



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 04:22 am BST

PDB ID : 9F62 / pdb_00009f62
EMDB ID : EMD-50210
Title : Subtomogram average of the Chlamydomonas reinhardtii mitochondrial respirasome I2 III4 IV6
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 5.44 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

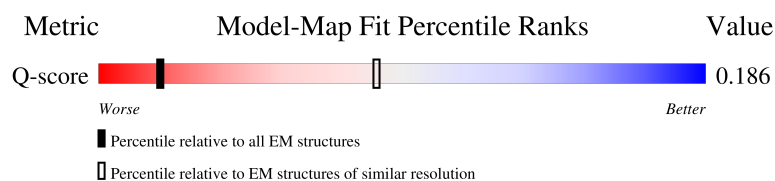
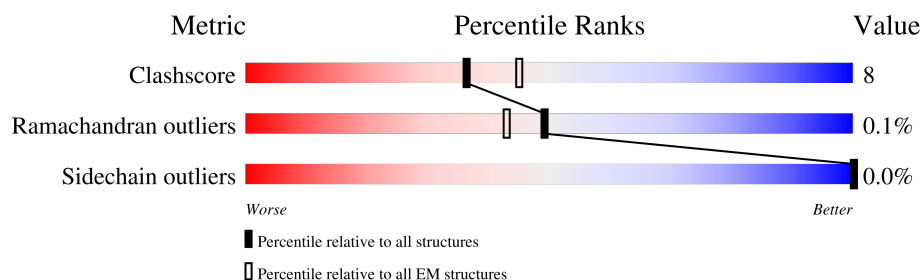
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.44 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	469 (4.94 - 5.94)

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	1A	381	
1	1B	381	
1	6A	381	
1	6B	381	

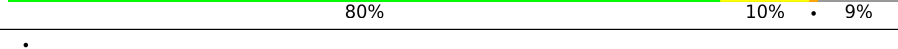
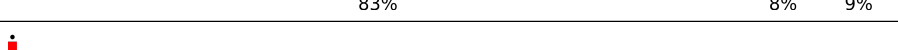
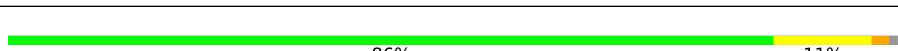
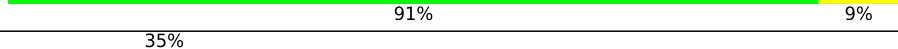
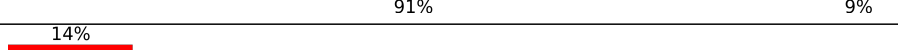
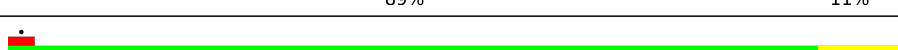
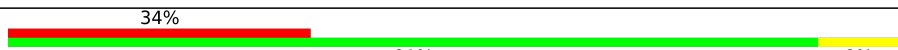
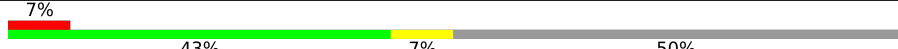
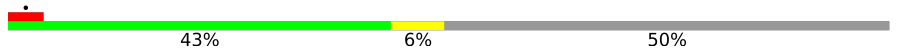
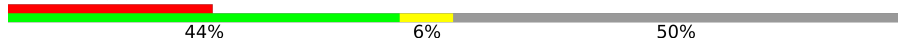
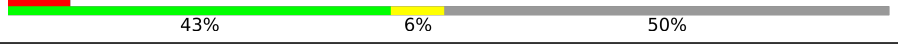
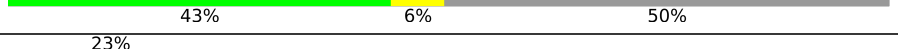
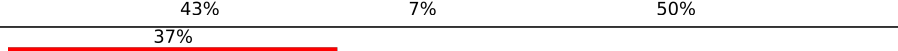
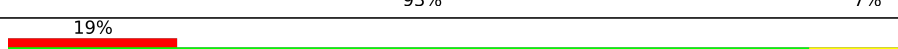
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Mol	Chain	Length	Quality of chain
2	1C	262	
2	1D	262	
2	6C	262	
2	6D	262	
3	1E	314	
3	1F	314	
3	6E	314	
3	6F	314	
4	1G	60	
4	1H	60	
4	6G	60	
4	6H	60	
5	1I	69	
5	1J	69	
5	6I	69	
5	6J	69	
6	1K	73	
6	1L	73	
6	6K	73	
6	6L	73	
7	1M	495	
7	1N	495	
7	6M	495	
7	6N	495	
8	1O	59	

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Mol	Chain	Length	Quality of chain
8	1P	59	
8	6O	59	
8	6P	59	
9	1Q	485	
9	1S	485	
9	6Q	485	
9	6S	485	
10	1R	123	
10	1T	123	
10	6R	123	
10	6T	123	
11	2A	505	
11	3A	505	
11	4A	505	
11	7A	505	
11	8A	505	
11	9A	505	
12	2B	284	
12	3B	284	
12	4B	284	
12	7B	284	
12	8B	284	
12	9B	284	
13	2C	153	
13	3C	153	

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Mol	Chain	Length	Quality of chain
13	4C	153	88% 90%10%
13	7C	153	37% 90%10%
13	8C	153	19% 90%10%
13	9C	153	89% 90%10%
14	2D	382	15% 64%6%30%
14	3D	382	8% 64%5%30%
14	4D	382	46% 64%6%30%
14	7D	382	15% 64%6%30%
14	8D	382	8% 64%5%30%
14	9D	382	47% 64%6%30%
15	2E	175	7% 49%..49%
15	3E	175	7% 49%.49%
15	4E	175	45% 49%.49%
15	7E	175	7% 49%..49%
15	8E	175	5% 49%.49%
15	9E	175	46% 48%.49%
16	2F	96	17% 81%8%10%
16	3F	96	18% 80%9%10%
16	4F	96	51% 83%6%10%
16	7F	96	18% 81%8%10%
16	8F	96	18% 80%9%10%
16	9F	96	50% 85%.10%
17	2G	125	27% 62%11%27%
17	3G	125	26% 65%8%27%
17	4G	125	58% 65%8%27%

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Mol	Chain	Length	Quality of chain
17	7G	125	
17	8G	125	
17	9G	125	
18	2H	148	
18	3H	148	
18	4H	148	
18	7H	148	
18	8H	148	
18	9H	148	
19	2I	101	
19	3I	101	
19	4I	101	
19	7I	101	
19	8I	101	
19	9I	101	
20	2J	105	
20	3J	105	
20	4J	105	
20	7J	105	
20	8J	105	
20	9J	105	
21	2K	58	
21	3K	58	
21	4K	58	
21	7K	58	

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Mol	Chain	Length	Quality of chain
21	8K	58	
21	9K	58	
22	2L	87	
22	3L	87	
22	4L	87	
22	7L	87	
22	8L	87	
22	9L	87	
23	5A	282	
23	A	282	
24	5B	484	
24	B	484	
25	5C	733	
25	C	733	
26	5D	282	
26	D	282	
27	5E	467	
27	E	467	
28	5F	164	
28	F	164	
29	5G	231	
29	G	231	
30	5H	118	
30	H	118	
31	5I	165	

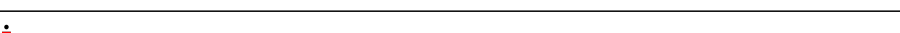
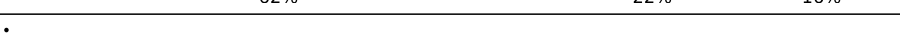
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Mol	Chain	Length	Quality of chain
31	I	165	
32	5J	128	
32	5r	128	
32	J	128	
32	r	128	
33	5K	138	
33	K	138	
34	5L	187	
34	L	187	
35	5M	154	
35	M	154	
36	5N	156	
36	N	156	
37	5O	101	
37	O	101	
38	5P	397	
38	P	397	
39	5Q	292	
39	Q	292	
40	5R	387	
40	R	387	
41	5S	279	
41	S	279	
42	5T	443	
42	T	443	

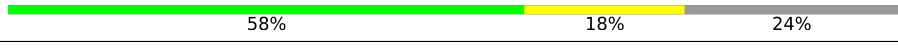
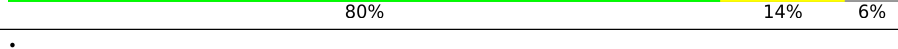
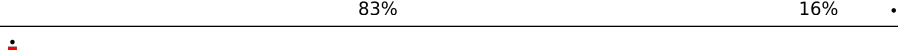
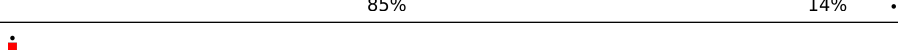
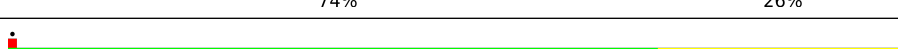
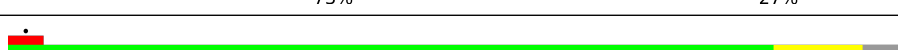
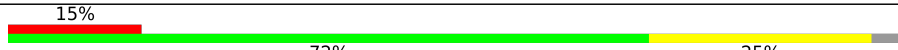
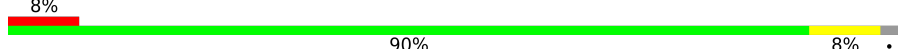
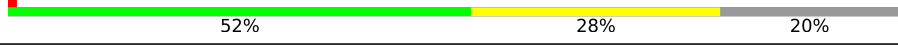
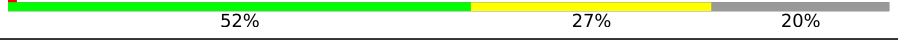
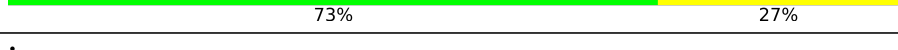
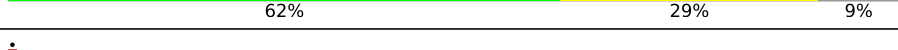
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Mol	Chain	Length	Quality of chain
43	5U	227	
43	U	227	
44	5V	546	
44	V	546	
45	5W	162	
45	W	162	
46	5X	149	
46	X	149	
47	5Y	64	
47	Y	64	
48	5Z	124	
48	Z	124	
49	5a	129	
49	a	129	
50	5b	172	
50	b	172	
51	5c	67	
51	c	67	
52	5d	86	
52	d	86	
53	5e	219	
53	e	219	
54	5f	65	
54	f	65	
55	5g	55	

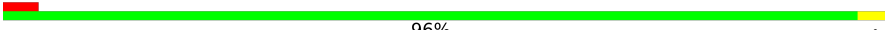
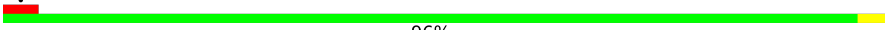
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Mol	Chain	Length	Quality of chain
55	g	55	
56	5h	142	
56	h	142	
57	5i	81	
57	i	81	
58	5j	86	
58	j	86	
59	5k	117	
59	k	117	
60	5l	121	
60	l	121	
61	5m	142	
61	m	142	
62	5n	106	
62	n	106	
63	5o	155	
63	o	155	
64	5p	130	
64	p	130	
65	5q	197	
65	q	197	
66	5s	312	
66	s	312	
67	5t	279	
67	t	279	

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Mol	Chain	Length	Quality of chain
68	5u	229	
68	u	229	
69	5v	45	
69	v	45	
70	5w	109	
70	w	109	
71	5x	157	
71	x	157	
72	5y	118	
72	y	118	

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
74	HEC	1E	401	X	-	-	-
74	HEC	1F	501	X	-	-	-
74	HEC	6E	401	X	-	-	-
74	HEC	6F	501	X	-	-	-
79	CUA	2C	301	-	-	X	-
79	CUA	3C	301	-	-	X	-
79	CUA	4C	301	-	-	X	-
79	CUA	7C	301	-	-	X	-
79	CUA	8C	301	-	-	X	-
79	CUA	9C	301	-	-	X	-
80	FES	5A	301	-	-	X	-
80	FES	A	301	-	-	X	-

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 292492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	1B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	6A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	6B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	1D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	6C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	6D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	1F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	6E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	6F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		

- Molecule 4 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	1H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	6G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	6H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	1J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	6I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	6J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	1L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	6K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	6L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		

- Molecule 7 is a protein called MPP-Beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	1N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	6M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	6N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	1P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	6O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	6P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		

- Molecule 9 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	1S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	6Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	6S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	1T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	6R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	6T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	3A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	4A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	7A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	8A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	9A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	3B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	4B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	7B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	8B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	9B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		

- Molecule 13 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	3C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	4C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	7C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	8C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	9C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	3D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	4D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	7D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	8D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	9D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		

- Molecule 15 is a protein called Cox5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	3E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	4E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	7E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	8E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	9E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		

- Molecule 16 is a protein called Cox5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	3F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	4F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	7F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	8F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	9F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

- Molecule 17 is a protein called Cox6a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	3G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	4G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	7G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	8G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	9G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		

- Molecule 18 is a protein called Cox6b.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	3H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	4H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	7H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	8H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	9H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		

- Molecule 19 is a protein called Cox7c.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	2I	72	Total	C	N	O	0	0
			594	393	98	103		
19	3I	72	Total	C	N	O	0	0
			594	393	98	103		

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Mol	Chain	Residues	Atoms				AltConf	Trace
19	4I	72	Total	C	N	O	0	0
			594	393	98	103		
19	7I	72	Total	C	N	O	0	0
			594	393	98	103		
19	8I	72	Total	C	N	O	0	0
			594	393	98	103		
19	9I	72	Total	C	N	O	0	0
			594	393	98	103		

- Molecule 20 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	3J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	4J	101	Total	C	N	O	S	0	0
			790	506	140	141	3		
20	7J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	8J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	9J	101	Total	C	N	O	S	0	0
			790	506	140	141	3		

- Molecule 21 is a protein called Cox7a.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	2K	47	Total	C	N	O	0	0
			382	249	63	70		
21	3K	47	Total	C	N	O	0	0
			382	249	63	70		
21	4K	47	Total	C	N	O	0	0
			382	249	63	70		
21	7K	47	Total	C	N	O	0	0
			382	249	63	70		
21	8K	47	Total	C	N	O	0	0
			382	249	63	70		
21	9K	47	Total	C	N	O	0	0
			382	249	63	70		

- Molecule 22 is a protein called CoxIn.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		
22	3L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	4L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	7L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		
22	8L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	9L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		
23	A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		
24	B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		
25	C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		
26	D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5E	386	Total	C	N	O	S	0	0
			3107	1986	540	558	23		
27	E	386	Total	C	N	O	S	0	0
			3107	1986	540	558	23		

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		
28	F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		

- Molecule 29 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		
29	G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		

- Molecule 30 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		
30	H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
32	5r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		
32	J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
32	r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		
33	K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		
34	L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		
35	M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		
36	N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		
37	O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		

- Molecule 38 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		
38	P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		
39	Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		
40	R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		
42	T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		

- Molecule 43 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		
43	U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		
44	V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		
45	W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		

- Molecule 46 is a protein called ASH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		
46	X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		

- Molecule 47 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		
47	Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		

- Molecule 48 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		
48	Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		

- Molecule 49 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		
49	a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		

- Molecule 50 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		
50	b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		

- Molecule 51 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		
51	c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		

- Molecule 52 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		
52	d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		

- Molecule 53 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		
53	e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		

- Molecule 54 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		
54	f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		

- Molecule 55 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		
55	g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		

- Molecule 56 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		
56	h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		

- Molecule 57 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		
57	i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		
58	j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	5k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		
59	k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		

- Molecule 60 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	5l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		
60	l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	5m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		
61	m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		

- Molecule 62 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		
62	n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		

- Molecule 63 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		
63	o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		

- Molecule 64 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	5p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		
64	p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		

- Molecule 65 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	5q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		
65	q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		

- Molecule 66 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	5s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		
66	s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		

- Molecule 67 is a protein called CAG2 - CA-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	5t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		
67	t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		

- Molecule 68 is a protein called CAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	5u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		
68	u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		

- Molecule 69 is a protein called P10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	5v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		
69	v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		

- Molecule 70 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		
70	w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		

- Molecule 71 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		
71	x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		

- Molecule 72 is a protein called NUOP7.

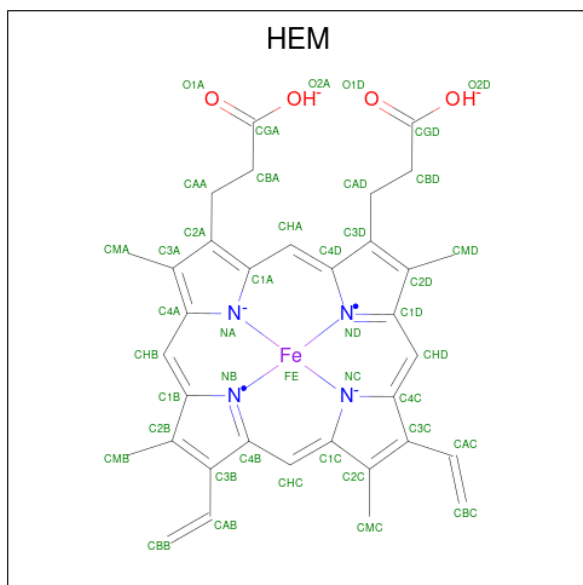
Mol	Chain	Residues	Atoms					AltConf	Trace
72	5y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

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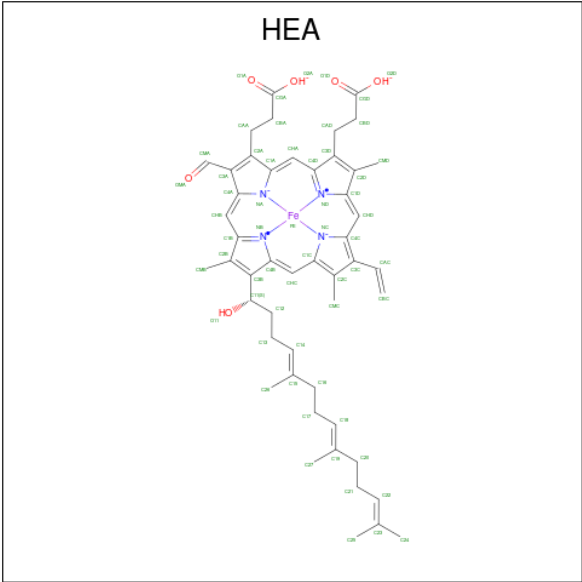
Mol	Chain	Residues	Atoms					AltConf	Trace
72	y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

- Molecule 73 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
73	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 74 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
76	2A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	2A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	3A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	3A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	7A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	7A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	9A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	9A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

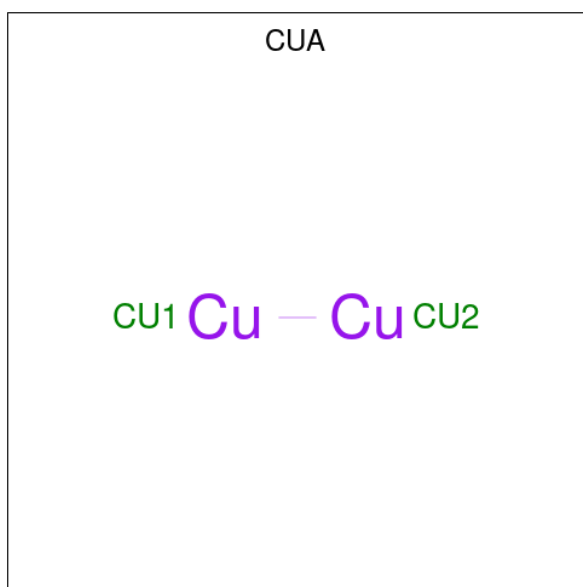
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	2A	1	Total 1	Cu 1	0
77	3A	1	Total 1	Cu 1	0
77	4A	1	Total 1	Cu 1	0
77	7A	1	Total 1	Cu 1	0
77	8A	1	Total 1	Cu 1	0
77	9A	1	Total 1	Cu 1	0

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

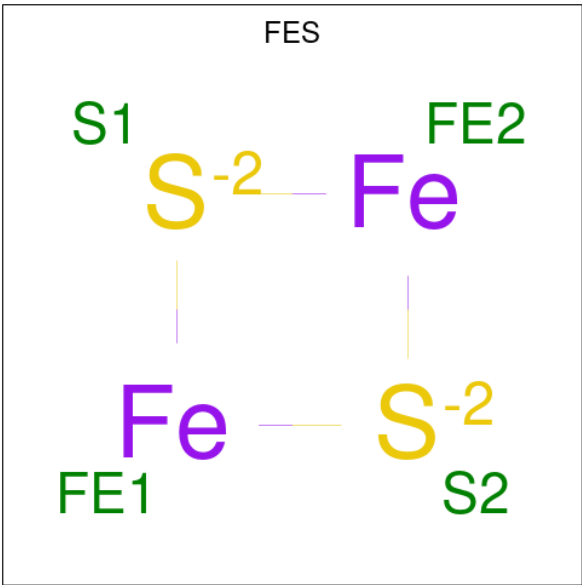
Mol	Chain	Residues	Atoms		AltConf
78	2A	1	Total 1	Mg 1	0
78	3A	1	Total 1	Mg 1	0
78	4A	1	Total 1	Mg 1	0
78	7A	1	Total 1	Mg 1	0
78	8A	1	Total 1	Mg 1	0
78	9A	1	Total 1	Mg 1	0

- Molecule 79 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



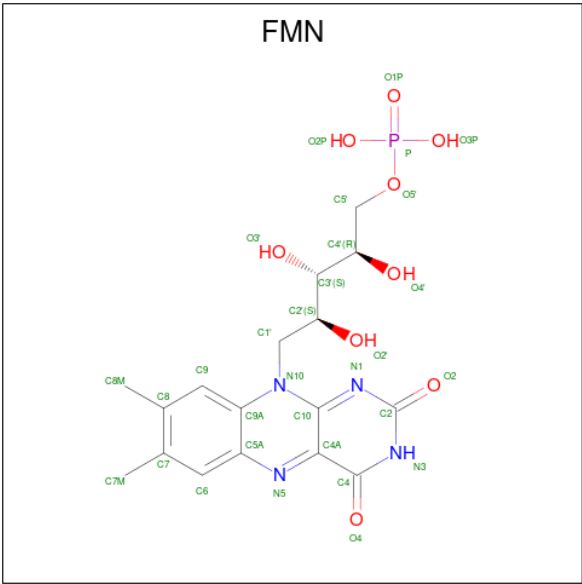
Mol	Chain	Residues	Atoms		AltConf
79	2C	1	Total 2	Cu 2	0
79	3C	1	Total 2	Cu 2	0
79	4C	1	Total 2	Cu 2	0
79	7C	1	Total 2	Cu 2	0
79	8C	1	Total 2	Cu 2	0
79	9C	1	Total 2	Cu 2	0

- Molecule 80 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



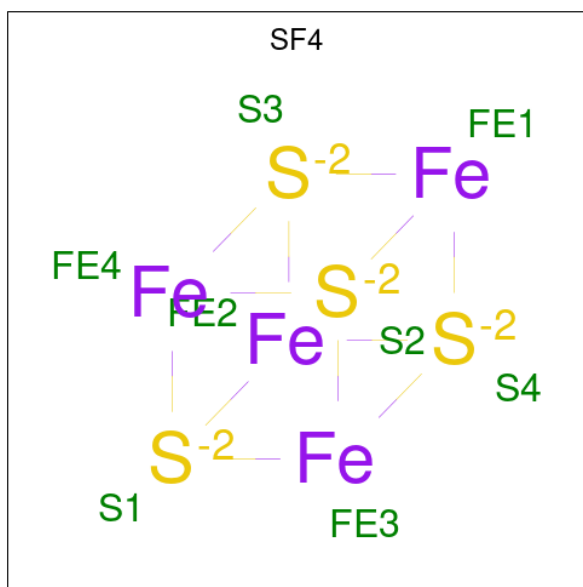
Mol	Chain	Residues	Atoms			AltConf
80	5A	1	Total	Fe	S	0
			4	2	2	
80	5C	1	Total	Fe	S	0
			4	2	2	
80	A	1	Total	Fe	S	0
			4	2	2	
80	C	1	Total	Fe	S	0
			4	2	2	

- Molecule 81 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
81	5B	1	Total	C	N	O	P	0
			31	17	4	9	1	
81	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 82 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



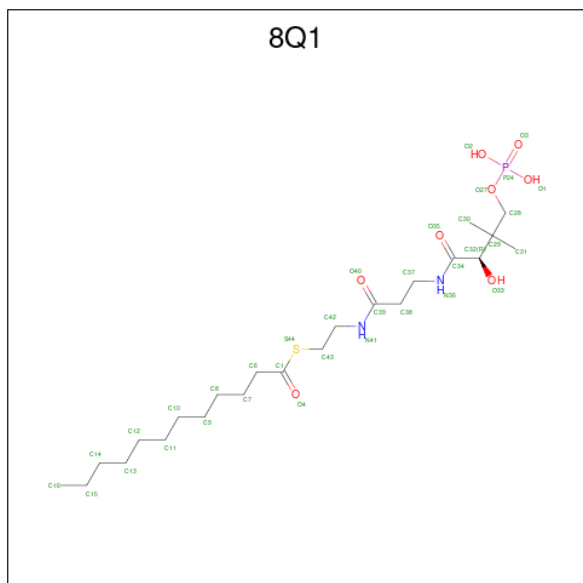
Mol	Chain	Residues	Atoms			AltConf
82	5B	1	Total	Fe	S	0
			8	4	4	
82	5C	1	Total	Fe	S	0
			8	4	4	
82	5C	1	Total	Fe	S	0
			8	4	4	
82	5F	1	Total	Fe	S	0
			8	4	4	
82	5G	1	Total	Fe	S	0
			8	4	4	
82	5G	1	Total	Fe	S	0
			8	4	4	
82	B	1	Total	Fe	S	0
			8	4	4	
82	C	1	Total	Fe	S	0
			8	4	4	
82	C	1	Total	Fe	S	0
			8	4	4	
82	F	1	Total	Fe	S	0
			8	4	4	

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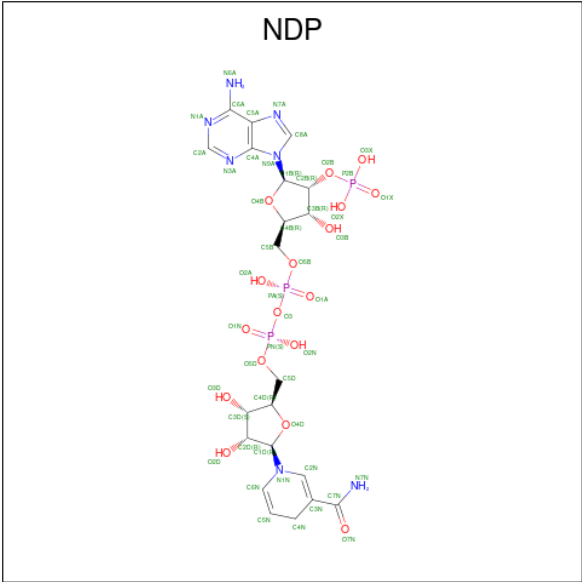
Mol	Chain	Residues	Atoms			AltConf
82	G	1	Total	Fe	S	0
			8	4	4	
82	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 83 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



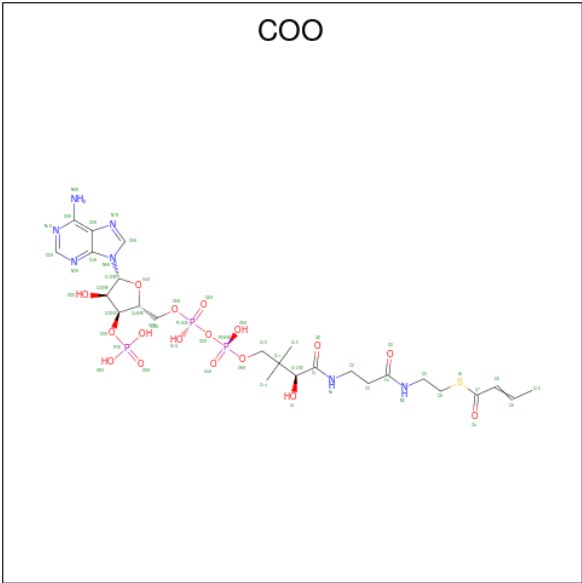
Mol	Chain	Residues	Atoms						AltConf
83	5J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	5k	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	k	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
84	5P	1	Total	C	N	O	P	0
			48	21	7	17	3	
84	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 85 is CROTONYL COENZYME A (CCD ID: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).

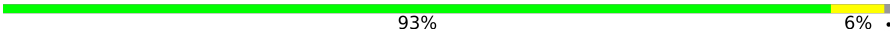


Mol	Chain	Residues	Atoms						AltConf
85	5s	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	
85	s	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

3 Residue-property plots [i](#)

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

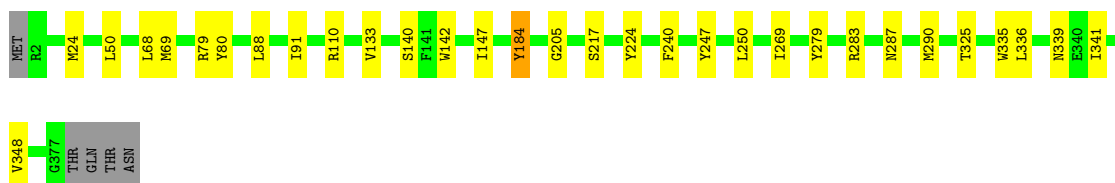
- Molecule 1: Cytochrome b

Chain 1A: 



- Molecule 1: Cytochrome b

Chain 1B: 



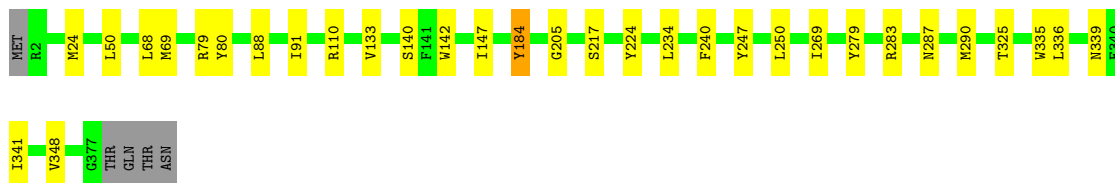
- Molecule 1: Cytochrome b

Chain 6A: 

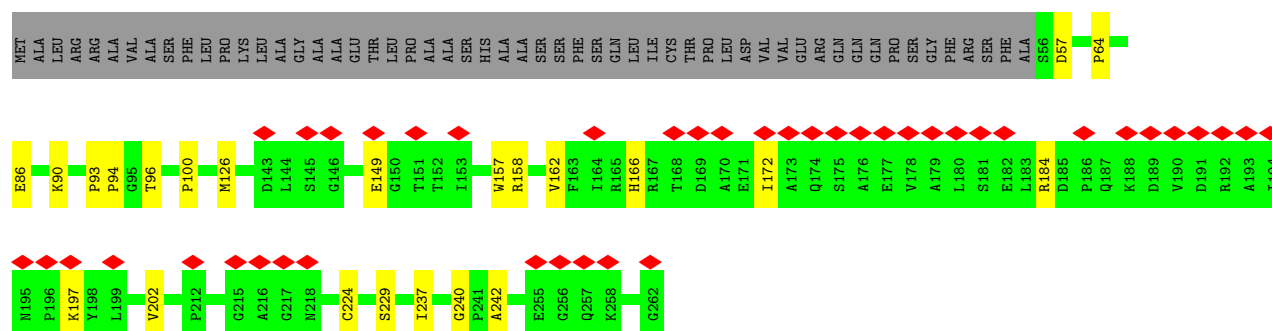
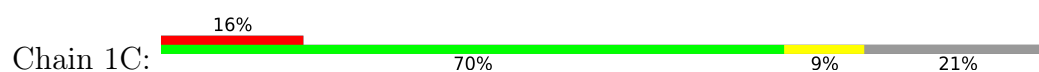


- Molecule 1: Cytochrome b

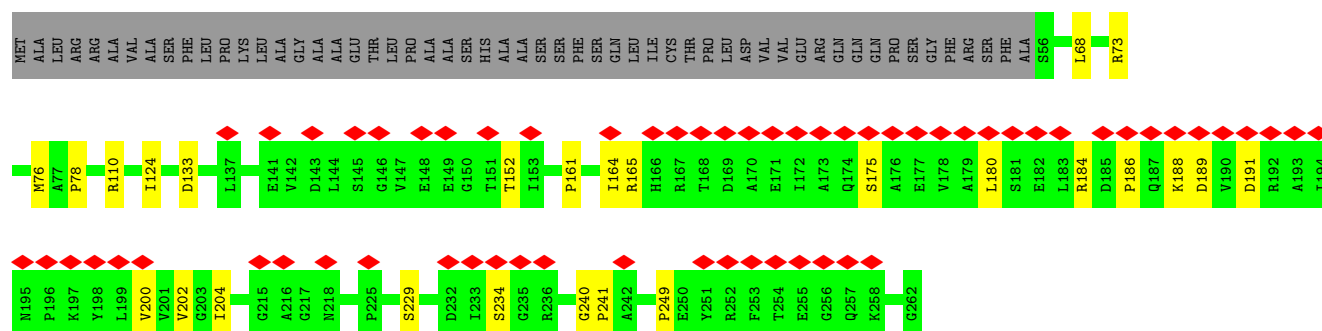
Chain 6B: 



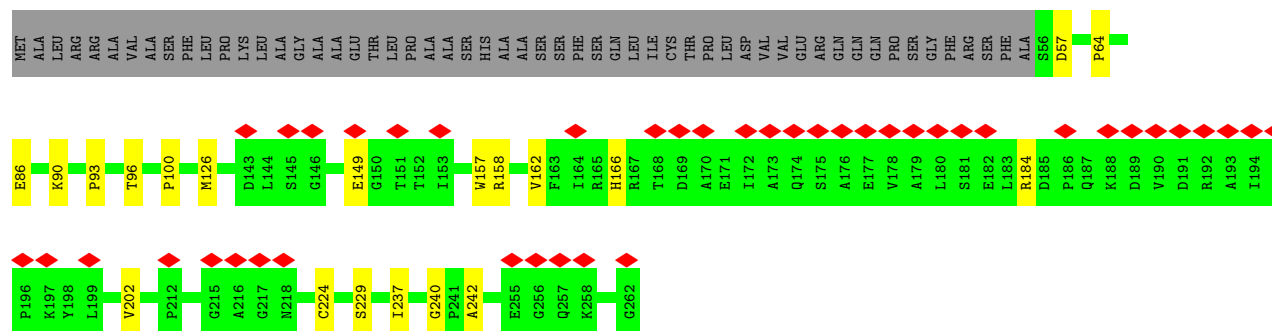
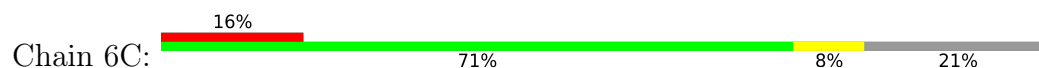
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



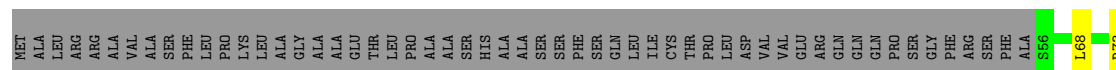
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

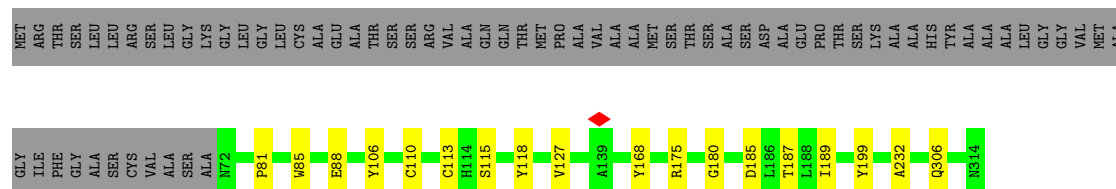


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

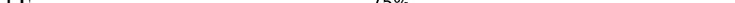


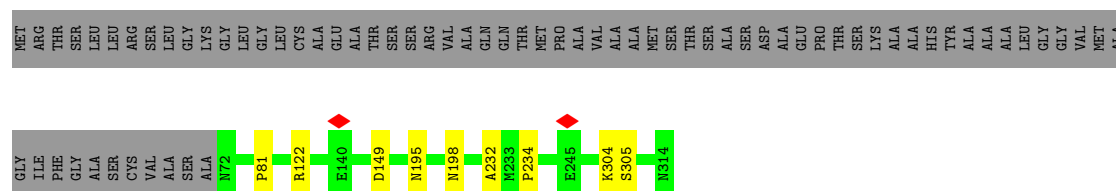
- Molecule 3: Cytochrome c1

Chain 1E:  72% 6% 23%

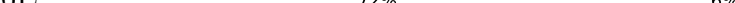


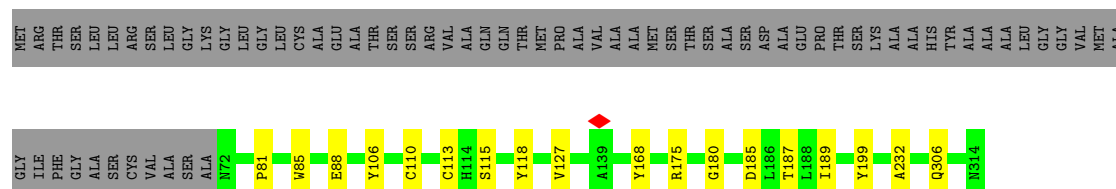
- Molecule 3: Cytochrome c1

Chain 1F:  75% 23%

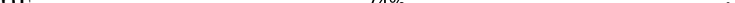


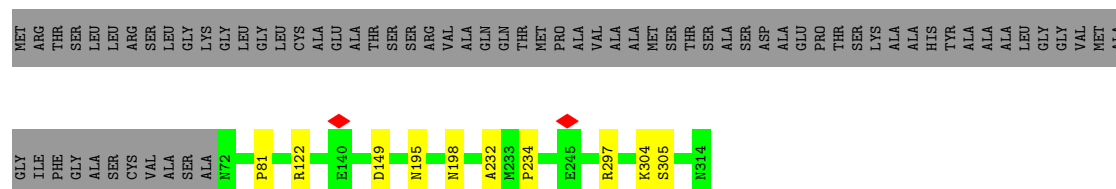
- Molecule 3: Cytochrome c1

Chain 6E:  72% 6% 23%

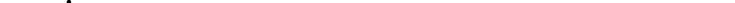


- Molecule 3: Cytochrome c1

Chain 6F:  74% 23%



- Molecule 4: Complex III subunit 9

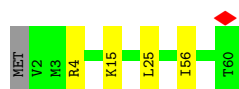
Chain 1G:  93% 5%



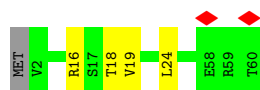
- Molecule 4: Complex III subunit 9



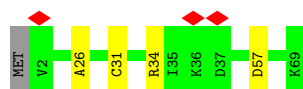
- Molecule 4: Complex III subunit 9



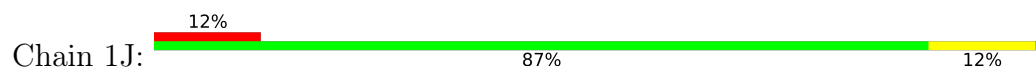
- Molecule 4: Complex III subunit 9



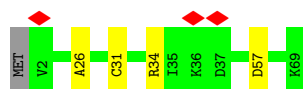
- Molecule 5: Cytochrome b-c1 complex subunit 6



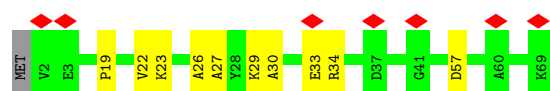
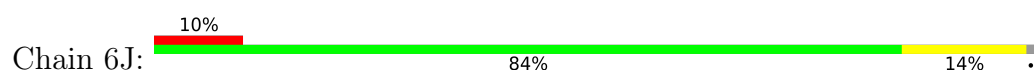
- Molecule 5: Cytochrome b-c1 complex subunit 6



- Molecule 5: Cytochrome b-c1 complex subunit 6



- Molecule 5: Cytochrome b-c1 complex subunit 6



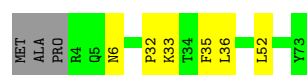
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



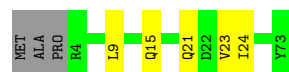
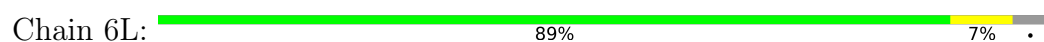
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



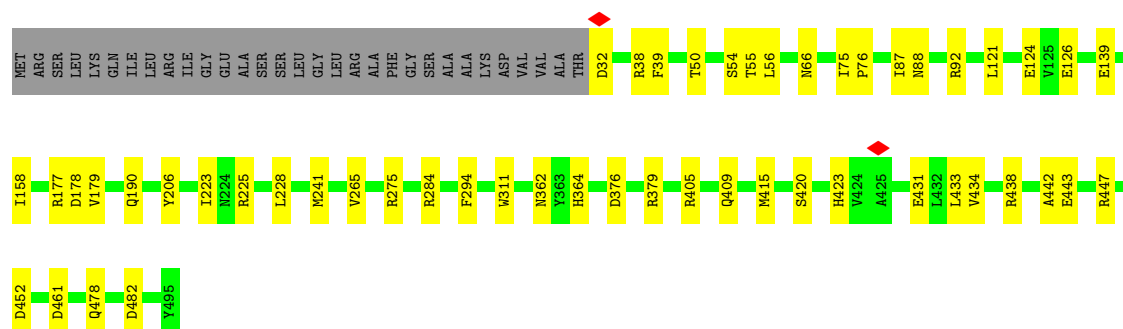
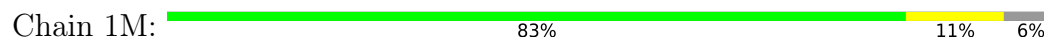
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

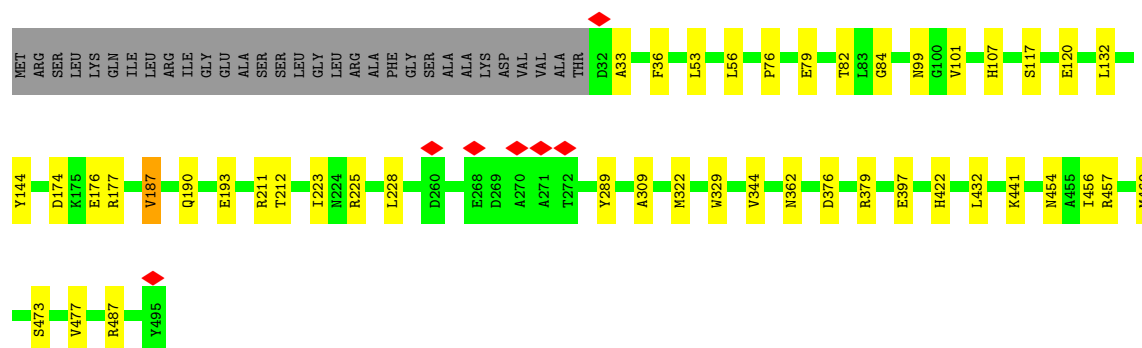


- Molecule 7: MPP-Beta



- Molecule 7: MPP-Beta

Chain 1N: 



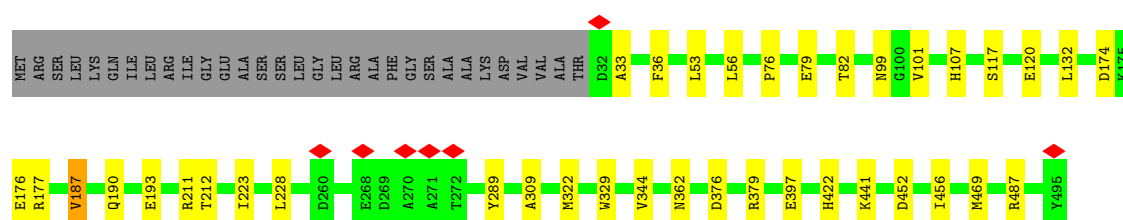
• Molecule 7: MPP-Beta

Chain 6M: 



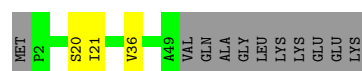
• Molecule 7: MPP-Beta

Chain 6N: 



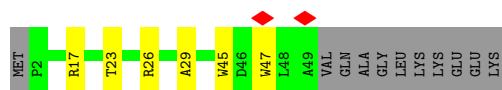
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 10O: 

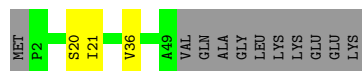
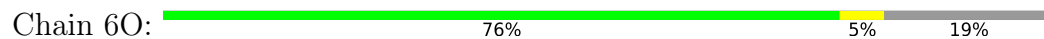


• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

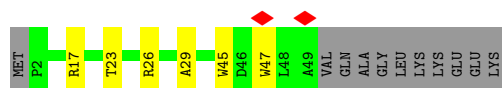
Chain 1P: 



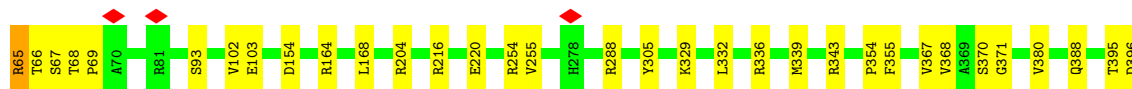
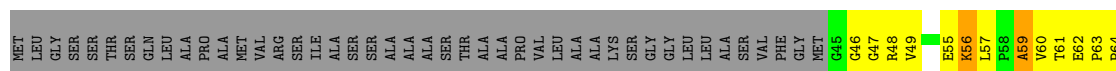
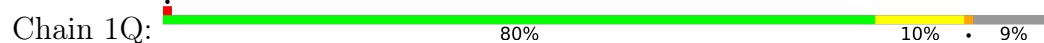
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



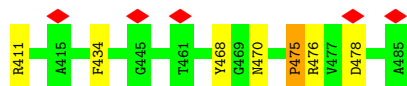
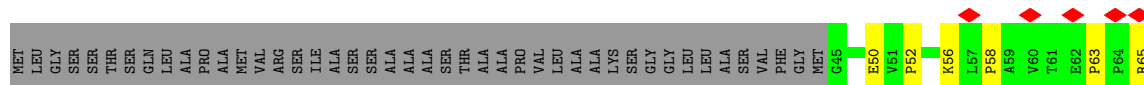
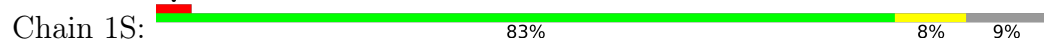
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



- Molecule 9: Alpha-MPP

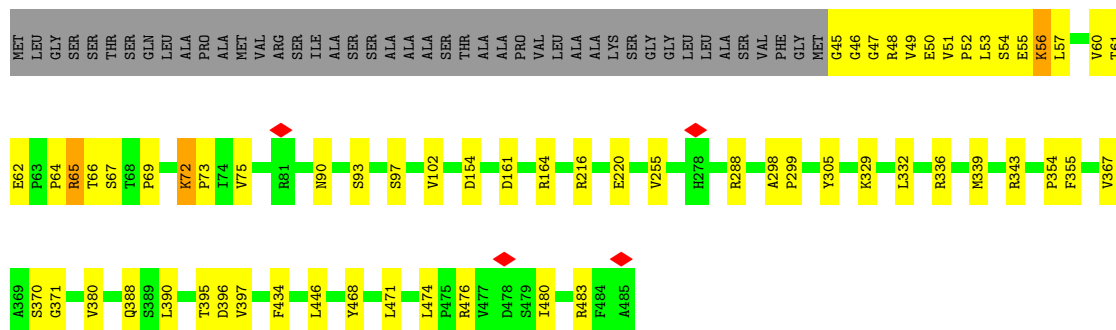


- Molecule 9: Alpha-MPP



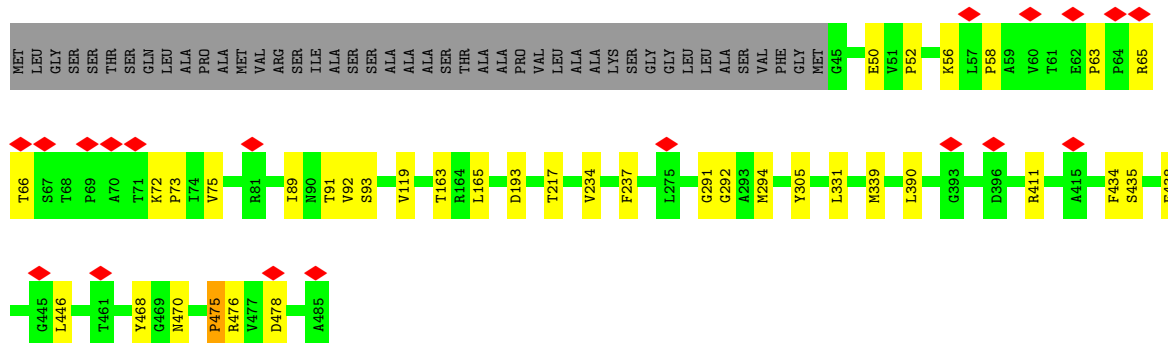
- Molecule 9: Alpha-MPP

Chain 6Q: 



• Molecule 9: Alpha-MPP

Chain 6S: 



• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1R: 



• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1T: 



• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6R: 



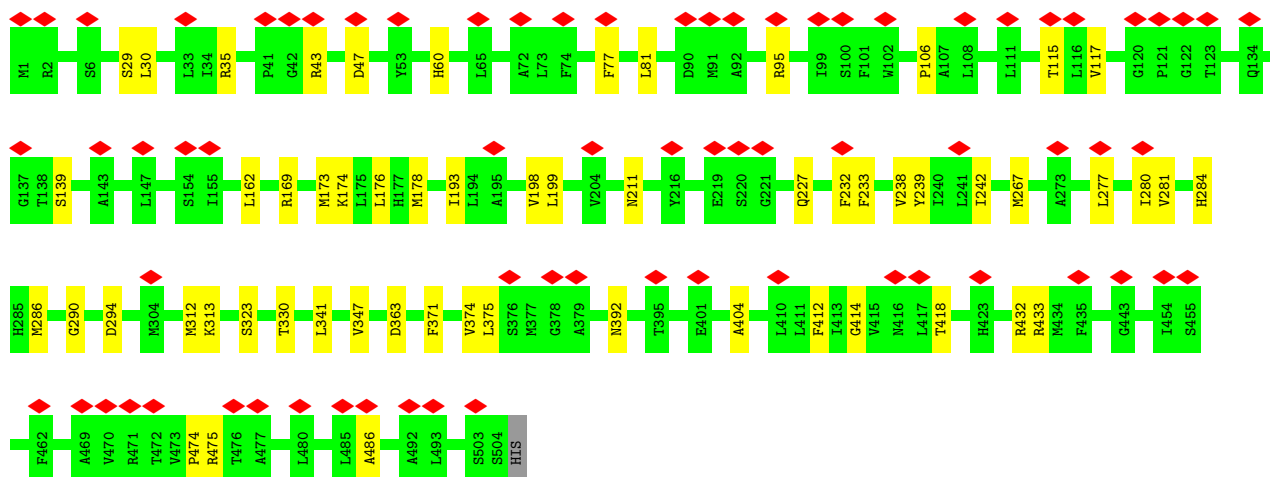
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6T:  88% 10% ..



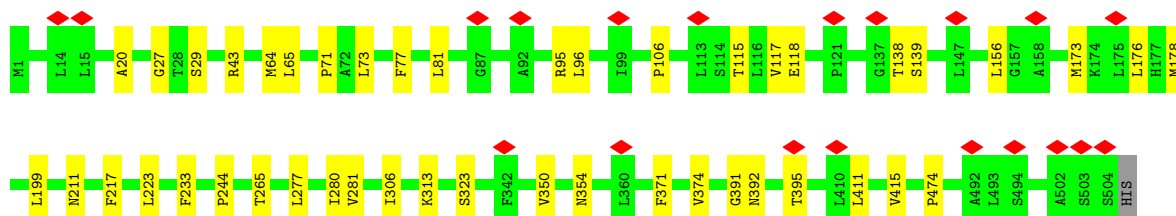
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 2A:  14% 89% 11%



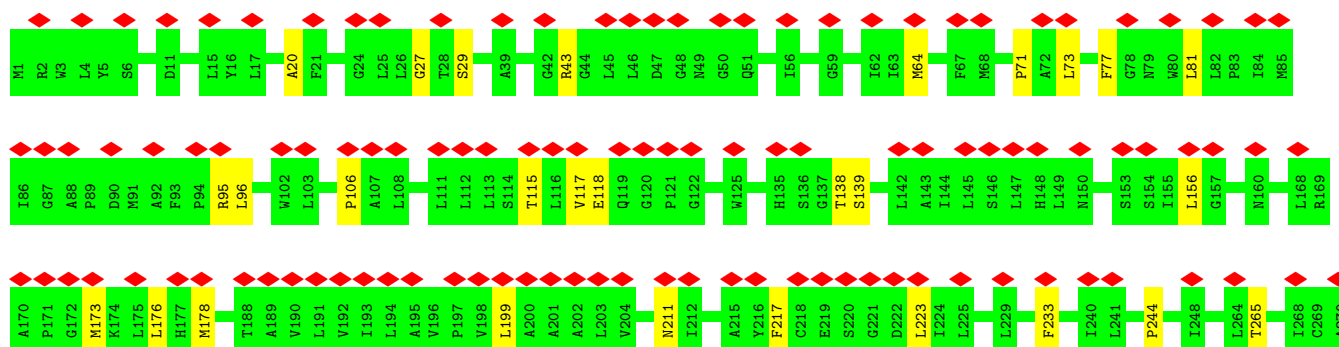
• Molecule 11: Cytochrome c oxidase subunit 1

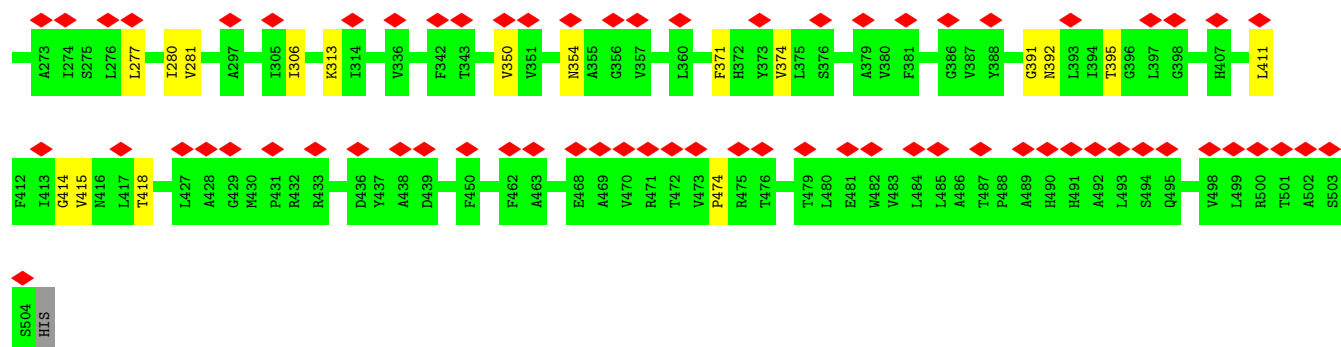
Chain 3A:  91% 9%



• Molecule 11: Cytochrome c oxidase subunit 1

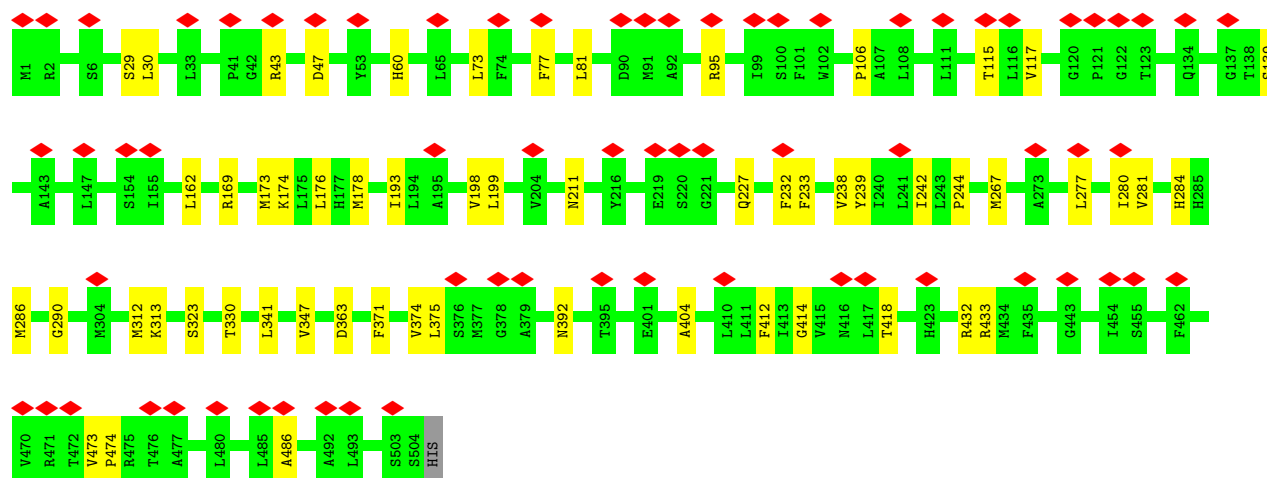
Chain 4A:  35% 91% 9%





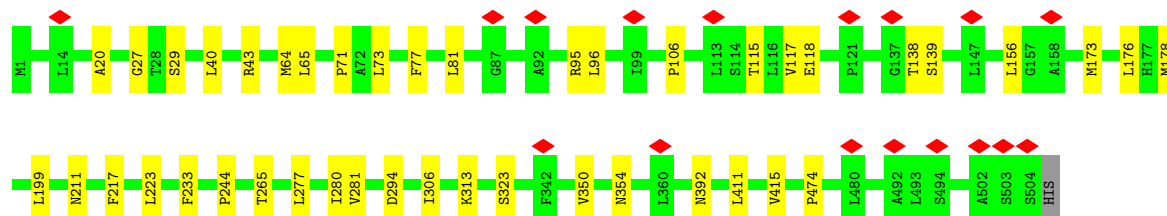
- Molecule 11: Cytochrome c oxidase subunit 1

Chain 7A: 14% 89% 11%



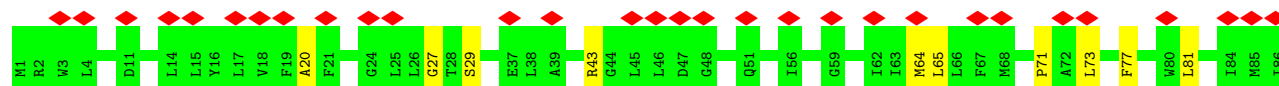
- Molecule 11: Cytochrome c oxidase subunit 1

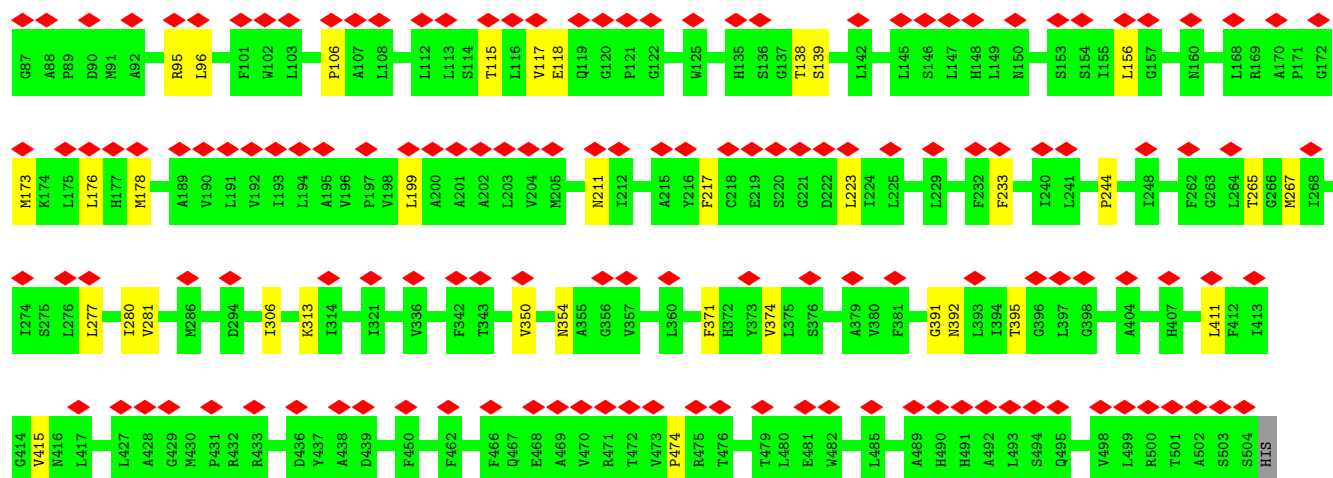
Chain 8A: 91% 9%



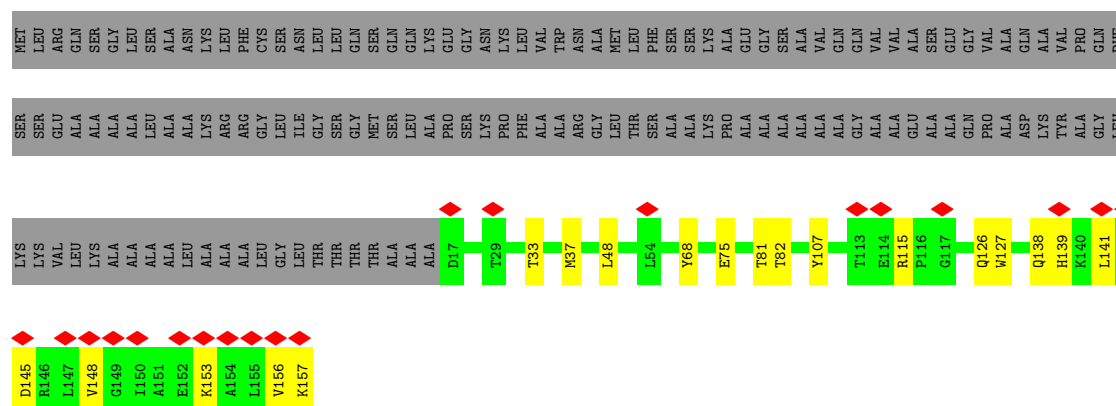
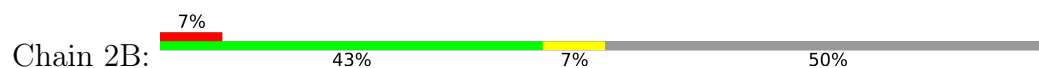
- Molecule 11: Cytochrome c oxidase subunit 1

Chain 9A: 34% 91% 9%

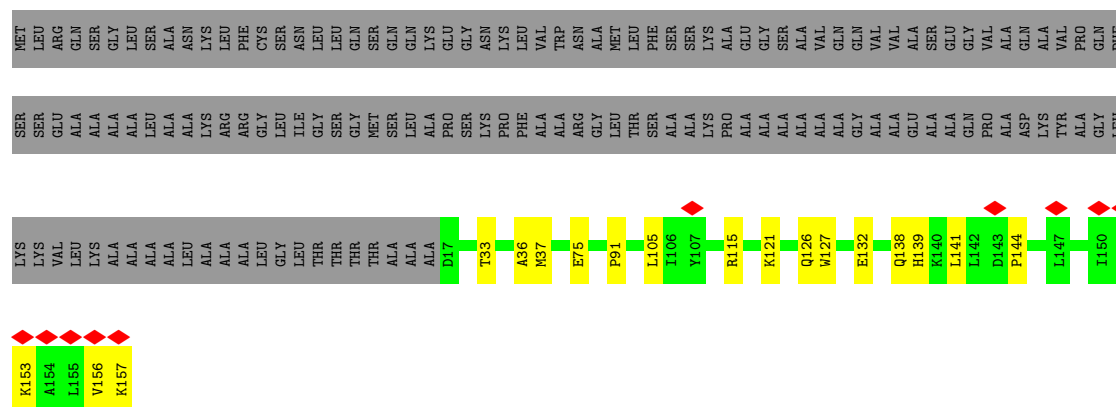




• Molecule 12: Cytochrome c oxidase polypeptide II

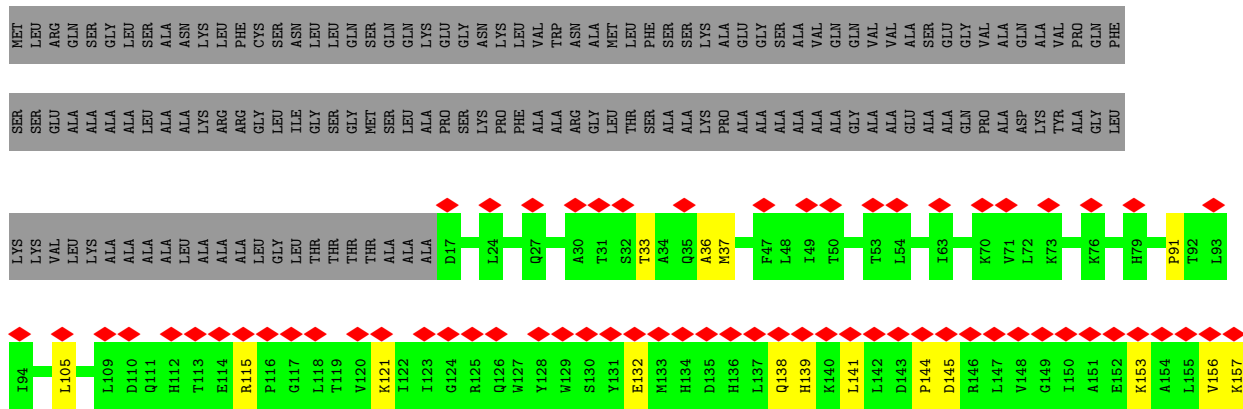


• Molecule 12: Cytochrome c oxidase polypeptide II

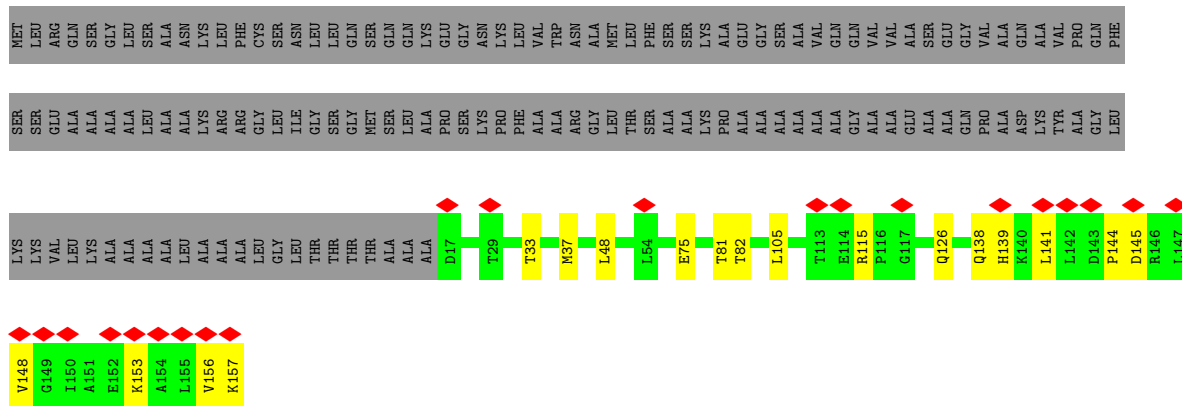


• Molecule 12: Cytochrome c oxidase polypeptide II

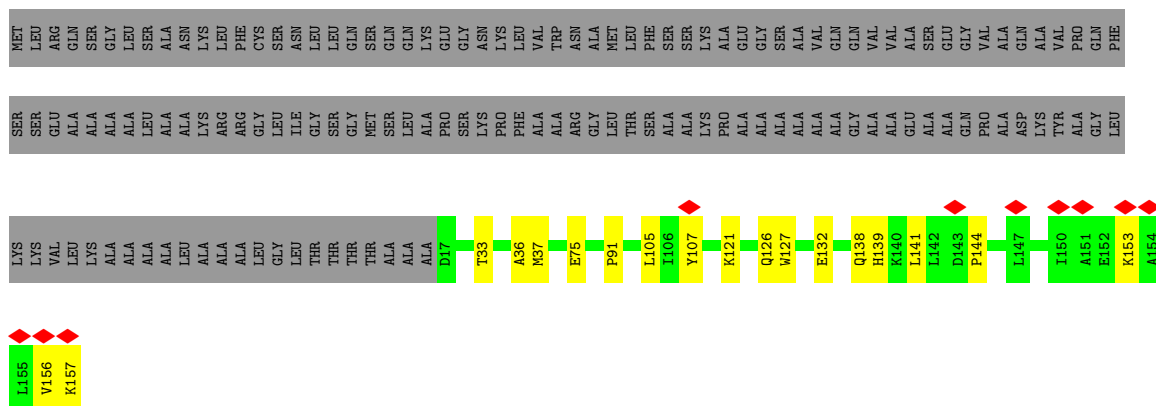




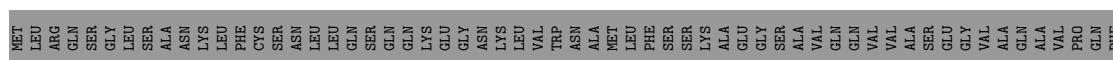
- Molecule 12: Cytochrome c oxidase polypeptide II

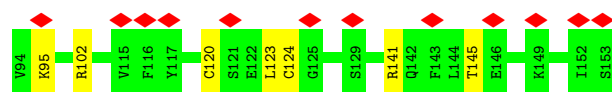


- Molecule 12: Cytochrome c oxidase polypeptide II

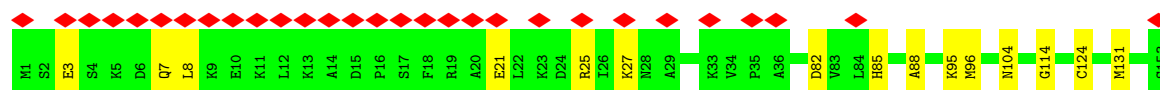


- Molecule 12: Cytochrome c oxidase polypeptide II

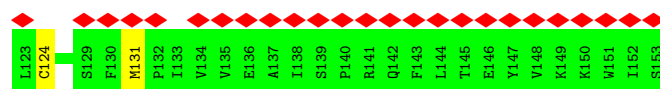
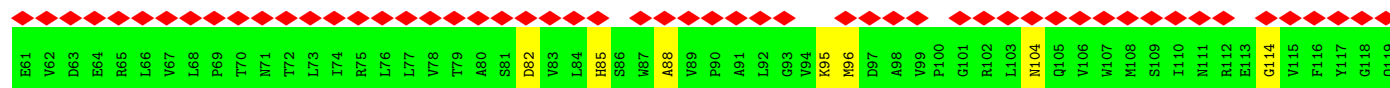
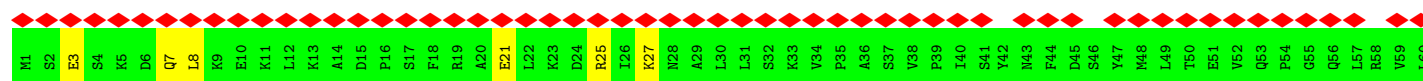
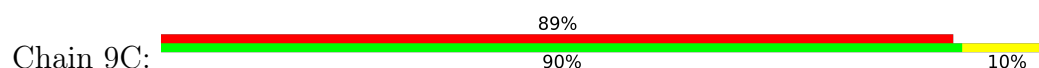




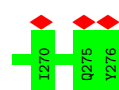
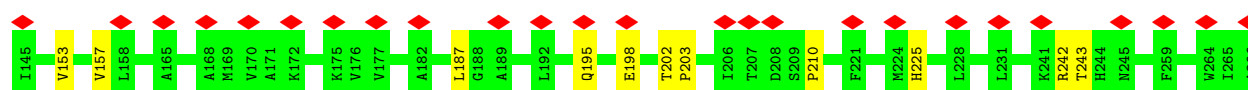
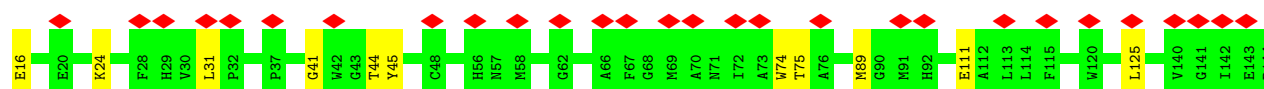
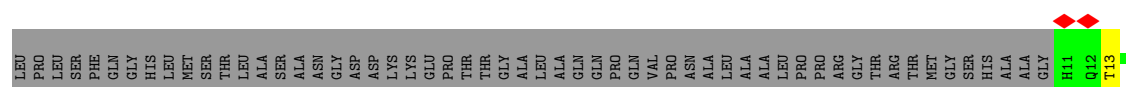
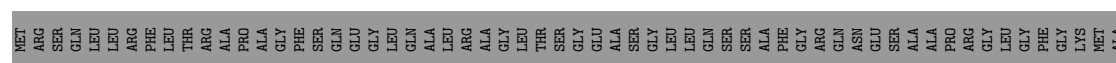
- Molecule 13: cytochrome-c oxidase



- Molecule 13: cytochrome-c oxidase

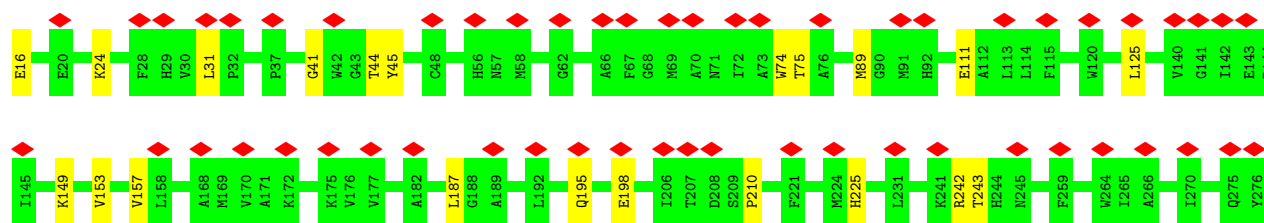


- Molecule 14: Cytochrome c oxidase subunit 3

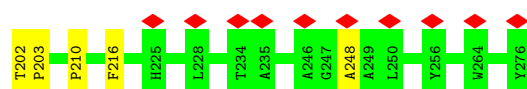
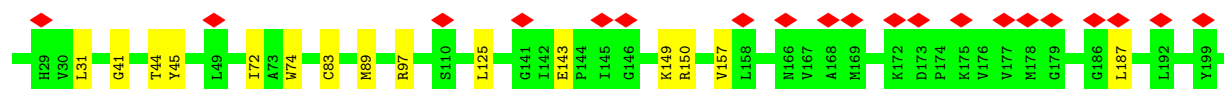
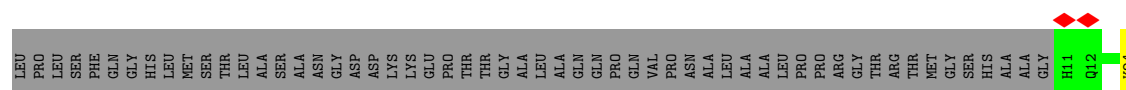
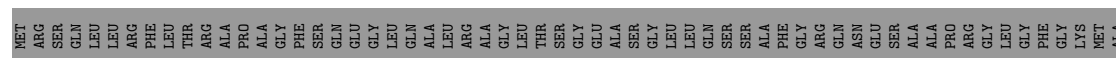


- Molecule 14: Cytochrome c oxidase subunit 3

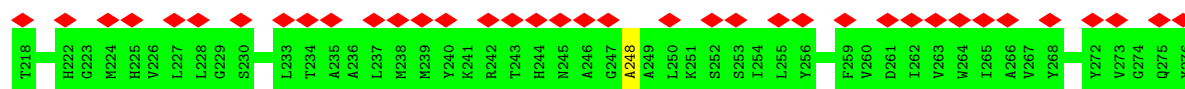
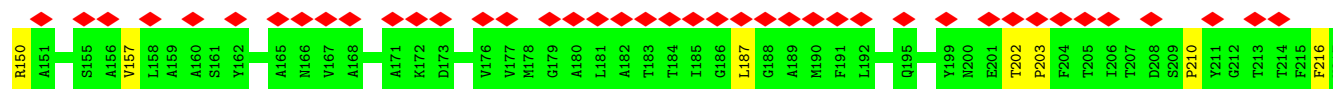
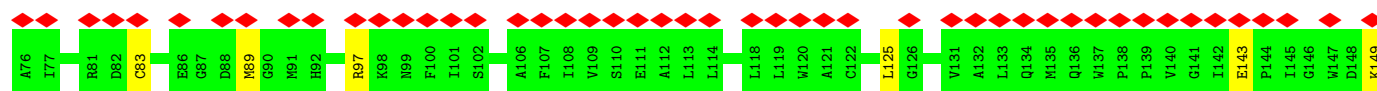
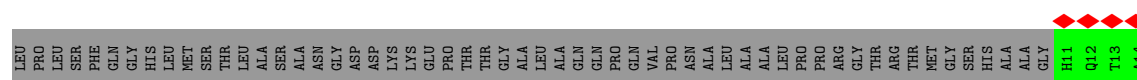
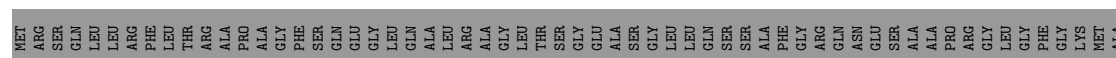




• Molecule 14: Cytochrome c oxidase subunit 3



• Molecule 14: Cytochrome c oxidase subunit 3



• Molecule 15: Cox5b



MET ASN ARG LEU GLY SER LEU LEU LEU ALA ARG ALA ALA ARG THR CYS SER ARG ARG TRP THR THR ALA ALA SER GLY VAL PRO PRO ALA LEU SER ALA VAL ILE VAL GLN PHE ALA ALA GLN ALA ARG SER LEU HIS THR LEU THR CYS GLN GLY ALA

PRO ALA GLU ALA LYS PRO SER ALA LEU LEU ALA ALA PRO PRO ARG LYS Y15 R16 P17 D20 A27 W28 F34 E38 E58 T61 D70 G71 D97 V98 L99 E100 A101 I102 E103 G104 GLY ALA ASP LYS LYS LYS LYS LYS

• Molecule 15: Cox5b



MET ASN ARG LEU GLY SER LEU LEU LEU ALA ARG ALA ALA ARG THR CYS SER ARG ARG TRP THR THR ALA ALA SER GLY VAL PRO PRO ALA LEU SER ALA VAL ILE VAL GLN PHE ALA ALA GLN ALA ARG SER LEU HIS THR LEU THR CYS GLN GLY ALA

PRO ALA GLU ALA LYS PRO SER ALA LEU LEU ALA ALA PRO PRO ARG LYS Y15 A27 W28 E38 E47 A48 D70 H88 V89 E90 Y91 I92 V95 V98 L99 E100 A101 I102 E103 G104 GLY ALA ASP LYS LYS LYS LYS LYS

• Molecule 15: Cox5b



MET ASN ARG LEU GLY SER LEU LEU LEU ALA ARG ALA ALA ARG THR CYS SER ARG ARG TRP THR THR ALA ALA SER GLY VAL PRO PRO ALA LEU SER ALA VAL ILE VAL GLN PHE ALA ALA GLN ALA ARG SER LEU HIS THR LEU THR CYS GLN GLY ALA

PRO ALA GLU ALA LYS PRO SER ALA LEU LEU ALA ALA PRO PRO ARG LYS Y15 R16 P17 L18 G19 D20 K21 E22 W24 H25 E26 A27 W28 E31 D32 K33 F34 G35 T36 E37 E38 D39 P40 T41 T42 V43 P44 S45 L46 E47 A48 E49 R50 T51 T55 E58 D59 E60 T61 L62

V63 V64 V65 G66 L68 K69 D70 G71 P73 P74 P75 R75 Q76 F77 V78 E79 N80 G81 E82 F83 Y84 V85 L86 K87 H88 V89 E90 Y91 I92 K93 K94 V95 G96 D97 V98 L99 E100 A101 I102 E103 G104 GLY ALA ASP LYS LYS LYS LYS LYS

• Molecule 15: Cox5b



MET ASN ARG LEU GLY SER LEU LEU LEU ALA ARG ALA ALA ARG THR CYS SER ARG ARG TRP THR THR ALA ALA SER GLY VAL PRO PRO ALA LEU SER ALA VAL ILE VAL GLN PHE ALA ALA GLN ALA ARG SER LEU HIS THR LEU THR CYS GLN GLY ALA

PRO ALA GLU ALA LYS PRO SER ALA LEU LEU ALA ALA PRO PRO ARG LYS Y15 R16 P17 D20 A27 W28 F34 E38 A48 E58 T61 D70 G71 D97 V98 L99 E100 A101 I102 E103 G104 GLY ALA ASP LYS LYS LYS LYS LYS

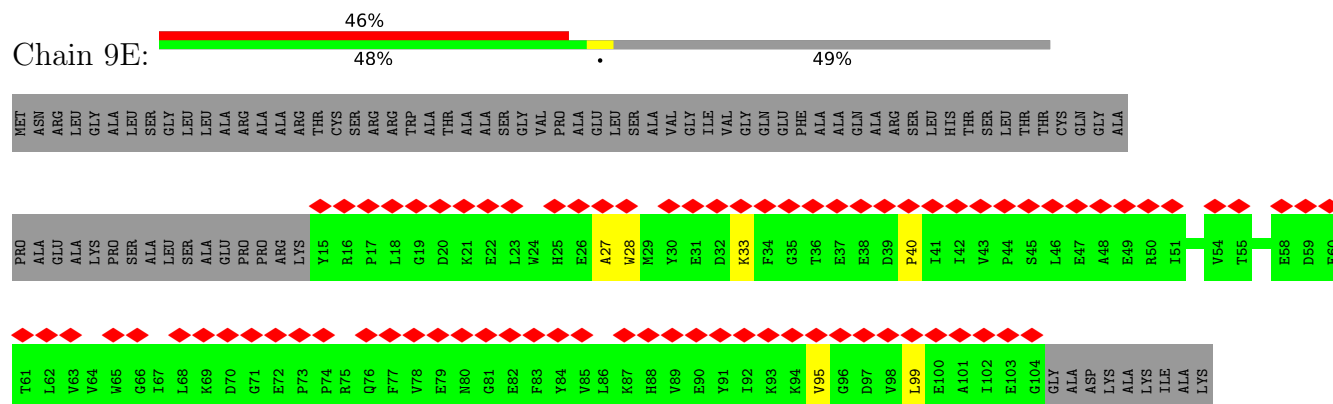
• Molecule 15: Cox5b



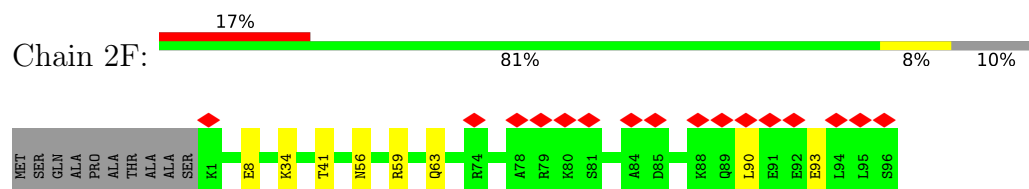
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PRO ALA GLU ALA LYS PRO SER ALA LEU LEU ALA ALA PRO PRO ARG LYS Y15 A27 W28 E38 A48 D70 H88 V89 E90 V95 L99 E100 A101 I102 E103 G104 GLY ALA ASP LYS LYS LYS LYS LYS

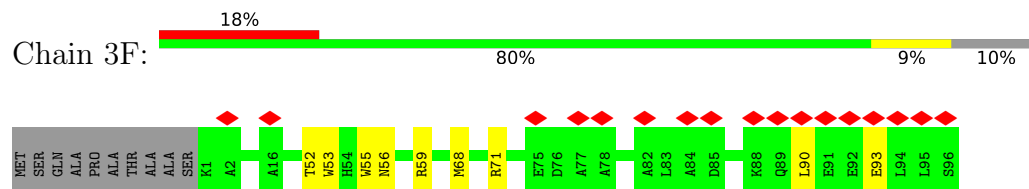
Chain 9E:



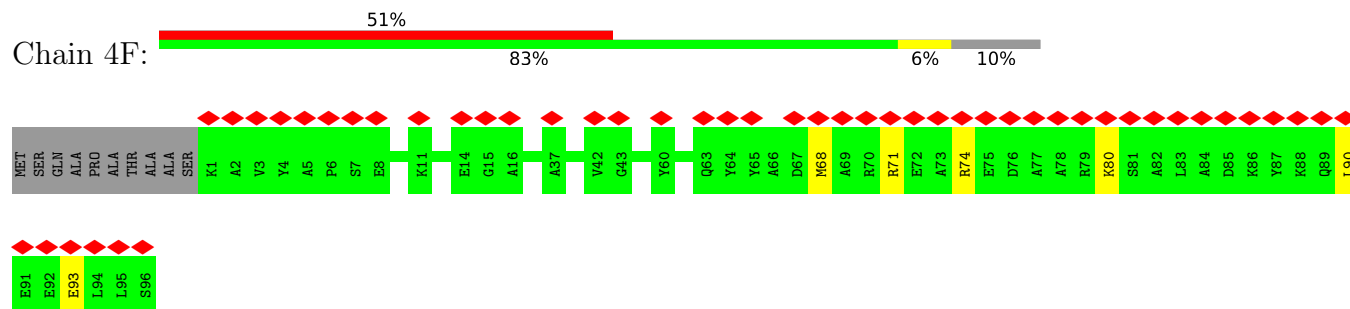
Chain 2F:



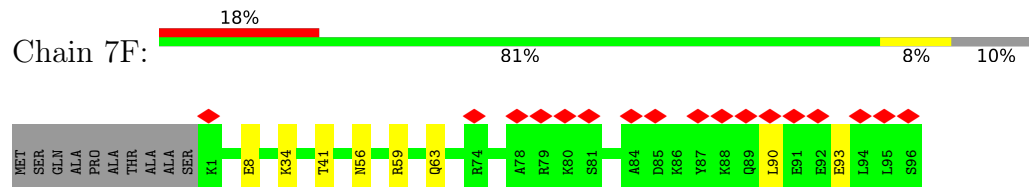
Chain 3F:



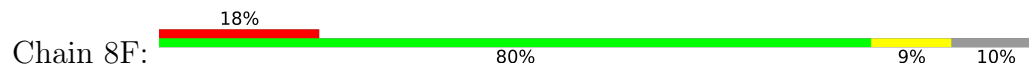
Chain 4F:



Chain 7F:

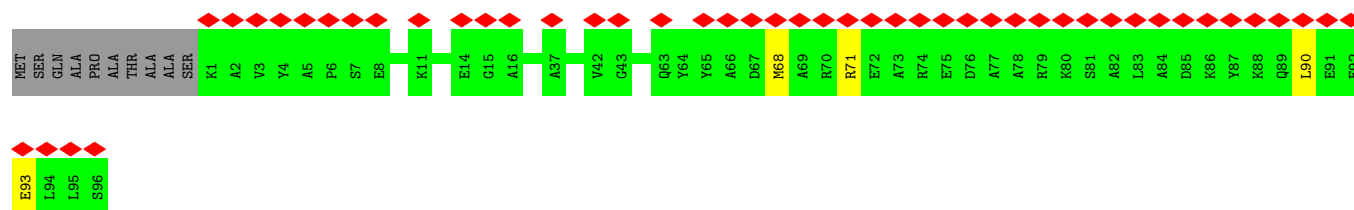
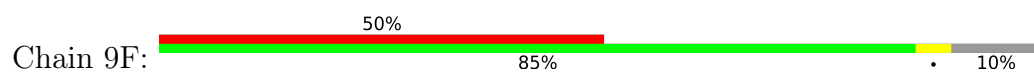


Chain 8F:

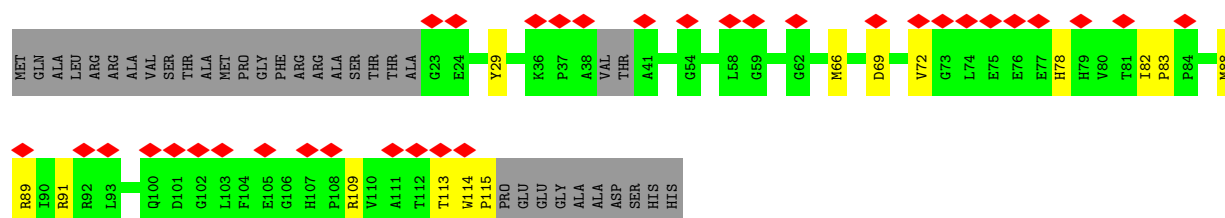




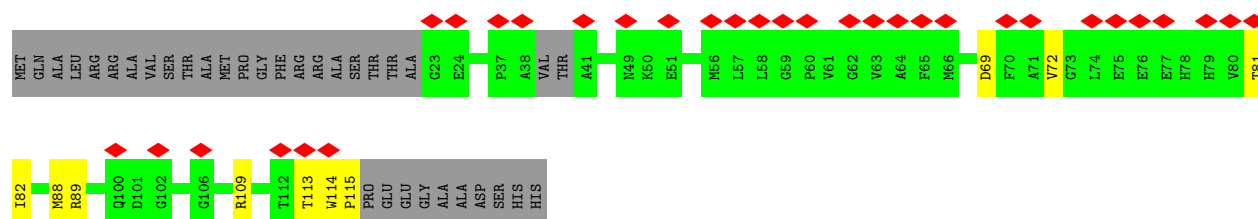
- Molecule 16: Cox5c



- Molecule 17: Cox6a



- Molecule 17: Cox6a

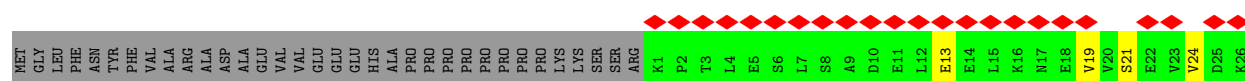


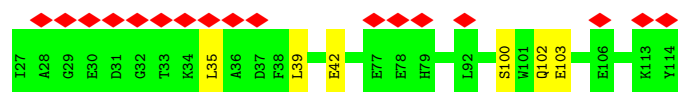
- Molecule 17: Cox6a



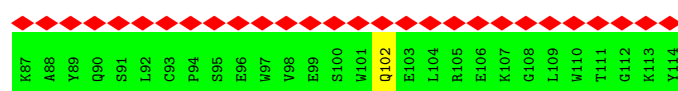
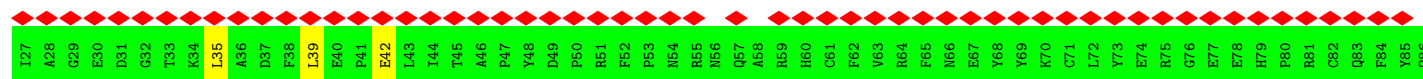
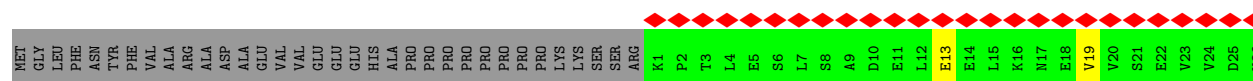
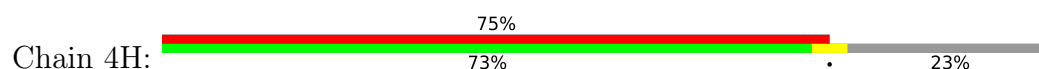
- Molecule 17: Cox6a



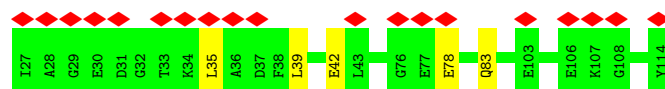
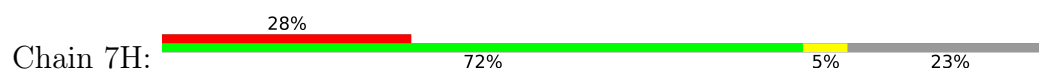




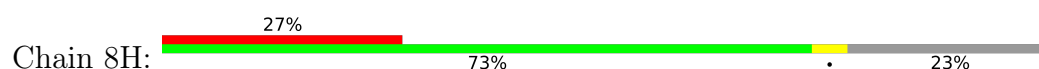
• Molecule 18: Cox6b



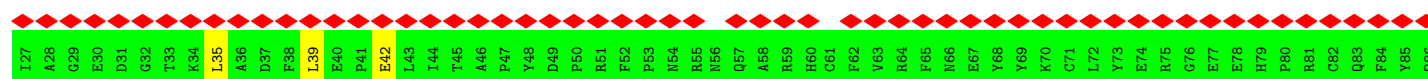
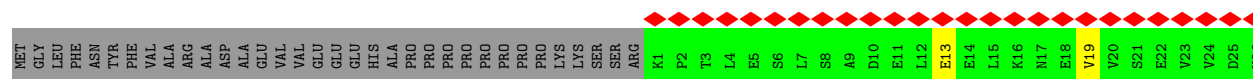
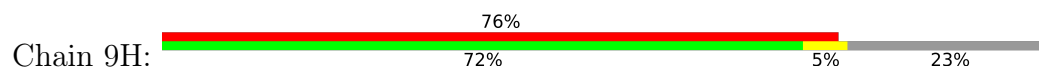
• Molecule 18: Cox6b

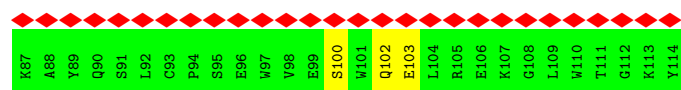


• Molecule 18: Cox6b

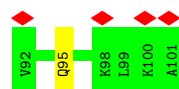
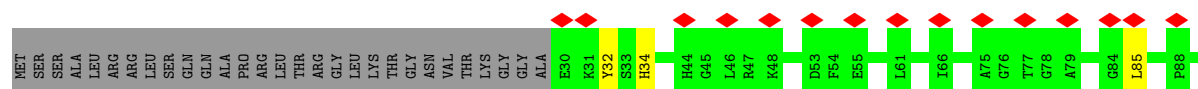


• Molecule 18: Cox6b

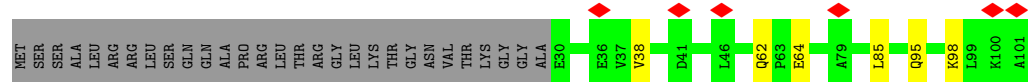




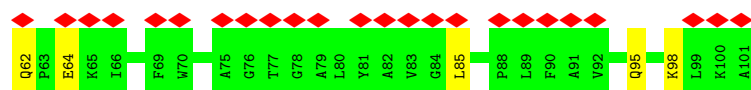
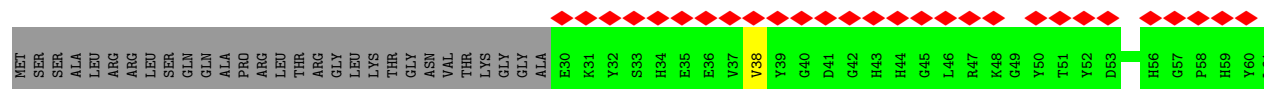
• Molecule 19: Cox7c



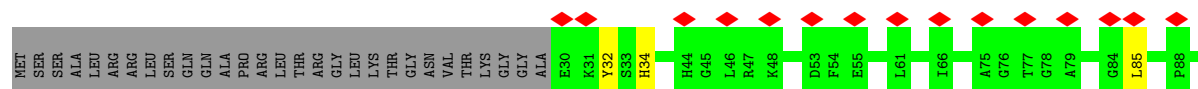
• Molecule 19: Cox7c



• Molecule 19: Cox7c

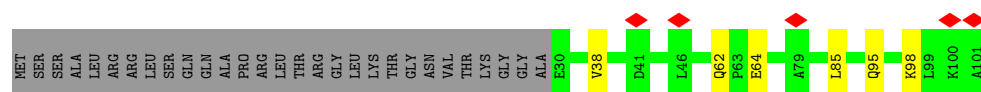


• Molecule 19: Cox7c

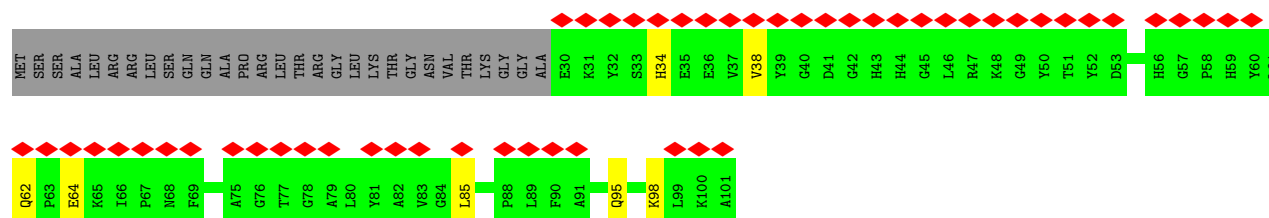


• Molecule 19: Cox7c

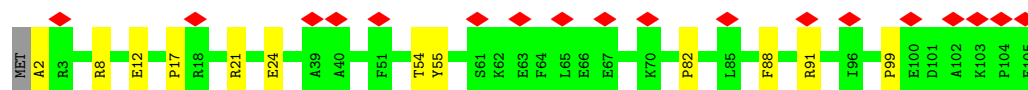




- Molecule 19: Cox7c



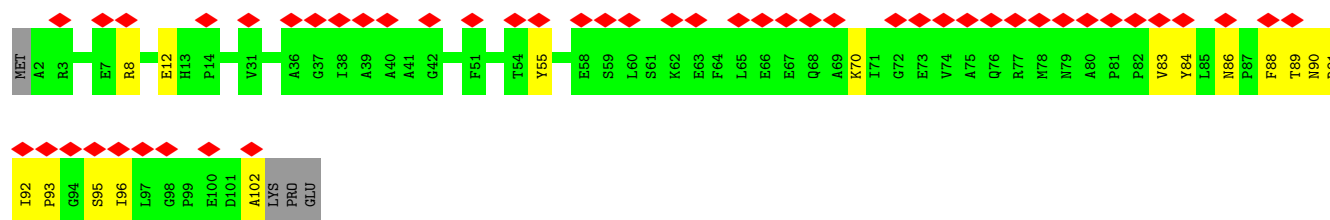
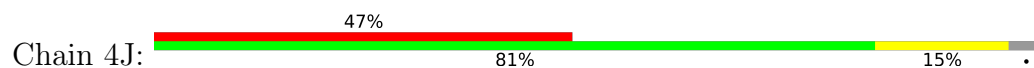
- Molecule 20: Cytochrome c oxidase subunit



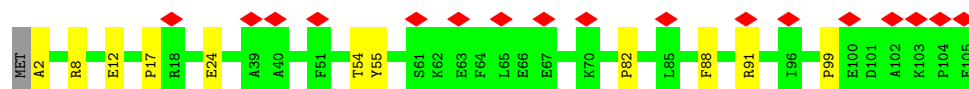
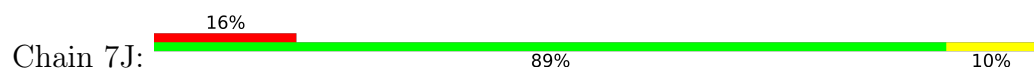
- Molecule 20: Cytochrome c oxidase subunit



- Molecule 20: Cytochrome c oxidase subunit



- Molecule 20: Cytochrome c oxidase subunit



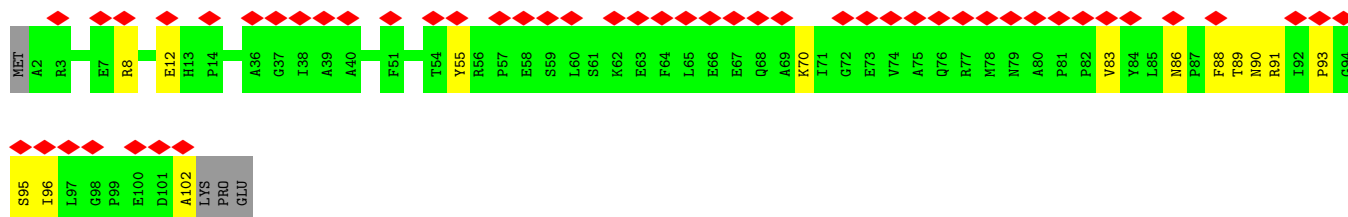
- Molecule 20: Cytochrome c oxidase subunit

Chain 8J:  91% 8%



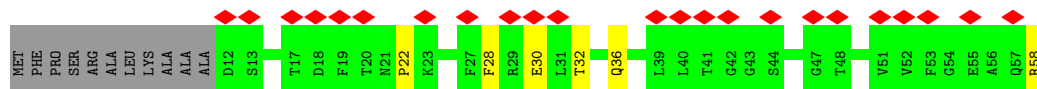
- Molecule 20: Cytochrome c oxidase subunit

Chain 9J:  48% 83% 13%



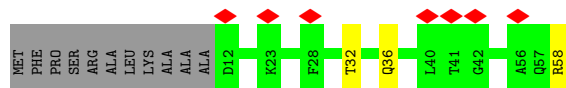
- Molecule 21: Cox7a

Chain 2K:  40% 71% 10% 19%



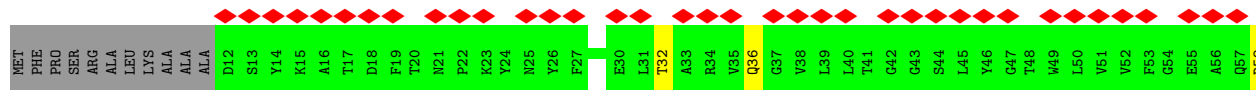
- Molecule 21: Cox7a

Chain 3K:  12% 76% 5% 19%



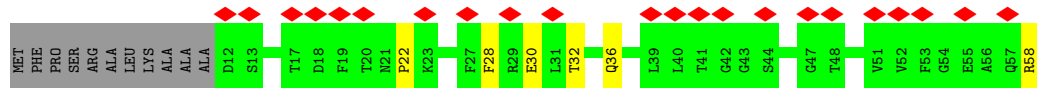
- Molecule 21: Cox7a

Chain 4K:  64% 76% 5% 19%



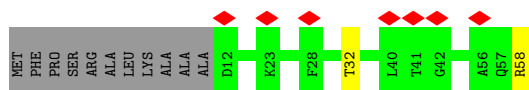
- Molecule 21: Cox7a

Chain 7K:  38% 71% 10% 19%

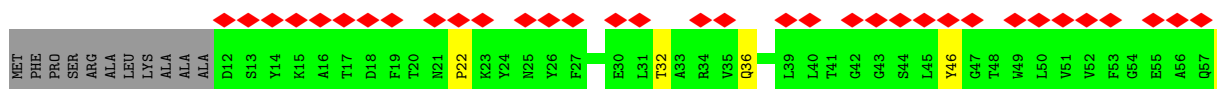
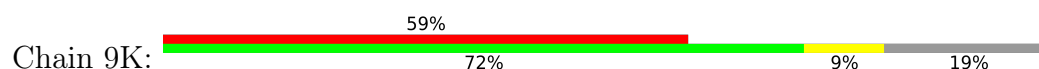


- Molecule 21: Cox7a

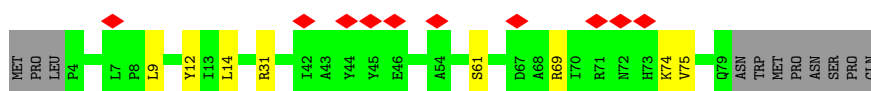
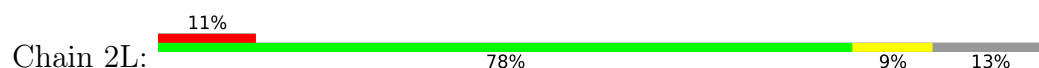
Chain 8K:  12% 78% 19%



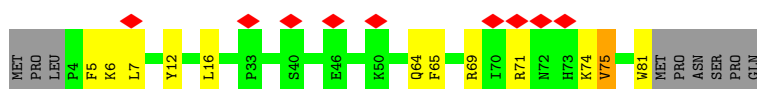
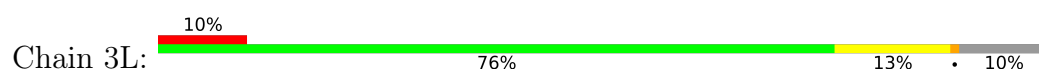
● Molecule 21: Cox7a



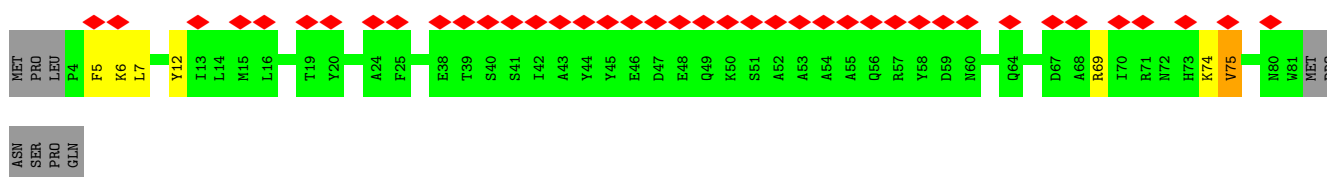
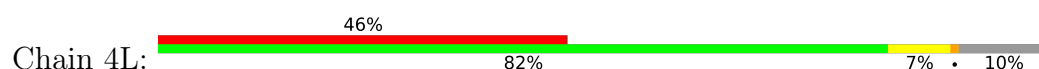
● Molecule 22: CoxIn



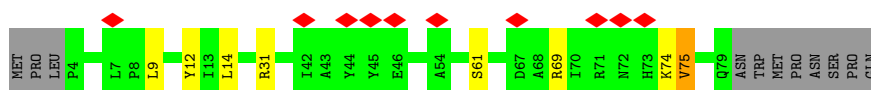
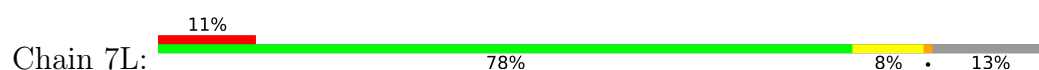
● Molecule 22: CoxIn



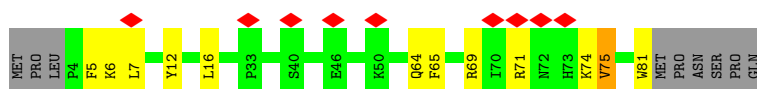
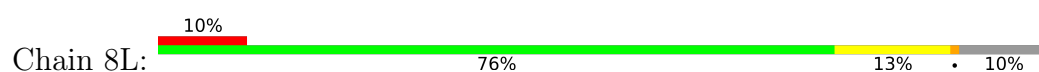
● Molecule 22: CoxIn



● Molecule 22: CoxIn

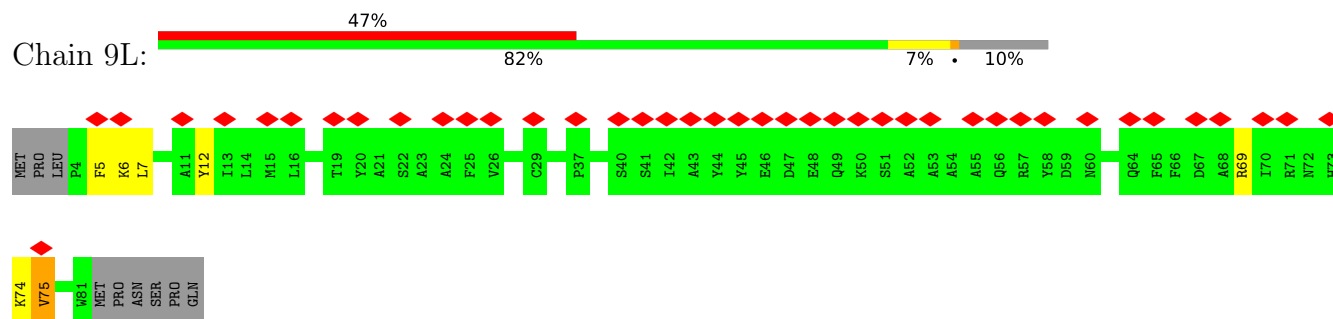


● Molecule 22: CoxIn



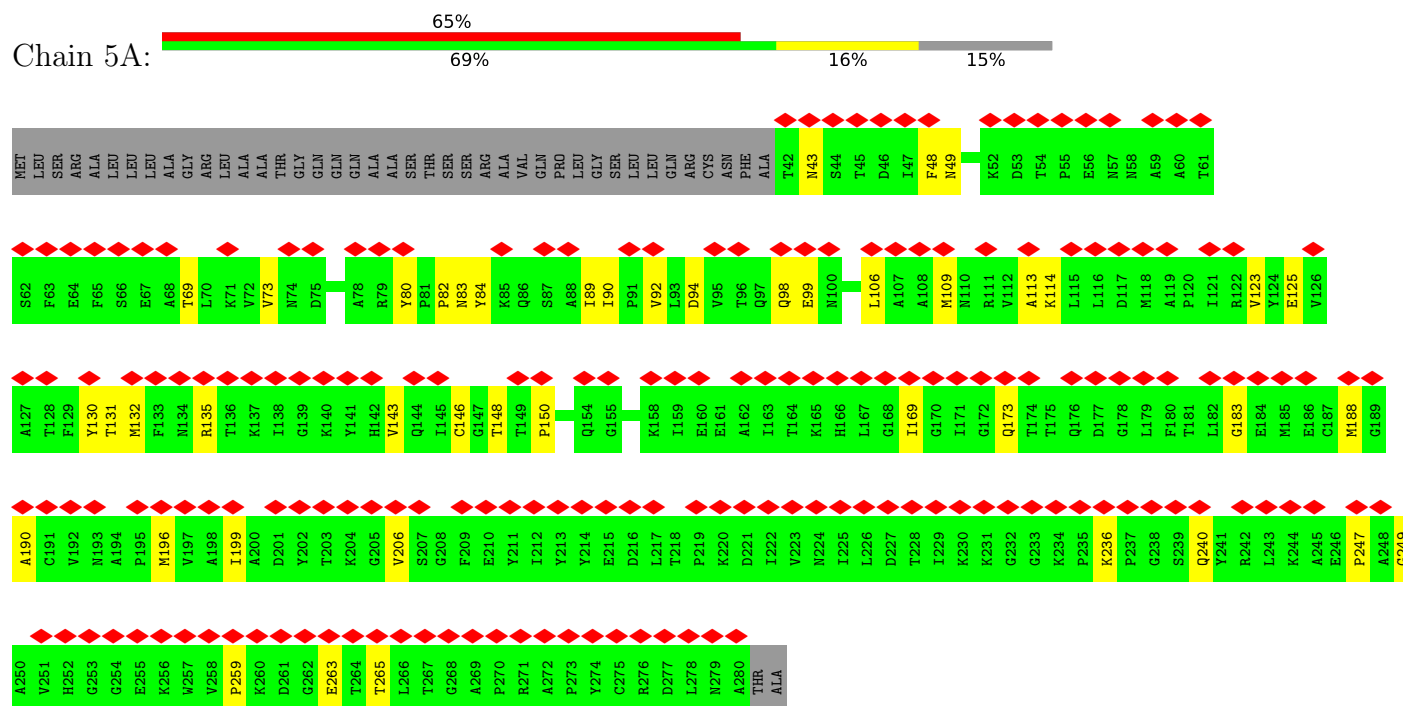
- Molecule 22: CoxIn

Chain 9L:



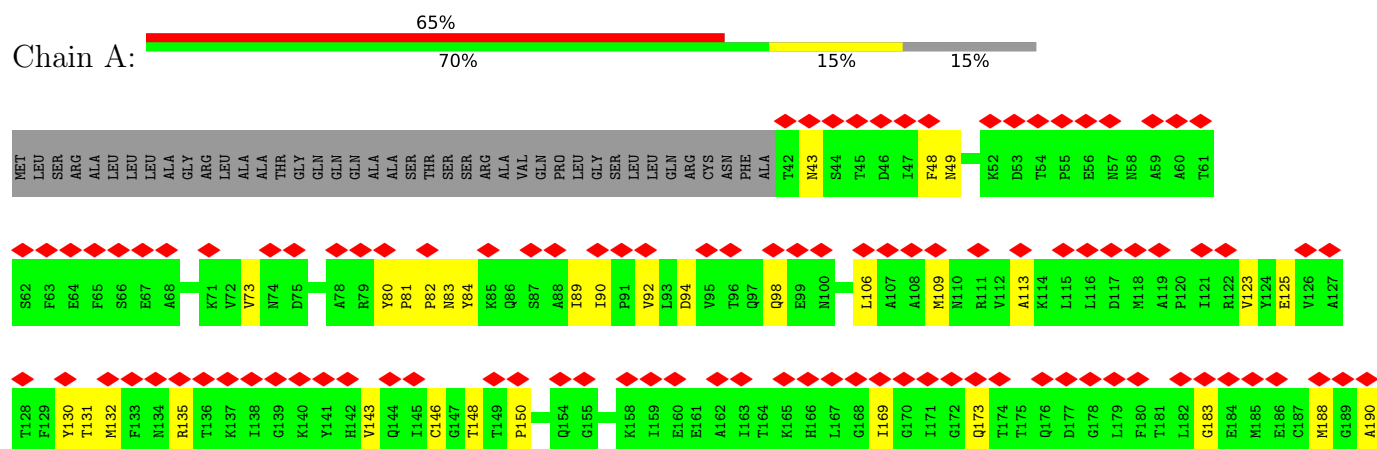
- Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

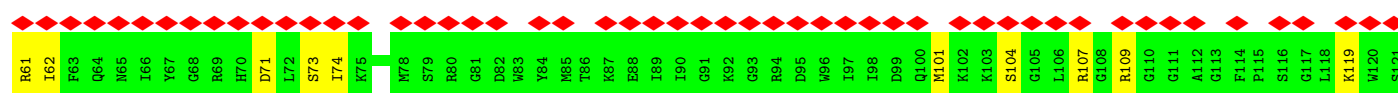
Chain 5A:

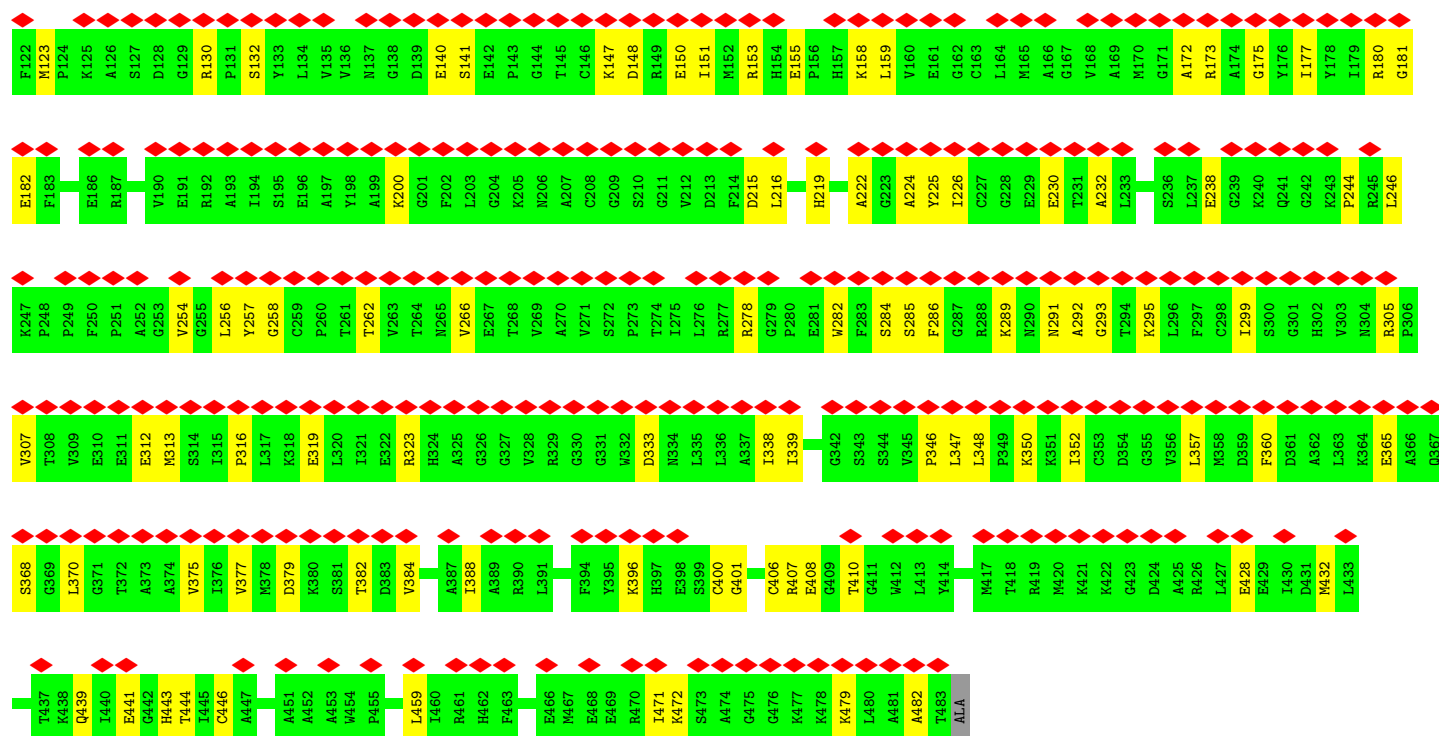


- Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain A:

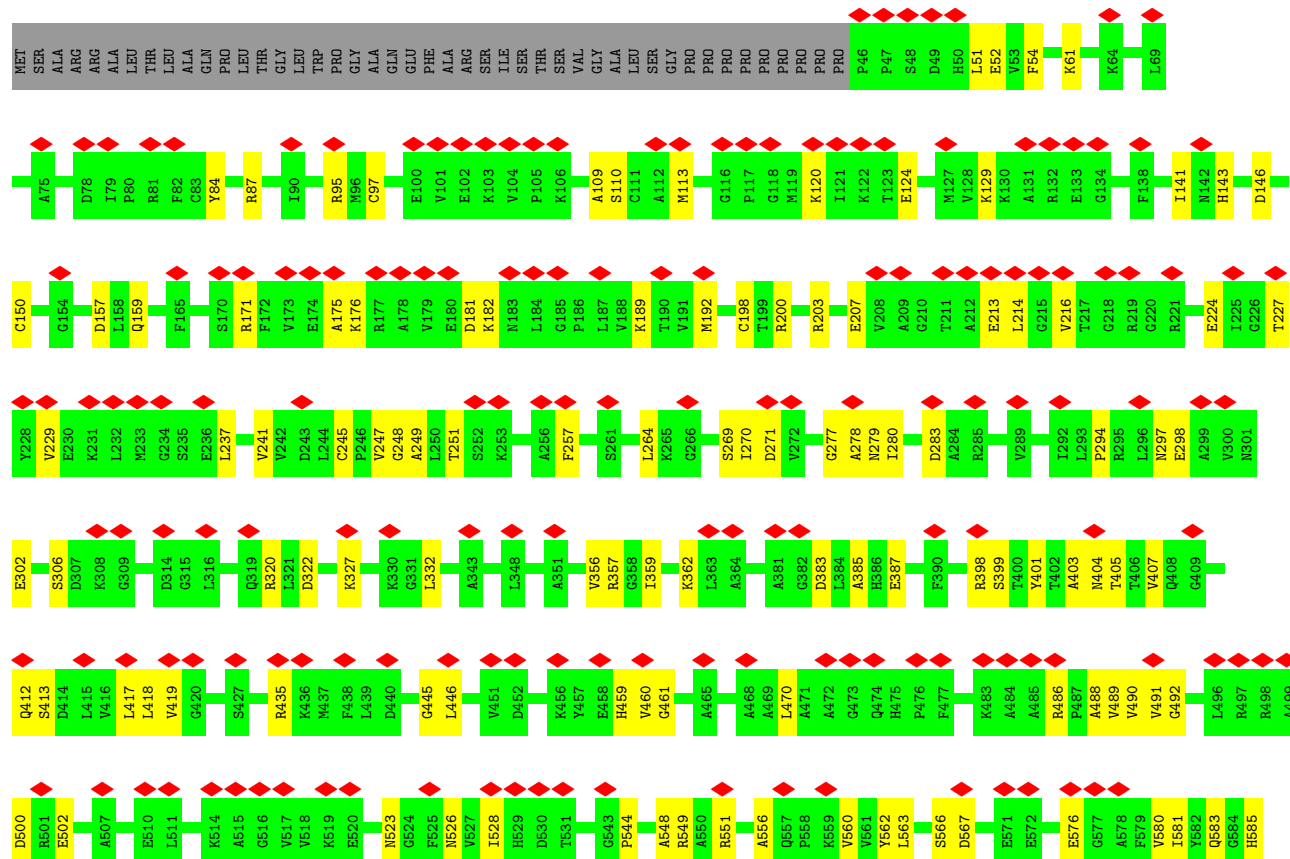


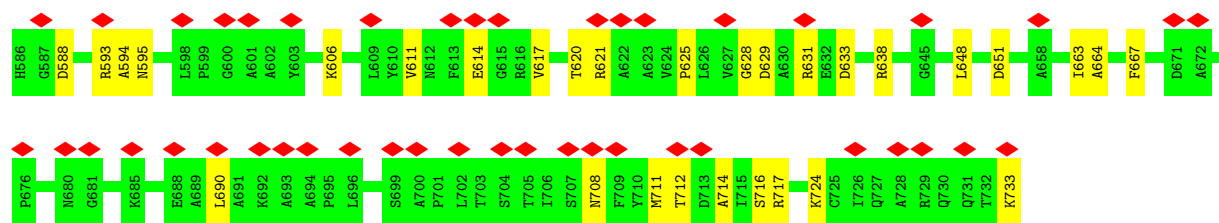




• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

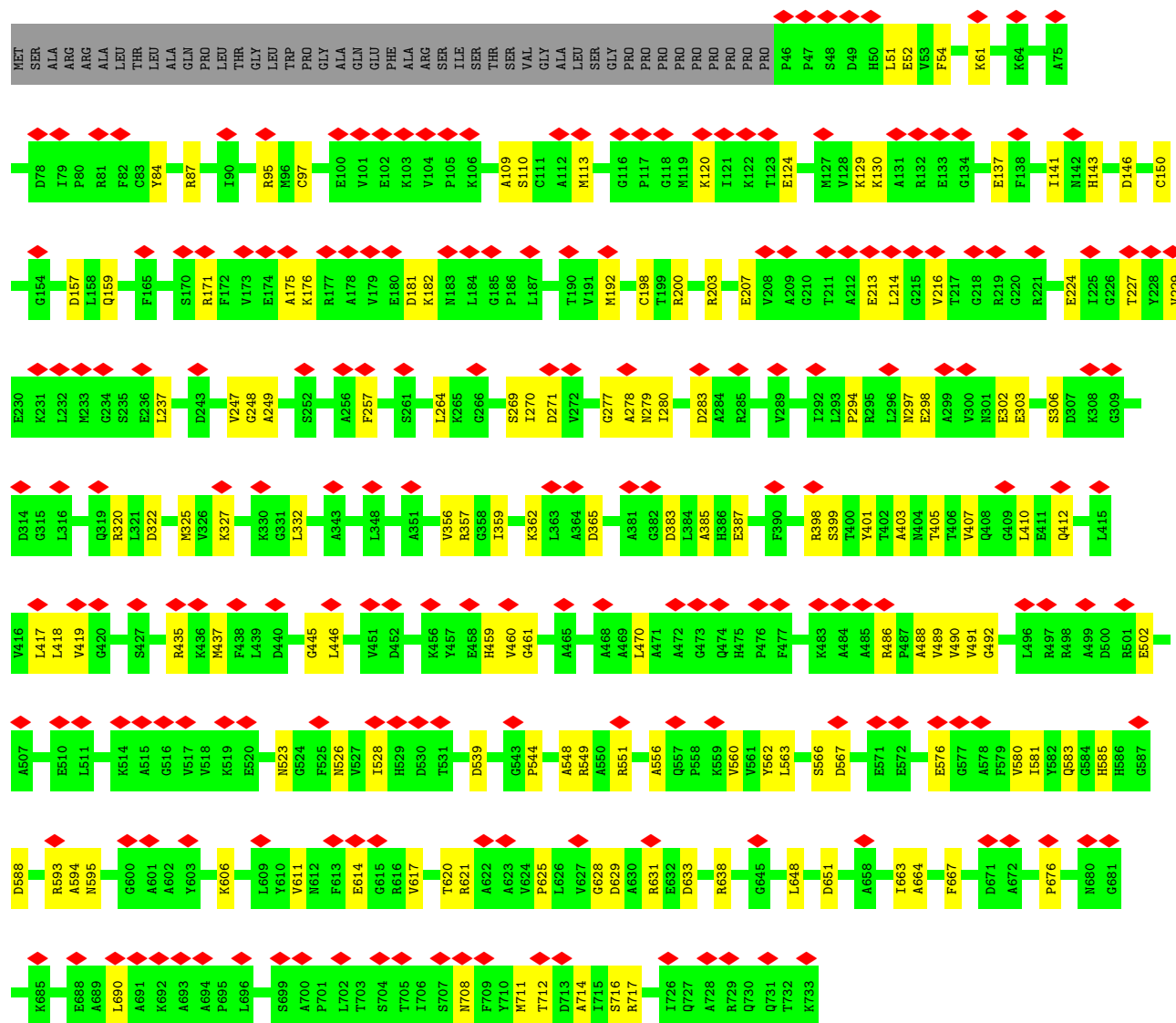
Chain 5C: 29% 74% 20% 6%





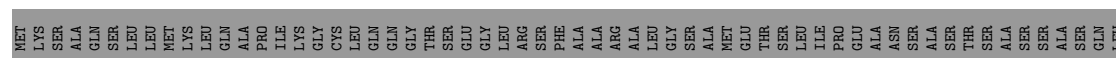
• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

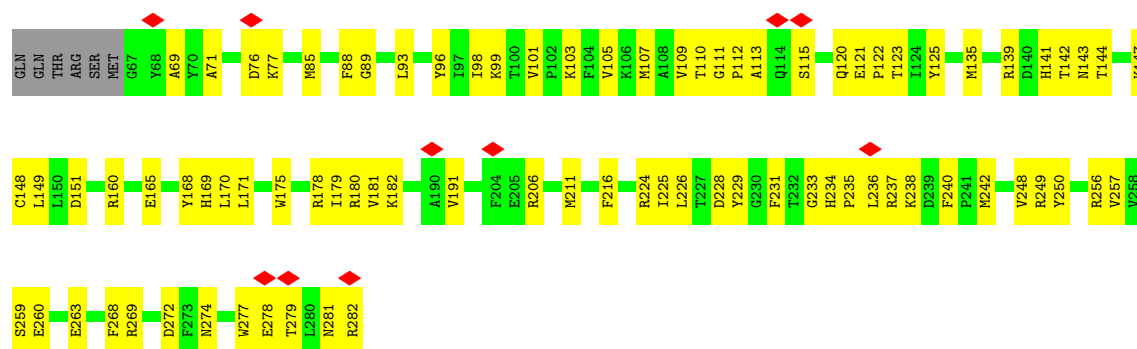
Chain C: 28% 74% 20% 6%



• Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

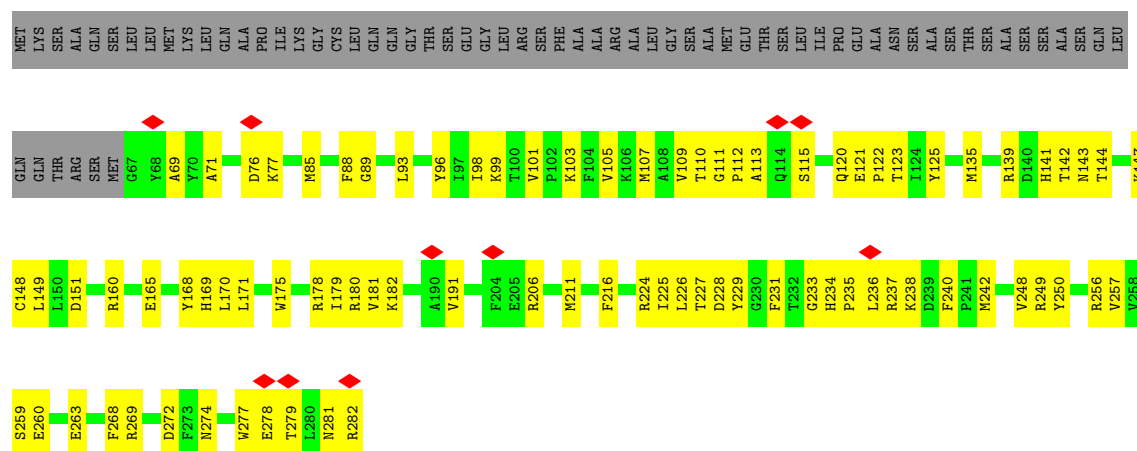
Chain 5D: 47% 29% 23%





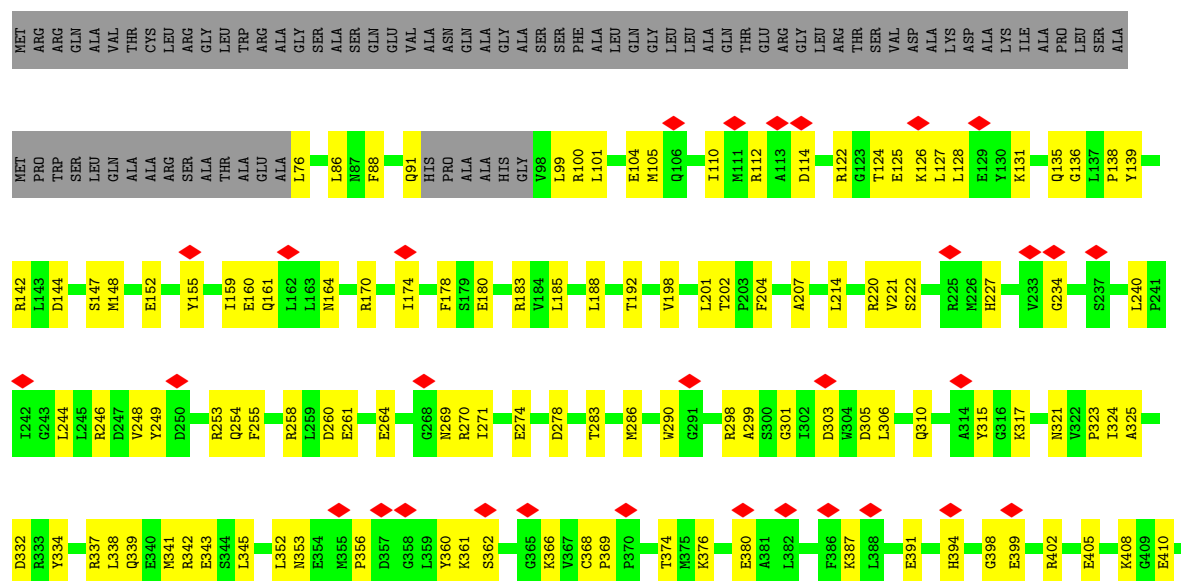
- Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

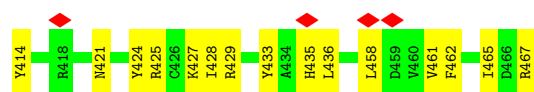
Chain D: 47% 30% 23%



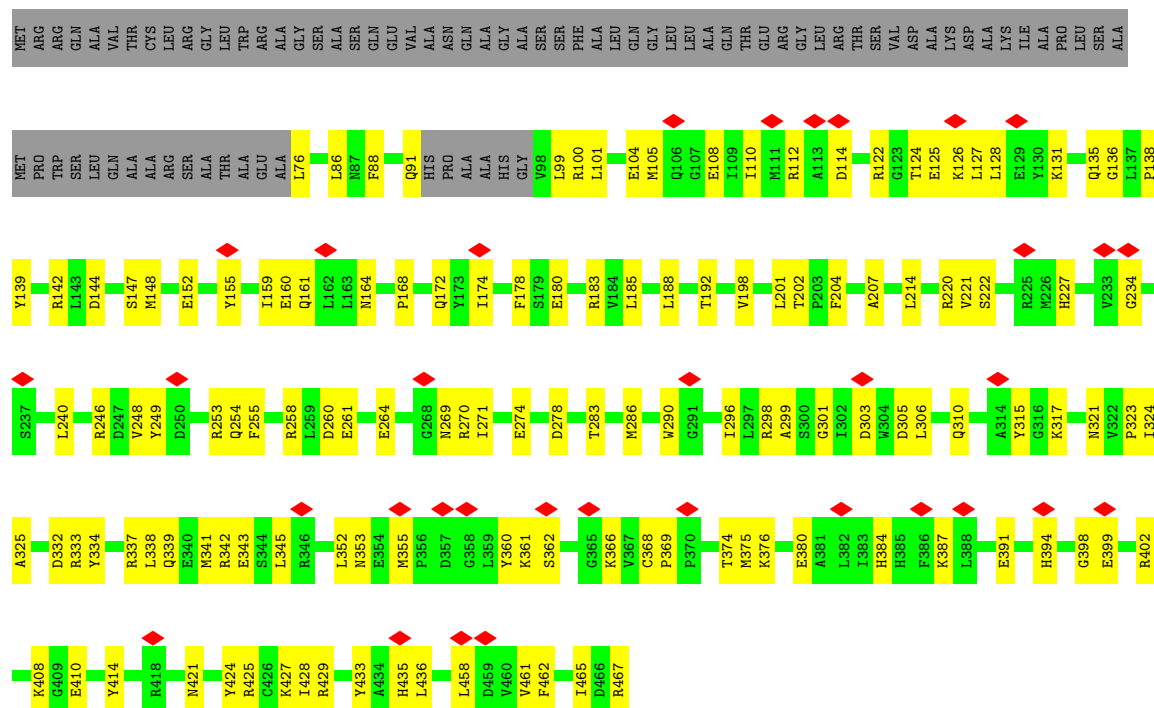
- Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain 5E: 7% 55% 28% 17%

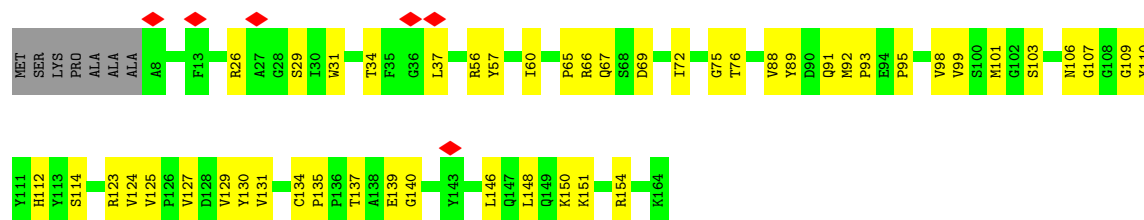




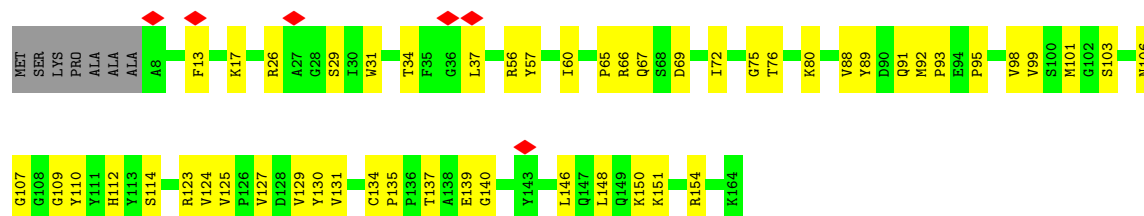
- Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit



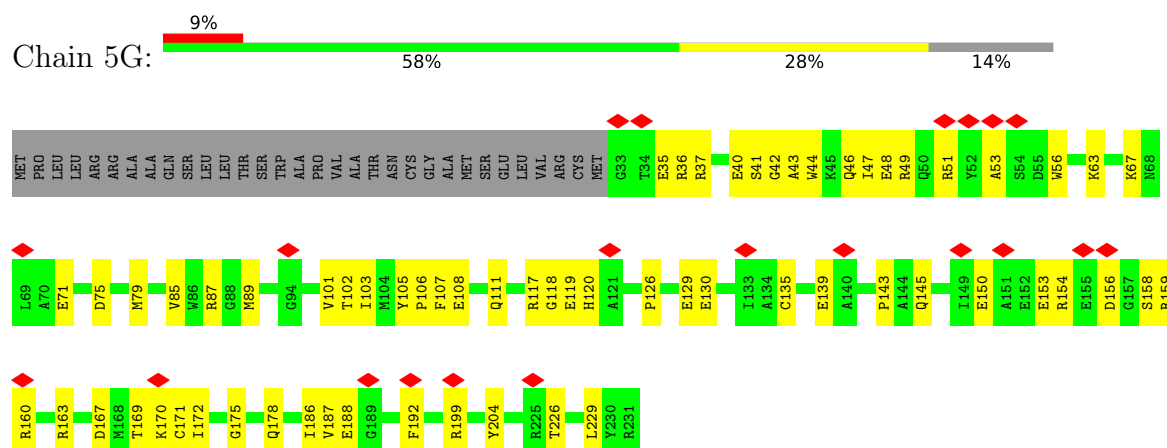
- Molecule 28: NADH:ubiquinone oxidoreductase subunit 10



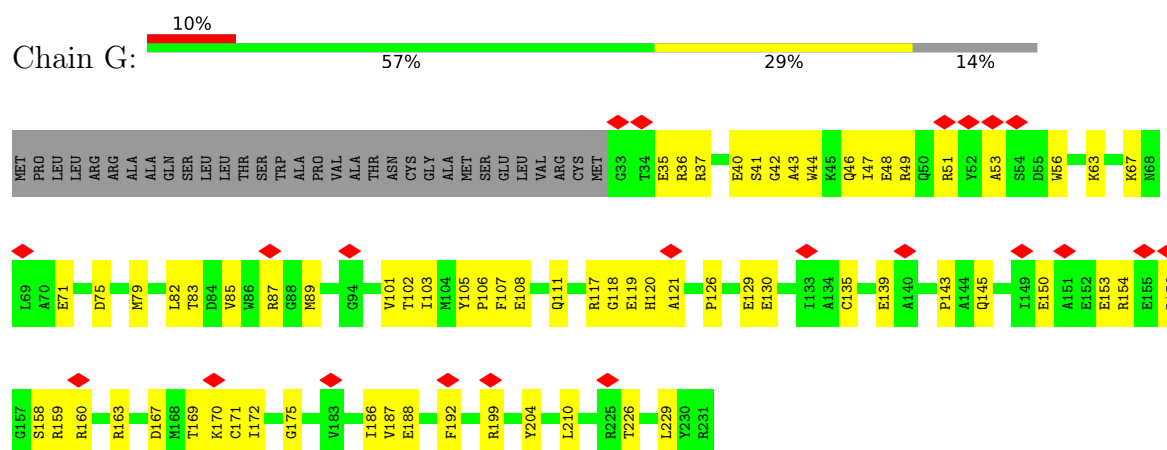
- Molecule 28: NADH:ubiquinone oxidoreductase subunit 10



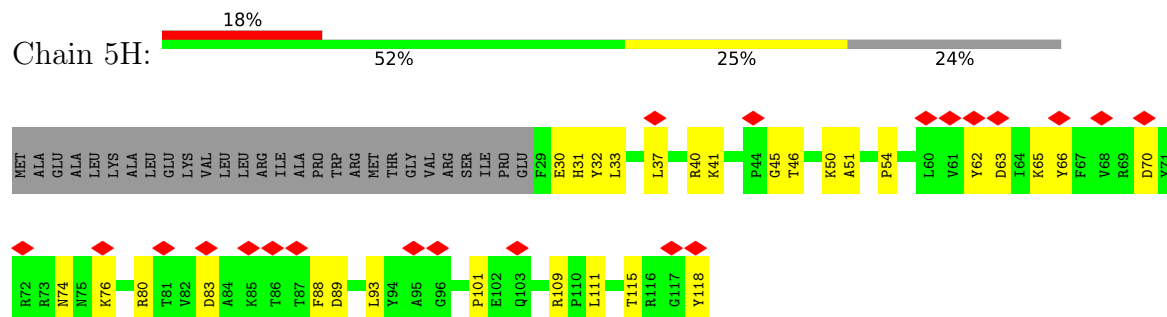
- Molecule 29: NADH:ubiquinone oxidoreductase subunit 8



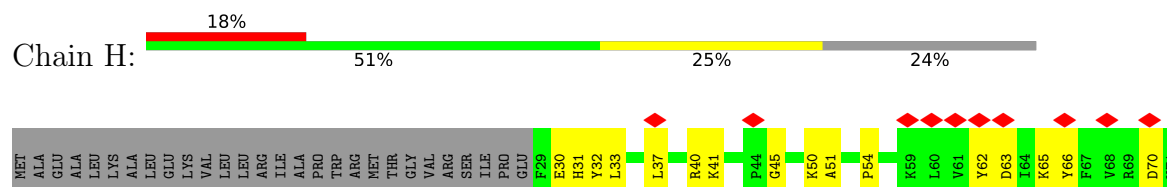
- Molecule 29: NADH:ubiquinone oxidoreductase subunit 8

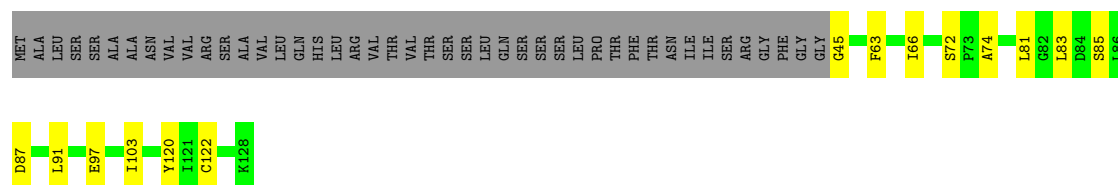


- Molecule 30: B14.5a

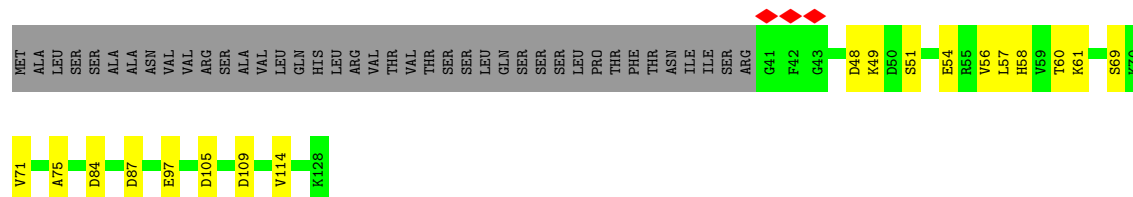


- Molecule 30: B14.5a

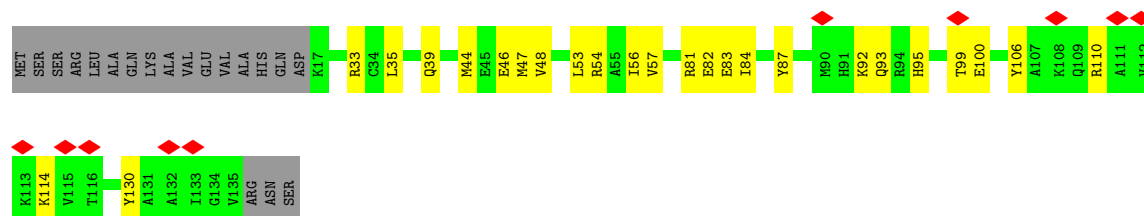




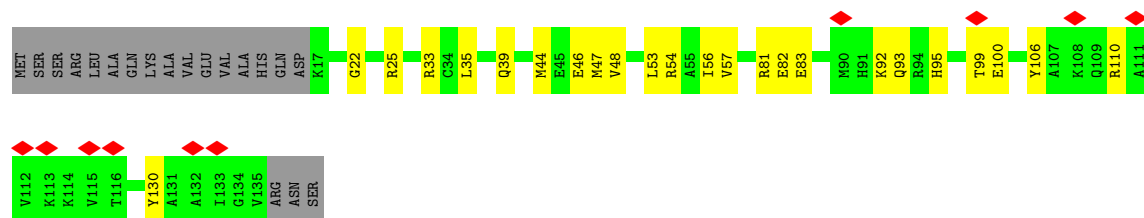
- Molecule 32: Acyl carrier protein



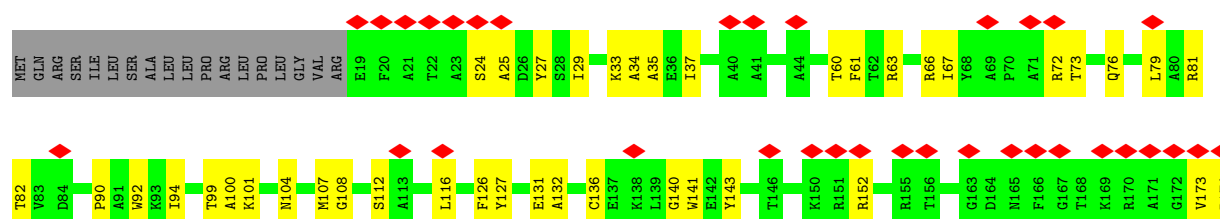
- Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

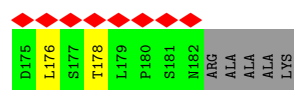


- Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

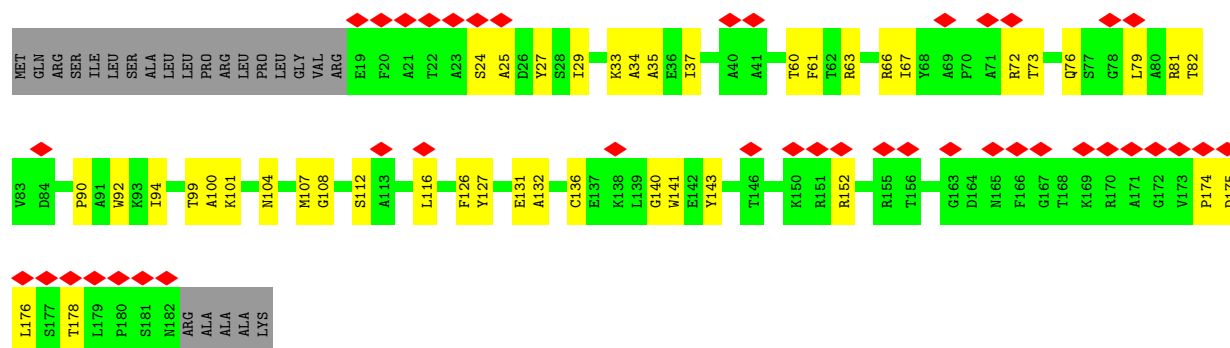


- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

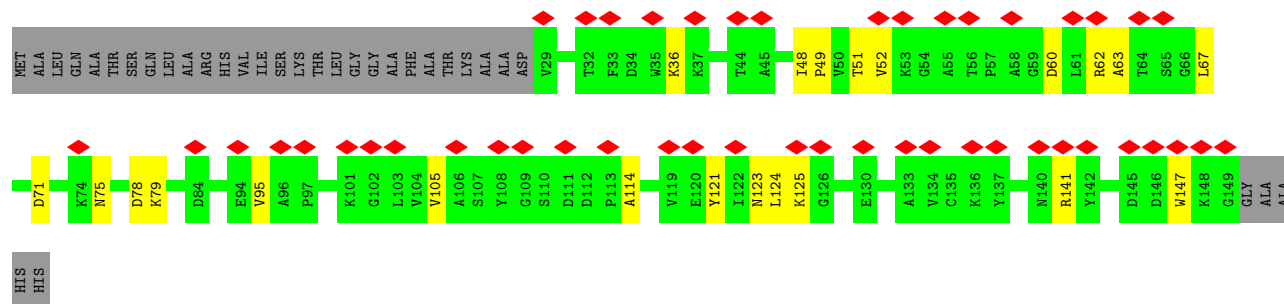




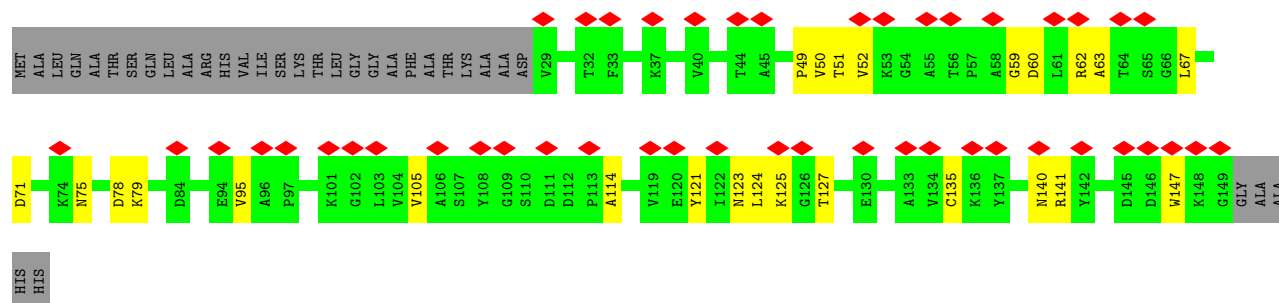
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



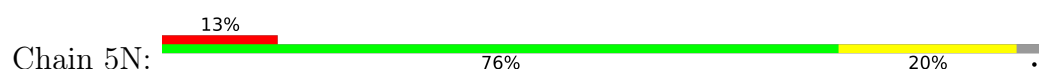
- Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

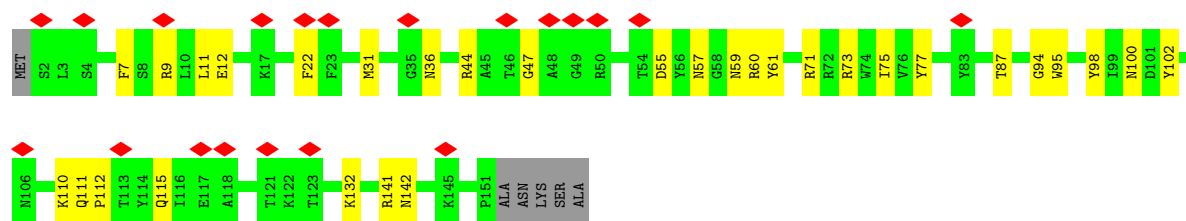


- Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

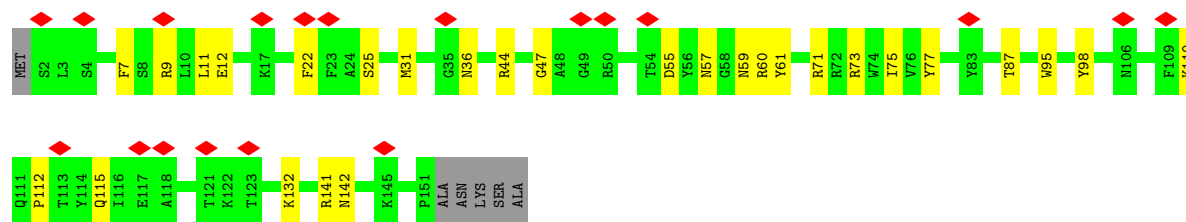
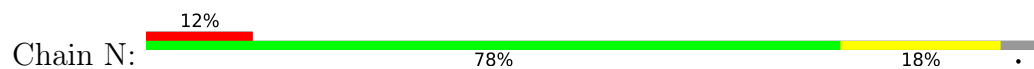


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

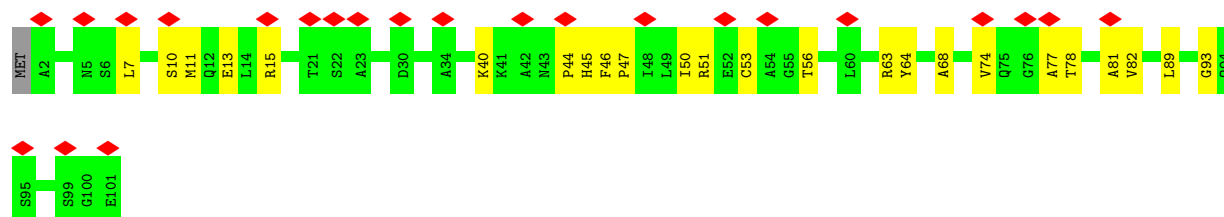
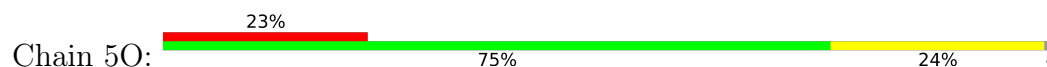




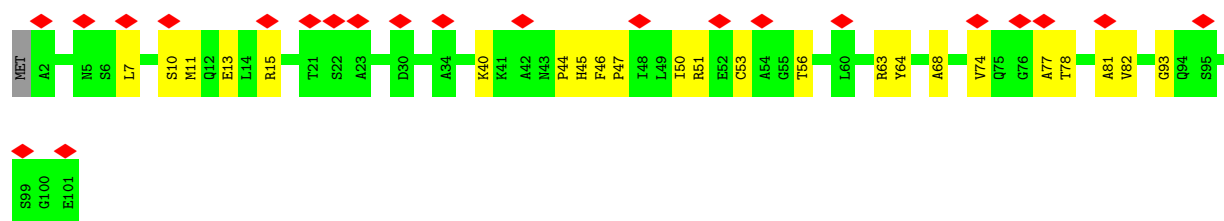
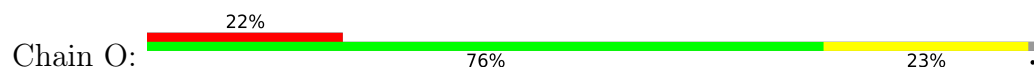
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



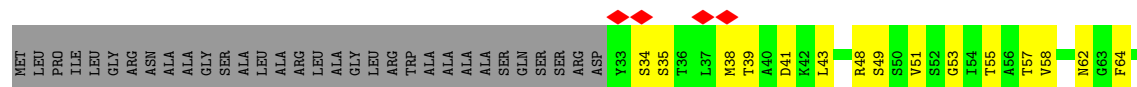
- Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit

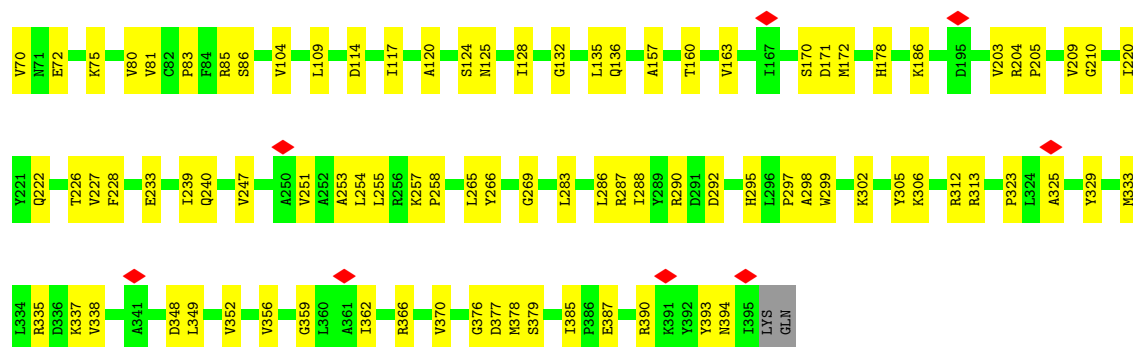


- Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit



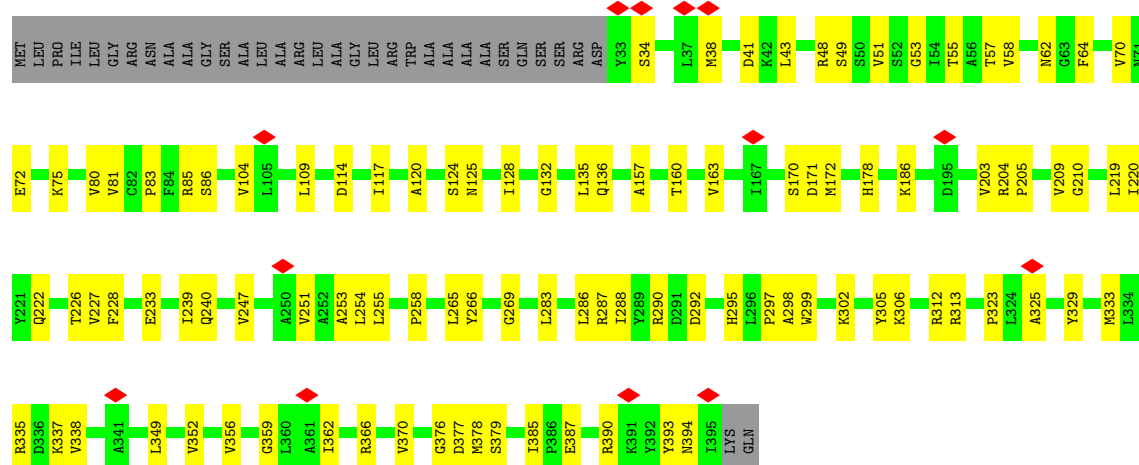
- Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit





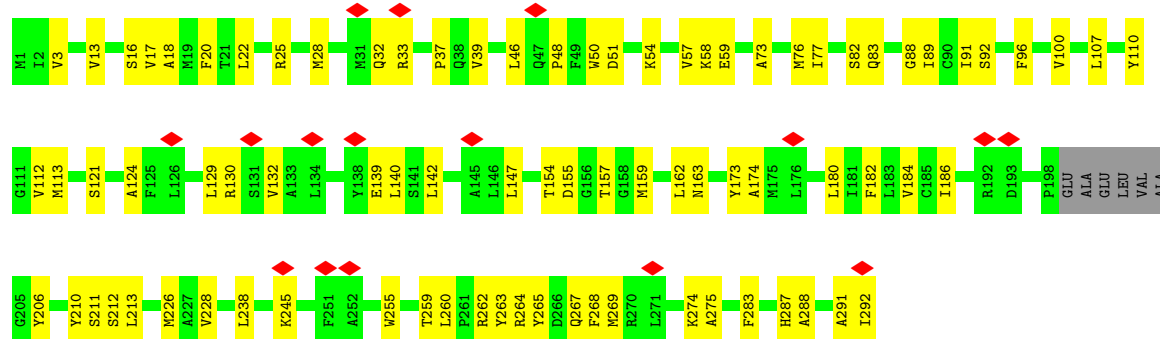
- Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P: 66% 25% 9%



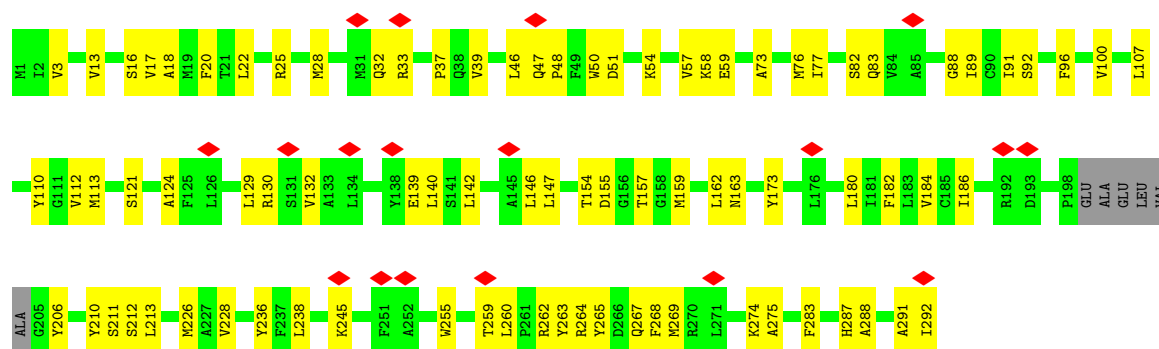
- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

Chain 5Q: 5% 70% 28%

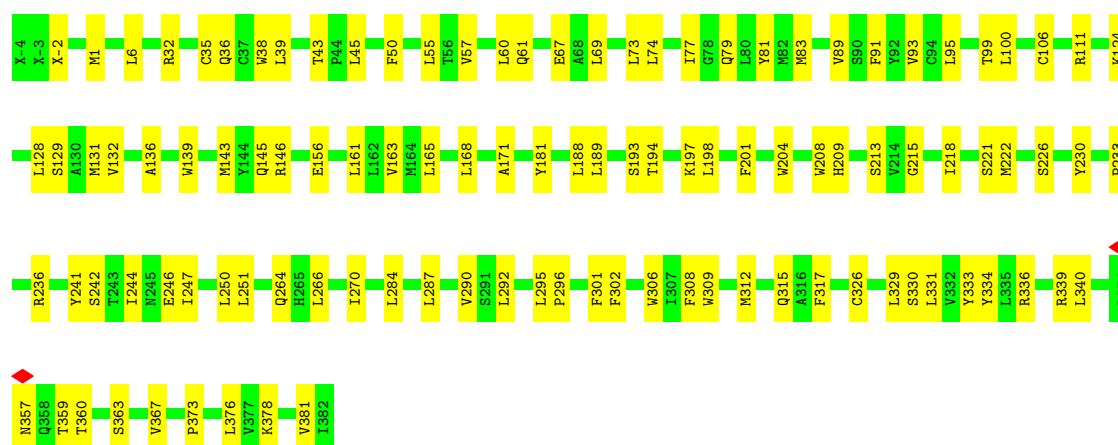


- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

Chain Q: 6% 69% 29%



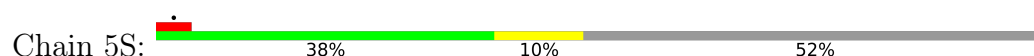
• Molecule 40: NADH-ubiquinone oxidoreductase chain 2



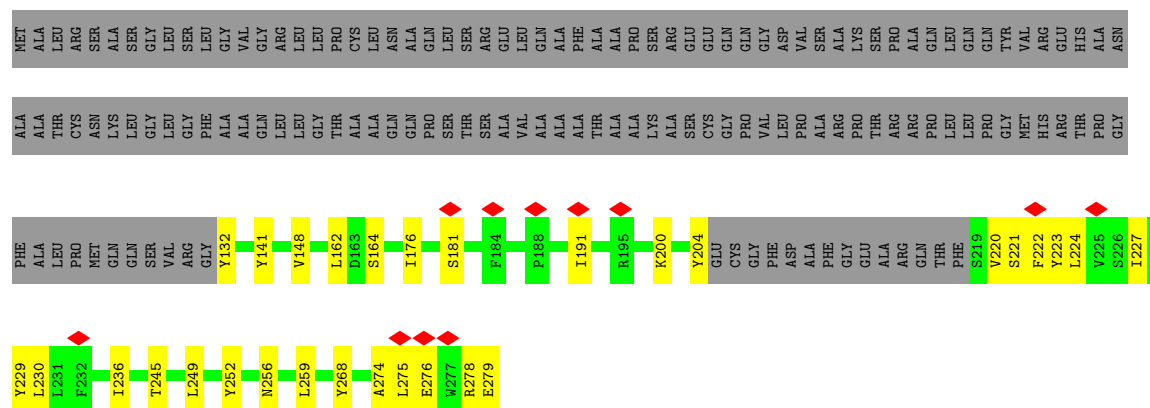
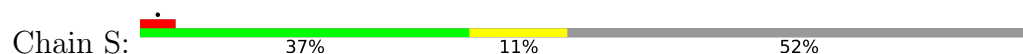
• Molecule 40: NADH-ubiquinone oxidoreductase chain 2



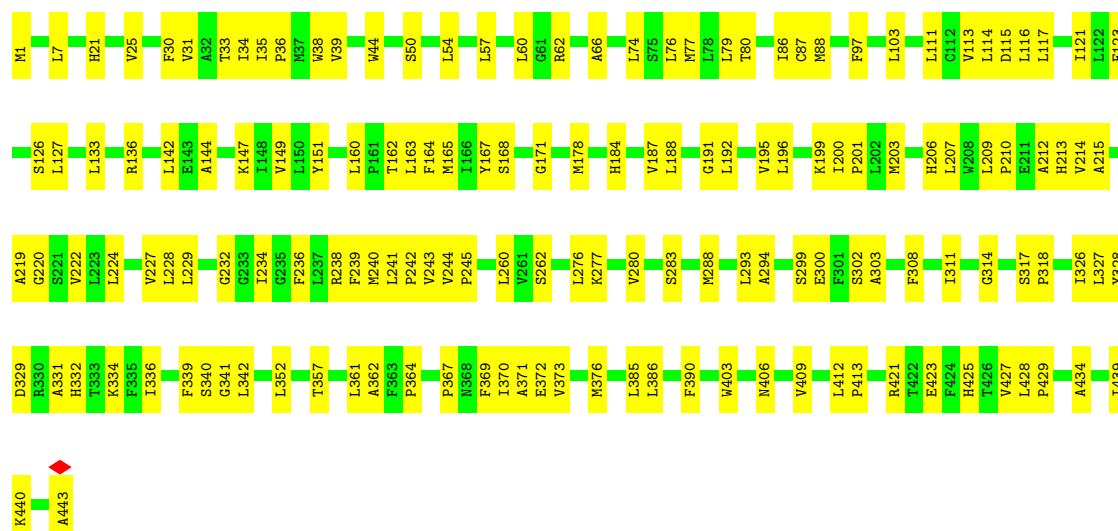
• Molecule 41: NADH-ubiquinone oxidoreductase chain 3



- Molecule 41: NADH-ubiquinone oxidoreductase chain 3

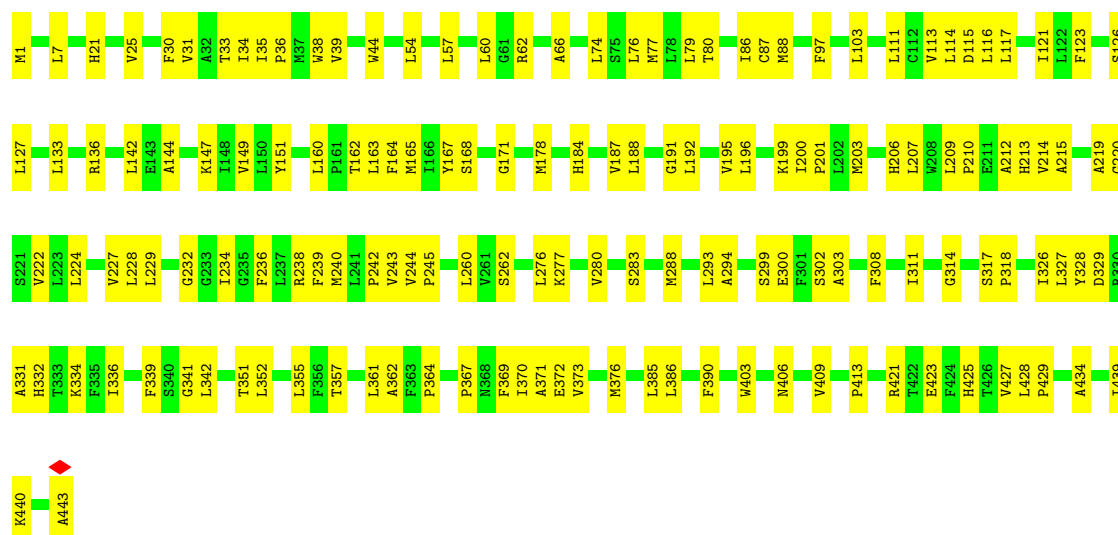


- Molecule 42: NADH-ubiquinone oxidoreductase chain 4



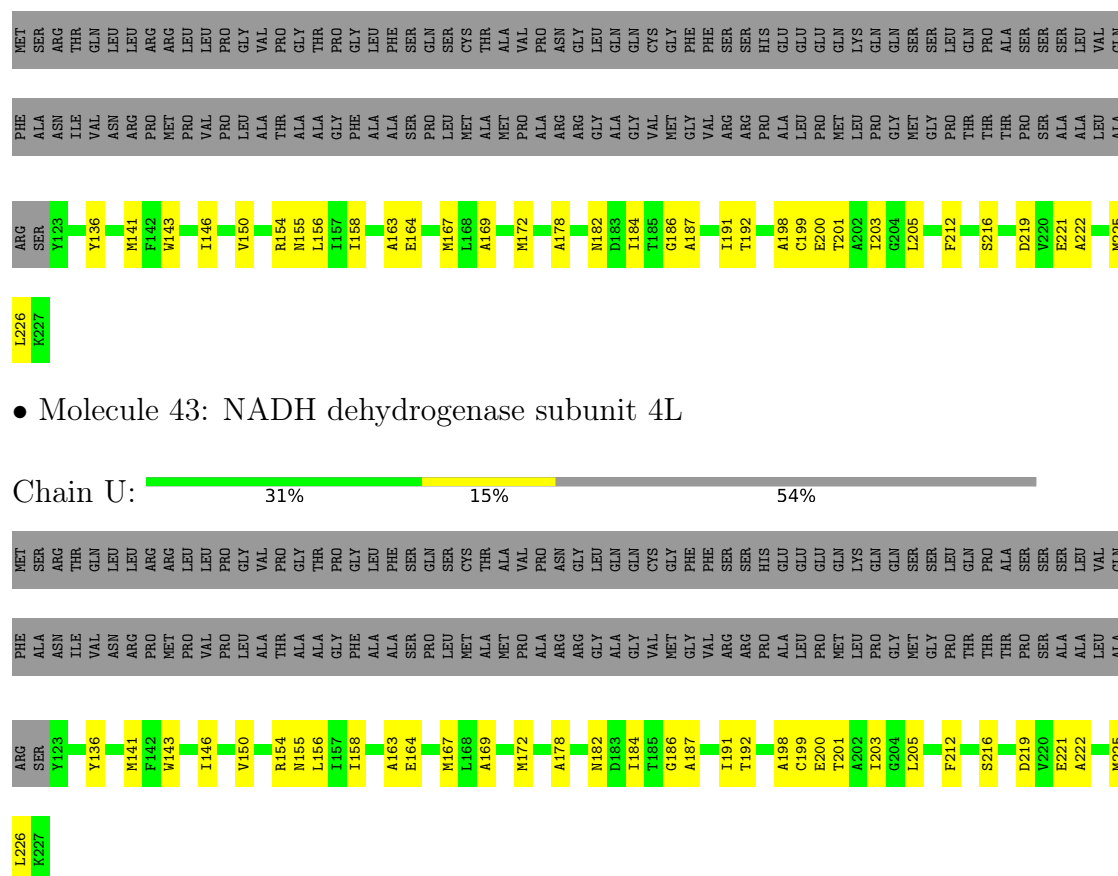
- Molecule 42: NADH-ubiquinone oxidoreductase chain 4

Chain T:  66% 34%



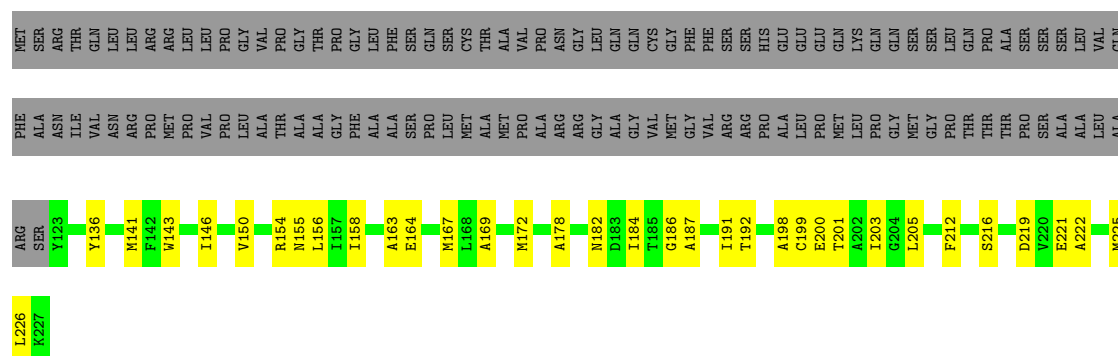
- Molecule 43: NADH dehydrogenase subunit 4L

Chain 5U:  31% 15% 54%



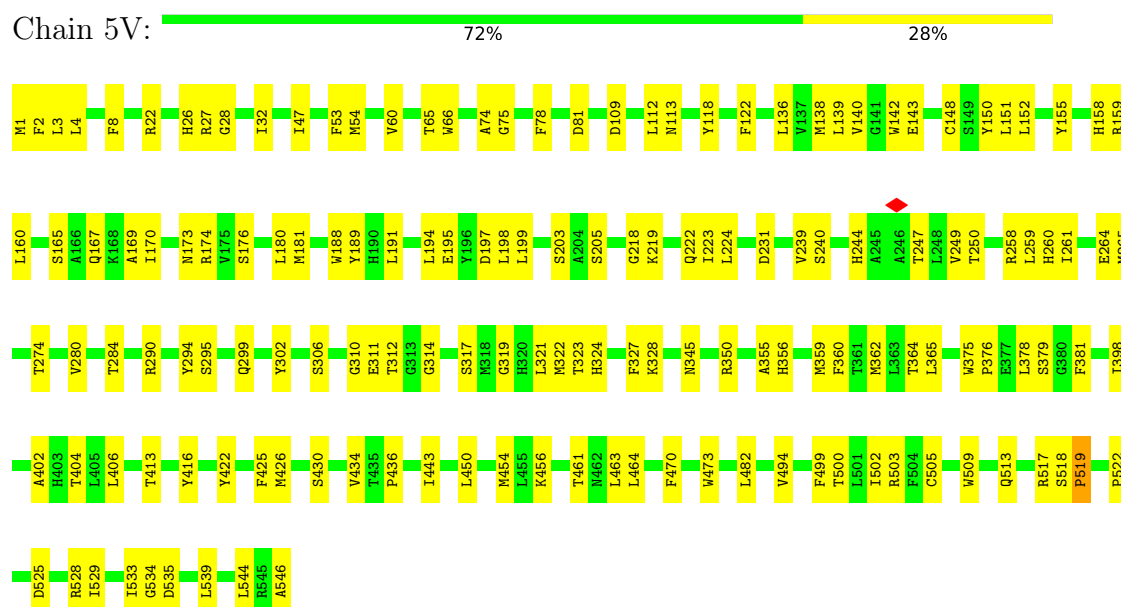
- Molecule 43: NADH dehydrogenase subunit 4L

Chain U:  31% 15% 54%



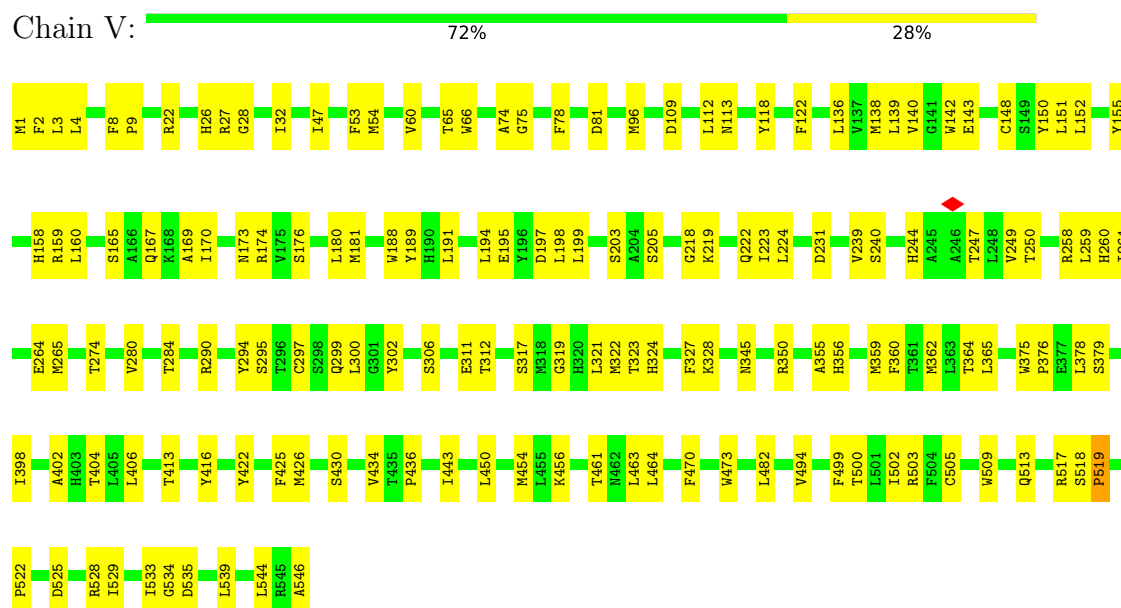
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain 5V:



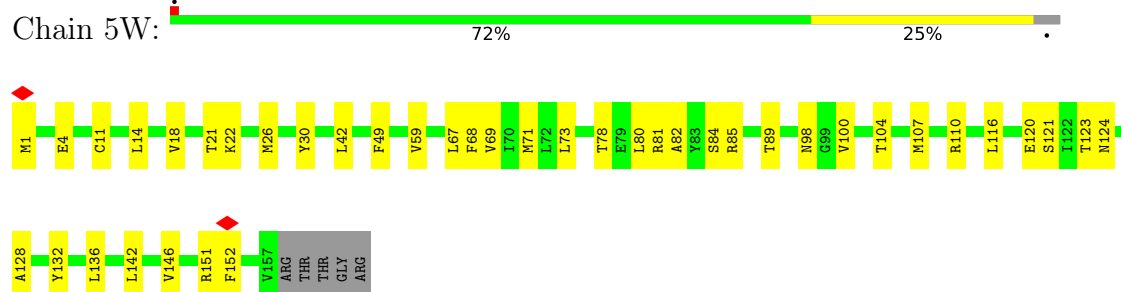
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain V:



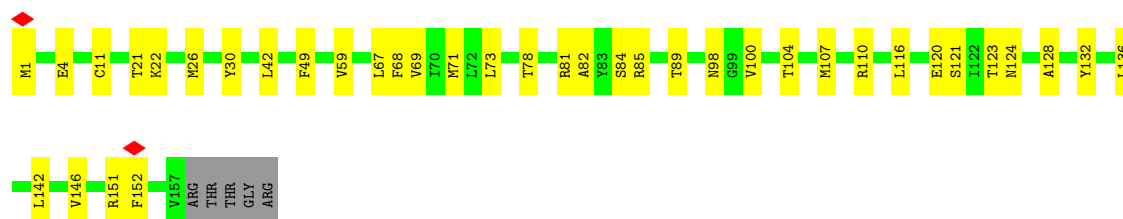
- Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain 5W:



- Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain W:  73% 23%



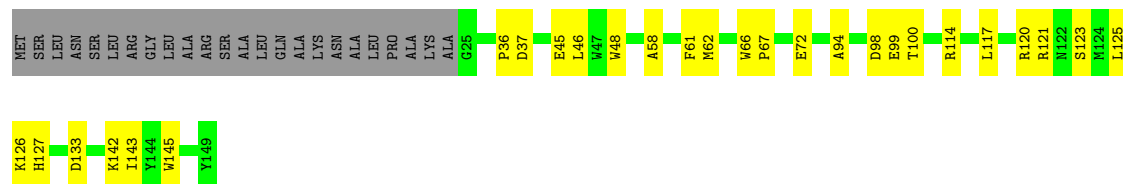
- Molecule 46: ASHI

Chain 5X:  64% 19% 16%



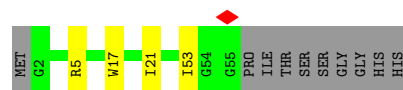
- Molecule 46: ASHI

Chain X:  66% 18% 16%



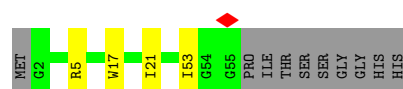
- Molecule 47: P9

Chain 5Y:  78% 6% 16%



- Molecule 47: P9

Chain Y:  78% 6% 16%

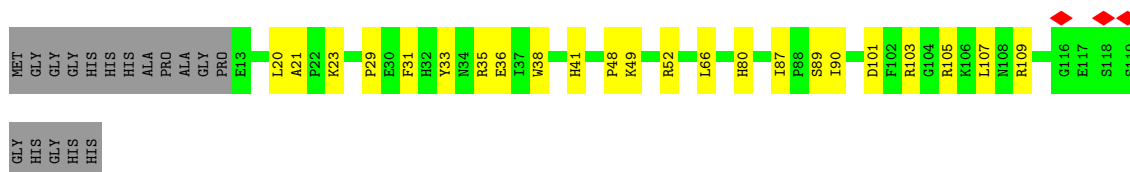


- Molecule 48: KFYI

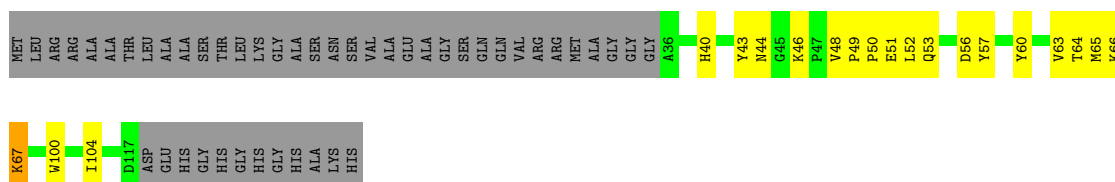
Chain 5Z:  71% 15% 14%



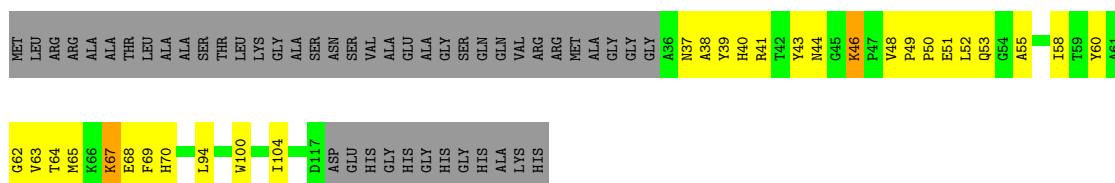
• Molecule 48: KFYI



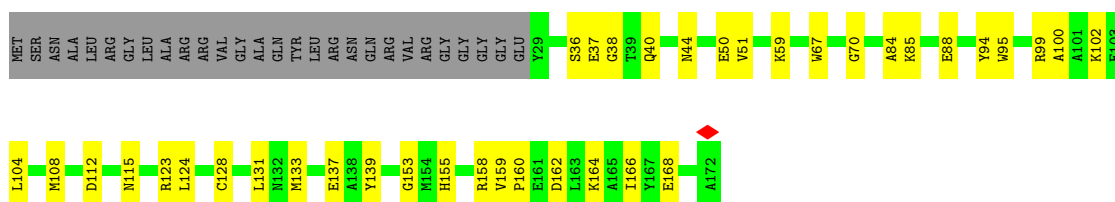
• Molecule 49: AGGG



• Molecule 49: AGGG



• Molecule 50: ESSS

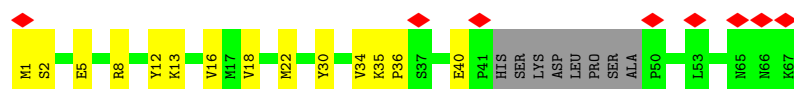


• Molecule 50: ESSS

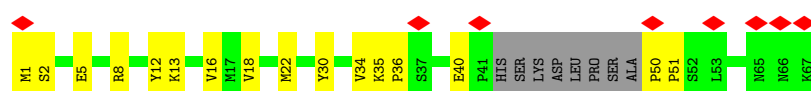




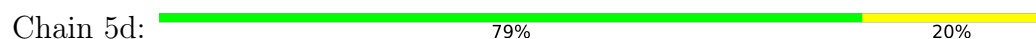
- Molecule 51: B9



- Molecule 51: B9



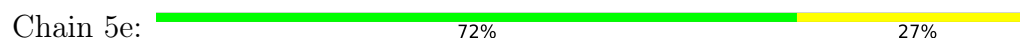
- Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit



- Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit



- Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

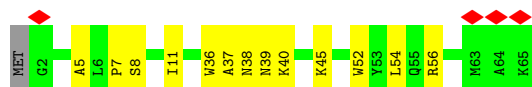
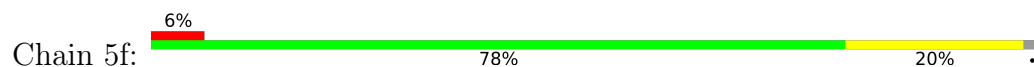


- Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

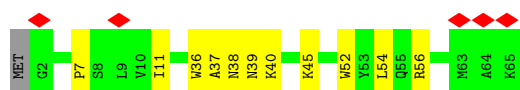
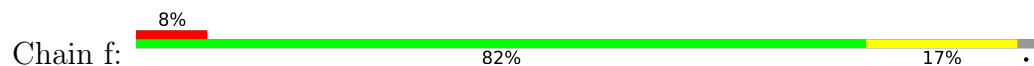




- Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit



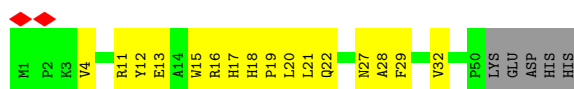
- Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit



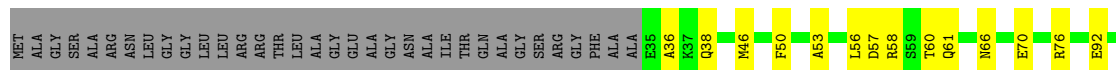
- Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit



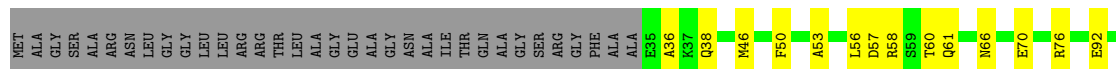
- Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit



- Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

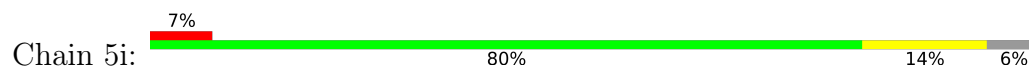


- Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

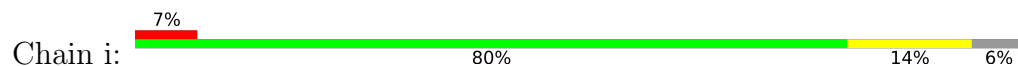




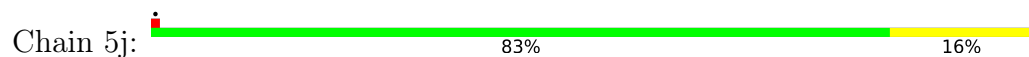
- Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like



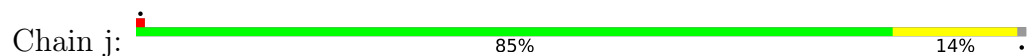
- Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like



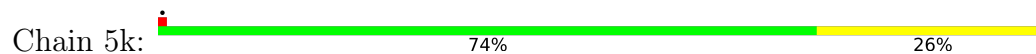
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



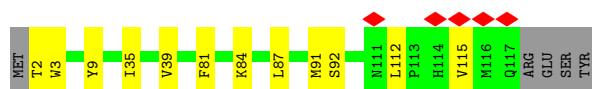
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





- Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain 5l: 86% 10%



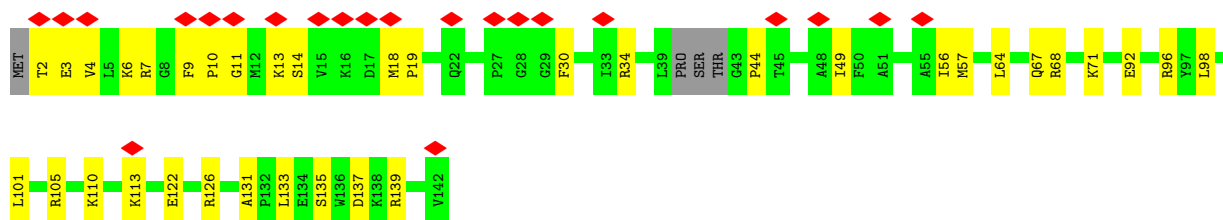
- Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain l: 85% 11%



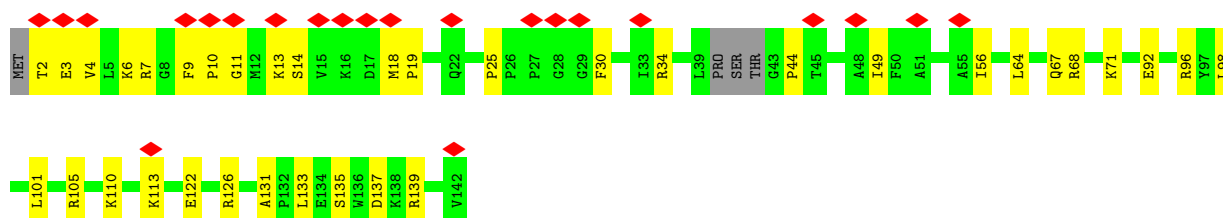
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain 5m: 15% 72% 25%



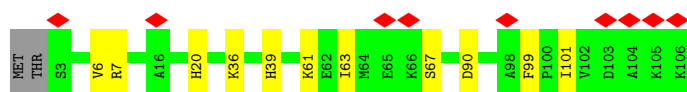
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain m: 15% 72% 25%

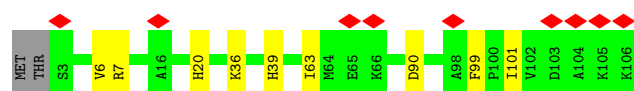
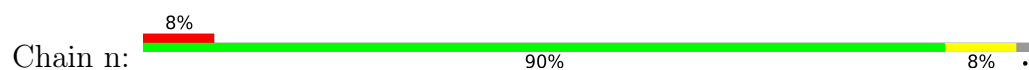


- Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

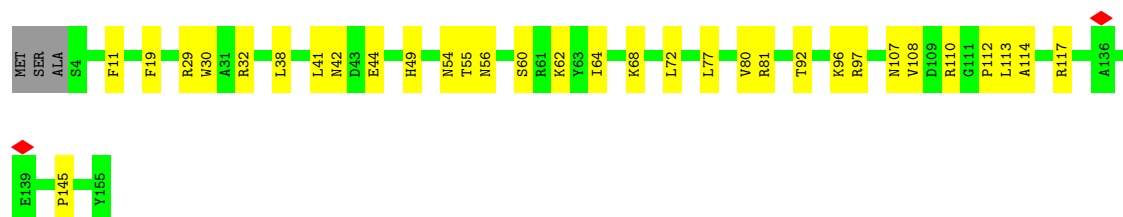
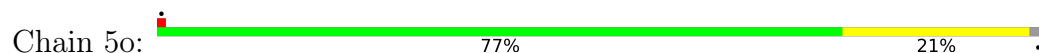
Chain 5n: 8% 88% 10%



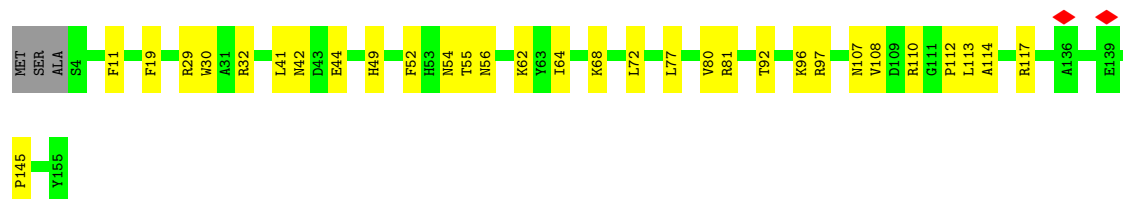
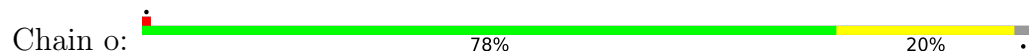
- Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit



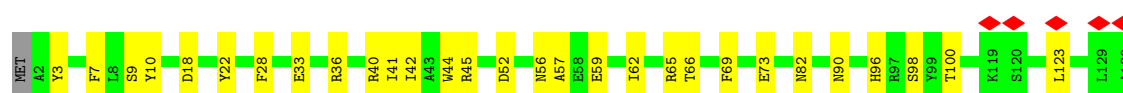
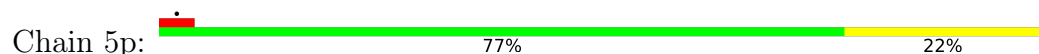
- Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



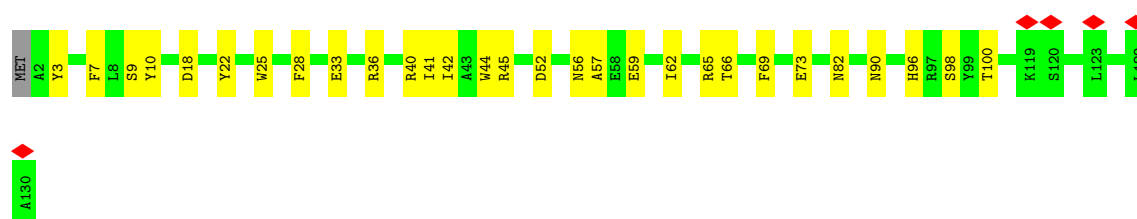
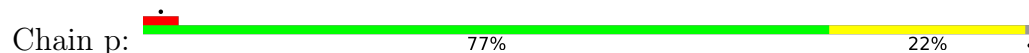
- Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



- Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

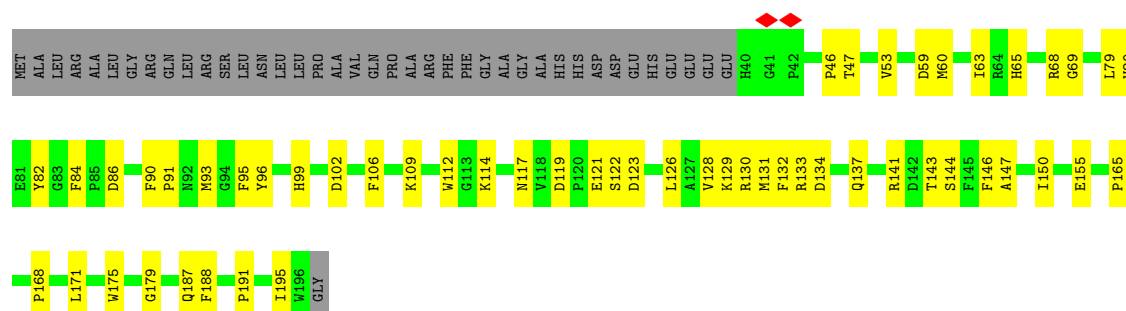


- Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

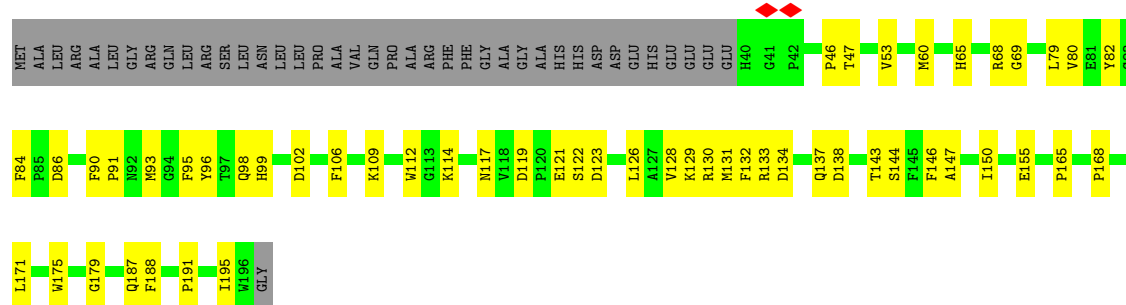


- Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

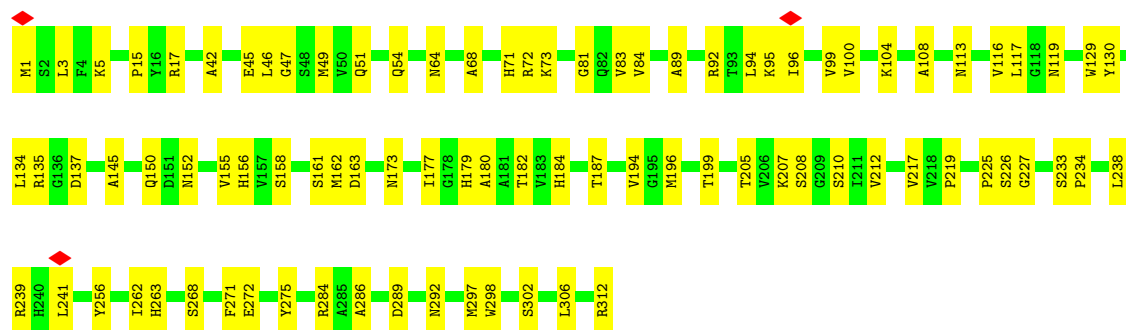




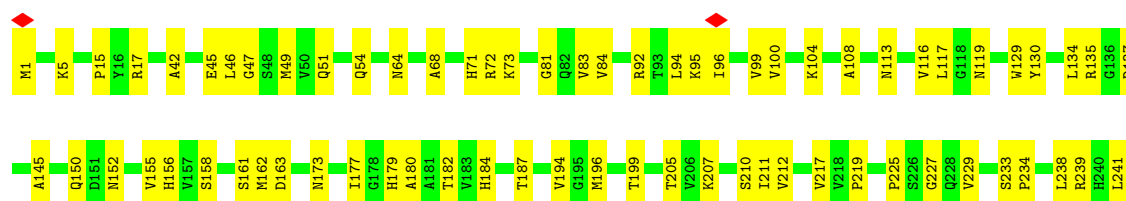
- Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

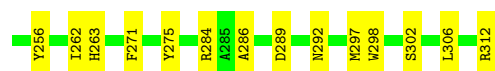


- Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

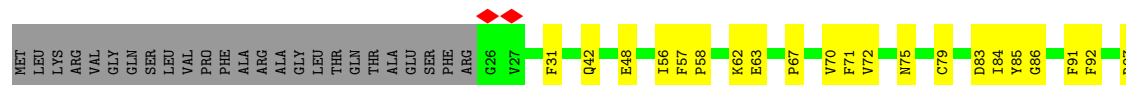


- Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

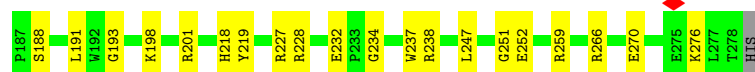
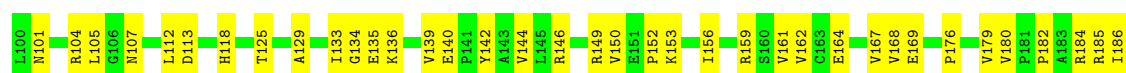




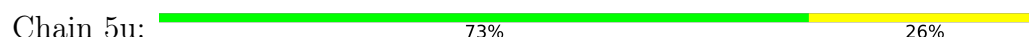
• Molecule 67: CAG2 - CA-like



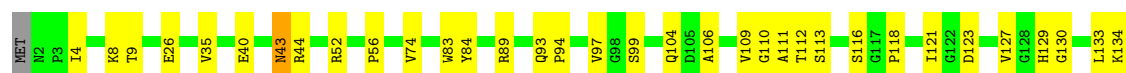
• Molecule 67: CAG2 - CA-like



• Molecule 68: CAG1

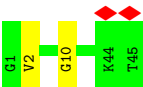


• Molecule 68: CAG1

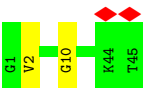




• Molecule 69: P10



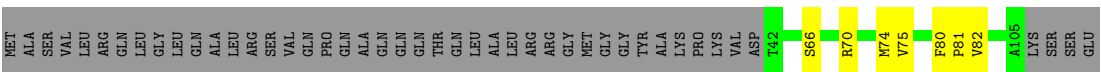
• Molecule 69: P10



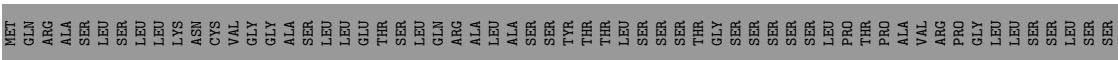
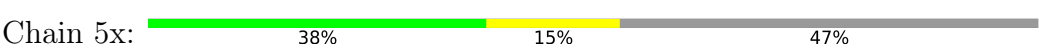
• Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



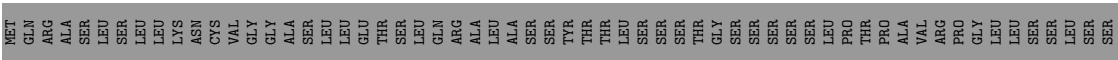
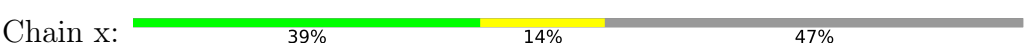
• Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



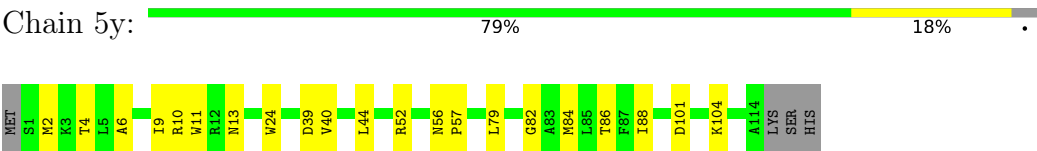
• Molecule 71: NUOP8



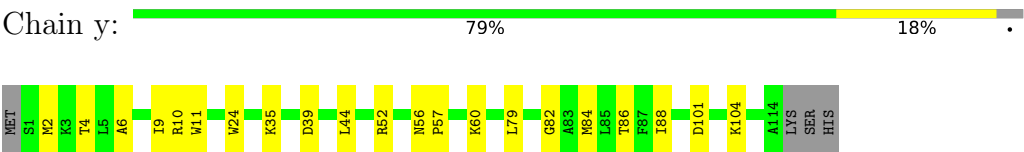
• Molecule 71: NUOP8



● Molecule 72: NUOP7



● Molecule 72: NUOP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	14488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	143.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.803	Depositor
Minimum map value	-0.297	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	550.08, 550.08, 550.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.9100001, 1.9100001, 1.9100001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HEA, COO, NDP, CUA, SF4, HEC, MG, CU, ZN, 8Q1, HEM, 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	1A	0.25	0/3060	0.48	1/4187 (0.0%)
1	1B	0.26	0/3060	0.48	1/4187 (0.0%)
1	6A	0.26	0/3060	0.48	1/4187 (0.0%)
1	6B	0.26	0/3060	0.48	1/4187 (0.0%)
2	1C	0.18	0/1643	0.36	0/2233
2	1D	0.17	0/1643	0.34	0/2233
2	6C	0.19	0/1643	0.36	0/2233
2	6D	0.18	0/1643	0.33	0/2233
3	1E	0.24	0/1953	0.43	1/2654 (0.0%)
3	1F	0.22	0/1953	0.38	0/2654
3	6E	0.24	0/1953	0.43	1/2654 (0.0%)
3	6F	0.22	0/1953	0.38	0/2654
4	1G	0.23	0/496	0.41	0/667
4	1H	0.22	0/496	0.39	0/667
4	6G	0.24	0/496	0.41	0/667
4	6H	0.22	0/496	0.39	0/667
5	1I	0.23	0/567	0.45	0/766
5	1J	0.21	0/567	0.39	0/766
5	6I	0.23	0/567	0.45	0/766
5	6J	0.21	0/567	0.39	0/766
6	1K	0.26	0/609	0.44	0/817
6	1L	0.22	0/609	0.42	0/817
6	6K	0.26	0/609	0.44	0/817
6	6L	0.22	0/609	0.42	0/817
7	1M	0.23	0/3723	0.42	0/5046
7	1N	0.22	0/3723	0.38	0/5046
7	6M	0.23	0/3723	0.42	0/5046
7	6N	0.22	0/3723	0.39	0/5046
8	1O	0.20	0/385	0.44	0/531
8	1P	0.21	0/385	0.52	0/531
8	6O	0.20	0/385	0.43	0/531
8	6P	0.21	0/385	0.51	0/531

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	1Q	0.30	0/3258	0.51	1/4439 (0.0%)
9	1S	0.21	0/3258	0.43	1/4439 (0.0%)
9	6Q	0.29	0/3258	0.49	0/4439
9	6S	0.21	0/3258	0.43	1/4439 (0.0%)
10	1R	0.28	0/996	0.59	3/1349 (0.2%)
10	1T	0.28	0/996	0.50	2/1349 (0.1%)
10	6R	0.28	0/996	0.59	3/1349 (0.2%)
10	6T	0.28	0/996	0.50	2/1349 (0.1%)
11	2A	0.26	0/4011	0.51	3/5484 (0.1%)
11	3A	0.27	0/4011	0.54	1/5484 (0.0%)
11	4A	0.27	0/4011	0.54	1/5484 (0.0%)
11	7A	0.26	0/4011	0.51	3/5484 (0.1%)
11	8A	0.27	0/4011	0.54	1/5484 (0.0%)
11	9A	0.28	0/4011	0.54	1/5484 (0.0%)
12	2B	0.24	0/1204	0.45	0/1641
12	3B	0.24	0/1204	0.46	0/1641
12	4B	0.24	0/1204	0.46	0/1641
12	7B	0.24	0/1204	0.45	0/1641
12	8B	0.24	0/1204	0.46	0/1641
12	9B	0.24	0/1204	0.46	0/1641
13	2C	0.21	0/1237	0.41	0/1676
13	3C	0.25	0/1237	0.46	0/1676
13	4C	0.25	0/1237	0.46	0/1676
13	7C	0.21	0/1237	0.41	0/1676
13	8C	0.24	0/1237	0.46	0/1676
13	9C	0.25	0/1237	0.46	0/1676
14	2D	0.24	0/2152	0.47	0/2937
14	3D	0.24	0/2152	0.49	0/2937
14	4D	0.24	0/2152	0.49	0/2937
14	7D	0.24	0/2152	0.47	0/2937
14	8D	0.24	0/2152	0.49	0/2937
14	9D	0.25	0/2152	0.49	0/2937
15	2E	0.24	0/757	0.62	3/1029 (0.3%)
15	3E	0.24	0/757	0.61	2/1029 (0.2%)
15	4E	0.25	0/757	0.61	2/1029 (0.2%)
15	7E	0.24	0/757	0.62	3/1029 (0.3%)
15	8E	0.25	0/757	0.61	2/1029 (0.2%)
15	9E	0.25	0/757	0.61	2/1029 (0.2%)
16	2F	0.19	0/726	0.35	0/974
16	3F	0.19	0/726	0.38	0/974
16	4F	0.19	0/726	0.38	0/974
16	7F	0.19	0/726	0.35	0/974
16	8F	0.19	0/726	0.38	0/974

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	9F	0.19	0/726	0.38	0/974
17	2G	0.27	0/762	0.57	0/1038
17	3G	0.27	0/762	0.52	0/1038
17	4G	0.27	0/762	0.52	0/1038
17	7G	0.27	0/762	0.57	0/1038
17	8G	0.27	0/762	0.52	0/1038
17	9G	0.27	0/762	0.52	0/1038
18	2H	0.20	0/980	0.42	0/1325
18	3H	0.23	0/980	0.52	1/1325 (0.1%)
18	4H	0.23	0/980	0.52	1/1325 (0.1%)
18	7H	0.20	0/980	0.42	0/1325
18	8H	0.23	0/980	0.52	1/1325 (0.1%)
18	9H	0.23	0/980	0.52	1/1325 (0.1%)
19	2I	0.24	0/619	0.46	0/839
19	3I	0.21	0/619	0.45	0/839
19	4I	0.22	0/619	0.45	0/839
19	7I	0.24	0/619	0.47	0/839
19	8I	0.21	0/619	0.45	0/839
19	9I	0.22	0/619	0.45	0/839
20	2J	0.21	0/839	0.39	0/1143
20	3J	0.23	0/839	0.43	0/1143
20	4J	0.23	0/812	0.42	0/1108
20	7J	0.22	0/839	0.39	0/1143
20	8J	0.23	0/839	0.43	0/1143
20	9J	0.23	0/812	0.42	0/1108
21	2K	0.20	0/392	0.39	0/531
21	3K	0.24	0/392	0.40	0/531
21	4K	0.24	0/392	0.41	0/531
21	7K	0.20	0/392	0.39	0/531
21	8K	0.24	0/392	0.40	0/531
21	9K	0.24	0/392	0.41	0/531
22	2L	0.25	0/621	0.58	1/841 (0.1%)
22	3L	0.27	0/645	0.57	1/875 (0.1%)
22	4L	0.28	0/645	0.57	1/875 (0.1%)
22	7L	0.26	0/621	0.58	1/841 (0.1%)
22	8L	0.27	0/645	0.57	1/875 (0.1%)
22	9L	0.27	0/645	0.57	1/875 (0.1%)
23	5A	0.11	0/1878	0.28	0/2549
23	A	0.11	0/1878	0.29	0/2549
24	5B	0.11	0/3400	0.26	0/4573
24	B	0.10	0/3400	0.27	0/4573
25	5C	0.11	0/5272	0.27	0/7143
25	C	0.11	0/5272	0.27	0/7143

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	5D	0.11	0/1843	0.31	0/2506
26	D	0.11	0/1843	0.31	0/2506
27	5E	0.12	0/3181	0.29	0/4303
27	E	0.11	0/3181	0.29	0/4303
28	5F	0.12	0/1258	0.31	0/1706
28	F	0.11	0/1258	0.31	0/1706
29	5G	0.12	0/1648	0.31	0/2222
29	G	0.11	0/1648	0.31	0/2222
30	5H	0.10	0/773	0.31	0/1046
30	H	0.10	0/773	0.31	0/1046
31	5I	0.10	0/1061	0.27	0/1441
31	I	0.10	0/1061	0.27	0/1441
32	5J	0.12	0/649	0.31	0/875
32	5r	0.11	0/673	0.27	0/906
32	J	0.12	0/649	0.31	0/875
32	r	0.10	0/673	0.27	0/906
33	5K	0.11	0/1007	0.30	0/1348
33	K	0.11	0/1007	0.30	0/1348
34	5L	0.11	0/1306	0.30	0/1769
34	L	0.10	0/1306	0.30	0/1769
35	5M	0.11	0/936	0.27	0/1276
35	M	0.10	0/936	0.27	0/1276
36	5N	0.10	0/1277	0.26	0/1735
36	N	0.10	0/1277	0.26	0/1735
37	5O	0.11	0/772	0.31	0/1037
37	O	0.11	0/772	0.31	0/1037
38	5P	0.12	0/2879	0.31	0/3905
38	P	0.12	0/2879	0.31	0/3905
39	5Q	0.15	0/2234	0.36	0/3034
39	Q	0.15	0/2234	0.36	0/3034
40	5R	0.14	0/3075	0.36	0/4191
40	R	0.14	0/3075	0.36	0/4191
41	5S	0.14	0/1106	0.32	0/1512
41	S	0.14	0/1106	0.32	0/1512
42	5T	0.13	0/3533	0.31	0/4825
42	T	0.13	0/3533	0.31	0/4825
43	5U	0.13	0/819	0.31	0/1112
43	U	0.13	0/819	0.30	0/1112
44	5V	0.13	0/4258	0.31	0/5792
44	V	0.12	0/4258	0.31	0/5792
45	5W	0.13	0/1239	0.36	0/1686
45	W	0.13	0/1239	0.36	0/1686
46	5X	0.12	0/1081	0.33	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
46	X	0.11	0/1081	0.33	0/1479
47	5Y	0.12	0/411	0.30	0/557
47	Y	0.11	0/411	0.31	0/557
48	5Z	0.11	0/894	0.28	0/1218
48	Z	0.11	0/894	0.28	0/1218
49	5a	0.41	0/698	0.57	0/949
49	a	0.44	0/698	0.59	0/949
50	5b	0.12	0/1201	0.30	0/1623
50	b	0.11	0/1201	0.31	0/1623
51	5c	0.12	0/463	0.29	0/623
51	c	0.11	0/463	0.29	0/623
52	5d	0.18	0/721	0.33	0/968
52	d	0.18	0/721	0.33	0/968
53	5e	0.13	0/1688	0.30	0/2301
53	e	0.13	0/1688	0.30	0/2301
54	5f	0.11	0/547	0.23	0/740
54	f	0.10	0/547	0.23	0/740
55	5g	0.27	0/433	0.54	0/587
55	g	0.11	0/433	0.32	0/587
56	5h	0.12	0/948	0.30	0/1285
56	h	0.11	0/948	0.30	0/1285
57	5i	0.10	0/644	0.25	0/860
57	i	0.10	0/644	0.25	0/860
58	5j	0.09	0/732	0.26	0/983
58	j	0.09	0/732	0.26	0/983
59	5k	0.12	0/1011	0.27	0/1361
59	k	0.11	0/1011	0.27	0/1361
60	5l	0.12	0/936	0.29	0/1278
60	l	0.11	0/936	0.29	0/1278
61	5m	0.11	0/1155	0.26	0/1558
61	m	0.11	0/1155	0.26	0/1558
62	5n	0.11	0/886	0.24	0/1188
62	n	0.10	0/886	0.24	0/1188
63	5o	0.12	0/1265	0.33	0/1705
63	o	0.12	0/1265	0.33	0/1705
64	5p	0.12	0/1095	0.29	0/1480
64	p	0.12	0/1095	0.29	0/1480
65	5q	0.12	0/1308	0.30	0/1779
65	q	0.12	0/1308	0.30	0/1779
66	5s	0.12	0/2353	0.30	0/3202
66	s	0.12	0/2353	0.30	0/3202
67	5t	0.11	0/2043	0.28	0/2778
67	t	0.11	0/2043	0.28	0/2778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	5u	0.13	0/1730	0.31	0/2341
68	u	0.13	0/1730	0.31	0/2341
69	5v	0.11	0/369	0.26	0/498
69	v	0.11	0/369	0.26	0/498
70	5w	0.12	0/521	0.30	0/702
70	w	0.12	0/521	0.30	0/702
71	5x	0.12	0/727	0.28	0/994
71	x	0.12	0/727	0.28	0/994
72	5y	0.15	0/963	0.30	0/1313
72	y	0.14	0/963	0.30	0/1313
All	All	0.20	0/298402	0.40	53/405254 (0.0%)

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	1A	0	1
1	1B	0	1
1	6A	0	1
1	6B	0	1
17	3G	0	1
17	4G	0	1
17	8G	0	1
17	9G	0	1
53	5e	0	1
53	e	0	1
All	All	0	10

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1R	10	LEU	CA-C-N	-10.11	107.20	119.84
10	1R	10	LEU	C-N-CA	-10.11	107.20	119.84
10	6R	10	LEU	CA-C-N	-10.07	107.25	119.84
10	6R	10	LEU	C-N-CA	-10.07	107.25	119.84
9	1Q	59	ALA	N-CA-C	-9.56	95.01	109.83
10	6T	5	LEU	N-CA-C	-8.38	101.83	110.97
10	1T	5	LEU	N-CA-C	-8.37	101.85	110.97
22	8L	75	VAL	N-CA-C	-7.12	106.07	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	75	VAL	N-CA-C	-7.08	106.10	112.90
22	4L	75	VAL	N-CA-C	-7.02	106.16	112.90
22	9L	75	VAL	N-CA-C	-6.98	106.20	112.90
22	7L	75	VAL	N-CA-C	-6.68	106.29	112.43
22	2L	75	VAL	N-CA-C	-6.67	106.30	112.43
15	2E	27	ALA	CA-C-N	6.56	134.07	121.54
15	2E	27	ALA	C-N-CA	6.56	134.07	121.54
15	7E	27	ALA	CA-C-N	6.56	134.06	121.54
15	7E	27	ALA	C-N-CA	6.56	134.06	121.54
11	2A	176	LEU	N-CA-C	-6.52	107.19	114.62
11	7A	176	LEU	N-CA-C	-6.48	107.24	114.62
15	8E	27	ALA	CA-C-N	6.24	133.45	121.54
15	8E	27	ALA	C-N-CA	6.24	133.45	121.54
15	4E	27	ALA	CA-C-N	6.23	133.44	121.54
15	4E	27	ALA	C-N-CA	6.23	133.44	121.54
15	9E	27	ALA	CA-C-N	6.22	133.43	121.54
15	9E	27	ALA	C-N-CA	6.22	133.43	121.54
15	3E	27	ALA	CA-C-N	6.22	133.43	121.54
15	3E	27	ALA	C-N-CA	6.22	133.43	121.54
10	6R	9	ALA	N-CA-C	-6.14	104.69	111.82
10	1R	9	ALA	N-CA-C	-6.13	104.71	111.82
11	3A	176	LEU	N-CA-C	-6.07	107.10	114.75
11	4A	176	LEU	N-CA-C	-6.07	107.11	114.75
11	9A	176	LEU	N-CA-C	-6.06	107.11	114.75
11	8A	176	LEU	N-CA-C	-6.03	107.15	114.75
1	1A	184	TYR	N-CA-C	-5.98	104.84	111.36
1	6A	184	TYR	N-CA-C	-5.93	104.90	111.36
3	1E	127	VAL	N-CA-C	-5.55	107.46	112.12
9	1S	234	VAL	N-CA-C	-5.51	107.01	111.91
9	6S	234	VAL	N-CA-C	-5.50	107.02	111.91
3	6E	127	VAL	N-CA-C	-5.48	107.52	112.12
18	4H	102	GLN	N-CA-CB	5.35	118.58	110.28
18	8H	102	GLN	N-CA-CB	5.35	118.57	110.28
18	9H	102	GLN	N-CA-CB	5.33	118.55	110.28
18	3H	102	GLN	N-CA-CB	5.33	118.54	110.28
11	2A	486	ALA	CA-C-N	5.24	131.13	121.70
11	2A	486	ALA	C-N-CA	5.24	131.13	121.70
11	7A	486	ALA	CA-C-N	5.22	131.09	121.70
11	7A	486	ALA	C-N-CA	5.22	131.09	121.70
15	2E	28	TRP	N-CA-C	-5.13	99.88	110.80
15	7E	28	TRP	N-CA-C	-5.13	99.88	110.80
10	6T	4	LEU	N-CA-C	-5.11	107.02	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1T	4	LEU	N-CA-C	-5.08	107.05	113.20
1	1B	184	TYR	N-CA-C	-5.08	105.45	111.69
1	6B	184	TYR	N-CA-C	-5.07	105.45	111.69

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	184	TYR	Sidechain
1	1B	184	TYR	Sidechain
17	3G	114	TRP	Peptide
17	4G	114	TRP	Peptide
53	5e	147	MET	Peptide
1	6A	184	TYR	Sidechain
1	6B	184	TYR	Sidechain
17	8G	114	TRP	Peptide
17	9G	114	TRP	Peptide
53	e	147	MET	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	1A	2958	0	2955	13	0
1	1B	2958	0	2955	18	0
1	6A	2958	0	2955	15	0
1	6B	2958	0	2955	19	0
2	1C	1602	0	1577	14	0
2	1D	1602	0	1577	16	0
2	6C	1602	0	1577	12	0
2	6D	1602	0	1577	16	0
3	1E	1898	0	1800	11	0
3	1F	1898	0	1800	8	0
3	6E	1898	0	1800	11	0
3	6F	1898	0	1800	9	0
4	1G	486	0	490	3	0
4	1H	486	0	490	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	6G	486	0	490	4	0
4	6H	486	0	490	3	0
5	1I	550	0	501	6	0
5	1J	550	0	501	20	0
5	6I	550	0	501	6	0
5	6J	550	0	501	58	0
6	1K	594	0	590	8	0
6	1L	594	0	590	4	0
6	6K	594	0	590	8	0
6	6L	594	0	590	5	0
7	1M	3646	0	3555	52	0
7	1N	3646	0	3555	29	0
7	6M	3646	0	3555	64	0
7	6N	3646	0	3555	25	0
8	1O	371	0	372	2	0
8	1P	371	0	372	5	0
8	6O	371	0	372	2	0
8	6P	371	0	372	5	0
9	1Q	3204	0	3271	95	0
9	1S	3204	0	3271	26	0
9	6Q	3204	0	3271	130	0
9	6S	3204	0	3271	24	0
10	1R	980	0	1005	17	0
10	1T	980	0	1005	26	0
10	6R	980	0	1005	18	0
10	6T	980	0	1005	26	0
11	2A	3888	0	3936	38	0
11	3A	3888	0	3936	36	0
11	4A	3888	0	3936	35	0
11	7A	3888	0	3936	37	0
11	8A	3888	0	3936	36	0
11	9A	3888	0	3936	36	0
12	2B	1169	0	1191	25	0
12	3B	1169	0	1191	14	0
12	4B	1169	0	1191	13	0
12	7B	1169	0	1191	23	0
12	8B	1169	0	1191	15	0
12	9B	1169	0	1191	15	0
13	2C	1212	0	1243	12	0
13	3C	1212	0	1243	12	0
13	4C	1212	0	1243	12	0
13	7C	1212	0	1243	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	8C	1212	0	1243	12	0
13	9C	1212	0	1243	12	0
14	2D	2079	0	2039	15	0
14	3D	2079	0	2039	14	0
14	4D	2079	0	2039	15	0
14	7D	2079	0	2039	15	0
14	8D	2079	0	2039	14	0
14	9D	2079	0	2039	16	0
15	2E	737	0	706	21	0
15	3E	737	0	706	1	0
15	4E	737	0	706	1	0
15	7E	737	0	706	21	0
15	8E	737	0	706	1	0
15	9E	737	0	706	2	0
16	2F	706	0	683	26	0
16	3F	706	0	685	37	0
16	4F	706	0	685	5	0
16	7F	706	0	683	27	0
16	8F	706	0	685	37	0
16	9F	706	0	685	2	0
17	2G	733	0	708	11	0
17	3G	733	0	708	5	0
17	4G	733	0	708	5	0
17	7G	733	0	708	10	0
17	8G	733	0	708	8	0
17	9G	733	0	708	6	0
18	2H	954	0	900	7	0
18	3H	954	0	900	7	0
18	4H	954	0	900	5	0
18	7H	954	0	900	6	0
18	8H	954	0	900	6	0
18	9H	954	0	900	7	0
19	2I	594	0	553	4	0
19	3I	594	0	553	5	0
19	4I	594	0	553	5	0
19	7I	594	0	553	4	0
19	8I	594	0	553	5	0
19	9I	594	0	553	6	0
20	2J	816	0	807	10	0
20	3J	816	0	807	6	0
20	4J	790	0	781	60	0
20	7J	816	0	807	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	8J	816	0	807	6	0
20	9J	790	0	781	25	0
21	2K	382	0	367	6	0
21	3K	382	0	367	3	0
21	4K	382	0	367	3	0
21	7K	382	0	367	6	0
21	8K	382	0	367	3	0
21	9K	382	0	367	5	0
22	2L	605	0	588	12	0
22	3L	627	0	604	48	0
22	4L	627	0	604	14	0
22	7L	605	0	588	13	0
22	8L	627	0	604	48	0
22	9L	627	0	604	14	0
23	5A	1839	0	1827	36	0
23	A	1839	0	1827	33	0
24	5B	3331	0	3328	76	0
24	B	3331	0	3328	75	0
25	5C	5175	0	5182	97	0
25	C	5175	0	5182	98	0
26	5D	1790	0	1740	72	0
26	D	1790	0	1740	75	0
27	5E	3107	0	3083	112	0
27	E	3107	0	3083	114	0
28	5F	1225	0	1224	38	0
28	F	1225	0	1224	41	0
29	5G	1615	0	1551	67	0
29	G	1615	0	1551	69	0
30	5H	750	0	751	26	0
30	H	750	0	751	26	0
31	5I	1044	0	1046	23	0
31	I	1044	0	1046	23	0
32	5J	640	0	629	11	0
32	5r	663	0	647	32	0
32	J	640	0	629	10	0
32	r	663	0	647	29	0
33	5K	986	0	1017	23	0
33	K	986	0	1017	24	0
34	5L	1275	0	1243	36	0
34	L	1275	0	1243	38	0
35	5M	913	0	909	15	0
35	M	913	0	909	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5N	1235	0	1161	22	0
36	N	1235	0	1161	20	0
37	5O	761	0	759	18	0
37	O	761	0	759	17	0
38	5P	2823	0	2854	71	0
38	P	2823	0	2854	70	0
39	5Q	2179	0	2241	74	0
39	Q	2179	0	2241	75	0
40	5R	3014	0	3082	89	0
40	R	3014	0	3082	94	0
41	5S	1071	0	1035	34	0
41	S	1071	0	1035	37	0
42	5T	3434	0	3590	110	0
42	T	3434	0	3590	109	0
43	5U	805	0	812	30	0
43	U	805	0	812	29	0
44	5V	4152	0	4212	107	0
44	V	4152	0	4212	110	0
45	5W	1210	0	1275	48	0
45	W	1210	0	1275	46	0
46	5X	1037	0	981	27	0
46	X	1037	0	981	25	0
47	5Y	405	0	404	7	0
47	Y	405	0	404	7	0
48	5Z	861	0	826	14	0
48	Z	861	0	826	17	0
49	5a	674	0	620	28	0
49	a	674	0	620	45	0
50	5b	1169	0	1144	32	0
50	b	1169	0	1144	30	0
51	5c	453	0	475	10	0
51	c	453	0	475	11	0
52	5d	699	0	670	16	0
52	d	699	0	670	17	0
53	5e	1639	0	1618	61	0
53	e	1639	0	1618	63	0
54	5f	532	0	524	12	0
54	f	532	0	524	11	0
55	5g	416	0	402	53	0
55	g	416	0	400	65	0
56	5h	915	0	866	20	0
56	h	915	0	866	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	5i	633	0	612	8	0
57	i	633	0	612	9	0
58	5j	712	0	684	11	0
58	j	712	0	684	9	0
59	5k	984	0	980	30	0
59	k	984	0	980	26	0
60	5l	904	0	875	7	0
60	l	904	0	875	8	0
61	5m	1126	0	1148	30	0
61	m	1126	0	1148	30	0
62	5n	864	0	839	10	0
62	n	864	0	839	8	0
63	5o	1240	0	1222	30	0
63	o	1240	0	1222	29	0
64	5p	1069	0	1014	63	0
64	p	1069	0	1014	64	0
65	5q	1268	0	1209	42	0
65	q	1268	0	1209	42	0
66	5s	2302	0	2299	105	0
66	s	2302	0	2299	101	0
67	5t	1997	0	1985	60	0
67	t	1997	0	1985	57	0
68	5u	1698	0	1686	46	0
68	u	1698	0	1686	44	0
69	5v	361	0	359	2	0
69	v	361	0	359	2	0
70	5w	508	0	494	7	0
70	w	508	0	494	7	0
71	5x	699	0	662	29	0
71	x	699	0	662	31	0
72	5y	932	0	950	19	0
72	y	932	0	950	21	0
73	1A	86	0	60	0	0
73	1B	86	0	60	2	0
73	6A	86	0	60	1	0
73	6B	86	0	60	2	0
74	1E	43	0	32	3	0
74	1F	43	0	32	2	0
74	6E	43	0	32	3	0
74	6F	43	0	32	2	0
75	1M	1	0	0	0	0
75	1N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	5s	1	0	0	0	0
75	6M	1	0	0	0	0
75	6N	1	0	0	0	0
75	s	1	0	0	0	0
76	2A	120	0	108	2	0
76	3A	120	0	108	3	0
76	4A	120	0	108	3	0
76	7A	120	0	108	2	0
76	8A	120	0	108	3	0
76	9A	120	0	108	3	0
77	2A	1	0	0	0	0
77	3A	1	0	0	0	0
77	4A	1	0	0	0	0
77	7A	1	0	0	0	0
77	8A	1	0	0	0	0
77	9A	1	0	0	0	0
78	2A	1	0	0	0	0
78	3A	1	0	0	0	0
78	4A	1	0	0	0	0
78	7A	1	0	0	0	0
78	8A	1	0	0	0	0
78	9A	1	0	0	0	0
79	2C	2	0	0	3	0
79	3C	2	0	0	2	0
79	4C	2	0	0	2	0
79	7C	2	0	0	3	0
79	8C	2	0	0	2	0
79	9C	2	0	0	2	0
80	5A	4	0	0	2	0
80	5C	4	0	0	1	0
80	A	4	0	0	2	0
80	C	4	0	0	1	0
81	5B	31	0	19	2	0
81	B	31	0	19	2	0
82	5B	8	0	0	0	0
82	5C	16	0	0	1	0
82	5F	8	0	0	1	0
82	5G	16	0	0	1	0
82	B	8	0	0	0	0
82	C	16	0	0	1	0
82	F	8	0	0	1	0
82	G	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	5J	35	0	0	1	0
83	5k	35	0	0	0	0
83	J	35	0	0	1	0
83	k	35	0	0	0	0
84	5P	48	0	26	4	0
84	P	48	0	26	4	0
85	5s	53	0	37	8	0
85	s	53	0	37	9	0
All	All	292492	0	289480	4480	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 8.

All (4480) 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)
66:5s:92:ARG:CD	15:7E:34:PHE:CD2	1.77	1.68
64:5p:10:TYR:CD2	16:8F:59:ARG:HD3	1.24	1.65
16:3F:59:ARG:HD3	64:p:10:TYR:CD2	1.24	1.65
9:6Q:60:VAL:CG2	55:g:11:ARG:HG2	1.22	1.62
11:8A:265:THR:HG21	22:8L:5:PHE:CE2	1.39	1.58
15:2E:34:PHE:CD2	66:s:92:ARG:CD	1.77	1.57
11:9A:265:THR:HG21	22:9L:5:PHE:CE2	1.39	1.57
11:3A:265:THR:HG21	22:3L:5:PHE:CE2	1.39	1.56
11:4A:265:THR:HG21	22:4L:5:PHE:CE2	1.39	1.56
9:6Q:62:GLU:HB2	55:g:11:ARG:CB	1.12	1.54
15:2E:34:PHE:CZ	66:s:92:ARG:NH1	1.75	1.53
66:5s:92:ARG:NH1	15:7E:34:PHE:CZ	1.75	1.53
13:7C:120:CYS:SG	79:7C:301:CUA:CU2	1.01	1.51
9:6Q:60:VAL:HG22	55:g:11:ARG:CG	1.35	1.50
13:2C:120:CYS:SG	79:2C:301:CUA:CU2	1.01	1.49
66:5s:92:ARG:NH1	15:7E:34:PHE:CE1	1.80	1.49
15:2E:34:PHE:CE1	66:s:92:ARG:NH1	1.80	1.48
66:5s:92:ARG:HD2	15:7E:34:PHE:CE2	1.49	1.46
15:2E:34:PHE:CE2	66:s:92:ARG:HD2	1.49	1.46
16:3F:59:ARG:CD	64:p:10:TYR:CG	2.00	1.44
15:2E:34:PHE:CD2	66:s:92:ARG:HD2	0.91	1.43
64:5p:10:TYR:CG	16:8F:59:ARG:CD	2.00	1.43
66:5s:92:ARG:HD2	15:7E:34:PHE:CD2	0.91	1.42
5:1J:23:LYS:CD	20:9J:90:ASN:O	1.65	1.41
9:6Q:62:GLU:CA	55:g:11:ARG:HB3	1.51	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6Q:62:GLU:CB	55:g:11:ARG:HB3	0.91	1.38
64:5p:10:TYR:CG	16:8F:59:ARG:HD2	1.56	1.36
16:3F:59:ARG:HD2	64:p:10:TYR:CG	1.56	1.36
20:4J:96:ILE:CG1	5:6J:26:ALA:O	1.72	1.35
9:1Q:57:LEU:O	9:1Q:60:VAL:HG13	1.28	1.34
9:6Q:67:SER:HB3	32:r:69:SER:CA	1.57	1.32
66:5s:92:ARG:CD	15:7E:34:PHE:CG	2.12	1.32
16:3F:59:ARG:CD	64:p:10:TYR:CD2	2.12	1.31
5:1J:23:LYS:HD3	20:9J:90:ASN:O	1.21	1.31
15:2E:34:PHE:CG	66:s:92:ARG:CD	2.12	1.31
9:6Q:62:GLU:HB2	55:g:11:ARG:CA	1.62	1.30
9:6Q:62:GLU:HG2	55:g:11:ARG:O	1.11	1.29
9:6Q:67:SER:CB	32:r:69:SER:HA	1.63	1.29
22:3L:81:TRP:HZ2	64:p:10:TYR:CZ	1.51	1.28
64:5p:10:TYR:CZ	22:8L:81:TRP:HZ2	1.51	1.27
20:4J:90:ASN:O	5:6J:23:LYS:HD2	1.19	1.27
9:6Q:62:GLU:OE1	55:g:11:ARG:HB2	1.13	1.27
13:3C:124:CYS:SG	79:3C:301:CUA:CU1	1.27	1.25
13:4C:124:CYS:SG	79:4C:301:CUA:CU1	1.27	1.25
20:4J:96:ILE:HD11	5:6J:30:ALA:N	1.50	1.24
9:6Q:62:GLU:CB	55:g:11:ARG:CB	1.82	1.24
15:2E:34:PHE:CG	66:s:92:ARG:HD2	1.70	1.24
22:3L:81:TRP:CZ2	64:p:10:TYR:OH	1.87	1.23
13:9C:124:CYS:SG	79:9C:301:CUA:CU1	1.27	1.23
64:5p:10:TYR:CD2	16:8F:59:ARG:CD	2.12	1.23
13:8C:124:CYS:SG	79:8C:301:CUA:CU1	1.27	1.23
66:5s:92:ARG:HD2	15:7E:34:PHE:CG	1.70	1.22
20:4J:90:ASN:HB3	5:6J:23:LYS:CD	1.69	1.22
9:1Q:60:VAL:HG21	55:5g:11:ARG:CG	1.69	1.21
64:5p:10:TYR:OH	22:8L:81:TRP:HZ2	1.20	1.20
66:5s:49:MET:SD	12:7B:81:THR:CG2	2.30	1.20
12:2B:81:THR:CG2	66:s:49:MET:SD	2.30	1.19
38:5P:295:HIS:O	10:6T:4:LEU:CD1	1.91	1.19
64:5p:10:TYR:OH	22:8L:81:TRP:CZ2	1.87	1.19
9:6Q:62:GLU:OE1	55:g:11:ARG:CB	1.90	1.19
20:4J:90:ASN:CB	5:6J:23:LYS:HD3	1.73	1.18
10:1T:4:LEU:CD1	38:P:295:HIS:O	1.91	1.18
16:3F:59:ARG:HD3	64:p:10:TYR:CG	1.70	1.18
16:3F:53:TRP:HB2	64:p:3:TYR:CE2	1.79	1.17
64:5p:3:TYR:CE2	16:8F:53:TRP:HB2	1.79	1.17
64:5p:10:TYR:CG	16:8F:59:ARG:HD3	1.70	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3L:81:TRP:HZ2	64:p:10:TYR:OH	1.20	1.17
9:6Q:60:VAL:CG2	55:g:11:ARG:CG	2.02	1.17
55:5g:8:GLN:CD	55:5g:11:ARG:NH2	2.04	1.15
20:4J:93:PRO:HG3	5:6J:27:ALA:HA	1.26	1.14
66:5s:49:MET:SD	12:7B:81:THR:HG22	1.87	1.14
9:6Q:62:GLU:CG	55:g:11:ARG:C	2.22	1.13
9:6Q:62:GLU:CG	55:g:11:ARG:O	1.95	1.13
66:5s:92:ARG:CZ	15:7E:34:PHE:CE1	2.31	1.13
16:3F:55:TRP:HB3	64:p:7:PHE:HE1	1.12	1.12
15:2E:34:PHE:CE1	66:s:92:ARG:CZ	2.31	1.11
9:6Q:62:GLU:HG2	55:g:11:ARG:C	1.75	1.11
5:1J:26:ALA:O	20:9J:96:ILE:HG13	1.48	1.11
12:2B:81:THR:HG22	66:s:49:MET:SD	1.87	1.10
64:5p:7:PHE:CE1	16:8F:55:TRP:HB3	1.87	1.10
11:8A:265:THR:CG2	22:8L:5:PHE:CE2	2.34	1.10
11:9A:265:THR:CG2	22:9L:5:PHE:CE2	2.35	1.10
16:3F:55:TRP:HB3	64:p:7:PHE:CE1	1.87	1.10
20:4J:96:ILE:HG12	5:6J:30:ALA:HB2	1.13	1.09
11:4A:265:THR:CG2	22:4L:5:PHE:CE2	2.35	1.09
9:1Q:67:SER:HB2	32:5r:69:SER:HA	1.34	1.08
9:6Q:61:THR:N	55:g:11:ARG:HD3	1.56	1.08
17:7G:78:HIS:O	17:7G:109:ARG:NH1	1.85	1.08
11:3A:265:THR:CG2	22:3L:5:PHE:CE2	2.35	1.08
64:5p:7:PHE:HE1	16:8F:55:TRP:HB3	1.12	1.08
20:4J:96:ILE:HG13	5:6J:26:ALA:C	1.78	1.08
20:4J:96:ILE:HG21	5:6J:26:ALA:HB1	1.29	1.08
5:1J:23:LYS:HD2	20:9J:90:ASN:O	1.45	1.07
17:2G:78:HIS:O	17:2G:109:ARG:NH1	1.85	1.07
10:1T:4:LEU:HD13	38:P:295:HIS:O	1.49	1.06
15:2E:34:PHE:CD1	66:s:92:ARG:CZ	2.39	1.06
22:3L:81:TRP:CZ2	64:p:10:TYR:CE2	2.43	1.06
20:4J:95:SER:HB2	5:6J:30:ALA:HB1	1.09	1.06
64:5p:10:TYR:CE2	22:8L:81:TRP:CZ2	2.43	1.05
16:7F:63:GLN:NE2	22:8L:71:ARG:NE	2.03	1.05
66:5s:92:ARG:CZ	15:7E:34:PHE:CD1	2.39	1.05
38:5P:295:HIS:O	10:6T:4:LEU:HD13	1.49	1.04
16:2F:63:GLN:NE2	22:3L:71:ARG:NE	2.03	1.04
11:3A:265:THR:HG21	22:3L:5:PHE:CD2	1.92	1.04
20:4J:96:ILE:HG21	5:6J:26:ALA:CB	1.87	1.04
11:8A:265:THR:HG21	22:8L:5:PHE:CD2	1.92	1.04
20:4J:102:ALA:O	5:6J:29:LYS:CE	2.05	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4A:265:THR:HG21	22:4L:5:PHE:CD2	1.92	1.04
5:1J:30:ALA:HB2	20:9J:96:ILE:HG12	1.07	1.03
7:1M:54:SER:HA	9:1Q:65:ARG:NH1	1.73	1.03
64:5p:7:PHE:CE1	16:8F:55:TRP:CB	2.41	1.03
9:1Q:60:VAL:CG2	55:5g:11:ARG:HG2	1.87	1.03
16:3F:55:TRP:CB	64:p:7:PHE:CE1	2.41	1.02
11:9A:265:THR:HG21	22:9L:5:PHE:CD2	1.92	1.01
9:6Q:62:GLU:CG	55:g:11:ARG:HB3	1.90	1.01
9:1Q:60:VAL:HG21	55:5g:11:ARG:HG2	1.02	1.01
64:5p:10:TYR:HE2	22:8L:81:TRP:CH2	1.78	1.01
10:1T:4:LEU:HA	10:1T:7:GLN:HB3	1.43	1.00
22:3L:81:TRP:CH2	64:p:10:TYR:HE2	1.78	1.00
5:1J:30:ALA:HB2	20:9J:96:ILE:CG1	1.89	1.00
16:3F:59:ARG:HD2	64:p:10:TYR:CD1	1.97	0.99
10:6T:4:LEU:HA	10:6T:7:GLN:HB3	1.43	0.99
9:1Q:57:LEU:O	9:1Q:60:VAL:CG1	2.09	0.98
64:5p:10:TYR:CD1	16:8F:59:ARG:HD2	1.97	0.98
23:5A:80:TYR:HH	24:5B:219:HIS:HD1	1.06	0.98
20:4J:102:ALA:O	5:6J:29:LYS:HE3	1.62	0.98
20:4J:95:SER:HB2	5:6J:30:ALA:CB	1.92	0.97
66:5s:92:ARG:HD3	15:7E:34:PHE:CD2	1.99	0.97
9:1Q:60:VAL:HG11	55:5g:11:ARG:HD3	1.47	0.96
55:5g:8:GLN:OE1	55:5g:11:ARG:NH2	1.97	0.96
20:4J:96:ILE:HG13	5:6J:26:ALA:O	0.80	0.96
23:A:80:TYR:HH	24:B:219:HIS:HD1	1.05	0.96
9:1Q:67:SER:CB	32:5r:69:SER:HA	1.95	0.96
7:6M:442:ALA:HB3	9:6Q:61:THR:HG22	1.45	0.95
10:1T:4:LEU:HA	10:1T:7:GLN:CB	1.96	0.95
10:6T:4:LEU:HA	10:6T:7:GLN:CB	1.96	0.94
20:4J:96:ILE:HG12	5:6J:30:ALA:CB	1.97	0.94
20:4J:90:ASN:O	5:6J:23:LYS:CD	2.14	0.94
16:3F:59:ARG:HD3	64:p:10:TYR:CE2	2.03	0.94
9:1Q:62:GLU:HB2	55:5g:11:ARG:HB3	1.48	0.94
64:5p:7:PHE:HE1	16:8F:55:TRP:CB	1.78	0.94
66:5s:92:ARG:NE	15:7E:34:PHE:CG	2.37	0.93
15:2E:34:PHE:CG	66:s:92:ARG:NE	2.37	0.93
20:4J:93:PRO:CG	5:6J:27:ALA:HA	1.97	0.93
15:2E:34:PHE:CD2	66:s:92:ARG:HD3	1.99	0.93
64:5p:10:TYR:CE2	16:8F:59:ARG:HD3	2.03	0.92
16:2F:56:ASN:OD1	22:3L:65:PHE:HA	1.69	0.92
22:3L:81:TRP:HZ2	64:p:10:TYR:CE2	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7F:56:ASN:OD1	22:8L:65:PHE:HA	1.69	0.92
11:3A:265:THR:HG21	22:3L:5:PHE:CZ	2.05	0.92
9:1Q:60:VAL:CG1	55:5g:11:ARG:HD3	2.00	0.91
9:6Q:61:THR:H	55:g:11:ARG:HD3	1.17	0.91
20:4J:96:ILE:CG2	5:6J:26:ALA:HB1	1.99	0.91
11:4A:265:THR:HG21	22:4L:5:PHE:CZ	2.05	0.91
11:9A:265:THR:HG21	22:9L:5:PHE:CZ	2.05	0.91
9:1Q:62:GLU:HG2	55:5g:11:ARG:O	1.71	0.90
66:5s:49:MET:SD	12:7B:81:THR:HG21	2.09	0.90
16:3F:55:TRP:CB	64:p:7:PHE:HE1	1.78	0.90
11:8A:265:THR:HG21	22:8L:5:PHE:CZ	2.05	0.90
64:5p:10:TYR:CE2	22:8L:81:TRP:HZ2	1.81	0.90
5:1J:33:GLU:OE2	20:9J:95:SER:HB3	1.73	0.89
55:5g:8:GLN:CD	55:5g:11:ARG:HH21	1.77	0.89
12:2B:81:THR:HG21	66:s:49:MET:SD	2.09	0.89
16:4F:74:ARG:HH12	5:6J:34:ARG:HA	1.36	0.89
20:4J:102:ALA:C	5:6J:29:LYS:HG3	1.97	0.89
16:7F:63:GLN:NE2	22:8L:71:ARG:CZ	2.35	0.89
22:3L:81:TRP:CH2	64:p:10:TYR:CE2	2.61	0.89
16:2F:63:GLN:NE2	22:3L:71:ARG:CZ	2.35	0.88
9:6Q:60:VAL:HG21	55:g:11:ARG:HA	1.53	0.88
9:6Q:62:GLU:CD	55:g:11:ARG:C	2.41	0.88
5:1J:30:ALA:N	20:9J:96:ILE:HD11	1.88	0.88
10:6T:4:LEU:CA	10:6T:7:GLN:HB3	2.04	0.87
49:5a:60:TYR:HB3	55:5g:18:HIS:CD2	2.10	0.87
49:a:58:ILE:HG12	49:a:67:LYS:HD3	1.55	0.87
7:6M:312:THR:HB	9:6Q:52:PRO:HD3	1.56	0.87
10:1T:4:LEU:CA	10:1T:7:GLN:HB3	2.03	0.87
15:2E:17:PRO:HB3	67:t:252:GLU:OE2	1.75	0.87
16:3F:59:ARG:HD2	64:p:10:TYR:CB	2.05	0.87
9:6Q:67:SER:CB	32:r:69:SER:CA	2.35	0.86
16:3F:59:ARG:CD	64:p:10:TYR:CB	2.54	0.86
55:5g:10:GLU:HG2	59:5k:41:TYR:OH	1.76	0.86
20:4J:96:ILE:HD11	5:6J:29:LYS:C	1.99	0.86
9:6Q:67:SER:HB2	32:r:69:SER:CB	2.06	0.86
67:5t:252:GLU:OE2	15:7E:17:PRO:HB3	1.75	0.86
55:5g:4:VAL:HB	55:5g:8:GLN:HE21	1.41	0.85
64:5p:10:TYR:CB	16:8F:59:ARG:HD2	2.04	0.85
9:6Q:60:VAL:HG23	55:g:11:ARG:CG	2.06	0.85
11:4A:265:THR:CG2	22:4L:5:PHE:CD2	2.58	0.85
49:5a:65:MET:SD	55:5g:21:LEU:HG	2.16	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:5p:10:TYR:CZ	22:8L:81:TRP:CZ2	2.42	0.84
7:1M:39:PHE:CE1	49:5a:50:PRO:HB2	2.12	0.84
66:5s:42:ALA:HB2	22:7L:12:TYR:CE1	2.13	0.84
22:2L:12:TYR:CE1	66:s:42:ALA:HB2	2.13	0.84
9:6Q:61:THR:N	55:g:11:ARG:CD	2.35	0.84
44:V:113:ASN:HD21	48:Z:41:HIS:HB2	1.40	0.84
44:5V:113:ASN:HD21	48:5Z:41:HIS:HB2	1.40	0.84
64:5p:10:TYR:CB	16:8F:59:ARG:CD	2.54	0.84
42:T:201:PRO:HD3	42:T:229:LEU:HD22	1.60	0.84
16:7F:56:ASN:HD21	22:8L:64:GLN:HG3	1.43	0.84
9:6Q:62:GLU:CA	55:g:11:ARG:CB	2.29	0.83
55:5g:8:GLN:CD	55:5g:11:ARG:HH22	1.81	0.83
64:5p:10:TYR:CE2	22:8L:81:TRP:CH2	2.61	0.83
53:e:99:LYS:HB3	72:y:2:MET:HE2	1.61	0.83
9:1Q:65:ARG:HB2	32:5r:68:ALA:HB2	1.59	0.83
10:1R:7:GLN:O	10:1R:10:LEU:HB3	1.79	0.83
20:4J:96:ILE:CD1	5:6J:30:ALA:N	2.40	0.83
10:6R:7:GLN:O	10:6R:10:LEU:HB3	1.79	0.82
7:1M:54:SER:HA	9:1Q:65:ARG:HH11	1.44	0.82
22:3L:81:TRP:HH2	64:p:10:TYR:HE2	1.26	0.82
9:1Q:61:THR:HB	9:1Q:65:ARG:NH2	1.95	0.82
42:5T:201:PRO:HD3	42:5T:229:LEU:HD22	1.60	0.82
5:1J:26:ALA:HB1	20:9J:96:ILE:HG21	1.61	0.82
11:8A:265:THR:CG2	22:8L:5:PHE:CD2	2.58	0.82
7:6M:54:SER:O	9:6Q:65:ARG:HA	1.79	0.82
20:4J:95:SER:HB3	5:6J:33:GLU:OE2	1.78	0.81
64:5p:10:TYR:HE2	22:8L:81:TRP:HH2	1.26	0.81
16:3F:55:TRP:HB2	64:p:7:PHE:CE1	2.15	0.81
9:6Q:57:LEU:HD13	72:y:60:LYS:HD2	1.63	0.81
11:3A:265:THR:CG2	22:3L:5:PHE:CD2	2.59	0.81
53:5e:99:LYS:HB3	72:5y:2:MET:HE2	1.61	0.81
5:1I:26:ALA:CB	47:Y:53:ILE:HG21	2.10	0.81
9:6Q:62:GLU:CD	55:g:11:ARG:CB	2.54	0.80
9:6Q:67:SER:HB3	32:r:69:SER:HA	0.85	0.80
7:1M:54:SER:O	9:1Q:65:ARG:HA	1.82	0.80
20:4J:70:LYS:O	5:6J:19:PRO:HB3	1.82	0.80
16:2F:56:ASN:HD21	22:3L:64:GLN:HG3	1.42	0.80
22:3L:81:TRP:CZ2	64:p:10:TYR:CZ	2.42	0.80
47:5Y:53:ILE:HG21	5:6I:26:ALA:CB	2.10	0.80
49:a:60:TYR:HB3	55:g:18:HIS:CD2	2.17	0.80
9:6Q:67:SER:CB	32:r:69:SER:CB	2.58	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:5s:92:ARG:HD3	15:7E:34:PHE:CG	2.15	0.80
20:4J:96:ILE:CG1	5:6J:30:ALA:HB2	2.04	0.79
20:4J:102:ALA:O	5:6J:29:LYS:HE2	1.82	0.79
15:2E:34:PHE:CG	66:s:92:ARG:HD3	2.15	0.79
11:9A:265:THR:CG2	22:9L:5:PHE:CD2	2.59	0.79
9:6Q:62:GLU:HA	55:g:11:ARG:CB	2.13	0.79
9:6Q:64:PRO:HG2	32:r:61:LYS:CB	2.13	0.78
16:3F:53:TRP:CB	64:p:3:TYR:CE2	2.65	0.78
64:5p:7:PHE:CE1	16:8F:55:TRP:HB2	2.15	0.78
7:6M:442:ALA:CB	9:6Q:61:THR:HG22	2.14	0.78
20:4J:102:ALA:HB1	5:6J:29:LYS:HG3	1.64	0.78
16:7F:63:GLN:HE22	22:8L:71:ARG:NE	1.81	0.78
41:S:224:LEU:HD12	45:W:151:ARG:HH22	1.49	0.78
64:5p:3:TYR:CE2	16:8F:53:TRP:CB	2.65	0.77
7:6M:312:THR:HA	9:6Q:51:VAL:HG23	1.65	0.77
9:6Q:62:GLU:CG	55:g:11:ARG:CB	2.57	0.77
26:D:170:LEU:HB2	26:D:179:ILE:HG22	1.67	0.77
9:1Q:60:VAL:HG11	55:5g:11:ARG:CD	2.14	0.77
42:T:243:VAL:HG12	42:T:244:VAL:HG13	1.67	0.77
36:N:44:ARG:NH2	36:N:71:ARG:O	2.18	0.77
15:2E:34:PHE:CD1	66:s:92:ARG:NE	2.53	0.77
41:5S:224:LEU:HD12	45:5W:151:ARG:HH22	1.49	0.77
36:5N:44:ARG:NH2	36:5N:71:ARG:O	2.18	0.76
16:2F:63:GLN:HE22	22:3L:71:ARG:CZ	1.98	0.76
42:5T:243:VAL:HG12	42:5T:244:VAL:HG13	1.67	0.76
66:5s:46:LEU:HA	22:7L:9:LEU:HD21	1.67	0.76
66:s:182:THR:HB	66:s:199:THR:HA	1.68	0.76
26:5D:170:LEU:HB2	26:5D:179:ILE:HG22	1.67	0.76
16:2F:63:GLN:HE22	22:3L:71:ARG:NE	1.81	0.76
20:4J:93:PRO:HG3	5:6J:27:ALA:CA	2.10	0.76
66:5s:182:THR:HB	66:5s:199:THR:HA	1.68	0.76
13:2C:124:CYS:SG	79:2C:301:CUA:CU1	1.75	0.75
20:4J:102:ALA:HB1	5:6J:29:LYS:CG	2.15	0.75
68:u:84:TYR:OH	68:u:213:HIS:ND1	2.19	0.75
29:5G:42:GLY:O	39:5Q:264:ARG:NH1	2.19	0.75
9:6Q:64:PRO:HG2	32:r:61:LYS:HB2	1.67	0.75
13:7C:124:CYS:SG	79:7C:301:CUA:CU1	1.75	0.75
66:5s:49:MET:HE1	12:7B:81:THR:C	2.11	0.75
66:5s:92:ARG:NE	15:7E:34:PHE:CD1	2.53	0.75
12:2B:81:THR:C	66:s:49:MET:HE1	2.11	0.75
13:8C:124:CYS:HG	79:8C:301:CUA:CU1	0.42	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2L:9:LEU:HD21	66:s:46:LEU:HA	1.67	0.74
16:7F:63:GLN:HE22	22:8L:71:ARG:CZ	1.99	0.74
40:5R:331:LEU:HD21	42:5T:149:VAL:HG12	1.69	0.74
59:5k:57:GLU:OE1	7:6M:275:ARG:NH2	2.21	0.74
9:1Q:60:VAL:CB	55:5g:11:ARG:CD	2.66	0.74
29:G:42:GLY:O	39:Q:264:ARG:NH1	2.19	0.74
38:5P:295:HIS:O	10:6T:4:LEU:HD11	1.85	0.74
7:6M:312:THR:CB	9:6Q:52:PRO:HD3	2.18	0.74
9:6Q:62:GLU:HA	55:g:11:ARG:HB3	1.66	0.74
66:5s:306:LEU:HD11	67:5t:259:ARG:HB3	1.69	0.74
67:t:149:ARG:HB2	67:t:167:VAL:HG22	1.70	0.73
45:5W:78:THR:O	45:5W:82:ALA:HB3	1.88	0.73
44:V:323:THR:HG1	44:V:379:SER:HG	1.26	0.73
13:4C:124:CYS:HG	79:4C:301:CUA:CU1	0.41	0.73
44:5V:323:THR:HG1	44:5V:379:SER:HG	1.29	0.73
13:9C:124:CYS:HG	79:9C:301:CUA:CU1	0.41	0.73
7:6M:77:PHE:HZ	9:6Q:69:PRO:O	1.70	0.73
66:s:71:HIS:CE1	68:u:212:GLU:HB3	2.24	0.73
33:5K:106:TYR:O	33:5K:110:ARG:HB2	1.88	0.73
45:W:78:THR:O	45:W:82:ALA:HB3	1.88	0.73
7:1M:275:ARG:NH2	59:k:57:GLU:OE1	2.21	0.73
20:4J:102:ALA:C	5:6J:29:LYS:HE2	2.12	0.73
40:R:331:LEU:HD21	42:T:149:VAL:HG12	1.69	0.73
9:1Q:62:GLU:HG2	55:5g:11:ARG:C	2.13	0.73
65:5q:93:MET:O	65:5q:130:ARG:NH2	2.22	0.73
67:5t:149:ARG:HB2	67:5t:167:VAL:HG22	1.70	0.72
37:O:13:GLU:HG3	37:O:47:PRO:HB2	1.71	0.72
49:a:58:ILE:CG1	49:a:67:LYS:HD3	2.19	0.72
13:3C:124:CYS:HG	79:3C:301:CUA:CU1	0.41	0.72
55:5g:8:GLN:HB2	55:5g:11:ARG:HH21	1.53	0.72
16:7F:56:ASN:OD1	22:8L:65:PHE:CA	2.37	0.72
9:1Q:64:PRO:CB	32:5r:61:LYS:HB2	2.19	0.72
33:K:106:TYR:O	33:K:110:ARG:HB2	1.88	0.72
66:5s:71:HIS:CE1	68:5u:212:GLU:HB3	2.24	0.72
68:5u:84:TYR:HH	68:5u:213:HIS:HD1	0.73	0.72
66:s:306:LEU:HD11	67:t:259:ARG:HB3	1.69	0.72
16:2F:56:ASN:OD1	22:3L:65:PHE:CA	2.37	0.72
46:5X:66:TRP:O	59:5k:74:ARG:NH1	2.23	0.72
65:5q:126:LEU:O	71:5x:72:TYR:OH	2.08	0.72
7:1M:39:PHE:HE1	49:5a:50:PRO:HB2	1.54	0.72
9:1Q:60:VAL:HB	55:5g:11:ARG:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:5s:92:ARG:CD	15:7E:34:PHE:HD2	1.95	0.71
62:n:39:HIS:ND1	64:p:100:THR:O	2.23	0.71
66:5s:42:ALA:CB	22:7L:12:TYR:CD1	2.74	0.71
62:5n:39:HIS:ND1	64:5p:100:THR:O	2.23	0.71
65:q:93:MET:O	65:q:130:ARG:NH2	2.22	0.71
10:1T:4:LEU:HD11	38:P:295:HIS:O	1.85	0.71
27:E:376:LYS:NZ	35:M:114:ALA:O	2.23	0.71
37:5O:13:GLU:HG3	37:5O:47:PRO:HB2	1.71	0.71
37:5O:13:GLU:HB3	37:5O:63:ARG:HB3	1.73	0.71
44:5V:295:SER:OG	44:5V:328:LYS:NZ	2.24	0.71
46:X:66:TRP:O	59:k:74:ARG:NH1	2.23	0.71
65:q:126:LEU:O	71:x:72:TYR:OH	2.08	0.71
22:2L:12:TYR:CD1	66:s:42:ALA:CB	2.74	0.71
20:4J:96:ILE:HG21	5:6J:26:ALA:CA	2.21	0.71
37:O:13:GLU:HB3	37:O:63:ARG:HB3	1.73	0.71
9:1Q:60:VAL:CG2	55:5g:11:ARG:CG	2.60	0.70
44:5V:65:THR:HA	44:5V:75:GLY:HA2	1.72	0.70
44:5V:81:ASP:OD2	44:5V:258:ARG:NH1	2.22	0.70
16:7F:63:GLN:HE21	22:8L:71:ARG:NE	1.88	0.70
58:5j:78:LYS:HG2	58:5j:83:LEU:HD12	1.73	0.70
42:T:203:MET:HG2	42:T:206:HIS:CE1	2.26	0.70
44:V:65:THR:HA	44:V:75:GLY:HA2	1.72	0.70
27:5E:91:GLN:NE2	28:5F:34:THR:O	2.24	0.70
9:6Q:62:GLU:HB2	55:g:11:ARG:CG	2.13	0.70
40:R:-2:UNK:HA	40:R:1:MET:HE2	1.72	0.70
42:T:329:ASP:OD1	56:h:58:ARG:NH2	2.23	0.70
40:5R:-2:UNK:HA	40:5R:1:MET:HE2	1.72	0.70
42:5T:203:MET:HG2	42:5T:206:HIS:CE1	2.26	0.70
47:5Y:53:ILE:HG21	5:6I:26:ALA:HB2	1.73	0.70
65:5q:65:HIS:HD1	65:5q:82:TYR:HH	1.39	0.70
20:4J:84:TYR:CE2	5:6J:26:ALA:HB2	2.27	0.70
20:4J:96:ILE:HD11	5:6J:30:ALA:H	1.53	0.70
44:5V:359:MET:HE2	55:5g:27:ASN:HD22	1.57	0.70
42:5T:329:ASP:OD1	56:5h:58:ARG:NH2	2.23	0.70
29:G:163:ARG:NH2	34:L:107:MET:O	2.25	0.70
48:Z:49:LYS:HA	50:b:38:GLY:HA3	1.73	0.70
44:5V:413:THR:HA	44:5V:416:TYR:CE2	2.27	0.70
48:5Z:49:LYS:HA	50:5b:38:GLY:HA3	1.73	0.70
65:5q:147:ALA:HA	65:5q:150:ILE:HD12	1.72	0.70
11:7A:375:LEU:HD13	76:7A:602:HEA:HAC	1.74	0.70
27:E:91:GLN:NE2	28:F:34:THR:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5G:163:ARG:NH2	34:5L:107:MET:O	2.25	0.70
44:V:295:SER:OG	44:V:328:LYS:NZ	2.24	0.70
9:1Q:60:VAL:HB	55:5g:11:ARG:CD	2.21	0.69
66:5s:45:GLU:HB3	22:7L:9:LEU:HD13	1.74	0.69
20:4J:90:ASN:HB3	5:6J:23:LYS:HD3	0.81	0.69
38:5P:254:LEU:HD21	38:5P:265:LEU:HD22	1.74	0.69
66:5s:68:ALA:HB3	66:5s:117:LEU:HG	1.74	0.69
68:5u:43:ASN:HD22	68:5u:43:ASN:C	2.00	0.69
38:P:254:LEU:HD21	38:P:265:LEU:HD22	1.74	0.69
44:V:413:THR:HA	44:V:416:TYR:CE2	2.27	0.69
58:j:78:LYS:HG2	58:j:83:LEU:HD12	1.73	0.69
65:q:147:ALA:HA	65:q:150:ILE:HD12	1.72	0.69
5:1I:26:ALA:HB2	47:Y:53:ILE:HG21	1.74	0.69
9:1Q:49:VAL:HG21	9:1Q:56:LYS:HE2	1.75	0.69
38:5P:135:LEU:HD21	38:5P:323:PRO:HA	1.75	0.69
44:5V:203:SER:OG	46:5X:121:ARG:NH1	2.26	0.69
67:t:75:ASN:HD21	67:t:92:PHE:HB3	1.57	0.69
29:5G:120:HIS:CD2	82:5G:302:SF4:S2	2.86	0.69
38:P:62:ASN:ND2	38:P:86:SER:OG	2.25	0.69
67:5t:75:ASN:HD21	67:5t:92:PHE:HB3	1.57	0.69
7:6M:121:LEU:HB3	9:6Q:339:MET:HE1	1.74	0.69
29:G:48:GLU:HA	29:G:51:ARG:HE	1.58	0.69
43:U:154:ARG:HB3	43:U:158:ILE:HD13	1.74	0.69
66:s:284:ARG:NH1	66:s:302:SER:O	2.26	0.69
67:t:142:TYR:OH	68:u:106:ALA:O	2.09	0.69
7:1M:442:ALA:HB2	9:1Q:61:THR:CG2	2.22	0.69
11:2A:375:LEU:HD13	76:2A:601:HEA:HAC	1.74	0.69
20:4J:102:ALA:CB	5:6J:29:LYS:HG3	2.22	0.69
29:G:89:MET:O	39:Q:255:TRP:NE1	2.26	0.69
44:V:359:MET:HE2	55:g:27:ASN:HD22	1.57	0.69
16:2F:63:GLN:HE21	22:3L:71:ARG:NE	1.88	0.69
44:V:203:SER:OG	46:X:121:ARG:NH1	2.26	0.69
49:a:49:PRO:HG2	49:a:52:LEU:HD12	1.74	0.69
9:1Q:65:ARG:O	32:5r:68:ALA:HB1	1.92	0.69
16:2F:56:ASN:OD1	22:3L:64:GLN:C	2.36	0.69
67:5t:182:PRO:O	67:5t:184:ARG:NH1	2.26	0.69
38:5P:62:ASN:ND2	38:5P:86:SER:OG	2.25	0.68
9:6Q:57:LEU:HD13	72:y:60:LYS:CD	2.23	0.68
10:1T:8:VAL:O	10:1T:11:PRO:HD2	1.93	0.68
24:5B:155:GLU:HG3	24:5B:158:LYS:HB2	1.74	0.68
43:5U:154:ARG:HB3	43:5U:158:ILE:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7F:56:ASN:OD1	22:8L:64:GLN:C	2.36	0.68
66:s:68:ALA:HB3	66:s:117:LEU:HG	1.74	0.68
16:2F:56:ASN:HB2	22:3L:65:PHE:HD1	1.59	0.68
26:5D:274:ASN:O	34:5L:81:ARG:NH2	2.27	0.68
66:5s:284:ARG:NH1	66:5s:302:SER:O	2.26	0.68
26:D:274:ASN:O	34:L:81:ARG:NH2	2.27	0.68
38:P:135:LEU:HD21	38:P:323:PRO:HA	1.75	0.68
49:a:40:HIS:N	49:a:64:THR:O	2.26	0.68
61:5m:3:GLU:HA	61:5m:6:LYS:HD3	1.76	0.68
65:5q:65:HIS:ND1	65:5q:82:TYR:OH	2.26	0.68
49:a:44:ASN:H	32:r:58:HIS:CG	2.11	0.68
67:t:182:PRO:O	67:t:184:ARG:NH1	2.26	0.68
49:a:60:TYR:CD2	55:g:18:HIS:HA	2.28	0.68
24:B:155:GLU:HG3	24:B:158:LYS:HB2	1.74	0.68
7:1M:39:PHE:CE1	49:5a:50:PRO:CB	2.77	0.68
9:6Q:62:GLU:CB	55:g:11:ARG:C	2.63	0.68
41:5S:252:TYR:O	41:5S:256:ASN:ND2	2.26	0.68
44:5V:430:SER:HA	55:5g:16:ARG:NH1	2.09	0.68
7:6M:54:SER:HB3	9:6Q:66:THR:OG1	1.94	0.68
7:6M:314:PRO:HB3	9:6Q:49:VAL:O	1.94	0.68
27:E:125:GLU:HA	27:E:128:LEU:HD12	1.76	0.68
27:E:332:ASP:OD1	29:G:36:ARG:NH2	2.27	0.68
41:S:220:VAL:HA	41:S:223:TYR:HD2	1.57	0.68
29:G:120:HIS:CD2	82:G:302:SF4:S2	2.86	0.68
28:5F:66:ARG:HB3	39:5Q:211:SER:HB3	1.75	0.68
9:6Q:62:GLU:CB	55:g:11:ARG:CA	2.48	0.68
10:6T:8:VAL:O	10:6T:11:PRO:HD2	1.93	0.68
23:A:43:ASN:ND2	23:A:131:THR:O	2.26	0.68
28:F:95:PRO:O	39:Q:58:LYS:NZ	2.27	0.68
9:1Q:60:VAL:CG1	55:5g:11:ARG:CD	2.72	0.67
23:5A:43:ASN:ND2	23:5A:131:THR:O	2.26	0.67
40:5R:264:GLN:HB2	40:5R:381:VAL:HG21	1.76	0.67
41:5S:220:VAL:HA	41:5S:223:TYR:HD2	1.57	0.67
44:V:81:ASP:OD2	44:V:258:ARG:NH1	2.22	0.67
16:2F:56:ASN:ND2	22:3L:64:GLN:HG3	2.09	0.67
22:2L:9:LEU:HD13	66:s:45:GLU:HB3	1.74	0.67
7:1M:121:LEU:HB3	9:1Q:339:MET:HE1	1.74	0.67
53:5e:146:PRO:HG2	53:5e:149:GLN:HE21	1.59	0.67
53:5e:11:SER:HB3	63:5o:112:PRO:HG3	1.75	0.67
44:V:3:LEU:HD21	44:V:60:VAL:HG11	1.77	0.67
56:h:92:GLU:HA	56:h:95:TRP:CD1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:m:3:GLU:HA	61:m:6:LYS:HD3	1.76	0.67
55:5g:8:GLN:NE2	55:5g:11:ARG:HH22	1.92	0.67
60:5l:112:LEU:HB3	60:5l:115:VAL:HB	1.76	0.67
34:L:72:ARG:NH1	34:L:73:THR:O	2.28	0.67
53:e:146:PRO:HG2	53:e:149:GLN:HE21	1.58	0.67
20:4J:84:TYR:HE2	5:6J:26:ALA:HB2	1.57	0.67
27:5E:376:LYS:NZ	35:5M:114:ALA:O	2.23	0.67
29:5G:89:MET:O	39:5Q:255:TRP:NE1	2.26	0.67
34:5L:72:ARG:NH1	34:5L:73:THR:O	2.28	0.67
44:5V:3:LEU:HD21	44:5V:60:VAL:HG11	1.77	0.67
16:7F:56:ASN:ND2	22:8L:64:GLN:HG3	2.09	0.67
40:R:264:GLN:HB2	40:R:381:VAL:HG21	1.77	0.67
10:1T:4:LEU:HA	10:1T:7:GLN:HB2	1.76	0.67
20:4J:90:ASN:C	5:6J:23:LYS:HD2	2.14	0.67
27:5E:332:ASP:OD1	29:5G:36:ARG:NH2	2.27	0.67
41:S:230:LEU:HD11	43:U:198:ALA:HB1	1.77	0.67
68:u:43:ASN:C	68:u:43:ASN:HD22	1.99	0.67
13:2C:120:CYS:HG	79:2C:301:CUA:CU2	1.05	0.67
27:5E:125:GLU:HA	27:5E:128:LEU:HD12	1.76	0.67
27:5E:436:LEU:HD22	27:5E:465:ILE:HD13	1.77	0.67
29:5G:48:GLU:HA	29:5G:51:ARG:HE	1.58	0.67
24:B:119:LYS:NZ	81:B:502:FMN:O1P	2.28	0.67
28:F:66:ARG:HB3	39:Q:211:SER:HB3	1.75	0.67
32:J:66:ILE:HD11	32:J:81:LEU:HD22	1.75	0.67
37:O:40:LYS:NZ	37:O:46:PHE:O	2.28	0.67
56:5h:92:GLU:HA	56:5h:95:TRP:CD1	2.29	0.67
42:T:200:ILE:HG23	42:T:288:MET:HB3	1.77	0.67
9:6Q:60:VAL:HG21	55:g:11:ARG:CA	2.22	0.66
41:S:252:TYR:O	41:S:256:ASN:ND2	2.26	0.66
53:e:11:SER:HB3	63:o:112:PRO:HG3	1.75	0.66
32:5J:66:ILE:HD11	32:5J:81:LEU:HD22	1.76	0.66
27:E:436:LEU:HD22	27:E:465:ILE:HD13	1.77	0.66
31:I:71:VAL:HG22	31:I:127:ALA:HB2	1.77	0.66
44:V:322:MET:HB3	44:V:456:LYS:HE3	1.77	0.66
66:s:135:ARG:NH1	66:s:137:ASP:OD2	2.29	0.66
5:1J:30:ALA:HB1	20:9J:95:SER:HB2	1.77	0.66
39:5Q:163:ASN:ND2	54:5f:37:ALA:O	2.29	0.66
25:5C:663:ILE:HG12	37:5O:15:ARG:HH12	1.61	0.66
53:5e:143:MET:HG2	6:6K:32:PRO:HB3	1.78	0.66
28:5F:67:GLN:NE2	39:5Q:210:TYR:O	2.29	0.66
28:5F:95:PRO:O	39:5Q:58:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5I:71:VAL:HG22	31:5I:127:ALA:HB2	1.77	0.66
42:5T:200:ILE:HG23	42:5T:288:MET:HB3	1.77	0.66
68:5u:127:VAL:HA	68:5u:144:ILE:HB	1.76	0.66
40:5R:241:TYR:HA	40:5R:244:ILE:HD12	1.77	0.66
9:6Q:62:GLU:CD	55:g:12:TYR:N	2.53	0.66
60:l:112:LEU:HB3	60:l:115:VAL:HB	1.76	0.66
24:5B:119:LYS:NZ	81:5B:501:FMN:O1P	2.28	0.66
37:5O:40:LYS:NZ	37:5O:46:PHE:O	2.28	0.66
41:5S:230:LEU:HD11	43:5U:198:ALA:HB1	1.77	0.66
28:F:67:GLN:NE2	39:Q:210:TYR:O	2.29	0.66
49:5a:44:ASN:H	32:5r:58:HIS:CG	2.14	0.66
16:7F:56:ASN:HB2	22:8L:65:PHE:HD1	1.58	0.66
43:U:219:ASP:HB3	43:U:222:ALA:HB2	1.78	0.66
7:1M:443:GLU:HA	9:1Q:59:ALA:HB1	1.77	0.66
24:B:62:ILE:O	24:B:158:LYS:NZ	2.25	0.66
6:1K:33:LYS:HD3	53:e:144:GLY:HA2	1.76	0.65
7:1M:50:THR:CG2	9:1Q:63:PRO:HG3	2.26	0.65
43:5U:219:ASP:HB3	43:5U:222:ALA:HB2	1.78	0.65
64:5p:7:PHE:CD2	16:8F:52:THR:HG23	2.31	0.65
66:5s:135:ARG:NH1	66:5s:137:ASP:OD2	2.29	0.65
42:T:192:LEU:HD13	42:T:240:MET:HG3	1.78	0.65
68:u:127:VAL:HA	68:u:144:ILE:HB	1.76	0.65
6:1K:32:PRO:HB3	53:e:143:MET:HG2	1.78	0.65
9:1Q:49:VAL:HG11	9:1Q:55:GLU:HA	1.78	0.65
13:7C:120:CYS:HG	79:7C:301:CUA:CU2	1.04	0.65
25:C:84:TYR:O	25:C:200:ARG:NH2	2.27	0.65
27:5E:188:LEU:HG	27:5E:341:MET:HE1	1.78	0.65
40:5R:373:PRO:HA	40:5R:376:LEU:HB2	1.78	0.65
66:5s:92:ARG:CD	15:7E:34:PHE:CE2	2.41	0.65
27:E:410:GLU:O	27:E:429:ARG:NH1	2.29	0.65
7:1M:447:ARG:HH22	9:1Q:49:VAL:HG12	1.60	0.65
16:3F:52:THR:HG23	64:p:7:PHE:CD2	2.31	0.65
25:5C:84:TYR:O	25:5C:200:ARG:NH2	2.28	0.65
45:5W:81:ARG:HB3	45:5W:85:ARG:HB3	1.77	0.65
25:C:320:ARG:HH21	25:C:585:HIS:HB2	1.61	0.65
39:Q:110:TYR:OH	45:W:59:VAL:O	2.13	0.65
10:1R:8:VAL:O	10:1R:11:PRO:HD2	1.96	0.65
16:4F:74:ARG:NH1	5:6J:34:ARG:HA	2.10	0.65
42:5T:192:LEU:HD13	42:5T:240:MET:HG3	1.78	0.65
53:5e:144:GLY:HA2	6:6K:33:LYS:HD3	1.76	0.65
54:5f:36:TRP:O	54:5f:40:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5i:58:ARG:NH1	61:5m:122:GLU:OE1	2.29	0.65
25:C:663:ILE:HG12	37:O:15:ARG:HH12	1.61	0.65
27:E:188:LEU:HG	27:E:341:MET:HE1	1.78	0.65
22:2L:12:TYR:CD1	66:s:42:ALA:HB1	2.32	0.65
24:5B:62:ILE:O	24:5B:158:LYS:NZ	2.25	0.65
44:5V:322:MET:HB3	44:5V:456:LYS:HE3	1.77	0.65
53:5e:77:ARG:HB3	71:5x:22:LYS:HZ2	1.61	0.65
66:5s:42:ALA:HB1	22:7L:12:TYR:CD1	2.32	0.65
26:D:178:ARG:NH2	27:E:410:GLU:OE2	2.30	0.65
40:R:241:TYR:HA	40:R:244:ILE:HD12	1.77	0.65
45:W:81:ARG:HB3	45:W:85:ARG:HB3	1.77	0.65
49:a:39:TYR:HE2	49:a:41:ARG:HD2	1.62	0.65
25:5C:198:CYS:O	25:5C:203:ARG:NH2	2.29	0.65
9:6S:50:GLU:HG2	9:6S:52:PRO:HD2	1.79	0.65
10:6T:4:LEU:HA	10:6T:7:GLN:HB2	1.76	0.65
57:i:58:ARG:NH1	61:m:122:GLU:OE1	2.30	0.65
50:5b:108:MET:SD	63:5o:97:ARG:NH1	2.70	0.65
49:a:44:ASN:HD22	32:r:54:GLU:CD	2.05	0.65
12:2B:81:THR:O	66:s:49:MET:HE1	1.97	0.65
26:5D:178:ARG:NH2	27:5E:410:GLU:OE2	2.30	0.65
67:5t:168:VAL:HA	67:5t:186:ILE:HB	1.79	0.65
44:V:22:ARG:NH2	50:b:44:ASN:O	2.26	0.65
7:6M:312:THR:HB	9:6Q:52:PRO:CD	2.27	0.65
7:6M:447:ARG:HG3	9:6Q:55:GLU:CD	2.22	0.65
25:C:198:CYS:O	25:C:203:ARG:NH2	2.29	0.65
27:5E:410:GLU:O	27:5E:429:ARG:NH1	2.29	0.64
53:5e:179:ARG:NH2	53:5e:211:ASP:OD2	2.30	0.64
66:5s:182:THR:OG1	68:5u:147:ASN:OD1	2.14	0.64
10:6R:8:VAL:O	10:6R:11:PRO:HD2	1.96	0.64
35:M:95:VAL:O	35:M:141:ARG:NH2	2.30	0.64
44:V:53:PHE:HB3	44:V:54:MET:HE2	1.79	0.64
50:b:108:MET:SD	63:o:97:ARG:NH1	2.70	0.64
25:5C:320:ARG:HH21	25:5C:585:HIS:HB2	1.61	0.64
27:5E:112:ARG:NH1	27:5E:114:ASP:OD2	2.30	0.64
24:B:232:ALA:HB2	24:B:244:PRO:HG3	1.79	0.64
25:C:544:PRO:O	25:C:549:ARG:NH1	2.30	0.64
27:E:278:ASP:OD2	29:G:41:SER:OG	2.15	0.64
40:R:146:ARG:NE	40:R:156:GLU:OE2	2.27	0.64
40:R:373:PRO:HA	40:R:376:LEU:HB2	1.78	0.64
43:U:212:PHE:O	43:U:216:SER:OG	2.14	0.64
66:s:196:MET:SD	85:s:401:COO:H52	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1J:27:ALA:HA	20:9J:93:PRO:HG3	1.79	0.64
39:5Q:110:TYR:OH	45:5W:59:VAL:O	2.13	0.64
26:D:269:ARG:O	29:G:145:GLN:NE2	2.30	0.64
9:1S:50:GLU:HG2	9:1S:52:PRO:HD2	1.79	0.64
11:4A:474:PRO:HG3	20:4J:8:ARG:HE	1.63	0.64
24:5B:401:GLY:HA2	24:5B:407:ARG:HB2	1.79	0.64
25:5C:544:PRO:O	25:5C:549:ARG:NH1	2.30	0.64
27:5E:278:ASP:OD2	29:5G:41:SER:OG	2.15	0.64
29:5G:229:LEU:HD13	30:5H:51:ALA:H	1.62	0.64
9:6Q:60:VAL:HG23	55:g:11:ARG:HG3	1.76	0.64
68:u:109:VAL:HG11	68:u:121:ILE:HD11	1.79	0.64
9:1Q:64:PRO:CB	32:5r:61:LYS:CB	2.75	0.64
11:3A:474:PRO:HG3	20:3J:8:ARG:HE	1.63	0.64
28:5F:124:VAL:HG12	28:5F:125:VAL:HG13	1.80	0.64
29:5G:158:SER:OG	29:5G:160:ARG:NE	2.25	0.64
24:B:401:GLY:HA2	24:B:407:ARG:HB2	1.78	0.64
25:C:563:LEU:HD22	25:C:566:SER:HB2	1.80	0.64
66:s:104:LYS:HE2	66:s:108:ALA:HB3	1.80	0.64
67:t:168:VAL:HA	67:t:186:ILE:HB	1.79	0.64
9:1Q:64:PRO:HB3	32:5r:61:LYS:CB	2.27	0.64
29:G:47:ILE:HG21	41:S:278:ARG:HH22	1.61	0.64
39:Q:163:ASN:ND2	54:f:37:ALA:O	2.29	0.64
35:5M:95:VAL:O	35:5M:141:ARG:NH2	2.30	0.64
25:C:157:ASP:OD1	26:D:277:TRP:NE1	2.29	0.64
66:s:182:THR:OG1	68:u:147:ASN:OD1	2.14	0.64
9:1Q:64:PRO:HB3	32:5r:61:LYS:HB3	1.80	0.64
34:5L:72:ARG:NH1	34:5L:76:GLN:O	2.30	0.64
7:6M:54:SER:O	9:6Q:66:THR:N	2.29	0.64
28:F:124:VAL:HG12	28:F:125:VAL:HG13	1.79	0.64
9:1Q:60:VAL:HG21	55:5g:11:ARG:CD	2.28	0.64
25:5C:563:LEU:HD22	25:5C:566:SER:HB2	1.80	0.64
26:5D:269:ARG:O	29:5G:145:GLN:NE2	2.30	0.64
64:5p:10:TYR:HB2	16:8F:59:ARG:NH1	2.13	0.64
27:E:112:ARG:NH1	27:E:114:ASP:OD2	2.30	0.64
33:K:99:THR:HG23	33:K:100:GLU:HG3	1.80	0.64
45:W:1:MET:HG2	45:W:4:GLU:HB2	1.80	0.64
24:5B:173:ARG:HG2	34:5L:176:LEU:HD13	1.80	0.63
24:5B:232:ALA:HB2	24:5B:244:PRO:HG3	1.79	0.63
65:5q:128:VAL:HA	65:5q:131:MET:HE2	1.80	0.63
66:5s:161:SER:OG	66:5s:163:ASP:OD1	2.16	0.63
9:6Q:62:GLU:HB2	55:g:11:ARG:C	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:286:PHE:HB3	24:B:312:GLU:HG3	1.79	0.63
27:E:161:GLN:OE1	27:E:402:ARG:NH1	2.31	0.63
34:L:72:ARG:NH1	34:L:76:GLN:O	2.30	0.63
16:3F:59:ARG:CD	64:p:10:TYR:CD1	2.67	0.63
25:5C:157:ASP:OD1	26:5D:277:TRP:NE1	2.29	0.63
64:5p:3:TYR:HB2	16:8F:56:ASN:HD22	1.64	0.63
66:5s:104:LYS:HE2	66:5s:108:ALA:HB3	1.80	0.63
3:6E:118:TYR:HB2	3:6E:187:THR:HG21	1.80	0.63
25:C:270:ILE:HG22	25:C:620:THR:HG22	1.80	0.63
37:O:64:TYR:HB2	37:O:68:ALA:HB3	1.81	0.63
68:u:143:LEU:HB2	68:u:199:LEU:HD11	1.81	0.63
16:3F:59:ARG:NH1	64:p:10:TYR:HB2	2.13	0.63
27:5E:161:GLN:OE1	27:5E:402:ARG:NH1	2.31	0.63
66:5s:49:MET:HE1	12:7B:81:THR:O	1.97	0.63
11:9A:474:PRO:HG3	20:9J:8:ARG:HE	1.63	0.63
49:a:55:ALA:O	49:a:67:LYS:HG3	1.97	0.63
53:e:148:PRO:HG2	72:y:11:TRP:HB3	1.79	0.63
3:1E:118:TYR:HB2	3:1E:187:THR:HG21	1.80	0.63
41:5S:223:TYR:HE1	45:5W:69:VAL:HG22	1.63	0.63
53:5e:148:PRO:HG2	72:5y:11:TRP:HB3	1.79	0.63
68:5u:109:VAL:HG11	68:5u:121:ILE:HD11	1.79	0.63
9:6Q:216:ARG:HH22	9:6S:470:ASN:HB2	1.64	0.63
28:F:56:ARG:HG2	39:Q:39:VAL:HG23	1.81	0.63
38:P:393:TYR:HB2	45:W:81:ARG:HG3	1.80	0.63
44:V:169:ALA:O	44:V:173:ASN:ND2	2.32	0.63
9:1Q:68:THR:H	32:5r:69:SER:HB3	1.63	0.63
27:5E:155:TYR:CZ	27:5E:159:ILE:HD11	2.34	0.63
29:5G:47:ILE:HG21	41:5S:278:ARG:HH22	1.62	0.63
27:E:427:LYS:NZ	27:E:428:ILE:O	2.32	0.63
56:h:38:GLN:NE2	56:h:56:LEU:O	2.30	0.63
40:5R:91:PHE:CZ	40:5R:95:LEU:HD11	2.34	0.63
44:5V:259:LEU:HB3	44:5V:261:ILE:HG12	1.79	0.63
65:5q:79:LEU:HD22	65:5q:84:PHE:HE2	1.64	0.63
2:6D:180:LEU:HB3	2:6D:186:PRO:HB3	1.80	0.63
29:G:229:LEU:HD13	30:H:51:ALA:H	1.62	0.63
36:N:12:GLU:OE1	36:N:60:ARG:NH2	2.32	0.63
44:V:259:LEU:HB3	44:V:261:ILE:HG12	1.79	0.63
53:e:179:ARG:NH2	53:e:211:ASP:OD2	2.30	0.63
16:3F:53:TRP:HA	64:p:3:TYR:CD2	2.33	0.63
27:5E:222:SER:O	29:5G:117:ARG:NH1	2.32	0.63
65:5q:188:PHE:O	67:5t:104:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6Q:46:GLY:H	9:6Q:48:ARG:HH22	1.47	0.63
27:E:222:SER:O	29:G:117:ARG:NH1	2.32	0.63
65:q:128:VAL:HA	65:q:131:MET:HE2	1.80	0.63
16:3F:56:ASN:HD22	64:p:3:TYR:HB2	1.64	0.63
24:5B:286:PHE:HB3	24:5B:312:GLU:HG3	1.79	0.63
29:5G:163:ARG:HH22	34:5L:108:GLY:HA3	1.64	0.63
40:5R:226:SER:HB3	40:5R:329:LEU:HD23	1.81	0.63
44:5V:53:PHE:HB3	44:5V:54:MET:HE2	1.79	0.63
24:B:299:ILE:HA	24:B:375:VAL:HB	1.81	0.63
40:R:91:PHE:CZ	40:R:95:LEU:HD11	2.34	0.63
27:5E:427:LYS:NZ	27:5E:428:ILE:O	2.31	0.63
33:5K:99:THR:HG23	33:5K:100:GLU:HG3	1.80	0.63
64:5p:3:TYR:CD2	16:8F:53:TRP:HA	2.34	0.63
68:5u:143:LEU:HB2	68:5u:199:LEU:HD11	1.81	0.63
9:6Q:60:VAL:CG2	55:g:11:ARG:HA	2.28	0.63
11:8A:474:PRO:HG3	20:8J:8:ARG:HE	1.63	0.63
40:R:226:SER:HB3	40:R:329:LEU:HD23	1.81	0.63
65:q:79:LEU:HD22	65:q:84:PHE:HE2	1.64	0.63
66:s:161:SER:OG	66:s:163:ASP:OD1	2.16	0.63
9:1Q:216:ARG:HH22	9:1S:470:ASN:HB2	1.64	0.62
16:3F:55:TRP:CB	64:p:7:PHE:CZ	2.82	0.62
28:5F:56:ARG:HG2	39:5Q:39:VAL:HG23	1.81	0.62
38:5P:393:TYR:HB2	45:5W:81:ARG:HG3	1.80	0.62
40:5R:36:GLN:HG3	40:5R:60:LEU:HD12	1.81	0.62
53:5e:211:ASP:HB3	53:5e:214:GLN:HG3	1.82	0.62
24:B:173:ARG:HG2	34:L:176:LEU:HD13	1.80	0.62
27:E:155:TYR:CZ	27:E:159:ILE:HD11	2.34	0.62
63:o:62:LYS:NZ	63:o:108:VAL:O	2.32	0.62
26:5D:111:GLY:N	26:5D:121:GLU:O	2.27	0.62
9:6Q:62:GLU:CB	55:g:11:ARG:O	2.46	0.62
25:C:124:GLU:O	25:C:129:LYS:NZ	2.33	0.62
25:C:207:GLU:O	25:C:435:ARG:NE	2.32	0.62
26:D:237:ARG:O	27:E:126:LYS:NZ	2.29	0.62
42:T:242:PRO:HA	53:e:10:PRO:HG2	1.79	0.62
54:f:38:ASN:O	54:f:40:LYS:NZ	2.32	0.62
67:t:238:ARG:NH2	68:u:26:GLU:OE1	2.27	0.62
24:5B:379:ASP:OD1	24:5B:382:THR:OG1	2.17	0.62
24:B:379:ASP:OD1	24:B:382:THR:OG1	2.17	0.62
67:5t:142:TYR:OH	68:5u:106:ALA:O	2.09	0.62
67:5t:238:ARG:NH2	68:5u:26:GLU:OE1	2.27	0.62
25:5C:270:ILE:HG22	25:5C:620:THR:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5N:132:LYS:HB3	36:5N:141:ARG:HD2	1.80	0.62
37:5O:64:TYR:HB2	37:5O:68:ALA:HB3	1.81	0.62
42:5T:242:PRO:HA	53:5e:10:PRO:HG2	1.79	0.62
63:5o:62:LYS:NZ	63:5o:108:VAL:O	2.32	0.62
64:5p:10:TYR:CD1	16:8F:59:ARG:CD	2.67	0.62
67:5t:162:VAL:HA	67:5t:180:VAL:HB	1.81	0.62
30:H:31:HIS:ND1	30:H:32:TYR:O	2.30	0.62
60:l:87:LEU:HG	60:l:91:MET:HE2	1.82	0.62
27:5E:274:GLU:HB3	39:5Q:267:GLN:HE22	1.65	0.62
44:5V:22:ARG:NH2	50:5b:44:ASN:O	2.26	0.62
10:6T:2:THR:N	10:6T:5:LEU:HB2	2.14	0.62
16:2F:56:ASN:OD1	22:3L:65:PHE:N	2.32	0.62
29:5G:44:TRP:HB2	41:5S:278:ARG:HD2	1.81	0.62
29:5G:108:GLU:OE2	36:5N:44:ARG:NH1	2.33	0.62
40:5R:67:GLU:OE2	41:5S:268:TYR:OH	2.17	0.62
45:5W:1:MET:HG2	45:5W:4:GLU:HB2	1.80	0.62
67:5t:97:ARG:NH1	67:5t:99:ASP:OD2	2.33	0.62
26:D:269:ARG:NH1	29:G:139:GLU:OE2	2.33	0.62
36:N:132:LYS:HB3	36:N:141:ARG:HD2	1.80	0.62
65:q:188:PHE:O	67:t:104:ARG:NH2	2.31	0.62
68:u:9:THR:OG1	68:u:52:ARG:NH1	2.33	0.62
7:1M:442:ALA:HB2	9:1Q:61:THR:HG22	1.81	0.62
26:5D:269:ARG:NH1	29:5G:139:GLU:OE2	2.33	0.62
40:5R:146:ARG:NE	40:5R:156:GLU:OE2	2.27	0.62
44:5V:375:TRP:HB3	44:5V:378:LEU:HD12	1.81	0.62
44:5V:518:SER:OG	44:5V:519:PRO:HD3	2.00	0.62
35:M:49:PRO:HB2	35:M:62:ARG:HB3	1.80	0.62
40:R:67:GLU:OE2	41:S:268:TYR:OH	2.17	0.62
53:e:211:ASP:HB3	53:e:214:GLN:HG3	1.81	0.62
10:1T:2:THR:N	10:1T:5:LEU:HB2	2.14	0.62
35:5M:49:PRO:HB2	35:5M:62:ARG:HB3	1.80	0.62
36:5N:12:GLU:OE1	36:5N:60:ARG:NH2	2.32	0.62
29:G:46:GLN:OE1	29:G:49:ARG:NH2	2.33	0.62
29:G:150:GLU:HB2	29:G:163:ARG:HB3	1.82	0.62
41:S:223:TYR:HE1	45:W:69:VAL:HG22	1.63	0.62
67:t:56:ILE:HD11	67:t:72:VAL:HG21	1.82	0.62
1:1A:213:ASN:HD22	10:1R:41:PRO:HD2	1.65	0.62
67:5t:234:GLY:O	67:5t:237:TRP:NE1	2.32	0.62
7:6N:79:GLU:HG2	9:6S:411:ARG:HD3	1.82	0.62
15:2E:34:PHE:CE2	66:s:92:ARG:CD	2.41	0.61
38:5P:287:ARG:HB3	38:5P:378:MET:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:8A:43:ARG:HB2	20:8J:55:TYR:HB3	1.82	0.61
24:B:71:ASP:OD2	24:B:73:SER:OG	2.17	0.61
29:G:108:GLU:OE2	36:N:44:ARG:NH1	2.32	0.61
44:V:375:TRP:HB3	44:V:378:LEU:HD12	1.81	0.61
67:t:162:VAL:HA	67:t:180:VAL:HB	1.81	0.61
24:5B:299:ILE:HA	24:5B:375:VAL:HB	1.81	0.61
25:5C:124:GLU:O	25:5C:129:LYS:NZ	2.33	0.61
38:P:81:VAL:HA	38:P:104:VAL:HB	1.82	0.61
5:1J:30:ALA:CA	20:9J:96:ILE:HD11	2.31	0.61
38:5P:81:VAL:HA	38:5P:104:VAL:HB	1.81	0.61
43:5U:212:PHE:O	43:5U:216:SER:OG	2.14	0.61
24:B:141:SER:HB2	24:B:225:TYR:HD1	1.64	0.61
27:E:185:LEU:HD21	27:E:214:LEU:HB2	1.82	0.61
29:G:44:TRP:HB2	41:S:278:ARG:HD2	1.81	0.61
44:V:518:SER:OG	44:V:519:PRO:HD3	2.00	0.61
9:1Q:60:VAL:HG11	55:5g:11:ARG:CG	2.29	0.61
11:3A:43:ARG:HB2	20:3J:55:TYR:HB3	1.82	0.61
24:5B:141:SER:HB2	24:5B:225:TYR:HD1	1.64	0.61
42:5T:162:THR:HG22	42:5T:187:VAL:HG12	1.82	0.61
53:5e:99:LYS:HB3	72:5y:2:MET:CE	2.30	0.61
68:5u:9:THR:OG1	68:5u:52:ARG:NH1	2.33	0.61
1:6A:213:ASN:HD22	10:6R:41:PRO:HD2	1.65	0.61
7:6M:77:PHE:CZ	9:6Q:69:PRO:O	2.53	0.61
9:6Q:64:PRO:HG2	32:r:61:LYS:HB3	1.82	0.61
16:7F:56:ASN:OD1	22:8L:65:PHE:N	2.32	0.61
29:G:163:ARG:HH22	34:L:108:GLY:HA3	1.64	0.61
16:3F:59:ARG:HD2	64:p:10:TYR:HB2	1.81	0.61
11:9A:43:ARG:HB2	20:9J:55:TYR:HB3	1.82	0.61
65:q:65:HIS:HD1	65:q:82:TYR:HH	1.38	0.61
2:1D:180:LEU:HB3	2:1D:186:PRO:HB3	1.80	0.61
29:5G:46:GLN:OE1	29:5G:49:ARG:NH2	2.33	0.61
55:5g:18:HIS:HB3	55:5g:21:LEU:HB2	1.83	0.61
27:E:86:LEU:HD22	27:E:105:MET:HE1	1.82	0.61
40:R:36:GLN:HG3	40:R:60:LEU:HD12	1.81	0.61
11:4A:43:ARG:HB2	20:4J:55:TYR:HB3	1.82	0.61
29:5G:150:GLU:HB2	29:5G:163:ARG:HB3	1.82	0.61
44:5V:529:ILE:HG23	44:5V:533:ILE:HD12	1.83	0.61
1:6A:282:LEU:HB2	1:6A:295:ILE:HD11	1.83	0.61
15:2E:34:PHE:HB3	66:s:92:ARG:HD3	1.82	0.61
25:5C:207:GLU:O	25:5C:435:ARG:NE	2.32	0.61
27:5E:105:MET:HG3	27:5E:110:ILE:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5V:136:LEU:HD23	44:5V:194:LEU:HD13	1.82	0.61
44:5V:169:ALA:O	44:5V:173:ASN:ND2	2.32	0.61
64:5p:7:PHE:CZ	16:8F:55:TRP:CB	2.83	0.61
44:V:136:LEU:HD23	44:V:194:LEU:HD13	1.82	0.61
67:t:84:ILE:HA	67:t:105:LEU:HB3	1.83	0.61
9:1Q:62:GLU:CB	55:5g:11:ARG:HB3	2.28	0.61
50:5b:99:ARG:HA	50:5b:102:LYS:HE2	1.82	0.61
25:C:638:ARG:HD3	25:C:648:LEU:HB2	1.83	0.61
26:D:225:ILE:HG23	26:D:226:LEU:HG	1.82	0.61
27:5E:86:LEU:HD22	27:5E:105:MET:HE1	1.82	0.60
67:5t:84:ILE:HA	67:5t:105:LEU:HB3	1.83	0.60
5:6I:31:CYS:HA	5:6I:34:ARG:HE	1.66	0.60
11:7A:47:ASP:HA	20:7J:54:THR:HG21	1.83	0.60
38:P:239:ILE:HG22	38:P:337:LYS:HB3	1.83	0.60
42:T:162:THR:HG22	42:T:187:VAL:HG12	1.82	0.60
5:1I:31:CYS:HA	5:1I:34:ARG:HE	1.66	0.60
23:5A:263:GLU:O	24:5B:305:ARG:NH2	2.35	0.60
60:5l:87:LEU:HG	60:5l:91:MET:HE2	1.81	0.60
11:8A:106:PRO:HB3	14:8D:45:TYR:HB2	1.84	0.60
27:E:105:MET:HG3	27:E:110:ILE:HA	1.83	0.60
67:t:97:ARG:NH1	67:t:99:ASP:OD2	2.33	0.60
68:u:129:HIS:HB2	68:u:146:MET:HE3	1.83	0.60
25:5C:97:CYS:O	25:5C:110:SER:OG	2.19	0.60
25:5C:362:LYS:NZ	25:5C:712:THR:O	2.34	0.60
34:5L:101:LYS:HG2	34:5L:112:SER:HB2	1.83	0.60
44:5V:250:THR:HB	44:5V:321:LEU:HD11	1.84	0.60
56:5h:38:GLN:NE2	56:5h:56:LEU:O	2.30	0.60
1:6A:139:MET:HE1	1:6A:269:ILE:HA	1.84	0.60
23:A:263:GLU:O	24:B:305:ARG:NH2	2.35	0.60
25:C:362:LYS:NZ	25:C:712:THR:O	2.34	0.60
25:C:490:VAL:HG22	25:C:526:ASN:HB2	1.83	0.60
36:N:73:ARG:NH1	36:N:95:TRP:O	2.34	0.60
52:5d:76:ARG:HD3	64:5p:41:ILE:HD11	1.83	0.60
66:5s:196:MET:SD	85:5s:401:COO:H52	2.41	0.60
7:6M:54:SER:HA	9:6Q:64:PRO:O	2.02	0.60
7:6N:177:ARG:NH2	7:6N:223:ILE:O	2.35	0.60
27:E:462:PHE:HA	27:E:465:ILE:HB	1.84	0.60
57:i:27:ARG:HB2	57:i:35:ARG:HD3	1.83	0.60
1:1A:282:LEU:HB2	1:1A:295:ILE:HD11	1.83	0.60
26:5D:225:ILE:HG23	26:5D:226:LEU:HG	1.82	0.60
27:5E:185:LEU:HD21	27:5E:214:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:5a:46:LYS:HE2	32:5r:54:GLU:OE2	2.02	0.60
49:a:44:ASN:HD22	32:r:54:GLU:HG3	1.65	0.60
11:4A:106:PRO:HB3	14:4D:45:TYR:HB2	1.84	0.60
25:5C:490:VAL:HG22	25:5C:526:ASN:HB2	1.83	0.60
28:5F:93:PRO:HB2	39:5Q:59:GLU:HB3	1.84	0.60
39:5Q:155:ASP:OD2	54:5f:39:ASN:ND2	2.34	0.60
44:5V:356:HIS:HA	44:5V:434:VAL:HG13	1.82	0.60
53:5e:173:LYS:HA	53:5e:176:LYS:HG3	1.82	0.60
1:6B:50:LEU:HD22	1:6B:68:LEU:HD21	1.84	0.60
38:P:222:GLN:O	38:P:226:THR:OG1	2.18	0.60
38:P:287:ARG:HB3	38:P:378:MET:HG2	1.82	0.60
41:S:276:GLU:OE1	41:S:278:ARG:NH2	2.34	0.60
42:T:385:LEU:HD13	56:h:107:LEU:HD11	1.83	0.60
67:t:234:GLY:O	67:t:237:TRP:NE1	2.32	0.60
16:2F:56:ASN:HD21	22:3L:64:GLN:CG	2.15	0.60
14:4D:149:LYS:HG3	14:4D:150:ARG:H	1.67	0.60
24:5B:60:ASP:HA	24:5B:278:ARG:HH12	1.66	0.60
27:5E:353:ASN:OD1	61:5m:30:PHE:N	2.34	0.60
65:5q:86:ASP:HA	65:5q:187:GLN:HB2	1.83	0.60
67:5t:56:ILE:HD11	67:5t:72:VAL:HG21	1.82	0.60
67:5t:266:ARG:NH1	67:5t:270:GLU:OE2	2.35	0.60
20:7J:88:PHE:O	20:7J:91:ARG:NH1	2.34	0.60
26:D:211:MET:HB3	26:D:236:LEU:HD12	1.83	0.60
44:V:356:HIS:HA	44:V:434:VAL:HG13	1.82	0.60
49:a:40:HIS:O	49:a:64:THR:N	2.34	0.60
53:e:173:LYS:HA	53:e:176:LYS:HG3	1.82	0.60
65:q:68:ARG:NH1	67:t:125:THR:O	2.35	0.60
65:q:86:ASP:HA	65:q:187:GLN:HB2	1.83	0.60
66:s:196:MET:HG2	85:s:401:COO:H51	1.83	0.60
67:t:266:ARG:NH1	67:t:270:GLU:OE2	2.35	0.60
1:1A:139:MET:HE1	1:1A:269:ILE:HA	1.84	0.60
7:1N:79:GLU:HG2	9:1S:411:ARG:HD3	1.82	0.60
10:1T:4:LEU:HD23	10:1T:4:LEU:H	1.66	0.60
26:5D:178:ARG:NH1	27:5E:310:GLN:OE1	2.35	0.60
26:5D:206:ARG:NH2	26:5D:224:ARG:O	2.34	0.60
31:5I:80:GLU:OE1	31:5I:85:ARG:NH2	2.34	0.60
38:5P:385:ILE:O	38:5P:390:ARG:NH2	2.33	0.60
42:5T:385:LEU:HD13	56:5h:107:LEU:HD11	1.83	0.60
50:5b:112:ASP:OD1	63:5o:97:ARG:NH2	2.35	0.60
64:5p:10:TYR:HB2	16:8F:59:ARG:CZ	2.32	0.60
44:V:250:THR:HB	44:V:321:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:168:TYR:HB2	26:5D:181:VAL:HB	1.83	0.60
29:5G:226:THR:HG21	30:5H:45:GLY:HA2	1.84	0.60
42:5T:162:THR:HB	42:5T:188:LEU:HA	1.84	0.60
27:E:435:HIS:HB3	27:E:458:LEU:HD22	1.83	0.60
31:I:80:GLU:OE1	31:I:85:ARG:NH2	2.34	0.60
53:e:99:LYS:HB3	72:y:2:MET:CE	2.30	0.60
11:2A:47:ASP:HA	20:2J:54:THR:HG21	1.83	0.60
41:5S:276:GLU:OE1	41:5S:278:ARG:NH2	2.34	0.60
68:5u:129:HIS:HB2	68:5u:146:MET:HE3	1.83	0.60
10:6T:4:LEU:HD23	10:6T:4:LEU:H	1.66	0.60
14:8D:149:LYS:HG3	14:8D:150:ARG:H	1.67	0.60
26:D:206:ARG:NH2	26:D:224:ARG:O	2.35	0.60
27:E:274:GLU:HB3	39:Q:267:GLN:HE22	1.65	0.60
44:V:189:TYR:O	63:o:117:ARG:NE	2.35	0.60
29:5G:37:ARG:NH1	29:5G:75:ASP:OD1	2.34	0.59
36:5N:73:ARG:NH1	36:5N:95:TRP:O	2.34	0.59
42:5T:342:LEU:HB2	42:5T:409:VAL:HA	1.84	0.59
57:5i:27:ARG:HB2	57:5i:35:ARG:HD3	1.83	0.59
66:5s:92:ARG:HD3	15:7E:34:PHE:CB	2.31	0.59
22:8L:5:PHE:CG	22:8L:6:LYS:N	2.70	0.59
50:b:112:ASP:OD1	63:o:97:ARG:NH2	2.35	0.59
11:2A:281:VAL:O	11:2A:284:HIS:ND1	2.24	0.59
66:5s:207:LYS:HG3	66:5s:225:PRO:HA	1.84	0.59
22:9L:5:PHE:CG	22:9L:6:LYS:N	2.70	0.59
26:D:178:ARG:NH1	27:E:310:GLN:OE1	2.35	0.59
27:E:142:ARG:NH2	28:F:134:CYS:SG	2.70	0.59
34:L:101:LYS:HG2	34:L:112:SER:HB2	1.83	0.59
39:Q:155:ASP:OD2	54:f:39:ASN:ND2	2.34	0.59
44:V:529:ILE:HG23	44:V:533:ILE:HD12	1.83	0.59
61:m:96:ARG:NE	62:n:6:VAL:O	2.35	0.59
20:2J:88:PHE:O	20:2J:91:ARG:NH1	2.35	0.59
23:5A:80:TYR:OH	24:5B:219:HIS:ND1	2.21	0.59
44:5V:189:TYR:O	63:5o:117:ARG:NE	2.35	0.59
39:Q:18:ALA:HB1	39:Q:48:PRO:HB2	1.85	0.59
66:s:15:PRO:HB2	66:s:275:TYR:HE2	1.67	0.59
11:3A:392:ASN:ND2	20:3J:12:GLU:OE1	2.35	0.59
22:4L:5:PHE:CG	22:4L:6:LYS:N	2.70	0.59
26:5D:211:MET:HB3	26:5D:236:LEU:HD12	1.82	0.59
38:5P:222:GLN:O	38:5P:226:THR:OG1	2.18	0.59
67:5t:144:VAL:HB	67:5t:161:VAL:HG12	1.84	0.59
29:G:37:ARG:NH1	29:G:75:ASP:OD1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:44:ASN:HD22	32:r:54:GLU:CG	2.16	0.59
50:b:99:ARG:HA	50:b:102:LYS:HE2	1.82	0.59
7:1N:177:ARG:NH2	7:1N:223:ILE:O	2.35	0.59
15:2E:34:PHE:CB	66:s:92:ARG:HD3	2.31	0.59
14:3D:149:LYS:HG3	14:3D:150:ARG:H	1.67	0.59
25:5C:638:ARG:HD3	25:5C:648:LEU:HB2	1.83	0.59
38:5P:64:PHE:HZ	38:5P:210:GLY:HA3	1.67	0.59
48:5Z:23:LYS:NZ	48:5Z:31:PHE:O	2.34	0.59
29:G:85:VAL:HG22	39:Q:260:LEU:HD21	1.84	0.59
54:f:36:TRP:O	54:f:40:LYS:NZ	2.29	0.59
67:t:62:LYS:NZ	67:t:99:ASP:O	2.34	0.59
67:t:144:VAL:HB	67:t:161:VAL:HG12	1.84	0.59
7:1M:447:ARG:NH2	9:1Q:49:VAL:HG12	2.17	0.59
11:4A:392:ASN:ND2	20:4J:12:GLU:OE1	2.35	0.59
42:5T:116:LEU:HB2	42:5T:178:MET:HE1	1.83	0.59
66:5s:92:ARG:HD3	15:7E:34:PHE:HB3	1.82	0.59
11:8A:392:ASN:ND2	20:8J:12:GLU:OE1	2.35	0.59
42:T:162:THR:HB	42:T:188:LEU:HA	1.84	0.59
52:d:76:ARG:HD3	64:p:41:ILE:HD11	1.83	0.59
66:s:150:GLN:HE22	85:s:401:COO:H9	1.68	0.59
11:3A:106:PRO:HB3	14:3D:45:TYR:HB2	1.84	0.59
27:5E:435:HIS:HB3	27:5E:458:LEU:HD22	1.83	0.59
44:5V:65:THR:OG1	44:5V:74:ALA:O	2.19	0.59
67:5t:62:LYS:NZ	67:5t:99:ASP:O	2.34	0.59
11:9A:392:ASN:ND2	20:9J:12:GLU:OE1	2.35	0.59
25:C:419:VAL:HB	25:C:491:VAL:HG22	1.85	0.59
28:F:93:PRO:HB2	39:Q:59:GLU:HB3	1.84	0.59
38:P:385:ILE:O	38:P:390:ARG:NH2	2.33	0.59
42:T:116:LEU:HB2	42:T:178:MET:HE1	1.83	0.59
44:V:319:GLY:HA2	44:V:461:THR:HG21	1.85	0.59
22:3L:5:PHE:CG	22:3L:6:LYS:N	2.70	0.59
20:4J:84:TYR:OH	5:6J:22:VAL:HB	2.02	0.59
42:5T:245:PRO:HB2	56:5h:135:LEU:HD11	1.85	0.59
49:5a:57:TYR:HB3	49:5a:64:THR:CG2	2.33	0.59
66:5s:150:GLN:HE22	85:5s:401:COO:H9	1.68	0.59
7:6M:66:ASN:ND2	7:6M:265:VAL:O	2.31	0.59
7:6M:177:ARG:NH2	7:6M:223:ILE:O	2.36	0.59
24:B:482:ALA:HB2	61:m:10:PRO:HB2	1.84	0.59
40:R:100:LEU:HD13	43:U:200:GLU:HG2	1.85	0.59
66:s:207:LYS:HG3	66:s:225:PRO:HA	1.84	0.59
61:5m:110:LYS:O	61:5m:113:LYS:NZ	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:9A:106:PRO:HB3	14:9D:45:TYR:HB2	1.84	0.59
26:D:113:ALA:HA	26:D:121:GLU:HB2	1.85	0.59
27:E:286:MET:O	27:E:290:TRP:N	2.35	0.59
63:o:107:ASN:HA	63:o:110:ARG:HD3	1.85	0.59
16:2F:59:ARG:NH1	22:3L:65:PHE:O	2.36	0.59
26:5D:256:ARG:HD3	33:5K:95:HIS:HB3	1.85	0.59
40:5R:100:LEU:HD13	43:5U:200:GLU:HG2	1.85	0.59
64:5p:10:TYR:HB2	16:8F:59:ARG:HD2	1.81	0.59
65:5q:68:ARG:NH1	67:5t:125:THR:O	2.35	0.59
14:9D:149:LYS:HG3	14:9D:150:ARG:H	1.67	0.59
49:a:46:LYS:HE2	32:r:54:GLU:OE2	2.01	0.59
1:1B:50:LEU:HD22	1:1B:68:LEU:HD21	1.84	0.58
9:1Q:61:THR:HB	9:1Q:65:ARG:HH21	1.68	0.58
38:5P:41:ASP:HB2	38:5P:53:GLY:HA3	1.85	0.58
9:6Q:60:VAL:CG2	55:g:11:ARG:CA	2.80	0.58
49:a:65:MET:SD	55:g:18:HIS:ND1	2.76	0.58
24:5B:482:ALA:HB2	61:5m:10:PRO:HB2	1.84	0.58
39:5Q:89:ILE:HD11	39:5Q:228:VAL:HG13	1.85	0.58
52:5d:31:ARG:NH1	67:5t:228:ARG:O	2.37	0.58
6:6L:15:GLN:HB2	7:6N:289:TYR:HB3	1.84	0.58
16:7F:41:THR:HG21	22:8L:16:LEU:HD11	1.86	0.58
24:B:60:ASP:HA	24:B:278:ARG:HH12	1.66	0.58
26:D:168:TYR:HB2	26:D:181:VAL:HB	1.83	0.58
35:M:75:ASN:HB3	35:M:78:ASP:HB2	1.85	0.58
48:Z:23:LYS:NZ	48:Z:31:PHE:O	2.34	0.58
49:a:44:ASN:O	49:a:46:LYS:NZ	2.37	0.58
38:5P:239:ILE:HG22	38:5P:337:LYS:HB3	1.83	0.58
49:5a:49:PRO:HG2	49:5a:52:LEU:HB2	1.86	0.58
66:5s:15:PRO:HB2	66:5s:275:TYR:HE2	1.67	0.58
16:7F:59:ARG:NH1	22:8L:65:PHE:O	2.36	0.58
52:d:31:ARG:NH1	67:t:228:ARG:O	2.36	0.58
67:t:83:ASP:HB2	67:t:104:ARG:HA	1.85	0.58
25:5C:419:VAL:HB	25:5C:491:VAL:HG22	1.85	0.58
27:5E:462:PHE:HA	27:5E:465:ILE:HB	1.84	0.58
31:5I:41:ARG:HH12	31:5I:105:ASP:CG	2.12	0.58
36:5N:112:PRO:HG2	36:5N:115:GLN:HB2	1.86	0.58
54:5f:38:ASN:O	54:5f:40:LYS:NZ	2.32	0.58
65:5q:60:MET:HE3	65:5q:165:PRO:HA	1.86	0.58
9:6Q:56:LYS:HE3	9:6Q:57:LEU:H	1.67	0.58
11:7A:211:ASN:O	21:7K:58:ARG:NH2	2.33	0.58
35:M:51:THR:OG1	35:M:60:ASP:OD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:T:342:LEU:HB2	42:T:409:VAL:HA	1.84	0.58
11:4A:211:ASN:O	21:4K:58:ARG:NH2	2.36	0.58
38:5P:288:ILE:HG22	38:5P:290:ARG:H	1.68	0.58
39:5Q:18:ALA:HB1	39:5Q:48:PRO:HB2	1.85	0.58
42:5T:79:LEU:HD21	42:5T:314:GLY:HA3	1.84	0.58
29:G:226:THR:HG21	30:H:45:GLY:HA2	1.84	0.58
39:Q:89:ILE:HD11	39:Q:228:VAL:HG13	1.85	0.58
66:s:51:GLN:HG2	66:s:54:GLN:HE21	1.68	0.58
16:3F:59:ARG:CZ	64:p:10:TYR:HB2	2.32	0.58
35:5M:75:ASN:HB3	35:5M:78:ASP:HB2	1.85	0.58
53:5e:12:SER:HB2	56:5h:138:GLU:HB2	1.85	0.58
28:F:72:ILE:HG12	28:F:99:VAL:HB	1.86	0.58
53:e:59:ILE:HG21	53:e:108:GLY:HA3	1.84	0.58
16:2F:41:THR:HG21	22:3L:16:LEU:HD11	1.85	0.58
53:5e:81:THR:HG23	53:5e:82:LEU:HD12	1.86	0.58
26:5D:113:ALA:HA	26:5D:121:GLU:HB2	1.85	0.58
39:5Q:140:LEU:HD11	41:5S:229:TYR:HA	1.85	0.58
1:6A:71:ASP:OD2	3:6F:122:ARG:NH2	2.37	0.58
26:D:236:LEU:HD23	27:E:126:LYS:HB2	1.85	0.58
38:P:64:PHE:HZ	38:P:210:GLY:HA3	1.67	0.58
6:1L:15:GLN:HB2	7:1N:289:TYR:HB3	1.84	0.58
26:5D:237:ARG:O	27:5E:126:LYS:NZ	2.29	0.58
28:5F:72:ILE:HG12	28:5F:99:VAL:HB	1.86	0.58
41:5S:245:THR:HG22	45:5W:123:THR:HA	1.86	0.58
44:5V:205:SER:OG	46:5X:145:TRP:O	2.22	0.58
53:5e:59:ILE:HG21	53:5e:108:GLY:HA3	1.84	0.58
26:D:281:ASN:O	26:D:282:ARG:NH1	2.34	0.58
31:I:41:ARG:HH12	31:I:105:ASP:CG	2.12	0.58
52:d:76:ARG:NH1	53:e:192:ASP:HA	2.19	0.58
9:6Q:67:SER:CB	32:r:69:SER:HB3	2.34	0.58
25:C:97:CYS:O	25:C:110:SER:OG	2.19	0.58
25:C:109:ALA:O	25:C:113:MET:N	2.33	0.58
42:T:79:LEU:HD21	42:T:314:GLY:HA3	1.84	0.58
65:q:60:MET:HE3	65:q:165:PRO:HA	1.86	0.58
26:D:77:LYS:O	30:H:109:ARG:NH2	2.36	0.57
27:E:353:ASN:OD1	61:m:30:PHE:N	2.33	0.57
38:P:288:ILE:HG22	38:P:290:ARG:H	1.69	0.57
40:R:36:GLN:HG2	40:R:57:VAL:HG13	1.86	0.57
46:X:61:PHE:HE1	46:X:67:PRO:HD2	1.69	0.57
53:e:12:SER:HB2	56:h:138:GLU:HB2	1.85	0.57
7:1M:66:ASN:ND2	7:1M:265:VAL:O	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:236:LEU:HD23	27:5E:126:LYS:HB2	1.85	0.57
27:5E:408:LYS:HE2	27:5E:461:VAL:HG23	1.86	0.57
45:5W:89:THR:HG21	53:5e:90:ALA:HB2	1.86	0.57
26:D:111:GLY:N	26:D:121:GLU:O	2.27	0.57
29:G:158:SER:OG	29:G:160:ARG:NE	2.25	0.57
39:Q:140:LEU:HD11	41:S:229:TYR:HA	1.85	0.57
44:5V:319:GLY:HA2	44:5V:461:THR:HG21	1.85	0.57
46:5X:120:ARG:O	46:5X:123:SER:OG	2.20	0.57
12:7B:139:HIS:HB3	18:7H:39:LEU:HD22	1.86	0.57
24:B:58:ASP:HA	24:B:61:ARG:HG3	1.86	0.57
26:D:256:ARG:HD3	33:K:95:HIS:HB3	1.85	0.57
38:P:41:ASP:HB2	38:P:53:GLY:HA3	1.85	0.57
66:s:17:ARG:HG3	68:u:35:VAL:HG22	1.85	0.57
25:5C:257:PHE:HD2	29:5G:153:GLU:HB3	1.69	0.57
61:5m:135:SER:OG	61:5m:137:ASP:OD1	2.21	0.57
64:5p:62:ILE:HB	64:5p:73:GLU:HG2	1.86	0.57
43:U:155:ASN:H	43:U:158:ILE:HD13	1.69	0.57
44:V:205:SER:OG	46:X:145:TRP:O	2.22	0.57
53:e:81:THR:HG23	53:e:82:LEU:HD12	1.86	0.57
12:2B:156:VAL:HG13	12:2B:157:LYS:HG2	1.87	0.57
27:5E:306:LEU:HB2	27:5E:405:GLU:HB2	1.86	0.57
29:5G:85:VAL:HG22	39:5Q:260:LEU:HD21	1.84	0.57
42:5T:364:PRO:HB3	44:5V:140:VAL:HG22	1.85	0.57
49:5a:44:ASN:HD22	32:5r:54:GLU:CD	2.13	0.57
49:5a:57:TYR:HB3	49:5a:64:THR:HG21	1.87	0.57
63:5o:107:ASN:HA	63:5o:110:ARG:HD3	1.85	0.57
32:5r:56:VAL:O	32:5r:60:THR:OG1	2.20	0.57
27:E:306:LEU:HB2	27:E:405:GLU:HB2	1.86	0.57
33:K:39:GLN:NE2	33:K:48:VAL:O	2.37	0.57
36:N:112:PRO:HG2	36:N:115:GLN:HB2	1.85	0.57
42:T:245:PRO:HB2	56:h:135:LEU:HD11	1.85	0.57
44:V:2:PHE:HA	44:V:47:ILE:HD11	1.87	0.57
44:V:525:ASP:HA	44:V:528:ARG:HG2	1.86	0.57
64:p:65:ARG:NE	64:p:66:THR:O	2.38	0.57
27:5E:361:LYS:NZ	27:5E:369:PRO:O	2.35	0.57
52:5d:76:ARG:NH1	53:5e:192:ASP:HA	2.19	0.57
66:5s:156:HIS:HB3	66:5s:184:HIS:HD2	1.70	0.57
27:E:270:ARG:NH2	29:G:79:MET:O	2.28	0.57
55:g:18:HIS:HB3	55:g:21:LEU:HB2	1.85	0.57
1:1B:110:ARG:NH1	1:1B:205:GLY:O	2.38	0.57
12:2B:139:HIS:HB3	18:2H:39:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:279:THR:O	26:5D:282:ARG:NH1	2.30	0.57
29:5G:102:THR:O	36:5N:71:ARG:NH1	2.37	0.57
66:5s:51:GLN:HG2	66:5s:54:GLN:HE21	1.68	0.57
67:5t:133:ILE:HA	67:5t:150:VAL:HB	1.87	0.57
9:6Q:46:GLY:H	9:6Q:48:ARG:NH2	2.02	0.57
11:8A:173:MET:HE3	11:8A:178:MET:HG2	1.87	0.57
37:O:78:THR:H	37:O:81:ALA:HB3	1.70	0.57
46:X:120:ARG:O	46:X:123:SER:OG	2.20	0.57
67:t:191:LEU:HD23	67:t:201:ARG:HG2	1.87	0.57
11:2A:211:ASN:O	21:2K:58:ARG:NH2	2.33	0.57
41:5S:148:VAL:HG12	54:5f:56:ARG:HB3	1.85	0.57
46:5X:61:PHE:HE1	46:5X:67:PRO:HD2	1.69	0.57
66:5s:17:ARG:HG3	68:5u:35:VAL:HG22	1.85	0.57
66:5s:150:GLN:NE2	85:5s:401:COO:H9	2.20	0.57
68:5u:152:GLU:HB2	68:5u:170:GLU:HG3	1.85	0.57
11:8A:211:ASN:O	21:8K:58:ARG:NH2	2.36	0.57
26:D:110:THR:HA	26:D:122:PRO:HA	1.86	0.57
41:S:148:VAL:HG12	54:f:56:ARG:HB3	1.86	0.57
66:s:156:HIS:HB3	66:s:184:HIS:HD2	1.70	0.57
9:1Q:65:ARG:O	32:5r:68:ALA:CB	2.52	0.57
24:5B:58:ASP:HA	24:5B:61:ARG:HG3	1.86	0.57
42:5T:280:VAL:O	42:5T:283:SER:OG	2.22	0.57
44:5V:2:PHE:HA	44:5V:47:ILE:HD11	1.87	0.57
66:5s:187:THR:HB	66:5s:205:THR:HG23	1.86	0.57
68:5u:104:GLN:HB3	68:5u:129:HIS:CD2	2.40	0.57
10:6R:4:LEU:O	10:6R:8:VAL:HG23	2.05	0.57
12:7B:156:VAL:HG13	12:7B:157:LYS:HG2	1.86	0.57
27:E:264:GLU:OE1	29:G:87:ARG:NH1	2.38	0.57
29:G:102:THR:O	36:N:71:ARG:NH1	2.37	0.57
42:T:364:PRO:HB3	44:V:140:VAL:HG22	1.85	0.57
44:V:546:ALA:N	65:q:123:ASP:OD1	2.37	0.57
64:p:62:ILE:HB	64:p:73:GLU:HG2	1.86	0.57
4:1H:16:ARG:HB2	4:1H:19:VAL:HG22	1.87	0.57
10:1R:4:LEU:O	10:1R:8:VAL:HG23	2.05	0.57
64:5p:65:ARG:NE	64:5p:66:THR:O	2.38	0.57
45:W:89:THR:HG21	53:e:90:ALA:HB2	1.86	0.57
46:X:45:GLU:CD	56:h:76:ARG:HH12	2.13	0.57
61:m:135:SER:OG	61:m:137:ASP:OD1	2.21	0.57
7:1M:177:ARG:NH2	7:1M:223:ILE:O	2.36	0.56
15:2E:34:PHE:HD2	66:s:92:ARG:CD	1.95	0.56
38:5P:114:ASP:HA	38:5P:117:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5V:525:ASP:HA	44:5V:528:ARG:HG2	1.86	0.56
61:5m:96:ARG:NE	62:5n:6:VAL:O	2.35	0.56
67:5t:159:ARG:HB2	68:5u:149:ILE:HD11	1.87	0.56
68:5u:110:GLY:O	68:5u:134:LYS:HA	2.05	0.56
26:D:250:TYR:HB2	26:D:257:VAL:HG22	1.87	0.56
40:R:378:LYS:HD2	42:T:62:ARG:HG3	1.87	0.56
41:S:245:THR:HG22	45:W:123:THR:HA	1.86	0.56
43:U:219:ASP:O	43:U:221:GLU:N	2.38	0.56
32:r:56:VAL:O	32:r:60:THR:OG1	2.20	0.56
68:u:110:GLY:O	68:u:134:LYS:HA	2.05	0.56
68:u:152:GLU:HB2	68:u:170:GLU:HG3	1.85	0.56
17:3G:82:ILE:HG21	17:3G:88:MET:HE2	1.87	0.56
27:5E:264:GLU:OE1	29:5G:87:ARG:NH1	2.38	0.56
42:5T:195:VAL:O	42:5T:199:LYS:HG3	2.04	0.56
46:5X:45:GLU:CD	56:5h:76:ARG:HH12	2.13	0.56
49:5a:67:LYS:HG2	55:5g:20:LEU:HD11	1.87	0.56
27:E:366:LYS:HD2	30:H:66:TYR:CZ	2.40	0.56
31:I:116:LEU:HA	31:I:119:LEU:HD12	1.87	0.56
39:Q:139:GLU:HA	39:Q:142:LEU:HD12	1.86	0.56
46:X:46:LEU:O	46:X:58:ALA:N	2.38	0.56
56:h:61:GLN:HG3	59:k:102:ILE:HD11	1.87	0.56
64:p:52:ASP:O	64:p:56:ASN:ND2	2.38	0.56
23:5A:83:ASN:HD21	34:5L:174:PRO:HA	1.70	0.56
26:5D:250:TYR:HB2	26:5D:257:VAL:HG22	1.87	0.56
27:5E:465:ILE:O	27:5E:467:ARG:NH1	2.39	0.56
29:5G:167:ASP:OD1	29:5G:169:THR:OG1	2.17	0.56
33:5K:39:GLN:NE2	33:5K:48:VAL:O	2.38	0.56
34:5L:79:LEU:O	34:5L:82:THR:OG1	2.22	0.56
37:5O:78:THR:H	37:5O:81:ALA:HB3	1.70	0.56
38:5P:227:VAL:HG23	38:5P:228:PHE:HD1	1.70	0.56
40:5R:301:PHE:HE2	42:5T:121:ILE:HG12	1.70	0.56
43:5U:219:ASP:O	43:5U:221:GLU:N	2.38	0.56
44:5V:247:THR:O	44:5V:249:VAL:N	2.38	0.56
59:5k:17:ARG:NH2	32:5r:109:ASP:OD2	2.38	0.56
67:5t:191:LEU:HD23	67:5t:201:ARG:HG2	1.87	0.56
3:6E:306:GLN:O	10:6T:75:LYS:NZ	2.33	0.56
9:6Q:476:ARG:HH11	9:6S:292:GLY:HA3	1.70	0.56
17:8G:82:ILE:HG21	17:8G:88:MET:HE2	1.87	0.56
30:H:70:ASP:O	30:H:74:ASN:ND2	2.30	0.56
34:L:79:LEU:O	34:L:82:THR:OG1	2.22	0.56
67:t:133:ILE:HA	67:t:150:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1Q:476:ARG:HH11	9:1S:292:GLY:HA3	1.70	0.56
16:3F:55:TRP:HB3	64:p:7:PHE:CZ	2.39	0.56
20:4J:102:ALA:C	5:6J:29:LYS:CE	2.75	0.56
24:5B:150:GLU:OE2	24:5B:153:ARG:NH2	2.38	0.56
30:5H:31:HIS:ND1	30:5H:32:TYR:O	2.30	0.56
38:5P:233:GLU:OE2	38:5P:298:ALA:N	2.37	0.56
1:6B:110:ARG:NH1	1:6B:205:GLY:O	2.38	0.56
9:6Q:67:SER:HB3	32:r:69:SER:N	2.16	0.56
23:A:83:ASN:HD21	34:L:174:PRO:HA	1.70	0.56
42:T:195:VAL:O	42:T:199:LYS:HG3	2.04	0.56
27:5E:286:MET:O	27:5E:290:TRP:N	2.35	0.56
40:5R:36:GLN:HG2	40:5R:57:VAL:HG13	1.86	0.56
42:5T:352:LEU:HD13	42:5T:427:VAL:HG11	1.88	0.56
67:5t:83:ASP:HB2	67:5t:104:ARG:HA	1.85	0.56
22:9L:7:LEU:HB2	22:9L:12:TYR:OH	2.06	0.56
40:R:181:TYR:HA	40:R:189:LEU:HD11	1.86	0.56
16:2F:56:ASN:OD1	22:3L:64:GLN:O	2.23	0.56
22:3L:7:LEU:HB2	22:3L:12:TYR:OH	2.06	0.56
17:4G:82:ILE:HG21	17:4G:88:MET:HE2	1.87	0.56
39:5Q:139:GLU:HA	39:5Q:142:LEU:HD12	1.86	0.56
40:5R:181:TYR:HA	40:5R:189:LEU:HD11	1.86	0.56
44:5V:546:ALA:N	65:5q:123:ASP:OD1	2.37	0.56
1:6A:24:MET:HE2	1:6A:217:SER:HB3	1.88	0.56
16:7F:56:ASN:OD1	22:8L:64:GLN:O	2.23	0.56
17:9G:82:ILE:HG21	17:9G:88:MET:HE2	1.87	0.56
25:C:182:LYS:NZ	25:C:224:GLU:OE2	2.32	0.56
27:E:408:LYS:HE2	27:E:461:VAL:HG23	1.86	0.56
36:N:36:ASN:HB2	39:Q:39:VAL:HG13	1.88	0.56
38:P:227:VAL:HG23	38:P:228:PHE:HD1	1.70	0.56
44:V:247:THR:O	44:V:249:VAL:N	2.38	0.56
24:5B:230:GLU:HG3	81:5B:501:FMN:H3'	1.87	0.56
40:5R:360:THR:OG1	52:5d:21:LYS:NZ	2.39	0.56
43:5U:155:ASN:H	43:5U:158:ILE:HD13	1.69	0.56
55:5g:10:GLU:OE2	59:5k:37:TYR:HB3	2.06	0.56
10:6T:2:THR:O	10:6T:5:LEU:HB3	2.06	0.56
26:D:228:ASP:HB3	26:D:231:PHE:HB2	1.88	0.56
27:E:192:THR:HB	27:E:204:PHE:HA	1.88	0.56
38:P:125:ASN:HA	38:P:163:VAL:HA	1.88	0.56
40:R:74:LEU:HD23	40:R:77:ILE:HD12	1.88	0.56
66:s:187:THR:HB	66:s:205:THR:HG23	1.86	0.56
7:1M:55:THR:HG22	9:1Q:66:THR:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1T:2:THR:O	10:1T:5:LEU:HB3	2.06	0.56
26:5D:228:ASP:HB3	26:5D:231:PHE:HB2	1.88	0.56
41:5S:227:ILE:HD12	45:5W:151:ARG:HE	1.71	0.56
46:5X:46:LEU:O	46:5X:58:ALA:N	2.38	0.56
4:6H:16:ARG:HB2	4:6H:19:VAL:HG22	1.87	0.56
11:7A:281:VAL:O	11:7A:284:HIS:ND1	2.24	0.56
38:P:157:ALA:O	38:P:160:THR:OG1	2.24	0.56
50:b:124:LEU:HD13	50:b:166:ILE:HG21	1.88	0.56
9:1Q:60:VAL:HG21	55:5g:11:ARG:CB	2.35	0.56
16:3F:59:ARG:NE	64:p:10:TYR:CB	2.69	0.56
27:5E:192:THR:HB	27:5E:204:PHE:HA	1.88	0.56
29:5G:167:ASP:O	29:5G:171:CYS:N	2.39	0.56
44:5V:306:SER:HB3	44:5V:317:SER:HB2	1.88	0.56
55:5g:4:VAL:HB	55:5g:8:GLN:NE2	2.16	0.56
56:5h:61:GLN:HG3	59:5k:102:ILE:HD11	1.87	0.56
16:7F:56:ASN:HD21	22:8L:64:GLN:CG	2.15	0.56
24:B:150:GLU:OE2	24:B:153:ARG:NH2	2.38	0.56
38:P:114:ASP:HA	38:P:117:ILE:HD12	1.87	0.56
40:R:360:THR:OG1	52:d:21:LYS:NZ	2.39	0.56
44:V:306:SER:HB3	44:V:317:SER:HB2	1.88	0.56
7:1M:50:THR:HG22	9:1Q:63:PRO:HG3	1.87	0.56
7:1M:442:ALA:HB2	9:1Q:61:THR:HG23	1.87	0.56
19:3I:62:GLN:NE2	19:3I:64:GLU:OE2	2.40	0.56
27:5E:366:LYS:HD2	30:5H:66:TYR:CZ	2.41	0.56
39:5Q:154:THR:O	61:5m:71:LYS:NZ	2.34	0.56
44:5V:197:ASP:HB3	63:5o:80:VAL:HG11	1.88	0.56
53:5e:143:MET:O	6:6K:36:LEU:HD11	2.06	0.56
65:5q:191:PRO:O	67:5t:85:TYR:OH	2.14	0.56
1:6B:283:ARG:HH21	1:6B:341:ILE:HG12	1.71	0.56
24:B:230:GLU:HG3	81:B:502:FMN:H3'	1.87	0.56
25:C:257:PHE:HD2	29:G:153:GLU:HB3	1.69	0.56
39:Q:154:THR:O	61:m:71:LYS:NZ	2.34	0.56
42:T:260:LEU:HD11	42:T:386:LEU:HD22	1.88	0.56
68:u:104:GLN:HB3	68:u:129:HIS:CD2	2.40	0.56
9:1Q:47:GLY:O	9:1Q:48:ARG:NE	2.39	0.55
27:5E:274:GLU:HB3	39:5Q:267:GLN:NE2	2.21	0.55
28:5F:31:TRP:N	28:5F:69:ASP:OD2	2.36	0.55
28:5F:129:VAL:HG21	28:5F:148:LEU:HB2	1.87	0.55
9:6Q:62:GLU:HB2	55:g:11:ARG:HA	1.76	0.55
25:C:638:ARG:NH2	25:C:651:ASP:OD1	2.40	0.55
42:T:7:LEU:HD23	42:T:36:PRO:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:224:ARG:N	33:5K:82:GLU:OE2	2.24	0.55
36:5N:36:ASN:HB2	39:5Q:39:VAL:HG13	1.88	0.55
39:5Q:57:VAL:HG12	41:5S:191:ILE:HD12	1.88	0.55
42:5T:123:PHE:CZ	42:5T:199:LYS:HD3	2.42	0.55
42:5T:341:GLY:HA3	42:5T:413:PRO:HA	1.88	0.55
50:5b:124:LEU:HD13	50:5b:166:ILE:HG21	1.88	0.55
66:5s:83:VAL:HG22	66:5s:100:VAL:HG22	1.88	0.55
19:8I:62:GLN:NE2	19:8I:64:GLU:OE2	2.40	0.55
11:9A:173:MET:HE3	11:9A:178:MET:HG2	1.87	0.55
27:E:465:ILE:O	27:E:467:ARG:NH1	2.39	0.55
28:F:89:TYR:HA	28:F:92:MET:HG3	1.87	0.55
42:T:341:GLY:HA3	42:T:413:PRO:HA	1.88	0.55
42:T:352:LEU:HD13	42:T:427:VAL:HG11	1.88	0.55
53:e:79:PRO:HG2	53:e:82:LEU:HB2	1.88	0.55
9:1Q:65:ARG:HH11	9:1Q:65:ARG:HA	1.72	0.55
11:3A:173:MET:HE3	11:3A:178:MET:HG2	1.87	0.55
22:3L:69:ARG:HB2	22:3L:74:LYS:HB2	1.88	0.55
25:5C:159:GLN:NE2	82:5C:803:SF4:S2	2.80	0.55
44:5V:223:ILE:HG13	44:5V:224:LEU:HG	1.89	0.55
64:5p:7:PHE:CZ	16:8F:55:TRP:HB3	2.40	0.55
66:5s:72:ARG:NH1	66:5s:73:LYS:O	2.39	0.55
22:8L:7:LEU:HB2	22:8L:12:TYR:OH	2.06	0.55
40:R:230:TYR:OH	44:V:544:LEU:O	2.23	0.55
41:S:227:ILE:HD12	45:W:151:ARG:HE	1.71	0.55
64:p:96:HIS:NE2	64:p:98:SER:OG	2.39	0.55
14:3D:97:ARG:HG2	14:3D:248:ALA:HB2	1.88	0.55
11:4A:173:MET:HE3	11:4A:178:MET:HG2	1.87	0.55
25:5C:182:LYS:NZ	25:5C:224:GLU:OE2	2.32	0.55
27:5E:88:PHE:HB3	27:5E:101:LEU:HB2	1.89	0.55
28:5F:89:TYR:HA	28:5F:92:MET:HG3	1.87	0.55
38:5P:378:MET:N	38:5P:378:MET:SD	2.79	0.55
42:5T:7:LEU:HD23	42:5T:36:PRO:HG3	1.89	0.55
44:5V:398:ILE:HD11	46:5X:94:ALA:HB2	1.88	0.55
7:6M:443:GLU:HG3	9:6Q:55:GLU:OE1	2.07	0.55
26:D:148:CYS:HB3	26:D:171:LEU:HB3	1.89	0.55
27:E:274:GLU:HB3	39:Q:267:GLN:NE2	2.21	0.55
40:R:301:PHE:HE2	42:T:121:ILE:HG12	1.70	0.55
42:T:123:PHE:CZ	42:T:199:LYS:HD3	2.42	0.55
43:U:205:LEU:HD22	45:W:69:VAL:HG11	1.88	0.55
66:s:162:MET:HE1	68:u:192:ARG:HH21	1.71	0.55
14:3D:157:VAL:HG13	14:3D:187:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5C:638:ARG:NH2	25:5C:651:ASP:OD1	2.39	0.55
26:5D:77:LYS:O	30:5H:109:ARG:NH2	2.36	0.55
31:5I:116:LEU:HA	31:5I:119:LEU:HD12	1.87	0.55
37:5O:11:MET:HG3	37:5O:46:PHE:HZ	1.71	0.55
38:5P:125:ASN:HA	38:5P:163:VAL:HA	1.88	0.55
38:5P:203:VAL:HG12	38:5P:205:PRO:HD3	1.89	0.55
66:5s:196:MET:HG2	85:5s:401:COO:H51	1.89	0.55
9:6Q:476:ARG:NH1	9:6S:291:GLY:O	2.40	0.55
12:7B:126:GLN:NE2	13:7C:124:CYS:O	2.35	0.55
14:8D:157:VAL:HG13	14:8D:187:LEU:HD22	1.89	0.55
22:8L:69:ARG:HB2	22:8L:74:LYS:HB2	1.88	0.55
14:9D:202:THR:HG21	14:9D:216:PHE:HZ	1.72	0.55
24:B:439:GLN:OE1	25:C:171:ARG:NH2	2.40	0.55
28:F:31:TRP:N	28:F:69:ASP:OD2	2.36	0.55
28:F:103:SER:HA	28:F:106:ASN:HB2	1.89	0.55
44:V:65:THR:OG1	44:V:74:ALA:O	2.19	0.55
67:t:159:ARG:HB2	68:u:149:ILE:HD11	1.87	0.55
4:1G:15:LYS:NZ	7:1M:461:ASP:OD2	2.39	0.55
20:4J:102:ALA:C	5:6J:29:LYS:CG	2.76	0.55
26:5D:110:THR:HA	26:5D:122:PRO:HA	1.86	0.55
38:5P:376:GLY:HA3	38:5P:378:MET:HE1	1.89	0.55
16:7F:56:ASN:HB2	22:8L:65:PHE:CD1	2.41	0.55
22:9L:5:PHE:CD2	22:9L:6:LYS:O	2.60	0.55
24:B:140:GLU:OE2	24:B:148:ASP:N	2.36	0.55
29:G:101:VAL:HG12	30:H:33:LEU:HD22	1.88	0.55
38:P:376:GLY:HA3	38:P:378:MET:HE1	1.89	0.55
1:1A:71:ASP:OD2	3:1F:122:ARG:NH2	2.37	0.55
14:2D:75:THR:OG1	21:2K:36:GLN:OE1	2.25	0.55
26:5D:148:CYS:HB3	26:5D:171:LEU:HB3	1.88	0.55
29:5G:101:VAL:HG12	30:5H:33:LEU:HD22	1.88	0.55
30:5H:70:ASP:O	30:5H:74:ASN:ND2	2.30	0.55
40:5R:74:LEU:HD23	40:5R:77:ILE:HD12	1.88	0.55
66:5s:162:MET:HE1	68:5u:192:ARG:HH21	1.71	0.55
19:9I:62:GLN:NE2	19:9I:64:GLU:OE2	2.40	0.55
39:Q:57:VAL:HG12	41:S:191:ILE:HD12	1.88	0.55
40:R:124:LYS:NZ	71:x:27:SER:OG	2.39	0.55
65:q:65:HIS:ND1	65:q:82:TYR:OH	2.26	0.55
66:s:83:VAL:HG22	66:s:100:VAL:HG22	1.89	0.55
9:1Q:476:ARG:NH1	9:1S:291:GLY:O	2.40	0.55
13:2C:3:GLU:O	13:2C:7:GLN:N	2.38	0.55
14:3D:89:MET:HG3	19:3I:38:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4L:7:LEU:HB2	22:4L:12:TYR:OH	2.06	0.55
40:5R:367:VAL:HG11	52:5d:20:LEU:HD22	1.89	0.55
44:5V:109:ASP:OD1	44:5V:155:TYR:OH	2.25	0.55
53:5e:203:THR:HB	53:5e:207:VAL:HB	1.89	0.55
4:6G:15:LYS:NZ	7:6M:461:ASP:OD2	2.39	0.55
14:7D:75:THR:OG1	21:7K:36:GLN:OE1	2.25	0.55
38:P:378:MET:N	38:P:378:MET:SD	2.79	0.55
40:R:367:VAL:HG11	52:d:20:LEU:HD22	1.88	0.55
42:T:328:TYR:O	42:T:332:HIS:N	2.36	0.55
42:T:376:MET:HE1	44:V:181:MET:HG2	1.88	0.55
44:V:398:ILE:HD11	46:X:94:ALA:HB2	1.88	0.55
46:X:123:SER:O	46:X:126:LYS:NZ	2.40	0.55
53:e:16:ARG:HG3	53:e:17:GLU:HG3	1.89	0.55
61:m:110:LYS:O	61:m:113:LYS:NZ	2.30	0.55
66:s:84:VAL:HG23	66:s:99:VAL:HG23	1.89	0.55
1:1A:24:MET:HE2	1:1A:217:SER:HB3	1.88	0.55
9:1S:56:LYS:HB3	9:1S:58:PRO:HD2	1.89	0.55
14:4D:97:ARG:HG2	14:4D:248:ALA:HB2	1.88	0.55
38:5P:390:ARG:O	38:5P:394:ASN:N	2.40	0.55
40:5R:378:LYS:HD2	42:5T:62:ARG:HG3	1.87	0.55
42:5T:260:LEU:HD11	42:5T:386:LEU:HD22	1.88	0.55
64:5p:96:HIS:NE2	64:5p:98:SER:OG	2.39	0.55
32:5r:75:ALA:H	32:5r:114:VAL:HB	1.72	0.55
71:5x:51:PHE:HB2	71:5x:56:LEU:HD21	1.89	0.55
9:6S:56:LYS:HB3	9:6S:58:PRO:HD2	1.89	0.55
24:B:254:VAL:HG13	24:B:258:GLY:HA2	1.89	0.55
27:E:88:PHE:HB3	27:E:101:LEU:HB2	1.89	0.55
16:3F:53:TRP:HA	64:p:3:TYR:HD2	1.72	0.55
24:5B:109:ARG:HD2	24:5B:295:LYS:HE2	1.89	0.55
11:7A:238:VAL:HB	76:7A:601:HEA:HAC	1.89	0.55
11:7A:392:ASN:ND2	20:7J:12:GLU:OE1	2.40	0.55
14:8D:89:MET:HG3	19:8I:38:VAL:HG21	1.89	0.55
22:8L:5:PHE:CD2	22:8L:6:LYS:O	2.60	0.55
25:C:159:GLN:NE2	82:C:801:SF4:S2	2.80	0.55
26:D:180:ARG:HD3	26:D:182:LYS:HE3	1.89	0.55
38:P:170:SER:HB3	38:P:204:ARG:HG2	1.89	0.55
53:e:203:THR:HB	53:e:207:VAL:HB	1.89	0.55
1:1B:283:ARG:HH21	1:1B:341:ILE:HG12	1.71	0.54
14:4D:202:THR:HG21	14:4D:216:PHE:HZ	1.72	0.54
28:5F:103:SER:HA	28:5F:106:ASN:HB2	1.89	0.54
38:5P:136:GLN:OE1	38:5P:313:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5Q:265:TYR:HA	39:5Q:268:PHE:CZ	2.43	0.54
40:5R:124:LYS:NZ	71:5x:27:SER:OG	2.39	0.54
53:5e:79:PRO:HG2	53:5e:82:LEU:HB2	1.88	0.54
64:5p:10:TYR:CB	16:8F:59:ARG:NE	2.69	0.54
9:6Q:67:SER:HB2	32:r:69:SER:HB2	1.85	0.54
10:6R:41:PRO:HG3	10:6R:51:LEU:HD12	1.89	0.54
39:Q:265:TYR:HA	39:Q:268:PHE:CZ	2.42	0.54
40:R:106:CYS:HA	40:R:188:LEU:HD13	1.89	0.54
40:R:193:SER:HA	40:R:197:LYS:HE2	1.89	0.54
11:2A:474:PRO:HG3	20:2J:8:ARG:HE	1.72	0.54
22:4L:5:PHE:CD2	22:4L:6:LYS:O	2.60	0.54
24:5B:339:ILE:HG12	24:5B:347:LEU:HB3	1.90	0.54
38:5P:157:ALA:O	38:5P:160:THR:OG1	2.24	0.54
42:5T:376:MET:HE1	44:5V:181:MET:HG2	1.88	0.54
44:5V:142:TRP:CD1	44:5V:219:LYS:HZ2	2.25	0.54
49:5a:44:ASN:O	49:5a:46:LYS:NZ	2.40	0.54
2:6D:68:LEU:HB3	2:6D:73:ARG:HE	1.73	0.54
7:6M:39:PHE:CE1	49:a:50:PRO:HB3	2.42	0.54
11:7A:474:PRO:HG3	20:7J:8:ARG:HE	1.72	0.54
24:B:289:LYS:O	24:B:291:ASN:ND2	2.40	0.54
26:D:272:ASP:OD2	34:L:81:ARG:NH1	2.35	0.54
27:E:399:GLU:OE1	27:E:414:TYR:OH	2.25	0.54
28:F:129:VAL:HG21	28:F:148:LEU:HB2	1.87	0.54
38:P:136:GLN:OE1	38:P:313:ARG:NH1	2.40	0.54
44:V:150:TYR:HB2	44:V:170:ILE:HD11	1.89	0.54
44:V:223:ILE:HG13	44:V:224:LEU:HG	1.89	0.54
59:k:17:ARG:NH2	32:r:109:ASP:OD2	2.38	0.54
32:r:75:ALA:H	32:r:114:VAL:HB	1.72	0.54
9:1Q:60:VAL:CB	55:5g:11:ARG:HD3	2.32	0.54
13:4C:114:GLY:HA2	20:4J:83:VAL:HG11	1.90	0.54
19:4I:62:GLN:NE2	19:4I:64:GLU:OE2	2.39	0.54
22:4L:69:ARG:HB2	22:4L:74:LYS:HB2	1.88	0.54
38:5P:171:ASP:OD1	38:5P:172:MET:N	2.41	0.54
13:8C:114:GLY:HA2	20:8J:83:VAL:HG11	1.90	0.54
14:8D:97:ARG:HG2	14:8D:248:ALA:HB2	1.88	0.54
14:9D:97:ARG:HG2	14:9D:248:ALA:HB2	1.88	0.54
40:R:128:LEU:O	40:R:131:MET:HG3	2.07	0.54
6:1K:36:LEU:HD11	53:e:143:MET:O	2.06	0.54
14:4D:89:MET:HG3	19:4I:38:VAL:HG21	1.89	0.54
14:4D:157:VAL:HG13	14:4D:187:LEU:HD22	1.89	0.54
7:6M:431:GLU:OE1	7:6M:438:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:9C:114:GLY:HA2	20:9J:83:VAL:HG11	1.90	0.54
38:P:70:VAL:HG13	38:P:80:VAL:HG11	1.90	0.54
40:R:233:PRO:HG3	65:q:130:ARG:NH2	2.22	0.54
42:T:147:LYS:O	42:T:151:TYR:HD1	1.90	0.54
44:V:197:ASP:HB3	63:o:80:VAL:HG11	1.88	0.54
63:o:92:THR:HG22	63:o:96:LYS:HE3	1.90	0.54
7:1M:431:GLU:OE1	7:1M:438:ARG:NH1	2.39	0.54
25:5C:143:HIS:O	25:5C:176:LYS:NZ	2.35	0.54
66:5s:84:VAL:HG23	66:5s:99:VAL:HG23	1.89	0.54
17:7G:78:HIS:O	17:7G:109:ARG:CZ	2.55	0.54
11:9A:211:ASN:O	21:9K:58:ARG:NH2	2.36	0.54
66:s:72:ARG:NH1	66:s:73:LYS:O	2.39	0.54
71:x:51:PHE:HB2	71:x:56:LEU:HD21	1.89	0.54
2:1D:68:LEU:HB3	2:1D:73:ARG:HE	1.73	0.54
13:3C:114:GLY:HA2	20:3J:83:VAL:HG11	1.90	0.54
16:3F:55:TRP:HB2	64:p:7:PHE:CZ	2.43	0.54
29:5G:117:ARG:HD2	29:5G:175:GLY:HA3	1.89	0.54
38:5P:70:VAL:HG13	38:5P:80:VAL:HG11	1.90	0.54
26:D:88:PHE:HE1	30:H:88:PHE:HZ	1.56	0.54
31:I:98:VAL:O	31:I:102:ASN:ND2	2.30	0.54
37:O:11:MET:HG3	37:O:46:PHE:HZ	1.72	0.54
38:P:233:GLU:OE2	38:P:298:ALA:N	2.37	0.54
42:T:44:TRP:O	50:b:85:LYS:NZ	2.40	0.54
44:V:240:SER:O	44:V:244:HIS:ND1	2.40	0.54
22:2L:69:ARG:HB2	22:2L:74:LYS:HB2	1.90	0.54
22:3L:5:PHE:CD2	22:3L:6:LYS:O	2.60	0.54
24:5B:254:VAL:HG13	24:5B:258:GLY:HA2	1.89	0.54
26:5D:88:PHE:HE1	30:5H:88:PHE:HZ	1.55	0.54
42:5T:147:LYS:O	42:5T:151:TYR:HD1	1.90	0.54
64:5p:52:ASP:O	64:5p:56:ASN:ND2	2.38	0.54
7:6N:82:THR:HG21	7:6N:422:HIS:HA	1.89	0.54
14:9D:89:MET:HG3	19:9I:38:VAL:HG21	1.89	0.54
22:9L:69:ARG:HB2	22:9L:74:LYS:HB2	1.88	0.54
24:B:175:GLY:N	24:B:215:ASP:O	2.39	0.54
25:C:460:VAL:HG11	25:C:470:LEU:HD22	1.90	0.54
25:C:548:ALA:HA	25:C:551:ARG:HE	1.73	0.54
34:L:127:TYR:N	34:L:131:GLU:OE1	2.40	0.54
38:P:203:VAL:HG12	38:P:205:PRO:HD3	1.88	0.54
32:r:57:LEU:HD22	32:r:71:VAL:HG12	1.90	0.54
66:s:150:GLN:NE2	85:s:401:COO:H9	2.22	0.54
11:2A:238:VAL:HB	76:2A:602:HEA:HAC	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5K:93:GLN:HB2	33:5K:95:HIS:ND1	2.23	0.54
43:5U:172:MET:HG2	45:5W:42:LEU:HD11	1.90	0.54
64:5p:3:TYR:O	16:8F:56:ASN:ND2	2.41	0.54
32:5r:57:LEU:HD22	32:5r:71:VAL:HG12	1.90	0.54
43:U:146:ILE:O	71:x:32:TYR:OH	2.26	0.54
56:h:60:THR:HG22	59:k:100:LYS:HD2	1.90	0.54
10:1T:4:LEU:C	10:1T:7:GLN:HB3	2.33	0.54
16:3F:56:ASN:ND2	64:p:3:TYR:O	2.41	0.54
24:5B:439:GLN:OE1	25:5C:171:ARG:NH2	2.40	0.54
25:5C:227:THR:OG1	25:5C:229:VAL:O	2.22	0.54
40:5R:233:PRO:HG3	65:5q:130:ARG:NH2	2.22	0.54
43:5U:146:ILE:O	71:5x:32:TYR:OH	2.26	0.54
56:5h:60:THR:HG22	59:5k:100:LYS:HD2	1.90	0.54
66:5s:130:TYR:OH	66:5s:263:HIS:ND1	2.36	0.54
24:B:339:ILE:HG12	24:B:347:LEU:HB3	1.90	0.54
38:P:390:ARG:O	38:P:394:ASN:N	2.40	0.54
43:U:172:MET:HG2	45:W:42:LEU:HD11	1.90	0.54
3:1E:306:GLN:O	10:1T:75:LYS:NZ	2.33	0.54
9:1Q:60:VAL:CG2	55:5g:11:ARG:CD	2.85	0.54
11:2A:392:ASN:ND2	20:2J:12:GLU:OE1	2.40	0.54
20:4J:70:LYS:O	5:6J:19:PRO:CB	2.55	0.54
24:5B:71:ASP:OD2	24:5B:73:SER:OG	2.17	0.54
25:5C:548:ALA:HA	25:5C:551:ARG:HE	1.73	0.54
25:5C:708:ASN:ND2	25:5C:711:MET:HB2	2.23	0.54
26:5D:180:ARG:HD3	26:5D:182:LYS:HE3	1.89	0.54
35:5M:51:THR:OG1	35:5M:60:ASP:OD1	2.21	0.54
39:5Q:46:LEU:HB3	39:5Q:50:TRP:NE1	2.22	0.54
40:5R:193:SER:HA	40:5R:197:LYS:HE2	1.89	0.54
43:5U:205:LEU:HD22	45:5W:69:VAL:HG11	1.88	0.54
9:6Q:73:PRO:HG2	9:6Q:90:ASN:O	2.08	0.54
1:1B:24:MET:HE3	1:1B:217:SER:HB3	1.90	0.53
7:1M:54:SER:O	9:1Q:65:ARG:CA	2.55	0.53
12:2B:81:THR:CB	66:s:49:MET:SD	2.96	0.53
16:2F:41:THR:HG21	22:3L:16:LEU:CD1	2.39	0.53
14:3D:202:THR:HG21	14:3D:216:PHE:HZ	1.72	0.53
11:8A:95:ARG:NH2	14:8D:83:CYS:SG	2.81	0.53
14:8D:202:THR:HG21	14:8D:216:PHE:HZ	1.72	0.53
25:C:143:HIS:O	25:C:176:LYS:NZ	2.35	0.53
38:P:43:LEU:HB2	38:P:51:VAL:HB	1.89	0.53
39:Q:46:LEU:HB3	39:Q:50:TRP:NE1	2.22	0.53
45:W:121:SER:HB3	45:W:124:ASN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:b:133:MET:HE2	50:b:137:GLU:HB3	1.91	0.53
16:2F:63:GLN:NE2	22:3L:71:ARG:HE	2.04	0.53
11:3A:95:ARG:NH2	14:3D:83:CYS:SG	2.81	0.53
20:4J:90:ASN:CB	5:6J:23:LYS:CD	2.56	0.53
24:5B:289:LYS:O	24:5B:291:ASN:ND2	2.40	0.53
24:5B:406:CYS:O	24:5B:410:THR:HG23	2.09	0.53
38:5P:170:SER:HB3	38:5P:204:ARG:HG2	1.89	0.53
42:5T:44:TRP:O	50:5b:85:LYS:NZ	2.40	0.53
44:5V:150:TYR:HB2	44:5V:170:ILE:HD11	1.89	0.53
44:5V:324:HIS:HA	44:5V:327:PHE:CZ	2.43	0.53
48:5Z:48:PRO:HA	50:5b:40:GLN:HB2	1.89	0.53
9:6Q:154:ASP:OD1	9:6Q:154:ASP:N	2.41	0.53
46:X:99:GLU:HG2	46:X:127:HIS:HB3	1.90	0.53
7:1N:56:LEU:O	9:1S:65:ARG:NH1	2.42	0.53
40:5R:128:LEU:O	40:5R:131:MET:HG3	2.07	0.53
49:5a:49:PRO:HG2	49:5a:52:LEU:HD12	1.90	0.53
50:5b:133:MET:HE2	50:5b:137:GLU:HB3	1.91	0.53
10:6T:7:GLN:OE1	10:6T:8:VAL:HG13	2.09	0.53
16:7F:41:THR:HG21	22:8L:16:LEU:CD1	2.39	0.53
26:D:224:ARG:N	33:K:82:GLU:OE2	2.24	0.53
33:K:106:TYR:O	33:K:110:ARG:CB	2.56	0.53
38:P:171:ASP:OD1	38:P:172:MET:N	2.41	0.53
40:R:330:SER:HA	40:R:333:TYR:CE2	2.43	0.53
53:e:178:TYR:O	53:e:179:ARG:NH1	2.31	0.53
7:1N:82:THR:HG21	7:1N:422:HIS:HA	1.89	0.53
9:1Q:60:VAL:CB	55:5g:11:ARG:HD2	2.36	0.53
24:5B:175:GLY:N	24:5B:215:ASP:O	2.39	0.53
27:5E:399:GLU:OE1	27:5E:414:TYR:OH	2.25	0.53
39:5Q:113:MET:SD	45:5W:67:LEU:HD23	2.48	0.53
44:5V:240:SER:O	44:5V:244:HIS:ND1	2.40	0.53
53:5e:178:TYR:O	53:5e:179:ARG:NH1	2.31	0.53
63:5o:92:THR:HG22	63:5o:96:LYS:HE3	1.90	0.53
10:6T:4:LEU:C	10:6T:7:GLN:HB3	2.33	0.53
14:9D:157:VAL:HG13	14:9D:187:LEU:HD22	1.88	0.53
22:9L:5:PHE:CD2	22:9L:6:LYS:N	2.77	0.53
25:C:576:GLU:HA	25:C:593:ARG:HH21	1.74	0.53
29:G:117:ARG:HD2	29:G:175:GLY:HA3	1.89	0.53
34:L:136:CYS:O	34:L:140:GLY:N	2.41	0.53
41:S:164:SER:HB2	54:f:45:LYS:HG2	1.91	0.53
1:1A:57:HIS:ND1	1:1A:58:VAL:O	2.41	0.53
11:2A:77:PHE:O	11:2A:81:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5E:142:ARG:NH2	28:5F:134:CYS:SG	2.70	0.53
32:5J:97:GLU:OE2	33:5K:54:ARG:NH1	2.33	0.53
34:5L:136:CYS:O	34:5L:140:GLY:N	2.41	0.53
44:5V:188:TRP:O	63:5o:117:ARG:NH2	2.42	0.53
46:5X:123:SER:O	46:5X:126:LYS:NZ	2.40	0.53
49:5a:49:PRO:CG	49:5a:52:LEU:HD12	2.39	0.53
53:5e:16:ARG:HG3	53:5e:17:GLU:HG3	1.89	0.53
7:6N:56:LEU:O	9:6S:65:ARG:NH1	2.42	0.53
17:7G:82:ILE:HG21	17:7G:88:MET:HE2	1.90	0.53
24:B:109:ARG:HD2	24:B:295:LYS:HE2	1.89	0.53
26:D:122:PRO:HG2	26:D:179:ILE:HG13	1.90	0.53
27:E:174:ILE:HG12	27:E:240:LEU:HD11	1.91	0.53
28:F:56:ARG:HA	39:Q:37:PRO:HA	1.91	0.53
42:T:327:LEU:O	42:T:331:ALA:HB3	2.08	0.53
44:V:142:TRP:CD1	44:V:219:LYS:HZ1	2.25	0.53
10:1T:7:GLN:OE1	10:1T:8:VAL:HG13	2.08	0.53
28:5F:56:ARG:NH2	28:5F:57:TYR:OH	2.42	0.53
29:5G:51:ARG:NH2	66:5s:312:ARG:O	2.40	0.53
31:5I:128:ARG:HD3	67:5t:276:LYS:HA	1.91	0.53
33:5K:44:MET:HA	33:5K:47:MET:HE2	1.90	0.53
40:5R:124:LYS:HD3	71:5x:28:LEU:HB2	1.91	0.53
42:5T:327:LEU:O	42:5T:331:ALA:HB3	2.08	0.53
53:5e:199:PRO:HG3	64:5p:44:TRP:CD1	2.44	0.53
1:6A:57:HIS:ND1	1:6A:58:VAL:O	2.41	0.53
7:6M:312:THR:C	9:6Q:51:VAL:CG2	2.81	0.53
22:7L:69:ARG:HB2	22:7L:74:LYS:HB2	1.90	0.53
24:B:406:CYS:O	24:B:410:THR:HG23	2.09	0.53
28:F:56:ARG:NH2	28:F:57:TYR:OH	2.42	0.53
29:G:167:ASP:OD1	29:G:169:THR:OG1	2.17	0.53
39:Q:113:MET:SD	45:W:67:LEU:HD23	2.48	0.53
25:5C:109:ALA:O	25:5C:113:MET:N	2.33	0.53
38:5P:43:LEU:HB2	38:5P:51:VAL:HB	1.89	0.53
66:5s:49:MET:SD	12:7B:81:THR:CB	2.96	0.53
9:6S:193:ASP:OD1	9:6S:193:ASP:N	2.42	0.53
11:9A:95:ARG:NH2	14:9D:83:CYS:SG	2.81	0.53
24:B:284:SER:HA	24:B:292:ALA:HB1	1.91	0.53
41:S:222:PHE:HB3	45:W:68:PHE:CZ	2.44	0.53
44:V:109:ASP:OD1	44:V:155:TYR:OH	2.25	0.53
44:V:188:TRP:O	63:o:117:ARG:NH2	2.42	0.53
58:j:3:ASP:OD1	58:j:3:ASP:N	2.41	0.53
9:1Q:56:LYS:HD3	9:1Q:56:LYS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:5R:106:CYS:HA	40:5R:188:LEU:HD13	1.89	0.53
41:5S:164:SER:HB2	54:5f:45:LYS:HG2	1.91	0.53
42:5T:80:THR:HG22	42:5T:227:VAL:HG22	1.90	0.53
42:5T:328:TYR:O	42:5T:332:HIS:N	2.36	0.53
55:5g:8:GLN:CB	55:5g:11:ARG:HH21	2.19	0.53
64:5p:7:PHE:CZ	16:8F:55:TRP:HB2	2.43	0.53
27:E:299:ALA:HA	27:E:325:ALA:HB3	1.90	0.53
40:R:215:GLY:HA2	40:R:218:ILE:HD12	1.91	0.53
44:V:1:MET:HA	44:V:4:LEU:HD12	1.91	0.53
44:V:324:HIS:HA	44:V:327:PHE:CZ	2.43	0.53
50:b:100:ALA:HB1	63:o:68:LYS:HG3	1.91	0.53
3:1F:305:SER:OG	6:1L:21:GLN:NE2	2.42	0.53
7:1M:87:ILE:HG12	7:1M:241:MET:HG2	1.91	0.53
9:1Q:154:ASP:OD1	9:1Q:154:ASP:N	2.41	0.53
11:3A:211:ASN:O	21:3K:58:ARG:NH2	2.36	0.53
11:4A:95:ARG:NH2	14:4D:83:CYS:SG	2.81	0.53
24:5B:439:GLN:O	24:5B:443:HIS:ND1	2.42	0.53
26:5D:122:PRO:HG2	26:5D:179:ILE:HG13	1.90	0.53
49:5a:60:TYR:CD2	55:5g:18:HIS:HA	2.43	0.53
29:G:43:ALA:O	41:S:278:ARG:NH1	2.42	0.53
29:G:51:ARG:NH2	66:s:312:ARG:O	2.40	0.53
42:T:439:ILE:HG22	42:T:440:LYS:HG2	1.90	0.53
11:2A:323:SER:OG	12:2B:75:GLU:OE1	2.27	0.53
12:2B:126:GLN:NE2	13:2C:124:CYS:O	2.35	0.53
14:3D:74:TRP:HE1	21:3K:32:THR:HG21	1.74	0.53
41:5S:222:PHE:HB3	45:5W:68:PHE:CZ	2.44	0.53
44:5V:494:VAL:HG12	69:5v:2:VAL:HB	1.90	0.53
67:5t:112:LEU:HD12	67:5t:140:GLU:HA	1.91	0.53
24:B:439:GLN:O	24:B:443:HIS:ND1	2.42	0.53
42:T:80:THR:HG22	42:T:227:VAL:HG22	1.90	0.53
44:V:494:VAL:HG12	69:v:2:VAL:HB	1.90	0.53
44:V:519:PRO:HA	70:w:74:MET:SD	2.50	0.53
17:2G:78:HIS:O	17:2G:109:ARG:CZ	2.55	0.52
29:5G:67:LYS:N	29:5G:71:GLU:OE1	2.36	0.52
31:5I:61:ARG:NH1	31:5I:103:GLU:HA	2.24	0.52
42:5T:133:LEU:HD21	42:5T:220:GLY:HA3	1.92	0.52
45:5W:121:SER:HB3	45:5W:124:ASN:HB2	1.89	0.52
11:7A:106:PRO:HB3	14:7D:45:TYR:HB2	1.91	0.52
14:7D:195:GLN:NE2	14:7D:198:GLU:OE1	2.41	0.52
22:8L:5:PHE:CD2	22:8L:6:LYS:N	2.77	0.52
23:A:169:ILE:HB	23:A:173:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:398:ARG:HA	25:C:401:TYR:CZ	2.44	0.52
33:K:44:MET:HA	33:K:47:MET:HE2	1.90	0.52
33:K:93:GLN:HB2	33:K:95:HIS:ND1	2.23	0.52
17:2G:82:ILE:HG21	17:2G:88:MET:HE2	1.90	0.52
14:4D:74:TRP:HE1	21:4K:32:THR:HG21	1.74	0.52
40:5R:330:SER:HA	40:5R:333:TYR:CE2	2.43	0.52
11:7A:77:PHE:O	11:7A:81:LEU:HB2	2.09	0.52
11:7A:323:SER:OG	12:7B:75:GLU:OE1	2.27	0.52
28:F:60:ILE:HD11	39:Q:25:ARG:NH1	2.24	0.52
36:N:9:ARG:NH1	36:N:47:GLY:O	2.42	0.52
40:R:330:SER:HA	40:R:333:TYR:CZ	2.44	0.52
53:e:77:ARG:HB3	71:x:22:LYS:HZ1	1.73	0.52
10:1R:41:PRO:HG3	10:1R:51:LEU:HD12	1.89	0.52
11:2A:106:PRO:HB3	14:2D:45:TYR:HB2	1.91	0.52
25:5C:280:ILE:HG22	25:5C:294:PRO:HA	1.92	0.52
27:5E:122:ARG:NH2	27:5E:142:ARG:O	2.31	0.52
65:5q:129:LYS:HE2	71:5x:16:LEU:HA	1.91	0.52
66:5s:113:ASN:HD21	66:5s:130:TYR:HB3	1.74	0.52
13:8C:8:LEU:HD22	18:8H:19:VAL:HG21	1.91	0.52
14:9D:74:TRP:HE1	21:9K:32:THR:HG21	1.74	0.52
34:L:63:ARG:NH2	34:L:99:THR:OG1	2.42	0.52
40:R:45:LEU:HA	40:R:50:PHE:HE2	1.74	0.52
60:l:81:PHE:O	60:l:84:LYS:HG3	2.10	0.52
66:s:113:ASN:HD21	66:s:130:TYR:HB3	1.74	0.52
8:1P:17:ARG:NH1	10:1T:112:GLY:O	2.42	0.52
14:2D:195:GLN:NE2	14:2D:198:GLU:OE1	2.42	0.52
24:5B:284:SER:HA	24:5B:292:ALA:HB1	1.91	0.52
25:5C:460:VAL:HG11	25:5C:470:LEU:HD22	1.90	0.52
26:5D:76:ASP:N	26:5D:76:ASP:OD1	2.42	0.52
27:5E:299:ALA:HA	27:5E:325:ALA:HB3	1.90	0.52
42:5T:439:ILE:HG22	42:5T:440:LYS:HG2	1.91	0.52
64:5p:3:TYR:HE2	16:8F:53:TRP:HB2	1.63	0.52
9:6Q:61:THR:OG1	55:g:11:ARG:NH1	2.43	0.52
14:8D:74:TRP:HE1	21:8K:32:THR:HG21	1.74	0.52
31:I:128:ARG:HD3	67:t:276:LYS:HA	1.91	0.52
48:Z:48:PRO:HA	50:b:40:GLN:HB2	1.89	0.52
65:q:191:PRO:O	67:t:85:TYR:OH	2.14	0.52
66:s:64:ASN:ND2	67:t:48:GLU:O	2.38	0.52
10:1T:2:THR:O	10:1T:6:LYS:HG3	2.09	0.52
22:3L:5:PHE:CD2	22:3L:6:LYS:N	2.77	0.52
27:5E:174:ILE:HG12	27:5E:240:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5G:119:GLU:OE2	29:5G:204:TYR:OH	2.24	0.52
30:5H:101:PRO:HG3	31:5I:107:ALA:HB1	1.91	0.52
39:5Q:96:PHE:HA	39:5Q:162:LEU:HB2	1.91	0.52
44:5V:519:PRO:HA	70:5w:74:MET:SD	2.50	0.52
1:6B:24:MET:HE3	1:6B:217:SER:HB3	1.90	0.52
9:6Q:62:GLU:CB	55:g:11:ARG:CG	2.79	0.52
10:6T:2:THR:O	10:6T:6:LYS:HG3	2.09	0.52
13:7C:25:ARG:NH1	18:7H:13:GLU:OE2	2.43	0.52
23:A:106:LEU:HA	23:A:109:MET:HE3	1.91	0.52
39:Q:96:PHE:HA	39:Q:162:LEU:HB2	1.91	0.52
53:e:199:PRO:HG3	64:p:44:TRP:CD1	2.44	0.52
25:5C:398:ARG:HA	25:5C:401:TYR:CZ	2.45	0.52
28:5F:60:ILE:HD11	39:5Q:25:ARG:NH1	2.24	0.52
29:5G:43:ALA:O	41:5S:278:ARG:NH1	2.42	0.52
40:5R:45:LEU:HA	40:5R:50:PHE:HE2	1.74	0.52
40:5R:340:LEU:HD21	65:5q:96:TYR:HA	1.92	0.52
50:5b:100:ALA:HB1	63:5o:68:LYS:HG3	1.91	0.52
50:5b:115:ASN:OD1	50:5b:139:TYR:OH	2.27	0.52
55:5g:7:PHE:CE1	32:5r:62:HIS:HB2	2.45	0.52
59:5k:110:GLU:HG3	59:5k:111:TYR:CE2	2.45	0.52
7:6M:87:ILE:HG12	7:6M:241:MET:HG2	1.91	0.52
11:9A:20:ALA:HB2	11:9A:71:PRO:HB2	1.92	0.52
25:C:280:ILE:HG22	25:C:294:PRO:HA	1.92	0.52
31:I:61:ARG:NH1	31:I:103:GLU:HA	2.24	0.52
40:R:213:SER:HB2	53:e:206:ALA:H	1.75	0.52
42:T:133:LEU:HD21	42:T:220:GLY:HA3	1.91	0.52
44:V:513:GLN:OE1	44:V:513:GLN:N	2.36	0.52
50:b:115:ASN:OD1	50:b:139:TYR:OH	2.26	0.52
59:k:110:GLU:HG3	59:k:111:TYR:CE2	2.45	0.52
11:4A:20:ALA:HB2	11:4A:71:PRO:HB2	1.92	0.52
20:4J:96:ILE:HD12	5:6J:29:LYS:HB2	1.91	0.52
27:5E:324:ILE:O	31:5I:47:TYR:OH	2.24	0.52
33:5K:106:TYR:O	33:5K:110:ARG:CB	2.56	0.52
34:5L:63:ARG:NH2	34:5L:99:THR:OG1	2.42	0.52
44:5V:1:MET:HA	44:5V:4:LEU:HD12	1.91	0.52
46:5X:99:GLU:HG2	46:5X:127:HIS:HB3	1.91	0.52
58:5j:61:LYS:O	58:5j:65:LYS:HG3	2.10	0.52
65:5q:137:GLN:HB3	71:5x:23:GLU:HA	1.92	0.52
3:6F:304:LYS:NZ	10:6R:74:CYS:O	2.43	0.52
11:7A:414:GLY:O	11:7A:418:THR:OG1	2.26	0.52
49:a:41:ARG:HG2	49:a:63:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5T:168:SER:O	64:5p:40:ARG:NH1	2.43	0.52
42:5T:326:ILE:HG12	42:5T:423:GLU:HG2	1.92	0.52
49:5a:51:GLU:HG3	49:5a:52:LEU:HG	1.92	0.52
3:6E:115:SER:OG	3:6E:185:ASP:OD1	2.28	0.52
7:6M:206:TYR:O	7:6M:284:ARG:NH2	2.41	0.52
7:6M:314:PRO:HD3	9:6Q:50:GLU:HA	1.92	0.52
13:9C:8:LEU:HD22	18:9H:19:VAL:HG21	1.91	0.52
25:C:708:ASN:ND2	25:C:711:MET:HB2	2.23	0.52
38:P:302:LYS:O	38:P:306:LYS:N	2.42	0.52
64:p:56:ASN:HB3	64:p:59:GLU:HG3	1.92	0.52
3:1F:304:LYS:NZ	10:1R:74:CYS:O	2.43	0.52
11:2A:117:VAL:O	11:2A:139:SER:OG	2.28	0.52
13:2C:25:ARG:NH1	18:2H:13:GLU:OE2	2.43	0.52
35:5M:147:TRP:H	35:5M:147:TRP:CD1	2.28	0.52
40:5R:330:SER:HA	40:5R:333:TYR:CZ	2.44	0.52
16:7F:63:GLN:NE2	22:8L:71:ARG:HE	2.04	0.52
24:B:471:ILE:O	61:m:13:LYS:NZ	2.43	0.52
25:C:356:VAL:HG22	25:C:560:VAL:HB	1.92	0.52
40:R:124:LYS:HD3	71:x:28:LEU:HB2	1.91	0.52
43:U:143:TRP:CG	45:W:98:ASN:HB3	2.45	0.52
56:h:119:SER:OG	63:o:110:ARG:NH2	2.43	0.52
68:u:109:VAL:HG22	68:u:133:LEU:HB2	1.92	0.52
7:1N:99:ASN:HD21	7:1N:211:ARG:HB3	1.74	0.52
13:4C:8:LEU:HD22	18:4H:19:VAL:HG21	1.91	0.52
22:4L:5:PHE:CD2	22:4L:6:LYS:N	2.77	0.52
36:5N:9:ARG:NH1	36:5N:47:GLY:O	2.42	0.52
58:5j:3:ASP:N	58:5j:3:ASP:OD1	2.41	0.52
3:6F:305:SER:OG	6:6L:21:GLN:NE2	2.42	0.52
42:T:1:MET:HE3	42:T:60:LEU:HD11	1.92	0.52
72:y:6:ALA:HA	72:y:9:ILE:HD12	1.92	0.52
3:1E:115:SER:OG	3:1E:185:ASP:OD1	2.28	0.51
9:1Q:388:GLN:NE2	9:1Q:483:ARG:O	2.44	0.51
13:4C:3:GLU:O	13:4C:7:GLN:N	2.41	0.51
23:5A:169:ILE:HB	23:5A:173:GLN:HB2	1.91	0.51
28:5F:56:ARG:HA	39:5Q:37:PRO:HA	1.91	0.51
30:5H:37:LEU:HD22	30:5H:41:LYS:HE3	1.92	0.51
40:5R:136:ALA:HB2	40:5R:163:VAL:HG21	1.92	0.51
40:5R:215:GLY:HA2	40:5R:218:ILE:HD12	1.91	0.51
67:5t:83:ASP:O	67:5t:105:LEU:N	2.43	0.51
7:6M:178:ASP:N	7:6M:178:ASP:OD1	2.43	0.51
25:C:327:LYS:HA	25:C:332:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:E:183:ARG:NH2	27:E:405:GLU:O	2.42	0.51
42:T:168:SER:O	64:p:40:ARG:NH1	2.43	0.51
44:V:482:LEU:HD23	72:y:84:MET:HB3	1.92	0.51
9:1Q:102:VAL:HG22	9:1Q:255:VAL:HG22	1.92	0.51
11:3A:350:VAL:O	11:3A:354:ASN:ND2	2.43	0.51
38:5P:302:LYS:O	38:5P:306:LYS:N	2.42	0.51
42:5T:293:LEU:HD23	42:5T:390:PHE:HE2	1.74	0.51
44:5V:482:LEU:HD23	72:5y:84:MET:HB3	1.92	0.51
64:5p:3:TYR:HD2	16:8F:53:TRP:HA	1.72	0.51
65:5q:130:ARG:HG3	71:5x:72:TYR:OH	2.11	0.51
66:5s:42:ALA:CB	22:7L:12:TYR:CE1	2.88	0.51
20:7J:17:PRO:HG2	20:7J:24:GLU:HB3	1.92	0.51
13:9C:21:GLU:OE2	13:9C:25:ARG:NH2	2.43	0.51
26:D:71:ALA:HA	27:E:303:ASP:HB2	1.93	0.51
44:V:434:VAL:O	49:a:38:ALA:HB2	2.10	0.51
57:i:32:ILE:O	57:i:36:ARG:N	2.42	0.51
62:n:20:HIS:HA	62:n:101:ILE:HG23	1.92	0.51
65:q:133:ARG:NH2	65:q:134:ASP:OD2	2.43	0.51
1:1B:336:LEU:HD11	1:1B:348:VAL:HG12	1.92	0.51
7:1M:88:ASN:HB2	7:1M:433:LEU:HD22	1.93	0.51
22:2L:12:TYR:CE1	66:s:42:ALA:CB	2.88	0.51
25:5C:279:ASN:CG	25:5C:297:ASN:HD22	2.18	0.51
25:5C:327:LYS:HA	25:5C:332:LEU:HA	1.92	0.51
26:5D:272:ASP:OD1	34:5L:81:ARG:NH2	2.44	0.51
53:5e:69:GLN:NE2	71:5x:68:VAL:O	2.44	0.51
56:5h:100:PHE:HZ	70:5w:75:VAL:HG21	1.76	0.51
64:5p:56:ASN:HB3	64:5p:59:GLU:HG3	1.92	0.51
68:5u:109:VAL:HG22	68:5u:133:LEU:HB2	1.92	0.51
1:6B:336:LEU:HD11	1:6B:348:VAL:HG12	1.92	0.51
11:9A:350:VAL:O	11:9A:354:ASN:ND2	2.43	0.51
29:G:167:ASP:O	29:G:171:CYS:N	2.39	0.51
30:H:101:PRO:HG3	31:I:107:ALA:HB1	1.91	0.51
40:R:340:LEU:HD21	65:q:96:TYR:HA	1.92	0.51
52:d:64:ARG:HG2	52:d:67:ARG:NH2	2.26	0.51
65:q:53:VAL:O	65:q:69:GLY:N	2.24	0.51
66:s:130:TYR:OH	66:s:263:HIS:ND1	2.36	0.51
10:1T:4:LEU:H	10:1T:4:LEU:CD2	2.23	0.51
13:4C:21:GLU:OE2	13:4C:25:ARG:NH2	2.43	0.51
16:4F:68:MET:HG3	16:4F:71:ARG:HH12	1.76	0.51
25:5C:576:GLU:HA	25:5C:593:ARG:HH21	1.74	0.51
40:5R:230:TYR:OH	44:5V:544:LEU:O	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5U:163:ALA:O	43:5U:167:MET:HG2	2.11	0.51
68:5u:167:TYR:HB3	68:5u:183:SER:HA	1.92	0.51
72:5y:101:ASP:HA	72:5y:104:LYS:HB3	1.91	0.51
11:7A:173:MET:HE3	11:7A:178:MET:HG2	1.92	0.51
11:7A:267:MET:SD	11:7A:313:LYS:NZ	2.81	0.51
11:8A:350:VAL:O	11:8A:354:ASN:ND2	2.43	0.51
29:G:67:LYS:O	51:c:8:ARG:NE	2.44	0.51
30:H:37:LEU:HD22	30:H:41:LYS:HE3	1.92	0.51
42:T:214:VAL:HG13	42:T:277:LYS:HD3	1.93	0.51
59:k:19:TYR:HE1	59:k:43:LEU:HG	1.75	0.51
67:t:83:ASP:O	67:t:105:LEU:N	2.43	0.51
3:1E:199:TYR:OH	74:1E:401:HEC:O2A	2.28	0.51
16:2F:34:LYS:HE3	22:3L:12:TYR:CE2	2.46	0.51
23:5A:89:ILE:HG23	23:5A:90:ILE:HD12	1.92	0.51
25:5C:356:VAL:HG22	25:5C:560:VAL:HB	1.92	0.51
27:5E:180:GLU:OE2	27:5E:315:TYR:OH	2.20	0.51
29:5G:67:LYS:O	51:5c:8:ARG:NE	2.44	0.51
44:5V:26:HIS:HB3	44:5V:112:LEU:HD23	1.93	0.51
59:5k:69:LEU:HD23	72:5y:44:LEU:HB3	1.93	0.51
7:6M:88:ASN:HB2	7:6M:433:LEU:HD22	1.93	0.51
12:8B:156:VAL:HG13	12:8B:157:LYS:HG2	1.92	0.51
13:8C:3:GLU:O	13:8C:7:GLN:N	2.41	0.51
13:8C:21:GLU:OE2	13:8C:25:ARG:NH2	2.43	0.51
24:B:348:LEU:HD22	24:B:352:ILE:HG21	1.92	0.51
25:C:279:ASN:CG	25:C:297:ASN:HD22	2.18	0.51
28:F:139:GLU:HB3	29:G:192:PHE:HE2	1.76	0.51
34:L:90:PRO:HA	34:L:127:TYR:HA	1.93	0.51
40:R:136:ALA:HB2	40:R:163:VAL:HG21	1.92	0.51
65:q:129:LYS:HE2	71:x:16:LEU:HA	1.91	0.51
70:w:66:SER:HB3	70:w:70:ARG:HH11	1.76	0.51
12:3B:156:VAL:HG13	12:3B:157:LYS:HG2	1.92	0.51
11:4A:350:VAL:O	11:4A:354:ASN:ND2	2.43	0.51
26:5D:160:ARG:NH1	26:5D:165:GLU:OE2	2.44	0.51
26:5D:248:VAL:HA	26:5D:259:SER:HA	1.93	0.51
27:5E:270:ARG:NH2	29:5G:79:MET:O	2.28	0.51
34:5L:127:TYR:N	34:5L:131:GLU:OE1	2.40	0.51
42:5T:66:ALA:O	42:5T:114:LEU:N	2.44	0.51
59:5k:19:TYR:HE1	59:5k:43:LEU:HG	1.75	0.51
9:6Q:49:VAL:CG2	9:6Q:56:LYS:HG3	2.40	0.51
42:T:293:LEU:HD23	42:T:390:PHE:HE2	1.74	0.51
68:u:167:TYR:HB3	68:u:183:SER:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2F:56:ASN:HB2	22:3L:65:PHE:CD1	2.41	0.51
28:5F:139:GLU:HB3	29:5G:192:PHE:HE2	1.76	0.51
40:5R:168:LEU:HD13	40:5R:247:ILE:HD11	1.92	0.51
7:6N:107:HIS:HB3	7:6N:176:GLU:HG2	1.93	0.51
11:8A:64:MET:HE1	76:8A:601:HEA:H172	1.93	0.51
23:A:89:ILE:HG23	23:A:90:ILE:HD12	1.92	0.51
26:D:248:VAL:HA	26:D:259:SER:HA	1.93	0.51
27:E:324:ILE:O	31:I:47:TYR:OH	2.24	0.51
33:K:83:GLU:OE2	33:K:92:LYS:NZ	2.40	0.51
42:T:224:LEU:HD23	42:T:228:LEU:HD12	1.93	0.51
46:X:58:ALA:HB3	46:X:62:MET:HE1	1.93	0.51
48:Z:87:ILE:HD12	48:Z:89:SER:HB2	1.93	0.51
58:j:3:ASP:CG	58:j:80:ARG:HH22	2.19	0.51
72:y:101:ASP:HA	72:y:104:LYS:HB3	1.91	0.51
2:1C:93:PRO:O	2:1C:96:THR:OG1	2.25	0.51
7:1M:420:SER:HG	7:1M:423:HIS:HD1	1.57	0.51
38:5P:58:VAL:HG22	38:5P:128:ILE:HB	1.92	0.51
38:5P:257:LYS:NZ	38:5P:348:ASP:O	2.31	0.51
40:5R:363:SER:OG	52:5d:24:GLN:NE2	2.39	0.51
42:5T:1:MET:HE3	42:5T:60:LEU:HD11	1.92	0.51
62:5n:20:HIS:HA	62:5n:101:ILE:HG23	1.92	0.51
66:5s:116:VAL:HG22	66:5s:134:LEU:HB2	1.93	0.51
7:6M:53:LEU:O	9:6Q:65:ARG:NH1	2.41	0.51
7:6N:99:ASN:HD21	7:6N:211:ARG:HB3	1.74	0.51
9:6Q:102:VAL:HG22	9:6Q:255:VAL:HG22	1.92	0.51
23:A:48:PHE:O	23:A:135:ARG:NH1	2.36	0.51
29:G:67:LYS:N	29:G:71:GLU:OE1	2.36	0.51
29:G:89:MET:HG2	39:Q:259:THR:HG21	1.93	0.51
44:V:26:HIS:HB3	44:V:112:LEU:HD23	1.93	0.51
67:t:112:LEU:HD12	67:t:140:GLU:HA	1.92	0.51
76:3A:601:HEA:H243	12:3B:91:PRO:HB3	1.93	0.51
20:4J:102:ALA:O	5:6J:29:LYS:HB3	2.11	0.51
23:5A:48:PHE:O	23:5A:135:ARG:NH1	2.36	0.51
23:5A:106:LEU:HA	23:5A:109:MET:HE3	1.91	0.51
33:5K:83:GLU:OE2	33:5K:92:LYS:NZ	2.40	0.51
39:5Q:155:ASP:OD1	39:5Q:157:THR:OG1	2.24	0.51
40:5R:213:SER:HB2	53:5e:206:ALA:H	1.75	0.51
43:5U:143:TRP:CG	45:5W:98:ASN:HB3	2.45	0.51
46:5X:58:ALA:HB3	46:5X:62:MET:HE1	1.93	0.51
48:5Z:87:ILE:HD12	48:5Z:89:SER:HB2	1.93	0.51
55:5g:10:GLU:OE1	59:5k:37:TYR:CD2	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:5l:81:PHE:O	60:5l:84:LYS:HG3	2.10	0.51
9:6Q:60:VAL:CG2	55:g:11:ARG:CB	2.84	0.51
10:6T:4:LEU:H	10:6T:4:LEU:CD2	2.23	0.51
16:9F:68:MET:HG3	16:9F:71:ARG:HH12	1.76	0.51
29:G:129:GLU:OE1	29:G:130:GLU:N	2.43	0.51
37:O:53:CYS:HB3	37:O:56:THR:HG21	1.93	0.51
53:e:69:GLN:NE2	71:x:68:VAL:O	2.44	0.51
58:j:61:LYS:O	58:j:65:LYS:HG3	2.10	0.51
1:1B:88:LEU:HD12	1:1B:240:PHE:HD1	1.76	0.51
17:2G:69:ASP:HA	17:2G:72:VAL:HG12	1.93	0.51
11:3A:64:MET:HE1	76:3A:604:HEA:H172	1.93	0.51
12:3B:144:PRO:HB2	13:3C:27:LYS:HE3	1.93	0.51
12:4B:156:VAL:HG13	12:4B:157:LYS:HG2	1.92	0.51
24:5B:180:ARG:NE	24:5B:182:GLU:OE1	2.41	0.51
31:5I:98:VAL:O	31:5I:102:ASN:ND2	2.30	0.51
32:5J:72:SER:OG	32:5J:74:ALA:O	2.29	0.51
32:5J:103:ILE:H	33:5K:33:ARG:NH2	2.09	0.51
58:5j:3:ASP:CG	58:5j:80:ARG:HH22	2.19	0.51
7:6M:437:ARG:NH2	9:6Q:54:SER:HA	2.25	0.51
25:C:227:THR:OG1	25:C:229:VAL:O	2.22	0.51
26:D:160:ARG:NH1	26:D:165:GLU:OE2	2.44	0.51
42:T:200:ILE:HD12	42:T:236:PHE:HE2	1.76	0.51
42:T:326:ILE:HG12	42:T:423:GLU:HG2	1.92	0.51
5:1I:26:ALA:HA	47:Y:53:ILE:CG2	2.41	0.50
9:1Q:49:VAL:CG2	9:1Q:56:LYS:HE2	2.41	0.50
9:1S:475:PRO:O	9:1S:476:ARG:NE	2.37	0.50
13:3C:8:LEU:HD22	18:3H:19:VAL:HG21	1.91	0.50
29:5G:89:MET:HG2	39:5Q:259:THR:HG21	1.93	0.50
8:6P:17:ARG:NH1	10:6T:112:GLY:O	2.43	0.50
12:7B:153:LYS:HA	12:7B:156:VAL:HG12	1.93	0.50
14:7D:111:GLU:OE1	14:7D:225:HIS:NE2	2.33	0.50
11:8A:20:ALA:HB2	11:8A:71:PRO:HB2	1.92	0.50
76:8A:604:HEA:H243	12:8B:91:PRO:HB3	1.93	0.50
12:8B:144:PRO:HB2	13:8C:27:LYS:HE3	1.93	0.50
12:9B:156:VAL:HG13	12:9B:157:LYS:HG2	1.92	0.50
26:D:89:GLY:HA2	26:D:93:LEU:HB2	1.92	0.50
26:D:279:THR:O	26:D:282:ARG:NH1	2.30	0.50
32:J:72:SER:OG	32:J:74:ALA:O	2.29	0.50
65:q:137:GLN:HB3	71:x:23:GLU:HA	1.92	0.50
11:2A:173:MET:HE3	11:2A:178:MET:HG2	1.92	0.50
12:4B:144:PRO:HB2	13:4C:27:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5B:348:LEU:HD22	24:5B:352:ILE:HG21	1.92	0.50
26:5D:71:ALA:HA	27:5E:303:ASP:HB2	1.92	0.50
27:5E:248:VAL:HG12	27:5E:352:LEU:HD11	1.94	0.50
9:6Q:62:GLU:OE1	55:g:11:ARG:CA	2.57	0.50
9:6Q:388:GLN:NE2	9:6Q:483:ARG:O	2.44	0.50
26:D:76:ASP:OD1	26:D:76:ASP:N	2.42	0.50
35:M:147:TRP:CD1	35:M:147:TRP:H	2.28	0.50
42:T:213:HIS:NE2	42:T:224:LEU:HB3	2.26	0.50
43:U:163:ALA:O	43:U:167:MET:HG2	2.11	0.50
56:h:57:ASP:H	56:h:60:THR:HG1	1.56	0.50
60:l:2:THR:OG1	60:l:3:TRP:N	2.45	0.50
65:q:130:ARG:HG3	71:x:72:TYR:OH	2.10	0.50
66:s:116:VAL:HG22	66:s:134:LEU:HB2	1.93	0.50
2:1D:152:THR:OG1	2:1D:165:ARG:NH1	2.37	0.50
2:1D:189:ASP:OD1	2:1D:234:SER:OG	2.27	0.50
12:2B:153:LYS:HA	12:2B:156:VAL:HG12	1.93	0.50
20:3J:88:PHE:O	20:3J:91:ARG:NH1	2.44	0.50
12:4B:141:LEU:HD21	18:4H:35:LEU:HD13	1.94	0.50
24:5B:132:SER:HB2	24:5B:172:ALA:HA	1.93	0.50
24:5B:471:ILE:O	61:5m:13:LYS:NZ	2.43	0.50
27:5E:317:LYS:HG3	30:5H:111:LEU:HD23	1.94	0.50
39:5Q:275:ALA:HA	51:5c:16:VAL:HG11	1.94	0.50
42:5T:224:LEU:HD23	42:5T:228:LEU:HD12	1.93	0.50
56:5h:119:SER:OG	63:5o:110:ARG:NH2	2.43	0.50
65:5q:133:ARG:NH2	65:5q:134:ASP:OD2	2.43	0.50
9:6Q:72:LYS:HZ2	9:6Q:72:LYS:HB3	1.75	0.50
11:8A:96:LEU:HD11	11:8A:156:LEU:HD22	1.94	0.50
20:9J:88:PHE:O	20:9J:91:ARG:NH1	2.44	0.50
25:C:213:GLU:HG2	25:C:214:LEU:HG	1.94	0.50
42:T:66:ALA:O	42:T:114:LEU:N	2.44	0.50
42:T:425:HIS:O	42:T:429:PRO:HD3	2.11	0.50
59:k:69:LEU:HD23	72:y:44:LEU:HB3	1.93	0.50
9:1Q:471:LEU:HD11	9:1Q:474:LEU:HD13	1.94	0.50
11:3A:20:ALA:HB2	11:3A:71:PRO:HB2	1.92	0.50
25:5C:502:GLU:HG3	25:5C:690:LEU:HB3	1.93	0.50
34:5L:90:PRO:HA	34:5L:127:TYR:HA	1.93	0.50
70:5w:66:SER:HB3	70:5w:70:ARG:HH11	1.76	0.50
1:6B:88:LEU:HD12	1:6B:240:PHE:HD1	1.76	0.50
23:A:148:THR:HG22	23:A:150:PRO:HD2	1.93	0.50
38:P:58:VAL:HG22	38:P:128:ILE:HB	1.92	0.50
42:T:443:ALA:O	50:b:94:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:X:72:GLU:OE2	70:w:70:ARG:NH2	2.45	0.50
7:1M:206:TYR:O	7:1M:284:ARG:NH2	2.41	0.50
14:2D:125:LEU:HD13	14:2D:210:PRO:HB3	1.93	0.50
20:2J:17:PRO:HG2	20:2J:24:GLU:HB3	1.92	0.50
27:5E:255:PHE:HD2	27:5E:345:LEU:HD13	1.77	0.50
29:5G:56:TRP:HZ2	51:5c:13:LYS:HE2	1.76	0.50
34:5L:90:PRO:HD3	34:5L:127:TYR:CZ	2.47	0.50
40:5R:330:SER:HB3	40:5R:334:TYR:CE2	2.47	0.50
42:5T:200:ILE:HD12	42:5T:236:PHE:HE2	1.76	0.50
42:5T:406:ASN:OD1	44:5V:150:TYR:OH	2.28	0.50
42:5T:425:HIS:O	42:5T:429:PRO:HD3	2.12	0.50
62:5n:20:HIS:CD2	62:5n:101:ILE:HA	2.47	0.50
66:5s:271:PHE:CE1	68:5u:40:GLU:HA	2.47	0.50
13:7C:3:GLU:O	13:7C:7:GLN:N	2.38	0.50
24:B:60:ASP:OD1	24:B:278:ARG:NH2	2.45	0.50
25:C:629:ASP:OD1	25:C:631:ARG:NH1	2.44	0.50
26:D:272:ASP:OD1	34:L:81:ARG:NH2	2.44	0.50
27:E:248:VAL:HG12	27:E:352:LEU:HD11	1.94	0.50
27:E:255:PHE:HD2	27:E:345:LEU:HD13	1.77	0.50
29:G:119:GLU:OE2	29:G:204:TYR:OH	2.24	0.50
39:Q:96:PHE:CE2	45:W:49:PHE:HB2	2.46	0.50
39:Q:275:ALA:HA	51:c:16:VAL:HG11	1.94	0.50
56:h:100:PHE:HZ	70:w:75:VAL:HG21	1.76	0.50
65:q:91:PRO:HG3	65:q:175:TRP:CZ3	2.47	0.50
6:1K:32:PRO:HB3	53:e:143:MET:CG	2.41	0.50
7:1N:107:HIS:HB3	7:1N:176:GLU:HG2	1.93	0.50
11:2A:371:PHE:HA	11:2A:374:VAL:HG22	1.93	0.50
11:4A:64:MET:HE1	76:4A:602:HEA:H172	1.93	0.50
20:4J:96:ILE:HG21	5:6J:26:ALA:HA	1.94	0.50
25:5C:403:ALA:HA	25:5C:526:ASN:HA	1.94	0.50
38:5P:171:ASP:H	38:5P:186:LYS:HD3	1.77	0.50
47:5Y:53:ILE:CG2	5:6I:26:ALA:HA	2.41	0.50
55:5g:13:GLU:OE1	59:5k:33:ARG:NE	2.42	0.50
65:5q:80:VAL:HG12	65:5q:188:PHE:HD1	1.77	0.50
72:5y:6:ALA:HA	72:5y:9:ILE:HD12	1.92	0.50
2:6C:93:PRO:O	2:6C:96:THR:OG1	2.26	0.50
16:7F:34:LYS:HE3	22:8L:12:TYR:CE2	2.46	0.50
16:8F:68:MET:HG3	16:8F:71:ARG:HH12	1.76	0.50
25:C:502:GLU:HG3	25:C:690:LEU:HB3	1.93	0.50
27:E:361:LYS:NZ	27:E:369:PRO:O	2.35	0.50
40:R:330:SER:HB3	40:R:334:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:T:428:LEU:HD23	50:b:67:TRP:HH2	1.75	0.50
62:n:20:HIS:CD2	62:n:101:ILE:HA	2.47	0.50
11:2A:43:ARG:HB2	20:2J:55:TYR:HB3	1.94	0.50
16:3F:68:MET:HG3	16:3F:71:ARG:HH12	1.76	0.50
23:5A:148:THR:HG22	23:5A:150:PRO:HD2	1.93	0.50
26:5D:89:GLY:HA2	26:5D:93:LEU:HB2	1.92	0.50
38:5P:297:PRO:HB2	38:5P:299:TRP:CD1	2.47	0.50
42:5T:362:ALA:HB1	42:5T:372:GLU:HG2	1.93	0.50
53:5e:210:SER:HB2	53:5e:214:GLN:HE22	1.76	0.50
68:5u:216:ILE:HG22	68:5u:217:MET:HE2	1.94	0.50
11:9A:96:LEU:HD11	11:9A:156:LEU:HD22	1.94	0.50
27:E:180:GLU:OE2	27:E:315:TYR:OH	2.20	0.50
30:H:83:ASP:HB2	31:I:149:VAL:HG21	1.94	0.50
33:K:39:GLN:HG3	33:K:44:MET:HB2	1.94	0.50
38:P:171:ASP:H	38:P:186:LYS:HD3	1.77	0.50
46:X:98:ASP:OD1	46:X:100:THR:OG1	2.24	0.50
46:X:133:ASP:OD1	46:X:133:ASP:N	2.44	0.50
66:s:271:PHE:CE1	68:u:40:GLU:HA	2.47	0.50
68:u:99:SER:N	68:u:123:ASP:OD1	2.45	0.50
68:u:216:ILE:HG22	68:u:217:MET:HE2	1.94	0.50
2:1D:78:PRO:HD2	7:1N:212:THR:HG21	1.94	0.50
27:5E:274:GLU:OE2	29:5G:40:GLU:HG2	2.11	0.50
27:5E:433:TYR:HD1	27:5E:465:ILE:HG23	1.77	0.50
30:5H:83:ASP:HB2	31:5I:149:VAL:HG21	1.93	0.50
40:5R:309:TRP:HD1	42:5T:164:PHE:HB3	1.77	0.50
52:5d:64:ARG:HG2	52:5d:67:ARG:NH2	2.26	0.50
68:5u:99:SER:N	68:5u:123:ASP:OD1	2.45	0.50
7:6M:39:PHE:CE1	49:a:50:PRO:CB	2.95	0.50
11:7A:117:VAL:O	11:7A:139:SER:OG	2.29	0.50
12:8B:141:LEU:HD21	18:8H:35:LEU:HD13	1.94	0.50
11:9A:64:MET:HE1	76:9A:603:HEA:H172	1.93	0.50
11:9A:77:PHE:O	11:9A:81:LEU:HB2	2.12	0.50
12:9B:144:PRO:HB2	13:9C:27:LYS:HE3	1.93	0.50
25:C:412:GLN:O	25:C:486:ARG:NE	2.35	0.50
27:E:274:GLU:OE2	29:G:40:GLU:HG2	2.11	0.50
27:E:317:LYS:HG3	30:H:111:LEU:HD23	1.94	0.50
29:G:153:GLU:HG2	35:M:63:ALA:HB3	1.94	0.50
44:V:60:VAL:N	44:V:78:PHE:O	2.42	0.50
9:1S:478:ASP:N	9:1S:478:ASP:OD1	2.45	0.50
13:2C:21:GLU:OE2	13:2C:25:ARG:NH2	2.44	0.50
76:4A:604:HEA:H243	12:4B:91:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5K:39:GLN:HG3	33:5K:44:MET:HB2	1.94	0.50
39:5Q:96:PHE:CE2	45:5W:49:PHE:HB2	2.46	0.50
39:5Q:129:LEU:HD21	45:5W:71:MET:HE3	1.94	0.50
52:5d:22:ASN:ND2	52:5d:28:ALA:O	2.44	0.50
65:5q:53:VAL:O	65:5q:69:GLY:N	2.24	0.50
65:5q:109:LYS:HA	65:5q:112:TRP:CE2	2.47	0.50
2:6C:86:GLU:HB3	2:6C:90:LYS:HD3	1.93	0.50
25:C:95:ARG:N	80:C:803:FES:S1	2.84	0.50
38:P:57:THR:HG21	38:P:120:ALA:HB1	1.94	0.50
3:1E:175:ARG:NH1	3:1E:180:GLY:O	2.43	0.49
24:5B:140:GLU:OE2	24:5B:148:ASP:N	2.36	0.49
26:5D:272:ASP:OD2	34:5L:81:ARG:NH1	2.35	0.49
26:5D:281:ASN:O	26:5D:282:ARG:NH1	2.34	0.49
44:5V:165:SER:OG	44:5V:231:ASP:HB3	2.12	0.49
44:5V:513:GLN:OE1	44:5V:513:GLN:N	2.36	0.49
45:5W:107:MET:HB3	45:5W:110:ARG:HB2	1.94	0.49
61:5m:44:PRO:HB2	61:5m:49:ILE:HD11	1.94	0.49
67:5t:139:VAL:HA	67:5t:156:ILE:HB	1.94	0.49
9:6Q:305:TYR:HB2	9:6Q:468:TYR:HB3	1.94	0.49
14:7D:125:LEU:HD13	14:7D:210:PRO:HB3	1.93	0.49
24:B:132:SER:HB2	24:B:172:ALA:HA	1.93	0.49
26:D:135:MET:HE1	26:D:149:LEU:HD13	1.94	0.49
50:b:88:GLU:OE1	63:o:29:ARG:NH1	2.45	0.49
52:d:22:ASN:ND2	52:d:28:ALA:O	2.44	0.49
53:e:210:SER:HB2	53:e:214:GLN:HE22	1.76	0.49
2:1C:86:GLU:HB3	2:1C:90:LYS:HD3	1.93	0.49
11:3A:77:PHE:O	11:3A:81:LEU:HB2	2.12	0.49
11:3A:96:LEU:HD11	11:3A:156:LEU:HD22	1.94	0.49
25:5C:629:ASP:OD1	25:5C:631:ARG:NH1	2.44	0.49
37:5O:53:CYS:HB3	37:5O:56:THR:HG21	1.93	0.49
39:5Q:147:LEU:HD11	41:5S:236:ILE:HG23	1.94	0.49
40:5R:89:VAL:O	40:5R:93:VAL:HG23	2.12	0.49
42:5T:214:VAL:HG13	42:5T:277:LYS:HD3	1.93	0.49
42:5T:428:LEU:HD23	50:5b:67:TRP:HH2	1.76	0.49
55:5g:8:GLN:CG	55:5g:11:ARG:HH21	2.24	0.49
1:6B:79:ARG:NH1	73:6B:401:HEM:O2D	2.39	0.49
7:6M:56:LEU:O	9:6Q:65:ARG:CZ	2.60	0.49
9:6Q:471:LEU:HD11	9:6Q:474:LEU:HD13	1.94	0.49
11:7A:371:PHE:HA	11:7A:374:VAL:HG22	1.93	0.49
29:G:56:TRP:HZ2	51:c:13:LYS:HE2	1.76	0.49
30:H:63:ASP:OD2	30:H:65:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:P:83:PRO:HB2	38:P:109:LEU:HD22	1.94	0.49
39:Q:91:ILE:HG22	39:Q:91:ILE:O	2.12	0.49
39:Q:129:LEU:HD21	45:W:71:MET:HE3	1.94	0.49
40:R:168:LEU:HD13	40:R:247:ILE:HD11	1.92	0.49
42:T:362:ALA:HB1	42:T:372:GLU:HG2	1.93	0.49
48:Z:103:ARG:NH2	58:j:36:ASP:OD1	2.34	0.49
65:q:109:LYS:HA	65:q:112:TRP:CE2	2.47	0.49
12:4B:33:THR:HG22	12:4B:37:MET:HE3	1.94	0.49
20:4J:96:ILE:CD1	5:6J:29:LYS:HB2	2.42	0.49
23:5A:190:ALA:HB3	23:5A:196:MET:HG2	1.94	0.49
44:5V:158:HIS:O	59:5k:91:SER:OG	2.29	0.49
44:5V:222:GLN:HA	44:5V:274:THR:HG21	1.93	0.49
65:5q:91:PRO:HG3	65:5q:175:TRP:CZ3	2.47	0.49
65:5q:91:PRO:HG2	65:5q:171:LEU:HD22	1.94	0.49
65:5q:114:LYS:HE3	65:5q:155:GLU:HB2	1.94	0.49
66:5s:158:SER:HB3	66:5s:184:HIS:HE1	1.77	0.49
71:5x:27:SER:O	71:5x:31:ASN:ND2	2.45	0.49
3:6F:149:ASP:N	3:6F:149:ASP:OD1	2.46	0.49
24:B:282:TRP:O	24:B:285:SER:OG	2.25	0.49
42:T:103:LEU:HD23	42:T:126:SER:HB2	1.94	0.49
44:V:302:TYR:CD1	44:V:406:LEU:HD22	2.47	0.49
67:t:71:PHE:HB2	67:t:227:ARG:HG3	1.94	0.49
9:1Q:65:ARG:HB2	32:5r:68:ALA:CB	2.35	0.49
15:2E:34:PHE:CB	66:s:92:ARG:CD	2.83	0.49
12:3B:33:THR:HG22	12:3B:37:MET:HE3	1.94	0.49
20:4J:102:ALA:CA	5:6J:29:LYS:HG3	2.42	0.49
23:5A:113:ALA:HB2	23:5A:123:VAL:HG21	1.95	0.49
25:5C:213:GLU:HG2	25:5C:214:LEU:HG	1.94	0.49
26:5D:168:TYR:N	26:5D:181:VAL:O	2.44	0.49
27:5E:201:LEU:HD12	39:5Q:28:MET:HE2	1.94	0.49
38:5P:57:THR:HG21	38:5P:120:ALA:HB1	1.94	0.49
44:5V:60:VAL:N	44:5V:78:PHE:O	2.42	0.49
53:5e:143:MET:CG	6:6K:32:PRO:HB3	2.41	0.49
55:5g:29:PHE:HB3	55:5g:32:VAL:HG21	1.93	0.49
60:5l:2:THR:OG1	60:5l:3:TRP:N	2.45	0.49
67:5t:71:PHE:HB2	67:5t:227:ARG:HG3	1.94	0.49
7:6M:54:SER:C	9:6Q:65:ARG:NH1	2.71	0.49
9:6Q:395:THR:O	9:6Q:397:VAL:N	2.45	0.49
11:7A:115:THR:O	19:7I:95:GLN:NE2	2.38	0.49
13:7C:21:GLU:OE2	13:7C:25:ARG:NH2	2.44	0.49
27:E:201:LEU:HD12	39:Q:28:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:F:151:LYS:O	28:F:154:ARG:HG2	2.13	0.49
29:G:229:LEU:HD22	30:H:50:LYS:HE2	1.94	0.49
40:R:198:LEU:HA	40:R:266:LEU:HD21	1.94	0.49
58:j:47:SER:OG	58:j:51:LYS:NZ	2.45	0.49
61:m:44:PRO:HB2	61:m:49:ILE:HD11	1.94	0.49
12:3B:141:LEU:HD21	18:3H:35:LEU:HD13	1.94	0.49
13:3C:21:GLU:OE2	13:3C:25:ARG:NH2	2.43	0.49
28:5F:109:GLY:HA2	29:5G:170:LYS:HA	1.95	0.49
29:5G:129:GLU:OE1	29:5G:130:GLU:N	2.43	0.49
42:5T:103:LEU:HD23	42:5T:126:SER:HB2	1.94	0.49
42:5T:213:HIS:NE2	42:5T:224:LEU:HB3	2.26	0.49
46:5X:72:GLU:OE2	70:5w:70:ARG:NH2	2.45	0.49
56:5h:50:PHE:CE1	67:5t:176:PRO:HD3	2.47	0.49
7:6M:58:GLU:OE2	9:6Q:65:ARG:HD2	2.12	0.49
7:6N:376:ASP:HB2	7:6N:379:ARG:HH21	1.78	0.49
11:8A:77:PHE:O	11:8A:81:LEU:HB2	2.12	0.49
25:C:270:ILE:HD12	25:C:279:ASN:HA	1.94	0.49
25:C:405:THR:OG1	25:C:523:ASN:O	2.20	0.49
28:F:107:GLY:O	28:F:112:HIS:ND1	2.35	0.49
34:L:24:SER:HA	34:L:29:ILE:HD11	1.94	0.49
34:L:90:PRO:HD3	34:L:127:TYR:CZ	2.47	0.49
35:M:105:VAL:HB	35:M:124:LEU:HD11	1.95	0.49
49:a:65:MET:SD	55:g:21:LEU:HG	2.52	0.49
55:g:29:PHE:HB3	55:g:32:VAL:HG21	1.93	0.49
57:i:45:ASP:OD1	61:m:126:ARG:NH1	2.45	0.49
9:1S:193:ASP:OD1	9:1S:193:ASP:N	2.42	0.49
39:5Q:91:ILE:HG22	39:5Q:91:ILE:O	2.12	0.49
64:5p:57:ALA:HA	64:5p:82:ASN:HB3	1.94	0.49
9:6Q:60:VAL:HG22	55:g:11:ARG:CB	2.28	0.49
11:7A:43:ARG:HB2	20:7J:55:TYR:HB3	1.94	0.49
22:7L:31:ARG:NH2	22:7L:61:SER:OG	2.34	0.49
76:9A:602:HEA:H243	12:9B:91:PRO:HB3	1.93	0.49
25:C:418:LEU:HB2	25:C:446:LEU:HA	1.95	0.49
40:R:309:TRP:HD1	42:T:164:PHE:HB3	1.77	0.49
42:T:280:VAL:O	42:T:283:SER:OG	2.23	0.49
44:V:158:HIS:O	59:k:91:SER:OG	2.29	0.49
44:V:222:GLN:HA	44:V:274:THR:HG21	1.93	0.49
53:e:16:ARG:N	63:o:42:ASN:OD1	2.34	0.49
67:t:139:VAL:HA	67:t:156:ILE:HB	1.94	0.49
71:x:27:SER:O	71:x:31:ASN:ND2	2.45	0.49
10:1R:5:LEU:HA	10:1R:8:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4J:96:ILE:CD1	5:6J:26:ALA:O	2.53	0.49
29:5G:229:LEU:HD22	30:5H:50:LYS:HE2	1.94	0.49
41:5S:249:LEU:HD21	51:5c:35:LYS:HE2	1.95	0.49
3:6E:199:TYR:OH	74:6E:401:HEC:O2A	2.28	0.49
25:C:298:GLU:HG3	34:L:152:ARG:HG3	1.94	0.49
26:D:109:VAL:O	26:D:123:THR:N	2.45	0.49
65:q:80:VAL:HG12	65:q:188:PHE:HD1	1.77	0.49
65:q:114:LYS:HE3	65:q:155:GLU:HB2	1.94	0.49
66:s:238:LEU:HG	66:s:239:ARG:HG3	1.95	0.49
2:1D:161:PRO:HD2	2:1D:204:ILE:HD11	1.95	0.49
2:1D:188:LYS:HG3	2:1D:191:ASP:H	1.78	0.49
7:1M:178:ASP:N	7:1M:178:ASP:OD1	2.43	0.49
7:1M:442:ALA:CB	9:1Q:61:THR:HG23	2.42	0.49
7:1N:309:ALA:O	7:1N:362:ASN:ND2	2.43	0.49
9:1Q:329:LYS:HE3	9:1Q:355:PHE:HA	1.95	0.49
9:1Q:395:THR:O	9:1Q:397:VAL:N	2.45	0.49
11:4A:77:PHE:O	11:4A:81:LEU:HB2	2.12	0.49
14:4D:125:LEU:HD13	14:4D:210:PRO:HB3	1.95	0.49
24:5B:60:ASP:OD1	24:5B:278:ARG:NH2	2.45	0.49
25:5C:270:ILE:HD12	25:5C:279:ASN:HA	1.94	0.49
25:5C:298:GLU:HG3	34:5L:152:ARG:HG3	1.94	0.49
26:5D:135:MET:HE1	26:5D:149:LEU:HD13	1.94	0.49
27:5E:425:ARG:HH22	27:5E:427:LYS:HD3	1.78	0.49
28:5F:151:LYS:O	28:5F:154:ARG:HG2	2.13	0.49
41:5S:221:SER:HB3	41:5S:279:GLU:O	2.12	0.49
58:5j:47:SER:OG	58:5j:51:LYS:NZ	2.45	0.49
71:5x:13:TRP:HA	71:5x:16:LEU:HD12	1.94	0.49
12:9B:33:THR:HG22	12:9B:37:MET:HE3	1.94	0.49
29:G:35:GLU:HG3	29:G:63:LYS:HB2	1.95	0.49
32:J:103:ILE:H	33:K:33:ARG:NH2	2.09	0.49
41:S:249:LEU:HD21	51:c:35:LYS:HE2	1.95	0.49
49:a:49:PRO:HB2	49:a:51:GLU:CD	2.38	0.49
49:a:51:GLU:HG2	49:a:52:LEU:HG	1.94	0.49
66:s:129:TRP:CD1	66:s:150:GLN:HA	2.48	0.49
11:3A:115:THR:O	19:3I:95:GLN:NE2	2.39	0.49
38:5P:83:PRO:HB2	38:5P:109:LEU:HD22	1.94	0.49
44:5V:302:TYR:CD1	44:5V:406:LEU:HD22	2.47	0.49
44:5V:534:GLY:O	44:5V:539:LEU:N	2.38	0.49
2:6D:188:LYS:HG3	2:6D:191:ASP:H	1.78	0.49
12:8B:33:THR:HG22	12:8B:37:MET:HE3	1.94	0.49
23:A:190:ALA:HB3	23:A:196:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:606:LYS:NZ	25:C:633:ASP:OD2	2.41	0.49
32:J:97:GLU:OE2	33:K:54:ARG:NH1	2.33	0.49
38:P:297:PRO:HB2	38:P:299:TRP:CD1	2.47	0.49
40:R:1:MET:HG3	60:l:92:SER:HB2	1.95	0.49
40:R:145:GLN:OE1	45:W:110:ARG:NH2	2.46	0.49
45:W:107:MET:HB3	45:W:110:ARG:HB2	1.93	0.49
48:Z:80:HIS:CG	63:o:81:ARG:HB3	2.48	0.49
66:s:158:SER:HB3	66:s:184:HIS:HE1	1.77	0.49
29:5G:153:GLU:HG2	35:5M:63:ALA:HB3	1.94	0.49
38:5P:171:ASP:HA	84:5P:401:NDP:H5N	1.95	0.49
40:5R:145:GLN:OE1	45:5W:110:ARG:NH2	2.46	0.49
42:5T:443:ALA:O	50:5b:94:TYR:OH	2.29	0.49
45:5W:128:ALA:HA	45:5W:132:TYR:HD1	1.78	0.49
57:5i:45:ASP:OD1	61:5m:126:ARG:NH1	2.45	0.49
57:5i:63:GLU:OE1	57:5i:66:ARG:NH1	2.42	0.49
26:D:278:GLU:OE2	26:D:279:THR:N	2.46	0.49
27:E:433:TYR:HD1	27:E:465:ILE:HG23	1.77	0.49
39:Q:147:LEU:HD11	41:S:236:ILE:HG23	1.94	0.49
44:V:176:SER:HB3	44:V:218:GLY:HA3	1.95	0.49
3:1F:149:ASP:N	3:1F:149:ASP:OD1	2.46	0.48
7:1N:376:ASP:HB2	7:1N:379:ARG:HH21	1.78	0.48
20:4J:93:PRO:HD3	5:6J:27:ALA:HB2	1.94	0.48
27:5E:338:LEU:O	27:5E:342:ARG:HG2	2.13	0.48
42:5T:117:LEU:HB2	42:5T:163:LEU:HD21	1.95	0.48
57:5i:32:ILE:O	57:5i:36:ARG:N	2.42	0.48
12:9B:141:LEU:HD21	18:9H:35:LEU:HD13	1.94	0.48
29:G:154:ARG:HB3	29:G:156:ASP:OD1	2.13	0.48
59:k:105:TYR:O	59:k:113:LYS:NZ	2.46	0.48
2:1C:184:ARG:NH1	2:1C:240:GLY:O	2.47	0.48
3:1E:232:ALA:HB3	74:1E:401:HEC:HBD2	1.96	0.48
9:1Q:305:TYR:HB2	9:1Q:468:TYR:HB3	1.94	0.48
11:4A:73:LEU:HB3	11:4A:244:PRO:HB2	1.95	0.48
26:5D:149:LEU:HD12	26:5D:169:HIS:O	2.13	0.48
31:5I:67:ALA:O	31:5I:71:VAL:HG23	2.13	0.48
59:5k:105:TYR:O	59:5k:113:LYS:NZ	2.46	0.48
66:5s:150:GLN:HE22	85:5s:401:COO:C9	2.25	0.48
17:7G:69:ASP:HA	17:7G:72:VAL:HG12	1.93	0.48
25:C:403:ALA:HA	25:C:526:ASN:HA	1.94	0.48
25:C:580:VAL:N	25:C:595:ASN:OD1	2.37	0.48
41:S:221:SER:HB3	41:S:279:GLU:O	2.12	0.48
44:V:138:MET:HE1	44:V:180:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:h:50:PHE:CE1	67:t:176:PRO:HD3	2.47	0.48
65:q:91:PRO:HG2	65:q:171:LEU:HD22	1.94	0.48
11:2A:199:LEU:HB2	11:2A:233:PHE:CG	2.48	0.48
26:5D:109:VAL:O	26:5D:123:THR:N	2.45	0.48
29:5G:35:GLU:HG3	29:5G:63:LYS:HB2	1.95	0.48
29:5G:154:ARG:HB3	29:5G:156:ASP:OD1	2.13	0.48
40:5R:139:TRP:HH2	45:5W:104:THR:HG22	1.79	0.48
40:5R:168:LEU:HB3	40:5R:247:ILE:HG12	1.95	0.48
65:5q:47:THR:HA	67:5t:184:ARG:HA	1.96	0.48
85:5s:401:COO:H121	85:5s:401:COO:C8A	2.44	0.48
2:6D:78:PRO:HD2	7:6N:212:THR:HG21	1.94	0.48
25:C:237:LEU:HD23	25:C:306:SER:HA	1.95	0.48
26:D:142:THR:N	31:I:126:GLU:OE1	2.45	0.48
26:D:211:MET:C	26:D:234:HIS:HB3	2.39	0.48
28:F:37:LEU:HB2	28:F:75:GLY:HA3	1.95	0.48
44:V:404:THR:HG23	72:y:88:ILE:HG22	1.95	0.48
64:p:57:ALA:HA	64:p:82:ASN:HB3	1.94	0.48
25:5C:237:LEU:HD23	25:5C:306:SER:HA	1.95	0.48
25:5C:269:SER:N	25:5C:280:ILE:O	2.33	0.48
34:5L:104:ASN:OD1	34:5L:107:MET:N	2.43	0.48
38:5P:377:ASP:HB3	45:5W:22:LYS:HZ2	1.78	0.48
40:5R:181:TYR:O	40:5R:236:ARG:NH1	2.36	0.48
44:5V:518:SER:O	44:5V:522:PRO:HG2	2.14	0.48
53:5e:144:GLY:HA2	6:6K:33:LYS:CD	2.42	0.48
65:5q:102:ASP:OD2	65:5q:146:PHE:HB3	2.14	0.48
66:5s:42:ALA:O	22:7L:9:LEU:HD11	2.13	0.48
67:5t:134:GLY:N	67:5t:150:VAL:O	2.47	0.48
9:6Q:329:LYS:HE3	9:6Q:355:PHE:HA	1.95	0.48
11:8A:73:LEU:HB3	11:8A:244:PRO:HB2	1.95	0.48
23:A:113:ALA:HB2	23:A:123:VAL:HG21	1.95	0.48
26:D:149:LEU:HD12	26:D:169:HIS:O	2.14	0.48
26:D:249:ARG:NE	26:D:260:GLU:OE1	2.46	0.48
38:P:132:GLY:O	84:P:401:NDP:H8A	2.13	0.48
38:P:171:ASP:HA	84:P:401:NDP:H5N	1.95	0.48
40:R:315:GLN:HB3	40:R:317:PHE:CZ	2.48	0.48
42:T:184:HIS:HB3	53:e:174:TYR:CE2	2.49	0.48
44:V:165:SER:OG	44:V:231:ASP:HB3	2.12	0.48
3:1F:81:PRO:HG3	5:1J:57:ASP:HB3	1.95	0.48
26:5D:211:MET:C	26:5D:234:HIS:HB3	2.39	0.48
27:5E:183:ARG:NH2	27:5E:405:GLU:O	2.42	0.48
40:5R:171:ALA:HB3	40:5R:221:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5T:403:TRP:HB2	44:5V:167:GLN:HE22	1.78	0.48
44:5V:284:THR:HG21	44:5V:505:CYS:HB3	1.96	0.48
66:5s:129:TRP:CD1	66:5s:150:GLN:HA	2.48	0.48
11:7A:199:LEU:HB2	11:7A:233:PHE:CG	2.49	0.48
25:C:87:ARG:NH2	25:C:298:GLU:OE2	2.46	0.48
26:D:69:ALA:O	27:E:303:ASP:N	2.42	0.48
27:E:261:GLU:OE1	39:Q:33:ARG:NH2	2.43	0.48
38:P:220:ILE:HD12	38:P:286:LEU:HD11	1.96	0.48
40:R:132:VAL:HG22	71:x:39:MET:HE3	1.95	0.48
32:r:48:ASP:OD1	32:r:51:SER:OG	2.22	0.48
1:1A:35:LEU:HD22	1:1A:236:LEU:HD13	1.95	0.48
2:1C:149:GLU:HA	2:1C:166:HIS:HB3	1.96	0.48
5:1J:26:ALA:CB	20:9J:96:ILE:HG21	2.40	0.48
25:5C:95:ARG:N	80:5C:801:FES:S1	2.84	0.48
26:5D:103:LYS:HB2	31:5I:138:PRO:O	2.14	0.48
30:5H:63:ASP:OD2	30:5H:65:LYS:NZ	2.45	0.48
35:5M:105:VAL:HB	35:5M:124:LEU:HD11	1.95	0.48
73:6B:401:HEM:HHD	73:6B:401:HEM:HBC2	1.95	0.48
13:9C:3:GLU:O	13:9C:7:GLN:N	2.41	0.48
26:D:229:TYR:OH	27:E:100:ARG:NH1	2.42	0.48
28:F:109:GLY:HA2	29:G:170:LYS:HA	1.95	0.48
38:P:387:GLU:O	38:P:390:ARG:HG2	2.13	0.48
40:R:89:VAL:O	40:R:93:VAL:HG23	2.12	0.48
44:V:518:SER:O	44:V:522:PRO:HG2	2.14	0.48
59:k:72:ARG:NH2	72:y:39:ASP:O	2.41	0.48
71:x:13:TRP:HA	71:x:16:LEU:HD12	1.94	0.48
9:1S:91:THR:HG22	9:1S:93:SER:H	1.79	0.48
22:2L:9:LEU:HD11	66:s:42:ALA:O	2.13	0.48
11:3A:118:GLU:O	19:3I:98:LYS:NZ	2.46	0.48
43:5U:187:ALA:O	43:5U:191:ILE:HG12	2.14	0.48
44:5V:176:SER:HB3	44:5V:218:GLY:HA3	1.95	0.48
51:5c:18:VAL:HG12	51:5c:22:MET:HE2	1.95	0.48
7:6N:309:ALA:O	7:6N:362:ASN:ND2	2.43	0.48
9:6Q:354:PRO:HA	9:6Q:367:VAL:HA	1.96	0.48
14:8D:125:LEU:HD13	14:8D:210:PRO:HB3	1.95	0.48
14:9D:125:LEU:HD13	14:9D:210:PRO:HB3	1.95	0.48
27:E:321:ASN:N	27:E:343:GLU:OE1	2.38	0.48
42:T:403:TRP:HB2	44:V:167:GLN:HE22	1.78	0.48
45:W:128:ALA:HA	45:W:132:TYR:HD1	1.78	0.48
49:a:48:VAL:O	49:a:53:GLN:NE2	2.47	0.48
65:q:47:THR:HA	67:t:184:ARG:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5C:583:GLN:NE2	25:5C:633:ASP:OD1	2.44	0.48
28:5F:37:LEU:HB2	28:5F:75:GLY:HA3	1.96	0.48
29:5G:49:ARG:O	29:5G:53:ALA:N	2.47	0.48
34:5L:29:ILE:O	34:5L:33:LYS:HG2	2.13	0.48
39:5Q:129:LEU:O	41:5S:222:PHE:HE2	1.96	0.48
42:5T:184:HIS:HB3	53:5e:174:TYR:CE2	2.49	0.48
48:5Z:80:HIS:CG	63:5o:81:ARG:HB3	2.48	0.48
3:6F:234:PRO:HD2	74:6F:501:HEC:HBC2	1.96	0.48
10:6R:10:LEU:HD23	10:6R:10:LEU:C	2.39	0.48
11:7A:290:GLY:O	13:7C:102:ARG:NH2	2.47	0.48
27:E:271:ILE:HD12	39:Q:260:LEU:HD22	1.96	0.48
27:E:425:ARG:HH22	27:E:427:LYS:HD3	1.78	0.48
34:L:34:ALA:HA	34:L:37:ILE:HG13	1.96	0.48
40:R:139:TRP:HH2	45:W:104:THR:HG22	1.78	0.48
42:T:222:VAL:HG13	42:T:318:PRO:HB3	1.96	0.48
42:T:336:ILE:HA	42:T:339:PHE:HD2	1.79	0.48
43:U:136:TYR:OH	45:W:100:VAL:O	2.19	0.48
48:Z:52:ARG:NH2	50:b:37:GLU:OE2	2.46	0.48
66:s:210:SER:OG	66:s:225:PRO:O	2.32	0.48
11:4A:96:LEU:HD11	11:4A:156:LEU:HD22	1.94	0.48
25:5C:418:LEU:HB2	25:5C:446:LEU:HA	1.95	0.48
26:5D:112:PRO:O	27:5E:161:GLN:NE2	2.47	0.48
26:5D:263:GLU:HB3	38:5P:49:SER:HB2	1.96	0.48
26:5D:278:GLU:OE2	26:5D:279:THR:N	2.46	0.48
30:5H:80:ARG:N	31:5I:149:VAL:O	2.47	0.48
38:5P:135:LEU:HD13	38:5P:312:ARG:HH12	1.79	0.48
40:5R:198:LEU:HA	40:5R:266:LEU:HD21	1.94	0.48
42:5T:127:LEU:HD11	42:5T:149:VAL:HA	1.96	0.48
44:5V:159:ARG:NH1	59:5k:87:GLY:O	2.39	0.48
67:5t:67:PRO:HG2	67:5t:70:VAL:HB	1.96	0.48
1:6A:35:LEU:HD22	1:6A:236:LEU:HD13	1.95	0.48
2:6D:175:SER:HB2	2:6D:234:SER:HB2	1.96	0.48
3:6F:81:PRO:HG3	5:6J:57:ASP:HB3	1.95	0.48
26:D:112:PRO:O	27:E:161:GLN:NE2	2.47	0.48
26:D:263:GLU:HB3	38:P:49:SER:HB2	1.96	0.48
29:G:49:ARG:O	29:G:53:ALA:N	2.47	0.48
42:T:117:LEU:HB2	42:T:163:LEU:HD21	1.95	0.48
44:V:139:LEU:O	44:V:143:GLU:HG2	2.14	0.48
44:V:159:ARG:NH1	59:k:87:GLY:O	2.39	0.48
53:e:188:GLU:OE1	53:e:188:GLU:N	2.47	0.48
68:u:56:PRO:HB3	68:u:74:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1J:29:LYS:HE3	20:9J:102:ALA:O	2.14	0.48
10:1T:49:GLU:OE2	10:1T:52:ARG:NH1	2.47	0.48
11:2A:115:THR:O	19:2I:95:GLN:NE2	2.39	0.48
27:5E:387:LYS:NZ	27:5E:391:GLU:OE1	2.36	0.48
39:5Q:82:SER:OG	39:5Q:83:GLN:OE1	2.32	0.48
48:5Z:52:ARG:NH2	50:5b:37:GLU:OE2	2.46	0.48
50:5b:88:GLU:OE1	63:5o:29:ARG:NH1	2.45	0.48
2:6D:161:PRO:HD2	2:6D:204:ILE:HD11	1.95	0.48
7:6N:53:LEU:HB2	9:6S:63:PRO:HG3	1.95	0.48
25:C:387:GLU:OE2	25:C:567:ASP:N	2.47	0.48
27:E:271:ILE:HG12	39:Q:263:TYR:CZ	2.49	0.48
27:E:301:GLY:N	27:E:325:ALA:O	2.47	0.48
29:G:135:CYS:HA	29:G:159:ARG:HH21	1.79	0.48
39:Q:3:VAL:HG13	41:S:176:ILE:HD11	1.96	0.48
39:Q:129:LEU:O	41:S:222:PHE:HE2	1.96	0.48
39:Q:291:ALA:O	61:m:68:ARG:NH1	2.46	0.48
55:g:18:HIS:O	55:g:22:GLN:HG3	2.14	0.48
3:1F:234:PRO:HD2	74:1F:501:HEC:HBC2	1.96	0.47
10:1T:4:LEU:HD23	10:1T:4:LEU:N	2.29	0.47
27:5E:261:GLU:OE2	39:5Q:33:ARG:NH1	2.39	0.47
34:5L:24:SER:HA	34:5L:29:ILE:HD11	1.94	0.47
40:5R:1:MET:HG3	60:5l:92:SER:HB2	1.95	0.47
46:5X:133:ASP:OD1	46:5X:133:ASP:N	2.44	0.47
59:5k:33:ARG:HG2	59:5k:37:TYR:CE1	2.49	0.47
65:5q:129:LYS:HE3	71:5x:16:LEU:HD23	1.96	0.47
66:5s:208:SER:O	66:5s:226:SER:OG	2.30	0.47
71:5x:9:THR:O	71:5x:13:TRP:HD1	1.97	0.47
9:6S:91:THR:HG22	9:6S:93:SER:H	1.79	0.47
14:7D:13:THR:OG1	14:7D:16:GLU:OE1	2.32	0.47
11:9A:118:GLU:O	19:9I:98:LYS:NZ	2.46	0.47
36:N:22:PHE:HZ	36:N:31:MET:HE1	1.79	0.47
40:R:168:LEU:HB3	40:R:247:ILE:HG12	1.95	0.47
44:V:518:SER:HG	44:V:519:PRO:HD3	1.78	0.47
45:W:26:MET:HE2	45:W:30:TYR:CZ	2.49	0.47
49:a:41:ARG:HG2	49:a:63:VAL:CG1	2.44	0.47
59:k:33:ARG:HG2	59:k:37:TYR:CE1	2.49	0.47
67:t:67:PRO:HG2	67:t:70:VAL:HB	1.96	0.47
71:x:9:THR:O	71:x:13:TRP:HD1	1.97	0.47
6:1K:33:LYS:CD	53:e:144:GLY:HA2	2.42	0.47
11:2A:290:GLY:O	13:2C:102:ARG:NH2	2.47	0.47
25:5C:611:VAL:HG22	25:5C:617:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:107:MET:HB3	26:5D:125:TYR:HB2	1.96	0.47
27:5E:271:ILE:HG12	39:5Q:263:TYR:CZ	2.48	0.47
29:5G:135:CYS:HA	29:5G:159:ARG:HH21	1.79	0.47
38:5P:387:GLU:O	38:5P:390:ARG:HG2	2.13	0.47
39:5Q:113:MET:HE3	39:5Q:132:VAL:HG11	1.95	0.47
44:5V:463:LEU:HB3	58:5j:37:TYR:HE2	1.80	0.47
48:5Z:101:ASP:OD1	48:5Z:105:ARG:N	2.47	0.47
56:5h:124:ARG:HH22	63:5o:113:LEU:HD23	1.79	0.47
11:7A:239:TYR:HA	11:7A:242:ILE:HG22	1.96	0.47
25:C:417:LEU:N	25:C:488:ALA:O	2.47	0.47
25:C:583:GLN:NE2	25:C:633:ASP:OD1	2.44	0.47
27:E:338:LEU:O	27:E:342:ARG:HG2	2.13	0.47
40:R:171:ALA:HB3	40:R:221:SER:HA	1.96	0.47
52:d:44:TYR:CZ	52:d:48:LYS:HD2	2.50	0.47
68:u:209:LEU:O	68:u:213:HIS:HD2	1.97	0.47
3:1E:85:TRP:HB2	3:1E:88:GLU:HG3	1.96	0.47
10:1R:10:LEU:HD23	10:1R:10:LEU:C	2.39	0.47
11:3A:73:LEU:HB3	11:3A:244:PRO:HB2	1.95	0.47
26:5D:274:ASN:HB3	34:5L:81:ARG:HH21	1.79	0.47
28:5F:107:GLY:O	28:5F:112:HIS:ND1	2.35	0.47
40:5R:93:VAL:HG21	45:5W:136:LEU:HD11	1.96	0.47
40:5R:132:VAL:HG22	71:5x:39:MET:HE3	1.95	0.47
42:5T:317:SER:OG	42:5T:318:PRO:HD3	2.15	0.47
44:5V:404:THR:HG23	72:5y:88:ILE:HG22	1.95	0.47
50:5b:51:VAL:HB	59:5k:104:ASN:HD21	1.79	0.47
58:5j:37:TYR:OH	58:5j:41:ARG:NH1	2.38	0.47
59:5k:26:LEU:O	59:5k:30:SER:OG	2.22	0.47
66:5s:150:GLN:HB3	66:5s:179:HIS:ND1	2.29	0.47
67:5t:146:ARG:HG2	67:5t:164:GLU:HG3	1.96	0.47
2:6D:164:ILE:HG12	2:6D:200:VAL:HG22	1.96	0.47
10:6T:82:ASP:OD1	10:6T:82:ASP:N	2.47	0.47
23:A:265:THR:OG1	24:B:58:ASP:OD1	2.33	0.47
28:F:29:SER:OG	39:Q:51:ASP:OD1	2.29	0.47
30:H:80:ARG:N	31:I:149:VAL:O	2.47	0.47
31:I:67:ALA:O	31:I:71:VAL:HG23	2.13	0.47
39:Q:155:ASP:OD1	39:Q:157:THR:OG1	2.24	0.47
39:Q:283:PHE:O	39:Q:287:HIS:ND1	2.48	0.47
40:R:93:VAL:HG21	45:W:136:LEU:HD11	1.96	0.47
42:T:87:CYS:HB3	42:T:219:ALA:HB1	1.97	0.47
44:V:434:VAL:CG1	49:a:38:ALA:HB3	2.44	0.47
2:1C:224:CYS:HB2	2:1C:229:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5C:87:ARG:NH2	25:5C:298:GLU:OE2	2.46	0.47
27:5E:271:ILE:HD12	39:5Q:260:LEU:HD22	1.96	0.47
28:5F:146:LEU:O	28:5F:150:LYS:HG2	2.15	0.47
40:5R:287:LEU:HA	40:5R:290:VAL:HG22	1.97	0.47
68:5u:209:LEU:O	68:5u:213:HIS:HD2	1.97	0.47
25:C:269:SER:N	25:C:280:ILE:O	2.33	0.47
26:D:274:ASN:HB3	34:L:81:ARG:HH21	1.79	0.47
27:E:269:ASN:HD21	27:E:271:ILE:HG13	1.79	0.47
34:L:29:ILE:O	34:L:33:LYS:HG2	2.13	0.47
35:M:67:LEU:O	35:M:79:LYS:NZ	2.38	0.47
38:P:135:LEU:HD13	38:P:312:ARG:HH12	1.79	0.47
39:Q:82:SER:OG	39:Q:83:GLN:OE1	2.32	0.47
42:T:317:SER:OG	42:T:318:PRO:HD3	2.14	0.47
42:T:370:ILE:HD11	44:V:66:TRP:CE2	2.50	0.47
42:T:385:LEU:HD22	70:w:82:VAL:HG22	1.96	0.47
43:U:187:ALA:O	43:U:191:ILE:HG12	2.14	0.47
44:V:284:THR:HG21	44:V:505:CYS:HB3	1.96	0.47
53:e:88:LYS:HA	53:e:91:GLN:HG2	1.97	0.47
65:q:102:ASP:OD2	65:q:146:PHE:HB3	2.13	0.47
3:1E:113:CYS:SG	3:1E:168:TYR:OH	2.72	0.47
7:1N:53:LEU:HB2	9:1S:63:PRO:HG3	1.95	0.47
11:2A:277:LEU:HD23	11:2A:280:ILE:HD11	1.97	0.47
14:2D:13:THR:OG1	14:2D:16:GLU:OE1	2.32	0.47
19:2I:32:TYR:HE1	21:2K:30:GLU:HG3	1.80	0.47
13:3C:3:GLU:O	13:3C:7:GLN:N	2.41	0.47
14:3D:125:LEU:HD13	14:3D:210:PRO:HB3	1.95	0.47
76:4A:602:HEA:H132	76:4A:602:HEA:HHC	1.96	0.47
17:4G:113:THR:C	17:4G:115:PRO:HD2	2.40	0.47
25:5C:357:ARG:HA	25:5C:383:ASP:HB3	1.97	0.47
25:5C:412:GLN:O	25:5C:486:ARG:NE	2.35	0.47
27:5E:127:LEU:HD11	28:5F:114:SER:HB2	1.97	0.47
30:5H:76:LYS:HG2	34:5L:25:ALA:HB1	1.97	0.47
42:5T:50:SER:OG	50:5b:88:GLU:O	2.30	0.47
44:5V:518:SER:HG	44:5V:519:PRO:HD3	1.78	0.47
48:5Z:103:ARG:NH2	58:5j:36:ASP:OD1	2.34	0.47
52:5d:44:TYR:CZ	52:5d:48:LYS:HD2	2.50	0.47
56:5h:57:ASP:H	56:5h:60:THR:HG1	1.57	0.47
68:5u:56:PRO:HB3	68:5u:74:VAL:HB	1.95	0.47
7:6M:312:THR:O	9:6Q:52:PRO:HD2	2.14	0.47
14:7D:41:GLY:O	14:7D:44:THR:OG1	2.26	0.47
76:8A:601:HEA:HHC	76:8A:601:HEA:H132	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:711:MET:HA	25:C:716:SER:HB2	1.96	0.47
26:D:107:MET:HB3	26:D:125:TYR:HB2	1.96	0.47
30:H:85:LYS:NZ	31:I:143:ALA:O	2.29	0.47
40:R:284:LEU:HD11	52:d:20:LEU:HD21	1.96	0.47
42:T:357:THR:O	42:T:361:LEU:HG	2.15	0.47
49:a:69:PHE:CG	49:a:70:HIS:N	2.83	0.47
56:h:124:ARG:HH22	63:o:113:LEU:HD23	1.79	0.47
73:1B:401:HEM:HHD	73:1B:401:HEM:HBC2	1.95	0.47
7:1M:405:ARG:NH1	7:1M:409:GLN:OE1	2.40	0.47
9:1Q:56:LYS:HD3	9:1Q:56:LYS:H	1.78	0.47
9:1S:331:LEU:HD13	9:1S:390:LEU:HD11	1.97	0.47
11:2A:330:THR:HG21	11:2A:404:ALA:HB1	1.96	0.47
13:2C:8:LEU:HD22	18:2H:19:VAL:HG21	1.96	0.47
14:2D:111:GLU:OE1	14:2D:225:HIS:NE2	2.33	0.47
76:3A:604:HEA:HH2	76:3A:604:HEA:H132	1.96	0.47
13:4C:96:MET:SD	13:4C:104:ASN:HB3	2.55	0.47
26:5D:249:ARG:NE	26:5D:260:GLU:OE1	2.46	0.47
34:5L:34:ALA:HA	34:5L:37:ILE:HG13	1.96	0.47
42:5T:33:THR:O	42:5T:36:PRO:HD2	2.14	0.47
42:5T:336:ILE:HA	42:5T:339:PHE:HD2	1.79	0.47
43:5U:150:VAL:HA	43:5U:226:LEU:HD13	1.97	0.47
44:5V:8:PHE:CE1	48:5Z:66:LEU:HD12	2.50	0.47
44:5V:139:LEU:O	44:5V:143:GLU:HG2	2.14	0.47
44:5V:260:HIS:NE2	44:5V:311:GLU:HG3	2.30	0.47
45:5W:26:MET:HE2	45:5W:30:TYR:CZ	2.49	0.47
46:5X:98:ASP:OD1	46:5X:100:THR:OG1	2.25	0.47
53:5e:88:LYS:HA	53:5e:91:GLN:HG2	1.97	0.47
53:5e:122:ARG:NH1	53:5e:126:ASP:OD2	2.47	0.47
59:5k:110:GLU:HG3	59:5k:111:TYR:CD2	2.50	0.47
68:5u:145:GLY:HA3	68:5u:164:ALA:HA	1.97	0.47
10:6R:5:LEU:HA	10:6R:8:VAL:HB	1.94	0.47
13:9C:96:MET:SD	13:9C:104:ASN:HB3	2.55	0.47
44:V:260:HIS:NE2	44:V:311:GLU:HG3	2.30	0.47
44:V:534:GLY:O	44:V:539:LEU:N	2.38	0.47
59:k:68:GLU:OE2	72:y:35:LYS:NZ	2.43	0.47
59:k:110:GLU:HG3	59:k:111:TYR:CD2	2.50	0.47
63:o:30:TRP:CD1	64:p:22:TYR:HB2	2.50	0.47
66:s:95:LYS:O	66:s:95:LYS:HD2	2.14	0.47
85:s:401:COO:C8A	85:s:401:COO:H121	2.44	0.47
2:1C:100:PRO:HA	4:1G:4:ARG:HH11	1.80	0.47
9:1Q:332:LEU:HD13	9:1Q:367:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2A:239:TYR:HA	11:2A:242:ILE:HG22	1.96	0.47
14:2D:153:VAL:HG12	17:2G:66:MET:HE3	1.97	0.47
16:3F:56:ASN:ND2	64:p:3:TYR:HB2	2.30	0.47
23:5A:265:THR:OG1	24:5B:61:ARG:NE	2.48	0.47
25:5C:150:CYS:SG	25:5C:248:GLY:HA3	2.55	0.47
25:5C:387:GLU:OE2	25:5C:567:ASP:N	2.47	0.47
25:5C:711:MET:HA	25:5C:716:SER:HB2	1.96	0.47
27:5E:283:THR:HG22	31:5I:53:HIS:ND1	2.30	0.47
27:5E:337:ARG:O	27:5E:341:MET:HG3	2.15	0.47
34:5L:60:THR:HG23	34:5L:116:LEU:HD11	1.97	0.47
38:5P:132:GLY:O	84:5P:401:NDP:H8A	2.13	0.47
40:5R:292:LEU:HB3	40:5R:334:TYR:CZ	2.50	0.47
40:5R:315:GLN:HB3	40:5R:317:PHE:CZ	2.48	0.47
42:5T:30:PHE:CD2	42:5T:34:ILE:HD11	2.49	0.47
42:5T:222:VAL:HG13	42:5T:318:PRO:HB3	1.96	0.47
42:5T:328:TYR:CD1	42:5T:334:LYS:HG3	2.50	0.47
44:5V:138:MET:HE1	44:5V:180:LEU:HD11	1.95	0.47
44:5V:312:THR:HG23	44:5V:464:LEU:HD21	1.96	0.47
53:5e:165:ASP:OD1	71:5x:54:ARG:NE	2.48	0.47
64:5p:42:ILE:HG22	64:5p:45:ARG:HH21	1.80	0.47
66:5s:238:LEU:HG	66:5s:239:ARG:HG3	1.95	0.47
2:6C:149:GLU:HA	2:6C:166:HIS:HB3	1.96	0.47
2:6D:189:ASP:OD1	2:6D:234:SER:OG	2.27	0.47
3:6E:232:ALA:HB3	74:6E:401:HEC:HBD2	1.96	0.47
7:6M:312:THR:CA	9:6Q:51:VAL:HG23	2.39	0.47
9:6S:331:LEU:HD13	9:6S:390:LEU:HD11	1.97	0.47
10:6T:57:ASP:OD1	10:6T:57:ASP:N	2.48	0.47
16:7F:63:GLN:HE21	22:8L:71:ARG:HE	1.59	0.47
23:A:265:THR:OG1	24:B:61:ARG:NE	2.48	0.47
25:C:150:CYS:SG	25:C:248:GLY:HA3	2.55	0.47
27:E:337:ARG:O	27:E:341:MET:HG3	2.15	0.47
27:E:387:LYS:NZ	27:E:391:GLU:OE1	2.36	0.47
28:F:69:ASP:HA	39:Q:58:LYS:HZ1	1.79	0.47
30:H:76:LYS:HG2	34:L:25:ALA:HB1	1.97	0.47
33:K:53:LEU:HA	33:K:56:ILE:HD12	1.97	0.47
38:P:387:GLU:HA	38:P:390:ARG:CZ	2.45	0.47
39:Q:113:MET:HE3	39:Q:132:VAL:HG11	1.95	0.47
42:T:30:PHE:CD2	42:T:34:ILE:HD11	2.49	0.47
42:T:76:LEU:HD12	42:T:234:ILE:HD12	1.96	0.47
42:T:328:TYR:CD1	42:T:334:LYS:HG3	2.49	0.47
44:V:463:LEU:HB3	58:j:37:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:e:165:ASP:OD1	71:x:54:ARG:NE	2.48	0.47
65:q:168:PRO:HG3	65:q:179:GLY:HA3	1.96	0.47
66:s:150:GLN:HE22	85:s:401:COO:C9	2.28	0.47
71:x:8:ASN:OD1	71:x:9:THR:N	2.47	0.47
2:1D:175:SER:HB2	2:1D:234:SER:HB2	1.96	0.47
7:1M:376:ASP:OD1	7:1M:376:ASP:N	2.47	0.47
10:1T:2:THR:OG1	10:1T:3:SER:N	2.48	0.47
27:5E:301:GLY:N	27:5E:325:ALA:O	2.47	0.47
39:5Q:291:ALA:O	61:5m:68:ARG:NH1	2.46	0.47
40:5R:39:LEU:O	40:5R:43:THR:OG1	2.31	0.47
40:5R:284:LEU:HD11	52:5d:20:LEU:HD21	1.96	0.47
42:5T:66:ALA:HB1	64:5p:28:PHE:HZ	1.80	0.47
44:5V:375:TRP:CD2	44:5V:376:PRO:HD2	2.50	0.47
53:5e:16:ARG:HB3	56:5h:139:ARG:NH2	2.30	0.47
63:5o:30:TRP:CD1	64:5p:22:TYR:HB2	2.50	0.47
71:5x:8:ASN:OD1	71:5x:9:THR:N	2.47	0.47
1:6A:80:TYR:O	1:6A:84:ASN:ND2	2.39	0.47
7:6N:132:LEU:HD12	9:6S:339:MET:HG2	1.97	0.47
9:6Q:72:LYS:HB3	9:6Q:72:LYS:NZ	2.30	0.47
13:8C:96:MET:SD	13:8C:104:ASN:HB3	2.55	0.47
11:9A:73:LEU:HB3	11:9A:244:PRO:HB2	1.95	0.47
25:C:182:LYS:HD3	25:C:192:MET:HG3	1.97	0.47
25:C:611:VAL:HG22	25:C:617:VAL:HA	1.96	0.47
33:K:35:LEU:HD11	33:K:57:VAL:HG21	1.97	0.47
34:L:60:THR:HG23	34:L:116:LEU:HD11	1.97	0.47
42:T:127:LEU:HD11	42:T:149:VAL:HA	1.96	0.47
50:b:123:ARG:NH1	50:b:162:ASP:OD1	2.48	0.47
53:e:122:ARG:NH1	53:e:126:ASP:OD2	2.47	0.47
61:m:9:PHE:HE2	61:m:19:PRO:HD3	1.80	0.47
68:u:178:GLU:OE1	68:u:180:TRP:NE1	2.46	0.47
12:4B:153:LYS:HA	12:4B:156:VAL:HG12	1.97	0.47
24:5B:428:GLU:OE2	61:5m:14:SER:OG	2.31	0.47
30:5H:80:ARG:NE	31:5I:151:ASP:OD2	2.30	0.47
38:5P:220:ILE:HD12	38:5P:286:LEU:HD11	1.96	0.47
39:5Q:238:LEU:HD13	39:5Q:245:LYS:HG2	1.97	0.47
40:5R:218:ILE:HG22	40:5R:222:MET:HE2	1.97	0.47
43:5U:156:LEU:HD11	43:5U:225:MET:HE3	1.97	0.47
50:5b:123:ARG:NH1	50:5b:162:ASP:OD1	2.48	0.47
50:5b:128:CYS:HB3	50:5b:133:MET:HB2	1.97	0.47
51:5c:2:SER:N	51:5c:5:GLU:OE1	2.46	0.47
51:5c:30:TYR:HA	51:5c:34:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:5k:6:VAL:HA	59:5k:9:LEU:HG	1.97	0.47
61:5m:9:PHE:HE2	61:5m:19:PRO:HD3	1.80	0.47
63:5o:30:TRP:H	64:5p:18:ASP:CG	2.22	0.47
10:6T:2:THR:C	10:6T:5:LEU:HB3	2.39	0.47
28:F:146:LEU:O	28:F:150:LYS:HG2	2.15	0.47
39:Q:46:LEU:HD13	39:Q:50:TRP:HZ2	1.80	0.47
40:R:38:TRP:HH2	40:R:77:ILE:HD11	1.80	0.47
40:R:181:TYR:O	40:R:236:ARG:NH1	2.36	0.47
42:T:66:ALA:HB1	64:p:28:PHE:HZ	1.79	0.47
42:T:209:LEU:HG	42:T:213:HIS:CD2	2.50	0.47
44:V:295:SER:O	44:V:299:GLN:HG2	2.15	0.47
44:V:312:THR:HG23	44:V:464:LEU:HD21	1.96	0.47
49:a:44:ASN:CG	32:r:58:HIS:HB2	2.40	0.47
51:c:18:VAL:HG12	51:c:22:MET:HE2	1.95	0.47
52:d:21:LYS:HD3	52:d:35:ILE:HG21	1.97	0.47
66:s:150:GLN:HB3	66:s:179:HIS:ND1	2.30	0.47
10:1T:2:THR:C	10:1T:5:LEU:HB3	2.39	0.47
10:1T:4:LEU:O	10:1T:8:VAL:HG22	2.15	0.47
14:4D:143:GLU:HB2	14:4D:203:PRO:HG2	1.97	0.47
28:5F:29:SER:OG	39:5Q:51:ASP:OD1	2.29	0.47
36:5N:22:PHE:HZ	36:5N:31:MET:HE1	1.79	0.47
40:5R:222:MET:HB3	40:5R:326:CYS:SG	2.55	0.47
42:5T:87:CYS:HB3	42:5T:219:ALA:HB1	1.97	0.47
42:5T:209:LEU:HG	42:5T:213:HIS:CD2	2.50	0.47
53:5e:16:ARG:N	63:5o:42:ASN:OD1	2.34	0.47
55:5g:13:GLU:HA	55:5g:15:TRP:NE1	2.30	0.47
65:5q:168:PRO:HG3	65:5q:179:GLY:HA3	1.96	0.47
66:5s:64:ASN:ND2	67:5t:48:GLU:O	2.38	0.47
68:5u:150:ILE:HA	68:5u:168:VAL:HB	1.96	0.47
2:6C:184:ARG:NH1	2:6C:240:GLY:O	2.47	0.47
9:6Q:47:GLY:O	9:6Q:48:ARG:NE	2.47	0.47
10:6R:9:ALA:O	10:6R:10:LEU:C	2.58	0.47
11:8A:118:GLU:O	19:8I:98:LYS:NZ	2.46	0.47
14:8D:143:GLU:HB2	14:8D:203:PRO:HG2	1.97	0.47
40:R:218:ILE:HG22	40:R:222:MET:HE2	1.97	0.47
41:S:223:TYR:HB3	45:W:151:ARG:HH21	1.80	0.47
42:T:33:THR:O	42:T:36:PRO:HD2	2.14	0.47
42:T:167:TYR:O	42:T:171:GLY:N	2.48	0.47
53:e:16:ARG:HB3	56:h:139:ARG:NH2	2.30	0.47
67:t:146:ARG:HG2	67:t:164:GLU:HG3	1.97	0.47
7:1N:397:GLU:OE2	8:1P:23:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1T:82:ASP:OD1	10:1T:82:ASP:N	2.47	0.46
12:2B:144:PRO:HB2	13:2C:27:LYS:HE3	1.96	0.46
20:4J:88:PHE:O	20:4J:91:ARG:NH1	2.44	0.46
24:5B:101:MET:O	24:5B:104:SER:OG	2.31	0.46
25:5C:264:LEU:HD13	25:5C:283:ASP:HB3	1.97	0.46
26:5D:115:SER:HA	26:5D:178:ARG:HH11	1.81	0.46
27:5E:124:THR:HA	27:5E:127:LEU:HD12	1.97	0.46
27:5E:269:ASN:HD21	27:5E:271:ILE:HG13	1.80	0.46
36:5N:57:ASN:ND2	36:5N:87:THR:O	2.48	0.46
42:5T:136:ARG:NH1	42:5T:215:ALA:O	2.36	0.46
42:5T:167:TYR:O	42:5T:171:GLY:N	2.48	0.46
44:5V:295:SER:O	44:5V:299:GLN:HG2	2.15	0.46
66:5s:95:LYS:HD2	66:5s:95:LYS:O	2.14	0.46
13:7C:8:LEU:HD22	18:7H:19:VAL:HG21	1.96	0.46
11:8A:277:LEU:HD23	11:8A:280:ILE:HD11	1.97	0.46
12:8B:153:LYS:HA	12:8B:156:VAL:HG12	1.97	0.46
20:8J:88:PHE:O	20:8J:91:ARG:NH1	2.44	0.46
26:D:103:LYS:HB2	31:I:138:PRO:O	2.14	0.46
27:E:122:ARG:NH2	27:E:142:ARG:O	2.31	0.46
42:T:31:VAL:HA	42:T:34:ILE:HD12	1.97	0.46
51:c:30:TYR:HA	51:c:34:VAL:HB	1.96	0.46
59:k:6:VAL:HA	59:k:9:LEU:HG	1.97	0.46
68:u:4:ILE:HG22	68:u:8:LYS:HE3	1.97	0.46
1:1A:336:LEU:HD11	1:1A:348:VAL:HG12	1.98	0.46
22:2L:9:LEU:HD11	66:s:46:LEU:N	2.30	0.46
26:5D:235:PRO:HA	26:5D:240:PHE:CD1	2.50	0.46
42:5T:76:LEU:HD12	42:5T:234:ILE:HD12	1.96	0.46
42:5T:113:VAL:HG22	42:5T:115:ASP:H	1.80	0.46
44:5V:450:LEU:O	44:5V:454:MET:HG3	2.15	0.46
50:5b:131:LEU:HD21	50:5b:160:PRO:HD3	1.97	0.46
56:5h:36:ALA:HB2	56:5h:53:ALA:HB3	1.97	0.46
1:6A:336:LEU:HD11	1:6A:348:VAL:HG12	1.98	0.46
9:6Q:332:LEU:HD13	9:6Q:367:VAL:HB	1.97	0.46
25:C:247:VAL:HG23	25:C:249:ALA:H	1.80	0.46
25:C:264:LEU:HD13	25:C:283:ASP:HB3	1.97	0.46
31:I:105:ASP:N	31:I:105:ASP:OD1	2.48	0.46
40:R:38:TRP:CZ3	40:R:73:LEU:HD13	2.51	0.46
40:R:93:VAL:HG22	43:U:192:THR:HG21	1.97	0.46
40:R:222:MET:HB3	40:R:326:CYS:SG	2.55	0.46
44:V:191:LEU:HD22	44:V:199:LEU:HD22	1.98	0.46
48:Z:101:ASP:OD1	48:Z:105:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:h:36:ALA:HB2	56:h:53:ALA:HB3	1.97	0.46
12:3B:36:ALA:HB1	22:3L:75:VAL:HG11	1.98	0.46
13:3C:96:MET:SD	13:3C:104:ASN:HB3	2.55	0.46
24:5B:130:ARG:NH1	24:5B:258:GLY:O	2.43	0.46
31:5I:105:ASP:OD1	31:5I:105:ASP:N	2.48	0.46
38:5P:292:ASP:OD2	47:5Y:5:ARG:NH1	2.48	0.46
39:5Q:46:LEU:HD13	39:5Q:50:TRP:HZ2	1.80	0.46
44:5V:355:ALA:HB2	55:5g:20:LEU:O	2.16	0.46
53:5e:51:TYR:O	53:5e:55:ASN:ND2	2.46	0.46
55:5g:9:TRP:CH2	32:5r:94:ALA:HB2	2.50	0.46
3:6E:85:TRP:HB2	3:6E:88:GLU:HG3	1.96	0.46
10:6T:49:GLU:OE2	10:6T:52:ARG:NH1	2.47	0.46
12:7B:33:THR:HG22	12:7B:37:MET:HE3	1.97	0.46
11:9A:117:VAL:HG11	11:9A:138:THR:HB	1.97	0.46
23:A:132:MET:HE1	24:B:181:GLY:HA3	1.96	0.46
27:E:127:LEU:HD11	28:F:114:SER:HB2	1.97	0.46
36:N:57:ASN:ND2	36:N:87:THR:O	2.48	0.46
38:P:292:ASP:OD2	47:Y:5:ARG:NH1	2.48	0.46
40:R:287:LEU:HA	40:R:290:VAL:HG22	1.97	0.46
40:R:292:LEU:HB3	40:R:334:TYR:CZ	2.50	0.46
42:T:421:ARG:NH2	50:b:50:GLU:OE1	2.36	0.46
44:V:8:PHE:CE1	48:Z:66:LEU:HD12	2.50	0.46
45:W:49:PHE:HB3	45:W:120:GLU:OE2	2.15	0.46
49:a:60:TYR:CE2	55:g:17:HIS:C	2.93	0.46
53:e:183:PRO:HA	53:e:192:ASP:HB2	1.96	0.46
7:1M:55:THR:CG2	9:1Q:66:THR:HB	2.46	0.46
9:1Q:354:PRO:HA	9:1Q:367:VAL:HA	1.96	0.46
17:3G:113:THR:C	17:3G:115:PRO:HD2	2.40	0.46
17:4G:69:ASP:HA	17:4G:72:VAL:HG12	1.98	0.46
25:5C:182:LYS:HD3	25:5C:192:MET:HG3	1.97	0.46
32:5J:103:ILE:O	33:5K:33:ARG:NH2	2.48	0.46
33:5K:35:LEU:HD11	33:5K:57:VAL:HG21	1.97	0.46
34:5L:61:PHE:HD1	34:5L:141:TRP:CD1	2.34	0.46
38:5P:387:GLU:HA	38:5P:390:ARG:CZ	2.45	0.46
39:5Q:3:VAL:HG13	41:5S:176:ILE:HD11	1.96	0.46
53:5e:9:THR:HG21	63:5o:55:THR:HG23	1.98	0.46
53:5e:183:PRO:HA	53:5e:192:ASP:HB2	1.96	0.46
68:5u:4:ILE:HG22	68:5u:8:LYS:HE3	1.97	0.46
14:7D:153:VAL:HG12	17:7G:66:MET:HE3	1.97	0.46
19:7I:32:TYR:HE1	21:7K:30:GLU:HG3	1.79	0.46
12:8B:36:ALA:HB1	22:8L:75:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:9A:603:HEA:H132	76:9A:603:HEA:HHC	1.96	0.46
27:E:283:THR:HG22	31:I:53:HIS:ND1	2.30	0.46
40:R:79:GLN:O	40:R:83:MET:HG3	2.16	0.46
46:X:37:ASP:OD1	46:X:37:ASP:N	2.47	0.46
49:a:60:TYR:CD1	55:g:19:PRO:HD3	2.50	0.46
50:b:88:GLU:HG2	50:b:95:TRP:HB2	1.97	0.46
65:q:129:LYS:HE3	71:x:16:LEU:HD23	1.96	0.46
66:s:196:MET:SD	85:s:401:COO:C5	3.03	0.46
7:1M:32:ASP:OD1	7:1M:32:ASP:N	2.49	0.46
17:2G:83:PRO:HB3	17:2G:114:TRP:CZ2	2.51	0.46
25:5C:297:ASN:O	25:5C:302:GLU:N	2.46	0.46
28:5F:65:PRO:HG3	28:5F:88:VAL:HG13	1.97	0.46
41:5S:223:TYR:HB3	45:5W:151:ARG:HH21	1.80	0.46
43:5U:164:GLU:OE2	43:5U:201:THR:OG1	2.33	0.46
2:6D:184:ARG:NH1	2:6D:240:GLY:O	2.39	0.46
7:6M:312:THR:O	9:6Q:51:VAL:HG22	2.15	0.46
12:7B:145:ASP:OD1	12:7B:145:ASP:N	2.48	0.46
17:9G:113:THR:C	17:9G:115:PRO:HD2	2.40	0.46
25:C:52:GLU:OE2	25:C:61:LYS:NZ	2.48	0.46
25:C:357:ARG:HA	25:C:383:ASP:HB3	1.97	0.46
39:Q:212:SER:OG	39:Q:213:LEU:N	2.49	0.46
44:V:430:SER:HA	55:g:16:ARG:NH1	2.30	0.46
50:b:51:VAL:HB	59:k:104:ASN:HD21	1.79	0.46
50:b:131:LEU:HD21	50:b:160:PRO:HD3	1.97	0.46
53:e:51:TYR:O	53:e:55:ASN:ND2	2.46	0.46
64:p:42:ILE:HG22	64:p:45:ARG:HH21	1.80	0.46
67:t:91:PHE:HB3	67:t:113:ASP:OD1	2.16	0.46
67:t:134:GLY:N	67:t:150:VAL:O	2.47	0.46
68:u:145:GLY:HA3	68:u:164:ALA:HA	1.97	0.46
7:1N:132:LEU:HD12	9:1S:339:MET:HG2	1.97	0.46
12:2B:33:THR:HG22	12:2B:37:MET:HE3	1.97	0.46
12:4B:36:ALA:HB1	22:4L:75:VAL:HG11	1.98	0.46
40:5R:38:TRP:HH2	40:5R:77:ILE:HD11	1.80	0.46
42:5T:31:VAL:HA	42:5T:34:ILE:HD12	1.97	0.46
49:5a:48:VAL:O	49:5a:53:GLN:NE2	2.48	0.46
66:5s:46:LEU:N	22:7L:9:LEU:HD11	2.30	0.46
2:6C:126:MET:HE3	2:6C:126:MET:HB3	1.81	0.46
7:6N:397:GLU:OE2	8:6P:23:THR:OG1	2.33	0.46
13:7C:141:ARG:O	13:7C:145:THR:OG1	2.29	0.46
17:8G:113:THR:C	17:8G:115:PRO:HD2	2.40	0.46
24:B:472:LYS:HA	61:m:13:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:365:ASP:OD1	25:C:365:ASP:N	2.47	0.46
26:D:235:PRO:HA	26:D:240:PHE:CD1	2.50	0.46
31:I:48:VAL:HG23	31:I:50:ILE:HG13	1.98	0.46
38:P:38:MET:SD	38:P:255:LEU:HB3	2.56	0.46
56:h:38:GLN:O	56:h:46:MET:N	2.42	0.46
11:3A:277:LEU:HD23	11:3A:280:ILE:HD11	1.97	0.46
23:5A:265:THR:OG1	24:5B:58:ASP:OD1	2.33	0.46
24:5B:282:TRP:O	24:5B:285:SER:OG	2.25	0.46
26:5D:142:THR:N	31:5I:126:GLU:OE1	2.45	0.46
42:5T:327:LEU:O	42:5T:331:ALA:CB	2.64	0.46
42:5T:357:THR:O	42:5T:361:LEU:HG	2.15	0.46
42:5T:370:ILE:HD11	44:5V:66:TRP:CE2	2.50	0.46
43:5U:150:VAL:HG21	71:5x:32:TYR:CE2	2.51	0.46
2:6C:224:CYS:HB2	2:6C:229:SER:HB2	1.96	0.46
9:6Q:67:SER:HB2	32:r:69:SER:HB3	1.89	0.46
11:7A:330:THR:HG21	11:7A:404:ALA:HB1	1.96	0.46
12:7B:144:PRO:HB2	13:7C:27:LYS:HE3	1.96	0.46
17:7G:83:PRO:HB3	17:7G:114:TRP:CZ2	2.51	0.46
12:9B:153:LYS:HA	12:9B:156:VAL:HG12	1.97	0.46
14:9D:143:GLU:HB2	14:9D:203:PRO:HG2	1.97	0.46
32:J:103:ILE:O	33:K:33:ARG:NH2	2.48	0.46
34:L:61:PHE:HD1	34:L:141:TRP:CD1	2.34	0.46
57:i:63:GLU:OE1	57:i:66:ARG:NH1	2.42	0.46
2:1D:76:MET:HE2	7:1N:187:VAL:HA	1.98	0.46
2:1D:164:ILE:HG12	2:1D:200:VAL:HG22	1.96	0.46
3:1F:232:ALA:HB3	74:1F:501:HEC:HBD2	1.98	0.46
22:3L:81:TRP:CE2	64:p:10:TYR:OH	2.47	0.46
14:4D:41:GLY:O	14:4D:44:THR:OG1	2.30	0.46
33:5K:114:LYS:HD2	33:5K:114:LYS:HA	1.73	0.46
38:5P:35:SER:O	38:5P:39:THR:OG1	2.26	0.46
42:5T:86:ILE:HD11	42:5T:429:PRO:HG2	1.97	0.46
45:5W:49:PHE:HB3	45:5W:120:GLU:OE2	2.16	0.46
46:5X:61:PHE:CE1	46:5X:67:PRO:HD2	2.48	0.46
50:5b:88:GLU:HG2	50:5b:95:TRP:HB2	1.97	0.46
55:5g:18:HIS:O	55:5g:22:GLN:HG3	2.15	0.46
56:5h:38:GLN:O	56:5h:46:MET:N	2.42	0.46
66:5s:49:MET:CE	12:7B:82:THR:HA	2.46	0.46
66:5s:256:TYR:OH	85:5s:401:COO:C9	2.63	0.46
9:6Q:57:LEU:CD1	72:y:60:LYS:HD2	2.41	0.46
11:9A:117:VAL:O	11:9A:139:SER:OG	2.34	0.46
11:9A:277:LEU:HD23	11:9A:280:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:112:PRO:HB2	27:E:161:GLN:HE21	1.81	0.46
27:E:124:THR:HA	27:E:127:LEU:HD12	1.97	0.46
28:F:65:PRO:HG3	28:F:88:VAL:HG13	1.97	0.46
34:L:104:ASN:OD1	34:L:107:MET:N	2.43	0.46
42:T:113:VAL:HG22	42:T:115:ASP:H	1.80	0.46
42:T:406:ASN:OD1	44:V:150:TYR:OH	2.28	0.46
43:U:156:LEU:HD11	43:U:225:MET:HE3	1.96	0.46
44:V:375:TRP:CD2	44:V:376:PRO:HD2	2.50	0.46
68:u:150:ILE:HA	68:u:168:VAL:HB	1.96	0.46
16:2F:63:GLN:HE21	22:3L:71:ARG:HE	1.59	0.46
20:4J:102:ALA:O	5:6J:29:LYS:CG	2.64	0.46
23:5A:132:MET:HE1	24:5B:181:GLY:HA3	1.97	0.46
23:5A:188:MET:N	80:5A:301:FES:S2	2.87	0.46
24:5B:123:MET:SD	24:5B:262:THR:OG1	2.74	0.46
25:5C:52:GLU:OE2	25:5C:61:LYS:NZ	2.48	0.46
25:5C:407:VAL:HG23	25:5C:614:GLU:OE1	2.16	0.46
26:5D:69:ALA:O	27:5E:303:ASP:N	2.42	0.46
26:5D:88:PHE:CD1	30:5H:93:LEU:HD13	2.51	0.46
38:5P:38:MET:SD	38:5P:255:LEU:HB3	2.56	0.46
39:5Q:22:LEU:HB2	39:5Q:48:PRO:HG3	1.98	0.46
42:5T:385:LEU:HD22	70:5w:82:VAL:HG22	1.96	0.46
52:5d:21:LYS:HD3	52:5d:35:ILE:HG21	1.97	0.46
54:5f:5:ALA:O	54:5f:8:SER:OG	2.31	0.46
68:5u:155:GLU:HB3	68:5u:173:THR:HG23	1.98	0.46
72:5y:84:MET:O	72:5y:88:ILE:HG13	2.16	0.46
17:9G:69:ASP:HA	17:9G:72:VAL:HG12	1.98	0.46
24:B:428:GLU:OE2	61:m:14:SER:OG	2.31	0.46
27:E:99:LEU:HG	27:E:101:LEU:HG	1.98	0.46
29:G:51:ARG:HH12	41:S:276:GLU:HG3	1.81	0.46
32:J:85:SER:OG	83:J:200:8Q1:O1	2.29	0.46
38:P:240:GLN:HB2	38:P:338:VAL:HG12	1.98	0.46
39:Q:238:LEU:HD13	39:Q:245:LYS:HG2	1.97	0.46
43:U:164:GLU:OE2	43:U:201:THR:OG1	2.33	0.46
46:X:61:PHE:CE1	46:X:67:PRO:HD2	2.48	0.46
1:1A:80:TYR:O	1:1A:84:ASN:ND2	2.39	0.46
11:4A:199:LEU:HB2	11:4A:233:PHE:CG	2.51	0.46
26:5D:112:PRO:HB2	27:5E:161:GLN:HE21	1.80	0.46
26:5D:229:TYR:OH	27:5E:100:ARG:NH1	2.42	0.46
27:5E:104:GLU:HB2	27:5E:112:ARG:HB3	1.97	0.46
27:5E:188:LEU:HD22	27:5E:207:ALA:HB1	1.98	0.46
27:5E:278:ASP:CG	29:5G:46:GLN:HG3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5F:75:GLY:HA2	82:5F:201:SF4:S4	2.56	0.46
46:5X:37:ASP:OD1	46:5X:37:ASP:N	2.47	0.46
7:6M:312:THR:CA	9:6Q:52:PRO:HD3	2.46	0.46
11:7A:277:LEU:HD23	11:7A:280:ILE:HD11	1.97	0.46
19:7I:34:HIS:CD2	21:7K:22:PRO:HG3	2.51	0.46
11:8A:117:VAL:O	11:8A:139:SER:OG	2.34	0.46
24:B:319:GLU:O	24:B:323:ARG:HG2	2.16	0.46
26:D:99:LYS:HD2	26:D:99:LYS:HA	1.75	0.46
26:D:115:SER:HA	26:D:178:ARG:HH11	1.81	0.46
38:P:209:VAL:HG21	38:P:356:VAL:HG13	1.98	0.46
39:Q:22:LEU:HB2	39:Q:48:PRO:HG3	1.98	0.46
50:b:128:CYS:HB3	50:b:133:MET:HB2	1.97	0.46
1:1A:88:LEU:HD12	1:1A:240:PHE:HD1	1.81	0.45
1:1B:79:ARG:NH1	73:1B:401:HEM:O2D	2.39	0.45
7:1M:54:SER:HA	9:1Q:65:ARG:HH12	1.69	0.45
9:1Q:57:LEU:HD21	55:5g:11:ARG:HG3	1.97	0.45
9:1Q:64:PRO:C	9:1Q:65:ARG:NH1	2.74	0.45
11:4A:117:VAL:HG11	11:4A:138:THR:HB	1.98	0.45
23:5A:98:GLN:HB2	23:5A:206:VAL:HG22	1.98	0.45
24:5B:319:GLU:O	24:5B:323:ARG:HG2	2.15	0.45
25:5C:247:VAL:HG23	25:5C:249:ALA:H	1.80	0.45
9:6Q:61:THR:H	55:g:11:ARG:CD	2.05	0.45
9:6S:305:TYR:HB2	9:6S:468:TYR:HB3	1.97	0.45
11:9A:115:THR:O	19:9I:95:GLN:NE2	2.39	0.45
26:D:168:TYR:N	26:D:181:VAL:O	2.45	0.45
39:Q:265:TYR:O	39:Q:269:MET:HG2	2.16	0.45
42:T:86:ILE:HD11	42:T:429:PRO:HG2	1.97	0.45
43:U:150:VAL:HA	43:U:226:LEU:HD13	1.97	0.45
44:V:355:ALA:HB2	55:g:20:LEU:O	2.15	0.45
53:e:75:PHE:HA	53:e:78:LEU:HG	1.98	0.45
27:5E:148:MET:SD	27:5E:148:MET:N	2.89	0.45
27:5E:160:GLU:OE2	27:5E:234:GLY:N	2.34	0.45
27:5E:334:TYR:CZ	27:5E:338:LEU:HD11	2.51	0.45
36:5N:61:TYR:CE2	36:5N:75:ILE:HD12	2.52	0.45
39:5Q:283:PHE:O	39:5Q:287:HIS:ND1	2.48	0.45
40:5R:79:GLN:O	40:5R:83:MET:HG3	2.16	0.45
49:5a:60:TYR:HB3	55:5g:18:HIS:HD2	1.70	0.45
52:5d:20:LEU:HA	52:5d:23:VAL:HB	1.99	0.45
63:5o:44:GLU:CD	63:5o:54:ASN:HD22	2.24	0.45
66:5s:210:SER:OG	66:5s:225:PRO:O	2.32	0.45
68:5u:97:VAL:HG22	68:5u:121:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6D:76:MET:HE2	7:6N:187:VAL:HA	1.98	0.45
11:7A:95:ARG:HG3	14:7D:31:LEU:HD13	1.98	0.45
11:9A:313:LYS:HE3	11:9A:313:LYS:HB3	1.82	0.45
24:B:441:GLU:O	24:B:443:HIS:ND1	2.49	0.45
26:D:88:PHE:CD1	30:H:93:LEU:HD13	2.51	0.45
27:E:104:GLU:HB2	27:E:112:ARG:HB3	1.97	0.45
36:N:61:TYR:CE2	36:N:75:ILE:HD12	2.52	0.45
38:P:377:ASP:HB3	45:W:22:LYS:HZ2	1.81	0.45
40:R:128:LEU:HD21	71:x:32:TYR:HA	1.98	0.45
43:U:150:VAL:HG21	71:x:32:TYR:CE2	2.51	0.45
44:V:450:LEU:O	44:V:454:MET:HG3	2.15	0.45
68:u:155:GLU:HB3	68:u:173:THR:HG23	1.98	0.45
7:1N:117:SER:OG	7:1N:120:GLU:OE1	2.33	0.45
13:3C:82:ASP:OD1	13:3C:82:ASP:N	2.49	0.45
14:3D:143:GLU:HB2	14:3D:203:PRO:HG2	1.97	0.45
25:5C:413:SER:OG	25:5C:486:ARG:O	2.25	0.45
33:5K:53:LEU:HA	33:5K:56:ILE:HD12	1.97	0.45
53:5e:188:GLU:OE1	53:5e:188:GLU:N	2.47	0.45
2:6C:100:PRO:HA	4:6G:4:ARG:HH11	1.80	0.45
7:6M:179:VAL:HG21	9:6Q:343:ARG:HH12	1.80	0.45
28:F:75:GLY:HA2	82:F:201:SF4:S4	2.57	0.45
38:P:253:ALA:HB3	38:P:349:LEU:HD13	1.98	0.45
38:P:283:LEU:O	38:P:287:ARG:N	2.49	0.45
42:T:35:ILE:O	42:T:39:VAL:HG23	2.17	0.45
63:o:30:TRP:H	64:p:18:ASP:CG	2.22	0.45
66:s:156:HIS:O	66:s:184:HIS:HA	2.17	0.45
11:2A:162:LEU:HD12	11:2A:193:ILE:HD12	1.98	0.45
19:2I:34:HIS:CD2	21:2K:22:PRO:HG3	2.51	0.45
12:3B:153:LYS:HA	12:3B:156:VAL:HG12	1.97	0.45
11:4A:277:LEU:HD23	11:4A:280:ILE:HD11	1.97	0.45
27:5E:122:ARG:HD3	28:5F:76:THR:HG21	1.97	0.45
27:5E:374:THR:HG23	61:5m:2:THR:HG21	1.97	0.45
38:5P:209:VAL:HG21	38:5P:356:VAL:HG13	1.97	0.45
40:5R:38:TRP:CZ3	40:5R:73:LEU:HD13	2.51	0.45
11:8A:217:PHE:HB3	11:8A:223:LEU:HD23	1.99	0.45
11:8A:313:LYS:HE3	11:8A:313:LYS:HB3	1.82	0.45
23:A:98:GLN:HB2	23:A:206:VAL:HG22	1.99	0.45
27:E:76:LEU:HG	33:K:81:ARG:NH1	2.32	0.45
37:O:7:LEU:HD23	37:O:7:LEU:O	2.17	0.45
49:a:65:MET:SD	55:g:18:HIS:CE1	3.10	0.45
72:y:84:MET:O	72:y:88:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1Q:68:THR:OG1	9:1Q:69:PRO:HD2	2.17	0.45
9:1S:305:TYR:HB2	9:1S:468:TYR:HB3	1.97	0.45
21:2K:28:PHE:O	21:2K:32:THR:OG1	2.34	0.45
11:3A:117:VAL:HG11	11:3A:138:THR:HB	1.98	0.45
24:5B:401:GLY:O	24:5B:407:ARG:HD3	2.17	0.45
27:5E:99:LEU:HG	27:5E:101:LEU:HG	1.98	0.45
27:5E:321:ASN:N	27:5E:343:GLU:OE1	2.38	0.45
38:5P:283:LEU:O	38:5P:287:ARG:N	2.49	0.45
42:5T:201:PRO:HD2	42:5T:288:MET:HG3	1.99	0.45
44:5V:191:LEU:HD22	44:5V:199:LEU:HD22	1.97	0.45
64:5p:3:TYR:HB2	16:8F:56:ASN:ND2	2.30	0.45
1:6A:88:LEU:HD12	1:6A:240:PHE:HD1	1.81	0.45
10:6T:4:LEU:HD23	10:6T:4:LEU:N	2.29	0.45
10:6T:4:LEU:O	10:6T:8:VAL:HG22	2.16	0.45
11:8A:117:VAL:HG11	11:8A:138:THR:HB	1.98	0.45
11:8A:199:LEU:HB2	11:8A:233:PHE:CG	2.51	0.45
11:9A:95:ARG:HG3	14:9D:31:LEU:HD13	1.99	0.45
14:9D:60:THR:OG1	21:9K:46:TYR:OH	2.30	0.45
24:B:180:ARG:NE	24:B:182:GLU:OE1	2.40	0.45
26:D:141:HIS:CD2	26:D:143:ASN:HB2	2.51	0.45
26:D:242:MET:HE1	26:D:268:PHE:CG	2.52	0.45
27:E:122:ARG:HD3	28:F:76:THR:HG21	1.98	0.45
39:Q:88:GLY:HA2	39:Q:92:SER:HB2	1.98	0.45
43:U:141:MET:HE2	43:U:169:ALA:HB2	1.99	0.45
44:V:118:TYR:CZ	44:V:151:LEU:HD13	2.51	0.45
46:X:114:ARG:HH12	46:X:125:LEU:HB3	1.82	0.45
49:a:68:GLU:CD	49:a:70:HIS:HE1	2.25	0.45
68:u:97:VAL:HG22	68:u:121:ILE:HB	1.99	0.45
10:1R:9:ALA:O	10:1R:10:LEU:C	2.58	0.45
12:2B:82:THR:HA	66:s:49:MET:CE	2.46	0.45
16:2F:90:LEU:HA	16:2F:93:GLU:HB2	1.98	0.45
23:5A:146:CYS:HB2	23:5A:188:MET:HG3	1.98	0.45
24:5B:472:LYS:HA	61:5m:13:LYS:HD2	1.97	0.45
25:5C:146:ASP:O	25:5C:150:CYS:N	2.48	0.45
25:5C:398:ARG:HD2	37:5O:51:ARG:HD2	1.99	0.45
26:5D:141:HIS:CD2	26:5D:143:ASN:HB2	2.51	0.45
26:5D:141:HIS:HD2	26:5D:144:THR:HG23	1.82	0.45
31:5I:48:VAL:HG23	31:5I:50:ILE:HG13	1.97	0.45
34:5L:92:TRP:HB2	34:5L:126:PHE:HB2	1.99	0.45
44:5V:422:TYR:CD1	44:5V:426:MET:HB2	2.52	0.45
45:5W:80:LEU:HD12	45:5W:80:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:5W:128:ALA:HA	45:5W:132:TYR:CD1	2.52	0.45
53:5e:146:PRO:HG2	53:5e:149:GLN:NE2	2.30	0.45
65:5q:121:GLU:OE1	72:5y:10:ARG:NH1	2.49	0.45
70:5w:80:PHE:CG	70:5w:81:PRO:HD3	2.52	0.45
7:6M:48:ASP:OD2	49:a:62:GLY:N	2.50	0.45
7:6N:452:ASP:OD1	7:6N:452:ASP:N	2.48	0.45
23:A:143:VAL:O	23:A:183:GLY:N	2.50	0.45
25:C:181:ASP:C	25:C:182:LYS:HD2	2.42	0.45
25:C:320:ARG:NH2	25:C:585:HIS:HB2	2.31	0.45
40:R:363:SER:OG	52:d:24:GLN:NE2	2.39	0.45
49:a:41:ARG:NH2	55:g:15:TRP:NE1	2.64	0.45
10:1R:24:VAL:O	10:1R:28:LEU:N	2.50	0.45
11:2A:95:ARG:HG3	14:2D:31:LEU:HD13	1.98	0.45
12:3B:139:HIS:HB3	18:3H:39:LEU:HD22	1.99	0.45
17:3G:69:ASP:HA	17:3G:72:VAL:HG12	1.98	0.45
29:5G:51:ARG:HH12	41:5S:276:GLU:HG3	1.81	0.45
39:5Q:88:GLY:HA2	39:5Q:92:SER:HB2	1.98	0.45
43:5U:143:TRP:CD2	45:5W:98:ASN:HB3	2.52	0.45
54:5f:7:PRO:O	54:5f:11:ILE:HG13	2.17	0.45
59:5k:26:LEU:HD12	59:5k:43:LEU:HD22	1.99	0.45
66:5s:177:ILE:HA	66:5s:194:VAL:HB	1.99	0.45
7:6M:225:ARG:HA	7:6M:228:LEU:HD12	1.99	0.45
14:7D:24:LYS:HG3	17:7G:29:TYR:CZ	2.52	0.45
11:8A:95:ARG:HG3	14:8D:31:LEU:HD13	1.99	0.45
11:9A:199:LEU:HB2	11:9A:233:PHE:CG	2.51	0.45
12:9B:36:ALA:HB1	22:9L:75:VAL:HG11	1.98	0.45
12:9B:139:HIS:HB3	18:9H:39:LEU:HD22	1.99	0.45
15:9E:33:LYS:NZ	15:9E:40:PRO:O	2.43	0.45
25:C:146:ASP:O	25:C:150:CYS:N	2.48	0.45
26:D:85:MET:HE2	26:D:175:TRP:CE2	2.52	0.45
27:E:202:THR:HA	39:Q:32:GLN:HG2	1.99	0.45
27:E:380:GLU:OE1	27:E:380:GLU:N	2.50	0.45
53:e:9:THR:HG21	63:o:55:THR:HG23	1.98	0.45
54:f:54:LEU:HB3	62:n:7:ARG:NH2	2.31	0.45
63:o:44:GLU:CD	63:o:54:ASN:HD22	2.24	0.45
66:s:150:GLN:OE1	66:s:179:HIS:N	2.50	0.45
7:1M:179:VAL:HG21	9:1Q:343:ARG:HH12	1.80	0.45
9:1Q:380:VAL:HG11	9:1Q:480:ILE:HD12	1.99	0.45
14:2D:41:GLY:O	14:2D:44:THR:OG1	2.26	0.45
14:2D:157:VAL:HG13	14:2D:187:LEU:HD22	1.99	0.45
12:4B:139:HIS:HB3	18:4H:39:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5B:441:GLU:O	24:5B:443:HIS:ND1	2.49	0.45
28:5F:26:ARG:CZ	28:5F:95:PRO:HG3	2.47	0.45
40:5R:93:VAL:HG22	43:5U:192:THR:HG21	1.97	0.45
42:5T:203:MET:SD	42:5T:262:SER:HA	2.57	0.45
43:5U:205:LEU:HD23	43:5U:205:LEU:HA	1.86	0.45
44:5V:118:TYR:CZ	44:5V:151:LEU:HD13	2.52	0.45
53:5e:9:THR:OG1	53:5e:10:PRO:HD3	2.17	0.45
54:5f:54:LEU:HB3	62:5n:7:ARG:NH2	2.32	0.45
66:5s:150:GLN:OE1	66:5s:179:HIS:N	2.50	0.45
67:5t:91:PHE:HB3	67:5t:113:ASP:OD1	2.16	0.45
23:A:132:MET:HE2	24:B:182:GLU:CD	2.42	0.45
25:C:407:VAL:HG23	25:C:614:GLU:OE1	2.16	0.45
27:E:148:MET:N	27:E:148:MET:SD	2.90	0.45
27:E:227:HIS:CD2	28:F:135:PRO:HD3	2.52	0.45
27:E:278:ASP:CG	29:G:46:GLN:HG3	2.41	0.45
42:T:38:TRP:CZ2	50:b:70:GLY:HA2	2.52	0.45
66:s:177:ILE:HA	66:s:194:VAL:HB	1.99	0.45
11:3A:117:VAL:O	11:3A:139:SER:OG	2.34	0.45
11:4A:95:ARG:HG3	14:4D:31:LEU:HD13	1.99	0.45
11:4A:117:VAL:O	11:4A:139:SER:OG	2.34	0.45
26:5D:98:ILE:HA	26:5D:105:VAL:HG21	1.99	0.45
29:5G:46:GLN:CD	29:5G:49:ARG:HH21	2.25	0.45
39:5Q:265:TYR:O	39:5Q:269:MET:HG2	2.16	0.45
40:5R:81:TYR:HB3	64:5p:69:PHE:CE1	2.51	0.45
40:5R:251:LEU:HD23	40:5R:251:LEU:HA	1.87	0.45
48:5Z:33:TYR:CZ	48:5Z:35:ARG:HG2	2.51	0.45
53:5e:75:PHE:HA	53:5e:78:LEU:HG	1.98	0.45
66:5s:156:HIS:O	66:5s:184:HIS:HA	2.17	0.45
1:6B:224:TYR:OH	7:6M:482:ASP:OD2	2.30	0.45
9:6Q:93:SER:O	9:6Q:164:ARG:NH1	2.49	0.45
9:6S:217:THR:HG23	9:6S:294:MET:HE3	1.99	0.45
24:B:123:MET:SD	24:B:262:THR:OG1	2.74	0.45
24:B:346:PRO:HD2	24:B:368:SER:HA	1.99	0.45
28:F:26:ARG:CZ	28:F:95:PRO:HG3	2.47	0.45
42:T:88:MET:HE1	42:T:97:PHE:HA	1.99	0.45
44:V:28:GLY:O	44:V:32:ILE:HG12	2.17	0.45
45:W:69:VAL:O	45:W:73:LEU:HB2	2.17	0.45
11:3A:199:LEU:HB2	11:3A:233:PHE:CG	2.51	0.45
24:5B:177:ILE:HD11	24:5B:216:LEU:HD21	1.99	0.45
27:5E:76:LEU:HG	33:5K:81:ARG:NH1	2.32	0.45
27:5E:380:GLU:N	27:5E:380:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5P:240:GLN:HB2	38:5P:338:VAL:HG12	1.98	0.45
45:5W:69:VAL:O	45:5W:73:LEU:HB2	2.17	0.45
53:5e:30:GLY:HA2	53:5e:216:TRP:HE1	1.81	0.45
3:6E:113:CYS:SG	3:6E:168:TYR:OH	2.73	0.45
3:6E:175:ARG:NH1	3:6E:180:GLY:O	2.43	0.45
7:6M:452:ASP:N	7:6M:452:ASP:OD1	2.50	0.45
9:6S:435:SER:OG	9:6S:438:GLU:OE1	2.24	0.45
24:B:388:ILE:HG13	24:B:459:LEU:HD13	1.99	0.45
27:E:188:LEU:HD22	27:E:207:ALA:HB1	1.98	0.45
27:E:254:GLN:O	27:E:258:ARG:HG2	2.17	0.45
27:E:334:TYR:CZ	27:E:338:LEU:HD11	2.51	0.45
27:E:374:THR:HG23	61:m:2:THR:HG21	1.97	0.45
30:H:89:ASP:OD1	30:H:89:ASP:N	2.47	0.45
38:P:390:ARG:HA	38:P:393:TYR:CZ	2.52	0.45
39:Q:226:MET:HE3	39:Q:226:MET:HB3	1.79	0.45
40:R:39:LEU:O	40:R:43:THR:OG1	2.31	0.45
67:t:218:HIS:NE2	68:u:112:THR:O	2.41	0.45
11:3A:27:GLY:HA3	11:3A:64:MET:SD	2.58	0.44
12:4B:115:ARG:HD2	12:4B:115:ARG:HA	1.89	0.44
26:5D:191:VAL:O	26:5D:216:PHE:HA	2.17	0.44
27:5E:254:GLN:O	27:5E:258:ARG:HG2	2.17	0.44
28:5F:130:TYR:CE2	29:5G:199:ARG:HB2	2.53	0.44
38:5P:85:ARG:NH2	84:5P:401:NDP:O3X	2.49	0.44
38:5P:247:VAL:O	38:5P:251:VAL:HG23	2.17	0.44
38:5P:390:ARG:HA	38:5P:393:TYR:CE2	2.52	0.44
38:5P:390:ARG:HA	38:5P:393:TYR:CZ	2.52	0.44
39:5Q:159:MET:HB2	60:5l:9:TYR:CZ	2.51	0.44
39:5Q:212:SER:OG	39:5Q:213:LEU:N	2.49	0.44
40:5R:45:LEU:HA	40:5R:50:PHE:CE2	2.52	0.44
42:5T:421:ARG:NH2	50:5b:50:GLU:OE1	2.36	0.44
43:5U:141:MET:SD	45:5W:11:CYS:HB3	2.58	0.44
44:5V:280:VAL:HG21	44:5V:509:TRP:CZ2	2.53	0.44
59:5k:29:TRP:CD1	59:5k:75:HIS:HD2	2.35	0.44
64:5p:33:GLU:OE2	64:5p:36:ARG:NH2	2.48	0.44
68:5u:43:ASN:C	68:5u:43:ASN:ND2	2.71	0.44
2:6D:152:THR:OG1	2:6D:165:ARG:NH1	2.37	0.44
7:6M:32:ASP:OD1	7:6M:32:ASP:N	2.49	0.44
7:6M:405:ARG:NH1	7:6M:409:GLN:OE1	2.40	0.44
7:6N:174:ASP:OD1	7:6N:177:ARG:NH1	2.45	0.44
10:6T:2:THR:OG1	10:6T:3:SER:N	2.48	0.44
14:7D:74:TRP:HE1	21:7K:32:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:7G:78:HIS:HB2	17:7G:109:ARG:NH2	2.32	0.44
12:8B:121:LYS:HB2	12:8B:132:GLU:HB2	1.99	0.44
11:9A:27:GLY:HA3	11:9A:64:MET:SD	2.57	0.44
23:A:146:CYS:HB2	23:A:188:MET:HG3	1.99	0.44
27:E:283:THR:HG23	27:E:286:MET:HE2	1.99	0.44
38:P:85:ARG:NH2	84:P:401:NDP:O3X	2.49	0.44
39:Q:159:MET:HB2	60:l:9:TYR:CZ	2.51	0.44
39:Q:288:ALA:O	39:Q:292:ILE:HG12	2.17	0.44
42:T:327:LEU:O	42:T:331:ALA:CB	2.64	0.44
44:V:422:TYR:CD1	44:V:426:MET:HB2	2.52	0.44
46:X:121:ARG:NE	46:X:143:ILE:HG12	2.32	0.44
53:e:9:THR:OG1	53:e:10:PRO:HD3	2.17	0.44
65:q:144:SER:O	71:x:17:ARG:NH2	2.41	0.44
66:s:158:SER:HB3	66:s:184:HIS:CE1	2.52	0.44
66:s:194:VAL:HA	66:s:212:VAL:HB	1.99	0.44
70:w:66:SER:HB3	70:w:70:ARG:NH1	2.32	0.44
6:1L:23:VAL:HG12	6:1L:24:ILE:HG23	1.98	0.44
9:1S:163:THR:HG22	9:1S:165:LEU:H	1.82	0.44
23:5A:69:THR:OG1	23:5A:99:GLU:OE1	2.29	0.44
25:5C:418:LEU:N	25:5C:445:GLY:O	2.43	0.44
25:5C:606:LYS:NZ	25:5C:633:ASP:OD2	2.41	0.44
38:5P:253:ALA:HB3	38:5P:349:LEU:HD13	1.98	0.44
40:5R:128:LEU:HD21	71:5x:32:TYR:HA	1.98	0.44
42:5T:35:ILE:O	42:5T:39:VAL:HG23	2.16	0.44
44:5V:28:GLY:O	44:5V:32:ILE:HG12	2.17	0.44
6:6L:23:VAL:HG12	6:6L:24:ILE:HG23	1.98	0.44
9:6Q:471:LEU:HD21	9:6Q:474:LEU:HB2	2.00	0.44
9:6S:478:ASP:N	9:6S:478:ASP:OD1	2.45	0.44
12:9B:115:ARG:HD2	12:9B:115:ARG:HA	1.89	0.44
23:A:249:GLY:HA3	23:A:259:PRO:HA	1.99	0.44
24:B:401:GLY:O	24:B:407:ARG:HD3	2.17	0.44
25:C:297:ASN:O	25:C:302:GLU:N	2.45	0.44
25:C:398:ARG:HD2	37:O:51:ARG:HD2	1.99	0.44
25:C:625:PRO:HG3	34:L:101:LYS:HB2	1.98	0.44
27:E:144:ASP:OD2	27:E:147:SER:OG	2.31	0.44
37:O:10:SER:HB2	37:O:93:GLY:HA3	1.98	0.44
40:R:81:TYR:HB3	64:p:69:PHE:CE1	2.52	0.44
43:U:143:TRP:CD2	45:W:98:ASN:HB3	2.52	0.44
51:c:2:SER:N	51:c:5:GLU:OE1	2.46	0.44
52:d:20:LEU:HA	52:d:23:VAL:HB	1.99	0.44
32:r:84:ASP:OD1	32:r:87:ASP:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1Q:93:SER:O	9:1Q:164:ARG:NH1	2.49	0.44
14:2D:24:LYS:HG3	17:2G:29:TYR:CZ	2.52	0.44
12:3B:115:ARG:HD2	12:3B:115:ARG:HA	1.89	0.44
11:4A:217:PHE:HB3	11:4A:223:LEU:HD23	1.99	0.44
23:5A:130:TYR:CD1	24:5B:222:ALA:HB3	2.52	0.44
25:5C:405:THR:OG1	25:5C:523:ASN:O	2.20	0.44
25:5C:500:ASP:OD1	25:5C:500:ASP:N	2.44	0.44
27:5E:227:HIS:CD2	28:5F:135:PRO:HD3	2.52	0.44
27:5E:362:SER:HB3	27:5E:368:CYS:SG	2.57	0.44
28:5F:91:GLN:HA	41:5S:200:LYS:HG3	2.00	0.44
37:5O:10:SER:HB2	37:5O:93:GLY:HA3	1.99	0.44
39:5Q:226:MET:HE3	39:5Q:226:MET:HB3	1.79	0.44
42:5T:293:LEU:HD23	42:5T:390:PHE:CE2	2.53	0.44
57:5i:52:ARG:NH2	61:5m:131:ALA:O	2.48	0.44
61:5m:98:LEU:HD23	61:5m:101:LEU:HD12	1.99	0.44
70:5w:66:SER:HB3	70:5w:70:ARG:NH1	2.32	0.44
7:6M:56:LEU:O	9:6Q:65:ARG:NE	2.50	0.44
12:7B:115:ARG:HA	12:7B:115:ARG:HD2	1.84	0.44
25:C:279:ASN:OD1	25:C:297:ASN:ND2	2.48	0.44
26:D:99:LYS:NZ	30:H:86:THR:O	2.44	0.44
26:D:141:HIS:HD2	26:D:144:THR:HG23	1.82	0.44
28:F:91:GLN:HA	41:S:200:LYS:HG3	2.00	0.44
33:K:110:ARG:CZ	38:P:352:VAL:HG11	2.47	0.44
42:T:294:ALA:O	42:T:302:SER:HB2	2.18	0.44
48:Z:33:TYR:CZ	48:Z:35:ARG:HG2	2.51	0.44
66:s:116:VAL:HA	66:s:134:LEU:O	2.18	0.44
70:w:80:PHE:CG	70:w:81:PRO:HD3	2.52	0.44
9:1Q:471:LEU:HD21	9:1Q:474:LEU:HB2	1.99	0.44
10:1R:82:ASP:OD1	10:1R:82:ASP:N	2.50	0.44
17:2G:78:HIS:HB2	17:2G:109:ARG:NH2	2.32	0.44
11:3A:217:PHE:HB3	11:3A:223:LEU:HD23	1.98	0.44
12:4B:105:LEU:HB2	22:4L:75:VAL:HG13	2.00	0.44
13:4C:82:ASP:OD1	13:4C:82:ASP:N	2.50	0.44
24:5B:388:ILE:HG13	24:5B:459:LEU:HD13	1.99	0.44
26:5D:99:LYS:HD2	26:5D:99:LYS:HA	1.76	0.44
26:5D:238:LYS:HE3	27:5E:424:TYR:CZ	2.53	0.44
27:5E:202:THR:HA	39:5Q:32:GLN:HG2	1.99	0.44
33:5K:110:ARG:CZ	38:5P:352:VAL:HG11	2.47	0.44
38:5P:359:GLY:O	38:5P:362:ILE:HG22	2.17	0.44
40:5R:194:THR:HG22	40:5R:270:ILE:HG12	2.00	0.44
42:5T:207:LEU:O	42:5T:210:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:5X:114:ARG:HH12	46:5X:125:LEU:HB3	1.82	0.44
59:5k:72:ARG:NH2	72:5y:39:ASP:O	2.41	0.44
1:6A:207:THR:OG1	73:6A:401:HEM:O1D	2.32	0.44
4:6H:18:THR:HG21	8:6P:29:ALA:HB1	1.99	0.44
7:6M:376:ASP:OD1	7:6M:379:ARG:NH1	2.50	0.44
9:6S:475:PRO:O	9:6S:476:ARG:NE	2.37	0.44
12:9B:121:LYS:HB2	12:9B:132:GLU:HB2	1.99	0.44
42:T:195:VAL:HG23	42:T:196:LEU:HG	1.98	0.44
42:T:201:PRO:HD2	42:T:288:MET:HG3	1.99	0.44
43:U:154:ARG:NH1	45:W:21:THR:O	2.51	0.44
54:f:7:PRO:O	54:f:11:ILE:HG13	2.17	0.44
61:m:98:LEU:HD23	61:m:101:LEU:HD12	1.99	0.44
1:1A:287:ASN:HB3	1:1A:290:MET:HB2	1.99	0.44
2:1C:64:PRO:HB3	7:1M:294:PHE:HE2	1.83	0.44
6:1K:35:PHE:CE2	53:e:143:MET:HE1	2.52	0.44
7:1M:225:ARG:HA	7:1M:228:LEU:HD12	1.99	0.44
9:1Q:62:GLU:OE2	32:5r:62:HIS:CD2	2.70	0.44
9:1Q:64:PRO:CB	32:5r:61:LYS:HB3	2.43	0.44
9:1S:119:VAL:HG11	9:1S:237:PHE:CE2	2.53	0.44
10:1T:2:THR:N	10:1T:5:LEU:CB	2.80	0.44
11:3A:95:ARG:HG3	14:3D:31:LEU:HD13	1.99	0.44
23:5A:132:MET:HE2	24:5B:182:GLU:CD	2.42	0.44
27:5E:283:THR:HG23	27:5E:286:MET:HE2	1.99	0.44
39:5Q:288:ALA:O	39:5Q:292:ILE:HG12	2.17	0.44
40:5R:308:PHE:HD2	42:5T:160:LEU:HD23	1.83	0.44
43:5U:141:MET:HE2	43:5U:169:ALA:HB2	1.99	0.44
44:5V:473:TRP:NE1	49:5a:100:TRP:O	2.51	0.44
66:5s:42:ALA:HB2	22:7L:12:TYR:CZ	2.52	0.44
66:5s:94:LEU:HD12	66:5s:96:ILE:HG12	2.00	0.44
3:6F:232:ALA:HB3	74:6F:501:HEC:HBD2	1.98	0.44
9:6Q:46:GLY:N	9:6Q:48:ARG:NH2	2.65	0.44
10:6R:7:GLN:O	10:6R:11:PRO:CD	2.66	0.44
9:6S:119:VAL:HG11	9:6S:237:PHE:CE2	2.53	0.44
17:8G:69:ASP:HA	17:8G:72:VAL:HG12	1.98	0.44
25:C:51:LEU:HD23	25:C:51:LEU:H	1.82	0.44
25:C:401:TYR:OH	37:O:51:ARG:NH2	2.51	0.44
26:D:238:LYS:HE3	27:E:424:TYR:CZ	2.53	0.44
34:L:175:ASP:OD1	34:L:175:ASP:N	2.48	0.44
38:P:240:GLN:HG2	38:P:269:GLY:N	2.32	0.44
38:P:247:VAL:O	38:P:251:VAL:HG23	2.17	0.44
42:T:203:MET:SD	42:T:262:SER:HA	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:V:195:GLU:O	44:V:199:LEU:HG	2.18	0.44
51:c:1:MET:HB2	51:c:5:GLU:HB2	2.00	0.44
7:1M:54:SER:O	9:1Q:65:ARG:HD3	2.18	0.44
11:2A:363:ASP:HA	11:2A:432:ARG:HD3	2.00	0.44
16:2F:56:ASN:CG	22:3L:65:PHE:CD1	2.96	0.44
16:2F:63:GLN:NE2	22:3L:71:ARG:CD	2.79	0.44
18:2H:78:GLU:HA	18:2H:83:GLN:HE22	1.83	0.44
11:3A:411:LEU:O	11:3A:415:VAL:HG22	2.18	0.44
16:3F:53:TRP:CA	64:p:3:TYR:CD2	3.01	0.44
25:5C:181:ASP:C	25:5C:182:LYS:HD2	2.42	0.44
25:5C:714:ALA:HA	25:5C:717:ARG:HB2	1.99	0.44
36:5N:111:GLN:OE1	36:5N:115:GLN:NE2	2.41	0.44
38:5P:240:GLN:HG2	38:5P:269:GLY:N	2.32	0.44
41:5S:227:ILE:HG21	45:5W:151:ARG:HG3	2.00	0.44
42:5T:38:TRP:CZ2	50:5b:70:GLY:HA2	2.52	0.44
9:6Q:380:VAL:HG11	9:6Q:480:ILE:HD12	1.99	0.44
11:8A:411:LEU:O	11:8A:415:VAL:HG22	2.18	0.44
11:9A:267:MET:SD	11:9A:313:LYS:NZ	2.85	0.44
12:9B:126:GLN:HA	12:9B:127:TRP:HA	1.77	0.44
25:C:562:TYR:HD1	25:C:581:ILE:HB	1.83	0.44
27:E:398:GLY:HA2	34:L:27:TYR:CG	2.53	0.44
39:Q:73:ALA:O	39:Q:77:ILE:N	2.41	0.44
42:T:30:PHE:O	42:T:34:ILE:HG13	2.18	0.44
45:W:89:THR:H	53:e:89:GLN:NE2	2.16	0.44
45:W:128:ALA:HA	45:W:132:TYR:CD1	2.52	0.44
47:Y:17:TRP:O	47:Y:21:ILE:HG12	2.18	0.44
52:d:76:ARG:NH2	53:e:190:TRP:O	2.51	0.44
55:g:13:GLU:HA	55:g:15:TRP:NE1	2.32	0.44
10:1R:8:VAL:C	10:1R:11:PRO:HD2	2.43	0.44
11:2A:227:GLN:HB2	11:2A:286:MET:HE3	2.00	0.44
11:4A:411:LEU:O	11:4A:415:VAL:HG22	2.18	0.44
20:4J:96:ILE:HD11	5:6J:30:ALA:CA	2.38	0.44
25:5C:401:TYR:OH	37:5O:51:ARG:NH2	2.51	0.44
25:5C:417:LEU:N	25:5C:488:ALA:O	2.47	0.44
25:5C:580:VAL:HB	25:5C:594:ALA:HA	2.00	0.44
27:5E:391:GLU:OE2	27:5E:394:HIS:NE2	2.49	0.44
28:5F:101:MET:HA	28:5F:131:VAL:HB	2.00	0.44
38:5P:204:ARG:NH1	38:5P:266:TYR:OH	2.41	0.44
40:5R:35:CYS:SG	40:5R:73:LEU:HD11	2.58	0.44
40:5R:296:PRO:HA	40:5R:301:PHE:CG	2.53	0.44
43:5U:154:ARG:NH1	45:5W:21:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5c:1:MET:HB2	51:5c:5:GLU:HB2	2.00	0.44
32:5r:84:ASP:OD1	32:5r:87:ASP:N	2.40	0.44
66:5s:194:VAL:HA	66:5s:212:VAL:HB	1.99	0.44
68:5u:106:ALA:O	68:5u:130:GLY:HA2	2.17	0.44
7:6N:101:VAL:HG23	7:6N:228:LEU:HD23	2.00	0.44
16:7F:56:ASN:CB	22:8L:65:PHE:CD1	3.01	0.44
12:8B:105:LEU:HB2	22:8L:75:VAL:HG13	2.00	0.44
14:8D:41:GLY:O	14:8D:44:THR:OG1	2.30	0.44
24:B:316:PRO:HA	24:B:357:LEU:HA	2.00	0.44
24:B:479:LYS:HG3	61:m:11:GLY:HA3	2.00	0.44
25:C:130:LYS:HA	25:C:130:LYS:HD2	1.85	0.44
27:E:362:SER:HB3	27:E:368:CYS:SG	2.57	0.44
34:L:33:LYS:C	34:L:35:ALA:H	2.26	0.44
40:R:38:TRP:CH2	40:R:77:ILE:HD11	2.53	0.44
50:b:164:LYS:NZ	50:b:168:GLU:OE2	2.46	0.44
53:e:30:GLY:HA2	53:e:216:TRP:HE1	1.81	0.44
53:e:58:LEU:HD22	71:x:51:PHE:CD2	2.53	0.44
53:e:77:ARG:HD2	71:x:22:LYS:HZ1	1.83	0.44
57:i:52:ARG:NH2	61:m:131:ALA:O	2.48	0.44
59:k:26:LEU:HD12	59:k:43:LEU:HD22	1.99	0.44
63:o:11:PHE:HE2	63:o:41:LEU:HD11	1.82	0.44
2:1D:184:ARG:NH1	2:1D:240:GLY:O	2.39	0.44
4:1H:18:THR:HG21	8:1P:29:ALA:HB1	1.99	0.44
9:1Q:355:PHE:HE2	9:1Q:368:VAL:HG23	1.83	0.44
11:3A:265:THR:HG22	22:3L:5:PHE:CD2	2.52	0.44
16:3F:59:ARG:CZ	64:p:10:TYR:CB	2.96	0.44
11:4A:27:GLY:HA3	11:4A:64:MET:SD	2.58	0.44
23:5A:143:VAL:O	23:5A:183:GLY:N	2.50	0.44
24:5B:267:GLU:OE1	24:5B:295:LYS:NZ	2.51	0.44
33:5K:53:LEU:O	33:5K:57:VAL:HG23	2.18	0.44
40:5R:204:TRP:NE1	40:5R:208:TRP:HD1	2.16	0.44
42:5T:294:ALA:O	42:5T:302:SER:HB2	2.18	0.44
53:5e:143:MET:HE1	6:6K:35:PHE:CE2	2.52	0.44
66:5s:92:ARG:CG	15:7E:34:PHE:CD2	2.86	0.44
66:5s:116:VAL:HA	66:5s:134:LEU:O	2.18	0.44
66:5s:196:MET:SD	85:5s:401:COO:C5	3.06	0.44
66:5s:286:ALA:O	66:5s:292:ASN:ND2	2.51	0.44
11:7A:162:LEU:HD12	11:7A:193:ILE:HD12	1.98	0.44
11:7A:227:GLN:HB2	11:7A:286:MET:HE3	2.00	0.44
11:7A:363:ASP:HA	11:7A:432:ARG:HD3	2.00	0.44
12:8B:139:HIS:HB3	18:8H:39:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:9A:217:PHE:HB3	11:9A:223:LEU:HD23	1.98	0.44
24:B:130:ARG:NH1	24:B:258:GLY:O	2.43	0.44
43:U:141:MET:SD	45:W:11:CYS:HB3	2.58	0.44
51:c:36:PRO:HA	51:c:40:GLU:HB2	2.00	0.44
2:1C:126:MET:HE3	2:1C:126:MET:HB3	1.81	0.44
7:1M:92:ARG:NH1	7:1M:139:GLU:OE2	2.49	0.44
7:1N:174:ASP:OD1	7:1N:177:ARG:NH1	2.45	0.44
7:1N:432:LEU:HD23	7:1N:432:LEU:HA	1.89	0.44
9:1Q:64:PRO:CG	32:5r:61:LYS:HB2	2.47	0.44
20:4J:92:ILE:HD11	5:6J:23:LYS:HG2	2.00	0.44
24:5B:479:LYS:HG3	61:5m:11:GLY:HA3	2.00	0.44
25:5C:625:PRO:HG3	34:5L:101:LYS:HB2	1.98	0.44
32:5J:85:SER:OG	83:5J:200:8Q1:O1	2.29	0.44
40:5R:111:ARG:NH2	66:5s:289:ASP:OD1	2.51	0.44
40:5R:242:SER:O	40:5R:246:GLU:HG2	2.18	0.44
41:5S:274:ALA:HB1	45:5W:152:PHE:CE1	2.53	0.44
45:5W:84:SER:OG	53:5e:84:ARG:NH2	2.50	0.44
47:5Y:17:TRP:O	47:5Y:21:ILE:HG12	2.18	0.44
62:5n:61:LYS:HE3	62:5n:61:LYS:HB3	1.79	0.44
1:6A:147:ILE:HD13	1:6A:147:ILE:HA	1.80	0.44
9:6S:163:THR:HG22	9:6S:165:LEU:H	1.82	0.44
22:9L:5:PHE:CE2	22:9L:6:LYS:O	2.71	0.44
24:B:177:ILE:HG13	24:B:216:LEU:HD11	2.00	0.44
27:E:298:ARG:HH21	27:E:305:ASP:HA	1.82	0.44
27:E:391:GLU:OE2	27:E:394:HIS:NE2	2.49	0.44
33:K:53:LEU:O	33:K:57:VAL:HG23	2.18	0.44
39:Q:259:THR:HG23	39:Q:260:LEU:HG	2.00	0.44
39:Q:274:LYS:HE3	41:S:275:LEU:HB2	2.00	0.44
43:U:178:ALA:O	43:U:182:ASN:N	2.51	0.44
44:V:280:VAL:HG21	44:V:509:TRP:CZ2	2.53	0.44
45:W:84:SER:OG	53:e:84:ARG:NH2	2.50	0.44
59:k:29:TRP:CD1	59:k:75:HIS:HD2	2.36	0.44
68:u:106:ALA:O	68:u:130:GLY:HA2	2.17	0.44
7:1M:376:ASP:OD1	7:1M:379:ARG:NH1	2.50	0.43
11:2A:267:MET:SD	11:2A:313:LYS:NZ	2.81	0.43
12:2B:115:ARG:HD2	12:2B:115:ARG:HA	1.84	0.43
23:5A:249:GLY:HA3	23:5A:259:PRO:HA	1.99	0.43
26:5D:101:VAL:O	26:5D:105:VAL:HG23	2.18	0.43
39:5Q:112:VAL:HG13	39:5Q:206:TYR:CG	2.54	0.43
39:5Q:259:THR:HG23	39:5Q:260:LEU:HG	2.00	0.43
40:5R:295:LEU:HD23	40:5R:295:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5S:162:LEU:HB3	61:5m:139:ARG:CZ	2.48	0.43
42:5T:77:MET:HG3	42:5T:111:LEU:HD13	2.00	0.43
42:5T:88:MET:HE1	42:5T:97:PHE:HA	1.99	0.43
66:5s:158:SER:HB3	66:5s:184:HIS:CE1	2.52	0.43
21:7K:28:PHE:O	21:7K:32:THR:OG1	2.34	0.43
15:9E:95:VAL:HG13	15:9E:99:LEU:HG	2.00	0.43
23:A:84:TYR:CZ	24:B:257:TYR:HB3	2.54	0.43
26:D:98:ILE:HA	26:D:105:VAL:HG21	1.99	0.43
26:D:191:VAL:O	26:D:216:PHE:HA	2.17	0.43
26:D:269:ARG:NH2	29:G:145:GLN:O	2.51	0.43
29:G:56:TRP:CH2	51:c:12:TYR:HE2	2.36	0.43
40:R:204:TRP:NE1	40:R:208:TRP:HD1	2.16	0.43
40:R:233:PRO:O	65:q:98:GLN:NE2	2.39	0.43
63:o:72:LEU:HD23	63:o:72:LEU:HA	1.87	0.43
66:s:81:GLY:N	66:s:119:ASN:OD1	2.27	0.43
2:1D:133:ASP:OD1	2:1D:133:ASP:N	2.50	0.43
10:1R:7:GLN:O	10:1R:11:PRO:CD	2.66	0.43
16:2F:56:ASN:CB	22:3L:65:PHE:CD1	3.01	0.43
22:2L:31:ARG:NH2	22:2L:61:SER:OG	2.34	0.43
25:5C:51:LEU:HD23	25:5C:51:LEU:H	1.82	0.43
37:5O:7:LEU:O	37:5O:7:LEU:HD23	2.17	0.43
39:5Q:274:LYS:HE3	41:5S:275:LEU:HB2	2.00	0.43
40:5R:38:TRP:CH2	40:5R:77:ILE:HD11	2.53	0.43
40:5R:363:SER:O	40:5R:367:VAL:HG23	2.18	0.43
46:5X:121:ARG:NE	46:5X:143:ILE:HG12	2.32	0.43
50:5b:104:LEU:HD21	63:5o:72:LEU:HG	2.00	0.43
52:5d:76:ARG:NH2	53:5e:190:TRP:O	2.51	0.43
55:5g:10:GLU:CD	59:5k:37:TYR:HB3	2.43	0.43
65:5q:99:HIS:HB3	65:5q:195:ILE:HD11	2.00	0.43
1:6B:234:LEU:HD23	1:6B:234:LEU:HA	1.88	0.43
9:6Q:355:PHE:HE2	9:6Q:368:VAL:HG23	1.83	0.43
20:8J:86:ASN:HB3	20:8J:89:THR:HG22	2.01	0.43
25:C:714:ALA:HA	25:C:717:ARG:HB2	1.99	0.43
28:F:130:TYR:CE2	29:G:199:ARG:HB2	2.53	0.43
34:L:92:TRP:HB2	34:L:126:PHE:HB2	1.99	0.43
38:P:34:SER:O	38:P:258:PRO:HB3	2.18	0.43
41:S:162:LEU:HB3	61:m:139:ARG:CZ	2.48	0.43
44:V:473:TRP:NE1	49:a:100:TRP:O	2.50	0.43
61:m:64:LEU:O	61:m:67:GLN:HG3	2.18	0.43
5:1J:19:PRO:HB3	20:9J:70:LYS:O	2.19	0.43
7:1M:56:LEU:HD11	7:1M:415:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1N:441:LYS:HE3	7:1N:441:LYS:HB3	1.76	0.43
9:1Q:204:ARG:HA	9:1Q:204:ARG:HD3	1.89	0.43
25:5C:567:ASP:OD2	25:5C:588:ASP:HB3	2.18	0.43
26:5D:242:MET:HE1	26:5D:268:PHE:CG	2.52	0.43
30:5H:54:PRO:HA	61:5m:7:ARG:HD3	2.00	0.43
38:5P:34:SER:O	38:5P:258:PRO:HB3	2.18	0.43
39:5Q:76:MET:HG2	41:5S:181:SER:HB2	2.01	0.43
40:5R:312:MET:HG2	42:5T:165:MET:HB2	1.99	0.43
44:5V:160:LEU:HD11	46:5X:48:TRP:CD2	2.53	0.43
44:5V:310:GLY:O	44:5V:314:GLY:N	2.50	0.43
49:5a:56:ASP:OD2	49:5a:66:LYS:NZ	2.51	0.43
64:5p:3:TYR:CD2	16:8F:53:TRP:CA	3.01	0.43
68:5u:142:VAL:HG11	68:5u:156:ILE:HG21	2.00	0.43
68:5u:178:GLU:OE1	68:5u:180:TRP:NE1	2.46	0.43
2:6C:64:PRO:HB3	7:6M:294:PHE:HE2	1.83	0.43
7:6M:54:SER:C	9:6Q:65:ARG:HH12	2.25	0.43
14:7D:157:VAL:HG13	14:7D:187:LEU:HD22	1.99	0.43
16:7F:90:LEU:HA	16:7F:93:GLU:HB2	1.99	0.43
24:B:177:ILE:HD11	24:B:216:LEU:HD21	1.99	0.43
27:E:178:PHE:HZ	27:E:221:VAL:HG11	1.84	0.43
32:J:45:GLY:N	32:J:122:CYS:O	2.52	0.43
36:N:7:PHE:O	36:N:11:LEU:HD23	2.18	0.43
38:P:359:GLY:O	38:P:362:ILE:HG22	2.17	0.43
38:P:390:ARG:HA	38:P:393:TYR:CE2	2.52	0.43
44:V:517:ARG:HH21	46:X:66:TRP:HZ2	1.65	0.43
57:i:14:TYR:OH	64:p:90:ASN:HB3	2.19	0.43
65:q:129:LYS:HB3	71:x:72:TYR:HE1	1.82	0.43
9:1S:217:THR:HG23	9:1S:294:MET:HE3	1.99	0.43
11:4A:391:GLY:O	11:4A:395:THR:OG1	2.35	0.43
28:5F:98:VAL:HB	28:5F:127:VAL:HA	2.01	0.43
42:5T:195:VAL:HG23	42:5T:196:LEU:HG	1.99	0.43
42:5T:207:LEU:HD11	44:5V:535:ASP:HB3	2.00	0.43
2:6C:237:ILE:HD13	2:6C:242:ALA:HB3	2.01	0.43
7:6M:56:LEU:HD11	7:6M:415:MET:HE1	2.00	0.43
9:6Q:64:PRO:CG	32:r:61:LYS:HB3	2.49	0.43
9:6S:75:VAL:HG21	9:6S:434:PHE:HD2	1.82	0.43
16:7F:56:ASN:CG	22:8L:65:PHE:CD1	2.96	0.43
23:A:80:TYR:OH	24:B:219:HIS:ND1	2.21	0.43
27:E:271:ILE:HG23	39:Q:263:TYR:CD1	2.54	0.43
41:S:274:ALA:HB1	45:W:152:PHE:CE1	2.53	0.43
66:s:286:ALA:O	66:s:292:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:t:247:LEU:HD22	67:t:252:GLU:HB2	2.00	0.43
2:1C:237:ILE:HD13	2:1C:242:ALA:HB3	2.00	0.43
3:1E:81:PRO:HG3	5:1I:57:ASP:HB3	2.00	0.43
7:1N:76:PRO:HG2	9:1S:92:VAL:HG21	2.01	0.43
7:1N:454:ASN:OD1	7:1N:457:ARG:NH2	2.50	0.43
12:2B:81:THR:HG22	66:s:49:MET:CE	2.47	0.43
20:4J:86:ASN:HB3	20:4J:89:THR:HG22	2.01	0.43
24:5B:346:PRO:HD2	24:5B:368:SER:HA	1.99	0.43
25:5C:271:ASP:HB3	25:5C:278:ALA:H	1.83	0.43
26:5D:85:MET:HE2	26:5D:175:TRP:CE2	2.52	0.43
27:5E:298:ARG:HH21	27:5E:305:ASP:HA	1.83	0.43
29:5G:105:TYR:CD1	29:5G:106:PRO:HA	2.54	0.43
34:5L:33:LYS:C	34:5L:35:ALA:H	2.26	0.43
37:5O:50:ILE:O	37:5O:51:ARG:NH1	2.40	0.43
38:5P:85:ARG:HH21	84:5P:401:NDP:P2B	2.42	0.43
49:5a:40:HIS:O	49:5a:63:VAL:HG13	2.17	0.43
63:5o:19:PHE:CD2	63:5o:49:HIS:HB3	2.54	0.43
65:5q:59:ASP:OD1	65:5q:63:ILE:N	2.30	0.43
67:5t:142:TYR:HB3	67:5t:159:ARG:HD2	2.01	0.43
68:5u:223:LYS:HB3	68:5u:223:LYS:HE2	1.86	0.43
10:6R:82:ASP:OD1	10:6R:82:ASP:N	2.50	0.43
11:7A:341:LEU:HD11	11:7A:412:PHE:HE1	1.84	0.43
11:8A:27:GLY:HA3	11:8A:64:MET:SD	2.58	0.43
23:A:130:TYR:CD1	24:B:222:ALA:HB3	2.52	0.43
25:C:580:VAL:HB	25:C:594:ALA:HA	2.00	0.43
27:E:99:LEU:HD22	27:E:462:PHE:HZ	1.84	0.43
28:F:101:MET:HA	28:F:131:VAL:HB	2.00	0.43
29:G:46:GLN:CD	29:G:49:ARG:HH21	2.25	0.43
30:H:37:LEU:HD22	30:H:41:LYS:HG3	2.00	0.43
31:I:144:ASP:OD1	31:I:144:ASP:N	2.42	0.43
34:L:99:THR:HG22	34:L:100:ALA:N	2.33	0.43
42:T:191:GLY:O	42:T:195:VAL:HG22	2.19	0.43
42:T:207:LEU:HD11	44:V:535:ASP:HB3	2.00	0.43
44:V:160:LEU:HD11	46:X:48:TRP:CD2	2.53	0.43
46:X:114:ARG:NH1	46:X:125:LEU:HB3	2.34	0.43
48:Z:21:ALA:O	48:Z:35:ARG:NH1	2.52	0.43
9:1S:72:LYS:HD2	9:1S:73:PRO:HD2	2.00	0.43
14:2D:74:TRP:HE1	21:2K:32:THR:HG21	1.82	0.43
12:3B:121:LYS:HB2	12:3B:132:GLU:HB2	1.99	0.43
12:4B:121:LYS:HB2	12:4B:132:GLU:HB2	1.99	0.43
24:5B:177:ILE:HG13	24:5B:216:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5B:316:PRO:HA	24:5B:357:LEU:HA	1.99	0.43
25:5C:492:GLY:HA2	25:5C:528:ILE:HG12	2.01	0.43
26:5D:224:ARG:HH22	26:5D:233:GLY:H	1.66	0.43
29:5G:56:TRP:CH2	51:5c:12:TYR:HE2	2.36	0.43
48:5Z:21:ALA:O	48:5Z:35:ARG:NH1	2.52	0.43
53:5e:58:LEU:HD22	71:5x:51:PHE:CD2	2.53	0.43
65:5q:46:PRO:HB2	67:5t:185:ARG:O	2.19	0.43
65:5q:129:LYS:HB3	71:5x:72:TYR:HE1	1.82	0.43
1:6A:287:ASN:HB3	1:6A:290:MET:HB2	1.99	0.43
6:6L:9:LEU:HD21	10:6R:67:ARG:HD3	2.01	0.43
8:6P:45:TRP:HB2	8:6P:47:TRP:H	1.83	0.43
12:7B:141:LEU:HD21	18:7H:35:LEU:HD13	2.00	0.43
26:D:101:VAL:O	26:D:105:VAL:HG23	2.18	0.43
26:D:224:ARG:HH22	26:D:233:GLY:H	1.66	0.43
27:E:160:GLU:OE2	27:E:234:GLY:N	2.34	0.43
31:I:33:ASP:N	31:I:33:ASP:OD1	2.51	0.43
34:L:33:LYS:HE2	34:L:33:LYS:HB3	1.89	0.43
38:P:329:TYR:CE1	38:P:333:MET:HE3	2.53	0.43
40:R:111:ARG:NH2	66:s:289:ASP:OD1	2.51	0.43
40:R:309:TRP:NE1	42:T:168:SER:OG	2.49	0.43
41:S:132:TYR:HD1	45:W:1:MET:HE2	1.83	0.43
44:V:360:PHE:CD2	44:V:443:ILE:HG23	2.53	0.43
68:u:142:VAL:HG11	68:u:156:ILE:HG21	2.00	0.43
11:2A:294:ASP:OD1	12:2B:107:TYR:OH	2.28	0.43
11:4A:118:GLU:O	19:4I:98:LYS:NZ	2.46	0.43
29:5G:118:GLY:H	29:5G:188:GLU:HB3	1.84	0.43
32:5J:45:GLY:N	32:5J:122:CYS:O	2.52	0.43
38:5P:290:ARG:HH21	47:5Y:5:ARG:HG2	1.83	0.43
39:5Q:22:LEU:HD22	39:5Q:48:PRO:HD3	2.01	0.43
44:5V:517:ARG:HH21	46:5X:66:TRP:HZ2	1.65	0.43
64:5p:123:LEU:HD23	64:5p:123:LEU:HA	1.90	0.43
66:5s:134:LEU:HG	66:5s:155:VAL:HB	2.01	0.43
67:5t:118:HIS:O	67:5t:146:ARG:HA	2.19	0.43
67:5t:135:GLU:HG3	67:5t:152:PRO:HB3	2.00	0.43
2:6C:57:ASP:OD1	7:6M:190:GLN:NE2	2.51	0.43
9:6Q:62:GLU:CD	55:g:11:ARG:HB3	2.31	0.43
17:7G:89:ARG:O	17:7G:89:ARG:HG2	2.18	0.43
25:C:567:ASP:OD2	25:C:588:ASP:HB3	2.18	0.43
38:P:204:ARG:NH1	38:P:266:TYR:OH	2.41	0.43
39:Q:22:LEU:HD22	39:Q:48:PRO:HD3	2.01	0.43
39:Q:121:SER:HB2	39:Q:124:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:R:69:LEU:O	40:R:73:LEU:HG	2.19	0.43
40:R:194:THR:HG22	40:R:270:ILE:HG12	2.00	0.43
40:R:296:PRO:HA	40:R:301:PHE:CG	2.53	0.43
40:R:308:PHE:HD2	42:T:160:LEU:HD23	1.83	0.43
40:R:339:ARG:HD2	42:T:142:LEU:HD22	2.01	0.43
1:1B:224:TYR:OH	7:1M:482:ASP:OD2	2.30	0.43
17:2G:89:ARG:O	17:2G:89:ARG:HG2	2.18	0.43
12:3B:138:GLN:HE21	18:3H:42:GLU:HB3	1.84	0.43
15:4E:95:VAL:HG13	15:4E:99:LEU:HG	2.00	0.43
23:5A:114:LYS:HB2	23:5A:114:LYS:HE3	1.87	0.43
25:5C:551:ARG:HB3	25:5C:556:ALA:HB3	2.01	0.43
25:5C:621:ARG:HE	34:5L:66:ARG:NE	2.16	0.43
31:5I:33:ASP:OD1	31:5I:33:ASP:N	2.51	0.43
42:5T:30:PHE:O	42:5T:34:ILE:HG13	2.18	0.43
45:5W:89:THR:H	53:5e:89:GLN:NE2	2.16	0.43
63:5o:11:PHE:HE2	63:5o:41:LEU:HD11	1.82	0.43
66:5s:271:PHE:HE1	68:5u:40:GLU:HA	1.84	0.43
71:5x:77:TYR:HA	71:5x:80:LYS:HD2	2.00	0.43
18:7H:78:GLU:HA	18:7H:83:GLN:HE22	1.83	0.43
11:8A:265:THR:HG22	22:8L:5:PHE:CD2	2.52	0.43
11:9A:411:LEU:O	11:9A:415:VAL:HG22	2.18	0.43
25:C:459:HIS:NE2	25:C:461:GLY:O	2.52	0.43
37:O:11:MET:HE2	37:O:11:MET:HB3	1.92	0.43
38:P:255:LEU:HD23	38:P:255:LEU:HA	1.88	0.43
38:P:305:TYR:CE2	38:P:325:ALA:HA	2.53	0.43
46:X:117:LEU:HD11	58:j:25:HIS:HA	2.01	0.43
49:a:65:MET:SD	55:g:18:HIS:CG	3.11	0.43
53:e:146:PRO:HG2	53:e:149:GLN:NE2	2.29	0.43
65:q:46:PRO:HB2	67:t:185:ARG:O	2.19	0.43
66:s:94:LEU:HD12	66:s:96:ILE:HG12	2.00	0.43
66:s:179:HIS:HE2	67:t:118:HIS:CD2	2.37	0.43
9:1Q:46:GLY:H	9:1Q:48:ARG:NH1	2.17	0.43
10:1T:2:THR:CA	10:1T:5:LEU:HB3	2.49	0.43
15:2E:17:PRO:CB	67:t:252:GLU:OE2	2.59	0.43
25:5C:562:TYR:HD1	25:5C:581:ILE:HB	1.83	0.43
26:5D:250:TYR:HA	26:5D:257:VAL:HA	2.01	0.43
29:5G:167:ASP:HB3	29:5G:170:LYS:HB3	2.00	0.43
38:5P:305:TYR:CE2	38:5P:325:ALA:HA	2.53	0.43
39:5Q:121:SER:HB2	39:5Q:124:ALA:HB3	2.01	0.43
42:5T:196:LEU:HD22	42:5T:232:GLY:HA2	2.01	0.43
43:5U:136:TYR:OH	45:5W:100:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5V:195:GLU:O	44:5V:199:LEU:HG	2.18	0.43
56:5h:97:LEU:O	56:5h:101:THR:OG1	2.32	0.43
9:6Q:446:LEU:HD12	9:6Q:446:LEU:HA	1.92	0.43
10:6R:8:VAL:C	10:6R:11:PRO:HD2	2.43	0.43
11:7A:162:LEU:HD23	11:7A:162:LEU:HA	1.85	0.43
12:7B:138:GLN:HE21	18:7H:42:GLU:HB3	1.84	0.43
11:9A:65:LEU:HD23	11:9A:65:LEU:HA	1.92	0.43
24:B:238:GLU:HG3	24:B:256:LEU:HD12	2.01	0.43
28:F:98:VAL:HB	28:F:127:VAL:HA	2.00	0.43
30:H:54:PRO:HA	61:m:7:ARG:HD3	2.00	0.43
38:P:72:GLU:O	38:P:75:LYS:HG2	2.18	0.43
39:Q:76:MET:HG2	41:S:181:SER:HB2	2.01	0.43
39:Q:107:LEU:HD22	45:W:59:VAL:HG11	2.01	0.43
40:R:242:SER:O	40:R:246:GLU:HG2	2.18	0.43
40:R:247:ILE:HD12	40:R:250:LEU:HD12	2.01	0.43
42:T:54:LEU:HB3	42:T:57:LEU:HD21	2.01	0.43
42:T:77:MET:HG3	42:T:111:LEU:HD13	2.00	0.43
59:k:50:SER:HA	59:k:53:LEU:HD13	2.01	0.43
66:s:145:ALA:N	66:s:173:ASN:OD1	2.37	0.43
2:1C:57:ASP:OD1	7:1M:190:GLN:NE2	2.51	0.43
7:1M:452:ASP:OD1	7:1M:452:ASP:N	2.50	0.43
9:1S:78:SER:OG	9:1S:264:HIS:NE2	2.41	0.43
23:5A:84:TYR:CZ	24:5B:257:TYR:HB3	2.53	0.43
23:5A:94:ASP:O	23:5A:98:GLN:OE1	2.37	0.43
25:5C:417:LEU:HB3	25:5C:489:VAL:HG22	2.01	0.43
30:5H:89:ASP:OD1	30:5H:89:ASP:N	2.47	0.43
36:5N:7:PHE:O	36:5N:11:LEU:HD23	2.18	0.43
38:5P:72:GLU:O	38:5P:75:LYS:HG2	2.18	0.43
42:5T:54:LEU:HB3	42:5T:57:LEU:HD21	2.01	0.43
43:5U:184:ILE:HG12	45:5W:128:ALA:CB	2.49	0.43
44:5V:350:ARG:NH1	32:5r:97:GLU:OE2	2.30	0.43
44:5V:362:MET:HE1	55:5g:28:ALA:HA	2.01	0.43
49:5a:44:ASN:HD22	32:5r:54:GLU:HG3	1.83	0.43
51:5c:36:PRO:HA	51:5c:40:GLU:HB2	2.00	0.43
64:5p:10:TYR:CB	16:8F:59:ARG:CZ	2.96	0.43
67:5t:252:GLU:OE2	15:7E:17:PRO:CB	2.59	0.43
72:5y:56:ASN:N	72:5y:57:PRO:HD2	2.34	0.43
1:6B:147:ILE:HD13	1:6B:147:ILE:HA	1.81	0.43
2:6C:162:VAL:HG22	2:6C:202:VAL:HG22	2.01	0.43
3:6E:81:PRO:HG3	5:6I:57:ASP:HB3	2.00	0.43
7:6M:364:HIS:CE1	7:6M:434:VAL:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6M:443:GLU:HG3	9:6Q:55:GLU:CB	2.49	0.43
12:9B:105:LEU:HB2	22:9L:75:VAL:HG13	2.00	0.43
24:B:107:ARG:H	24:B:109:ARG:HH12	1.67	0.43
24:B:360:PHE:CZ	24:B:370:LEU:HD22	2.54	0.43
25:C:271:ASP:HB3	25:C:278:ALA:H	1.84	0.43
27:E:323:PRO:HB3	27:E:339:GLN:HB3	2.01	0.43
32:J:83:LEU:HB3	32:J:87:ASP:HB2	2.01	0.43
40:R:363:SER:O	40:R:367:VAL:HG23	2.18	0.43
42:T:207:LEU:O	42:T:210:PRO:HD2	2.18	0.43
55:g:12:TYR:CD2	55:g:13:GLU:HG3	2.53	0.43
66:s:227:GLY:C	66:s:241:LEU:HD23	2.44	0.43
9:1Q:168:LEU:CD1	49:5a:50:PRO:HG3	2.49	0.42
10:1T:57:ASP:N	10:1T:57:ASP:OD1	2.48	0.42
13:3C:85:HIS:ND1	13:3C:131:MET:HE1	2.35	0.42
27:5E:178:PHE:HZ	27:5E:221:VAL:HG11	1.84	0.42
27:5E:271:ILE:HG23	39:5Q:263:TYR:CD1	2.54	0.42
39:5Q:180:LEU:O	39:5Q:184:VAL:HG23	2.18	0.42
43:5U:178:ALA:O	43:5U:182:ASN:N	2.51	0.42
46:5X:117:LEU:HD11	58:5j:25:HIS:HA	2.01	0.42
50:5b:100:ALA:HB2	63:5o:64:ILE:HG23	2.01	0.42
66:5s:49:MET:CE	12:7B:81:THR:HG22	2.47	0.42
66:5s:81:GLY:N	66:5s:119:ASN:OD1	2.27	0.42
7:6M:376:ASP:OD1	7:6M:376:ASP:N	2.48	0.42
15:8E:95:VAL:HG13	15:8E:99:LEU:HG	2.00	0.42
22:8L:5:PHE:CE2	22:8L:6:LYS:O	2.71	0.42
11:9A:265:THR:HG22	22:9L:5:PHE:CD2	2.52	0.42
13:9C:85:HIS:ND1	13:9C:131:MET:HE1	2.34	0.42
25:C:325:MET:HE2	25:C:325:MET:HB3	1.94	0.42
27:E:91:GLN:O	41:S:204:TYR:OH	2.37	0.42
27:E:192:THR:HG21	27:E:207:ALA:HB3	2.01	0.42
38:P:290:ARG:HH21	47:Y:5:ARG:HG2	1.83	0.42
42:T:276:LEU:O	42:T:280:VAL:HG23	2.19	0.42
50:b:100:ALA:HB2	63:o:64:ILE:HG23	2.01	0.42
58:j:37:TYR:OH	58:j:41:ARG:NH1	2.38	0.42
66:s:217:VAL:HB	66:s:233:SER:HA	2.01	0.42
7:1M:364:HIS:CE1	7:1M:434:VAL:HG23	2.53	0.42
12:2B:138:GLN:HE21	18:2H:42:GLU:HB3	1.84	0.42
12:3B:105:LEU:HB2	22:3L:75:VAL:HG13	2.00	0.42
22:3L:5:PHE:CE2	22:3L:6:LYS:O	2.71	0.42
22:4L:5:PHE:CE2	22:4L:6:LYS:O	2.71	0.42
25:5C:359:ILE:HG12	25:5C:385:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:269:ARG:NH2	29:5G:145:GLN:O	2.51	0.42
30:5H:37:LEU:HD22	30:5H:41:LYS:HG3	2.00	0.42
38:5P:329:TYR:CE1	38:5P:333:MET:HE3	2.53	0.42
39:5Q:107:LEU:HD22	45:5W:59:VAL:HG11	2.01	0.42
40:5R:357:ASN:O	40:5R:360:THR:HG23	2.19	0.42
44:5V:122:PHE:HD1	44:5V:148:CYS:HB2	1.84	0.42
62:5n:63:ILE:HA	62:5n:99:PHE:CE2	2.54	0.42
66:5s:179:HIS:HE2	67:5t:118:HIS:CD2	2.37	0.42
67:5t:58:PRO:HB3	67:5t:63:GLU:HG3	2.01	0.42
9:6Q:60:VAL:CG2	55:g:11:ARG:HG3	2.18	0.42
9:6S:72:LYS:HD2	9:6S:73:PRO:HD2	2.00	0.42
11:7A:198:VAL:HG11	11:7A:232:PHE:HD2	1.83	0.42
11:7A:473:VAL:HA	11:7A:474:PRO:HD3	1.88	0.42
14:9D:41:GLY:O	14:9D:44:THR:OG1	2.30	0.42
25:C:621:ARG:HE	34:L:66:ARG:NE	2.16	0.42
29:G:118:GLY:N	29:G:188:GLU:HB3	2.35	0.42
31:I:73:SER:HA	31:I:76:LYS:HZ2	1.85	0.42
42:T:293:LEU:HD23	42:T:390:PHE:CE2	2.53	0.42
42:T:361:LEU:O	44:V:174:ARG:NH2	2.52	0.42
53:e:170:LEU:HD23	53:e:170:LEU:HA	1.92	0.42
53:e:179:ARG:NE	53:e:213:GLY:O	2.52	0.42
60:l:35:ILE:O	60:l:39:VAL:HG23	2.19	0.42
63:o:19:PHE:CD2	63:o:49:HIS:HB3	2.54	0.42
66:s:1:MET:H1	66:s:5:LYS:HD2	1.84	0.42
67:t:118:HIS:O	67:t:146:ARG:HA	2.19	0.42
67:t:135:GLU:HG3	67:t:152:PRO:HB3	2.00	0.42
71:x:77:TYR:HA	71:x:80:LYS:HD2	2.00	0.42
8:1P:45:TRP:HB2	8:1P:47:TRP:H	1.83	0.42
9:1S:66:THR:HA	9:1S:67:SER:HA	1.83	0.42
9:1S:75:VAL:HG21	9:1S:434:PHE:HD2	1.82	0.42
12:2B:145:ASP:OD1	12:2B:145:ASP:N	2.48	0.42
15:3E:95:VAL:HG13	15:3E:99:LEU:HG	2.00	0.42
26:5D:105:VAL:O	31:5I:145:TYR:OH	2.34	0.42
26:5D:139:ARG:HG2	26:5D:147:LYS:HD3	2.01	0.42
31:5I:117:GLU:HA	31:5I:120:ILE:HD12	2.02	0.42
41:5S:132:TYR:HD1	45:5W:1:MET:HE2	1.83	0.42
42:5T:144:ALA:HB1	42:5T:212:ALA:HA	2.01	0.42
44:5V:360:PHE:CD2	44:5V:443:ILE:HG23	2.53	0.42
53:5e:8:ASN:ND2	53:5e:10:PRO:HD2	2.35	0.42
57:5i:16:TRP:H	57:5i:16:TRP:HE3	1.68	0.42
67:5t:247:LEU:HD22	67:5t:252:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:8B:138:GLN:HE21	18:8H:42:GLU:HB3	1.84	0.42
13:8C:85:HIS:ND1	13:8C:131:MET:HE1	2.35	0.42
23:A:94:ASP:O	23:A:98:GLN:OE1	2.37	0.42
24:B:159:LEU:HD13	24:B:266:VAL:HG13	2.01	0.42
24:B:365:GLU:N	24:B:365:GLU:OE1	2.53	0.42
24:B:444:THR:OG1	24:B:446:CYS:O	2.37	0.42
27:E:260:ASP:OD2	61:m:34:ARG:NH1	2.51	0.42
27:E:360:TYR:CD2	27:E:361:LYS:HG3	2.55	0.42
28:F:110:TYR:CD1	29:G:172:ILE:HD13	2.54	0.42
33:K:46:GLU:HG3	38:P:366:ARG:NH1	2.34	0.42
39:Q:180:LEU:O	39:Q:184:VAL:HG23	2.18	0.42
40:R:312:MET:HG2	42:T:165:MET:HB2	1.99	0.42
41:S:227:ILE:HG21	45:W:151:ARG:HG3	2.00	0.42
42:T:369:PHE:O	42:T:373:VAL:HG23	2.19	0.42
43:U:184:ILE:HG12	45:W:128:ALA:CB	2.49	0.42
44:V:434:VAL:HG12	44:V:436:PRO:HD3	2.01	0.42
49:a:40:HIS:HB3	49:a:64:THR:HB	2.01	0.42
52:d:70:TYR:CD2	52:d:72:ILE:HD11	2.54	0.42
59:k:17:ARG:CZ	32:r:105:ASP:HB3	2.50	0.42
67:t:142:TYR:HB3	67:t:159:ARG:HD2	2.01	0.42
67:t:193:GLY:O	67:t:198:LYS:N	2.49	0.42
1:1A:147:ILE:HD13	1:1A:147:ILE:HA	1.80	0.42
7:1M:126:GLU:OE1	9:1Q:336:ARG:NH1	2.53	0.42
11:2A:341:LEU:HD11	11:2A:412:PHE:HE1	1.84	0.42
11:3A:65:LEU:HD23	11:3A:65:LEU:HA	1.92	0.42
14:3D:41:GLY:O	14:3D:44:THR:OG1	2.30	0.42
13:4C:85:HIS:ND1	13:4C:131:MET:HE1	2.34	0.42
24:5B:365:GLU:OE1	24:5B:365:GLU:N	2.53	0.42
27:5E:261:GLU:OE1	39:5Q:33:ARG:NH2	2.43	0.42
32:5J:83:LEU:HB3	32:5J:87:ASP:HB2	2.01	0.42
33:5K:130:TYR:CD1	34:5L:100:ALA:HB2	2.54	0.42
60:5l:35:ILE:O	60:5l:39:VAL:HG23	2.19	0.42
1:6B:325:THR:HG23	6:6K:52:LEU:HD13	2.02	0.42
16:7F:63:GLN:NE2	22:8L:71:ARG:CD	2.79	0.42
17:8G:89:ARG:HG2	17:8G:89:ARG:O	2.20	0.42
27:E:131:LYS:HG3	27:E:139:TYR:HE2	1.84	0.42
27:E:198:VAL:O	39:Q:262:ARG:HG2	2.19	0.42
35:M:71:ASP:OD1	36:N:142:ASN:N	2.46	0.42
39:Q:96:PHE:O	39:Q:100:VAL:HG23	2.20	0.42
40:R:35:CYS:SG	40:R:73:LEU:HD11	2.58	0.42
40:R:357:ASN:O	40:R:360:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:37:ASN:OD1	49:a:39:TYR:CE1	2.72	0.42
65:q:119:ASP:HB3	65:q:122:SER:HB3	2.02	0.42
9:1Q:46:GLY:H	9:1Q:48:ARG:HH12	1.68	0.42
11:2A:414:GLY:O	11:2A:418:THR:OG1	2.26	0.42
11:4A:115:THR:O	19:4I:95:GLN:NE2	2.39	0.42
14:4D:44:THR:HA	14:4D:72:ILE:HD11	2.02	0.42
26:5D:96:TYR:HH	26:5D:141:HIS:CE1	2.37	0.42
26:5D:151:ASP:N	26:5D:151:ASP:OD1	2.52	0.42
27:5E:360:TYR:CD2	27:5E:361:LYS:HG3	2.55	0.42
27:5E:398:GLY:HA2	34:5L:27:TYR:CG	2.53	0.42
28:5F:110:TYR:CD1	29:5G:172:ILE:HD13	2.54	0.42
37:5O:44:PRO:HG2	37:5O:45:HIS:CE1	2.55	0.42
39:5Q:96:PHE:O	39:5Q:100:VAL:HG23	2.20	0.42
42:5T:213:HIS:CE1	42:5T:224:LEU:HB3	2.54	0.42
42:5T:241:LEU:HD23	42:5T:241:LEU:HA	1.89	0.42
42:5T:361:LEU:O	44:5V:174:ARG:NH2	2.52	0.42
62:5n:67:SER:O	62:5n:67:SER:OG	2.30	0.42
67:5t:86:GLY:HA3	67:5t:107:ASN:CG	2.45	0.42
72:5y:52:ARG:O	72:5y:57:PRO:HD3	2.20	0.42
2:6D:229:SER:HB3	2:6D:241:PRO:HD2	2.02	0.42
4:6G:25:LEU:HD12	8:6O:36:VAL:HG12	2.01	0.42
9:6Q:97:SER:OG	9:6Q:161:ASP:OD1	2.36	0.42
25:C:492:GLY:HA2	25:C:528:ILE:HG12	2.01	0.42
29:G:167:ASP:HB3	29:G:170:LYS:HB3	2.00	0.42
32:J:103:ILE:HG23	32:J:120:TYR:OH	2.20	0.42
38:P:379:SER:OG	45:W:84:SER:HB2	2.20	0.42
39:Q:112:VAL:HG13	39:Q:206:TYR:CG	2.54	0.42
41:S:141:TYR:OH	61:m:92:GLU:OE1	2.38	0.42
42:T:44:TRP:HA	42:T:74:LEU:HD21	2.02	0.42
44:V:365:LEU:HD23	44:V:425:PHE:HE2	1.85	0.42
44:V:500:THR:HA	44:V:503:ARG:HG2	2.02	0.42
65:q:121:GLU:OE1	72:y:10:ARG:NH1	2.49	0.42
66:s:134:LEU:HG	66:s:155:VAL:HB	2.01	0.42
67:t:58:PRO:HB3	67:t:63:GLU:HG3	2.01	0.42
67:t:219:TYR:HE1	68:u:112:THR:HB	1.85	0.42
7:1N:469:MET:HE1	7:1N:487:ARG:HA	2.01	0.42
9:1Q:64:PRO:HB2	32:5r:61:LYS:CB	2.49	0.42
11:2A:198:VAL:HG11	11:2A:232:PHE:HD2	1.83	0.42
11:2A:312:MET:SD	22:2L:14:LEU:HD11	2.60	0.42
12:2B:145:ASP:HA	12:2B:148:VAL:HB	2.01	0.42
14:3D:75:THR:OG1	21:3K:36:GLN:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:5A:73:VAL:HG13	23:5A:92:VAL:HG22	2.01	0.42
24:5B:226:ILE:HG12	24:5B:400:CYS:HB3	2.00	0.42
25:5C:459:HIS:NE2	25:5C:461:GLY:O	2.52	0.42
25:5C:664:ALA:HB3	25:5C:667:PHE:CD2	2.55	0.42
28:5F:92:MET:HE2	28:5F:92:MET:HB3	1.88	0.42
29:5G:156:ASP:HA	35:5M:52:VAL:HG22	2.01	0.42
34:5L:99:THR:HG22	34:5L:100:ALA:N	2.34	0.42
40:5R:339:ARG:HD2	42:5T:142:LEU:HD22	2.01	0.42
44:5V:136:LEU:O	44:5V:140:VAL:HG23	2.20	0.42
44:5V:198:LEU:HD11	63:5o:77:LEU:HG	2.02	0.42
44:5V:500:THR:HA	44:5V:503:ARG:HG2	2.02	0.42
59:5k:26:LEU:HD23	59:5k:26:LEU:HA	1.85	0.42
61:5m:64:LEU:O	61:5m:67:GLN:HG3	2.18	0.42
32:5r:70:LYS:HA	32:5r:70:LYS:HD3	1.91	0.42
66:5s:227:GLY:C	66:5s:241:LEU:HD23	2.44	0.42
68:5u:113:SER:HB2	68:5u:116:SER:HB3	2.01	0.42
13:9C:25:ARG:NH1	18:9H:13:GLU:OE2	2.53	0.42
23:A:236:LYS:HE3	23:A:240:GLN:HA	2.02	0.42
25:C:417:LEU:HB3	25:C:489:VAL:HG22	2.01	0.42
25:C:551:ARG:HB3	25:C:556:ALA:HB3	2.01	0.42
25:C:664:ALA:HB3	25:C:667:PHE:CD2	2.55	0.42
27:E:394:HIS:CE1	27:E:421:ASN:HB3	2.55	0.42
31:I:125:GLU:HG2	31:I:128:ARG:NH2	2.34	0.42
33:K:46:GLU:HG2	33:K:47:MET:SD	2.60	0.42
38:P:219:LEU:HD23	38:P:219:LEU:HA	1.91	0.42
39:Q:173:TYR:HB3	61:m:56:ILE:HG22	2.02	0.42
42:T:136:ARG:NH1	42:T:215:ALA:O	2.36	0.42
43:U:141:MET:HE2	43:U:141:MET:HB3	1.91	0.42
44:V:136:LEU:O	44:V:140:VAL:HG23	2.20	0.42
53:e:26:GLU:HG2	53:e:196:PRO:HA	2.02	0.42
66:s:162:MET:HE1	68:u:192:ARG:NH2	2.35	0.42
66:s:219:PRO:HG3	66:s:234:PRO:HB2	2.01	0.42
66:s:262:ILE:HG12	67:t:31:PHE:HZ	1.85	0.42
68:u:225:ALA:HA	68:u:228:PHE:CZ	2.54	0.42
72:y:52:ARG:O	72:y:57:PRO:HD3	2.20	0.42
72:y:56:ASN:N	72:y:57:PRO:HD2	2.34	0.42
2:1C:162:VAL:HG22	2:1C:202:VAL:HG22	2.01	0.42
3:1F:195:ASN:OD1	3:1F:198:ASN:ND2	2.52	0.42
5:1J:30:ALA:HB2	20:9J:96:ILE:CD1	2.49	0.42
7:1M:311:TRP:NE1	7:1M:362:ASN:O	2.53	0.42
8:1P:23:THR:HA	8:1P:26:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3A:323:SER:OG	12:3B:75:GLU:OE1	2.35	0.42
13:3C:25:ARG:NH1	18:3H:13:GLU:OE2	2.53	0.42
24:5B:444:THR:OG1	24:5B:446:CYS:O	2.37	0.42
25:5C:580:VAL:N	25:5C:595:ASN:OD1	2.37	0.42
27:5E:170:ARG:NH1	27:5E:356:PRO:O	2.52	0.42
27:5E:198:VAL:O	39:5Q:262:ARG:HG2	2.19	0.42
31:5I:125:GLU:HG2	31:5I:128:ARG:NH2	2.34	0.42
40:5R:69:LEU:O	40:5R:73:LEU:HG	2.19	0.42
42:5T:369:PHE:O	42:5T:373:VAL:HG23	2.19	0.42
44:5V:365:LEU:HD23	44:5V:425:PHE:HE2	1.85	0.42
46:5X:36:PRO:HB3	72:5y:24:TRP:CD2	2.55	0.42
59:5k:34:HIS:HA	59:5k:37:TYR:CD2	2.55	0.42
64:5p:3:TYR:CD2	16:8F:53:TRP:CB	3.02	0.42
66:5s:262:ILE:HG12	67:5t:31:PHE:HZ	1.84	0.42
72:5y:82:GLY:O	72:5y:86:THR:HG22	2.19	0.42
1:6B:287:ASN:HB3	1:6B:290:MET:HB2	2.01	0.42
12:9B:138:GLN:HE21	18:9H:42:GLU:HB3	1.84	0.42
24:B:432:MET:HG3	25:C:171:ARG:HD2	2.02	0.42
28:F:123:ARG:NH1	38:P:48:ARG:HD3	2.35	0.42
29:G:105:TYR:CD1	29:G:106:PRO:HA	2.54	0.42
36:N:55:ASP:OD1	36:N:59:ASN:N	2.53	0.42
44:V:96:MET:HE2	44:V:96:MET:HB3	1.93	0.42
66:s:152:ASN:O	66:s:180:ALA:HA	2.20	0.42
69:v:10:GLY:O	72:y:79:LEU:HA	2.20	0.42
1:1B:69:MET:HE1	1:1B:80:TYR:CZ	2.55	0.42
2:1C:157:TRP:CE2	2:1C:158:ARG:HD3	2.55	0.42
7:1M:75:ILE:HA	7:1M:76:PRO:HD3	1.93	0.42
12:2B:141:LEU:HD21	18:2H:35:LEU:HD13	2.01	0.42
24:5B:360:PHE:CZ	24:5B:370:LEU:HD22	2.54	0.42
34:5L:94:ILE:HD11	34:5L:132:ALA:HB1	2.01	0.42
42:5T:238:ARG:HA	53:5e:3:PHE:CE1	2.55	0.42
62:5n:36:LYS:HA	62:5n:36:LYS:HD2	1.63	0.42
63:5o:32:ARG:NE	63:5o:60:SER:OG	2.50	0.42
32:5r:96:GLU:OE2	32:5r:103:ILE:N	2.36	0.42
66:5s:3:LEU:HD12	66:5s:3:LEU:HA	1.89	0.42
66:5s:217:VAL:HB	66:5s:233:SER:HA	2.01	0.42
3:6F:297:ARG:HD3	6:6L:24:ILE:HG22	2.02	0.42
7:6N:190:GLN:HB2	7:6N:193:GLU:HG2	2.02	0.42
10:6R:24:VAL:O	10:6R:28:LEU:N	2.49	0.42
14:7D:149:LYS:HD2	14:7D:149:LYS:HA	1.89	0.42
13:8C:25:ARG:NH1	18:8H:13:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:9A:29:SER:HB2	19:9I:85:LEU:HD23	2.02	0.42
14:9D:44:THR:HA	14:9D:72:ILE:HD11	2.02	0.42
24:B:226:ILE:HG12	24:B:400:CYS:HB3	2.00	0.42
25:C:271:ASP:O	25:C:277:GLY:HA2	2.20	0.42
28:F:92:MET:HE2	28:F:92:MET:HB3	1.88	0.42
29:G:105:TYR:CG	29:G:106:PRO:HA	2.55	0.42
39:Q:16:SER:O	39:Q:20:PHE:CD2	2.72	0.42
42:T:144:ALA:HB1	42:T:212:ALA:HA	2.01	0.42
44:V:152:LEU:HD22	44:V:239:VAL:HG22	2.02	0.42
46:X:36:PRO:HB3	72:y:24:TRP:CD2	2.55	0.42
50:b:104:LEU:HD21	63:o:72:LEU:HG	2.00	0.42
66:s:47:GLY:O	66:s:51:GLN:HB2	2.20	0.42
67:t:86:GLY:HA3	67:t:107:ASN:CG	2.45	0.42
67:t:136:LYS:HE2	67:t:153:LYS:HG2	2.01	0.42
68:u:94:PRO:HG2	68:u:118:PRO:HB3	2.01	0.42
1:1B:133:VAL:HA	1:1B:140:SER:HB3	2.02	0.42
1:1B:279:TYR:CZ	1:1B:283:ARG:HD2	2.55	0.42
3:1E:106:TYR:HA	3:1E:110:CYS:SG	2.59	0.42
9:1Q:220:GLU:OE2	9:1Q:288:ARG:NH2	2.53	0.42
10:1R:7:GLN:O	10:1R:11:PRO:HD2	2.20	0.42
11:3A:29:SER:HB2	19:3I:85:LEU:HD23	2.02	0.42
14:3D:44:THR:HA	14:3D:72:ILE:HD11	2.01	0.42
20:3J:86:ASN:HB3	20:3J:89:THR:HG22	2.01	0.42
11:4A:29:SER:HB2	19:4I:85:LEU:HD23	2.02	0.42
24:5B:107:ARG:H	24:5B:109:ARG:HH12	1.67	0.42
39:5Q:13:VAL:O	39:5Q:17:VAL:HG23	2.20	0.42
39:5Q:182:PHE:CE2	39:5Q:186:ILE:HD11	2.55	0.42
42:5T:191:GLY:O	42:5T:195:VAL:HG22	2.19	0.42
44:5V:152:LEU:HD22	44:5V:239:VAL:HG22	2.02	0.42
44:5V:470:PHE:HB3	49:5a:104:ILE:HD11	2.02	0.42
52:5d:76:ARG:HH12	53:5e:192:ASP:HA	1.84	0.42
56:5h:66:ASN:O	56:5h:70:GLU:HG2	2.20	0.42
57:5i:14:TYR:OH	64:5p:90:ASN:HB3	2.18	0.42
65:5q:119:ASP:HB3	65:5q:122:SER:HB3	2.01	0.42
66:5s:162:MET:HE1	68:5u:192:ARG:NH2	2.35	0.42
68:5u:94:PRO:HG2	68:5u:118:PRO:HB3	2.02	0.42
1:6B:279:TYR:CZ	1:6B:283:ARG:HD2	2.55	0.42
2:6D:133:ASP:OD1	2:6D:133:ASP:N	2.50	0.42
3:6E:106:TYR:HA	3:6E:110:CYS:SG	2.59	0.42
7:6M:39:PHE:HE1	49:a:50:PRO:HB2	1.85	0.42
7:6N:117:SER:OG	7:6N:120:GLU:OE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6O:20:SER:OG	8:6O:21:ILE:N	2.53	0.42
9:6Q:370:SER:OG	9:6Q:371:GLY:N	2.53	0.42
12:7B:145:ASP:HA	12:7B:148:VAL:HB	2.01	0.42
23:A:188:MET:N	80:A:301:FES:S2	2.87	0.42
24:B:293:GLY:O	24:B:313:MET:HB2	2.20	0.42
25:C:87:ARG:NE	25:C:303:GLU:OE1	2.51	0.42
26:D:139:ARG:HG2	26:D:147:LYS:HD3	2.01	0.42
26:D:250:TYR:HA	26:D:257:VAL:HA	2.01	0.42
27:E:136:GLY:O	27:E:139:TYR:HB2	2.20	0.42
29:G:82:LEU:HB2	29:G:83:THR:H	1.71	0.42
40:R:45:LEU:HA	40:R:50:PHE:CE2	2.52	0.42
45:W:142:LEU:O	45:W:146:VAL:HG23	2.20	0.42
48:Z:90:ILE:HG23	48:Z:109:ARG:HH21	1.84	0.42
53:e:8:ASN:ND2	53:e:10:PRO:HD2	2.35	0.42
57:i:16:TRP:H	57:i:16:TRP:HE3	1.68	0.42
66:s:51:GLN:HG2	66:s:54:GLN:NE2	2.33	0.42
72:y:82:GLY:O	72:y:86:THR:HG22	2.19	0.42
4:1G:25:LEU:HD12	8:1O:36:VAL:HG12	2.01	0.42
7:1M:311:TRP:CD1	7:1M:434:VAL:HG21	2.55	0.42
7:1N:101:VAL:HG23	7:1N:228:LEU:HD23	2.00	0.42
8:1O:20:SER:OG	8:1O:21:ILE:N	2.53	0.42
22:2L:12:TYR:CZ	66:s:42:ALA:HB2	2.52	0.42
11:3A:313:LYS:HB3	11:3A:313:LYS:HE3	1.83	0.42
13:4C:25:ARG:NH1	18:4H:13:GLU:OE2	2.53	0.42
24:5B:74:ILE:HD13	24:5B:200:LYS:HD2	2.01	0.42
24:5B:238:GLU:HG3	24:5B:256:LEU:HD12	2.01	0.42
27:5E:136:GLY:O	27:5E:139:TYR:HB2	2.20	0.42
27:5E:253:ARG:O	30:5H:30:GLU:HG3	2.20	0.42
27:5E:323:PRO:HB3	27:5E:339:GLN:HB3	2.01	0.42
39:5Q:16:SER:O	39:5Q:20:PHE:CD2	2.72	0.42
40:5R:99:THR:HG21	40:5R:129:SER:HB3	2.02	0.42
42:5T:238:ARG:HG3	53:5e:3:PHE:CZ	2.55	0.42
45:5W:89:THR:H	53:5e:89:GLN:HE22	1.68	0.42
46:5X:114:ARG:NH1	46:5X:125:LEU:HB3	2.34	0.42
46:5X:142:LYS:HB2	63:5o:145:PRO:HG3	2.01	0.42
48:5Z:90:ILE:HG23	48:5Z:109:ARG:HH21	1.84	0.42
53:5e:179:ARG:NE	53:5e:213:GLY:O	2.53	0.42
59:5k:61:LYS:HD2	59:5k:61:LYS:HA	1.87	0.42
66:5s:1:MET:H1	66:5s:5:LYS:HD2	1.84	0.42
10:6T:2:THR:CA	10:6T:5:LEU:HB3	2.49	0.42
11:7A:312:MET:SD	22:7L:14:LEU:HD11	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7D:242:ARG:HG2	14:7D:243:THR:HG23	2.02	0.42
13:9C:82:ASP:OD1	13:9C:82:ASP:N	2.49	0.42
16:9F:90:LEU:HA	16:9F:93:GLU:HB2	2.02	0.42
23:A:143:VAL:HG22	23:A:199:ILE:HG12	2.02	0.42
27:E:108:GLU:OE2	41:S:221:SER:OG	2.37	0.42
27:E:387:LYS:HB3	27:E:387:LYS:HE3	1.90	0.42
35:M:124:LEU:O	35:M:127:THR:OG1	2.31	0.42
37:O:44:PRO:HG2	37:O:45:HIS:CE1	2.55	0.42
37:O:77:ALA:HB1	37:O:81:ALA:HB3	2.01	0.42
44:V:122:PHE:HD1	44:V:148:CYS:HB2	1.84	0.42
44:V:362:MET:HE1	55:g:28:ALA:HA	2.02	0.42
44:V:434:VAL:HB	49:a:38:ALA:HB3	2.02	0.42
49:a:51:GLU:OE1	49:a:51:GLU:N	2.38	0.42
56:h:66:ASN:O	56:h:70:GLU:HG2	2.20	0.42
67:t:247:LEU:O	67:t:251:GLY:N	2.53	0.42
72:y:2:MET:O	72:y:4:THR:HG23	2.20	0.42
6:1K:6:ASN:OD1	7:1M:478:GLN:NE2	2.40	0.41
17:4G:89:ARG:O	17:4G:89:ARG:HG2	2.20	0.41
25:5C:175:ALA:HA	35:5M:121:TYR:CZ	2.55	0.41
27:5E:192:THR:HG21	27:5E:207:ALA:HB3	2.01	0.41
28:5F:106:ASN:HB3	29:5G:169:THR:HB	2.01	0.41
29:5G:120:HIS:HB3	29:5G:186:ILE:HD11	2.02	0.41
30:5H:62:TYR:OH	61:5m:4:VAL:HG21	2.20	0.41
35:5M:71:ASP:OD1	36:5N:142:ASN:N	2.46	0.41
38:5P:379:SER:OG	45:5W:84:SER:HB2	2.20	0.41
41:5S:162:LEU:HD11	54:5f:52:TRP:CZ3	2.55	0.41
41:5S:162:LEU:HD21	54:5f:52:TRP:CE3	2.55	0.41
44:5V:142:TRP:CE2	44:5V:219:LYS:HG3	2.55	0.41
49:5a:49:PRO:HA	49:5a:50:PRO:HD3	1.92	0.41
50:5b:59:LYS:HE3	50:5b:59:LYS:HB2	1.80	0.41
52:5d:70:TYR:CD2	52:5d:72:ILE:HD11	2.54	0.41
53:5e:58:LEU:HD21	71:5x:56:LEU:HD23	2.02	0.41
1:6B:69:MET:HE1	1:6B:80:TYR:CZ	2.55	0.41
1:6B:247:TYR:HB3	1:6B:250:LEU:HB2	2.02	0.41
7:6M:311:TRP:NE1	7:6M:362:ASN:O	2.53	0.41
7:6N:469:MET:HE1	7:6N:487:ARG:HA	2.01	0.41
20:9J:86:ASN:HB3	20:9J:89:THR:HG22	2.00	0.41
26:D:96:TYR:HH	26:D:141:HIS:CE1	2.38	0.41
26:D:227:THR:O	28:F:80:LYS:NZ	2.36	0.41
28:F:106:ASN:HB3	29:G:169:THR:HB	2.01	0.41
29:G:120:HIS:HB3	29:G:186:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:O:74:VAL:HB	37:O:82:VAL:HG12	2.02	0.41
40:R:161:LEU:O	40:R:165:LEU:HG	2.20	0.41
48:Z:23:LYS:NZ	48:Z:29:PRO:O	2.53	0.41
50:b:84:ALA:O	64:p:9:SER:HB2	2.19	0.41
60:l:104:ASN:OD1	60:l:104:ASN:N	2.53	0.41
65:q:99:HIS:HB3	65:q:195:ILE:HD11	2.00	0.41
1:1B:147:ILE:HA	1:1B:147:ILE:HD13	1.81	0.41
6:1L:9:LEU:HD21	10:1R:67:ARG:HD3	2.01	0.41
7:1N:33:ALA:HB3	7:1N:36:PHE:HB2	2.03	0.41
9:1S:65:ARG:HD3	9:1S:65:ARG:HA	1.87	0.41
11:2A:433:ARG:HD3	13:2C:123:LEU:HD22	2.01	0.41
12:2B:68:TYR:OH	20:2J:24:GLU:OE2	2.36	0.41
18:2H:54:ASN:OD1	18:2H:54:ASN:N	2.50	0.41
11:3A:391:GLY:O	11:3A:395:THR:OG1	2.35	0.41
12:4B:138:GLN:HE21	18:4H:42:GLU:HB3	1.84	0.41
23:5A:148:THR:HB	80:5A:301:FES:S1	2.61	0.41
24:5B:147:LYS:O	24:5B:151:ILE:HG13	2.20	0.41
27:5E:148:MET:O	27:5E:152:GLU:HG3	2.20	0.41
33:5K:46:GLU:HG2	33:5K:47:MET:SD	2.60	0.41
35:5M:123:ASN:HD21	35:5M:125:LYS:HG2	1.85	0.41
40:5R:165:LEU:HD22	40:5R:251:LEU:HD11	2.02	0.41
42:5T:276:LEU:O	42:5T:280:VAL:HG23	2.19	0.41
66:5s:47:GLY:O	66:5s:51:GLN:HB2	2.20	0.41
67:5t:136:LYS:HE2	67:5t:153:LYS:HG2	2.01	0.41
67:5t:219:TYR:HE1	68:5u:112:THR:HB	1.85	0.41
2:6C:157:TRP:CE2	2:6C:158:ARG:HD3	2.55	0.41
7:6M:126:GLU:OE1	9:6Q:336:ARG:NH1	2.53	0.41
7:6N:329:TRP:HB2	7:6N:344:VAL:HG13	2.02	0.41
11:8A:29:SER:HB2	19:8I:85:LEU:HD23	2.02	0.41
24:B:101:MET:O	24:B:104:SER:OG	2.31	0.41
25:C:175:ALA:HA	35:M:121:TYR:CZ	2.55	0.41
27:E:366:LYS:HA	27:E:384:HIS:HD2	1.85	0.41
29:G:156:ASP:HA	35:M:52:VAL:HG22	2.01	0.41
33:K:130:TYR:CD1	34:L:100:ALA:HB2	2.54	0.41
34:L:33:LYS:HG2	34:L:33:LYS:H	1.70	0.41
34:L:67:ILE:HD12	34:L:143:TYR:HB2	2.02	0.41
35:M:123:ASN:HD21	35:M:125:LYS:HG2	1.85	0.41
40:R:336:ARG:HD2	65:q:95:PHE:HD2	1.85	0.41
62:n:63:ILE:HA	62:n:99:PHE:CE2	2.54	0.41
65:q:128:VAL:HG12	65:q:132:PHE:CE2	2.55	0.41
85:s:401:COO:N1A	67:t:179:VAL:HG11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1M:38:ARG:H	7:1M:38:ARG:HG2	1.73	0.41
7:1N:322:MET:HG3	7:1N:456:ILE:HD12	2.01	0.41
11:2A:30:LEU:HB3	11:2A:60:HIS:HB2	2.02	0.41
11:2A:169:ARG:HH21	11:2A:174:LYS:HA	1.86	0.41
20:2J:21:ARG:NH2	20:2J:24:GLU:O	2.52	0.41
24:5B:159:LEU:HD13	24:5B:266:VAL:HG13	2.01	0.41
24:5B:338:ILE:HG12	24:5B:377:VAL:HG22	2.02	0.41
27:5E:135:GLN:O	27:5E:138:PRO:HD2	2.21	0.41
27:5E:220:ARG:NH2	30:5H:40:ARG:HG3	2.35	0.41
40:5R:161:LEU:O	40:5R:165:LEU:HG	2.20	0.41
44:5V:160:LEU:HD11	46:5X:48:TRP:CE2	2.56	0.41
46:5X:109:TYR:OH	58:5j:25:HIS:O	2.26	0.41
49:5a:44:ASN:HD22	32:5r:54:GLU:CG	2.33	0.41
49:5a:65:MET:HE2	49:5a:65:MET:HB3	1.94	0.41
59:5k:50:SER:HA	59:5k:53:LEU:HD13	2.01	0.41
61:5m:7:ARG:HB2	61:5m:18:MET:SD	2.60	0.41
66:5s:49:MET:SD	12:7B:81:THR:HB	2.60	0.41
66:5s:219:PRO:HG3	66:5s:234:PRO:HB2	2.01	0.41
67:5t:112:LEU:HD11	67:5t:219:TYR:CZ	2.55	0.41
68:5u:123:ASP:N	68:5u:140:ASP:OD1	2.29	0.41
68:5u:225:ALA:HA	68:5u:228:PHE:CZ	2.54	0.41
69:5v:10:GLY:O	72:5y:79:LEU:HA	2.20	0.41
72:5y:2:MET:O	72:5y:4:THR:HG23	2.20	0.41
7:6M:311:TRP:CD1	7:6M:434:VAL:HG21	2.55	0.41
23:A:49:ASN:HB2	25:C:224:GLU:OE1	2.20	0.41
24:B:246:LEU:HD21	25:C:95:ARG:HH22	1.85	0.41
29:G:107:PHE:CE1	36:N:77:TYR:HD2	2.38	0.41
42:T:184:HIS:CD2	53:e:175:MET:HG2	2.55	0.41
42:T:196:LEU:HD22	42:T:232:GLY:HA2	2.01	0.41
44:V:27:ARG:NH2	50:b:36:SER:OG	2.36	0.41
61:m:7:ARG:HB2	61:m:18:MET:SD	2.60	0.41
1:1A:49:LEU:HD11	2:1D:124:ILE:HG23	2.02	0.41
2:1D:229:SER:HB3	2:1D:241:PRO:HD2	2.02	0.41
7:1N:329:TRP:HB2	7:1N:344:VAL:HG13	2.02	0.41
17:2G:91:ARG:HD3	17:2G:91:ARG:HA	1.95	0.41
12:3B:126:GLN:HA	12:3B:127:TRP:HA	1.77	0.41
16:4F:90:LEU:HA	16:4F:93:GLU:HB2	2.02	0.41
24:5B:333:ASP:HA	24:5B:350:LYS:HE3	2.02	0.41
24:5B:408:GLU:HB3	25:5C:141:ILE:HD11	2.02	0.41
25:5C:724:LYS:HD3	35:5M:48:ILE:HG21	2.02	0.41
27:5E:99:LEU:HD22	27:5E:462:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5E:125:GLU:OE2	27:5E:427:LYS:HD2	2.21	0.41
27:5E:394:HIS:CE1	27:5E:421:ASN:HB3	2.55	0.41
28:5F:137:THR:OG1	28:5F:140:GLY:N	2.48	0.41
37:5O:74:VAL:HB	37:5O:82:VAL:HG12	2.02	0.41
37:5O:77:ALA:HB1	37:5O:81:ALA:HB3	2.01	0.41
42:5T:21:HIS:O	42:5T:25:VAL:HG23	2.20	0.41
45:5W:142:LEU:O	45:5W:146:VAL:HG23	2.20	0.41
47:5Y:53:ILE:HG21	5:6I:26:ALA:CA	2.49	0.41
67:5t:247:LEU:O	67:5t:251:GLY:N	2.53	0.41
7:6M:75:ILE:HA	7:6M:76:PRO:HD3	1.93	0.41
7:6N:76:PRO:HG2	9:6S:92:VAL:HG21	2.01	0.41
7:6N:322:MET:HG3	7:6N:456:ILE:HD12	2.01	0.41
17:7G:113:THR:O	17:7G:115:PRO:HD3	2.20	0.41
24:B:74:ILE:HD13	24:B:200:LYS:HD2	2.01	0.41
24:B:408:GLU:HB3	25:C:141:ILE:HD11	2.02	0.41
25:C:359:ILE:HG12	25:C:385:ALA:HB3	2.01	0.41
26:D:141:HIS:HB3	26:D:144:THR:OG1	2.21	0.41
27:E:220:ARG:NH2	30:H:40:ARG:HG3	2.35	0.41
28:F:137:THR:OG1	28:F:140:GLY:N	2.48	0.41
29:G:118:GLY:H	29:G:188:GLU:HB3	1.84	0.41
29:G:210:LEU:HD23	29:G:210:LEU:HA	1.93	0.41
30:H:115:THR:HB	30:H:118:TYR:O	2.20	0.41
31:I:117:GLU:HA	31:I:120:ILE:HD12	2.01	0.41
34:L:94:ILE:HD11	34:L:132:ALA:HB1	2.01	0.41
38:P:178:HIS:CD2	38:P:335:ARG:HH11	2.38	0.41
40:R:99:THR:HG21	40:R:129:SER:HB3	2.02	0.41
40:R:330:SER:HB3	40:R:334:TYR:HE2	1.85	0.41
42:T:239:PHE:C	42:T:242:PRO:HD2	2.45	0.41
43:U:178:ALA:HB2	43:U:186:GLY:HA3	2.01	0.41
43:U:199:CYS:O	43:U:203:ILE:HG12	2.20	0.41
44:V:364:THR:HG23	44:V:450:LEU:HD11	2.02	0.41
44:V:499:PHE:HD1	44:V:502:ILE:HD12	1.85	0.41
45:W:78:THR:HA	45:W:82:ALA:HB3	2.02	0.41
48:Z:20:LEU:HD11	48:Z:36:GLU:HG3	2.03	0.41
48:Z:101:ASP:HB3	48:Z:107:LEU:HD11	2.01	0.41
49:a:60:TYR:HB3	55:g:18:HIS:HD2	1.77	0.41
53:e:77:ARG:HB3	71:x:22:LYS:NZ	2.35	0.41
7:1M:447:ARG:HG3	9:1Q:55:GLU:OE1	2.20	0.41
24:5B:432:MET:HG3	25:5C:171:ARG:HD2	2.01	0.41
29:5G:111:GLN:HA	36:5N:98:TYR:HB2	2.02	0.41
44:5V:364:THR:HG23	44:5V:450:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5Z:101:ASP:HB3	48:5Z:107:LEU:HD11	2.01	0.41
50:5b:84:ALA:O	64:5p:9:SER:HB2	2.20	0.41
54:5f:52:TRP:O	54:5f:56:ARG:HG2	2.21	0.41
66:5s:92:ARG:CD	15:7E:34:PHE:CB	2.83	0.41
66:5s:152:ASN:O	66:5s:180:ALA:HA	2.20	0.41
6:6K:6:ASN:OD1	7:6M:478:GLN:NE2	2.40	0.41
10:6T:2:THR:N	10:6T:5:LEU:CB	2.80	0.41
13:7C:82:ASP:OD1	13:7C:82:ASP:N	2.54	0.41
13:8C:82:ASP:OD1	13:8C:82:ASP:N	2.50	0.41
14:8D:44:THR:HA	14:8D:72:ILE:HD11	2.02	0.41
17:8G:81:THR:HA	17:8G:109:ARG:O	2.21	0.41
13:9C:88:ALA:HB2	13:9C:95:LYS:HG3	2.02	0.41
24:B:338:ILE:HG12	24:B:377:VAL:HG22	2.02	0.41
27:E:135:GLN:O	27:E:138:PRO:HD2	2.21	0.41
38:P:85:ARG:HH21	84:P:401:NDP:P2B	2.42	0.41
39:Q:54:LYS:HE3	39:Q:54:LYS:HB3	1.87	0.41
39:Q:182:PHE:CE2	39:Q:186:ILE:HD11	2.55	0.41
40:R:359:THR:O	40:R:359:THR:HG22	2.21	0.41
42:T:213:HIS:CE1	42:T:224:LEU:HB3	2.54	0.41
43:U:158:ILE:H	43:U:158:ILE:HD12	1.86	0.41
44:V:142:TRP:CE2	44:V:219:LYS:HG3	2.55	0.41
44:V:198:LEU:HD11	63:o:77:LEU:HG	2.02	0.41
65:q:106:PHE:HA	65:q:143:THR:O	2.20	0.41
68:u:89:ARG:NH1	68:u:112:THR:HG21	2.36	0.41
1:1B:335:TRP:O	1:1B:339:ASN:ND2	2.54	0.41
5:1J:29:LYS:HG3	20:9J:102:ALA:HB1	2.03	0.41
16:2F:8:GLU:OE2	20:2J:2:ALA:N	2.54	0.41
16:3F:90:LEU:HA	16:3F:93:GLU:HB2	2.02	0.41
11:4A:414:GLY:O	11:4A:418:THR:OG1	2.32	0.41
14:4D:75:THR:OG1	21:4K:36:GLN:OE1	2.38	0.41
25:5C:322:ASP:HB2	25:5C:628:GLY:HA3	2.03	0.41
27:5E:144:ASP:OD2	27:5E:147:SER:OG	2.31	0.41
27:5E:246:ARG:HH21	27:5E:249:TYR:HD2	1.68	0.41
29:5G:105:TYR:CG	29:5G:106:PRO:HA	2.55	0.41
29:5G:107:PHE:CE1	36:5N:77:TYR:HD2	2.38	0.41
30:5H:115:THR:HB	30:5H:118:TYR:O	2.20	0.41
32:5J:103:ILE:HG23	32:5J:120:TYR:OH	2.20	0.41
33:5K:46:GLU:HG3	38:5P:366:ARG:NH1	2.34	0.41
36:5N:55:ASP:OD1	36:5N:59:ASN:N	2.53	0.41
38:5P:55:THR:HB	38:5P:124:SER:HA	2.03	0.41
42:5T:44:TRP:HA	42:5T:74:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5T:184:HIS:CD2	53:5e:175:MET:HG2	2.55	0.41
42:5T:308:PHE:HD2	42:5T:371:ALA:HB2	1.85	0.41
44:5V:27:ARG:NH2	50:5b:36:SER:OG	2.36	0.41
55:5g:4:VAL:HG23	55:5g:4:VAL:O	2.21	0.41
59:5k:17:ARG:CZ	32:5r:105:ASP:HB3	2.50	0.41
62:5n:90:ASP:OD1	62:5n:90:ASP:N	2.52	0.41
67:5t:218:HIS:NE2	68:5u:112:THR:O	2.41	0.41
1:6B:133:VAL:HA	1:6B:140:SER:HB3	2.01	0.41
1:6B:335:TRP:O	1:6B:339:ASN:ND2	2.54	0.41
9:6Q:390:LEU:HD23	9:6Q:390:LEU:HA	1.93	0.41
10:6R:51:LEU:HD23	10:6R:51:LEU:HA	1.95	0.41
11:7A:433:ARG:HD3	13:7C:123:LEU:HD22	2.01	0.41
14:9D:75:THR:OG1	21:9K:36:GLN:OE1	2.38	0.41
23:A:73:VAL:HG13	23:A:92:VAL:HG22	2.01	0.41
23:A:247:PRO:HG3	24:B:307:VAL:HG21	2.03	0.41
29:G:121:ALA:N	29:G:187:VAL:O	2.53	0.41
40:R:143:MET:HE2	40:R:156:GLU:HB2	2.03	0.41
41:S:162:LEU:HD11	54:f:52:TRP:CZ3	2.55	0.41
42:T:79:LEU:HD22	42:T:311:ILE:HA	2.03	0.41
44:V:160:LEU:HD11	46:X:48:TRP:CE2	2.56	0.41
53:e:58:LEU:HD22	71:x:51:PHE:HD2	1.85	0.41
1:1B:325:THR:HG23	6:1K:52:LEU:HD13	2.02	0.41
7:1M:124:GLU:HG2	7:1M:158:ILE:HD11	2.02	0.41
11:3A:371:PHE:HA	11:3A:374:VAL:HG22	2.03	0.41
23:5A:143:VAL:HG22	23:5A:199:ILE:HG12	2.02	0.41
23:5A:247:PRO:HG3	24:5B:307:VAL:HG21	2.03	0.41
24:5B:246:LEU:HD21	25:5C:95:ARG:HH22	1.85	0.41
27:5E:160:GLU:O	27:5E:164:ASN:N	2.53	0.41
31:5I:144:ASP:OD1	31:5I:144:ASP:N	2.42	0.41
40:5R:6:LEU:HA	40:5R:38:TRP:HE1	1.85	0.41
40:5R:247:ILE:HD12	40:5R:250:LEU:HD12	2.01	0.41
43:5U:178:ALA:HB2	43:5U:186:GLY:HA3	2.01	0.41
65:5q:90:PHE:CZ	65:5q:102:ASP:HB3	2.55	0.41
67:5t:101:ASN:ND2	67:5t:129:ALA:HB3	2.36	0.41
71:5x:52:PRO:HA	71:5x:53:PRO:HD3	1.94	0.41
3:6E:189:ILE:HG12	74:6E:401:HEC:HMA2	2.03	0.41
20:7J:82:PRO:HG2	20:7J:99:PRO:HD2	2.03	0.41
11:8A:294:ASP:OD1	12:8B:107:TYR:OH	2.37	0.41
17:9G:81:THR:HA	17:9G:109:ARG:O	2.21	0.41
23:A:82:PRO:HD3	34:L:178:THR:HG23	2.03	0.41
24:B:147:LYS:O	24:B:151:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:137:GLU:O	25:C:141:ILE:HG23	2.21	0.41
39:Q:13:VAL:O	39:Q:17:VAL:HG23	2.20	0.41
49:a:39:TYR:HB2	49:a:65:MET:HG2	2.01	0.41
51:c:50:PRO:HA	51:c:51:PRO:HD2	1.99	0.41
54:f:52:TRP:O	54:f:56:ARG:HG2	2.21	0.41
62:n:90:ASP:OD1	62:n:90:ASP:N	2.52	0.41
67:t:112:LEU:HD11	67:t:219:TYR:CZ	2.55	0.41
1:1B:88:LEU:HD23	1:1B:91:ILE:HD12	2.03	0.41
1:1B:247:TYR:HB3	1:1B:250:LEU:HB2	2.02	0.41
7:1N:84:GLY:HA3	7:1N:144:TYR:HA	2.03	0.41
7:1N:190:GLN:HB2	7:1N:193:GLU:HG2	2.02	0.41
9:1Q:370:SER:OG	9:1Q:371:GLY:N	2.53	0.41
11:2A:475:ARG:HA	11:2A:475:ARG:HD2	1.91	0.41
11:3A:281:VAL:HG21	11:3A:306:ILE:HD11	2.03	0.41
13:3C:88:ALA:HB2	13:3C:95:LYS:HG3	2.02	0.41
23:5A:49:ASN:HB2	25:5C:224:GLU:OE1	2.20	0.41
23:5A:236:LYS:HE3	23:5A:240:GLN:HA	2.02	0.41
25:5C:271:ASP:O	25:5C:277:GLY:HA2	2.20	0.41
26:5D:110:THR:HG22	26:5D:120:GLN:HB3	2.03	0.41
29:5G:118:GLY:N	29:5G:188:GLU:HB3	2.35	0.41
34:5L:67:ILE:HD12	34:5L:143:TYR:HB2	2.02	0.41
35:5M:67:LEU:O	35:5M:79:LYS:NZ	2.38	0.41
38:5P:64:PHE:CZ	38:5P:210:GLY:HA3	2.53	0.41
38:5P:178:HIS:CD2	38:5P:335:ARG:HH11	2.38	0.41
39:5Q:54:LYS:HE3	39:5Q:54:LYS:HB3	1.87	0.41
42:5T:340:SER:OG	42:5T:412:LEU:O	2.34	0.41
44:5V:264:GLU:HG2	44:5V:265:MET:N	2.36	0.41
44:5V:402:ALA:O	44:5V:406:LEU:HG	2.21	0.41
45:5W:78:THR:HA	45:5W:82:ALA:HB3	2.02	0.41
53:5e:72:TYR:CE2	71:5x:30:THR:HA	2.56	0.41
61:5m:101:LEU:O	61:5m:105:ARG:HG2	2.20	0.41
65:5q:141:ARG:HD2	65:5q:141:ARG:HA	1.87	0.41
66:5s:135:ARG:HD2	68:5u:213:HIS:CE1	2.56	0.41
67:5t:169:GLU:HB3	67:5t:188:SER:HB2	2.03	0.41
7:6M:312:THR:O	9:6Q:52:PRO:CD	2.69	0.41
7:6N:33:ALA:HB3	7:6N:36:PHE:HB2	2.03	0.41
7:6N:441:LYS:HB3	7:6N:441:LYS:HE3	1.76	0.41
8:6P:23:THR:HA	8:6P:26:ARG:HG2	2.02	0.41
16:7F:8:GLU:OE2	20:7J:2:ALA:N	2.54	0.41
11:8A:281:VAL:HG21	11:8A:306:ILE:HD11	2.03	0.41
27:E:148:MET:O	27:E:152:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:E:160:GLU:O	27:E:164:ASN:N	2.53	0.41
30:H:62:TYR:OH	61:m:4:VAL:HG21	2.20	0.41
32:J:63:PHE:HE2	32:J:91:LEU:HD13	1.86	0.41
35:M:135:CYS:N	35:M:140:ASN:O	2.52	0.41
37:O:50:ILE:O	37:O:51:ARG:NH1	2.40	0.41
40:R:6:LEU:HA	40:R:38:TRP:HE1	1.85	0.41
40:R:278:ASN:HB3	40:R:359:THR:HG21	2.02	0.41
42:T:238:ARG:HA	53:e:3:PHE:CE1	2.55	0.41
46:X:142:LYS:HB2	63:o:145:PRO:HG3	2.01	0.41
49:a:94:LEU:HD23	49:a:94:LEU:HA	1.92	0.41
50:b:149:LYS:HB2	50:b:149:LYS:HE3	1.91	0.41
53:e:58:LEU:HD21	71:x:56:LEU:HD23	2.02	0.41
59:k:78:PRO:HB2	59:k:80:ILE:HD11	2.03	0.41
65:q:138:ASP:OD1	65:q:138:ASP:N	2.45	0.41
67:t:57:PHE:CZ	67:t:79:CYS:HB3	2.56	0.41
2:1D:110:ARG:HB3	4:1H:24:LEU:HD21	2.03	0.41
5:1I:26:ALA:CA	47:Y:53:ILE:HG21	2.49	0.41
9:1Q:103:GLU:HB2	9:1Q:254:ARG:HB3	2.02	0.41
10:1R:5:LEU:HD12	10:1R:8:VAL:HB	2.02	0.41
14:2D:242:ARG:HG2	14:2D:243:THR:HG23	2.02	0.41
11:4A:265:THR:HG22	22:4L:5:PHE:CD2	2.51	0.41
23:5A:82:PRO:HD3	34:5L:178:THR:HG23	2.03	0.41
24:5B:396:LYS:HA	24:5B:410:THR:HB	2.03	0.41
25:5C:189:LYS:N	25:5C:251:THR:O	2.44	0.41
25:5C:320:ARG:NH2	25:5C:585:HIS:HB2	2.31	0.41
27:5E:131:LYS:HG3	27:5E:139:TYR:HE2	1.84	0.41
27:5E:260:ASP:OD2	61:5m:34:ARG:NH1	2.51	0.41
28:5F:123:ARG:NH1	38:5P:48:ARG:HD3	2.35	0.41
29:5G:103:ILE:HA	36:5N:71:ARG:HH11	1.86	0.41
29:5G:126:PRO:HB3	36:5N:110:LYS:NZ	2.36	0.41
29:5G:178:GLN:HE21	29:5G:187:VAL:HG12	1.86	0.41
32:5J:63:PHE:HE2	32:5J:91:LEU:HD13	1.86	0.41
37:5O:51:ARG:HD3	37:5O:51:ARG:HA	1.88	0.41
40:5R:32:ARG:HD3	40:5R:61:GLN:HA	2.02	0.41
40:5R:197:LYS:O	40:5R:201:PHE:HD2	2.04	0.41
40:5R:209:HIS:HD1	53:5e:202:ASP:CG	2.28	0.41
42:5T:367:PRO:HD3	42:5T:434:ALA:O	2.21	0.41
43:5U:158:ILE:H	43:5U:158:ILE:HD12	1.86	0.41
44:5V:290:ARG:HG2	44:5V:294:TYR:CE2	2.56	0.41
44:5V:434:VAL:HG12	44:5V:436:PRO:HD3	2.02	0.41
44:5V:464:LEU:HD23	44:5V:464:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5d:11:MET:HG2	52:5d:40:MET:HB3	2.02	0.41
53:5e:26:GLU:HG2	53:5e:196:PRO:HA	2.02	0.41
63:5o:11:PHE:CE2	63:5o:41:LEU:HD11	2.56	0.41
63:5o:110:ARG:HG2	63:5o:114:ALA:HB3	2.02	0.41
65:5q:144:SER:O	71:5x:17:ARG:NH2	2.41	0.41
66:5s:268:SER:OG	67:5t:42:GLN:OE1	2.38	0.41
67:5t:57:PHE:CZ	67:5t:79:CYS:HB3	2.56	0.41
67:5t:177:ASN:HB2	68:5u:149:ILE:HD12	2.03	0.41
67:5t:187:PRO:HB2	67:5t:190:GLU:OE1	2.21	0.41
68:5u:89:ARG:NH1	68:5u:112:THR:HG21	2.36	0.41
2:6D:110:ARG:HB3	4:6H:24:LEU:HD21	2.03	0.41
5:6J:29:LYS:HA	5:6J:29:LYS:HD2	1.83	0.41
7:6M:124:GLU:HG2	7:6M:158:ILE:HD11	2.02	0.41
9:6Q:45:GLY:CA	9:6Q:48:ARG:HH12	2.34	0.41
9:6Q:220:GLU:OE2	9:6Q:288:ARG:NH2	2.53	0.41
9:6Q:298:ALA:HA	9:6Q:299:PRO:HD3	1.93	0.41
10:6R:5:LEU:HD12	10:6R:8:VAL:HB	2.02	0.41
9:6S:75:VAL:HG22	9:6S:89:ILE:HB	2.03	0.41
14:7D:89:MET:HE3	14:7D:89:MET:HB3	1.99	0.41
11:8A:65:LEU:HD23	11:8A:65:LEU:HA	1.92	0.41
12:8B:138:GLN:NE2	18:8H:42:GLU:OE1	2.54	0.41
16:8F:90:LEU:HA	16:8F:93:GLU:HB2	2.02	0.41
11:9A:391:GLY:O	11:9A:395:THR:OG1	2.35	0.41
12:9B:138:GLN:NE2	18:9H:42:GLU:OE1	2.54	0.41
19:9I:34:HIS:CD2	21:9K:22:PRO:HG3	2.56	0.41
25:C:399:SER:HB3	25:C:676:PRO:HB2	2.03	0.41
25:C:410:LEU:HG	25:C:437:MET:HE1	2.03	0.41
26:D:110:THR:HG22	26:D:120:GLN:HB3	2.03	0.41
26:D:256:ARG:HD3	33:K:95:HIS:CB	2.51	0.41
27:E:135:GLN:HG2	29:G:143:PRO:HB3	2.02	0.41
27:E:246:ARG:HH21	27:E:249:TYR:HD2	1.68	0.41
29:G:103:ILE:HA	36:N:71:ARG:HH11	1.86	0.41
39:Q:130:ARG:HG2	39:Q:265:TYR:CD1	2.56	0.41
40:R:197:LYS:O	40:R:201:PHE:HD2	2.04	0.41
40:R:302:PHE:HB3	40:R:306:TRP:CZ3	2.56	0.41
41:S:162:LEU:HD21	54:f:52:TRP:CE3	2.55	0.41
42:T:21:HIS:O	42:T:25:VAL:HG23	2.20	0.41
42:T:238:ARG:HG3	53:e:3:PHE:CZ	2.55	0.41
42:T:367:PRO:HD3	42:T:434:ALA:O	2.21	0.41
44:V:8:PHE:HB3	44:V:9:PRO:HD3	2.03	0.41
44:V:290:ARG:HG2	44:V:294:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:V:402:ALA:O	44:V:406:LEU:HG	2.21	0.41
48:Z:38:TRP:HA	50:b:45:GLY:HA3	2.03	0.41
50:b:152:LEU:HD12	50:b:152:LEU:HA	1.75	0.41
52:d:11:MET:HG2	52:d:40:MET:HB3	2.02	0.41
53:e:72:TYR:CE2	71:x:30:THR:HA	2.56	0.41
53:e:165:ASP:OD2	71:x:54:ARG:NH2	2.41	0.41
53:e:219:TYR:OH	57:i:36:ARG:NH2	2.46	0.41
59:k:21:THR:HA	59:k:24:LYS:HD2	2.03	0.41
59:k:34:HIS:HA	59:k:37:TYR:CD2	2.55	0.41
63:o:32:ARG:NH2	63:o:56:ASN:O	2.53	0.41
65:q:117:ASN:HD21	71:x:12:ASN:ND2	2.19	0.41
66:s:256:TYR:OH	85:s:401:COO:C9	2.69	0.41
68:u:43:ASN:C	68:u:43:ASN:ND2	2.71	0.41
68:u:113:SER:HB2	68:u:116:SER:HB3	2.01	0.41
15:2E:34:PHE:CE2	66:s:92:ARG:CG	3.02	0.41
18:3H:21:SER:HA	18:3H:24:VAL:HG22	2.03	0.41
17:4G:81:THR:HA	17:4G:109:ARG:O	2.21	0.41
36:5N:94:GLY:HA3	36:5N:100:ASN:HD21	1.86	0.41
37:5O:89:LEU:HD23	37:5O:89:LEU:HA	1.93	0.41
39:5Q:173:TYR:HB3	61:5m:56:ILE:HG22	2.02	0.41
40:5R:336:ARG:HD2	65:5q:95:PHE:HD2	1.85	0.41
40:5R:359:THR:HG22	40:5R:359:THR:O	2.21	0.41
45:5W:116:LEU:HD11	61:5m:133:LEU:HB3	2.02	0.41
64:5p:3:TYR:CE2	16:8F:53:TRP:CA	3.04	0.41
65:5q:117:ASN:HD21	71:5x:12:ASN:ND2	2.19	0.41
65:5q:128:VAL:HG12	65:5q:132:PHE:CE2	2.55	0.41
66:5s:51:GLN:HG2	66:5s:54:GLN:NE2	2.33	0.41
2:6D:202:VAL:HG23	2:6D:249:PRO:HD3	2.03	0.41
4:6G:56:ILE:HD13	4:6G:56:ILE:HA	1.89	0.41
11:7A:73:LEU:HB3	11:7A:244:PRO:HB2	2.03	0.41
17:8G:91:ARG:HD3	17:8G:91:ARG:HA	1.93	0.41
17:9G:89:ARG:HG2	17:9G:89:ARG:O	2.20	0.41
24:B:147:LYS:HE2	24:B:295:LYS:NZ	2.36	0.41
24:B:224:ALA:HB1	24:B:226:ILE:HG22	2.03	0.41
24:B:396:LYS:HA	24:B:410:THR:HB	2.03	0.41
29:G:111:GLN:HA	36:N:98:TYR:HB2	2.02	0.41
29:G:126:PRO:HB3	36:N:110:LYS:NZ	2.36	0.41
40:R:158:PHE:O	40:R:162:LEU:HG	2.21	0.41
40:R:184:ILE:HD12	40:R:184:ILE:H	1.85	0.41
40:R:295:LEU:HD23	40:R:295:LEU:HA	1.82	0.41
42:T:299:SER:OG	42:T:300:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:T:351:THR:O	42:T:355:LEU:HG	2.21	0.41
44:V:470:PHE:HB3	49:a:104:ILE:HD11	2.02	0.41
52:d:25:GLU:OE1	52:d:27:LYS:NZ	2.42	0.41
67:t:101:ASN:ND2	67:t:129:ALA:HB3	2.36	0.41
67:t:169:GLU:HB3	67:t:188:SER:HB2	2.03	0.41
68:u:83:TRP:CD1	68:u:104:GLN:HA	2.56	0.41
68:u:93:GLN:HB2	68:u:111:ALA:HB3	2.03	0.41
11:2A:35:ARG:HD2	11:2A:35:ARG:HA	1.84	0.40
12:2B:81:THR:HB	66:s:49:MET:SD	2.61	0.40
14:2D:89:MET:HE3	14:2D:89:MET:HB3	1.99	0.40
16:3F:53:TRP:CB	64:p:3:TYR:CD2	3.02	0.40
17:3G:81:THR:HA	17:3G:109:ARG:O	2.21	0.40
17:3G:89:ARG:O	17:3G:89:ARG:HG2	2.20	0.40
13:4C:88:ALA:HB2	13:4C:95:LYS:HG3	2.02	0.40
16:4F:80:LYS:HA	16:4F:80:LYS:HD3	1.94	0.40
20:4J:95:SER:CB	5:6J:33:GLU:OE2	2.60	0.40
23:5A:83:ASN:ND2	34:5L:173:VAL:O	2.54	0.40
23:5A:188:MET:HA	24:5B:180:ARG:HH22	1.85	0.40
24:5B:293:GLY:O	24:5B:313:MET:HB2	2.20	0.40
25:5C:54:PHE:HB2	25:5C:120:LYS:HD3	2.03	0.40
27:5E:135:GLN:HG2	29:5G:143:PRO:HB3	2.02	0.40
27:5E:324:ILE:HD13	27:5E:324:ILE:HA	1.98	0.40
42:5T:79:LEU:HD22	42:5T:311:ILE:HA	2.03	0.40
50:5b:164:LYS:NZ	50:5b:168:GLU:OE2	2.46	0.40
58:5j:22:VAL:HG13	58:5j:34:TYR:CE2	2.56	0.40
59:5k:78:PRO:HB2	59:5k:80:ILE:HD11	2.03	0.40
63:5o:32:ARG:NH2	63:5o:56:ASN:O	2.53	0.40
1:6A:88:LEU:HD23	1:6A:88:LEU:HA	1.88	0.40
7:6M:54:SER:O	9:6Q:65:ARG:NH1	2.54	0.40
7:6M:163:LEU:HD23	7:6M:163:LEU:HA	1.96	0.40
11:7A:30:LEU:HB3	11:7A:60:HIS:HB2	2.02	0.40
11:8A:40:LEU:HD23	11:8A:40:LEU:HA	1.95	0.40
11:8A:115:THR:O	19:8I:95:GLN:NE2	2.39	0.40
11:8A:323:SER:OG	12:8B:75:GLU:OE1	2.35	0.40
13:8C:88:ALA:HB2	13:8C:95:LYS:HG3	2.02	0.40
11:9A:371:PHE:HA	11:9A:374:VAL:HG22	2.03	0.40
25:C:322:ASP:HB2	25:C:628:GLY:HA3	2.03	0.40
25:C:418:LEU:N	25:C:445:GLY:O	2.43	0.40
26:D:144:THR:OG1	26:D:144:THR:O	2.39	0.40
27:E:253:ARG:O	30:H:30:GLU:HG3	2.20	0.40
27:E:355:MET:HB3	61:m:25:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K:22:GLY:O	33:K:25:ARG:HG2	2.22	0.40
40:R:32:ARG:HD3	40:R:61:GLN:HA	2.02	0.40
40:R:361:LEU:HD12	52:d:17:PHE:HZ	1.86	0.40
61:m:101:LEU:O	61:m:105:ARG:HG2	2.20	0.40
63:o:110:ARG:HG2	63:o:114:ALA:HB3	2.02	0.40
65:q:90:PHE:CZ	65:q:102:ASP:HB3	2.55	0.40
66:s:135:ARG:HD2	68:u:213:HIS:CE1	2.56	0.40
66:s:297:MET:HG3	66:s:298:TRP:CD2	2.56	0.40
71:x:48:ALA:HA	71:x:51:PHE:CD2	2.56	0.40
9:1Q:62:GLU:CD	32:5r:62:HIS:HD2	2.29	0.40
10:1R:3:SER:HA	10:1R:6:LYS:HE2	2.03	0.40
11:2A:162:LEU:HD23	11:2A:162:LEU:HA	1.85	0.40
11:2A:347:VAL:HB	12:2B:48:LEU:HD13	2.03	0.40
12:2B:127:TRP:CG	13:2C:127:ASN:HB2	2.56	0.40
17:2G:113:THR:O	17:2G:115:PRO:HD3	2.20	0.40
20:4J:84:TYR:CE1	5:6J:22:VAL:HB	2.56	0.40
25:5C:399:SER:HB2	25:5C:404:ASN:HD21	1.86	0.40
27:5E:244:LEU:O	27:5E:248:VAL:HG23	2.22	0.40
33:5K:84:ILE:HD12	33:5K:87:TYR:HD2	1.87	0.40
41:5S:141:TYR:OH	61:5m:92:GLU:OE1	2.38	0.40
44:5V:378:LEU:H	44:5V:381:PHE:HB3	1.87	0.40
50:5b:155:HIS:HB2	63:5o:38:LEU:HD13	2.04	0.40
50:5b:158:ARG:NH2	56:5h:140:GLN:OE1	2.41	0.40
1:6B:88:LEU:HD23	1:6B:91:ILE:HD12	2.03	0.40
9:6Q:75:VAL:HG21	9:6Q:434:PHE:HD2	1.86	0.40
10:6R:3:SER:HA	10:6R:6:LYS:HE2	2.03	0.40
11:7A:347:VAL:HB	12:7B:48:LEU:HD13	2.03	0.40
13:7C:88:ALA:HB2	13:7C:95:LYS:HG3	2.03	0.40
23:A:125:GLU:HG2	25:C:216:VAL:O	2.21	0.40
24:B:333:ASP:HA	24:B:350:LYS:HE3	2.02	0.40
26:D:211:MET:CB	26:D:236:LEU:HD12	2.51	0.40
27:E:168:PRO:O	27:E:172:GLN:HG3	2.21	0.40
42:T:303:ALA:HB3	53:e:5:GLY:HA2	2.03	0.40
42:T:308:PHE:HD2	42:T:371:ALA:HB2	1.85	0.40
45:W:116:LEU:HD11	61:m:133:LEU:HB3	2.02	0.40
32:r:49:LYS:HE3	32:r:49:LYS:HB2	1.94	0.40
1:1B:287:ASN:HB3	1:1B:290:MET:HB2	2.01	0.40
3:1E:189:ILE:HG12	74:1E:401:HEC:HMA2	2.03	0.40
9:1S:75:VAL:HG22	9:1S:89:ILE:HB	2.03	0.40
20:2J:82:PRO:HG2	20:2J:99:PRO:HD2	2.03	0.40
11:4A:281:VAL:HG21	11:4A:306:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4A:371:PHE:HA	11:4A:374:VAL:HG22	2.03	0.40
23:5A:125:GLU:HG2	25:5C:216:VAL:O	2.21	0.40
24:5B:224:ALA:HB1	24:5B:226:ILE:HG22	2.03	0.40
26:5D:141:HIS:HB3	26:5D:144:THR:OG1	2.21	0.40
40:5R:55:LEU:HD21	40:5R:194:THR:HB	2.04	0.40
40:5R:302:PHE:HB3	40:5R:306:TRP:CZ3	2.56	0.40
40:5R:330:SER:HB3	40:5R:334:TYR:HE2	1.85	0.40
42:5T:239:PHE:C	42:5T:242:PRO:HD2	2.45	0.40
42:5T:299:SER:OG	42:5T:300:GLU:N	2.54	0.40
43:5U:199:CYS:O	43:5U:203:ILE:HG12	2.20	0.40
65:5q:106:PHE:HA	65:5q:143:THR:O	2.20	0.40
66:5s:145:ALA:N	66:5s:173:ASN:OD1	2.37	0.40
66:5s:272:GLU:OE2	67:5t:253:TYR:OH	2.30	0.40
66:5s:297:MET:HG3	66:5s:298:TRP:CD2	2.56	0.40
67:5t:232:GLU:HG2	68:5u:44:ARG:CZ	2.52	0.40
71:5x:48:ALA:HA	71:5x:51:PHE:CD2	2.56	0.40
1:6A:49:LEU:HD11	2:6D:124:ILE:HG23	2.02	0.40
1:6B:142:TRP:HB3	1:6B:269:ILE:HD13	2.03	0.40
9:6S:446:LEU:HD23	9:6S:446:LEU:HA	1.94	0.40
11:7A:169:ARG:HH21	11:7A:174:LYS:HA	1.86	0.40
12:8B:126:GLN:HA	12:8B:127:TRP:HA	1.77	0.40
14:9D:24:LYS:HG3	17:9G:29:TYR:CZ	2.56	0.40
23:A:148:THR:HB	80:A:301:FES:S1	2.61	0.40
27:E:296:ILE:HG12	27:E:333:ARG:HD3	2.03	0.40
40:R:209:HIS:NE2	40:R:211:ASP:OD1	2.55	0.40
41:S:259:LEU:HD23	41:S:259:LEU:HA	1.96	0.40
44:V:264:GLU:HG2	44:V:265:MET:N	2.36	0.40
44:V:345:ASN:ND2	44:V:350:ARG:HB2	2.37	0.40
44:V:350:ARG:NH1	32:r:97:GLU:OE2	2.30	0.40
45:W:89:THR:H	53:e:89:GLN:HE22	1.68	0.40
56:h:97:LEU:O	56:h:101:THR:OG1	2.32	0.40
62:n:36:LYS:HD2	62:n:36:LYS:HA	1.63	0.40
63:o:52:PHE:CD2	64:p:25:TRP:HZ2	2.40	0.40
66:s:297:MET:HG3	66:s:298:TRP:CE2	2.57	0.40
67:t:232:GLU:HG2	68:u:44:ARG:CZ	2.51	0.40
2:1C:93:PRO:HA	2:1C:94:PRO:HD3	1.97	0.40
7:1N:473:SER:HB3	7:1N:477:VAL:HG11	2.03	0.40
16:3F:53:TRP:CA	64:p:3:TYR:CE2	3.04	0.40
11:4A:313:LYS:HE3	11:4A:313:LYS:HB3	1.82	0.40
12:4B:145:ASP:OD1	12:4B:145:ASP:N	2.54	0.40
25:5C:241:VAL:O	25:5C:245:CYS:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5C:264:LEU:HD22	25:5C:283:ASP:HB3	2.03	0.40
25:5C:733:LYS:HE2	35:5M:36:LYS:NZ	2.37	0.40
39:5Q:73:ALA:O	39:5Q:77:ILE:N	2.41	0.40
39:5Q:130:ARG:HG2	39:5Q:265:TYR:CD1	2.56	0.40
42:5T:303:ALA:HB3	53:5e:5:GLY:HA2	2.03	0.40
43:5U:141:MET:HE2	43:5U:141:MET:HB3	1.91	0.40
44:5V:499:PHE:HD1	44:5V:502:ILE:HD12	1.85	0.40
45:5W:14:LEU:O	45:5W:18:VAL:HG23	2.21	0.40
45:5W:151:ARG:C	45:5W:151:ARG:HD3	2.46	0.40
53:5e:148:PRO:HG3	72:5y:13:ASN:HB3	2.04	0.40
67:5t:146:ARG:NH1	67:5t:164:GLU:OE2	2.42	0.40
9:6Q:50:GLU:OE2	9:6Q:53:LEU:HD22	2.21	0.40
10:6R:7:GLN:O	10:6R:11:PRO:HD2	2.20	0.40
11:7A:29:SER:HB2	19:7I:85:LEU:HA	2.03	0.40
12:7B:105:LEU:HB2	22:7L:75:VAL:HG13	2.04	0.40
16:7F:63:GLN:HE22	22:8L:71:ARG:CD	2.35	0.40
11:9A:281:VAL:HG21	11:9A:306:ILE:HD11	2.03	0.40
23:A:81:PRO:HA	23:A:82:PRO:HD3	1.99	0.40
25:C:54:PHE:HB2	25:C:120:LYS:HD3	2.03	0.40
25:C:398:ARG:NH2	25:C:539:ASP:OD2	2.47	0.40
27:E:375:MET:HE3	27:E:375:MET:HB3	1.95	0.40
28:F:13:PHE:CE1	28:F:17:LYS:HE3	2.57	0.40
39:Q:22:LEU:HD13	39:Q:47:GLN:HB3	2.03	0.40
39:Q:146:LEU:HD13	39:Q:236:TYR:CE2	2.57	0.40
44:V:297:CYS:HA	44:V:300:LEU:HD12	2.04	0.40
59:k:61:LYS:HD2	59:k:61:LYS:HA	1.87	0.40
64:p:33:GLU:OE2	64:p:36:ARG:NH2	2.48	0.40
66:s:211:ILE:HB	66:s:229:VAL:HG22	2.04	0.40
1:1B:142:TRP:HB3	1:1B:269:ILE:HD13	2.03	0.40
2:1C:172:ILE:HD11	2:1C:197:LYS:HA	2.03	0.40
2:1D:202:VAL:HG23	2:1D:249:PRO:HD3	2.03	0.40
5:1J:26:ALA:O	20:9J:96:ILE:CG1	2.41	0.40
5:1J:29:LYS:HB3	20:9J:102:ALA:O	2.21	0.40
7:1N:225:ARG:HA	7:1N:228:LEU:HD12	2.03	0.40
9:1S:343:ARG:HA	9:1S:343:ARG:HD3	1.93	0.40
11:2A:29:SER:HB2	19:2I:85:LEU:HA	2.03	0.40
14:2D:202:THR:HA	14:2D:203:PRO:HD3	1.99	0.40
16:3F:53:TRP:HB2	64:p:3:TYR:HE2	1.63	0.40
18:3H:100:SER:HA	18:3H:103:GLU:HG2	2.04	0.40
14:4D:65:MET:HE2	14:4D:65:MET:HB3	1.93	0.40
24:5B:147:LYS:HE2	24:5B:295:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5D:148:CYS:O	26:5D:171:LEU:N	2.43	0.40
27:5E:414:TYR:HB3	27:5E:427:LYS:HB3	2.03	0.40
30:5H:46:THR:HG23	36:5N:102:TYR:CZ	2.57	0.40
32:5J:47:LEU:HD23	32:5J:47:LEU:HA	1.96	0.40
39:5Q:174:ALA:HA	61:5m:57:MET:HA	2.03	0.40
40:5R:143:MET:HE2	40:5R:156:GLU:HB2	2.03	0.40
44:5V:345:ASN:ND2	44:5V:350:ARG:HB2	2.37	0.40
46:5X:74:TYR:HE1	72:5y:40:VAL:HA	1.87	0.40
50:5b:153:GLY:HA3	50:5b:159:VAL:HG23	2.04	0.40
53:5e:58:LEU:HD22	71:5x:51:PHE:HD2	1.85	0.40
66:5s:89:ALA:HA	66:5s:92:ARG:NE	2.36	0.40
3:6F:195:ASN:OD1	3:6F:198:ASN:ND2	2.52	0.40
14:8D:24:LYS:HG3	17:8G:29:TYR:CZ	2.57	0.40
17:8G:95:GLY:O	21:8K:58:ARG:NH1	2.55	0.40
12:9B:93:LEU:HA	12:9B:96:VAL:HG12	2.04	0.40
18:9H:100:SER:HA	18:9H:103:GLU:HG2	2.04	0.40
24:B:384:VAL:O	24:B:388:ILE:HG12	2.22	0.40
26:D:151:ASP:OD1	26:D:151:ASP:N	2.52	0.40
33:K:93:GLN:HB2	33:K:95:HIS:CE1	2.57	0.40
35:M:50:VAL:HB	35:M:59:GLY:HA2	2.03	0.40
36:N:22:PHE:O	36:N:25:SER:OG	2.38	0.40
38:P:55:THR:HB	38:P:124:SER:HA	2.03	0.40
40:R:55:LEU:HD21	40:R:194:THR:HB	2.04	0.40
40:R:165:LEU:HD22	40:R:251:LEU:HD11	2.02	0.40
45:W:151:ARG:HD3	45:W:151:ARG:C	2.46	0.40
55:g:4:VAL:O	55:g:4:VAL:HG23	2.21	0.40
59:k:26:LEU:HD23	59:k:26:LEU:HA	1.85	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	1A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	1B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
1	6A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	6B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
2	1C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	1D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
2	6C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	6D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
3	1E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	1F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
3	6E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	6F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
4	1G	57/60 (95%)	57 (100%)	0	0	100	100
4	1H	57/60 (95%)	57 (100%)	0	0	100	100
4	6G	57/60 (95%)	57 (100%)	0	0	100	100
4	6H	57/60 (95%)	57 (100%)	0	0	100	100
5	1I	66/69 (96%)	66 (100%)	0	0	100	100
5	1J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
5	6I	66/69 (96%)	66 (100%)	0	0	100	100
5	6J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	1K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	1L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
6	6K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	6L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
7	1M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	1N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	77
7	6M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	6N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	77
8	1O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	1P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
8	6O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	6P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1Q	439/485 (90%)	419 (95%)	19 (4%)	1 (0%)	43	77
9	1S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	63
9	6Q	439/485 (90%)	416 (95%)	22 (5%)	1 (0%)	43	77
9	6S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	63
10	1R	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
10	1T	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
10	6R	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
10	6T	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
11	2A	502/505 (99%)	487 (97%)	15 (3%)	0	100	100
11	3A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	4A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	7A	502/505 (99%)	488 (97%)	14 (3%)	0	100	100
11	8A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	9A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
12	2B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100
12	3B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	4B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	7B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100
12	8B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	9B	139/284 (49%)	135 (97%)	4 (3%)	0	100	100
13	2C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
13	3C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	4C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	7C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
13	8C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	9C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
14	2D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
14	3D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
14	4D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
14	7D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
14	8D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	9D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
15	2E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	3E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	4E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	7E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	8E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	9E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
16	2F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
16	3F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	4F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	7F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
16	8F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	9F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
17	2G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
17	3G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
17	4G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
17	7G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
17	8G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
17	9G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
18	2H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	3H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	4H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	7H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	8H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	9H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
19	2I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	3I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	4I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	7I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	8I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	9I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	3J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	4J	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
20	7J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	8J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	9J	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
21	2K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	3K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	4K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	7K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	8K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	9K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
22	2L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
22	3L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
22	4L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
22	7L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
22	8L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
22	9L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
23	5A	237/282 (84%)	232 (98%)	5 (2%)	0	100	100
23	A	237/282 (84%)	232 (98%)	5 (2%)	0	100	100
24	5B	433/484 (90%)	425 (98%)	8 (2%)	0	100	100
24	B	433/484 (90%)	425 (98%)	8 (2%)	0	100	100
25	5C	686/733 (94%)	668 (97%)	18 (3%)	0	100	100
25	C	686/733 (94%)	668 (97%)	18 (3%)	0	100	100
26	5D	214/282 (76%)	204 (95%)	10 (5%)	0	100	100
26	D	214/282 (76%)	205 (96%)	9 (4%)	0	100	100
27	5E	382/467 (82%)	367 (96%)	15 (4%)	0	100	100
27	E	382/467 (82%)	367 (96%)	15 (4%)	0	100	100
28	5F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
28	F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
29	5G	197/231 (85%)	190 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	G	197/231 (85%)	190 (96%)	7 (4%)	0	100	100
30	5H	88/118 (75%)	83 (94%)	5 (6%)	0	100	100
30	H	88/118 (75%)	83 (94%)	5 (6%)	0	100	100
31	5I	133/165 (81%)	131 (98%)	2 (2%)	0	100	100
31	I	133/165 (81%)	131 (98%)	2 (2%)	0	100	100
32	5J	82/128 (64%)	79 (96%)	3 (4%)	0	100	100
32	5r	86/128 (67%)	81 (94%)	5 (6%)	0	100	100
32	J	82/128 (64%)	80 (98%)	2 (2%)	0	100	100
32	r	86/128 (67%)	81 (94%)	5 (6%)	0	100	100
33	5K	117/138 (85%)	114 (97%)	3 (3%)	0	100	100
33	K	117/138 (85%)	114 (97%)	3 (3%)	0	100	100
34	5L	162/187 (87%)	157 (97%)	5 (3%)	0	100	100
34	L	162/187 (87%)	157 (97%)	5 (3%)	0	100	100
35	5M	119/154 (77%)	114 (96%)	5 (4%)	0	100	100
35	M	119/154 (77%)	114 (96%)	5 (4%)	0	100	100
36	5N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
36	N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
37	5O	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	O	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	5P	361/397 (91%)	351 (97%)	9 (2%)	1 (0%)	36	71
38	P	361/397 (91%)	351 (97%)	9 (2%)	1 (0%)	36	71
39	5Q	282/292 (97%)	272 (96%)	10 (4%)	0	100	100
39	Q	282/292 (97%)	272 (96%)	10 (4%)	0	100	100
40	5R	381/387 (98%)	365 (96%)	16 (4%)	0	100	100
40	R	381/387 (98%)	366 (96%)	15 (4%)	0	100	100
41	5S	130/279 (47%)	129 (99%)	1 (1%)	0	100	100
41	S	130/279 (47%)	129 (99%)	1 (1%)	0	100	100
42	5T	441/443 (100%)	428 (97%)	13 (3%)	0	100	100
42	T	441/443 (100%)	428 (97%)	13 (3%)	0	100	100
43	5U	103/227 (45%)	101 (98%)	2 (2%)	0	100	100
43	U	103/227 (45%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	5V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	77
44	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	77
45	5W	155/162 (96%)	148 (96%)	7 (4%)	0	100	100
45	W	155/162 (96%)	149 (96%)	6 (4%)	0	100	100
46	5X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
46	X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
47	5Y	52/64 (81%)	52 (100%)	0	0	100	100
47	Y	52/64 (81%)	52 (100%)	0	0	100	100
48	5Z	105/124 (85%)	103 (98%)	2 (2%)	0	100	100
48	Z	105/124 (85%)	103 (98%)	2 (2%)	0	100	100
49	5a	80/129 (62%)	79 (99%)	0	1 (1%)	9	40
49	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	9	40
50	5b	142/172 (83%)	140 (99%)	2 (1%)	0	100	100
50	b	142/172 (83%)	141 (99%)	1 (1%)	0	100	100
51	5c	55/67 (82%)	51 (93%)	4 (7%)	0	100	100
51	c	55/67 (82%)	51 (93%)	4 (7%)	0	100	100
52	5d	83/86 (96%)	83 (100%)	0	0	100	100
52	d	83/86 (96%)	83 (100%)	0	0	100	100
53	5e	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
53	e	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
54	5f	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	f	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
55	5g	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
55	g	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
56	5h	106/142 (75%)	98 (92%)	8 (8%)	0	100	100
56	h	106/142 (75%)	98 (92%)	8 (8%)	0	100	100
57	5i	74/81 (91%)	74 (100%)	0	0	100	100
57	i	74/81 (91%)	74 (100%)	0	0	100	100
58	5j	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
58	j	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
59	5k	115/117 (98%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	k	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
60	5l	114/121 (94%)	113 (99%)	1 (1%)	0	100	100
60	l	114/121 (94%)	113 (99%)	1 (1%)	0	100	100
61	5m	134/142 (94%)	132 (98%)	2 (2%)	0	100	100
61	m	134/142 (94%)	132 (98%)	2 (2%)	0	100	100
62	5n	102/106 (96%)	102 (100%)	0	0	100	100
62	n	102/106 (96%)	102 (100%)	0	0	100	100
63	5o	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
63	o	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
64	5p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
64	p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
65	5q	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
65	q	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
66	5s	310/312 (99%)	299 (96%)	11 (4%)	0	100	100
66	s	310/312 (99%)	299 (96%)	11 (4%)	0	100	100
67	5t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
67	t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
68	5u	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
68	u	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
69	5v	43/45 (96%)	43 (100%)	0	0	100	100
69	v	43/45 (96%)	43 (100%)	0	0	100	100
70	5w	62/109 (57%)	62 (100%)	0	0	100	100
70	w	62/109 (57%)	62 (100%)	0	0	100	100
71	5x	81/157 (52%)	81 (100%)	0	0	100	100
71	x	81/157 (52%)	81 (100%)	0	0	100	100
72	5y	112/118 (95%)	112 (100%)	0	0	100	100
72	y	112/118 (95%)	112 (100%)	0	0	100	100
All	All	36512/43212 (84%)	35417 (97%)	1075 (3%)	20 (0%)	49	82

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP

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Mol	Chain	Res	Type
15	2E	28	TRP
15	3E	28	TRP
15	4E	28	TRP
9	6Q	396	ASP
15	7E	28	TRP
15	8E	28	TRP
15	9E	28	TRP
49	5a	43	TYR
49	a	43	TYR
9	1S	66	THR
9	6S	66	THR
38	5P	370	VAL
38	P	370	VAL
7	1N	187	VAL
9	1S	475	PRO
7	6N	187	VAL
9	6S	475	PRO
44	5V	519	PRO
44	V	519	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	1A	312/317 (98%)	312 (100%)	0	100	100
1	1B	312/317 (98%)	312 (100%)	0	100	100
1	6A	312/317 (98%)	312 (100%)	0	100	100
1	6B	312/317 (98%)	312 (100%)	0	100	100
2	1C	171/213 (80%)	171 (100%)	0	100	100
2	1D	171/213 (80%)	171 (100%)	0	100	100
2	6C	171/213 (80%)	171 (100%)	0	100	100
2	6D	171/213 (80%)	171 (100%)	0	100	100
3	1E	191/238 (80%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1F	191/238 (80%)	191 (100%)	0	100	100
3	6E	191/238 (80%)	191 (100%)	0	100	100
3	6F	191/238 (80%)	191 (100%)	0	100	100
4	1G	52/53 (98%)	52 (100%)	0	100	100
4	1H	52/53 (98%)	52 (100%)	0	100	100
4	6G	52/53 (98%)	52 (100%)	0	100	100
4	6H	52/53 (98%)	52 (100%)	0	100	100
5	1I	58/59 (98%)	58 (100%)	0	100	100
5	1J	58/59 (98%)	58 (100%)	0	100	100
5	6I	58/59 (98%)	58 (100%)	0	100	100
5	6J	58/59 (98%)	58 (100%)	0	100	100
6	1K	62/64 (97%)	62 (100%)	0	100	100
6	1L	62/64 (97%)	62 (100%)	0	100	100
6	6K	62/64 (97%)	62 (100%)	0	100	100
6	6L	62/64 (97%)	62 (100%)	0	100	100
7	1M	390/413 (94%)	390 (100%)	0	100	100
7	1N	390/413 (94%)	390 (100%)	0	100	100
7	6M	390/413 (94%)	390 (100%)	0	100	100
7	6N	390/413 (94%)	390 (100%)	0	100	100
8	1O	38/47 (81%)	38 (100%)	0	100	100
8	1P	38/47 (81%)	38 (100%)	0	100	100
8	6O	38/47 (81%)	38 (100%)	0	100	100
8	6P	38/47 (81%)	38 (100%)	0	100	100
9	1Q	333/362 (92%)	331 (99%)	2 (1%)	78	81
9	1S	333/362 (92%)	333 (100%)	0	100	100
9	6Q	333/362 (92%)	330 (99%)	3 (1%)	70	77
9	6S	333/362 (92%)	333 (100%)	0	100	100
10	1R	106/107 (99%)	106 (100%)	0	100	100
10	1T	106/107 (99%)	106 (100%)	0	100	100
10	6R	106/107 (99%)	106 (100%)	0	100	100
10	6T	106/107 (99%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2A	408/409 (100%)	408 (100%)	0	100	100
11	3A	408/409 (100%)	408 (100%)	0	100	100
11	4A	408/409 (100%)	408 (100%)	0	100	100
11	7A	408/409 (100%)	408 (100%)	0	100	100
11	8A	408/409 (100%)	408 (100%)	0	100	100
11	9A	408/409 (100%)	408 (100%)	0	100	100
12	2B	132/224 (59%)	132 (100%)	0	100	100
12	3B	132/224 (59%)	132 (100%)	0	100	100
12	4B	132/224 (59%)	132 (100%)	0	100	100
12	7B	132/224 (59%)	132 (100%)	0	100	100
12	8B	132/224 (59%)	132 (100%)	0	100	100
12	9B	132/224 (59%)	132 (100%)	0	100	100
13	2C	137/137 (100%)	137 (100%)	0	100	100
13	3C	137/137 (100%)	137 (100%)	0	100	100
13	4C	137/137 (100%)	137 (100%)	0	100	100
13	7C	137/137 (100%)	137 (100%)	0	100	100
13	8C	137/137 (100%)	137 (100%)	0	100	100
13	9C	137/137 (100%)	137 (100%)	0	100	100
14	2D	211/294 (72%)	211 (100%)	0	100	100
14	3D	211/294 (72%)	211 (100%)	0	100	100
14	4D	211/294 (72%)	211 (100%)	0	100	100
14	7D	211/294 (72%)	211 (100%)	0	100	100
14	8D	211/294 (72%)	211 (100%)	0	100	100
14	9D	211/294 (72%)	211 (100%)	0	100	100
15	2E	79/137 (58%)	79 (100%)	0	100	100
15	3E	79/137 (58%)	79 (100%)	0	100	100
15	4E	79/137 (58%)	79 (100%)	0	100	100
15	7E	79/137 (58%)	79 (100%)	0	100	100
15	8E	79/137 (58%)	79 (100%)	0	100	100
15	9E	79/137 (58%)	79 (100%)	0	100	100
16	2F	66/72 (92%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	3F	66/72 (92%)	66 (100%)	0	100	100
16	4F	66/72 (92%)	66 (100%)	0	100	100
16	7F	66/72 (92%)	66 (100%)	0	100	100
16	8F	66/72 (92%)	66 (100%)	0	100	100
16	9F	66/72 (92%)	66 (100%)	0	100	100
17	2G	75/100 (75%)	75 (100%)	0	100	100
17	3G	75/100 (75%)	75 (100%)	0	100	100
17	4G	75/100 (75%)	75 (100%)	0	100	100
17	7G	75/100 (75%)	75 (100%)	0	100	100
17	8G	75/100 (75%)	75 (100%)	0	100	100
17	9G	75/100 (75%)	75 (100%)	0	100	100
18	2H	103/132 (78%)	103 (100%)	0	100	100
18	3H	103/132 (78%)	103 (100%)	0	100	100
18	4H	103/132 (78%)	103 (100%)	0	100	100
18	7H	103/132 (78%)	103 (100%)	0	100	100
18	8H	103/132 (78%)	103 (100%)	0	100	100
18	9H	103/132 (78%)	103 (100%)	0	100	100
19	2I	58/80 (72%)	58 (100%)	0	100	100
19	3I	58/80 (72%)	58 (100%)	0	100	100
19	4I	58/80 (72%)	58 (100%)	0	100	100
19	7I	58/80 (72%)	58 (100%)	0	100	100
19	8I	58/80 (72%)	58 (100%)	0	100	100
19	9I	58/80 (72%)	58 (100%)	0	100	100
20	2J	83/84 (99%)	83 (100%)	0	100	100
20	3J	83/84 (99%)	83 (100%)	0	100	100
20	4J	80/84 (95%)	80 (100%)	0	100	100
20	7J	83/84 (99%)	83 (100%)	0	100	100
20	8J	83/84 (99%)	83 (100%)	0	100	100
20	9J	80/84 (95%)	80 (100%)	0	100	100
21	2K	39/46 (85%)	39 (100%)	0	100	100
21	3K	39/46 (85%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	4K	39/46 (85%)	39 (100%)	0	100	100
21	7K	39/46 (85%)	39 (100%)	0	100	100
21	8K	39/46 (85%)	39 (100%)	0	100	100
21	9K	39/46 (85%)	39 (100%)	0	100	100
22	2L	63/74 (85%)	63 (100%)	0	100	100
22	3L	65/74 (88%)	65 (100%)	0	100	100
22	4L	65/74 (88%)	65 (100%)	0	100	100
22	7L	63/74 (85%)	63 (100%)	0	100	100
22	8L	65/74 (88%)	65 (100%)	0	100	100
22	9L	65/74 (88%)	65 (100%)	0	100	100
23	5A	197/228 (86%)	197 (100%)	0	100	100
23	A	197/228 (86%)	197 (100%)	0	100	100
24	5B	344/377 (91%)	344 (100%)	0	100	100
24	B	344/377 (91%)	344 (100%)	0	100	100
25	5C	537/572 (94%)	537 (100%)	0	100	100
25	C	537/572 (94%)	537 (100%)	0	100	100
26	5D	196/248 (79%)	196 (100%)	0	100	100
26	D	196/248 (79%)	196 (100%)	0	100	100
27	5E	332/388 (86%)	332 (100%)	0	100	100
27	E	332/388 (86%)	332 (100%)	0	100	100
28	5F	129/133 (97%)	129 (100%)	0	100	100
28	F	129/133 (97%)	129 (100%)	0	100	100
29	5G	172/198 (87%)	172 (100%)	0	100	100
29	G	172/198 (87%)	172 (100%)	0	100	100
30	5H	82/105 (78%)	82 (100%)	0	100	100
30	H	82/105 (78%)	82 (100%)	0	100	100
31	5I	111/134 (83%)	111 (100%)	0	100	100
31	I	111/134 (83%)	111 (100%)	0	100	100
32	5J	71/108 (66%)	71 (100%)	0	100	100
32	5r	72/108 (67%)	72 (100%)	0	100	100
32	J	71/108 (66%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	r	72/108 (67%)	72 (100%)	0	100	100
33	5K	106/122 (87%)	106 (100%)	0	100	100
33	K	106/122 (87%)	106 (100%)	0	100	100
34	5L	130/148 (88%)	130 (100%)	0	100	100
34	L	130/148 (88%)	130 (100%)	0	100	100
35	5M	100/121 (83%)	100 (100%)	0	100	100
35	M	100/121 (83%)	100 (100%)	0	100	100
36	5N	128/132 (97%)	128 (100%)	0	100	100
36	N	128/132 (97%)	128 (100%)	0	100	100
37	5O	80/81 (99%)	80 (100%)	0	100	100
37	O	80/81 (99%)	80 (100%)	0	100	100
38	5P	305/327 (93%)	305 (100%)	0	100	100
38	P	305/327 (93%)	305 (100%)	0	100	100
39	5Q	230/234 (98%)	230 (100%)	0	100	100
39	Q	230/234 (98%)	230 (100%)	0	100	100
40	5R	321/321 (100%)	321 (100%)	0	100	100
40	R	321/321 (100%)	321 (100%)	0	100	100
41	5S	111/217 (51%)	111 (100%)	0	100	100
41	S	111/217 (51%)	111 (100%)	0	100	100
42	5T	374/374 (100%)	374 (100%)	0	100	100
42	T	374/374 (100%)	374 (100%)	0	100	100
43	5U	84/180 (47%)	84 (100%)	0	100	100
43	U	84/180 (47%)	84 (100%)	0	100	100
44	5V	439/439 (100%)	439 (100%)	0	100	100
44	V	439/439 (100%)	439 (100%)	0	100	100
45	5W	131/135 (97%)	131 (100%)	0	100	100
45	W	131/135 (97%)	131 (100%)	0	100	100
46	5X	105/122 (86%)	105 (100%)	0	100	100
46	X	105/122 (86%)	105 (100%)	0	100	100
47	5Y	38/46 (83%)	38 (100%)	0	100	100
47	Y	38/46 (83%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	5Z	93/102 (91%)	93 (100%)	0	100	100
48	Z	93/102 (91%)	93 (100%)	0	100	100
49	5a	68/98 (69%)	67 (98%)	1 (2%)	57	70
49	a	68/98 (69%)	66 (97%)	2 (3%)	37	57
50	5b	119/138 (86%)	119 (100%)	0	100	100
50	b	119/138 (86%)	119 (100%)	0	100	100
51	5c	49/56 (88%)	49 (100%)	0	100	100
51	c	49/56 (88%)	49 (100%)	0	100	100
52	5d	63/64 (98%)	63 (100%)	0	100	100
52	d	63/64 (98%)	63 (100%)	0	100	100
53	5e	163/164 (99%)	163 (100%)	0	100	100
53	e	163/164 (99%)	163 (100%)	0	100	100
54	5f	52/53 (98%)	52 (100%)	0	100	100
54	f	52/53 (98%)	52 (100%)	0	100	100
55	5g	40/45 (89%)	40 (100%)	0	100	100
55	g	40/45 (89%)	40 (100%)	0	100	100
56	5h	91/110 (83%)	91 (100%)	0	100	100
56	h	91/110 (83%)	91 (100%)	0	100	100
57	5i	65/67 (97%)	65 (100%)	0	100	100
57	i	65/67 (97%)	65 (100%)	0	100	100
58	5j	72/73 (99%)	72 (100%)	0	100	100
58	j	72/73 (99%)	72 (100%)	0	100	100
59	5k	102/102 (100%)	102 (100%)	0	100	100
59	k	102/102 (100%)	102 (100%)	0	100	100
60	5l	94/99 (95%)	94 (100%)	0	100	100
60	l	94/99 (95%)	94 (100%)	0	100	100
61	5m	118/122 (97%)	118 (100%)	0	100	100
61	m	118/122 (97%)	118 (100%)	0	100	100
62	5n	92/94 (98%)	92 (100%)	0	100	100
62	n	92/94 (98%)	92 (100%)	0	100	100
63	5o	130/132 (98%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	o	130/132 (98%)	130 (100%)	0	100	100
64	5p	109/110 (99%)	109 (100%)	0	100	100
64	p	109/110 (99%)	109 (100%)	0	100	100
65	5q	135/165 (82%)	135 (100%)	0	100	100
65	q	135/165 (82%)	135 (100%)	0	100	100
66	5s	243/243 (100%)	243 (100%)	0	100	100
66	s	243/243 (100%)	243 (100%)	0	100	100
67	5t	212/233 (91%)	212 (100%)	0	100	100
67	t	212/233 (91%)	212 (100%)	0	100	100
68	5u	180/181 (99%)	179 (99%)	1 (1%)	78	81
68	u	180/181 (99%)	179 (99%)	1 (1%)	78	81
69	5v	38/38 (100%)	38 (100%)	0	100	100
69	v	38/38 (100%)	38 (100%)	0	100	100
70	5w	55/91 (60%)	55 (100%)	0	100	100
70	w	55/91 (60%)	55 (100%)	0	100	100
71	5x	70/130 (54%)	70 (100%)	0	100	100
71	x	70/130 (54%)	70 (100%)	0	100	100
72	5y	102/106 (96%)	102 (100%)	0	100	100
72	y	102/106 (96%)	102 (100%)	0	100	100
All	All	30538/35054 (87%)	30528 (100%)	10 (0%)	100	100

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	1Q	56	LYS
9	1Q	65	ARG
49	5a	67	LYS
68	5u	43	ASN
9	6Q	56	LYS
9	6Q	65	ARG
9	6Q	72	LYS
49	a	46	LYS
49	a	67	LYS
68	u	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (249) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	53	HIS
1	1A	66	GLN
1	1A	213	ASN
1	1A	339	ASN
1	1A	376	HIS
1	1B	8	GLN
1	1B	108	GLN
1	1B	173	ASN
1	1B	215	GLN
1	1B	261	ASN
1	1B	268	HIS
1	1B	287	ASN
2	1C	207	HIS
2	1D	88	ASN
3	1E	79	HIS
4	1G	11	GLN
5	1J	12	GLN
5	1J	20	HIS
6	1L	26	GLN
7	1M	190	GLN
7	1M	224	ASN
7	1M	422	HIS
7	1N	49	HIS
7	1N	99	ASN
7	1N	165	ASN
7	1N	190	GLN
7	1N	198	HIS
7	1N	291	HIS
9	1Q	166	ASN
9	1Q	211	ASN
9	1Q	225	HIS
10	1R	95	GLN
9	1S	130	ASN
9	1S	202	GLN
9	1S	211	ASN
11	2A	490	HIS
12	2B	111	GLN
14	2D	21	HIS
14	2D	222	HIS
14	2D	275	GLN
16	2F	19	HIS

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Mol	Chain	Res	Type
16	2F	63	GLN
22	2L	56	GLN
22	2L	72	ASN
11	3A	104	ASN
11	3A	150	ASN
11	3A	285	HIS
11	3A	416	ASN
12	3B	111	GLN
15	3E	88	HIS
16	3F	56	ASN
16	3F	63	GLN
20	3J	86	ASN
11	4A	104	ASN
11	4A	150	ASN
11	4A	416	ASN
12	4B	111	GLN
15	4E	88	HIS
16	4F	19	HIS
16	4F	63	GLN
20	4J	86	ASN
22	4L	73	HIS
23	5A	74	ASN
23	5A	110	ASN
23	5A	142	HIS
23	5A	154	GLN
23	5A	176	GLN
23	5A	224	ASN
23	5A	252	HIS
24	5B	402	GLN
25	5C	297	ASN
25	5C	319	GLN
25	5C	338	GLN
25	5C	422	ASN
25	5C	431	ASN
25	5C	443	GLN
25	5C	474	GLN
25	5C	708	ASN
26	5D	143	ASN
26	5D	281	ASN
27	5E	187	HIS
27	5E	238	GLN
27	5E	269	ASN

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Mol	Chain	Res	Type
27	5E	437	GLN
28	5F	147	GLN
30	5H	75	ASN
30	5H	106	ASN
31	5I	136	ASN
37	5O	17	HIS
37	5O	75	GLN
38	5P	71	ASN
38	5P	93	HIS
38	5P	168	HIS
39	5Q	47	GLN
39	5Q	267	GLN
40	5R	23	ASN
41	5S	147	HIS
42	5T	298	GLN
44	5V	113	ASN
44	5V	190	HIS
45	5W	54	ASN
45	5W	140	ASN
47	5Y	26	GLN
48	5Z	41	HIS
48	5Z	54	ASN
49	5a	44	ASN
50	5b	155	HIS
52	5d	36	HIS
53	5e	8	ASN
53	5e	89	GLN
53	5e	149	GLN
56	5h	78	HIS
60	5l	114	HIS
62	5n	29	HIS
63	5o	54	ASN
64	5p	90	ASN
65	5q	40	HIS
65	5q	77	GLN
65	5q	92	ASN
32	5r	62	HIS
66	5s	62	GLN
66	5s	71	HIS
66	5s	146	ASN
67	5t	245	GLN
68	5u	2	ASN

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Mol	Chain	Res	Type
71	5x	12	ASN
72	5y	56	ASN
1	6A	53	HIS
1	6A	66	GLN
1	6A	213	ASN
1	6A	339	ASN
1	6A	376	HIS
1	6B	8	GLN
1	6B	108	GLN
1	6B	173	ASN
1	6B	215	GLN
1	6B	261	ASN
1	6B	268	HIS
1	6B	287	ASN
2	6D	88	ASN
3	6E	79	HIS
4	6G	11	GLN
5	6J	12	GLN
5	6J	20	HIS
6	6K	5	GLN
6	6L	26	GLN
7	6M	190	GLN
7	6M	224	ASN
7	6M	227	GLN
7	6M	422	HIS
7	6N	49	HIS
7	6N	99	ASN
7	6N	165	ASN
7	6N	190	GLN
7	6N	291	HIS
9	6Q	166	ASN
9	6Q	211	ASN
9	6Q	225	HIS
10	6R	95	GLN
9	6S	198	GLN
9	6S	202	GLN
9	6S	211	ASN
11	7A	251	GLN
11	7A	490	HIS
12	7B	111	GLN
12	7B	112	HIS
14	7D	21	HIS

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Mol	Chain	Res	Type
14	7D	275	GLN
16	7F	63	GLN
18	7H	83	GLN
22	7L	56	GLN
22	7L	72	ASN
11	8A	104	ASN
11	8A	150	ASN
11	8A	416	ASN
12	8B	111	GLN
15	8E	88	HIS
16	8F	56	ASN
16	8F	63	GLN
11	9A	104	ASN
11	9A	150	ASN
11	9A	285	HIS
11	9A	416	ASN
12	9B	111	GLN
15	9E	88	HIS
16	9F	19	HIS
16	9F	63	GLN
22	9L	73	HIS
23	A	74	ASN
23	A	110	ASN
23	A	142	HIS
23	A	154	GLN
23	A	176	GLN
23	A	252	HIS
24	B	402	GLN
25	C	297	ASN
25	C	319	GLN
25	C	338	GLN
25	C	422	ASN
25	C	431	ASN
25	C	443	GLN
25	C	474	GLN
26	D	143	ASN
26	D	281	ASN
27	E	238	GLN
27	E	269	ASN
27	E	437	GLN
28	F	147	GLN
30	H	75	ASN

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Mol	Chain	Res	Type
30	H	106	ASN
31	I	136	ASN
37	O	17	HIS
37	O	75	GLN
38	P	71	ASN
39	Q	47	GLN
39	Q	267	GLN
40	R	23	ASN
41	S	147	HIS
42	T	298	GLN
44	V	113	ASN
44	V	190	HIS
45	W	54	ASN
45	W	140	ASN
48	Z	41	HIS
48	Z	54	ASN
49	a	44	ASN
49	a	70	HIS
50	b	155	HIS
52	d	36	HIS
53	e	8	ASN
53	e	89	GLN
53	e	149	GLN
56	h	78	HIS
59	k	65	HIS
60	l	114	HIS
62	n	29	HIS
63	o	54	ASN
64	p	90	ASN
65	q	40	HIS
65	q	77	GLN
65	q	92	ASN
66	s	62	GLN
66	s	71	HIS
66	s	146	ASN
67	t	245	GLN
68	u	2	ASN
68	u	45	HIS
68	u	53	HIS
71	x	12	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 74 ligands modelled in this entry, 18 are monoatomic - leaving 56 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	$\# Z > 2$
79	CUA	2C	301	-	0,1,1	-	-	-		
82	SF4	C	802	25	0,12,12	-	-	-		
82	SF4	5G	301	29	0,12,12	-	-	-		
73	HEM	1B	402	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	9 (13%)
73	HEM	6B	402	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	9 (13%)
76	HEA	9A	603	11	66,67,67	2.40	23 (34%)	78,103,103	2.60	31 (39%)
83	8Q1	k	200	-	31,34,34	1.74	5 (16%)	40,43,43	1.68	7 (17%)
76	HEA	4A	602	11	66,67,67	2.39	23 (34%)	78,103,103	2.58	30 (38%)
76	HEA	4A	604	11	66,67,67	2.39	26 (39%)	78,103,103	2.55	33 (42%)
82	SF4	5B	502	24	0,12,12	-	-	-		
74	HEC	6F	501	3	50,50,50	1.76	4 (8%)	68,82,82	1.53	12 (17%)
73	HEM	1A	401	1	50,50,50	1.49	7 (14%)	66,82,82	1.38	7 (10%)
74	HEC	6E	401	3	50,50,50	1.84	5 (10%)	68,82,82	1.45	7 (10%)
79	CUA	3C	301	13	0,1,1	-	-	-		
81	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.17	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	SF4	5G	302	29	0,12,12	-	-	-		
76	HEA	2A	601	11	66,67,67	2.46	23 (34%)	78,103,103	2.58	32 (41%)
85	COO	s	401	-	48,55,55	1.10	4 (8%)	68,81,81	4.02	17 (25%)
76	HEA	7A	602	11	66,67,67	2.46	24 (36%)	78,103,103	2.59	32 (41%)
80	FES	5C	801	25	0,4,4	-	-	-		
82	SF4	B	501	24	0,12,12	-	-	-		
80	FES	C	803	25	0,4,4	-	-	-		
74	HEC	1F	501	3	50,50,50	1.77	4 (8%)	68,82,82	1.53	12 (17%)
76	HEA	2A	602	11	66,67,67	2.44	26 (39%)	78,103,103	2.54	32 (41%)
84	NDP	P	401	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	13 (19%)
82	SF4	G	301	29	0,12,12	-	-	-		
73	HEM	6B	401	1	50,50,50	1.43	8 (16%)	66,82,82	1.37	10 (15%)
74	HEC	1E	401	3	50,50,50	1.84	5 (10%)	68,82,82	1.44	8 (11%)
76	HEA	7A	601	11	66,67,67	2.44	26 (39%)	78,103,103	2.54	30 (38%)
80	FES	A	301	23	0,4,4	-	-	-		
76	HEA	9A	602	11	66,67,67	2.39	24 (36%)	78,103,103	2.55	33 (42%)
82	SF4	5C	803	25	0,12,12	-	-	-		
73	HEM	1B	401	1	50,50,50	1.43	8 (16%)	66,82,82	1.36	10 (15%)
76	HEA	8A	604	11	66,67,67	2.39	24 (36%)	78,103,103	2.54	33 (42%)
79	CUA	8C	301	13	0,1,1	-	-	-		
76	HEA	3A	604	11	66,67,67	2.40	23 (34%)	78,103,103	2.60	30 (38%)
83	8Q1	5J	200	-	31,34,34	1.72	5 (16%)	40,43,43	1.54	5 (12%)
76	HEA	8A	601	11	66,67,67	2.40	23 (34%)	78,103,103	2.59	30 (38%)
83	8Q1	5k	200	-	31,34,34	1.75	6 (19%)	40,43,43	1.68	7 (17%)
76	HEA	3A	601	11	66,67,67	2.39	25 (37%)	78,103,103	2.54	33 (42%)
82	SF4	F	201	28	0,12,12	-	-	-		
73	HEM	6A	402	1	50,50,50	1.49	7 (14%)	66,82,82	1.39	8 (12%)
82	SF4	C	801	25	0,12,12	-	-	-		
85	COO	5s	401	-	48,55,55	1.10	4 (8%)	68,81,81	4.01	17 (25%)
82	SF4	5F	201	28	0,12,12	-	-	-		
84	NDP	5P	401	-	49,52,52	2.22	6 (12%)	66,80,80	1.65	13 (19%)
81	FMN	5B	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.16	7 (14%)
82	SF4	G	302	29	0,12,12	-	-	-		
73	HEM	1A	402	1	50,50,50	1.31	7 (14%)	66,82,82	1.30	8 (12%)
80	FES	5A	301	23	0,4,4	-	-	-		
82	SF4	5C	802	25	0,12,12	-	-	-		
83	8Q1	J	200	-	31,34,34	1.72	6 (19%)	40,43,43	1.55	5 (12%)
79	CUA	4C	301	13	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	CUA	7C	301	-	0,1,1	-	-	-		
79	CUA	9C	301	13	0,1,1	-	-	-		
73	HEM	6A	401	1	50,50,50	1.31	7 (14%)	66,82,82	1.29	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SF4	C	802	25	-	-	0/6/5/5
82	SF4	5G	301	29	-	-	0/6/5/5
73	HEM	1B	402	1	-	4/14/54/54	-
73	HEM	6B	402	1	-	4/14/54/54	-
76	HEA	9A	603	11	-	4/36/76/76	-
83	8Q1	k	200	-	-	21/41/41/41	-
76	HEA	4A	602	11	-	4/36/76/76	-
76	HEA	4A	604	11	-	9/36/76/76	-
82	SF4	5B	502	24	-	-	0/6/5/5
74	HEC	6E	401	3	1/1/3/7	2/14/54/54	-
73	HEM	1A	401	1	-	3/14/54/54	-
74	HEC	6F	501	3	1/1/3/7	2/14/54/54	-
81	FMN	B	502	-	-	5/18/18/18	0/3/3/3
85	COO	s	401	-	-	22/54/70/70	0/3/3/3
82	SF4	5G	302	29	-	-	0/6/5/5
76	HEA	2A	601	11	-	7/36/76/76	-
76	HEA	7A	602	11	-	7/36/76/76	-
80	FES	5C	801	25	-	-	0/1/1/1
82	SF4	B	501	24	-	-	0/6/5/5
80	FES	C	803	25	-	-	0/1/1/1
74	HEC	1F	501	3	1/1/3/7	2/14/54/54	-
76	HEA	2A	602	11	-	10/36/76/76	-
84	NDP	P	401	-	-	8/34/77/77	0/5/5/5
82	SF4	G	301	29	-	-	0/6/5/5
73	HEM	6B	401	1	-	4/14/54/54	-
74	HEC	1E	401	3	1/1/3/7	2/14/54/54	-
76	HEA	7A	601	11	-	10/36/76/76	-
80	FES	A	301	23	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	HEA	9A	602	11	-	9/36/76/76	-
82	SF4	5C	803	25	-	-	0/6/5/5
73	HEM	1B	401	1	-	4/14/54/54	-
76	HEA	8A	604	11	-	9/36/76/76	-
76	HEA	3A	604	11	-	4/36/76/76	-
83	8Q1	5J	200	-	-	7/41/41/41	-
76	HEA	8A	601	11	-	4/36/76/76	-
83	8Q1	5k	200	-	-	21/41/41/41	-
76	HEA	3A	601	11	-	9/36/76/76	-
82	SF4	F	201	28	-	-	0/6/5/5
73	HEM	6A	402	1	-	3/14/54/54	-
82	SF4	C	801	25	-	-	0/6/5/5
82	SF4	5F	201	28	-	-	0/6/5/5
84	NDP	5P	401	-	-	8/34/77/77	0/5/5/5
81	FMN	5B	501	-	-	5/18/18/18	0/3/3/3
82	SF4	G	302	29	-	-	0/6/5/5
73	HEM	1A	402	1	-	4/14/54/54	-
80	FES	5A	301	23	-	-	0/1/1/1
82	SF4	5C	802	25	-	-	0/6/5/5
83	8Q1	J	200	-	-	7/41/41/41	-
85	COO	5s	401	-	-	22/54/70/70	0/3/3/3
73	HEM	6A	401	1	-	4/14/54/54	-

All (411) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	P	401	NDP	P2B-O2B	12.50	1.82	1.59
84	5P	401	NDP	P2B-O2B	12.47	1.82	1.59
74	1E	401	HEC	C3D-C2D	7.84	1.53	1.36
74	6E	401	HEC	C3D-C2D	7.83	1.53	1.36
74	1F	501	HEC	C3D-C2D	7.75	1.53	1.36
74	6F	501	HEC	C3D-C2D	7.71	1.53	1.36
83	5k	200	8Q1	C34-N36	5.85	1.46	1.33
83	k	200	8Q1	C34-N36	5.81	1.46	1.33
76	7A	602	HEA	C3B-C2B	5.67	1.47	1.34
76	2A	601	HEA	C3B-C2B	5.67	1.47	1.34
83	J	200	8Q1	C34-N36	5.61	1.45	1.33
83	5J	200	8Q1	C34-N36	5.60	1.45	1.33
76	2A	602	HEA	FE-NB	5.59	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7A	602	HEA	FE-ND	5.59	2.12	1.94
76	7A	601	HEA	FE-NB	5.59	2.12	1.94
76	2A	601	HEA	FE-ND	5.56	2.12	1.94
76	4A	602	HEA	FE-ND	5.53	2.12	1.94
76	9A	603	HEA	FE-ND	5.52	2.12	1.94
76	7A	601	HEA	FE-ND	5.51	2.11	1.94
76	2A	602	HEA	FE-ND	5.50	2.11	1.94
76	8A	601	HEA	FE-ND	5.49	2.11	1.94
76	3A	604	HEA	C3B-C2B	5.49	1.47	1.34
76	4A	604	HEA	FE-NB	5.48	2.11	1.94
76	3A	604	HEA	FE-ND	5.48	2.11	1.94
76	3A	601	HEA	FE-NB	5.46	2.11	1.94
76	9A	603	HEA	C3B-C2B	5.46	1.47	1.34
76	8A	601	HEA	C3B-C2B	5.45	1.47	1.34
76	9A	602	HEA	FE-NB	5.45	2.11	1.94
76	8A	604	HEA	FE-NB	5.45	2.11	1.94
76	4A	602	HEA	C3B-C2B	5.41	1.46	1.34
76	8A	601	HEA	FE-NB	5.40	2.11	1.94
76	2A	601	HEA	FE-NB	5.39	2.11	1.94
76	3A	604	HEA	FE-NB	5.39	2.11	1.94
76	7A	602	HEA	FE-NB	5.38	2.11	1.94
76	4A	602	HEA	FE-NB	5.37	2.11	1.94
76	3A	601	HEA	FE-ND	5.37	2.11	1.94
76	9A	603	HEA	FE-NB	5.36	2.11	1.94
76	8A	604	HEA	FE-ND	5.36	2.11	1.94
76	9A	602	HEA	FE-ND	5.35	2.11	1.94
76	4A	604	HEA	FE-ND	5.35	2.11	1.94
83	5k	200	8Q1	C39-N41	5.33	1.45	1.33
76	3A	601	HEA	C3B-C2B	5.33	1.46	1.34
83	k	200	8Q1	C39-N41	5.32	1.45	1.33
83	5J	200	8Q1	C39-N41	5.32	1.45	1.33
76	8A	604	HEA	C3B-C2B	5.32	1.46	1.34
76	9A	602	HEA	C3B-C2B	5.31	1.46	1.34
83	J	200	8Q1	C39-N41	5.30	1.45	1.33
76	4A	604	HEA	C3B-C2B	5.29	1.46	1.34
76	2A	602	HEA	C3A-C2A	5.18	1.47	1.36
76	7A	601	HEA	C3A-C2A	5.16	1.47	1.36
76	7A	601	HEA	C3B-C2B	5.16	1.46	1.34
76	2A	602	HEA	C3B-C2B	5.12	1.46	1.34
76	2A	601	HEA	C3D-C2D	4.94	1.47	1.36
76	7A	602	HEA	C3D-C2D	4.94	1.47	1.36
76	7A	601	HEA	C3D-C2D	4.91	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	6F	501	HEC	FE-ND	4.90	2.10	1.94
74	1F	501	HEC	FE-ND	4.89	2.10	1.94
76	8A	604	HEA	C3A-C2A	4.88	1.47	1.36
76	2A	602	HEA	C3D-C2D	4.86	1.47	1.36
76	3A	601	HEA	C3A-C2A	4.82	1.47	1.36
76	8A	601	HEA	C3A-C2A	4.81	1.47	1.36
76	8A	604	HEA	C3D-C2D	4.80	1.46	1.36
76	3A	604	HEA	C3A-C2A	4.80	1.47	1.36
76	2A	601	HEA	C3A-C2A	4.80	1.47	1.36
76	7A	602	HEA	FE-NC	4.79	2.11	1.95
76	9A	602	HEA	C3A-C2A	4.79	1.47	1.36
76	7A	602	HEA	C3A-C2A	4.79	1.47	1.36
76	9A	602	HEA	C3D-C2D	4.77	1.46	1.36
76	3A	601	HEA	C3D-C2D	4.77	1.46	1.36
76	4A	602	HEA	C3A-C2A	4.77	1.47	1.36
76	4A	604	HEA	C3A-C2A	4.76	1.47	1.36
76	4A	604	HEA	C3D-C2D	4.76	1.46	1.36
76	9A	603	HEA	C3A-C2A	4.76	1.46	1.36
76	2A	601	HEA	FE-NC	4.75	2.11	1.95
76	9A	603	HEA	C3D-C2D	4.73	1.46	1.36
76	3A	604	HEA	C3D-C2D	4.70	1.46	1.36
76	2A	602	HEA	FE-NC	4.69	2.11	1.95
76	7A	601	HEA	FE-NC	4.68	2.11	1.95
76	4A	602	HEA	C3D-C2D	4.67	1.46	1.36
74	1F	501	HEC	FE-NB	4.67	2.09	1.94
74	6F	501	HEC	FE-NB	4.66	2.09	1.94
76	8A	601	HEA	C3D-C2D	4.66	1.46	1.36
74	6E	401	HEC	FE-NB	4.66	2.09	1.94
74	1E	401	HEC	FE-NB	4.64	2.09	1.94
76	3A	601	HEA	FE-NC	4.64	2.10	1.95
76	8A	604	HEA	FE-NC	4.62	2.10	1.95
76	9A	602	HEA	FE-NC	4.59	2.10	1.95
76	4A	604	HEA	FE-NC	4.57	2.10	1.95
76	9A	603	HEA	FE-NC	4.56	2.10	1.95
76	3A	604	HEA	FE-NC	4.55	2.10	1.95
76	4A	602	HEA	FE-NC	4.55	2.10	1.95
76	8A	601	HEA	FE-NC	4.54	2.10	1.95
76	2A	601	HEA	CHC-C4B	4.52	1.47	1.38
76	7A	602	HEA	CHC-C4B	4.51	1.47	1.38
85	s	401	COO	C5A-C4A	4.49	1.47	1.39
76	8A	601	HEA	CHC-C4B	4.47	1.47	1.38
76	3A	604	HEA	CHC-C4B	4.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	5s	401	COO	C5A-C4A	4.44	1.47	1.39
76	9A	603	HEA	CHC-C4B	4.44	1.47	1.38
76	8A	604	HEA	CHC-C4B	4.44	1.47	1.38
76	4A	604	HEA	CHC-C4B	4.43	1.47	1.38
76	3A	601	HEA	CHC-C4B	4.43	1.47	1.38
76	4A	602	HEA	CHC-C4B	4.42	1.47	1.38
76	9A	602	HEA	CHC-C4B	4.41	1.47	1.38
76	7A	602	HEA	CHA-C1A	4.37	1.46	1.38
76	2A	602	HEA	CHD-C1D	4.35	1.47	1.38
76	7A	602	HEA	CHB-C4A	4.35	1.46	1.38
76	7A	601	HEA	CHD-C1D	4.35	1.47	1.38
74	1E	401	HEC	FE-ND	4.34	2.08	1.94
74	6E	401	HEC	FE-ND	4.34	2.08	1.94
76	2A	601	HEA	CHB-C4A	4.32	1.46	1.38
76	2A	601	HEA	CHA-C1A	4.31	1.46	1.38
76	4A	604	HEA	CHD-C1D	4.23	1.47	1.38
76	2A	601	HEA	CHD-C1D	4.22	1.47	1.38
76	3A	601	HEA	CHD-C1D	4.21	1.47	1.38
76	8A	604	HEA	CHD-C1D	4.21	1.47	1.38
76	7A	602	HEA	CHD-C1D	4.20	1.47	1.38
76	7A	601	HEA	CHC-C4B	4.17	1.47	1.38
76	9A	602	HEA	CHD-C1D	4.17	1.47	1.38
76	2A	602	HEA	CHC-C4B	4.16	1.47	1.38
76	8A	601	HEA	CHD-C1D	4.16	1.47	1.38
76	2A	602	HEA	C1A-NA	4.15	1.47	1.39
76	7A	601	HEA	C1A-NA	4.14	1.47	1.39
76	2A	602	HEA	CHB-C4A	4.13	1.46	1.38
76	7A	601	HEA	CHB-C4A	4.13	1.46	1.38
76	8A	601	HEA	CHB-C4A	4.13	1.46	1.38
76	9A	603	HEA	CHD-C1D	4.12	1.46	1.38
76	4A	602	HEA	CHB-C4A	4.11	1.46	1.38
76	3A	604	HEA	CHB-C4A	4.10	1.46	1.38
76	3A	604	HEA	CHD-C1D	4.09	1.46	1.38
76	4A	602	HEA	CHD-C1D	4.09	1.46	1.38
76	2A	602	HEA	CHA-C1A	4.09	1.46	1.38
76	9A	603	HEA	CHB-C4A	4.09	1.46	1.38
76	8A	604	HEA	CHB-C4A	4.08	1.46	1.38
76	7A	601	HEA	CHA-C1A	4.08	1.46	1.38
84	5P	401	NDP	PN-O5D	4.07	1.75	1.59
76	9A	602	HEA	C1A-NA	4.07	1.47	1.39
76	4A	604	HEA	CHB-C4A	4.06	1.46	1.38
84	P	401	NDP	PN-O5D	4.06	1.75	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7A	602	HEA	C1A-NA	4.05	1.47	1.39
76	3A	601	HEA	CHB-C4A	4.04	1.46	1.38
76	3A	601	HEA	C1A-NA	4.03	1.47	1.39
76	8A	604	HEA	C1A-NA	4.03	1.47	1.39
76	2A	601	HEA	C1A-NA	4.03	1.47	1.39
76	9A	602	HEA	CHB-C4A	4.02	1.46	1.38
73	1A	401	HEM	FE-NC	3.99	2.08	1.95
73	1A	401	HEM	FE-NA	3.99	2.08	1.95
73	6A	402	HEM	FE-NA	3.98	2.08	1.95
73	6A	402	HEM	FE-NC	3.98	2.08	1.95
76	2A	602	HEA	C4A-NA	3.98	1.47	1.39
76	4A	604	HEA	C1A-NA	3.97	1.47	1.39
76	4A	604	HEA	CHA-C1A	3.95	1.46	1.38
76	7A	601	HEA	C4A-NA	3.92	1.47	1.39
76	8A	604	HEA	CHA-C1A	3.91	1.46	1.38
76	3A	601	HEA	CHA-C1A	3.91	1.46	1.38
76	9A	603	HEA	C4A-NA	3.90	1.47	1.39
76	4A	602	HEA	C4A-NA	3.87	1.47	1.39
81	5B	501	FMN	C4A-N5	3.86	1.38	1.30
81	B	502	FMN	C4A-N5	3.86	1.38	1.30
76	9A	602	HEA	CHA-C1A	3.86	1.45	1.38
76	3A	604	HEA	C4A-NA	3.81	1.47	1.39
76	8A	601	HEA	C1A-NA	3.79	1.47	1.39
76	8A	601	HEA	C4A-NA	3.78	1.47	1.39
76	9A	603	HEA	CHA-C1A	3.77	1.45	1.38
76	3A	604	HEA	C1A-NA	3.74	1.47	1.39
76	7A	602	HEA	CHC-C1C	3.73	1.47	1.39
76	3A	604	HEA	CHA-C1A	3.73	1.45	1.38
76	2A	601	HEA	C4A-NA	3.72	1.47	1.39
76	7A	602	HEA	C4A-NA	3.72	1.47	1.39
76	4A	602	HEA	CHA-C1A	3.71	1.45	1.38
76	2A	601	HEA	CHC-C1C	3.69	1.47	1.39
76	4A	602	HEA	C1A-NA	3.67	1.46	1.39
76	8A	601	HEA	CHA-C1A	3.66	1.45	1.38
76	9A	603	HEA	C1A-NA	3.66	1.46	1.39
76	8A	604	HEA	C4A-NA	3.65	1.46	1.39
74	6E	401	HEC	FE-NC	3.64	2.07	1.95
76	3A	601	HEA	C4A-NA	3.64	1.46	1.39
76	4A	604	HEA	C4A-NA	3.63	1.46	1.39
74	1E	401	HEC	FE-NC	3.63	2.07	1.95
76	8A	601	HEA	CHC-C1C	3.63	1.47	1.39
76	2A	602	HEA	CHD-C4C	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7A	601	HEA	CHD-C4C	3.62	1.47	1.39
76	9A	602	HEA	C4A-NA	3.62	1.46	1.39
76	3A	604	HEA	CHC-C1C	3.62	1.47	1.39
76	9A	603	HEA	CHC-C1C	3.57	1.47	1.39
76	4A	602	HEA	CHC-C1C	3.54	1.47	1.39
76	9A	603	HEA	CHD-C4C	3.44	1.47	1.39
76	3A	604	HEA	CHD-C4C	3.44	1.47	1.39
73	1B	402	HEM	FE-NB	3.44	2.05	1.94
76	9A	602	HEA	CHD-C4C	3.42	1.47	1.39
76	4A	604	HEA	CHD-C4C	3.42	1.47	1.39
76	4A	602	HEA	CHD-C4C	3.42	1.47	1.39
73	6B	402	HEM	FE-NB	3.41	2.05	1.94
76	8A	601	HEA	CHD-C4C	3.41	1.47	1.39
76	7A	601	HEA	CHB-C1B	3.40	1.47	1.39
76	9A	602	HEA	CHC-C1C	3.40	1.47	1.39
76	7A	602	HEA	CHD-C4C	3.39	1.47	1.39
76	2A	601	HEA	CHD-C4C	3.39	1.47	1.39
73	6B	401	HEM	FE-NA	3.39	2.06	1.95
76	4A	604	HEA	CHC-C1C	3.38	1.47	1.39
73	1B	401	HEM	FE-NA	3.37	2.06	1.95
76	2A	602	HEA	CHB-C1B	3.36	1.46	1.39
76	3A	601	HEA	CHD-C4C	3.35	1.46	1.39
76	8A	604	HEA	CHD-C4C	3.35	1.46	1.39
76	8A	604	HEA	CHC-C1C	3.35	1.46	1.39
76	3A	601	HEA	CHC-C1C	3.33	1.46	1.39
73	6B	401	HEM	FE-NC	3.31	2.06	1.95
73	1B	401	HEM	FE-NC	3.31	2.06	1.95
76	7A	601	HEA	CHC-C1C	3.29	1.46	1.39
73	1A	401	HEM	FE-ND	3.27	2.05	1.94
73	1B	401	HEM	CAB-C3B	3.27	1.56	1.47
76	2A	602	HEA	CHC-C1C	3.25	1.46	1.39
73	6A	402	HEM	FE-ND	3.23	2.04	1.94
73	6B	401	HEM	CAB-C3B	3.23	1.56	1.47
76	2A	601	HEA	CHB-C1B	3.23	1.46	1.39
76	7A	602	HEA	CHB-C1B	3.23	1.46	1.39
76	2A	601	HEA	CHA-C4D	3.18	1.46	1.39
76	8A	604	HEA	CHB-C1B	3.16	1.46	1.39
76	2A	602	HEA	CHA-C4D	3.15	1.46	1.39
76	3A	601	HEA	CHB-C1B	3.15	1.46	1.39
76	7A	602	HEA	CHA-C4D	3.14	1.46	1.39
76	7A	601	HEA	CHA-C4D	3.14	1.46	1.39
76	4A	604	HEA	CHB-C1B	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7A	602	HEA	C4B-C3B	3.12	1.49	1.44
76	3A	604	HEA	CHB-C1B	3.11	1.46	1.39
76	9A	602	HEA	CHB-C1B	3.11	1.46	1.39
76	9A	603	HEA	CHB-C1B	3.11	1.46	1.39
73	6B	402	HEM	CAB-C3B	3.09	1.55	1.47
76	8A	601	HEA	C1D-ND	-3.09	1.35	1.40
76	4A	602	HEA	CHB-C1B	3.09	1.46	1.39
76	7A	602	HEA	C1D-ND	-3.07	1.35	1.40
76	2A	601	HEA	C1D-ND	-3.07	1.35	1.40
76	8A	601	HEA	CHB-C1B	3.06	1.46	1.39
73	6A	402	HEM	CAB-C3B	3.06	1.55	1.47
74	1E	401	HEC	FE-NA	3.06	2.05	1.95
84	5P	401	NDP	O2B-C2B	-3.06	1.33	1.44
74	6E	401	HEC	FE-NA	3.06	2.05	1.95
73	1B	402	HEM	CAB-C3B	3.06	1.55	1.47
76	2A	601	HEA	C4B-C3B	3.06	1.49	1.44
76	4A	602	HEA	C1D-ND	-3.06	1.35	1.40
84	P	401	NDP	O2B-C2B	-3.06	1.33	1.44
76	9A	603	HEA	C1D-ND	-3.05	1.35	1.40
76	3A	601	HEA	CHA-C4D	3.04	1.46	1.39
76	9A	602	HEA	CHA-C4D	3.03	1.46	1.39
76	4A	604	HEA	CHA-C4D	3.02	1.46	1.39
73	1A	401	HEM	CAB-C3B	3.02	1.55	1.47
76	8A	601	HEA	C4B-C3B	3.00	1.49	1.44
76	3A	604	HEA	CHA-C4D	3.00	1.46	1.39
76	8A	604	HEA	CHA-C4D	3.00	1.46	1.39
76	8A	601	HEA	CHA-C4D	2.99	1.46	1.39
73	1A	402	HEM	CAB-C3B	2.99	1.55	1.47
76	4A	602	HEA	C4B-C3B	2.99	1.49	1.44
73	6A	401	HEM	CAB-C3B	2.98	1.55	1.47
76	3A	604	HEA	C4B-C3B	2.98	1.49	1.44
76	3A	604	HEA	C1D-ND	-2.98	1.35	1.40
73	1A	402	HEM	FE-ND	2.97	2.04	1.94
73	1B	402	HEM	CAC-C3C	2.97	1.55	1.47
76	4A	602	HEA	CHA-C4D	2.96	1.46	1.39
76	9A	603	HEA	C4B-C3B	2.96	1.49	1.44
73	6B	402	HEM	CAC-C3C	2.95	1.55	1.47
73	6A	401	HEM	FE-ND	2.95	2.04	1.94
73	6B	401	HEM	CAC-C3C	2.93	1.55	1.47
73	6A	401	HEM	CAC-C3C	2.93	1.55	1.47
76	9A	603	HEA	CHA-C4D	2.92	1.45	1.39
73	1B	401	HEM	CAC-C3C	2.92	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	6A	402	HEM	CAC-C3C	2.91	1.55	1.47
73	1A	402	HEM	CAC-C3C	2.91	1.55	1.47
76	9A	602	HEA	C4B-C3B	2.90	1.49	1.44
73	1A	401	HEM	CAC-C3C	2.90	1.55	1.47
73	1B	401	HEM	FE-ND	2.89	2.03	1.94
76	8A	604	HEA	C1D-ND	-2.88	1.35	1.40
73	6B	401	HEM	FE-ND	2.88	2.03	1.94
76	9A	602	HEA	C1D-ND	-2.87	1.35	1.40
76	3A	601	HEA	C1D-ND	-2.86	1.35	1.40
76	4A	604	HEA	C4B-C3B	2.85	1.49	1.44
76	4A	604	HEA	C1D-ND	-2.83	1.35	1.40
76	8A	601	HEA	C4B-NB	-2.81	1.35	1.40
76	3A	601	HEA	C4B-C3B	2.80	1.49	1.44
73	6B	402	HEM	FE-ND	2.80	2.03	1.94
76	8A	604	HEA	C4B-C3B	2.79	1.49	1.44
76	3A	604	HEA	C4B-NB	-2.78	1.35	1.40
73	1B	402	HEM	FE-ND	2.78	2.03	1.94
76	7A	601	HEA	C1D-ND	-2.77	1.35	1.40
76	2A	601	HEA	C1C-C2C	2.76	1.49	1.43
76	2A	602	HEA	C4B-NB	-2.74	1.35	1.40
76	4A	602	HEA	C4B-NB	-2.73	1.35	1.40
76	9A	603	HEA	C4B-NB	-2.73	1.35	1.40
76	2A	602	HEA	C1D-ND	-2.73	1.35	1.40
76	7A	601	HEA	C4B-NB	-2.73	1.35	1.40
85	s	401	COO	C5A-C6A	2.72	1.48	1.41
76	8A	604	HEA	C4B-NB	-2.72	1.35	1.40
73	6B	402	HEM	FE-NA	2.71	2.04	1.95
76	3A	604	HEA	C4C-NC	-2.71	1.34	1.39
76	9A	602	HEA	C4B-NB	-2.71	1.35	1.40
85	5s	401	COO	C5A-C6A	2.71	1.48	1.41
76	7A	602	HEA	C1C-C2C	2.71	1.49	1.43
76	4A	602	HEA	C4C-NC	-2.70	1.34	1.39
73	1B	402	HEM	FE-NA	2.69	2.04	1.95
76	3A	601	HEA	C4B-NB	-2.68	1.35	1.40
76	9A	603	HEA	C4C-NC	-2.68	1.34	1.39
76	8A	601	HEA	C4C-NC	-2.68	1.34	1.39
76	4A	604	HEA	C4B-NB	-2.68	1.35	1.40
85	s	401	COO	C8A-N7A	2.54	1.36	1.31
84	P	401	NDP	C5A-C4A	2.53	1.43	1.39
83	5k	200	8Q1	C6-C1	2.53	1.53	1.50
83	k	200	8Q1	C1-S44	2.53	1.82	1.76
84	5P	401	NDP	C5A-C4A	2.53	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	J	200	8Q1	C6-C1	2.52	1.53	1.50
83	5k	200	8Q1	C1-S44	2.52	1.82	1.76
83	5J	200	8Q1	C6-C1	2.51	1.53	1.50
83	k	200	8Q1	C6-C1	2.51	1.53	1.50
83	J	200	8Q1	C1-S44	2.50	1.82	1.76
83	5J	200	8Q1	C1-S44	2.50	1.82	1.76
76	7A	602	HEA	C4B-NB	-2.49	1.36	1.40
76	2A	601	HEA	C4C-NC	-2.48	1.34	1.39
73	6B	401	HEM	FE-NB	2.48	2.02	1.94
81	B	502	FMN	C10-N1	2.47	1.38	1.33
73	1B	401	HEM	FE-NB	2.47	2.02	1.94
81	5B	501	FMN	C10-N1	2.46	1.38	1.33
76	7A	602	HEA	C4C-NC	-2.46	1.35	1.39
85	5s	401	COO	C8A-N7A	2.45	1.36	1.31
73	1A	402	HEM	FE-NC	2.44	2.03	1.95
76	9A	602	HEA	C4C-NC	-2.43	1.35	1.39
76	2A	601	HEA	C4D-C3D	2.43	1.49	1.45
73	6A	401	HEM	FE-NC	2.42	2.03	1.95
76	2A	602	HEA	C3C-C4C	2.42	1.48	1.42
76	2A	601	HEA	C4B-NB	-2.41	1.36	1.40
76	8A	601	HEA	C1C-C2C	2.41	1.48	1.43
76	4A	602	HEA	C1C-C2C	2.41	1.48	1.43
76	3A	601	HEA	C4C-NC	-2.41	1.35	1.39
84	P	401	NDP	C2A-N1A	2.40	1.38	1.33
76	2A	602	HEA	C4B-C3B	2.40	1.48	1.44
84	5P	401	NDP	C2A-N1A	2.40	1.38	1.33
76	9A	603	HEA	C1C-C2C	2.40	1.48	1.43
76	3A	604	HEA	C1C-C2C	2.39	1.48	1.43
76	4A	604	HEA	C4C-NC	-2.38	1.35	1.39
76	7A	601	HEA	C3C-C4C	2.37	1.48	1.42
76	8A	604	HEA	C4C-NC	-2.37	1.35	1.39
76	7A	602	HEA	C4D-C3D	2.36	1.49	1.45
73	6A	401	HEM	FE-NB	2.31	2.02	1.94
76	2A	602	HEA	C1C-NC	-2.30	1.35	1.39
76	9A	603	HEA	C4D-C3D	2.28	1.49	1.45
76	7A	601	HEA	C4B-C3B	2.27	1.48	1.44
76	7A	601	HEA	C1C-NC	-2.27	1.35	1.39
73	1B	402	HEM	FE-NC	2.27	2.02	1.95
73	6B	402	HEM	FE-NC	2.26	2.02	1.95
76	8A	604	HEA	C3C-C4C	2.26	1.48	1.42
73	1A	402	HEM	FE-NB	2.26	2.01	1.94
76	3A	604	HEA	C4D-C3D	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	8A	601	HEA	C4D-C3D	2.24	1.48	1.45
73	1A	402	HEM	FE-NA	2.24	2.02	1.95
76	4A	604	HEA	C1C-C2C	2.23	1.48	1.43
73	6A	401	HEM	FE-NA	2.23	2.02	1.95
76	3A	601	HEA	C3C-C4C	2.22	1.48	1.42
76	4A	602	HEA	C4D-C3D	2.22	1.48	1.45
76	3A	601	HEA	C1C-C2C	2.19	1.48	1.43
76	9A	602	HEA	C1C-C2C	2.19	1.48	1.43
83	k	200	8Q1	O40-C39	-2.18	1.18	1.23
76	8A	604	HEA	C1C-C2C	2.18	1.48	1.43
85	s	401	COO	C5A-N7A	-2.18	1.34	1.39
76	8A	604	HEA	C1D-C2D	2.18	1.48	1.44
76	3A	601	HEA	C1D-C2D	2.17	1.48	1.44
76	9A	602	HEA	C1C-NC	-2.17	1.35	1.39
76	8A	601	HEA	C1C-NC	-2.17	1.35	1.39
76	2A	602	HEA	C1D-C2D	2.16	1.48	1.44
73	6A	402	HEM	FE-NB	2.16	2.01	1.94
76	4A	604	HEA	C1D-C2D	2.15	1.48	1.44
76	4A	604	HEA	C1C-NC	-2.15	1.35	1.39
83	5k	200	8Q1	O40-C39	-2.14	1.18	1.23
76	9A	603	HEA	C1C-NC	-2.14	1.35	1.39
76	2A	602	HEA	C4C-NC	-2.14	1.35	1.39
76	7A	601	HEA	C4C-NC	-2.14	1.35	1.39
76	4A	604	HEA	C3C-C4C	2.13	1.47	1.42
85	5s	401	COO	C5A-N7A	-2.13	1.35	1.39
76	9A	602	HEA	C3C-C4C	2.13	1.47	1.42
76	7A	601	HEA	C1D-C2D	2.12	1.48	1.44
73	1A	401	HEM	FE-NB	2.12	2.01	1.94
76	3A	604	HEA	C1C-NC	-2.12	1.35	1.39
83	5J	200	8Q1	O40-C39	-2.11	1.19	1.23
83	J	200	8Q1	O40-C39	-2.11	1.19	1.23
76	3A	601	HEA	C1C-NC	-2.11	1.35	1.39
73	6B	401	HEM	C3C-C2C	-2.10	1.33	1.37
76	9A	602	HEA	C1D-C2D	2.09	1.48	1.44
73	1B	402	HEM	C2A-C3A	-2.09	1.33	1.38
74	6F	501	HEC	FE-NA	2.09	2.02	1.95
74	1F	501	HEC	FE-NA	2.09	2.02	1.95
76	2A	602	HEA	C1A-C2A	2.09	1.48	1.45
76	8A	604	HEA	C1C-NC	-2.08	1.35	1.39
76	4A	604	HEA	C4D-ND	-2.08	1.34	1.38
76	7A	601	HEA	C1A-C2A	2.08	1.48	1.45
73	6B	402	HEM	C2A-C3A	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	2A	602	HEA	C1C-C2C	2.07	1.48	1.43
76	4A	602	HEA	C1C-NC	-2.07	1.35	1.39
76	7A	601	HEA	C1C-C2C	2.06	1.48	1.43
73	1A	402	HEM	C2A-C3A	-2.05	1.33	1.38
76	2A	602	HEA	C1B-C2B	2.05	1.48	1.44
76	3A	601	HEA	C4D-ND	-2.05	1.34	1.38
76	7A	601	HEA	C1B-C2B	2.04	1.48	1.44
76	2A	601	HEA	C1D-C2D	2.03	1.48	1.44
73	1B	401	HEM	C3C-C2C	-2.03	1.33	1.37
83	5k	200	8Q1	O35-C34	-2.03	1.19	1.23
76	7A	602	HEA	C1D-C2D	2.03	1.48	1.44
73	6A	401	HEM	C2A-C3A	-2.03	1.33	1.38
76	7A	602	HEA	C3C-C4C	2.03	1.47	1.42
73	1B	401	HEM	C2A-C3A	-2.02	1.33	1.38
73	1A	401	HEM	CMC-C2C	2.02	1.55	1.50
84	5P	401	NDP	O5D-C5D	-2.02	1.37	1.44
73	6A	402	HEM	C2A-C3A	-2.02	1.33	1.38
76	4A	604	HEA	C1B-NB	-2.01	1.34	1.38
73	6B	401	HEM	C2A-C3A	-2.01	1.33	1.38
83	J	200	8Q1	O35-C34	-2.00	1.19	1.23

All (584) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	s	401	COO	C15-C11-C12	-19.15	77.00	108.23
85	5s	401	COO	C15-C11-C12	-19.15	77.00	108.23
85	s	401	COO	C15-C11-C13	-16.74	79.80	108.82
85	5s	401	COO	C15-C11-C13	-16.71	79.86	108.82
85	s	401	COO	C15-C11-C14	-15.20	78.19	109.17
85	5s	401	COO	C15-C11-C14	-15.19	78.20	109.17
76	2A	601	HEA	C3C-C4C-NC	7.27	114.72	110.25
76	9A	602	HEA	C3C-C4C-NC	7.17	114.66	110.25
76	4A	604	HEA	C3C-C4C-NC	7.14	114.64	110.25
76	7A	602	HEA	C3C-C4C-NC	7.11	114.62	110.25
76	8A	604	HEA	C3C-C4C-NC	7.01	114.56	110.25
76	3A	604	HEA	C3C-C4C-NC	6.98	114.55	110.25
76	3A	601	HEA	C3C-C4C-NC	6.98	114.54	110.25
76	9A	603	HEA	C3C-C4C-NC	6.97	114.54	110.25
76	8A	601	HEA	C3C-C4C-NC	6.95	114.53	110.25
76	3A	604	HEA	C3D-C4D-ND	6.91	117.05	110.36
84	P	401	NDP	PN-O3-PA	-6.91	109.11	132.83
84	5P	401	NDP	PN-O3-PA	-6.89	109.18	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	8A	601	HEA	C3D-C4D-ND	6.86	117.00	110.36
76	4A	602	HEA	C3C-C4C-NC	6.85	114.46	110.25
76	9A	603	HEA	C3D-C4D-ND	6.83	116.97	110.36
76	2A	602	HEA	C3D-C4D-ND	6.79	116.93	110.36
76	4A	602	HEA	C3D-C4D-ND	6.79	116.93	110.36
76	7A	601	HEA	C3D-C4D-ND	6.74	116.88	110.36
76	2A	601	HEA	C3D-C4D-ND	6.72	116.86	110.36
76	7A	602	HEA	C3D-C4D-ND	6.71	116.86	110.36
76	7A	601	HEA	C3C-C4C-NC	6.39	114.18	110.25
76	2A	602	HEA	C3C-C4C-NC	6.33	114.14	110.25
74	6E	401	HEC	C1D-ND-C4D	6.29	111.57	105.07
74	1E	401	HEC	C1D-ND-C4D	6.21	111.49	105.07
76	9A	602	HEA	C3D-C4D-ND	6.15	116.32	110.36
76	8A	604	HEA	C3D-C4D-ND	6.13	116.29	110.36
76	3A	601	HEA	C3D-C4D-ND	6.13	116.29	110.36
76	4A	604	HEA	C3D-C4D-ND	6.12	116.29	110.36
85	s	401	COO	C5A-C4A-N3A	-6.05	118.86	126.75
85	5s	401	COO	C5A-C4A-N3A	-6.01	118.90	126.75
83	J	200	8Q1	C6-C1-S44	5.89	120.32	113.46
83	k	200	8Q1	C6-C1-S44	5.83	120.24	113.46
83	5J	200	8Q1	C6-C1-S44	5.81	120.22	113.46
83	5k	200	8Q1	C6-C1-S44	5.79	120.20	113.46
76	4A	602	HEA	C2B-C1B-NB	5.77	116.79	109.88
76	7A	602	HEA	C3C-C2C-C1C	-5.76	100.21	107.16
76	2A	601	HEA	C3C-C2C-C1C	-5.73	100.24	107.16
76	3A	604	HEA	C2B-C1B-NB	5.73	116.74	109.88
76	9A	603	HEA	C2B-C1B-NB	5.73	116.74	109.88
76	3A	604	HEA	C3C-C2C-C1C	-5.72	100.26	107.16
76	8A	601	HEA	C3C-C2C-C1C	-5.71	100.27	107.16
76	8A	604	HEA	C2D-C1D-ND	5.71	116.60	109.84
76	9A	602	HEA	C2D-C1D-ND	5.69	116.58	109.84
76	9A	603	HEA	C3C-C2C-C1C	-5.68	100.31	107.16
76	4A	602	HEA	C3C-C2C-C1C	-5.68	100.31	107.16
76	4A	604	HEA	C2D-C1D-ND	5.67	116.56	109.84
76	3A	601	HEA	C2D-C1D-ND	5.67	116.56	109.84
76	8A	601	HEA	C2B-C1B-NB	5.66	116.66	109.88
76	2A	601	HEA	C2B-C1B-NB	5.65	116.64	109.88
76	7A	602	HEA	C2D-C1D-ND	5.64	116.53	109.84
76	7A	602	HEA	C2B-C1B-NB	5.64	116.64	109.88
76	2A	601	HEA	C2D-C1D-ND	5.64	116.52	109.84
76	7A	601	HEA	C3B-C4B-NB	5.63	116.51	109.84
76	2A	602	HEA	C3B-C4B-NB	5.57	116.44	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	3A	601	HEA	C2B-C1B-NB	5.49	116.46	109.88
76	4A	604	HEA	C2B-C1B-NB	5.48	116.45	109.88
74	6F	501	HEC	C1D-ND-C4D	5.47	110.73	105.07
74	1F	501	HEC	C1D-ND-C4D	5.46	110.72	105.07
76	7A	601	HEA	C3C-C2C-C1C	-5.46	100.57	107.16
76	9A	602	HEA	C2B-C1B-NB	5.45	116.41	109.88
76	8A	604	HEA	C2B-C1B-NB	5.44	116.39	109.88
76	9A	603	HEA	C2D-C1D-ND	5.44	116.28	109.84
76	8A	601	HEA	C2D-C1D-ND	5.41	116.24	109.84
76	9A	602	HEA	C3C-C2C-C1C	-5.40	100.64	107.16
76	2A	602	HEA	C3C-C2C-C1C	-5.40	100.64	107.16
76	4A	604	HEA	C3C-C2C-C1C	-5.37	100.68	107.16
76	4A	602	HEA	C2D-C1D-ND	5.37	116.20	109.84
76	3A	604	HEA	C2D-C1D-ND	5.36	116.19	109.84
76	3A	601	HEA	C3C-C2C-C1C	-5.34	100.71	107.16
76	8A	604	HEA	C3C-C2C-C1C	-5.32	100.73	107.16
76	9A	603	HEA	C2A-C1A-NA	5.29	115.47	110.32
76	7A	601	HEA	C2D-C1D-ND	5.28	116.09	109.84
76	2A	602	HEA	C2D-C1D-ND	5.26	116.08	109.84
76	3A	604	HEA	C2A-C1A-NA	5.23	115.41	110.32
76	4A	602	HEA	C2A-C1A-NA	5.16	115.35	110.32
76	8A	601	HEA	C2A-C1A-NA	5.16	115.34	110.32
76	8A	604	HEA	C1D-C2D-C3D	-5.14	101.55	106.96
76	4A	604	HEA	C1D-C2D-C3D	-5.12	101.57	106.96
76	3A	601	HEA	C1D-C2D-C3D	-5.12	101.57	106.96
76	8A	604	HEA	C3B-C4B-NB	5.09	115.86	109.84
76	3A	601	HEA	C3B-C4B-NB	5.06	115.84	109.84
76	9A	602	HEA	C3B-C4B-NB	5.03	115.81	109.84
76	9A	602	HEA	C1D-C2D-C3D	-5.02	101.68	106.96
76	4A	604	HEA	C3B-C4B-NB	5.00	115.76	109.84
76	7A	601	HEA	C2B-C1B-NB	4.99	115.86	109.88
76	2A	602	HEA	C2B-C1B-NB	4.99	115.85	109.88
76	7A	602	HEA	C3B-C4B-NB	4.98	115.74	109.84
76	2A	601	HEA	C3B-C4B-NB	4.97	115.72	109.84
85	5s	401	COO	C14-C11-C12	4.95	116.30	108.23
85	s	401	COO	C14-C11-C12	4.93	116.28	108.23
76	3A	604	HEA	C3B-C4B-NB	4.88	115.62	109.84
76	8A	601	HEA	C3B-C4B-NB	4.84	115.58	109.84
76	9A	603	HEA	C3B-C4B-NB	4.82	115.55	109.84
76	4A	602	HEA	C3B-C4B-NB	4.79	115.51	109.84
76	7A	601	HEA	C2C-C1C-NC	4.77	117.34	110.08
76	2A	602	HEA	C2C-C1C-NC	4.73	117.28	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	4A	604	HEA	C2A-C1A-NA	4.69	114.89	110.32
76	8A	601	HEA	C4A-NA-C1A	-4.66	100.78	105.35
76	3A	604	HEA	C4A-NA-C1A	-4.66	100.78	105.35
85	s	401	COO	N3A-C4A-N9A	4.64	134.73	127.08
76	8A	604	HEA	C2A-C1A-NA	4.64	114.84	110.32
76	9A	603	HEA	C4A-NA-C1A	-4.62	100.82	105.35
76	3A	601	HEA	C2A-C1A-NA	4.61	114.81	110.32
76	9A	602	HEA	C2A-C1A-NA	4.59	114.79	110.32
85	5s	401	COO	N3A-C4A-N9A	4.58	134.62	127.08
76	4A	604	HEA	C4A-NA-C1A	-4.57	100.88	105.35
76	7A	602	HEA	C2A-C1A-NA	4.56	114.76	110.32
76	8A	604	HEA	C4A-NA-C1A	-4.56	100.88	105.35
76	4A	602	HEA	C4A-NA-C1A	-4.55	100.89	105.35
76	3A	601	HEA	C4A-NA-C1A	-4.53	100.92	105.35
76	9A	602	HEA	C4A-NA-C1A	-4.52	100.92	105.35
76	2A	601	HEA	C2A-C1A-NA	4.51	114.71	110.32
76	9A	602	HEA	C2C-C1C-NC	4.48	116.91	110.08
76	8A	604	HEA	C2C-C1C-NC	4.47	116.88	110.08
76	4A	604	HEA	C2C-C1C-NC	4.46	116.87	110.08
76	2A	602	HEA	C13-C12-C11	-4.45	107.66	114.35
76	7A	602	HEA	C4A-NA-C1A	-4.45	100.99	105.35
73	1A	401	HEM	C3B-C2B-C1B	4.45	109.78	106.49
73	6A	402	HEM	C3B-C2B-C1B	4.45	109.78	106.49
76	3A	601	HEA	C2C-C1C-NC	4.43	116.83	110.08
76	2A	602	HEA	C2A-C1A-NA	4.42	114.62	110.32
76	7A	601	HEA	C13-C12-C11	-4.40	107.73	114.35
76	7A	601	HEA	C2A-C1A-NA	4.40	114.61	110.32
76	2A	601	HEA	C4A-NA-C1A	-4.36	101.08	105.35
76	7A	602	HEA	C2C-C1C-NC	4.28	116.59	110.08
76	8A	601	HEA	C2C-C1C-NC	4.24	116.54	110.08
76	9A	603	HEA	C2C-C1C-NC	4.22	116.50	110.08
76	3A	604	HEA	C2C-C1C-NC	4.21	116.49	110.08
76	2A	601	HEA	C2C-C1C-NC	4.21	116.48	110.08
76	4A	602	HEA	C2C-C1C-NC	4.17	116.44	110.08
76	2A	602	HEA	C1D-C2D-C3D	-4.10	102.64	106.96
76	7A	601	HEA	C1D-C2D-C3D	-4.09	102.65	106.96
76	2A	602	HEA	C4A-NA-C1A	-4.09	101.34	105.35
85	s	401	COO	C14-C11-C13	4.07	115.88	108.82
85	5s	401	COO	C14-C11-C13	4.07	115.88	108.82
76	7A	601	HEA	C4A-NA-C1A	-4.06	101.37	105.35
73	1A	401	HEM	CMB-C2B-C1B	-4.05	118.87	125.04
73	6A	402	HEM	CMB-C2B-C1B	-4.02	118.92	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7A	602	HEA	C1D-C2D-C3D	-3.85	102.91	106.96
83	5k	200	8Q1	C32-C34-N36	3.83	124.21	116.58
83	k	200	8Q1	C32-C34-N36	3.83	124.20	116.58
76	2A	601	HEA	C1D-C2D-C3D	-3.80	102.96	106.96
85	s	401	COO	C2A-N3A-C4A	3.80	120.72	111.75
85	5s	401	COO	C2A-N3A-C4A	3.76	120.64	111.75
76	3A	604	HEA	CHA-C4D-ND	-3.71	120.39	124.42
76	9A	603	HEA	C27-C19-C20	3.71	121.51	115.27
76	8A	601	HEA	CHA-C4D-ND	-3.71	120.39	124.42
76	3A	604	HEA	C4D-C3D-C2D	-3.69	101.51	106.90
76	8A	601	HEA	C4D-C3D-C2D	-3.69	101.52	106.90
76	9A	603	HEA	C1D-C2D-C3D	-3.69	103.08	106.96
76	9A	603	HEA	C3A-C2A-C1A	-3.68	103.56	107.08
76	9A	603	HEA	C4D-C3D-C2D	-3.68	101.54	106.90
76	4A	602	HEA	CHA-C4D-ND	-3.67	120.43	124.42
76	3A	604	HEA	C27-C19-C20	3.66	121.43	115.27
76	9A	603	HEA	CHA-C4D-ND	-3.66	120.44	124.42
76	2A	601	HEA	C4D-C3D-C2D	-3.65	101.57	106.90
76	3A	604	HEA	C3A-C2A-C1A	-3.65	103.59	107.08
76	4A	602	HEA	C1D-C2D-C3D	-3.65	103.12	106.96
76	8A	601	HEA	C27-C19-C20	3.65	121.40	115.27
76	8A	601	HEA	C1D-C2D-C3D	-3.65	103.12	106.96
76	4A	602	HEA	C4D-C3D-C2D	-3.64	101.59	106.90
76	4A	602	HEA	C27-C19-C20	3.64	121.40	115.27
76	3A	604	HEA	C1D-C2D-C3D	-3.64	103.13	106.96
76	8A	601	HEA	C3A-C2A-C1A	-3.62	103.62	107.08
76	7A	602	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
76	4A	602	HEA	C3A-C2A-C1A	-3.61	103.63	107.08
76	4A	602	HEA	C1B-C2B-C3B	-3.59	102.50	106.80
76	7A	601	HEA	C3A-C2A-C1A	-3.59	103.65	107.08
83	J	200	8Q1	O4-C1-C6	-3.59	119.75	123.99
76	2A	602	HEA	C3A-C2A-C1A	-3.58	103.66	107.08
76	3A	604	HEA	C1B-C2B-C3B	-3.55	102.55	106.80
76	4A	604	HEA	CAD-CBD-CGD	-3.55	105.97	113.60
76	3A	601	HEA	CAD-CBD-CGD	-3.54	105.99	113.60
76	9A	602	HEA	CAD-CBD-CGD	-3.54	105.99	113.60
76	9A	602	HEA	C3A-C2A-C1A	-3.53	103.70	107.08
76	8A	604	HEA	CAD-CBD-CGD	-3.53	106.00	113.60
76	8A	601	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
76	9A	603	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
76	4A	604	HEA	C3A-C2A-C1A	-3.52	103.72	107.08
85	5s	401	COO	C4A-C5A-N7A	-3.51	106.34	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	5J	200	8Q1	O4-C1-C6	-3.51	119.85	123.99
85	s	401	COO	C4A-C5A-N7A	-3.48	106.38	110.62
74	6F	501	HEC	CAA-CBA-CGA	-3.48	106.11	113.60
83	k	200	8Q1	O4-C1-C6	-3.48	119.88	123.99
74	1F	501	HEC	CAA-CBA-CGA	-3.47	106.13	113.60
76	7A	602	HEA	CHA-C4D-ND	-3.47	120.65	124.42
76	8A	604	HEA	C3A-C2A-C1A	-3.45	103.78	107.08
76	2A	601	HEA	CHA-C4D-ND	-3.45	120.67	124.42
76	3A	604	HEA	CAD-C3D-C4D	3.45	130.68	124.66
83	5k	200	8Q1	O4-C1-C6	-3.44	119.92	123.99
76	3A	601	HEA	C3A-C2A-C1A	-3.44	103.79	107.08
76	8A	601	HEA	CAD-C3D-C4D	3.43	130.66	124.66
76	4A	602	HEA	CAD-C3D-C4D	3.40	130.60	124.66
76	9A	603	HEA	CAD-C3D-C4D	3.39	130.58	124.66
76	7A	601	HEA	C4D-C3D-C2D	-3.35	102.02	106.90
76	2A	601	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
76	2A	602	HEA	C4D-C3D-C2D	-3.33	102.05	106.90
76	7A	602	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
84	5P	401	NDP	O2B-P2B-O1X	-3.32	96.57	109.39
76	4A	604	HEA	C1B-C2B-C3B	-3.32	102.83	106.80
84	P	401	NDP	O2B-P2B-O1X	-3.32	96.59	109.39
76	3A	601	HEA	C1B-C2B-C3B	-3.31	102.84	106.80
76	8A	604	HEA	C1B-C2B-C3B	-3.29	102.86	106.80
76	9A	602	HEA	C1B-C2B-C3B	-3.28	102.88	106.80
76	7A	601	HEA	CMB-C2B-C1B	3.27	130.02	125.04
76	2A	602	HEA	CMB-C2B-C1B	3.25	129.98	125.04
76	8A	604	HEA	C13-C12-C11	-3.24	109.47	114.35
76	3A	601	HEA	C13-C12-C11	-3.24	109.49	114.35
76	9A	602	HEA	C13-C12-C11	-3.21	109.53	114.35
73	1A	401	HEM	CHB-C1B-NB	3.20	128.32	124.37
73	6A	402	HEM	CHB-C1B-NB	3.19	128.31	124.37
76	7A	602	HEA	C3A-C2A-C1A	-3.18	104.04	107.08
76	2A	601	HEA	C3A-C2A-C1A	-3.18	104.04	107.08
76	4A	604	HEA	C13-C12-C11	-3.17	109.59	114.35
73	6B	401	HEM	C4C-NC-C1C	3.16	108.44	105.35
73	1B	401	HEM	C3B-C2B-C1B	3.14	108.82	106.49
73	6B	401	HEM	C3B-C2B-C1B	3.14	108.81	106.49
76	7A	602	HEA	C4B-C3B-C2B	-3.14	102.05	107.41
85	5s	401	COO	P1A-O3A-P2A	-3.14	122.06	132.83
73	1B	401	HEM	C4C-NC-C1C	3.13	108.41	105.35
85	s	401	COO	P1A-O3A-P2A	-3.13	122.09	132.83
76	2A	601	HEA	C4B-C3B-C2B	-3.12	102.09	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	2A	602	HEA	C4B-C3B-C2B	-3.11	102.10	107.41
76	7A	601	HEA	C1B-C2B-C3B	-3.10	103.09	106.80
76	7A	601	HEA	C4B-C3B-C2B	-3.08	102.14	107.41
85	s	401	COO	N1A-C2A-N3A	-3.08	123.78	128.60
85	5s	401	COO	N1A-C2A-N3A	-3.08	123.79	128.60
76	3A	601	HEA	C4B-C3B-C2B	-3.06	102.19	107.41
76	2A	602	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
76	8A	604	HEA	C4B-C3B-C2B	-3.06	102.19	107.41
76	9A	602	HEA	C4B-C3B-C2B	-3.05	102.20	107.41
76	4A	604	HEA	C4B-C3B-C2B	-3.04	102.22	107.41
81	5B	501	FMN	C4-N3-C2	-2.99	120.12	125.64
76	2A	602	HEA	CAD-CBD-CGD	-2.98	107.19	113.60
84	5P	401	NDP	PA-O5B-C5B	-2.98	104.20	121.68
84	P	401	NDP	PA-O5B-C5B	-2.97	104.26	121.68
76	7A	602	HEA	C27-C19-C20	2.97	120.27	115.27
76	3A	604	HEA	C4B-C3B-C2B	-2.97	102.34	107.41
76	8A	601	HEA	C4B-C3B-C2B	-2.96	102.35	107.41
73	1A	402	HEM	C4D-ND-C1D	2.96	108.13	105.07
76	2A	601	HEA	CAD-C3D-C4D	2.96	129.83	124.66
76	7A	602	HEA	CAD-C3D-C4D	2.96	129.83	124.66
76	2A	601	HEA	C27-C19-C20	2.95	120.24	115.27
73	6A	401	HEM	C4D-ND-C1D	2.95	108.12	105.07
73	1B	401	HEM	C4D-ND-C1D	2.95	108.12	105.07
73	6B	401	HEM	C4D-ND-C1D	2.95	108.12	105.07
76	7A	601	HEA	CAD-CBD-CGD	-2.94	107.27	113.60
81	B	502	FMN	C4-N3-C2	-2.94	120.21	125.64
85	s	401	COO	C5A-N7A-C8A	2.94	107.68	103.51
76	9A	603	HEA	C4B-C3B-C2B	-2.93	102.41	107.41
85	s	401	COO	C3X-C2X-C1X	2.92	106.36	99.89
84	P	401	NDP	PN-O5D-C5D	-2.92	104.58	121.68
84	5P	401	NDP	PN-O5D-C5D	-2.91	104.59	121.68
85	5s	401	COO	C3X-C2X-C1X	2.91	106.33	99.89
85	5s	401	COO	C5A-N7A-C8A	2.90	107.64	103.51
76	7A	602	HEA	C1D-ND-C4D	-2.90	102.08	105.07
76	2A	601	HEA	C1D-ND-C4D	-2.89	102.08	105.07
76	4A	602	HEA	C4B-C3B-C2B	-2.89	102.48	107.41
76	3A	604	HEA	C1D-ND-C4D	-2.87	102.11	105.07
76	8A	601	HEA	C1D-ND-C4D	-2.87	102.11	105.07
85	5s	401	COO	C10-C9-C8	-2.87	119.68	125.34
73	6A	402	HEM	C4D-ND-C1D	2.86	108.03	105.07
85	s	401	COO	C10-C9-C8	-2.86	119.70	125.34
76	9A	603	HEA	C1D-ND-C4D	-2.85	102.12	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	1A	401	HEM	C4D-ND-C1D	2.85	108.02	105.07
76	7A	602	HEA	CMC-C2C-C1C	2.85	129.71	125.37
76	2A	602	HEA	C13-C14-C15	-2.82	120.86	127.66
74	1F	501	HEC	C4A-NA-C1A	2.82	108.11	105.35
76	7A	601	HEA	CHC-C1C-C2C	-2.81	119.29	127.24
76	7A	602	HEA	CHB-C4A-NA	-2.81	121.40	124.44
76	2A	601	HEA	CMC-C2C-C1C	2.81	129.65	125.37
76	4A	602	HEA	C1D-ND-C4D	-2.81	102.17	105.07
76	7A	601	HEA	C13-C14-C15	-2.81	120.90	127.66
76	2A	602	HEA	CHC-C1C-C2C	-2.80	119.33	127.24
76	7A	602	HEA	CAD-CBD-CGD	-2.80	107.59	113.60
74	6F	501	HEC	C4A-NA-C1A	2.79	108.08	105.35
76	2A	601	HEA	CAD-CBD-CGD	-2.79	107.60	113.60
85	s	401	COO	C4A-N9A-C8A	2.77	108.73	105.73
74	1E	401	HEC	CAA-CBA-CGA	-2.77	107.64	113.60
76	3A	604	HEA	CHB-C1B-C2B	-2.77	120.66	124.98
73	1B	402	HEM	C4D-ND-C1D	2.75	107.92	105.07
76	4A	602	HEA	CHB-C1B-C2B	-2.75	120.68	124.98
76	2A	601	HEA	CHB-C4A-NA	-2.75	121.47	124.44
74	6F	501	HEC	CBB-CAB-C3B	2.75	120.00	112.43
74	6E	401	HEC	CAA-CBA-CGA	-2.74	107.71	113.60
76	8A	604	HEA	CMD-C2D-C1D	2.74	129.21	125.04
73	1A	402	HEM	CMC-C2C-C1C	-2.74	119.89	124.71
76	8A	604	HEA	C27-C19-C20	2.74	119.87	115.27
74	1F	501	HEC	CBB-CAB-C3B	2.73	119.97	112.43
73	6A	401	HEM	CMC-C2C-C1C	-2.72	119.92	124.71
76	8A	601	HEA	CHB-C1B-C2B	-2.71	120.74	124.98
73	6B	402	HEM	C4D-ND-C1D	2.71	107.87	105.07
76	3A	601	HEA	CMD-C2D-C1D	2.71	129.16	125.04
76	3A	601	HEA	C27-C19-C20	2.71	119.82	115.27
76	9A	602	HEA	C27-C19-C20	2.70	119.82	115.27
76	8A	601	HEA	CAD-CBD-CGD	-2.70	107.80	113.60
76	9A	603	HEA	CHB-C1B-C2B	-2.70	120.77	124.98
76	4A	604	HEA	CMD-C2D-C1D	2.69	129.14	125.04
76	4A	604	HEA	CHA-C4D-C3D	-2.69	120.88	124.84
73	1B	401	HEM	CAC-C3C-C4C	2.69	131.38	124.90
76	2A	602	HEA	C1D-ND-C4D	-2.68	102.30	105.07
76	4A	604	HEA	C27-C19-C20	2.68	119.78	115.27
76	8A	601	HEA	C13-C14-C15	-2.68	121.20	127.66
76	3A	601	HEA	CHA-C4D-C3D	-2.68	120.90	124.84
73	6B	402	HEM	C4A-NA-C1A	2.68	107.97	105.35
85	5s	401	COO	C4A-N9A-C8A	2.67	108.63	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	9A	602	HEA	CMD-C2D-C1D	2.67	129.11	125.04
76	7A	602	HEA	C13-C14-C15	-2.67	121.24	127.66
76	3A	604	HEA	CAD-CBD-CGD	-2.67	107.87	113.60
76	7A	602	HEA	C26-C15-C16	2.66	119.75	115.27
76	3A	604	HEA	C13-C14-C15	-2.66	121.25	127.66
76	4A	602	HEA	CAD-CBD-CGD	-2.66	107.88	113.60
76	9A	603	HEA	C13-C14-C15	-2.66	121.26	127.66
76	9A	603	HEA	CAD-CBD-CGD	-2.65	107.89	113.60
76	4A	602	HEA	C13-C14-C15	-2.65	121.27	127.66
73	1B	402	HEM	C4A-NA-C1A	2.65	107.94	105.35
76	9A	602	HEA	CHA-C4D-C3D	-2.65	120.95	124.84
76	2A	601	HEA	C26-C15-C16	2.64	119.72	115.27
76	9A	602	HEA	C1D-ND-C4D	-2.64	102.34	105.07
76	8A	604	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
76	2A	601	HEA	C13-C14-C15	-2.64	121.31	127.66
76	7A	601	HEA	C1D-ND-C4D	-2.64	102.35	105.07
76	9A	602	HEA	C4D-C3D-C2D	-2.63	103.06	106.90
76	2A	602	HEA	C27-C19-C20	2.63	119.69	115.27
73	6B	401	HEM	CAC-C3C-C4C	2.63	131.24	124.90
83	k	200	8Q1	C43-S44-C1	2.62	110.04	101.87
76	7A	601	HEA	C27-C19-C20	2.61	119.66	115.27
76	8A	604	HEA	C1D-ND-C4D	-2.61	102.38	105.07
81	5B	501	FMN	C4A-C4-N3	2.61	119.81	113.19
73	1A	402	HEM	C4A-NA-C1A	2.60	107.89	105.35
83	5k	200	8Q1	C43-S44-C1	2.60	109.96	101.87
74	1F	501	HEC	C2A-C1A-NA	-2.59	107.80	110.32
76	7A	601	HEA	C4B-NB-C1B	-2.59	102.40	105.07
81	B	502	FMN	C4A-C4-N3	2.58	119.75	113.19
76	4A	604	HEA	C1D-ND-C4D	-2.58	102.41	105.07
76	3A	601	HEA	C1D-ND-C4D	-2.58	102.41	105.07
74	6F	501	HEC	C2A-C1A-NA	-2.57	107.82	110.32
76	9A	602	HEA	CHC-C1C-C2C	-2.57	119.97	127.24
76	9A	603	HEA	CMD-C2D-C1D	2.57	128.95	125.04
76	3A	601	HEA	C4D-C3D-C2D	-2.56	103.16	106.90
76	4A	604	HEA	C4D-C3D-C2D	-2.56	103.16	106.90
76	8A	601	HEA	CMD-C2D-C1D	2.56	128.94	125.04
76	8A	604	HEA	C4D-C3D-C2D	-2.56	103.17	106.90
74	6E	401	HEC	CAB-C3B-C4B	-2.55	121.50	124.81
84	P	401	NDP	O3X-P2B-O2X	2.55	117.37	107.64
76	4A	604	HEA	CHC-C1C-C2C	-2.55	120.05	127.24
84	5P	401	NDP	O3X-P2B-O2X	2.54	117.36	107.64
73	6A	401	HEM	C4A-NA-C1A	2.54	107.84	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	J	200	8Q1	C43-S44-C1	2.54	109.78	101.87
76	2A	602	HEA	C4B-NB-C1B	-2.53	102.45	105.07
76	4A	602	HEA	CMD-C2D-C1D	2.53	128.89	125.04
76	3A	601	HEA	CHC-C1C-C2C	-2.53	120.09	127.24
76	3A	604	HEA	CMD-C2D-C1D	2.53	128.89	125.04
83	5J	200	8Q1	C43-S44-C1	2.53	109.73	101.87
76	8A	601	HEA	CHB-C4A-NA	-2.52	121.71	124.44
74	1E	401	HEC	CAB-C3B-C4B	-2.52	121.54	124.81
76	8A	604	HEA	CHC-C1C-C2C	-2.52	120.12	127.24
76	2A	601	HEA	CHB-C1B-C2B	-2.50	121.08	124.98
76	7A	602	HEA	CHB-C1B-C2B	-2.49	121.08	124.98
76	3A	601	HEA	C26-C15-C16	2.48	119.44	115.27
76	9A	603	HEA	CHB-C4A-NA	-2.48	121.76	124.44
81	B	502	FMN	C4A-C10-N10	2.47	120.09	116.48
81	5B	501	FMN	C4A-C10-N10	2.46	120.08	116.48
76	9A	602	HEA	C26-C15-C16	2.46	119.42	115.27
74	1F	501	HEC	CAC-C3C-C4C	-2.46	121.50	124.92
76	9A	603	HEA	CBA-CAA-C2A	-2.46	105.80	112.63
74	6F	501	HEC	CAC-C3C-C4C	-2.46	121.50	124.92
76	8A	604	HEA	C13-C14-C15	-2.46	121.75	127.66
76	4A	604	HEA	C13-C14-C15	-2.46	121.75	127.66
76	4A	602	HEA	CHB-C4A-NA	-2.45	121.78	124.44
84	P	401	NDP	N3A-C4A-N9A	2.45	131.13	127.08
76	3A	604	HEA	CHB-C4A-NA	-2.45	121.79	124.44
76	8A	601	HEA	CBA-CAA-C2A	-2.45	105.82	112.63
81	5B	501	FMN	O4-C4-C4A	-2.45	120.10	126.60
76	3A	604	HEA	CBA-CAA-C2A	-2.45	105.82	112.63
76	4A	602	HEA	CBA-CAA-C2A	-2.45	105.83	112.63
76	2A	602	HEA	CHA-C4D-C3D	-2.45	121.24	124.84
76	8A	604	HEA	C26-C15-C16	2.44	119.38	115.27
73	6A	402	HEM	CHD-C1D-ND	2.44	127.07	124.42
76	9A	602	HEA	C13-C14-C15	-2.44	121.79	127.66
76	7A	601	HEA	CHA-C4D-C3D	-2.44	121.26	124.84
73	1A	401	HEM	CHD-C1D-ND	2.43	127.06	124.42
81	B	502	FMN	O4-C4-C4A	-2.43	120.15	126.60
84	5P	401	NDP	N3A-C4A-N9A	2.43	131.09	127.08
76	4A	604	HEA	C26-C15-C16	2.43	119.36	115.27
76	3A	601	HEA	C13-C14-C15	-2.42	121.82	127.66
83	5k	200	8Q1	O35-C34-N36	-2.42	117.80	122.99
74	1E	401	HEC	C4A-NA-C1A	2.42	107.72	105.35
74	6E	401	HEC	C4A-NA-C1A	2.41	107.71	105.35
76	2A	602	HEA	CHB-C1B-NB	-2.41	121.80	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	k	200	8Q1	O35-C34-N36	-2.40	117.83	122.99
84	5P	401	NDP	C2A-N1A-C6A	-2.40	114.65	118.77
73	6A	401	HEM	C2A-C1A-NA	-2.39	107.47	110.15
73	1A	402	HEM	C2A-C1A-NA	-2.39	107.47	110.15
76	2A	602	HEA	CHA-C4D-ND	-2.38	121.83	124.42
73	6B	402	HEM	C1B-NB-C4B	2.38	107.53	105.07
73	1B	402	HEM	C3D-C4D-ND	-2.38	107.52	110.17
84	P	401	NDP	C2A-N1A-C6A	-2.38	114.69	118.77
73	6A	402	HEM	C1B-NB-C4B	2.37	107.53	105.07
76	7A	601	HEA	CHB-C1B-NB	-2.37	121.84	124.42
76	3A	601	HEA	CMB-C2B-C1B	2.37	128.65	125.04
73	1B	401	HEM	CAC-C3C-C2C	-2.37	120.81	128.60
76	4A	604	HEA	CMB-C2B-C1B	2.37	128.64	125.04
85	s	401	COO	C6A-C5A-N7A	2.36	136.42	132.02
73	1A	401	HEM	C1B-NB-C4B	2.36	107.51	105.07
73	1B	402	HEM	C1B-NB-C4B	2.36	107.51	105.07
85	5s	401	COO	C6A-C5A-N7A	2.36	136.41	132.02
76	8A	604	HEA	CMB-C2B-C1B	2.36	128.63	125.04
73	6B	401	HEM	CHD-C4C-C3C	2.35	129.28	125.26
74	6F	501	HEC	CAC-C3C-C2C	2.35	130.63	126.86
73	6B	402	HEM	C3D-C4D-ND	-2.35	107.55	110.17
76	7A	601	HEA	CHA-C4D-ND	-2.35	121.86	124.42
76	7A	602	HEA	C25-C23-C24	2.34	119.77	114.60
76	9A	602	HEA	CMB-C2B-C1B	2.33	128.59	125.04
74	1F	501	HEC	CAC-C3C-C2C	2.33	130.59	126.86
73	6A	401	HEM	C3D-C4D-ND	-2.33	107.57	110.17
76	2A	601	HEA	C25-C23-C24	2.33	119.74	114.60
76	4A	604	HEA	CHB-C1B-C2B	-2.33	121.34	124.98
73	6B	401	HEM	CAC-C3C-C2C	-2.33	120.94	128.60
76	7A	601	HEA	C4C-NC-C1C	-2.33	103.07	105.35
73	6A	402	HEM	C4C-NC-C1C	2.32	107.62	105.35
76	3A	601	HEA	C4B-NB-C1B	-2.32	102.67	105.07
73	1A	402	HEM	C3D-C4D-ND	-2.32	107.58	110.17
73	1A	401	HEM	C4C-NC-C1C	2.32	107.62	105.35
76	8A	604	HEA	CHB-C1B-C2B	-2.32	121.36	124.98
73	1B	401	HEM	CHD-C4C-C3C	2.32	129.22	125.26
84	P	401	NDP	C5A-C4A-N3A	-2.31	123.73	126.75
84	5P	401	NDP	O5D-PN-O1N	-2.31	100.03	109.07
76	8A	604	HEA	C4B-NB-C1B	-2.31	102.68	105.07
84	P	401	NDP	O5D-PN-O1N	-2.31	100.04	109.07
74	1E	401	HEC	C2A-C1A-NA	-2.30	108.08	110.32
76	4A	602	HEA	CMC-C2C-C3C	2.30	132.17	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	3A	601	HEA	CHB-C1B-C2B	-2.30	121.39	124.98
76	9A	603	HEA	CMC-C2C-C3C	2.29	132.14	126.59
76	9A	603	HEA	C4B-NB-C1B	-2.29	102.71	105.07
76	9A	602	HEA	C4B-NB-C1B	-2.29	102.71	105.07
76	8A	601	HEA	CMC-C2C-C3C	2.29	132.13	126.59
74	6F	501	HEC	C4B-NB-C1B	2.29	107.44	105.07
76	4A	602	HEA	C4B-NB-C1B	-2.28	102.71	105.07
85	s	401	COO	N9A-C8A-N7A	-2.28	110.79	113.91
76	3A	604	HEA	CMC-C2C-C3C	2.28	132.11	126.59
74	1F	501	HEC	C4B-NB-C1B	2.28	107.42	105.07
76	2A	601	HEA	C4B-NB-C1B	-2.27	102.72	105.07
76	8A	601	HEA	CHC-C1C-C2C	-2.27	120.82	127.24
73	1A	402	HEM	CMB-C2B-C1B	-2.27	121.58	125.04
76	2A	602	HEA	C4C-NC-C1C	-2.27	103.12	105.35
73	6A	401	HEM	CMB-C2B-C1B	-2.27	121.58	125.04
73	1A	402	HEM	C4C-NC-C1C	2.27	107.57	105.35
76	4A	604	HEA	C4B-NB-C1B	-2.27	102.73	105.07
76	4A	604	HEA	C4C-NC-C1C	-2.26	103.13	105.35
74	1E	401	HEC	CAD-CBD-CGD	-2.26	108.73	113.60
76	9A	603	HEA	C25-C23-C24	2.26	119.61	114.60
73	6A	401	HEM	C4C-NC-C1C	2.26	107.56	105.35
81	B	502	FMN	C10-C4A-N5	-2.26	120.06	124.86
84	5P	401	NDP	C5A-C4A-N3A	-2.26	123.80	126.75
76	7A	602	HEA	CHD-C1D-C2D	-2.26	120.45	126.73
76	3A	604	HEA	C4B-NB-C1B	-2.26	102.74	105.07
83	k	200	8Q1	C38-C39-N41	2.26	120.22	116.42
83	5k	200	8Q1	C38-C39-N41	2.26	120.22	116.42
84	5P	401	NDP	O2N-PN-O1N	2.26	123.39	112.24
76	4A	602	HEA	C25-C23-C24	2.26	119.58	114.60
76	9A	602	HEA	CHB-C1B-C2B	-2.26	121.46	124.98
76	3A	604	HEA	CHC-C1C-C2C	-2.25	120.87	127.24
74	6E	401	HEC	C2A-C1A-NA	-2.25	108.13	110.32
76	9A	603	HEA	CHC-C1C-C2C	-2.25	120.88	127.24
76	7A	602	HEA	C4B-NB-C1B	-2.25	102.75	105.07
84	P	401	NDP	O2N-PN-O1N	2.25	123.36	112.24
74	6E	401	HEC	CAD-CBD-CGD	-2.25	108.77	113.60
73	6B	402	HEM	C2A-C1A-NA	-2.25	107.64	110.15
76	2A	601	HEA	CHD-C1D-C2D	-2.24	120.50	126.73
76	8A	604	HEA	CBA-CAA-C2A	-2.24	106.40	112.63
73	6B	402	HEM	CMC-C2C-C1C	-2.24	120.76	124.71
84	5P	401	NDP	O4B-C4B-C3B	2.24	109.55	105.11
84	P	401	NDP	O4B-C4B-C3B	2.24	109.55	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	8A	601	HEA	C25-C23-C24	2.24	119.55	114.60
73	6B	401	HEM	C4A-NA-C1A	2.24	107.54	105.35
76	4A	602	HEA	CHC-C1C-C2C	-2.23	120.93	127.24
81	5B	501	FMN	C10-C4A-N5	-2.23	120.12	124.86
76	3A	601	HEA	CBA-CAA-C2A	-2.23	106.43	112.63
76	9A	602	HEA	C4C-NC-C1C	-2.23	103.16	105.35
74	6E	401	HEC	CHA-C4D-ND	2.23	126.84	124.42
76	4A	604	HEA	CMC-C2C-C3C	2.23	131.98	126.59
76	3A	604	HEA	C25-C23-C24	2.23	119.52	114.60
73	1B	401	HEM	C4A-NA-C1A	2.22	107.52	105.35
73	1B	402	HEM	CMC-C2C-C1C	-2.22	120.80	124.71
76	7A	601	HEA	CMC-C2C-C3C	2.22	131.96	126.59
73	1B	401	HEM	CBD-CAD-C3D	-2.21	106.47	112.63
76	7A	602	HEA	C4C-NC-C1C	-2.21	103.18	105.35
76	4A	604	HEA	CBA-CAA-C2A	-2.21	106.48	112.63
76	7A	602	HEA	CHA-C1A-NA	-2.21	122.05	124.44
73	1B	402	HEM	C2A-C1A-NA	-2.21	107.68	110.15
76	8A	604	HEA	CMC-C2C-C3C	2.20	131.92	126.59
76	9A	602	HEA	CBA-CAA-C2A	-2.20	106.52	112.63
76	2A	602	HEA	CMC-C2C-C3C	2.20	131.91	126.59
76	9A	602	HEA	CMC-C2C-C3C	2.19	131.90	126.59
85	5s	401	COO	N9A-C8A-N7A	-2.19	110.92	113.91
76	3A	601	HEA	CMC-C2C-C3C	2.19	131.89	126.59
73	6B	401	HEM	CBD-CAD-C3D	-2.19	106.55	112.63
74	1E	401	HEC	CHA-C4D-ND	2.18	126.79	124.42
76	8A	601	HEA	C4B-NB-C1B	-2.18	102.82	105.07
76	2A	601	HEA	C4C-NC-C1C	-2.18	103.21	105.35
76	8A	604	HEA	C4C-NC-C1C	-2.18	103.21	105.35
74	1F	501	HEC	C4C-NC-C1C	2.18	107.48	105.35
84	5P	401	NDP	C5B-C4B-C3B	-2.17	107.04	115.18
84	P	401	NDP	C5B-C4B-C3B	-2.16	107.07	115.18
73	1B	401	HEM	C3D-C4D-ND	-2.16	107.76	110.17
73	6B	402	HEM	CBD-CAD-C3D	-2.16	106.62	112.63
76	7A	601	HEA	CHD-C1D-C2D	-2.16	120.73	126.73
74	6F	501	HEC	C4C-NC-C1C	2.16	107.46	105.35
76	2A	602	HEA	CHD-C1D-C2D	-2.16	120.74	126.73
76	8A	604	HEA	CHD-C1D-C2D	-2.15	120.76	126.73
74	1F	501	HEC	CHA-C1A-NA	2.15	126.76	124.44
73	1B	402	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
76	2A	601	HEA	CHC-C1C-C2C	-2.14	121.19	127.24
76	3A	601	HEA	CHD-C1D-C2D	-2.14	120.80	126.73
76	7A	602	HEA	CHC-C1C-C2C	-2.13	121.21	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	5J	200	8Q1	C38-C39-N41	2.13	120.01	116.42
74	1F	501	HEC	CAD-CBD-CGD	-2.12	109.04	113.60
76	3A	604	HEA	C26-C15-C16	2.12	118.84	115.27
81	5B	501	FMN	C9A-C5A-N5	-2.12	120.13	122.43
73	6B	401	HEM	C3D-C4D-ND	-2.12	107.81	110.17
83	J	200	8Q1	C38-C39-N41	2.12	119.98	116.42
74	6F	501	HEC	CHA-C1A-NA	2.11	126.73	124.44
76	4A	604	HEA	CHD-C1D-C2D	-2.11	120.86	126.73
76	9A	603	HEA	C26-C15-C16	2.11	118.83	115.27
76	4A	602	HEA	C26-C15-C16	2.11	118.82	115.27
76	9A	602	HEA	C25-C23-C24	2.11	119.26	114.60
76	8A	601	HEA	C26-C15-C16	2.11	118.82	115.27
76	2A	601	HEA	CHA-C1A-NA	-2.11	122.16	124.44
74	6F	501	HEC	CAD-CBD-CGD	-2.11	109.07	113.60
76	8A	604	HEA	C25-C23-C24	2.11	119.25	114.60
76	9A	602	HEA	CHB-C1B-NB	-2.11	122.13	124.42
83	k	200	8Q1	O4-C1-S44	-2.11	119.88	122.61
81	B	502	FMN	C9A-C5A-N5	-2.11	120.14	122.43
76	7A	601	HEA	C26-C15-C16	2.10	118.81	115.27
83	5k	200	8Q1	O4-C1-S44	-2.10	119.88	122.61
76	7A	602	HEA	CBA-CAA-C2A	-2.10	106.79	112.63
76	3A	601	HEA	C4C-NC-C1C	-2.10	103.29	105.35
76	4A	604	HEA	C25-C23-C24	2.10	119.24	114.60
76	9A	602	HEA	CHB-C4A-NA	-2.10	122.17	124.44
76	2A	601	HEA	CBA-CAA-C2A	-2.10	106.80	112.63
76	9A	602	HEA	CHD-C1D-C2D	-2.09	120.91	126.73
76	3A	601	HEA	CHB-C1B-NB	-2.09	122.15	124.42
76	8A	601	HEA	CHD-C1D-C2D	-2.08	120.95	126.73
76	9A	603	HEA	CHD-C1D-C2D	-2.08	120.95	126.73
76	3A	601	HEA	C25-C23-C24	2.08	119.19	114.60
76	3A	601	HEA	CHB-C4A-NA	-2.07	122.20	124.44
83	5J	200	8Q1	O4-C1-S44	-2.07	119.93	122.61
76	2A	602	HEA	C26-C15-C16	2.07	118.75	115.27
83	J	200	8Q1	O4-C1-S44	-2.07	119.93	122.61
76	4A	602	HEA	CHD-C1D-C2D	-2.07	120.99	126.73
76	7A	602	HEA	CAA-CBA-CGA	-2.06	109.16	113.60
76	4A	604	HEA	CHB-C4A-NA	-2.06	122.21	124.44
76	3A	604	HEA	CHD-C1D-C2D	-2.06	121.02	126.73
76	8A	604	HEA	CHB-C4A-NA	-2.05	122.22	124.44
74	1F	501	HEC	CHD-C4C-NC	2.05	127.62	123.85
84	5P	401	NDP	C3B-C2B-C1B	-2.05	99.04	102.89
74	6F	501	HEC	CHD-C4C-NC	2.04	127.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B	502	FMN	C4A-C10-N1	-2.04	119.99	124.73
76	4A	604	HEA	CHB-C1B-NB	-2.04	122.20	124.42
81	5B	501	FMN	C4A-C10-N1	-2.04	120.00	124.73
76	2A	601	HEA	CAA-CBA-CGA	-2.04	109.22	113.60
84	P	401	NDP	C3B-C2B-C1B	-2.04	99.06	102.89
76	2A	602	HEA	C25-C23-C24	2.03	119.08	114.60
73	1B	401	HEM	CAA-CBA-CGA	-2.02	109.25	113.60
76	2A	602	HEA	CHA-C1A-NA	-2.02	122.25	124.44
73	6A	402	HEM	C2D-C1D-ND	-2.02	107.46	109.88
73	6B	402	HEM	CAC-C3C-C4C	-2.02	120.02	124.90
73	1B	402	HEM	CMB-C2B-C1B	-2.01	121.97	125.04
73	6B	401	HEM	CAA-CBA-CGA	-2.01	109.27	113.60
74	1E	401	HEC	C3C-C4C-NC	-2.01	107.90	110.15
73	1B	402	HEM	C3B-C2B-C1B	2.01	107.97	106.49
73	6B	402	HEM	CMB-C2B-C1B	-2.00	121.99	125.04
73	1A	402	HEM	CHB-C4A-NA	2.00	127.53	123.85
76	9A	603	HEA	CHA-C1A-C2A	-2.00	121.69	124.94
76	8A	604	HEA	CHB-C1B-NB	-2.00	122.24	124.42
76	7A	601	HEA	C25-C23-C24	2.00	119.02	114.60
76	2A	602	HEA	C17-C18-C19	-2.00	122.84	127.66

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
74	1E	401	HEC	NA
74	1F	501	HEC	NA
74	6E	401	HEC	NA
74	6F	501	HEC	NA

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
76	2A	601	HEA	C3B-C11-C12-C13
76	2A	601	HEA	O11-C11-C12-C13
76	2A	601	HEA	C15-C16-C17-C18
76	2A	602	HEA	C2A-C3A-CMA-OMA
76	3A	604	HEA	C3B-C11-C12-C13
76	3A	604	HEA	O11-C11-C12-C13
76	3A	604	HEA	C15-C16-C17-C18
76	3A	604	HEA	C19-C20-C21-C22
76	4A	602	HEA	C3B-C11-C12-C13
76	4A	602	HEA	O11-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
76	4A	602	HEA	C15-C16-C17-C18
76	4A	602	HEA	C19-C20-C21-C22
76	7A	601	HEA	C2A-C3A-CMA-OMA
76	7A	602	HEA	C3B-C11-C12-C13
76	7A	602	HEA	O11-C11-C12-C13
76	7A	602	HEA	C15-C16-C17-C18
76	8A	601	HEA	C3B-C11-C12-C13
76	8A	601	HEA	O11-C11-C12-C13
76	8A	601	HEA	C15-C16-C17-C18
76	8A	601	HEA	C19-C20-C21-C22
76	9A	603	HEA	C3B-C11-C12-C13
76	9A	603	HEA	O11-C11-C12-C13
76	9A	603	HEA	C15-C16-C17-C18
76	9A	603	HEA	C19-C20-C21-C22
83	5J	200	8Q1	C1-C6-C7-C8
83	5J	200	8Q1	O27-C28-C29-C32
83	5k	200	8Q1	O4-C1-S44-C43
83	5k	200	8Q1	C6-C1-S44-C43
83	5k	200	8Q1	C28-C29-C32-C34
83	5k	200	8Q1	C28-C29-C32-O33
83	5k	200	8Q1	C30-C29-C32-C34
83	5k	200	8Q1	C30-C29-C32-O33
83	5k	200	8Q1	C31-C29-C32-C34
83	5k	200	8Q1	C31-C29-C32-O33
83	5k	200	8Q1	O33-C32-C34-N36
83	5k	200	8Q1	C32-C34-N36-C37
83	5k	200	8Q1	C28-O27-P24-O1
83	J	200	8Q1	C1-C6-C7-C8
83	J	200	8Q1	O27-C28-C29-C32
83	k	200	8Q1	O4-C1-S44-C43
83	k	200	8Q1	C6-C1-S44-C43
83	k	200	8Q1	C28-C29-C32-C34
83	k	200	8Q1	C28-C29-C32-O33
83	k	200	8Q1	C30-C29-C32-C34
83	k	200	8Q1	C30-C29-C32-O33
83	k	200	8Q1	C31-C29-C32-C34
83	k	200	8Q1	C31-C29-C32-O33
83	k	200	8Q1	O33-C32-C34-N36
83	k	200	8Q1	C32-C34-N36-C37
83	k	200	8Q1	C28-O27-P24-O1
84	5P	401	NDP	C5B-O5B-PA-O1A
84	5P	401	NDP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
84	P	401	NDP	C5B-O5B-PA-O1A
84	P	401	NDP	C5B-O5B-PA-O2A
85	5s	401	COO	C14-C11-C13-O1
85	5s	401	COO	C12-C11-C13-O1
85	5s	401	COO	C14-C11-C13-C1
85	5s	401	COO	C12-C11-C13-C1
85	5s	401	COO	C13-C11-C12-O6A
85	5s	401	COO	C13-C1-N1-C2
85	5s	401	COO	O2-C1-N1-C2
85	5s	401	COO	C3-C4-N2-C5
85	5s	401	COO	O3-C4-N2-C5
85	5s	401	COO	O4-C7-S1-C6
85	5s	401	COO	C8-C7-S1-C6
85	5s	401	COO	S1-C7-C8-C9
85	s	401	COO	C14-C11-C13-O1
85	s	401	COO	C12-C11-C13-O1
85	s	401	COO	C14-C11-C13-C1
85	s	401	COO	C12-C11-C13-C1
85	s	401	COO	C13-C11-C12-O6A
85	s	401	COO	C13-C1-N1-C2
85	s	401	COO	O2-C1-N1-C2
85	s	401	COO	C3-C4-N2-C5
85	s	401	COO	O3-C4-N2-C5
85	s	401	COO	O4-C7-S1-C6
85	s	401	COO	C8-C7-S1-C6
85	s	401	COO	S1-C7-C8-C9
83	5k	200	8Q1	O35-C34-N36-C37
83	k	200	8Q1	O35-C34-N36-C37
84	5P	401	NDP	O4B-C4B-C5B-O5B
84	5P	401	NDP	C3B-C4B-C5B-O5B
84	P	401	NDP	O4B-C4B-C5B-O5B
84	P	401	NDP	C3B-C4B-C5B-O5B
84	5P	401	NDP	O4D-C1D-N1N-C6N
84	P	401	NDP	O4D-C1D-N1N-C6N
84	5P	401	NDP	O4D-C4D-C5D-O5D
84	P	401	NDP	O4D-C4D-C5D-O5D
73	1B	402	HEM	C2A-CAA-CBA-CGA
73	6B	402	HEM	C2A-CAA-CBA-CGA
76	2A	601	HEA	C19-C20-C21-C22
76	7A	602	HEA	C19-C20-C21-C22
83	5J	200	8Q1	O27-C28-C29-C30
83	5J	200	8Q1	O27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
83	J	200	8Q1	O27-C28-C29-C30
83	J	200	8Q1	O27-C28-C29-C31
85	5s	401	COO	C15-C11-C12-O6A
85	s	401	COO	C15-C11-C12-O6A
85	5s	401	COO	N2-C5-C6-S1
85	s	401	COO	N2-C5-C6-S1
83	5k	200	8Q1	C11-C10-C9-C8
83	k	200	8Q1	C11-C10-C9-C8
83	5k	200	8Q1	C6-C7-C8-C9
83	k	200	8Q1	C6-C7-C8-C9
73	1B	401	HEM	C2A-CAA-CBA-CGA
73	6B	401	HEM	C2A-CAA-CBA-CGA
76	3A	601	HEA	C2A-CAA-CBA-CGA
76	4A	604	HEA	C2A-CAA-CBA-CGA
76	8A	604	HEA	C2A-CAA-CBA-CGA
76	9A	602	HEA	C2A-CAA-CBA-CGA
85	5s	401	COO	O4-C7-C8-C9
85	s	401	COO	O4-C7-C8-C9
84	5P	401	NDP	C3D-C4D-C5D-O5D
84	P	401	NDP	C3D-C4D-C5D-O5D
83	5k	200	8Q1	O33-C32-C34-O35
83	k	200	8Q1	O33-C32-C34-O35
81	5B	501	FMN	C5'-O5'-P-O1P
81	B	502	FMN	C5'-O5'-P-O1P
85	5s	401	COO	P1A-O3A-P2A-O4A
85	s	401	COO	P1A-O3A-P2A-O4A
74	1F	501	HEC	C4B-C3B-CAB-CBB
73	1A	401	HEM	C2A-CAA-CBA-CGA
73	6A	402	HEM	C2A-CAA-CBA-CGA
74	6F	501	HEC	C4B-C3B-CAB-CBB
76	2A	601	HEA	C2A-C3A-CMA-OMA
76	3A	601	HEA	C2A-C3A-CMA-OMA
76	4A	604	HEA	C2A-C3A-CMA-OMA
76	7A	602	HEA	C2A-C3A-CMA-OMA
76	8A	604	HEA	C2A-C3A-CMA-OMA
76	9A	602	HEA	C2A-C3A-CMA-OMA
83	5k	200	8Q1	C28-O27-P24-O2
83	k	200	8Q1	C28-O27-P24-O2
73	1B	401	HEM	C4C-C3C-CAC-CBC
73	6B	401	HEM	C4C-C3C-CAC-CBC
74	1E	401	HEC	C2B-C3B-CAB-CBB
74	6E	401	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
76	2A	601	HEA	C4A-C3A-CMA-OMA
76	2A	602	HEA	C4A-C3A-CMA-OMA
76	3A	601	HEA	C4A-C3A-CMA-OMA
76	4A	604	HEA	C4A-C3A-CMA-OMA
76	7A	601	HEA	C4A-C3A-CMA-OMA
76	7A	602	HEA	C4A-C3A-CMA-OMA
76	8A	604	HEA	C4A-C3A-CMA-OMA
76	9A	602	HEA	C4A-C3A-CMA-OMA
83	5k	200	8Q1	O27-C28-C29-C30
83	5k	200	8Q1	O27-C28-C29-C31
83	k	200	8Q1	O27-C28-C29-C30
83	k	200	8Q1	O27-C28-C29-C31
85	5s	401	COO	C2X-C3X-O3X-P3X
85	s	401	COO	C2X-C3X-O3X-P3X
76	2A	601	HEA	C11-C12-C13-C14
76	7A	602	HEA	C11-C12-C13-C14
83	5k	200	8Q1	C28-O27-P24-O3
83	k	200	8Q1	C28-O27-P24-O3
85	5s	401	COO	P1A-O3A-P2A-O5A
85	s	401	COO	P1A-O3A-P2A-O5A
85	5s	401	COO	O2-C1-C13-C11
85	s	401	COO	O2-C1-C13-C11
85	5s	401	COO	N1-C1-C13-C11
85	s	401	COO	N1-C1-C13-C11
73	1A	402	HEM	CAD-CBD-CGD-O1D
73	6A	401	HEM	CAD-CBD-CGD-O1D
83	J	200	8Q1	C7-C8-C9-C10
83	5J	200	8Q1	C7-C8-C9-C10
81	5B	501	FMN	C3'-C4'-C5'-O5'
81	B	502	FMN	C3'-C4'-C5'-O5'
73	6B	402	HEM	CAA-CBA-CGA-O1A
73	1B	402	HEM	CAA-CBA-CGA-O1A
73	1B	402	HEM	CAA-CBA-CGA-O2A
73	6B	402	HEM	CAA-CBA-CGA-O2A
83	J	200	8Q1	C11-C12-C13-C14
83	5J	200	8Q1	C11-C12-C13-C14
76	7A	601	HEA	CAA-CBA-CGA-O2A
83	5J	200	8Q1	O4-C1-S44-C43
83	J	200	8Q1	O4-C1-S44-C43
76	2A	602	HEA	CAA-CBA-CGA-O2A
73	1A	402	HEM	CAA-CBA-CGA-O2A
73	6A	401	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
73	1A	402	HEM	CAA-CBA-CGA-O1A
73	6A	401	HEM	CAA-CBA-CGA-O1A
74	1F	501	HEC	C2B-C3B-CAB-CBB
74	6F	501	HEC	C2B-C3B-CAB-CBB
73	6B	401	HEM	CAD-CBD-CGD-O2D
76	2A	602	HEA	C4C-C3C-CAC-CBC
76	7A	601	HEA	C4C-C3C-CAC-CBC
76	2A	602	HEA	C26-C15-C16-C17
76	7A	601	HEA	C26-C15-C16-C17
73	1B	401	HEM	CAD-CBD-CGD-O2D
73	1B	401	HEM	CAD-CBD-CGD-O1D
73	6B	401	HEM	CAD-CBD-CGD-O1D
81	5B	501	FMN	C5'-O5'-P-O2P
81	B	502	FMN	C5'-O5'-P-O2P
85	5s	401	COO	C3X-O3X-P3X-O9A
85	s	401	COO	C3X-O3X-P3X-O9A
76	3A	601	HEA	C26-C15-C16-C17
76	4A	604	HEA	C26-C15-C16-C17
76	8A	604	HEA	C26-C15-C16-C17
76	9A	602	HEA	C26-C15-C16-C17
73	1A	401	HEM	CAD-CBD-CGD-O2D
73	6A	402	HEM	CAD-CBD-CGD-O2D
81	5B	501	FMN	O4'-C4'-C5'-O5'
81	B	502	FMN	O4'-C4'-C5'-O5'
76	2A	602	HEA	CAD-CBD-CGD-O2D
76	7A	601	HEA	CAD-CBD-CGD-O2D
74	6E	401	HEC	C4B-C3B-CAB-CBB
76	2A	602	HEA	CAA-CBA-CGA-O1A
76	7A	601	HEA	CAA-CBA-CGA-O1A
73	1A	402	HEM	CAD-CBD-CGD-O2D
73	6A	401	HEM	CAD-CBD-CGD-O2D
76	2A	602	HEA	CAD-CBD-CGD-O1D
76	3A	601	HEA	CAD-CBD-CGD-O2D
76	4A	604	HEA	CAD-CBD-CGD-O1D
76	4A	604	HEA	CAD-CBD-CGD-O2D
76	7A	601	HEA	CAD-CBD-CGD-O1D
76	8A	604	HEA	CAD-CBD-CGD-O1D
76	8A	604	HEA	CAD-CBD-CGD-O2D
76	9A	602	HEA	CAD-CBD-CGD-O1D
76	9A	602	HEA	CAD-CBD-CGD-O2D
74	1E	401	HEC	C4B-C3B-CAB-CBB
73	1A	401	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
76	3A	601	HEA	CAD-CBD-CGD-O1D
73	6A	402	HEM	CAD-CBD-CGD-O1D
84	5P	401	NDP	C5B-O5B-PA-O3
84	P	401	NDP	C5B-O5B-PA-O3
85	5s	401	COO	C3X-O3X-P3X-O8A
85	s	401	COO	C3X-O3X-P3X-O8A
76	3A	601	HEA	CAA-CBA-CGA-O2A
76	4A	604	HEA	CAA-CBA-CGA-O2A
76	8A	604	HEA	CAA-CBA-CGA-O2A
76	9A	602	HEA	CAA-CBA-CGA-O2A
76	2A	602	HEA	C19-C20-C21-C22
76	7A	601	HEA	C19-C20-C21-C22
76	2A	602	HEA	C2A-CAA-CBA-CGA
76	7A	601	HEA	C2A-CAA-CBA-CGA
83	5k	200	8Q1	C7-C8-C9-C10
83	k	200	8Q1	C7-C8-C9-C10
76	4A	604	HEA	CAA-CBA-CGA-O1A
76	8A	604	HEA	CAA-CBA-CGA-O1A
76	3A	601	HEA	C3B-C11-C12-C13
76	4A	604	HEA	C3B-C11-C12-C13
76	8A	604	HEA	C3B-C11-C12-C13
76	9A	602	HEA	C3B-C11-C12-C13
76	9A	602	HEA	CAA-CBA-CGA-O1A
76	3A	601	HEA	CAA-CBA-CGA-O1A
73	6B	402	HEM	CAD-CBD-CGD-O1D
83	5k	200	8Q1	C37-C38-C39-O40
83	k	200	8Q1	C37-C38-C39-O40
81	5B	501	FMN	N10-C1'-C2'-O2'
81	B	502	FMN	N10-C1'-C2'-O2'
73	1B	402	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

43 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	2C	301	CUA	3	0
76	9A	603	HEA	2	0
76	4A	602	HEA	2	0
76	4A	604	HEA	1	0
74	6F	501	HEC	2	0
74	6E	401	HEC	3	0
79	3C	301	CUA	2	0

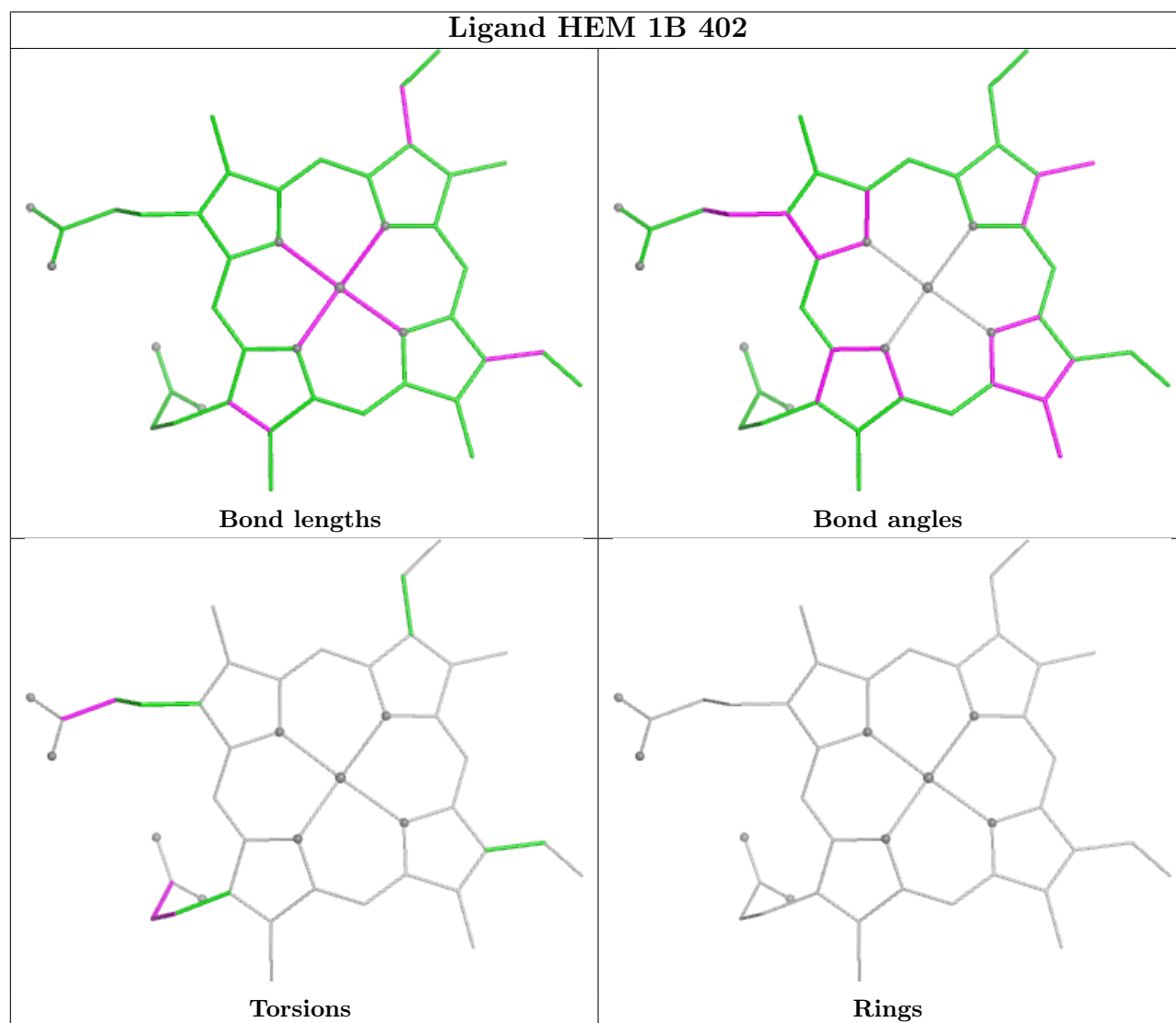
Continued on next page...

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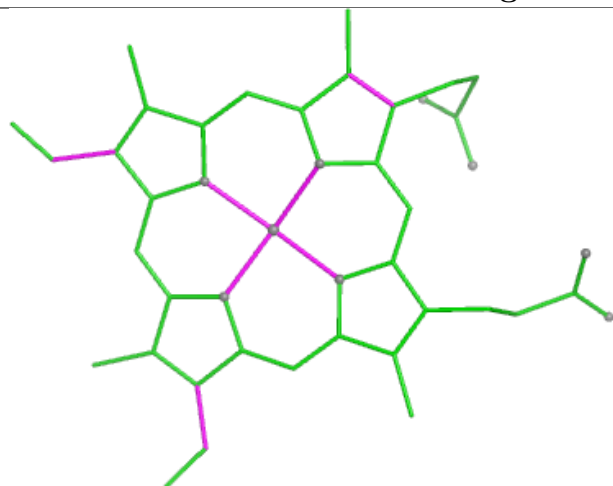
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	B	502	FMN	2	0
82	5G	302	SF4	1	0
76	2A	601	HEA	1	0
85	s	401	COO	9	0
76	7A	602	HEA	1	0
80	5C	801	FES	1	0
80	C	803	FES	1	0
74	1F	501	HEC	2	0
76	2A	602	HEA	1	0
84	P	401	NDP	4	0
73	6B	401	HEM	2	0
74	1E	401	HEC	3	0
76	7A	601	HEA	1	0
80	A	301	FES	2	0
76	9A	602	HEA	1	0
82	5C	803	SF4	1	0
73	1B	401	HEM	2	0
76	8A	604	HEA	1	0
79	8C	301	CUA	2	0
76	3A	604	HEA	2	0
83	5J	200	8Q1	1	0
76	8A	601	HEA	2	0
76	3A	601	HEA	1	0
82	F	201	SF4	1	0
82	C	801	SF4	1	0
85	5s	401	COO	8	0
82	5F	201	SF4	1	0
84	5P	401	NDP	4	0
81	5B	501	FMN	2	0
82	G	302	SF4	1	0
80	5A	301	FES	2	0
83	J	200	8Q1	1	0
79	4C	301	CUA	2	0
79	7C	301	CUA	3	0
79	9C	301	CUA	2	0
73	6A	401	HEM	1	0

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

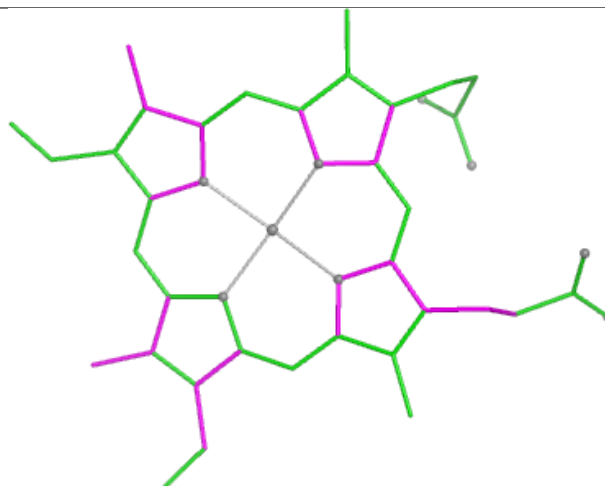
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



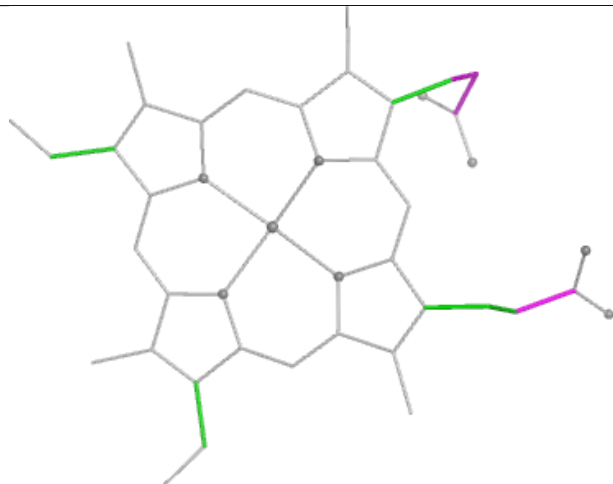
Ligand HEM 6B 402



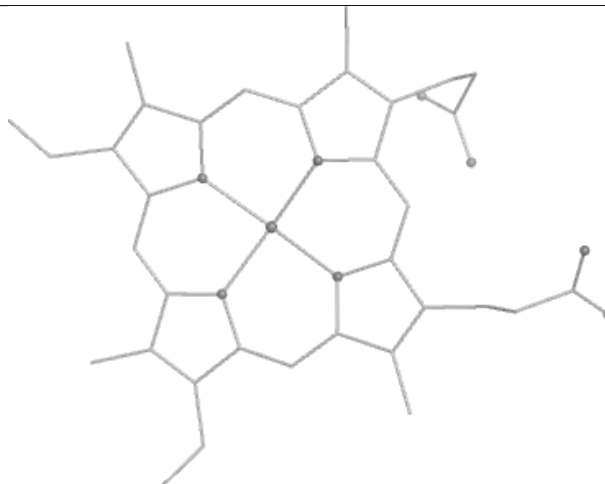
Bond lengths



Bond angles

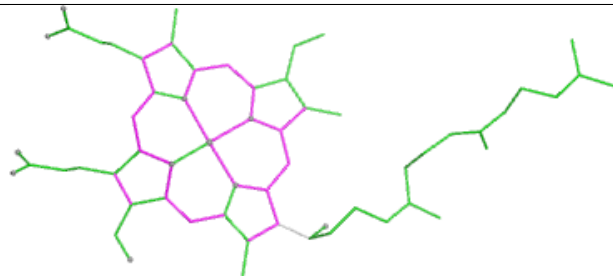


Torsions

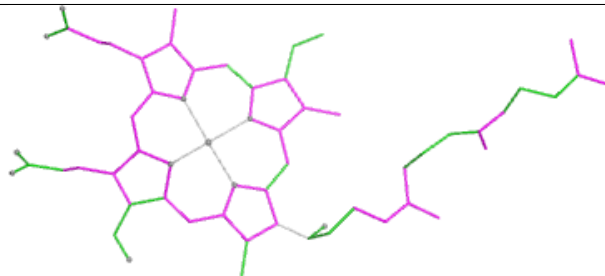


Rings

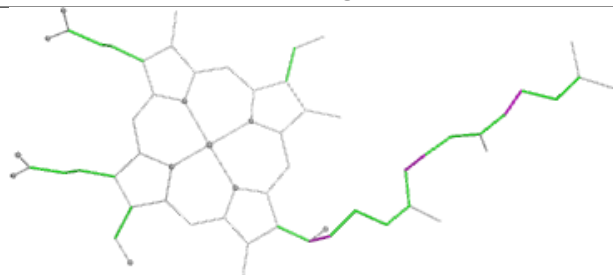
Ligand HEA 9A 603



Bond lengths



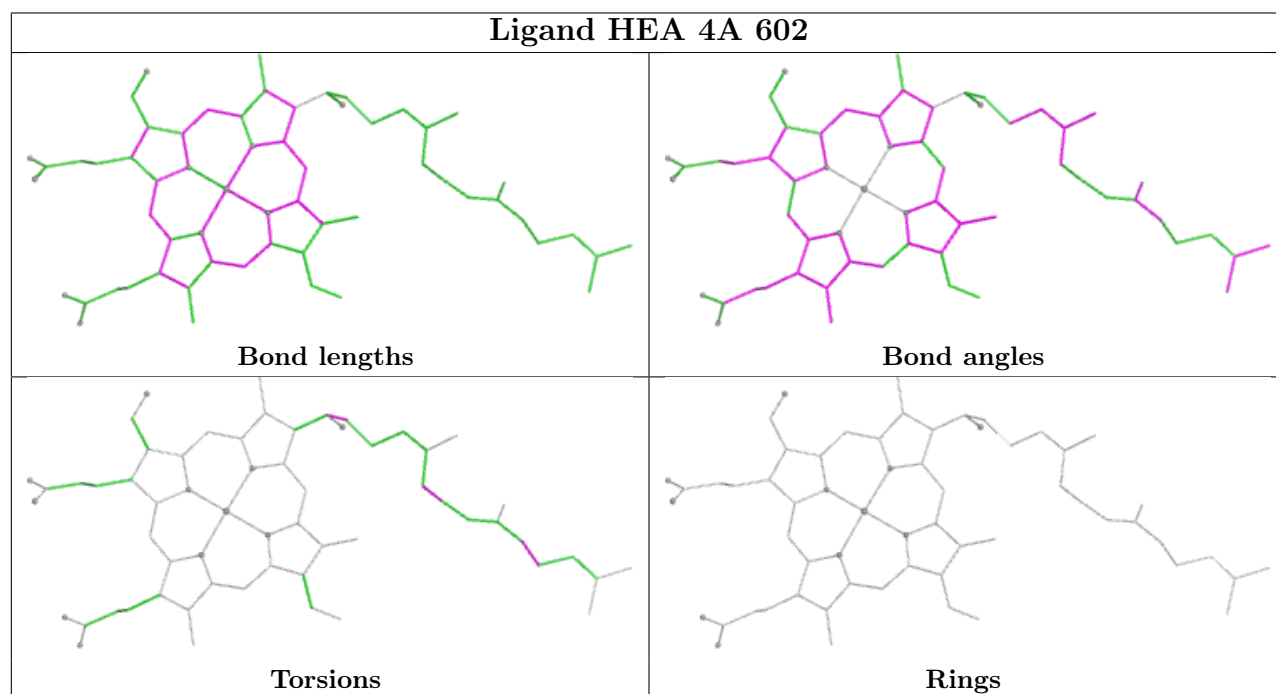
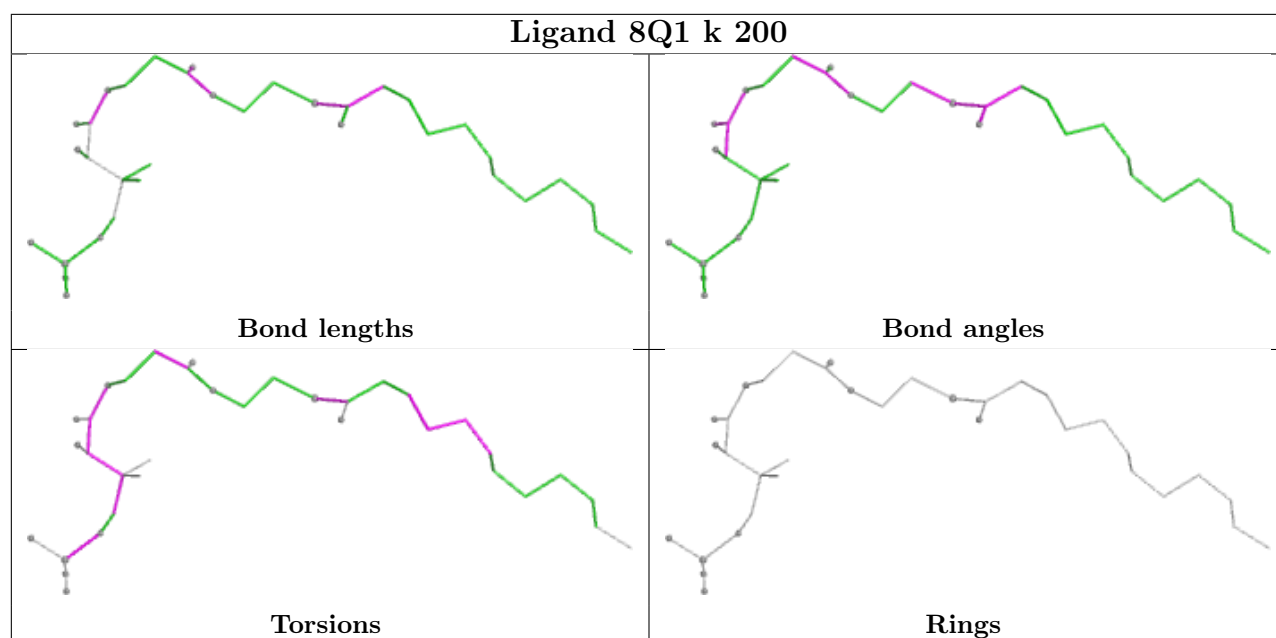
Bond angles

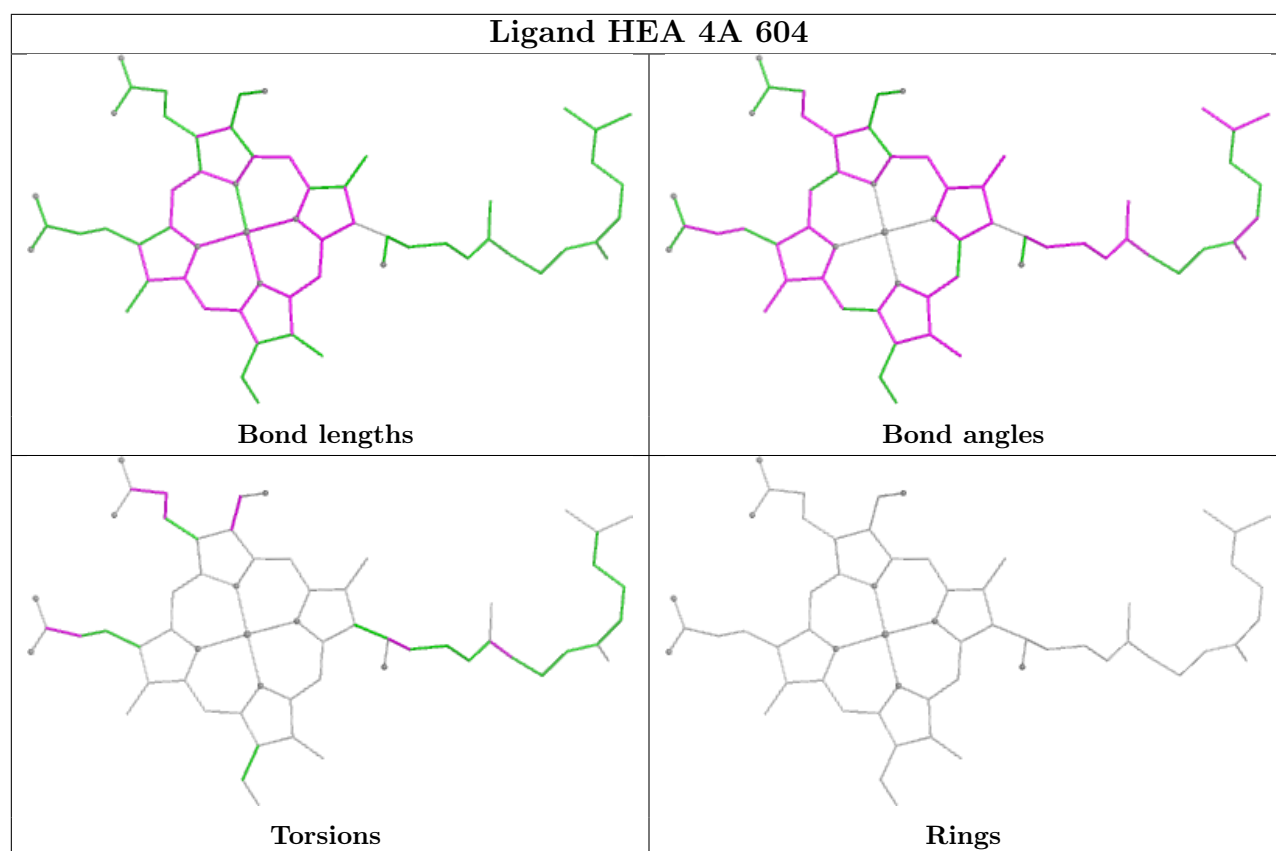


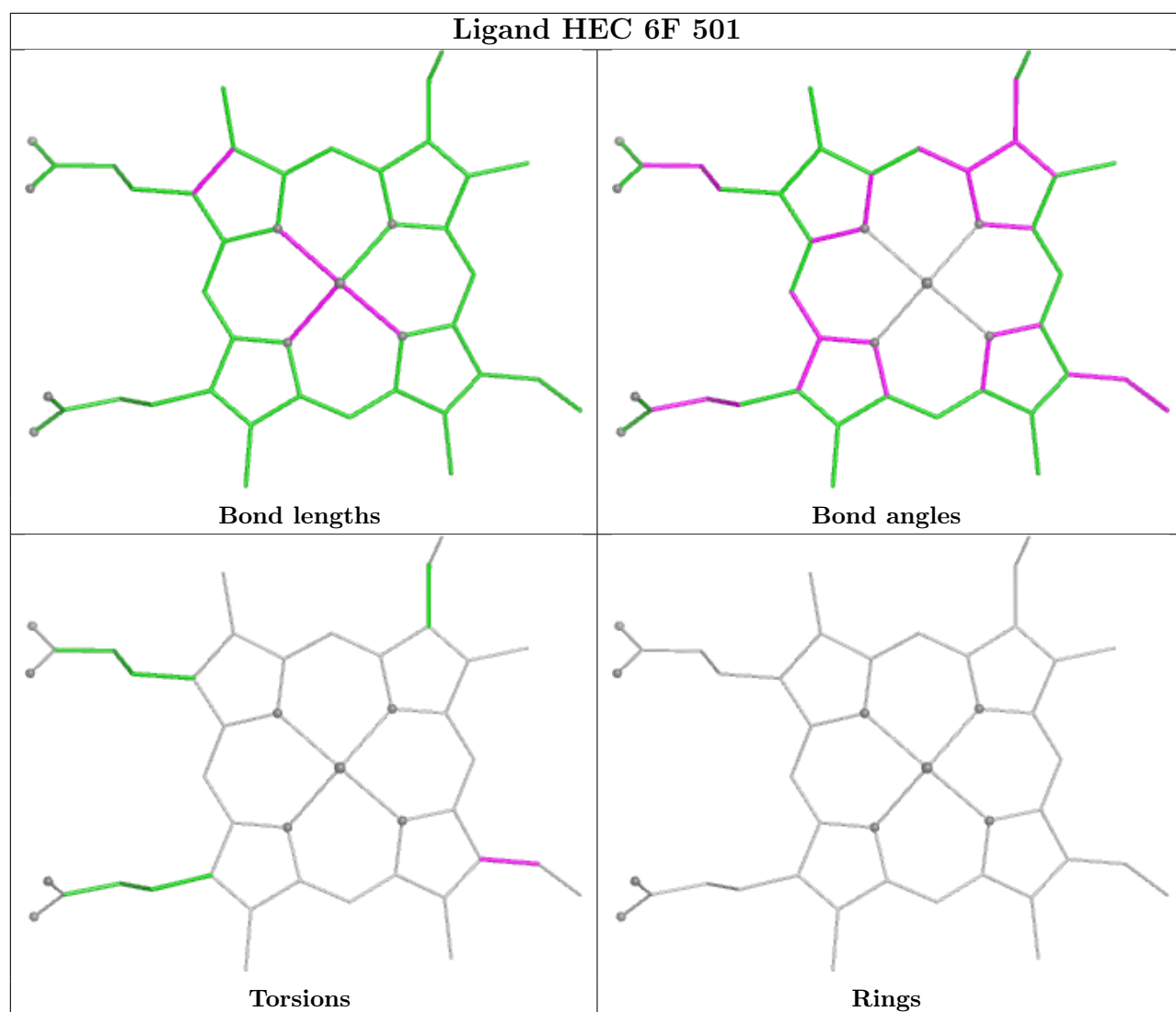
Torsions

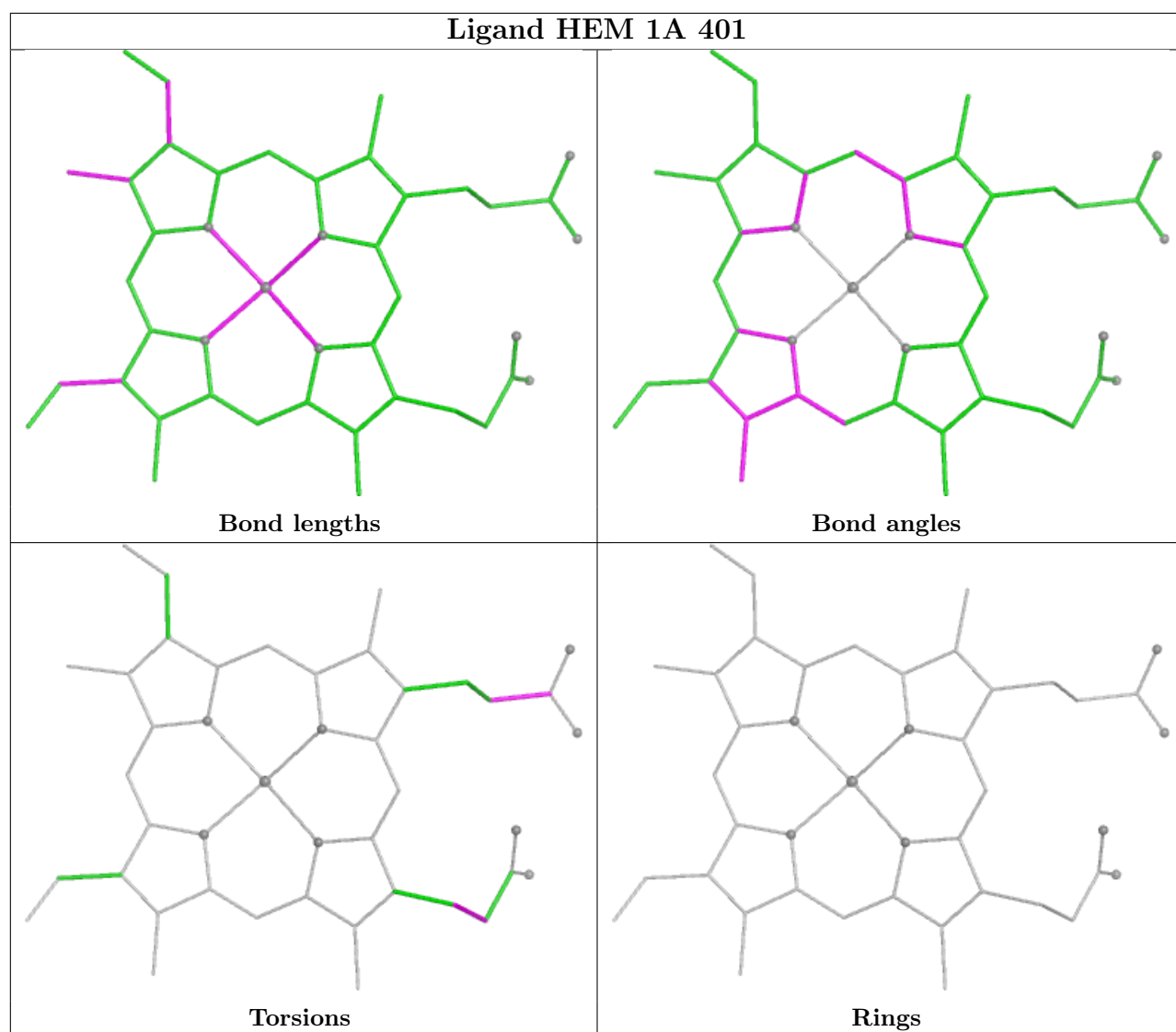


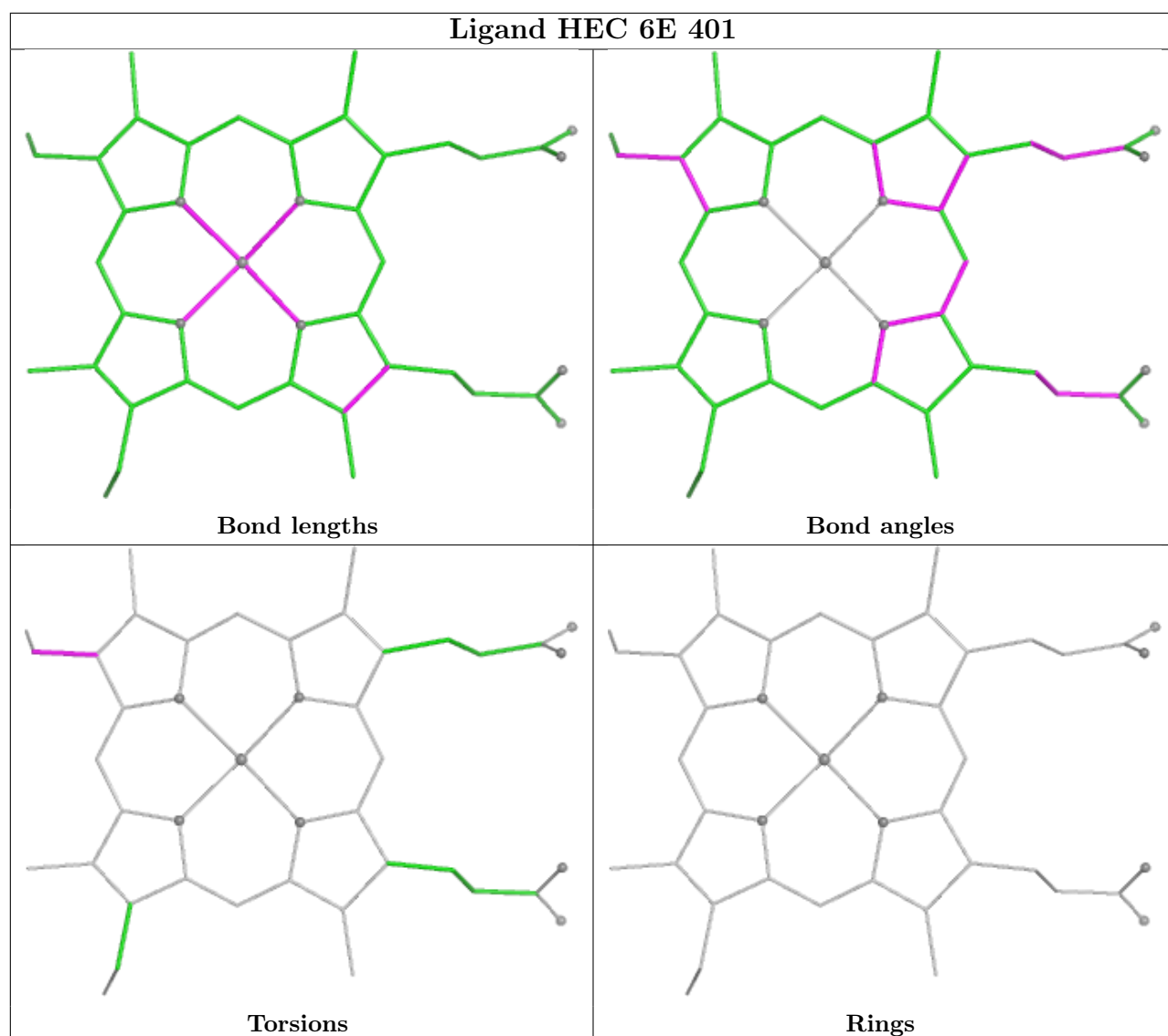
Rings

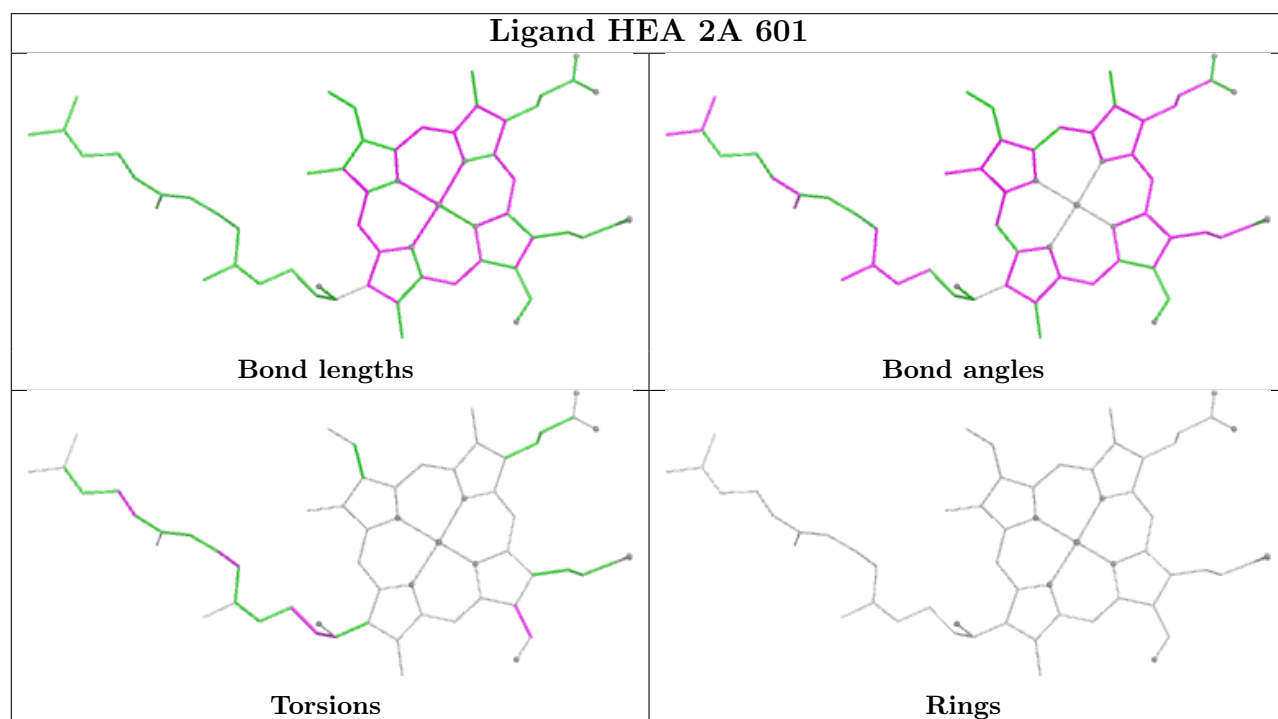
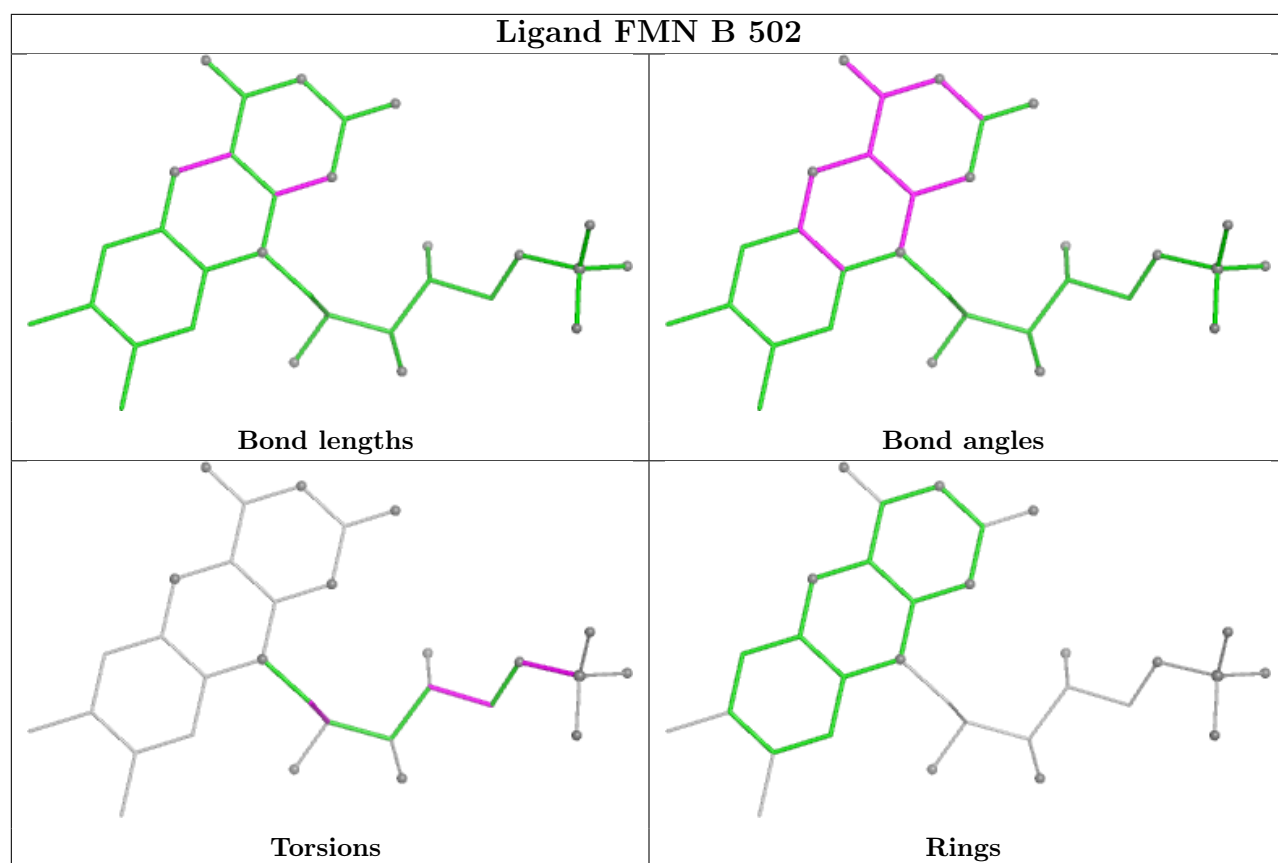


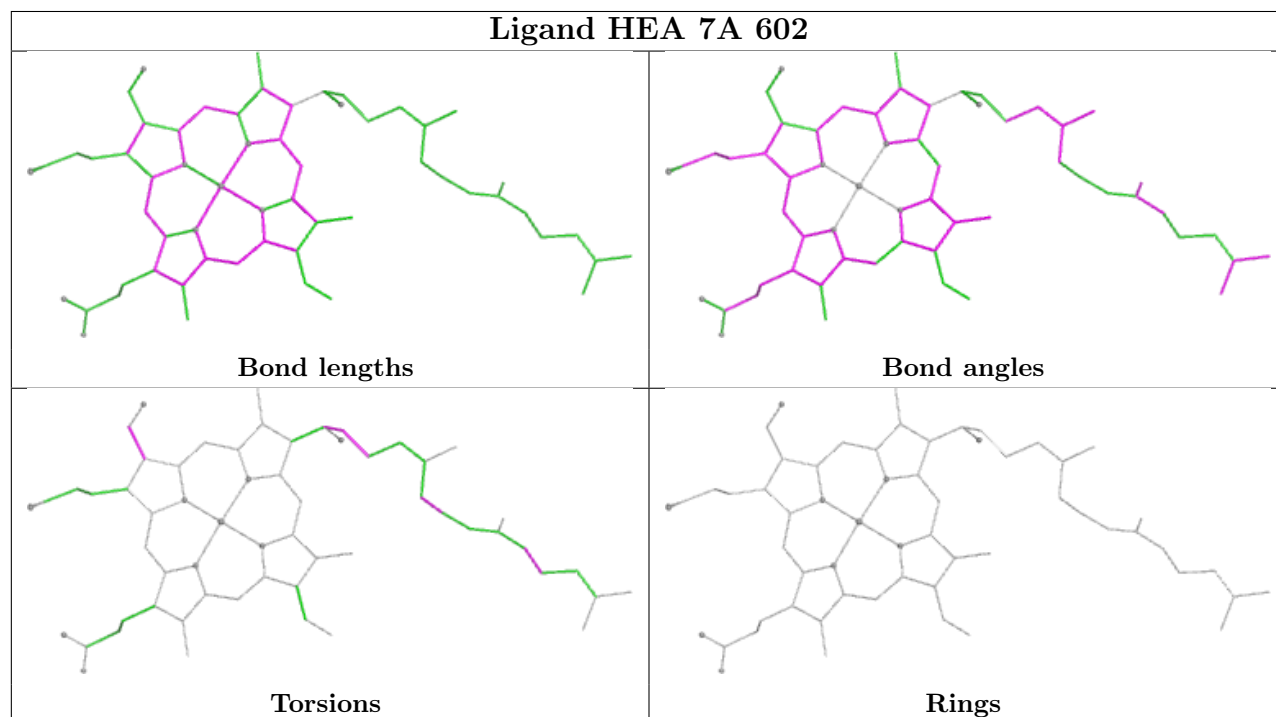
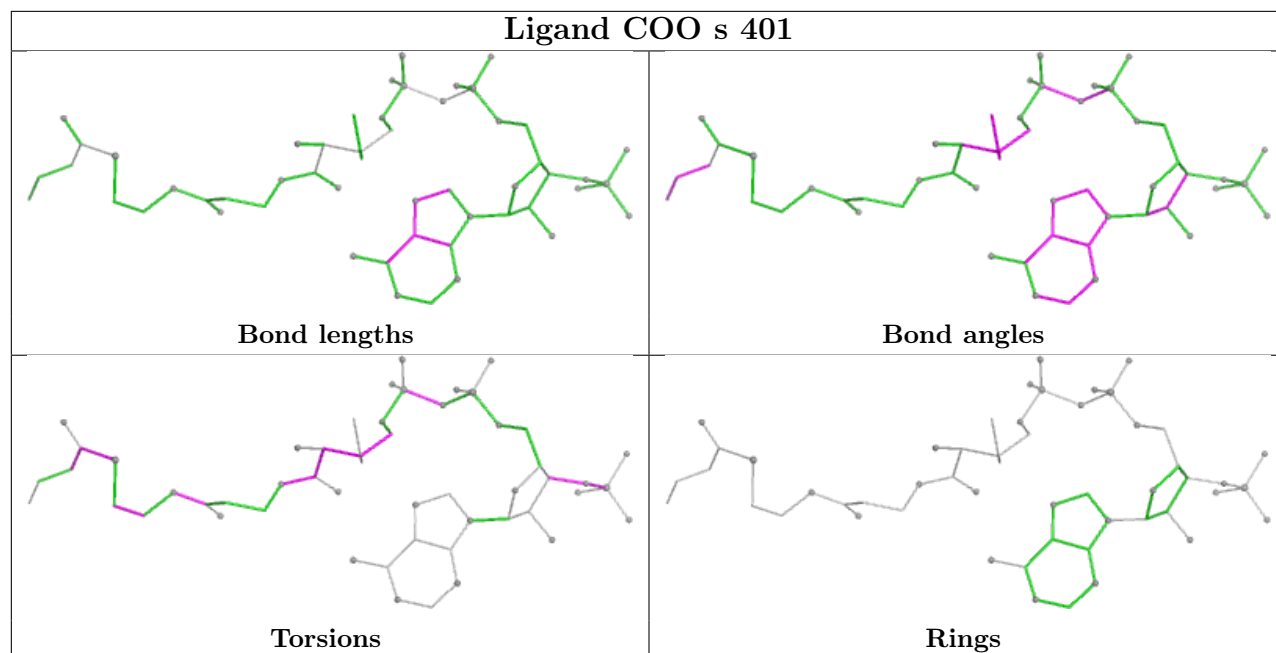


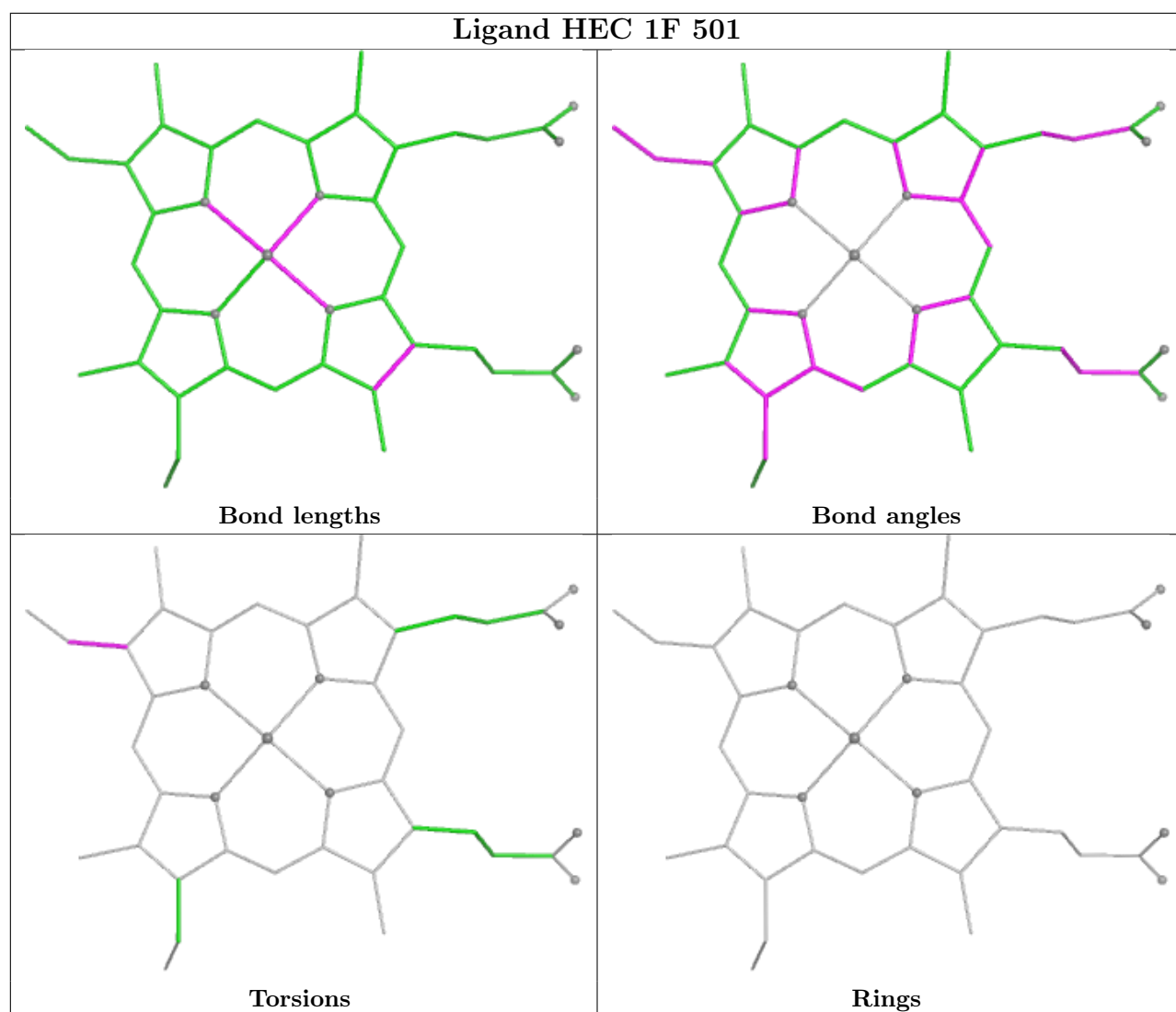


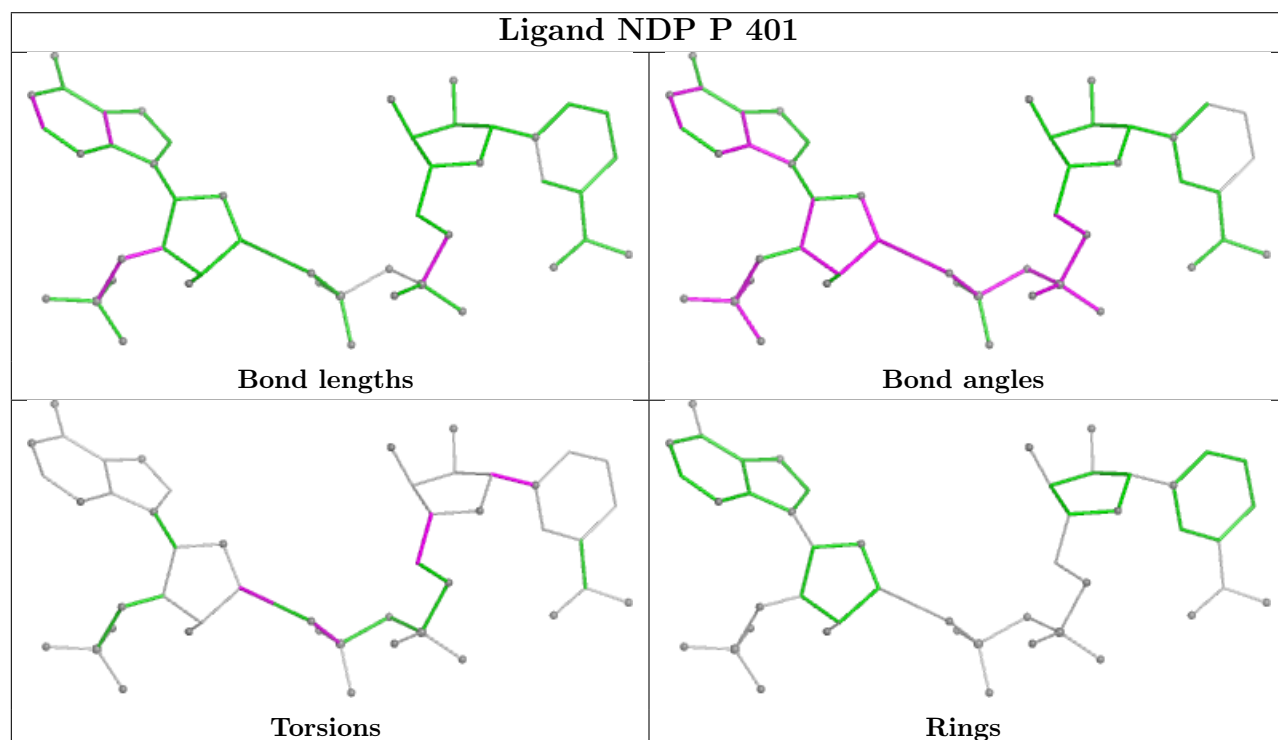
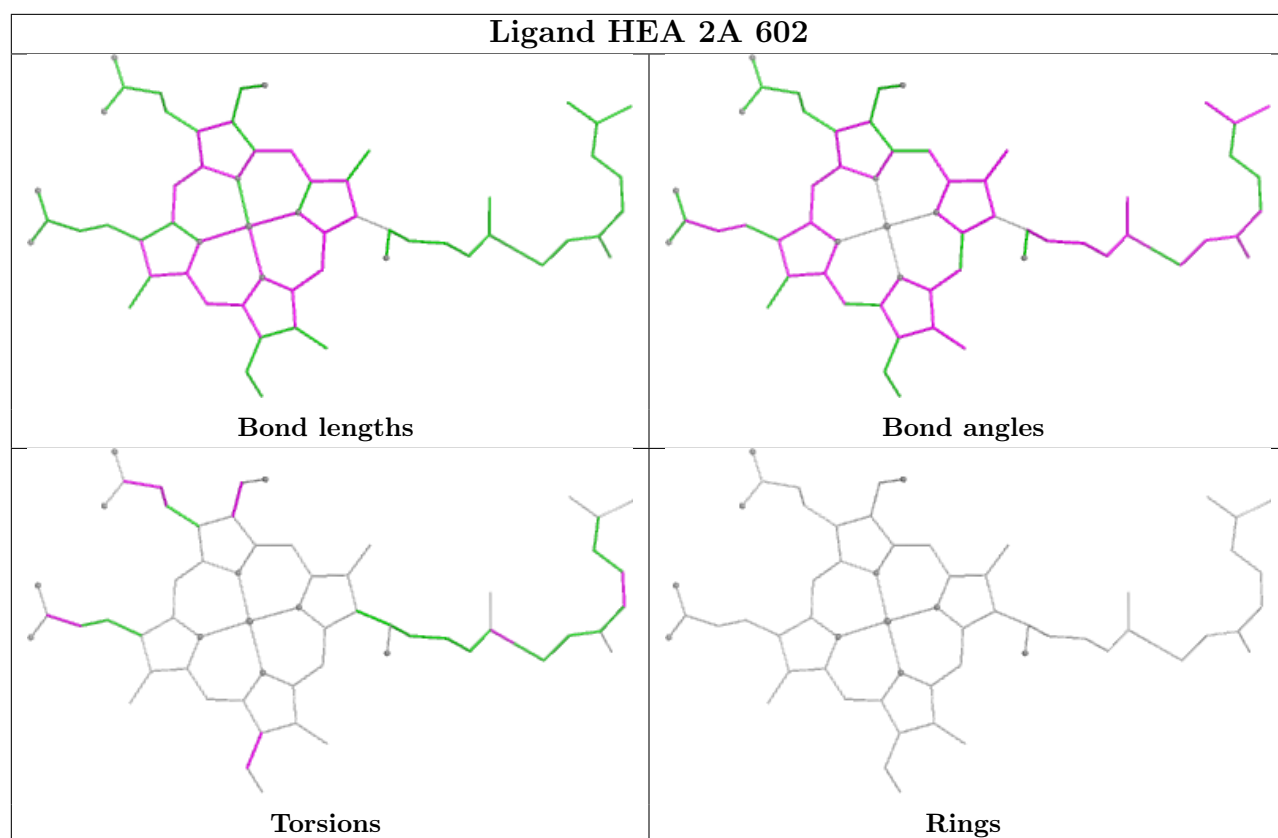


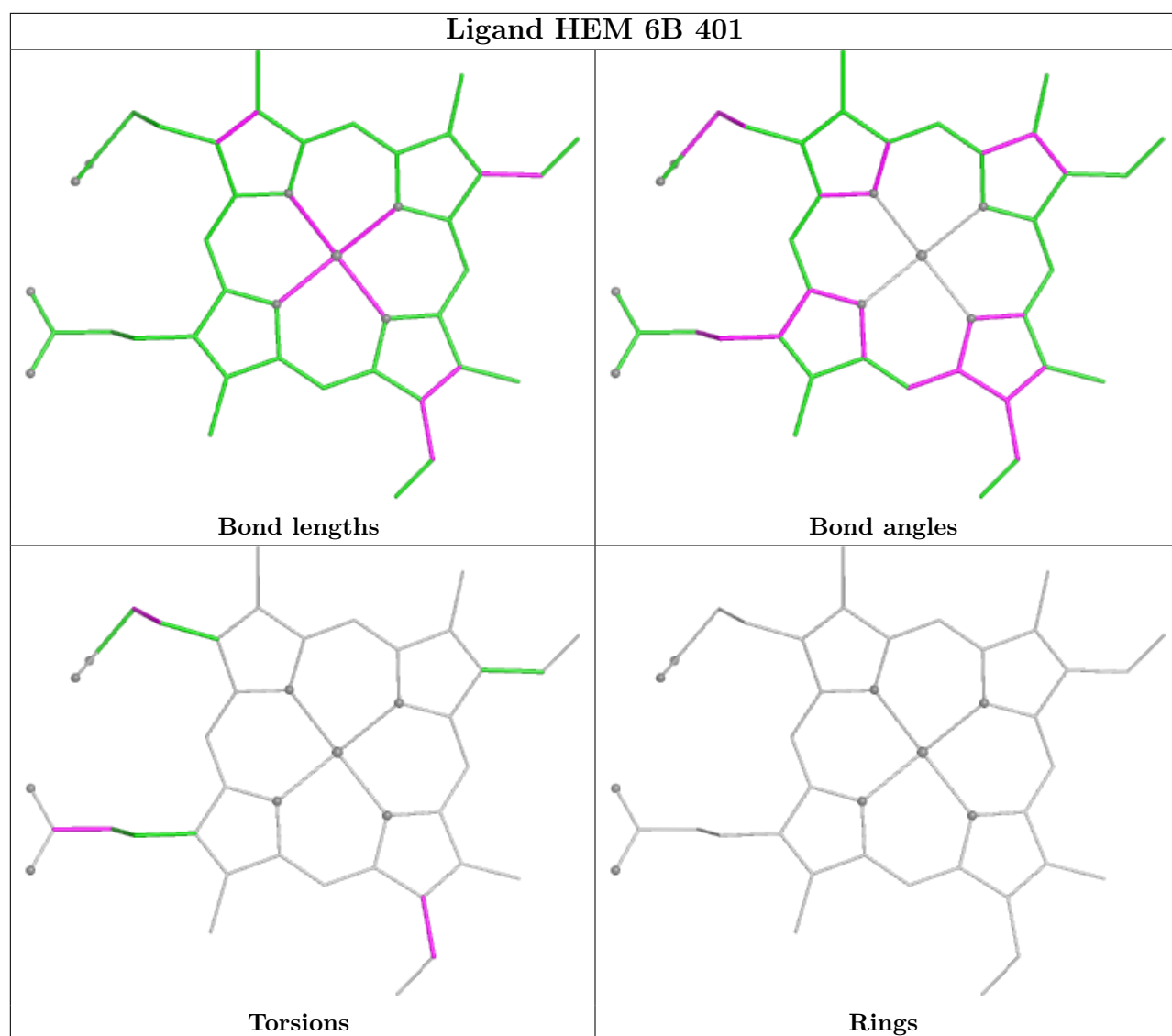


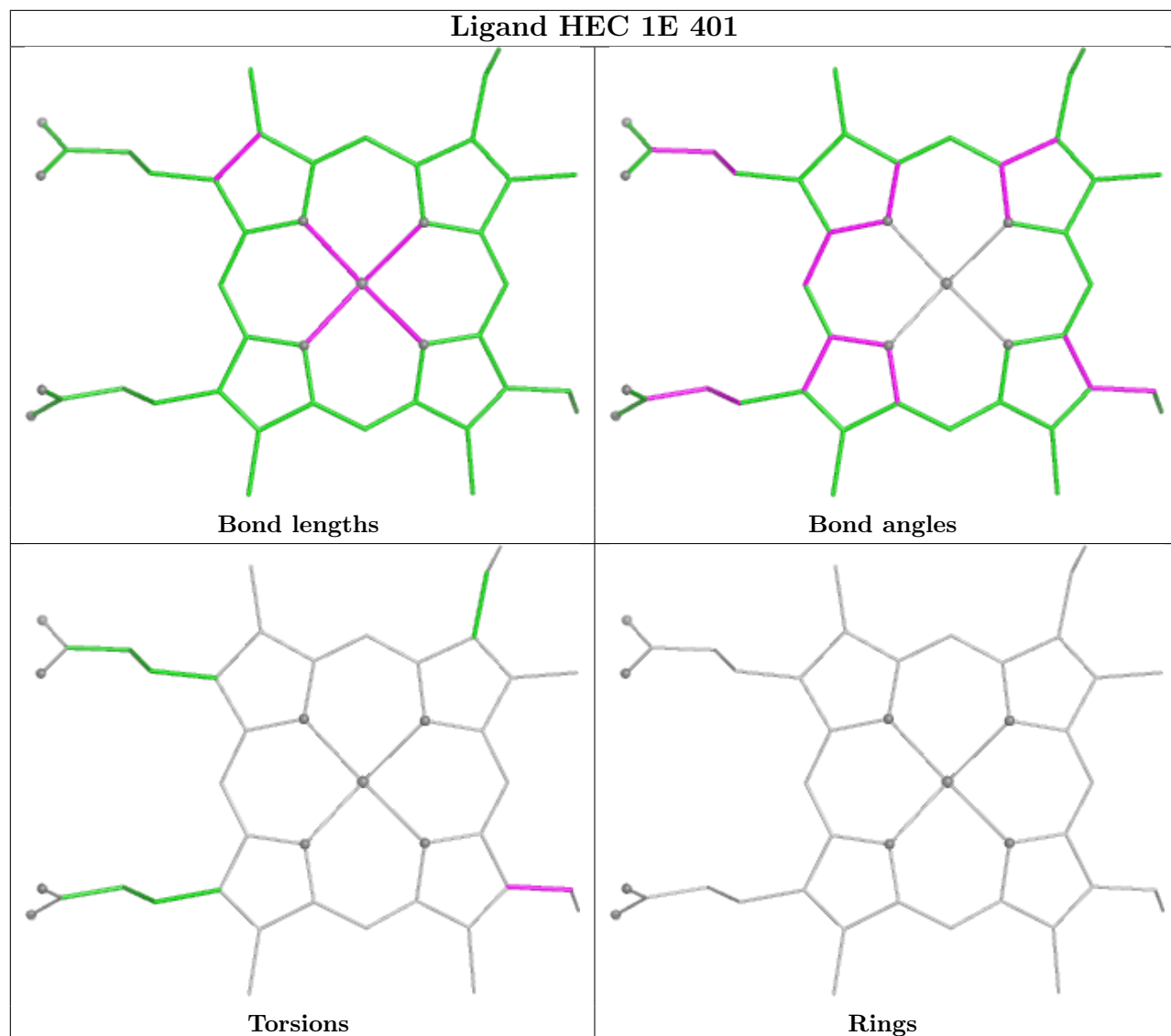


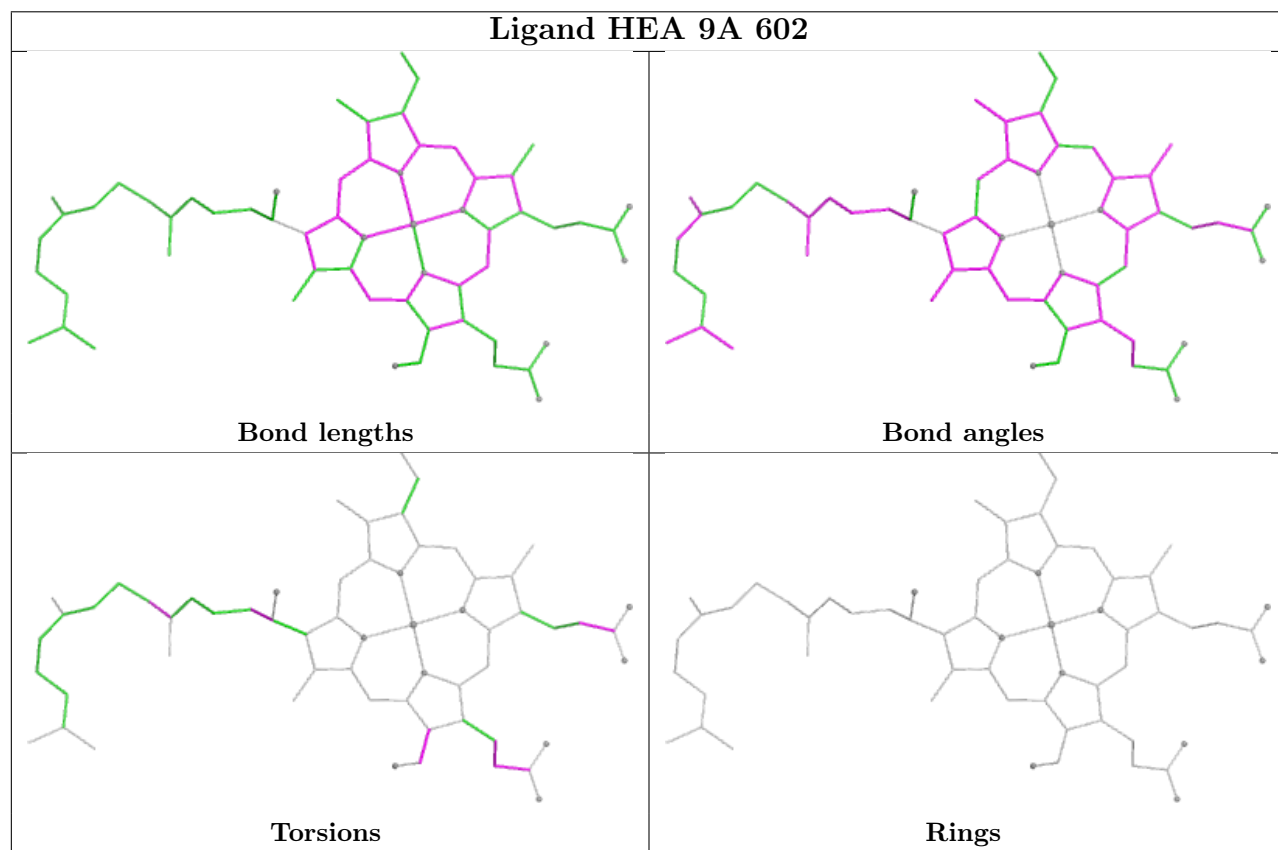
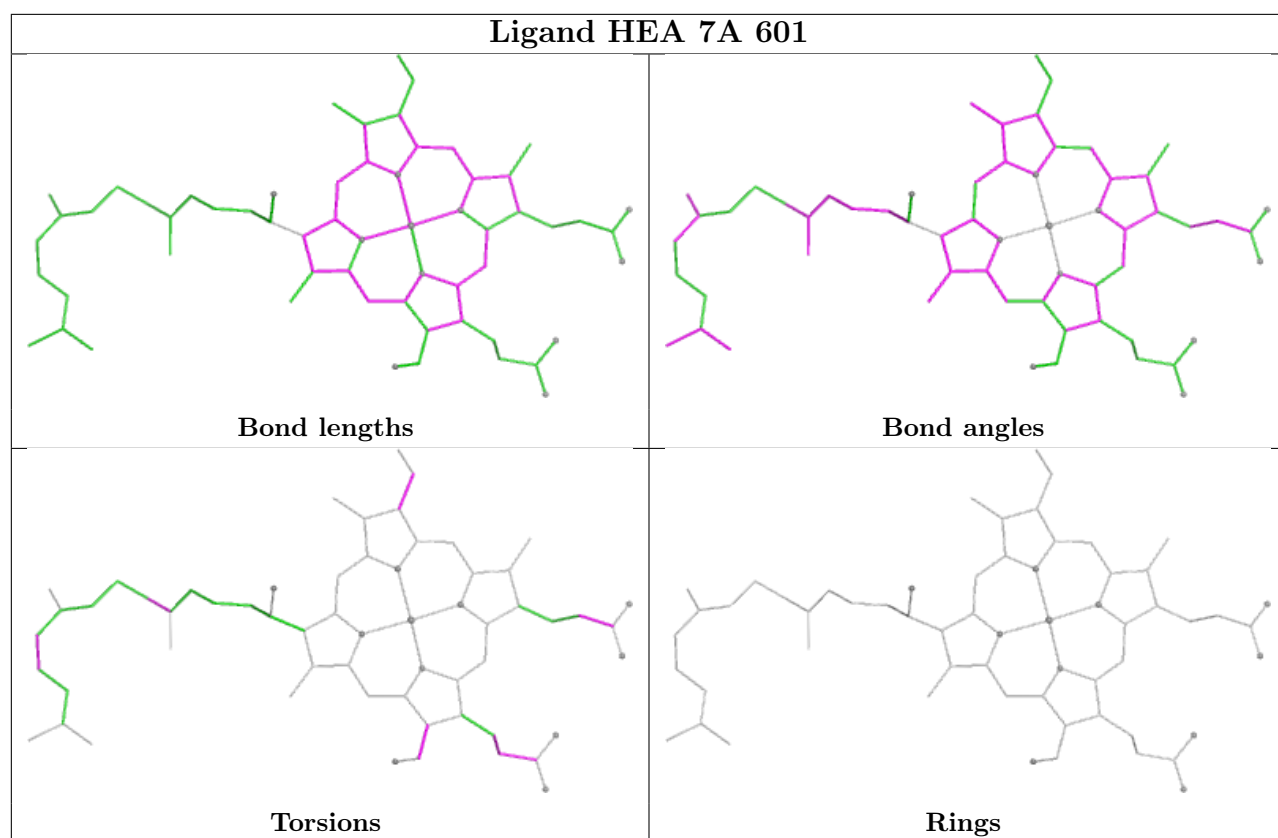




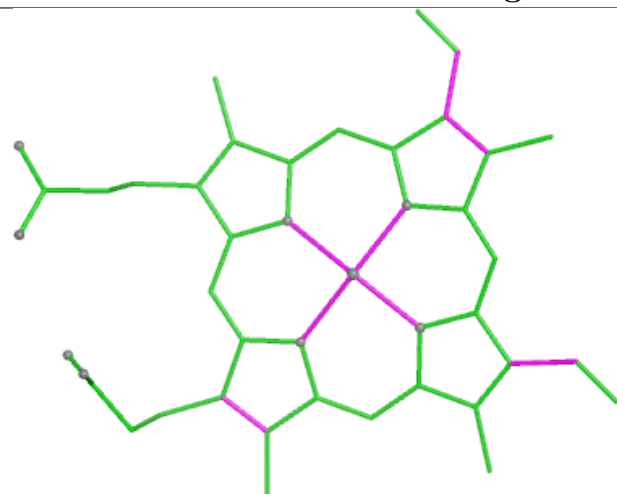




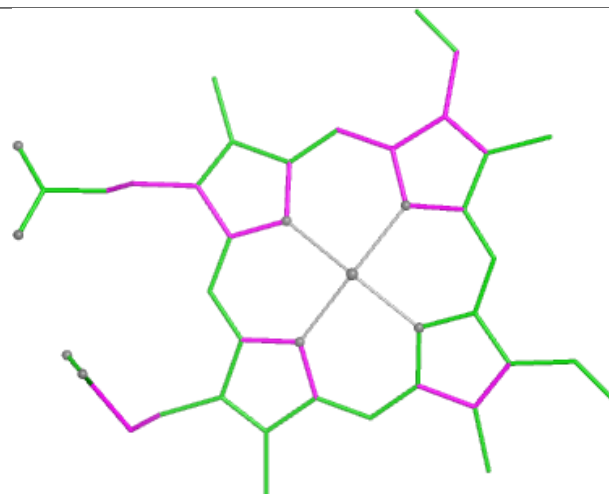




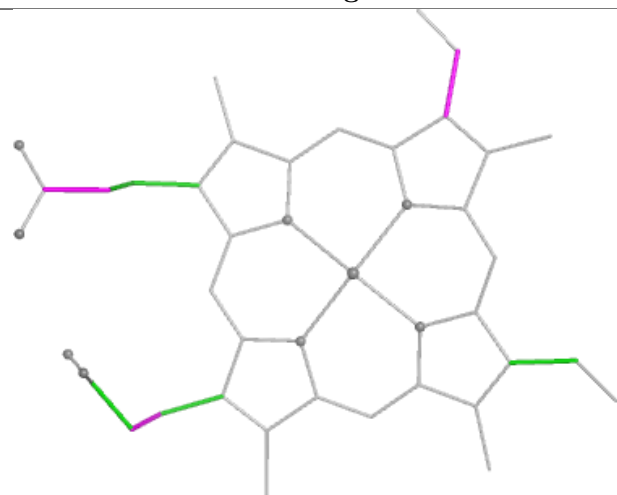
Ligand HEM 1B 401



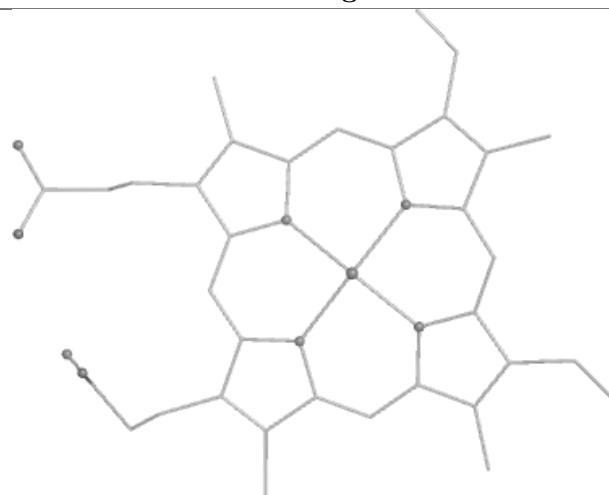
Bond lengths



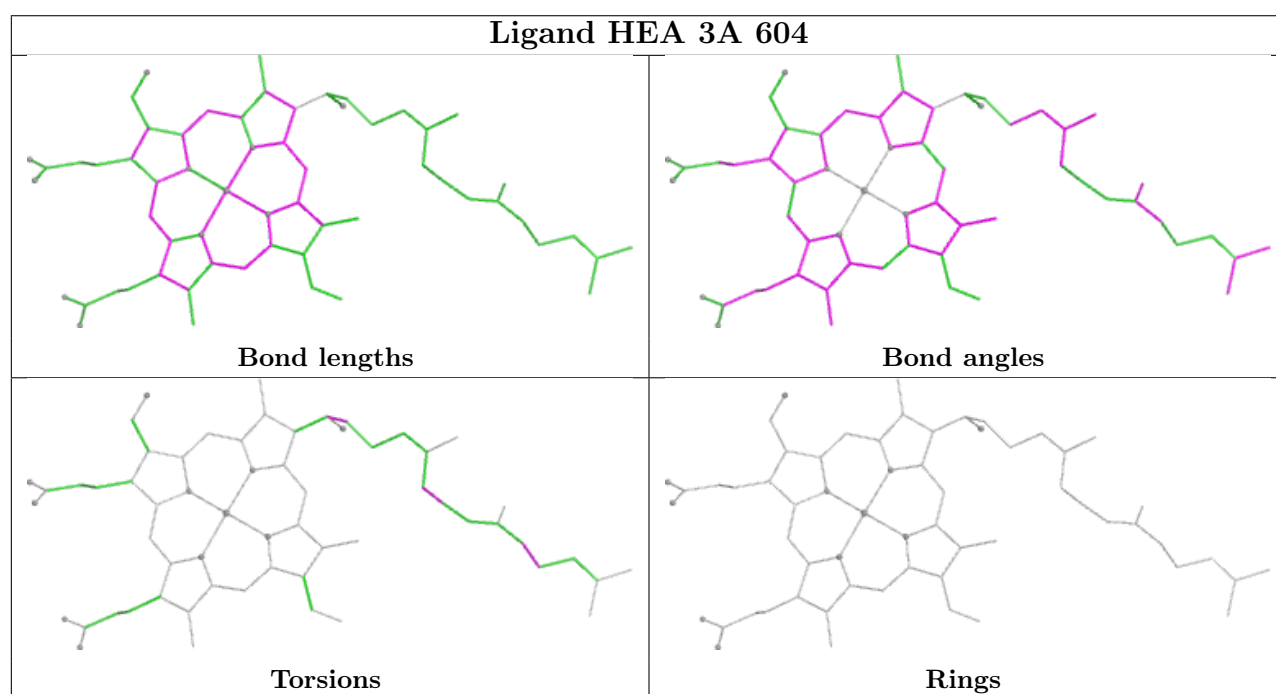
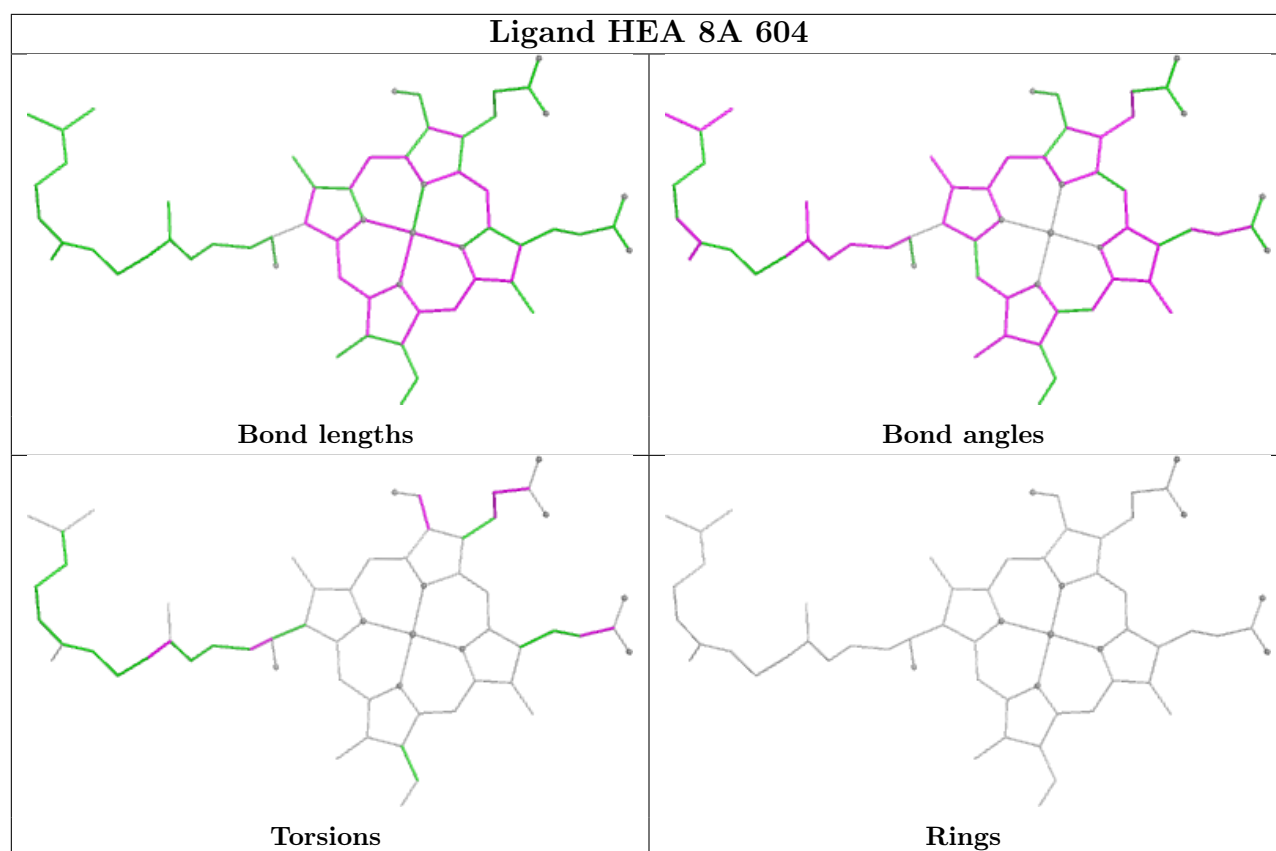
Bond angles

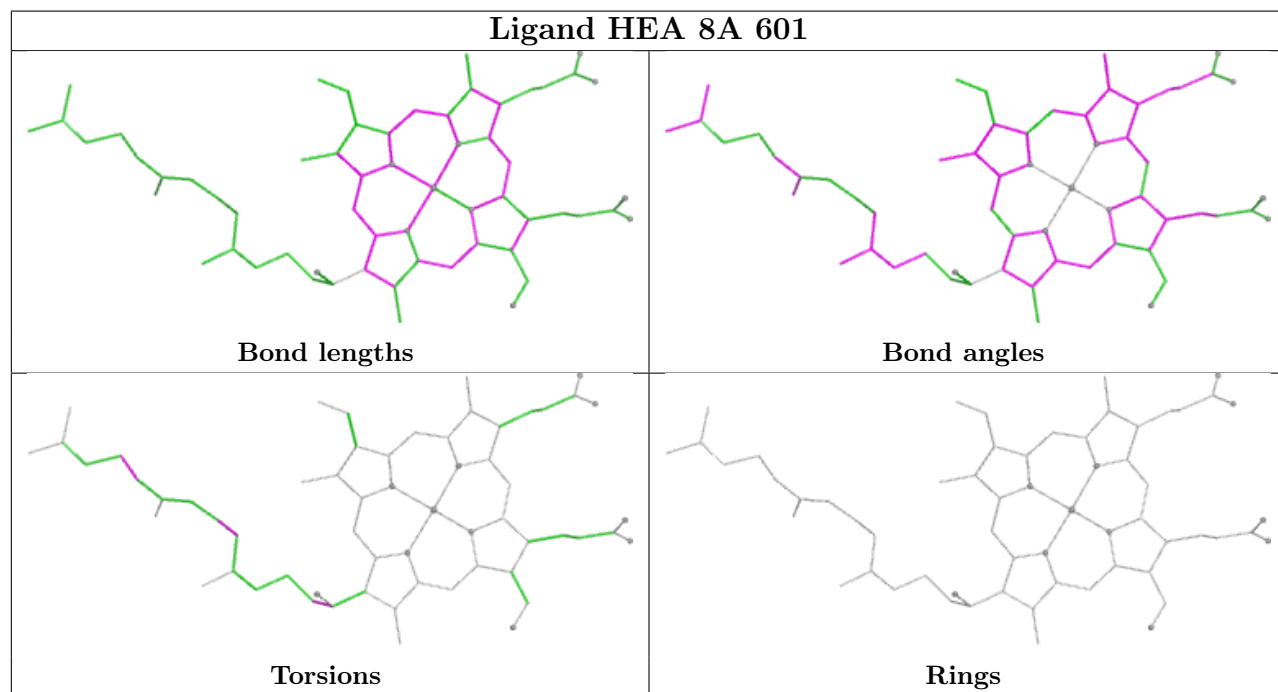
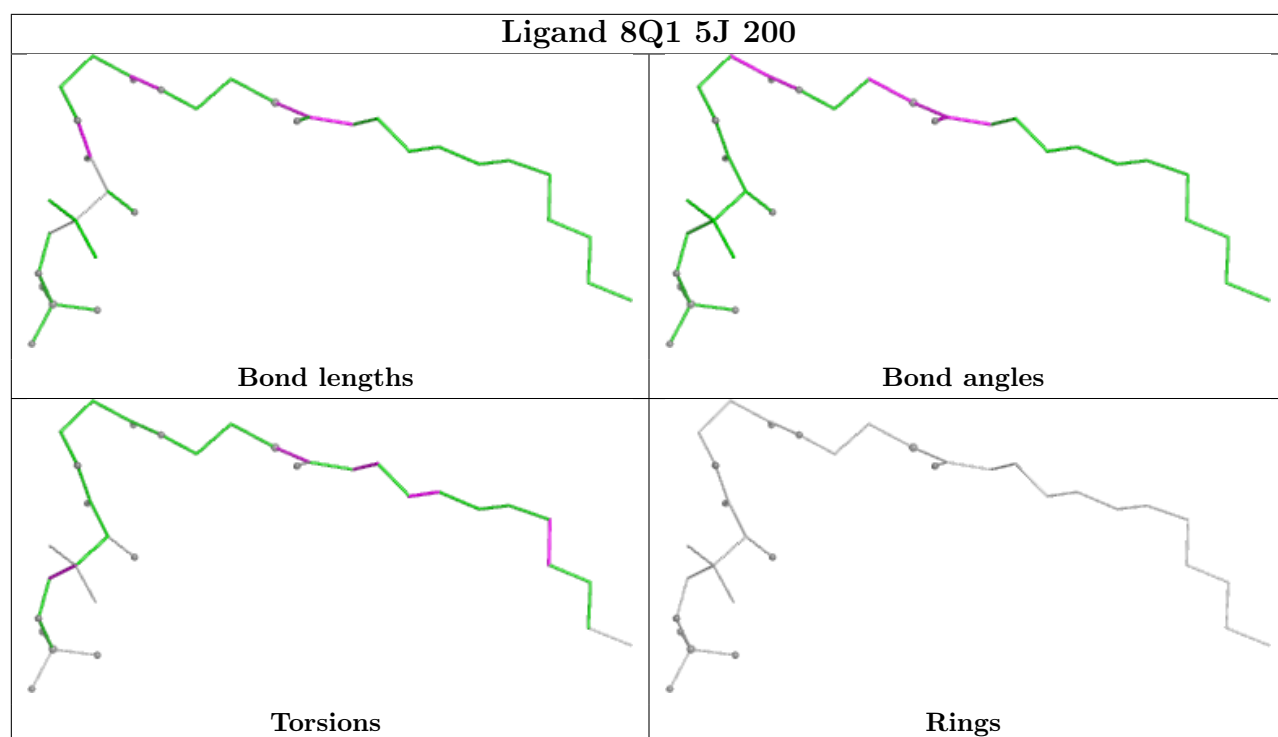


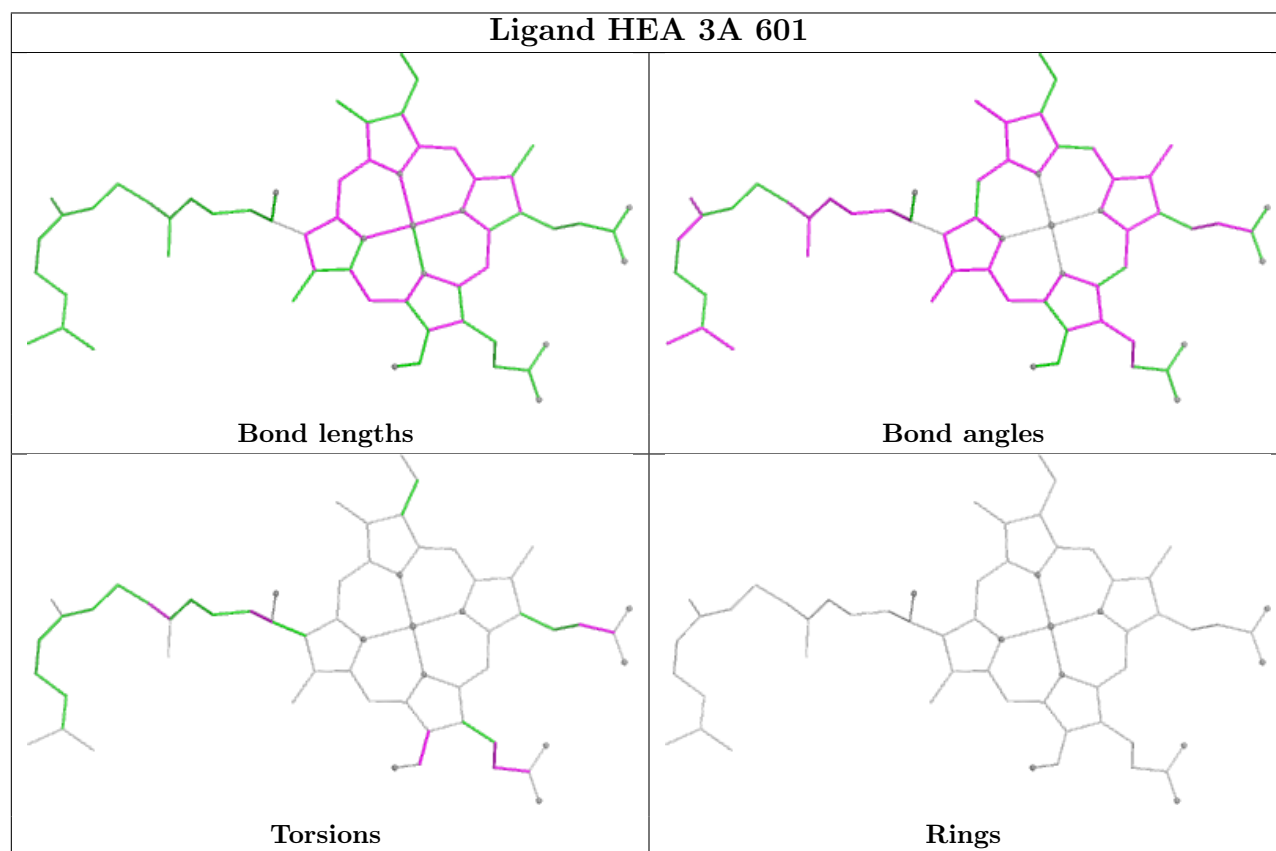
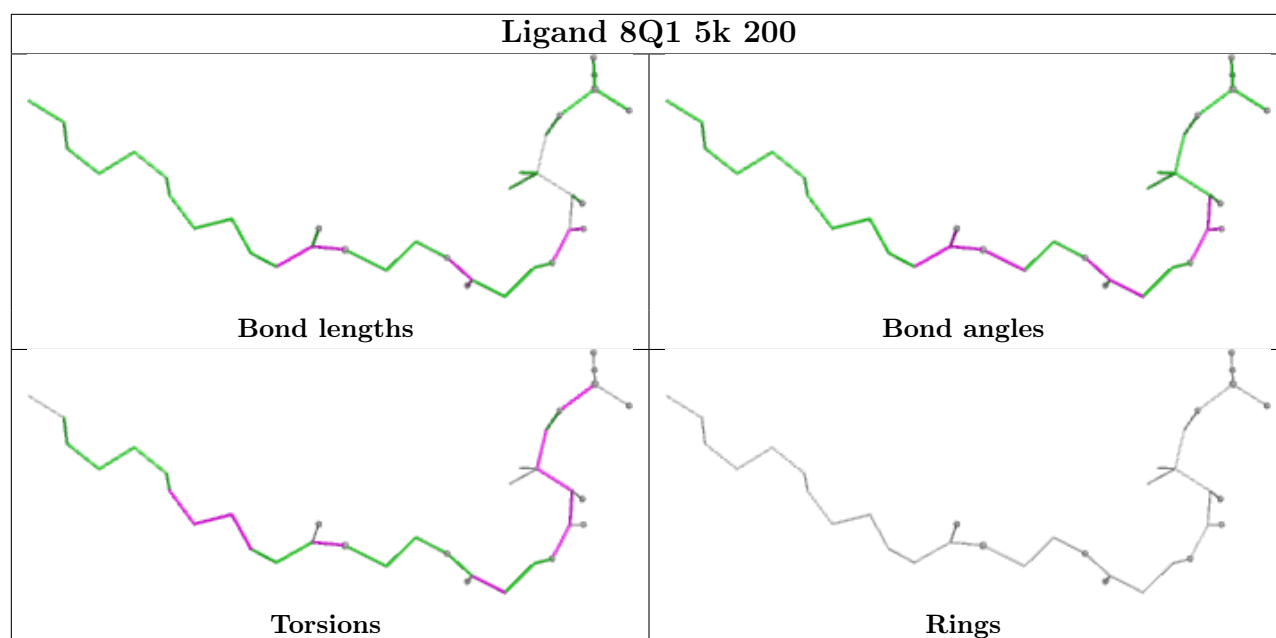
Torsions



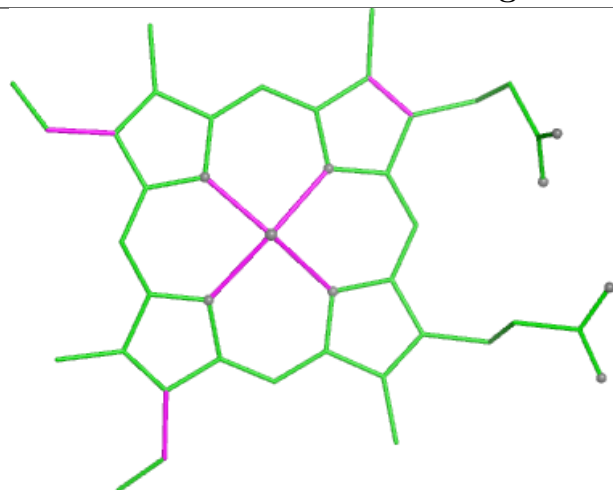
Rings



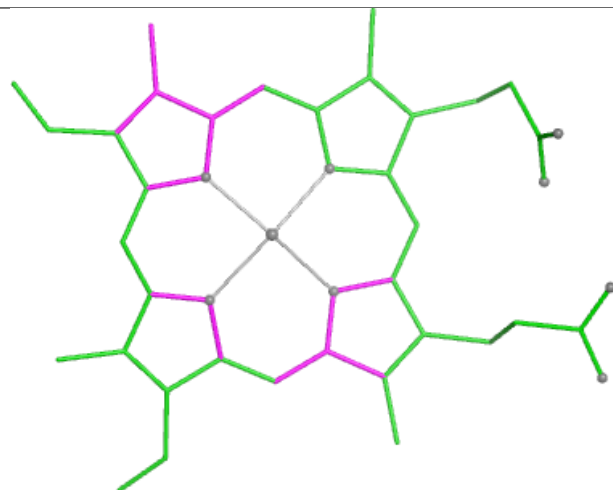




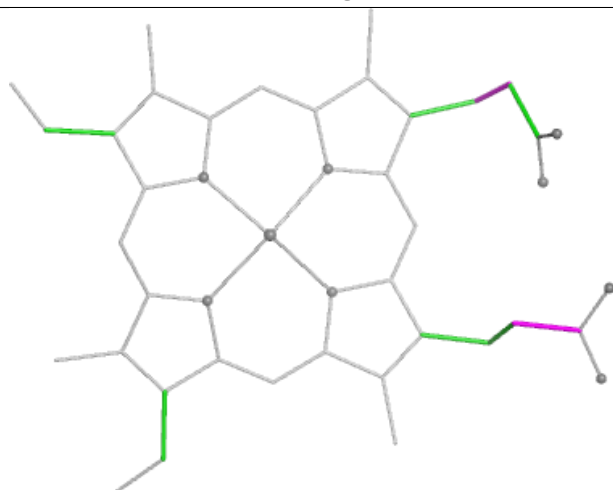
Ligand HEM 6A 402



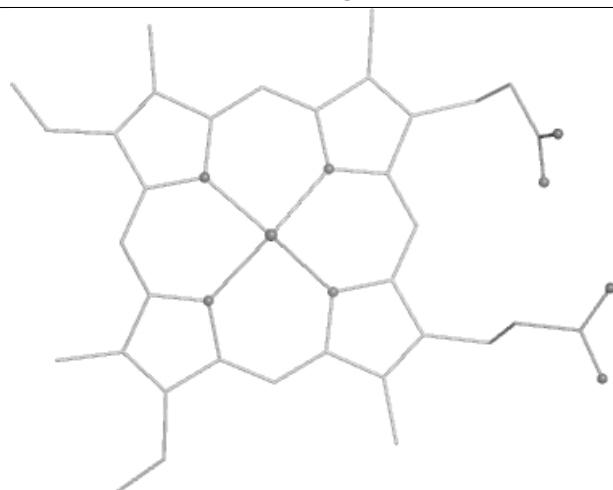
Bond lengths



Bond angles

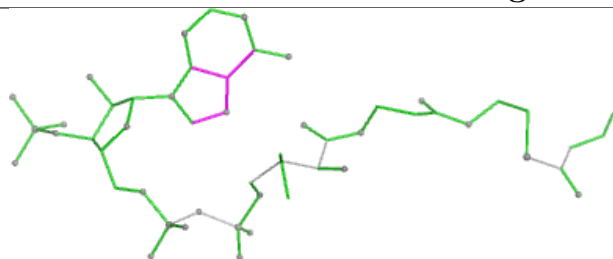


Torsions

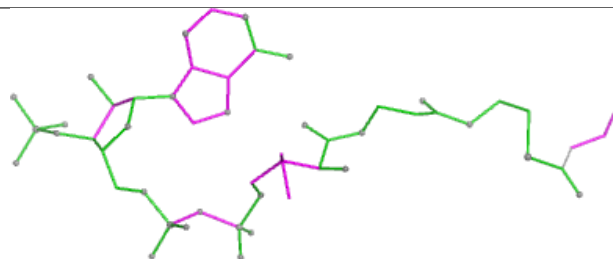


Rings

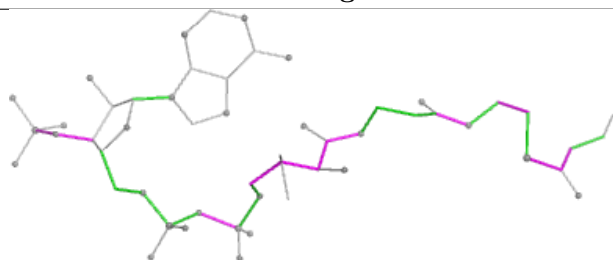
Ligand COO 5s 401



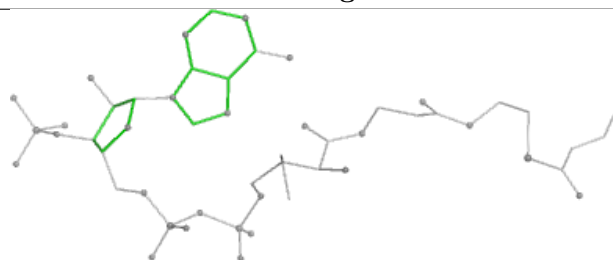
Bond lengths



Bond angles

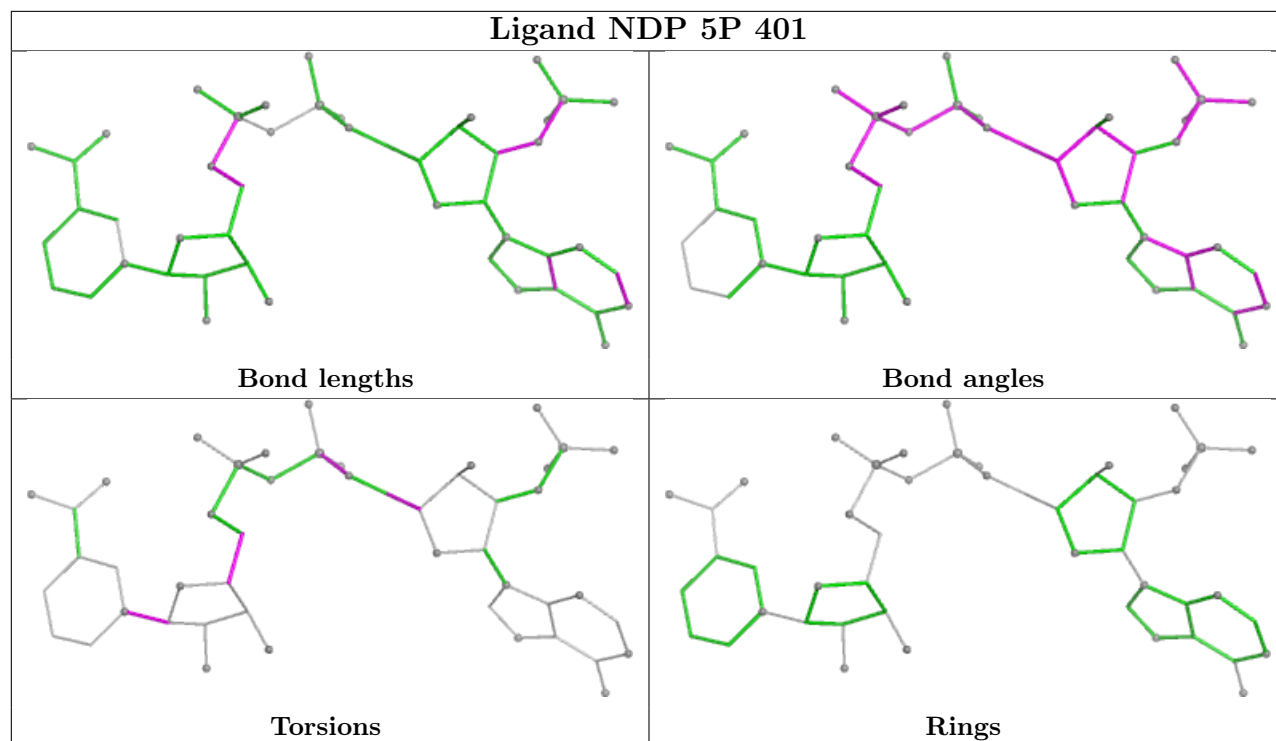


Torsions

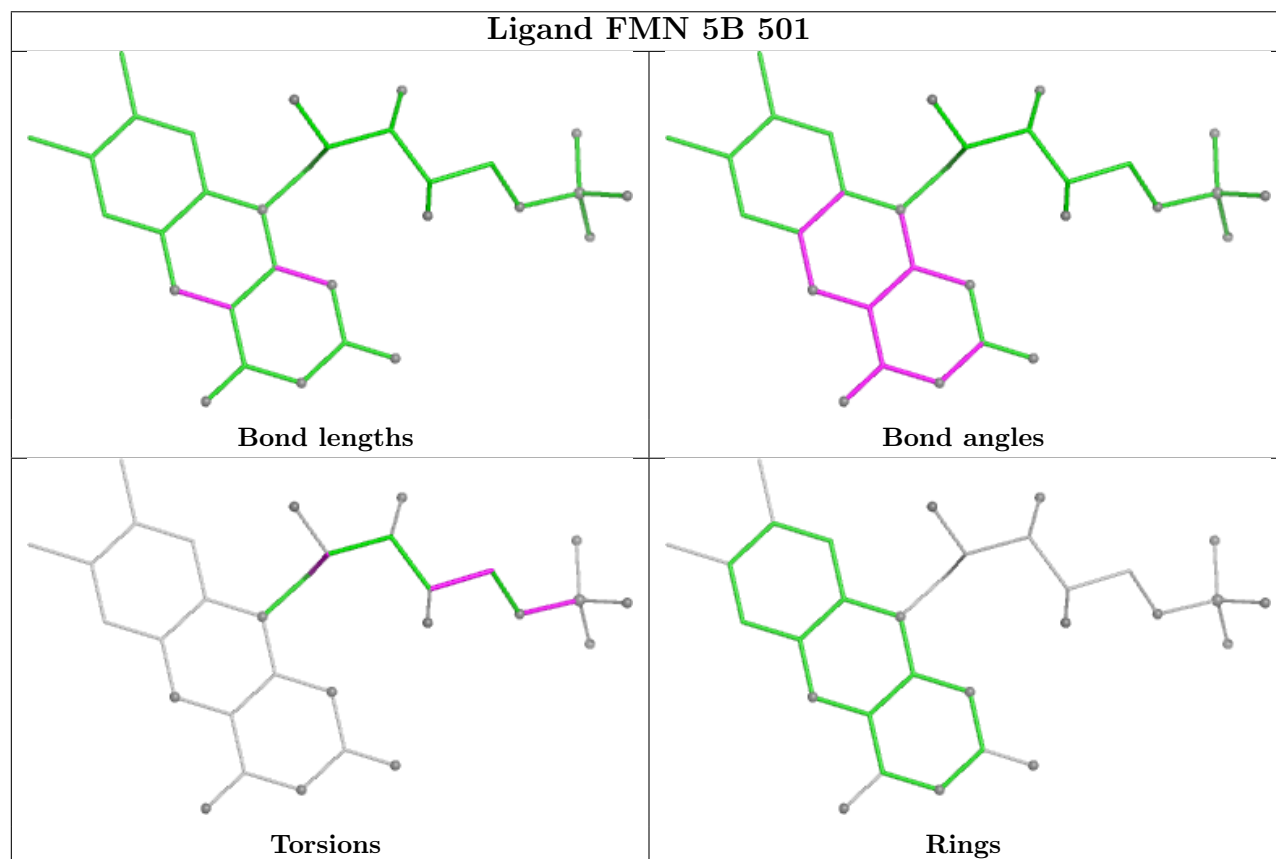


Rings

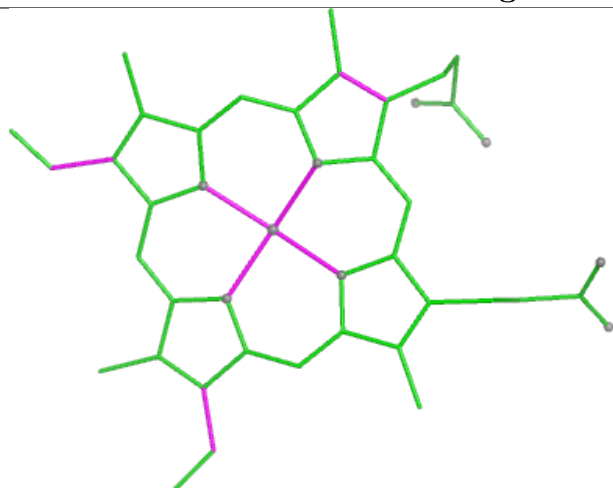
Ligand NDP 5P 401



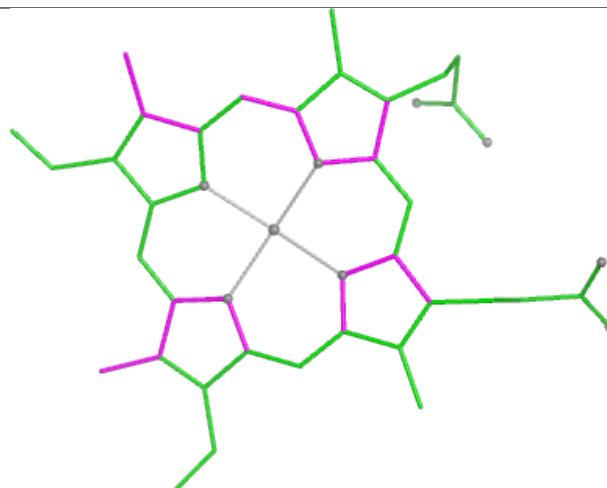
Ligand FMN 5B 501



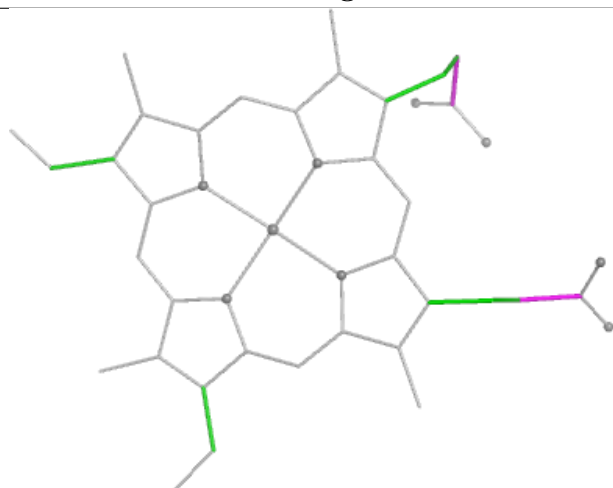
Ligand HEM 1A 402



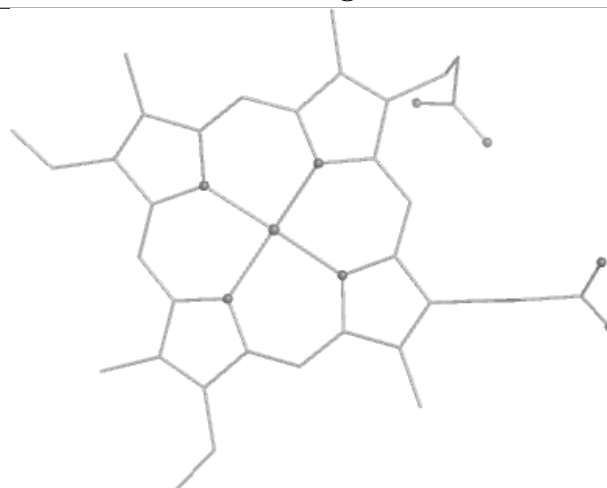
Bond lengths



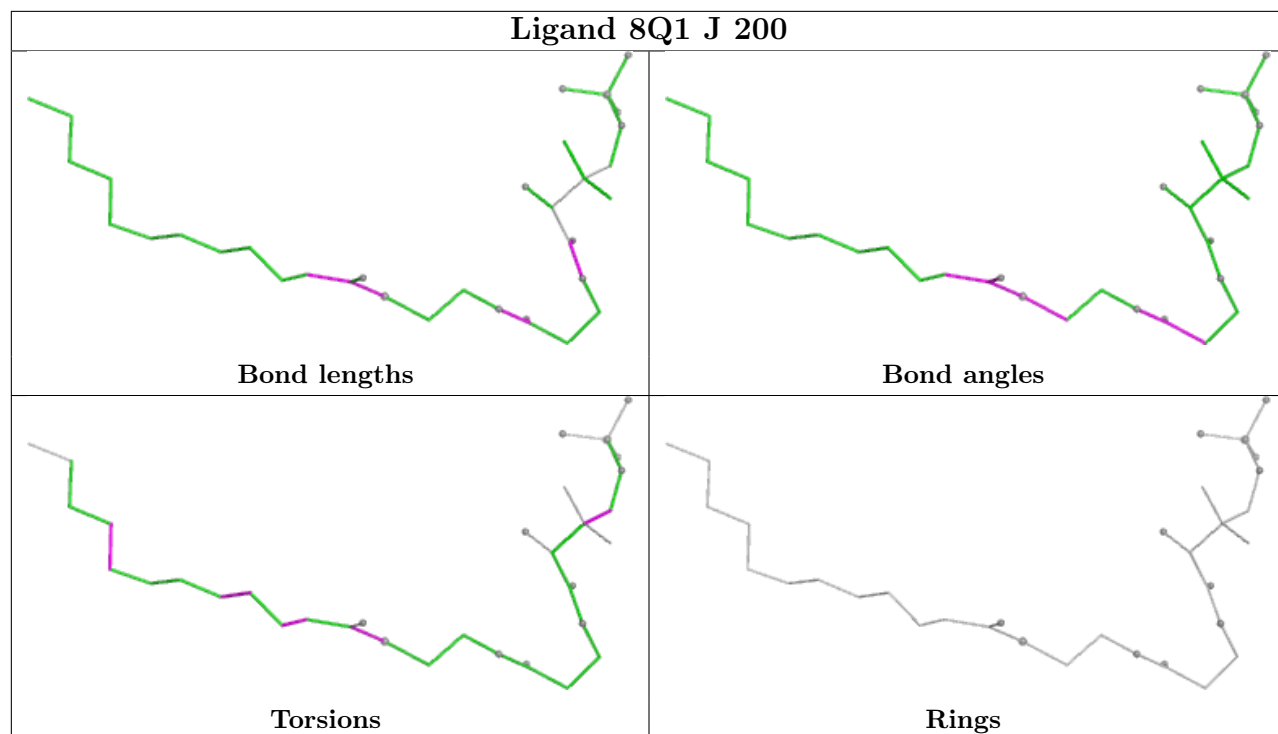
Bond angles

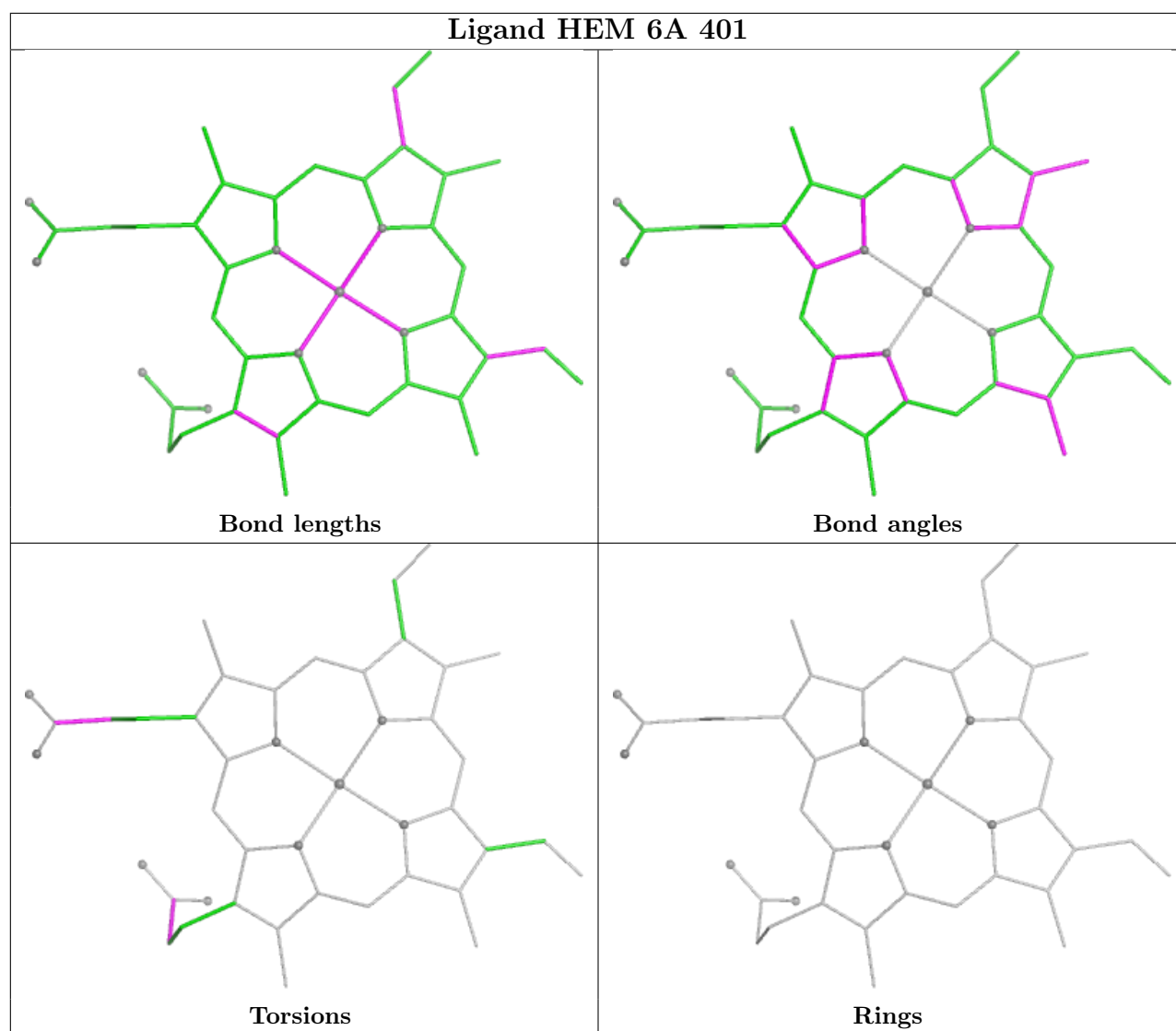


Torsions



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.

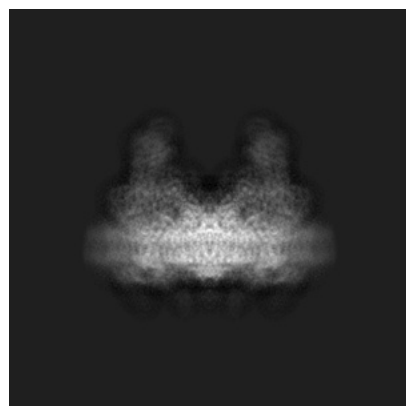
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50210. These allow visual inspection of the internal detail of the map and identification of artifacts.

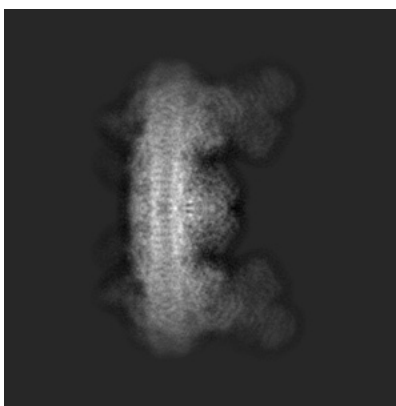
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

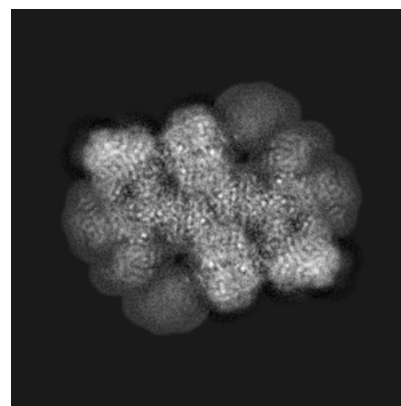
6.1.1 Primary map



X

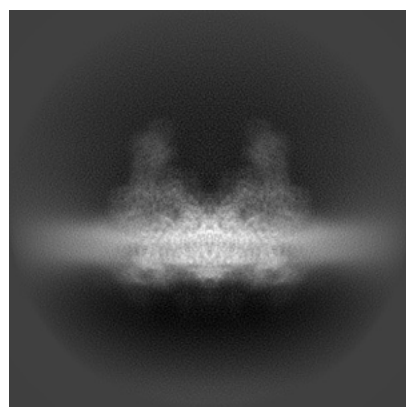


Y

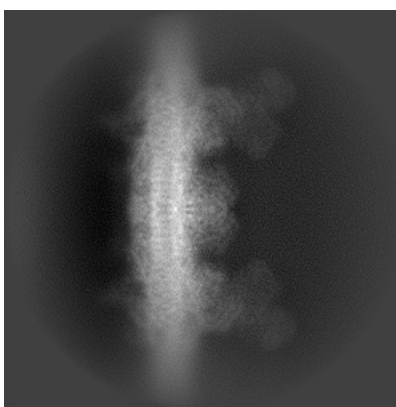


Z

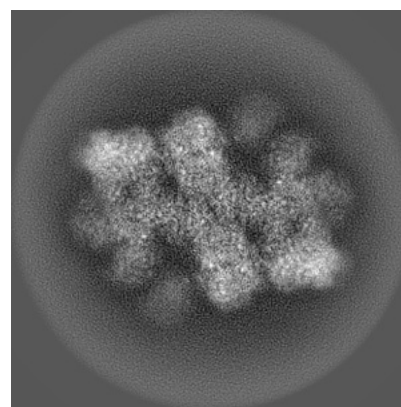
6.1.2 Raw map



X



Y

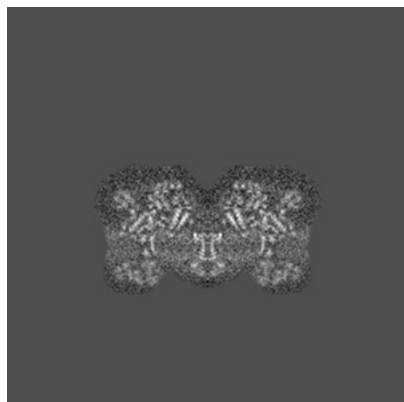


Z

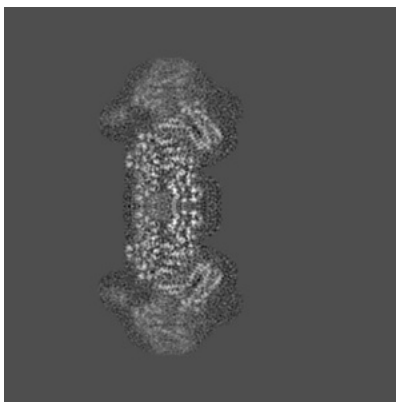
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

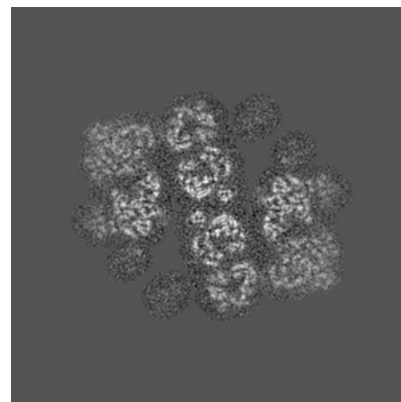
6.2.1 Primary map



X Index: 144

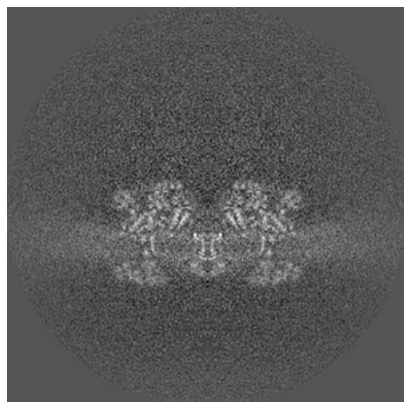


Y Index: 144

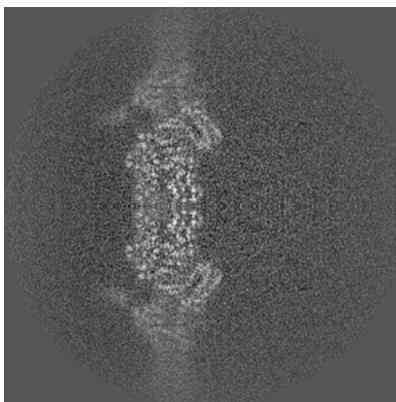


Z Index: 144

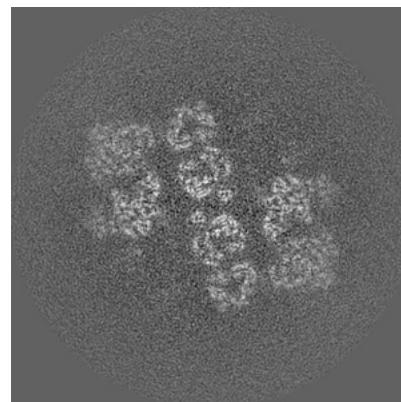
6.2.2 Raw map



X Index: 144



Y Index: 144

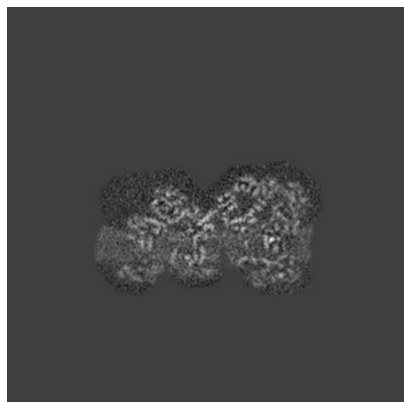


Z Index: 144

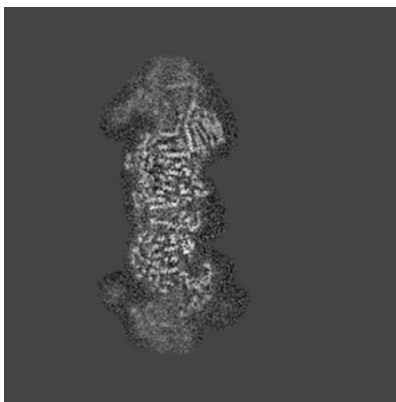
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

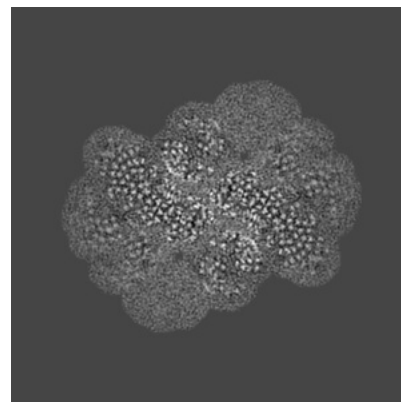
6.3.1 Primary map



X Index: 139

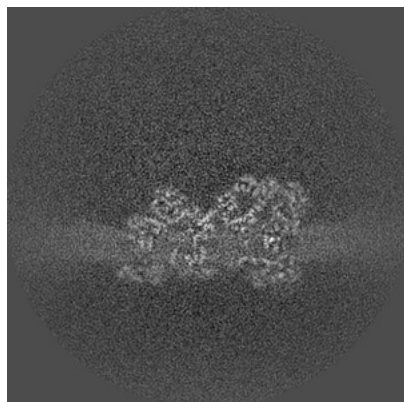


Y Index: 148

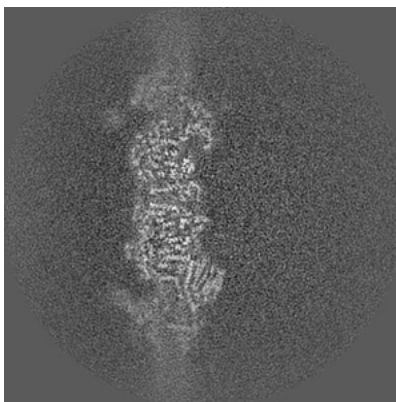


Z Index: 123

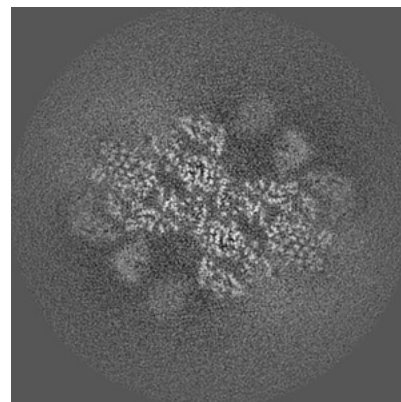
6.3.2 Raw map



X Index: 139



Y Index: 140

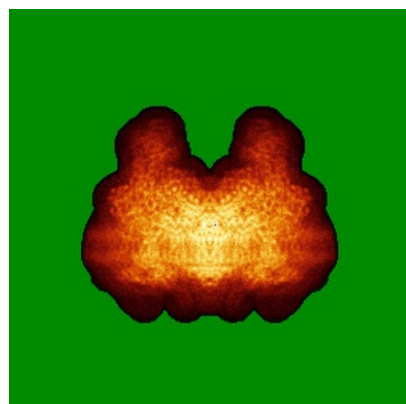


Z Index: 134

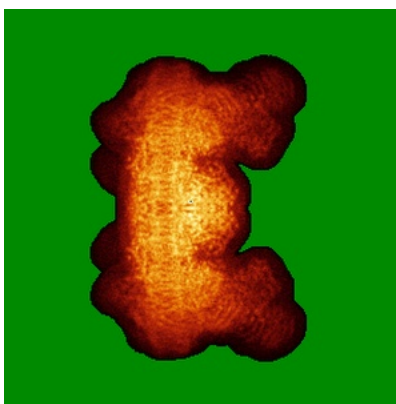
The images above show the largest variance slices of the map in three orthogonal directions.

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

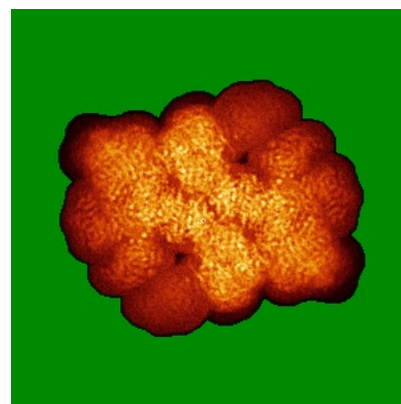
6.4.1 Primary map



X

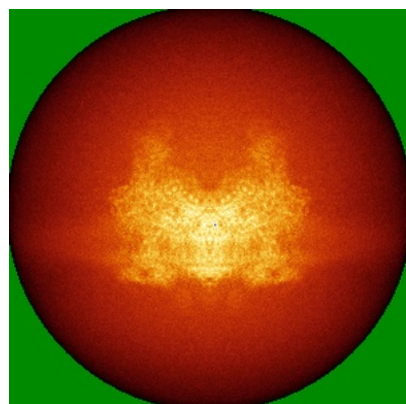


Y

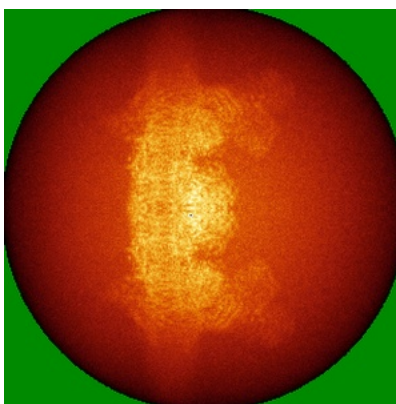


Z

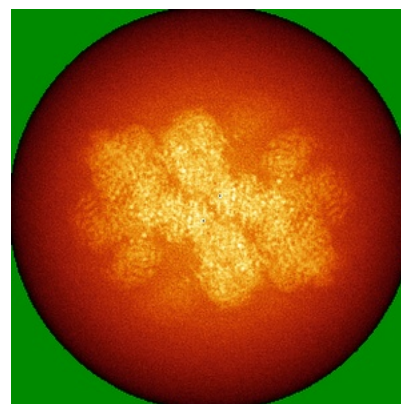
6.4.2 Raw map



X



Y

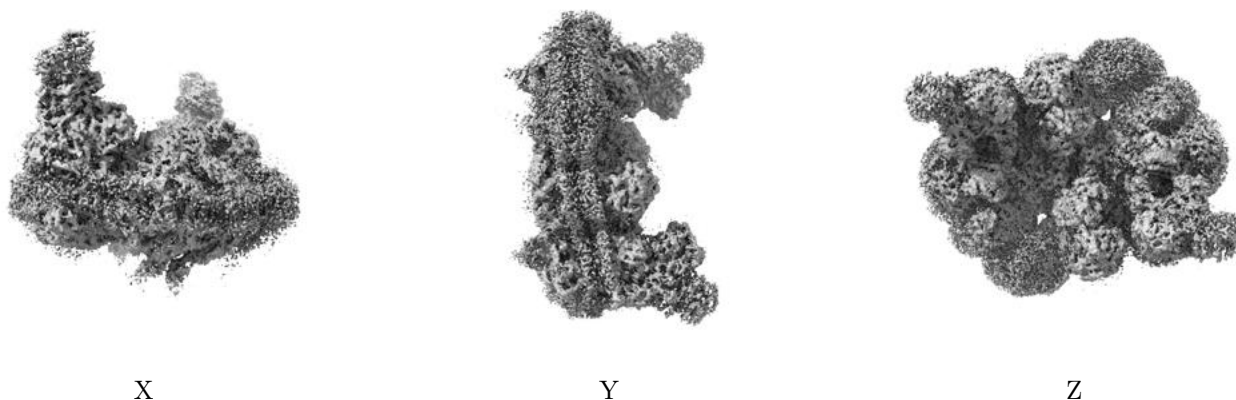


Z

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

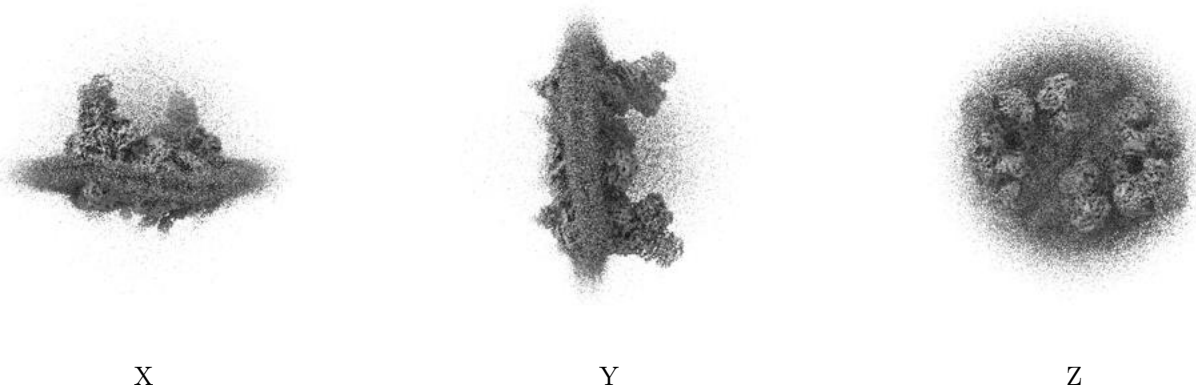
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

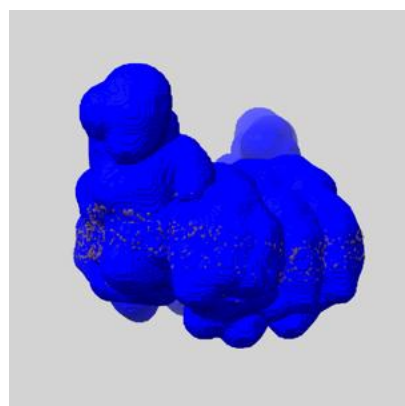
6.6 Mask visualisation [i](#)

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

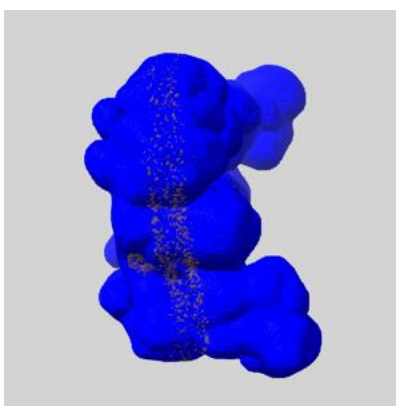
A mask typically either:

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

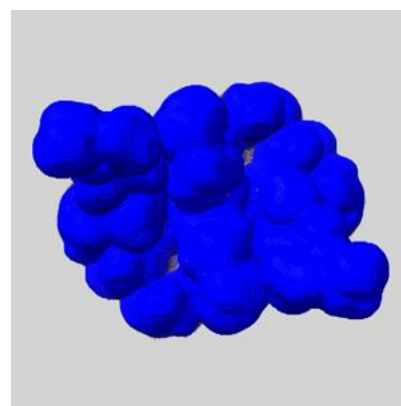
6.6.1 emd_50210_msk_1.map [i](#)



X



Y

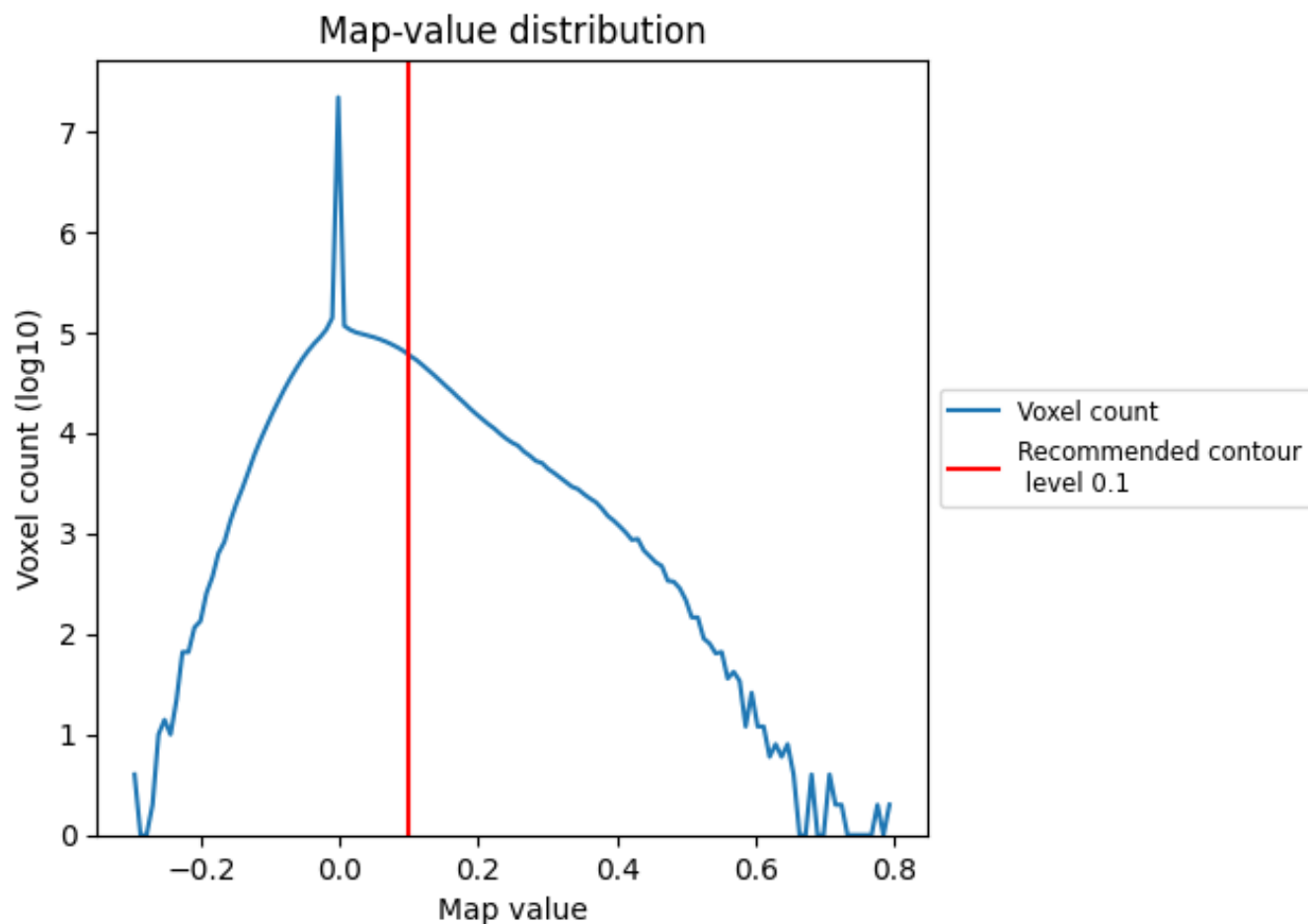


Z

7 Map analysis [i](#)

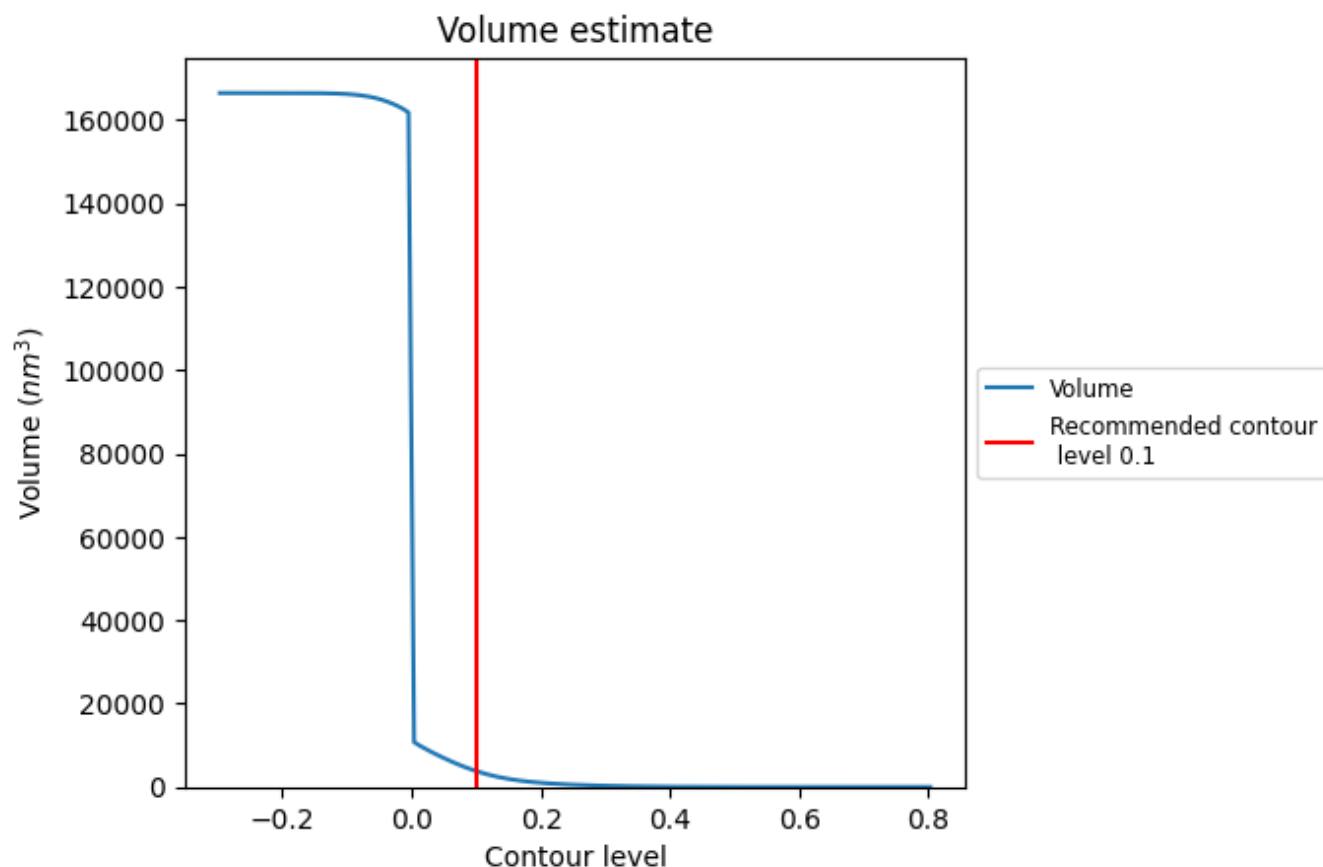
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

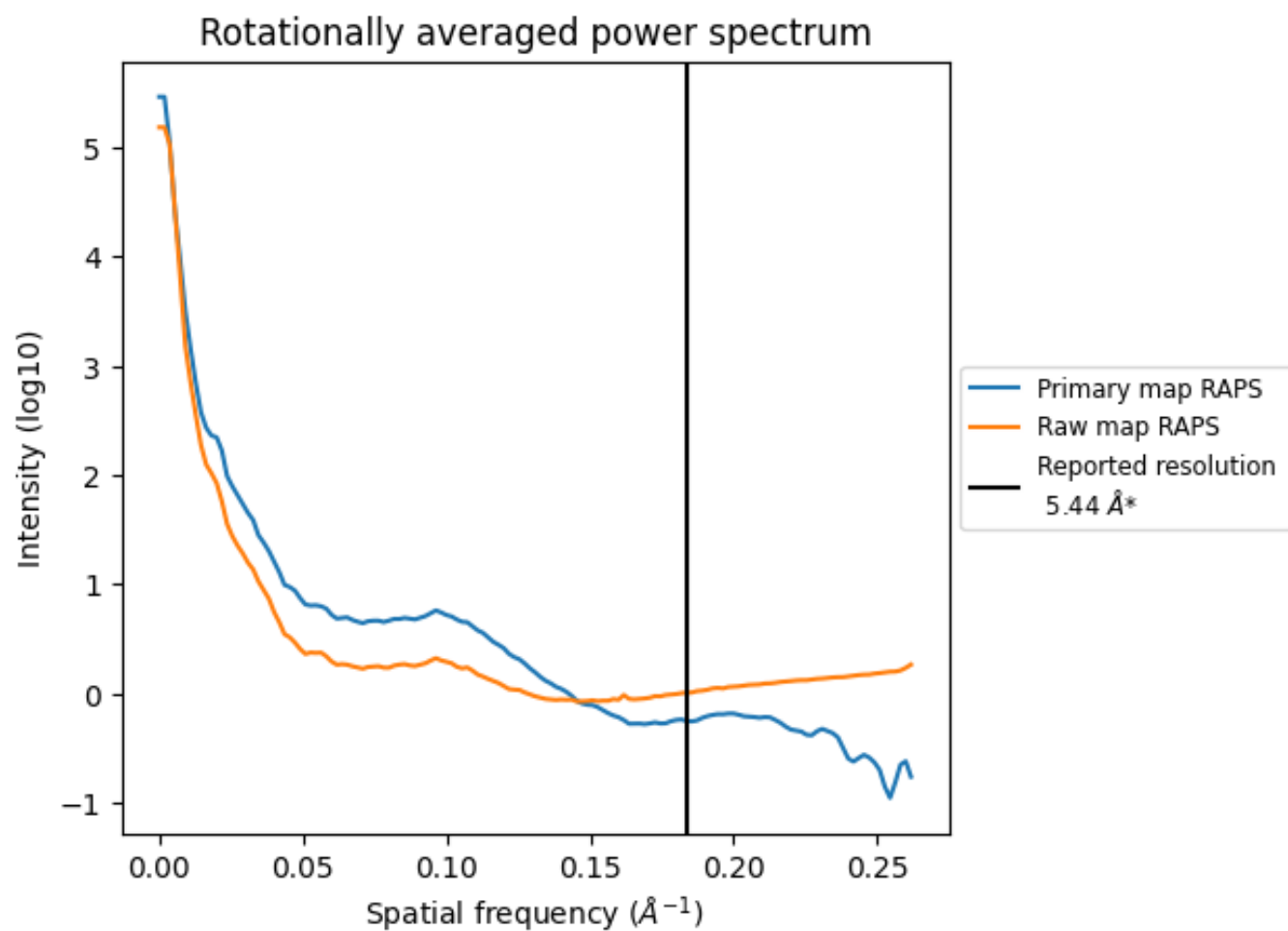
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3804 nm^3 ; this corresponds to an approximate mass of 3437 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 ⓘ

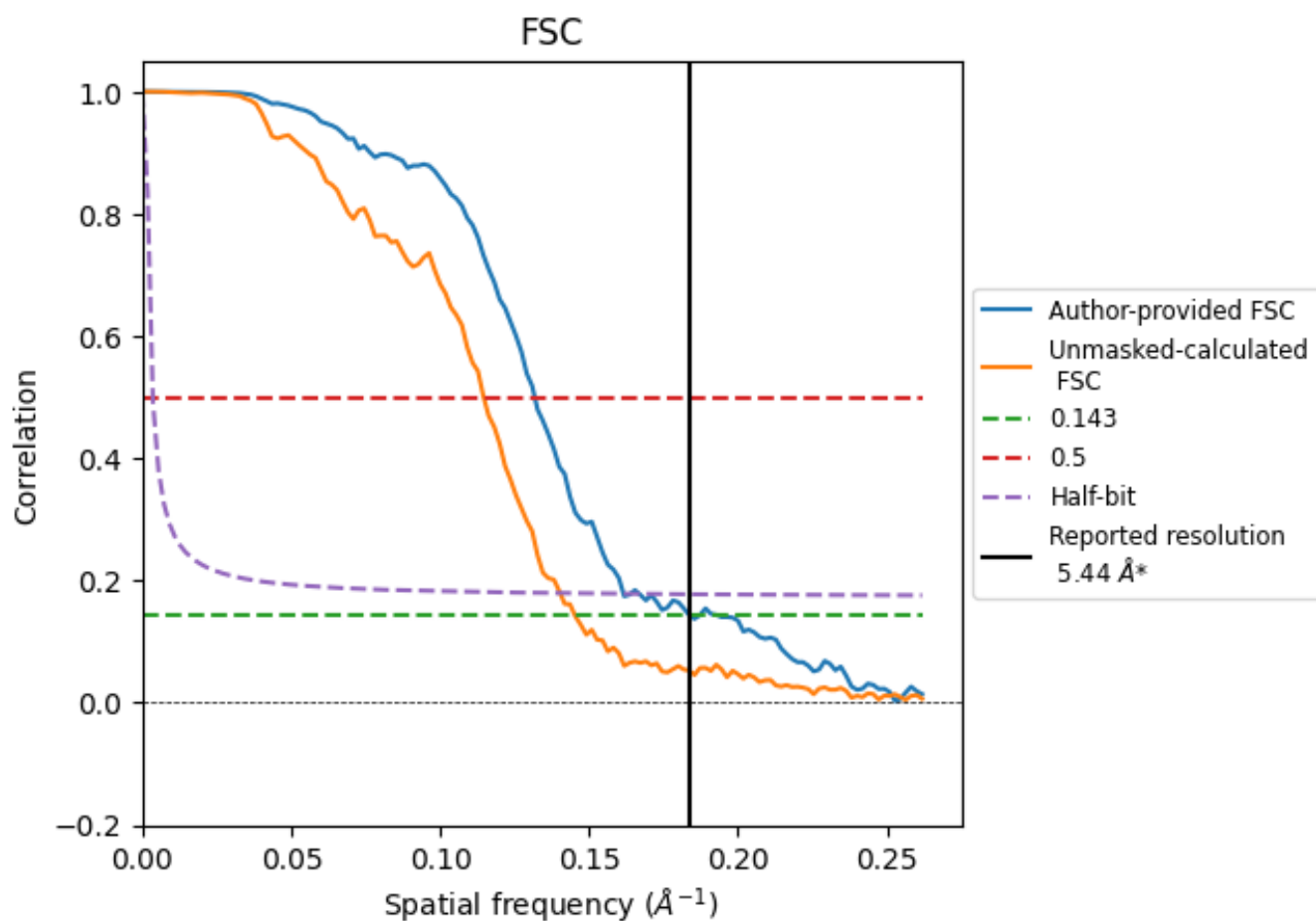


*Reported resolution corresponds to spatial frequency of 0.184 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.184 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

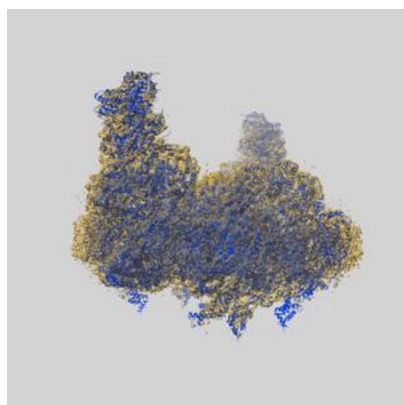
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.44	-	-
Author-provided FSC curve	5.45	7.59	6.19
Unmasked-calculated*	6.88	8.73	7.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.88 differs from the reported value 5.44 by more than 10 %

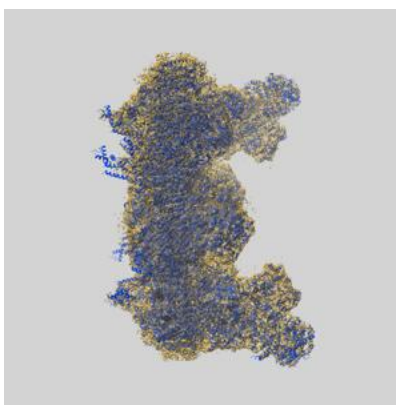
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50210 and PDB model 9F62. Per-residue inclusion information can be found in section 3 on page 38.

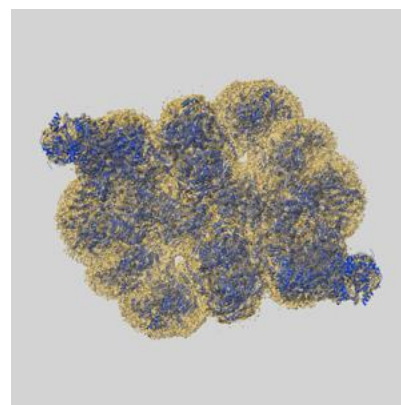
9.1 Map-model overlay [i](#)



X



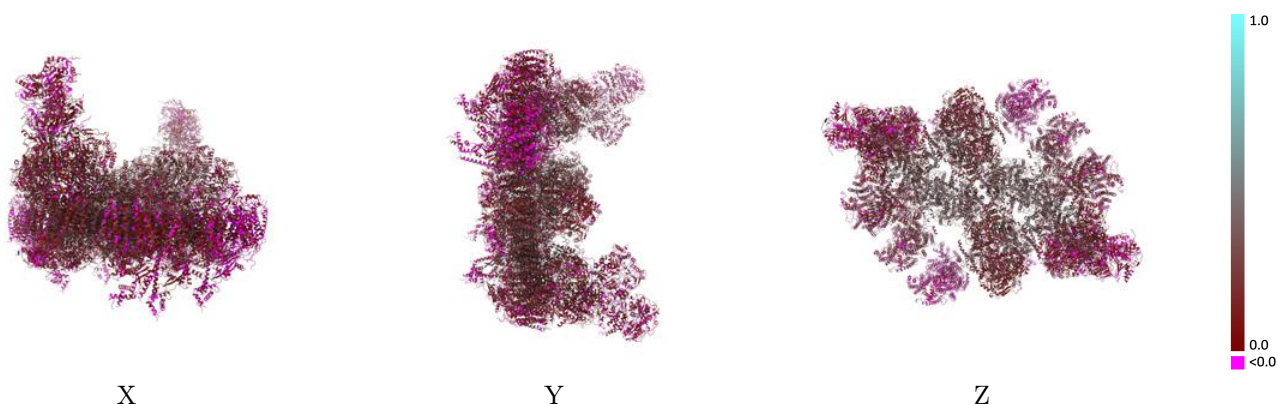
Y



Z

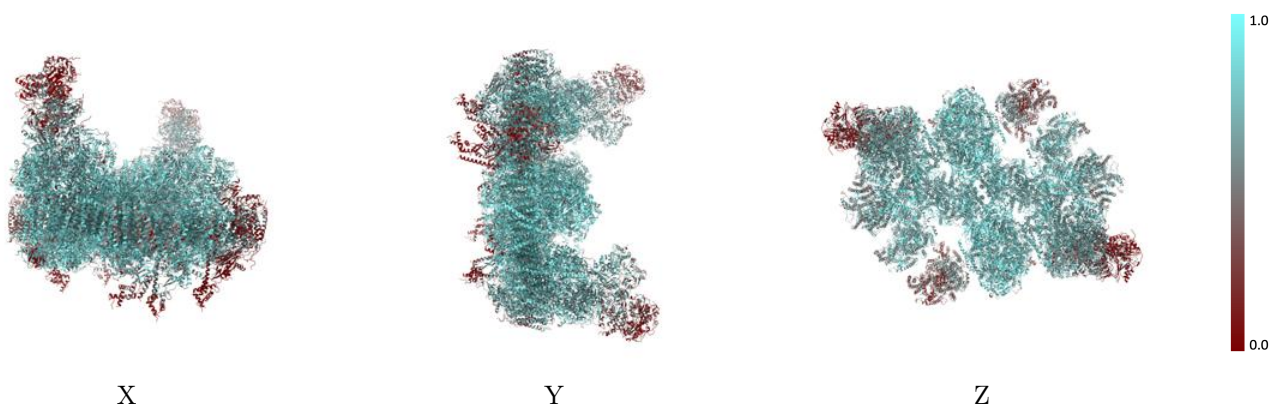
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



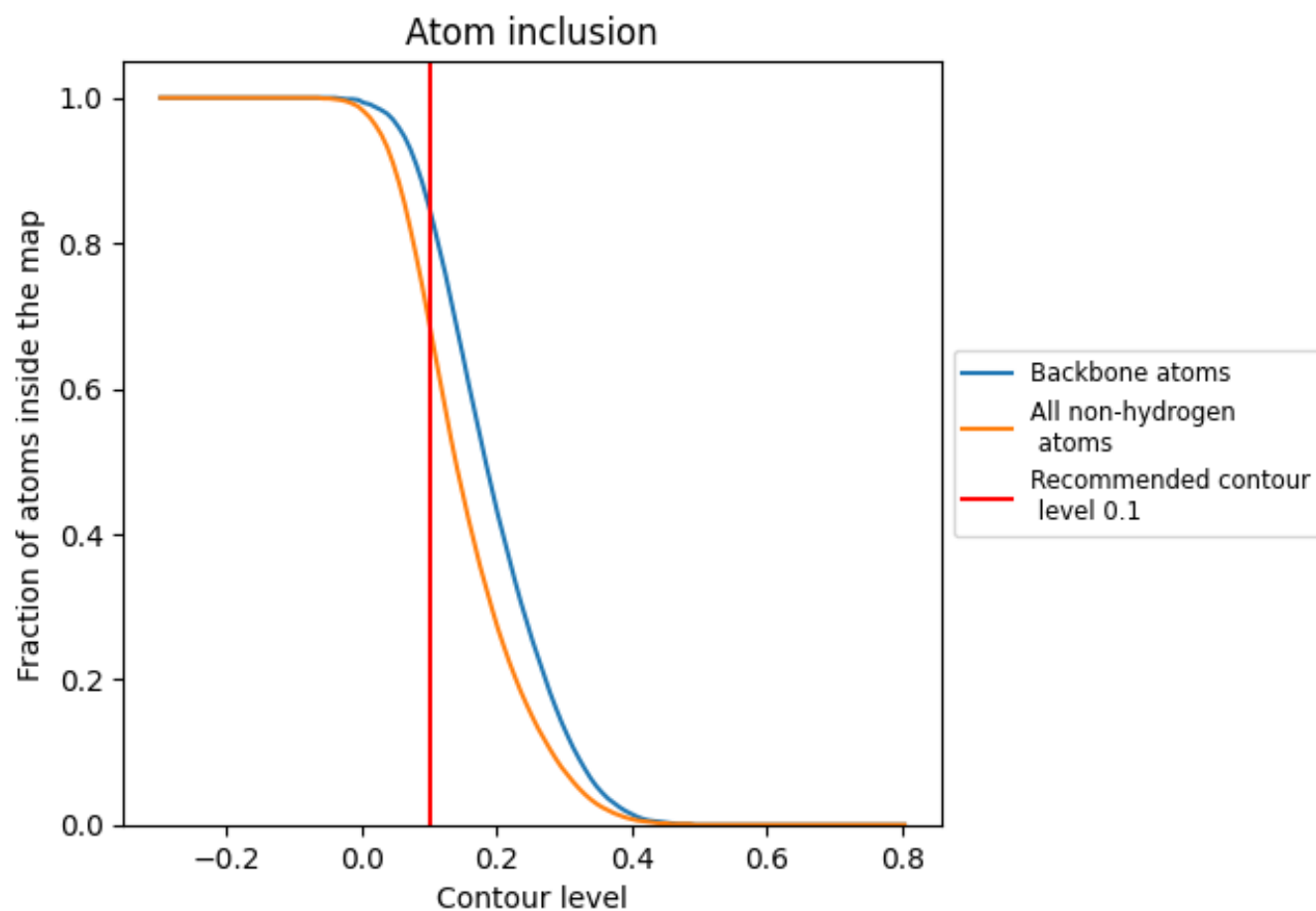
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.1860
1A	 0.8300	 0.2440
1B	 0.8460	 0.2770
1C	 0.6800	 0.1370
1D	 0.5770	 0.0990
1E	 0.8530	 0.2330
1F	 0.8120	 0.1950
1G	 0.8560	 0.2470
1H	 0.8220	 0.2080
1I	 0.8030	 0.1970
1J	 0.6890	 0.1300
1K	 0.8600	 0.2700
1L	 0.8030	 0.2010
1M	 0.8730	 0.2800
1N	 0.7910	 0.2110
1O	 0.8970	 0.2540
1P	 0.8370	 0.2270
1Q	 0.8430	 0.2440
1R	 0.8460	 0.2440
1S	 0.7830	 0.2070
1T	 0.8510	 0.2610
2A	 0.6240	 0.1410
2B	 0.6420	 0.1470
2C	 0.4820	 0.0880
2D	 0.5830	 0.1110
2E	 0.6350	 0.1480
2F	 0.6460	 0.1490
2G	 0.4980	 0.0960
2H	 0.4590	 0.0850
2I	 0.5360	 0.1070
2J	 0.6200	 0.1390
2K	 0.4070	 0.0790
2L	 0.6350	 0.1370
3A	 0.7430	 0.1530
3B	 0.7470	 0.1620



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Chain	Atom inclusion	Q-score
3C	 0.6530	 0.1570
3D	 0.6860	 0.1270
3E	 0.6960	 0.1110
3F	 0.6850	 0.1660
3G	 0.5420	 0.0910
3H	 0.4920	 0.0710
3I	 0.7410	 0.1140
3J	 0.8140	 0.1650
3K	 0.6580	 0.0910
3L	 0.6510	 0.1210
4A	 0.5160	 0.0480
4B	 0.4480	 0.0510
4C	 0.1580	 0.0530
4D	 0.3330	 0.0310
4E	 0.1600	 0.0580
4F	 0.3750	 0.1140
4G	 0.1930	 0.0230
4H	 0.0700	 0.0190
4I	 0.2660	 0.0090
4J	 0.4530	 0.0970
4K	 0.2340	 -0.0030
4L	 0.3770	 0.0120
5A	 0.2210	 0.1040
5B	 0.2100	 0.0750
5C	 0.5440	 0.1320
5D	 0.7210	 0.2010
5E	 0.6690	 0.1800
5F	 0.7330	 0.2060
5G	 0.6710	 0.1570
5H	 0.5780	 0.1630
5I	 0.6690	 0.1690
5J	 0.7740	 0.2420
5K	 0.7000	 0.1730
5L	 0.5610	 0.1690
5M	 0.4520	 0.1210
5N	 0.6910	 0.1840
5O	 0.6280	 0.1230
5P	 0.7620	 0.2020
5Q	 0.7000	 0.1810
5R	 0.8110	 0.2780
5S	 0.7140	 0.1920
5T	 0.8470	 0.3010

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Chain	Atom inclusion	Q-score
5U	 0.7940	 0.2470
5V	 0.8670	 0.2840
5W	 0.7650	 0.2310
5X	 0.9150	 0.3130
5Y	 0.8200	 0.2410
5Z	 0.8940	 0.2740
5a	 0.8880	 0.2630
5b	 0.8560	 0.2740
5c	 0.6960	 0.1900
5d	 0.8570	 0.2770
5e	 0.8920	 0.2900
5f	 0.7080	 0.1910
5g	 0.8570	 0.2170
5h	 0.9190	 0.3150
5i	 0.7980	 0.1940
5j	 0.8750	 0.2410
5k	 0.8810	 0.2970
5l	 0.8000	 0.2340
5m	 0.6540	 0.1690
5n	 0.6620	 0.1590
5o	 0.8560	 0.2530
5p	 0.8300	 0.2420
5q	 0.8920	 0.3070
5r	 0.8550	 0.2790
5s	 0.8380	 0.2330
5t	 0.8450	 0.2780
5u	 0.8500	 0.2590
5v	 0.8420	 0.2510
5w	 0.8890	 0.2930
5x	 0.8670	 0.2910
5y	 0.8940	 0.3060
6A	 0.8300	 0.2460
6B	 0.8460	 0.2780
6C	 0.6800	 0.1380
6D	 0.5780	 0.1010
6E	 0.8530	 0.2320
6F	 0.8160	 0.1990
6G	 0.8580	 0.2420
6H	 0.8250	 0.2090
6I	 0.7970	 0.1980
6J	 0.6960	 0.1340
6K	 0.8600	 0.2700

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Chain	Atom inclusion	Q-score
6L	 0.8040	 0.2080
6M	 0.8730	 0.2760
6N	 0.7920	 0.2110
6O	 0.8950	 0.2560
6P	 0.8390	 0.2230
6Q	 0.8430	 0.2420
6R	 0.8480	 0.2460
6S	 0.7840	 0.2060
6T	 0.8510	 0.2590
7A	 0.6240	 0.1410
7B	 0.6410	 0.1440
7C	 0.4840	 0.0880
7D	 0.5860	 0.1120
7E	 0.6330	 0.1540
7F	 0.6470	 0.1490
7G	 0.4960	 0.0920
7H	 0.4580	 0.0820
7I	 0.5450	 0.1100
7J	 0.6210	 0.1370
7K	 0.4070	 0.0860
7L	 0.6380	 0.1370
8A	 0.7430	 0.1550
8B	 0.7450	 0.1630
8C	 0.6500	 0.1610
8D	 0.6870	 0.1310
8E	 0.7040	 0.1150
8F	 0.6840	 0.1660
8G	 0.5370	 0.0930
8H	 0.4930	 0.0710
8I	 0.7440	 0.1130
8J	 0.8150	 0.1690
8K	 0.6580	 0.0900
8L	 0.6520	 0.1220
9A	 0.5170	 0.0460
9B	 0.4390	 0.0480
9C	 0.1540	 0.0600
9D	 0.3310	 0.0250
9E	 0.1620	 0.0610
9F	 0.3860	 0.1180
9G	 0.1990	 0.0270
9H	 0.0760	 0.0280
9I	 0.2770	 0.0130

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Chain	Atom inclusion	Q-score
9J	 0.4660	 0.1080
9K	 0.2670	 0.0010
9L	 0.3690	 0.0120
A	 0.2220	 0.1040
B	 0.2100	 0.0750
C	 0.5440	 0.1300
D	 0.7220	 0.2000
E	 0.6700	 0.1780
F	 0.7330	 0.2070
G	 0.6700	 0.1570
H	 0.5770	 0.1660
I	 0.6730	 0.1710
J	 0.7740	 0.2400
K	 0.7000	 0.1740
L	 0.5610	 0.1690
M	 0.4600	 0.1220
N	 0.6900	 0.1820
O	 0.6260	 0.1240
P	 0.7620	 0.2030
Q	 0.6980	 0.1810
R	 0.8110	 0.2780
S	 0.7130	 0.1940
T	 0.8480	 0.3000
U	 0.7930	 0.2490
V	 0.8670	 0.2800
W	 0.7630	 0.2330
X	 0.9160	 0.3100
Y	 0.8120	 0.2390
Z	 0.8950	 0.2740
a	 0.8960	 0.2610
b	 0.8590	 0.2740
c	 0.6980	 0.1940
d	 0.8540	 0.2740
e	 0.8920	 0.2910
f	 0.7000	 0.1870
g	 0.8690	 0.2330
h	 0.9190	 0.3140
i	 0.7880	 0.1910
j	 0.8700	 0.2390
k	 0.8810	 0.2960
l	 0.7990	 0.2350
m	 0.6570	 0.1750

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Chain	Atom inclusion	Q-score
n	 0.6620	 0.1630
o	 0.8540	 0.2530
p	 0.8280	 0.2440
q	 0.8930	 0.3050
r	 0.8560	 0.2790
s	 0.8390	 0.2360
t	 0.8470	 0.2810
u	 0.8510	 0.2620
v	 0.8480	 0.2420
w	 0.8970	 0.2890
x	 0.8670	 0.2900
y	 0.8940	 0.3020