



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 01:32 AM EDT

PDB ID : 8UCA / pdb_00008uca
EMDB ID : EMD-42122
Title : Formation of I2+III2 supercomplex rescues respiratory chain defects
Authors : Letts, J.A.; Padavannil, A.
Deposited on : 2023-09-26
Resolution : 3.70 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:

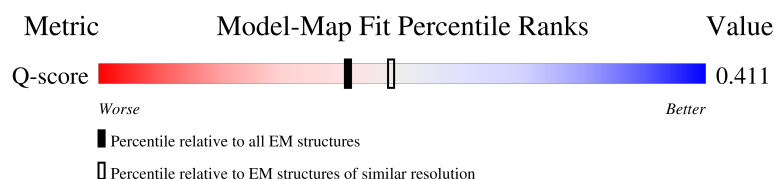
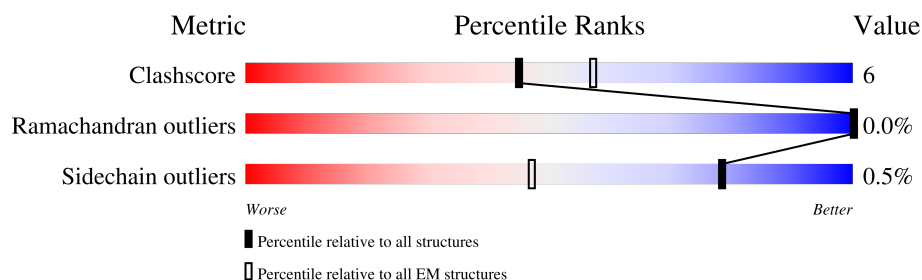
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	3	115	
1	3a	115	
2	S3	263	
2	s3	263	

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Mol	Chain	Length	Quality of chain
3	S2	463	
3	s2	463	
4	1	318	
4	1a	318	
5	6	172	
5	6a	172	
6	4L	98	
6	4l	98	
7	5	607	
7	5a	607	
8	4	459	
8	4a	459	
9	2	345	
9	2a	345	
10	AL	355	
10	al	355	
11	A9	377	
11	a9	377	
12	S4	175	
12	s4	175	
13	S6	116	
13	s6	116	
14	A2	99	
14	a2	99	
15	AB	156	

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Mol	Chain	Length	Quality of chain
15	AC	156	
15	ab	156	
15	ac	156	
16	A5	116	
16	a5	116	
17	A6	131	
17	a6	131	
18	A8	172	
18	a8	172	
19	AM	142	
19	am	142	
20	AO	144	
20	ao	144	
21	A1	70	
21	a1	70	
22	A3	84	
22	a3	84	
23	C1	76	
23	c1	76	
24	C2	120	
24	c2	120	
25	S5	106	
25	s5	106	
26	B1	57	
26	b1	57	

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Mol	Chain	Length	Quality of chain
27	BM	151	
27	bm	151	
28	B5	189	
28	b5	189	
29	B6	127	
29	b6	127	
30	B2	105	
30	b2	105	
31	B3	104	
31	b3	104	
32	B8	186	
32	b8	186	
33	B4	129	
33	b4	129	
34	B9	179	
34	b9	179	
35	B7	136	
35	b7	136	
36	BL	176	
36	bl	176	
37	AN	145	
37	an	145	
38	A7	112	
38	a7	112	
39	V3	104	

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Mol	Chain	Length	Quality of chain
39	v3	104	
40	3A	446	
40	3L	446	
41	3B	439	
41	3M	439	
42	3C	380	
42	3N	380	
43	3D	241	
43	3O	241	
44	3E	196	
44	3P	196	
45	3F	110	
45	3Q	110	
46	3G	81	
46	3R	81	
47	3H	76	
47	3S	76	
48	3J	63	
48	3U	63	
49	3K	56	
49	3V	56	
50	3T	78	
51	V1	457	
51	v1	457	
52	V2	244	

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Mol	Chain	Length	Quality of chain
52	v2	244	
53	S1	716	
53	s1	716	
54	S7	224	
54	s7	224	
55	S8	212	
55	s8	212	

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
62	HEC	3D	401	X	-	-	-
62	HEC	3O	401	X	-	-	-
64	SF4	S7	301	-	-	X	-
64	SF4	s7	301	-	-	X	-
64	SF4	s8	301	-	-	X	-

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 162102 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	113	Total	C	N	O	S	0	0
			914	622	131	155	6		
1	3a	111	Total	C	N	O	S	0	0
			893	607	128	152	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S3	206	Total	C	N	O	S	0	0
			1712	1105	294	310	3		
2	s3	205	Total	C	N	O	S	0	0
			1701	1099	290	309	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	423	Total	C	N	O	S	0	0
			3410	2180	586	620	24		
3	s2	421	Total	C	N	O	S	0	0
			3386	2165	581	616	24		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	317	Total	C	N	O	S	0	0
			2530	1700	383	426	21		
4	1a	316	Total	C	N	O	S	0	0
			2522	1695	382	425	20		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	170	Total	C	N	O	S	0	0
			1290	868	184	224	14		
5	6a	171	Total	C	N	O	S	0	0
			1298	873	185	225	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4L	97	Total	C	N	O	S	0	0
			729	473	111	135	10		
6	4l	97	Total	C	N	O	S	0	0
			727	471	111	135	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		
7	5a	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		
8	4a	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		
9	2a	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	al	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		
11	a9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		
12	s4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		
13	s6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		
14	a2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AB	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	AC	88	Total	C	N	O	S	0	0
			706	453	104	144	5		
15	ab	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	ac	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A5	114	Total	C	N	O	S	0	0
			927	604	154	166	3		
16	a5	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A6	112	Total	C	N	O	S	0	0
			957	612	178	161	6		
17	a6	111	Total	C	N	O	S	0	0
			950	607	177	160	6		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A8	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		
18	a8	170	Total	C	N	O	S	0	0
			1389	884	249	246	10		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		
19	am	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AO	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		
20	ao	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		
21	a1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		
22	a3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C1	49	Total	C	N	O	S	0	0
			407	266	70	70	1		
23	c1	45	Total	C	N	O	S	0	0
			377	247	65	64	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		
24	c2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		
25	s5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		
26	b1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BM	98	Total	C	N	O	S	0	0
			826	536	133	153	4		
27	bm	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		
28	b5	138	Total	C	N	O	S	0	0
			1158	760	193	202	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	94	Total	C	N	O	S	0	0
			783	511	137	132	3		
29	b6	90	Total	C	N	O	S	0	0
			761	495	133	130	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	64	Total	C	N	O	S	0	0
			555	365	92	97	1		
30	b2	63	Total	C	N	O	S	0	0
			545	359	89	96	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B3	70	Total	C	N	O	S	0	0
			569	376	99	92	2		
31	b3	71	Total	C	N	O	S	0	0
			573	378	100	93	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		
32	b8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B4	125	Total	C	N	O		0	0
			1044	673	188	183			
33	b4	125	Total	C	N	O		0	0
			1044	673	188	183			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B9	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		
34	b9	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	114	Total	C	N	O	S	0	0
			984	620	185	171	8		
35	b7	117	Total	C	N	O	S	0	0
			1005	634	189	174	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	167	Total	C	N	O	S	0	0
			1410	888	251	263	8		
36	bl	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AN	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		
37	an	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A7	92	Total	C	N	O	S	0	0
			741	469	139	130	3		
38	a7	70	Total	C	N	O	S	0	0
			560	350	108	100	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	V3	40	Total	C	N	O	0	0
			339	213	62	64		
39	v3	36	Total	C	N	O	0	0
			303	190	56	57		

- Molecule 40 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
40	3L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 41 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
41	3M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 42 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
42	3N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 43 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
43	3O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 44 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3E	80	Total	C	N	O	S	0	0
			602	374	100	126	2		
44	3P	81	Total	C	N	O	S	0	0
			610	380	101	127	2		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	3Q	99	Total	C	N	O	S	0	0
			879	563	156	157	3		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3G	79	Total	C	N	O	S	0	0
			670	432	123	114	1		
46	3R	71	Total	C	N	O		0	0
			600	389	112	99			

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
47	3S	66	Total	C	N	O	S	0	0
			545	333	101	106	5		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	3J	56	Total	C	N	O	0	0
			460	302	81	77		
48	3U	59	Total	C	N	O	0	0
			489	320	85	84		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3K	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
49	3V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3T	56	Total	C	N	O	S	0	0
			397	250	76	69	2		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochond-

drial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V1	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		
51	v1	422	Total	C	N	O	S	0	0
			3259	2053	584	600	22		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	209	Total	C	N	O	S	0	0
			1630	1038	273	308	11		
52	v2	192	Total	C	N	O	S	0	0
			1517	965	255	286	11		

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		
53	s1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		
54	s7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

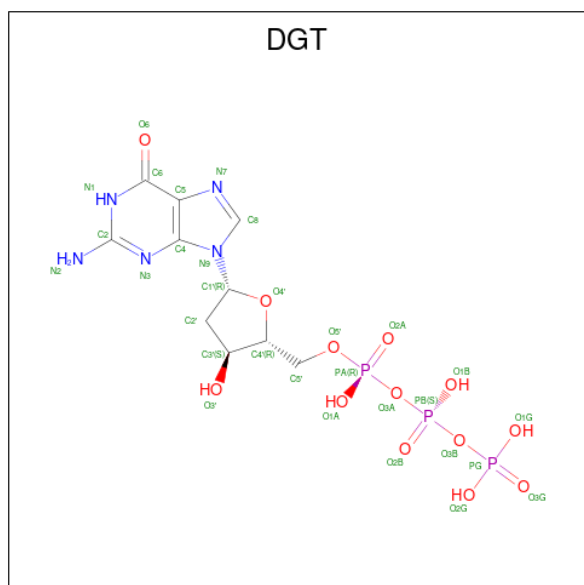
- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S8	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		
55	s8	164	Total	C	N	O	S	0	0
			1309	821	226	250	12		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

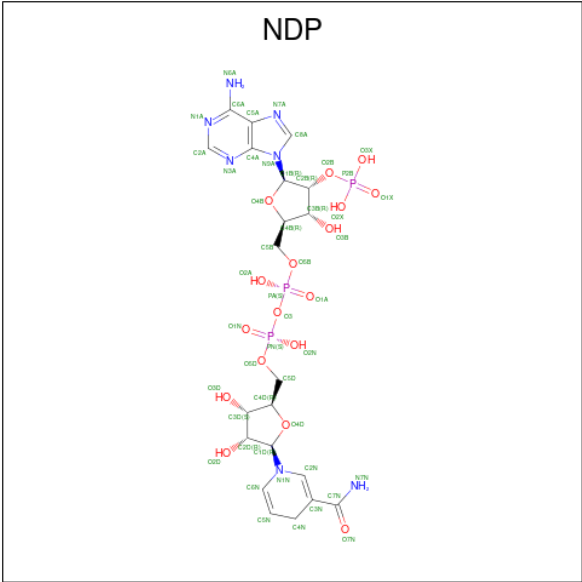
Mol	Chain	Residues	Atoms		AltConf
56	AL	1	Total	Mg	0
			1	1	
56	al	1	Total	Mg	0
			1	1	

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	AL	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	al	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

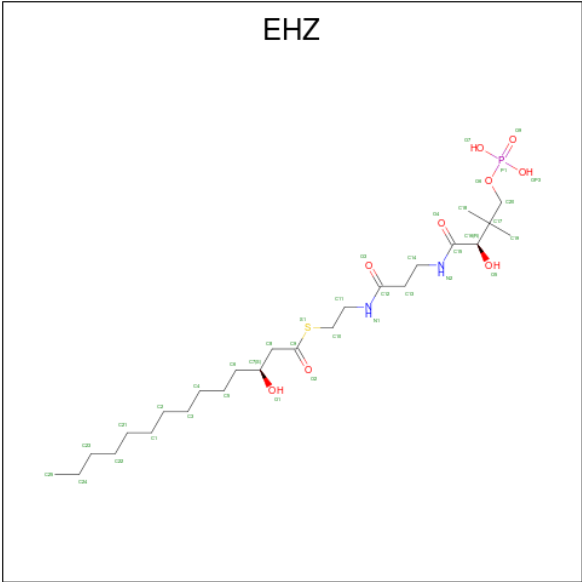


Mol	Chain	Residues	Atoms					AltConf
58	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	
58	a9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

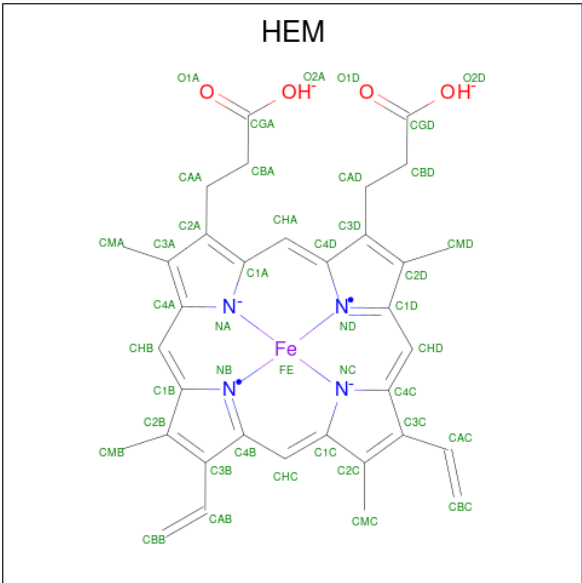
Mol	Chain	Residues	Atoms		AltConf
59	S6	1	Total	Zn	0
			1	1	
59	s6	1	Total	Zn	0
			1	1	

- Molecule 60 is {S}-[2-[3-[[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



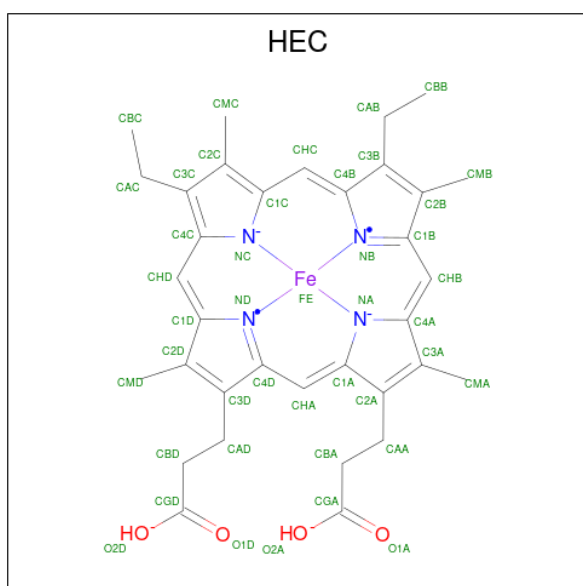
Mol	Chain	Residues	Atoms						AltConf
60	A6	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	B9	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	5a	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	a6	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 61 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



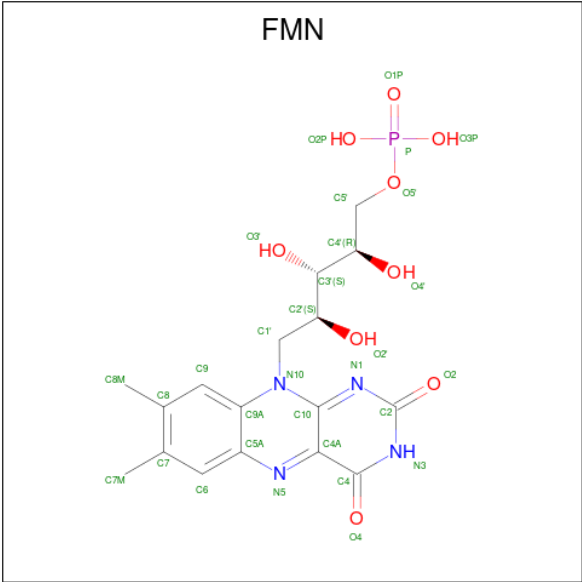
Mol	Chain	Residues	Atoms					AltConf
61	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 62 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



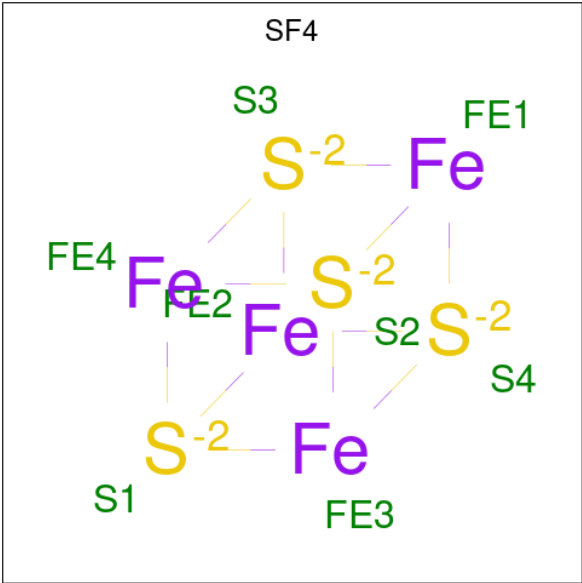
Mol	Chain	Residues	Atoms					AltConf
62	3D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	3O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 63 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
63	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	
63	v1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 64 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



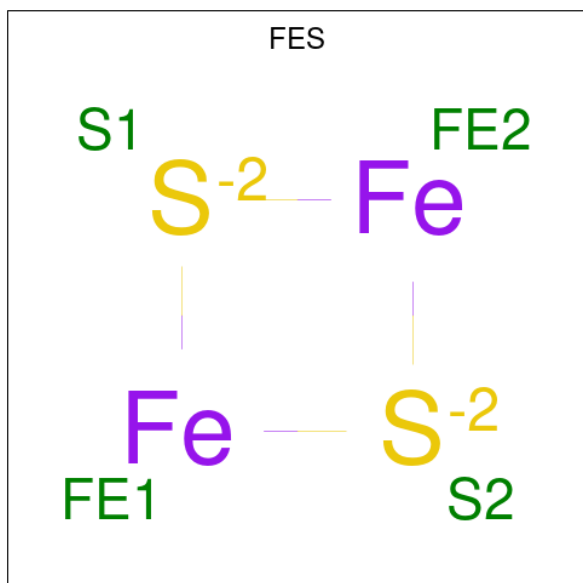
Mol	Chain	Residues	Atoms			AltConf
64	V1	1	Total	Fe	S	0
			8	4	4	
64	S1	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
64	S1	1	Total	Fe	S	0
			8	4	4	
64	S7	1	Total	Fe	S	0
			8	4	4	
64	S8	1	Total	Fe	S	0
			8	4	4	
64	S8	1	Total	Fe	S	0
			8	4	4	
64	v1	1	Total	Fe	S	0
			8	4	4	
64	s1	1	Total	Fe	S	0
			8	4	4	
64	s1	1	Total	Fe	S	0
			8	4	4	
64	s7	1	Total	Fe	S	0
			8	4	4	
64	s8	1	Total	Fe	S	0
			8	4	4	
64	s8	1	Total	Fe	S	0
			8	4	4	

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
65	V2	1	Total	Fe	S	0
			4	2	2	

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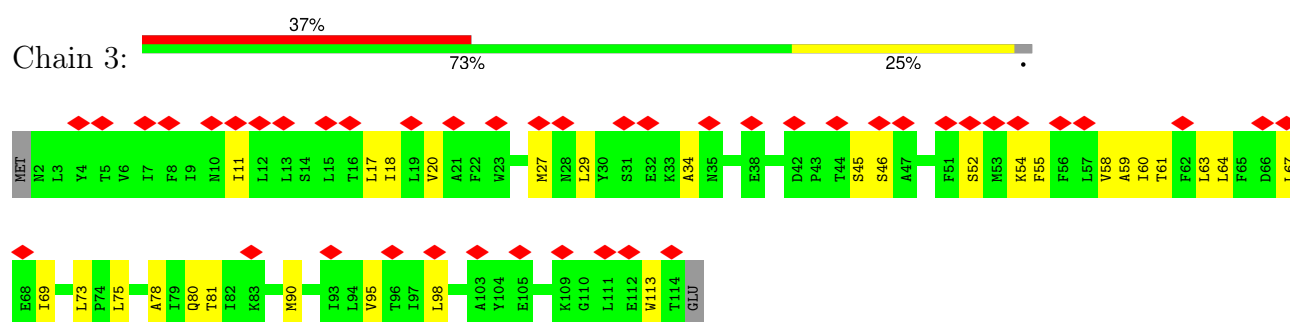
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Mol	Chain	Residues	Atoms			AltConf
65	S1	1	Total 4	Fe 2	S 2	0
65	v2	1	Total 4	Fe 2	S 2	0
65	s1	1	Total 4	Fe 2	S 2	0

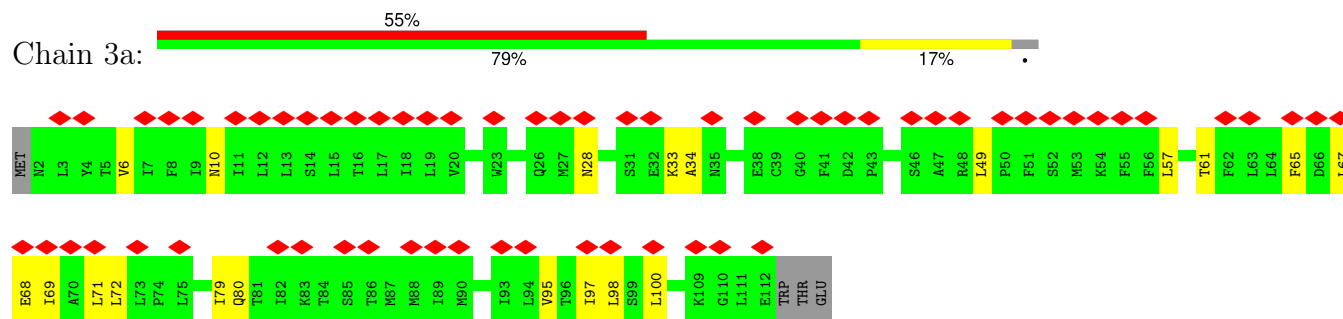
3 Residue-property plots

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

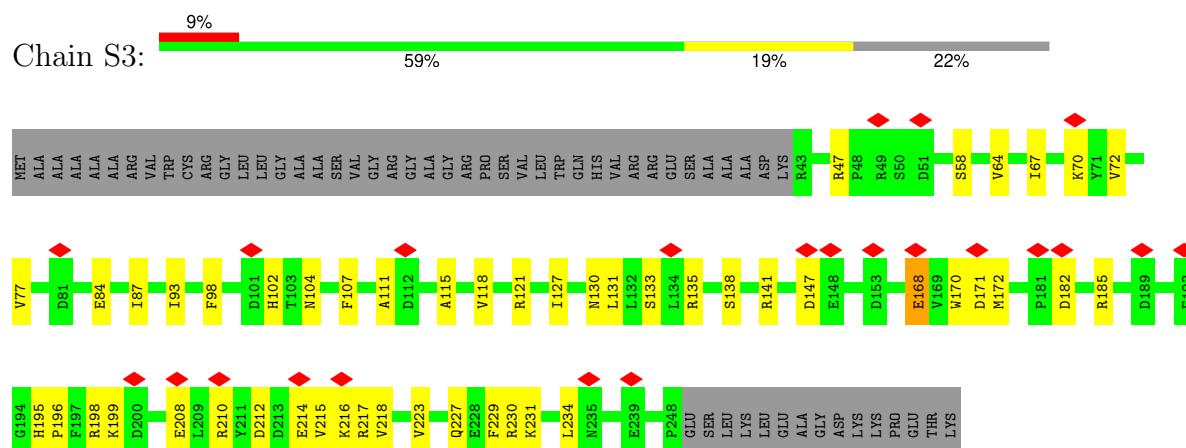
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



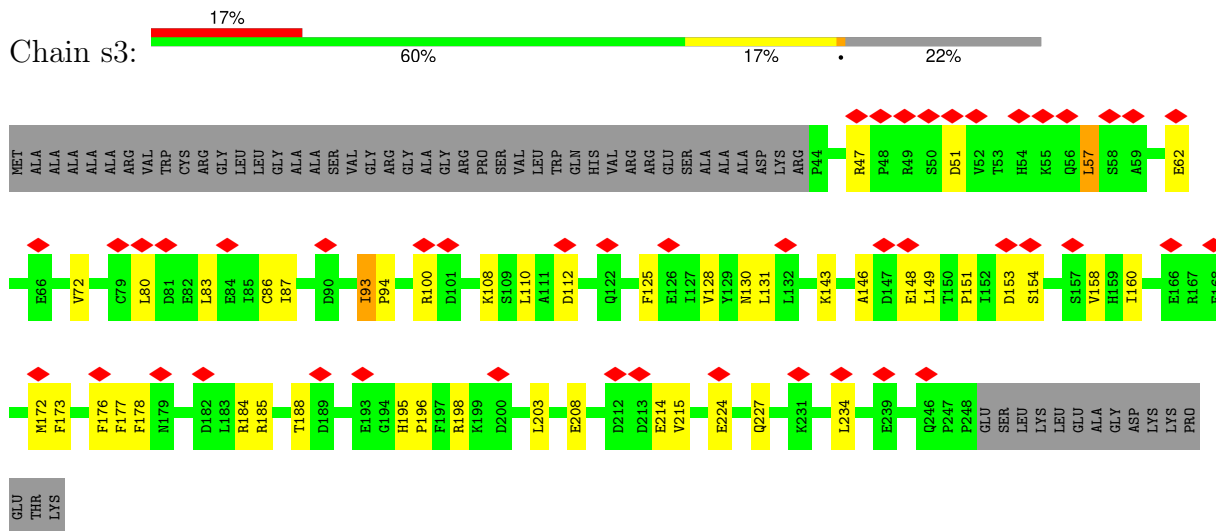
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



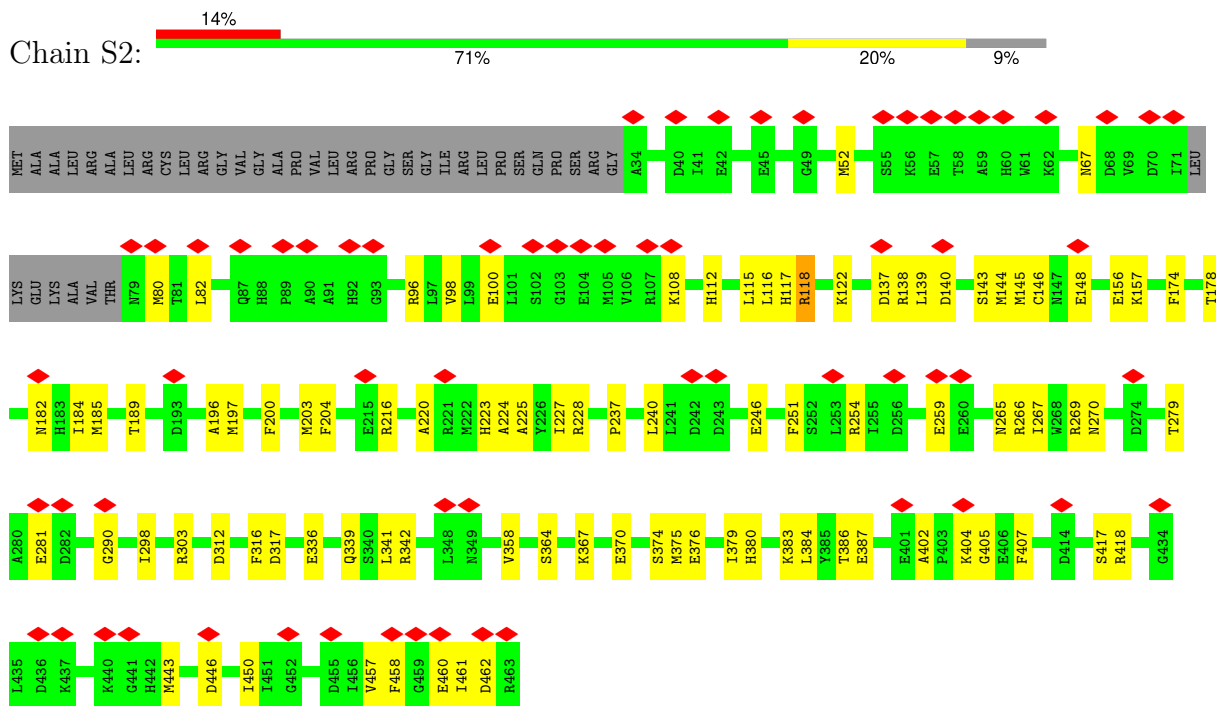
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

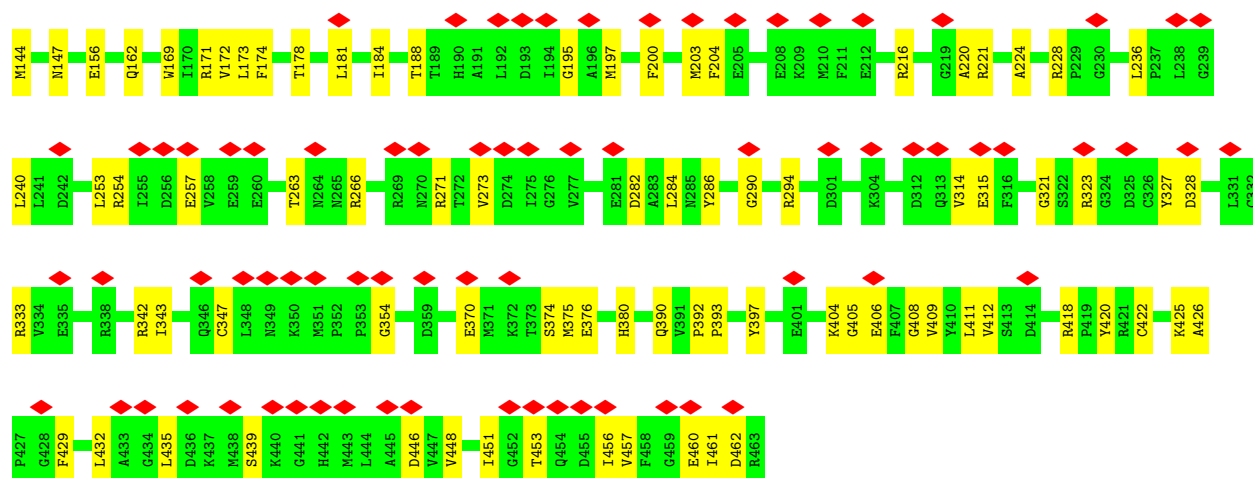


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

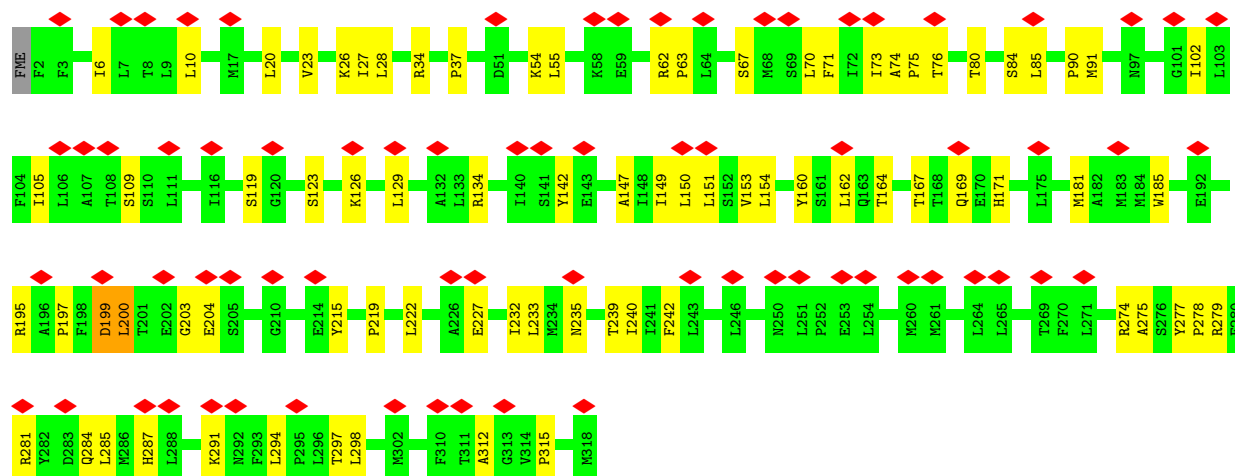
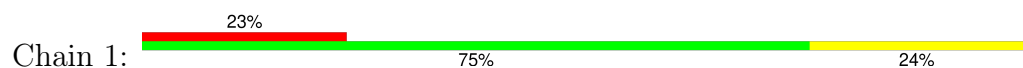


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

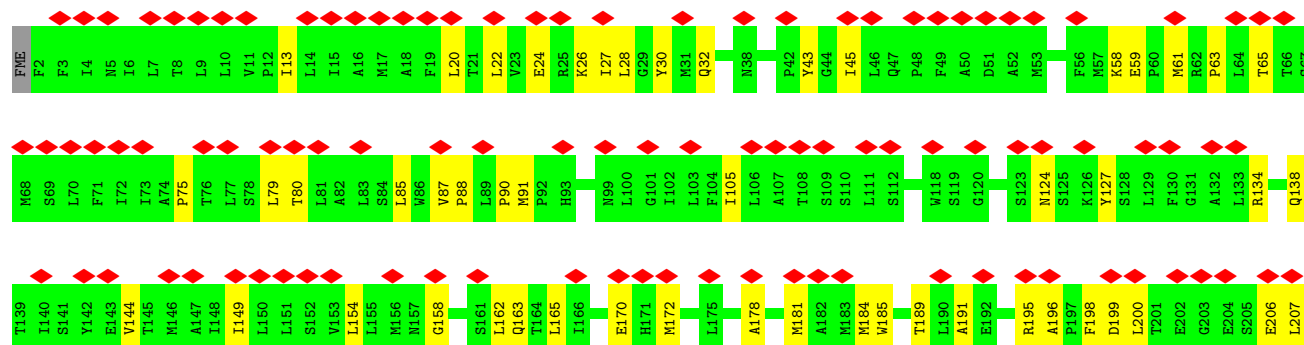
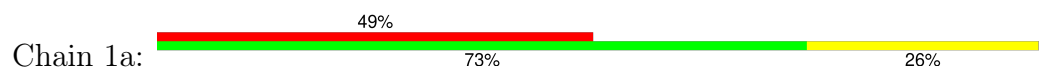


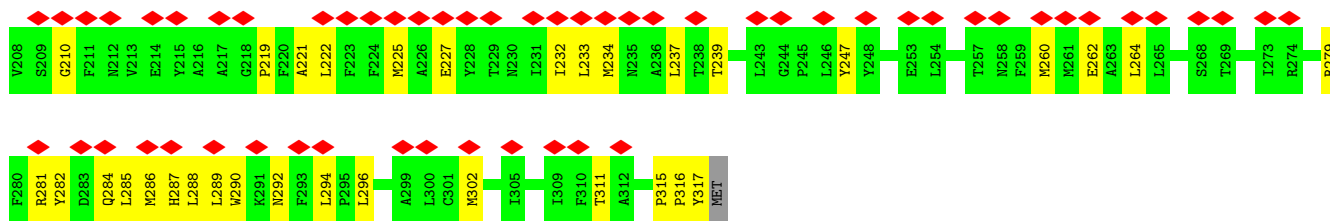


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

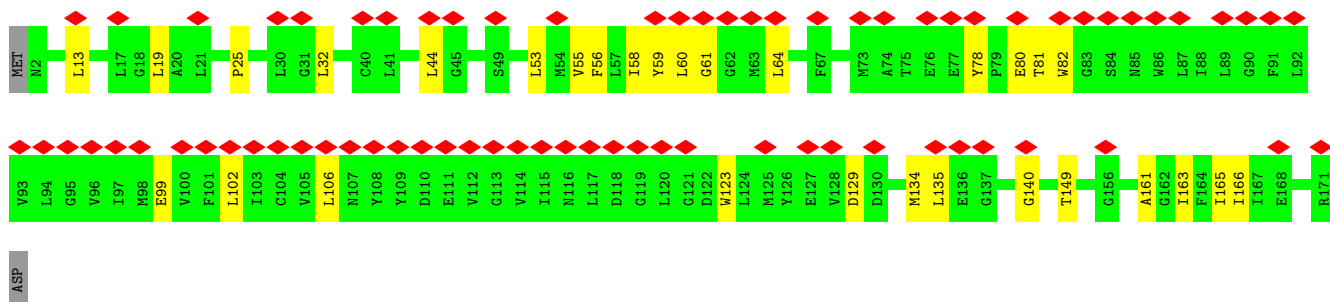
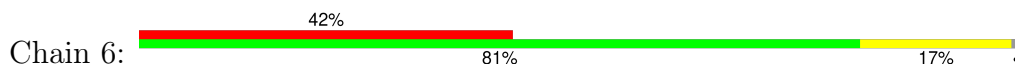


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

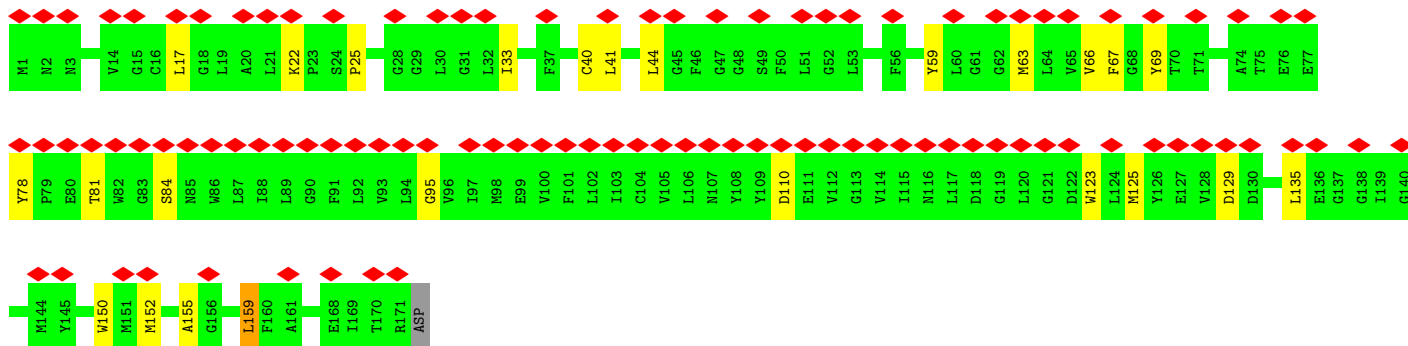
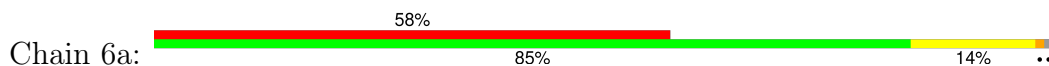




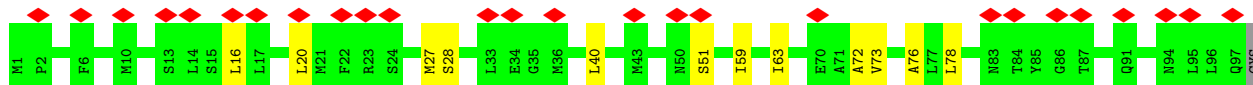
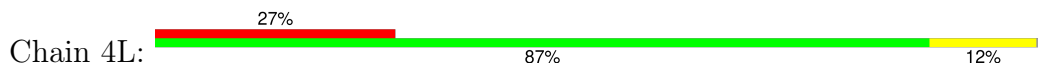
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6



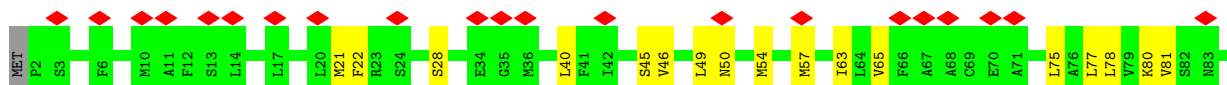
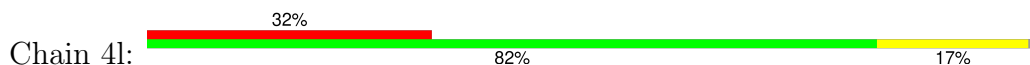
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6

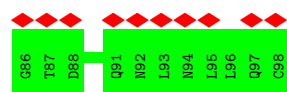


• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

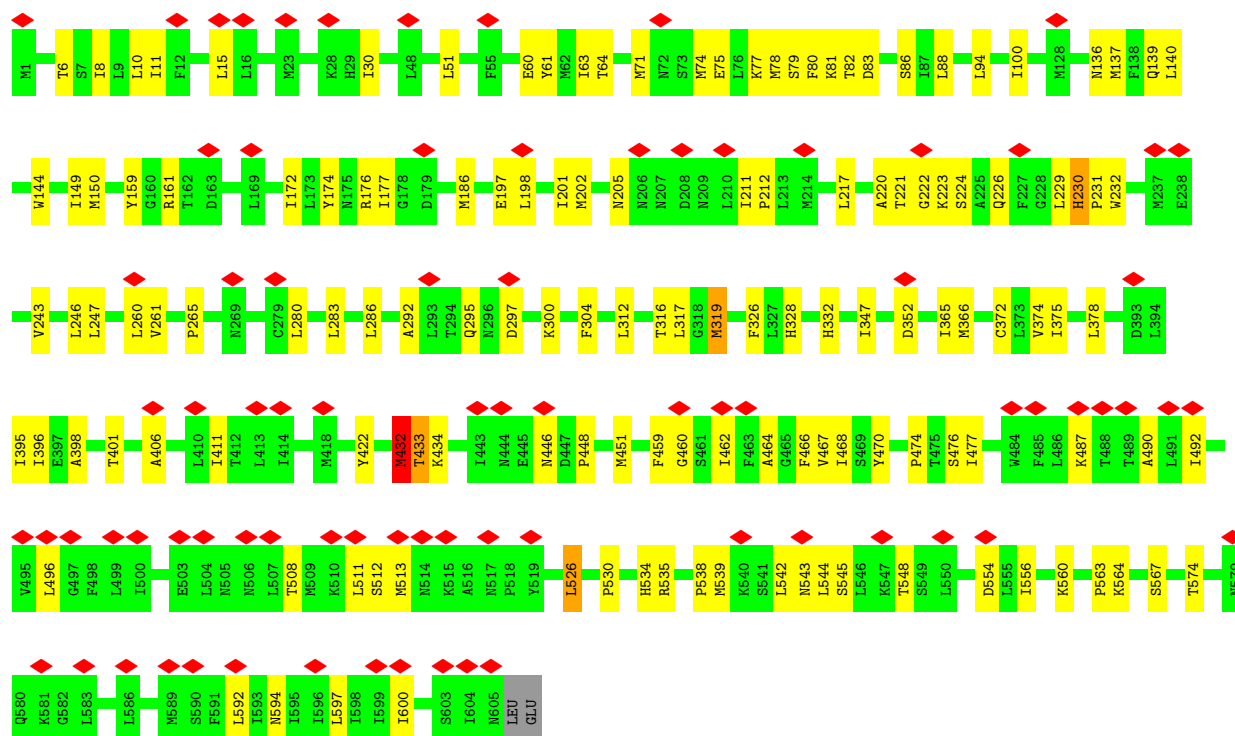
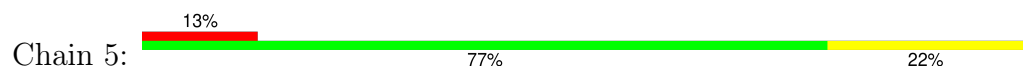


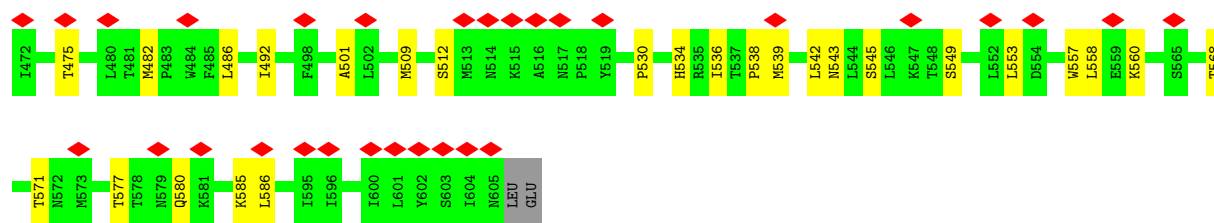
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L



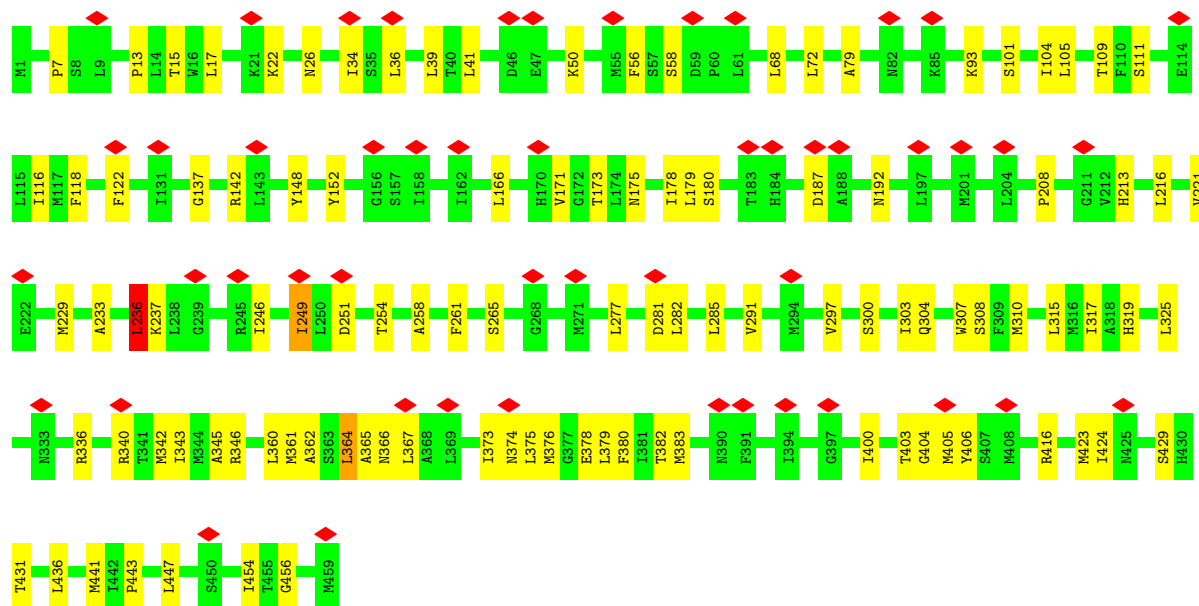
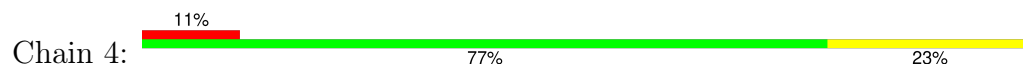


• Molecule 7: NADH-ubiquinone oxidoreductase chain 5

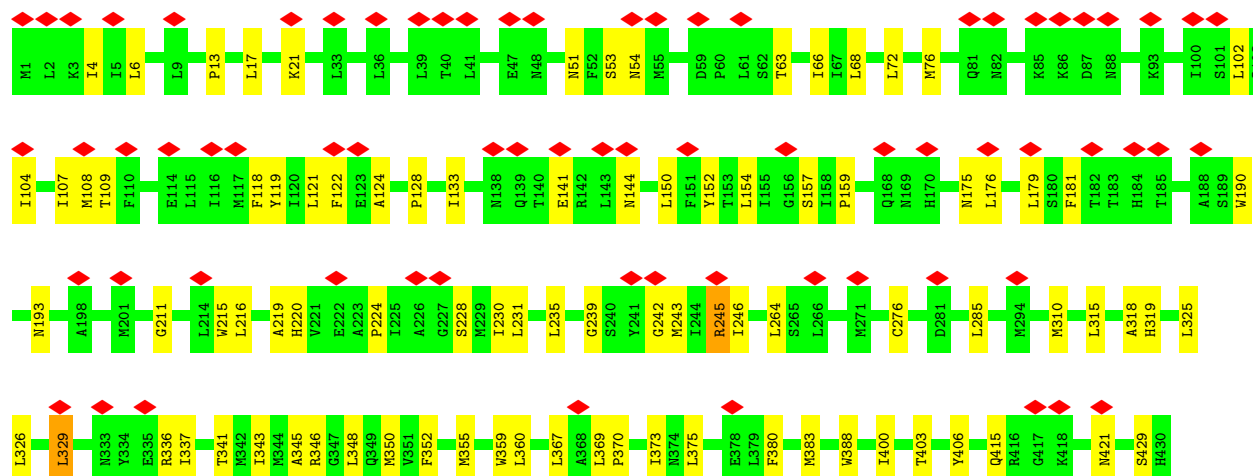
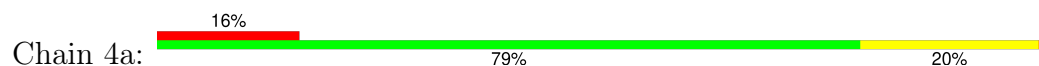


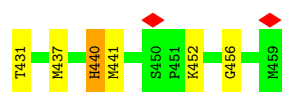


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

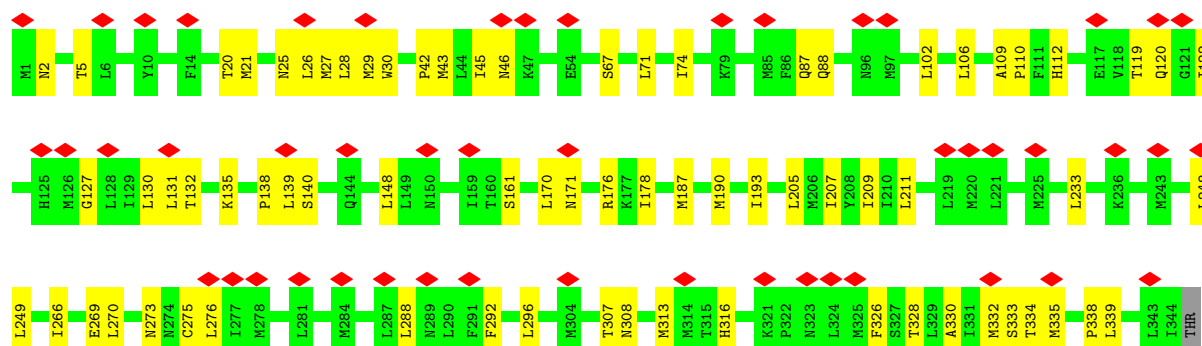
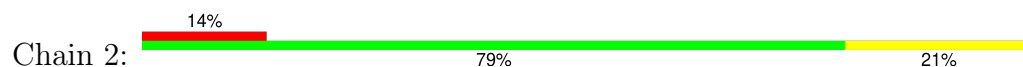


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

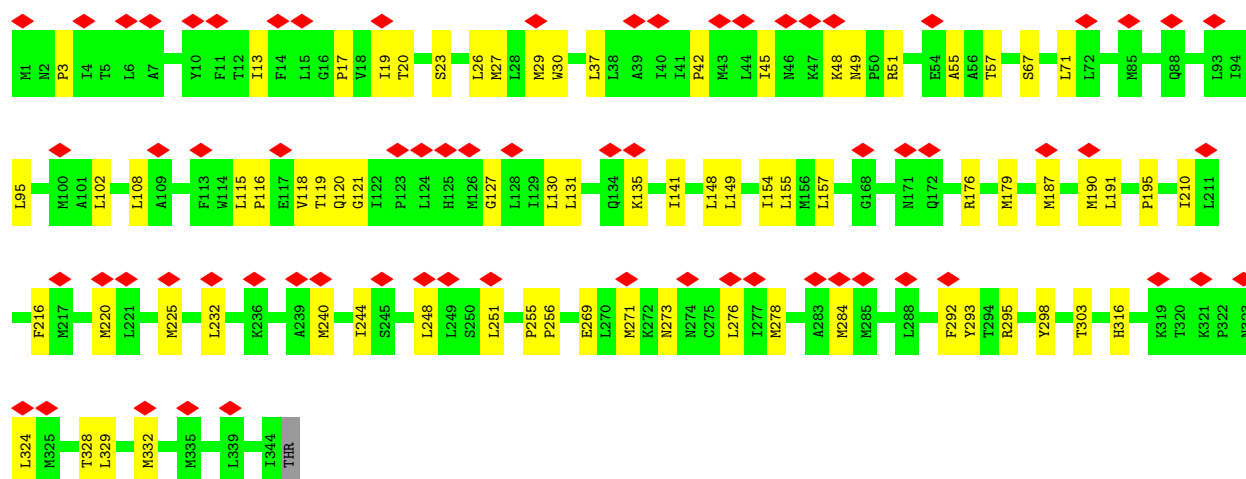
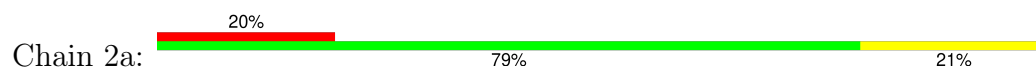




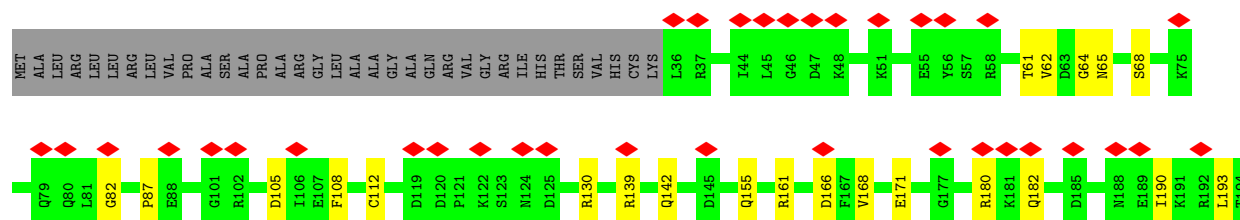
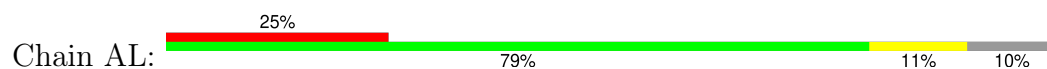
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

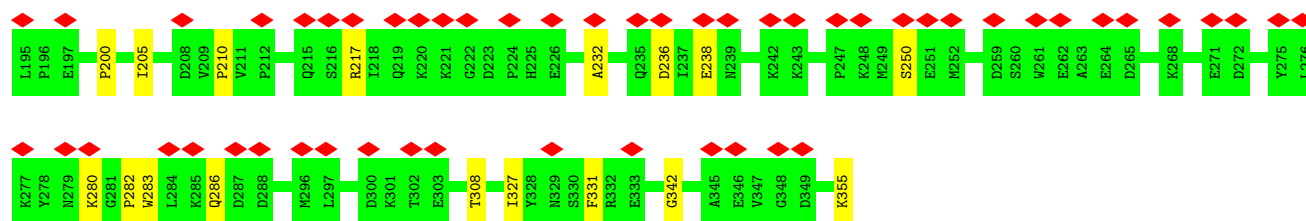


• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

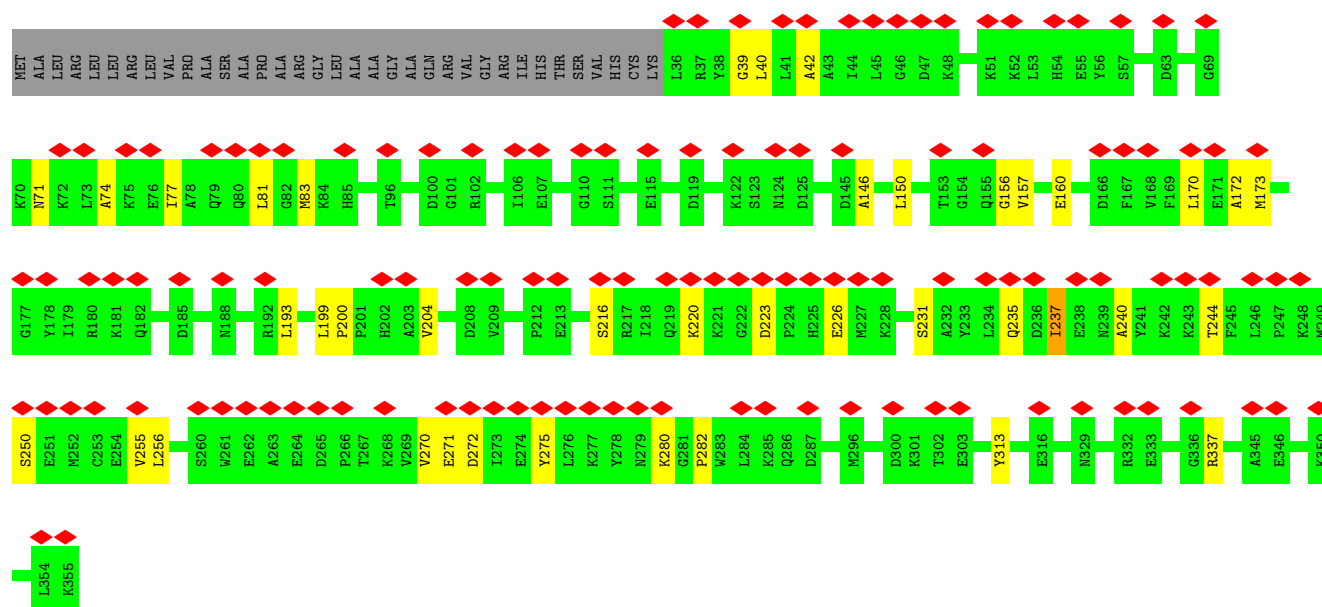
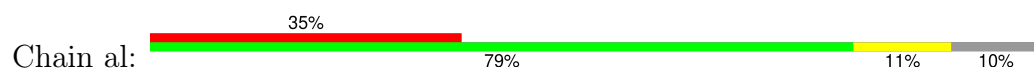


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

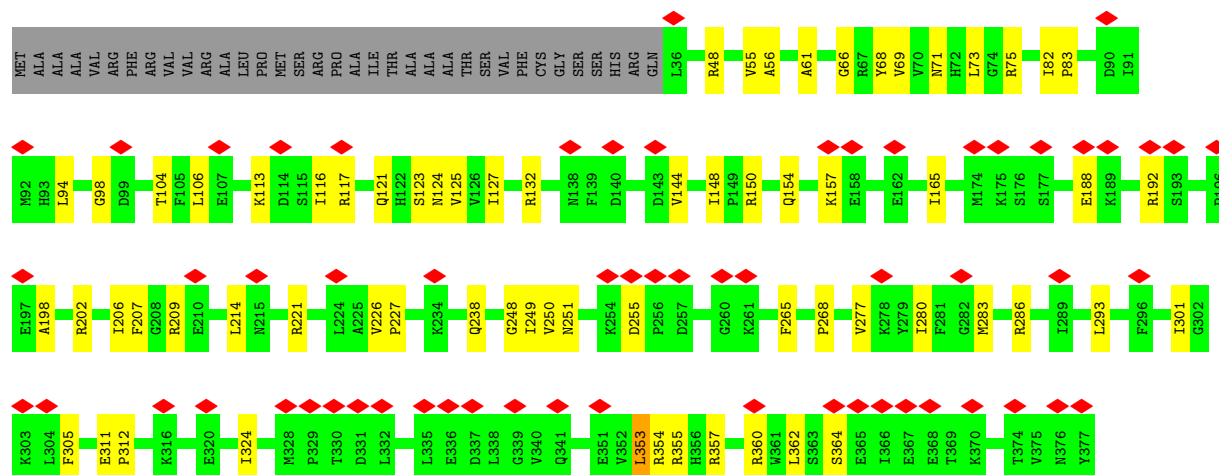
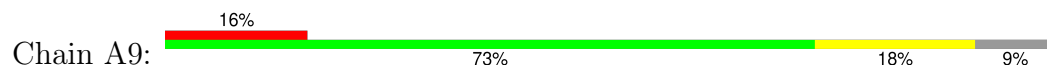




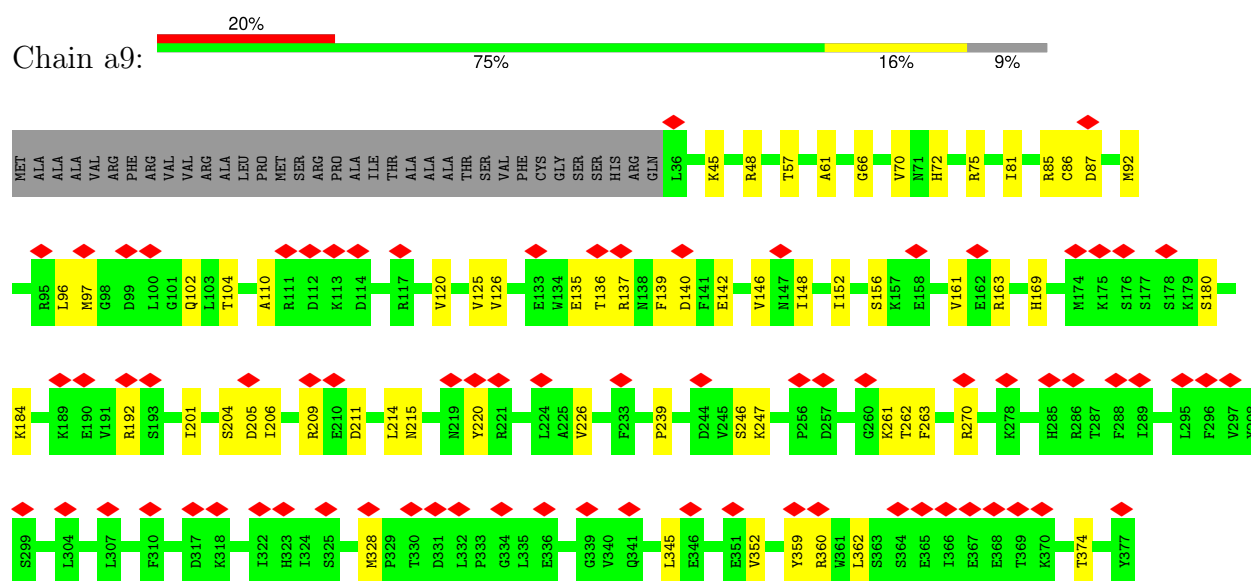
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



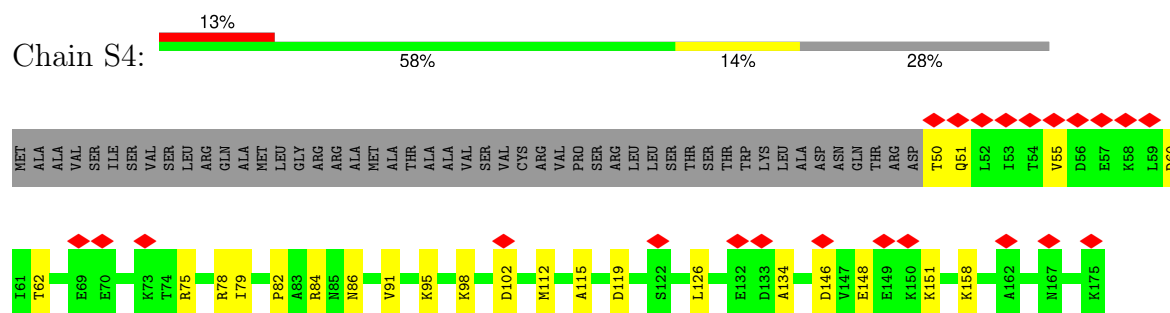
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



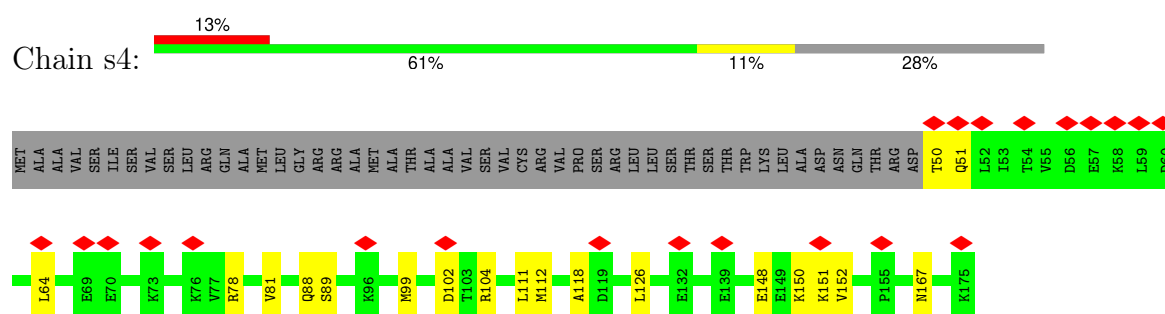
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



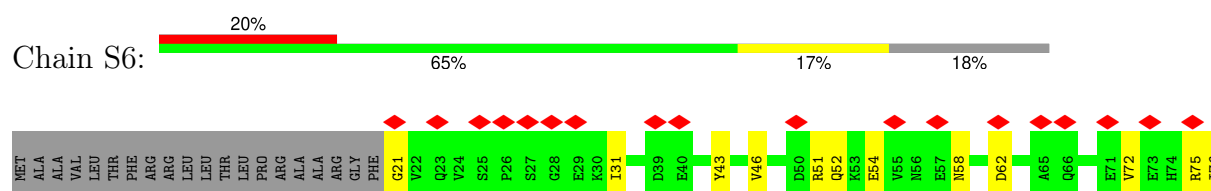
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

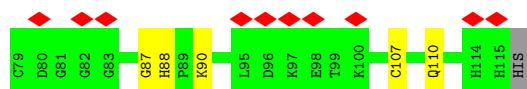
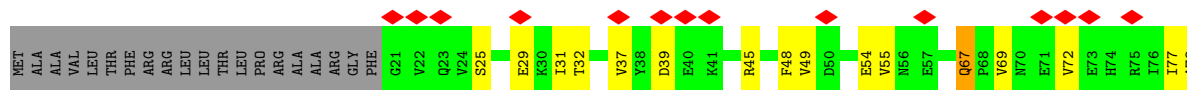


- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

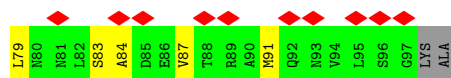
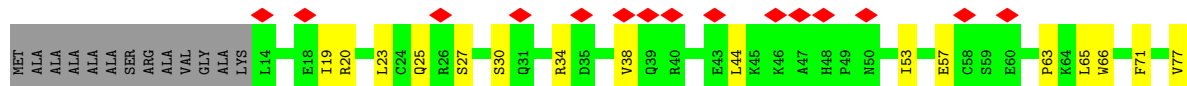




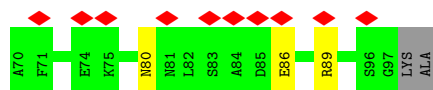
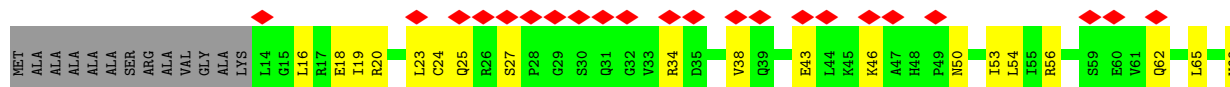
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



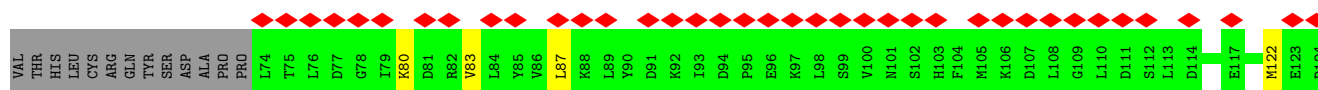
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 15: Acyl carrier protein, mitochondrial



- Molecule 15: Acyl carrier protein, mitochondrial



MET ALA SER ARG VAL LEU CYS ALA CYS VAL ARG ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO PRO LEU LEU LEU ALA ARG ARG PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU LEU ALA GLN VAL PRO GLY THR

VAL THR HIS LEU CYS ARG GLN TYR S69 D70 A71 P72 L76 D77 D81 Y85 L89 D94 P95 E96 M105 K106 Q115 V116 E117 M120 E123 D124 E125 D132 A135 E136 K137 L138 P141 Q142 E143 I144 V145 D146 D150 D153 V154 Y155 E156

- Molecule 15: Acyl carrier protein, mitochondrial



MET ALA SER ARG VAL LEU CYS ALA CYS VAL ASP ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO PRO LEU THR THR LEU ALA ALA ARG PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU LEU ALA GLN VAL PRO GLY THR

VAL THR HIS LEU CYS ARG GLN TYR L74 T75 L76 D77 G78 I79 K80 D81 R82 V83 L84 Y85 V86 L87 K88 L89 Y90 D91 K92 I93 D94 P95 E96 K97 S99 V100 N101 S102 H103 F104 M105 K106 D107 L108 G109 L110 D111 S112 L113 D114 Q115 V116 E117 I118 I119 M120

A121 M122 E123 D124 E125 F126 G127 F128 E129 I130 P131 D132 I133 D134 A135 E136 K137 L138 M139 C140 P141 Q142 E143 I144 V145 D146 Y147 I148 A149 D150 K151 LYS ASP VAL TYR GLU

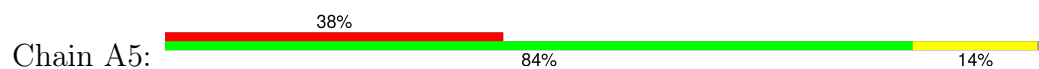
- Molecule 15: Acyl carrier protein, mitochondrial



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VAL THR HIS LEU CYS ARG GLN TYR S69 D70 A71 D77 D81 Y85 L89 Y90 D91 K92 D94 P95 E96 K97 M105 K106 D107 L108 S112 E117 E123 D124 E129 I130 P131 D132 I133 A135 E136 K137 L138 E143 D146 Y155 E156

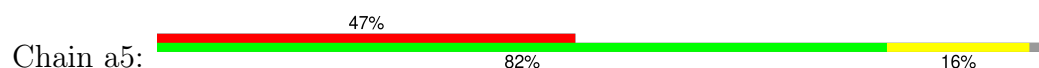
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

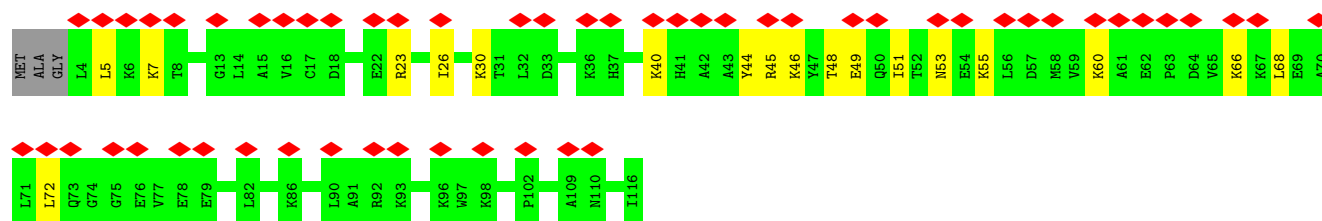


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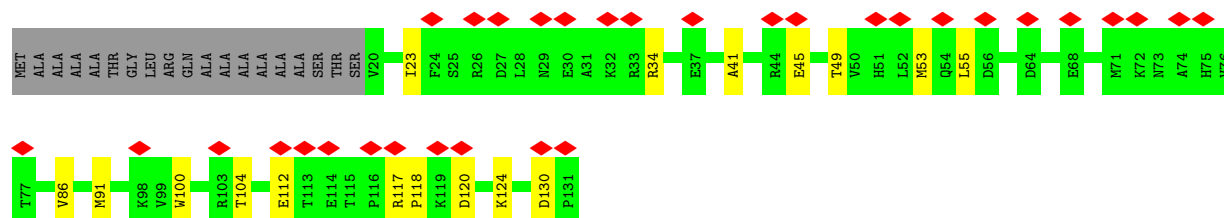
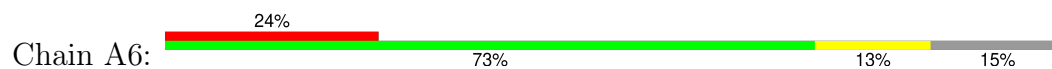
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- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

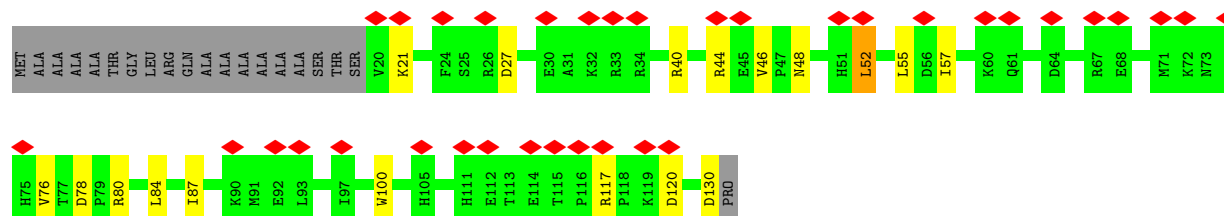
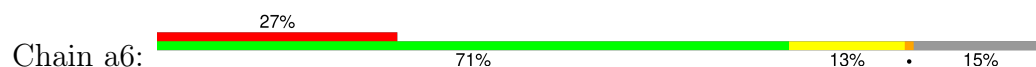




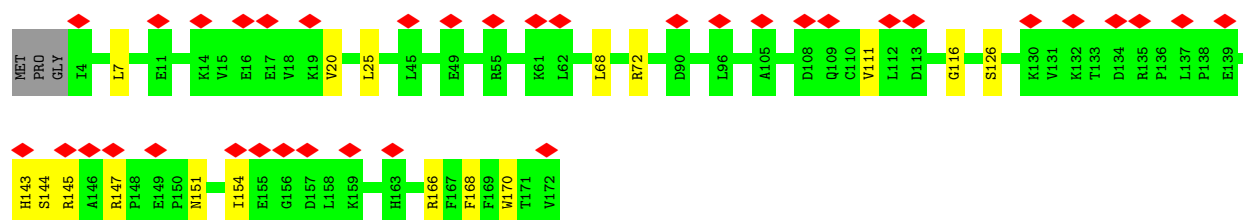
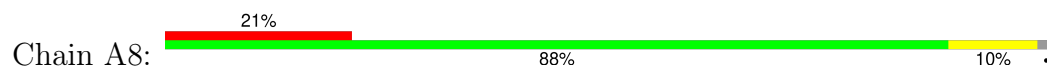
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



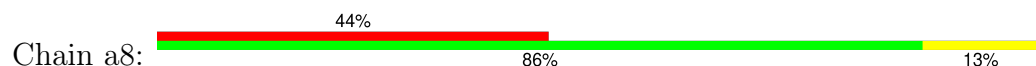
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

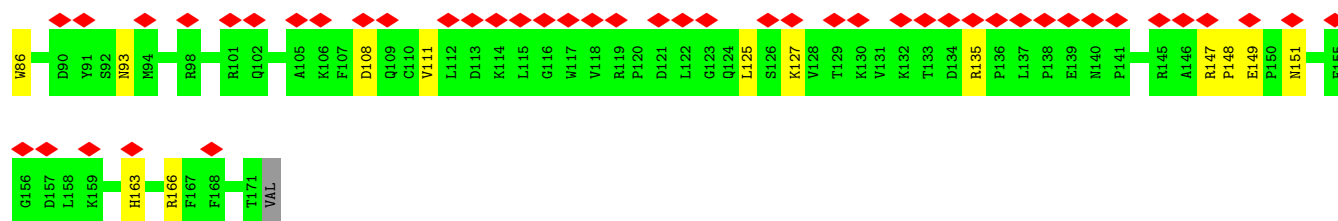


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

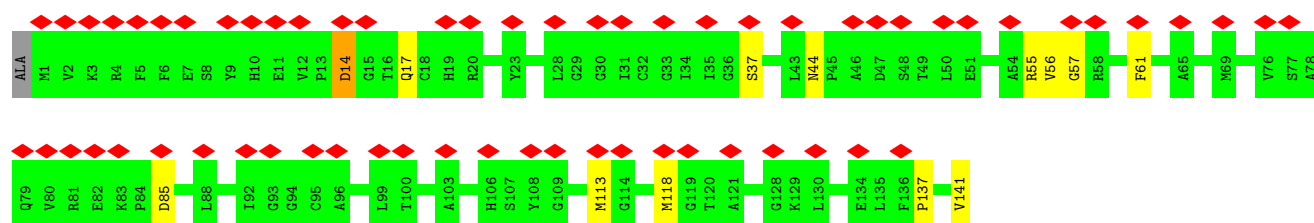


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

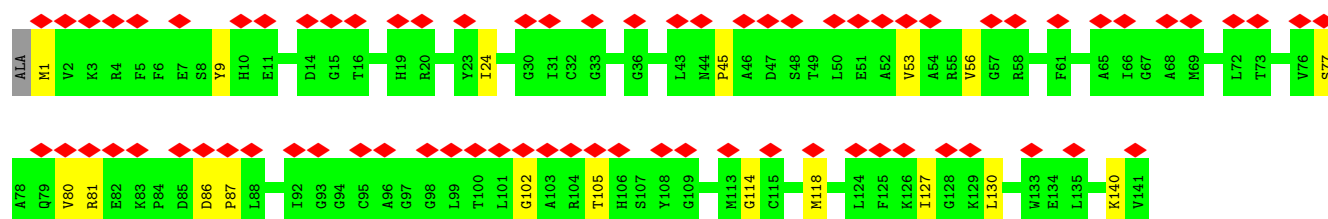
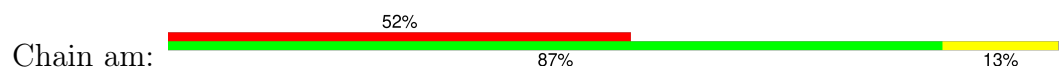




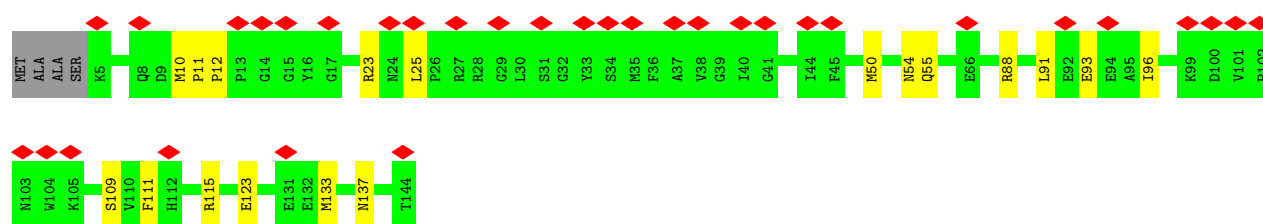
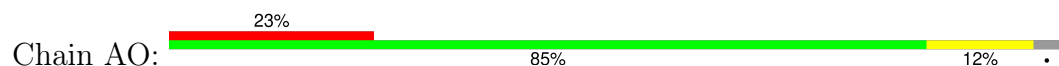
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



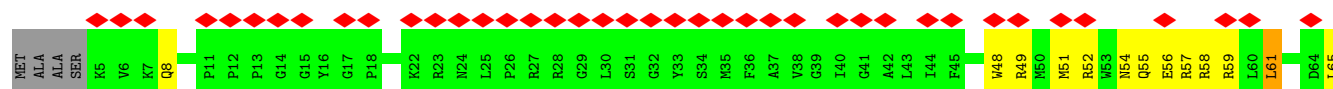
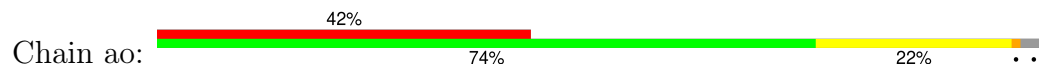
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

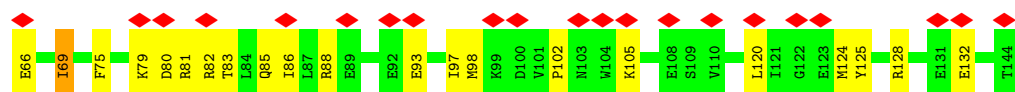


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

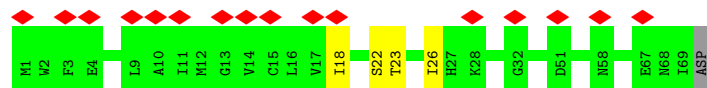


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

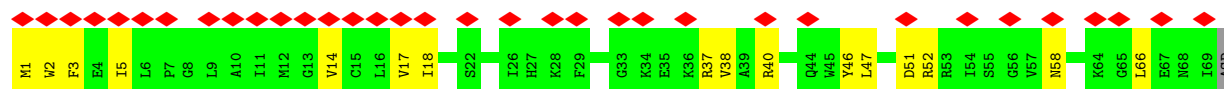
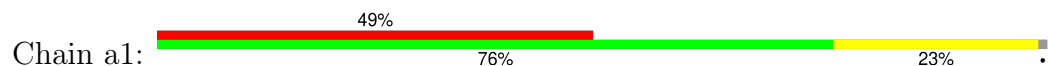




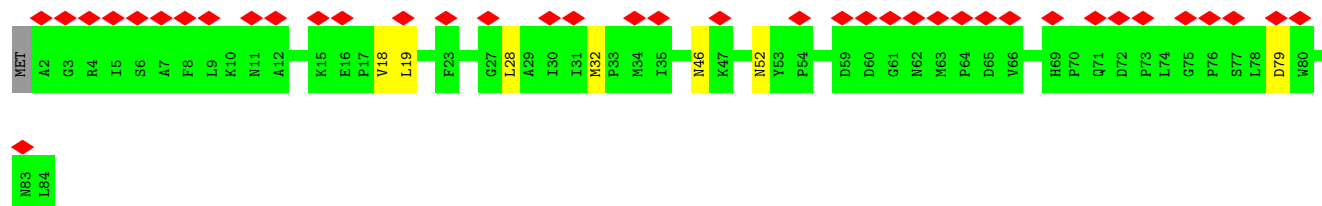
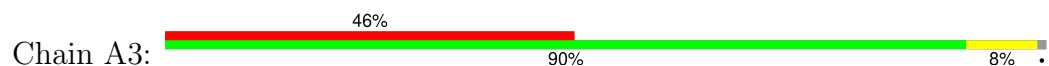
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



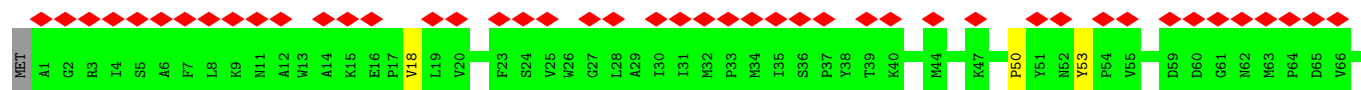
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



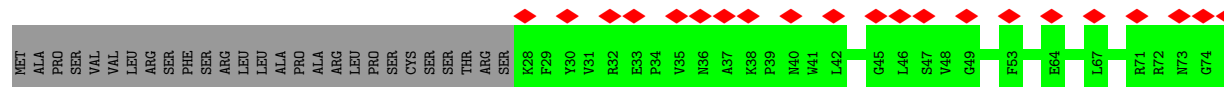
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

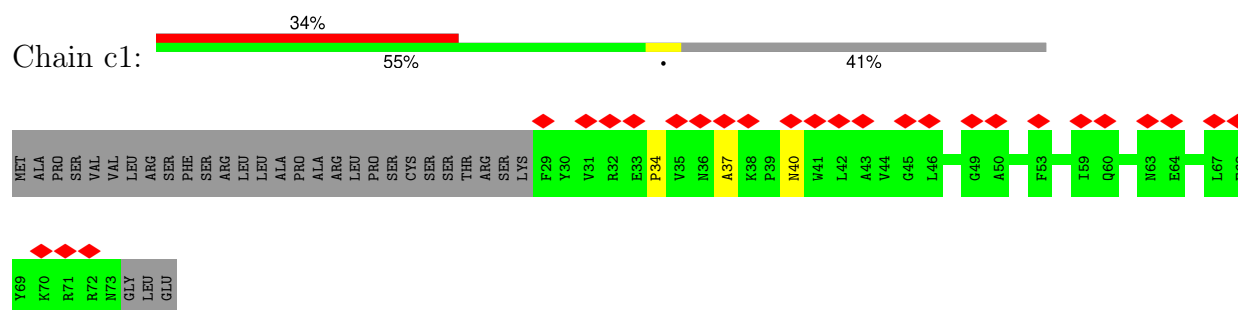


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

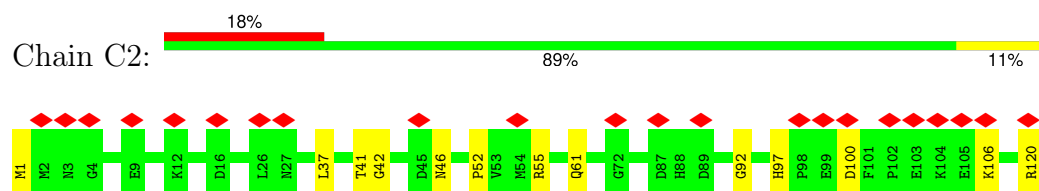




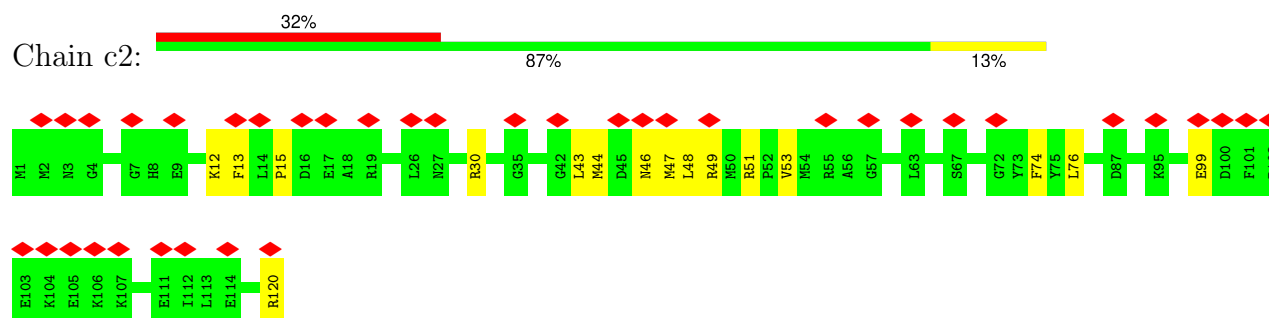
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



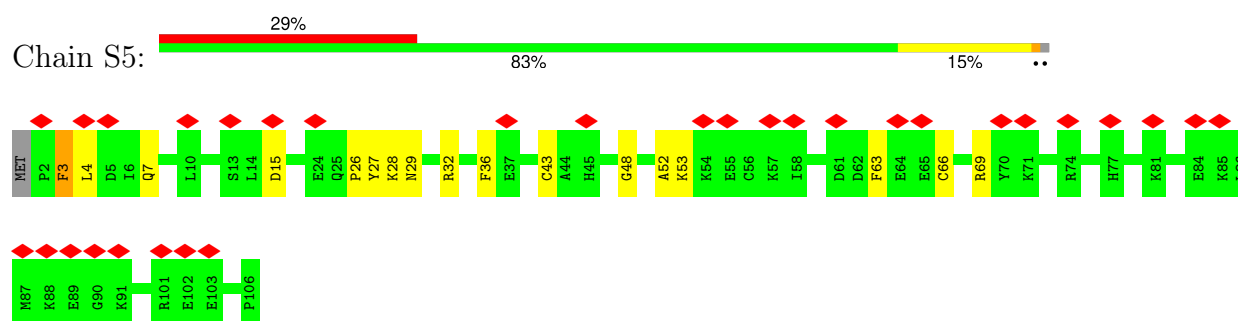
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



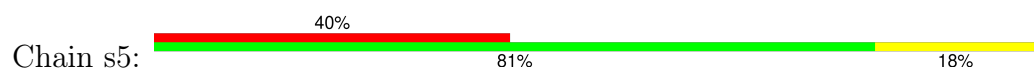
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



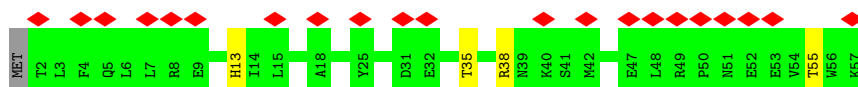
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



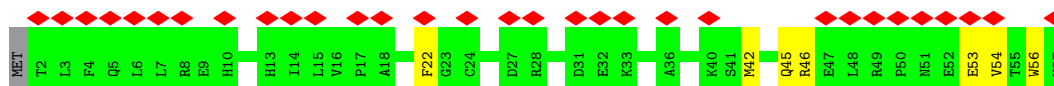
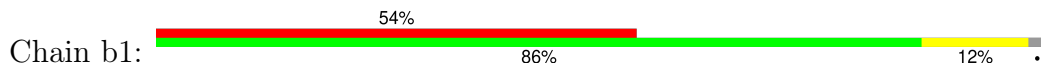
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



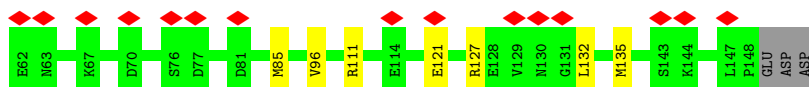
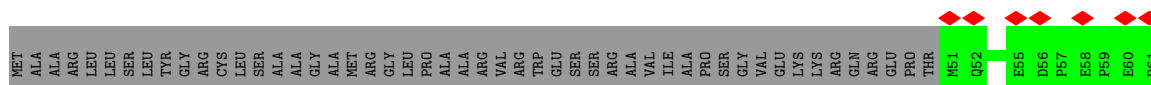
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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



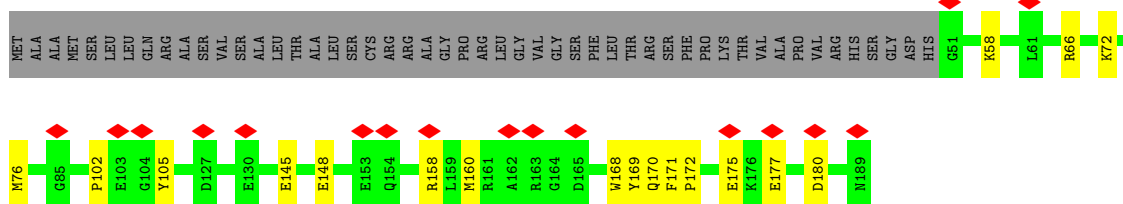
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



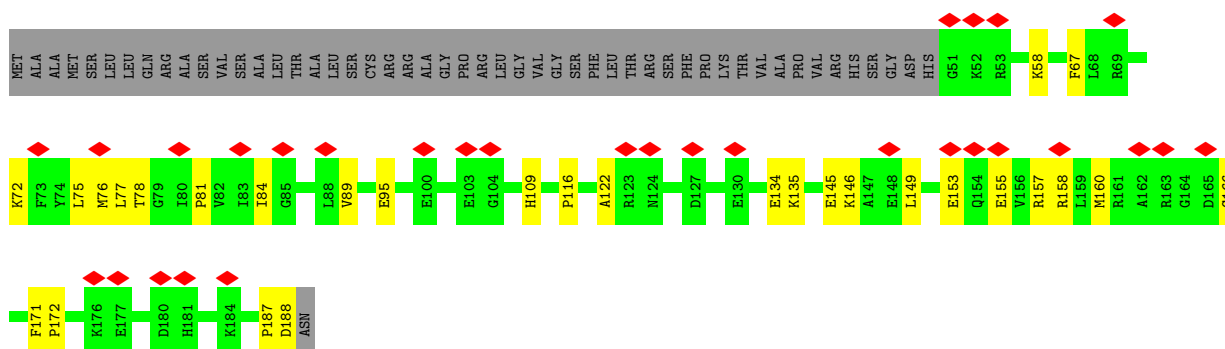
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



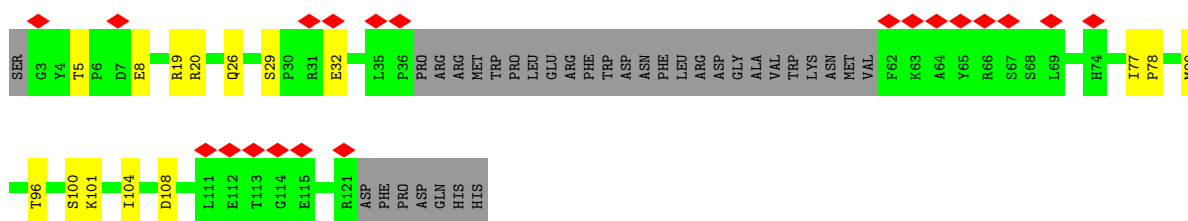
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



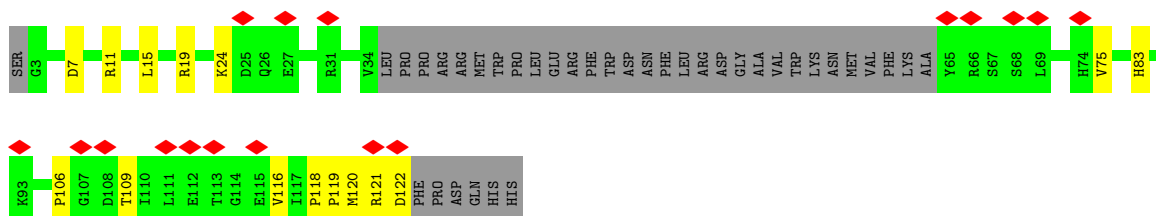
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



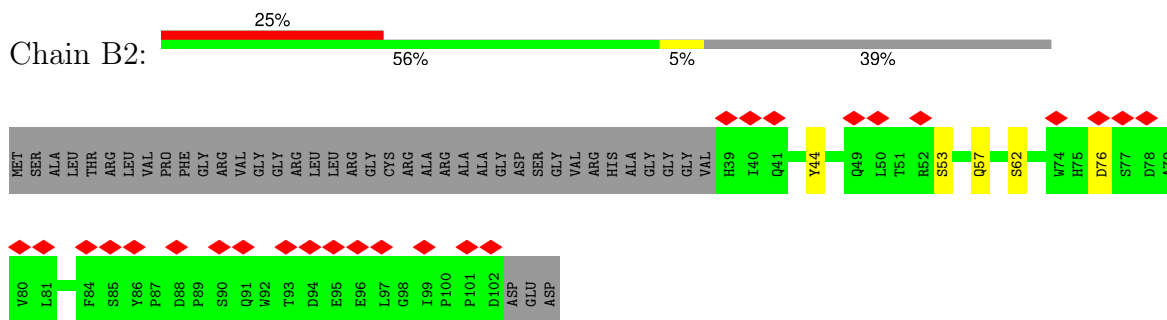
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



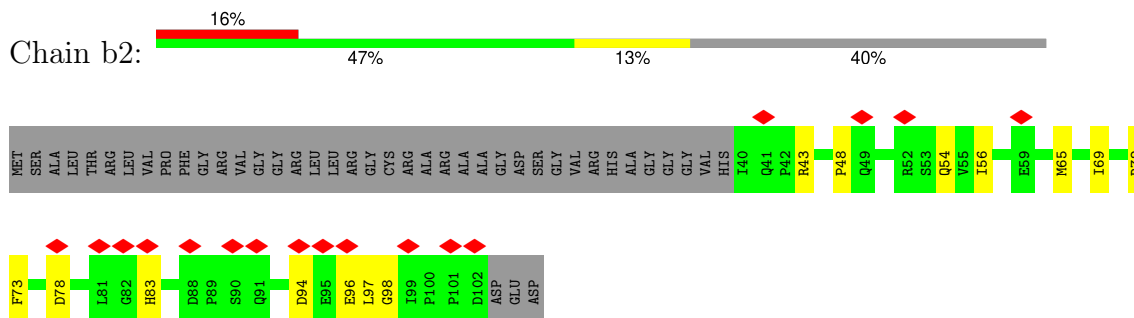
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



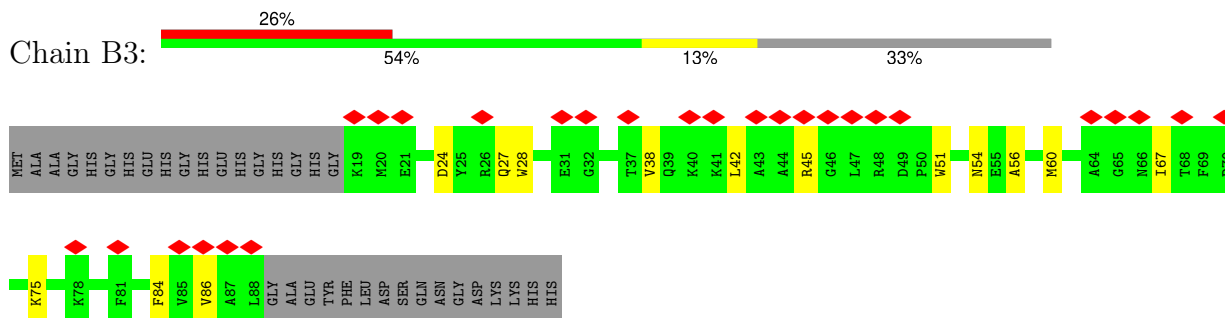
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



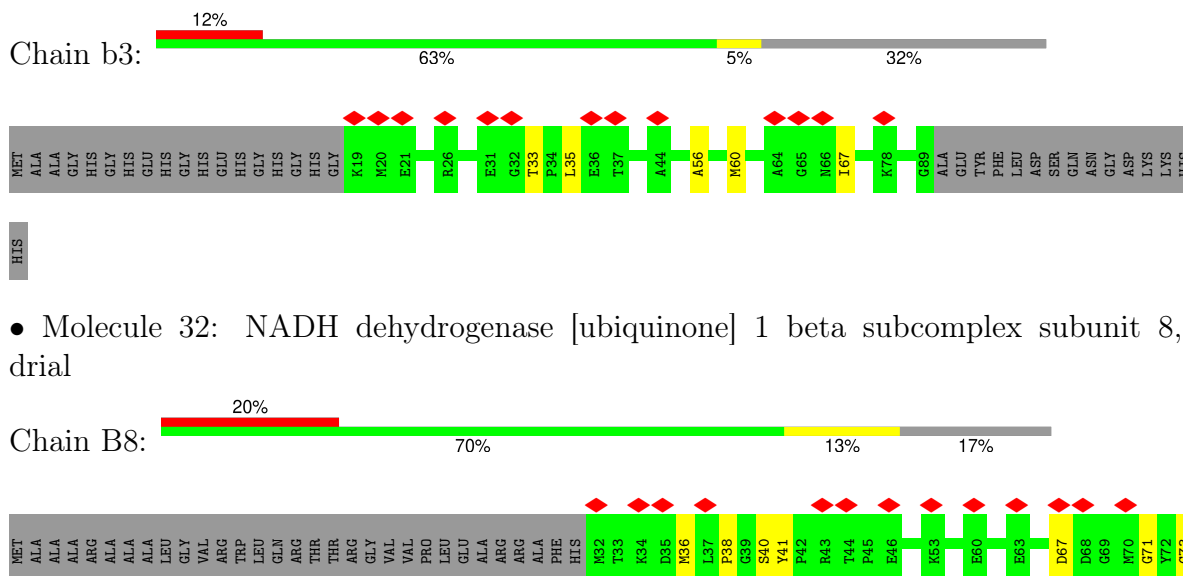
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

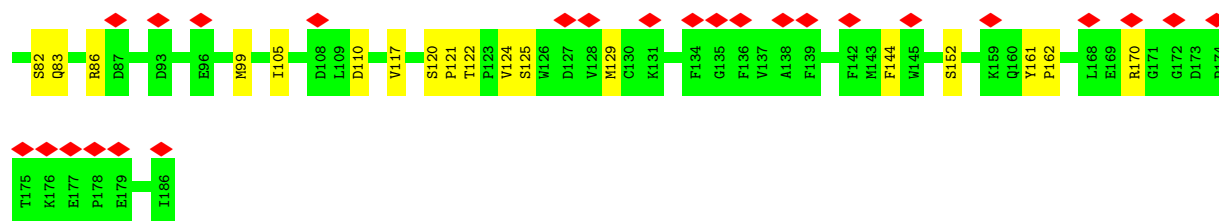


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

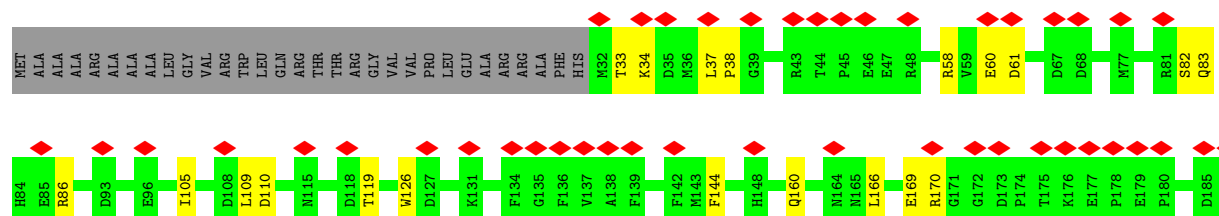
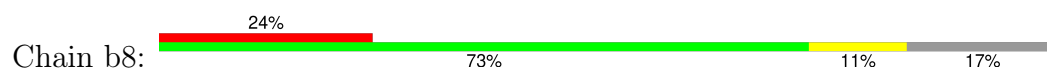


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

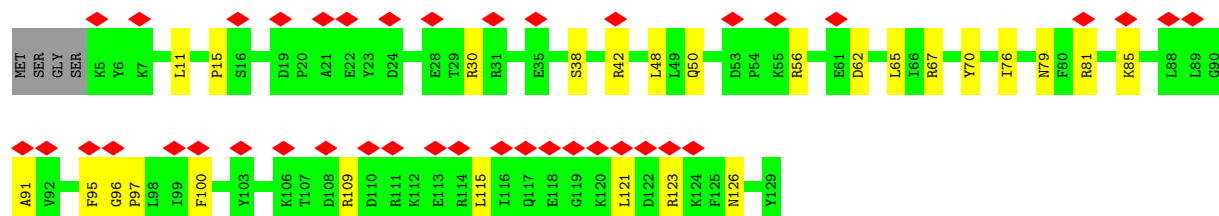
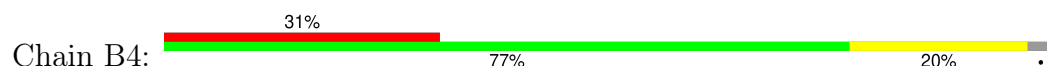




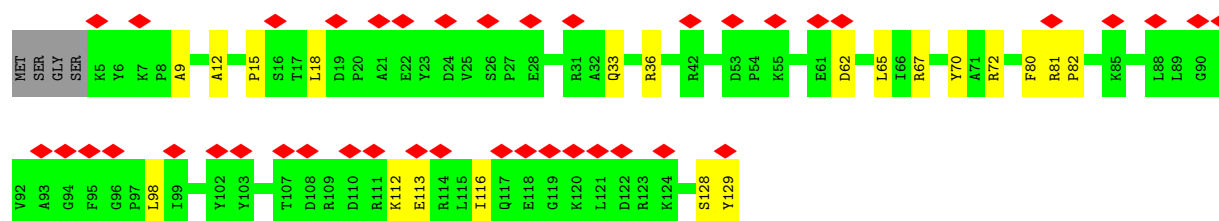
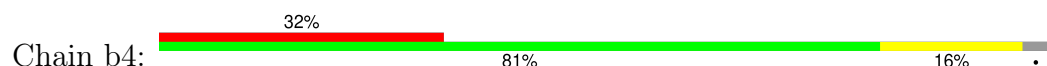
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



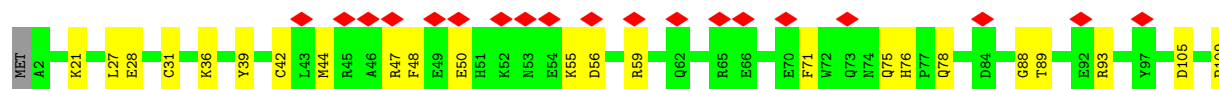
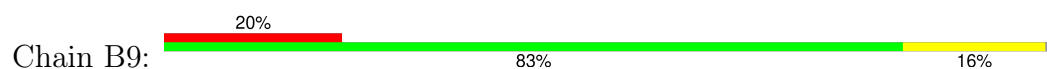
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

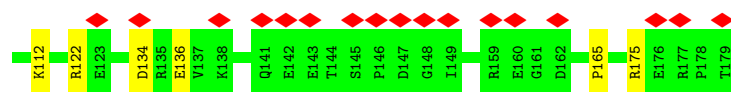


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

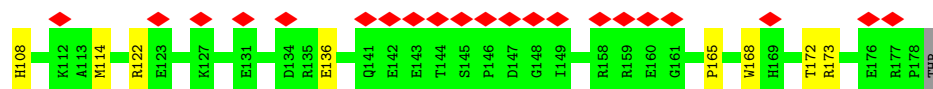
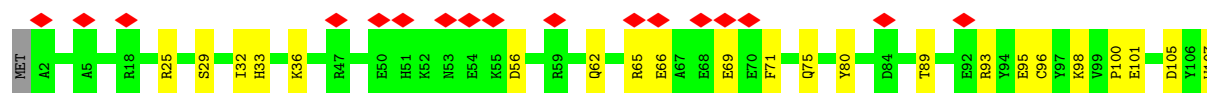
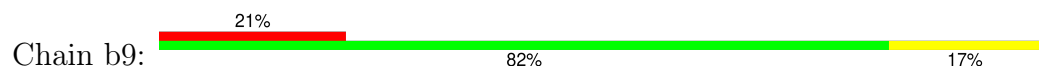


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

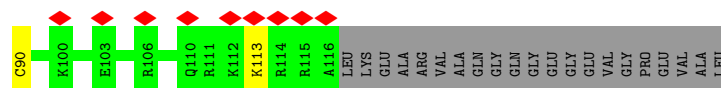
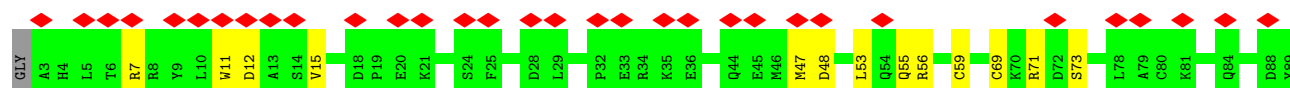
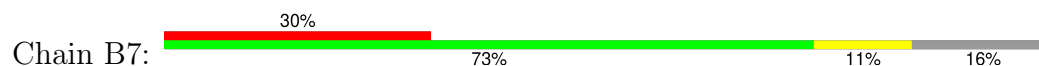




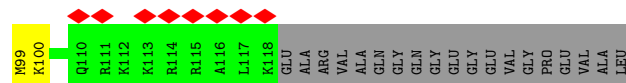
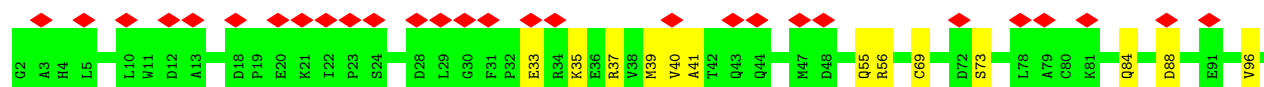
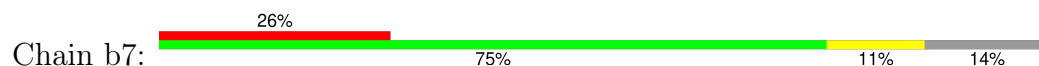
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



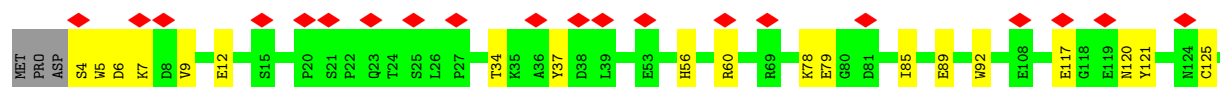
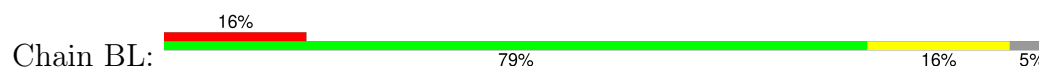
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



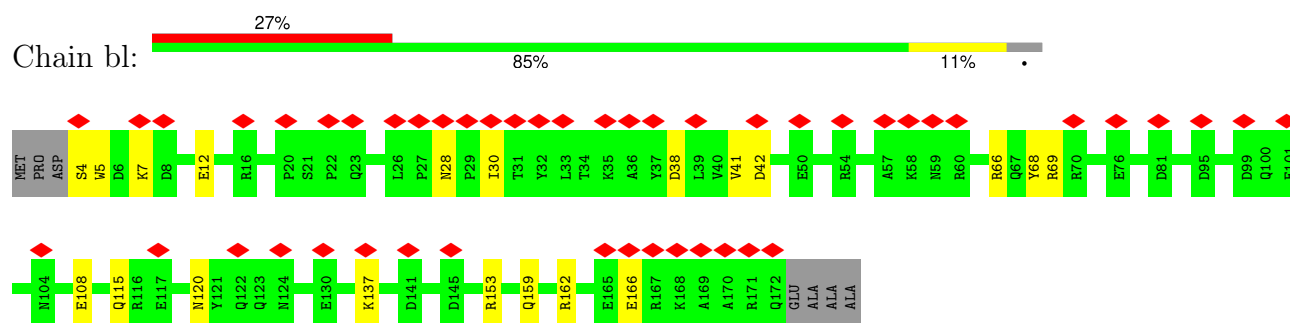
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



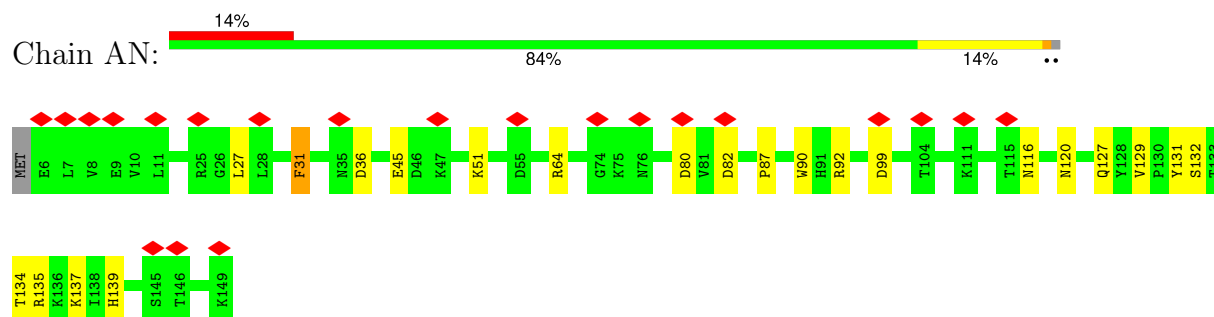
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



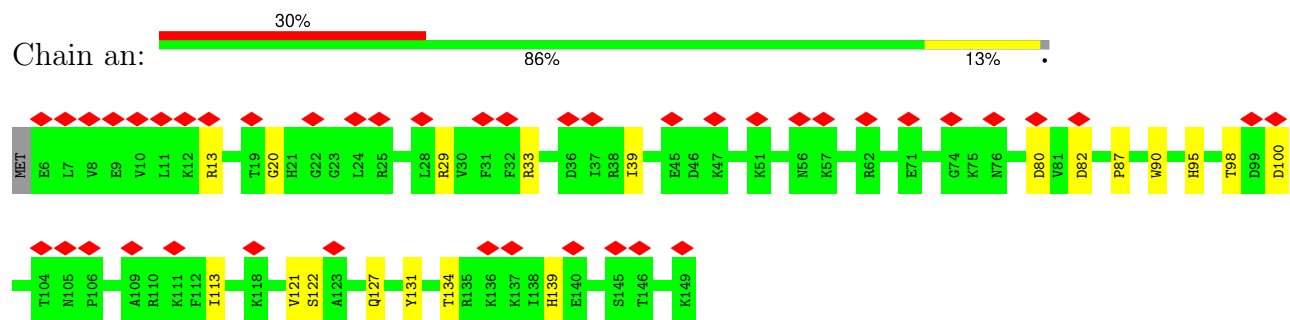
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



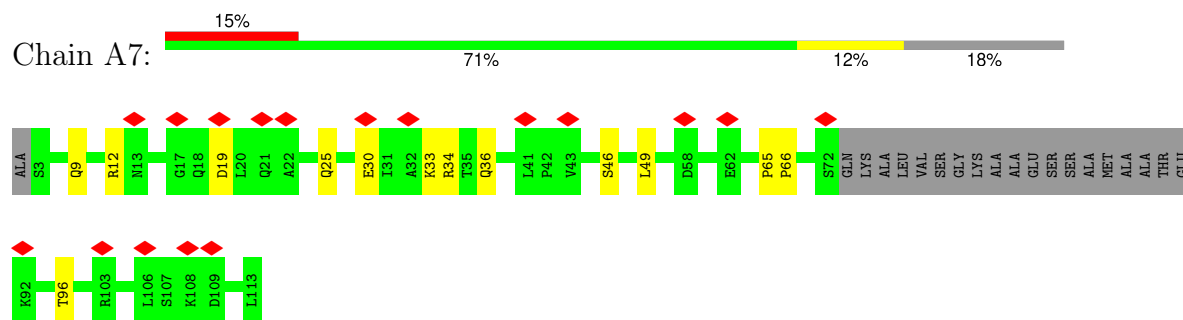
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



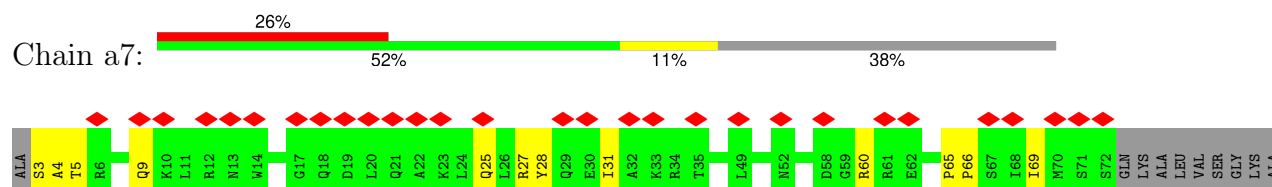
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



ALA
GLU
SER
SER
ALA
MET
ALA
ALA
THR
GLY
GLY
LYS
LYS
VAL
THR
PRO
ALA
VAL
PRO
PRO
MET
LYS
ARG
TRP
GLU
LEU
SER
LYS
GLN
PRO
TYR
LEU

- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET
ALA
VAL
SER
SER
LEU
LEU
LEU
ARG
GLY
GLY
ARG
ILE
ARG
ALA
LEU
LYS
LYS
ALA
VAL
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T66
L70
L71
H72
H73
L81
L85
D86
L87
S88
K89
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R91
L92
P93
Q94
P95
S96
S97
G98
R99
E100
E103
H104

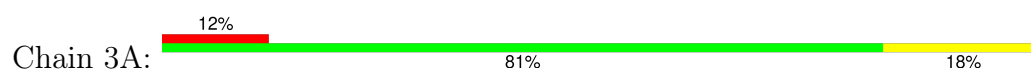
- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET
ALA
VAL
SER
SER
LEU
LEU
LEU
ARG
GLY
GLY
ARG
ILE
ARG
ALA
LEU
LYS
LYS
ALA
VAL
LEU
LEU
LEU
GLU
ALA
ARG
VAL
PHE
PRO
GLY
GLU
LEU
VAL
SER
VAL
VAL
ARG
LEU
SER
THR
GLU
SER
GLU
LYS
LYS
SER
SER
LYS
GLU
GLY
LYS
LYS
LEU
LEU
HIS
PRO
LYS
THR
GLN
SER
SER
VAL
VAL
LYS
LYS
GLU
PRO
GLU

PRO
THR
ASP
THR
THR
THR
TYR
K68
N69
L70
H73
H74
D74
L81
D82
L83
N84
D86
K89
F90
R91
R99
E100
R103
HIS

- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



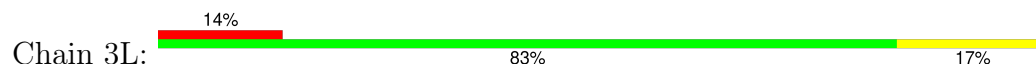
THR
A36
T37
F38
A39
Q40
A41
L42
Q43
S44
E47
L53
D54
R53
S64
S65
T70
V71
W74
R80
E84
K85
N86
N87
G88
F92
L93
E94
A97
F98
K99
G100
T101
K102
N103
V113
L120
A122
R126
L132
I133
K138
D139

V144
D149
I150
D158
E162
R165
D166
E174
N175
D176
A177
S178
Q199
S205
E206
R210
L211
T214
D215
L216
T217
D218
R222
V230
L231
A232
Q240
L245
A246
S252
E258
E259
D260
A261
V263
G264
L265
T266
E274
I275
R276
H277
R278

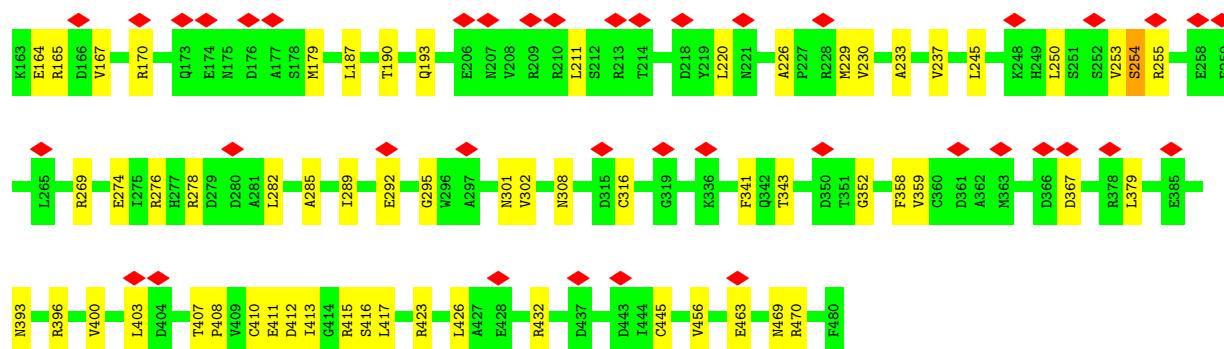
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T303
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Q305
V306
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N335
K336
L337
S349
D350
T351
G352
C360
D361
A362
M363
S364
M368
L372
E385
V388
K392
L395
R396
N397
A398
L399
T406
E411
D412
L417

L426
W429
I433
Q434
E435
V436
D437
A438
Q439
D443
I444
C445
S446
F449
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C453
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Q464
L465
M469
R472
S473
G474
E479
F480

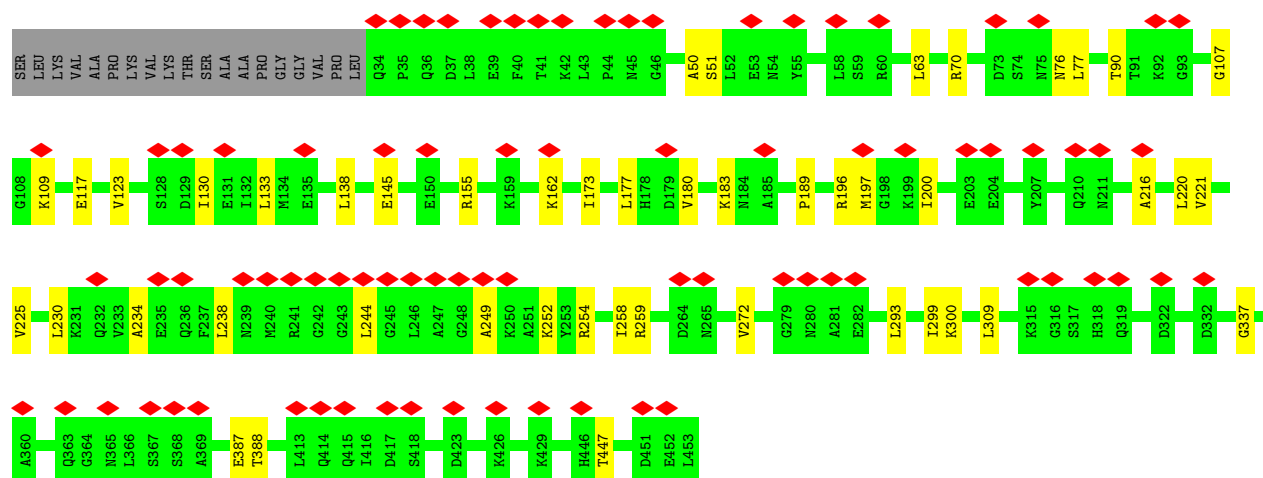
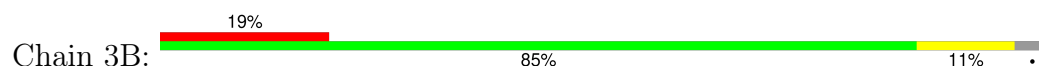
- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



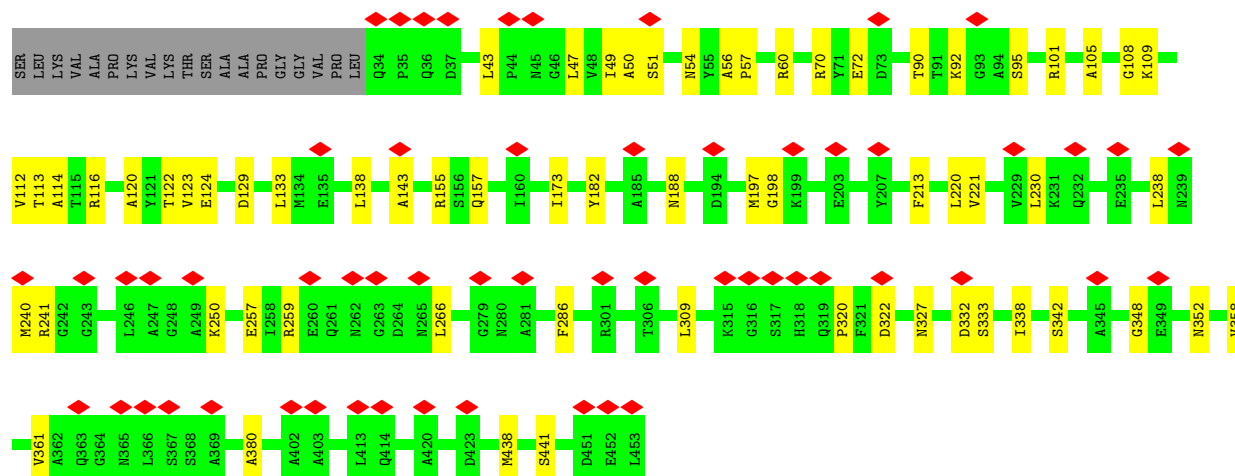
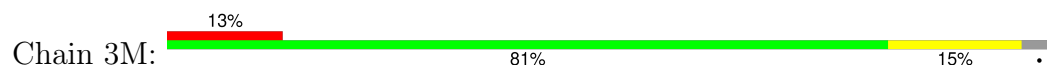
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N55
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D76
T83
E84
K85
L93
E94
K102
M103
M107
E110
E114
A118
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A135
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S159
E162



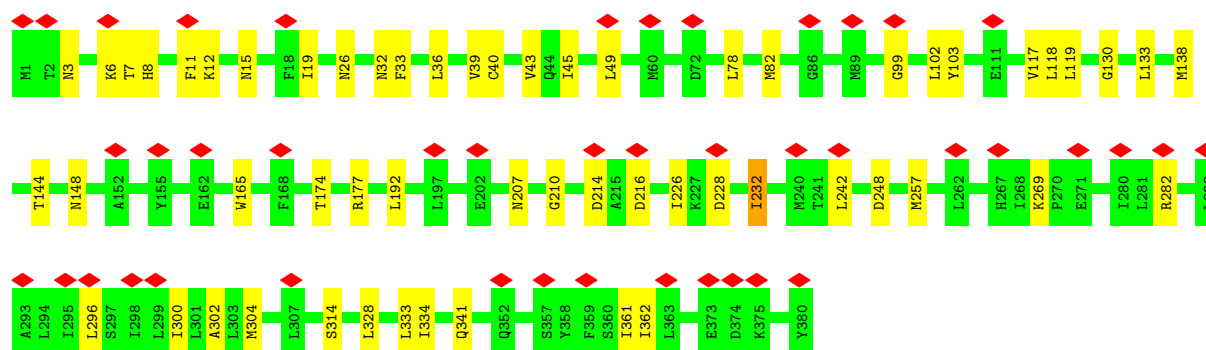
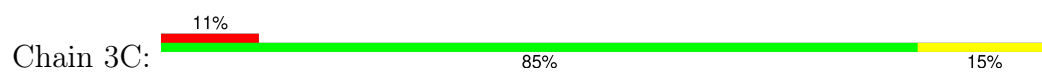
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



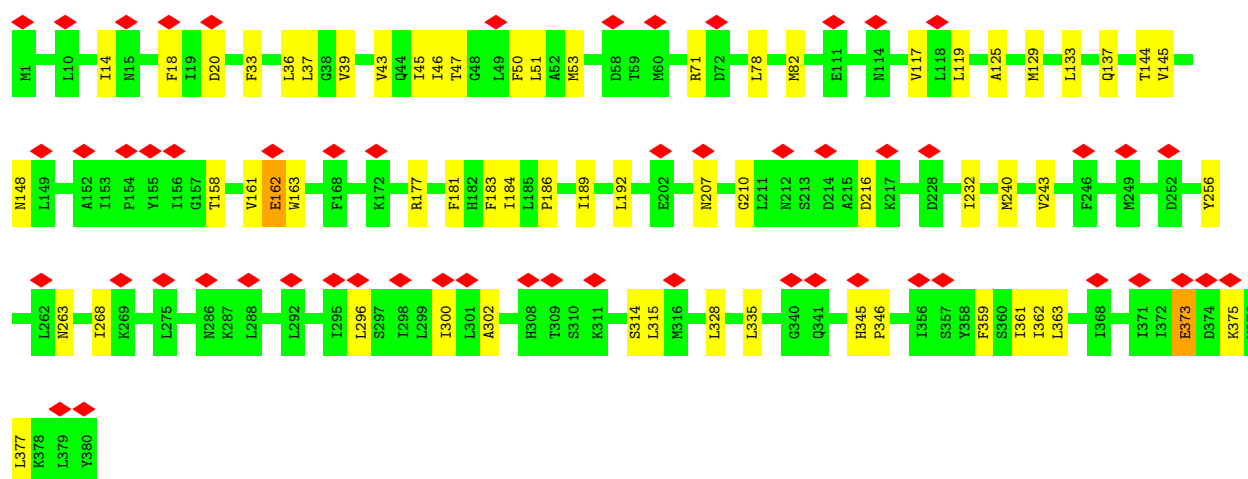
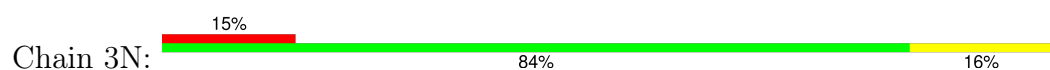
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



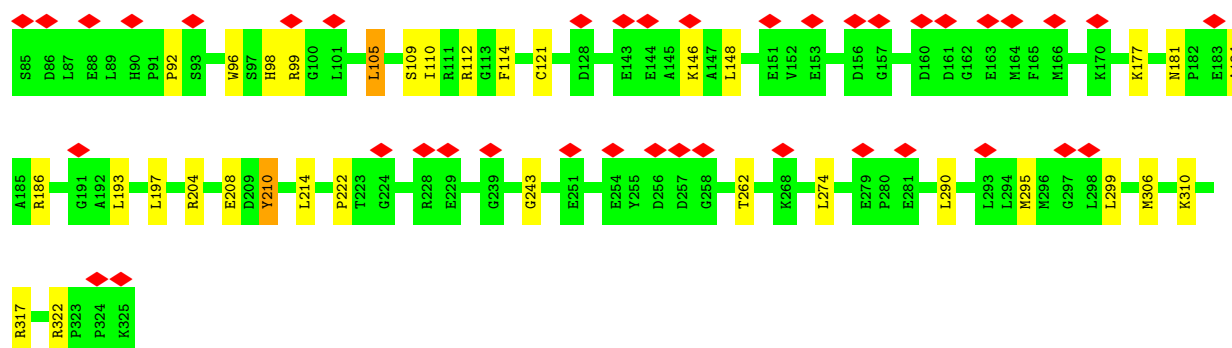
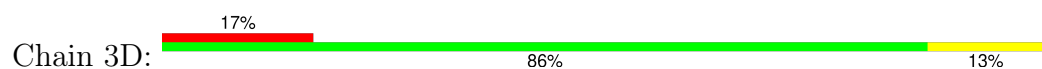
- Molecule 42: Cytochrome b



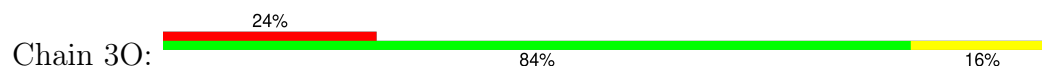
• Molecule 42: Cytochrome b

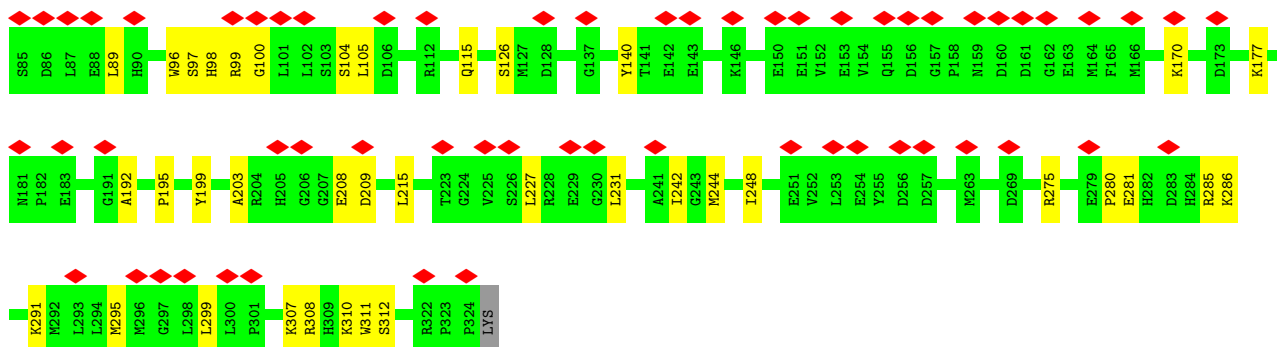


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

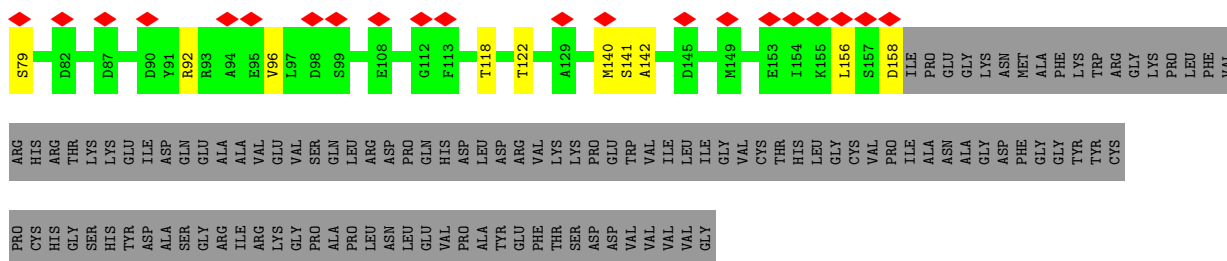
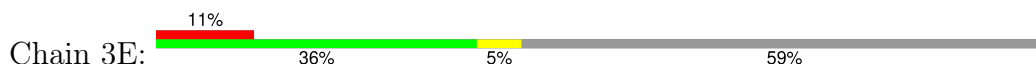


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

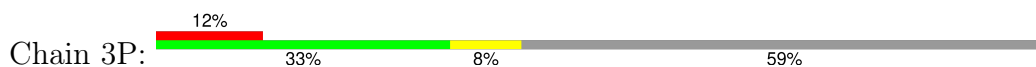




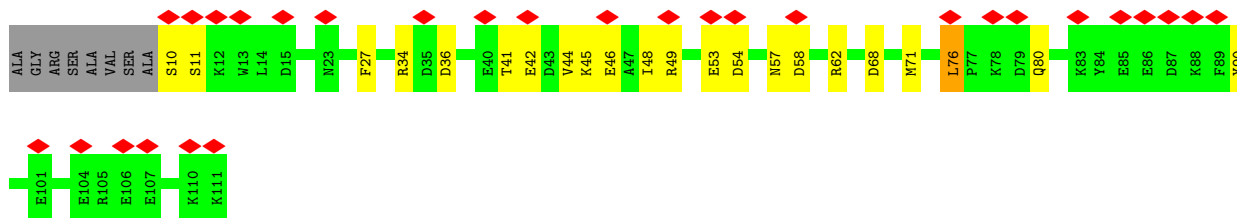
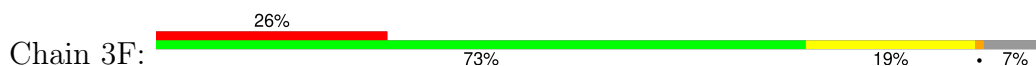
• Molecule 44: Cytochrome b-c1 complex subunit 9



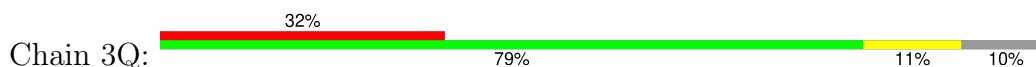
• Molecule 44: Cytochrome b-c1 complex subunit 9

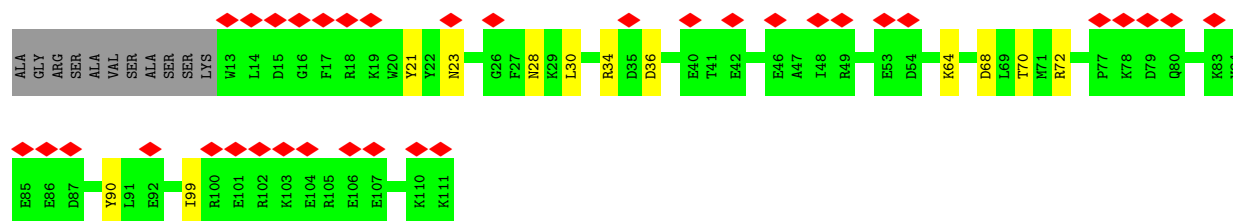


• Molecule 45: Cytochrome b-c1 complex subunit 7

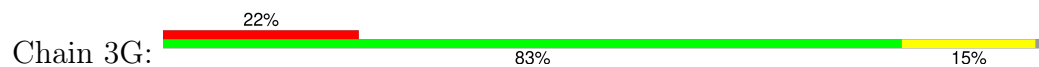


• Molecule 45: Cytochrome b-c1 complex subunit 7

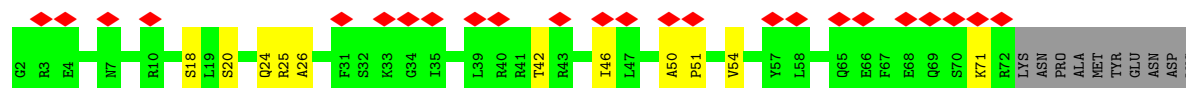
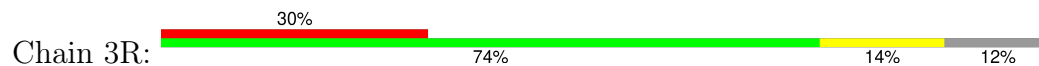




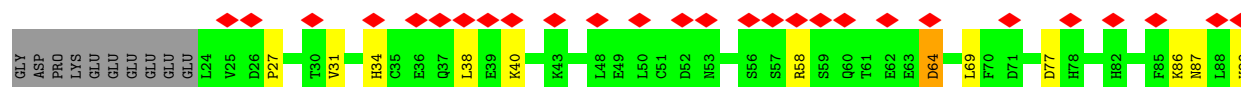
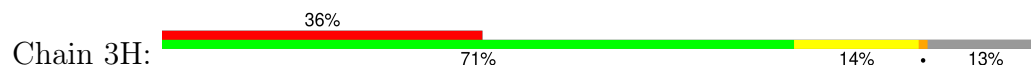
- Molecule 46: Cytochrome b-c1 complex subunit 8



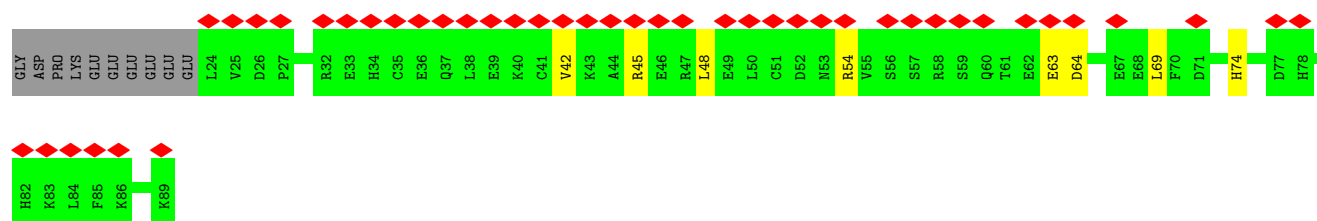
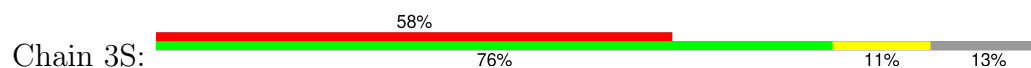
- Molecule 46: Cytochrome b-c1 complex subunit 8



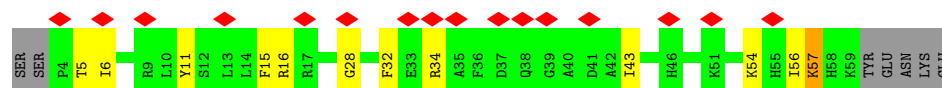
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



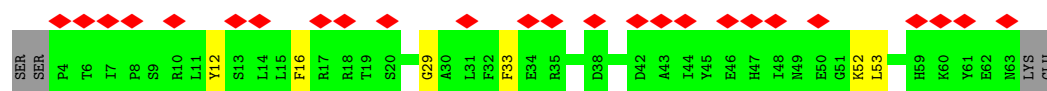
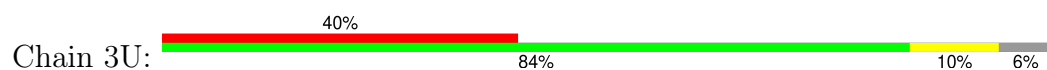
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



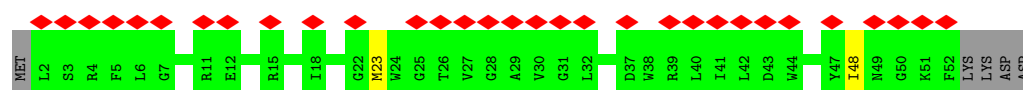
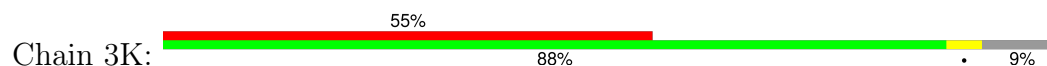
- Molecule 48: Cytochrome b-c1 complex subunit 9



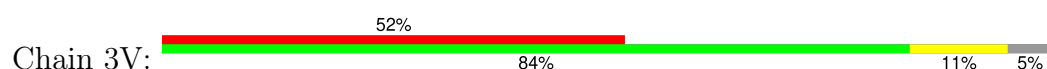
- Molecule 48: Cytochrome b-c1 complex subunit 9



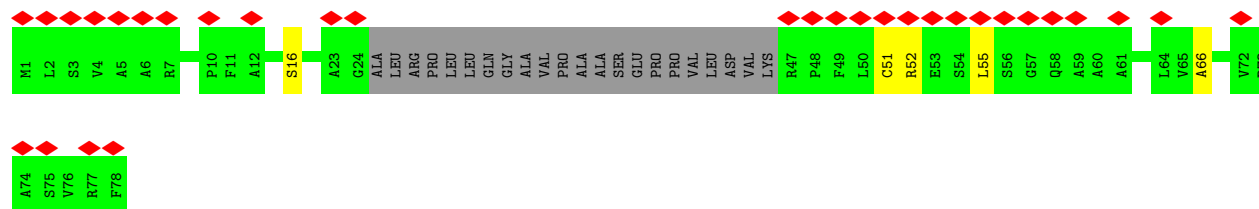
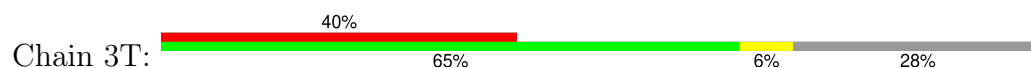
• Molecule 49: Cytochrome b-c1 complex subunit 10



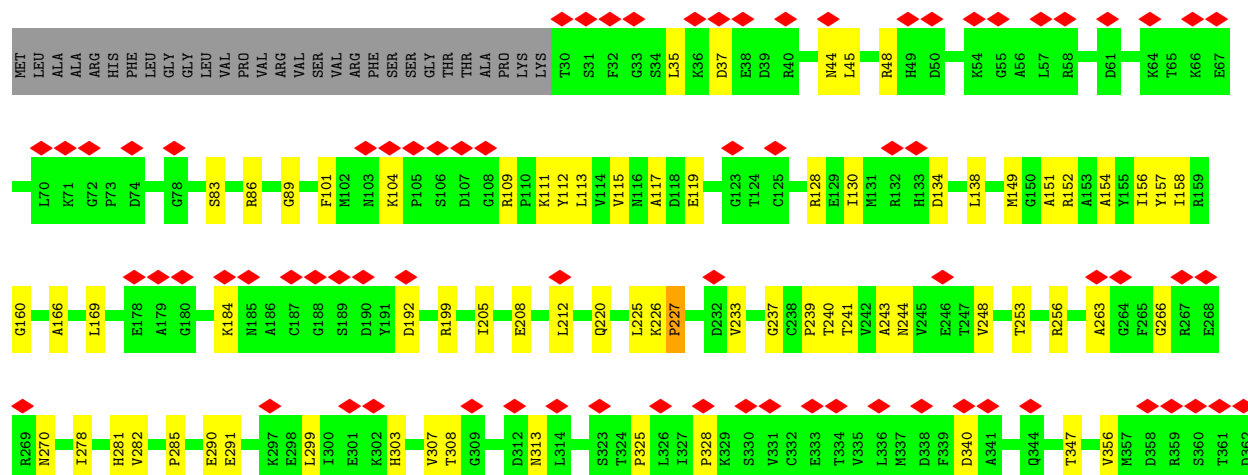
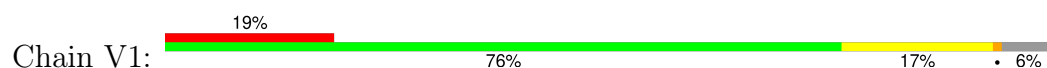
• Molecule 49: Cytochrome b-c1 complex subunit 10

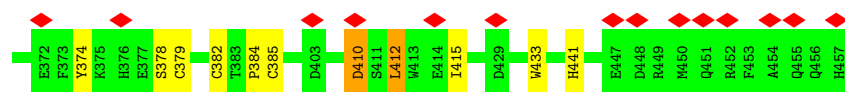


• Molecule 50: Cytochrome b-c1 complex subunit Rieske, mitochondrial



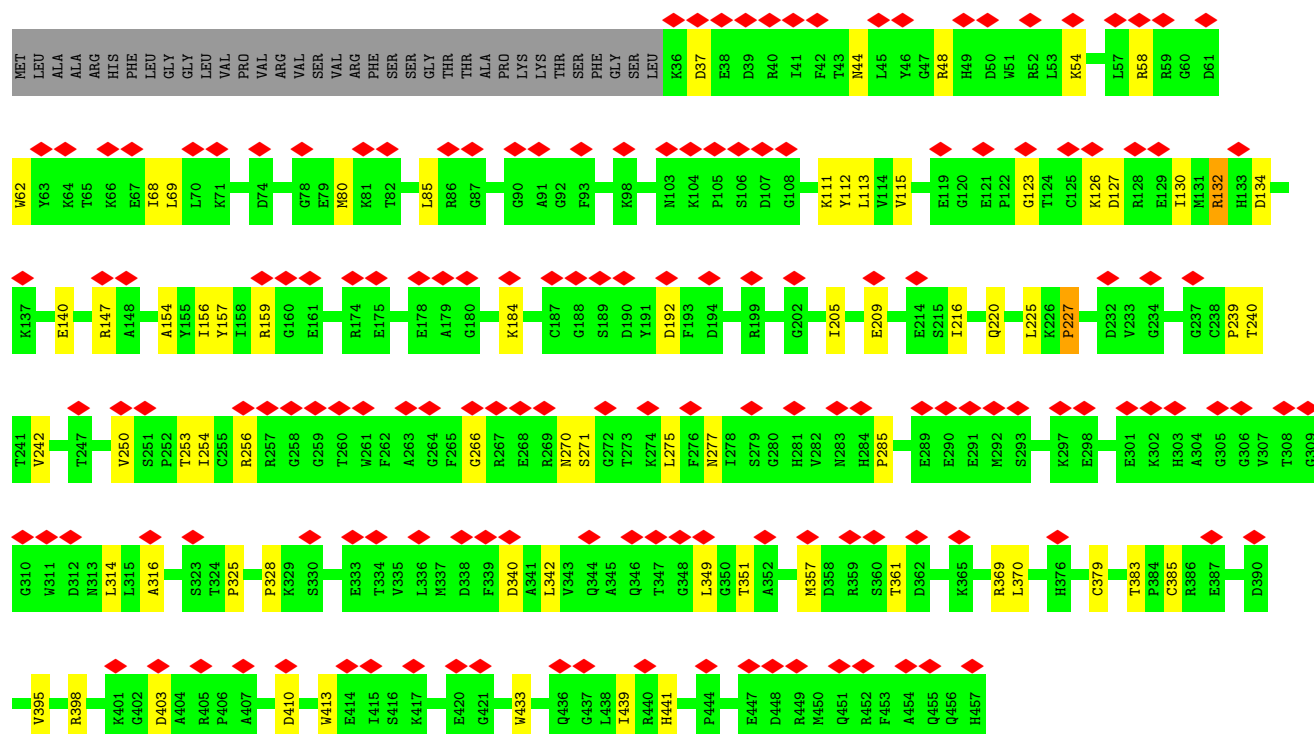
• Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





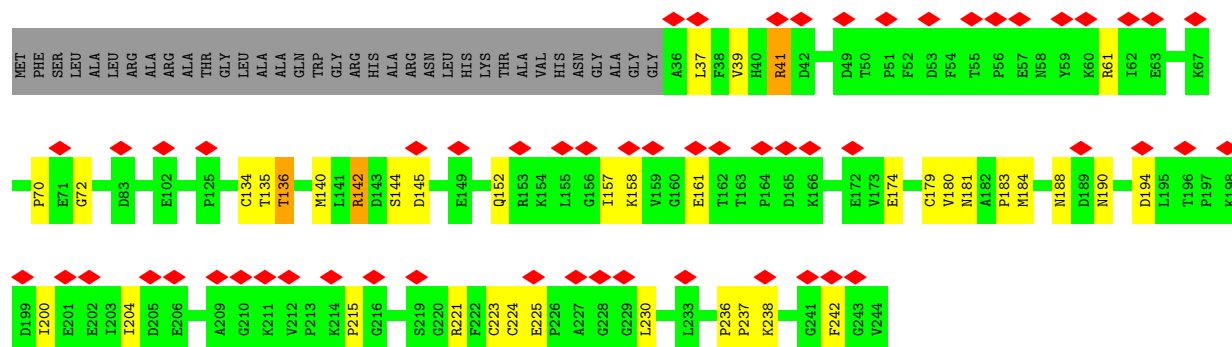
- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain v1: 34% 77% 15% 8%



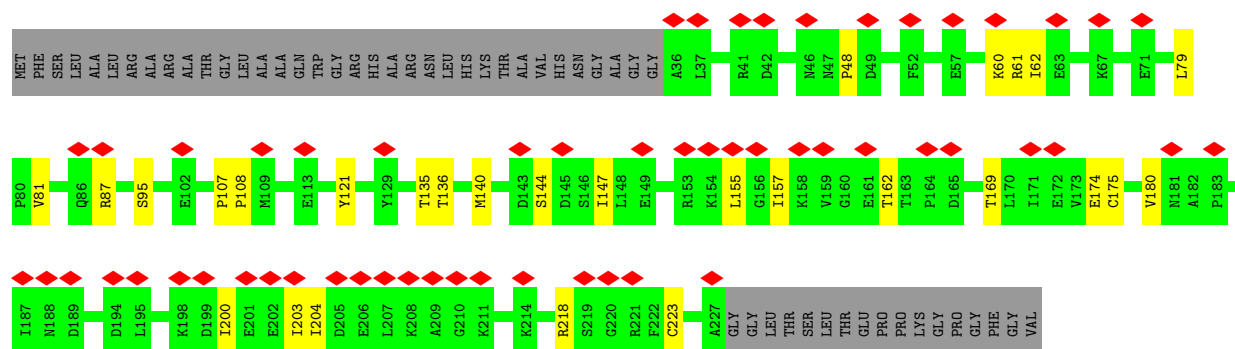
- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 23% 70% 14% 14%

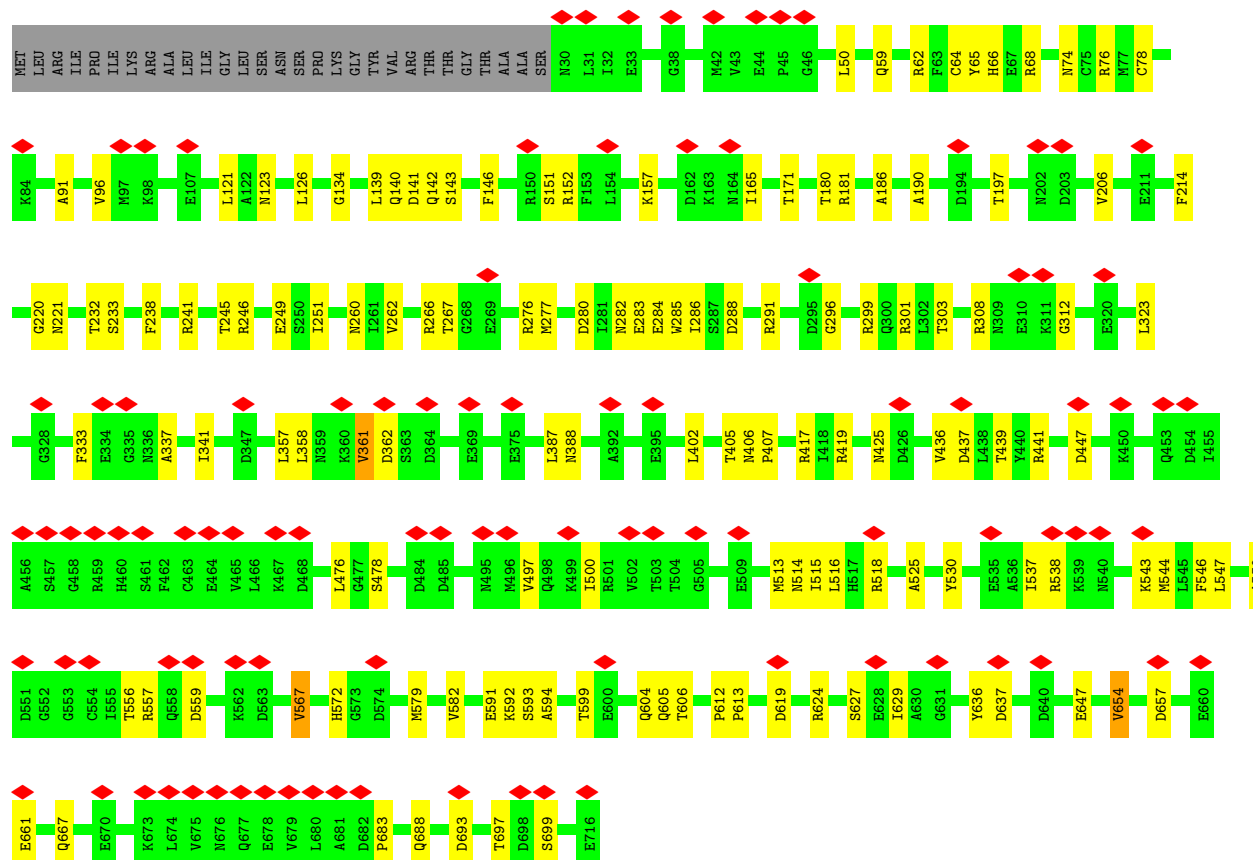
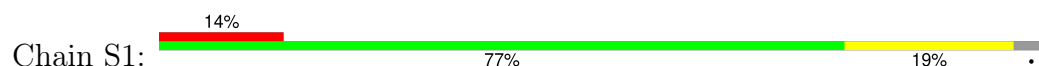


- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

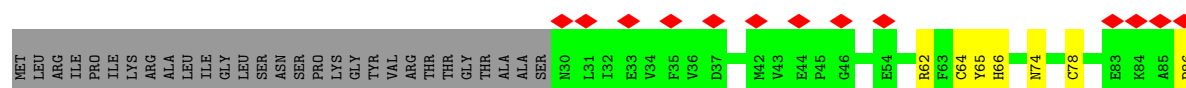
Chain v2: 23% 67% 11% 21%

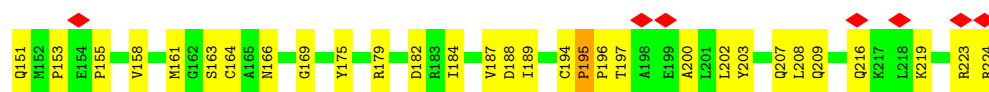


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

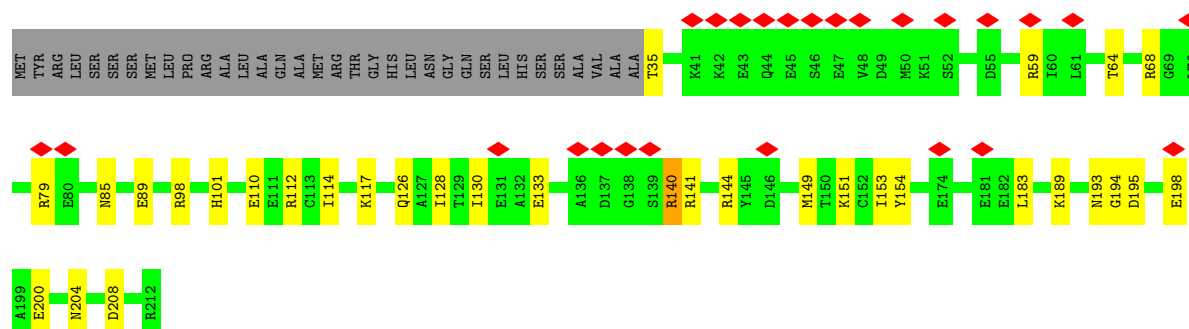


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

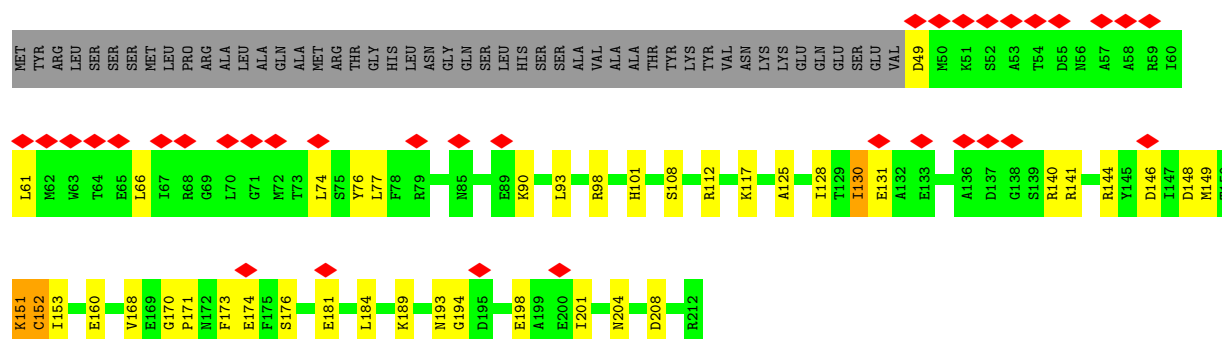




- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.227	Depositor
Minimum map value	-9.364	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.291	Depositor
Recommended contour level	3.4	Depositor
Map size ($\text{\AA}$)	249.92, 338.8, 238.48	wwPDB
Map dimensions	271, 385, 284	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FMN, FES, DGT, NDP, SF4, ZN, 2MR, HEM, EHZ, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	3	0.40	0/940	0.80	0/1285
1	3a	0.38	0/917	0.76	0/1252
2	S3	0.31	0/1762	0.68	0/2401
2	s3	0.30	0/1751	0.66	3/2386 (0.1%)
3	S2	0.33	0/3485	0.66	2/4720 (0.0%)
3	s2	0.33	0/3469	0.67	2/4698 (0.0%)
4	1	0.42	1/2607 (0.0%)	0.90	3/3564 (0.1%)
4	1a	0.38	0/2599	0.84	0/3554
5	6	0.34	0/1322	0.68	0/1799
5	6a	0.30	0/1330	0.68	0/1809
6	4L	0.38	0/740	0.73	0/1005
6	4l	0.34	0/738	0.71	0/1002
7	5	0.37	0/4913	0.79	6/6685 (0.1%)
7	5a	0.35	0/4913	0.76	2/6685 (0.0%)
8	4	0.41	0/3717	0.82	3/5062 (0.1%)
8	4a	0.37	0/3717	0.79	3/5062 (0.1%)
9	2	0.41	0/2756	0.84	2/3751 (0.1%)
9	2a	0.49	3/2756 (0.1%)	1.00	7/3751 (0.2%)
10	AL	0.25	0/2674	0.59	2/3626 (0.1%)
10	al	0.26	0/2674	0.58	0/3626
11	A9	0.27	0/2823	0.59	0/3828
11	a9	0.25	0/2823	0.58	0/3828
12	S4	0.21	0/1044	0.48	0/1409
12	s4	0.21	0/1044	0.49	0/1409
13	S6	0.22	0/762	0.50	0/1026
13	s6	0.23	0/762	0.53	2/1026 (0.2%)
14	A2	0.29	0/682	0.69	0/920
14	a2	0.24	0/682	0.64	0/920
15	AB	0.30	0/637	0.63	0/858
15	AC	0.31	0/718	0.70	0/970
15	ab	0.24	0/637	0.58	0/858
15	ac	0.24	0/718	0.59	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	A5	0.28	0/949	0.65	2/1286 (0.2%)
16	a5	0.30	0/945	0.64	0/1281
17	A6	0.31	0/980	0.69	2/1317 (0.2%)
17	a6	0.30	0/972	0.63	1/1305 (0.1%)
18	A8	0.31	0/1422	0.69	0/1921
18	a8	0.27	0/1427	0.63	0/1927
19	AM	0.32	0/1069	0.68	2/1449 (0.1%)
19	am	0.30	0/1069	0.62	0/1449
20	AO	0.25	0/1192	0.50	0/1608
20	ao	0.25	0/1192	0.56	2/1608 (0.1%)
21	A1	0.36	0/577	0.68	0/777
21	a1	0.48	1/577 (0.2%)	0.72	0/777
22	A3	0.26	0/671	0.55	0/921
22	a3	0.26	0/671	0.58	0/921
23	C1	0.26	0/418	0.53	0/567
23	c1	0.26	0/388	0.51	0/528
24	C2	0.27	0/1028	0.55	0/1387
24	c2	0.27	0/1028	0.58	0/1387
25	S5	0.25	0/900	0.57	0/1199
25	s5	0.26	0/900	0.65	0/1199
26	B1	0.26	0/495	0.56	0/667
26	b1	0.30	0/495	0.62	0/667
27	BM	0.26	0/854	0.57	0/1163
27	bm	0.29	0/863	0.64	1/1175 (0.1%)
28	B5	0.28	0/1201	0.61	0/1626
28	b5	0.28	0/1193	0.59	0/1615
29	B6	0.32	0/807	0.67	0/1096
29	b6	0.27	0/784	0.58	0/1063
30	B2	0.27	0/580	0.64	0/794
30	b2	0.23	0/569	0.53	0/779
31	B3	0.25	0/587	0.53	0/793
31	b3	0.25	0/591	0.51	0/798
32	B8	0.25	0/1356	0.57	0/1851
32	b8	0.25	0/1356	0.57	0/1851
33	B4	0.29	0/1073	0.54	1/1455 (0.1%)
33	b4	0.29	0/1073	0.53	0/1455
34	B9	0.28	0/1596	0.64	6/2162 (0.3%)
34	b9	0.24	0/1589	0.58	2/2152 (0.1%)
35	B7	0.23	0/1009	0.56	0/1355
35	b7	0.27	0/1030	0.60	0/1382
36	BL	0.27	0/1443	0.58	0/1951
36	bl	0.28	0/1463	0.55	0/1977
37	AN	0.26	0/1243	0.60	0/1692

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	an	0.24	0/1243	0.57	0/1692
38	A7	0.20	0/759	0.46	0/1027
38	a7	0.23	0/572	0.53	0/774
39	V3	0.24	0/349	0.62	0/473
39	v3	0.31	0/311	0.65	0/420
40	3A	0.30	0/3529	0.70	7/4793 (0.1%)
40	3L	0.33	0/3530	0.74	4/4793 (0.1%)
41	3B	0.27	0/3205	0.62	0/4332
41	3M	0.26	0/3205	0.59	0/4332
42	3C	0.31	0/3147	0.66	0/4297
42	3N	0.31	0/3147	0.67	3/4297 (0.1%)
43	3D	0.26	0/1978	0.60	1/2685 (0.0%)
43	3O	0.24	0/1968	0.53	0/2674
44	3E	0.26	0/609	0.59	0/821
44	3P	0.28	0/617	0.64	0/832
45	3F	0.25	0/922	0.53	0/1234
45	3Q	0.26	0/901	0.57	0/1207
46	3G	0.37	0/689	0.78	1/931 (0.1%)
46	3R	0.36	0/617	0.68	0/833
47	3H	0.31	0/552	0.70	2/739 (0.3%)
47	3S	0.26	0/552	0.67	0/739
48	3J	0.54	1/473 (0.2%)	0.85	1/637 (0.2%)
48	3U	0.28	0/503	0.56	0/678
49	3K	0.32	0/437	0.63	0/598
49	3V	0.33	0/454	0.58	0/619
50	3T	0.25	0/403	0.51	0/546
51	V1	0.34	0/3376	0.78	2/4561 (0.0%)
51	v1	0.35	0/3333	0.76	6/4503 (0.1%)
52	V2	0.40	0/1670	0.83	3/2276 (0.1%)
52	v2	0.39	0/1553	0.89	0/2116
53	S1	0.30	0/5377	0.73	9/7285 (0.1%)
53	s1	0.29	0/5377	0.70	6/7285 (0.1%)
54	S7	0.41	0/1272	0.87	0/1722
54	s7	0.36	0/1272	0.84	0/1722
55	S8	0.36	0/1438	0.81	1/1946 (0.1%)
55	s8	0.36	0/1337	0.79	2/1808 (0.1%)
All	All	0.32	6/165414 (0.0%)	0.69	104/224305 (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
2	S3	0	1
4	1	0	2
7	5a	0	1
8	4	0	2
18	A8	0	1
37	AN	0	1
41	3B	0	1
42	3C	0	1
51	V1	0	1
51	v1	0	2
52	V2	0	4
52	v2	0	1
54	S7	0	4
54	s7	0	3
All	All	0	25

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2a	255	PRO	CB-CG	-11.20	0.93	1.49
21	a1	18	ILE	C-N	9.06	1.45	1.34
9	2a	255	PRO	CG-CD	-7.88	1.24	1.50
48	3J	57	LYS	CA-C	6.53	1.61	1.52
9	2a	255	PRO	N-CA	5.90	1.58	1.46
4	1	74	ALA	C-N	5.20	1.40	1.34

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2a	255	PRO	CB-CG-CD	18.22	164.40	106.10
9	2a	255	PRO	N-CD-CG	-17.40	77.11	103.20
9	2a	255	PRO	CA-CB-CG	-16.77	72.64	104.50
10	AL	210	PRO	CA-C-N	10.80	127.05	120.24
10	AL	210	PRO	C-N-CA	10.80	127.05	120.24
9	2a	255	PRO	CA-N-CD	-8.28	100.41	112.00
9	2a	255	PRO	N-CA-C	7.61	119.98	110.70
7	5	432	MET	CA-C-N	7.44	135.75	121.54
7	5	432	MET	C-N-CA	7.44	135.75	121.54
34	B9	27	LEU	CA-C-N	7.37	135.62	121.54
34	B9	27	LEU	C-N-CA	7.37	135.62	121.54
7	5	526	LEU	CA-CB-CG	6.91	140.48	116.30
34	B9	56	ASP	CA-C-N	6.53	134.02	121.54
34	B9	56	ASP	C-N-CA	6.53	134.02	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	s1	361	VAL	CA-C-N	6.46	131.57	122.46
53	s1	361	VAL	C-N-CA	6.46	131.57	122.46
52	V2	180	VAL	N-CA-C	-6.46	107.58	113.71
40	3A	444	ILE	CG1-CB-CG2	-6.44	91.39	110.70
53	S1	283	GLU	CA-CB-CG	6.43	126.97	114.10
40	3L	250	LEU	CA-CB-CG	6.43	138.79	116.30
7	5a	230	HIS	N-CA-C	6.42	124.00	109.81
19	AM	17	GLN	CB-CG-CD	6.39	123.47	112.60
27	bm	112	MET	CA-CB-CG	6.39	126.88	114.10
40	3A	80	ARG	CA-C-N	6.38	131.93	122.74
40	3A	80	ARG	C-N-CA	6.38	131.93	122.74
53	S1	283	GLU	CB-CA-C	6.38	121.98	112.03
19	AM	17	GLN	CA-CB-CG	6.35	126.81	114.10
53	S1	361	VAL	CA-C-N	6.33	133.64	121.54
53	S1	361	VAL	C-N-CA	6.33	133.64	121.54
51	v1	314	LEU	CA-CB-CG	6.21	138.02	116.30
42	3N	373	GLU	CA-CB-CG	6.14	126.38	114.10
43	3D	210	TYR	CA-CB-CG	6.13	124.94	113.90
40	3A	349	SER	CA-C-N	6.13	133.25	121.54
40	3A	349	SER	C-N-CA	6.13	133.25	121.54
52	V2	41	ARG	CA-C-N	6.02	130.95	122.46
52	V2	41	ARG	C-N-CA	6.02	130.95	122.46
53	S1	654	VAL	N-CA-C	-5.94	106.47	113.42
20	ao	102	PRO	CA-C-N	5.92	132.84	121.54
20	ao	102	PRO	C-N-CA	5.92	132.84	121.54
51	v1	227	PRO	CA-C-N	-5.89	112.48	119.84
51	v1	227	PRO	C-N-CA	-5.89	112.48	119.84
8	4	406	TYR	CA-CB-CG	5.87	124.47	113.90
3	S2	375	MET	CB-CG-SD	5.85	130.24	112.70
8	4a	406	TYR	CA-CB-CG	5.83	124.40	113.90
34	b9	56	ASP	CA-C-N	5.81	132.63	121.54
34	b9	56	ASP	C-N-CA	5.81	132.63	121.54
13	s6	49	VAL	CA-C-N	5.80	131.65	122.61
13	s6	49	VAL	C-N-CA	5.80	131.65	122.61
40	3L	254	SER	CA-C-N	5.78	132.59	121.54
40	3L	254	SER	C-N-CA	5.78	132.59	121.54
7	5a	422	TYR	CA-CB-CG	5.78	124.30	113.90
51	v1	370	LEU	CA-CB-CG	5.75	136.43	116.30
42	3N	133	LEU	N-CA-C	5.62	122.24	109.81
55	S8	153	ILE	CA-CB-CG2	5.60	120.01	110.50
53	S1	697	THR	CA-C-N	5.59	132.22	121.54
53	S1	697	THR	C-N-CA	5.59	132.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	200	LEU	CA-C-N	5.56	132.16	121.54
4	1	200	LEU	C-N-CA	5.56	132.16	121.54
53	s1	697	THR	CA-C-N	5.56	132.15	121.54
53	s1	697	THR	C-N-CA	5.56	132.15	121.54
9	2a	190	MET	CA-CB-CG	5.52	125.14	114.10
40	3L	445	CYS	CA-CB-SG	5.46	126.95	114.40
34	B9	48	PHE	N-CA-CB	5.42	119.23	110.40
8	4	364	LEU	CA-CB-CG	5.39	135.18	116.30
7	5	422	TYR	CA-CB-CG	5.37	123.57	113.90
53	S1	126	LEU	CA-CB-CG	5.34	135.01	116.30
42	3N	162	GLU	CB-CG-CD	5.34	121.67	112.60
7	5	230	HIS	N-CA-C	5.33	120.92	113.57
4	1	142	TYR	CA-CB-CG	5.33	123.49	113.90
16	A5	115	PRO	CA-C-N	5.29	131.22	121.70
16	A5	115	PRO	C-N-CA	5.29	131.22	121.70
51	V1	226	LYS	N-CA-C	5.28	121.48	109.81
51	v1	132	ARG	CA-C-N	5.27	131.60	121.54
51	v1	132	ARG	C-N-CA	5.27	131.60	121.54
33	B4	96	GLY	N-CA-C	5.27	123.08	112.34
7	5	319	MET	CA-CB-CG	5.26	124.62	114.10
40	3A	85	LYS	CA-C-N	5.25	129.86	122.46
40	3A	85	LYS	C-N-CA	5.25	129.86	122.46
34	B9	28	GLU	CA-CB-CG	5.24	124.59	114.10
8	4	236	LEU	CA-CB-CG	5.23	134.61	116.30
8	4a	4	ILE	N-CA-C	-5.21	107.75	112.96
55	s8	151	LYS	CA-C-N	5.20	131.47	121.54
55	s8	151	LYS	C-N-CA	5.20	131.47	121.54
48	3J	56	ILE	CG1-CB-CG2	-5.20	95.10	110.70
2	s3	80	LEU	CA-C-N	5.18	129.77	122.46
2	s3	80	LEU	C-N-CA	5.18	129.77	122.46
17	A6	23	ILE	CA-C-N	5.16	131.40	121.54
17	A6	23	ILE	C-N-CA	5.16	131.40	121.54
9	2a	37	LEU	CA-CB-CG	5.16	134.37	116.30
8	4a	329	LEU	CA-CB-CG	5.16	134.35	116.30
53	s1	126	LEU	CA-CB-CG	5.15	134.32	116.30
17	a6	46	VAL	N-CA-C	5.13	119.96	108.88
2	s3	160	ILE	CG1-CB-CG2	-5.11	95.38	110.70
3	s2	273	VAL	CA-C-N	5.10	129.37	122.07
3	s2	273	VAL	C-N-CA	5.10	129.37	122.07
51	V1	130	ILE	CA-CB-CG1	5.08	119.03	110.40
53	s1	254	MET	CA-CB-CG	5.05	124.20	114.10
47	3H	87	ASN	CA-C-N	5.05	131.18	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3H	87	ASN	C-N-CA	5.05	131.18	121.54
9	2	339	LEU	CA-C-N	5.04	126.06	120.06
9	2	339	LEU	C-N-CA	5.04	126.06	120.06
46	3G	50	ALA	N-CA-C	5.03	120.93	109.81
53	S1	582	VAL	CG1-CB-CG2	-5.02	99.75	110.80
3	S2	139	LEU	CB-CG-CD1	-5.00	95.68	110.70

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1	154	LEU	Peptide
4	1	199	ASP	Peptide
41	3B	258	ILE	Peptide
42	3C	26	ASN	Peptide
8	4	249	ILE	Peptide
8	4	366	ASN	Peptide
7	5a	437	PHE	Peptide
18	A8	166	ARG	Sidechain
37	AN	120	ASN	Peptide
2	S3	70	LYS	Peptide
54	S7	153	PRO	Peptide
54	S7	193	GLY	Peptide
54	S7	194	CYS	Peptide
54	S7	195	PRO	Peptide
51	V1	227	PRO	Peptide
52	V2	136	THR	Peptide
52	V2	142	ARG	Peptide
52	V2	179	CYS	Peptide
52	V2	181	ASN	Peptide
54	s7	134	ALA	Peptide
54	s7	194	CYS	Peptide
54	s7	195	PRO	Peptide
51	v1	227	PRO	Peptide
51	v1	253	THR	Peptide
52	v2	87	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	914	0	952	25	0
1	3a	893	0	935	17	0
2	S3	1712	0	1667	37	0
2	s3	1701	0	1655	31	0
3	S2	3410	0	3348	71	0
3	s2	3386	0	3319	69	0
4	1	2530	0	2615	49	0
4	1a	2522	0	2606	62	0
5	6	1290	0	1304	21	0
5	6a	1298	0	1316	20	0
6	4L	729	0	764	12	0
6	4l	727	0	758	16	0
7	5	4790	0	4975	100	0
7	5a	4790	0	4973	73	0
8	4	3630	0	3854	70	0
8	4a	3630	0	3854	64	0
9	2	2694	0	2896	48	0
9	2a	2694	0	2896	48	0
10	AL	2607	0	2562	22	0
10	al	2607	0	2563	23	0
11	A9	2748	0	2765	44	0
11	a9	2748	0	2765	38	0
12	S4	1021	0	1022	19	0
12	s4	1021	0	1022	15	0
13	S6	748	0	721	16	0
13	s6	748	0	721	14	0
14	A2	671	0	688	14	0
14	a2	671	0	688	12	0
15	AB	628	0	627	4	0
15	AC	706	0	696	13	0
15	ab	628	0	627	12	0
15	ac	706	0	696	7	0
16	A5	927	0	968	11	0
16	a5	923	0	965	12	0
17	A6	957	0	979	12	0
17	a6	950	0	972	16	0
18	A8	1385	0	1370	14	0
18	a8	1389	0	1374	17	0
19	AM	1045	0	1034	9	0
19	am	1045	0	1034	11	0
20	AO	1161	0	1161	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	ao	1161	0	1161	31	0
21	A1	564	0	579	2	0
21	a1	564	0	579	11	0
22	A3	648	0	649	6	0
22	a3	648	0	652	5	0
23	C1	407	0	404	0	0
23	c1	377	0	371	2	0
24	C2	996	0	1001	10	0
24	c2	996	0	1001	11	0
25	S5	877	0	871	14	0
25	s5	877	0	869	17	0
26	B1	482	0	479	2	0
26	b1	482	0	479	6	0
27	BM	826	0	766	7	0
27	bm	835	0	772	9	0
28	B5	1166	0	1166	12	0
28	b5	1158	0	1160	20	0
29	B6	783	0	792	12	0
29	b6	761	0	769	11	0
30	B2	555	0	506	5	0
30	b2	545	0	499	10	0
31	B3	569	0	573	12	0
31	b3	573	0	576	3	0
32	B8	1302	0	1197	19	0
32	b8	1302	0	1197	15	0
33	B4	1044	0	1056	21	0
33	b4	1044	0	1056	15	0
34	B9	1541	0	1470	18	0
34	b9	1534	0	1463	19	0
35	B7	984	0	970	11	0
35	b7	1005	0	995	12	0
36	BL	1410	0	1379	21	0
36	bl	1430	0	1400	16	0
37	AN	1201	0	1158	17	0
37	an	1201	0	1158	14	0
38	A7	741	0	770	11	0
38	a7	560	0	579	8	0
39	V3	339	0	320	7	0
39	v3	303	0	290	6	0
40	3A	3459	0	3365	52	0
40	3L	3460	0	3365	46	0
41	3B	3154	0	3158	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	3M	3154	0	3158	41	0
42	3C	3046	0	3110	36	0
42	3N	3046	0	3111	36	0
43	3D	1919	0	1864	24	0
43	3O	1909	0	1849	28	0
44	3E	602	0	601	6	0
44	3P	610	0	612	10	0
45	3F	900	0	887	12	0
45	3Q	879	0	864	8	0
46	3G	670	0	666	9	0
46	3R	600	0	604	7	0
47	3H	545	0	529	8	0
47	3S	545	0	531	5	0
48	3J	460	0	464	8	0
48	3U	489	0	485	4	0
49	3K	421	0	418	2	0
49	3V	438	0	443	3	0
50	3T	397	0	418	5	0
51	V1	3301	0	3248	50	0
51	v1	3259	0	3212	44	0
52	V2	1630	0	1623	24	0
52	v2	1517	0	1509	19	0
53	S1	5290	0	5317	90	0
53	s1	5290	0	5317	93	0
54	S7	1241	0	1250	25	0
54	s7	1241	0	1248	37	0
55	S8	1408	0	1341	29	0
55	s8	1309	0	1261	36	0
56	AL	1	0	0	0	0
56	al	1	0	0	0	0
57	AL	31	0	12	1	0
57	al	31	0	12	0	0
58	A9	48	0	26	3	0
58	a9	48	0	25	1	0
59	S6	1	0	0	0	0
59	s6	1	0	0	0	0
60	5a	37	0	0	0	0
60	A6	37	0	0	0	0
60	B9	37	0	0	1	0
60	a6	37	0	0	0	0
61	3C	86	0	60	1	0
61	3N	86	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	3D	43	0	30	3	0
62	3O	43	0	30	2	0
63	V1	31	0	18	2	0
63	v1	31	0	19	0	0
64	S1	16	0	0	1	0
64	S7	8	0	0	3	0
64	S8	16	0	0	1	0
64	V1	8	0	0	1	0
64	s1	16	0	0	1	0
64	s7	8	0	0	2	0
64	s8	16	0	0	2	0
64	v1	8	0	0	1	0
65	S1	4	0	0	1	0
65	V2	4	0	0	1	0
65	s1	4	0	0	1	0
65	v2	4	0	0	1	0
All	All	162102	0	161959	2056	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 6.

All (2056) 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)
43:3D:121:CYS:SG	62:3D:401:HEC:CAB	2.02	1.45
43:3D:121:CYS:SG	62:3D:401:HEC:C3B	2.32	1.18
35:B7:7:ARG:O	35:B7:11:TRP:HB2	1.71	0.91
8:4a:13:PRO:O	8:4a:17:LEU:HB2	1.75	0.87
3:S2:223:HIS:CD2	64:S7:301:SF4:S1	2.69	0.86
4:1:281:ARG:O	4:1:285:LEU:HB2	1.76	0.85
55:S8:101:HIS:HE1	64:S8:301:SF4:S4	1.99	0.84
7:5a:273:ILE:O	7:5a:277:MET:HB2	1.78	0.84
36:BL:121:TYR:O	36:BL:125:CYS:HB2	1.76	0.83
7:5:243:VAL:O	7:5:247:LEU:HB2	1.78	0.82
3:S2:380:HIS:O	3:S2:384:LEU:HB2	1.78	0.82
42:3N:296:LEU:O	42:3N:300:ILE:HB	1.82	0.79
7:5:530:PRO:O	7:5:534:HIS:HB2	1.81	0.79
4:1:119:SER:O	4:1:123:SER:HB2	1.85	0.77
31:B3:56:ALA:O	31:B3:60:MET:HB3	1.85	0.77
55:s8:128:ILE:HA	55:s8:146:ASP:O	1.85	0.77
3:S2:223:HIS:NE2	64:S7:301:SF4:S1	2.57	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6a:59:TYR:O	5:6a:63:MET:HB2	1.85	0.76
5:6:55:VAL:O	5:6:59:TYR:HB2	1.86	0.75
20:ao:120:LEU:O	20:ao:124:MET:HB2	1.87	0.74
38:a7:3:SER:N	38:a7:28:TYR:HH	1.84	0.74
3:S2:223:HIS:CE1	54:S7:99:CYS:SG	2.82	0.73
11:A9:56:ALA:HA	11:A9:125:VAL:O	1.87	0.73
42:3C:99:GLY:O	42:3C:103:TYR:HB2	1.90	0.72
28:B5:72:LYS:O	28:B5:76:MET:HB2	1.89	0.71
16:A5:45:ARG:O	16:A5:49:GLU:HB2	1.90	0.71
55:s8:148:ASP:O	55:s8:152:CYS:HB2	1.90	0.71
41:3B:173:ILE:O	41:3B:177:LEU:HB2	1.90	0.70
2:S3:168:GLU:O	2:S3:172:MET:HB2	1.90	0.70
20:AO:50:MET:O	20:AO:54:ASN:HB2	1.91	0.70
53:S1:78:CYS:HB3	65:S1:803:FES:S2	2.32	0.70
53:s1:78:CYS:HB3	65:s1:803:FES:S2	2.32	0.69
8:4:68:LEU:O	8:4:72:LEU:HB2	1.92	0.69
24:c2:44:MET:O	24:c2:48:LEU:HB2	1.93	0.69
7:5:374:VAL:O	7:5:378:LEU:HB2	1.93	0.69
4:1:287:HIS:O	4:1:291:LYS:HB2	1.92	0.68
3:S2:200:PHE:O	3:S2:204:PHE:HB2	1.93	0.68
51:V1:208:GLU:O	51:V1:212:LEU:HB2	1.94	0.68
46:3R:42:THR:O	46:3R:46:ILE:HB	1.94	0.68
42:3C:144:THR:O	42:3C:148:ASN:HB2	1.94	0.68
7:5:63:ILE:O	7:5:79:SER:HA	1.94	0.67
7:5:544:LEU:O	7:5:548:THR:HB	1.94	0.67
7:5a:460:GLY:O	7:5a:464:ALA:HB2	1.95	0.67
55:s8:130:ILE:HA	55:s8:144:ARG:O	1.94	0.66
53:s1:404:GLY:HA3	53:s1:477:GLY:H	1.59	0.66
8:4a:239:GLY:O	8:4a:243:MET:HB2	1.96	0.66
5:6a:63:MET:O	5:6a:67:PHE:HB2	1.96	0.66
40:3L:118:ALA:HA	40:3L:134:LYS:O	1.95	0.66
30:b2:94:ASP:O	30:b2:98:GLY:HA2	1.96	0.66
42:3N:78:LEU:O	42:3N:82:MET:HB2	1.95	0.66
3:s2:195:GLY:HA3	4:1a:279:ARG:HB3	1.77	0.65
10:al:240:ALA:O	10:al:244:THR:HB	1.96	0.65
25:s5:95:PRO:O	25:s5:99:SER:HB2	1.96	0.64
7:5:220:ALA:O	7:5:224:SER:HB3	1.97	0.64
8:4a:175:ASN:O	8:4a:179:LEU:HB2	1.98	0.64
51:V1:113:LEU:O	51:V1:154:ALA:HA	1.97	0.64
39:V3:81:LEU:HB3	52:V2:61:ARG:HD3	1.80	0.63
4:1:134:ARG:HD3	4:1:200:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S2:223:HIS:NE2	54:S7:99:CYS:SG	2.71	0.63
4:1:90:PRO:HG3	4:1:162:LEU:HB3	1.81	0.63
9:2:42:PRO:O	9:2:46:ASN:HB3	1.99	0.63
3:s2:220:ALA:HB1	54:s7:195:PRO:HG2	1.81	0.62
5:6:102:LEU:O	5:6:106:LEU:HB2	1.99	0.62
41:3M:266:LEU:HA	41:3M:342:SER:O	1.99	0.62
40:3L:308:ASN:ND2	40:3L:343:THR:OG1	2.32	0.62
51:v1:113:LEU:O	51:v1:154:ALA:HA	2.00	0.62
34:B9:71:PHE:O	34:B9:75:GLN:HB3	2.00	0.62
17:a6:48:ASN:O	17:a6:52:LEU:HB3	1.99	0.62
33:b4:33:GLN:HG3	33:b4:36:ARG:HH21	1.65	0.62
46:3G:42:THR:O	46:3G:46:ILE:HB	1.99	0.62
3:S2:82:LEU:HD12	4:1:126:LYS:HB3	1.82	0.62
43:3O:295:MET:O	43:3O:299:LEU:HB2	2.00	0.62
8:4:118:PHE:O	8:4:122:PHE:HB2	2.00	0.61
3:s2:370:GLU:O	3:s2:374:SER:HB2	2.00	0.61
9:2:26:LEU:HB3	9:2:74:ILE:HG12	1.83	0.61
9:2:328:THR:O	9:2:332:MET:HB2	2.01	0.61
16:a5:49:GLU:O	16:a5:53:ASN:HB2	2.01	0.61
43:3O:281:GLU:O	43:3O:285:ARG:HB2	2.01	0.61
52:V2:183:PRO:HD2	52:V2:194:ASP:HA	1.83	0.61
8:4:254:THR:HG21	8:4:304:GLN:HE21	1.66	0.60
9:2:187:MET:HA	9:2:190:MET:HG2	1.83	0.60
30:B2:53:SER:O	30:B2:57:GLN:HB2	2.00	0.60
39:v3:81:LEU:HB3	52:v2:61:ARG:HD3	1.83	0.60
11:a9:86:CYS:SG	11:a9:87:ASP:N	2.74	0.60
48:3J:11:TYR:HA	48:3J:15:PHE:HB2	1.83	0.60
3:S2:100:GLU:HB3	3:S2:108:LYS:HB3	1.84	0.60
48:3U:29:GLY:O	48:3U:33:PHE:HB2	2.01	0.60
54:s7:99:CYS:HB2	64:s7:301:SF4:S1	2.42	0.60
2:S3:234:LEU:HD12	3:S2:418:ARG:HE	1.67	0.60
7:5a:243:VAL:O	7:5a:247:LEU:HB2	2.02	0.60
15:AC:117:GLU:HG2	31:B3:51:TRP:HE1	1.66	0.60
53:s1:170:LYS:HB2	53:s1:234:LYS:HG3	1.82	0.60
2:S3:199:LYS:HB3	12:S4:126:LEU:HD11	1.84	0.60
4:1a:138:GLN:HE21	4:1a:200:LEU:HB2	1.66	0.60
53:s1:593:SER:HA	53:s1:606:THR:O	2.02	0.60
6:4l:22:PHE:HB2	7:5a:585:LYS:HB3	1.84	0.59
20:ao:97:ILE:HG22	20:ao:98:MET:HG3	1.85	0.59
4:1:197:PRO:HG3	4:1:277:TYR:HB2	1.83	0.59
8:4a:325:LEU:HD21	8:4a:441:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3D:186:ARG:HG2	43:3D:193:LEU:HB2	1.85	0.59
53:s1:251:ILE:HD12	53:s1:604:GLN:HB2	1.85	0.59
9:2a:216:PHE:O	9:2a:220:MET:HB2	2.02	0.59
7:5:556:ILE:O	7:5:560:LYS:HB2	2.02	0.59
53:s1:337:ALA:HB1	53:s1:543:LYS:H	1.65	0.59
11:A9:251:ASN:O	11:A9:255:ASP:HB2	2.03	0.59
8:4a:336:ARG:HH21	8:4a:429:SER:HA	1.68	0.59
41:3B:234:ALA:O	41:3B:238:LEU:HB2	2.02	0.59
13:S6:104:CYS:HB3	13:S6:107:CYS:SG	2.42	0.59
2:s3:128:VAL:HG12	2:s3:143:LYS:HG2	1.85	0.59
20:ao:128:ARG:HE	20:ao:132:GLU:HG2	1.67	0.59
3:S2:98:VAL:HG11	17:A6:100:TRP:HE1	1.67	0.58
1:3a:68:GLU:HG2	5:6a:159:LEU:HD23	1.83	0.58
31:b3:56:ALA:O	31:b3:60:MET:HB3	2.03	0.58
42:3C:45:ILE:HA	61:3C:401:HEM:HAB	1.84	0.58
12:s4:99:MET:HB3	12:s4:126:LEU:HB2	1.84	0.58
1:3a:6:VAL:O	1:3a:10:ASN:HB2	2.02	0.58
3:s2:197:MET:SD	4:1a:32:GLN:NE2	2.76	0.58
8:4a:108:MET:HB3	8:4a:121:LEU:HD13	1.84	0.58
40:3A:301:ASN:O	40:3A:305:GLN:HB2	2.02	0.58
41:3M:320:PRO:HA	50:3T:52:ARG:HE	1.68	0.58
6:4L:16:LEU:O	6:4L:20:LEU:HB2	2.03	0.58
42:3C:78:LEU:O	42:3C:82:MET:HB3	2.04	0.58
10:al:146:ALA:HB1	10:al:157:VAL:HG21	1.85	0.58
51:V1:225:LEU:HD21	53:S1:76:ARG:HH22	1.69	0.58
11:A9:301:ILE:O	11:A9:305:PHE:HB2	2.04	0.58
2:S3:111:ALA:HB3	2:S3:130:ASN:HB3	1.85	0.58
2:s3:86:CYS:HA	2:s3:143:LYS:O	2.05	0.57
51:V1:385:CYS:HB3	64:V1:502:SF4:S3	2.44	0.57
4:1:20:LEU:HD22	4:1:232:ILE:HB	1.86	0.57
22:A3:28:LEU:O	22:A3:32:MET:HB2	2.03	0.57
2:s3:195:HIS:HB2	2:s3:198:ARG:HD2	1.85	0.57
11:A9:221:ARG:HD2	11:A9:286:ARG:HG3	1.87	0.57
10:al:223:ASP:HB3	10:al:226:GLU:HB2	1.86	0.57
55:s8:181:GLU:HA	55:s8:184:LEU:HD12	1.87	0.57
8:4a:150:LEU:O	8:4a:154:LEU:HB2	2.05	0.57
4:1:149:ILE:HG21	4:1:185:TRP:HB2	1.86	0.57
15:ac:93:ILE:HD11	15:ac:108:LEU:HD13	1.87	0.57
51:v1:68:ILE:HD11	51:v1:256:ARG:HB3	1.86	0.57
4:1a:90:PRO:HG3	4:1a:162:LEU:HB3	1.86	0.57
34:b9:136:GLU:HG2	34:b9:165:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c1:34:PRO:HG2	23:c1:37:ALA:HB2	1.87	0.57
53:S1:337:ALA:HB1	53:S1:543:LYS:H	1.69	0.57
7:5a:231:PRO:HB3	7:5a:530:PRO:HG3	1.85	0.57
7:5a:418:MET:HA	7:5a:421:MET:HB3	1.86	0.57
4:1:26:LYS:HG2	4:1:37:PRO:HD2	1.87	0.56
43:3D:222:PRO:HG3	47:3H:69:LEU:HD13	1.87	0.56
51:V1:112:TYR:HB2	51:V1:240:THR:HG22	1.85	0.56
52:V2:223:CYS:SG	52:V2:224:CYS:N	2.78	0.56
14:A2:65:LEU:HB2	14:A2:79:LEU:HD11	1.87	0.56
44:3P:98:ASP:HB3	44:3P:101:LYS:HG2	1.86	0.56
2:S3:47:ARG:HH12	3:S2:156:GLU:HG3	1.68	0.56
3:S2:254:ARG:HE	38:A7:25:GLN:HB3	1.70	0.56
5:6:166:ILE:HD11	6:4L:73:VAL:HA	1.87	0.56
29:B6:104:ILE:HB	35:B7:48:ASP:HB3	1.87	0.56
3:s2:144:MET:N	3:s2:144:MET:SD	2.78	0.56
4:1a:284:GLN:HA	4:1a:287:HIS:HB2	1.87	0.56
7:5a:221:THR:HG23	7:5a:226:GLN:HB2	1.87	0.56
42:3C:226:ILE:HD11	43:3D:306:MET:HE3	1.87	0.56
51:V1:35:LEU:HB2	51:V1:291:GLU:HB2	1.88	0.56
54:S7:198:ALA:O	54:S7:202:LEU:HB2	2.06	0.56
3:s2:426:ALA:HB3	3:s2:429:PHE:HB2	1.88	0.56
43:3D:92:PRO:HG3	47:3H:77:ASP:HB3	1.86	0.56
55:S8:110:GLU:OE2	55:S8:141:ARG:NH1	2.38	0.56
8:4:173:THR:HG22	8:4:175:ASN:H	1.70	0.56
53:s1:478:SER:HA	53:s1:481:LEU:HB2	1.87	0.56
4:1:23:VAL:O	4:1:27:ILE:HB	2.06	0.56
2:s3:224:GLU:HB2	12:s4:118:ALA:HA	1.87	0.56
7:5:433:THR:OG1	7:5:434:LYS:N	2.39	0.56
40:3A:360:CYS:SG	40:3A:361:ASP:N	2.79	0.56
40:3L:408:PRO:HA	40:3L:411:GLU:HB3	1.87	0.56
53:S1:476:LEU:HB3	53:S1:515:ILE:HG12	1.88	0.56
51:v1:112:TYR:HB2	51:v1:240:THR:HG22	1.87	0.56
1:3:90:MET:HE3	5:6:149:THR:HB	1.88	0.56
9:2:132:THR:HB	9:2:209:ILE:HG12	1.88	0.56
32:B8:40:SER:OG	32:B8:41:TYR:N	2.39	0.56
8:4:325:LEU:HD22	8:4:362:ALA:HB2	1.87	0.55
53:S1:262:VAL:HG23	53:S1:276:ARG:HB2	1.87	0.55
9:2:21:MET:HE2	25:S5:4:LEU:HG	1.89	0.55
37:AN:64:ARG:HH22	37:AN:99:ASP:HA	1.70	0.55
37:an:139:HIS:HB2	53:s1:299:ARG:HA	1.87	0.55
42:3N:45:ILE:HA	61:3N:401:HEM:HAB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v2:155:LEU:HB3	52:v2:157:ILE:HG12	1.88	0.55
53:s1:216:SER:HA	53:s1:691:ILE:HD11	1.87	0.55
3:s2:408:GLY:H	3:s2:425:LYS:HB3	1.71	0.55
9:2a:102:LEU:HD21	9:2a:141:ILE:HD12	1.88	0.55
25:s5:48:GLY:O	25:s5:52:ALA:HB2	2.06	0.55
3:S2:96:ARG:HB3	3:S2:112:HIS:HB2	1.87	0.55
7:5:292:ALA:HA	7:5:295:GLN:HB2	1.88	0.55
7:5a:296:ASN:HD22	7:5a:357:ARG:HE	1.55	0.55
12:S4:82:PRO:HG3	12:S4:98:LYS:HD2	1.88	0.55
39:V3:65:THR:OG1	39:V3:66:THR:N	2.39	0.55
41:3M:108:GLY:HA3	41:3M:124:GLU:O	2.06	0.55
42:3N:119:LEU:HD12	42:3N:192:LEU:HB3	1.89	0.55
3:S2:118:2MR:HD3	54:S7:136:THR:HG21	1.86	0.55
22:A3:52:ASN:ND2	25:S5:27:TYR:O	2.38	0.55
42:3C:282:ARG:NH2	42:3C:341:GLN:O	2.40	0.55
53:S1:591:GLU:HB3	53:S1:612:PRO:HD3	1.87	0.55
7:5:61:TYR:O	7:5:81:LYS:HA	2.06	0.55
20:AO:133:MET:SD	20:AO:137:ASN:ND2	2.80	0.55
51:V1:253:THR:HA	51:V1:256:ARG:HG2	1.89	0.55
40:3L:48:THR:OG1	40:3L:423:ARG:NH1	2.39	0.55
3:S2:140:ASP:OD1	3:S2:404:LYS:NZ	2.39	0.55
7:5:100:ILE:HG13	7:5:246:LEU:HB2	1.89	0.55
8:4:208:PRO:HG3	8:4:216:LEU:HD22	1.89	0.55
32:B8:125:SER:O	32:B8:129:MET:HB2	2.07	0.55
3:s2:254:ARG:HD2	38:a7:25:GLN:HB3	1.88	0.55
40:3L:295:GLY:O	40:3L:301:ASN:ND2	2.40	0.55
7:5:328:HIS:O	7:5:332:HIS:HB3	2.07	0.55
11:A9:83:PRO:HA	11:A9:106:LEU:O	2.07	0.55
8:4a:216:LEU:O	8:4a:220:HIS:HB2	2.07	0.55
10:al:275:TYR:HB3	16:a5:23:ARG:HH21	1.72	0.55
25:s5:97:HIS:HA	25:s5:102:GLU:HB3	1.88	0.55
40:3L:55:ASN:HD22	40:3L:253:VAL:H	1.52	0.55
27:BM:135:MET:SD	36:BL:142:ARG:NH1	2.80	0.54
40:3L:289:ILE:HG13	40:3L:456:VAL:HG22	1.89	0.54
7:5:365:ILE:HG22	7:5:366:MET:HG3	1.90	0.54
11:A9:227:PRO:HB3	11:A9:293:LEU:HD12	1.90	0.54
2:s3:62:GLU:HG3	38:a7:69:ILE:HD12	1.89	0.54
4:1:105:ILE:O	4:1:109:SER:HB3	2.07	0.54
9:2:30:TRP:NE1	9:2:67:SER:OG	2.41	0.54
40:3A:445:CYS:O	40:3A:449:PHE:HB2	2.06	0.54
40:3L:403:LEU:HD12	40:3L:426:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:140:LEU:O	7:5:144:TRP:HB2	2.07	0.54
24:C2:42:GLY:HA3	24:C2:61:GLN:HG2	1.90	0.54
4:1a:207:LEU:HD12	4:1a:210:GLY:HA2	1.90	0.54
7:5a:22:SER:HA	7:5a:27:ILE:HD12	1.90	0.54
40:3A:222:ARG:HH21	40:3A:263:PRO:HB3	1.72	0.54
48:3J:34:ARG:HD3	49:3K:48:ILE:HG23	1.90	0.54
43:3O:307:LYS:O	43:3O:311:TRP:HB2	2.08	0.54
55:S8:189:LYS:O	55:S8:193:ASN:HB2	2.07	0.54
55:s8:204:ASN:O	55:s8:208:ASP:HB2	2.07	0.54
21:A1:18:ILE:O	21:A1:22:SER:HB3	2.08	0.54
4:1a:221:ALA:O	4:1a:225:MET:HB2	2.08	0.54
8:4a:176:LEU:HD21	8:4a:245:ARG:HB3	1.89	0.54
9:2:122:ILE:O	9:2:176:ARG:NH1	2.40	0.54
14:A2:44:LEU:HD21	14:A2:91:MET:HE2	1.89	0.54
2:S3:171:ASP:HB2	2:S3:185:ARG:HA	1.90	0.54
8:4:36:LEU:HB2	27:BM:96:VAL:HG22	1.89	0.54
2:s3:153:ASP:OD1	2:s3:153:ASP:N	2.41	0.54
42:3C:32:ASN:ND2	42:3C:228:ASP:OD1	2.41	0.54
40:3L:140:LEU:HA	40:3L:143:VAL:HB	1.90	0.54
53:s1:186:ALA:HA	53:s1:190:ALA:HB3	1.89	0.54
54:s7:87:ARG:HB2	54:s7:209:GLN:HG3	1.90	0.54
8:4:254:THR:O	8:4:258:ALA:HB2	2.08	0.54
2:s3:112:ASP:HB2	2:s3:130:ASN:HB2	1.89	0.54
52:V2:136:THR:OG1	65:V2:301:FES:S2	2.64	0.54
9:2:127:GLY:O	9:2:131:LEU:HB2	2.07	0.54
8:4a:350:MET:HE2	34:b9:96:CYS:HA	1.90	0.54
40:3L:469:ASN:ND2	43:3O:310:LYS:O	2.41	0.54
53:S1:186:ALA:HA	53:S1:190:ALA:HB3	1.89	0.54
1:3:60:ILE:HG13	6:4L:76:ALA:HB2	1.90	0.53
9:2:20:THR:HG23	9:2:29:MET:HB2	1.89	0.53
19:AM:141:VAL:HG22	28:B5:158:ARG:HB2	1.89	0.53
28:B5:160:MET:HG2	28:B5:168:TRP:HB2	1.91	0.53
7:5a:316:THR:HG21	7:5a:395:ILE:HG12	1.88	0.53
8:4a:315:LEU:O	8:4a:319:HIS:HB3	2.07	0.53
5:6:55:VAL:HA	5:6:58:ILE:HG22	1.91	0.53
7:5:316:THR:HG21	7:5:395:ILE:HD12	1.91	0.53
11:A9:238:GLN:NE2	11:A9:268:PRO:O	2.42	0.53
40:3L:292:GLU:HA	40:3L:352:GLY:O	2.07	0.53
49:3V:30:VAL:HA	49:3V:33:VAL:HG12	1.90	0.53
52:V2:157:ILE:HG23	52:V2:161:GLU:HG3	1.90	0.53
9:2:248:LEU:HD11	9:2:296:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3L:278:ARG:NH1	40:3L:463:GLU:OE2	2.41	0.53
3:S2:376:GLU:O	3:S2:380:HIS:ND1	2.39	0.53
3:s2:143:SER:O	3:s2:147:ASN:ND2	2.42	0.53
3:s2:412:VAL:HG23	3:s2:420:TYR:HB3	1.91	0.53
11:a9:48:ARG:NH2	11:a9:96:LEU:O	2.42	0.53
41:3B:63:LEU:HD13	41:3B:220:LEU:HB2	1.91	0.53
51:V1:44:ASN:ND2	51:V1:48:ARG:O	2.42	0.53
4:1:203:GLY:O	4:1:279:ARG:NH1	2.42	0.53
3:s2:314:VAL:HB	3:s2:343:ILE:HD12	1.91	0.53
53:S1:68:ARG:NH2	53:S1:277:MET:SD	2.82	0.53
52:v2:140:MET:HA	52:v2:144:SER:H	1.74	0.53
12:S4:151:LYS:NZ	53:S1:657:ASP:OD2	2.41	0.53
2:s3:108:LYS:HB2	3:s2:284:LEU:HD22	1.91	0.53
4:1a:138:GLN:NE2	4:1a:198:PHE:O	2.41	0.53
7:5a:530:PRO:O	7:5a:534:HIS:HB3	2.09	0.53
15:ab:79:ILE:HD12	15:ab:145:VAL:HB	1.91	0.53
15:ac:123:GLU:HG2	15:ac:129:GLU:HA	1.90	0.53
53:s1:276:ARG:O	53:s1:282:ASN:ND2	2.42	0.53
3:S2:224:ALA:O	55:S8:98:ARG:NH2	2.42	0.53
7:5:261:VAL:HG11	7:5:326:PHE:HB2	1.91	0.53
8:4a:68:LEU:O	8:4a:72:LEU:HB2	2.08	0.53
15:ab:116:VAL:O	15:ab:120:MET:HB3	2.09	0.53
35:b7:69:CYS:O	35:b7:73:SER:HB3	2.09	0.53
44:3E:156:LEU:HD12	44:3E:158:ASP:H	1.74	0.53
53:S1:165:ILE:HG23	53:S1:214:PHE:HB3	1.91	0.53
54:s7:200:ALA:HB2	55:s8:173:PHE:HB2	1.90	0.53
3:S2:67:ASN:HB2	10:AL:193:LEU:HD22	1.91	0.53
13:S6:104:CYS:CB	13:S6:107:CYS:SG	2.96	0.53
10:a1:271:GLU:HG2	16:a5:26:ILE:HD13	1.91	0.53
40:3L:403:LEU:HD13	40:3L:423:ARG:HH21	1.73	0.53
3:s2:173:LEU:HD12	3:s2:347:CYS:HB3	1.90	0.53
3:s2:266:ARG:H	55:s8:66:LEU:HD21	1.73	0.53
6:4l:50:ASN:O	25:s5:32:ARG:NH1	2.42	0.53
9:2a:149:LEU:HD22	9:2a:154:ILE:HD11	1.90	0.53
11:a9:110:ALA:HB1	11:a9:148:ILE:HG12	1.91	0.53
53:S1:419:ARG:NH1	53:S1:439:THR:O	2.42	0.53
52:v2:200:ILE:HG23	52:v2:204:ILE:HD12	1.90	0.53
7:5:51:LEU:HD11	7:5:88:LEU:HD12	1.90	0.53
11:A9:113:LYS:HA	11:A9:116:ILE:HD12	1.89	0.53
14:A2:25:GLN:NE2	53:S1:661:GLU:O	2.40	0.53
15:AB:83:VAL:O	15:AB:87:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:V1:328:PRO:HB3	51:V1:441:HIS:HB3	1.91	0.53
8:4:229:MET:O	8:4:233:ALA:HB3	2.09	0.52
3:s2:93:GLY:HA3	54:s7:96:GLY:HA3	1.91	0.52
4:1a:65:THR:O	4:1a:124:ASN:ND2	2.40	0.52
40:3A:453:CYS:SG	40:3A:472:ARG:NH1	2.82	0.52
43:3D:295:MET:O	43:3D:299:LEU:HB2	2.09	0.52
45:3F:76:LEU:HB3	45:3F:80:GLN:HB3	1.90	0.52
51:V1:158:ILE:HG21	51:V1:166:ALA:HB2	1.90	0.52
53:S1:497:VAL:HG11	53:S1:513:MET:HB2	1.91	0.52
51:v1:385:CYS:HB3	64:v1:502:SF4:S3	2.50	0.52
7:5:174:TYR:HD2	7:5:232:TRP:HB3	1.73	0.52
12:S4:84:ARG:HH21	53:S1:277:MET:HE2	1.74	0.52
11:a9:169:HIS:HB2	11:a9:184:LYS:HZ2	1.73	0.52
41:3M:113:THR:HB	41:3M:120:ALA:HB3	1.92	0.52
42:3N:39:VAL:HG21	42:3N:232:ILE:HD11	1.92	0.52
53:S1:66:HIS:HB2	53:S1:181:ARG:HD3	1.91	0.52
53:s1:257:VAL:HG11	53:s1:413:LEU:HB3	1.91	0.52
54:s7:216:GLN:HB3	54:s7:219:LYS:HB3	1.91	0.52
3:S2:290:GLY:HA3	3:S2:405:GLY:HA2	1.90	0.52
6:4L:63:ILE:HD12	9:2:71:LEU:HD21	1.92	0.52
22:A3:52:ASN:HD22	25:S5:28:LYS:HE3	1.74	0.52
36:BL:6:ASP:N	36:BL:6:ASP:OD1	2.42	0.52
2:s3:153:ASP:HA	2:s3:178:PHE:HB2	1.92	0.52
3:s2:216:ARG:HH21	3:s2:240:LEU:HA	1.74	0.52
8:4a:264:LEU:HD13	33:b4:98:LEU:HD21	1.91	0.52
18:a8:163:HIS:O	28:b5:146:LYS:NZ	2.42	0.52
53:S1:165:ILE:HD12	53:S1:171:THR:HG21	1.91	0.52
53:s1:165:ILE:HG23	53:s1:214:PHE:HB3	1.90	0.52
2:S3:195:HIS:HB2	2:S3:198:ARG:HD2	1.92	0.52
4:1:28:LEU:HD22	4:1:275:ALA:HB2	1.90	0.52
40:3A:64:SER:OG	40:3A:65:SER:N	2.42	0.52
3:S2:143:SER:HB3	3:S2:182:ASN:HB2	1.91	0.52
20:AO:93:GLU:HA	20:AO:96:ILE:HD12	1.91	0.52
2:s3:100:ARG:NH1	2:s3:158:VAL:O	2.43	0.52
21:a1:1:MET:HE1	38:a7:4:ALA:HA	1.91	0.52
42:3C:177:ARG:NH2	44:3P:140:MET:O	2.42	0.52
47:3H:38:LEU:HD23	47:3H:40:LYS:H	1.74	0.52
40:3L:62:GLU:OE1	40:3L:423:ARG:NH1	2.42	0.52
41:3M:116:ARG:NH1	41:3M:188:ASN:O	2.43	0.52
51:v1:44:ASN:ND2	51:v1:48:ARG:O	2.41	0.52
2:S3:98:PHE:HB2	16:A5:94:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:137:MET:HB3	7:5:186:MET:HE2	1.91	0.52
7:5:432:MET:HG2	31:B3:67:ILE:HD11	1.91	0.52
7:5:474:PRO:O	35:B7:55:GLN:NE2	2.42	0.52
18:A8:147:ARG:NH1	25:S5:43:CYS:SG	2.82	0.52
4:1a:282:TYR:HA	4:1a:285:LEU:HB3	1.92	0.52
11:a9:142:GLU:O	11:a9:146:VAL:HB	2.10	0.52
43:3D:243:GLY:H	62:3D:401:HEC:HBD2	1.74	0.52
52:v2:147:ILE:HG13	52:v2:200:ILE:HD11	1.92	0.52
55:s8:194:GLY:O	55:s8:198:GLU:HB2	2.10	0.52
3:S2:144:MET:N	3:S2:144:MET:SD	2.82	0.52
11:A9:82:ILE:HD13	11:A9:94:LEU:HD23	1.92	0.52
39:V3:103:ARG:HH11	53:S1:441:ARG:HB3	1.75	0.52
11:a9:140:ASP:OD1	11:a9:140:ASP:N	2.43	0.52
12:s4:89:SER:O	53:s1:62:ARG:NH1	2.43	0.52
37:an:87:PRO:HG2	37:an:90:TRP:HB2	1.91	0.52
43:3O:126:SER:HB2	43:3O:177:LYS:HD2	1.91	0.52
51:V1:113:LEU:HD21	51:V1:248:VAL:HG11	1.92	0.52
8:4:456:GLY:O	27:BM:111:ARG:NH1	2.43	0.52
32:b8:61:ASP:OD2	33:b4:36:ARG:NH1	2.43	0.52
42:3C:334:ILE:HG12	46:3G:56:VAL:HG23	1.92	0.52
51:v1:328:PRO:HB3	51:v1:441:HIS:HB3	1.92	0.52
18:A8:7:LEU:O	20:AO:88:ARG:NH2	2.43	0.52
24:C2:52:PRO:HB3	24:C2:55:ARG:HE	1.75	0.52
7:5a:328:HIS:O	7:5a:332:HIS:HB3	2.10	0.52
7:5a:577:THR:O	7:5a:580:GLN:NE2	2.43	0.52
9:2a:51:ARG:HG2	9:2a:121:GLY:HA2	1.91	0.52
40:3L:141:PRO:HA	40:3L:245:LEU:HD21	1.92	0.52
40:3L:412:ASP:O	40:3L:416:SER:HB2	2.09	0.52
48:3U:12:TYR:HA	48:3U:16:PHE:HB2	1.92	0.52
53:s1:406:ASN:HD22	53:s1:436:VAL:HG11	1.74	0.52
15:AC:138:LEU:HD13	15:AC:144:ILE:HG13	1.92	0.52
1:3a:95:VAL:HG23	1:3a:98:LEU:HD23	1.91	0.52
3:s2:333:ARG:NH1	3:s2:453:THR:O	2.43	0.52
12:s4:88:GLN:NE2	53:s1:141:ASP:OD2	2.43	0.52
41:3M:173:ILE:HD11	41:3M:441:SER:HB3	1.92	0.52
51:V1:220:GLN:NE2	53:S1:197:THR:O	2.44	0.52
54:s7:97:LEU:HD11	54:s7:141:MET:HE2	1.91	0.52
3:S2:225:ALA:O	3:S2:228:ARG:NH1	2.43	0.51
7:5:574:THR:HG21	9:2:170:LEU:HB2	1.91	0.51
8:4:360:LEU:O	8:4:364:LEU:HB3	2.10	0.51
3:s2:55:SER:OG	3:s2:56:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5a:509:MET:SD	34:b9:33:HIS:ND1	2.83	0.51
9:2a:131:LEU:O	9:2a:135:LYS:NZ	2.43	0.51
43:3O:100:GLY:O	43:3O:286:LYS:NZ	2.43	0.51
51:V1:138:LEU:HD23	51:V1:169:LEU:HD21	1.92	0.51
53:S1:301:ARG:NH2	53:S1:591:GLU:OE1	2.43	0.51
53:S1:593:SER:HA	53:S1:606:THR:O	2.10	0.51
3:S2:138:ARG:NE	64:S7:301:SF4:S2	2.82	0.51
5:6:61:GLY:HA2	5:6:64:LEU:HD12	1.92	0.51
29:B6:29:SER:HB2	29:B6:32:GLU:HB2	1.91	0.51
8:4a:181:PHE:O	36:bl:153:ARG:NH1	2.43	0.51
39:V3:93:PRO:O	51:V1:152:ARG:NH2	2.43	0.51
9:2a:316:HIS:O	10:al:337:ARG:NH2	2.43	0.51
11:a9:81:ILE:HG22	11:a9:104:THR:HB	1.92	0.51
40:3L:393:ASN:OD1	40:3L:396:ARG:NH1	2.44	0.51
43:3O:227:LEU:HD12	43:3O:231:LEU:HB3	1.92	0.51
7:5:594:ASN:ND2	9:2:110:PRO:O	2.43	0.51
4:1a:22:LEU:HD11	4:1a:45:ILE:HA	1.91	0.51
9:2:130:LEU:O	9:2:135:LYS:NZ	2.44	0.51
15:AC:115:GLN:NE2	15:AC:135:ALA:O	2.43	0.51
4:1a:172:MET:HE3	20:ao:49:ARG:HB3	1.91	0.51
18:a8:166:ARG:NH1	28:b5:153:GLU:OE1	2.44	0.51
34:b9:71:PHE:O	34:b9:75:GLN:HB3	2.11	0.51
40:3A:446:SER:OG	48:3J:16:ARG:NH2	2.44	0.51
51:V1:111:LYS:HG2	51:V1:239:PRO:HG2	1.93	0.51
53:S1:437:ASP:OD1	53:S1:437:ASP:N	2.43	0.51
51:v1:111:LYS:HG2	51:v1:239:PRO:HG2	1.93	0.51
12:S4:75:ARG:NH2	12:S4:102:ASP:O	2.44	0.51
3:s2:446:ASP:OD2	4:1a:281:ARG:NH1	2.44	0.51
10:al:216:SER:OG	10:al:220:LYS:NZ	2.43	0.51
11:a9:204:SER:OG	11:a9:205:ASP:N	2.44	0.51
12:s4:64:LEU:HD21	17:a6:84:LEU:HD13	1.93	0.51
19:am:81:ARG:NH1	19:am:86:ASP:OD2	2.44	0.51
53:S1:280:ASP:O	53:S1:417:ARG:NH1	2.44	0.51
53:s1:64:CYS:SG	53:s1:65:TYR:N	2.84	0.51
2:S3:230:ARG:NH2	55:S8:128:ILE:O	2.44	0.51
4:1:70:LEU:HA	4:1:73:ILE:HG22	1.93	0.51
4:1:195:ARG:NH2	4:1:227:GLU:OE2	2.44	0.51
40:3A:144:VAL:HG11	40:3A:245:LEU:HB3	1.93	0.51
42:3C:39:VAL:HG21	42:3C:232:ILE:HD11	1.92	0.51
51:v1:220:GLN:NE2	53:s1:197:THR:O	2.44	0.51
8:4:236:LEU:HD23	8:4:237:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S6:75:ARG:HH21	13:S6:76:ILE:HD11	1.75	0.51
14:A2:83:SER:OG	14:A2:84:ALA:N	2.43	0.51
17:A6:41:ALA:O	17:A6:45:GLU:HB2	2.10	0.51
17:A6:117:ARG:HH21	17:A6:130:ASP:HB3	1.75	0.51
7:5a:560:LYS:HD3	33:b4:80:PHE:HE2	1.76	0.51
11:a9:192:ARG:NH2	11:a9:262:THR:OG1	2.42	0.51
28:b5:77:LEU:HD23	28:b5:78:THR:HG23	1.92	0.51
41:3B:50:ALA:O	41:3B:221:VAL:HA	2.11	0.51
53:S1:251:ILE:HD12	53:S1:604:GLN:HB2	1.91	0.51
53:S1:447:ASP:HB3	53:S1:683:PRO:HB3	1.91	0.51
54:s7:164:CYS:HA	54:s7:169:GLY:H	1.76	0.51
7:5:352:ASP:OD2	34:B9:93:ARG:NH1	2.44	0.51
8:4:300:SER:O	8:4:308:SER:OG	2.28	0.51
12:S4:78:ARG:HH21	12:S4:148:GLU:HG3	1.75	0.51
33:B4:97:PRO:HA	33:B4:100:PHE:HB3	1.93	0.51
3:s2:376:GLU:O	3:s2:380:HIS:ND1	2.42	0.51
4:1a:234:MET:HA	4:1a:237:LEU:HB2	1.93	0.51
8:4a:141:GLU:OE2	8:4a:144:ASN:ND2	2.44	0.51
9:2a:30:TRP:NE1	9:2a:67:SER:OG	2.44	0.51
53:S1:221:ASN:ND2	53:S1:286:ILE:O	2.43	0.51
51:v1:205:ILE:HG12	51:v1:379:CYS:HB3	1.93	0.51
7:5:161:ARG:NH2	34:B9:88:GLY:O	2.44	0.51
35:B7:47:MET:SD	36:BL:120:ASN:ND2	2.79	0.51
8:4a:380:PHE:HA	8:4a:383:MET:HG2	1.93	0.51
11:a9:85:ARG:HH22	54:s7:224:ARG:HG3	1.76	0.51
24:c2:46:ASN:OD1	24:c2:51:ARG:NH1	2.39	0.51
37:an:82:ASP:HB2	54:s7:203:TYR:HE1	1.75	0.51
42:3C:117:VAL:HG11	42:3C:302:ALA:HB2	1.93	0.51
43:3O:192:ALA:HB1	62:3O:401:HEC:HBD1	1.92	0.51
53:S1:50:LEU:HD21	53:S1:62:ARG:HE	1.74	0.51
53:s1:301:ARG:NH2	53:s1:591:GLU:OE1	2.44	0.51
9:2:109:ALA:HA	9:2:112:HIS:HB3	1.93	0.50
12:S4:75:ARG:NH1	12:S4:119:ASP:OD1	2.45	0.50
35:B7:59:CYS:HB2	35:B7:90:CYS:HB3	1.92	0.50
1:3a:34:ALA:HB1	4:1a:63:PRO:HA	1.93	0.50
10:al:71:ASN:ND2	10:al:160:GLU:OE1	2.44	0.50
13:s6:69:VAL:HG12	13:s6:110:GLN:HB2	1.92	0.50
18:a8:125:LEU:HB2	20:ao:66:GLU:HG2	1.93	0.50
19:am:1:MET:SD	19:am:1:MET:N	2.82	0.50
41:3M:43:LEU:HD12	41:3M:47:LEU:HD23	1.92	0.50
54:S7:169:GLY:HA2	55:S8:151:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s1:437:ASP:N	53:s1:437:ASP:OD1	2.43	0.50
1:3:54:LYS:HB3	1:3:113:TRP:HB3	1.93	0.50
1:3:95:VAL:HG13	4:1:298:LEU:HD22	1.92	0.50
2:S3:170:TRP:NE1	17:A6:91:MET:SD	2.77	0.50
2:S3:210:ARG:NH2	11:A9:71:ASN:OD1	2.44	0.50
10:AL:82:GLY:O	10:AL:155:GLN:NE2	2.44	0.50
11:a9:239:PRO:HG2	11:a9:345:LEU:HD22	1.92	0.50
45:3F:58:ASP:OD2	45:3F:62:ARG:NH1	2.43	0.50
13:S6:58:ASN:ND2	55:S8:195:ASP:OD2	2.44	0.50
20:AO:25:LEU:HG	55:S8:68:ARG:HH21	1.74	0.50
37:AN:27:LEU:O	37:AN:31:PHE:HB2	2.12	0.50
7:5a:145:GLU:OE2	7:5a:176:ARG:NH1	2.44	0.50
7:5a:396:ILE:O	7:5a:400:ASN:HB2	2.11	0.50
8:4a:437:MET:HA	8:4a:440:HIS:HB2	1.93	0.50
51:V1:290:GLU:OE2	51:V1:303:HIS:ND1	2.44	0.50
2:S3:107:PHE:HB3	2:S3:131:LEU:HB3	1.92	0.50
7:5:136:ASN:ND2	7:5:197:GLU:OE1	2.44	0.50
12:S4:78:ARG:NH1	53:S1:249:GLU:OE1	2.45	0.50
14:A2:79:LEU:HD22	14:A2:87:VAL:HG23	1.93	0.50
7:5a:142:ILE:HG12	8:4a:370:PRO:HB2	1.92	0.50
33:b4:62:ASP:HB2	33:b4:65:LEU:HB2	1.93	0.50
53:s1:594:ALA:O	53:s1:605:GLN:HA	2.11	0.50
6:4L:59:ILE:HG23	9:2:27:MET:HE2	1.93	0.50
10:AL:250:SER:O	10:AL:280:LYS:NZ	2.44	0.50
15:AC:89:LEU:HD13	31:B3:54:ASN:HA	1.94	0.50
33:B4:38:SER:OG	33:B4:42:ARG:NH1	2.45	0.50
36:BL:7:LYS:NZ	36:BL:12:GLU:O	2.44	0.50
1:3a:6:VAL:HG21	4:1a:87:VAL:HG11	1.92	0.50
3:s2:282:ASP:O	3:s2:286:TYR:HB2	2.10	0.50
43:3D:197:LEU:HB2	43:3D:274:LEU:HD11	1.94	0.50
51:V1:278:ILE:HD11	51:V1:299:LEU:HD22	1.92	0.50
51:V1:308:THR:O	51:V1:313:ASN:ND2	2.44	0.50
53:S1:647:GLU:HG2	53:S1:654:VAL:HG21	1.94	0.50
3:S2:402:ALA:HB2	3:S2:407:PHE:HB2	1.94	0.50
8:4:261:PHE:O	8:4:265:SER:HB3	2.11	0.50
11:A9:165:ILE:HG21	11:A9:249:ILE:HG23	1.94	0.50
2:s3:151:PRO:HB3	2:s3:176:PHE:HB3	1.92	0.50
7:5a:446:ASN:ND2	30:b2:54:GLN:OE1	2.45	0.50
9:2a:3:PRO:HB3	10:a1:40:LEU:HD11	1.94	0.50
18:a8:13:LEU:HD23	18:a8:57:LEU:HD11	1.93	0.50
24:c2:30:ARG:HH21	24:c2:76:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3A:58:ARG:O	40:3A:230:VAL:HA	2.12	0.50
52:V2:136:THR:OG1	52:V2:174:GLU:O	2.30	0.50
2:S3:118:VAL:HG21	2:S3:121:ARG:HH21	1.75	0.50
7:5:511:LEU:HD11	31:B3:38:VAL:HG22	1.94	0.50
8:4:101:SER:HA	8:4:104:ILE:HD12	1.94	0.50
8:4:360:LEU:O	8:4:364:LEU:CB	2.60	0.50
1:3a:10:ASN:HB3	4:1a:80:THR:HG23	1.94	0.50
6:4l:45:SER:O	6:4l:49:LEU:HB2	2.11	0.50
18:a8:23:ALA:HB3	18:a8:86:TRP:HE3	1.76	0.50
20:ao:52:ARG:NH1	20:ao:55:GLN:OE1	2.44	0.50
42:3N:377:LEU:O	45:3Q:34:ARG:NH1	2.45	0.50
51:V1:89:GLY:HA3	63:V1:501:FMN:H1'2	1.94	0.50
53:S1:220:GLY:HA3	53:S1:291:ARG:HD3	1.93	0.50
54:s7:219:LYS:HE3	54:s7:223:ARG:HE	1.77	0.50
55:s8:153:ILE:N	64:s8:301:SF4:S3	2.81	0.50
3:S2:116:LEU:HD21	54:S7:97:LEU:HG	1.94	0.50
11:A9:61:ALA:HB3	11:A9:82:ILE:HG23	1.94	0.50
4:1a:195:ARG:NH1	4:1a:227:GLU:OE2	2.44	0.50
22:a3:72:ASP:OD1	22:a3:72:ASP:N	2.39	0.50
32:b8:33:THR:O	32:b8:37:LEU:HB2	2.11	0.50
39:v3:86:ASP:O	39:v3:89:LYS:NZ	2.45	0.50
42:3C:102:LEU:HD21	42:3C:304:MET:HE3	1.93	0.50
53:S1:405:THR:HG21	53:S1:516:LEU:HD11	1.94	0.50
5:6:81:THR:OG1	5:6:82:TRP:N	2.45	0.50
9:2:25:ASN:HB3	9:2:28:LEU:HB2	1.92	0.50
9:2:139:LEU:HD23	9:2:205:LEU:HD22	1.94	0.50
9:2:269:GLU:O	9:2:273:ASN:ND2	2.45	0.50
10:AL:64:GLY:O	10:AL:161:ARG:NH1	2.45	0.50
4:1a:58:LYS:HA	54:s7:155:PRO:HG2	1.94	0.50
8:4a:388:TRP:O	33:b4:112:LYS:NZ	2.44	0.50
34:b9:62:GLN:OE1	34:b9:65:ARG:NH1	2.44	0.50
40:3A:451:ASP:OD1	40:3A:472:ARG:NH2	2.45	0.50
41:3M:70:ARG:NH1	41:3M:332:ASP:OD2	2.45	0.50
54:s7:182:ASP:OD1	54:s7:182:ASP:N	2.44	0.50
3:S2:312:ASP:N	3:S2:312:ASP:OD1	2.43	0.49
33:B4:50:GLN:O	33:B4:56:ARG:NH1	2.44	0.49
4:1a:26:LYS:NZ	4:1a:43:TYR:O	2.45	0.49
7:5a:306:THR:HB	7:5a:336:LYS:HG2	1.94	0.49
8:4a:400:ILE:HA	8:4a:403:THR:HG22	1.94	0.49
11:a9:135:GLU:HB2	11:a9:140:ASP:HA	1.94	0.49
14:a2:24:CYS:SG	14:a2:25:GLN:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a2:86:GLU:HA	14:a2:89:ARG:HG3	1.94	0.49
42:3N:43:VAL:HA	42:3N:46:ILE:HG22	1.94	0.49
8:4:56:PHE:HB3	8:4:111:SER:HB3	1.92	0.49
8:4:251:ASP:OD2	36:BL:154:LYS:NZ	2.44	0.49
31:B3:84:PHE:HB3	31:B3:86:VAL:HG22	1.94	0.49
3:s2:156:GLU:OE2	3:s2:171:ARG:NH2	2.45	0.49
3:s2:228:ARG:NH1	55:s8:160:GLU:OE2	2.46	0.49
7:5a:14:LEU:HD11	29:b6:75:VAL:HG22	1.94	0.49
12:s4:111:LEU:HD23	12:s4:112:MET:HB2	1.93	0.49
14:a2:27:SER:O	14:a2:34:ARG:NH2	2.45	0.49
41:3B:183:LYS:HD2	41:3B:252:LYS:HE3	1.94	0.49
40:3L:179:MET:HE1	40:3L:282:LEU:HD22	1.94	0.49
43:3O:199:TYR:O	43:3O:203:ALA:HB2	2.11	0.49
51:v1:126:LYS:HB2	51:v1:275:LEU:HD13	1.94	0.49
2:S3:98:PHE:O	2:S3:102:HIS:HB2	2.12	0.49
2:S3:229:PHE:O	53:S1:246:ARG:NH2	2.45	0.49
6:4L:40:LEU:HD13	9:2:71:LEU:HD23	1.94	0.49
8:4:317:ILE:HB	8:4:454:ILE:HD11	1.94	0.49
10:AL:68:SER:HA	10:AL:217:ARG:HH21	1.76	0.49
10:AL:200:PRO:O	10:AL:283:TRP:NE1	2.42	0.49
11:A9:123:SER:OG	11:A9:124:ASN:N	2.46	0.49
2:s3:214:GLU:OE1	11:a9:75:ARG:NH2	2.44	0.49
3:s2:253:LEU:O	3:s2:257:GLU:HB2	2.12	0.49
4:1a:20:LEU:HD22	4:1a:232:ILE:HB	1.94	0.49
4:1a:154:LEU:HD21	4:1a:165:LEU:HD11	1.94	0.49
8:4a:224:PRO:O	8:4a:228:SER:HB2	2.13	0.49
27:bm:101:THR:HA	27:bm:104:VAL:HG12	1.93	0.49
40:3A:126:ARG:NH1	40:3A:199:GLN:O	2.46	0.49
41:3B:70:ARG:NH2	41:3B:249:ALA:O	2.45	0.49
41:3B:162:LYS:HD2	41:3B:197:MET:HE1	1.93	0.49
48:3J:5:THR:OG1	48:3J:6:ILE:N	2.45	0.49
42:3N:137:GLN:NE2	42:3N:263:ASN:OD1	2.45	0.49
53:s1:647:GLU:HG2	53:s1:654:VAL:HG21	1.93	0.49
4:1:153:VAL:HG21	4:1:242:PHE:HE1	1.77	0.49
5:6:134:MET:O	25:S5:29:ASN:ND2	2.45	0.49
7:5:224:SER:OG	7:5:226:GLN:NE2	2.44	0.49
18:A8:143:HIS:HB2	20:AO:115:ARG:HB3	1.94	0.49
19:am:9:TYR:HB2	19:am:24:ILE:HG21	1.93	0.49
32:b8:110:ASP:OD2	33:b4:72:ARG:NH1	2.45	0.49
41:3M:90:THR:HG23	41:3M:95:SER:HA	1.93	0.49
43:3O:89:LEU:HD11	47:3S:74:HIS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3O:195:PRO:HG3	62:3O:401:HEC:HBA1	1.93	0.49
51:v1:285:PRO:HB2	52:v2:180:VAL:HG13	1.93	0.49
53:s1:281:ILE:HA	53:s1:391:ILE:HD13	1.94	0.49
7:5:446:ASN:HA	7:5:451:MET:HE3	1.94	0.49
9:2:326:PHE:O	9:2:330:ALA:HB2	2.12	0.49
11:A9:144:VAL:HA	11:A9:148:ILE:HD12	1.94	0.49
2:s3:173:PHE:O	2:s3:198:ARG:NH1	2.46	0.49
3:s2:66:TRP:HB2	10:al:193:LEU:HD11	1.93	0.49
4:1a:184:MET:HE1	4:1a:296:LEU:HB3	1.94	0.49
6:4l:54:MET:HB2	25:s5:26:PRO:HD2	1.94	0.49
7:5a:121:LEU:HD22	7:5a:246:LEU:HD23	1.95	0.49
9:2a:51:ARG:HD3	9:2a:120:GLN:HG3	1.94	0.49
36:bl:28:ASN:HB3	36:bl:30:ILE:HG12	1.95	0.49
51:V1:134:ASP:OD1	51:V1:134:ASP:N	2.46	0.49
53:S1:637:ASP:OD1	53:S1:637:ASP:N	2.46	0.49
53:s1:340:ALA:HA	53:s1:546:PHE:O	2.12	0.49
53:s1:682:ASP:N	53:s1:682:ASP:OD1	2.45	0.49
7:5:347:ILE:HG23	7:5:352:ASP:HA	1.95	0.49
24:C2:106:LYS:O	36:BL:78:LYS:NZ	2.46	0.49
37:AN:87:PRO:HG2	37:AN:90:TRP:HB2	1.95	0.49
4:1a:178:ALA:HB1	4:1a:181:MET:HB2	1.95	0.49
4:1a:286:MET:O	4:1a:290:TRP:HB2	2.12	0.49
8:4a:431:THR:HG22	28:b5:67:PHE:HB2	1.95	0.49
12:s4:78:ARG:HE	53:s1:607:LYS:HG3	1.77	0.49
29:b6:83:HIS:NE2	36:bl:42:ASP:OD1	2.45	0.49
40:3A:469:ASN:ND2	43:3D:310:LYS:O	2.45	0.49
48:3J:28:GLY:O	48:3J:32:PHE:HB2	2.13	0.49
41:3M:213:PHE:O	41:3M:241:ARG:NH1	2.46	0.49
2:S3:182:ASP:N	2:S3:182:ASP:OD1	2.46	0.49
7:5:198:LEU:HA	7:5:201:ILE:HG22	1.95	0.49
7:5:535:ARG:NH2	32:B8:120:SER:OG	2.45	0.49
8:4:166:LEU:HD22	9:2:276:LEU:HD11	1.94	0.49
8:4:297:VAL:HA	8:4:300:SER:HB3	1.94	0.49
10:AL:200:PRO:HG2	10:AL:282:PRO:HG2	1.94	0.49
34:B9:136:GLU:HG2	34:B9:165:PRO:HA	1.93	0.49
37:AN:80:ASP:OD1	54:S7:210:ARG:NH1	2.45	0.49
40:3A:397:ASN:ND2	41:3B:107:GLY:O	2.46	0.49
44:3E:141:SER:OG	44:3E:142:ALA:N	2.45	0.49
51:V1:115:VAL:HB	51:V1:156:ILE:HA	1.95	0.49
53:S1:238:PHE:HB3	55:S8:140:ARG:HE	1.77	0.49
3:S2:379:ILE:HD12	53:S1:140:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:260:LEU:HB2	7:5:317:LEU:HD11	1.94	0.49
7:5:574:THR:HB	9:2:171:ASN:HB2	1.93	0.49
8:4:105:LEU:O	8:4:109:THR:OG1	2.26	0.49
19:AM:57:GLY:O	19:AM:61:PHE:HB2	2.13	0.49
9:2a:324:LEU:HD23	24:c2:49:ARG:HH22	1.76	0.49
16:a5:40:LYS:O	16:a5:46:LYS:NZ	2.45	0.49
47:3H:64:ASP:OD1	47:3H:64:ASP:N	2.45	0.49
51:V1:37:ASP:N	51:V1:37:ASP:OD1	2.44	0.49
53:S1:693:ASP:OD1	53:S1:693:ASP:N	2.45	0.49
2:S3:227:GLN:OE1	2:S3:230:ARG:NH1	2.46	0.49
2:S3:231:LYS:H	53:S1:246:ARG:HH21	1.60	0.49
3:S2:148:GLU:HB3	3:S2:227:ILE:HB	1.94	0.49
7:5:144:TRP:O	7:5:223:LYS:NZ	2.44	0.49
33:B4:62:ASP:HB3	33:B4:65:LEU:HB2	1.94	0.49
4:1a:27:ILE:HD13	21:a1:5:ILE:HG12	1.94	0.49
10:a1:172:ALA:HB2	10:a1:237:ILE:HD11	1.95	0.49
34:b9:89:THR:O	34:b9:93:ARG:NH1	2.46	0.49
34:b9:105:ASP:OD1	34:b9:122:ARG:NH2	2.42	0.49
41:3B:76:ASN:OD1	41:3B:76:ASN:N	2.46	0.49
41:3B:109:LYS:O	41:3B:123:VAL:HA	2.13	0.49
42:3N:186:PRO:HA	42:3N:189:ILE:HB	1.95	0.49
44:3P:141:SER:OG	44:3P:142:ALA:N	2.46	0.49
54:s7:147:LYS:O	54:s7:151:GLN:NE2	2.44	0.49
8:4:443:PRO:O	8:4:447:LEU:HB2	2.13	0.49
10:AL:112:CYS:HB3	10:AL:130:ARG:HB3	1.95	0.49
13:S6:72:VAL:HG21	13:S6:77:ILE:HD12	1.95	0.49
30:B2:76:ASP:N	30:B2:76:ASP:OD1	2.46	0.49
31:B3:45:ARG:NH2	34:B9:39:TYR:OH	2.46	0.49
35:B7:53:LEU:HA	35:B7:56:ARG:HD2	1.95	0.49
6:4l:46:VAL:O	6:4l:50:ASN:HB2	2.12	0.49
12:s4:78:ARG:NH1	12:s4:148:GLU:OE1	2.45	0.49
14:a2:62:GLN:OE1	14:a2:80:ASN:ND2	2.46	0.49
15:ab:132:ASP:OD2	17:a6:40:ARG:NH1	2.46	0.49
44:3P:79:SER:OG	44:3P:80:HIS:N	2.45	0.49
52:v2:136:THR:OG1	65:v2:301:FES:S2	2.65	0.49
2:S3:230:ARG:NH2	55:S8:126:GLN:OE1	2.45	0.48
3:S2:115:LEU:O	54:S7:138:THR:OG1	2.31	0.48
11:A9:192:ARG:NH1	11:A9:198:ALA:O	2.45	0.48
15:AC:69:SER:OG	15:AC:70:ASP:N	2.46	0.48
22:A3:79:ASP:OD1	22:A3:79:ASP:N	2.46	0.48
33:B4:91:ALA:O	33:B4:95:PHE:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BL:4:SER:OG	36:BL:5:TRP:N	2.46	0.48
8:4a:456:GLY:O	27:bm:111:ARG:NH1	2.46	0.48
20:ao:82:ARG:NH1	20:ao:125:TYR:OH	2.46	0.48
21:a1:37:ARG:NH2	21:a1:51:ASP:OD2	2.46	0.48
29:b6:11:ARG:O	29:b6:15:LEU:HB2	2.12	0.48
42:3C:45:ILE:O	42:3C:49:LEU:HB2	2.13	0.48
42:3C:214:ASP:HB3	46:3G:8:LEU:HB3	1.94	0.48
42:3C:216:ASP:OD1	43:3D:317:ARG:NH2	2.46	0.48
53:s1:354:LEU:HD22	53:s1:548:LEU:HG	1.94	0.48
8:4:187:ASP:N	8:4:187:ASP:OD1	2.45	0.48
10:AL:139:ARG:NH1	10:AL:161:ARG:O	2.46	0.48
3:s2:96:ARG:HH22	17:a6:100:TRP:HA	1.78	0.48
4:1a:134:ARG:NH2	4:1a:206:GLU:OE1	2.47	0.48
10:al:81:LEU:HD23	10:al:83:MET:HG3	1.95	0.48
53:s1:131:CYS:O	53:s1:241:ARG:NH1	2.44	0.48
53:s1:239:THR:O	53:s1:266:ARG:NH2	2.42	0.48
2:S3:72:VAL:HA	2:S3:87:ILE:HG22	1.96	0.48
16:A5:44:TYR:O	16:A5:48:THR:OG1	2.30	0.48
38:A7:25:GLN:OE1	55:S8:79:ARG:NH1	2.46	0.48
9:2a:269:GLU:OE1	28:b5:157:ARG:NH2	2.46	0.48
31:b3:33:THR:HG22	31:b3:35:LEU:H	1.78	0.48
39:v3:84:ASN:OD1	39:v3:91:ARG:NH2	2.42	0.48
42:3N:158:THR:HA	42:3N:161:VAL:HG12	1.94	0.48
43:3O:97:SER:O	48:3U:52:LYS:NZ	2.47	0.48
51:V1:112:TYR:O	51:V1:240:THR:HA	2.12	0.48
53:s1:380:ASP:OD1	53:s1:380:ASP:N	2.43	0.48
53:s1:407:PRO:HD2	53:s1:438:LEU:HD11	1.95	0.48
55:s8:148:ASP:HB3	55:s8:151:LYS:HB2	1.96	0.48
3:S2:266:ARG:O	3:S2:270:ASN:HB2	2.13	0.48
7:5:8:ILE:HA	7:5:11:ILE:HD12	1.95	0.48
10:AL:327:ILE:O	10:AL:331:PHE:HB2	2.13	0.48
8:4a:276:CYS:HB3	8:4a:285:LEU:HG	1.95	0.48
9:2a:240:MET:O	9:2a:244:ILE:HB	2.13	0.48
13:s6:67:GLN:NE2	55:s8:108:SER:O	2.47	0.48
36:bl:162:ARG:NH1	36:bl:166:GLU:OE1	2.46	0.48
44:3P:93:ARG:HD2	44:3P:110:ARG:HG2	1.94	0.48
2:S3:196:PRO:O	3:S2:122:LYS:NZ	2.47	0.48
9:2:42:PRO:HA	9:2:45:ILE:HG22	1.96	0.48
1:3a:69:ILE:HA	1:3a:72:LEU:HB2	1.96	0.48
3:s2:221:ARG:HD2	54:s7:197:THR:HG23	1.96	0.48
17:a6:27:ASP:OD1	17:a6:27:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:bm:70:ASP:OD1	34:b9:108:HIS:NE2	2.47	0.48
40:3A:368:MET:O	40:3A:372:LEU:HB2	2.14	0.48
45:3F:54:ASP:OD1	45:3F:54:ASP:N	2.47	0.48
42:3N:47:THR:O	42:3N:51:LEU:HB2	2.12	0.48
52:V2:37:LEU:HB3	52:V2:41:ARG:HH21	1.79	0.48
53:S1:140:GLN:NE2	64:S1:801:SF4:S3	2.86	0.48
53:s1:66:HIS:HB2	53:s1:181:ARG:HD3	1.96	0.48
4:1:28:LEU:HD11	4:1:274:ARG:HH11	1.79	0.48
8:4:180:SER:O	36:BL:153:ARG:NH2	2.45	0.48
10:AL:139:ARG:NH1	10:AL:166:ASP:OD1	2.47	0.48
14:A2:27:SER:O	14:A2:34:ARG:NH2	2.44	0.48
2:s3:185:ARG:NH1	2:s3:188:THR:OG1	2.46	0.48
8:4a:53:SER:OG	8:4a:54:ASN:N	2.47	0.48
9:2a:273:ASN:O	19:am:140:LYS:NZ	2.47	0.48
15:ac:131:PRO:HG2	15:ac:134:ASP:HB2	1.95	0.48
19:am:87:PRO:HG3	19:am:127:ILE:HD13	1.95	0.48
25:s5:15:ASP:N	25:s5:15:ASP:OD1	2.47	0.48
51:V1:243:ALA:HA	63:V1:501:FMN:H5'2	1.94	0.48
53:s1:592:LYS:NZ	53:s1:619:ASP:OD2	2.46	0.48
7:5:564:LYS:HA	7:5:567:SER:HB3	1.95	0.48
8:4:36:LEU:HD13	27:BM:96:VAL:HA	1.95	0.48
14:A2:71:PHE:H	53:S1:362:ASP:HB3	1.79	0.48
34:B9:105:ASP:OD1	34:B9:122:ARG:NH2	2.46	0.48
5:6a:22:LYS:NZ	6:4l:21:MET:O	2.40	0.48
9:2a:154:ILE:HG21	9:2a:195:PRO:HD3	1.94	0.48
14:a2:19:ILE:HG23	14:a2:53:ILE:HA	1.96	0.48
19:am:114:GLY:O	19:am:118:MET:HB2	2.13	0.48
42:3C:6:LYS:O	42:3C:12:LYS:NZ	2.47	0.48
42:3C:210:GLY:HA3	42:3C:314:SER:HB3	1.95	0.48
41:3M:129:ASP:N	41:3M:129:ASP:OD1	2.45	0.48
44:3P:103:SER:OG	44:3P:104:LYS:N	2.45	0.48
53:S1:478:SER:O	53:S1:518:ARG:NH1	2.47	0.48
15:AC:141:PRO:HA	15:AC:144:ILE:HG22	1.96	0.48
3:s2:411:LEU:HD13	3:s2:422:CYS:HB3	1.94	0.48
4:1a:127:TYR:HD1	4:1a:207:LEU:HB3	1.79	0.48
11:a9:211:ASP:OD1	11:a9:211:ASP:N	2.46	0.48
40:3A:300:ASP:OD1	40:3A:300:ASP:N	2.37	0.48
42:3C:130:GLY:HA2	42:3C:133:LEU:HD12	1.96	0.48
40:3L:341:PHE:HB3	40:3L:358:PHE:HB3	1.96	0.48
53:S1:197:THR:HG22	53:S1:206:VAL:HG22	1.96	0.48
3:S2:281:GLU:OE2	16:A5:86:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S2:303:ARG:NH2	3:S2:336:GLU:OE2	2.47	0.48
8:4:26:ASN:OD1	26:B1:13:HIS:NE2	2.45	0.48
8:4:137:GLY:O	8:4:142:ARG:NH1	2.47	0.48
5:6a:129:ASP:HB3	5:6a:135:LEU:HD21	1.95	0.48
7:5a:153:LEU:HD21	8:4a:360:LEU:HD21	1.95	0.48
7:5a:512:SER:H	34:b9:36:LYS:HE3	1.78	0.48
8:4a:66:ILE:HG23	8:4a:107:ILE:HD11	1.96	0.48
14:a2:56:ARG:NH2	53:s1:379:THR:O	2.47	0.48
15:ac:97:LYS:NZ	15:ac:107:ASP:O	2.47	0.48
20:ao:56:GLU:HA	20:ao:59:ARG:HE	1.79	0.48
53:s1:518:ARG:HG3	53:s1:519:ILE:HG13	1.96	0.48
4:1:54:LYS:HD3	4:1:55:LEU:HG	1.96	0.48
8:4:171:VAL:HG21	8:4:179:LEU:HD21	1.95	0.48
9:2:43:MET:O	9:2:46:ASN:ND2	2.45	0.48
10:AL:105:ASP:HB2	10:AL:108:PHE:HD2	1.79	0.48
11:A9:132:ARG:NH1	58:A9:501:NDP:O2X	2.47	0.48
14:A2:19:ILE:HD13	14:A2:91:MET:HE1	1.95	0.48
21:a1:14:VAL:HA	21:a1:17:VAL:HG12	1.96	0.48
53:S1:296:GLY:O	53:S1:572:HIS:NE2	2.42	0.48
54:S7:146:ARG:NH1	54:S7:184:ILE:O	2.46	0.48
53:s1:419:ARG:NH1	53:s1:439:THR:O	2.47	0.48
55:s8:90:LYS:NZ	55:s8:174:GLU:OE2	2.47	0.48
3:S2:137:ASP:OD1	3:S2:137:ASP:N	2.46	0.47
5:6:129:ASP:HB3	5:6:135:LEU:HD21	1.96	0.47
36:BL:140:GLN:HG2	36:BL:144:LEU:HD22	1.96	0.47
4:1a:281:ARG:NE	4:1a:284:GLN:OE1	2.43	0.47
7:5a:460:GLY:O	7:5a:464:ALA:CB	2.62	0.47
18:a8:149:GLU:OE2	25:s5:51:ARG:NH1	2.47	0.47
41:3B:155:ARG:NH1	41:3B:200:ILE:O	2.47	0.47
3:S2:216:ARG:HE	3:S2:240:LEU:HD13	1.78	0.47
5:6:25:PRO:HG3	6:4L:28:SER:HB2	1.95	0.47
8:4:375:LEU:O	8:4:379:LEU:HB2	2.14	0.47
9:2:120:GLN:O	9:2:176:ARG:NH1	2.46	0.47
9:2:307:THR:OG1	9:2:308:ASN:N	2.47	0.47
11:A9:117:ARG:O	11:A9:121:GLN:HB3	2.14	0.47
13:S6:75:ARG:NH1	13:S6:96:ASP:OD2	2.48	0.47
14:A2:20:ARG:HB3	14:A2:66:TRP:O	2.15	0.47
8:4a:310:MET:HE3	8:4a:310:MET:HB3	1.79	0.47
9:2a:155:LEU:HD23	9:2a:278:MET:HG2	1.96	0.47
26:b1:42:MET:O	36:bl:69:ARG:NH1	2.46	0.47
35:b7:56:ARG:NH2	36:bl:120:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3A:74:TRP:HB2	40:3A:230:VAL:HG22	1.97	0.47
41:3M:60:ARG:NH2	41:3M:122:THR:OG1	2.47	0.47
53:S1:497:VAL:HA	53:S1:500:ILE:HB	1.96	0.47
54:S7:164:CYS:HA	54:S7:169:GLY:H	1.78	0.47
55:s8:140:ARG:O	55:s8:141:ARG:NH1	2.44	0.47
5:6:123:TRP:HH2	20:AO:123:GLU:HG3	1.79	0.47
8:4:221:VAL:O	8:4:340:ARG:NH1	2.48	0.47
11:A9:280:ILE:HG23	11:A9:353:LEU:HD11	1.95	0.47
14:A2:19:ILE:HD12	14:A2:53:ILE:HB	1.95	0.47
39:V3:94:GLN:HB3	52:V2:70:PRO:HA	1.96	0.47
8:4a:159:PRO:HG3	9:2a:284:MET:HE1	1.97	0.47
27:bm:138:ASN:HB3	36:bl:159:GLN:HE21	1.79	0.47
45:3Q:68:ASP:OD2	45:3Q:72:ARG:NH1	2.47	0.47
51:V1:160:GLY:O	51:V1:199:ARG:NH2	2.48	0.47
51:V1:410:ASP:OD1	51:V1:410:ASP:N	2.39	0.47
53:s1:197:THR:HG22	53:s1:206:VAL:HG22	1.96	0.47
53:s1:336:ASN:O	53:s1:365:ASN:ND2	2.47	0.47
2:S3:133:SER:HG	2:S3:138:SER:H	1.60	0.47
3:S2:443:MET:H	3:S2:446:ASP:HB2	1.79	0.47
5:6:78:TYR:HB3	11:A9:360:ARG:HD2	1.97	0.47
7:5:304:PHE:HZ	7:5:526:LEU:HD13	1.80	0.47
10:AL:342:GLY:O	10:AL:355:LYS:NZ	2.45	0.47
15:AB:136:GLU:OE1	15:AB:137:LYS:NZ	2.46	0.47
36:BL:164:LEU:HD23	36:BL:167:ARG:HE	1.79	0.47
2:s3:149:LEU:HG	17:a6:80:ARG:HH21	1.80	0.47
4:1a:317:TYR:O	21:a1:40:ARG:NH1	2.44	0.47
7:5a:136:ASN:HA	7:5a:197:GLU:HA	1.96	0.47
9:2a:108:LEU:HD23	9:2a:187:MET:HB3	1.96	0.47
11:a9:270:ARG:NH2	11:a9:328:MET:SD	2.82	0.47
40:3A:165:ARG:NH2	40:3A:211:LEU:O	2.48	0.47
43:3O:291:LYS:O	43:3O:295:MET:HB2	2.15	0.47
52:V2:134:CYS:SG	52:V2:135:THR:N	2.87	0.47
2:S3:208:GLU:OE1	54:S7:183:ARG:NH2	2.47	0.47
28:B5:175:GLU:HG3	28:B5:177:GLU:H	1.78	0.47
32:B8:38:PRO:HD3	33:B4:67:ARG:HG2	1.96	0.47
33:B4:30:ARG:HG3	40:3A:261:ALA:HB2	1.97	0.47
38:A7:9:GLN:OE1	38:A7:12:ARG:NH2	2.47	0.47
1:3a:28:ASN:O	1:3a:33:LYS:NZ	2.43	0.47
3:s2:117:HIS:ND1	3:s2:462:ASP:O	2.47	0.47
29:b6:19:ARG:HH21	34:b9:173:ARG:HE	1.63	0.47
29:b6:122:ASP:OD1	29:b6:122:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3C:40:CYS:HA	42:3C:43:VAL:HG12	1.97	0.47
47:3H:31:VAL:HA	47:3H:34:HIS:HB3	1.96	0.47
40:3L:316:CYS:O	41:3M:157:GLN:NE2	2.47	0.47
41:3M:50:ALA:HB3	41:3M:221:VAL:HG12	1.97	0.47
51:V1:266:GLY:N	51:V1:291:GLU:OE2	2.48	0.47
53:S1:64:CYS:SG	53:S1:65:TYR:N	2.88	0.47
53:S1:388:ASN:ND2	53:S1:513:MET:O	2.43	0.47
51:v1:54:LYS:O	51:v1:58:ARG:NH1	2.47	0.47
51:v1:126:LYS:NZ	51:v1:351:THR:O	2.44	0.47
1:3:58:VAL:HA	1:3:61:THR:HG22	1.97	0.47
4:1:294:LEU:HA	4:1:297:THR:HG22	1.96	0.47
9:2:119:THR:HG22	9:2:176:ARG:HB3	1.95	0.47
18:A8:144:SER:OG	18:A8:145:ARG:N	2.47	0.47
19:AM:85:ASP:OD1	19:AM:85:ASP:N	2.45	0.47
37:AN:82:ASP:N	37:AN:82:ASP:OD1	2.47	0.47
7:5a:482:MET:HB3	7:5a:486:LEU:HB3	1.96	0.47
8:4a:102:LEU:HD13	8:4a:128:PRO:HB2	1.96	0.47
10:a1:272:ASP:OD2	16:a5:30:LYS:NZ	2.47	0.47
30:b2:97:LEU:HD11	35:b7:100:LYS:HG3	1.97	0.47
36:bl:159:GLN:HG2	36:bl:162:ARG:HH21	1.80	0.47
40:3A:122:ALA:H	41:3B:300:LYS:HD2	1.78	0.47
43:3O:104:SER:OG	43:3O:105:LEU:N	2.46	0.47
51:V1:225:LEU:HB3	51:V1:227:PRO:HD2	1.96	0.47
54:S7:87:ARG:HB2	54:S7:209:GLN:HG3	1.97	0.47
1:3:52:SER:OG	1:3:54:LYS:NZ	2.47	0.47
1:3:60:ILE:HG23	6:4L:72:ALA:HB1	1.95	0.47
3:S2:220:ALA:HB2	55:S8:98:ARG:HE	1.79	0.47
4:1:67:SER:O	4:1:71:PHE:HB2	2.14	0.47
4:1:80:THR:O	4:1:84:SER:HB3	2.15	0.47
11:A9:104:THR:HG21	13:S6:46:VAL:HG13	1.96	0.47
12:S4:60:ASP:HB2	12:S4:62:THR:HG23	1.95	0.47
29:B6:108:ASP:OD2	35:B7:71:ARG:NH2	2.47	0.47
35:B7:69:CYS:O	35:B7:73:SER:HB2	2.14	0.47
37:AN:82:ASP:HB2	54:S7:203:TYR:HE1	1.80	0.47
39:V3:72:HIS:NE2	52:V2:215:PRO:O	2.48	0.47
4:1a:191:ALA:HB2	4:1a:198:PHE:HD2	1.80	0.47
12:s4:81:VAL:HG21	12:s4:150:LYS:HD3	1.95	0.47
25:s5:7:GLN:HE21	25:s5:14:LEU:HD12	1.80	0.47
28:b5:89:VAL:HG22	28:b5:116:PRO:HG2	1.97	0.47
32:b8:110:ASP:OD1	32:b8:110:ASP:N	2.45	0.47
40:3A:392:LYS:HG2	40:3A:433:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3B:216:ALA:HB3	41:3B:244:LEU:HA	1.96	0.47
41:3M:109:LYS:HG2	41:3M:124:GLU:HG2	1.97	0.47
46:3R:25:ARG:HH11	46:3R:26:ALA:H	1.61	0.47
53:S1:123:ASN:HD22	53:S1:157:LYS:HA	1.79	0.47
53:s1:426:ASP:OD1	53:s1:426:ASP:N	2.46	0.47
32:B8:67:ASP:O	33:B4:81:ARG:NH2	2.48	0.47
7:5a:538:PRO:O	7:5a:542:LEU:HB2	2.15	0.47
8:4a:326:LEU:HA	8:4a:329:LEU:HD22	1.97	0.47
13:s6:32:THR:HG22	13:s6:55:VAL:HG22	1.96	0.47
32:b8:38:PRO:HD3	33:b4:67:ARG:HG2	1.95	0.47
42:3C:39:VAL:HG11	42:3C:232:ILE:HG12	1.96	0.47
40:3L:367:ASP:OD1	40:3L:367:ASP:N	2.48	0.47
45:3Q:30:LEU:HD21	45:3Q:70:THR:HG23	1.97	0.47
53:S1:546:PHE:HB2	53:S1:567:VAL:HG22	1.96	0.47
53:s1:693:ASP:OD1	53:s1:693:ASP:N	2.45	0.47
11:A9:357:ARG:NH2	11:A9:364:SER:O	2.48	0.47
24:C2:97:HIS:HB3	24:C2:100:ASP:HB2	1.96	0.47
3:s2:236:LEU:HD13	3:s2:240:LEU:HD23	1.97	0.47
7:5a:60:GLU:OE2	7:5a:81:LYS:NZ	2.48	0.47
7:5a:204:SER:HB3	7:5a:266:LEU:HD11	1.97	0.47
9:2a:210:ILE:HD12	9:2a:329:LEU:HD22	1.95	0.47
12:s4:50:THR:OG1	12:s4:51:GLN:N	2.46	0.47
40:3A:446:SER:O	48:3J:16:ARG:NH2	2.45	0.47
42:3C:296:LEU:O	42:3C:300:ILE:HB	2.15	0.47
42:3N:240:MET:HA	42:3N:243:VAL:HG12	1.96	0.47
4:1:199:ASP:OD1	4:1:279:ARG:NH1	2.48	0.47
11:A9:226:VAL:HG11	11:A9:277:VAL:HG11	1.97	0.47
13:S6:21:GLY:N	13:S6:62:ASP:OD2	2.48	0.47
13:S6:106:TYR:O	55:S8:141:ARG:NH2	2.48	0.47
17:A6:120:ASP:OD1	17:A6:120:ASP:N	2.45	0.47
32:B8:86:ARG:NH1	32:B8:99:MET:SD	2.81	0.47
3:s2:120:THR:HG21	3:s2:139:LEU:HD21	1.97	0.47
4:1a:75:PRO:HG2	4:1a:219:PRO:HB3	1.97	0.47
6:4l:78:LEU:HA	6:4l:81:VAL:HG12	1.97	0.47
7:5a:386:LEU:HD21	30:b2:65:MET:HE2	1.96	0.47
7:5a:553:LEU:HA	7:5a:557:TRP:HB2	1.96	0.47
25:s5:47:ILE:HG13	25:s5:51:ARG:HB3	1.97	0.47
42:3C:304:MET:HE1	42:3C:362:ILE:HD12	1.95	0.47
51:V1:374:TYR:O	51:V1:378:SER:HB3	2.15	0.47
53:S1:308:ARG:NH1	53:S1:312:GLY:O	2.48	0.47
51:v1:209:GLU:HA	51:v1:242:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:75:LEU:HA	1:3:78:ALA:HB3	1.96	0.46
4:1:85:LEU:HB2	4:1:233:LEU:HD21	1.95	0.46
7:5:398:ALA:HA	7:5:401:THR:HG22	1.97	0.46
15:AC:115:GLN:NE2	15:AC:138:LEU:O	2.47	0.46
24:C2:120:ARG:O	33:B4:109:ARG:NH1	2.46	0.46
27:BM:127:ARG:HD3	27:BM:132:LEU:HB3	1.96	0.46
28:B5:145:GLU:HA	28:B5:148:GLU:HG2	1.95	0.46
28:B5:180:ASP:OD1	28:B5:180:ASP:N	2.42	0.46
2:s3:234:LEU:HD12	3:s2:418:ARG:HH11	1.80	0.46
3:s2:224:ALA:O	55:s8:98:ARG:NH2	2.46	0.46
4:1a:59:GLU:HB3	54:s7:153:PRO:HB2	1.97	0.46
7:5a:62:MET:HB3	36:bl:115:GLN:HG2	1.96	0.46
8:4a:119:TYR:HE1	8:4a:157:SER:HB2	1.80	0.46
8:4a:345:ALA:HB1	8:4a:348:LEU:HD11	1.97	0.46
18:a8:47:ARG:HH21	28:b5:187:PRO:HB2	1.81	0.46
24:c2:44:MET:HA	24:c2:47:MET:HG2	1.97	0.46
40:3L:37:THR:OG1	40:3L:38:PHE:N	2.47	0.46
43:3O:215:LEU:HB3	43:3O:248:ILE:HD11	1.97	0.46
54:S7:112:TYR:HD2	54:S7:198:ALA:HB3	1.80	0.46
55:s8:189:LYS:O	55:s8:193:ASN:HB2	2.15	0.46
3:S2:185:MET:SD	3:S2:189:THR:OG1	2.73	0.46
7:5:82:THR:HA	7:5:86:SER:HB3	1.96	0.46
7:5:161:ARG:NH1	34:B9:89:THR:O	2.48	0.46
8:4:118:PHE:O	8:4:122:PHE:CB	2.63	0.46
9:2:106:LEU:HG	9:2:138:PRO:HB2	1.97	0.46
1:3a:97:ILE:HA	1:3a:100:LEU:HB2	1.97	0.46
2:s3:72:VAL:HA	2:s3:87:ILE:HG22	1.96	0.46
4:1a:27:ILE:HD11	55:s8:77:LEU:HD13	1.96	0.46
14:a2:18:GLU:OE2	14:a2:20:ARG:NH1	2.48	0.46
15:ab:115:GLN:NE2	15:ab:138:LEU:O	2.47	0.46
42:3C:33:PHE:HA	42:3C:36:LEU:HB2	1.97	0.46
40:3L:411:GLU:O	40:3L:415:ARG:HB2	2.15	0.46
53:S1:266:ARG:HH12	55:S8:117:LYS:HE2	1.80	0.46
54:S7:182:ASP:OD1	54:S7:182:ASP:N	2.45	0.46
53:s1:319:TRP:HE1	53:s1:615:LEU:HB3	1.80	0.46
7:5:222:GLY:HA2	7:5:229:LEU:HD22	1.97	0.46
24:C2:42:GLY:O	24:C2:46:ASN:ND2	2.47	0.46
35:B7:15:VAL:HG12	35:B7:113:LYS:HG3	1.97	0.46
2:s3:57:LEU:HB3	2:s3:83:LEU:HD21	1.96	0.46
4:1a:315:PRO:HG3	20:ao:54:ASN:HD21	1.79	0.46
8:4a:231:LEU:HA	8:4a:235:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2a:42:PRO:HA	9:2a:45:ILE:HG22	1.96	0.46
32:b8:169:GLU:OE1	35:b7:56:ARG:NH1	2.48	0.46
40:3L:226:ALA:HA	40:3L:229:MET:HB2	1.97	0.46
42:3N:14:ILE:O	42:3N:18:PHE:HB2	2.15	0.46
49:3V:45:VAL:HG12	49:3V:47:TYR:H	1.81	0.46
51:V1:48:ARG:NH1	52:V2:225:GLU:OE2	2.49	0.46
53:s1:261:ILE:HG23	53:s1:273:ILE:HG23	1.97	0.46
53:s1:588:ALA:H	53:s1:591:GLU:HB2	1.80	0.46
3:S2:174:PHE:O	3:S2:178:THR:OG1	2.31	0.46
11:A9:69:VAL:O	11:A9:73:LEU:HB2	2.16	0.46
18:A8:7:LEU:HD23	20:AO:91:LEU:HD13	1.97	0.46
3:s2:290:GLY:HA3	3:s2:405:GLY:HA2	1.97	0.46
17:a6:55:LEU:HD13	17:a6:57:ILE:HD11	1.98	0.46
18:a8:53:PRO:HB3	20:ao:80:ASP:HB2	1.96	0.46
51:V1:101:PHE:O	51:V1:104:LYS:NZ	2.48	0.46
53:S1:59:GLN:OE1	53:S1:62:ARG:NH1	2.43	0.46
53:s1:86:PRO:O	53:s1:108:LYS:NZ	2.48	0.46
55:s8:74:LEU:HD12	55:s8:77:LEU:HD21	1.96	0.46
3:S2:317:ASP:OD2	3:S2:342:ARG:NH2	2.48	0.46
4:1:164:THR:HA	4:1:167:THR:HG22	1.96	0.46
18:A8:144:SER:OG	18:A8:147:ARG:NH2	2.49	0.46
2:s3:154:SER:HB3	2:s3:177:PHE:HB3	1.98	0.46
3:s2:184:ILE:HG23	3:s2:203:MET:HB3	1.98	0.46
5:6a:81:THR:H	5:6a:84:SER:HB2	1.80	0.46
7:5a:97:THR:HG21	7:5a:125:LEU:HD22	1.96	0.46
7:5a:357:ARG:HG2	34:b9:32:ILE:HG23	1.98	0.46
9:2a:115:LEU:HA	9:2a:118:VAL:HG12	1.96	0.46
13:s6:31:ILE:HG12	13:s6:37:VAL:HB	1.98	0.46
25:s5:33:CYS:HB3	25:s5:36:PHE:HB2	1.98	0.46
45:3F:46:GLU:OE2	45:3F:49:ARG:NH1	2.49	0.46
53:s1:134:GLY:HA3	53:s1:241:ARG:HD2	1.96	0.46
54:s7:158:VAL:HB	54:s7:187:VAL:HA	1.98	0.46
2:S3:218:VAL:O	17:A6:104:THR:OG1	2.33	0.46
3:S2:458:PHE:HA	3:S2:461:ILE:HG12	1.97	0.46
36:BL:79:GLU:HA	36:BL:85:ILE:HD11	1.98	0.46
3:s2:254:ARG:NE	55:s8:76:TYR:OH	2.48	0.46
5:6a:155:ALA:HB1	6:4l:65:VAL:HG11	1.96	0.46
8:4a:109:THR:OG1	8:4a:121:LEU:O	2.34	0.46
10:al:200:PRO:HG2	10:al:282:PRO:HG2	1.98	0.46
11:a9:70:VAL:HG12	11:a9:97:MET:HG3	1.98	0.46
28:b5:155:GLU:HB2	28:b5:158:ARG:HH21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3A:303:THR:HA	40:3A:306:VAL:HG12	1.98	0.46
43:3D:210:TYR:O	43:3D:214:LEU:HB2	2.15	0.46
42:3N:125:ALA:O	42:3N:129:MET:HB2	2.16	0.46
51:v1:369:ARG:HE	52:v2:136:THR:HA	1.81	0.46
53:s1:401:LEU:HA	53:s1:430:ALA:O	2.16	0.46
4:1:284:GLN:HA	4:1:287:HIS:HB2	1.98	0.46
5:6:161:ALA:O	5:6:165:ILE:HB	2.16	0.46
6:4L:27:MET:HE2	6:4L:78:LEU:HD13	1.97	0.46
7:5:75:GLU:HG3	7:5:77:LYS:HD3	1.98	0.46
7:5:172:ILE:O	7:5:176:ARG:HB2	2.15	0.46
8:4:315:LEU:O	8:4:319:HIS:HB3	2.15	0.46
10:AL:87:PRO:O	10:AL:142:GLN:NE2	2.42	0.46
4:1a:149:ILE:HG21	4:1a:185:TRP:HB2	1.98	0.46
4:1a:189:THR:OG1	4:1a:234:MET:SD	2.70	0.46
4:1a:260:MET:HE3	4:1a:264:LEU:HB3	1.97	0.46
7:5a:237:MET:HE1	7:5a:248:HIS:HB2	1.98	0.46
15:ac:81:ASP:O	15:ac:85:TYR:HB2	2.15	0.46
20:ao:82:ARG:NH2	21:a1:46:TYR:OH	2.48	0.46
27:bm:93:PHE:HD2	28:b5:75:LEU:HD13	1.81	0.46
45:3F:41:THR:OG1	45:3F:42:GLU:N	2.47	0.46
42:3N:163:TRP:O	42:3N:177:ARG:NH1	2.48	0.46
43:3O:308:ARG:O	43:3O:312:SER:HB2	2.15	0.46
53:s1:546:PHE:HB2	53:s1:567:VAL:HG22	1.98	0.46
2:S3:212:ASP:OD2	11:A9:75:ARG:NH1	2.49	0.46
7:5:319:MET:HB2	7:5:319:MET:HE3	1.75	0.46
12:S4:158:LYS:HA	12:S4:158:LYS:HD3	1.76	0.46
13:S6:51:ARG:HD3	37:AN:129:VAL:HG11	1.98	0.46
32:B8:110:ASP:OD1	32:B8:110:ASP:N	2.47	0.46
37:AN:135:ARG:NH2	55:S8:133:GLU:OE1	2.48	0.46
1:3a:33:LYS:HG2	4:1a:61:MET:HE1	1.97	0.46
13:s6:39:ASP:O	13:s6:45:ARG:NH1	2.49	0.46
16:a5:5:LEU:O	16:a5:7:LYS:NZ	2.48	0.46
24:c2:120:ARG:NH1	33:b4:113:GLU:OE1	2.49	0.46
28:b5:145:GLU:O	28:b5:149:LEU:HB2	2.16	0.46
32:b8:105:ILE:HG23	32:b8:109:LEU:HD22	1.96	0.46
37:an:20:GLY:HA3	37:an:39:ILE:HG13	1.96	0.46
40:3A:88:GLY:O	40:3A:92:PHE:HB2	2.15	0.46
40:3A:292:GLU:HA	40:3A:352:GLY:O	2.16	0.46
41:3B:90:THR:HG23	41:3B:145:GLU:HB2	1.97	0.46
40:3L:193:GLN:O	40:3L:269:ARG:NH2	2.44	0.46
40:3L:400:VAL:HG21	41:3M:57:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3N:71:ARG:HG3	43:3O:280:PRO:HG2	1.98	0.46
52:V2:152:GLN:NE2	52:V2:158:LYS:O	2.49	0.46
55:S8:204:ASN:O	55:S8:208:ASP:HB2	2.15	0.46
3:S2:80:MET:HE2	3:S2:80:MET:HB3	1.78	0.46
4:1:312:ALA:O	20:AO:55:GLN:NE2	2.49	0.46
8:4:277:LEU:HD21	8:4:405:MET:HB3	1.98	0.46
15:AC:85:TYR:OH	31:B3:28:TRP:NE1	2.43	0.46
15:AC:153:ASP:OD2	29:B6:19:ARG:NH2	2.48	0.46
16:A5:38:PHE:O	16:A5:45:ARG:NH2	2.49	0.46
25:S5:66:CYS:HA	25:S5:69:ARG:HE	1.80	0.46
2:s3:125:PHE:HB2	2:s3:146:ALA:HB3	1.98	0.46
3:s2:315:GLU:O	3:s2:342:ARG:NH2	2.48	0.46
4:1a:289:LEU:O	4:1a:294:LEU:N	2.49	0.46
30:b2:78:ASP:HB3	30:b2:83:HIS:HA	1.98	0.46
46:3G:51:PRO:HA	46:3G:54:VAL:HB	1.97	0.46
51:V1:325:PRO:HG2	51:V1:347:THR:HA	1.98	0.46
53:S1:142:GLN:O	53:S1:146:PHE:HB2	2.16	0.46
53:S1:333:PHE:HD2	53:S1:544:MET:HB2	1.81	0.46
53:S1:572:HIS:O	53:S1:699:SER:OG	2.34	0.46
51:v1:159:ARG:NH2	52:v2:175:CYS:O	2.49	0.46
53:s1:292:PHE:HB3	53:s1:706:THR:HG21	1.98	0.46
53:s1:390:THR:HG22	53:s1:659:ILE:HD13	1.98	0.46
3:S2:358:VAL:HG12	3:S2:364:SER:HB3	1.96	0.46
9:2:207:ILE:O	9:2:211:LEU:HB2	2.16	0.46
11:A9:188:GLU:OE2	11:A9:202:ARG:NE	2.45	0.46
2:s3:148:GLU:HG2	2:s3:149:LEU:HD22	1.97	0.46
3:s2:432:LEU:HD22	3:s2:456:ILE:HG21	1.98	0.46
4:1a:311:THR:OG1	20:ao:51:MET:SD	2.66	0.46
5:6a:150:TRP:HE1	9:2a:19:ILE:HD11	1.81	0.46
8:4a:76:MET:HE1	8:4a:230:ILE:HD13	1.98	0.46
36:bl:4:SER:OG	36:bl:5:TRP:N	2.49	0.46
42:3C:248:ASP:N	42:3C:248:ASP:OD1	2.47	0.46
42:3N:33:PHE:HA	42:3N:36:LEU:HB2	1.98	0.46
54:s7:163:SER:OG	64:s7:301:SF4:S3	2.70	0.46
55:s8:168:VAL:HG21	55:s8:201:ILE:HG21	1.98	0.46
3:S2:196:ALA:HB2	4:1:278:PRO:HB3	1.98	0.45
3:S2:383:LYS:NZ	53:S1:141:ASP:OD1	2.43	0.45
7:5:297:ASP:HB2	7:5:300:LYS:HB2	1.96	0.45
11:A9:248:GLY:HA3	11:A9:265:PHE:HZ	1.81	0.45
12:S4:50:THR:OG1	12:S4:51:GLN:N	2.47	0.45
36:BL:56:HIS:O	36:BL:60:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s2:80:MET:N	3:s2:80:MET:SD	2.89	0.45
7:5a:393:ASP:O	7:5a:397:GLU:HB2	2.17	0.45
32:b8:83:GLN:HE22	32:b8:86:ARG:HH21	1.64	0.45
40:3A:113:VAL:HG11	40:3A:120:LEU:HD11	1.97	0.45
40:3A:426:LEU:HA	40:3A:429:TRP:HB2	1.97	0.45
41:3M:322:ASP:HB2	50:3T:55:LEU:HB3	1.98	0.45
42:3N:359:PHE:HA	42:3N:362:ILE:HG22	1.98	0.45
51:v1:325:PRO:HD3	51:v1:433:TRP:HB3	1.98	0.45
53:s1:220:GLY:HA3	53:s1:291:ARG:HD3	1.98	0.45
53:s1:266:ARG:HD2	53:s1:267:THR:HG23	1.98	0.45
3:S2:185:MET:O	3:S2:189:THR:OG1	2.34	0.45
36:BL:92:TRP:HH2	36:BL:150:TYR:HB2	1.81	0.45
1:3a:80:GLN:OE1	20:ao:58:ARG:NH1	2.48	0.45
3:s2:271:ARG:HD3	4:1a:284:GLN:HE22	1.82	0.45
3:s2:404:LYS:HZ1	3:s2:457:VAL:HG22	1.80	0.45
4:1a:105:ILE:HG21	4:1a:237:LEU:HD11	1.98	0.45
11:a9:136:THR:OG1	11:a9:137:ARG:N	2.50	0.45
13:s6:88:HIS:HD2	13:s6:107:CYS:SG	2.28	0.45
20:ao:69:ILE:HD11	22:a3:53:TYR:HA	1.97	0.45
36:bl:66:ARG:HH11	36:bl:68:TYR:HE1	1.64	0.45
47:3S:54:ARG:NH2	47:3S:63:GLU:OE1	2.47	0.45
51:V1:119:GLU:OE2	51:V1:128:ARG:N	2.49	0.45
53:s1:538:ARG:NH1	53:s1:559:ASP:OD2	2.49	0.45
1:3:80:GLN:NE2	4:1:315:PRO:O	2.49	0.45
3:S2:246:GLU:HG3	38:A7:30:GLU:HB3	1.98	0.45
7:5:231:PRO:HB3	7:5:530:PRO:HG3	1.98	0.45
17:A6:34:ARG:HG2	17:A6:86:VAL:HG11	1.98	0.45
34:B9:31:CYS:HB3	34:B9:36:LYS:HB3	1.97	0.45
2:s3:215:VAL:O	11:a9:209:ARG:NH2	2.49	0.45
5:6a:78:TYR:HB3	11:a9:360:ARG:HD2	1.97	0.45
7:5a:536:ILE:HD12	32:b8:126:TRP:HZ2	1.82	0.45
11:a9:61:ALA:HA	11:a9:66:GLY:HA3	1.97	0.45
11:a9:72:HIS:ND1	11:a9:246:SER:OG	2.50	0.45
20:ao:48:TRP:HD1	20:ao:51:MET:HE3	1.80	0.45
43:3D:109:SER:OG	43:3D:112:ARG:NH2	2.50	0.45
41:3M:72:GLU:O	41:3M:188:ASN:ND2	2.50	0.45
42:3N:145:VAL:HG21	42:3N:268:ILE:HG12	1.98	0.45
42:3N:373:GLU:OE1	45:3Q:21:TYR:OH	2.32	0.45
53:S1:74:ASN:OD1	53:S1:180:THR:OG1	2.33	0.45
51:v1:250:VAL:HG13	51:v1:254:ILE:HD11	1.97	0.45
51:v1:410:ASP:OD1	51:v1:410:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:492:ILE:O	7:5:496:LEU:HB2	2.16	0.45
8:4:7:PRO:HB2	8:4:34:ILE:HD11	1.98	0.45
13:S6:52:GLN:HG3	37:AN:127:GLN:H	1.81	0.45
15:AC:120:MET:HE1	34:B9:21:LYS:HA	1.97	0.45
31:B3:42:LEU:HD11	34:B9:42:CYS:HB2	1.97	0.45
3:s2:174:PHE:O	3:s2:178:THR:OG1	2.31	0.45
7:5a:367:PRO:O	7:5a:371:SER:HB3	2.16	0.45
8:4a:104:ILE:O	8:4a:108:MET:HB2	2.17	0.45
9:2a:298:TYR:O	9:2a:303:THR:OG1	2.31	0.45
37:an:134:THR:HB	55:s8:144:ARG:HB2	1.98	0.45
42:3C:165:TRP:O	42:3C:174:THR:OG1	2.34	0.45
44:3E:118:THR:O	44:3E:122:THR:OG1	2.33	0.45
40:3L:164:GLU:HA	40:3L:167:VAL:HB	1.98	0.45
47:3S:64:ASP:OD1	47:3S:64:ASP:N	2.49	0.45
54:S7:206:LEU:HB3	54:S7:210:ARG:HH21	1.80	0.45
55:s8:49:ASP:N	55:s8:49:ASP:OD1	2.50	0.45
7:5:539:MET:O	7:5:543:ASN:HB2	2.16	0.45
16:A5:52:THR:O	16:A5:56:LEU:HB2	2.17	0.45
34:B9:50:GLU:OE2	34:B9:59:ARG:NH2	2.49	0.45
2:s3:172:MET:HA	2:s3:196:PRO:HD2	1.99	0.45
11:a9:92:MET:HE2	54:s7:188:ASP:HA	1.99	0.45
37:an:122:SER:OG	54:s7:207:GLN:OE1	2.33	0.45
40:3L:58:ARG:O	40:3L:230:VAL:HA	2.17	0.45
51:V1:109:ARG:NH1	51:V1:237:GLY:O	2.50	0.45
53:S1:406:ASN:ND2	53:S1:688:GLN:O	2.48	0.45
51:v1:123:GLY:O	51:v1:277:ASN:ND2	2.49	0.45
53:s1:406:ASN:OD1	53:s1:406:ASN:N	2.49	0.45
2:S3:216:LYS:HE2	11:A9:209:ARG:HD3	1.98	0.45
3:S2:279:THR:HG23	16:A5:13:GLY:HA3	1.97	0.45
8:4:187:ASP:OD1	8:4:192:ASN:ND2	2.49	0.45
11:A9:48:ARG:NH2	11:A9:98:GLY:O	2.49	0.45
20:AO:10:MET:HE2	20:AO:10:MET:HB3	1.83	0.45
36:BL:34:THR:HA	36:BL:37:TYR:HB3	1.99	0.45
3:s2:204:PHE:HE2	54:s7:105:MET:HB3	1.81	0.45
5:6a:63:MET:HA	5:6a:66:VAL:HG12	1.98	0.45
7:5a:101:MET:HE3	7:5a:101:MET:HB3	1.77	0.45
12:s4:167:ASN:O	39:v3:99:ARG:NH1	2.49	0.45
43:3D:98:HIS:NE2	43:3D:208:GLU:OE2	2.45	0.45
46:3R:20:SER:O	46:3R:24:GLN:NE2	2.46	0.45
54:S7:103:GLU:HA	54:S7:106:HIS:HB2	1.98	0.45
53:s1:74:ASN:OD1	53:s1:180:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:361:MET:HB3	8:4:441:MET:HE3	1.98	0.45
8:4:431:THR:OG1	28:B5:66:ARG:NH1	2.48	0.45
10:AL:282:PRO:O	10:AL:286:GLN:NE2	2.50	0.45
13:S6:87:GLY:HA2	55:S8:112:ARG:HH12	1.82	0.45
29:B6:101:LYS:HE2	29:B6:101:LYS:HB2	1.79	0.45
37:AN:45:GLU:OE1	37:AN:51:LYS:NZ	2.49	0.45
3:s2:263:THR:O	3:s2:327:TYR:OH	2.34	0.45
4:1a:85:LEU:HB3	4:1a:233:LEU:HD11	1.99	0.45
9:2a:179:MET:HE1	9:2a:251:LEU:HD11	1.99	0.45
11:a9:136:THR:HG23	11:a9:139:PHE:H	1.81	0.45
40:3A:230:VAL:HG11	40:3A:417:LEU:HB3	1.99	0.45
53:S1:303:THR:HG22	53:S1:613:PRO:HG2	1.99	0.45
51:v1:134:ASP:OD1	51:v1:134:ASP:N	2.47	0.45
53:s1:643:ARG:NH1	53:s1:656:TYR:OH	2.50	0.45
54:s7:146:ARG:NH1	54:s7:184:ILE:O	2.49	0.45
3:S2:386:THR:OG1	3:S2:387:GLU:N	2.50	0.45
7:5:15:LEU:HD21	7:5:94:LEU:HD21	1.97	0.45
7:5:448:PRO:HA	7:5:451:MET:HB2	1.98	0.45
19:AM:118:MET:HB3	19:AM:118:MET:HE2	1.86	0.45
24:C2:1:MET:HA	28:B5:169:TYR:H	1.82	0.45
7:5a:328:HIS:O	7:5a:332:HIS:CB	2.64	0.45
8:4a:124:ALA:HA	9:2a:256:PRO:HD3	1.98	0.45
15:ab:83:VAL:HA	15:ab:86:VAL:HG12	1.98	0.45
20:ao:80:ASP:HA	20:ao:83:THR:HG22	1.97	0.45
32:b8:58:ARG:NH1	32:b8:60:GLU:OE1	2.49	0.45
40:3A:97:ALA:HB1	40:3A:150:ILE:HG23	1.99	0.45
41:3B:70:ARG:HD3	41:3B:117:GLU:HG3	1.99	0.45
43:3D:322:ARG:NH2	44:3E:79:SER:O	2.50	0.45
40:3L:410:CYS:HA	40:3L:413:ILE:HG22	1.98	0.45
41:3M:309:LEU:HD11	41:3M:338:ILE:HD12	1.99	0.45
53:s1:160:VAL:H	53:s1:174:THR:HG22	1.82	0.45
53:s1:308:ARG:NH1	53:s1:312:GLY:O	2.47	0.45
7:5:88:LEU:HD11	7:5:468:ILE:HD12	1.99	0.45
7:5:512:SER:OG	7:5:513:MET:N	2.50	0.45
8:4:36:LEU:HA	8:4:39:LEU:HD12	1.99	0.45
11:A9:150:ARG:O	11:A9:154:GLN:HB2	2.17	0.45
11:A9:206:ILE:H	58:A9:501:NDP:H42N	1.82	0.45
4:1a:239:THR:HG23	4:1a:262:GLU:HG2	1.98	0.45
7:5a:326:PHE:HA	7:5a:329:ILE:HD12	1.98	0.45
9:2a:17:PRO:HA	9:2a:20:THR:HG22	1.99	0.45
23:c1:40:ASN:OD1	23:c1:40:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b7:39:MET:HG3	35:b7:41:ALA:H	1.81	0.45
37:an:29:ARG:O	37:an:33:ARG:HB2	2.17	0.45
40:3A:71:VAL:HA	40:3A:232:ALA:O	2.16	0.45
43:3D:290:LEU:HD21	48:3J:43:ILE:HG23	1.99	0.45
52:V2:238:LYS:HE3	52:V2:242:PHE:HB3	1.98	0.45
55:s8:101:HIS:H	55:s8:149:MET:HE1	1.82	0.45
55:s8:125:ALA:HB1	55:s8:151:LYS:HB3	1.98	0.45
3:S2:265:ASN:O	3:S2:269:ARG:HB2	2.16	0.45
7:5:202:MET:HE2	7:5:265:PRO:HG2	1.98	0.45
34:B9:109:PRO:HA	34:B9:112:LYS:HB2	1.99	0.45
8:4a:63:THR:HA	8:4a:66:ILE:HB	1.99	0.45
15:ac:85:TYR:O	15:ac:89:LEU:HB2	2.17	0.45
40:3A:58:ARG:NH2	40:3A:417:LEU:O	2.50	0.45
41:3B:50:ALA:HB3	41:3B:221:VAL:HG12	1.99	0.45
42:3C:138:MET:HE2	42:3C:269:LYS:H	1.81	0.45
52:V2:200:ILE:HG23	52:V2:204:ILE:HD12	1.98	0.45
53:S1:387:LEU:N	53:S1:599:THR:O	2.46	0.45
54:s7:169:GLY:HA2	55:s8:151:LYS:HA	1.99	0.45
1:3:73:LEU:O	4:1:160:TYR:OH	2.30	0.44
4:1:102:ILE:HG23	4:1:150:LEU:HD13	1.99	0.44
5:6:56:PHE:O	5:6:60:LEU:HB2	2.17	0.44
7:5:6:THR:O	7:5:10:LEU:HB2	2.16	0.44
8:4:282:LEU:HB2	8:4:342:MET:HG3	1.98	0.44
8:4:378:GLU:O	8:4:382:THR:OG1	2.30	0.44
9:2:338:PRO:HA	18:A8:170:TRP:HZ2	1.82	0.44
34:B9:55:LYS:NZ	40:3A:53:LEU:O	2.49	0.44
7:5a:261:VAL:O	7:5a:264:HIS:ND1	2.49	0.44
8:4a:352:PHE:HB3	8:4a:355:MET:HB3	1.99	0.44
10:al:77:ILE:HG13	10:al:270:VAL:HG22	1.99	0.44
41:3M:155:ARG:HD3	41:3M:198:GLY:HA2	1.97	0.44
45:3Q:23:ASN:OD1	45:3Q:28:ASN:ND2	2.48	0.44
51:v1:369:ARG:NH2	52:v2:174:GLU:OE1	2.50	0.44
3:S2:52:MET:HE3	3:S2:52:MET:HB3	1.82	0.44
8:4:41:LEU:HD23	8:4:58:SER:HB2	1.98	0.44
9:2:87:GLN:HE21	9:2:87:GLN:HB2	1.60	0.44
38:A7:46:SER:O	38:A7:46:SER:OG	2.35	0.44
20:ao:128:ARG:NH2	25:s5:102:GLU:OE2	2.51	0.44
26:b1:45:GLN:O	36:bl:69:ARG:NH2	2.51	0.44
40:3A:121:ASN:HB3	40:3A:132:LEU:HB2	2.00	0.44
45:3F:27:PHE:HE2	45:3F:34:ARG:HA	1.83	0.44
53:S1:245:THR:HG22	53:S1:266:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S1:594:ALA:O	53:S1:605:GLN:HA	2.18	0.44
53:s1:566:ILE:O	53:s1:581:ASP:N	2.46	0.44
55:s8:170:GLY:HA2	55:s8:171:PRO:HD3	1.86	0.44
2:S3:58:SER:HA	2:S3:77:VAL:HG21	2.00	0.44
10:AL:190:ILE:HD12	10:AL:308:THR:HA	1.99	0.44
26:B1:35:THR:OG1	26:B1:38:ARG:NH1	2.50	0.44
7:5a:545:SER:HA	7:5a:549:SER:HB3	1.99	0.44
15:ab:84:LEU:O	15:ab:88:LYS:HB2	2.17	0.44
41:3B:197:MET:HE3	41:3B:197:MET:HB2	1.84	0.44
40:3L:302:VAL:HG21	40:3L:432:ARG:HB3	1.99	0.44
51:V1:184:LYS:HD2	51:V1:192:ASP:HB3	1.99	0.44
51:V1:285:PRO:HG3	52:V2:142:ARG:HH22	1.82	0.44
53:s1:66:HIS:NE2	53:s1:284:GLU:OE1	2.48	0.44
3:S2:145:MET:HA	3:S2:148:GLU:HB2	1.98	0.44
7:5:217:LEU:HD11	7:5:280:LEU:HD13	2.00	0.44
7:5:460:GLY:O	7:5:464:ALA:CB	2.65	0.44
8:4:208:PRO:HG2	8:4:291:VAL:HA	1.98	0.44
17:A6:53:MET:HB3	17:A6:55:LEU:HG	1.98	0.44
2:s3:184:ARG:NH1	3:s2:110:ASP:OD2	2.50	0.44
4:1a:30:TYR:HE2	21:a1:2:TRP:HA	1.82	0.44
7:5a:283:LEU:HB2	32:b8:144:PHE:HE2	1.83	0.44
8:4a:242:GLY:O	8:4a:246:ILE:HB	2.18	0.44
18:a8:47:ARG:NH2	28:b5:188:ASP:OD1	2.44	0.44
47:3H:86:LYS:HB2	47:3H:89:LYS:HD3	2.00	0.44
41:3M:101:ARG:O	41:3M:105:ALA:HB3	2.17	0.44
44:3P:87:ASP:OD1	44:3P:87:ASP:N	2.49	0.44
53:s1:140:GLN:NE2	64:s1:801:SF4:S3	2.91	0.44
1:3:69:ILE:HD12	4:1:147:ALA:HB3	2.00	0.44
4:1:6:ILE:O	4:1:10:LEU:HB2	2.16	0.44
11:a9:48:ARG:O	11:a9:102:GLN:NE2	2.49	0.44
11:a9:152:ILE:O	11:a9:156:SER:HB3	2.18	0.44
16:a5:44:TYR:O	16:a5:48:THR:OG1	2.33	0.44
40:3A:310:ILE:HD11	40:3A:388:VAL:HA	1.99	0.44
42:3N:144:THR:O	42:3N:148:ASN:HB2	2.18	0.44
52:v2:162:THR:HB	52:v2:169:THR:HG22	1.99	0.44
54:s7:137:LEU:HD11	54:s7:145:LEU:HD22	1.99	0.44
2:S3:215:VAL:HG11	2:S3:217:ARG:HH11	1.82	0.44
7:5:63:ILE:HB	7:5:80:PHE:HB2	2.00	0.44
8:4:175:ASN:HB3	8:4:178:ILE:HB	2.00	0.44
8:4:400:ILE:HA	8:4:403:THR:HG22	2.00	0.44
9:2:333:SER:OG	9:2:334:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A5:49:GLU:O	16:A5:53:ASN:ND2	2.46	0.44
29:B6:90:MET:HE3	29:B6:90:MET:HB2	1.79	0.44
17:a6:76:VAL:HG22	17:a6:78:ASP:H	1.83	0.44
18:a8:71:PHE:HA	18:a8:74:ILE:HG22	2.00	0.44
27:bm:127:ARG:HD3	27:bm:134:ILE:HA	2.00	0.44
32:b8:82:SER:HB3	32:b8:119:THR:H	1.83	0.44
37:an:98:THR:OG1	37:an:100:ASP:OD1	2.35	0.44
44:3E:92:ARG:HA	46:3G:24:GLN:HA	2.00	0.44
40:3L:165:ARG:NH2	40:3L:211:LEU:O	2.45	0.44
51:V1:205:ILE:HG12	51:V1:379:CYS:HB3	1.98	0.44
51:v1:132:ARG:HH21	52:v2:223:CYS:HB3	1.82	0.44
53:s1:142:GLN:O	53:s1:146:PHE:HB2	2.17	0.44
53:s1:344:GLY:N	53:s1:521:SER:OG	2.49	0.44
3:S2:146:CYS:H	3:S2:178:THR:HG21	1.83	0.44
8:4:116:ILE:HG21	18:A8:168:PHE:HB3	1.99	0.44
13:S6:54:GLU:O	37:AN:131:TYR:OH	2.35	0.44
9:2a:176:ARG:NH1	9:2a:225:MET:SD	2.91	0.44
16:a5:51:ILE:HG13	16:a5:55:LYS:HE2	2.00	0.44
36:bl:38:ASP:HA	36:bl:41:VAL:HG22	1.99	0.44
37:an:121:VAL:HG13	37:an:127:GLN:HA	2.00	0.44
42:3C:257:MET:SD	43:3D:204:ARG:NH1	2.91	0.44
48:3J:54:LYS:H	48:3J:54:LYS:HG3	1.64	0.44
53:S1:592:LYS:NZ	53:S1:619:ASP:OD2	2.51	0.44
51:v1:403:ASP:OD1	51:v1:403:ASP:N	2.41	0.44
1:3:80:GLN:O	25:S5:27:TYR:OH	2.35	0.44
3:S2:370:GLU:O	3:S2:374:SER:OG	2.34	0.44
7:5:64:THR:O	29:B6:96:THR:OG1	2.36	0.44
8:4:13:PRO:O	8:4:17:LEU:HB2	2.18	0.44
14:A2:65:LEU:HB3	14:A2:77:VAL:HB	2.00	0.44
29:B6:5:THR:HG23	29:B6:8:GLU:H	1.83	0.44
8:4a:318:ALA:HB2	8:4a:373:ILE:HG13	1.99	0.44
9:2a:26:LEU:HA	9:2a:29:MET:HG2	1.99	0.44
43:3D:262:THR:HG21	47:3H:27:PRO:HD2	1.99	0.44
40:3L:193:GLN:OE1	44:3P:92:ARG:NH2	2.49	0.44
53:S1:78:CYS:SG	53:S1:91:ALA:N	2.90	0.44
53:S1:402:LEU:HD22	53:S1:407:PRO:HG2	1.99	0.44
53:S1:425:ASN:OD1	53:S1:425:ASN:N	2.51	0.44
52:v2:107:PRO:HA	52:v2:108:PRO:HD3	1.86	0.44
53:s1:349:GLU:HG2	53:s1:646:LEU:HD11	1.99	0.44
8:4:336:ARG:HH22	8:4:429:SER:HA	1.83	0.44
8:4:360:LEU:HG	8:4:364:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:102:LEU:HD22	9:2:138:PRO:HB3	2.00	0.44
15:AB:122:MET:O	15:AB:126:PHE:HB2	2.17	0.44
4:1a:79:LEU:HD22	4:1a:222:LEU:HD22	1.99	0.44
14:a2:50:ASN:OD1	14:a2:50:ASN:N	2.46	0.44
20:ao:75:PHE:HZ	21:a1:47:LEU:HD13	1.83	0.44
39:v3:85:LEU:HD21	52:v2:60:LYS:HG2	2.00	0.44
41:3B:51:SER:OG	41:3B:225:VAL:O	2.35	0.44
42:3C:15:ASN:HA	42:3C:19:ILE:HB	2.00	0.44
43:3O:209:ASP:OD1	43:3O:209:ASP:N	2.49	0.44
53:S1:579:MET:HE2	53:S1:579:MET:HB3	1.95	0.44
51:v1:112:TYR:O	51:v1:240:THR:HA	2.18	0.44
7:5:186:MET:HE3	7:5:186:MET:HB2	1.73	0.43
15:AC:76:LEU:HD11	29:B6:20:ARG:HH21	1.83	0.43
25:S5:48:GLY:O	25:S5:52:ALA:CB	2.66	0.43
27:BM:85:MET:HE3	27:BM:85:MET:HB3	1.83	0.43
7:5a:89:PHE:HZ	7:5a:251:THR:HA	1.82	0.43
7:5a:128:MET:HG2	7:5a:251:THR:HB	1.99	0.43
7:5a:171:ALA:O	7:5a:175:ASN:HB2	2.18	0.43
10:al:74:ALA:HA	10:al:77:ILE:HG22	2.00	0.43
14:a2:43:GLU:HA	14:a2:46:LYS:HG2	1.99	0.43
20:ao:81:ARG:O	25:s5:105:ARG:NH2	2.50	0.43
26:b1:56:TRP:HH2	28:b5:134:GLU:HB2	1.82	0.43
28:b5:160:MET:HE1	28:b5:166:GLY:HA3	2.00	0.43
37:an:80:ASP:OD1	37:an:80:ASP:N	2.41	0.43
42:3C:118:LEU:HD22	42:3C:192:LEU:HD21	2.00	0.43
45:3F:44:VAL:O	45:3F:48:ILE:HB	2.18	0.43
51:V1:149:MET:SD	51:V1:241:THR:OG1	2.69	0.43
7:5:542:LEU:HA	7:5:545:SER:HB2	2.00	0.43
10:AL:139:ARG:NH2	57:AL:502:DGT:N7	2.66	0.43
13:S6:90:LYS:HE2	13:S6:90:LYS:HB3	1.87	0.43
19:AM:14:ASP:OD1	19:AM:14:ASP:N	2.50	0.43
32:B8:82:SER:OG	32:B8:83:GLN:N	2.51	0.43
1:3a:71:LEU:HB3	5:6a:152:MET:HE1	2.00	0.43
14:a2:23:LEU:HD11	14:a2:34:ARG:HG3	2.01	0.43
16:a5:45:ARG:O	16:a5:49:GLU:HB2	2.18	0.43
22:a3:18:VAL:HG13	55:s8:61:LEU:HD21	2.00	0.43
33:b4:128:SER:OG	33:b4:129:TYR:N	2.51	0.43
53:S1:538:ARG:NH1	53:S1:559:ASP:OD2	2.51	0.43
51:v1:225:LEU:HD22	53:s1:93:ALA:HB3	2.00	0.43
7:5:211:ILE:HG23	7:5:212:PRO:HD3	2.00	0.43
20:AO:109:SER:OG	20:AO:111:PHE:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5a:176:ARG:NH2	8:4a:367:LEU:O	2.51	0.43
8:4a:337:ILE:HD13	8:4a:345:ALA:HB2	2.00	0.43
8:4a:452:LYS:H	8:4a:452:LYS:HG2	1.62	0.43
35:b7:33:GLU:O	35:b7:35:LYS:NZ	2.48	0.43
51:V1:325:PRO:HD3	51:V1:433:TRP:HB3	1.98	0.43
52:V2:184:MET:HE2	52:V2:184:MET:HB2	1.88	0.43
53:s1:78:CYS:SG	53:s1:91:ALA:N	2.91	0.43
54:s7:161:MET:HG2	54:s7:196:PRO:HG2	2.00	0.43
55:s8:101:HIS:CD2	64:s8:301:SF4:S1	3.11	0.43
3:S2:417:SER:O	3:S2:417:SER:OG	2.36	0.43
5:6:19:LEU:HD22	5:6:32:LEU:HD13	2.00	0.43
6:4L:51:SER:HA	25:S5:32:ARG:HH21	1.82	0.43
7:5:556:ILE:HD12	33:B4:76:ILE:HG22	2.00	0.43
8:4:179:LEU:HD22	8:4:249:ILE:HD12	1.99	0.43
11:A9:61:ALA:HA	11:A9:66:GLY:HA3	2.00	0.43
12:S4:91:VAL:HG12	12:S4:95:LYS:HG3	2.01	0.43
28:B5:102:PRO:HG2	28:B5:105:TYR:HB3	1.99	0.43
4:1a:158:GLY:HA3	4:1a:315:PRO:HB2	2.01	0.43
20:ao:69:ILE:HD12	20:ao:69:ILE:HA	1.86	0.43
30:b2:72:ARG:HD3	30:b2:72:ARG:HA	1.85	0.43
32:b8:34:LYS:NZ	33:b4:70:TYR:OH	2.50	0.43
34:b9:101:GLU:OE2	34:b9:122:ARG:NE	2.52	0.43
34:b9:168:TRP:O	34:b9:172:THR:HB	2.19	0.43
40:3A:86:ASN:HA	40:3A:211:LEU:HD21	1.99	0.43
41:3B:77:LEU:HD11	41:3B:189:PRO:HD2	1.99	0.43
41:3B:254:ARG:HH12	41:3M:259:ARG:HD3	1.84	0.43
42:3C:207:ASN:OD1	42:3C:210:GLY:N	2.47	0.43
41:3M:257:GLU:HG3	41:3M:438:MET:HB3	2.01	0.43
42:3N:314:SER:OG	42:3N:315:LEU:N	2.51	0.43
7:5:83:ASP:N	7:5:83:ASP:OD1	2.51	0.43
33:B4:123:ARG:HD2	36:BL:144:LEU:HD21	1.99	0.43
2:s3:203:LEU:HD12	3:s2:122:LYS:HG3	2.00	0.43
4:1a:289:LEU:HD23	4:1a:289:LEU:HA	1.88	0.43
7:5a:426:ILE:O	7:5a:430:VAL:HB	2.18	0.43
11:a9:359:TYR:HA	11:a9:362:LEU:HB2	1.98	0.43
13:s6:45:ARG:O	13:s6:48:PHE:HB2	2.19	0.43
18:a8:151:ASN:OD1	18:a8:151:ASN:N	2.51	0.43
34:b9:66:GLU:HA	34:b9:69:GLU:HG2	2.00	0.43
40:3A:70:THR:HA	40:3A:133:ILE:O	2.19	0.43
42:3N:50:PHE:HA	42:3N:53:MET:HE2	2.00	0.43
50:3T:16:SER:O	50:3T:16:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s1:395:GLU:OE2	53:s1:420:LYS:NZ	2.43	0.43
53:s1:403:VAL:HA	53:s1:432:ILE:HB	1.99	0.43
2:S3:147:ASP:OD1	2:S3:147:ASP:N	2.51	0.43
7:5:79:SER:N	7:5:139:GLN:OE1	2.48	0.43
7:5:286:LEU:HD22	7:5:411:ILE:HD11	1.99	0.43
7:5:328:HIS:O	7:5:332:HIS:CB	2.66	0.43
7:5:466:PHE:O	7:5:470:TYR:HB2	2.18	0.43
7:5:594:ASN:HA	7:5:597:LEU:HB2	1.99	0.43
12:S4:115:ALA:HB2	53:S1:267:THR:HB	2.00	0.43
18:A8:111:VAL:O	18:A8:116:GLY:N	2.49	0.43
32:B8:38:PRO:HD2	33:B4:70:TYR:HD2	1.84	0.43
35:B7:12:ASP:OD1	35:B7:12:ASP:N	2.44	0.43
3:s2:169:TRP:HA	3:s2:172:VAL:HG12	1.99	0.43
3:s2:460:GLU:HG2	3:s2:461:ILE:HG13	2.00	0.43
7:5a:108:MET:HB2	7:5a:114:ILE:HD13	2.00	0.43
8:4a:72:LEU:O	8:4a:76:MET:N	2.51	0.43
9:2a:108:LEU:HD11	9:2a:191:LEU:HD22	2.00	0.43
10:a1:250:SER:O	10:a1:280:LYS:NZ	2.51	0.43
20:ao:65:LEU:HD23	22:a3:50:PRO:HD2	2.00	0.43
27:bm:112:MET:HB3	27:bm:112:MET:HE3	1.71	0.43
40:3A:214:THR:HA	40:3A:217:THR:HG22	2.01	0.43
40:3A:337:LEU:O	40:3A:364:SER:OG	2.37	0.43
43:3D:177:LYS:HE2	43:3D:177:LYS:HB2	1.79	0.43
46:3G:53:PHE:HA	46:3G:56:VAL:HG12	1.99	0.43
49:3K:23:MET:HE3	49:3K:23:MET:HB2	1.83	0.43
51:V1:83:SER:HA	51:V1:263:ALA:HB2	2.01	0.43
51:V1:111:LYS:HB2	51:V1:151:ALA:HA	2.00	0.43
51:v1:270:ASN:ND2	51:v1:340:ASP:OD1	2.51	0.43
51:v1:383:THR:HG21	53:s1:120:LEU:HG	2.00	0.43
53:s1:388:ASN:ND2	53:s1:513:MET:O	2.47	0.43
54:s7:107:MET:HE3	54:s7:114:MET:HG2	2.00	0.43
2:S3:210:ARG:HD2	11:A9:48:ARG:HH11	1.84	0.43
3:S2:223:HIS:HE1	54:S7:99:CYS:SG	2.40	0.43
3:S2:367:LYS:HE2	3:S2:367:LYS:HB2	1.85	0.43
4:1:169:GLN:NE2	4:1:240:ILE:O	2.52	0.43
8:4:307:TRP:NE1	8:4:383:MET:SD	2.92	0.43
9:2:102:LEU:O	9:2:106:LEU:HB2	2.17	0.43
15:AC:132:ASP:HA	15:AC:135:ALA:HB3	2.00	0.43
18:A8:126:SER:O	18:A8:126:SER:OG	2.36	0.43
11:a9:126:VAL:HG12	11:a9:161:VAL:HG21	2.01	0.43
19:am:130:LEU:HD23	19:am:130:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b6:106:PRO:HB3	29:b6:119:PRO:HA	2.01	0.43
40:3A:406:THR:OG1	41:3B:387:GLU:OE2	2.36	0.43
40:3L:170:ARG:HH21	50:3T:51:CYS:HA	1.83	0.43
51:V1:412:LEU:HA	51:V1:415:ILE:HG12	2.00	0.43
52:V2:236:PRO:HA	52:V2:237:PRO:HD3	1.87	0.43
55:S8:149:MET:SD	55:S8:154:TYR:OH	2.71	0.43
51:v1:340:ASP:OD1	51:v1:340:ASP:N	2.51	0.43
54:s7:146:ARG:HA	54:s7:146:ARG:HD2	1.81	0.43
1:3:73:LEU:HD23	4:1:151:LEU:HD13	2.01	0.43
2:S3:214:GLU:HA	11:A9:68:TYR:HE1	1.84	0.43
3:S2:216:ARG:HH11	38:A7:34:ARG:HH21	1.67	0.43
9:2:2:ASN:HD21	9:2:5:THR:HG23	1.84	0.43
9:2:193:ILE:HB	9:2:266:ILE:HG12	2.01	0.43
12:S4:112:MET:O	55:S8:144:ARG:NH1	2.51	0.43
14:A2:38:VAL:O	53:S1:667:GLN:NE2	2.51	0.43
19:AM:113:MET:HE2	19:AM:113:MET:HB2	1.81	0.43
32:B8:170:ARG:HD3	32:B8:170:ARG:HA	1.78	0.43
7:5a:147:VAL:HB	7:5a:252:MET:HG2	2.00	0.43
7:5a:347:ILE:HG23	7:5a:352:ASP:HA	2.00	0.43
9:2a:292:PHE:HB3	9:2a:295:ARG:HH21	1.84	0.43
17:a6:21:LYS:HA	17:a6:21:LYS:HD2	1.86	0.43
20:ao:79:LYS:HB3	20:ao:79:LYS:HE3	1.85	0.43
24:c2:12:LYS:HB3	24:c2:15:PRO:HG3	2.00	0.43
37:an:113:ILE:HG12	55:s8:198:GLU:HB3	2.01	0.43
43:3D:105:LEU:HB3	43:3D:110:ILE:HD11	1.99	0.43
45:3F:68:ASP:HA	45:3F:71:MET:HE2	2.01	0.43
40:3L:133:ILE:HD13	40:3L:143:VAL:HG13	2.01	0.43
41:3M:92:LYS:HE2	41:3M:143:ALA:HB1	2.01	0.43
55:S8:59:ARG:HA	55:S8:64:THR:HG22	2.01	0.43
55:S8:114:ILE:O	55:S8:140:ARG:NH1	2.52	0.43
1:3:27:MET:HE1	4:1:62:ARG:HE	1.84	0.43
7:5:476:SER:OG	7:5:477:ILE:N	2.51	0.43
10:AL:65:ASN:HD21	10:AL:238:GLU:HB2	1.84	0.43
10:AL:168:VAL:HA	10:AL:171:GLU:HG2	2.01	0.43
11:A9:283:MET:HG2	11:A9:357:ARG:HH12	1.84	0.43
2:s3:51:ASP:OD1	2:s3:51:ASP:N	2.51	0.43
2:s3:227:GLN:HG2	55:s8:151:LYS:HZ1	1.84	0.43
5:6a:123:TRP:HZ3	20:ao:120:LEU:HD12	1.84	0.43
7:5a:313:MET:HG3	7:5a:328:HIS:HD2	1.82	0.43
13:s6:25:SER:HG	13:s6:29:GLU:H	1.65	0.43
26:b1:53:GLU:HG2	26:b1:54:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b5:81:PRO:HA	28:b5:84:ILE:HG22	2.00	0.43
41:3B:259:ARG:NH1	41:3B:447:THR:O	2.52	0.43
41:3M:240:MET:H	41:3M:240:MET:HG2	1.57	0.43
43:3O:170:LYS:HD3	43:3O:170:LYS:HA	1.78	0.43
46:3R:51:PRO:HA	46:3R:54:VAL:HG22	1.99	0.43
51:V1:270:ASN:ND2	51:V1:340:ASP:OD1	2.52	0.43
53:S1:288:ASP:HA	53:S1:291:ARG:HG2	2.00	0.43
54:S7:113:ASP:OD2	54:S7:116:ARG:N	2.49	0.43
55:S8:200:GLU:OE2	55:S8:204:ASN:ND2	2.47	0.43
3:S2:251:PHE:HD2	3:S2:341:LEU:HD21	1.84	0.43
7:5:60:GLU:H	29:B6:100:SER:HB3	1.84	0.43
7:5:487:LYS:HE2	7:5:487:LYS:HB2	1.83	0.43
17:A6:118:PRO:O	17:A6:124:LYS:NZ	2.48	0.43
31:B3:24:ASP:OD1	31:B3:24:ASP:N	2.48	0.43
7:5a:291:CYS:HB2	7:5a:304:PHE:HE2	1.83	0.43
10:a1:231:SER:O	10:a1:235:GLN:HB2	2.19	0.43
17:a6:55:LEU:HD23	17:a6:55:LEU:HA	1.90	0.43
18:a8:127:LYS:HD2	22:a3:76:PRO:HD2	2.00	0.43
40:3A:58:ARG:HB2	40:3A:230:VAL:HG12	2.00	0.43
40:3A:120:LEU:HD13	41:3B:299:ILE:HG23	2.01	0.43
40:3L:70:THR:OG1	40:3L:410:CYS:SG	2.72	0.43
41:3M:286:PHE:HB3	41:3M:327:ASN:HD21	1.84	0.43
42:3N:37:LEU:HD13	61:3N:402:HEM:HBB2	2.01	0.43
42:3N:216:ASP:HB2	45:3Q:64:LYS:HG3	1.99	0.43
53:S1:357:LEU:HD23	53:S1:627:SER:HB2	2.01	0.43
51:v1:69:LEU:O	51:v1:147:ARG:NH1	2.52	0.43
51:v1:266:GLY:HA3	51:v1:271:SER:HA	2.00	0.43
51:v1:342:LEU:HD12	51:v1:349:LEU:HB2	2.01	0.43
52:v2:203:ILE:HD11	52:v2:218:ARG:HD2	2.01	0.43
54:s7:202:LEU:HD23	54:s7:202:LEU:HA	1.91	0.43
1:3:64:LEU:HD12	5:6:163:ILE:HD13	2.01	0.42
7:5:64:THR:HA	7:5:78:MET:O	2.19	0.42
7:5:205:ASN:ND2	36:BL:121:TYR:OH	2.51	0.42
9:2:187:MET:HE2	9:2:187:MET:HB3	1.84	0.42
10:AL:232:ALA:O	10:AL:236:ASP:HB2	2.19	0.42
37:AN:137:LYS:HE2	37:AN:137:LYS:HB2	1.94	0.42
3:s2:98:VAL:HG21	17:a6:100:TRP:HE1	1.84	0.42
7:5a:363:THR:HG21	31:b3:67:ILE:HG21	2.01	0.42
9:2a:271:MET:HE1	9:2a:276:LEU:HA	2.01	0.42
12:s4:104:ARG:NH2	17:a6:130:ASP:OD1	2.49	0.42
42:3C:328:LEU:HB2	42:3C:361:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3L:70:THR:HG21	40:3L:407:THR:HG22	2.00	0.42
46:3R:46:ILE:O	46:3R:50:ALA:HB3	2.18	0.42
53:s1:304:GLU:HG2	53:s1:615:LEU:HD12	2.01	0.42
53:s1:478:SER:O	53:s1:518:ARG:NH1	2.52	0.42
55:s8:131:GLU:O	55:s8:144:ARG:HB3	2.18	0.42
5:6:80:GLU:OE1	11:A9:360:ARG:NH1	2.52	0.42
7:5:535:ARG:HB3	33:B4:11:LEU:HD22	2.02	0.42
12:S4:146:ASP:OD2	53:S1:605:GLN:NE2	2.52	0.42
37:AN:139:HIS:HB2	53:S1:299:ARG:HA	2.01	0.42
38:A7:19:ASP:OD1	38:A7:19:ASP:N	2.51	0.42
2:s3:110:LEU:HA	2:s3:131:LEU:HG	2.01	0.42
4:1a:316:PRO:HG3	20:ao:57:ARG:HB3	2.00	0.42
7:5a:421:MET:HA	7:5a:501:ALA:HB2	2.01	0.42
8:4a:54:ASN:N	8:4a:54:ASN:OD1	2.51	0.42
9:2a:95:LEU:HD13	9:2a:148:LEU:HB3	2.01	0.42
18:a8:108:ASP:HA	18:a8:111:VAL:HG12	2.00	0.42
28:b5:58:LYS:HB2	34:b9:107:TRP:HZ2	1.84	0.42
35:b7:96:VAL:HA	35:b7:99:MET:HE3	1.99	0.42
41:3B:180:VAL:HA	41:3B:254:ARG:HE	1.83	0.42
46:3G:18:SER:OG	46:3G:19:LEU:N	2.52	0.42
53:S1:388:ASN:H	53:S1:514:ASN:HB3	1.84	0.42
55:S8:194:GLY:O	55:S8:198:GLU:HB2	2.19	0.42
54:s7:97:LEU:O	54:s7:136:THR:OG1	2.31	0.42
3:S2:117:HIS:NE2	54:S7:175:TYR:OH	2.43	0.42
3:S2:457:VAL:HG23	3:S2:460:GLU:HG2	2.00	0.42
4:1:204:GLU:OE2	54:S7:122:ARG:NH1	2.43	0.42
15:AC:125:GLU:OE2	30:B2:44:TYR:OH	2.37	0.42
38:A7:49:LEU:HD13	53:S1:152:ARG:HB2	2.00	0.42
25:s5:48:GLY:O	25:s5:52:ALA:CB	2.67	0.42
32:b8:160:GLN:OE1	35:b7:37:ARG:NH2	2.51	0.42
37:an:95:HIS:HB3	55:s8:93:LEU:HB2	2.01	0.42
40:3A:274:GLU:HB3	46:3G:18:SER:HB3	2.01	0.42
51:V1:382:CYS:HB3	51:V1:384:PRO:HD2	2.01	0.42
52:V2:145:ASP:OD1	52:V2:145:ASP:N	2.52	0.42
53:S1:323:LEU:HB3	53:S1:629:ILE:HG21	2.00	0.42
51:v1:157:TYR:HB2	51:v1:216:ILE:HD11	2.01	0.42
5:6:13:LEU:HD23	5:6:99:GLU:HG3	2.01	0.42
5:6:44:LEU:HD11	5:6:53:LEU:HG	2.00	0.42
8:4:304:GLN:O	36:BL:148:ALA:N	2.52	0.42
8:4:336:ARG:HA	8:4:336:ARG:HD3	1.89	0.42
8:4:343:ILE:O	8:4:346:ARG:NH1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A9:324:ILE:HD12	11:A9:324:ILE:HA	1.97	0.42
58:A9:501:NDP:O2N	58:A9:501:NDP:O7N	2.37	0.42
13:S6:107:CYS:SG	13:S6:108:GLY:N	2.92	0.42
32:B8:161:TYR:HA	32:B8:162:PRO:HD3	1.90	0.42
3:s2:84:PHE:O	4:1a:127:TYR:OH	2.38	0.42
7:5a:586:LEU:HD21	19:am:45:PRO:HG3	2.02	0.42
8:4a:51:ASN:O	28:b5:135:LYS:NZ	2.52	0.42
8:4a:118:PHE:O	8:4a:122:PHE:CB	2.67	0.42
10:al:39:GLY:H	10:al:42:ALA:HB3	1.83	0.42
11:a9:220:TYR:HB3	11:a9:226:VAL:HG12	2.01	0.42
12:s4:102:ASP:N	12:s4:102:ASP:OD1	2.49	0.42
13:s6:77:ILE:HD12	13:s6:77:ILE:HA	1.91	0.42
15:ab:88:LYS:HB2	15:ab:88:LYS:HE2	1.90	0.42
28:b5:72:LYS:O	28:b5:76:MET:HB2	2.19	0.42
29:b6:118:PRO:HA	29:b6:119:PRO:HD3	1.85	0.42
34:b9:114:MET:HE2	34:b9:114:MET:HB3	1.90	0.42
41:3B:51:SER:HB2	41:3B:230:LEU:HD23	2.02	0.42
42:3C:8:HIS:HB3	42:3C:11:PHE:HB2	2.01	0.42
42:3C:8:HIS:O	42:3C:12:LYS:N	2.53	0.42
40:3L:187:LEU:HA	40:3L:190:THR:HG22	2.02	0.42
42:3N:117:VAL:HG21	42:3N:302:ALA:HB2	2.01	0.42
45:3Q:36:ASP:OD1	45:3Q:90:TYR:OH	2.37	0.42
51:V1:117:ALA:HB3	51:V1:157:TYR:O	2.19	0.42
53:S1:341:ILE:HD11	53:S1:537:ILE:HG13	2.01	0.42
51:v1:184:LYS:HD2	51:v1:192:ASP:HB3	2.00	0.42
53:s1:387:LEU:HA	53:s1:514:ASN:HB2	2.01	0.42
5:6:140:GLY:HA2	25:S5:26:PRO:HG3	2.01	0.42
7:5:71:MET:HG2	8:4:380:PHE:HE2	1.84	0.42
7:5:221:THR:HG22	7:5:226:GLN:HB2	2.01	0.42
7:5:554:ASP:OD1	8:4:213:HIS:NE2	2.49	0.42
8:4:307:TRP:HA	8:4:310:MET:HE2	2.00	0.42
9:2:170:LEU:HD11	9:2:288:LEU:HD13	2.00	0.42
11:A9:127:ILE:HG23	11:A9:165:ILE:HB	2.00	0.42
20:AO:25:LEU:HD12	20:AO:25:LEU:HA	1.94	0.42
21:A1:23:THR:HA	21:A1:26:ILE:HG22	2.02	0.42
25:S5:7:GLN:NE2	25:S5:15:ASP:OD1	2.52	0.42
25:S5:53:LYS:HE3	25:S5:53:LYS:HB2	1.82	0.42
4:1a:170:GLU:HG2	4:1a:247:TYR:H	1.85	0.42
7:5a:346:ILE:O	7:5a:350:LEU:HB2	2.18	0.42
11:a9:201:ILE:HD13	11:a9:263:PHE:HB2	2.01	0.42
11:a9:206:ILE:HG12	58:a9:501:NDP:H42N	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s6:87:GLY:HA2	55:s8:112:ARG:HH12	1.84	0.42
15:ab:90:TYR:OH	15:ab:117:GLU:OE1	2.38	0.42
18:a8:82:PHE:HD2	21:a1:66:LEU:HD11	1.84	0.42
24:c2:43:LEU:HD22	24:c2:53:VAL:HG12	2.00	0.42
40:3A:85:LYS:HG2	40:3A:210:ARG:HH22	1.84	0.42
43:3O:96:TRP:HB2	43:3O:99:ARG:HB2	2.01	0.42
47:3S:48:LEU:HD21	47:3S:69:LEU:HD12	2.02	0.42
53:S1:134:GLY:HA3	53:S1:241:ARG:HD2	2.00	0.42
53:S1:260:ASN:OD1	53:S1:276:ARG:NH2	2.53	0.42
51:v1:369:ARG:NE	52:v2:135:THR:O	2.53	0.42
53:s1:637:ASP:OD1	53:s1:637:ASP:N	2.52	0.42
1:3:18:ILE:HD12	4:1:76:THR:HB	2.01	0.42
1:3:63:LEU:HD22	6:4L:72:ALA:HB2	2.02	0.42
32:B8:73:GLY:HA3	33:B4:79:ASN:HD22	1.83	0.42
8:4a:152:TYR:HD2	8:4a:215:TRP:HB3	1.84	0.42
17:a6:120:ASP:OD1	17:a6:120:ASP:N	2.53	0.42
25:s5:65:GLU:O	25:s5:69:ARG:HA	2.20	0.42
25:s5:102:GLU:H	25:s5:102:GLU:HG3	1.58	0.42
43:3D:96:TRP:H	43:3D:99:ARG:HB2	1.84	0.42
41:3M:54:ASN:HB2	41:3M:56:ALA:HB2	2.01	0.42
51:V1:86:ARG:NH1	51:V1:270:ASN:OD1	2.46	0.42
51:v1:37:ASP:OD1	51:v1:37:ASP:N	2.48	0.42
53:s1:627:SER:OG	53:s1:632:ILE:O	2.35	0.42
2:S3:64:VAL:HA	2:S3:67:ILE:HG22	2.01	0.42
2:S3:208:GLU:HB3	2:S3:223:VAL:HG23	2.01	0.42
3:S2:223:HIS:HD2	54:S7:194:CYS:HB3	1.85	0.42
4:1:34:ARG:HE	4:1:34:ARG:HB2	1.73	0.42
4:1:181:MET:HE3	4:1:181:MET:HB3	1.82	0.42
7:5:372:CYS:HA	7:5:375:ILE:HG22	2.02	0.42
8:4:424:ILE:HG13	33:B4:56:ARG:HH21	1.83	0.42
9:2:140:SER:HB2	25:S5:3:PHE:HD2	1.85	0.42
14:A2:30:SER:HB3	14:A2:63:PRO:HG3	2.01	0.42
18:A8:20:VAL:HG12	18:A8:25:LEU:HG	2.02	0.42
32:B8:121:PRO:HG3	33:B4:15:PRO:HB3	2.00	0.42
33:B4:123:ARG:HB3	33:B4:126:ASN:HB3	2.01	0.42
1:3a:65:PHE:HB3	4:1a:144:VAL:HG11	2.01	0.42
3:s2:117:HIS:NE2	54:s7:175:TYR:OH	2.41	0.42
3:s2:323:ARG:N	3:s2:328:ASP:OD2	2.53	0.42
3:s2:354:GLY:O	20:ao:8:GLN:NE2	2.44	0.42
5:6a:125:MET:N	5:6a:125:MET:SD	2.93	0.42
13:s6:54:GLU:O	37:an:131:TYR:OH	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b9:29:SER:HB2	34:b9:80:TYR:H	1.84	0.42
40:3L:285:ALA:O	40:3L:359:VAL:HA	2.18	0.42
41:3M:51:SER:HB3	41:3M:230:LEU:HD12	2.00	0.42
53:S1:406:ASN:HD21	53:S1:436:VAL:HG21	1.84	0.42
53:s1:569:GLN:HG2	53:s1:584:LEU:HB2	2.01	0.42
1:3:64:LEU:HA	1:3:67:LEU:HG	2.01	0.42
7:5:226:GLN:O	7:5:230:HIS:N	2.53	0.42
9:2:313:MET:HA	9:2:316:HIS:HB2	2.02	0.42
12:S4:86:ASN:HD21	53:S1:284:GLU:HB3	1.85	0.42
18:A8:151:ASN:ND2	28:B5:170:GLN:OE1	2.53	0.42
36:BL:117:GLU:HB3	36:BL:121:TYR:HA	2.02	0.42
5:6a:66:VAL:HG23	6:4l:75:LEU:HD21	2.02	0.42
7:5a:257:ILE:H	7:5a:257:ILE:HG12	1.69	0.42
7:5a:475:THR:HA	35:b7:55:GLN:HE22	1.84	0.42
9:2a:240:MET:HE3	9:2a:240:MET:HB3	1.89	0.42
20:ao:85:GLN:OE1	25:s5:105:ARG:NH2	2.52	0.42
30:b2:69:ILE:O	30:b2:73:PHE:HB2	2.20	0.42
41:3M:114:ALA:HB3	50:3T:66:ALA:HB3	2.01	0.42
41:3M:358:VAL:HA	41:3M:361:VAL:HG12	2.02	0.42
43:3O:98:HIS:NE2	43:3O:208:GLU:OE2	2.46	0.42
43:3O:115:GLN:OE1	43:3O:140:TYR:OH	2.37	0.42
43:3O:295:MET:HE1	48:3U:33:PHE:HE2	1.85	0.42
55:S8:117:LYS:HA	55:S8:130:ILE:HD11	2.02	0.42
53:s1:358:LEU:HA	53:s1:361:VAL:HG12	2.02	0.42
54:s7:189:ILE:HG21	54:s7:208:LEU:HB2	2.02	0.42
3:S2:379:ILE:HG21	53:S1:143:SER:HB3	2.02	0.42
4:1:215:TYR:HD2	4:1:219:PRO:HB2	1.85	0.42
8:4:50:LYS:HB2	8:4:58:SER:HB3	2.02	0.42
9:2:335:MET:HB2	24:C2:37:LEU:HD21	2.02	0.42
31:B3:24:ASP:OD1	31:B3:27:GLN:NE2	2.46	0.42
1:3a:79:ILE:HD12	1:3a:79:ILE:HA	1.94	0.42
3:s2:375:MET:HE3	53:s1:124:HIS:HB3	2.02	0.42
4:1a:61:MET:HG3	54:s7:126:ARG:HE	1.84	0.42
6:4l:63:ILE:HG12	9:2a:71:LEU:HD21	2.02	0.42
6:4l:77:LEU:HD21	9:2a:57:THR:HA	2.02	0.42
7:5a:361:ASN:HB2	7:5a:435:PRO:HB3	2.01	0.42
8:4a:359:TRP:CD1	8:4a:415:GLN:HE22	2.37	0.42
9:2a:27:MET:HE2	9:2a:27:MET:HB2	1.90	0.42
16:a5:66:LYS:HD3	16:a5:66:LYS:HA	1.83	0.42
27:bm:119:GLU:OE2	27:bm:122:ARG:NH2	2.53	0.42
28:b5:95:GLU:HA	28:b5:116:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b6:120:MET:H	29:b6:120:MET:HG2	1.66	0.42
40:3A:305:GLN:HB3	40:3A:395:LEU:HD11	2.01	0.42
40:3L:274:GLU:HG2	46:3R:18:SER:HB2	2.00	0.42
51:V1:282:VAL:HA	51:V1:307:VAL:HA	2.02	0.42
51:v1:357:MET:HB3	51:v1:361:THR:HG21	2.02	0.42
1:3:34:ALA:HB1	4:1:63:PRO:HA	2.02	0.42
1:3:81:THR:O	22:A3:46:ASN:ND2	2.53	0.42
4:1:75:PRO:HB2	4:1:222:LEU:HD23	2.02	0.42
7:5:149:ILE:HD13	7:5:149:ILE:HA	1.88	0.42
7:5:600:ILE:HD13	7:5:600:ILE:HA	1.96	0.42
30:B2:53:SER:O	30:B2:57:GLN:CB	2.68	0.42
3:s2:65:PRO:HD2	9:2a:51:ARG:HH12	1.84	0.42
4:1a:196:ALA:HA	4:1a:199:ASP:HB3	2.01	0.42
4:1a:302:MET:HE2	4:1a:302:MET:HB2	1.93	0.42
10:al:150:LEU:HD13	10:al:156:GLY:HA2	2.01	0.42
12:s4:150:LYS:HE2	12:s4:152:VAL:HG12	2.01	0.42
17:a6:84:LEU:HA	17:a6:87:ILE:HG22	2.02	0.42
20:ao:88:ARG:HA	20:ao:88:ARG:HD2	1.85	0.42
21:a1:3:PHE:HE2	37:an:13:ARG:HH21	1.68	0.42
32:b8:166:LEU:HB2	32:b8:170:ARG:HH21	1.85	0.42
41:3B:272:VAL:HG12	41:3B:337:GLY:HA3	2.02	0.42
53:S1:221:ASN:HD21	53:S1:286:ILE:H	1.67	0.42
53:S1:525:ALA:HB1	53:S1:530:TYR:HB2	2.02	0.42
54:S7:146:ARG:HA	54:S7:146:ARG:HD2	1.82	0.42
55:S8:149:MET:HB2	55:S8:183:LEU:HB3	2.02	0.42
53:s1:170:LYS:O	53:s1:231:LEU:HA	2.20	0.42
53:s1:266:ARG:HH12	55:s8:117:LYS:HE2	1.84	0.42
7:5:159:TYR:HB3	8:4:416:ARG:HG2	2.01	0.41
8:4:281:ASP:OD1	8:4:281:ASP:N	2.52	0.41
11:A9:157:LYS:HA	11:A9:157:LYS:HD2	1.86	0.41
12:S4:126:LEU:HD12	12:S4:126:LEU:HA	1.88	0.41
29:B6:26:GLN:OE1	34:B9:175:ARG:NH1	2.53	0.41
3:s2:392:PRO:HA	3:s2:393:PRO:HD3	1.89	0.41
3:s2:435:LEU:O	3:s2:439:SER:OG	2.37	0.41
4:1a:87:VAL:HG23	4:1a:88:PRO:HD3	2.02	0.41
7:5a:378:LEU:HA	7:5a:381:THR:HG22	2.01	0.41
8:4a:190:TRP:HA	8:4a:193:ASN:HB2	2.02	0.41
9:2a:29:MET:HE3	9:2a:141:ILE:HA	2.02	0.41
14:a2:54:LEU:HD21	53:s1:529:GLY:HA3	2.01	0.41
34:b9:95:GLU:HA	34:b9:98:LYS:HG3	2.01	0.41
42:3C:78:LEU:O	42:3C:82:MET:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3F:10:SER:OG	45:3F:11:SER:N	2.53	0.41
41:3M:49:ILE:HD12	41:3M:220:LEU:HB3	2.02	0.41
42:3N:345:HIS:HA	42:3N:346:PRO:HA	1.94	0.41
52:V2:194:ASP:OD2	52:V2:221:ARG:NH1	2.52	0.41
51:v1:316:ALA:HB3	51:v1:357:MET:HB2	2.01	0.41
4:1:20:LEU:HA	4:1:23:VAL:HG22	2.03	0.41
7:5:312:LEU:HD21	7:5:395:ILE:HG21	2.01	0.41
16:A5:33:ASP:HA	16:A5:36:LYS:HG2	2.01	0.41
2:s3:47:ARG:HA	3:s2:162:GLN:HB2	2.01	0.41
3:s2:390:GLN:O	38:a7:60:ARG:NH2	2.47	0.41
9:2a:328:THR:O	9:2a:332:MET:HB2	2.20	0.41
13:s6:78:ALA:HB1	13:s6:90:LYS:HG2	2.01	0.41
16:a5:68:LEU:O	16:a5:72:LEU:HB2	2.20	0.41
24:c2:99:GLU:H	24:c2:99:GLU:HG3	1.62	0.41
28:b5:171:PHE:HA	28:b5:172:PRO:HD3	1.89	0.41
36:bl:137:LYS:HE2	36:bl:137:LYS:HB2	1.92	0.41
53:S1:121:LEU:HD21	53:S1:139:LEU:HD21	2.01	0.41
53:S1:232:THR:OG1	53:S1:233:SER:N	2.54	0.41
51:v1:395:VAL:HG22	51:v1:398:ARG:HH12	1.85	0.41
52:v2:62:ILE:HD12	52:v2:81:VAL:HG22	2.02	0.41
2:S3:84:GLU:HA	2:S3:141:ARG:O	2.20	0.41
2:S3:93:ILE:HD13	2:S3:93:ILE:HA	1.94	0.41
3:S2:267:ILE:HB	4:1:278:PRO:HG2	2.00	0.41
7:5:477:ILE:HD11	35:B7:55:GLN:HA	2.01	0.41
11:A9:73:LEU:HD13	11:A9:250:VAL:HG22	2.01	0.41
11:A9:354:ARG:NH1	11:A9:362:LEU:O	2.53	0.41
37:AN:36:ASP:OD2	55:S8:85:ASN:ND2	2.50	0.41
4:1a:13:ILE:HD12	4:1a:13:ILE:HA	1.91	0.41
7:5a:295:GLN:HE21	7:5a:300:LYS:HB3	1.85	0.41
18:a8:83:THR:HA	18:a8:86:TRP:HD1	1.84	0.41
19:am:77:SER:HA	19:am:80:VAL:HG12	2.02	0.41
40:3A:53:LEU:HD11	40:3A:246:ALA:HB1	2.03	0.41
40:3A:278:ARG:NH2	40:3A:280:ASP:OD2	2.47	0.41
43:3D:146:LYS:HE3	43:3D:146:LYS:HB3	1.93	0.41
43:3D:181:ASN:OD1	43:3D:184:ALA:N	2.47	0.41
45:3F:53:GLU:OE2	45:3F:57:ASN:ND2	2.52	0.41
41:3M:101:ARG:O	41:3M:105:ALA:CB	2.69	0.41
43:3O:99:ARG:NH2	43:3O:209:ASP:OD1	2.49	0.41
46:3R:71:LYS:HA	46:3R:71:LYS:HD2	1.81	0.41
52:V2:140:MET:HA	52:V2:144:SER:HB2	2.03	0.41
52:v2:48:PRO:HA	52:v2:95:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S2:197:MET:H	3:S2:197:MET:HG2	1.72	0.41
7:5:538:PRO:HB2	32:B8:117:VAL:HB	2.02	0.41
19:AM:44:ASN:O	19:AM:55:ARG:NH1	2.54	0.41
28:B5:58:LYS:HB2	28:B5:58:LYS:HE3	1.87	0.41
4:1a:85:LEU:HD23	4:1a:105:ILE:HD12	2.03	0.41
5:6a:25:PRO:HG3	6:4l:28:SER:HB3	2.01	0.41
8:4a:370:PRO:HB3	8:4a:375:LEU:HD22	2.03	0.41
9:2a:19:ILE:O	9:2a:23:SER:HB3	2.20	0.41
11:a9:57:THR:HG21	11:a9:120:VAL:HG12	2.01	0.41
46:3G:80:ASN:O	47:3H:58:ARG:NH1	2.52	0.41
42:3N:207:ASN:OD1	42:3N:210:GLY:N	2.53	0.41
51:v1:80:MET:HE1	51:v1:85:LEU:HD12	2.02	0.41
53:s1:125:PRO:HD2	53:s1:175:ARG:HA	2.02	0.41
53:s1:406:ASN:HA	53:s1:407:PRO:HD3	1.95	0.41
3:S2:184:ILE:HG23	3:S2:203:MET:HB3	2.01	0.41
3:S2:237:PRO:HG2	3:S2:240:LEU:HB2	2.02	0.41
7:5:177:ILE:HB	7:5:229:LEU:HD21	2.03	0.41
7:5:508:THR:OG1	34:B9:36:LYS:NZ	2.51	0.41
16:A5:66:LYS:H	16:A5:66:LYS:HG2	1.72	0.41
27:BM:121:GLU:HA	36:BL:9:VAL:HG21	2.02	0.41
34:B9:44:MET:HE2	34:B9:44:MET:HB2	1.93	0.41
1:3a:49:LEU:HD23	1:3a:49:LEU:HA	1.96	0.41
3:s2:97:LEU:HD22	3:s2:109:CYS:HB2	2.02	0.41
5:6a:33:ILE:HD13	5:6a:33:ILE:HA	1.94	0.41
5:6a:40:CYS:O	5:6a:44:LEU:HB2	2.21	0.41
11:a9:261:LYS:HE3	11:a9:261:LYS:HB2	1.93	0.41
33:b4:9:ALA:HB3	33:b4:12:ALA:H	1.85	0.41
40:3L:233:ALA:HB1	40:3L:237:VAL:HG21	2.02	0.41
42:3N:14:ILE:HD13	42:3N:14:ILE:HA	1.96	0.41
49:3V:12:GLU:O	49:3V:16:ASN:HB2	2.20	0.41
53:s1:103:LEU:HB3	53:s1:106:SER:HB3	2.01	0.41
53:s1:255:ASP:OD1	53:s1:289:LYS:NZ	2.52	0.41
53:s1:301:ARG:HH12	53:s1:588:ALA:HB2	1.86	0.41
7:5:74:MET:HE3	7:5:74:MET:HB3	1.84	0.41
12:S4:112:MET:HE2	12:S4:112:MET:HB3	1.90	0.41
17:A6:49:THR:HG23	17:A6:53:MET:HE2	2.01	0.41
30:B2:62:SER:OG	31:B3:75:LYS:O	2.37	0.41
3:s2:294:ARG:O	3:s2:321:GLY:N	2.51	0.41
6:4l:80:LYS:HE3	9:2a:48:LYS:HD3	2.02	0.41
7:5a:125:LEU:HD12	7:5a:125:LEU:HA	1.92	0.41
8:4a:21:LYS:HA	8:4a:21:LYS:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a9:214:LEU:HD12	11:a9:352:VAL:HG11	2.03	0.41
11:a9:360:ARG:O	11:a9:360:ARG:NH1	2.49	0.41
30:b2:43:ARG:HD3	30:b2:48:PRO:HA	2.02	0.41
40:3A:450:TYR:OH	40:3A:480:PHE:O	2.39	0.41
42:3C:242:LEU:HD23	42:3C:242:LEU:HA	1.97	0.41
43:3D:114:PHE:HE2	43:3D:148:LEU:HD13	1.86	0.41
41:3M:123:VAL:HG11	41:3M:133:LEU:HB3	2.03	0.41
42:3N:359:PHE:O	42:3N:363:LEU:HB2	2.20	0.41
43:3O:281:GLU:O	43:3O:285:ARG:CB	2.69	0.41
55:S8:85:ASN:O	55:S8:89:GLU:N	2.44	0.41
51:v1:413:TRP:HB2	51:v1:439:ILE:HD13	2.01	0.41
7:5:224:SER:OG	7:5:224:SER:O	2.38	0.41
16:A5:93:LYS:HD3	16:A5:93:LYS:HA	1.84	0.41
28:B5:171:PHE:HA	28:B5:172:PRO:HD3	1.94	0.41
34:B9:76:HIS:ND1	34:B9:78:GLN:O	2.54	0.41
37:AN:116:ASN:OD1	37:AN:116:ASN:N	2.54	0.41
7:5a:558:LEU:HD11	8:4a:211:GLY:HA2	2.01	0.41
7:5a:568:THR:HA	7:5a:571:THR:HG22	2.02	0.41
14:a2:16:LEU:HD12	14:a2:69:TYR:HE1	1.86	0.41
18:a8:93:ASN:OD1	18:a8:93:ASN:N	2.44	0.41
18:a8:147:ARG:HD3	18:a8:148:PRO:HD2	2.02	0.41
35:b7:84:GLN:O	35:b7:88:ASP:HB2	2.20	0.41
38:a7:65:PRO:HA	38:a7:66:PRO:HD3	1.93	0.41
42:3N:328:LEU:HB2	42:3N:361:ILE:HG21	2.03	0.41
53:s1:303:THR:HB	53:s1:614:GLY:HA3	2.02	0.41
1:3:29:LEU:O	11:A9:355:ARG:NH1	2.54	0.41
1:3:98:LEU:HD23	4:1:298:LEU:HD11	2.03	0.41
4:1:235:ASN:O	4:1:239:THR:OG1	2.34	0.41
6:4L:20:LEU:HB3	7:5:592:LEU:HD12	2.03	0.41
14:A2:23:LEU:HB2	14:A2:57:GLU:HG3	2.01	0.41
17:A6:130:ASP:OD1	17:A6:130:ASP:N	2.54	0.41
1:3a:57:LEU:O	1:3a:61:THR:OG1	2.33	0.41
2:s3:93:ILE:HG13	2:s3:94:PRO:HD3	2.01	0.41
3:s2:50:ALA:HB2	3:s2:63:PRO:HA	2.02	0.41
3:s2:188:THR:HG23	3:s2:200:PHE:HA	2.03	0.41
7:5a:149:ILE:HG13	8:4a:369:LEU:HD13	2.02	0.41
8:4a:230:ILE:HD12	8:4a:230:ILE:HA	1.92	0.41
8:4a:421:ASN:HD22	34:b9:100:PRO:HG3	1.86	0.41
9:2a:127:GLY:HA2	9:2a:130:LEU:HB3	2.02	0.41
11:a9:125:VAL:HG12	11:a9:163:ARG:HB3	2.03	0.41
20:ao:61:LEU:O	20:ao:65:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a1:52:ARG:NH1	21:a1:58:ASN:OD1	2.44	0.41
38:a7:5:THR:O	38:a7:9:GLN:HB2	2.20	0.41
39:v3:68:LYS:HA	39:v3:68:LYS:HD3	1.93	0.41
45:3F:36:ASP:OD1	45:3F:90:TYR:OH	2.35	0.41
45:3F:45:LYS:HE2	45:3F:45:LYS:HB2	1.86	0.41
40:3L:93:LEU:HD11	40:3L:220:LEU:HB2	2.02	0.41
40:3L:274:GLU:OE1	40:3L:276:ARG:NE	2.54	0.41
45:3Q:99:ILE:HD13	45:3Q:99:ILE:HA	1.94	0.41
51:v1:115:VAL:HB	51:v1:156:ILE:HA	2.01	0.41
53:s1:407:PRO:HB2	53:s1:415:ASN:HB2	2.02	0.41
3:S2:376:GLU:HG3	53:S1:151:SER:HB3	2.03	0.41
7:5:149:ILE:HG22	7:5:150:MET:HE2	2.02	0.41
7:5:316:THR:HA	7:5:319:MET:HB3	2.02	0.41
7:5:464:ALA:HA	7:5:467:VAL:HG12	2.03	0.41
8:4:365:ALA:O	8:4:374:ASN:ND2	2.52	0.41
10:AL:180:ARG:HH21	10:AL:182:GLN:HE21	1.68	0.41
12:S4:79:ILE:HD12	12:S4:134:ALA:HB1	2.03	0.41
15:AB:80:LYS:HA	15:AB:80:LYS:HD3	1.90	0.41
17:A6:112:GLU:H	17:A6:112:GLU:HG2	1.68	0.41
37:AN:132:SER:OG	37:AN:134:THR:OG1	2.39	0.41
39:V3:97:SER:HB3	52:V2:72:GLY:HA3	2.03	0.41
3:s2:62:LYS:HD2	3:s2:62:LYS:HA	1.86	0.41
3:s2:397:TYR:OH	3:s2:406:GLU:OE2	2.37	0.41
3:s2:448:VAL:HA	3:s2:451:ILE:HG22	2.03	0.41
6:4l:54:MET:HA	6:4l:57:MET:HG3	2.03	0.41
7:5a:539:MET:O	7:5a:543:ASN:HB2	2.21	0.41
8:4a:133:ILE:HD13	8:4a:219:ALA:HB1	2.02	0.41
8:4a:348:LEU:H	8:4a:415:GLN:HA	1.86	0.41
9:2a:13:ILE:HD12	9:2a:13:ILE:HA	1.95	0.41
9:2a:108:LEU:HD13	9:2a:157:LEU:HB3	2.03	0.41
10:al:170:LEU:HA	10:al:173:MET:HE3	2.03	0.41
10:al:204:VAL:HB	10:al:255:VAL:HG12	2.03	0.41
11:a9:211:ASP:O	11:a9:215:ASN:ND2	2.51	0.41
13:s6:107:CYS:O	55:s8:141:ARG:NH2	2.54	0.41
19:am:53:VAL:HA	19:am:56:VAL:HG12	2.02	0.41
24:c2:13:PHE:HE2	24:c2:74:PHE:HB3	1.86	0.41
40:3A:276:ARG:HH21	40:3A:465:LEU:HD23	1.86	0.41
41:3B:76:ASN:HA	41:3B:196:ARG:HH12	1.86	0.41
41:3B:293:LEU:HB3	41:3B:309:LEU:HG	2.03	0.41
41:3M:138:LEU:HD11	41:3M:238:LEU:HB2	2.03	0.41
41:3M:348:GLY:O	41:3M:352:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3O:242:ILE:HG23	43:3O:244:MET:H	1.85	0.41
47:3S:42:VAL:HA	47:3S:45:ARG:HB3	2.03	0.41
51:V1:48:ARG:HH22	52:V2:230:LEU:HG	1.86	0.41
51:V1:281:HIS:H	52:V2:142:ARG:HD3	1.86	0.41
51:V1:307:VAL:HG11	51:V1:356:VAL:HG11	2.03	0.41
52:V2:190:ASN:HB3	52:V2:215:PRO:HB3	2.03	0.41
53:S1:358:LEU:HA	53:S1:361:VAL:HG12	2.03	0.41
53:S1:556:THR:OG1	53:S1:557:ARG:N	2.54	0.41
54:S7:160:SER:OG	54:S7:166:ASN:OD1	2.38	0.41
51:v1:127:ASP:HA	51:v1:130:ILE:HG22	2.01	0.41
53:s1:542:PRO:HG2	53:s1:545:LEU:HB2	2.02	0.41
53:s1:556:THR:OG1	53:s1:557:ARG:N	2.54	0.41
54:s7:163:SER:HA	54:s7:166:ASN:HD22	1.86	0.41
5:6:165:ILE:HG12	9:2:42:PRO:HG2	2.03	0.41
7:5:406:ALA:HB2	32:B8:152:SER:HB2	2.03	0.41
8:4:79:ALA:HB2	8:4:436:LEU:HD21	2.03	0.41
8:4:148:TYR:O	8:4:152:TYR:HB2	2.21	0.41
8:4:303:ILE:HD12	8:4:303:ILE:HA	1.96	0.41
9:2:88:GLN:HA	9:2:148:LEU:HD11	2.02	0.41
10:AL:62:VAL:HG12	10:AL:205:ILE:HB	2.03	0.41
11:A9:207:PHE:HD1	11:A9:214:LEU:HD11	1.86	0.41
18:A8:154:ILE:HG12	24:C2:92:GLY:HA3	2.02	0.41
22:A3:18:VAL:HG13	22:A3:19:LEU:HD12	2.03	0.41
33:B4:115:LEU:HB3	33:B4:121:LEU:HB2	2.03	0.41
38:A7:65:PRO:HA	38:A7:66:PRO:HD3	1.95	0.41
2:s3:208:GLU:OE2	54:s7:179:ARG:NH1	2.52	0.41
4:1a:24:GLU:O	4:1a:28:LEU:HB2	2.21	0.41
7:5a:492:ILE:HD13	7:5a:492:ILE:HA	1.97	0.41
8:4a:341:THR:HG22	8:4a:343:ILE:H	1.86	0.41
20:ao:83:THR:HA	20:ao:86:ILE:HG22	2.03	0.41
27:bm:117:ARG:NH1	36:bl:108:GLU:OE2	2.51	0.41
29:b6:109:THR:HG22	29:b6:116:VAL:HG22	2.03	0.41
30:b2:56:ILE:HD12	30:b2:56:ILE:HA	1.97	0.41
36:bl:7:LYS:HE3	36:bl:12:GLU:HB3	2.03	0.41
41:3B:130:ILE:HA	41:3B:133:LEU:HD12	2.03	0.41
41:3M:250:LYS:HA	41:3M:250:LYS:HD2	1.87	0.41
44:3P:120:THR:HA	44:3P:123:VAL:HG12	2.02	0.41
53:S1:624:ARG:NE	53:S1:636:TYR:O	2.50	0.41
53:s1:476:LEU:HD11	53:s1:489:ILE:HG22	2.02	0.41
1:3:17:LEU:HA	1:3:20:VAL:HG12	2.03	0.40
1:3:55:PHE:O	1:3:59:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S3:104:ASN:HB3	38:A7:96:THR:HG22	2.03	0.40
7:5:283:LEU:HB2	32:B8:144:PHE:HE2	1.85	0.40
8:4:345:ALA:HA	8:4:423:MET:HE1	2.03	0.40
9:2:249:LEU:HD23	9:2:249:LEU:HA	1.94	0.40
32:B8:71:GLY:HA3	33:B4:76:ILE:HG23	2.02	0.40
32:B8:122:THR:OG1	32:B8:124:VAL:O	2.35	0.40
36:BL:85:ILE:O	36:BL:89:GLU:HB2	2.20	0.40
38:A7:33:LYS:O	38:A7:36:GLN:NE2	2.49	0.40
4:1a:288:LEU:O	4:1a:292:ASN:HB2	2.21	0.40
17:a6:44:ARG:HD3	17:a6:44:ARG:HA	1.87	0.40
24:c2:120:ARG:HD2	33:b4:116:ILE:HG13	2.02	0.40
26:b1:46:ARG:HE	26:b1:46:ARG:HB3	1.60	0.40
30:b2:96:GLU:HG3	30:b2:97:LEU:HD12	2.03	0.40
40:3A:336:LYS:HD3	40:3A:336:LYS:HA	1.85	0.40
40:3L:58:ARG:HG2	40:3L:417:LEU:HD12	2.03	0.40
41:3M:197:MET:H	41:3M:197:MET:HG2	1.67	0.40
43:3O:208:GLU:OE1	43:3O:275:ARG:NH2	2.54	0.40
3:S2:339:GLN:OE1	3:S2:342:ARG:NE	2.53	0.40
7:5:378:LEU:HD12	7:5:378:LEU:HA	1.96	0.40
7:5:459:PHE:HA	7:5:462:ILE:HG22	2.03	0.40
8:4:15:THR:O	8:4:93:LYS:NZ	2.48	0.40
24:C2:37:LEU:O	24:C2:41:THR:OG1	2.32	0.40
25:S5:36:PHE:HB3	25:S5:63:PHE:HB2	2.03	0.40
32:B8:36:MET:HE3	32:B8:36:MET:HB2	1.90	0.40
3:s2:52:MET:SD	9:2a:295:ARG:NH1	2.94	0.40
7:5a:12:PHE:HE2	7:5a:130:ILE:HD13	1.87	0.40
12:s4:151:LYS:HB2	12:s4:151:LYS:HE2	1.89	0.40
15:ac:138:LEU:HD12	15:ac:138:LEU:HA	1.90	0.40
19:am:102:GLY:HA2	19:am:105:THR:HG22	2.04	0.40
28:b5:109:HIS:NE2	28:b5:122:ALA:O	2.54	0.40
29:b6:121:ARG:HB2	35:b7:40:VAL:HB	2.03	0.40
40:3A:37:THR:OG1	40:3A:38:PHE:N	2.54	0.40
40:3A:98:PHE:HB2	40:3A:99:LYS:HE3	2.02	0.40
42:3C:3:ASN:O	42:3C:7:THR:CB	2.69	0.40
40:3L:136:LEU:HD21	41:3M:380:ALA:HA	2.04	0.40
41:3M:43:LEU:HB2	41:3M:47:LEU:HB3	2.02	0.40
53:s1:177:ILE:HG13	53:s1:179:CYS:HB3	2.04	0.40
54:s7:113:ASP:OD2	54:s7:116:ARG:N	2.51	0.40
54:s7:207:GLN:NE2	55:s8:176:SER:O	2.49	0.40
7:5:396:ILE:HG21	7:5:490:ALA:HB2	2.03	0.40
8:4:22:LYS:O	8:4:26:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:367:LEU:HD12	8:4:404:GLY:HA2	2.03	0.40
9:2:178:ILE:HD11	9:2:292:PHE:HB2	2.02	0.40
9:2:275:CYS:HB2	19:AM:137:PRO:HG2	2.03	0.40
11:A9:55:VAL:HG11	13:S6:43:TYR:HB2	2.04	0.40
19:AM:37:SER:HB2	19:AM:56:VAL:HA	2.04	0.40
20:AO:11:PRO:HA	20:AO:12:PRO:HD3	1.96	0.40
20:AO:23:ARG:HE	20:AO:23:ARG:HB2	1.75	0.40
33:B4:48:LEU:HD23	33:B4:48:LEU:HA	1.98	0.40
33:B4:85:LYS:HA	33:B4:85:LYS:HD3	1.93	0.40
34:B9:47:ARG:NH2	60:B9:201:EHZ:O1	2.46	0.40
37:AN:92:ARG:HD3	55:S8:200:GLU:HG2	2.03	0.40
3:s2:115:LEU:O	54:s7:138:THR:OG1	2.38	0.40
5:6a:17:LEU:HD21	5:6a:95:GLY:HA3	2.03	0.40
5:6a:66:VAL:HA	5:6a:69:TYR:HB2	2.04	0.40
8:4a:245:ARG:HD2	8:4a:245:ARG:HA	1.76	0.40
9:2a:55:ALA:HB1	9:2a:118:VAL:HA	2.04	0.40
9:2a:116:PRO:HA	9:2a:119:THR:HG22	2.03	0.40
11:a9:45:LYS:HG3	17:a6:117:ARG:HH21	1.86	0.40
13:s6:72:VAL:HG13	13:s6:77:ILE:HD13	2.04	0.40
20:ao:93:GLU:OE1	25:s5:92:TYR:OH	2.39	0.40
33:b4:81:ARG:HA	33:b4:82:PRO:HD3	1.95	0.40
38:a7:27:ARG:HD2	38:a7:31:ILE:HD11	2.02	0.40
40:3A:298:ASN:HA	40:3A:299:PRO:HD3	1.88	0.40
40:3L:254:SER:OG	40:3L:255:ARG:N	2.40	0.40
41:3M:182:TYR:OH	41:3M:333:SER:O	2.37	0.40
42:3N:256:TYR:HB3	43:3O:199:TYR:HD2	1.86	0.40
42:3N:375:LYS:HB2	42:3N:375:LYS:HE2	1.84	0.40
1:3:45:SER:OG	1:3:46:SER:N	2.54	0.40
2:S3:115:ALA:HB2	2:S3:127:ILE:HD13	2.04	0.40
3:S2:316:PHE:O	55:S8:35:THR:OG1	2.39	0.40
4:1:129:LEU:HD12	4:1:129:LEU:HA	1.91	0.40
8:4:373:ILE:HA	8:4:376:MET:HB3	2.03	0.40
11:A9:311:GLU:HA	11:A9:312:PRO:HD3	1.96	0.40
1:3a:67:LEU:HG	6:4l:65:VAL:HG22	2.02	0.40
4:1a:294:LEU:HD12	4:1a:294:LEU:HA	1.89	0.40
5:6a:110:ASP:OD1	5:6a:110:ASP:N	2.51	0.40
8:4a:6:LEU:HD21	26:b1:22:PHE:HD2	1.86	0.40
9:2a:248:LEU:HD12	9:2a:293:TYR:HB3	2.03	0.40
15:ab:136:GLU:H	15:ab:136:GLU:HG3	1.71	0.40
15:ab:137:LYS:HE3	15:ab:137:LYS:HB3	1.95	0.40
20:ao:105:LYS:HE2	20:ao:105:LYS:HB2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b4:15:PRO:HG2	33:b4:18:LEU:HD12	2.04	0.40
40:3A:332:ALA:HA	40:3A:337:LEU:HD13	2.04	0.40
42:3N:181:PHE:HA	42:3N:184:ILE:HG22	2.03	0.40
44:3P:102:SER:OG	44:3P:103:SER:N	2.54	0.40
53:S1:282:ASN:ND2	53:S1:285:TRP:O	2.53	0.40
53:S1:547:LEU:HD12	53:S1:550:ALA:HB3	2.03	0.40
54:S7:158:VAL:HB	54:S7:187:VAL:HA	2.04	0.40
52:v2:79:LEU:O	52:v2:121:TYR:OH	2.38	0.40
53:s1:374:THR:HG22	53:s1:378:GLY:HA3	2.03	0.40
3:S2:383:LYS:NZ	3:S2:387:GLU:OE1	2.54	0.40
7:5:139:GLN:HE21	7:5:139:GLN:HB3	1.75	0.40
18:A8:68:LEU:O	18:A8:72:ARG:HB2	2.21	0.40
29:B6:77:ILE:HG23	29:B6:78:PRO:HD3	2.03	0.40
3:s2:41:ILE:HG23	10:a1:313:TYR:HB3	2.03	0.40
6:4l:40:LEU:HD21	9:2a:71:LEU:HB3	2.04	0.40
7:5a:191:LEU:HD23	7:5a:191:LEU:HA	1.97	0.40
7:5a:411:ILE:HA	7:5a:414:ILE:HG22	2.03	0.40
8:4a:343:ILE:O	8:4a:346:ARG:NE	2.52	0.40
11:a9:247:LYS:HA	11:a9:247:LYS:HD2	1.84	0.40
15:ab:82:ARG:NE	15:ab:125:GLU:OE2	2.46	0.40
15:ab:106:LYS:HD3	15:ab:106:LYS:HA	1.95	0.40
16:a5:60:LYS:HE2	16:a5:60:LYS:HB3	1.88	0.40
29:b6:24:LYS:HE2	29:b6:24:LYS:HB2	1.80	0.40
35:b7:39:MET:HE2	35:b7:39:MET:HB2	1.79	0.40
41:3B:138:LEU:HD13	41:3B:238:LEU:HD23	2.03	0.40
44:3E:140:MET:HE3	42:3N:163:TRP:HE1	1.87	0.40
40:3L:470:ARG:HH22	42:3N:20:ASP:HB3	1.85	0.40
41:3M:112:VAL:HA	41:3M:120:ALA:O	2.21	0.40
51:v1:62:TRP:N	51:v1:140:GLU:OE1	2.50	0.40
53:s1:587:ALA:HB3	53:s1:592:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
1	3a	109/115 (95%)	102 (94%)	7 (6%)	0	100	100
2	S3	204/263 (78%)	197 (97%)	7 (3%)	0	100	100
2	s3	203/263 (77%)	188 (93%)	15 (7%)	0	100	100
3	S2	418/463 (90%)	401 (96%)	17 (4%)	0	100	100
3	s2	416/463 (90%)	400 (96%)	16 (4%)	0	100	100
4	1	315/318 (99%)	294 (93%)	20 (6%)	1 (0%)	36	65
4	1a	314/318 (99%)	293 (93%)	20 (6%)	1 (0%)	36	65
5	6	168/172 (98%)	160 (95%)	8 (5%)	0	100	100
5	6a	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
6	4L	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
6	4l	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	5	603/607 (99%)	573 (95%)	28 (5%)	2 (0%)	36	65
7	5a	603/607 (99%)	562 (93%)	41 (7%)	0	100	100
8	4	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
8	4a	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
9	2	342/345 (99%)	331 (97%)	11 (3%)	0	100	100
9	2a	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
10	AL	318/355 (90%)	299 (94%)	19 (6%)	0	100	100
10	al	318/355 (90%)	304 (96%)	14 (4%)	0	100	100
11	A9	340/377 (90%)	321 (94%)	19 (6%)	0	100	100
11	a9	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
12	S4	124/175 (71%)	118 (95%)	6 (5%)	0	100	100
12	s4	124/175 (71%)	122 (98%)	2 (2%)	0	100	100
13	S6	93/116 (80%)	93 (100%)	0	0	100	100
13	s6	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
14	A2	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
14	a2	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
15	AB	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	AC	86/156 (55%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	ab	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	ac	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
16	A5	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
16	a5	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
17	A6	110/131 (84%)	105 (96%)	5 (4%)	0	100	100
17	a6	109/131 (83%)	103 (94%)	6 (6%)	0	100	100
18	A8	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
18	a8	168/172 (98%)	162 (96%)	6 (4%)	0	100	100
19	AM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
19	am	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
20	AO	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
20	ao	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
21	A1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
21	a1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
22	A3	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
22	a3	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
23	C1	47/76 (62%)	47 (100%)	0	0	100	100
23	c1	43/76 (57%)	42 (98%)	1 (2%)	0	100	100
24	C2	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
24	c2	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
25	S5	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
25	s5	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
26	B1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
26	b1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	BM	96/151 (64%)	93 (97%)	3 (3%)	0	100	100
27	bm	97/151 (64%)	93 (96%)	4 (4%)	0	100	100
28	B5	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
28	b5	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
29	B6	90/127 (71%)	89 (99%)	1 (1%)	0	100	100
29	b6	86/127 (68%)	83 (96%)	3 (4%)	0	100	100
30	B2	62/105 (59%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b2	61/105 (58%)	61 (100%)	0	0	100	100
31	B3	68/104 (65%)	65 (96%)	3 (4%)	0	100	100
31	b3	69/104 (66%)	66 (96%)	3 (4%)	0	100	100
32	B8	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
32	b8	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
33	B4	123/129 (95%)	121 (98%)	2 (2%)	0	100	100
33	b4	123/129 (95%)	118 (96%)	5 (4%)	0	100	100
34	B9	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
34	b9	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	B7	112/136 (82%)	110 (98%)	2 (2%)	0	100	100
35	b7	115/136 (85%)	109 (95%)	6 (5%)	0	100	100
36	BL	165/176 (94%)	159 (96%)	6 (4%)	0	100	100
36	bl	167/176 (95%)	159 (95%)	8 (5%)	0	100	100
37	AN	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
37	an	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
38	A7	88/112 (79%)	84 (96%)	4 (4%)	0	100	100
38	a7	68/112 (61%)	63 (93%)	5 (7%)	0	100	100
39	V3	38/104 (36%)	38 (100%)	0	0	100	100
39	v3	34/104 (33%)	34 (100%)	0	0	100	100
40	3A	443/446 (99%)	427 (96%)	16 (4%)	0	100	100
40	3L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
41	3B	418/439 (95%)	405 (97%)	13 (3%)	0	100	100
41	3M	418/439 (95%)	396 (95%)	22 (5%)	0	100	100
42	3C	378/380 (100%)	366 (97%)	12 (3%)	0	100	100
42	3N	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
43	3D	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
43	3O	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
44	3E	78/196 (40%)	76 (97%)	2 (3%)	0	100	100
44	3P	79/196 (40%)	73 (92%)	6 (8%)	0	100	100
45	3F	100/110 (91%)	97 (97%)	3 (3%)	0	100	100
45	3Q	97/110 (88%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	3G	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
46	3R	69/81 (85%)	63 (91%)	6 (9%)	0	100	100
47	3H	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
47	3S	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
48	3J	54/63 (86%)	52 (96%)	1 (2%)	1 (2%)	6	33
48	3U	57/63 (90%)	56 (98%)	1 (2%)	0	100	100
49	3K	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
49	3V	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
50	3T	52/78 (67%)	50 (96%)	2 (4%)	0	100	100
51	V1	426/457 (93%)	371 (87%)	55 (13%)	0	100	100
51	v1	420/457 (92%)	375 (89%)	45 (11%)	0	100	100
52	V2	207/244 (85%)	178 (86%)	28 (14%)	1 (0%)	24	56
52	v2	190/244 (78%)	176 (93%)	14 (7%)	0	100	100
53	S1	685/716 (96%)	620 (90%)	65 (10%)	0	100	100
53	s1	685/716 (96%)	619 (90%)	66 (10%)	0	100	100
54	S7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
54	s7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
55	S8	176/212 (83%)	158 (90%)	18 (10%)	0	100	100
55	s8	162/212 (76%)	145 (90%)	16 (10%)	1 (1%)	21	52
All	All	19905/22630 (88%)	18869 (95%)	1029 (5%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1	91	MET
7	5	433	THR
4	1a	91	MET
48	3J	57	LYS
55	s8	152	CYS
52	V2	188	ASN
7	5	563	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	102/104 (98%)	101 (99%)	1 (1%)	68	74
1	3a	100/104 (96%)	100 (100%)	0	100	100
2	S3	188/227 (83%)	186 (99%)	2 (1%)	65	73
2	s3	187/227 (82%)	185 (99%)	2 (1%)	65	73
3	S2	364/394 (92%)	359 (99%)	5 (1%)	59	70
3	s2	362/394 (92%)	359 (99%)	3 (1%)	73	76
4	1	279/279 (100%)	278 (100%)	1 (0%)	84	81
4	1a	278/279 (100%)	277 (100%)	1 (0%)	84	81
5	6	136/138 (99%)	136 (100%)	0	100	100
5	6a	137/138 (99%)	135 (98%)	2 (2%)	57	68
6	4L	87/88 (99%)	87 (100%)	0	100	100
6	4l	87/88 (99%)	87 (100%)	0	100	100
7	5	548/550 (100%)	546 (100%)	2 (0%)	84	81
7	5a	548/550 (100%)	543 (99%)	5 (1%)	70	75
8	4	415/415 (100%)	412 (99%)	3 (1%)	76	77
8	4a	415/415 (100%)	413 (100%)	2 (0%)	81	80
9	2	307/308 (100%)	304 (99%)	3 (1%)	68	74
9	2a	307/308 (100%)	305 (99%)	2 (1%)	76	77
10	AL	284/309 (92%)	283 (100%)	1 (0%)	84	81
10	al	284/309 (92%)	281 (99%)	3 (1%)	65	73
11	A9	299/325 (92%)	298 (100%)	1 (0%)	86	83
11	a9	299/325 (92%)	297 (99%)	2 (1%)	76	77
12	S4	112/153 (73%)	111 (99%)	1 (1%)	70	75
12	s4	112/153 (73%)	112 (100%)	0	100	100
13	S6	80/96 (83%)	79 (99%)	1 (1%)	61	71
13	s6	80/96 (83%)	79 (99%)	1 (1%)	61	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	A2	74/80 (92%)	74 (100%)	0	100	100
14	a2	74/80 (92%)	72 (97%)	2 (3%)	39	59
15	AB	72/135 (53%)	72 (100%)	0	100	100
15	AC	81/135 (60%)	81 (100%)	0	100	100
15	ab	72/135 (53%)	72 (100%)	0	100	100
15	ac	81/135 (60%)	80 (99%)	1 (1%)	63	72
16	A5	101/102 (99%)	101 (100%)	0	100	100
16	a5	101/102 (99%)	101 (100%)	0	100	100
17	A6	106/114 (93%)	106 (100%)	0	100	100
17	a6	105/114 (92%)	104 (99%)	1 (1%)	68	74
18	A8	152/154 (99%)	152 (100%)	0	100	100
18	a8	152/154 (99%)	151 (99%)	1 (1%)	76	77
19	AM	106/106 (100%)	105 (99%)	1 (1%)	70	75
19	am	106/106 (100%)	106 (100%)	0	100	100
20	AO	121/123 (98%)	121 (100%)	0	100	100
20	ao	121/123 (98%)	119 (98%)	2 (2%)	53	67
21	A1	59/60 (98%)	59 (100%)	0	100	100
21	a1	59/60 (98%)	58 (98%)	1 (2%)	53	67
22	A3	72/73 (99%)	72 (100%)	0	100	100
22	a3	72/73 (99%)	72 (100%)	0	100	100
23	C1	43/67 (64%)	43 (100%)	0	100	100
23	c1	40/67 (60%)	40 (100%)	0	100	100
24	C2	107/107 (100%)	107 (100%)	0	100	100
24	c2	107/107 (100%)	107 (100%)	0	100	100
25	S5	93/94 (99%)	92 (99%)	1 (1%)	65	73
25	s5	93/94 (99%)	93 (100%)	0	100	100
26	B1	52/53 (98%)	51 (98%)	1 (2%)	50	65
26	b1	52/53 (98%)	52 (100%)	0	100	100
27	BM	89/129 (69%)	89 (100%)	0	100	100
27	bm	90/129 (70%)	90 (100%)	0	100	100
28	B5	123/162 (76%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b5	122/162 (75%)	122 (100%)	0	100	100
29	B6	86/119 (72%)	86 (100%)	0	100	100
29	b6	85/119 (71%)	84 (99%)	1 (1%)	63	72
30	B2	60/87 (69%)	60 (100%)	0	100	100
30	b2	59/87 (68%)	59 (100%)	0	100	100
31	B3	55/78 (70%)	55 (100%)	0	100	100
31	b3	55/78 (70%)	55 (100%)	0	100	100
32	B8	140/161 (87%)	139 (99%)	1 (1%)	76	77
32	b8	140/161 (87%)	140 (100%)	0	100	100
33	B4	111/114 (97%)	111 (100%)	0	100	100
33	b4	111/114 (97%)	111 (100%)	0	100	100
34	B9	163/164 (99%)	162 (99%)	1 (1%)	78	79
34	b9	162/164 (99%)	161 (99%)	1 (1%)	78	79
35	B7	106/120 (88%)	106 (100%)	0	100	100
35	b7	108/120 (90%)	108 (100%)	0	100	100
36	BL	152/158 (96%)	152 (100%)	0	100	100
36	bl	154/158 (98%)	154 (100%)	0	100	100
37	AN	130/131 (99%)	129 (99%)	1 (1%)	73	76
37	an	130/131 (99%)	130 (100%)	0	100	100
38	A7	83/95 (87%)	83 (100%)	0	100	100
38	a7	63/95 (66%)	63 (100%)	0	100	100
39	V3	39/95 (41%)	39 (100%)	0	100	100
39	v3	35/95 (37%)	35 (100%)	0	100	100
40	3A	372/373 (100%)	371 (100%)	1 (0%)	86	83
40	3L	372/373 (100%)	371 (100%)	1 (0%)	86	83
41	3B	330/344 (96%)	329 (100%)	1 (0%)	86	83
41	3M	330/344 (96%)	330 (100%)	0	100	100
42	3C	332/332 (100%)	329 (99%)	3 (1%)	70	75
42	3N	332/332 (100%)	329 (99%)	3 (1%)	70	75
43	3D	206/206 (100%)	205 (100%)	1 (0%)	81	80
43	3O	205/206 (100%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	3E	69/166 (42%)	68 (99%)	1 (1%)	59	70
44	3P	70/166 (42%)	70 (100%)	0	100	100
45	3F	94/98 (96%)	93 (99%)	1 (1%)	65	73
45	3Q	91/98 (93%)	91 (100%)	0	100	100
46	3G	72/73 (99%)	72 (100%)	0	100	100
46	3R	64/73 (88%)	64 (100%)	0	100	100
47	3H	63/72 (88%)	62 (98%)	1 (2%)	55	68
47	3S	63/72 (88%)	63 (100%)	0	100	100
48	3J	47/54 (87%)	47 (100%)	0	100	100
48	3U	50/54 (93%)	49 (98%)	1 (2%)	48	64
49	3K	41/46 (89%)	41 (100%)	0	100	100
49	3V	43/46 (94%)	43 (100%)	0	100	100
50	3T	41/58 (71%)	41 (100%)	0	100	100
51	V1	343/366 (94%)	338 (98%)	5 (2%)	57	68
51	v1	338/366 (92%)	338 (100%)	0	100	100
52	V2	182/204 (89%)	181 (100%)	1 (0%)	81	80
52	v2	170/204 (83%)	170 (100%)	0	100	100
53	S1	579/602 (96%)	577 (100%)	2 (0%)	86	83
53	s1	579/602 (96%)	577 (100%)	2 (0%)	86	83
54	S7	131/185 (71%)	128 (98%)	3 (2%)	44	62
54	s7	131/185 (71%)	130 (99%)	1 (1%)	73	76
55	S8	145/178 (82%)	144 (99%)	1 (1%)	76	77
55	s8	138/178 (78%)	137 (99%)	1 (1%)	76	77
All	All	17545/19460 (90%)	17455 (100%)	90 (0%)	78	80

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	11	ILE
2	S3	135	ARG
2	S3	168	GLU
3	S2	157	LYS
3	S2	259	GLU
3	S2	298	ILE

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Mol	Chain	Res	Type
3	S2	450	ILE
3	S2	462	ASP
4	1	171	HIS
7	5	30	ILE
7	5	432	MET
8	4	236	LEU
8	4	246	ILE
8	4	285	LEU
9	2	161	SER
9	2	233	LEU
9	2	270	LEU
10	AL	61	THR
11	A9	353	LEU
12	S4	55	VAL
13	S6	31	ILE
19	AM	14	ASP
25	S5	3	PHE
26	B1	55	THR
32	B8	105	ILE
34	B9	134	ASP
37	AN	31	PHE
2	s3	57	LEU
2	s3	93	ILE
3	s2	124	ILE
3	s2	181	LEU
3	s2	409	VAL
4	1a	163	GLN
5	6a	41	LEU
5	6a	159	LEU
7	5a	77	LYS
7	5a	187	VAL
7	5a	210	LEU
7	5a	253	VAL
7	5a	361	ASN
8	4a	245	ARG
8	4a	440	HIS
9	2a	49	ASN
9	2a	232	LEU
10	al	199	LEU
10	al	237	ILE
10	al	256	LEU
11	a9	180	SER

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Mol	Chain	Res	Type
11	a9	374	THR
13	s6	67	GLN
14	a2	38	VAL
14	a2	65	LEU
15	ac	112	SER
17	a6	52	LEU
18	a8	135	ARG
20	ao	61	LEU
20	ao	69	ILE
21	a1	38	VAL
29	b6	7	ASP
34	b9	25	ARG
40	3A	399	LEU
41	3B	388	THR
42	3C	119	LEU
42	3C	232	ILE
42	3C	333	LEU
43	3D	105	LEU
44	3E	96	VAL
45	3F	76	LEU
47	3H	64	ASP
40	3L	379	LEU
42	3N	162	GLU
42	3N	183	PHE
42	3N	335	LEU
48	3U	53	LEU
51	V1	45	LEU
51	V1	233	VAL
51	V1	244	ASN
51	V1	410	ASP
51	V1	412	LEU
52	V2	39	VAL
53	S1	96	VAL
53	S1	567	VAL
54	S7	145	LEU
54	S7	202	LEU
54	S7	205	ILE
55	S8	140	ARG
53	s1	154	LEU
53	s1	514	ASN
54	s7	99	CYS
55	s8	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (213) such sidechains are listed below:

Mol	Chain	Res	Type
2	S3	54	HIS
2	S3	195	HIS
3	S2	36	GLN
3	S2	38	GLN
3	S2	250	ASN
3	S2	306	GLN
3	S2	313	GLN
3	S2	390	GLN
4	1	93	HIS
4	1	230	ASN
6	4L	50	ASN
6	4L	92	ASN
7	5	31	ASN
7	5	58	ASN
7	5	226	GLN
7	5	321	GLN
7	5	444	ASN
7	5	594	ASN
8	4	83	HIS
8	4	139	GLN
8	4	144	ASN
8	4	304	GLN
8	4	331	ASN
8	4	349	GLN
8	4	390	ASN
8	4	399	ASN
9	2	197	ASN
9	2	289	ASN
9	2	310	ASN
10	AL	65	ASN
10	AL	176	GLN
10	AL	235	GLN
11	A9	37	HIS
11	A9	38	HIS
11	A9	79	GLN
11	A9	216	HIS
12	S4	51	GLN
13	S6	36	GLN
14	A2	48	HIS
14	A2	50	ASN
15	AB	115	GLN

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Mol	Chain	Res	Type
15	AB	142	GLN
18	A8	151	ASN
19	AM	79	GLN
20	AO	24	ASN
20	AO	54	ASN
20	AO	137	ASN
21	A1	31	ASN
21	A1	68	ASN
22	A3	52	ASN
23	C1	60	GLN
24	C2	117	HIS
25	S5	29	ASN
25	S5	45	HIS
25	S5	77	HIS
26	B1	45	GLN
27	BM	138	ASN
27	BM	146	GLN
31	B3	39	GLN
31	B3	54	ASN
32	B8	115	ASN
32	B8	132	HIS
33	B4	126	ASN
34	B9	13	GLN
34	B9	139	GLN
35	B7	44	GLN
35	B7	76	ASN
35	B7	110	GLN
36	BL	123	GLN
36	BL	131	GLN
37	AN	91	HIS
39	V3	69	ASN
1	3a	108	GLN
2	s3	54	HIS
2	s3	163	ASN
2	s3	179	ASN
2	s3	235	ASN
3	s2	36	GLN
3	s2	88	HIS
3	s2	147	ASN
3	s2	234	GLN
3	s2	313	GLN
3	s2	349	ASN

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Mol	Chain	Res	Type
4	1a	93	HIS
4	1a	138	GLN
6	4l	83	ASN
6	4l	94	ASN
6	4l	97	GLN
7	5a	31	ASN
7	5a	56	HIS
7	5a	57	ASN
7	5a	135	ASN
7	5a	199	GLN
7	5a	295	GLN
7	5a	348	HIS
7	5a	446	ASN
7	5a	506	ASN
7	5a	572	ASN
8	4a	192	ASN
8	4a	374	ASN
9	2a	134	GLN
9	2a	223	ASN
9	2a	309	ASN
10	al	71	ASN
10	al	79	GLN
10	al	132	GLN
10	al	142	GLN
10	al	175	ASN
10	al	286	GLN
11	a9	37	HIS
11	a9	43	HIS
13	s6	36	GLN
14	a2	25	GLN
14	a2	80	ASN
15	ab	115	GLN
15	ac	142	GLN
19	am	79	GLN
20	ao	54	ASN
21	a1	31	ASN
24	c2	27	ASN
24	c2	59	HIS
25	s5	7	GLN
25	s5	25	GLN
27	bm	63	ASN
27	bm	146	GLN

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Mol	Chain	Res	Type
28	b5	124	ASN
30	b2	49	GLN
30	b2	83	HIS
31	b3	27	GLN
33	b4	52	ASN
33	b4	86	ASN
34	b9	12	HIS
34	b9	169	HIS
35	b7	76	ASN
36	b1	107	GLN
37	an	21	HIS
37	an	73	ASN
37	an	120	ASN
38	a7	21	GLN
38	a7	29	GLN
38	a7	51	ASN
40	3A	40	GLN
40	3A	43	GLN
40	3A	86	ASN
40	3A	103	ASN
40	3A	175	ASN
40	3A	207	ASN
40	3A	247	GLN
40	3A	323	HIS
40	3A	375	GLN
40	3A	464	GLN
41	3B	118	ASN
41	3B	139	ASN
41	3B	210	GLN
41	3B	261	GLN
41	3B	303	ASN
41	3B	311	GLN
41	3B	318	HIS
42	3C	15	ASN
42	3C	32	ASN
42	3C	255	ASN
42	3C	263	ASN
42	3C	267	HIS
42	3C	341	GLN
42	3C	345	HIS
43	3D	284	HIS
44	3E	80	HIS

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Mol	Chain	Res	Type
47	3H	74	HIS
47	3H	78	HIS
40	3L	175	ASN
40	3L	199	GLN
40	3L	221	ASN
41	3M	34	GLN
41	3M	170	GLN
41	3M	211	ASN
41	3M	236	GLN
41	3M	262	ASN
41	3M	311	GLN
43	3O	155	GLN
43	3O	240	GLN
43	3O	265	GLN
44	3P	135	GLN
45	3Q	57	ASN
46	3R	37	ASN
47	3S	37	GLN
49	3V	16	ASN
51	V1	164	ASN
51	V1	168	ASN
51	V1	281	HIS
51	V1	283	ASN
52	V2	152	GLN
53	S1	101	ASN
53	S1	406	ASN
53	S1	569	GLN
55	S8	172	ASN
51	v1	49	HIS
51	v1	168	ASN
51	v1	283	ASN
51	v1	284	HIS
51	v1	303	HIS
51	v1	418	GLN
52	v2	68	ASN
52	v2	89	ASN
53	s1	101	ASN
53	s1	140	GLN
53	s1	365	ASN
53	s1	384	ASN
53	s1	425	ASN
53	s1	495	ASN

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Mol	Chain	Res	Type
54	s7	151	GLN
54	s7	166	ASN
55	s8	193	ASN
55	s8	206	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
3	2MR	s2	118	3	3,4,13	0.83	0	2,4,15	1.27	0
3	2MR	S2	118	3	10,12,13	2.72	3 (30%)	5,13,15	7.36	4 (80%)

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
3	2MR	s2	118	3	-	1/1/2/15	-
3	2MR	S2	118	3	-	4/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S2	118	2MR	CZ-NE	5.73	1.46	1.34
3	S2	118	2MR	CZ-NH2	5.42	1.44	1.33
3	S2	118	2MR	CQ1-NH1	-2.49	1.41	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S2	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
3	S2	118	2MR	CD-NE-CZ	10.13	142.39	123.36
3	S2	118	2MR	CQ2-NH2-CZ	3.05	130.19	123.65
3	S2	118	2MR	CG-CD-NE	-2.38	105.52	112.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	s2	118	2MR	O-C-CA-CB
3	S2	118	2MR	CA-CB-CG-CD
3	S2	118	2MR	C-CA-CB-CG
3	S2	118	2MR	N-CA-CB-CG
3	S2	118	2MR	NE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S2	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	$\# Z > 2$
65	FES	V2	301	52	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	SF4	v1	502	51	0,12,12	-	-	-		
58	NDP	a9	501	11,54	51,52,52	0.33	0	71,80,80	0.43	0
63	FMN	v1	501	-	33,33,33	0.27	0	48,50,50	0.54	1 (2%)
64	SF4	S1	801	53	0,12,12	-	-	-		
60	EHZ	5a	701	7	31,36,37	0.25	0	36,44,47	1.14	1 (2%)
61	HEM	3N	402	42	50,50,50	1.37	7 (14%)	67,82,82	1.60	15 (22%)
64	SF4	S8	302	55	0,12,12	-	-	-		
61	HEM	3N	401	42	50,50,50	1.31	6 (12%)	67,82,82	1.61	12 (17%)
57	DGT	al	502	-	32,33,33	0.57	0	48,52,52	0.59	0
62	HEC	3O	401	43	50,50,50	1.31	6 (12%)	68,82,82	1.51	14 (20%)
64	SF4	S1	802	53	0,12,12	-	-	-		
60	EHZ	A6	201	-	31,36,37	0.20	0	36,44,47	1.26	1 (2%)
65	FES	s1	803	53	0,4,4	-	-	-		
65	FES	S1	803	53	0,4,4	-	-	-		
64	SF4	S7	301	54,3	0,12,12	-	-	-		
58	NDP	A9	501	-	51,52,52	0.32	0	71,80,80	0.42	0
65	FES	v2	301	52	0,4,4	-	-	-		
64	SF4	s8	302	55	0,12,12	-	-	-		
63	FMN	V1	501	51	33,33,33	0.30	0	48,50,50	0.48	0
64	SF4	s1	801	53	0,12,12	-	-	-		
62	HEC	3D	401	43	50,50,50	1.45	9 (18%)	68,82,82	1.77	18 (26%)
61	HEM	3C	401	42	50,50,50	1.31	8 (16%)	67,82,82	1.62	12 (17%)
57	DGT	AL	502	56	32,33,33	0.57	0	48,52,52	0.58	0
64	SF4	s8	301	55	0,12,12	-	-	-		
64	SF4	S8	301	55	0,12,12	-	-	-		
64	SF4	V1	502	51	0,12,12	-	-	-		
64	SF4	s7	301	54	0,12,12	-	-	-		
60	EHZ	B9	201	-	31,36,37	0.20	0	36,44,47	1.04	1 (2%)
61	HEM	3C	402	42	50,50,50	1.34	6 (12%)	67,82,82	1.62	16 (23%)
64	SF4	s1	802	53	0,12,12	-	-	-		
60	EHZ	a6	201	-	31,36,37	0.19	0	36,44,47	1.25	1 (2%)

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
65	FES	V2	301	52	-	-	0/1/1/1
64	SF4	v1	502	51	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	NDP	a9	501	11,54	-	10/34/77/77	0/5/5/5
63	FMN	v1	501	-	-	4/18/18/18	0/3/3/3
64	SF4	S1	801	53	-	-	0/6/5/5
60	EHZ	5a	701	7	-	4/42/44/45	-
61	HEM	3N	402	42	-	7/14/54/54	-
64	SF4	S8	302	55	-	-	0/6/5/5
61	HEM	3N	401	42	-	9/14/54/54	-
57	DGT	al	502	-	-	2/22/34/34	0/3/3/3
62	HEC	3O	401	43	1/1/3/7	5/14/54/54	-
64	SF4	S1	802	53	-	-	0/6/5/5
60	EHZ	A6	201	-	-	3/42/44/45	-
65	FES	s1	803	53	-	-	0/1/1/1
65	FES	S1	803	53	-	-	0/1/1/1
64	SF4	S7	301	54,3	-	-	0/6/5/5
58	NDP	A9	501	-	-	9/34/77/77	0/5/5/5
65	FES	v2	301	52	-	-	0/1/1/1
64	SF4	s8	302	55	-	-	0/6/5/5
63	FMN	V1	501	51	-	5/18/18/18	0/3/3/3
64	SF4	s1	801	53	-	-	0/6/5/5
61	HEM	3C	401	42	-	9/14/54/54	-
62	HEC	3D	401	43	1/1/3/7	7/14/54/54	-
57	DGT	AL	502	56	-	1/22/34/34	0/3/3/3
64	SF4	s8	301	55	-	-	0/6/5/5
64	SF4	S8	301	55	-	-	0/6/5/5
64	SF4	V1	502	51	-	-	0/6/5/5
64	SF4	s7	301	54	-	-	0/6/5/5
60	EHZ	B9	201	-	-	8/42/44/45	-
61	HEM	3C	402	42	-	7/14/54/54	-
64	SF4	s1	802	53	-	-	0/6/5/5
60	EHZ	a6	201	-	-	10/42/44/45	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	3C	402	HEM	C4D-ND	-3.81	1.33	1.40
61	3N	402	HEM	C4D-ND	-3.62	1.34	1.40
61	3N	401	HEM	C4D-ND	-3.58	1.34	1.40
61	3C	401	HEM	C4D-ND	-3.43	1.34	1.40
61	3C	401	HEM	C1B-NB	-3.43	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	3O	401	HEC	CBC-CAC	-3.41	1.37	1.51
62	3D	401	HEC	CBC-CAC	-3.41	1.37	1.51
61	3N	401	HEM	C1B-NB	-3.32	1.34	1.40
61	3N	402	HEM	C1B-NB	-3.30	1.34	1.40
61	3C	402	HEM	C1D-ND	-3.10	1.32	1.38
62	3D	401	HEC	CAC-C3C	3.03	1.58	1.51
62	3O	401	HEC	CAC-C3C	3.03	1.58	1.51
61	3C	402	HEM	C1C-C2C	-3.00	1.39	1.45
61	3C	402	HEM	C1B-NB	-2.98	1.35	1.40
61	3N	402	HEM	C1C-C2C	-2.96	1.39	1.45
61	3C	401	HEM	C1D-ND	-2.85	1.33	1.38
61	3N	401	HEM	C1D-ND	-2.84	1.33	1.38
61	3N	402	HEM	C1D-ND	-2.80	1.33	1.38
62	3D	401	HEC	O1A-CGA	2.74	1.31	1.22
61	3N	401	HEM	C1C-C2C	-2.66	1.40	1.45
62	3O	401	HEC	CBB-CAB	-2.55	1.40	1.51
61	3N	402	HEM	C3B-C4B	2.54	1.49	1.44
62	3D	401	HEC	CBB-CAB	-2.47	1.41	1.51
61	3C	401	HEM	C1C-C2C	-2.43	1.40	1.45
62	3D	401	HEC	CMB-C2B	2.41	1.55	1.50
61	3N	402	HEM	FE-NB	2.41	2.02	1.94
62	3O	401	HEC	CMD-C2D	2.40	1.55	1.50
62	3D	401	HEC	CMA-C3A	2.39	1.55	1.50
62	3O	401	HEC	CAB-C3B	2.39	1.57	1.51
62	3D	401	HEC	CAA-C2A	2.36	1.57	1.51
61	3N	401	HEM	FE-NB	2.31	2.02	1.94
61	3C	402	HEM	FE-NB	2.30	2.02	1.94
62	3O	401	HEC	CMB-C2B	2.26	1.55	1.50
62	3D	401	HEC	CAB-C3B	2.22	1.56	1.51
62	3D	401	HEC	CMD-C2D	2.18	1.55	1.50
61	3C	401	HEM	C3C-C4C	-2.16	1.42	1.46
61	3C	402	HEM	C4B-NB	-2.12	1.34	1.38
61	3C	401	HEM	FE-NB	2.11	2.01	1.94
61	3C	401	HEM	FE-ND	2.09	2.01	1.94
61	3N	401	HEM	FE-ND	2.07	2.01	1.94
61	3C	401	HEM	C4B-NB	-2.03	1.34	1.38
61	3N	402	HEM	FE-ND	2.01	2.01	1.94

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	a6	201	EHZ	C10-S1-C9	7.12	122.89	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	A6	201	EHZ	C10-S1-C9	6.83	122.02	101.84
60	5a	701	EHZ	C10-S1-C9	6.03	119.67	101.84
60	B9	201	EHZ	C10-S1-C9	5.84	119.11	101.84
61	3N	401	HEM	CHC-C4B-NB	4.69	129.47	124.42
61	3C	401	HEM	CHB-C1B-NB	4.65	130.12	124.37
61	3C	401	HEM	CHC-C4B-NB	4.62	129.40	124.42
61	3C	402	HEM	CHC-C4B-NB	4.61	129.39	124.42
61	3N	402	HEM	CHB-C1B-NB	4.48	129.90	124.37
61	3N	401	HEM	CHB-C1B-NB	4.45	129.87	124.37
62	3D	401	HEC	CMA-C3A-C4A	-4.18	117.37	124.73
61	3N	402	HEM	CHD-C4C-NC	4.05	128.86	124.45
62	3O	401	HEC	CBD-CAD-C3D	4.03	123.67	112.53
61	3N	401	HEM	CHD-C4C-NC	3.87	128.66	124.45
61	3C	402	HEM	CHD-C4C-NC	3.84	128.63	124.45
62	3D	401	HEC	C1D-ND-C4D	3.74	109.64	105.21
61	3C	401	HEM	CHD-C4C-NC	3.68	128.46	124.45
61	3C	402	HEM	CHB-C1B-NB	3.67	128.91	124.37
62	3D	401	HEC	C3D-C4D-ND	-3.64	106.83	110.35
62	3D	401	HEC	CBD-CAD-C3D	3.53	122.31	112.53
62	3D	401	HEC	CAA-CBA-CGA	3.52	123.00	113.67
61	3N	402	HEM	C4D-ND-C1D	3.48	109.33	105.21
62	3D	401	HEC	CBA-CAA-C2A	3.41	121.96	112.53
61	3C	401	HEM	C1B-NB-C4B	3.23	109.03	105.21
62	3O	401	HEC	CMD-C2D-C1D	-3.21	120.02	125.03
62	3D	401	HEC	CMA-C3A-C2A	3.20	134.80	126.15
61	3C	402	HEM	C4D-ND-C1D	3.14	108.92	105.21
61	3C	401	HEM	CHA-C4D-ND	3.08	128.18	124.37
61	3C	402	HEM	CHD-C1D-ND	3.08	127.74	124.42
61	3C	402	HEM	C1B-NB-C4B	2.99	108.75	105.21
62	3O	401	HEC	O1D-CGD-CBD	-2.96	113.71	123.09
61	3N	402	HEM	C1B-NB-C4B	2.89	108.62	105.21
61	3N	401	HEM	CHA-C4D-ND	2.85	127.89	124.37
62	3O	401	HEC	C1D-ND-C4D	2.82	108.55	105.21
61	3N	401	HEM	C4B-C3B-C2B	-2.76	104.74	107.28
62	3D	401	HEC	O1D-CGD-CBD	-2.76	114.34	123.09
61	3N	401	HEM	C1B-NB-C4B	2.75	108.46	105.21
61	3C	401	HEM	CHD-C1D-ND	2.74	127.38	124.42
61	3N	401	HEM	C4D-ND-C1D	2.73	108.44	105.21
61	3N	401	HEM	CHD-C1D-ND	2.72	127.34	124.42
63	v1	501	FMN	C4'-C3'-C2'	-2.71	109.06	113.57
61	3C	401	HEM	C4D-ND-C1D	2.71	108.41	105.21
61	3N	402	HEM	CHC-C4B-NB	2.70	127.33	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	3N	401	HEM	CHA-C1A-NA	2.70	128.75	123.86
61	3C	402	HEM	C3B-C4B-NB	-2.67	107.55	109.47
61	3N	401	HEM	C3B-C2B-C1B	2.67	108.42	106.41
61	3C	401	HEM	CHA-C1A-NA	2.63	128.64	123.86
62	3D	401	HEC	C2D-C1D-ND	-2.61	106.84	109.84
61	3C	402	HEM	C1C-CHC-C4B	-2.58	120.54	126.02
62	3D	401	HEC	CHA-C1A-NA	-2.56	121.66	124.45
61	3N	402	HEM	CHB-C1B-C2B	-2.54	119.73	126.95
61	3N	402	HEM	C3B-C4B-NB	-2.49	107.68	109.47
62	3D	401	HEC	CAA-C2A-C3A	2.49	132.53	127.87
61	3C	402	HEM	CBB-CAB-C3B	-2.48	115.16	127.53
61	3C	401	HEM	CHB-C1B-C2B	-2.47	119.92	126.95
62	3O	401	HEC	CAD-C3D-C4D	-2.47	120.40	124.70
62	3O	401	HEC	CAD-C3D-C2D	2.43	132.41	127.87
61	3N	402	HEM	CHD-C1D-ND	2.40	127.00	124.42
61	3C	402	HEM	C2A-C1A-NA	-2.40	107.49	110.15
62	3D	401	HEC	CMB-C2B-C1B	-2.40	121.29	125.03
62	3D	401	HEC	CMD-C2D-C1D	-2.38	121.31	125.03
61	3N	402	HEM	C3B-C2B-C1B	2.36	108.19	106.41
61	3C	402	HEM	C4A-CHB-C1B	-2.36	120.69	126.25
61	3N	402	HEM	C4A-CHB-C1B	-2.36	120.70	126.25
62	3O	401	HEC	C3B-C4B-NB	-2.33	107.62	110.17
61	3N	402	HEM	C4B-C3B-C2B	-2.32	105.14	107.28
61	3C	401	HEM	C3B-C4B-NB	-2.31	107.81	109.47
62	3O	401	HEC	C4B-NB-C1B	2.30	107.93	105.21
61	3N	401	HEM	CHB-C1B-C2B	-2.30	120.42	126.95
62	3D	401	HEC	CMB-C2B-C3B	2.29	132.34	126.15
62	3D	401	HEC	C3B-C4B-NB	-2.28	107.67	110.17
61	3N	402	HEM	CHA-C1A-NA	2.26	127.95	123.86
61	3C	401	HEM	C1C-CHC-C4B	-2.25	121.23	126.02
62	3O	401	HEC	O1A-CGA-CBA	-2.25	115.96	123.09
61	3N	401	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
62	3O	401	HEC	C3D-C4D-ND	-2.22	108.21	110.35
61	3N	402	HEM	CHA-C4D-ND	2.22	127.11	124.37
61	3C	402	HEM	CHB-C1B-C2B	-2.20	120.68	126.95
61	3C	402	HEM	CHA-C1A-NA	2.20	127.86	123.86
61	3N	402	HEM	C1C-CHC-C4B	-2.20	121.35	126.02
61	3C	402	HEM	CBD-CAD-C3D	2.19	118.58	112.53
62	3D	401	HEC	O2A-CGA-O1A	2.15	128.87	123.33
61	3C	401	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
62	3O	401	HEC	CMC-C2C-C3C	2.13	130.14	125.62
62	3D	401	HEC	CHD-C4C-C3C	2.13	129.95	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	3O	401	HEC	CMB-C2B-C1B	-2.11	121.73	125.03
61	3C	402	HEM	C4C-CHD-C1D	-2.11	121.54	126.02
61	3N	402	HEM	C2A-C1A-NA	-2.10	107.82	110.15
62	3O	401	HEC	C3C-C4C-NC	-2.08	107.84	110.15
62	3D	401	HEC	CMC-C2C-C3C	2.06	129.99	125.62
62	3O	401	HEC	CMD-C2D-C3D	2.02	131.61	126.15
61	3C	402	HEM	CAA-CBA-CGA	-2.02	108.32	113.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
62	3D	401	HEC	NA
62	3O	401	HEC	NA

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	al	502	DGT	PB-O3A-PA-O5'
58	A9	501	NDP	C5B-O5B-PA-O3
58	A9	501	NDP	C2N-C3N-C7N-O7N
58	A9	501	NDP	C2N-C3N-C7N-N7N
58	a9	501	NDP	C5D-O5D-PN-O3
58	a9	501	NDP	C5D-O5D-PN-O1N
58	a9	501	NDP	C5D-O5D-PN-O2N
58	a9	501	NDP	C2D-C1D-N1N-C2N
58	a9	501	NDP	C2N-C3N-C7N-N7N
60	A6	201	EHZ	O2-C9-S1-C10
60	A6	201	EHZ	C8-C9-S1-C10
60	B9	201	EHZ	O1-C7-C8-C9
60	B9	201	EHZ	O5-C16-C17-C19
60	B9	201	EHZ	O5-C16-C17-C20
60	a6	201	EHZ	O1-C7-C8-C9
60	a6	201	EHZ	O4-C15-C16-O5
60	a6	201	EHZ	C15-C16-C17-C18
60	a6	201	EHZ	C15-C16-C17-C19
60	a6	201	EHZ	C15-C16-C17-C20
61	3C	401	HEM	C2B-C3B-CAB-CBB
61	3C	401	HEM	C4B-C3B-CAB-CBB
61	3C	401	HEM	C2C-C3C-CAC-CBC
61	3C	401	HEM	C4C-C3C-CAC-CBC
61	3C	402	HEM	C2B-C3B-CAB-CBB
61	3C	402	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
61	3C	402	HEM	C2C-C3C-CAC-CBC
61	3C	402	HEM	C4C-C3C-CAC-CBC
61	3N	401	HEM	C2B-C3B-CAB-CBB
61	3N	401	HEM	C2C-C3C-CAC-CBC
61	3N	401	HEM	C4C-C3C-CAC-CBC
61	3N	402	HEM	C2C-C3C-CAC-CBC
61	3N	402	HEM	C4C-C3C-CAC-CBC
62	3D	401	HEC	C1A-C2A-CAA-CBA
62	3D	401	HEC	C3A-C2A-CAA-CBA
63	V1	501	FMN	C1'-C2'-C3'-O3'
63	V1	501	FMN	C1'-C2'-C3'-C4'
63	v1	501	FMN	C5'-O5'-P-O2P
63	v1	501	FMN	C5'-O5'-P-O3P
60	5a	701	EHZ	C13-C12-N1-C11
63	V1	501	FMN	O2'-C2'-C3'-C4'
61	3N	402	HEM	C2A-CAA-CBA-CGA
60	5a	701	EHZ	O3-C12-N1-C11
63	V1	501	FMN	O2'-C2'-C3'-O3'
58	a9	501	NDP	C2D-C1D-N1N-C6N
62	3O	401	HEC	C4D-C3D-CAD-CBD
62	3O	401	HEC	C2D-C3D-CAD-CBD
61	3N	401	HEM	C4B-C3B-CAB-CBB
58	a9	501	NDP	O4D-C1D-N1N-C2N
61	3C	401	HEM	C2A-CAA-CBA-CGA
61	3N	401	HEM	C2A-CAA-CBA-CGA
63	v1	501	FMN	C5'-O5'-P-O1P
60	B9	201	EHZ	O5-C16-C17-C18
58	A9	501	NDP	O4D-C1D-N1N-C6N
61	3C	402	HEM	C2A-CAA-CBA-CGA
62	3D	401	HEC	C2A-CAA-CBA-CGA
60	B9	201	EHZ	C15-C16-C17-C19
60	a6	201	EHZ	C19-C17-C20-O6
58	A9	501	NDP	C2B-O2B-P2B-O1X
57	AL	502	DGT	C5'-O5'-PA-O2A
57	al	502	DGT	C5'-O5'-PA-O2A
60	a6	201	EHZ	O5-C16-C17-C20
63	V1	501	FMN	C4'-C5'-O5'-P
58	A9	501	NDP	O4D-C4D-C5D-O5D
58	a9	501	NDP	O4B-C4B-C5B-O5B
60	5a	701	EHZ	O5-C16-C17-C19
58	A9	501	NDP	PN-O3-PA-O2A
60	A6	201	EHZ	C10-C11-N1-C12

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Mol	Chain	Res	Type	Atoms
60	a6	201	EHZ	N2-C15-C16-O5
60	B9	201	EHZ	C21-C1-C2-C3
61	3N	401	HEM	CAA-CBA-CGA-O1A
61	3N	402	HEM	CAD-CBD-CGD-O1D
61	3C	401	HEM	CAD-CBD-CGD-O1D
61	3N	401	HEM	CAA-CBA-CGA-O2A
61	3C	402	HEM	CAA-CBA-CGA-O1A
62	3O	401	HEC	CAD-CBD-CGD-O2D
58	a9	501	NDP	PA-O3-PN-O1N
61	3C	401	HEM	CAD-CBD-CGD-O2D
61	3N	402	HEM	CAD-CBD-CGD-O2D
60	B9	201	EHZ	C6-C7-C8-C9
61	3C	402	HEM	CAA-CBA-CGA-O2A
61	3N	401	HEM	CAD-CBD-CGD-O2D
62	3D	401	HEC	CAD-CBD-CGD-O1D
62	3D	401	HEC	CAA-CBA-CGA-O2A
62	3O	401	HEC	CAD-CBD-CGD-O1D
61	3C	401	HEM	CAA-CBA-CGA-O2A
61	3C	401	HEM	CAA-CBA-CGA-O1A
61	3N	401	HEM	CAD-CBD-CGD-O1D
60	a6	201	EHZ	O5-C16-C17-C18
58	A9	501	NDP	PN-O3-PA-O1A
62	3D	401	HEC	CAD-CBD-CGD-O2D
58	A9	501	NDP	C3D-C4D-C5D-O5D
61	3N	402	HEM	CAA-CBA-CGA-O1A
60	5a	701	EHZ	C22-C23-C24-C25
60	B9	201	EHZ	C15-C16-C17-C20
60	a6	201	EHZ	C18-C17-C20-O6
63	v1	501	FMN	N10-C1'-C2'-O2'
61	3N	402	HEM	CAA-CBA-CGA-O2A
62	3D	401	HEC	CAA-CBA-CGA-O1A
58	a9	501	NDP	O4D-C4D-C5D-O5D
62	3O	401	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

22 monomers are involved in 32 short contacts:

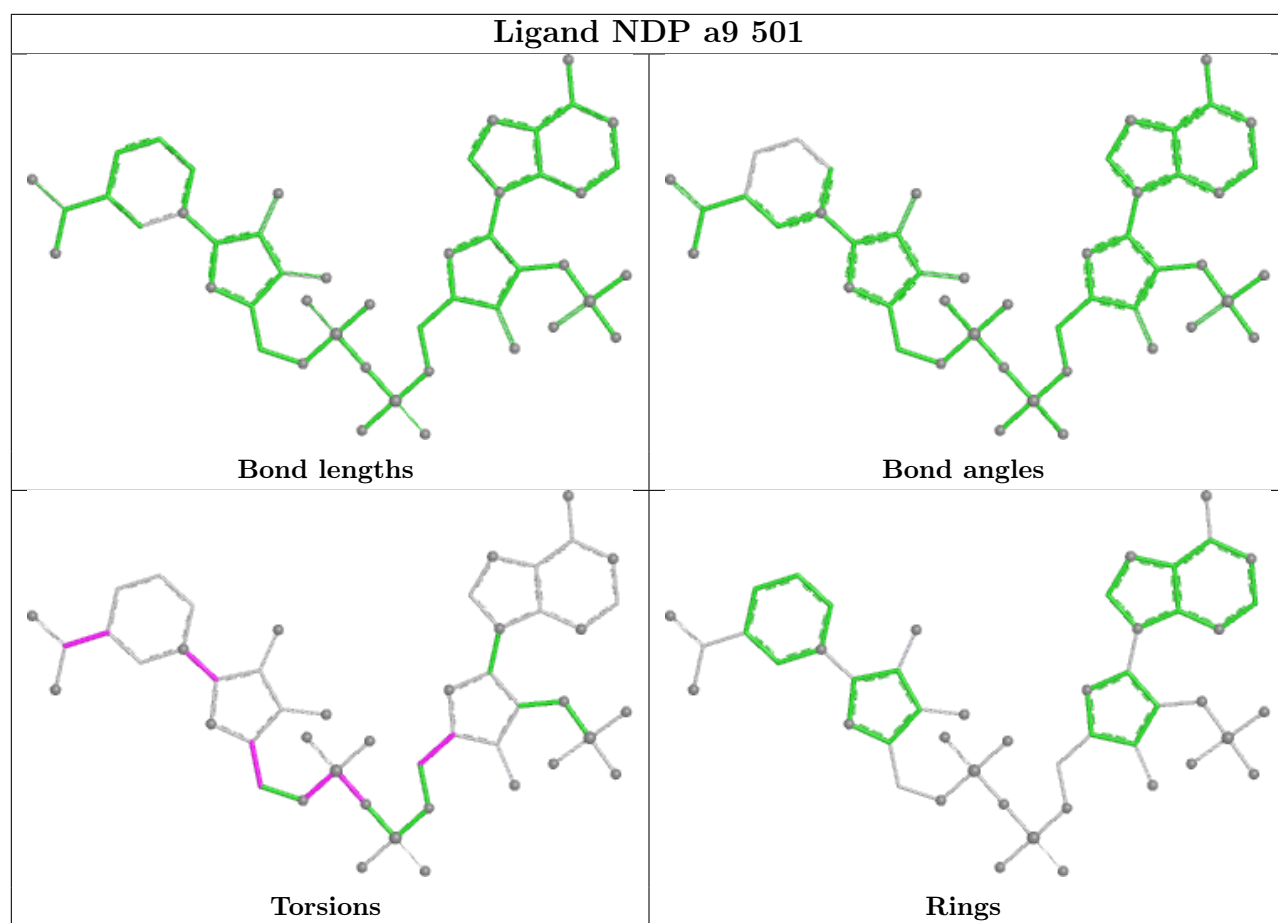
Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	V2	301	FES	1	0
64	v1	502	SF4	1	0
58	a9	501	NDP	1	0
64	S1	801	SF4	1	0

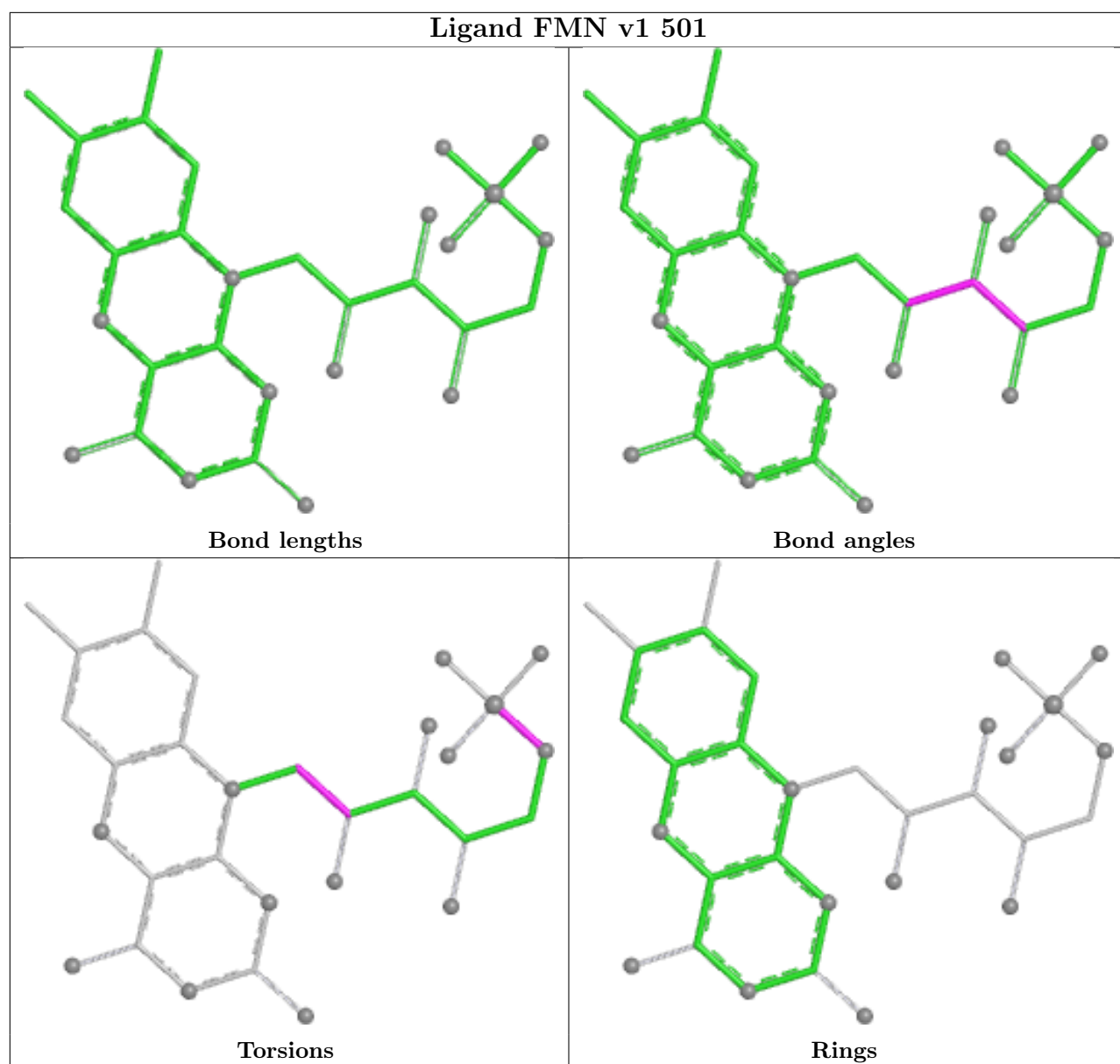
Continued on next page...

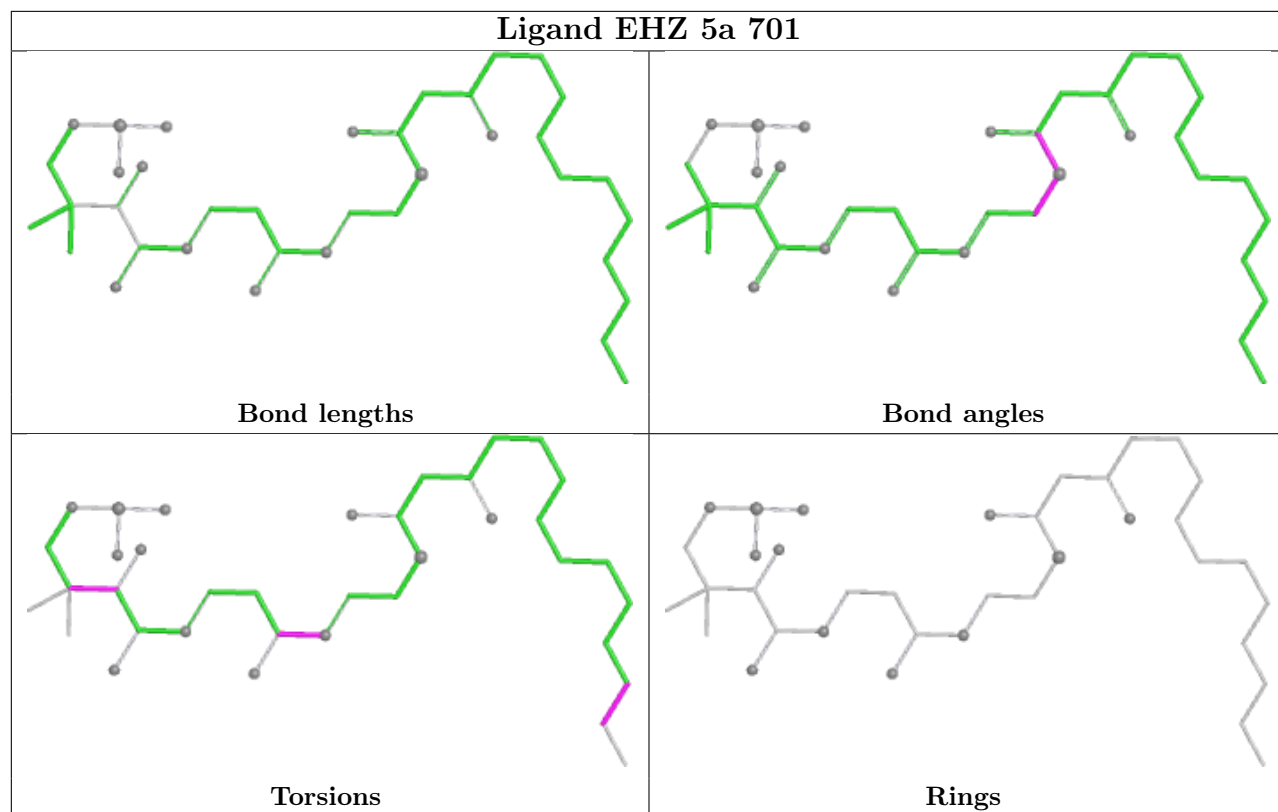
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	3N	402	HEM	1	0
61	3N	401	HEM	1	0
62	3O	401	HEC	2	0
65	s1	803	FES	1	0
65	S1	803	FES	1	0
64	S7	301	SF4	3	0
58	A9	501	NDP	3	0
65	v2	301	FES	1	0
63	V1	501	FMN	2	0
64	s1	801	SF4	1	0
62	3D	401	HEC	3	0
61	3C	401	HEM	1	0
57	AL	502	DGT	1	0
64	s8	301	SF4	2	0
64	S8	301	SF4	1	0
64	V1	502	SF4	1	0
64	s7	301	SF4	2	0
60	B9	201	EHZ	1	0

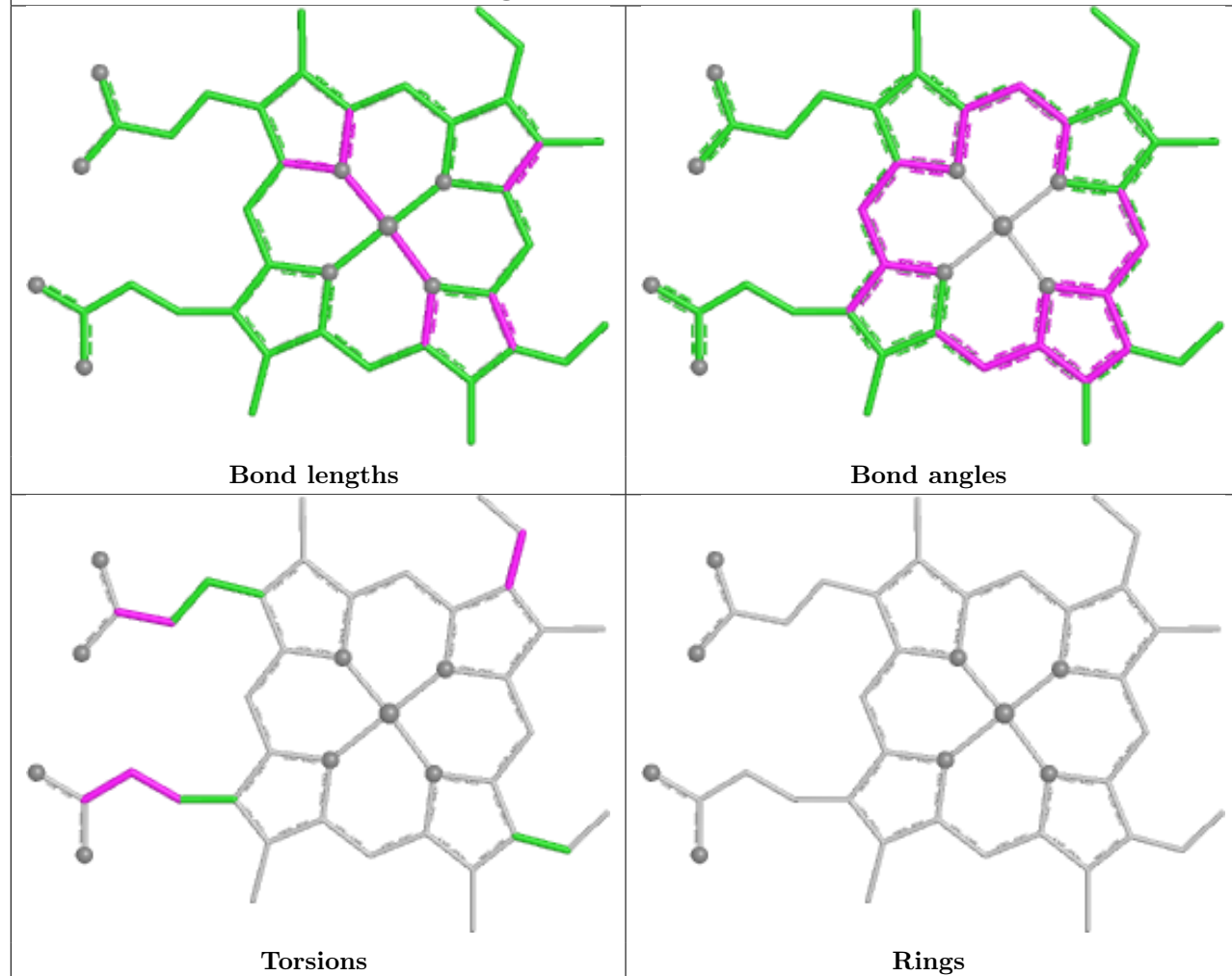
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



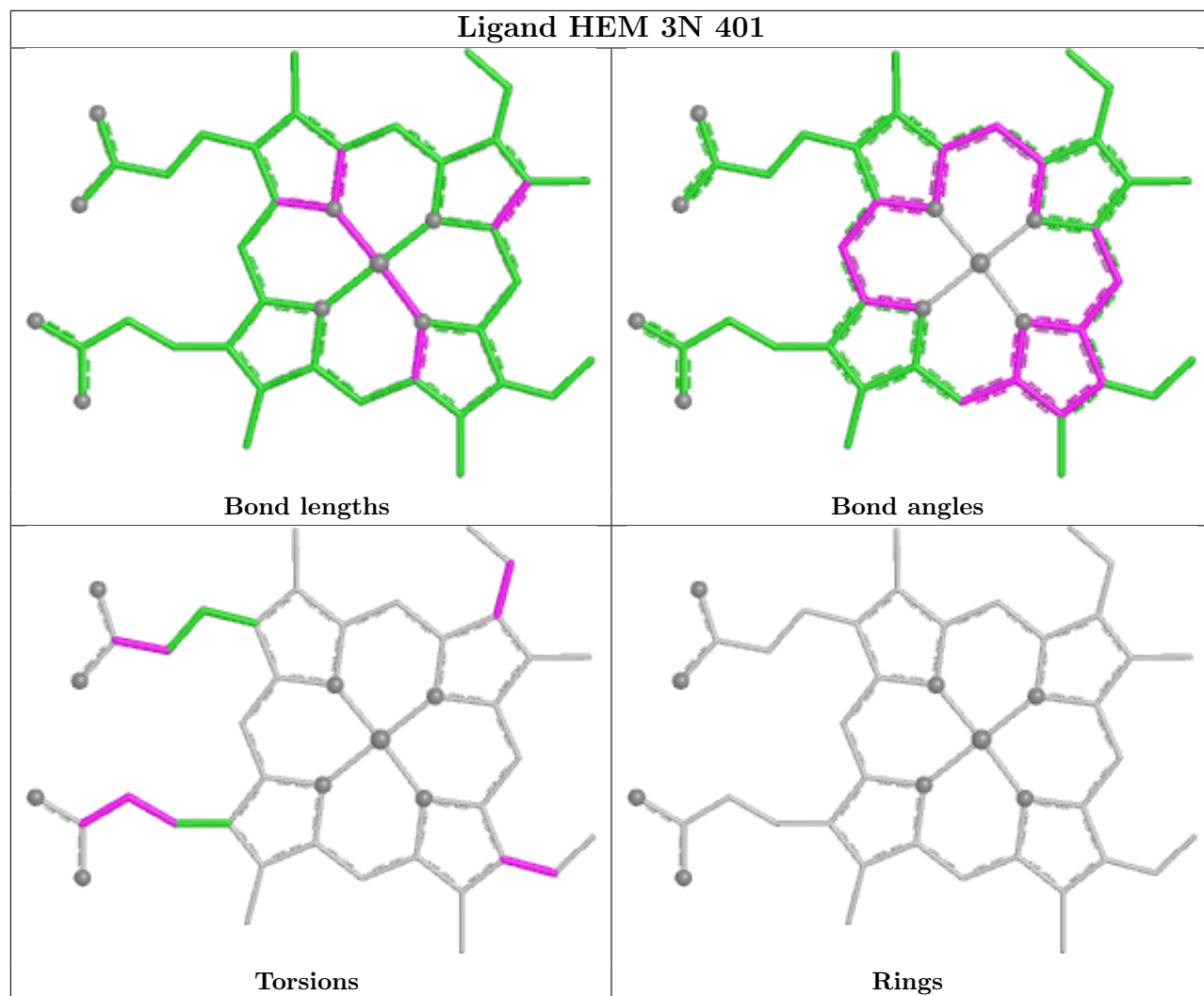


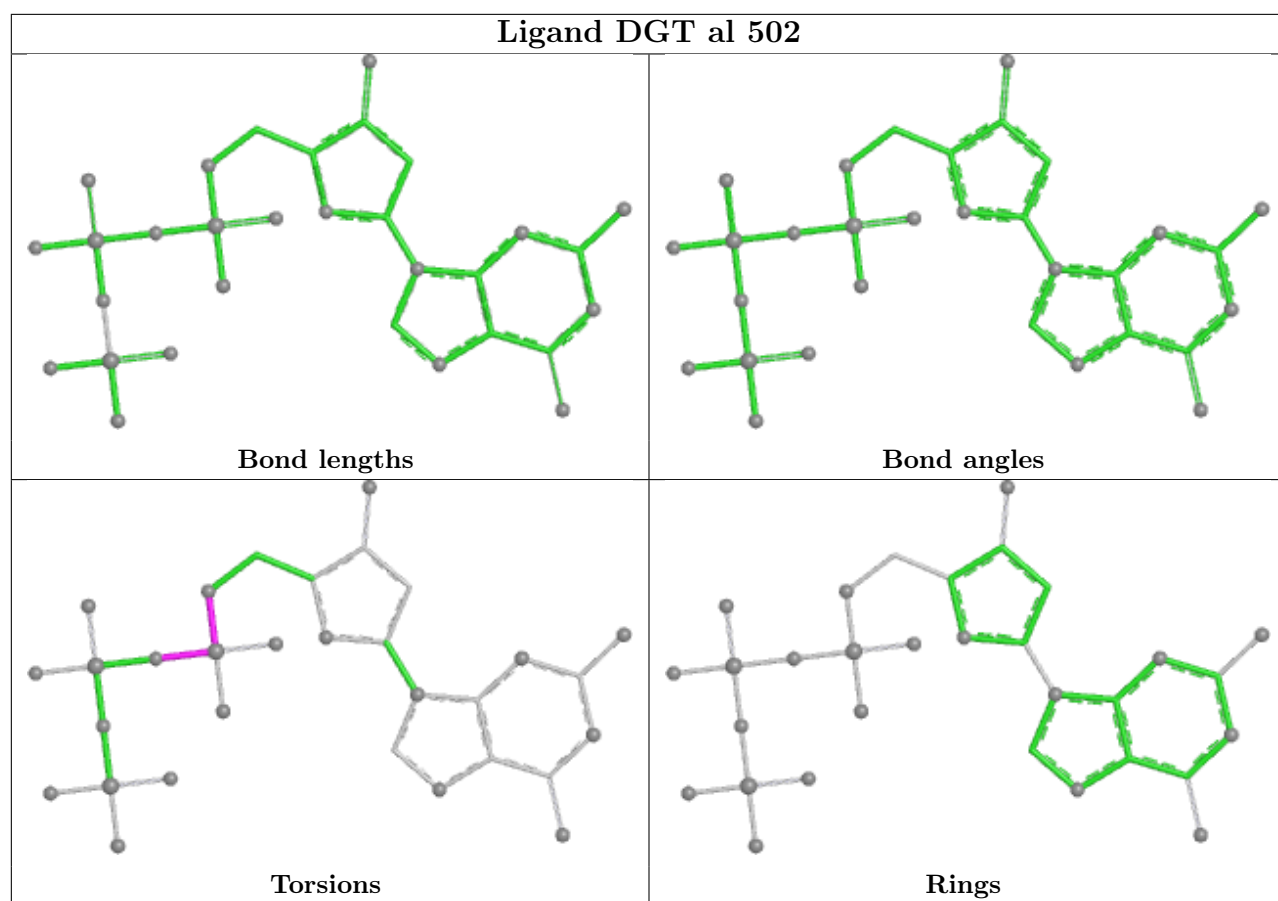


Ligand HEM 3N 402

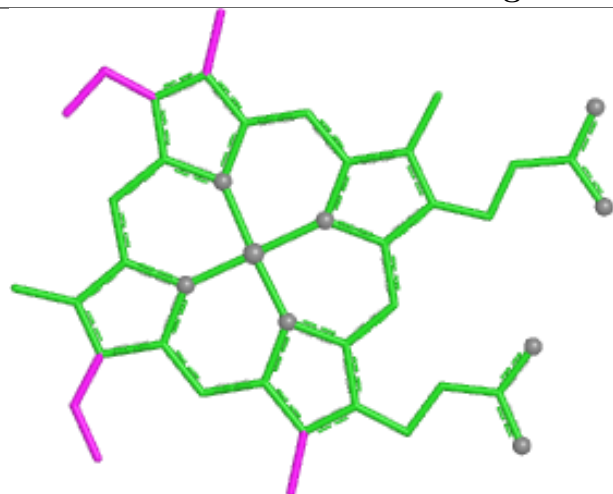


Ligand HEM 3N 401

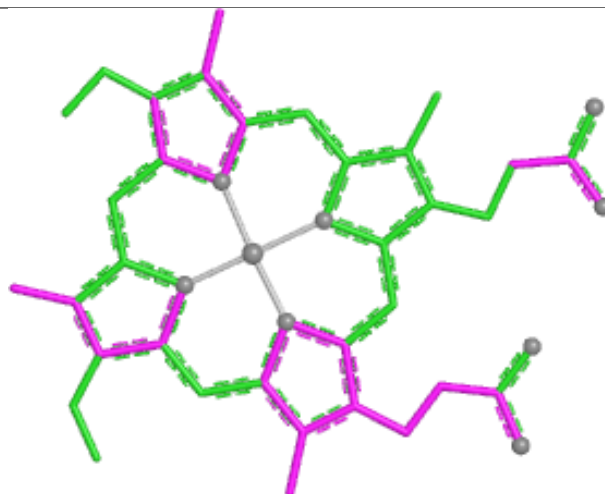




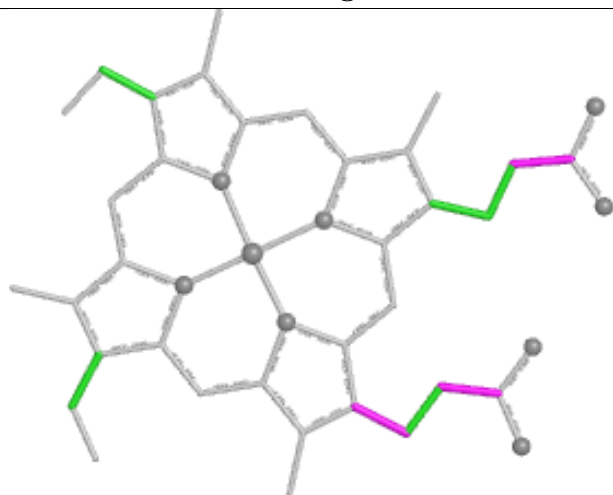
Ligand HEC 3O 401



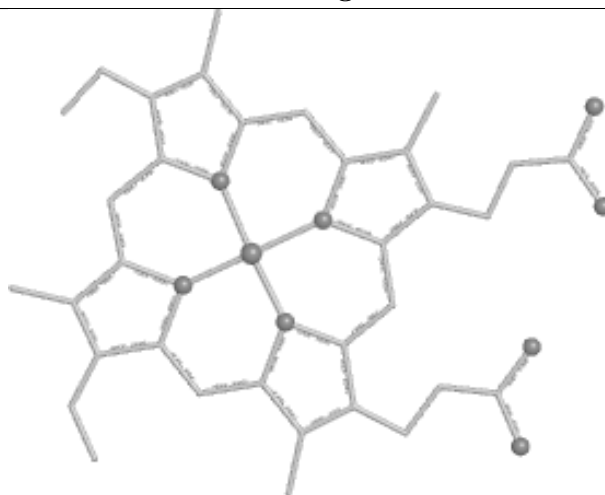
Bond lengths



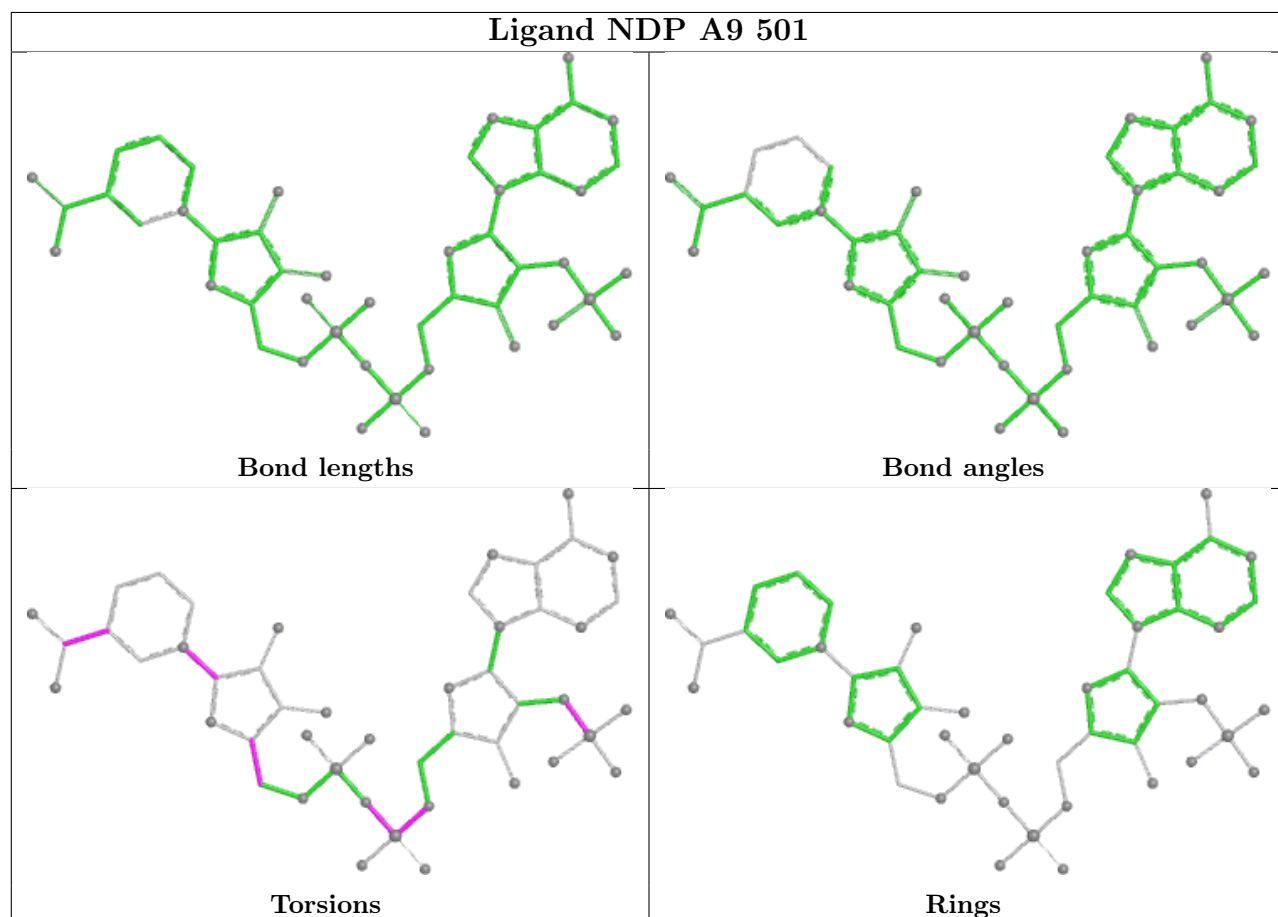
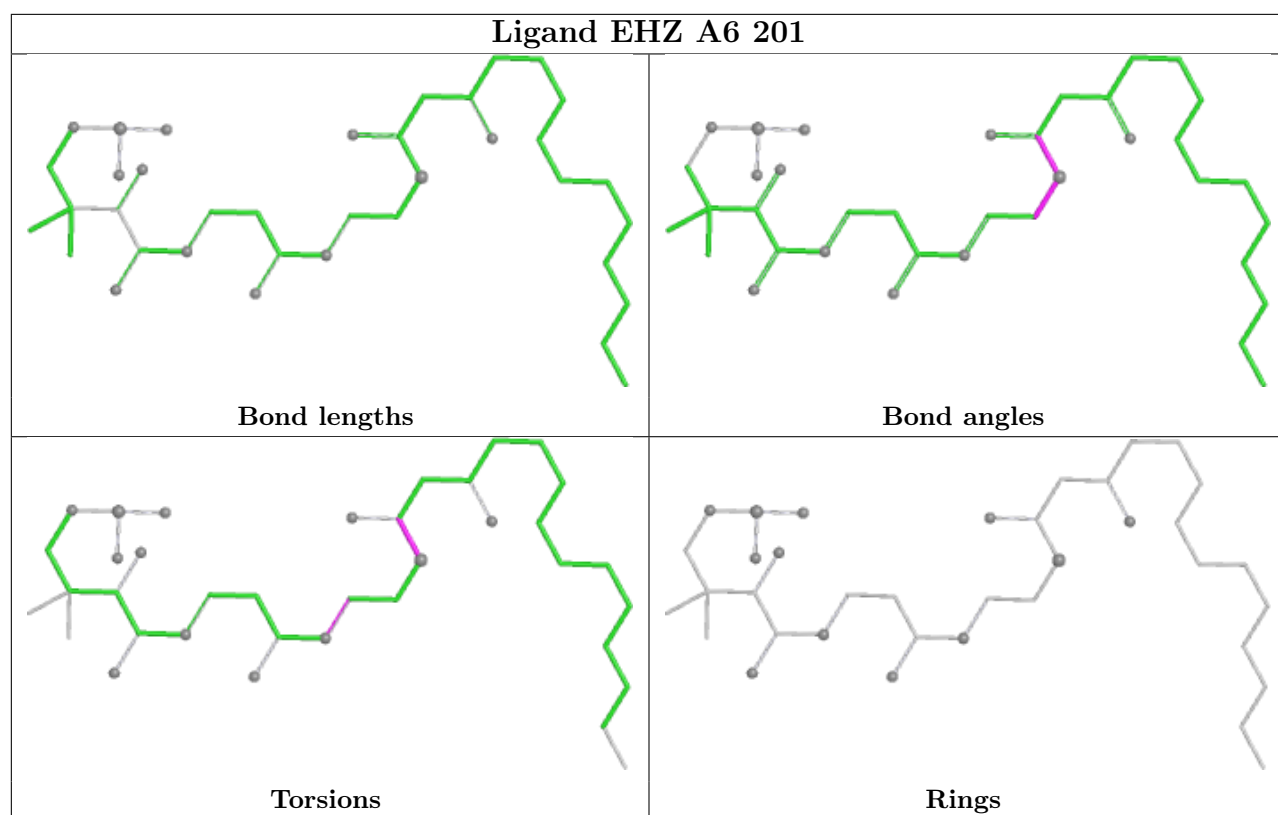
Bond angles

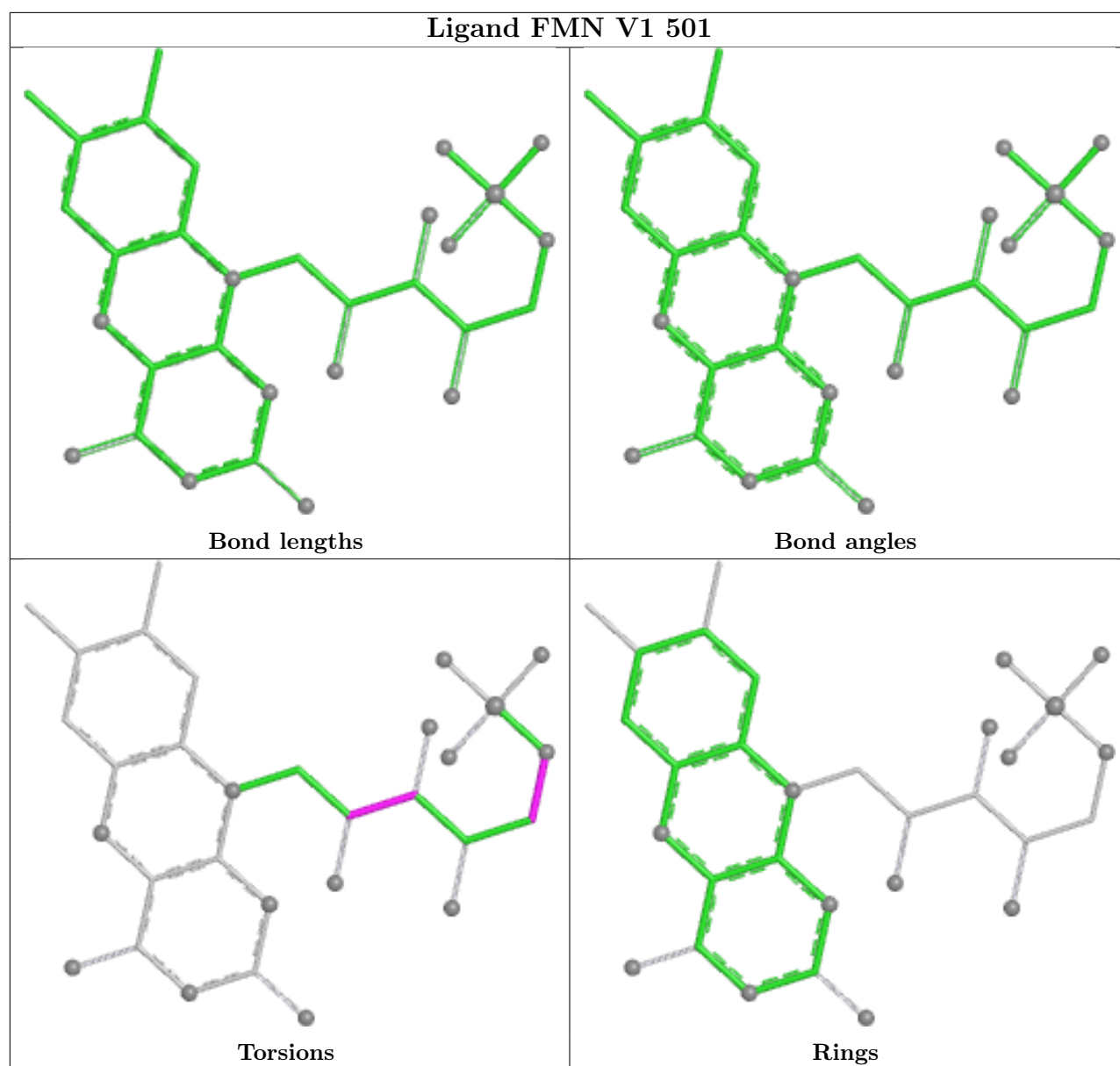


Torsions

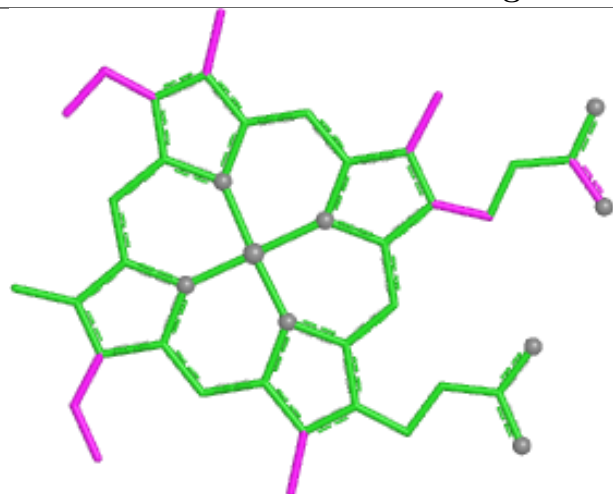


Rings

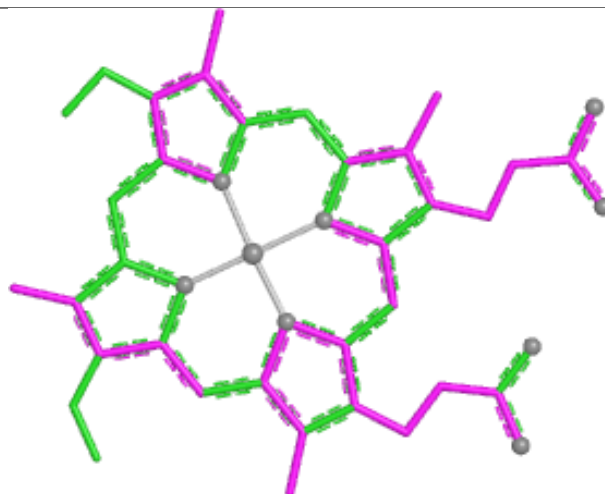




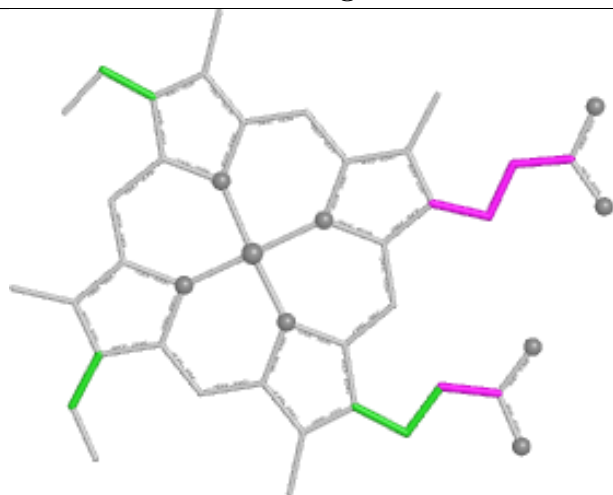
Ligand HEC 3D 401



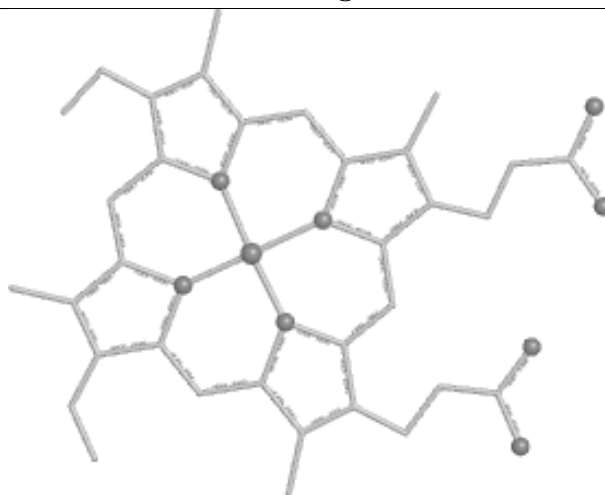
Bond lengths



Bond angles

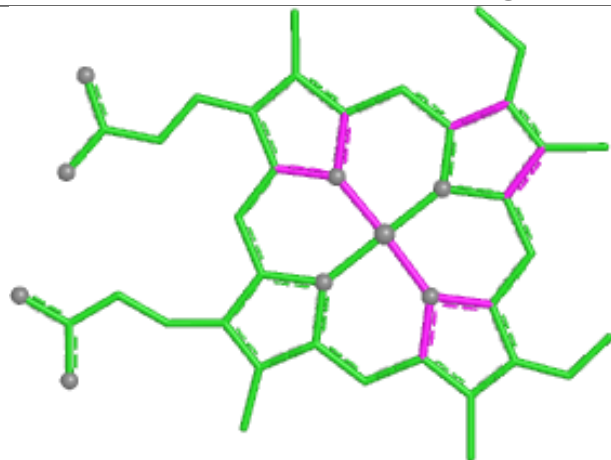


Torsions

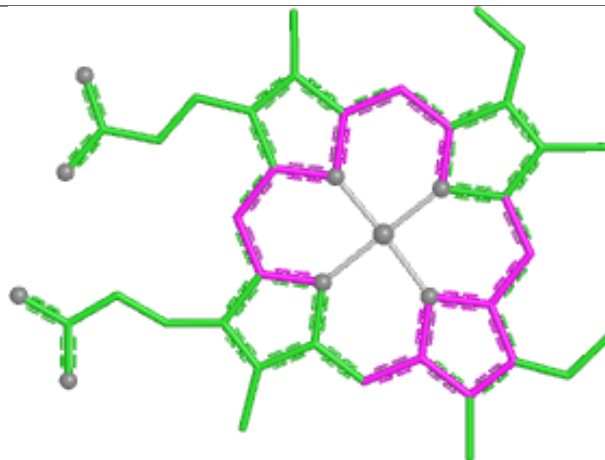


Rings

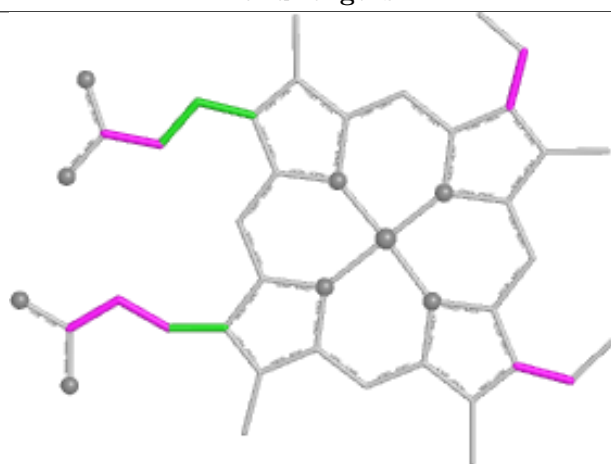
Ligand HEM 3C 401



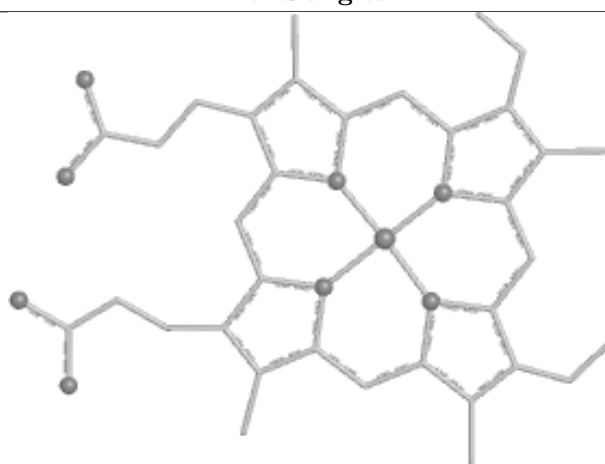
Bond lengths



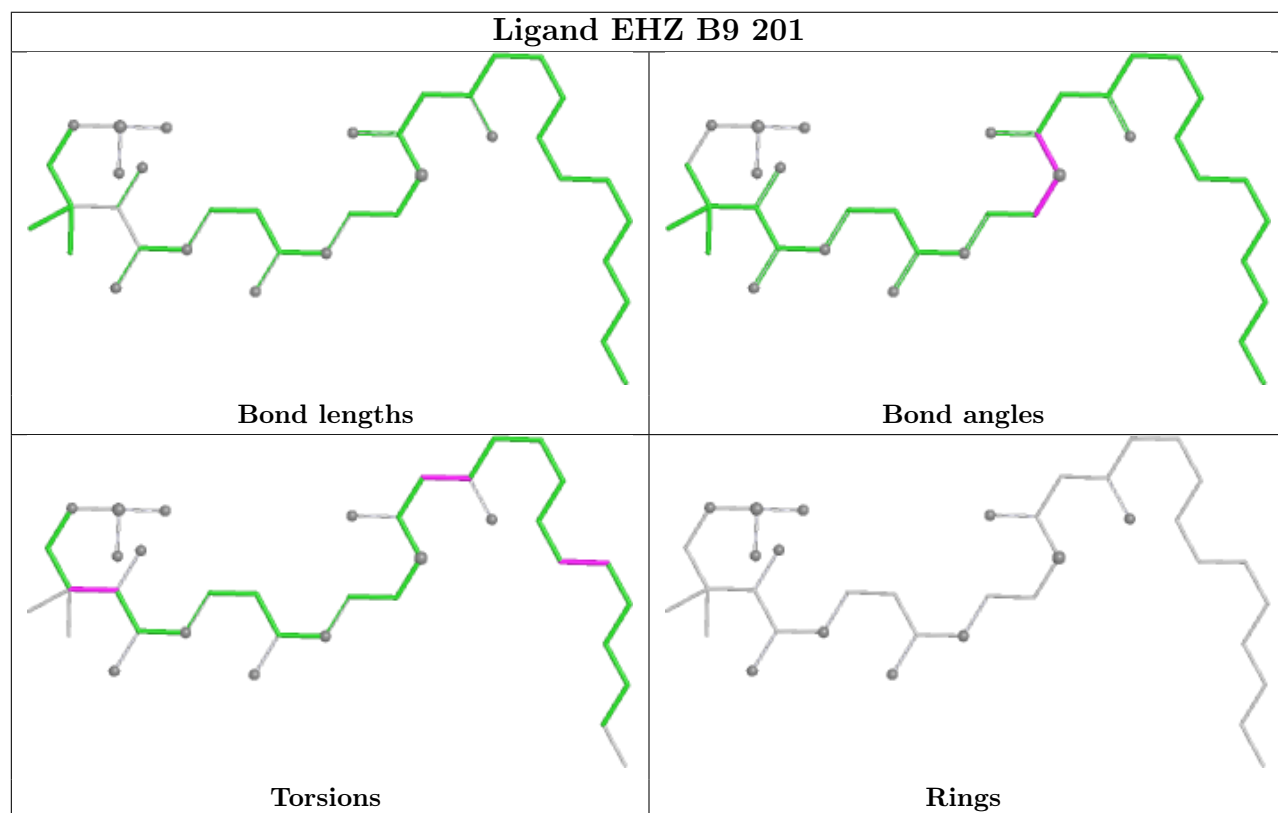
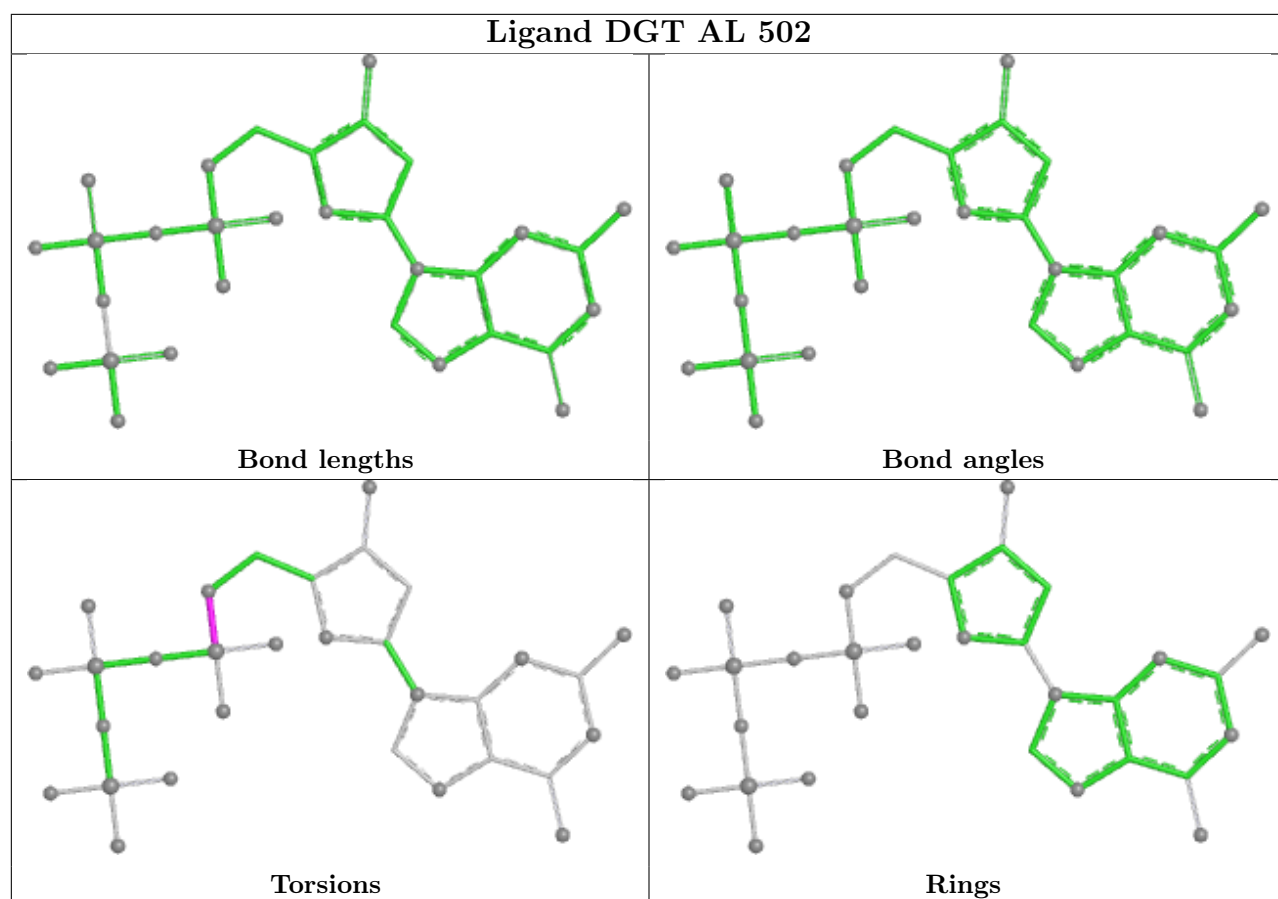
Bond angles

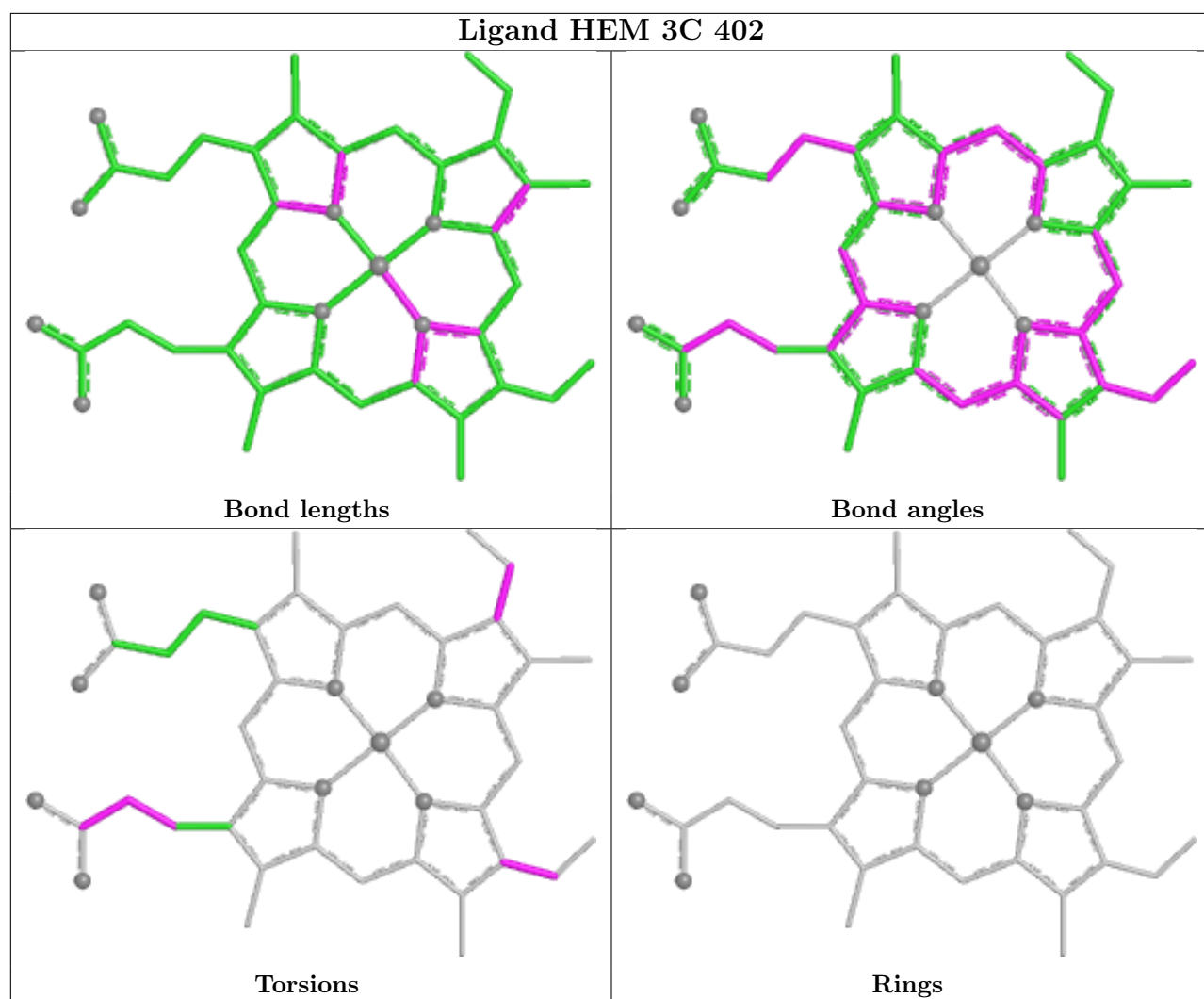


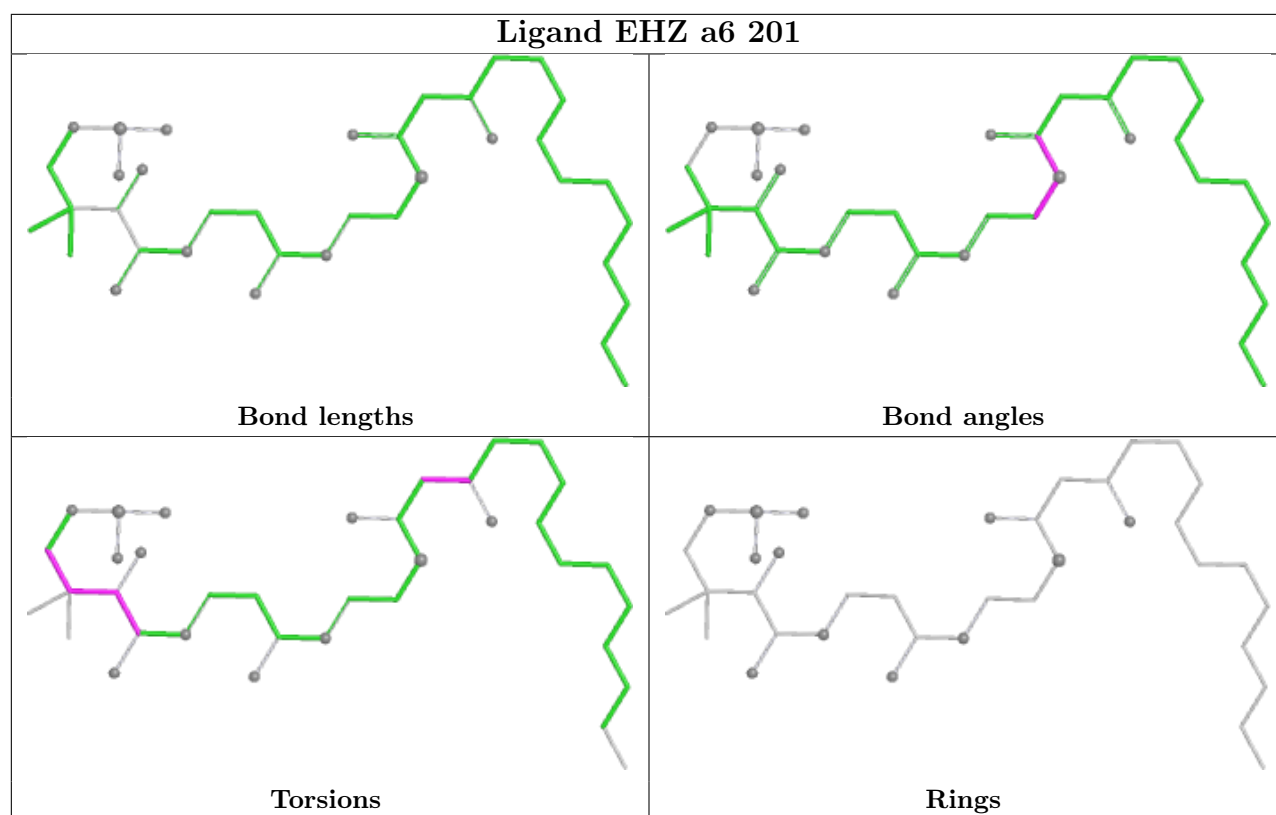
Torsions



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.

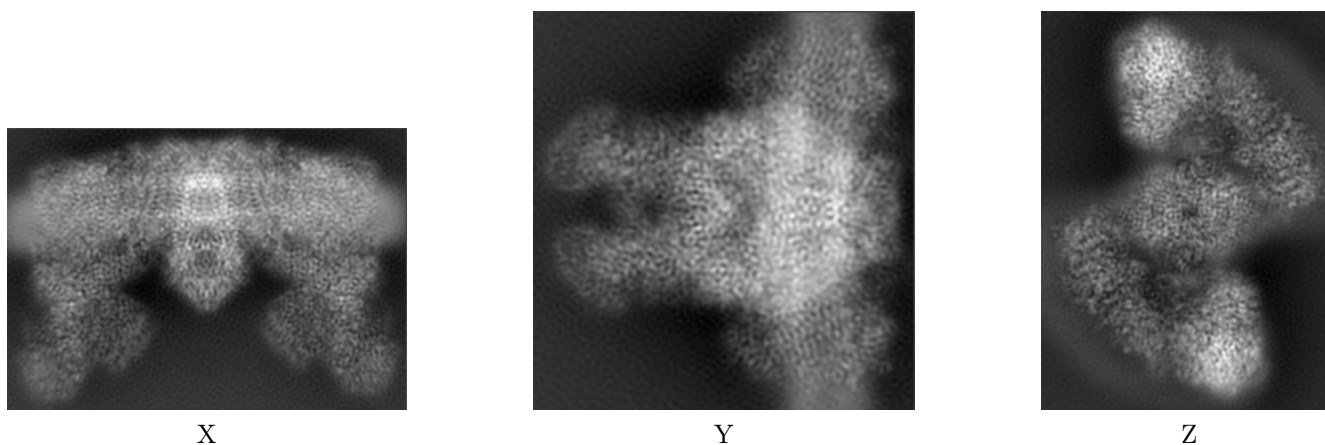
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42122. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

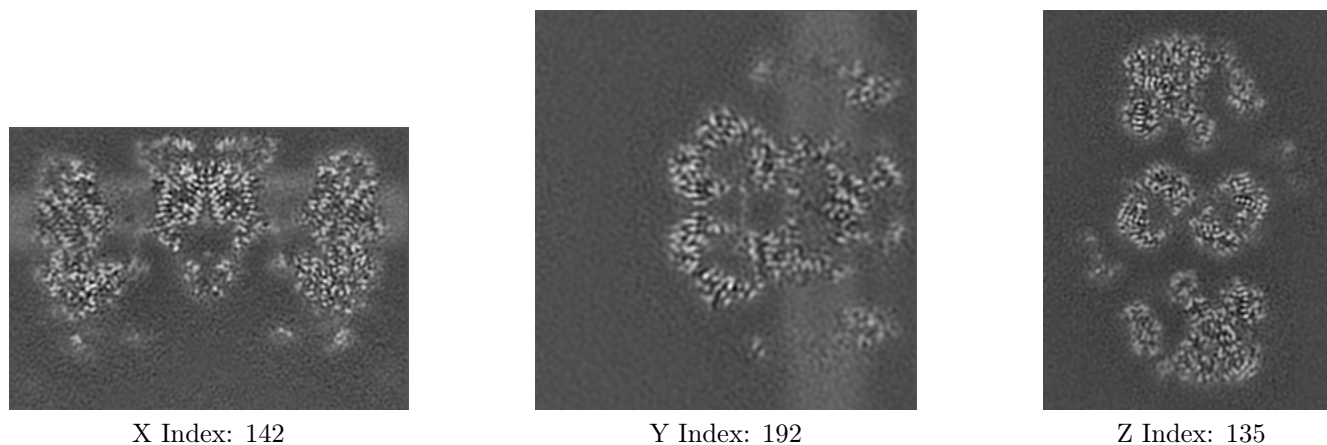
6.1.1 Primary map



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

6.2 Central slices [i](#)

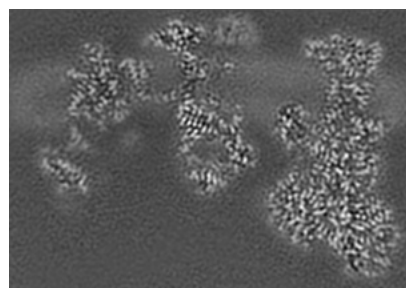
6.2.1 Primary map



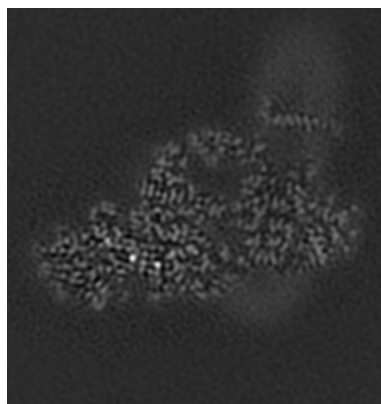
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

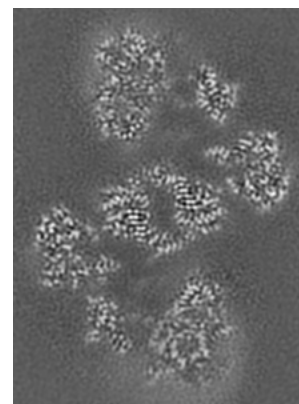
6.3.1 Primary map



X Index: 114



Y Index: 323

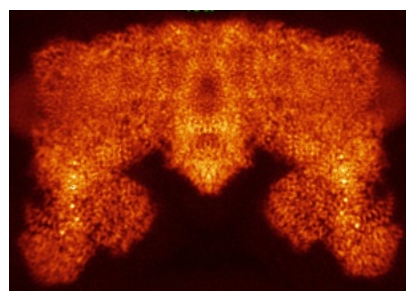


Z Index: 159

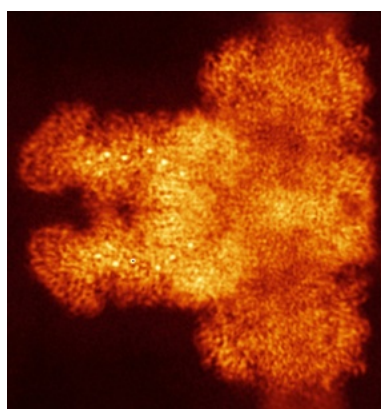
The images above show the largest variance slices of the map in three orthogonal directions.

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

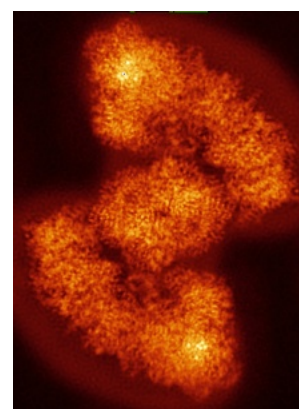
6.4.1 Primary map



X



Y

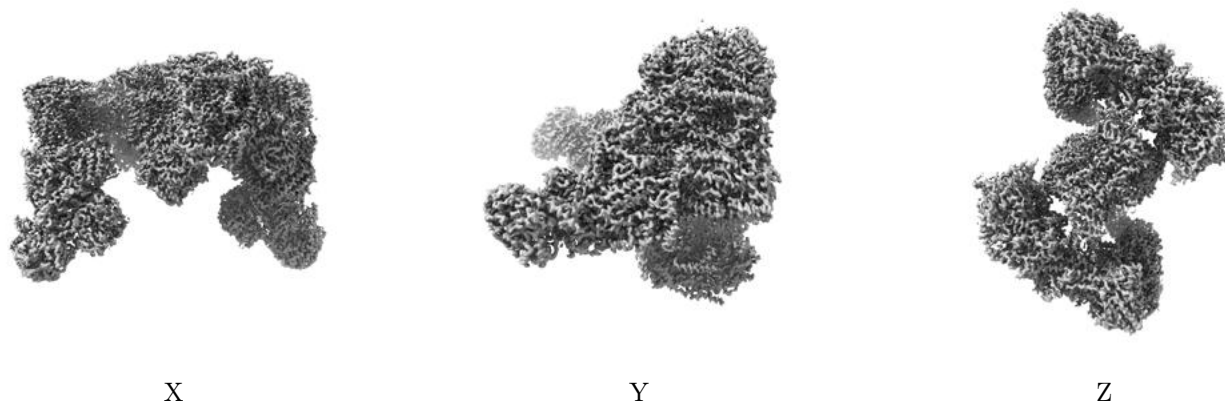


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

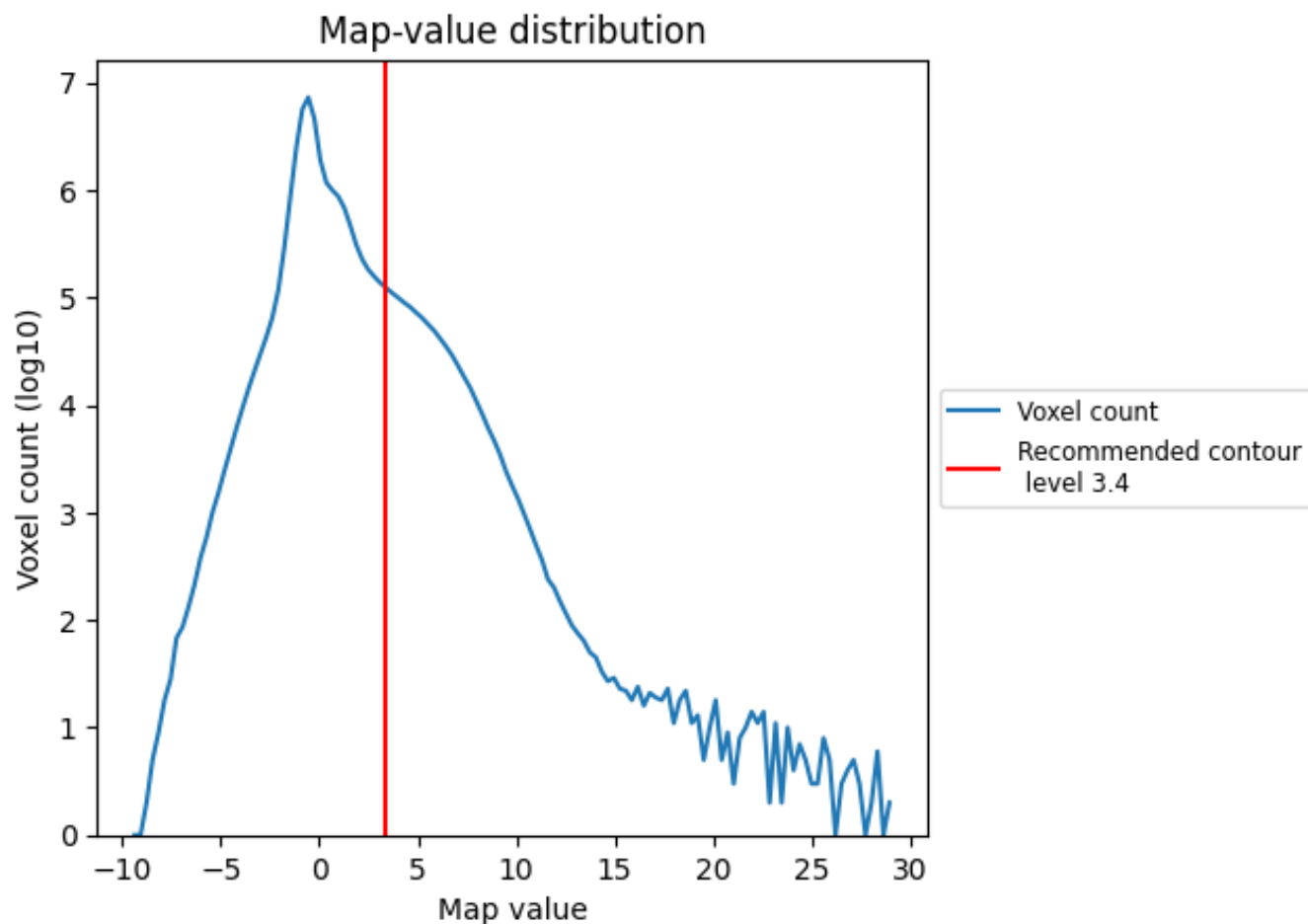
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

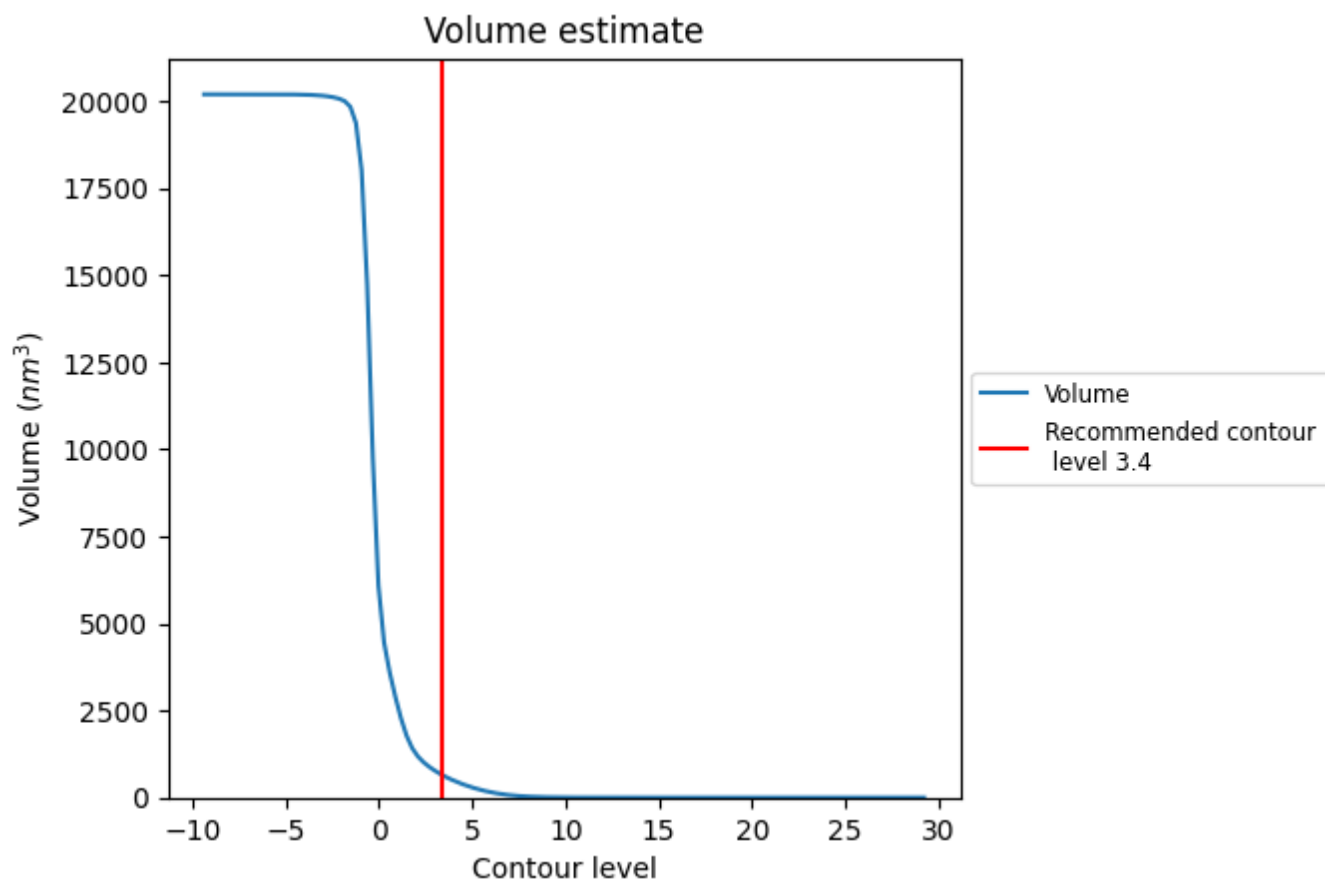
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 650 nm^3 ; this corresponds to an approximate mass of 587 kDa.

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

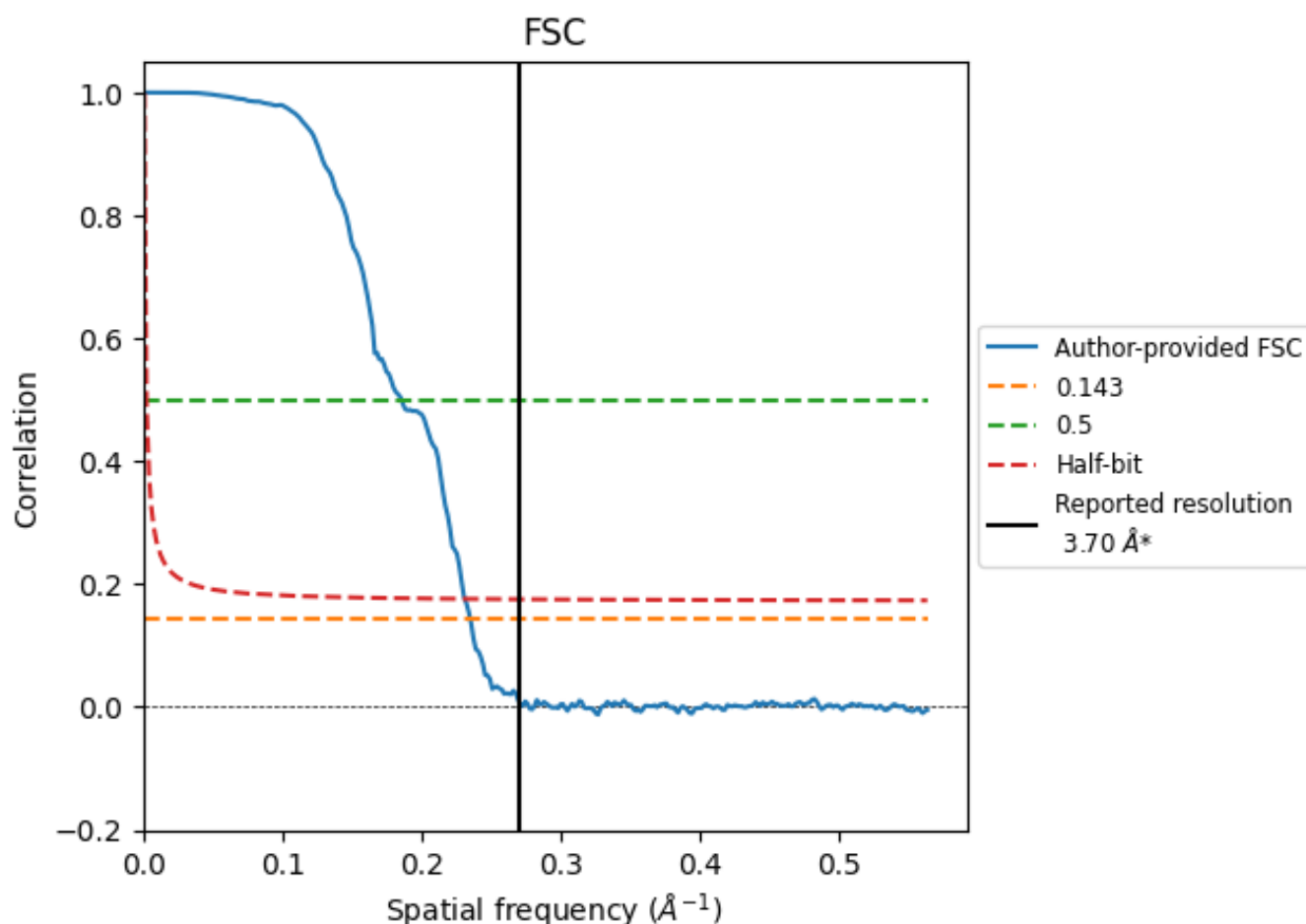
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

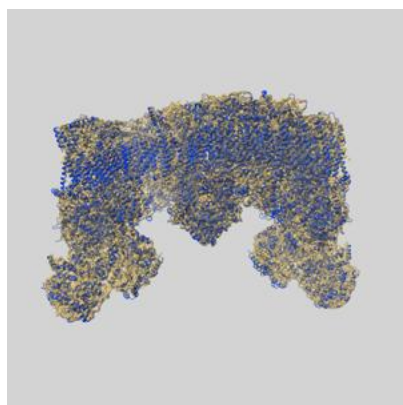
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	4.25	5.39	4.32
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.7 by more than 10 %

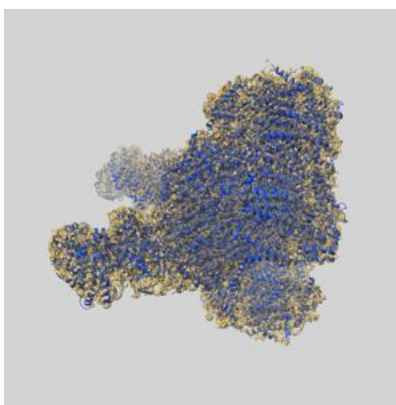
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42122 and PDB model 8UCA. Per-residue inclusion information can be found in section [3](#) on page [26](#).

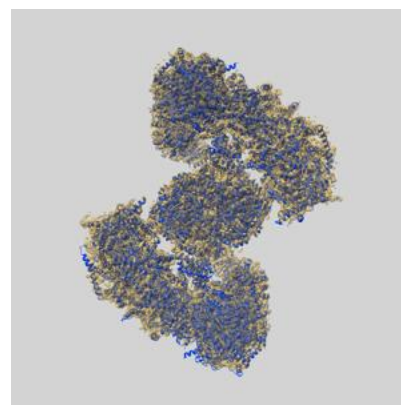
9.1 Map-model overlay [i](#)



X



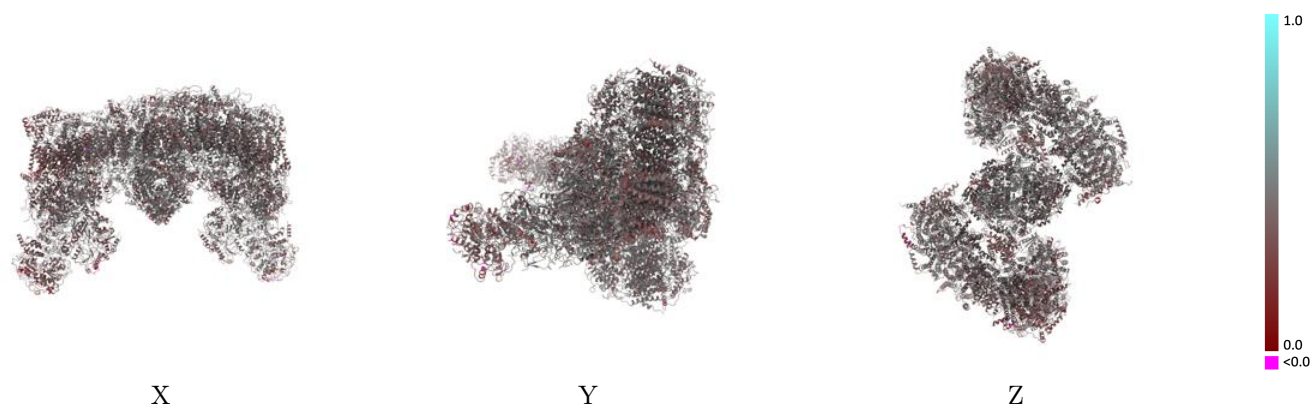
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4 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](#)



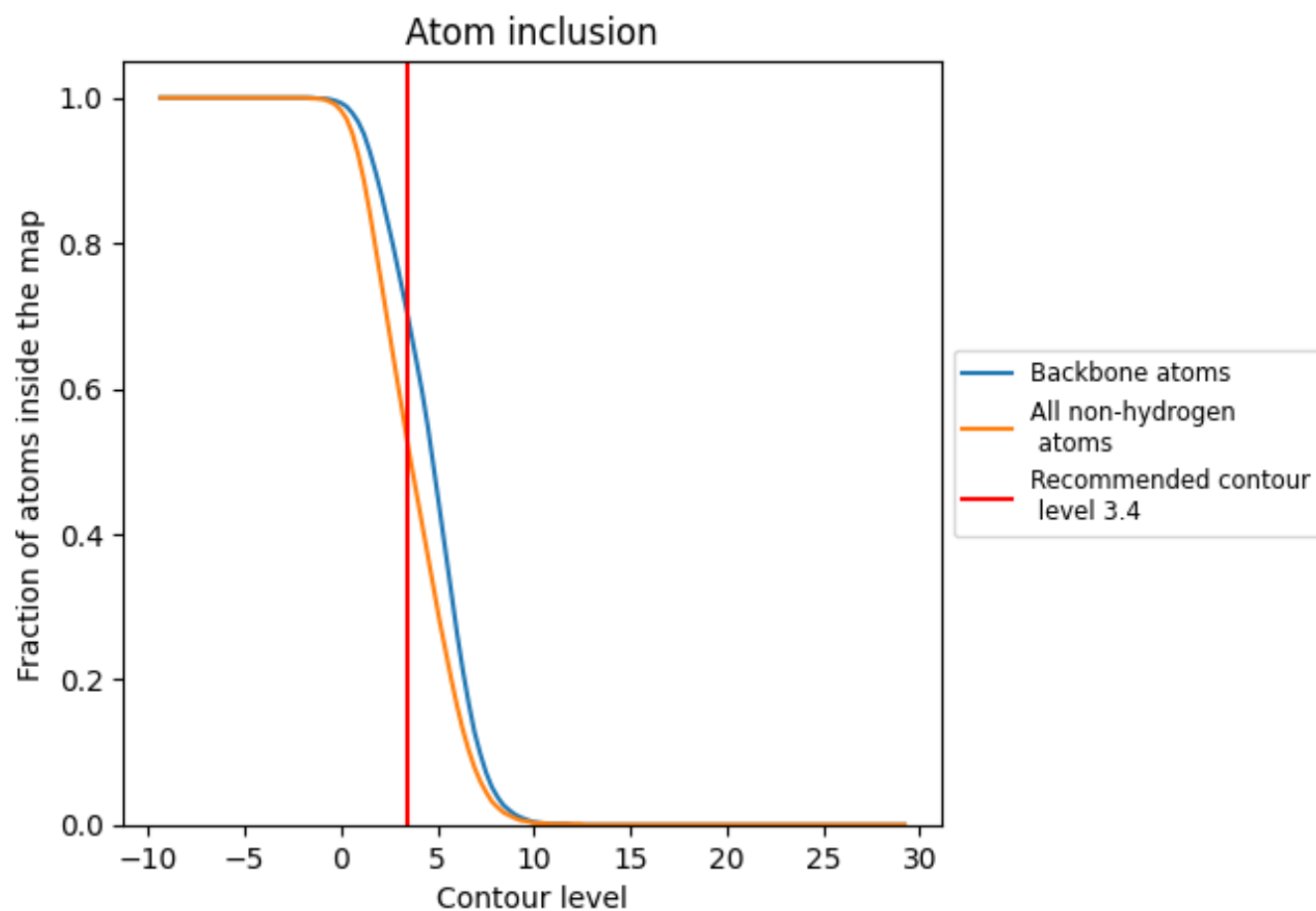
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.4110
1	 0.5210	 0.4050
1a	 0.3980	 0.3640
2	 0.5480	 0.4290
2a	 0.5150	 0.4220
3	 0.4490	 0.3920
3A	 0.6140	 0.4350
3B	 0.5740	 0.4260
3C	 0.5920	 0.4440
3D	 0.6190	 0.4400
3E	 0.5060	 0.4320
3F	 0.5480	 0.4460
3G	 0.5250	 0.4390
3H	 0.4370	 0.3540
3J	 0.5230	 0.4200
3K	 0.3370	 0.4010
3L	 0.6100	 0.4420
3M	 0.6080	 0.4430
3N	 0.5740	 0.4400
3O	 0.6000	 0.4380
3P	 0.4920	 0.4320
3Q	 0.4910	 0.4430
3R	 0.4900	 0.4270
3S	 0.2980	 0.3010
3T	 0.3250	 0.3810
3U	 0.4510	 0.3890
3V	 0.3610	 0.3500
3a	 0.3660	 0.3720
4	 0.5710	 0.4400
4L	 0.4940	 0.3990
4a	 0.5440	 0.4360
4l	 0.4650	 0.4130
5	 0.5710	 0.4280
5a	 0.5540	 0.4230
6	 0.4030	 0.3940



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Chain	Atom inclusion	Q-score
6a	 0.3330	 0.3610
A1	 0.5710	 0.3930
A2	 0.5350	 0.3830
A3	 0.4360	 0.3900
A5	 0.4740	 0.4070
A6	 0.5330	 0.4290
A7	 0.5730	 0.4530
A8	 0.5680	 0.4150
A9	 0.5830	 0.4350
AB	 0.2790	 0.3290
AC	 0.5610	 0.4100
AL	 0.5300	 0.4090
AM	 0.4050	 0.3950
AN	 0.6070	 0.4500
AO	 0.5450	 0.4120
B1	 0.4540	 0.4070
B2	 0.4670	 0.3660
B3	 0.5120	 0.4090
B4	 0.5100	 0.4150
B5	 0.5930	 0.4440
B6	 0.5750	 0.4330
B7	 0.4950	 0.3860
B8	 0.5450	 0.4300
B9	 0.5830	 0.4230
BL	 0.5800	 0.4180
BM	 0.5440	 0.4290
C1	 0.4070	 0.4080
C2	 0.5450	 0.4330
S1	 0.6080	 0.4110
S2	 0.5980	 0.4350
S3	 0.6310	 0.4510
S4	 0.5670	 0.4530
S5	 0.5270	 0.4110
S6	 0.5800	 0.4490
S7	 0.6000	 0.4040
S8	 0.6340	 0.4100
V1	 0.5730	 0.3660
V2	 0.5350	 0.3580
V3	 0.5210	 0.3920
a1	 0.4350	 0.3780
a2	 0.4740	 0.3900
a3	 0.2510	 0.3150

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Chain	Atom inclusion	Q-score
a5	 0.4020	 0.3610
a6	 0.4820	 0.4280
a7	 0.4450	 0.3780
a8	 0.4440	 0.3740
a9	 0.5320	 0.4220
ab	 0.1850	 0.2990
ac	 0.5540	 0.4370
al	 0.4470	 0.3890
am	 0.3710	 0.3860
an	 0.5170	 0.4170
ao	 0.4310	 0.3790
b1	 0.3650	 0.3860
b2	 0.5240	 0.4110
b3	 0.5820	 0.4150
b4	 0.5010	 0.4210
b5	 0.5430	 0.4240
b6	 0.5630	 0.4360
b7	 0.5070	 0.3960
b8	 0.5220	 0.4340
b9	 0.5740	 0.4340
bl	 0.5090	 0.3970
bm	 0.5130	 0.4180
c1	 0.3390	 0.3770
c2	 0.4940	 0.4180
s1	 0.5610	 0.3800
s2	 0.5210	 0.4040
s3	 0.5670	 0.4270
s4	 0.5520	 0.4300
s5	 0.4720	 0.4000
s6	 0.5510	 0.4290
s7	 0.5790	 0.3810
s8	 0.5730	 0.3740
v1	 0.4820	 0.3250
v2	 0.5020	 0.3540
v3	 0.5320	 0.3610