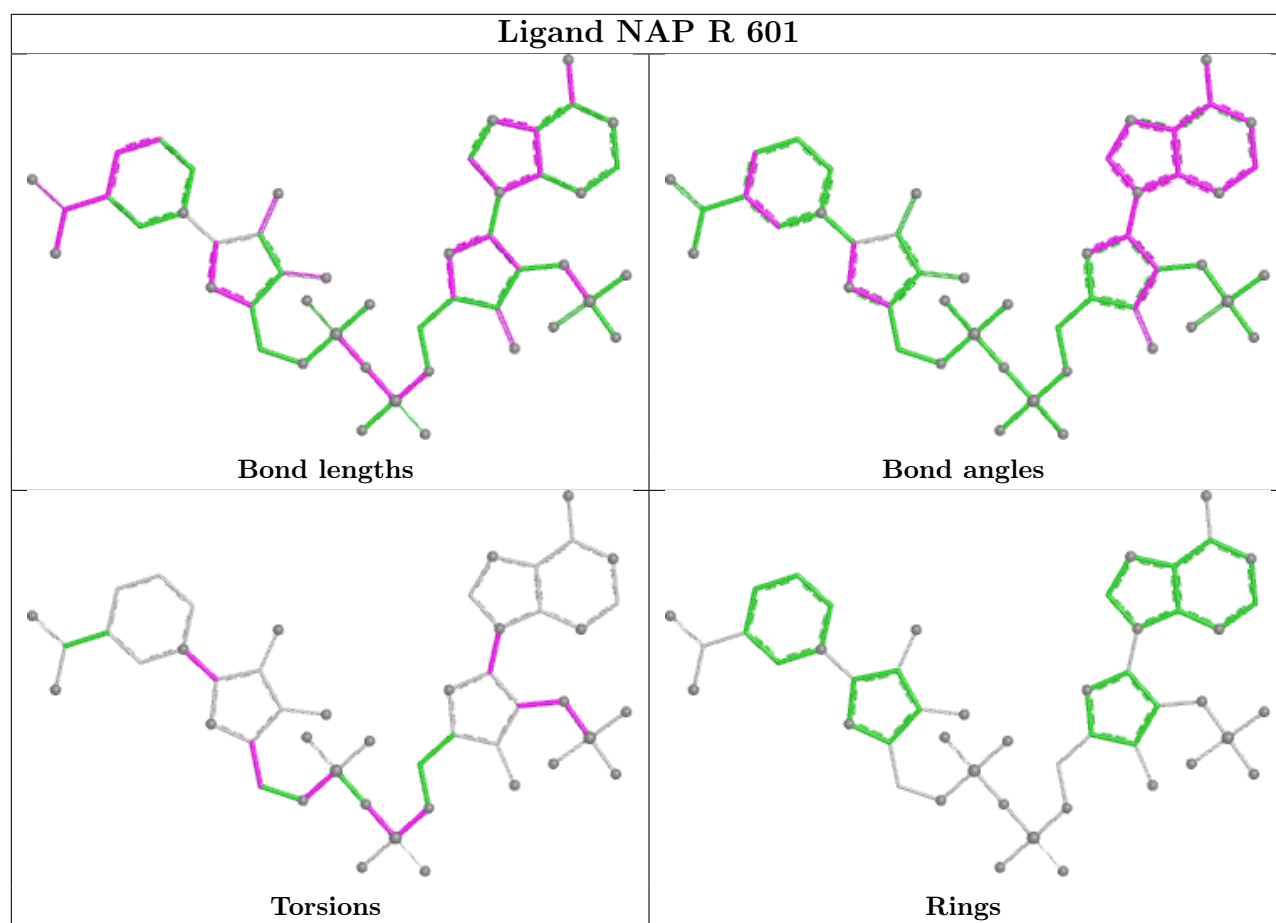
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

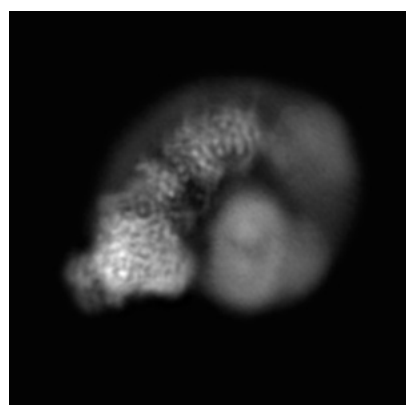
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30673. These allow visual inspection of the internal detail of the map and identification of artifacts.

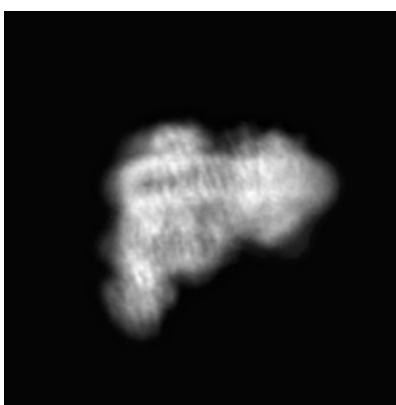
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

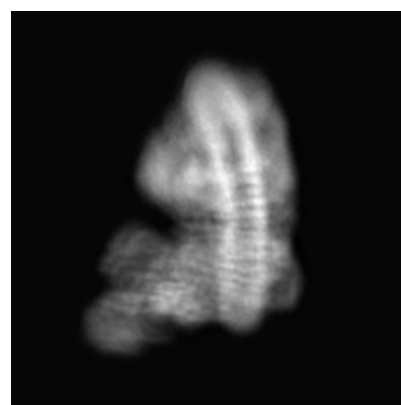
6.1.1 Primary map



X



Y

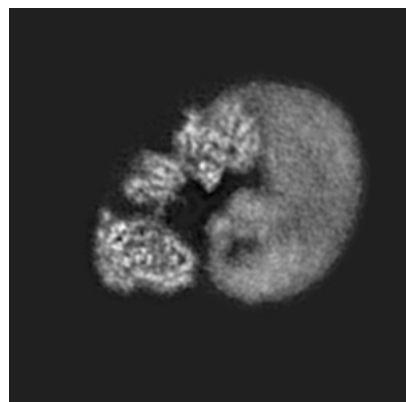


Z

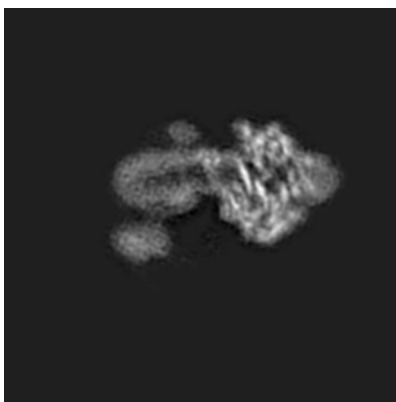
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

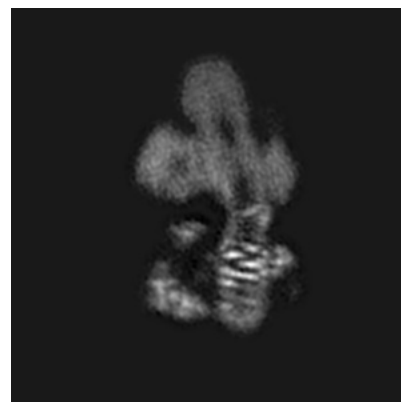
6.2.1 Primary map



X Index: 140



Y Index: 140

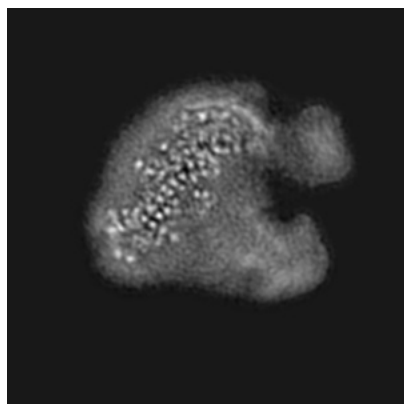


Z Index: 140

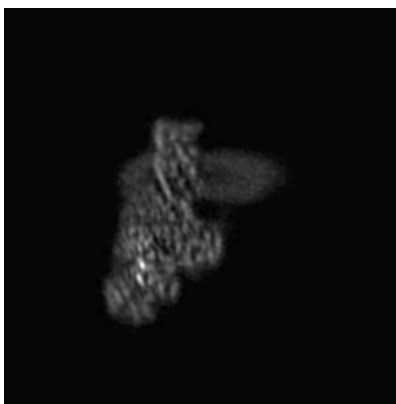
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

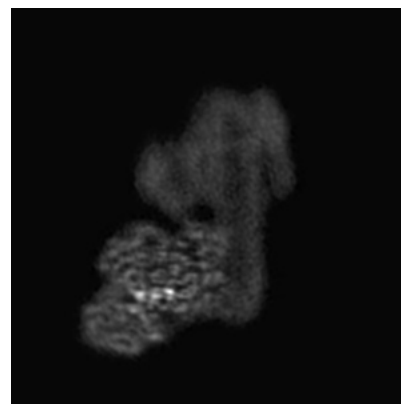
6.3.1 Primary map



X Index: 173



Y Index: 78

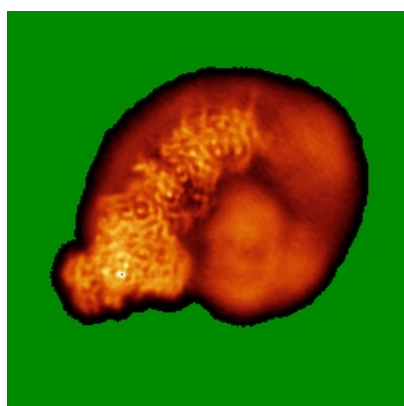


Z Index: 95

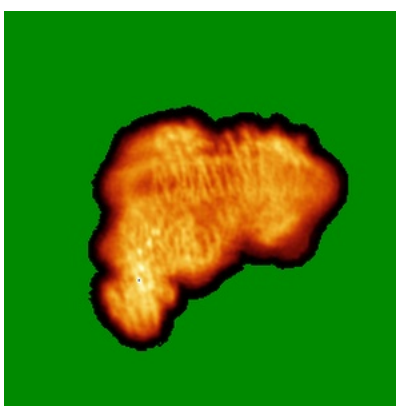
The images above show the largest variance slices of the map in three orthogonal directions.

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.

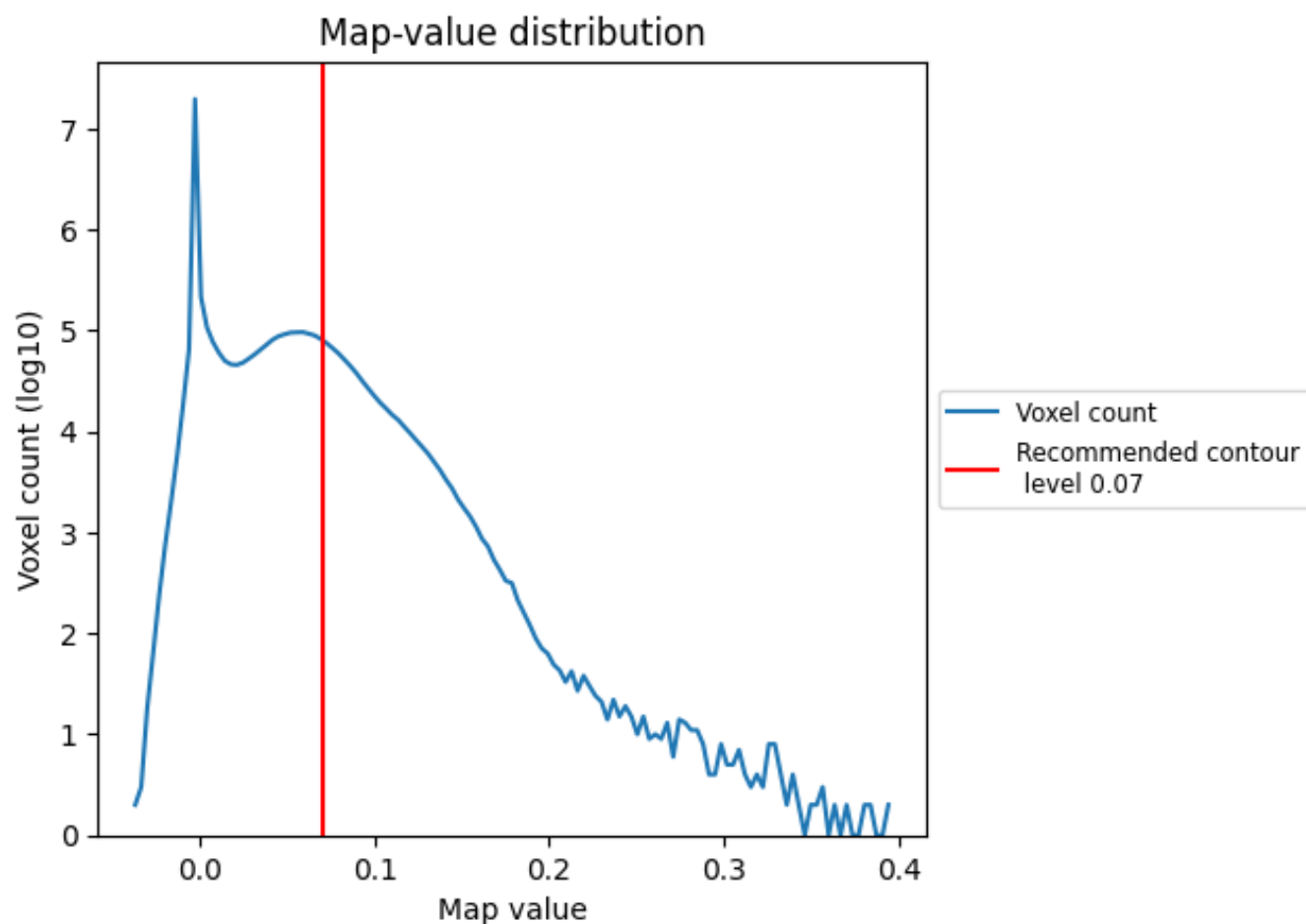
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

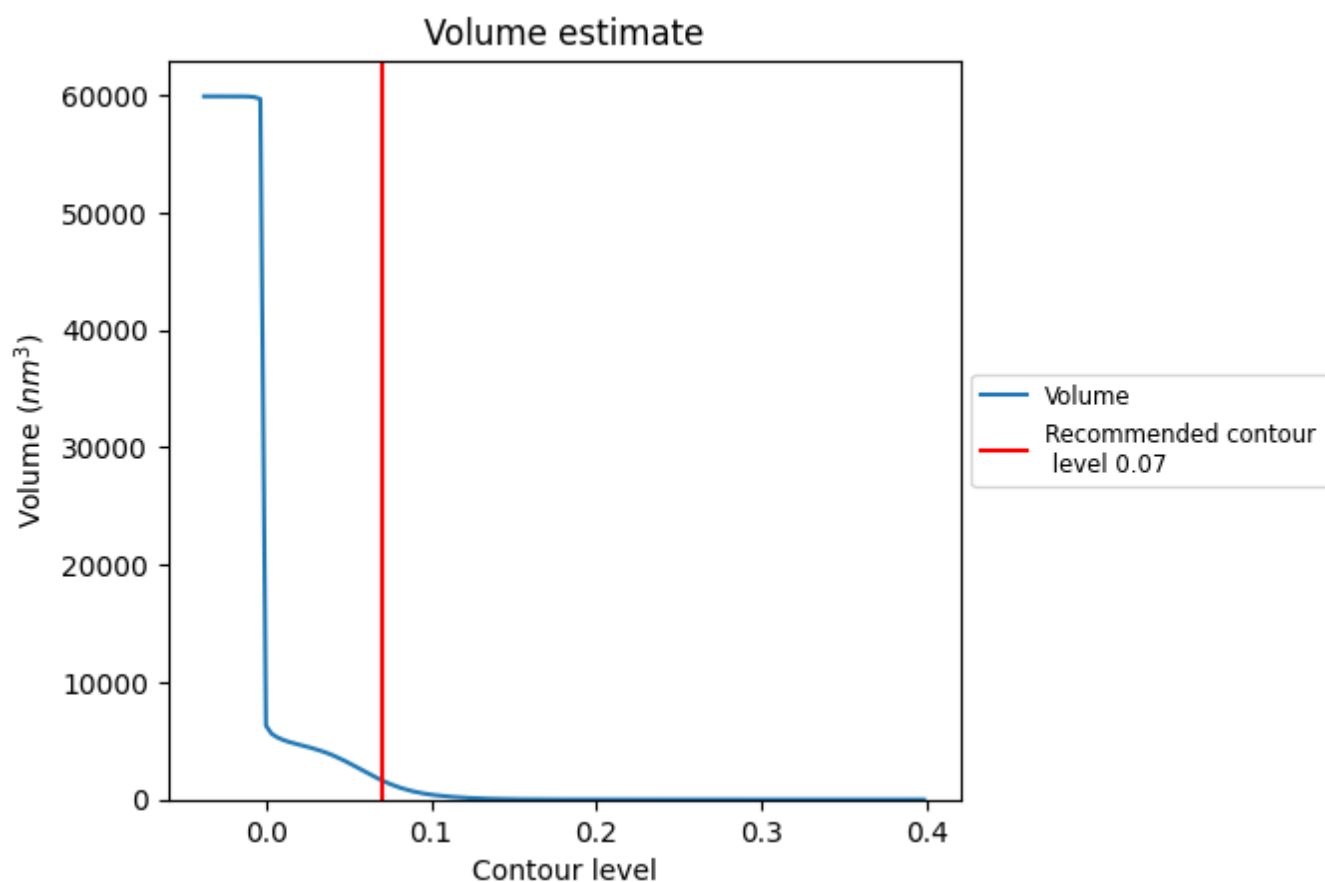
This section contains the results of statistical analysis of the map.

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.

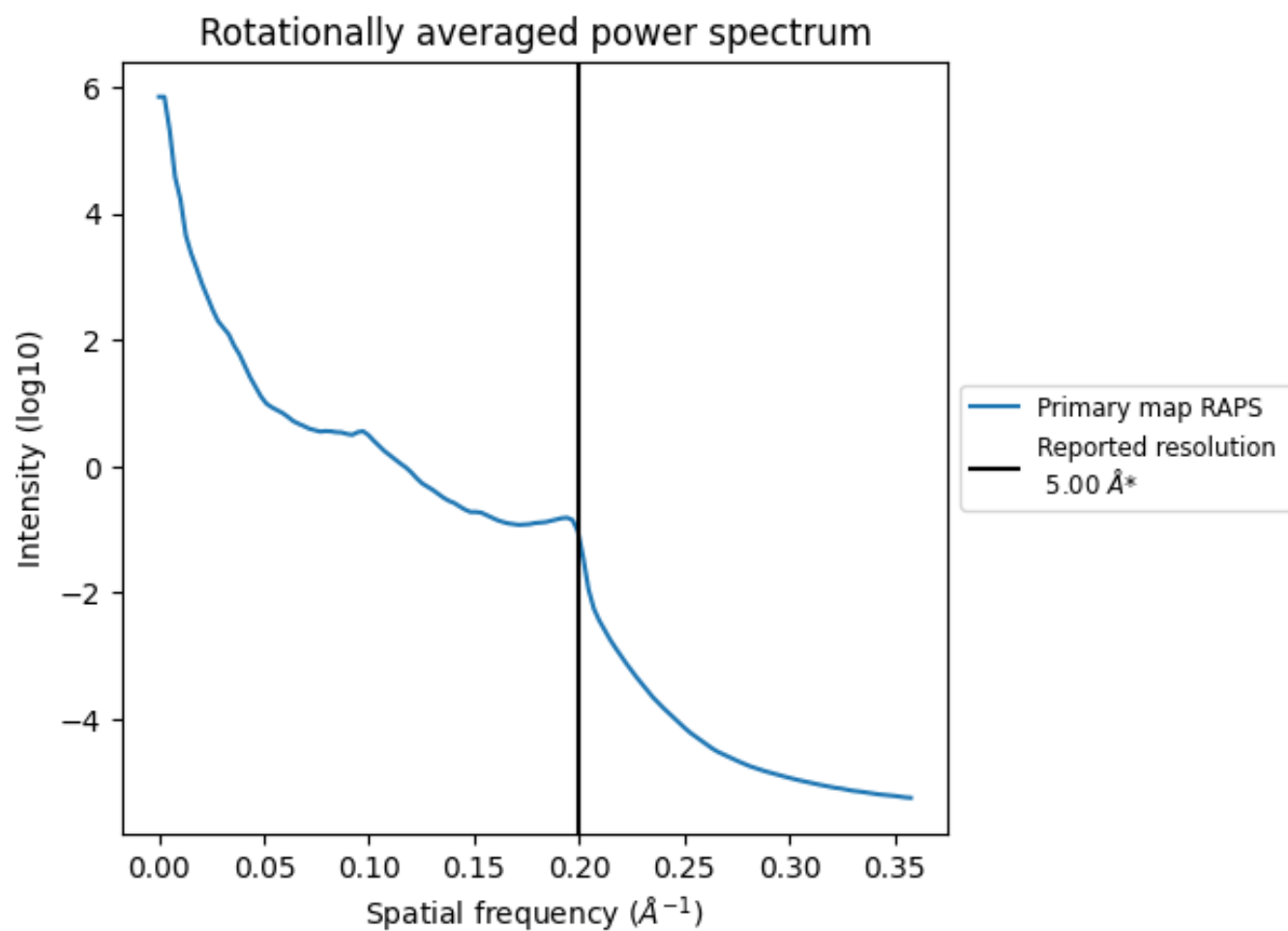
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1648 nm³; this corresponds to an approximate mass of 1489 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 0.200 Å⁻¹

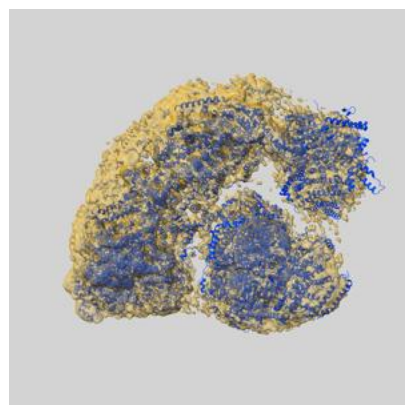
8 Fourier-Shell correlation

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

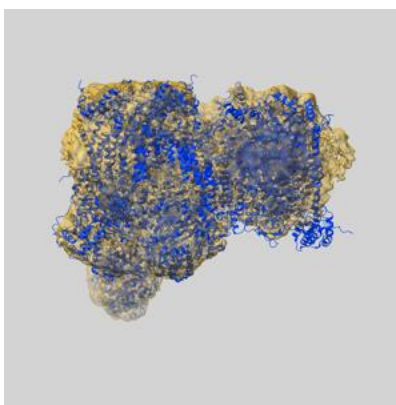
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30673 and PDB model 7DGQ. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

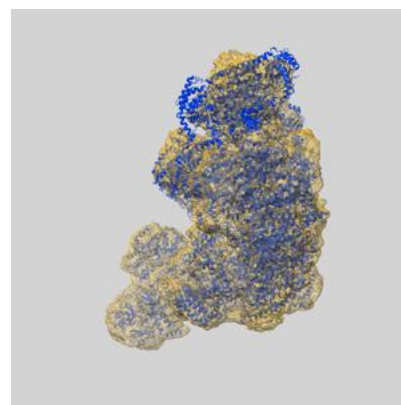
9.1 Map-model overlay [i](#)



X



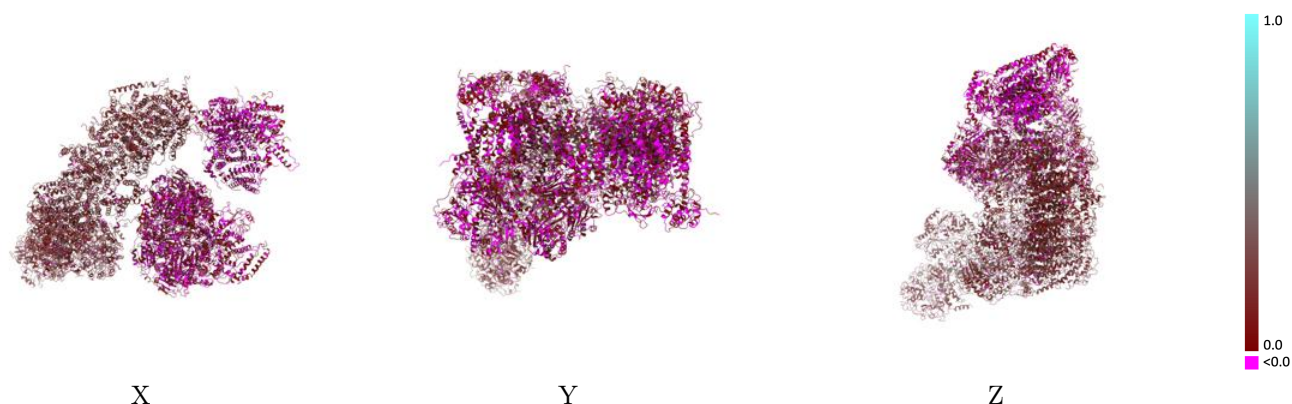
Y



Z

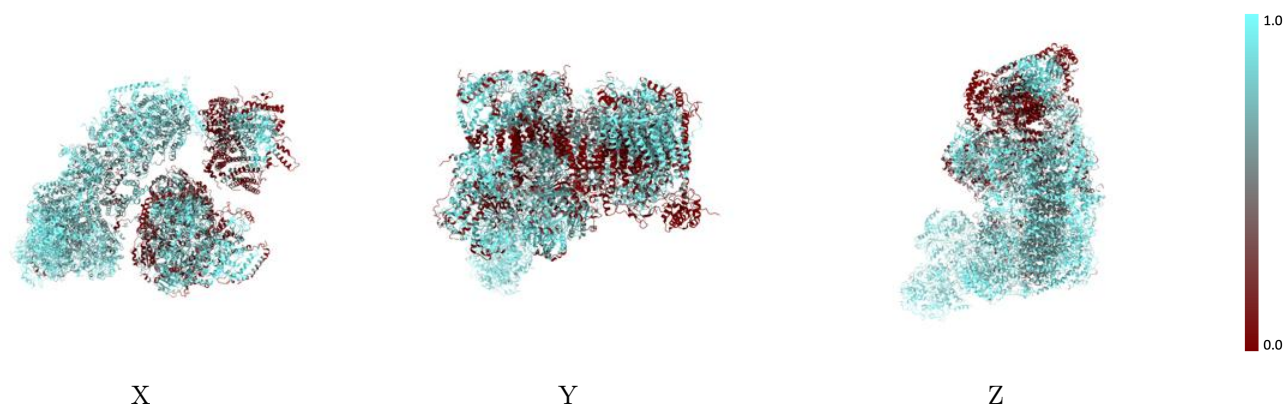
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



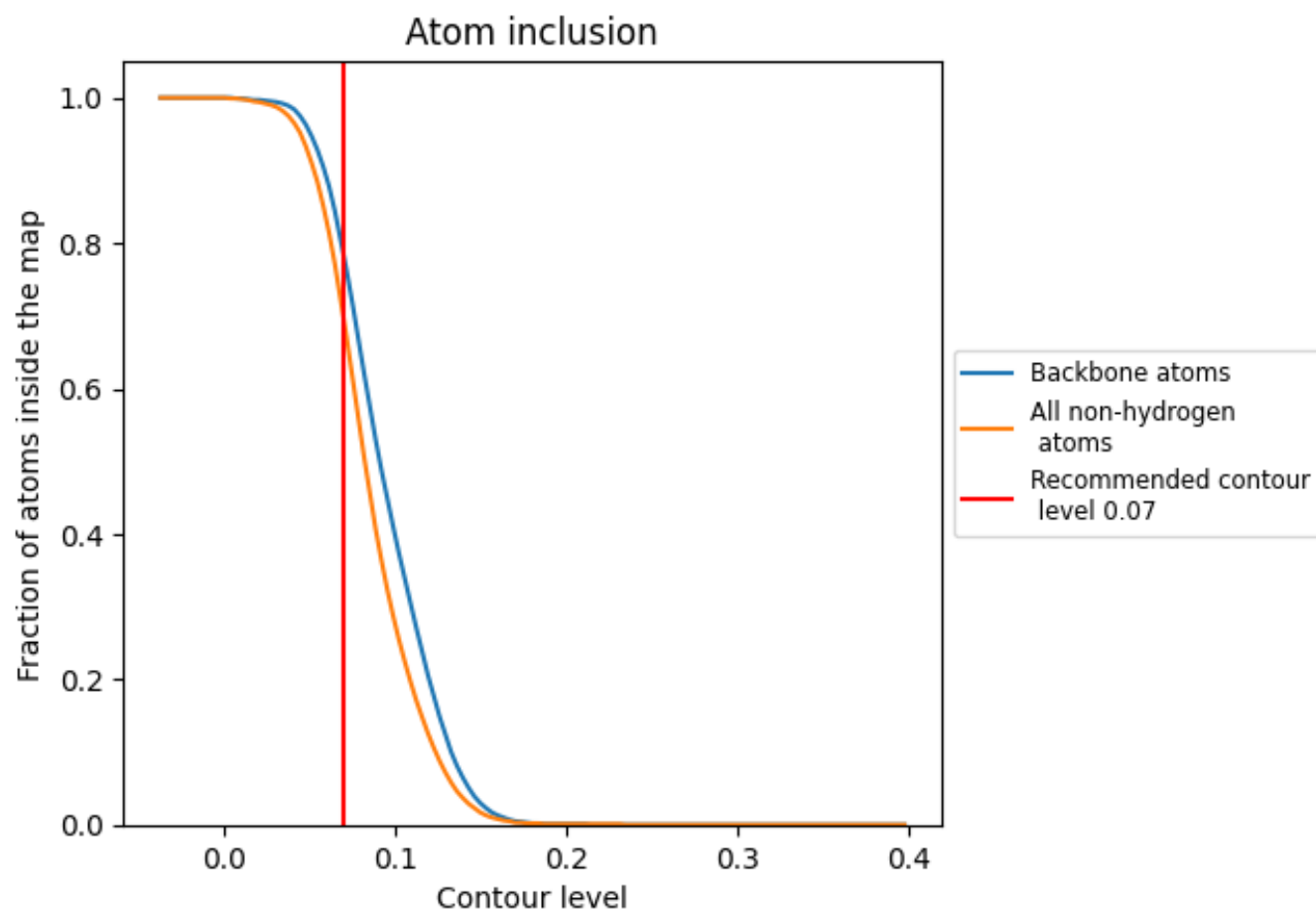
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% 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	 0.1370
1	 0.7230	 0.1890
2	 0.7400	 0.2030
3	 0.5620	 0.1640
4	 0.7340	 0.1990
5	 0.7100	 0.1980
6	 0.7260	 0.1730
7	 0.6960	 0.2000
8	 0.9590	 0.1910
9	 0.9320	 0.1940
A	 0.9350	 0.2080
A0	 0.2080	 0.0080
A1	 0.4260	 0.0540
A2	 0.3530	 0.1290
A3	 0.4260	 0.1100
A4	 0.2550	 0.0880
A5	 0.1520	 0.0210
A6	 0.1560	 -0.0070
A7	 0.1290	 0.0360
A8	 0.2350	 0.0120
A9	 0.2670	 0.0190
B	 0.8150	 0.2060
B2	 0.1040	 0.0280
B3	 0.2530	 0.0350
B4	 0.0250	 0.0460
B5	 0.3060	 0.0850
B6	 0.1840	 0.0610
B7	 0.2870	 0.0630
C	 0.9060	 0.2300
C0	 0.3150	 0.0330
C1	 0.6680	 0.0290
C2	 0.2380	 0.0360
C3	 0.5320	 0.0100
D	 0.8570	 0.2290
E	 0.9310	 0.2160



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Chain	Atom inclusion	Q-score
F	 0.9010	 0.1820
G	 0.8670	 0.2370
H	 0.8870	 0.2380
I	 0.7860	 0.1900
J	 0.8710	 0.1910
K	 0.9180	 0.1800
L	 0.8310	 0.2070
M	 0.5950	 0.1790
N	 0.9200	 0.2110
O	 0.8260	 0.2030
P	 0.8650	 0.2350
Q	 0.8940	 0.2120
R	 0.8110	 0.1950
S	 0.8080	 0.1830
T	 0.6510	 0.2090
U	 0.7060	 0.2000
V	 0.8730	 0.2090
W	 0.9360	 0.1850
X	 0.8610	 0.2150
Y	 0.9550	 0.2070
Z	 0.8570	 0.1800
a	 0.7880	 0.2130
b	 0.8670	 0.2180
c	 0.9450	 0.2240
d	 0.9700	 0.1850
e	 0.8140	 0.2280
f	 0.8950	 0.2100
g	 0.9180	 0.2010
h	 0.8660	 0.2000
i	 0.8940	 0.2010
j	 0.8150	 0.1980
k	 0.6740	 0.0470
l	 0.5390	 0.0510
m	 0.5360	 0.0590
o	 0.7830	 0.0660
p	 0.5510	 0.0480
q	 0.6250	 0.0590
r	 0.6620	 0.0710
s	 0.5900	 0.0660
t	 0.5810	 0.1060
u	 0.6010	 0.0350
v	 0.3040	 -0.0110

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Chain	Atom inclusion	Q-score
w	 0.5850	 0.0780
x	 0.7490	 0.0720
y	 0.5750	 0.0820
z	 0.6910	 0.0590