



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 06:41 pm BST

PDB ID : 6QC2 / pdb\_00006qc2  
EMDB ID : EMD-4494  
Title : Ovine respiratory supercomplex I+III2 open class 2  
Authors : Letts, J.A.; Sazanov, L.A.  
Deposited on : 2018-12-26  
Resolution : 4.20 Å(reported)  
Based on initial models : 1PPJ, 5LNK

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

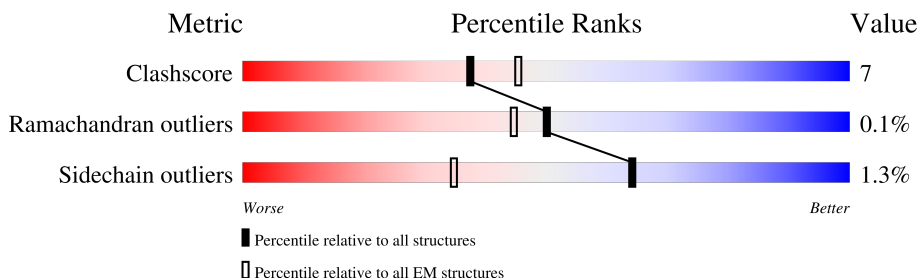
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	D3	115	<div> <div>48%</div> <div>68%</div> <div>10%</div> <div>22%</div> </div>
2	D1	318	<div> <div>37%</div> <div>68%</div> <div>24%</div> <div>7%</div> </div>
3	D6	175	<div> <div>56%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
4	4L	98	<div> <div>42%</div> <div>80%</div> <div>20%</div> </div>
5	D5	606	<div> <div>34%</div> <div>79%</div> <div>21%</div> </div>
6	D4	459	<div> <div>28%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
7	D2	347	<div> <div>26%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
8	AK	140	<div> <div>57%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	B5	143	
10	AA	88	
10	AB	88	
11	A8	171	
12	BJ	175	
13	AJ	320	
14	S5	105	
15	A3	83	
16	B3	97	
17	C2	120	
18	B4	128	
19	AM	143	
20	B6	127	
21	B7	119	
22	B9	178	
23	B2	72	
24	B8	158	
25	BK	125	
26	C1	49	
27	B1	57	
28	A1	70	
29	a1	446	
29	a3	446	
30	a2	439	
30	a4	439	

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Mol	Chain	Length	Quality of chain
31	b1	379	42% 99% .
31	b2	379	32% 99% .
32	c1	240	45% 98% .
32	c2	240	35% 98% ..
33	f1	196	88% 99% .
33	f2	196	88% 98% ..
34	d1	110	32% 88% 9%
34	d2	110	42% 89% 8%
35	q1	81	51% 90% 10%
35	q2	81	36% 91% 7%
36	h1	78	58% 81% 17%
36	h2	78	56% 81% 17%
37	x1	78	37% 42% 58%
37	x2	78	26% 38% 62%
38	i1	63	62% 86% 13%
38	i2	63	60% 90% 10%
39	V1	445	38% 74% 22%
40	V2	217	37% 75% 23%
41	S1	704	42% 72% 26%
42	S2	430	31% 78% 21%
43	S3	228	27% 74% 17% 9%
44	S7	179	21% 63% 23% 13%
45	S8	176	19% 69% 28% ..
46	V3	75	25% 39% 12% 45%
47	S6	96	33% 83% 15% ..

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Mol	Chain	Length	Quality of chain
48	S4	133	
49	A9	338	
50	A2	98	
51	A5	115	
52	A6	127	
53	A7	112	
54	AL	145	

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	SF4	S8	202	-	-	X	-
62	SF4	V1	500	-	-	X	-

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 96938 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	D3	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D1	296	Total	C	N	O	S	0	0
			2362	1599	358	386	19		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D6	168	Total	C	N	O	S	0	0
			1280	859	183	225	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D5	606	Total	C	N	O	S	0	0
			4805	3187	746	828	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D4	459	Total	C	N	O	S	0	0
			3646	2428	571	607	40		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 8 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		
10	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 12 is a protein called NDUF10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BJ	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 19 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	139	Total	C	N	O	S	0	0
			1143	733	200	201	9		

- Molecule 20 is a protein called NDUF6.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	B6	94	Total	C	N	O	S	0	0
			797	525	134	137	1		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 22 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 25 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 26 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 27 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	B1	52	Total	C	N	O	0	0
			449	296	79	74		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 28 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 29 is a protein called UQCRC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a1	439	Total	C	N	O	S	0	0
			3409	2132	603	654	20		
29	a3	444	Total	C	N	O	S	0	0
			3447	2153	608	666	20		

- Molecule 30 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a2	414	Total	C	N	O	S	0	0
			3126	1963	554	601	8		
30	a4	413	Total	C	N	O	S	0	0
			3122	1961	553	600	8		

- Molecule 31 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b1	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		
31	b2	378	Total	C	N	O	S	0	0
			3019	2029	471	498	21		

- Molecule 32 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c1	239	Total	C	N	O	S	0	0
			1909	1219	330	345	15		
32	c2	238	Total	C	N	O	S	0	0
			1903	1216	329	343	15		

- Molecule 33 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f1	196	Total	C	N	O	S	0	0
			1520	958	263	291	8		
33	f2	195	Total	C	N	O	S	0	0
			1514	955	262	289	8		

- Molecule 34 is a protein called UQCRB.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d1	100	Total	C	N	O	S	0	0
			886	566	159	159	2		
34	d2	101	Total	C	N	O	S	0	0
			888	566	159	161	2		

- Molecule 35 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q1	73	Total	C	N	O	S	0	0
			618	404	116	97	1		
35	q2	75	Total	C	N	O	S	0	0
			631	413	118	99	1		

- Molecule 36 is a protein called UQCRQH.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h1	65	Total	C	N	O	S	0	0
			532	324	96	107	5		
36	h2	65	Total	C	N	O	S	0	0
			532	324	96	107	5		

- Molecule 37 is a protein called UQCRFS1N.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	x1	33	Total	C	N	O	0	0
			164	98	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
37	x2	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 38 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	i1	55	Total	C	N	O	0	0
			459	303	80	76		
38	i2	57	Total	C	N	O	0	0
			473	312	82	79		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 40 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	V2	212	Total	C	N	O	S	0	0
			1647	1052	277	308	10		

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S1	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 42 is a protein called NDUF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S2	427	Total	C	N	O	S	0	0
			3435	2193	589	628	25		

- Molecule 43 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S3	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 44 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S7	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 45 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 46 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 47 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S4	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	A9	291	Total	C	N	O	S	0	0
			2301	1470	416	410	5		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

- Molecule 51 is a protein called NDUF5A5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

- Molecule 52 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

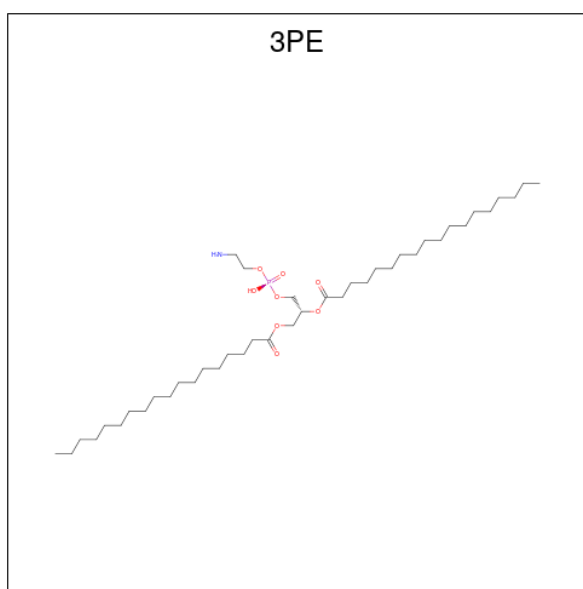
- Molecule 53 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A7	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

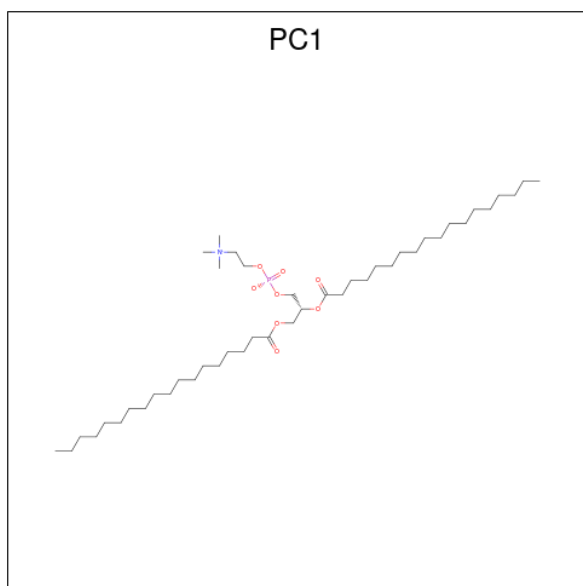
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AL	139	Total	C	N	O	S	0	0
			1160	746	209	201	4		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



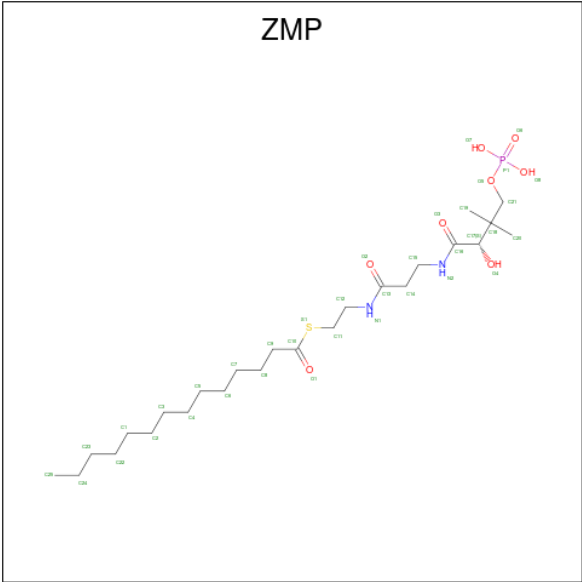
Mol	Chain	Residues	Atoms					AltConf
55	D1	1	Total	C	N	O	P	0
			32	22	1	8	1	
55	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	b2	1	Total	C	N	O	P	0
			29	19	1	8	1	
55	f2	1	Total	C	N	O	P	0
			23	13	1	8	1	

- Molecule 56 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



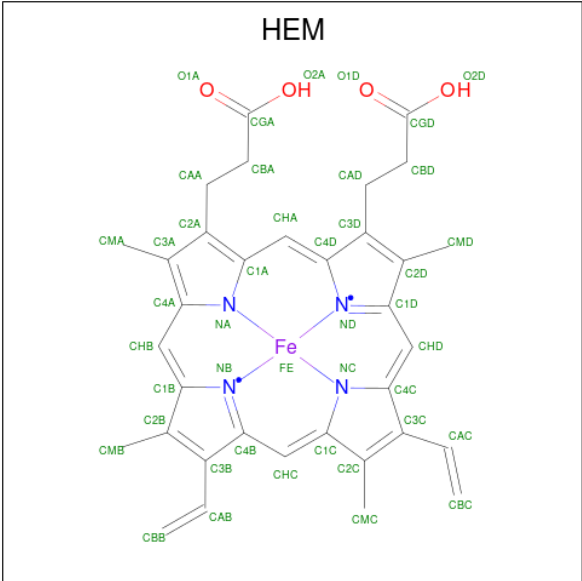
Mol	Chain	Residues	Atoms					AltConf
56	D4	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 57 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula:  $C_{25}H_{49}N_2O_8PS$ ).



Mol	Chain	Residues	Atoms						AltConf
57	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
57	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 58 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

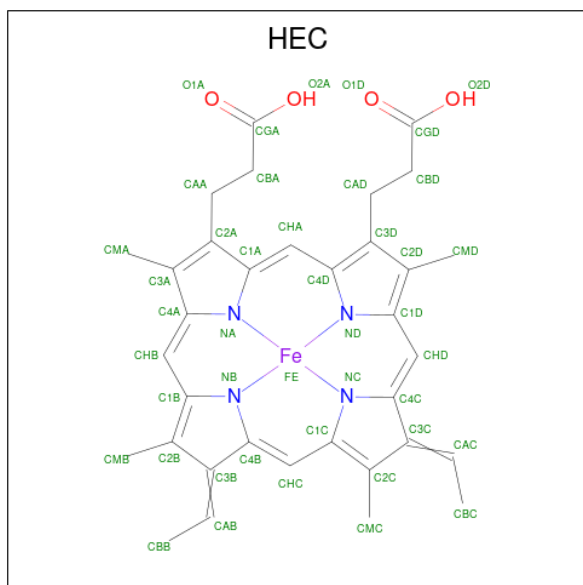




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Mol	Chain	Residues	Atoms					AltConf
58	b1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
58	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
58	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 59 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



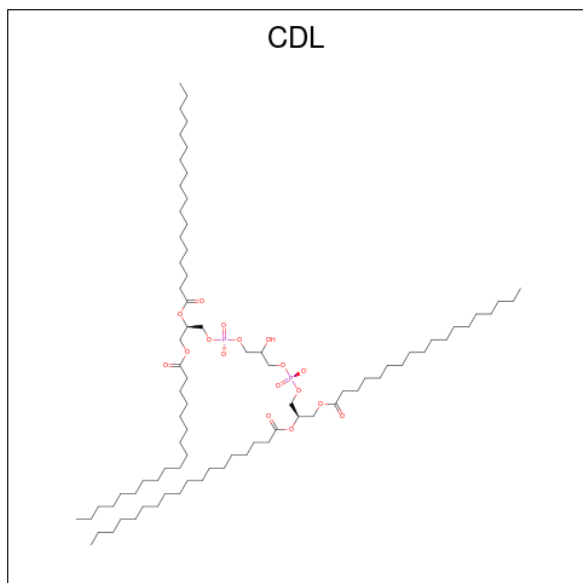
Mol	Chain	Residues	Atoms					AltConf
59	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
59	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 60 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



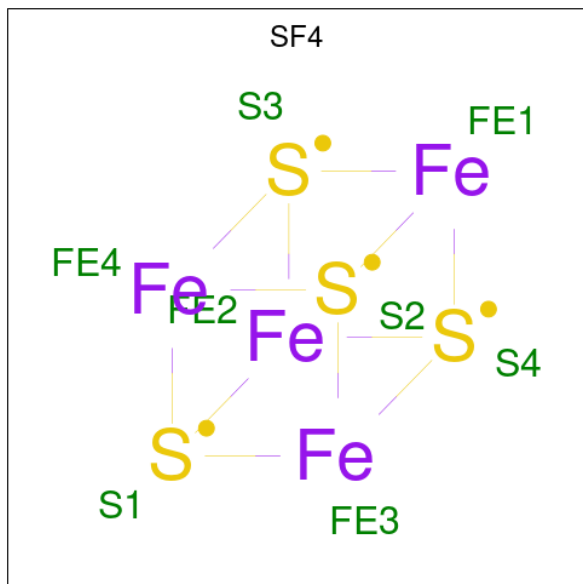
Mol	Chain	Residues	Atoms			AltConf
60	f1	1	Total	Fe	S	0
			4	2	2	
60	f2	1	Total	Fe	S	0
			4	2	2	
60	V2	1	Total	Fe	S	0
			4	2	2	
60	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 61 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
61	b2	1	Total	C	O	P	0
			38	19	17	2	
61	b2	1	Total	C	O	P	0
			41	22	17	2	
61	c2	1	Total	C	O	P	0
			41	22	17	2	

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
62	V1	1	Total	Fe	S	0
			8	4	4	
62	S1	1	Total	Fe	S	0
			8	4	4	
62	S1	1	Total	Fe	S	0
			8	4	4	
62	S7	1	Total	Fe	S	0
			8	4	4	
62	S8	1	Total	Fe	S	0
			8	4	4	
62	S8	1	Total	Fe	S	0
			8	4	4	

- Molecule 63 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).

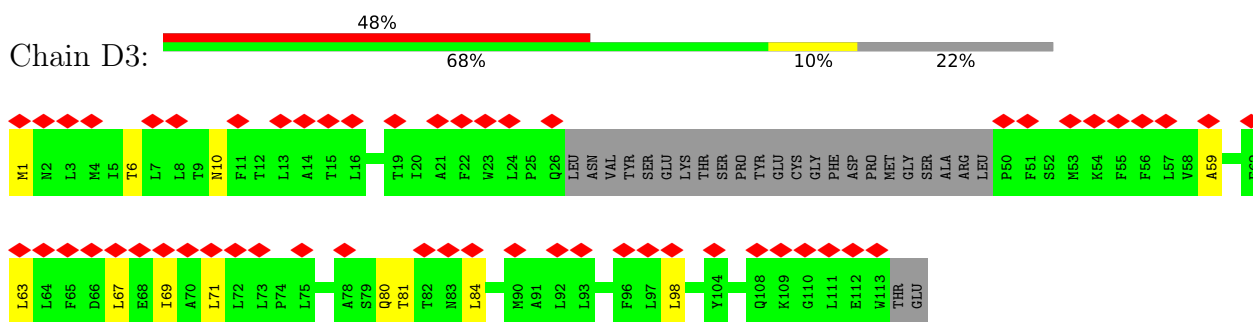


Mol	Chain	Residues	Atoms					AltConf
65	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

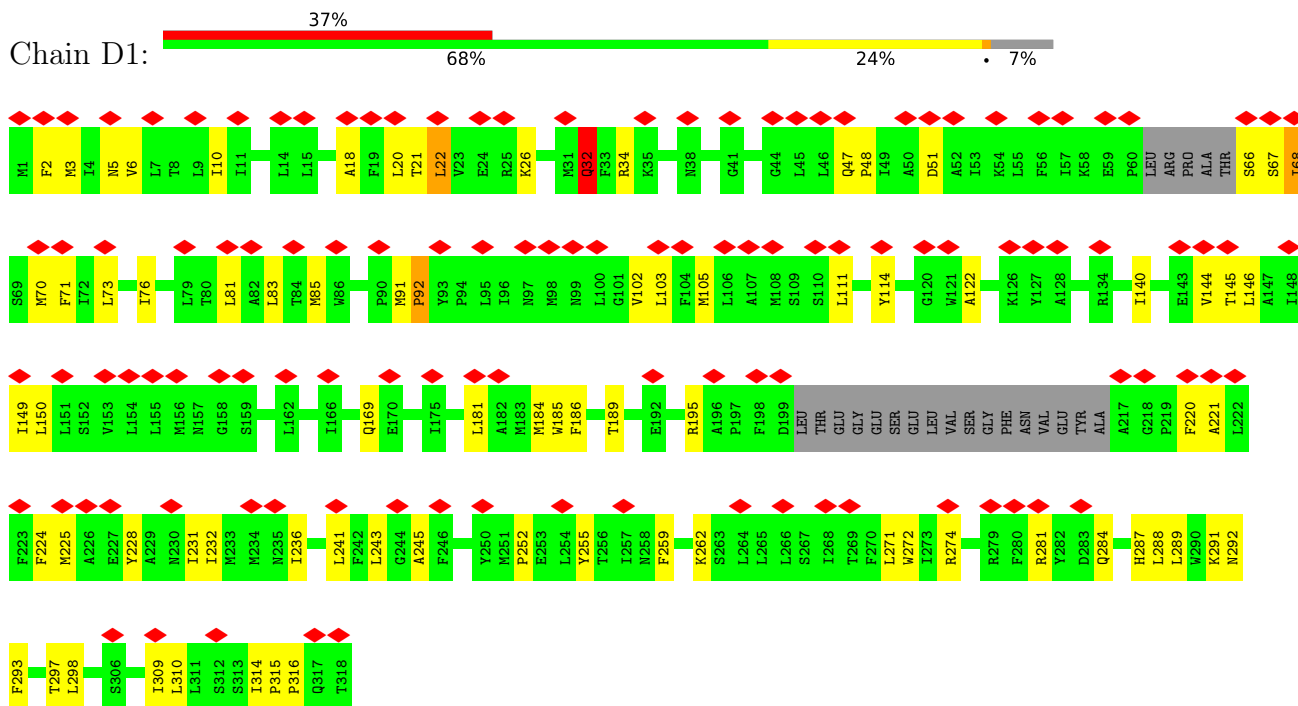
### 3 Residue-property plots

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.

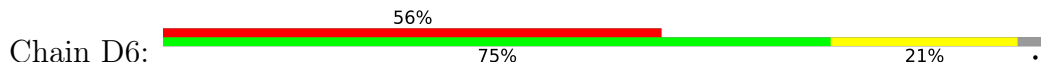
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

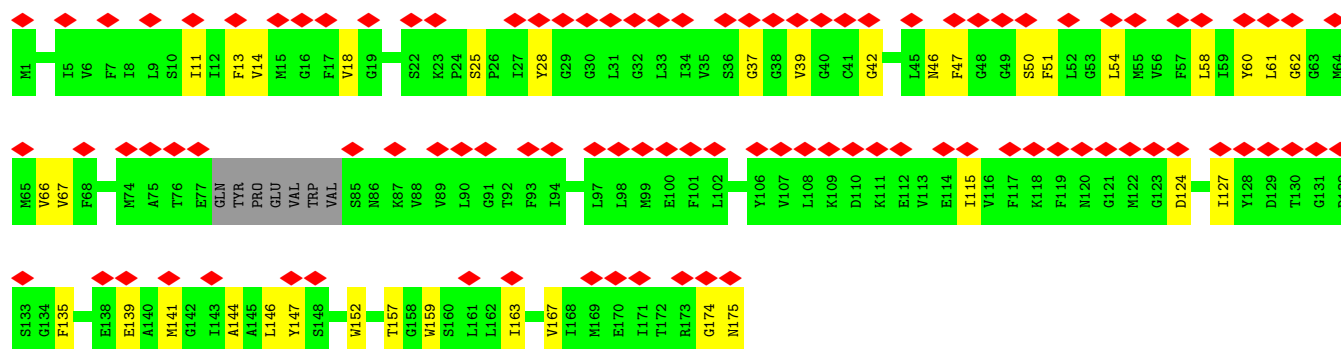


- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

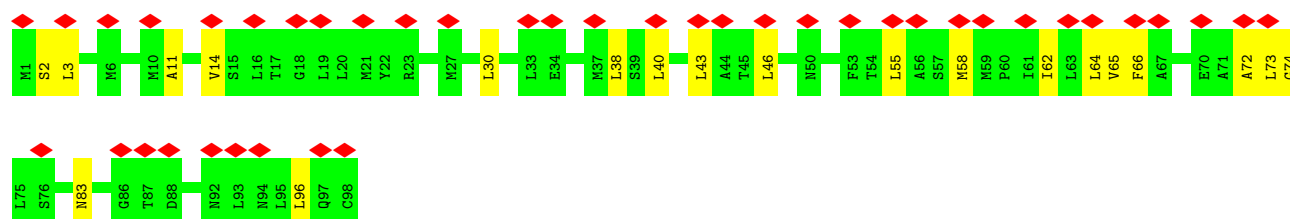
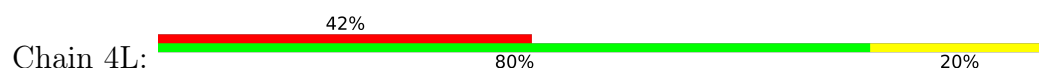


- Molecule 3: NADH-ubiquinone oxidoreductase chain 6

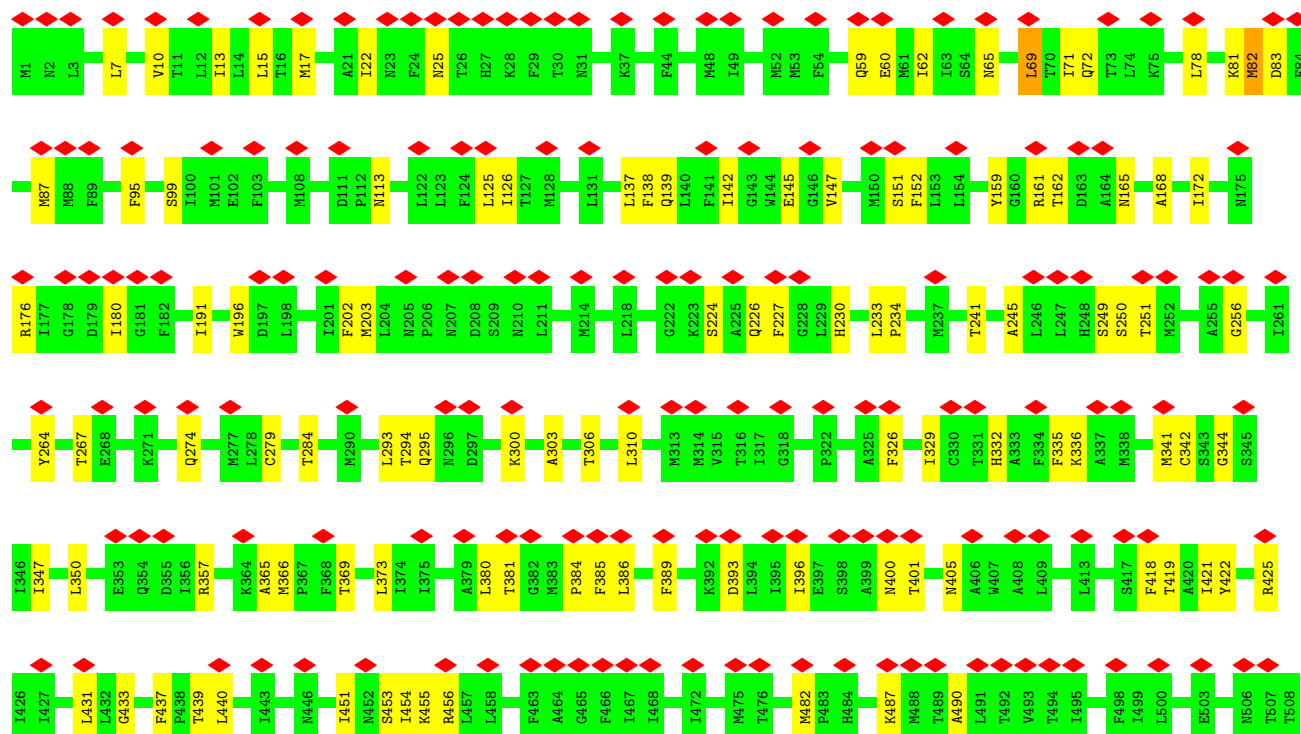
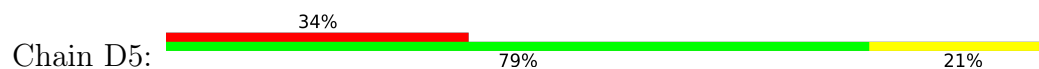


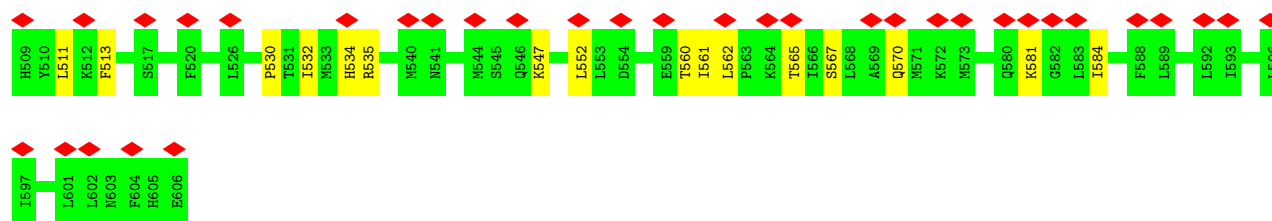


• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

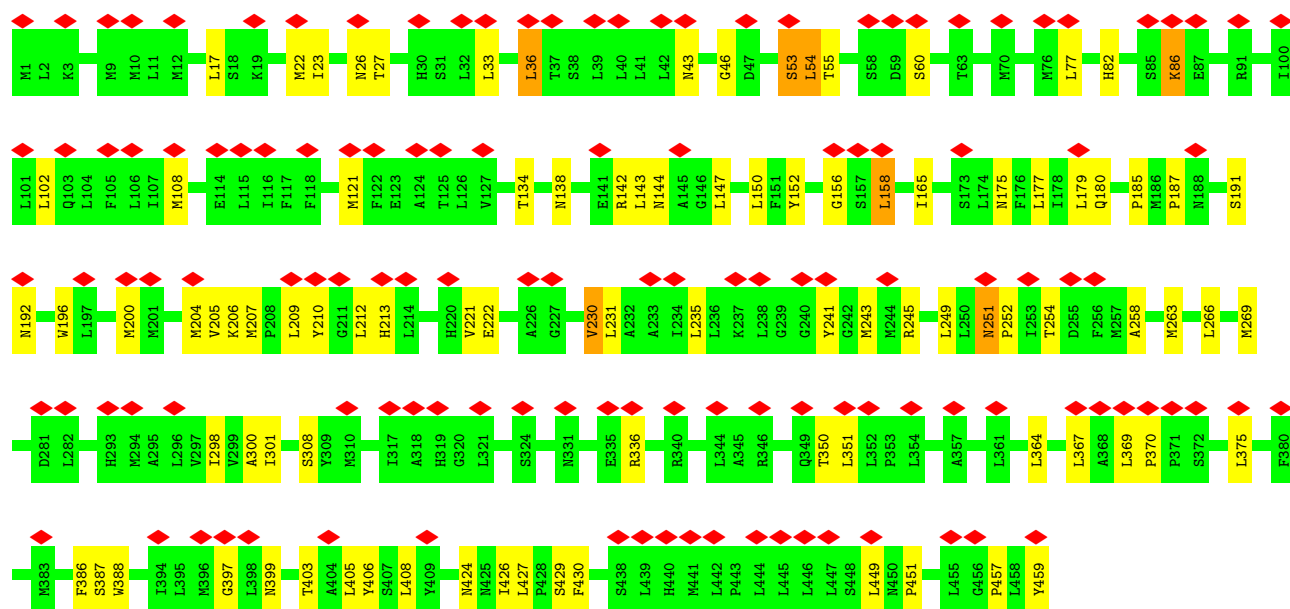
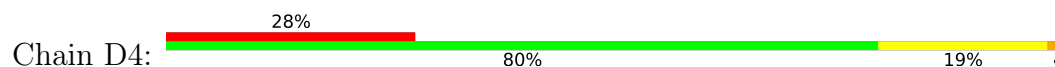


• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

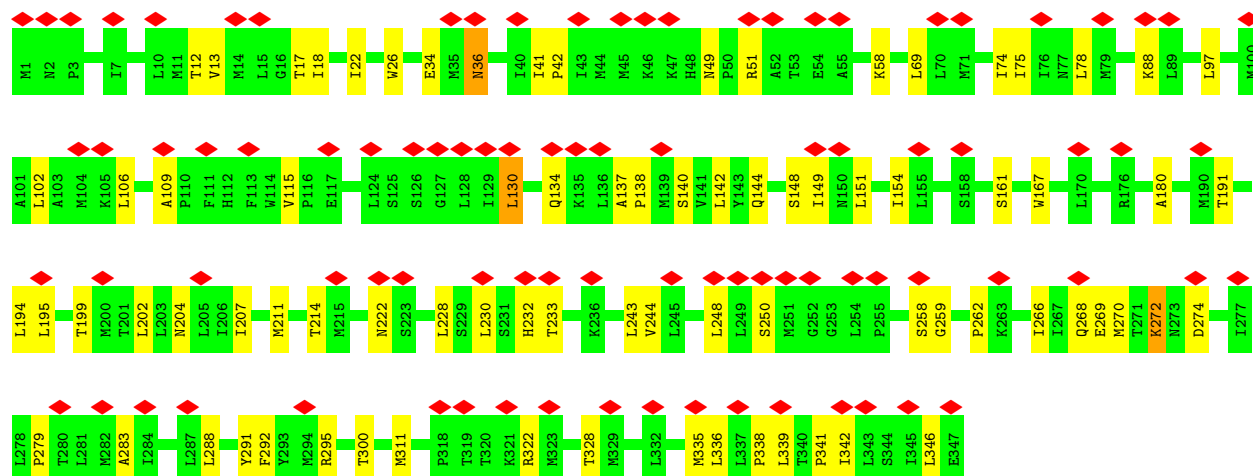
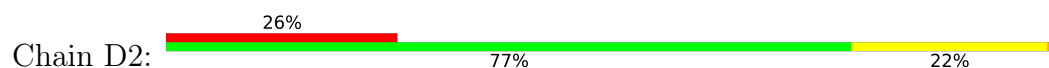




• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

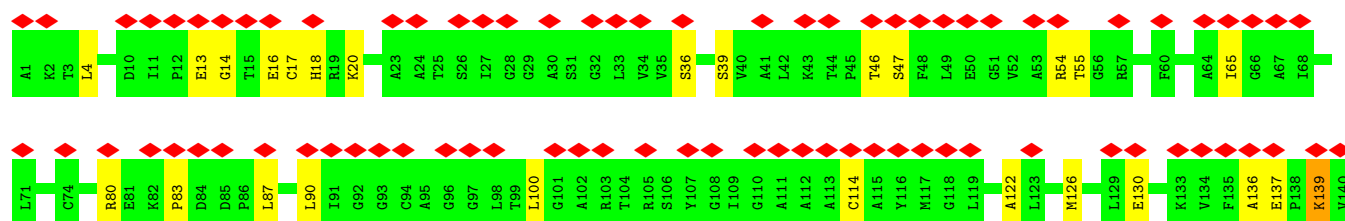
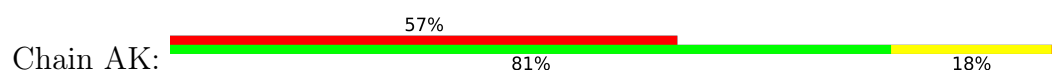


• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

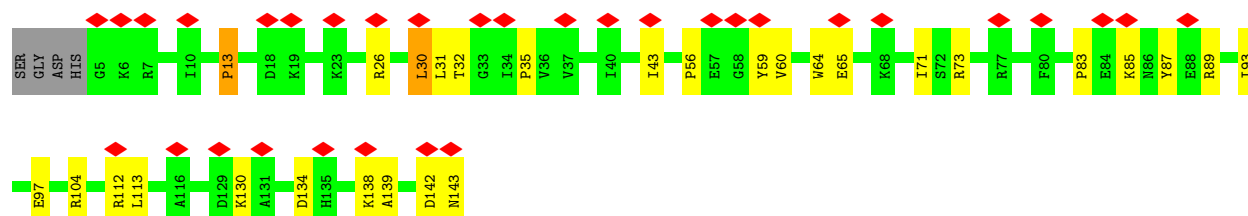
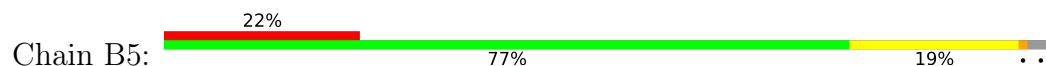


• Molecule 8: NDUFA11

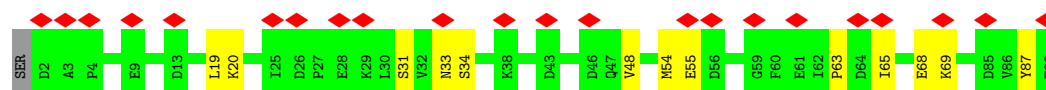
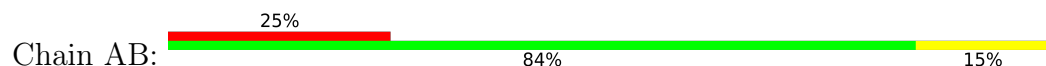




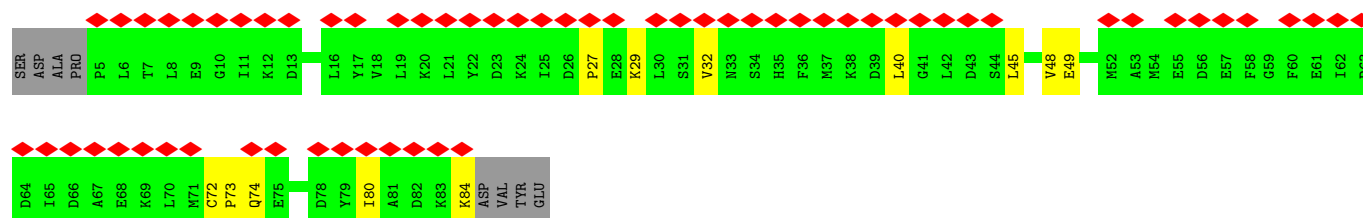
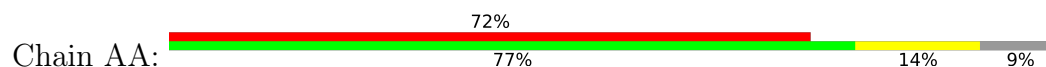
• Molecule 9: NADH:ubiquinone oxidoreductase subunit B5



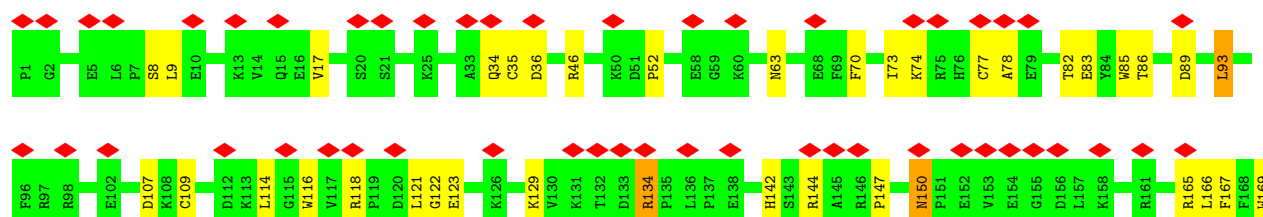
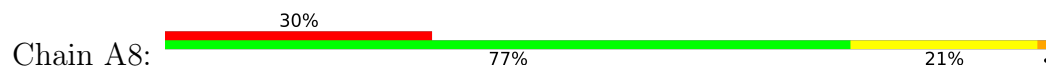
• Molecule 10: Acyl carrier protein



• Molecule 10: Acyl carrier protein

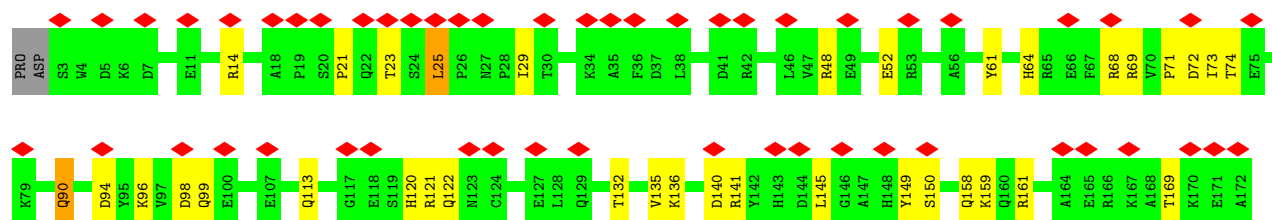
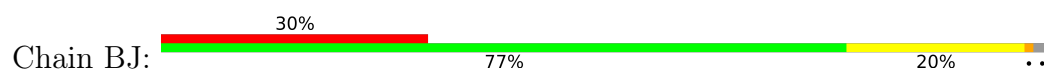


• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

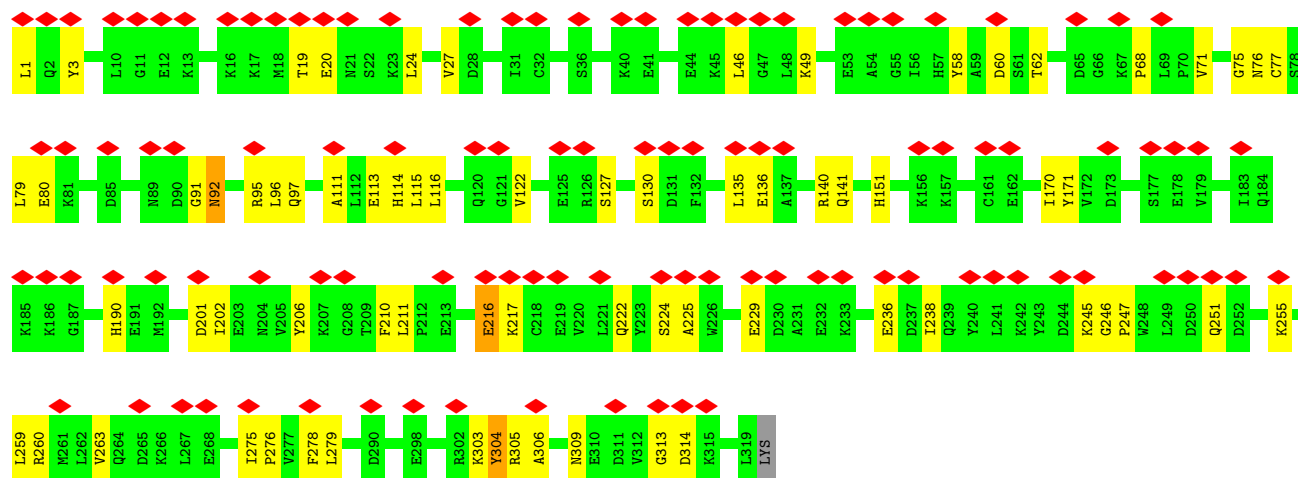
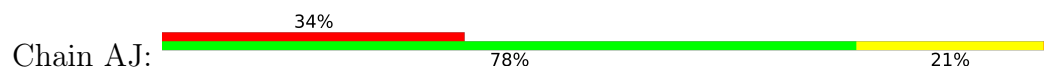




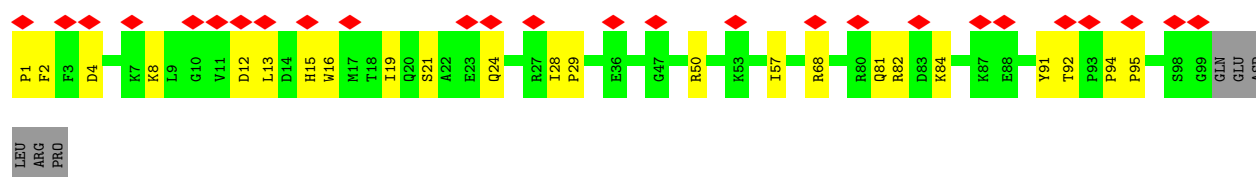
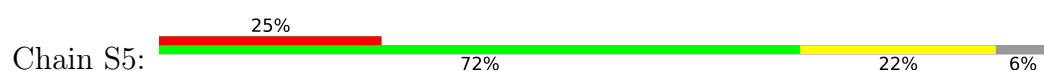
• Molecule 12: NDUFB10



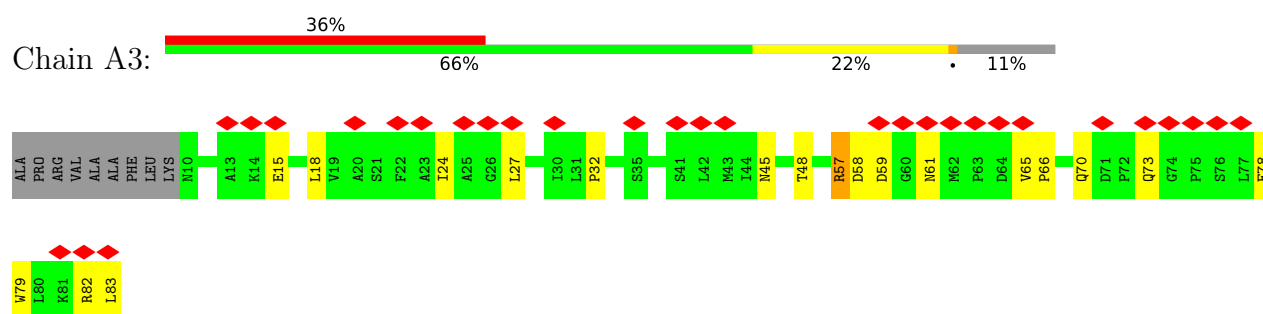
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



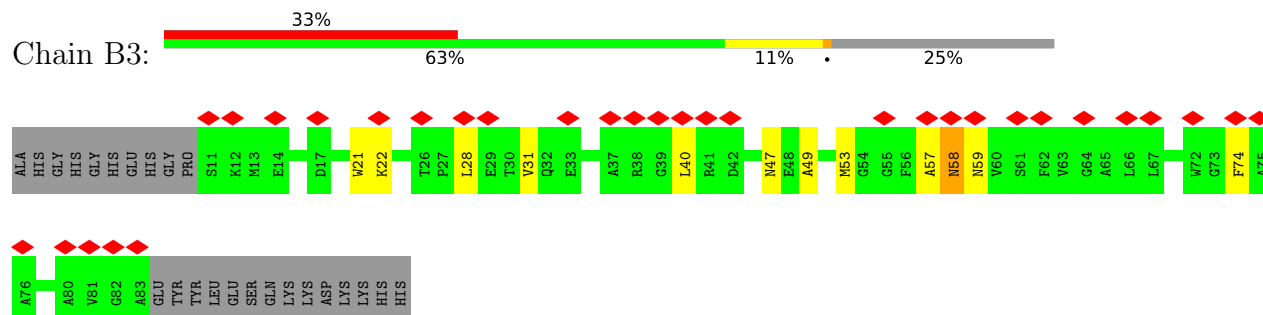
• Molecule 14: NADH:ubiquinone oxidoreductase subunit S5



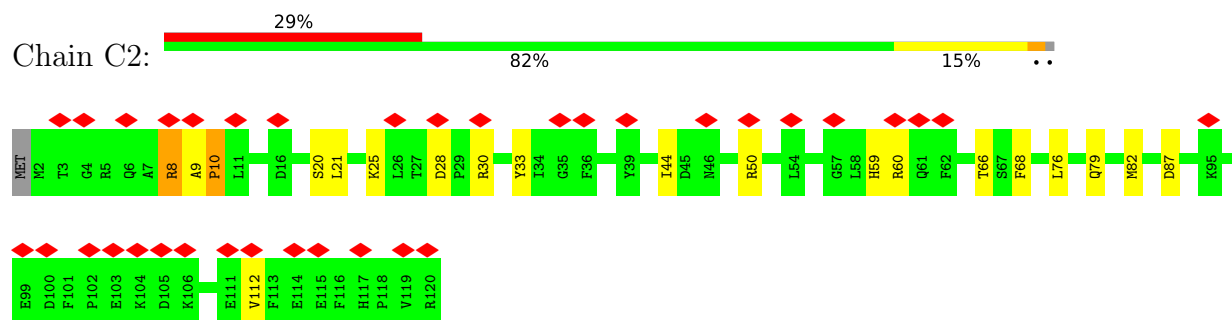
• Molecule 15: NADH:ubiquinone oxidoreductase subunit A3



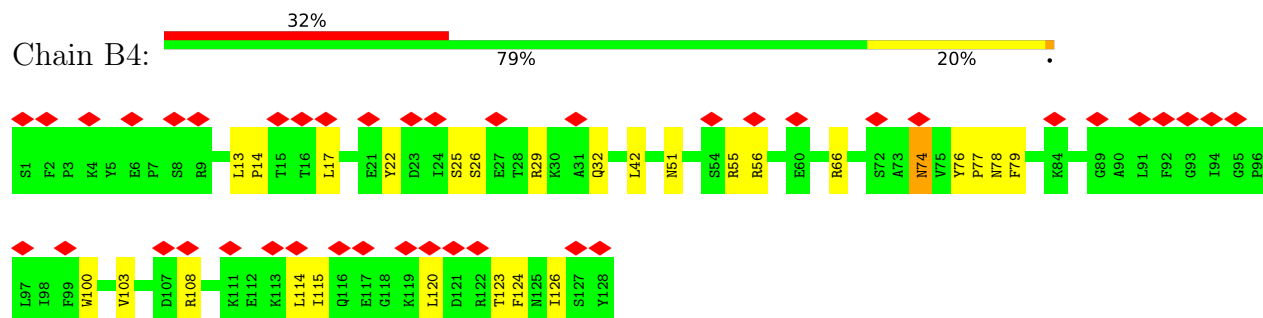
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B3



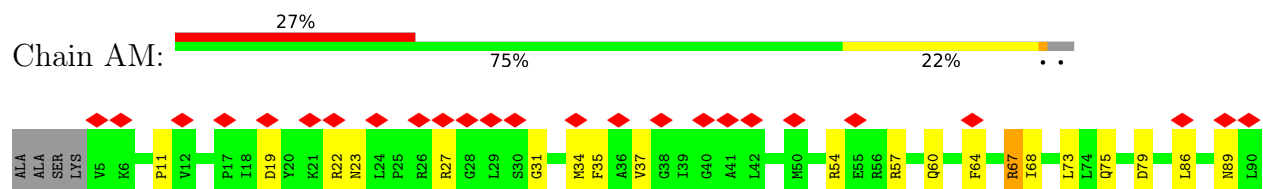
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

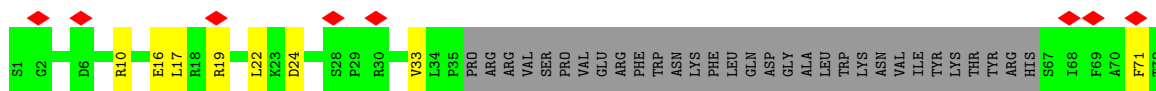


- Molecule 19: NDUFA13

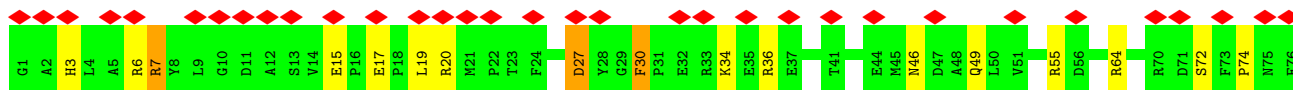
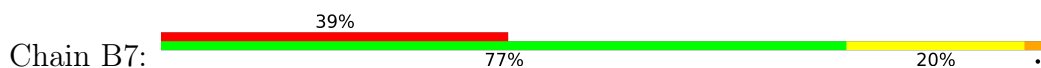




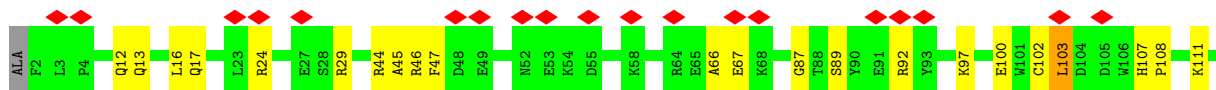
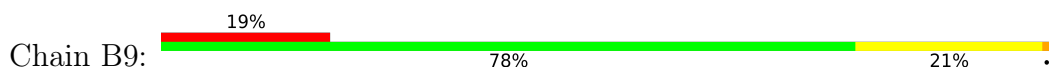
• Molecule 20: NDUFB6



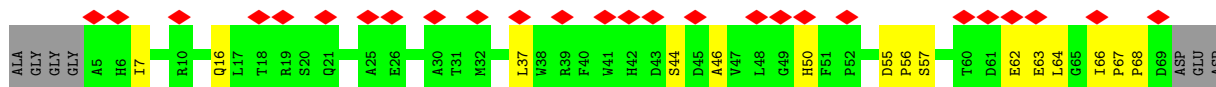
• Molecule 21: NADH:ubiquinone oxidoreductase subunit B7



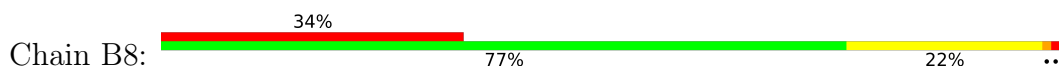
• Molecule 22: NADH:ubiquinone oxidoreductase subunit B9

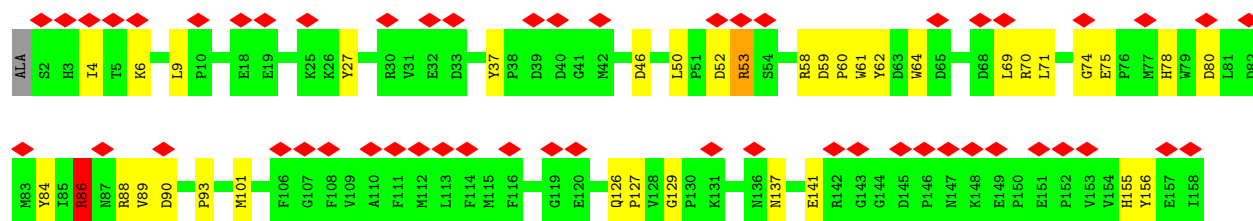


• Molecule 23: NADH:ubiquinone oxidoreductase subunit B2

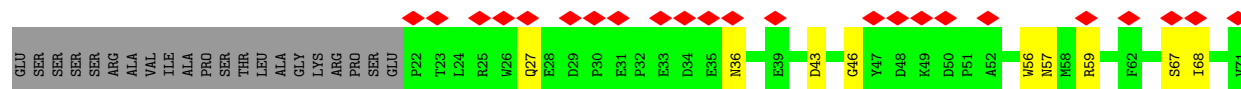


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

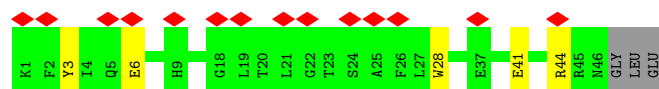
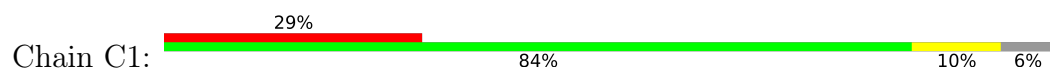




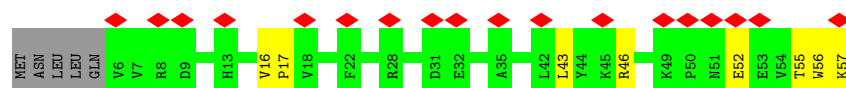
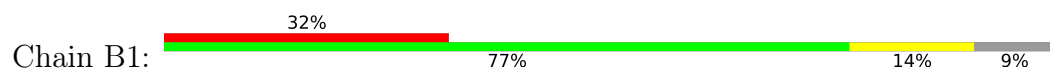
• Molecule 25: NDUFB1



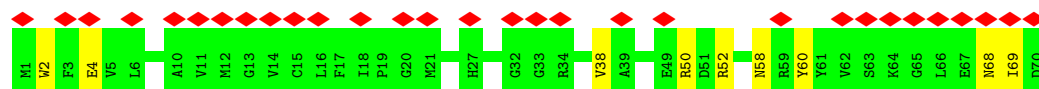
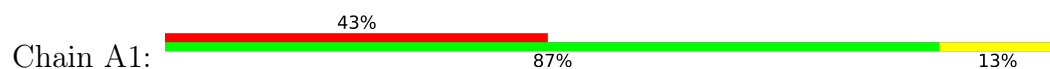
• Molecule 26: NDUFC1



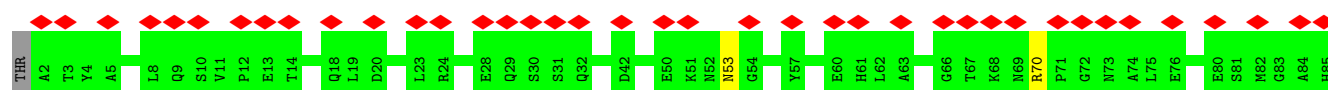
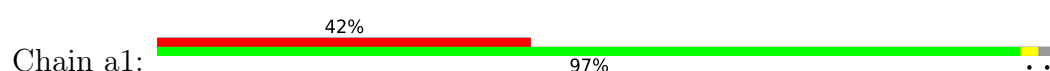
• Molecule 27: NDUFB1

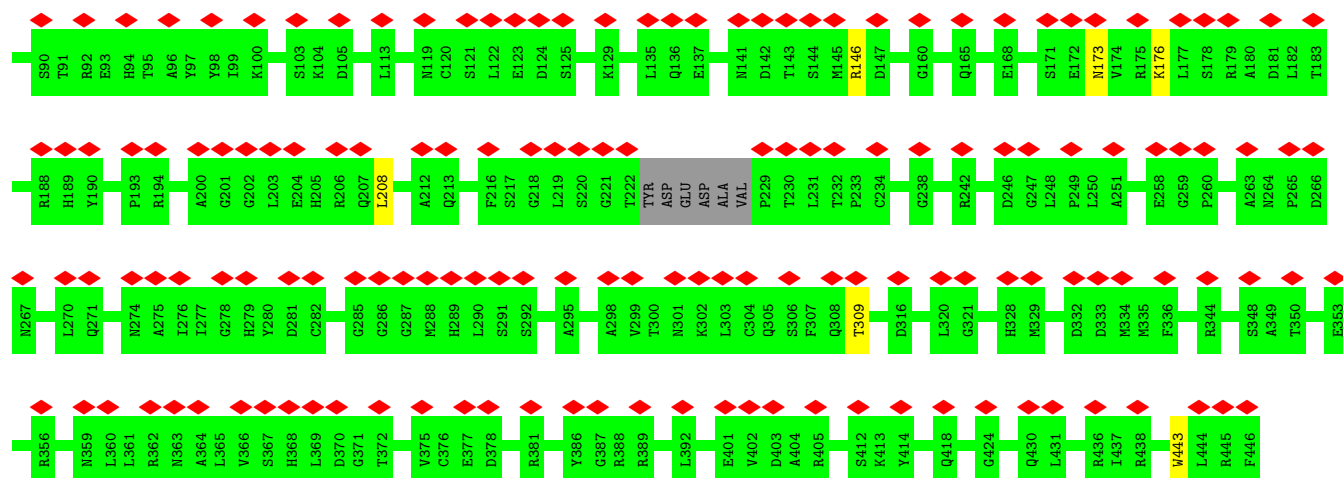


• Molecule 28: NDUFA1

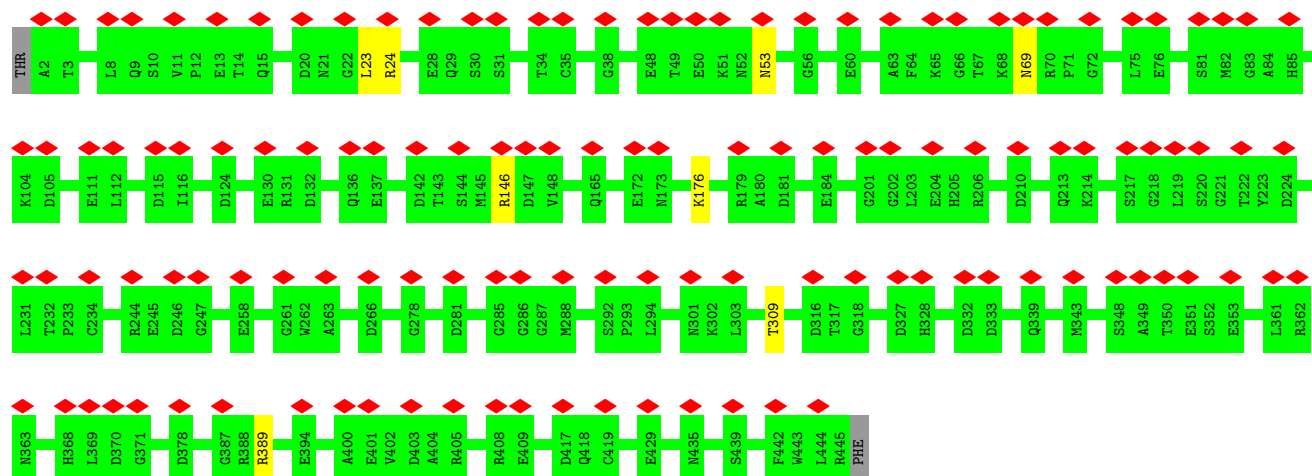


• Molecule 29: UQCRC1

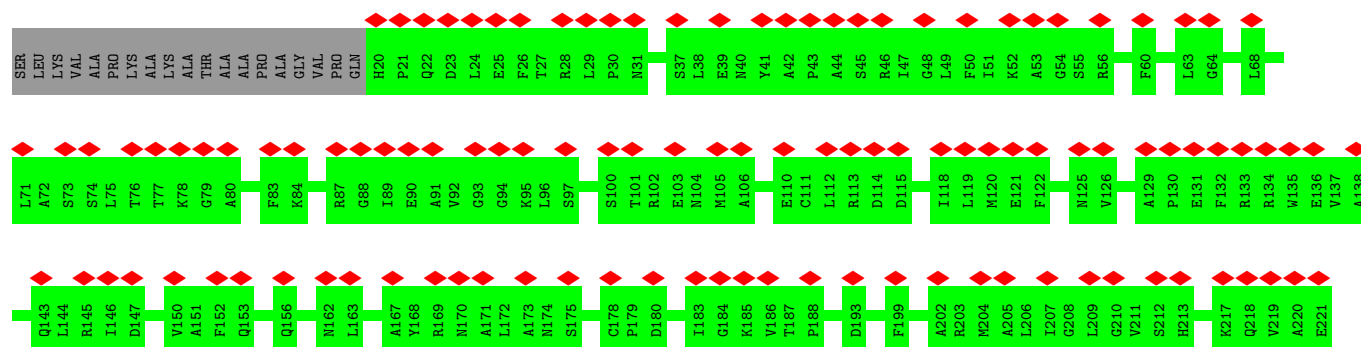


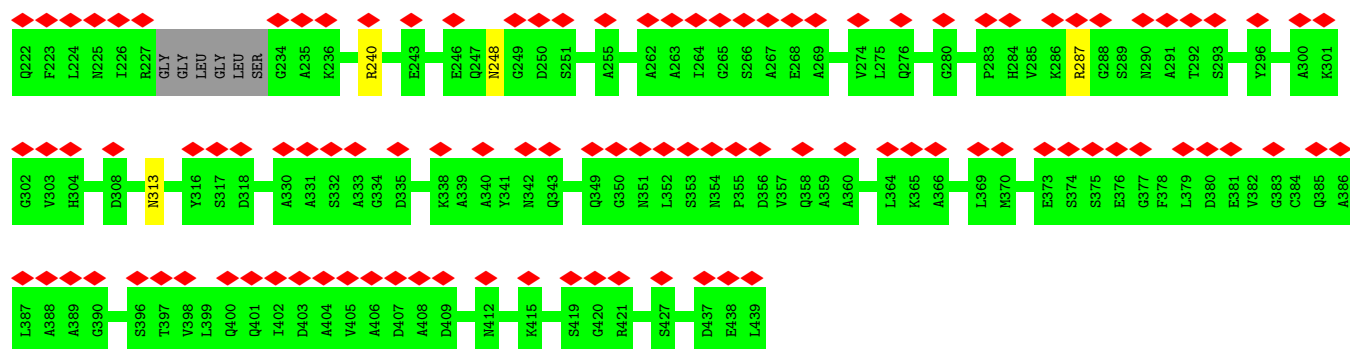


• Molecule 29: UQCRC1



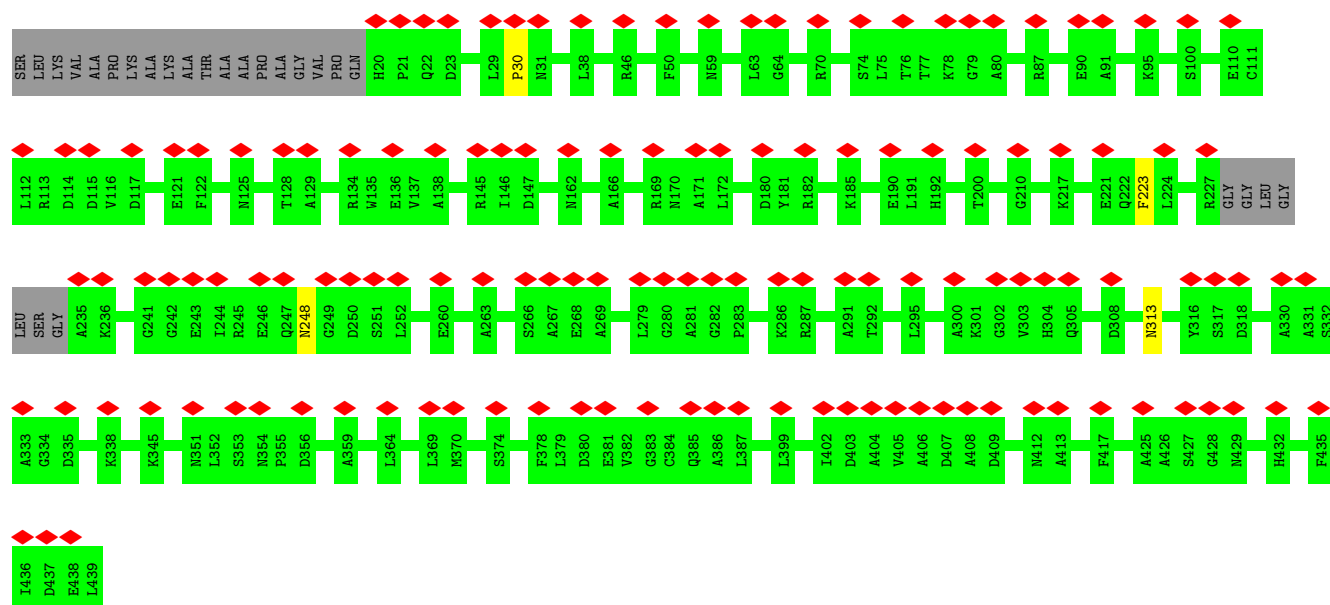
• Molecule 30: Ubiquinol-cytochrome c reductase core protein 2





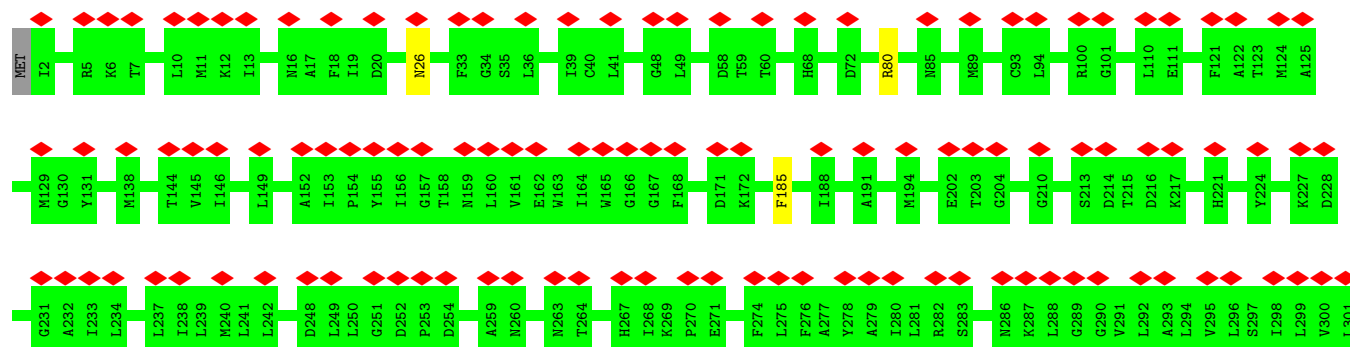
• Molecule 30: Ubiquinol-cytochrome c reductase core protein 2

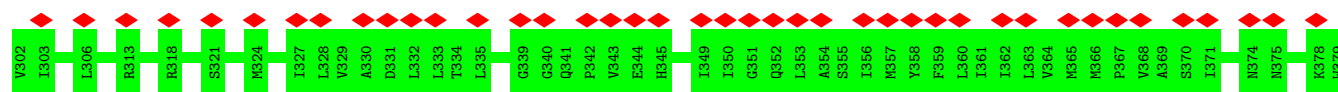
Chain a4: 31% 93% 6%



• Molecule 31: Cytochrome b

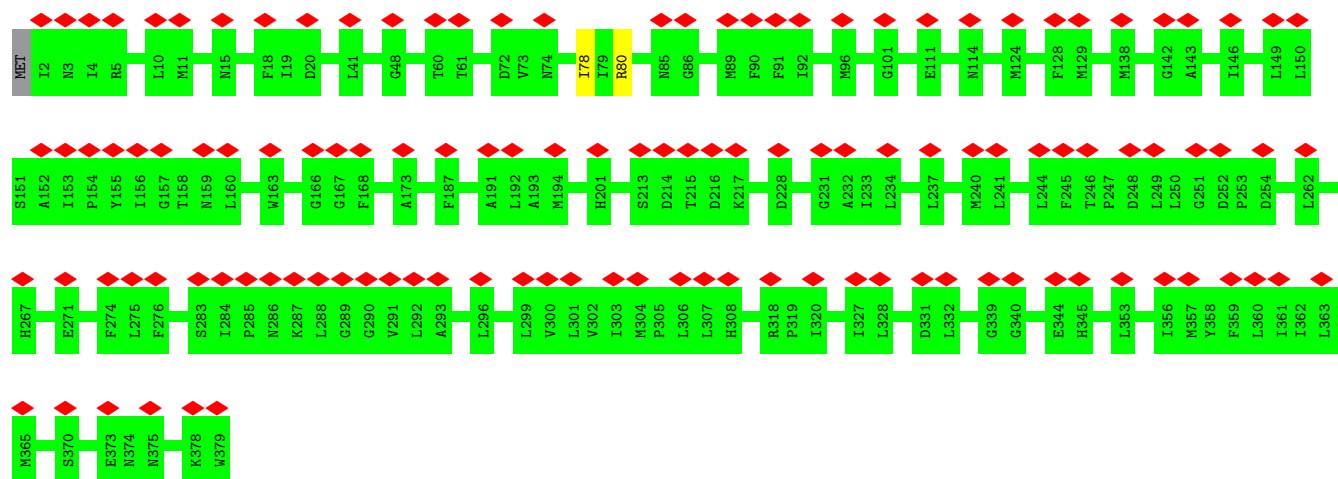
Chain b1: 42% 99%





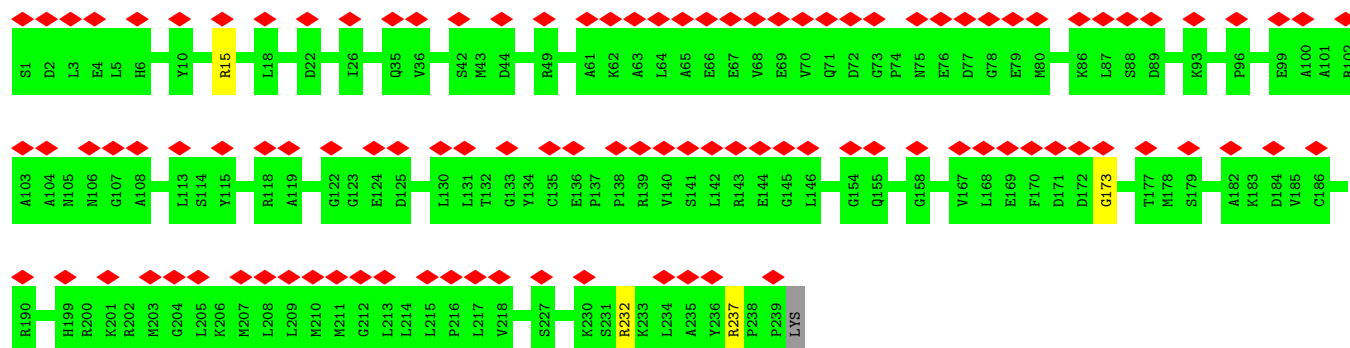
• Molecule 31: Cytochrome b

Chain b2: 32% 99%



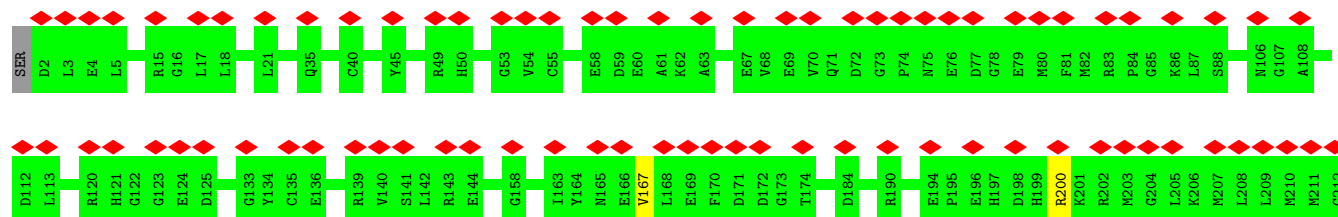
• Molecule 32: Cytochrome c1

Chain c1: 45% 98%

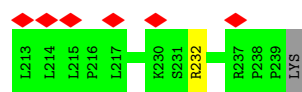


• Molecule 32: Cytochrome c1

Chain c2: 35% 98%







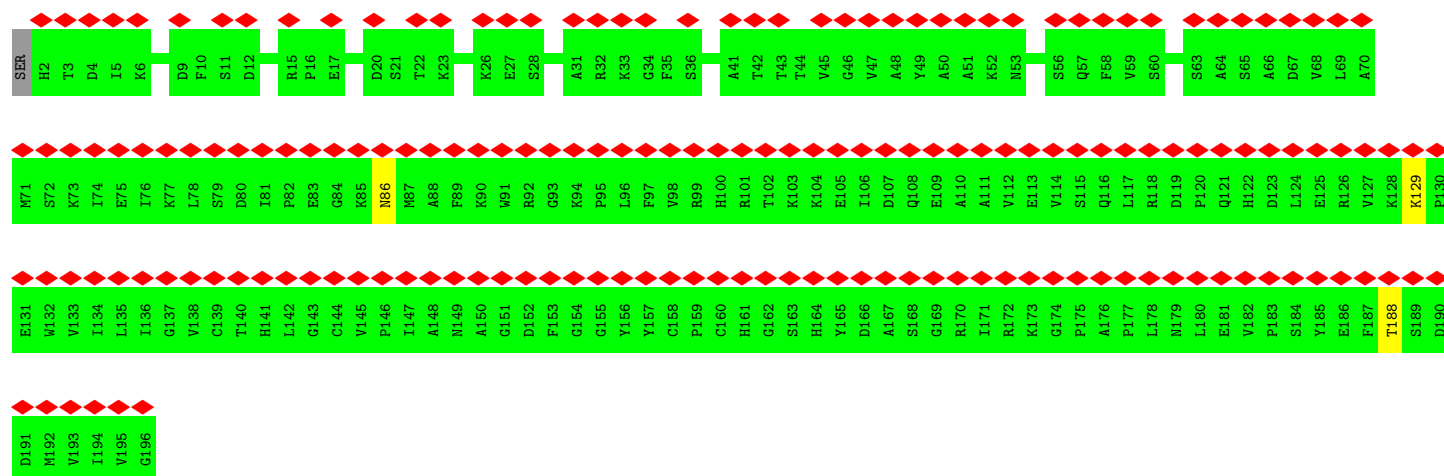
- Molecule 33: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain f1: 88% 99%



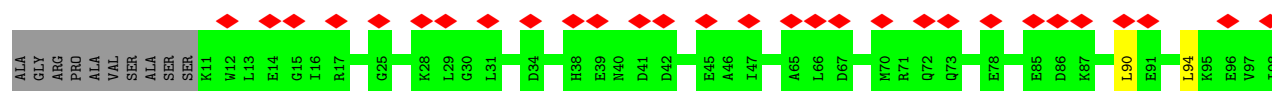
- Molecule 33: Cytochrome b-c1 complex subunit Rieske, mitochondrial

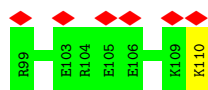
Chain f2: 88% 98%



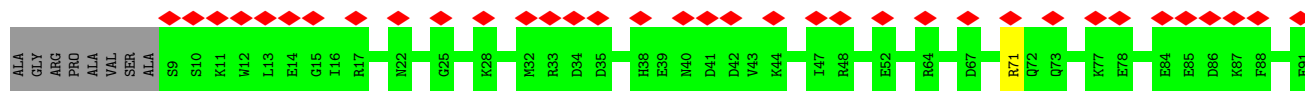
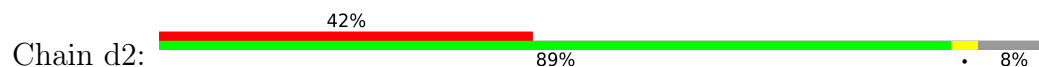
- Molecule 34: UQCRB

Chain d1: 32% 88% 9%

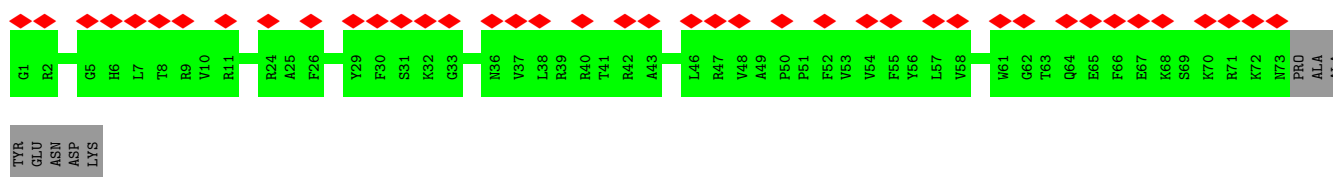
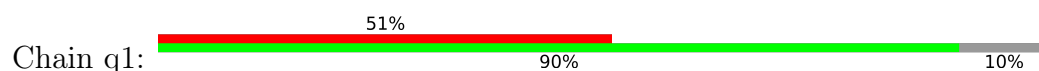




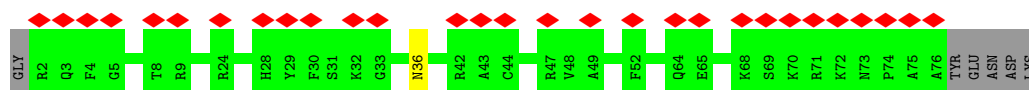
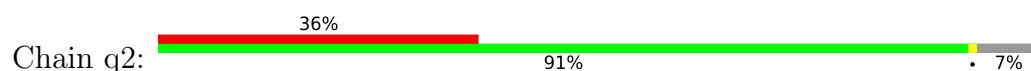
• Molecule 34: UQCRB



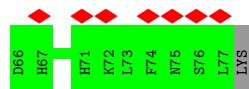
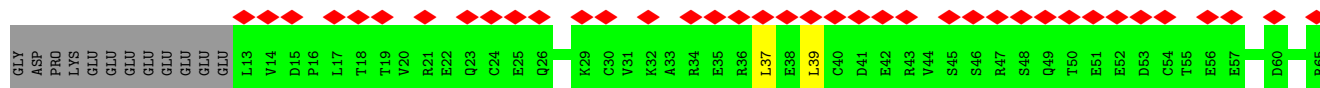
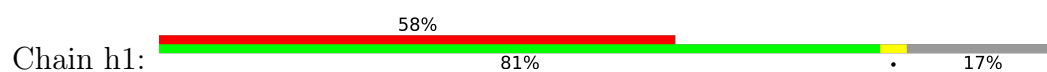
• Molecule 35: Ubiquinol-cytochrome c reductase complex III subunit VII



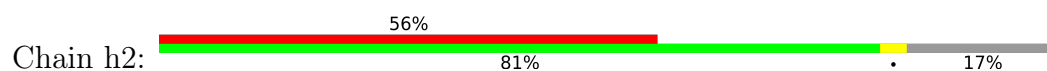
• Molecule 35: Ubiquinol-cytochrome c reductase complex III subunit VII

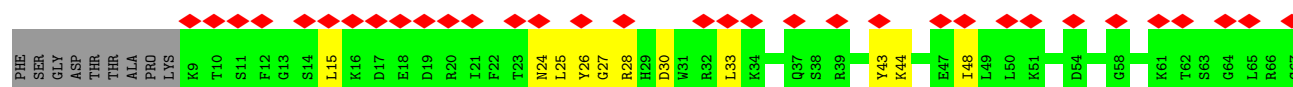


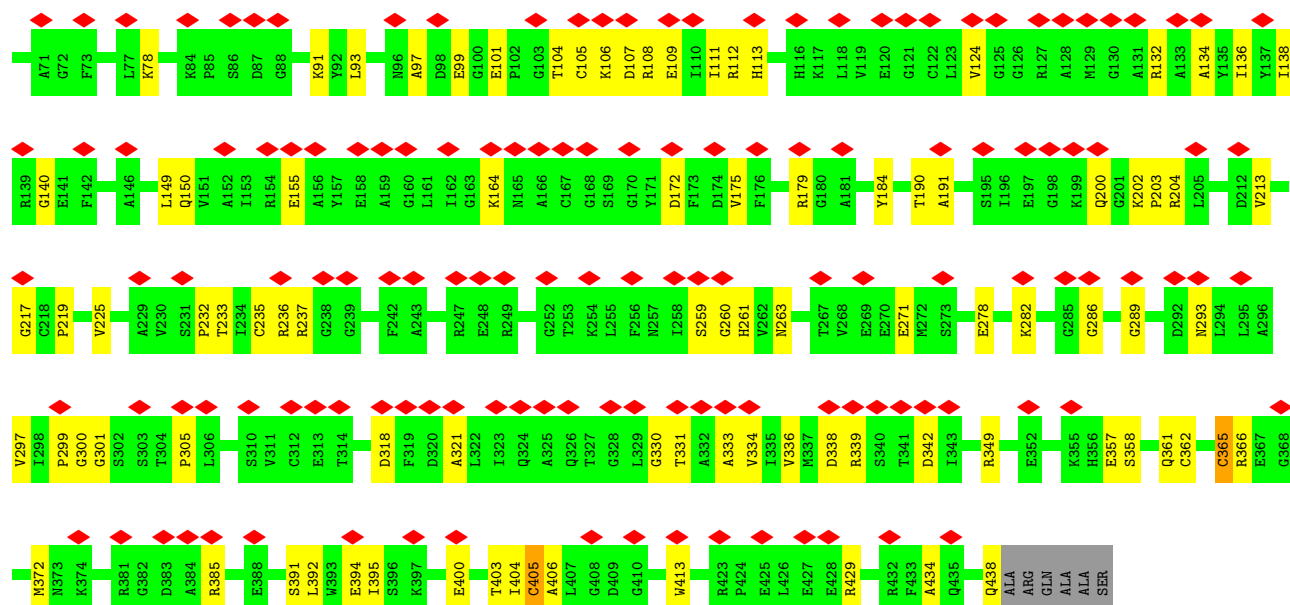
• Molecule 36: UQCRQH



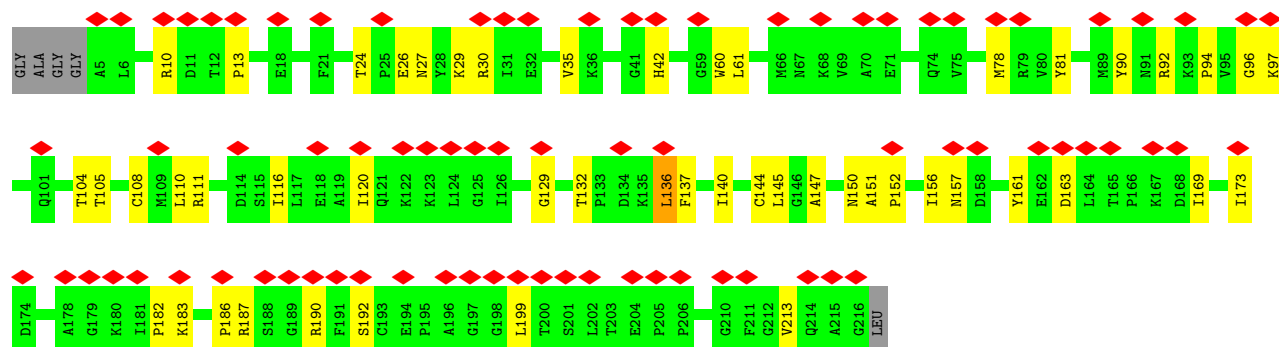
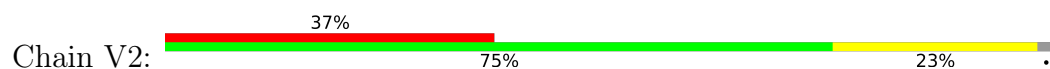
• Molecule 36: UQCRQH



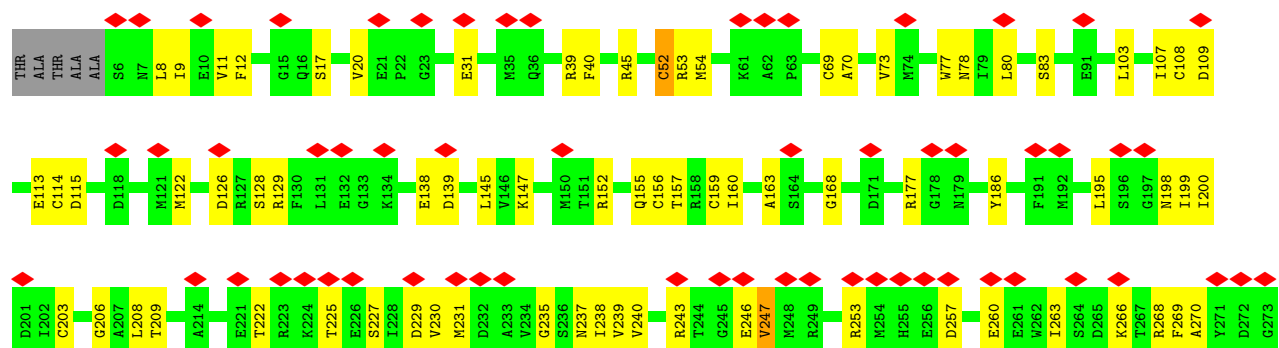
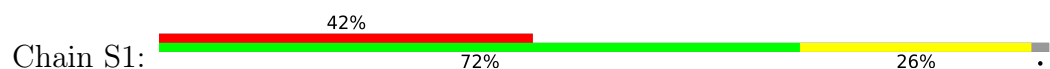


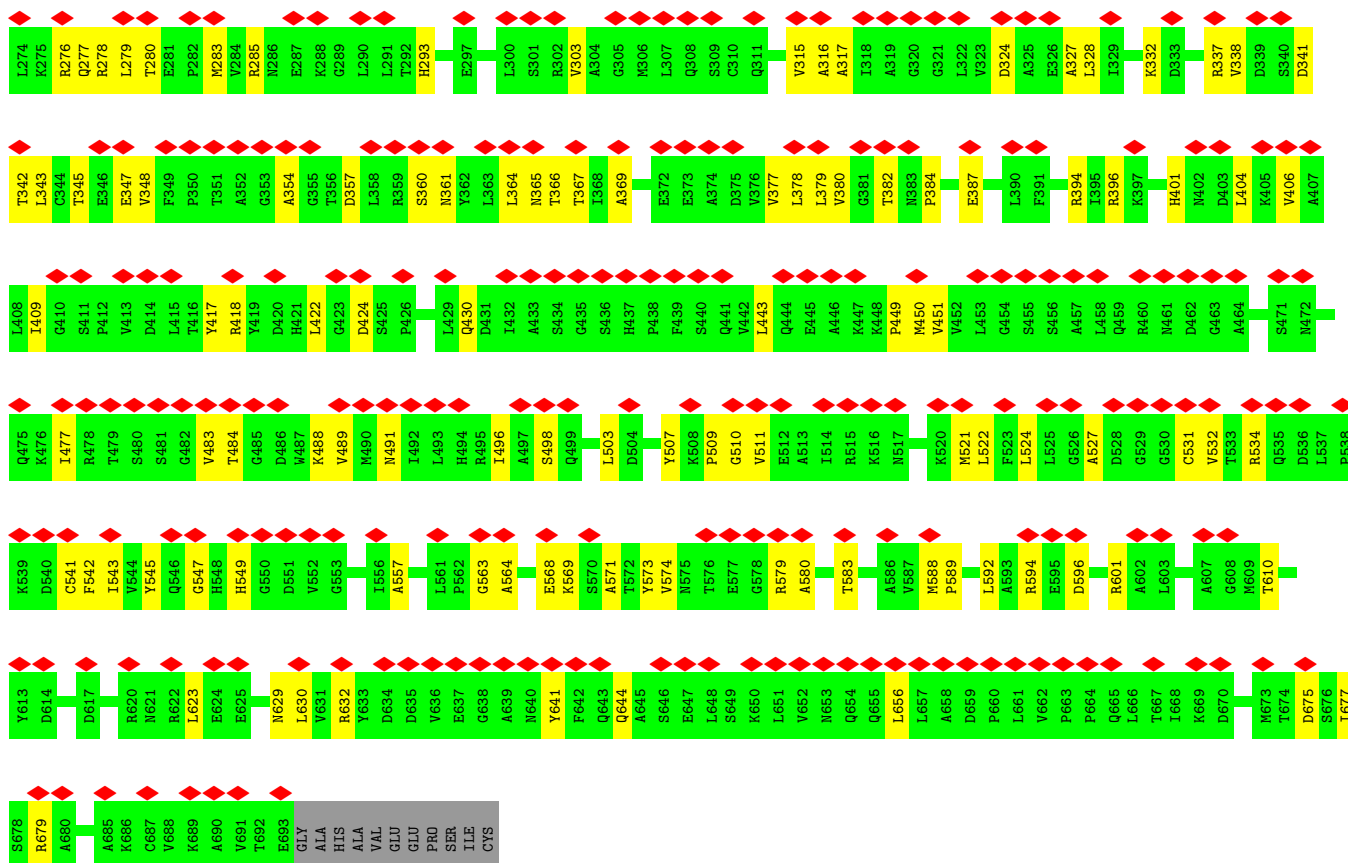


• Molecule 40: NDUFV2

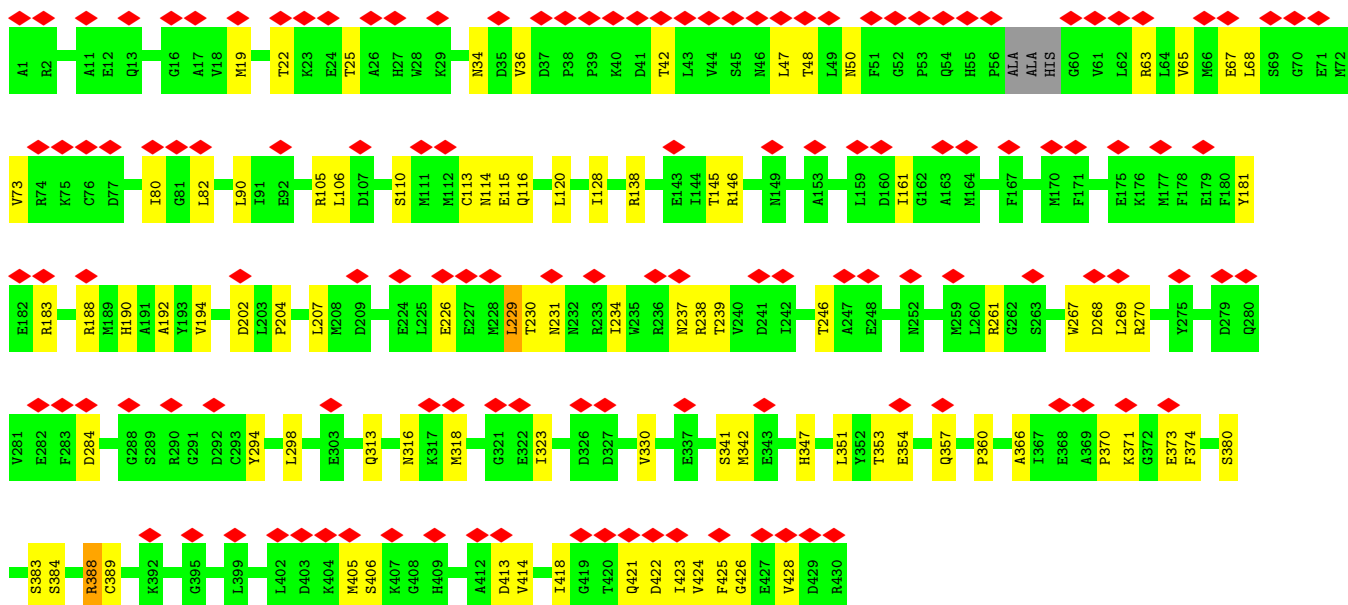
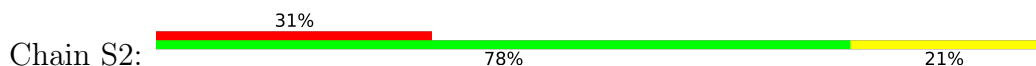


• Molecule 41: NADH:ubiquinone oxidoreductase core subunit S1



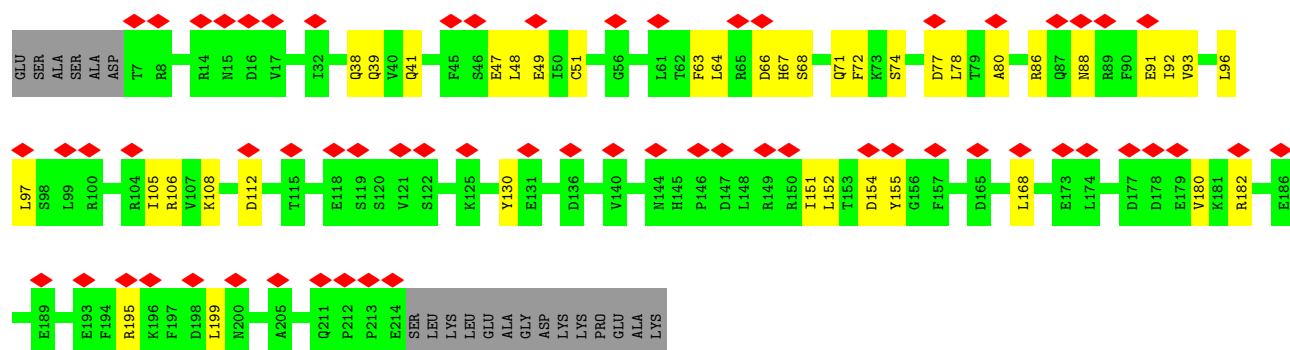


• Molecule 42: NDUFS2



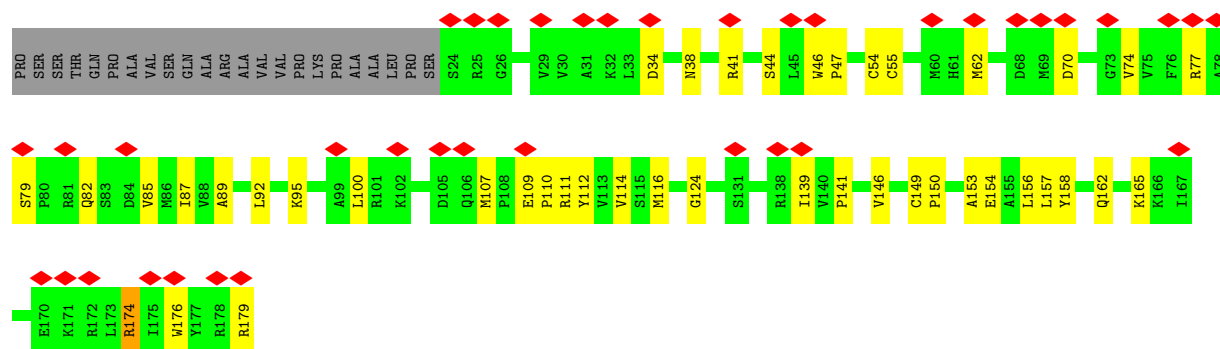
• Molecule 43: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3: 27% 74% 17% 9%



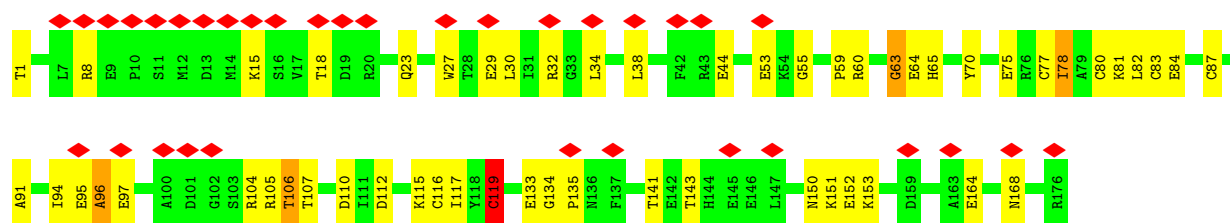
• Molecule 44: NDUF57

Chain S7: 21% 63% 23% 13%



• Molecule 45: NDUF58

Chain S8: 19% 69% 28%




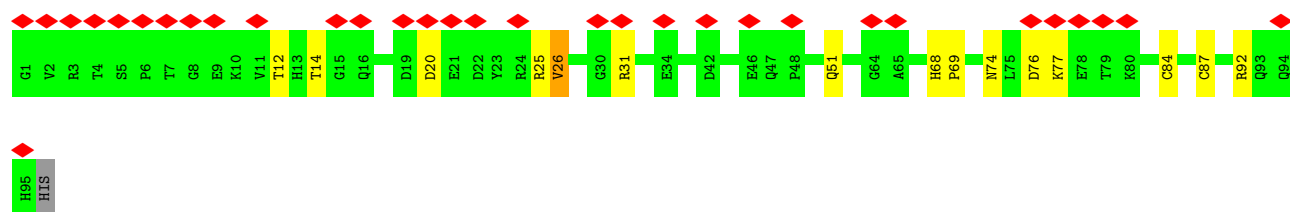
• Molecule 46: NDUFV3

Chain V3: 25% 39% 12% 45%




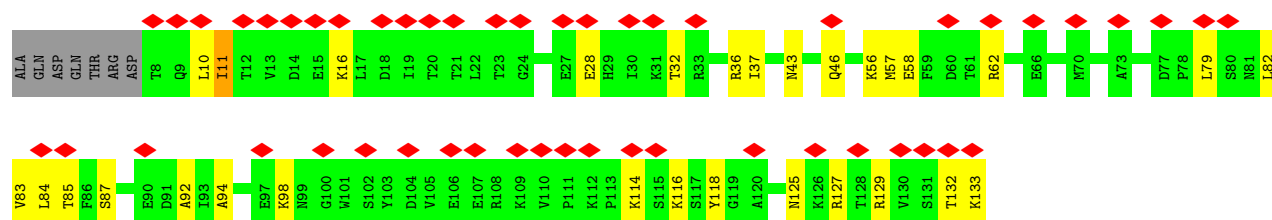
• Molecule 47: NDUF56

Chain S6: 



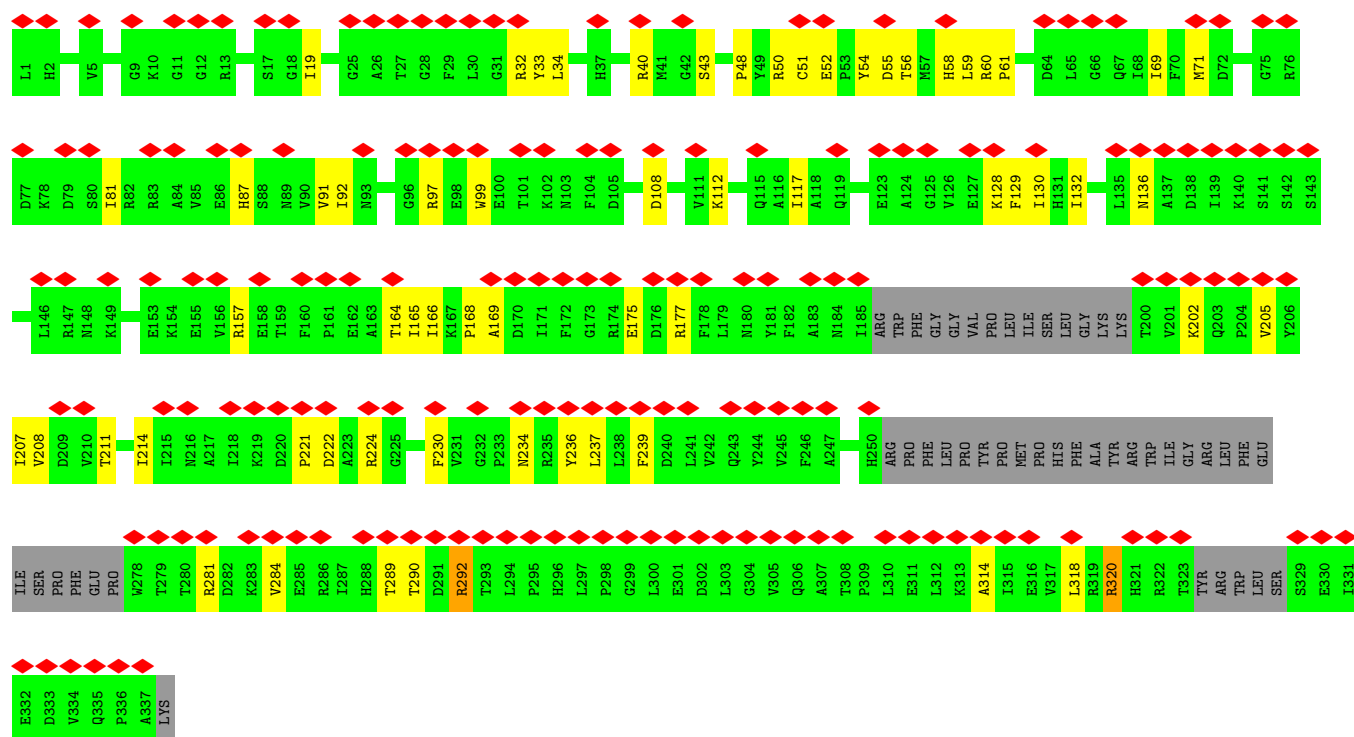
- Molecule 48: NADH:ubiquinone oxidoreductase subunit S4

Chain S4: 



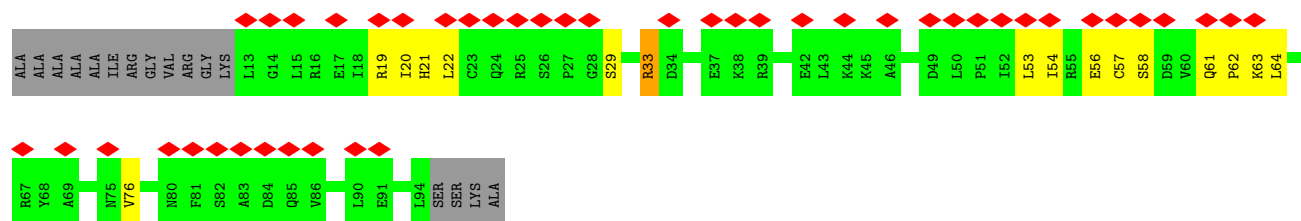
- Molecule 49: NADH:ubiquinone oxidoreductase subunit A9

Chain A9: 

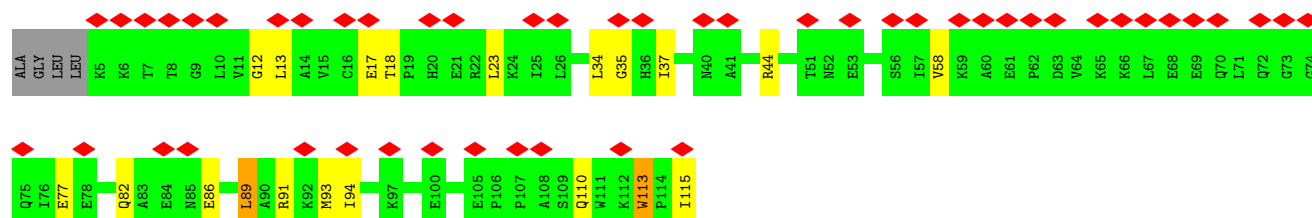
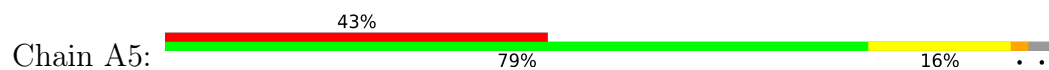


- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

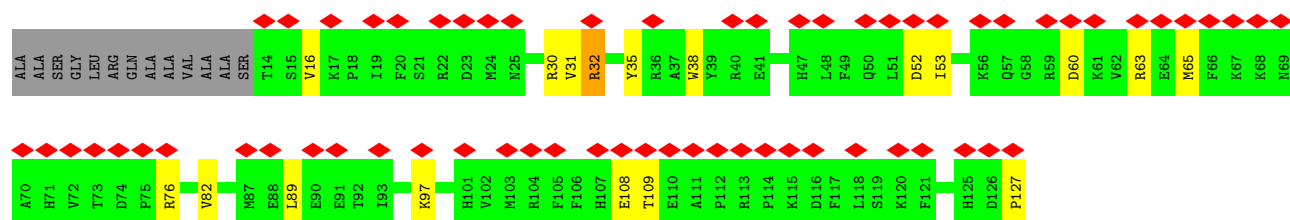
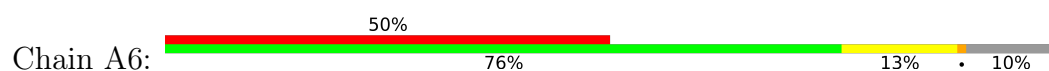
Chain A2: 



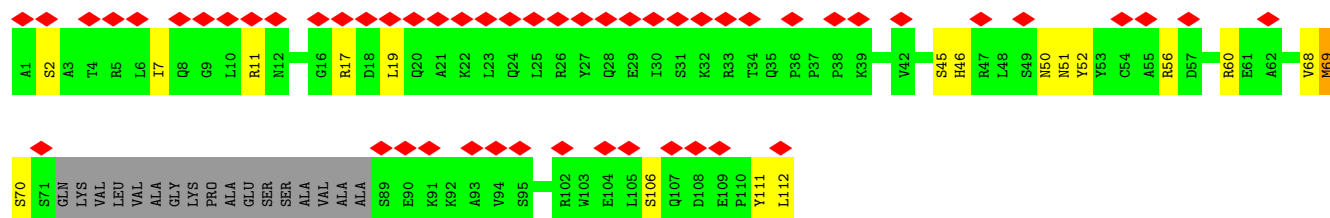
• Molecule 51: NDUFA5



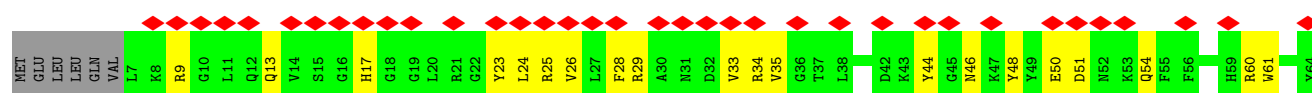
• Molecule 52: NADH:ubiquinone oxidoreductase subunit A6



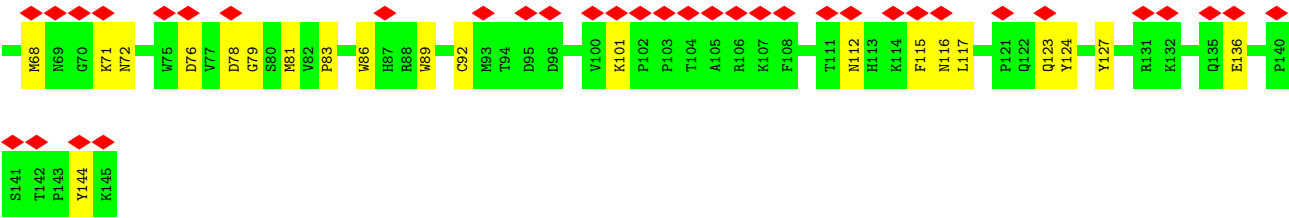
• Molecule 53: NDUFA7



• Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.153	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	D3	0.38	0/747	0.68	0/1022
2	D1	0.48	0/2432	0.74	1/3323 (0.0%)
3	D6	0.43	0/1309	0.72	1/1768 (0.1%)
4	4L	0.45	0/758	0.76	0/1024
5	D5	0.46	0/4933	0.76	5/6710 (0.1%)
6	D4	0.49	0/3740	0.77	5/5095 (0.1%)
7	D2	0.51	0/2788	0.73	1/3795 (0.0%)
8	AK	0.39	0/1046	0.69	1/1419 (0.1%)
9	B5	0.44	0/1189	0.63	1/1607 (0.1%)
10	AA	0.32	0/655	0.66	0/881
10	AB	0.42	0/714	0.66	0/963
11	A8	0.40	0/1441	0.70	1/1942 (0.1%)
12	BJ	0.43	0/1475	0.62	2/1989 (0.1%)
13	AJ	0.45	0/2644	0.69	3/3579 (0.1%)
14	S5	0.42	0/843	0.68	1/1128 (0.1%)
15	A3	0.37	0/602	0.70	0/828
16	B3	0.45	0/595	0.75	0/803
17	C2	0.48	0/1028	0.67	0/1388
18	B4	0.47	0/1085	0.68	1/1467 (0.1%)
19	AM	0.44	0/1172	0.66	1/1579 (0.1%)
20	B6	0.44	0/822	0.77	0/1118
21	B7	0.40	0/1051	0.68	2/1408 (0.1%)
22	B9	0.45	0/1568	0.64	1/2123 (0.0%)
23	B2	0.41	0/590	0.71	0/810
24	B8	0.51	1/1379 (0.1%)	0.75	2/1884 (0.1%)
25	BK	0.47	0/880	0.67	0/1196
26	C1	0.40	0/404	0.55	0/548
27	B1	0.39	0/462	0.59	0/624
28	A1	0.42	0/592	0.68	0/795
29	a1	0.38	0/3479	0.61	1/4719 (0.0%)
29	a3	0.42	0/3518	0.61	1/4776 (0.0%)
30	a2	0.35	0/3183	0.56	0/4313

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
30	a4	0.38	0/3179	0.60	0/4308
31	b1	0.42	0/3119	0.60	0/4268
31	b2	0.45	0/3119	0.62	0/4268
32	c1	0.39	0/1968	0.59	0/2672
32	c2	0.41	0/1962	0.59	0/2664
33	f1	0.32	0/1554	0.52	0/2101
33	f2	0.35	0/1548	0.57	0/2093
34	d1	0.38	0/906	0.60	2/1213 (0.2%)
34	d2	0.41	0/908	0.60	0/1218
35	q1	0.41	0/638	0.56	0/862
35	q2	0.47	0/652	0.63	0/883
36	h1	0.34	0/538	0.64	1/723 (0.1%)
36	h2	0.37	0/538	0.75	1/723 (0.1%)
38	i1	0.36	0/471	0.52	0/634
38	i2	0.35	0/486	0.53	0/655
39	V1	0.41	0/3386	0.66	0/4575
40	V2	0.39	0/1687	0.74	1/2295 (0.0%)
41	S1	0.41	0/5362	0.64	0/7266
42	S2	0.50	0/3525	0.67	1/4776 (0.0%)
43	S3	0.47	0/1776	0.64	0/2417
44	S7	0.51	0/1278	0.63	0/1728
45	S8	0.59	1/1445 (0.1%)	0.72	3/1956 (0.2%)
46	V3	0.38	0/355	0.69	0/480
47	S6	0.44	0/749	0.62	0/1009
48	S4	0.38	0/1047	0.60	0/1415
49	A9	0.37	0/2351	0.67	3/3181 (0.1%)
50	A2	0.33	0/676	0.65	0/911
51	A5	0.38	0/921	0.66	2/1249 (0.2%)
52	A6	0.37	0/993	0.59	0/1336
53	A7	0.33	0/775	0.65	0/1048
54	AL	0.41	0/1201	0.67	0/1632
All	All	0.43	2/98237 (0.0%)	0.66	45/133183 (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	D1	0	3
3	D6	0	2
5	D5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	D4	0	1
7	D2	0	1
8	AK	0	1
10	AB	0	1
11	A8	0	1
12	BJ	0	1
13	AJ	0	2
14	S5	0	1
15	A3	0	1
16	B3	0	4
17	C2	0	1
18	B4	0	2
20	B6	0	2
21	B7	0	1
23	B2	0	4
24	B8	0	2
26	C1	0	1
27	B1	0	1
29	a1	0	2
29	a3	0	1
30	a4	0	2
32	c1	0	2
32	c2	0	1
33	f2	0	2
39	V1	0	2
40	V2	0	2
41	S1	0	3
42	S2	0	4
45	S8	0	2
48	S4	0	1
51	A5	0	2
53	A7	0	2
All	All	0	63

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S8	119	CYS	CB-SG	-7.04	1.70	1.82
24	B8	46	ASP	C-N	-6.11	1.20	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D5	69	LEU	CA-CB-CG	7.97	133.64	115.30
22	B9	103	LEU	CA-CB-CG	7.63	132.85	115.30
40	V2	136	LEU	CA-CB-CG	7.56	132.70	115.30
51	A5	89	LEU	CA-CB-CG	7.55	132.68	115.30
45	S8	78	ILE	CG1-CB-CG2	-7.37	95.19	111.40
42	S2	106	LEU	CA-CB-CG	7.17	131.79	115.30
5	D5	78	LEU	CA-CB-CG	6.93	131.24	115.30
3	D6	146	LEU	CA-CB-CG	6.64	130.58	115.30
6	D4	36	LEU	CA-CB-CG	6.63	130.56	115.30
5	D5	386	LEU	CA-CB-CG	6.44	130.11	115.30
21	B7	19	LEU	CA-CB-CG	6.35	129.90	115.30
49	A9	222	ASP	CB-CG-OD1	6.32	123.99	118.30
45	S8	82	LEU	CB-CG-CD2	-6.30	100.28	111.00
21	B7	27	ASP	CB-CG-OD1	6.30	123.97	118.30
34	d1	90	LEU	CA-CB-CG	6.26	129.70	115.30
45	S8	96	ALA	C-N-CA	-6.21	106.18	121.70
29	a1	208	LEU	CA-CB-CG	6.17	129.48	115.30
29	a3	23	LEU	CA-CB-CG	6.10	129.33	115.30
49	A9	320	ARG	CA-CB-CG	6.08	126.78	113.40
36	h2	62	LEU	CA-CB-CG	6.08	129.29	115.30
18	B4	17	LEU	CA-CB-CG	6.07	129.26	115.30
6	D4	369	LEU	CA-CB-CG	6.06	129.23	115.30
7	D2	130	LEU	CA-CB-CG	5.91	128.90	115.30
2	D1	22	LEU	CA-CB-CG	5.75	128.53	115.30
12	BJ	25	LEU	C-N-CD	-5.72	108.02	120.60
6	D4	158	LEU	CA-CB-CG	5.70	128.41	115.30
34	d1	94	LEU	CA-CB-CG	5.42	127.76	115.30
12	BJ	21	PRO	C-N-CA	5.35	135.07	121.70
13	AJ	229	GLU	C-N-CA	5.35	135.07	121.70
49	A9	221	PRO	C-N-CA	5.32	135.01	121.70
8	AK	90	LEU	CA-CB-CG	5.32	127.53	115.30
6	D4	17	LEU	CA-CB-CG	5.32	127.53	115.30
13	AJ	275	ILE	C-N-CD	-5.28	108.98	120.60
24	B8	86	ARG	C-N-CA	5.27	134.88	121.70
9	B5	30	LEU	CA-CB-CG	5.22	127.32	115.30
19	AM	126	LEU	CA-CB-CG	5.22	127.30	115.30
36	h1	39	LEU	CA-CB-CG	5.16	127.17	115.30
24	B8	37	TYR	C-N-CD	-5.16	109.26	120.60
5	D5	511	LEU	CA-CB-CG	5.14	127.13	115.30
51	A5	89	LEU	CB-CG-CD2	-5.13	102.28	111.00
5	D5	125	LEU	CB-CG-CD2	5.11	119.69	111.00
11	A8	93	LEU	CA-CB-CG	5.10	127.03	115.30
13	AJ	304	TYR	CA-CB-CG	5.09	123.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S5	19	ILE	CG1-CB-CG2	-5.09	100.20	111.40
6	D4	230	VAL	CG1-CB-CG2	-5.08	102.77	110.90

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	A3	57	ARG	Peptide
51	A5	113	TRP	Peptide
51	A5	93	MET	Peptide
53	A7	68	VAL	Peptide
53	A7	69	MET	Peptide
11	A8	52	PRO	Peptide
10	AB	68	GLU	Peptide
13	AJ	216	GLU	Peptide
13	AJ	278	PHE	Peptide
8	AK	16	GLU	Peptide
27	B1	52	GLU	Peptide
23	B2	44	SER	Peptide
23	B2	56	PRO	Peptide
23	B2	63	GLU	Peptide
23	B2	67	PRO	Peptide
16	B3	21	TRP	Peptide
16	B3	22	LYS	Peptide
16	B3	57	ALA	Peptide
16	B3	58	ASN	Peptide
18	B4	123	THR	Peptide
18	B4	76	TYR	Peptide
20	B6	122	PHE	Peptide
20	B6	86	LYS	Peptide
21	B7	30	PHE	Peptide
24	B8	53	ARG	Peptide
24	B8	86	ARG	Peptide
12	BJ	150	SER	Peptide
26	C1	6	GLU	Peptide
17	C2	8	ARG	Peptide
2	D1	316	PRO	Peptide
2	D1	32	GLN	Peptide
2	D1	91	MET	Peptide
7	D2	272	LYS	Peptide
6	D4	53	SER	Peptide
5	D5	159	TYR	Peptide

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Mol	Chain	Res	Type	Group
5	D5	365	ALA	Peptide
3	D6	115	ILE	Peptide
3	D6	51	PHE	Peptide
41	S1	247	VAL	Peptide
41	S1	341	ASP	Peptide
41	S1	380	VAL	Peptide
42	S2	192	ALA	Peptide
42	S2	42	THR	Peptide
42	S2	68	LEU	Peptide
42	S2	73	VAL	Peptide
48	S4	11	ILE	Peptide
14	S5	92	THR	Peptide
45	S8	106	THR	Peptide
45	S8	63	GLY	Peptide
39	V1	105	CYS	Peptide
39	V1	331	THR	Peptide
40	V2	13	PRO	Peptide
40	V2	35	VAL	Peptide
29	a1	309	THR	Peptide
29	a1	443	TRP	Peptide
29	a3	309	THR	Peptide
30	a4	223	PHE	Peptide
30	a4	30	PRO	Peptide
32	c1	173	GLY	Peptide
32	c1	237	ARG	Peptide
32	c2	167	VAL	Peptide
33	f2	129	LYS	Peptide
33	f2	188	THR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D3	728	0	773	12	0
2	D1	2362	0	2480	54	0
3	D6	1280	0	1305	28	0
4	4L	748	0	794	16	0
5	D5	4805	0	4950	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D4	3646	0	3850	66	0
7	D2	2724	0	2930	59	0
8	AK	1025	0	1033	13	0
9	B5	1156	0	1177	22	0
10	AA	645	0	649	8	0
10	AB	702	0	692	9	0
11	A8	1404	0	1384	28	0
12	BJ	1441	0	1417	28	0
13	AJ	2583	0	2547	40	0
14	S5	822	0	820	19	0
15	A3	582	0	583	17	0
16	B3	578	0	570	5	0
17	C2	997	0	983	16	0
18	B4	1059	0	1062	19	0
19	AM	1143	0	1137	25	0
20	B6	797	0	817	19	0
21	B7	1026	0	995	22	0
22	B9	1515	0	1469	29	0
23	B2	563	0	509	10	0
24	B8	1324	0	1218	24	0
25	BK	853	0	800	21	0
26	C1	391	0	391	3	0
27	B1	449	0	453	6	0
28	A1	577	0	570	5	0
29	a1	3409	0	3322	0	0
29	a3	3447	0	3350	0	0
30	a2	3126	0	3093	0	0
30	a4	3122	0	3090	0	0
31	b1	3019	0	3082	0	0
31	b2	3019	0	3082	0	0
32	c1	1909	0	1858	0	0
32	c2	1903	0	1850	0	0
33	f1	1520	0	1505	0	0
33	f2	1514	0	1497	0	0
34	d1	886	0	883	0	0
34	d2	888	0	880	0	0
35	q1	618	0	628	0	0
35	q2	631	0	639	0	0
36	h1	532	0	509	0	0
36	h2	532	0	509	0	0
37	x1	164	0	40	0	0
37	x2	150	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i1	459	0	462	0	0
38	i2	473	0	477	0	0
39	V1	3312	0	3266	68	0
40	V2	1647	0	1657	32	0
41	S1	5275	0	5300	128	0
42	S2	3435	0	3377	60	0
43	S3	1726	0	1676	36	0
44	S7	1247	0	1256	35	0
45	S8	1414	0	1371	41	0
46	V3	345	0	323	9	0
47	S6	737	0	710	13	0
48	S4	1024	0	1023	23	0
49	A9	2301	0	2291	37	0
50	A2	665	0	678	10	0
51	A5	901	0	936	19	0
52	A6	969	0	980	21	0
53	A7	757	0	771	14	0
54	AL	1160	0	1125	26	0
55	D1	32	0	38	1	0
55	D4	40	0	54	3	0
55	D5	38	0	50	1	0
55	b2	29	0	32	0	0
55	f2	23	0	20	0	0
56	D4	28	0	30	0	0
57	AA	34	0	40	4	0
57	AB	31	0	34	6	0
58	b1	86	0	60	0	0
58	b2	86	0	60	0	0
59	c1	43	0	30	0	0
59	c2	43	0	30	0	0
60	S1	4	0	0	1	0
60	V2	4	0	0	0	0
60	f1	4	0	0	0	0
60	f2	4	0	0	0	0
61	b2	79	0	46	0	0
61	c2	41	0	26	0	0
62	S1	16	0	0	2	0
62	S7	8	0	0	0	0
62	S8	16	0	0	2	0
62	V1	8	0	0	3	0
63	V1	31	0	19	1	0
64	S6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	A9	48	0	26	4	0
All	All	96938	0	96494	1034	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 7.

All (1034) 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:S3:80:ALA:HA	43:S3:91:GLU:O	1.13	1.25
43:S3:38:GLN:HA	53:A7:70:SER:O	1.35	1.25
41:S1:449:PRO:O	41:S1:489:VAL:HA	1.60	1.02
43:S3:80:ALA:CA	43:S3:91:GLU:O	2.08	1.00
50:A2:21:HIS:O	50:A2:62:PRO:HA	1.64	0.95
52:A6:32:ARG:NH2	57:AA:101:ZMP:O7	2.05	0.90
43:S3:74:SER:HB3	43:S3:97:LEU:O	1.73	0.87
52:A6:32:ARG:HB2	52:A6:32:ARG:CZ	2.08	0.82
5:D5:83:ASP:O	5:D5:87:MET:HB2	1.79	0.81
49:A9:108:ASP:O	49:A9:112:LYS:HB3	1.81	0.80
12:BJ:169:THR:O	12:BJ:173:ALA:HB2	1.82	0.80
54:AL:25:ARG:O	54:AL:29:ARG:HB2	1.88	0.73
2:D1:195:ARG:HE	2:D1:274:ARG:HD3	1.54	0.73
2:D1:288:LEU:O	2:D1:292:ASN:HB2	1.88	0.73
19:AM:31:GLY:O	19:AM:35:PHE:HB2	1.88	0.72
6:D4:46:GLY:H	25:BK:84:ARG:HA	1.55	0.71
7:D2:88:LYS:HG3	7:D2:148:SER:HB3	1.71	0.71
43:S3:38:GLN:O	53:A7:70:SER:HA	1.89	0.71
39:V1:134:ALA:HB3	39:V1:175:VAL:HG12	1.73	0.70
42:S2:204:PRO:HD3	45:S8:60:ARG:HH22	1.57	0.69
43:S3:78:LEU:HA	43:S3:93:VAL:O	1.92	0.69
2:D1:67:SER:O	2:D1:70:MET:N	2.26	0.69
49:A9:289:THR:HG22	49:A9:290:THR:HG23	1.76	0.68
2:D1:102:VAL:HB	2:D1:150:LEU:HD21	1.73	0.68
49:A9:48:PRO:HA	49:A9:71:MET:O	1.94	0.68
5:D5:451:ILE:O	5:D5:455:LYS:HB2	1.94	0.67
2:D1:281:ARG:NH1	42:S2:413:ASP:OD2	2.27	0.67
6:D4:231:LEU:O	6:D4:235:LEU:HB2	1.94	0.66
10:AA:27:PRO:HG2	10:AA:29:LYS:HB2	1.78	0.66
13:AJ:202:ILE:O	13:AJ:206:TYR:HB2	1.95	0.66
44:S7:124:GLY:HA2	45:S8:115:LYS:HA	1.78	0.66
2:D1:149:ILE:HG23	2:D1:181:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:198:ASN:ND2	41:S1:263:ILE:O	2.27	0.65
45:S8:64:GLU:H	45:S8:134:GLY:H	1.44	0.65
12:BJ:161:ARG:NH2	25:BK:111:ASN:OD1	2.30	0.65
44:S7:158:TYR:OH	54:AL:116:ASN:ND2	2.28	0.65
39:V1:297:VAL:HG22	39:V1:336:VAL:HG12	1.78	0.65
3:D6:58:LEU:O	3:D6:62:GLY:HA3	1.96	0.64
55:D4:501:3PE:H291	7:D2:288:LEU:HD23	1.78	0.64
13:AJ:306:ALA:HA	13:AJ:309:ASN:HB2	1.80	0.64
6:D4:263:MET:SD	6:D4:263:MET:N	2.70	0.64
42:S2:347:HIS:O	42:S2:351:LEU:HB2	1.98	0.64
6:D4:457:PRO:HA	25:BK:84:ARG:HH22	1.63	0.64
8:AK:36:SER:HB2	8:AK:55:THR:HG22	1.80	0.64
47:S6:68:HIS:HE1	47:S6:87:CYS:SG	2.11	0.64
41:S1:52:CYS:SG	41:S1:53:ARG:N	2.70	0.64
45:S8:135:PRO:HG3	45:S8:164:GLU:HG2	1.79	0.64
15:A3:66:PRO:HB3	15:A3:73:GLN:HB2	1.80	0.63
6:D4:251:ASN:OD1	6:D4:251:ASN:N	2.32	0.63
6:D4:207:MET:HG3	6:D4:298:ILE:HD11	1.81	0.63
43:S3:80:ALA:HA	43:S3:91:GLU:C	2.14	0.63
19:AM:131:GLU:O	19:AM:135:SER:HB3	1.99	0.63
24:B8:4:ILE:HG22	24:B8:6:LYS:H	1.63	0.63
39:V1:394:GLU:OE1	41:S1:129:ARG:NH1	2.32	0.63
42:S2:371:LYS:NZ	42:S2:422:ASP:O	2.31	0.63
5:D5:203:MET:SD	12:BJ:113:GLN:NE2	2.72	0.63
39:V1:24:ASN:ND2	39:V1:30:ASP:O	2.32	0.63
41:S1:332:LYS:HD3	41:S1:507:TYR:HE1	1.64	0.63
41:S1:549:HIS:HE1	41:S1:677:ILE:HG12	1.64	0.63
40:V2:129:GLY:HA2	40:V2:140:ILE:HG22	1.81	0.62
52:A6:32:ARG:HB2	52:A6:32:ARG:NH1	2.13	0.62
41:S1:128:SER:HG	42:S2:341:SER:HG	1.47	0.62
7:D2:222:ASN:HD21	7:D2:233:THR:HG22	1.63	0.62
39:V1:213:VAL:HG13	39:V1:217:GLY:HA2	1.81	0.62
18:B4:74:ASN:ND2	18:B4:77:PRO:O	2.33	0.62
42:S2:105:ARG:NH1	44:S7:149:CYS:SG	2.72	0.62
6:D4:210:TYR:O	6:D4:213:HIS:ND1	2.33	0.62
7:D2:266:ILE:O	7:D2:270:MET:HB2	2.00	0.62
44:S7:85:VAL:HG12	44:S7:112:TYR:HB2	1.80	0.62
6:D4:204:MET:HB3	6:D4:209:LEU:HD22	1.82	0.62
41:S1:266:LYS:O	41:S1:270:ALA:HB2	1.99	0.62
41:S1:324:ASP:HA	41:S1:573:TYR:HE1	1.65	0.62
48:S4:118:TYR:OH	48:S4:133:LYS:NZ	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A9:157:ARG:HH21	49:A9:165:ILE:HD13	1.65	0.62
6:D4:177:LEU:O	6:D4:180:GLN:C	2.38	0.61
11:A8:129:LYS:HD2	15:A3:65:VAL:HG13	1.82	0.61
22:B9:125:LYS:HE2	22:B9:129:ARG:HH22	1.63	0.61
45:S8:53:GLU:OE2	54:AL:34:ARG:NH2	2.34	0.61
49:A9:51:CYS:SG	49:A9:52:GLU:N	2.73	0.61
7:D2:130:LEU:O	7:D2:134:GLN:HB2	2.00	0.61
6:D4:54:LEU:HA	9:B5:93:ILE:HD11	1.81	0.61
20:B6:109:ILE:HG22	20:B6:111:GLU:H	1.65	0.61
42:S2:388:ARG:NH1	42:S2:389:CYS:O	2.32	0.61
43:S3:38:GLN:CA	53:A7:70:SER:O	2.30	0.61
5:D5:342:CYS:HG	5:D5:369:THR:HG1	1.49	0.61
52:A6:32:ARG:CG	52:A6:32:ARG:HH11	2.14	0.61
1:D3:81:THR:O	15:A3:45:ASN:ND2	2.34	0.61
41:S1:377:VAL:O	41:S1:406:VAL:HA	2.01	0.61
13:AJ:111:ALA:HB1	13:AJ:122:VAL:HG21	1.83	0.61
42:S2:360:PRO:HA	42:S2:380:SER:O	2.00	0.61
51:A5:37:ILE:O	51:A5:44:ARG:NH1	2.33	0.61
12:BJ:145:LEU:HD13	12:BJ:149:TYR:HB3	1.81	0.60
42:S2:405:MET:SD	42:S2:421:GLN:NE2	2.73	0.60
2:D1:149:ILE:HG21	2:D1:185:TRP:HB2	1.82	0.60
40:V2:183:LYS:O	40:V2:187:ARG:NH1	2.32	0.60
5:D5:17:MET:HG2	20:B6:73:HIS:HE1	1.66	0.60
24:B8:88:ARG:HG3	24:B8:89:VAL:HG23	1.84	0.60
4:4L:55:LEU:HB2	14:S5:24:GLN:HG3	1.83	0.60
39:V1:362:CYS:N	62:V1:500:SF4:S2	2.74	0.60
49:A9:55:ASP:O	49:A9:58:HIS:ND1	2.32	0.60
49:A9:92:ILE:HG22	49:A9:130:ILE:HB	1.83	0.60
41:S1:114:CYS:SG	41:S1:115:ASP:N	2.74	0.60
51:A5:34:LEU:O	51:A5:44:ARG:NH1	2.35	0.60
2:D1:66:SER:N	2:D1:122:ALA:O	2.35	0.60
52:A6:32:ARG:HH11	52:A6:32:ARG:HG3	1.66	0.60
46:V3:57:ASP:O	46:V3:60:LYS:NZ	2.34	0.60
2:D1:22:LEU:HB3	2:D1:48:PRO:HG2	1.84	0.59
6:D4:254:THR:O	6:D4:258:ALA:HB3	2.02	0.59
39:V1:301:GLY:HA2	39:V1:333:ALA:HB3	1.83	0.59
45:S8:65:HIS:NE2	45:S8:116:CYS:SG	2.74	0.59
5:D5:191:ILE:HD12	6:D4:386:PHE:HD2	1.68	0.59
39:V1:434:ALA:O	39:V1:438:GLN:HB2	2.02	0.59
13:AJ:236:GLU:OE2	51:A5:91:ARG:NH1	2.34	0.59
7:D2:142:LEU:HB3	7:D2:194:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AJ:116:LEU:O	13:AJ:260:ARG:NH2	2.35	0.59
40:V2:27:ASN:OD1	40:V2:30:ARG:NH1	2.36	0.59
46:V3:38:TYR:HE2	46:V3:41:LEU:HB2	1.67	0.59
6:D4:370:PRO:HA	6:D4:375:LEU:HD13	1.85	0.59
39:V1:43:TYR:O	39:V1:236:ARG:NH1	2.36	0.59
47:S6:12:THR:OG1	47:S6:14:THR:O	2.21	0.59
13:AJ:91:GLY:O	13:AJ:95:ARG:NH2	2.36	0.59
19:AM:127:ARG:HG2	19:AM:131:GLU:HB2	1.85	0.59
2:D1:146:LEU:HG	2:D1:185:TRP:HE1	1.68	0.58
3:D6:159:TRP:HE1	7:D2:12:THR:HG22	1.67	0.58
41:S1:574:VAL:HG21	41:S1:630:LEU:HD22	1.84	0.58
41:S1:69:CYS:SG	41:S1:70:ALA:N	2.76	0.58
41:S1:317:ALA:HB3	41:S1:343:LEU:HG	1.84	0.58
43:S3:41:GLN:NE2	43:S3:49:GLU:OE1	2.37	0.58
45:S8:104:ARG:O	45:S8:105:ARG:NH1	2.36	0.58
50:A2:29:SER:OG	50:A2:33:ARG:NH1	2.36	0.58
43:S3:68:SER:HA	51:A5:82:GLN:HE21	1.68	0.58
3:D6:152:TRP:HB2	14:S5:13:LEU:HD12	1.85	0.58
3:D6:58:LEU:O	3:D6:62:GLY:CA	2.51	0.58
6:D4:177:LEU:O	6:D4:180:GLN:O	2.20	0.58
6:D4:269:MET:SD	6:D4:399:ASN:ND2	2.76	0.58
20:B6:100:LYS:HB3	21:B7:49:GLN:HE22	1.68	0.58
6:D4:221:VAL:HG23	6:D4:222:GLU:HG3	1.85	0.58
5:D5:267:THR:O	5:D5:274:GLN:NE2	2.36	0.58
39:V1:263:ASN:HB2	39:V1:286:GLY:H	1.69	0.58
49:A9:168:PRO:HA	49:A9:230:PHE:HB2	1.85	0.58
5:D5:547:LYS:O	5:D5:552:LEU:CB	2.51	0.58
21:B7:17:GLU:OE1	21:B7:20:ARG:NH2	2.37	0.58
41:S1:409:ILE:HG12	41:S1:422:LEU:HB2	1.86	0.58
41:S1:449:PRO:HG2	41:S1:489:VAL:HG22	1.85	0.58
3:D6:167:VAL:HG22	7:D2:42:PRO:HG2	1.84	0.58
39:V1:78:LYS:NZ	63:V1:501:FMN:O2P	2.37	0.58
41:S1:31:GLU:OE2	41:S1:39:ARG:NH1	2.37	0.58
44:S7:46:TRP:NE1	44:S7:82:GLN:O	2.37	0.58
22:B9:107:HIS:NE2	25:BK:43:ASP:OD1	2.36	0.57
41:S1:229:ASP:HB3	41:S1:235:GLY:HA2	1.86	0.57
40:V2:10:ARG:HE	47:S6:77:LYS:HD2	1.69	0.57
41:S1:569:LYS:NZ	41:S1:596:ASP:OD2	2.37	0.57
6:D4:388:TRP:O	18:B4:108:ARG:NH2	2.36	0.57
39:V1:44:LYS:HG3	40:V2:213:VAL:HG21	1.85	0.57
39:V1:261:HIS:HB2	40:V2:110:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:S2:371:LYS:HZ1	42:S2:424:VAL:HG13	1.69	0.57
54:AL:13:GLN:NE2	54:AL:33:VAL:O	2.37	0.57
40:V2:24:THR:HG22	40:V2:26:GLU:H	1.69	0.57
2:D1:92:PRO:HG3	2:D1:255:TYR:HD2	1.69	0.57
5:D5:15:LEU:HB3	5:D5:126:ILE:HG12	1.87	0.57
6:D4:336:ARG:HH21	6:D4:429:SER:HA	1.70	0.57
39:V1:349:ARG:HE	40:V2:105:THR:HA	1.69	0.57
45:S8:70:TYR:HH	47:S6:68:HIS:HD1	1.53	0.57
13:AJ:77:CYS:O	13:AJ:92:ASN:ND2	2.36	0.57
15:A3:79:TRP:HA	15:A3:82:ARG:HB2	1.87	0.57
53:A7:45:SER:O	53:A7:46:HIS:ND1	2.36	0.57
5:D5:82:MET:SD	5:D5:82:MET:N	2.78	0.56
11:A8:17:VAL:HG21	19:AM:73:LEU:HD21	1.86	0.56
24:B8:69:LEU:HB3	24:B8:71:LEU:HD23	1.87	0.56
41:S1:45:ARG:HD3	48:S4:114:LYS:HZ1	1.70	0.56
42:S2:424:VAL:HG23	42:S2:426:GLY:H	1.70	0.56
9:B5:73:ARG:NH2	12:BJ:61:TYR:O	2.39	0.56
11:A8:165:ARG:NH2	17:C2:87:ASP:OD1	2.38	0.56
21:B7:27:ASP:HA	21:B7:30:PHE:HB2	1.86	0.56
25:BK:82:ASP:HB2	25:BK:86:GLN:H	1.70	0.56
41:S1:163:ALA:O	41:S1:168:GLY:N	2.31	0.56
41:S1:357:ASP:HB3	50:A2:53:LEU:HA	1.87	0.56
47:S6:31:ARG:HH22	49:A9:69:ILE:HD11	1.70	0.56
2:D1:34:ARG:NH1	44:S7:70:ASP:OD2	2.32	0.56
25:BK:100:ARG:HD3	25:BK:107:LEU:HA	1.87	0.56
41:S1:443:LEU:HD23	41:S1:477:ILE:HD11	1.85	0.56
13:AJ:80:GLU:OE1	13:AJ:190:HIS:ND1	2.37	0.56
19:AM:138:GLY:O	19:AM:142:TYR:HB2	2.05	0.56
23:B2:46:ALA:O	23:B2:50:HIS:NE2	2.38	0.56
51:A5:17:GLU:HG2	51:A5:18:THR:HG23	1.86	0.56
13:AJ:202:ILE:O	13:AJ:206:TYR:CB	2.53	0.56
21:B7:34:LYS:NZ	24:B8:155:HIS:O	2.38	0.56
12:BJ:136:LYS:NZ	12:BJ:140:ASP:OD2	2.37	0.56
42:S2:347:HIS:O	42:S2:351:LEU:CB	2.54	0.56
10:AA:29:LYS:HE3	10:AA:40:LEU:HG	1.88	0.56
7:D2:269:GLU:HG2	7:D2:272:LYS:HE3	1.88	0.56
41:S1:531:CYS:SG	41:S1:532:VAL:N	2.79	0.56
26:C1:41:GLU:OE2	26:C1:44:ARG:NH2	2.38	0.56
11:A8:107:ASP:OD2	11:A8:118:ARG:NH1	2.39	0.55
12:BJ:68:ARG:NH1	27:B1:43:LEU:O	2.38	0.55
39:V1:289:GLY:HA3	39:V1:293:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:V2:147:ALA:HB1	40:V2:150:ASN:HD22	1.70	0.55
5:D5:227:PHE:H	5:D5:284:THR:HG22	1.71	0.55
5:D5:264:TYR:HA	5:D5:267:THR:HG22	1.87	0.55
42:S2:246:THR:HG23	51:A5:12:GLY:HA3	1.88	0.55
21:B7:34:LYS:HG3	24:B8:156:TYR:HA	1.89	0.55
5:D5:482:MET:SD	5:D5:487:LYS:NZ	2.80	0.55
7:D2:13:VAL:HG13	7:D2:36:ASN:HD21	1.71	0.55
40:V2:92:ARG:NH1	41:S1:186:TYR:OH	2.40	0.55
41:S1:377:VAL:HG22	41:S1:450:MET:HB3	1.88	0.55
49:A9:202:LYS:N	49:A9:236:TYR:O	2.40	0.55
52:A6:63:ARG:HB2	10:AA:45:LEU:HD21	1.87	0.55
50:A2:57:CYS:SG	50:A2:58:SER:N	2.79	0.55
54:AL:71:LYS:HD2	54:AL:115:PHE:HZ	1.70	0.55
49:A9:50:ARG:NE	65:A9:401:NDP:O3X	2.40	0.55
54:AL:51:ASP:OD2	54:AL:54:GLN:NE2	2.39	0.55
5:D5:547:LYS:O	5:D5:552:LEU:HB2	2.06	0.55
5:D5:584:ILE:HD11	7:D2:58:LYS:HE2	1.87	0.55
7:D2:49:ASN:HB3	42:S2:36:VAL:HG22	1.89	0.55
12:BJ:141:ARG:NH1	25:BK:109:GLU:O	2.40	0.55
41:S1:278:ARG:NH2	41:S1:568:GLU:OE1	2.39	0.55
41:S1:404:LEU:H	48:S4:127:ARG:HH22	1.54	0.55
42:S2:82:LEU:HD12	44:S7:95:LYS:HE3	1.89	0.55
5:D5:279:CYS:SG	5:D5:405:ASN:ND2	2.80	0.55
6:D4:27:THR:HB	6:D4:77:LEU:HD11	1.88	0.55
11:A8:144:ARG:HH22	14:S5:57:ILE:HD13	1.71	0.55
41:S1:592:LEU:O	41:S1:594:ARG:NH1	2.40	0.55
42:S2:47:LEU:O	42:S2:67:GLU:HA	2.07	0.55
5:D5:72:GLN:OE1	12:BJ:99:GLN:NE2	2.39	0.55
41:S1:12:PHE:HB2	41:S1:78:ASN:HA	1.87	0.55
2:D1:111:LEU:HD13	2:D1:114:TYR:HD2	1.71	0.55
7:D2:202:LEU:HD23	7:D2:346:LEU:HD21	1.88	0.55
10:AB:55:GLU:OE1	22:B9:24:ARG:NH2	2.39	0.55
19:AM:86:LEU:HD21	19:AM:118:PRO:HG3	1.89	0.55
39:V1:366:ARG:NH1	41:S1:155:GLN:OE1	2.39	0.55
48:S4:62:ARG:HH12	52:A6:127:PRO:HD2	1.72	0.55
24:B8:62:TYR:HD2	24:B8:64:TRP:HE3	1.54	0.54
5:D5:241:THR:HG21	5:D5:344:GLY:HA3	1.89	0.54
39:V1:391:SER:OG	41:S1:129:ARG:NH1	2.40	0.54
41:S1:366:THR:OG1	41:S1:491:ASN:ND2	2.41	0.54
42:S2:261:ARG:NH1	42:S2:267:TRP:O	2.40	0.54
44:S7:62:MET:HB3	44:S7:153:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D2:69:LEU:HD11	7:D2:97:LEU:HD22	1.90	0.54
15:A3:58:ASP:OD1	15:A3:58:ASP:N	2.41	0.54
40:V2:144:CYS:SG	40:V2:145:LEU:N	2.81	0.54
41:S1:278:ARG:HA	41:S1:549:HIS:HB3	1.88	0.54
2:D1:73:LEU:HA	2:D1:76:ILE:HG22	1.89	0.54
19:AM:23:ASN:O	53:A7:17:ARG:NH2	2.41	0.54
41:S1:534:ARG:NH1	41:S1:541:CYS:SG	2.81	0.54
7:D2:102:LEU:HD22	7:D2:138:PRO:HB3	1.90	0.54
8:AK:39:SER:HB2	8:AK:54:ARG:HH22	1.71	0.54
10:AB:31:SER:HB3	10:AB:34:SER:HB2	1.90	0.54
16:B3:40:LEU:HD21	22:B9:45:ALA:HB2	1.88	0.54
49:A9:136:ASN:HD22	49:A9:292:ARG:HD2	1.73	0.54
41:S1:316:ALA:O	41:S1:522:LEU:HA	2.08	0.54
17:C2:66:THR:OG1	26:C1:28:TRP:NE1	2.40	0.54
20:B6:122:PHE:HE1	21:B7:64:ARG:HD2	1.73	0.54
2:D1:228:TYR:HA	2:D1:231:ILE:HD12	1.89	0.54
11:A8:123:GLU:OE1	15:A3:70:GLN:NE2	2.40	0.54
45:S8:63:GLY:H	45:S8:133:GLU:HB3	1.73	0.54
2:D1:245:ALA:H	2:D1:255:TYR:HE1	1.55	0.54
40:V2:42:HIS:HD2	48:S4:129:ARG:HH12	1.54	0.54
41:S1:103:LEU:HD13	47:S6:69:PRO:HB2	1.90	0.54
4:4L:55:LEU:HD13	14:S5:24:GLN:HA	1.90	0.53
8:AK:80:ARG:HH12	8:AK:87:LEU:HB3	1.73	0.53
57:AB:101:ZMP:H8	22:B9:47:PHE:HE1	1.73	0.53
21:B7:108:LEU:O	21:B7:112:LYS:HB2	2.08	0.53
41:S1:257:ASP:OD2	41:S1:579:ARG:NH2	2.42	0.53
1:D3:98:LEU:HD22	2:D1:298:LEU:HD21	1.90	0.53
41:S1:159:CYS:HB2	41:S1:199:ILE:HD11	1.91	0.53
44:S7:109:GLU:O	49:A9:54:TYR:OH	2.19	0.53
7:D2:151:LEU:HD22	8:AK:136:ALA:HB2	1.89	0.53
7:D2:211:MET:O	7:D2:214:THR:OG1	2.23	0.53
42:S2:238:ARG:HG3	42:S2:239:THR:HG23	1.90	0.53
49:A9:34:LEU:HD11	49:A9:214:ILE:HG21	1.91	0.53
2:D1:26:LYS:NZ	28:A1:4:GLU:O	2.40	0.53
5:D5:380:LEU:HD23	5:D5:381:THR:HG23	1.90	0.53
6:D4:54:LEU:HD11	11:A8:170:THR:HG21	1.91	0.53
8:AK:122:ALA:O	8:AK:126:MET:HB2	2.09	0.53
17:C2:25:LYS:N	17:C2:28:ASP:OD2	2.42	0.53
21:B7:55:ARG:NH1	24:B8:141:GLU:OE2	2.42	0.53
45:S8:152:GLU:OE1	54:AL:127:TYR:OH	2.27	0.53
54:AL:46:ASN:ND2	54:AL:48:TYR:OH	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:157:THR:HG23	41:S1:160:ILE:HD12	1.90	0.53
41:S1:225:THR:HB	41:S1:240:VAL:HG23	1.89	0.53
41:S1:243:ARG:HH12	45:S8:95:GLU:HG3	1.72	0.53
45:S8:1:THR:HB	53:A7:106:SER:HB2	1.90	0.53
10:AA:80:ILE:O	10:AA:84:LYS:N	2.41	0.53
7:D2:292:PHE:HA	7:D2:295:ARG:HG2	1.90	0.53
13:AJ:141:GLN:NE2	13:AJ:201:ASP:OD2	2.40	0.53
41:S1:222:THR:HG22	41:S1:243:ARG:HB2	1.91	0.53
9:B5:43:ILE:HG13	9:B5:71:ILE:HD11	1.90	0.53
40:V2:96:GLY:HA3	40:V2:136:LEU:H	1.73	0.53
42:S2:229:LEU:HD23	42:S2:230:THR:H	1.74	0.53
45:S8:44:GLU:OE2	53:A7:2:SER:OG	2.26	0.53
50:A2:20:ILE:HB	50:A2:54:ILE:HG12	1.91	0.53
17:C2:30:ARG:HE	17:C2:76:LEU:HD11	1.73	0.53
48:S4:37:ILE:HD13	48:S4:92:ALA:HB1	1.91	0.53
51:A5:13:LEU:HD21	51:A5:77:GLU:HB3	1.91	0.53
6:D4:336:ARG:HB3	6:D4:426:ILE:HG22	1.91	0.53
7:D2:228:LEU:O	7:D2:232:HIS:ND1	2.38	0.53
43:S3:39:GLN:HB3	43:S3:51:CYS:HB2	1.90	0.53
43:S3:63:PHE:HD2	43:S3:64:LEU:HD12	1.74	0.53
54:AL:17:HIS:HD2	54:AL:35:VAL:HG21	1.74	0.53
1:D3:69:ILE:HD11	2:D1:144:VAL:HG13	1.91	0.52
12:BJ:122:GLN:HG3	21:B7:46:ASN:HD21	1.74	0.52
19:AM:31:GLY:O	19:AM:35:PHE:CB	2.56	0.52
39:V1:48:ILE:HD13	39:V1:235:CYS:HB3	1.89	0.52
39:V1:342:ASP:OD2	39:V1:429:ARG:NH2	2.42	0.52
41:S1:285:ARG:NH2	54:AL:144:TYR:O	2.42	0.52
42:S2:284:ASP:OD1	42:S2:284:ASP:N	2.41	0.52
2:D1:145:THR:HG23	2:D1:297:THR:HG21	1.90	0.52
5:D5:344:GLY:HA2	5:D5:347:ILE:HD12	1.90	0.52
41:S1:114:CYS:O	48:S4:46:GLN:NE2	2.42	0.52
49:A9:132:ILE:HD13	65:A9:401:NDP:H1D	1.92	0.52
2:D1:140:ILE:HD12	3:D6:66:VAL:HG11	1.91	0.52
45:S8:91:ALA:HB1	45:S8:112:ASP:H	1.75	0.52
2:D1:10:ILE:HB	2:D1:83:LEU:HD22	1.92	0.52
41:S1:122:MET:O	53:A7:60:ARG:NH2	2.43	0.52
49:A9:108:ASP:O	49:A9:112:LYS:CB	2.56	0.52
49:A9:237:LEU:HG	49:A9:239:PHE:H	1.73	0.52
11:A8:70:PHE:HA	11:A8:73:ILE:HG22	1.92	0.52
18:B4:42:LEU:HD13	24:B8:74:GLY:HA3	1.90	0.52
41:S1:632:ARG:NH1	50:A2:57:CYS:SG	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B2:62:GLU:HA	23:B2:66:ILE:H	1.73	0.52
28:A1:2:TRP:HH2	53:A7:7:ILE:HG21	1.74	0.52
42:S2:116:GLN:HG3	42:S2:138:ARG:HD3	1.91	0.52
50:A2:61:GLN:HB2	50:A2:63:LYS:HE3	1.91	0.52
27:B1:46:ARG:NH2	27:B1:55:THR:OG1	2.42	0.52
41:S1:315:VAL:HA	41:S1:521:MET:O	2.10	0.52
11:A8:74:LYS:HD2	28:A1:69:ILE:HG13	1.91	0.52
27:B1:16:VAL:HG23	27:B1:17:PRO:HD3	1.91	0.52
39:V1:109:GLU:OE2	39:V1:112:ARG:NH2	2.35	0.52
41:S1:316:ALA:HA	41:S1:342:THR:O	2.10	0.52
2:D1:284:GLN:NE2	42:S2:237:ASN:O	2.43	0.52
7:D2:207:ILE:HD13	7:D2:262:PRO:HD3	1.92	0.52
39:V1:91:LYS:HG2	39:V1:219:PRO:HG2	1.90	0.52
39:V1:140:GLY:O	39:V1:179:ARG:NH2	2.43	0.52
40:V2:132:THR:HG21	40:V2:137:PHE:H	1.74	0.52
42:S2:48:THR:HG22	42:S2:67:GLU:HG2	1.91	0.52
48:S4:56:LYS:HA	48:S4:84:LEU:O	2.09	0.52
5:D5:72:GLN:NE2	6:D4:459:TYR:OXT	2.43	0.52
5:D5:83:ASP:O	5:D5:87:MET:CB	2.57	0.52
5:D5:439:THR:OG1	5:D5:440:LEU:N	2.43	0.52
7:D2:144:GLN:HE21	14:S5:2:PHE:HB2	1.75	0.52
14:S5:8:LYS:HB2	17:C2:10:PRO:HG3	1.92	0.52
42:S2:146:ARG:HG3	42:S2:370:PRO:HG3	1.92	0.52
22:B9:153:LEU:HD13	22:B9:164:PRO:HG2	1.92	0.51
41:S1:257:ASP:O	41:S1:394:ARG:NH2	2.43	0.51
44:S7:47:PRO:HB3	44:S7:85:VAL:HG23	1.91	0.51
49:A9:97:ARG:HG3	49:A9:99:TRP:H	1.75	0.51
49:A9:166:ILE:HG23	49:A9:168:PRO:HD3	1.91	0.51
2:D1:66:SER:OG	2:D1:67:SER:N	2.41	0.51
57:AB:101:ZMP:O2	57:AB:101:ZMP:N2	2.44	0.51
12:BJ:159:LYS:HE2	25:BK:118:ILE:HD11	1.92	0.51
24:B8:53:ARG:NH2	24:B8:84:TYR:OH	2.41	0.51
39:V1:33:LEU:HD23	39:V1:155:GLU:HB3	1.92	0.51
41:S1:324:ASP:HB2	41:S1:327:ALA:H	1.73	0.51
45:S8:53:GLU:HG2	54:AL:61:TRP:HB3	1.92	0.51
52:A6:32:ARG:NH1	52:A6:32:ARG:CB	2.73	0.51
5:D5:145:GLU:HB2	6:D4:370:PRO:HB3	1.92	0.51
7:D2:269:GLU:HA	7:D2:272:LYS:HG2	1.91	0.51
12:BJ:159:LYS:NZ	17:C2:112:VAL:O	2.44	0.51
44:S7:41:ARG:HH12	44:S7:110:PRO:HB3	1.75	0.51
4:4L:62:ILE:HA	4:4L:65:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A8:35:CYS:SG	11:A8:36:ASP:N	2.82	0.51
22:B9:102:CYS:SG	22:B9:103:LEU:N	2.72	0.51
39:V1:136:ILE:HD13	39:V1:149:LEU:HD21	1.93	0.51
41:S1:80:LEU:HB3	41:S1:83:SER:HB3	1.92	0.51
2:D1:85:MET:HE1	2:D1:105:MET:HA	1.92	0.51
6:D4:205:VAL:HG22	6:D4:212:LEU:HD13	1.93	0.51
7:D2:243:LEU:HD21	17:C2:44:ILE:HD11	1.92	0.51
41:S1:564:ALA:HB3	41:S1:569:LYS:HD3	1.92	0.51
44:S7:116:MET:HA	44:S7:146:VAL:HG23	1.93	0.51
45:S8:59:PRO:O	45:S8:168:ASN:ND2	2.44	0.51
7:D2:274:ASP:N	8:AK:137:GLU:OE2	2.44	0.51
41:S1:568:GLU:HB3	41:S1:589:PRO:HG3	1.93	0.51
42:S2:161:ILE:HD11	42:S2:238:ARG:HE	1.75	0.51
45:S8:77:CYS:SG	45:S8:78:ILE:N	2.84	0.51
2:D1:310:LEU:HD21	15:A3:32:PRO:HA	1.93	0.51
2:D1:272:TRP:HE1	45:S8:38:LEU:HB2	1.76	0.51
5:D5:535:ARG:NE	24:B8:90:ASP:O	2.44	0.51
7:D2:295:ARG:HH12	42:S2:19:MET:HG2	1.75	0.51
9:B5:139:ALA:HB3	14:S5:28:ILE:HG22	1.93	0.51
15:A3:48:THR:HG21	19:AM:57:ARG:HH21	1.76	0.51
19:AM:34:MET:HA	19:AM:37:VAL:HG12	1.92	0.51
41:S1:337:ARG:NH1	41:S1:610:THR:O	2.44	0.51
46:V3:70:ARG:NH2	48:S4:125:ASN:O	2.44	0.51
52:A6:32:ARG:NH1	52:A6:32:ARG:CG	2.73	0.51
6:D4:82:HIS:O	6:D4:86:LYS:NZ	2.44	0.51
39:V1:305:PRO:HG3	39:V1:413:TRP:HB3	1.93	0.51
43:S3:77:ASP:O	43:S3:93:VAL:O	2.28	0.51
43:S3:182:ARG:NH1	52:A6:108:GLU:OE1	2.43	0.51
45:S8:83:CYS:O	45:S8:87:CYS:HB2	2.10	0.51
5:D5:224:SER:HB2	5:D5:310:LEU:HD23	1.93	0.50
10:AB:65:ILE:O	10:AB:69:LYS:NZ	2.44	0.50
39:V1:111:ILE:HD11	39:V1:149:LEU:HB2	1.93	0.50
41:S1:543:ILE:HD11	41:S1:557:ALA:HA	1.93	0.50
43:S3:78:LEU:HD22	43:S3:130:TYR:HB3	1.92	0.50
44:S7:165:LYS:NZ	54:AL:78:ASP:OD1	2.35	0.50
47:S6:20:ASP:OD1	47:S6:25:ARG:NH1	2.42	0.50
2:D1:271:LEU:HD23	2:D1:274:ARG:HH21	1.76	0.50
24:B8:52:ASP:OD1	24:B8:78:HIS:NE2	2.27	0.50
40:V2:42:HIS:CD2	48:S4:129:ARG:HH12	2.29	0.50
6:D4:102:LEU:HD21	6:D4:230:VAL:HG11	1.92	0.50
6:D4:243:MET:HG2	6:D4:301:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B9:97:LYS:HE2	22:B9:175:GLU:HA	1.92	0.50
54:AL:60:ARG:NH1	54:AL:92:CYS:SG	2.84	0.50
5:D5:161:ARG:NH2	22:B9:87:GLY:O	2.45	0.50
6:D4:300:ALA:O	6:D4:308:SER:OG	2.27	0.50
11:A8:166:LEU:HD23	11:A8:167:PHE:H	1.76	0.50
13:AJ:113:GLU:HB2	13:AJ:263:VAL:HG11	1.93	0.50
20:B6:89:VAL:HG22	20:B6:95:THR:HG21	1.93	0.50
22:B9:13:GLN:HE21	22:B9:17:GLN:HE21	1.59	0.50
41:S1:40:PHE:HE1	41:S1:115:ASP:HB3	1.76	0.50
41:S1:73:VAL:HA	41:S1:77:TRP:HE1	1.76	0.50
13:AJ:49:LYS:HD2	13:AJ:114:HIS:HE1	1.77	0.50
39:V1:362:CYS:SG	39:V1:404:ILE:N	2.82	0.50
40:V2:97:LYS:O	40:V2:157:ASN:ND2	2.44	0.50
42:S2:354:GLU:HA	43:S3:199:LEU:HD22	1.93	0.50
13:AJ:127:SER:O	13:AJ:130:SER:OG	2.29	0.50
39:V1:318:ASP:HB2	39:V1:321:ALA:HB3	1.93	0.50
48:S4:36:ARG:NH2	48:S4:58:GLU:OE1	2.42	0.50
51:A5:23:LEU:HD22	51:A5:58:VAL:HG11	1.94	0.50
5:D5:234:PRO:HB3	5:D5:300:LYS:HG2	1.94	0.50
14:S5:12:ASP:HB3	14:S5:15:HIS:HB2	1.93	0.50
41:S1:367:THR:HG22	41:S1:369:ALA:H	1.75	0.50
41:S1:511:VAL:HG11	41:S1:531:CYS:HB2	1.93	0.50
51:A5:37:ILE:HD11	51:A5:94:ILE:HA	1.94	0.50
5:D5:570:GLN:OE1	7:D2:167:TRP:NE1	2.45	0.50
39:V1:202:LYS:NZ	48:S4:132:THR:O	2.39	0.50
40:V2:110:LEU:HD23	40:V2:111:ARG:HG3	1.93	0.50
41:S1:623:LEU:HD11	41:S1:630:LEU:HD12	1.94	0.50
6:D4:53:SER:O	6:D4:55:THR:N	2.45	0.50
6:D4:175:ASN:ND2	9:B5:97:GLU:OE1	2.45	0.50
7:D2:17:THR:HG23	7:D2:137:ALA:HB2	1.94	0.50
39:V1:104:THR:HG22	39:V1:106:LYS:HB2	1.94	0.50
43:S3:88:ASN:HA	43:S3:112:ASP:HB3	1.94	0.50
14:S5:82:ARG:HH12	14:S5:95:PRO:HG2	1.76	0.49
42:S2:145:THR:OG1	42:S2:181:TYR:OH	2.29	0.49
6:D4:254:THR:O	6:D4:258:ALA:CB	2.59	0.49
19:AM:22:ARG:NE	42:S2:226:GLU:OE1	2.43	0.49
44:S7:34:ASP:OD1	44:S7:38:ASN:ND2	2.45	0.49
4:4L:73:LEU:HD21	7:D2:41:ILE:HG13	1.94	0.49
5:D5:433:GLY:O	16:B3:59:ASN:ND2	2.44	0.49
54:AL:117:LEU:HD13	54:AL:123:GLN:HA	1.93	0.49
1:D3:71:LEU:O	3:D6:147:TYR:OH	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D5:233:LEU:HG	5:D5:303:ALA:HB1	1.94	0.49
6:D4:350:THR:OG1	6:D4:351:LEU:N	2.46	0.49
9:B5:142:ASP:OD2	11:A8:46:ARG:NH2	2.44	0.49
41:S1:260:GLU:OE2	41:S1:394:ARG:NH1	2.45	0.49
5:D5:60:GLU:HB2	20:B6:99:LYS:HB3	1.95	0.49
7:D2:18:ILE:O	7:D2:22:ILE:HB	2.11	0.49
7:D2:338:PRO:O	11:A8:169:TRP:NE1	2.45	0.49
20:B6:17:LEU:HD11	22:B9:162:LEU:HD22	1.95	0.49
41:S1:279:LEU:HG	41:S1:549:HIS:H	1.76	0.49
5:D5:139:GLN:HA	5:D5:142:ILE:HD12	1.93	0.49
6:D4:459:TYR:O	12:BJ:96:LYS:NZ	2.43	0.49
41:S1:424:ASP:OD1	41:S1:424:ASP:N	2.44	0.49
42:S2:383:SER:OG	42:S2:384:SER:N	2.45	0.49
43:S3:151:ILE:HG22	43:S3:152:LEU:HG	1.94	0.49
1:D3:59:ALA:HB1	3:D6:67:VAL:HG13	1.94	0.49
9:B5:143:ASN:HD22	14:S5:29:PRO:HG3	1.77	0.49
41:S1:69:CYS:HB2	60:S1:803:FES:S2	2.52	0.49
6:D4:22:MET:O	6:D4:26:ASN:ND2	2.45	0.49
7:D2:109:ALA:HB2	7:D2:161:SER:HA	1.93	0.49
5:D5:224:SER:HB3	5:D5:256:GLY:HA3	1.95	0.49
13:AJ:217:LYS:HE2	13:AJ:247:PRO:HD3	1.94	0.49
13:AJ:217:LYS:HG2	13:AJ:246:GLY:HA2	1.95	0.49
15:A3:83:LEU:O	19:AM:54:ARG:NH2	2.45	0.49
41:S1:547:GLY:O	41:S1:563:GLY:N	2.46	0.49
44:S7:179:ARG:HA	49:A9:50:ARG:HH12	1.78	0.49
7:D2:230:LEU:HB3	7:D2:300:THR:HG21	1.95	0.49
11:A8:34:GLN:OE1	11:A8:116:TRP:NE1	2.46	0.49
1:D3:84:LEU:HD13	2:D1:309:ILE:HD11	1.94	0.48
6:D4:187:PRO:O	6:D4:192:ASN:ND2	2.43	0.48
14:S5:91:TYR:HD2	14:S5:94:PRO:HD2	1.77	0.48
17:C2:20:SER:OG	17:C2:21:LEU:N	3.14	0.48
39:V1:109:GLU:OE2	39:V1:113:HIS:NE2	2.43	0.48
45:S8:110:ASP:OD1	45:S8:150:ASN:ND2	2.46	0.48
9:B5:64:TRP:CD1	9:B5:65:GLU:HG3	2.48	0.48
17:C2:8:ARG:H	17:C2:9:ALA:HB3	1.78	0.48
15:A3:59:ASP:HB3	15:A3:61:ASN:H	1.78	0.48
22:B9:133:GLU:O	22:B9:137:LYS:HB2	2.13	0.48
39:V1:101:GLU:H	39:V1:184:TYR:HE1	1.60	0.48
12:BJ:69:ARG:NH1	12:BJ:90:GLN:OE1	2.47	0.48
39:V1:200:GLN:HE21	39:V1:202:LYS:HE3	1.79	0.48
41:S1:107:ILE:HG22	45:S8:104:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:503:LEU:HD21	41:S1:509:PRO:HG3	1.95	0.48
44:S7:77:ARG:HG3	44:S7:79:SER:H	1.77	0.48
5:D5:341:MET:HE3	5:D5:454:ILE:HD13	1.96	0.48
10:AB:48:VAL:HG21	22:B9:16:LEU:HD11	1.95	0.48
41:S1:354:ALA:O	41:S1:361:ASN:ND2	2.44	0.48
43:S3:80:ALA:HB2	43:S3:92:ILE:HD13	1.95	0.48
2:D1:18:ALA:O	2:D1:21:THR:OG1	2.26	0.48
42:S2:188:ARG:HH12	44:S7:153:ALA:H	1.62	0.48
2:D1:243:LEU:HD13	2:D1:262:LYS:HD3	1.95	0.48
2:D1:289:LEU:HA	2:D1:293:PHE:HD2	1.77	0.48
13:AJ:1:LEU:HD13	13:AJ:3:TYR:HB2	1.96	0.48
21:B7:7:ARG:HB2	21:B7:15:GLU:HG3	1.93	0.48
43:S3:38:GLN:O	53:A7:70:SER:CA	2.59	0.48
48:S4:57:MET:O	48:S4:83:VAL:HA	2.14	0.48
6:D4:147:LEU:HD21	7:D2:291:TYR:HE1	1.78	0.48
55:D4:501:3PE:N	7:D2:291:TYR:OH	2.46	0.48
11:A8:46:ARG:HH12	19:AM:75:GLN:HE21	1.62	0.48
41:S1:328:LEU:HD22	41:S1:507:TYR:HE2	1.79	0.48
42:S2:110:SER:OG	42:S2:114:ASN:OD1	2.28	0.48
2:D1:221:ALA:O	2:D1:225:MET:HB2	2.14	0.48
7:D2:137:ALA:O	7:D2:140:SER:OG	2.28	0.48
9:B5:138:LYS:HB3	14:S5:29:PRO:HD3	1.95	0.48
11:A8:134:ARG:O	15:A3:57:ARG:NH2	2.47	0.48
39:V1:299:PRO:HA	39:V1:334:VAL:HG12	1.96	0.48
40:V2:61:LEU:HD21	40:V2:90:TYR:HB3	1.94	0.48
44:S7:158:TYR:HE1	54:AL:79:GLY:H	1.62	0.48
39:V1:25:LEU:O	39:V1:113:HIS:NE2	2.46	0.47
39:V1:358:SER:OG	62:V1:500:SF4:S3	2.66	0.47
40:V2:116:ILE:HG23	40:V2:169:ILE:HD11	1.94	0.47
40:V2:186:PRO:HG2	40:V2:192:SER:HA	1.95	0.47
42:S2:110:SER:HB2	42:S2:113:CYS:HB2	1.96	0.47
42:S2:231:ASN:OD1	42:S2:294:TYR:OH	2.32	0.47
42:S2:268:ASP:OD2	42:S2:270:ARG:NH2	2.47	0.47
5:D5:547:LYS:O	5:D5:552:LEU:HB3	2.15	0.47
39:V1:138:ILE:HG22	39:V1:179:ARG:HA	1.95	0.47
41:S1:364:LEU:HG	41:S1:491:ASN:HB2	1.97	0.47
18:B4:51:ASN:HD22	22:B9:165:LEU:HD23	1.80	0.47
39:V1:372:MET:HG2	39:V1:392:LEU:HD11	1.95	0.47
41:S1:641:TYR:HB3	41:S1:644:GLN:HB2	1.96	0.47
9:B5:104:ARG:NH2	11:A8:166:LEU:O	2.47	0.47
13:AJ:305:ARG:HB2	17:C2:50:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AM:27:ARG:O	45:S8:32:ARG:NH2	2.48	0.47
10:AA:32:VAL:HB	10:AA:74:GLN:HB2	1.97	0.47
39:V1:124:VAL:HG21	39:V1:232:PRO:HA	1.95	0.47
43:S3:86:ARG:HD3	51:A5:110:GLN:HG3	1.96	0.47
2:D1:68:ILE:HA	2:D1:71:PHE:HB3	1.96	0.47
2:D1:186:PHE:O	2:D1:189:THR:OG1	2.29	0.47
5:D5:95:PHE:HZ	5:D5:456:ARG:HG2	1.80	0.47
5:D5:165:ASN:N	5:D5:165:ASN:OD1	2.46	0.47
5:D5:418:PHE:HA	5:D5:421:ILE:HG12	1.97	0.47
6:D4:403:THR:HA	6:D4:406:TYR:CE2	2.50	0.47
8:AK:17:CYS:SG	8:AK:18:HIS:N	2.87	0.47
19:AM:19:ASP:N	19:AM:19:ASP:OD1	2.47	0.47
19:AM:67:ARG:HD3	19:AM:68:ILE:HG13	1.97	0.47
22:B9:103:LEU:HB3	22:B9:121:ARG:HH12	1.78	0.47
42:S2:50:ASN:HD22	42:S2:65:VAL:HG22	1.80	0.47
43:S3:66:ASP:HB2	51:A5:89:LEU:HD23	1.96	0.47
49:A9:19:ILE:O	49:A9:43:SER:OG	2.32	0.47
49:A9:208:VAL:HA	49:A9:211:THR:HG22	1.95	0.47
13:AJ:306:ALA:HB1	26:C1:3:TYR:HE1	1.79	0.47
44:S7:162:GLN:OE1	54:AL:116:ASN:ND2	2.44	0.47
3:D6:50:SER:N	3:D6:139:GLU:OE2	2.48	0.47
7:D2:232:HIS:CE1	13:AJ:276:PRO:HG3	2.50	0.47
13:AJ:71:VAL:O	13:AJ:76:ASN:ND2	2.47	0.47
21:B7:3:HIS:CE1	24:B8:127:PRO:HD3	2.50	0.47
45:S8:27:TRP:HD1	45:S8:30:LEU:HD13	1.80	0.47
2:D1:66:SER:O	2:D1:70:MET:HB2	2.15	0.47
6:D4:60:SER:OG	25:BK:84:ARG:NH2	2.48	0.47
39:V1:109:GLU:HG3	39:V1:113:HIS:HD2	1.80	0.47
40:V2:120:ILE:HD13	40:V2:173:ILE:HD11	1.97	0.47
42:S2:406:SER:HB2	42:S2:414:VAL:HG22	1.96	0.47
43:S3:195:ARG:NE	45:S8:84:GLU:OE2	2.42	0.47
57:AB:101:ZMP:H19A	22:B9:12:GLN:HG3	1.97	0.46
39:V1:101:GLU:O	39:V1:104:THR:OG1	2.30	0.46
39:V1:392:LEU:HA	39:V1:395:ILE:HG22	1.96	0.46
5:D5:384:PRO:HA	5:D5:385:PHE:HA	1.57	0.46
10:AB:48:VAL:HG21	22:B9:16:LEU:HD21	1.97	0.46
41:S1:45:ARG:HE	41:S1:260:GLU:HB3	1.81	0.46
49:A9:130:ILE:HG12	49:A9:164:THR:HB	1.96	0.46
3:D6:14:VAL:HG22	4:4L:11:ALA:HB2	1.98	0.46
5:D5:10:VAL:HA	5:D5:13:ILE:HG22	1.96	0.46
57:AB:101:ZMP:H5A	22:B9:46:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D5:65:ASN:ND2	20:B6:84:TYR:OH	2.48	0.46
13:AJ:24:LEU:HG	13:AJ:115:LEU:HD22	1.98	0.46
23:B2:55:ASP:OD1	23:B2:55:ASP:N	2.48	0.46
5:D5:172:ILE:HG21	6:D4:408:LEU:HD22	1.96	0.46
5:D5:191:ILE:HD13	6:D4:387:SER:HB2	1.97	0.46
5:D5:245:ALA:O	5:D5:249:SER:CB	2.64	0.46
25:BK:80:LEU:HD11	25:BK:83:TYR:HB2	1.98	0.46
25:BK:100:ARG:HG2	25:BK:105:LEU:HD11	1.96	0.46
39:V1:300:GLY:HA2	39:V1:330:GLY:H	1.81	0.46
45:S8:96:ALA:HA	45:S8:106:THR:HA	1.97	0.46
52:A6:60:ASP:HA	52:A6:63:ARG:HG2	1.97	0.46
3:D6:18:VAL:HG22	4:4L:14:VAL:HG11	1.97	0.46
57:AB:101:ZMP:O7	22:B9:12:GLN:NE2	2.48	0.46
41:S1:227:SER:HB3	41:S1:238:ILE:O	2.15	0.46
41:S1:524:LEU:HB3	41:S1:527:ALA:HB2	1.97	0.46
5:D5:341:MET:SD	5:D5:453:SER:OG	2.65	0.46
13:AJ:46:LEU:HD21	13:AJ:238:ILE:HG21	1.98	0.46
13:AJ:60:ASP:HB3	13:AJ:68:PRO:HA	1.96	0.46
42:S2:234:ILE:HD12	42:S2:237:ASN:HB3	1.98	0.46
51:A5:35:GLY:HA2	51:A5:44:ARG:HH12	1.81	0.46
3:D6:124:ASP:N	3:D6:124:ASP:OD1	2.49	0.46
3:D6:163:ILE:HG13	7:D2:12:THR:HG21	1.97	0.46
5:D5:138:PHE:HB2	5:D5:196:TRP:HE1	1.80	0.46
49:A9:91:VAL:HG13	49:A9:129:PHE:HD1	1.80	0.46
5:D5:180:ILE:HD12	6:D4:397:GLY:HA3	1.97	0.46
23:B2:7:ILE:HD11	23:B2:16:GLN:HG3	1.98	0.46
39:V1:99:GLU:OE2	39:V1:107:ASP:N	2.49	0.46
54:AL:78:ASP:HB2	54:AL:81:MET:HG3	1.97	0.46
5:D5:295:GLN:H	5:D5:425:ARG:HH22	1.63	0.46
9:B5:32:THR:OG1	25:BK:67:SER:O	2.31	0.46
39:V1:357:GLU:HG2	41:S1:177:ARG:HH12	1.81	0.46
41:S1:430:GLN:HE21	41:S1:656:LEU:HD22	1.81	0.46
53:A7:51:ASN:HB2	53:A7:56:ARG:HH12	1.81	0.46
5:D5:373:LEU:HB3	5:D5:431:LEU:HD11	1.98	0.45
18:B4:66:ARG:HD3	24:B8:27:TYR:HE1	1.81	0.45
21:B7:111:LYS:HD3	23:B2:68:PRO:HB3	1.98	0.45
41:S1:360:SER:HA	41:S1:365:ASN:HD21	1.81	0.45
48:S4:28:GLU:O	48:S4:32:THR:HB	2.16	0.45
5:D5:326:PHE:HA	5:D5:329:ILE:HD12	1.97	0.45
9:B5:31:LEU:HD23	9:B5:32:THR:HG23	1.98	0.45
14:S5:1:PRO:HB2	14:S5:2:PHE:H	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S5:13:LEU:O	14:S5:16:TRP:NE1	2.45	0.45
25:BK:74:SER:O	25:BK:78:ALA:HB2	2.16	0.45
41:S1:449:PRO:O	41:S1:489:VAL:CA	2.48	0.45
41:S1:524:LEU:HB2	41:S1:545:TYR:HA	1.98	0.45
11:A8:142:HIS:ND1	19:AM:113:THR:O	2.37	0.45
12:BJ:72:ASP:OD2	12:BJ:74:THR:OG1	2.31	0.45
15:A3:59:ASP:HB3	15:A3:61:ASN:N	2.32	0.45
25:BK:68:ILE:HA	25:BK:72:LEU:HD13	1.98	0.45
40:V2:151:ALA:HB3	40:V2:163:ASP:HA	1.96	0.45
42:S2:269:LEU:HD11	42:S2:373:GLU:HG2	1.98	0.45
42:S2:313:GLN:HA	42:S2:316:ASN:HD22	1.82	0.45
44:S7:85:VAL:HA	44:S7:112:TYR:O	2.15	0.45
49:A9:33:TYR:HD2	49:A9:207:ILE:HG12	1.81	0.45
2:D1:236:ILE:HG23	2:D1:259:PHE:HZ	1.82	0.45
7:D2:339:LEU:HD23	7:D2:342:ILE:HG13	1.97	0.45
13:AJ:79:LEU:HD23	13:AJ:96:LEU:HD11	1.99	0.45
40:V2:108:CYS:HB3	40:V2:152:PRO:HB3	1.99	0.45
42:S2:115:GLU:HB3	42:S2:194:VAL:HB	1.97	0.45
45:S8:141:THR:HG22	45:S8:143:THR:H	1.82	0.45
52:A6:32:ARG:HG3	10:AA:48:VAL:HG21	1.98	0.45
5:D5:142:ILE:HA	6:D4:370:PRO:HB2	1.97	0.45
6:D4:191:SER:N	8:AK:130:GLU:OE1	2.49	0.45
11:A8:82:THR:HA	11:A8:85:TRP:CD1	2.52	0.45
13:AJ:313:GLY:HA3	13:AJ:314:ASP:HA	1.70	0.45
2:D1:2:PHE:HA	2:D1:5:ASN:HD22	1.81	0.45
6:D4:196:TRP:CE2	6:D4:200:MET:HG3	2.51	0.45
15:A3:78:GLU:OE1	15:A3:82:ARG:NH2	2.49	0.45
21:B7:102:GLU:OE1	23:B2:57:SER:N	2.43	0.45
39:V1:190:THR:HG21	39:V1:204:ARG:HB2	1.98	0.45
39:V1:278:GLU:O	39:V1:282:LYS:HB2	2.15	0.45
41:S1:382:THR:OG1	41:S1:387:GLU:OE1	2.25	0.45
39:V1:405:CYS:SG	39:V1:406:ALA:N	2.90	0.45
54:AL:17:HIS:CD2	54:AL:35:VAL:HG21	2.50	0.45
18:B4:100:TRP:HA	18:B4:103:VAL:HG22	1.98	0.45
40:V2:29:LYS:HE3	46:V3:56:LEU:HD11	1.98	0.45
45:S8:143:THR:HA	49:A9:60:ARG:HH22	1.82	0.45
5:D5:396:ILE:O	5:D5:400:ASN:HB2	2.16	0.45
12:BJ:72:ASP:OD1	12:BJ:73:ILE:N	2.50	0.45
39:V1:97:ALA:HA	39:V1:225:VAL:HG21	1.99	0.45
42:S2:204:PRO:HB3	45:S8:60:ARG:HH12	1.82	0.45
44:S7:165:LYS:HE2	54:AL:76:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A7:11:ARG:HB3	53:A7:19:LEU:HD13	1.97	0.45
5:D5:137:LEU:HB3	5:D5:196:TRP:HB2	1.99	0.45
7:D2:266:ILE:O	7:D2:270:MET:CB	2.65	0.45
8:AK:14:GLY:H	8:AK:83:PRO:HB3	1.82	0.45
11:A8:8:SER:OG	11:A8:9:LEU:N	2.49	0.45
12:BJ:64:HIS:HA	25:BK:91:ARG:HH12	1.81	0.45
18:B4:115:ILE:HG22	18:B4:120:LEU:HG	1.99	0.45
44:S7:154:GLU:OE2	45:S8:55:GLY:N	2.38	0.45
1:D3:67:LEU:HB3	4:4L:65:VAL:HG23	1.99	0.44
5:D5:532:ILE:HD11	24:B8:101:MET:HB3	1.99	0.44
20:B6:33:VAL:HG12	22:B9:114:TYR:HE1	1.81	0.44
39:V1:233:THR:HA	39:V1:236:ARG:HG2	2.00	0.44
41:S1:11:VAL:O	41:S1:17:SER:HA	2.15	0.44
41:S1:138:GLU:N	47:S6:74:ASN:HD22	2.15	0.44
43:S3:47:GLU:OE1	43:S3:106:ARG:NH1	2.35	0.44
43:S3:48:LEU:HB3	43:S3:105:ILE:HG22	1.98	0.44
49:A9:314:ALA:O	49:A9:318:LEU:HB2	2.17	0.44
51:A5:86:GLU:HA	51:A5:89:LEU:HG	1.99	0.44
53:A7:111:TYR:HA	53:A7:112:LEU:HA	1.75	0.44
5:D5:71:ILE:HG13	5:D5:72:GLN:H	1.83	0.44
6:D4:231:LEU:HA	6:D4:235:LEU:HD13	1.99	0.44
11:A8:93:LEU:HB3	28:A1:38:VAL:HG23	1.99	0.44
16:B3:28:LEU:HD23	16:B3:28:LEU:HA	1.87	0.44
18:B4:14:PRO:HB3	24:B8:93:PRO:HG3	1.98	0.44
18:B4:56:ARG:HH21	25:BK:36:ASN:HD22	1.64	0.44
21:B7:97:ARG:HB3	24:B8:129:GLY:H	1.82	0.44
5:D5:451:ILE:O	5:D5:455:LYS:CB	2.63	0.44
18:B4:22:TYR:OH	22:B9:67:GLU:OE1	2.33	0.44
19:AM:11:PRO:HG3	42:S2:318:MET:HB3	1.98	0.44
41:S1:145:LEU:HB3	41:S1:269:PHE:HE2	1.82	0.44
1:D3:10:ASN:HD21	2:D1:10:ILE:HG21	1.82	0.44
6:D4:165:ILE:HG21	7:D2:268:GLN:HA	1.99	0.44
6:D4:206:LYS:HD2	6:D4:206:LYS:HA	1.81	0.44
12:BJ:29:ILE:H	12:BJ:29:ILE:HG13	1.60	0.44
21:B7:6:ARG:NH2	21:B7:15:GLU:OE2	2.50	0.44
39:V1:191:ALA:HB2	39:V1:203:PRO:HG3	1.99	0.44
41:S1:401:HIS:HE1	48:S4:116:LYS:HE2	1.81	0.44
44:S7:55:CYS:HB3	44:S7:89:ALA:HB1	1.99	0.44
44:S7:62:MET:HG2	44:S7:156:LEU:HD23	2.00	0.44
44:S7:92:LEU:HD21	44:S7:139:ILE:HG13	1.99	0.44
45:S8:80:CYS:N	62:S8:202:SF4:S1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A9:56:THR:HA	49:A9:59:LEU:HG	2.00	0.44
49:A9:128:LYS:HE2	49:A9:224:ARG:HD3	2.00	0.44
54:AL:44:TYR:OH	54:AL:112:ASN:OD1	2.35	0.44
5:D5:562:LEU:HD23	5:D5:562:LEU:HA	1.79	0.44
7:D2:115:VAL:HG12	7:D2:180:ALA:HB1	1.98	0.44
9:B5:26:ARG:O	9:B5:30:LEU:HB2	2.18	0.44
9:B5:32:THR:HA	9:B5:35:PRO:HD2	1.99	0.44
10:AB:87:TYR:HB2	20:B6:22:LEU:HD23	1.99	0.44
11:A8:77:CYS:HA	11:A8:78:ALA:HA	1.71	0.44
43:S3:72:PHE:HB3	43:S3:96:LEU:HD23	2.00	0.44
44:S7:107:MET:O	44:S7:111:ARG:NH2	2.43	0.44
5:D5:294:THR:HA	5:D5:425:ARG:HH12	1.83	0.44
49:A9:177:ARG:NH2	65:A9:401:NDP:O3	2.51	0.44
65:A9:401:NDP:H2D	65:A9:401:NDP:H2N	1.80	0.44
50:A2:64:LEU:HB3	50:A2:76:VAL:HG23	1.99	0.44
54:AL:23:TYR:HA	54:AL:26:VAL:HG12	2.00	0.44
2:D1:92:PRO:HG2	2:D1:252:PRO:HB2	1.99	0.44
10:AB:20:LYS:HB2	10:AB:20:LYS:HE2	1.86	0.44
20:B6:102:ARG:HG2	21:B7:49:GLN:HB2	1.99	0.44
40:V2:182:PRO:HB2	40:V2:187:ARG:HH12	1.82	0.44
41:S1:280:THR:HG21	54:AL:136:GLU:HG2	2.00	0.44
44:S7:87:ILE:HG12	44:S7:114:VAL:HB	1.99	0.44
47:S6:26:VAL:HB	49:A9:87:HIS:HB2	1.99	0.44
48:S4:79:LEU:HD22	48:S4:82:LEU:HD11	2.00	0.44
5:D5:350:LEU:HD21	5:D5:437:PHE:HB2	2.00	0.44
41:S1:378:LEU:HG	41:S1:451:VAL:HG22	1.99	0.44
50:A2:22:LEU:HB2	50:A2:56:GLU:HG2	2.00	0.44
52:A6:31:VAL:HG21	57:AA:101:ZMP:H12A	1.98	0.44
5:D5:152:PHE:CD1	5:D5:168:ALA:HB1	2.53	0.44
11:A8:121:LEU:HA	11:A8:122:GLY:HA2	1.73	0.44
24:B8:59:ASP:HA	24:B8:60:PRO:HD3	1.89	0.44
41:S1:239:VAL:N	41:S1:253:ARG:HH12	2.16	0.44
41:S1:450:MET:HA	41:S1:489:VAL:O	2.17	0.44
5:D5:202:PHE:HB3	12:BJ:120:HIS:HE1	1.83	0.43
7:D2:244:VAL:O	7:D2:248:LEU:HB2	2.18	0.43
10:AB:19:LEU:HD23	10:AB:19:LEU:HA	1.83	0.43
23:B2:46:ALA:HA	23:B2:50:HIS:CE1	2.53	0.43
41:S1:266:LYS:O	41:S1:270:ALA:CB	2.66	0.43
55:D1:501:3PE:H271	3:D6:46:ASN:HD21	1.83	0.43
3:D6:141:MET:HA	3:D6:144:ALA:HB3	2.00	0.43
13:AJ:216:GLU:OE1	13:AJ:245:LYS:NZ	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B6:24:ASP:OD2	22:B9:124:TRP:NE1	2.49	0.43
20:B6:71:PHE:O	20:B6:75:LEU:HB2	2.17	0.43
20:B6:92:LYS:O	20:B6:95:THR:OG1	2.37	0.43
22:B9:100:GLU:O	22:B9:121:ARG:NH2	2.51	0.43
39:V1:164:LYS:HA	39:V1:172:ASP:HB3	2.00	0.43
39:V1:259:SER:OG	39:V1:260:GLY:N	2.51	0.43
41:S1:8:LEU:HA	41:S1:20:VAL:O	2.18	0.43
48:S4:28:GLU:O	48:S4:32:THR:CB	2.66	0.43
2:D1:287:HIS:CE1	2:D1:291:LYS:HD2	2.54	0.43
3:D6:60:TYR:CZ	4:4L:38:LEU:HB2	2.53	0.43
4:4L:2:SER:OG	4:4L:3:LEU:N	2.50	0.43
5:D5:419:THR:HA	5:D5:422:TYR:CE2	2.52	0.43
6:D4:23:ILE:H	6:D4:23:ILE:HG13	1.68	0.43
6:D4:449:LEU:HD23	6:D4:449:LEU:HA	1.88	0.43
7:D2:258:SER:HB2	7:D2:336:LEU:H	1.82	0.43
20:B6:117:PRO:HA	20:B6:118:PRO:HD3	1.87	0.43
39:V1:26:TYR:CZ	40:V2:199:LEU:HD11	2.53	0.43
41:S1:276:ARG:HG2	41:S1:277:GLN:HG3	1.99	0.43
1:D3:63:LEU:HD12	3:D6:67:VAL:HG21	1.99	0.43
5:D5:306:THR:HA	5:D5:336:LYS:HZ3	1.83	0.43
6:D4:156:GLY:HA3	6:D4:205:VAL:HG21	2.00	0.43
6:D4:351:LEU:HD23	9:B5:13:PRO:HB3	2.01	0.43
6:D4:424:ASN:OD1	18:B4:55:ARG:NH1	2.52	0.43
7:D2:328:THR:HG23	17:C2:68:PHE:HZ	1.84	0.43
8:AK:46:THR:HA	8:AK:47:SER:HA	1.75	0.43
13:AJ:75:GLY:HA3	13:AJ:76:ASN:HA	1.64	0.43
18:B4:124:PHE:HB2	18:B4:126:ILE:HD11	2.01	0.43
24:B8:58:ARG:NH2	24:B8:75:GLU:OE2	2.51	0.43
39:V1:27:GLY:H	39:V1:113:HIS:CE1	2.36	0.43
41:S1:138:GLU:H	47:S6:74:ASN:HD22	1.65	0.43
41:S1:588:MET:HA	41:S1:589:PRO:HD3	1.89	0.43
7:D2:270:MET:HG2	7:D2:279:PRO:HG3	1.99	0.43
19:AM:138:GLY:O	19:AM:142:TYR:CB	2.67	0.43
41:S1:108:CYS:SG	41:S1:109:ASP:N	2.92	0.43
41:S1:203:CYS:HB2	41:S1:208:LEU:HD12	1.99	0.43
1:D3:6:THR:HG22	2:D1:6:VAL:HG22	2.01	0.43
5:D5:161:ARG:NH1	22:B9:89:SER:O	2.52	0.43
5:D5:162:THR:HG21	24:B8:86:ARG:HE	1.83	0.43
14:S5:81:GLN:HA	14:S5:84:LYS:HG2	2.01	0.43
18:B4:114:LEU:HD22	18:B4:120:LEU:HD23	2.00	0.43
41:S1:113:GLU:OE2	48:S4:43:ASN:ND2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S3:93:VAL:HG13	43:S3:108:LYS:HG2	1.99	0.43
48:S4:114:LYS:HD3	48:S4:116:LYS:HE3	2.01	0.43
3:D6:25:SER:HB3	3:D6:28:TYR:HD2	1.84	0.43
7:D2:199:THR:HG23	7:D2:346:LEU:HD22	2.00	0.43
43:S3:180:VAL:HG23	43:S3:182:ARG:HG2	2.01	0.43
48:S4:87:SER:OG	51:A5:115:ILE:O	2.37	0.43
54:AL:24:LEU:O	54:AL:28:PHE:HB2	2.18	0.43
3:D6:157:THR:HA	4:4L:66:PHE:HZ	1.84	0.43
7:D2:102:LEU:HD23	7:D2:102:LEU:HA	1.84	0.43
57:AB:101:ZMP:H7A	22:B9:66:ALA:HA	2.01	0.43
12:BJ:158:GLN:HE22	25:BK:111:ASN:HA	1.84	0.43
18:B4:42:LEU:HD23	18:B4:42:LEU:HA	1.85	0.43
41:S1:11:VAL:HG12	41:S1:77:TRP:HB2	2.00	0.43
41:S1:225:THR:H	41:S1:239:VAL:HG23	1.83	0.43
42:S2:425:PHE:HA	42:S2:428:VAL:HB	2.00	0.43
52:A6:52:ASP:H	52:A6:53:ILE:HD12	1.84	0.43
54:AL:50:GLU:HB2	54:AL:89:TRP:HZ2	1.83	0.43
5:D5:401:THR:HG22	24:B8:126:GLN:HE22	1.84	0.43
6:D4:158:LEU:HD21	7:D2:283:ALA:HB1	2.01	0.43
7:D2:202:LEU:HB3	7:D2:346:LEU:HD11	2.00	0.43
13:AJ:259:LEU:HD23	13:AJ:259:LEU:HA	1.89	0.43
21:B7:36:ARG:HH22	21:B7:96:LYS:HD3	1.84	0.43
24:B8:50:LEU:HB2	24:B8:78:HIS:HD2	1.83	0.43
24:B8:78:HIS:HE1	24:B8:80:ASP:HB2	1.84	0.43
41:S1:126:ASP:N	41:S1:126:ASP:OD1	2.52	0.43
41:S1:483:VAL:HA	41:S1:484:THR:HA	1.59	0.43
1:D3:80:GLN:HA	15:A3:45:ASN:HD21	1.84	0.43
2:D1:20:LEU:HD22	2:D1:232:ILE:HD11	2.00	0.43
2:D1:314:ILE:HA	2:D1:315:PRO:HD3	1.83	0.43
3:D6:127:ILE:HG21	14:S5:68:ARG:HD2	2.01	0.43
13:AJ:224:SER:OG	13:AJ:225:ALA:N	2.52	0.43
39:V1:365:CYS:SG	39:V1:366:ARG:N	2.92	0.43
41:S1:195:LEU:HG	41:S1:198:ASN:HD22	1.83	0.43
41:S1:200:ILE:HD11	41:S1:268:ARG:HD3	2.01	0.43
41:S1:237:ASN:O	41:S1:253:ARG:HG2	2.19	0.43
42:S2:63:ARG:NH1	43:S3:155:TYR:OH	2.52	0.43
43:S3:155:TYR:HB3	52:A6:97:LYS:HE3	2.01	0.43
49:A9:169:ALA:HB3	49:A9:205:VAL:HG12	2.00	0.43
1:D3:63:LEU:HD22	4:4L:72:ALA:HB2	2.01	0.42
9:B5:64:TRP:HD1	9:B5:65:GLU:HG3	1.84	0.42
12:BJ:120:HIS:HB2	12:BJ:121:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S8:15:LYS:HA	45:S8:18:THR:HG22	2.01	0.42
46:V3:50:THR:O	46:V3:54:LEU:HB2	2.18	0.42
49:A9:234:ASN:HB3	49:A9:236:TYR:HD1	1.83	0.42
5:D5:293:LEU:HD21	5:D5:421:ILE:HG13	2.00	0.42
39:V1:233:THR:O	39:V1:237:ARG:HB2	2.19	0.42
47:S6:74:ASN:ND2	47:S6:76:ASP:OD2	2.50	0.42
2:D1:103:LEU:HD22	3:D6:54:LEU:HD13	2.00	0.42
5:D5:293:LEU:HD11	5:D5:421:ILE:HD11	2.01	0.42
5:D5:561:ILE:O	5:D5:565:THR:OG1	2.29	0.42
13:AJ:19:THR:OG1	13:AJ:20:GLU:N	2.48	0.42
18:B4:13:LEU:HD22	18:B4:14:PRO:HD2	2.00	0.42
39:V1:28:ARG:HD3	39:V1:28:ARG:HA	1.90	0.42
39:V1:150:GLN:HB3	46:V3:54:LEU:HD12	2.00	0.42
42:S2:105:ARG:CZ	45:S8:117:ILE:HD11	2.49	0.42
43:S3:78:LEU:CA	43:S3:93:VAL:O	2.65	0.42
45:S8:23:GLN:NE2	45:S8:29:GLU:OE1	2.52	0.42
50:A2:19:ARG:HA	50:A2:53:LEU:O	2.20	0.42
12:BJ:14:ARG:NH2	20:B6:98:GLU:OE2	2.39	0.42
21:B7:99:LYS:HG2	23:B2:57:SER:HB3	2.01	0.42
21:B7:107:LEU:O	21:B7:111:LYS:HB3	2.19	0.42
42:S2:423:ILE:HD13	42:S2:425:PHE:HE2	1.84	0.42
52:A6:16:VAL:HG11	52:A6:76:ARG:HD3	2.01	0.42
2:D1:32:GLN:OE1	2:D1:34:ARG:NH2	2.52	0.42
3:D6:42:GLY:O	3:D6:46:ASN:ND2	2.52	0.42
13:AJ:171:TYR:HD2	13:AJ:222:GLN:HG3	1.83	0.42
20:B6:16:GLU:HA	20:B6:19:ARG:HD2	2.01	0.42
40:V2:29:LYS:HG3	46:V3:56:LEU:HD11	2.01	0.42
42:S2:22:THR:H	42:S2:25:THR:HB	1.84	0.42
42:S2:230:THR:HG23	42:S2:298:LEU:HD21	2.00	0.42
42:S2:366:ALA:HA	42:S2:374:PHE:O	2.19	0.42
45:S8:97:GLU:H	45:S8:107:THR:HG23	1.85	0.42
2:D1:47:GLN:NE2	2:D1:51:ASP:OD1	2.53	0.42
2:D1:314:ILE:HG13	19:AM:57:ARG:HH12	1.84	0.42
3:D6:174:GLY:HA2	3:D6:175:ASN:HA	1.65	0.42
13:AJ:80:GLU:HB3	13:AJ:190:HIS:HD1	1.84	0.42
41:S1:52:CYS:SG	41:S1:54:MET:N	2.93	0.42
41:S1:378:LEU:HD13	41:S1:409:ILE:HD12	2.00	0.42
2:D1:47:GLN:HE22	44:S7:44:SER:HA	1.84	0.42
15:A3:24:ILE:HD12	15:A3:27:LEU:HD21	2.00	0.42
41:S1:147:LYS:HB3	41:S1:209:THR:HG23	2.00	0.42
41:S1:496:ILE:HG22	41:S1:498:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S4:56:LYS:HE2	48:S4:85:THR:HG22	2.02	0.42
54:AL:83:PRO:HG2	54:AL:86:TRP:HD1	1.84	0.42
5:D5:332:HIS:CE1	5:D5:336:LYS:HD2	2.55	0.42
5:D5:567:SER:OG	55:D4:501:3PE:O22	2.32	0.42
10:AB:63:PRO:HB3	24:B8:61:TRP:CD2	2.55	0.42
39:V1:361:GLN:N	62:V1:500:SF4:S2	2.93	0.42
41:S1:283:MET:HG2	41:S1:293:HIS:HA	2.02	0.42
42:S2:90:LEU:HD23	43:S3:168:LEU:HD11	2.01	0.42
43:S3:86:ARG:NH2	51:A5:110:GLN:O	2.53	0.42
3:D6:37:GLY:HA3	3:D6:61:LEU:HD11	2.02	0.42
4:4L:96:LEU:HD12	7:D2:51:ARG:HD2	2.02	0.42
55:D5:701:3PE:H332	6:D4:405:LEU:HD11	2.01	0.42
6:D4:33:LEU:HA	6:D4:36:LEU:HD13	2.02	0.42
16:B3:28:LEU:HA	16:B3:31:VAL:HG12	2.02	0.42
4:4L:66:PHE:HB3	7:D2:34:GLU:OE1	2.19	0.42
5:D5:22:ILE:HA	5:D5:25:ASN:HB2	2.00	0.42
5:D5:396:ILE:HD11	5:D5:490:ALA:HB2	2.02	0.42
17:C2:59:HIS:CE1	17:C2:60:ARG:HG3	2.54	0.42
18:B4:77:PRO:HA	18:B4:78:ASN:HA	1.68	0.42
41:S1:348:VAL:HG22	41:S1:510:GLY:HA2	2.02	0.42
41:S1:629:ASN:N	41:S1:629:ASN:OD1	2.52	0.42
44:S7:141:PRO:HB3	49:A9:61:PRO:HD3	2.02	0.42
44:S7:157:LEU:HD12	44:S7:157:LEU:HA	1.90	0.42
45:S8:75:GLU:OE2	45:S8:151:LYS:NZ	2.44	0.42
3:D6:13:PHE:HD1	3:D6:39:VAL:HG23	1.84	0.41
6:D4:427:LEU:HD11	25:BK:36:ASN:HB3	2.02	0.41
7:D2:341:PRO:HB2	17:C2:79:GLN:NE2	2.35	0.41
8:AK:13:GLU:HG2	8:AK:20:LYS:HZ1	1.85	0.41
11:A8:129:LYS:HB2	15:A3:58:ASP:HA	2.01	0.41
12:BJ:23:THR:HG22	21:B7:72:SER:HA	2.02	0.41
13:AJ:97:GLN:HG2	13:AJ:135:LEU:HD13	2.01	0.41
17:C2:82:MET:SD	17:C2:82:MET:N	4.23	0.41
21:B7:99:LYS:HB3	23:B2:64:LEU:HD21	2.01	0.41
25:BK:56:TRP:HA	25:BK:59:ARG:HH11	1.85	0.41
28:A1:52:ARG:HB3	28:A1:60:TYR:HB3	2.01	0.41
41:S1:156:CYS:N	62:S1:802:SF4:S4	2.93	0.41
41:S1:522:LEU:HD21	41:S1:543:ILE:HG22	2.02	0.41
49:A9:40:ARG:HH12	52:A6:109:THR:HG22	1.84	0.41
2:D1:169:GLN:NE2	2:D1:241:LEU:O	2.46	0.41
5:D5:7:LEU:HA	5:D5:10:VAL:HG22	2.01	0.41
11:A8:46:ARG:NH1	19:AM:79:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B4:25:SER:OG	18:B4:26:SER:N	2.52	0.41
22:B9:89:SER:HB3	22:B9:92:ARG:HB2	2.02	0.41
39:V1:15:LEU:HB2	39:V1:271:GLU:HG3	2.00	0.41
39:V1:400:GLU:OE2	39:V1:413:TRP:NE1	2.53	0.41
40:V2:60:TRP:CG	40:V2:94:PRO:HA	2.55	0.41
41:S1:139:ASP:N	41:S1:139:ASP:OD1	2.53	0.41
41:S1:345:THR:OG1	41:S1:347:GLU:O	2.31	0.41
41:S1:379:LEU:HD21	41:S1:384:PRO:HG2	2.01	0.41
42:S2:353:THR:OG1	42:S2:354:GLU:N	2.53	0.41
7:D2:250:SER:O	7:D2:259:GLY:HA3	2.21	0.41
9:B5:134:ASP:N	14:S5:21:SER:O	2.49	0.41
11:A8:83:GLU:HA	11:A8:86:THR:HG22	2.03	0.41
22:B9:108:PRO:HA	22:B9:111:LYS:HB2	2.03	0.41
44:S7:47:PRO:HD3	44:S7:74:VAL:HG13	2.01	0.41
45:S8:81:LYS:N	62:S8:202:SF4:S1	2.88	0.41
2:D1:272:TRP:CD2	45:S8:34:LEU:HD12	2.55	0.41
8:AK:65:ILE:HD11	8:AK:100:LEU:HD23	2.01	0.41
13:AJ:251:GLN:HB3	13:AJ:255:LYS:HB2	2.02	0.41
46:V3:72:SER:OG	46:V3:74:ARG:O	2.37	0.41
48:S4:10:LEU:HB3	48:S4:11:ILE:H	1.67	0.41
3:D6:135:PHE:HE2	19:AM:64:PHE:HE1	1.68	0.41
6:D4:266:LEU:HA	6:D4:266:LEU:HD23	1.85	0.41
6:D4:298:ILE:HD13	6:D4:298:ILE:HA	1.76	0.41
11:A8:150:ASN:HA	14:S5:50:ARG:HH22	1.85	0.41
12:BJ:25:LEU:HG	21:B7:74:PRO:HB2	2.02	0.41
41:S1:675:ASP:O	41:S1:679:ARG:HB2	2.20	0.41
42:S2:190:HIS:ND1	44:S7:150:PRO:HD3	2.36	0.41
42:S2:341:SER:OG	42:S2:342:MET:N	2.54	0.41
44:S7:34:ASP:OD2	44:S7:174:ARG:NE	2.49	0.41
52:A6:65:MET:HB3	57:AA:101:ZMP:H6	2.03	0.41
5:D5:99:SER:OG	5:D5:453:SER:OG	2.35	0.41
5:D5:172:ILE:O	5:D5:176:ARG:HG2	2.21	0.41
5:D5:335:PHE:HE2	5:D5:336:LYS:HE3	1.84	0.41
6:D4:179:LEU:HD21	6:D4:249:LEU:HD23	2.02	0.41
14:S5:4:ASP:HB2	17:C2:10:PRO:HB3	2.01	0.41
19:AM:103:TRP:CZ3	19:AM:105:VAL:HG12	2.56	0.41
41:S1:243:ARG:NH2	45:S8:94:ILE:O	2.54	0.41
41:S1:303:VAL:HG13	41:S1:542:PHE:HZ	1.86	0.41
41:S1:418:ARG:HG3	46:V3:75:HIS:CE1	2.55	0.41
42:S2:128:ILE:HD11	42:S2:330:VAL:HG21	2.03	0.41
5:D5:560:THR:HG21	18:B4:79:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BJ:132:THR:HA	12:BJ:135:VAL:HG12	2.03	0.41
13:AJ:136:GLU:O	13:AJ:140:ARG:HG2	2.21	0.41
20:B6:86:LYS:O	20:B6:90:THR:HB	2.19	0.41
39:V1:93:LEU:O	39:V1:134:ALA:HA	2.20	0.41
41:S1:246:GLU:HB3	41:S1:247:VAL:H	1.71	0.41
43:S3:154:ASP:OD1	43:S3:155:TYR:N	2.53	0.41
47:S6:51:GLN:HG2	47:S6:92:ARG:HB2	2.01	0.41
4:4L:40:LEU:HD22	7:D2:75:ILE:HD12	2.03	0.41
5:D5:147:VAL:O	5:D5:151:SER:OG	2.34	0.41
5:D5:513:PHE:HE1	22:B9:29:ARG:HG2	1.86	0.41
13:AJ:27:VAL:HG22	13:AJ:170:ILE:HD12	2.03	0.41
41:S1:396:ARG:NH1	41:S1:417:TYR:HB3	2.35	0.41
42:S2:183:ARG:HD2	42:S2:207:LEU:HD13	2.02	0.41
44:S7:100:LEU:HD23	44:S7:139:ILE:HG21	2.02	0.41
51:A5:34:LEU:HD11	51:A5:44:ARG:HA	2.02	0.41
3:D6:11:ILE:HD13	3:D6:11:ILE:HA	1.88	0.41
5:D5:245:ALA:O	5:D5:249:SER:OG	2.32	0.41
6:D4:108:MET:HB3	6:D4:121:MET:HG3	2.02	0.41
6:D4:430:PHE:CD1	25:BK:46:GLY:HA2	2.56	0.41
7:D2:335:MET:O	17:C2:33:TYR:OH	2.38	0.41
13:AJ:151:HIS:CD2	13:AJ:279:LEU:HD11	2.56	0.41
13:AJ:303:LYS:HG2	13:AJ:304:TYR:CD2	2.56	0.41
19:AM:129:GLY:H	19:AM:132:ILE:HD11	1.86	0.41
27:B1:55:THR:HG23	27:B1:56:TRP:HD1	1.86	0.41
39:V1:403:THR:OG1	39:V1:405:CYS:O	2.31	0.41
41:S1:9:ILE:HB	41:S1:20:VAL:HB	2.02	0.41
41:S1:206:GLY:N	62:S1:801:SF4:S2	2.85	0.41
41:S1:574:VAL:HG22	41:S1:580:ALA:HA	2.03	0.41
42:S2:354:GLU:OE2	42:S2:357:GLN:NE2	2.50	0.41
47:S6:84:CYS:HB3	47:S6:87:CYS:HB2	2.02	0.41
49:A9:32:ARG:NH2	49:A9:175:GLU:OE1	2.53	0.41
49:A9:81:ILE:HG21	49:A9:117:ILE:HG22	2.03	0.41
51:A5:113:TRP:O	51:A5:115:ILE:N	2.52	0.41
53:A7:50:ASN:O	53:A7:52:TYR:N	2.53	0.41
10:AA:72:CYS:HA	10:AA:73:PRO:HD3	1.91	0.41
2:D1:81:LEU:HD11	2:D1:111:LEU:HB3	2.02	0.41
3:D6:47:PHE:HD2	4:4L:46:LEU:HD22	1.86	0.41
5:D5:389:PHE:O	5:D5:393:ASP:HB2	2.21	0.41
6:D4:134:THR:O	6:D4:142:ARG:NH1	2.54	0.41
6:D4:241:TYR:OH	6:D4:245:ARG:NH2	2.50	0.41
20:B6:103:ILE:H	20:B6:103:ILE:HG13	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:V1:109:GLU:HG3	39:V1:113:HIS:CD2	2.56	0.41
40:V2:78:MET:HA	40:V2:81:TYR:HD2	1.86	0.41
40:V2:156:ILE:HG12	40:V2:161:TYR:HE2	1.86	0.41
43:S3:71:GLN:HE21	51:A5:82:GLN:HE22	1.69	0.41
45:S8:117:ILE:HG23	45:S8:119:CYS:SG	2.61	0.41
52:A6:30:ARG:HE	52:A6:82:VAL:HG11	1.85	0.41
2:D1:220:PHE:O	2:D1:224:PHE:CB	2.69	0.40
5:D5:62:ILE:HG22	5:D5:81:LYS:HB2	2.02	0.40
5:D5:530:PRO:O	5:D5:534:HIS:HB2	2.20	0.40
7:D2:149:ILE:HD12	7:D2:195:LEU:HD21	2.03	0.40
27:B1:57:LYS:HE2	27:B1:57:LYS:HB2	1.96	0.40
39:V1:99:GLU:OE2	39:V1:108:ARG:N	2.40	0.40
41:S1:230:VAL:HG23	41:S1:231:MET:HG3	2.03	0.40
45:S8:105:ARG:HD3	45:S8:105:ARG:HA	1.87	0.40
52:A6:35:TYR:OH	10:AA:49:GLU:OE2	2.32	0.40
6:D4:364:LEU:HD22	6:D4:367:LEU:HD22	2.03	0.40
7:D2:243:LEU:HA	7:D2:243:LEU:HD23	1.75	0.40
9:B5:60:VAL:HG11	27:B1:46:ARG:HD2	2.03	0.40
9:B5:112:ARG:HG3	9:B5:113:LEU:HD12	2.02	0.40
11:A8:85:TRP:O	11:A8:89:ASP:HB2	2.20	0.40
12:BJ:94:ASP:O	12:BJ:98:ASP:HB2	2.21	0.40
12:BJ:141:ARG:HD2	25:BK:112:CYS:H	1.87	0.40
13:AJ:210:PHE:HD2	13:AJ:211:LEU:HD22	1.86	0.40
15:A3:15:GLU:HB3	15:A3:18:LEU:HB2	2.02	0.40
16:B3:49:ALA:O	16:B3:53:MET:HG2	2.22	0.40
39:V1:338:ASP:OD1	39:V1:339:ARG:N	2.54	0.40
41:S1:571:ALA:N	41:S1:583:THR:OG1	2.40	0.40
45:S8:153:LYS:HB2	54:AL:124:TYR:CE1	2.57	0.40
52:A6:38:TRP:CD2	52:A6:89:LEU:HD12	2.56	0.40
2:D1:184:MET:HE2	2:D1:293:PHE:HD1	1.85	0.40
5:D5:250:SER:OG	5:D5:251:THR:N	2.54	0.40
6:D4:185:PRO:HB3	6:D4:252:PRO:HG3	2.03	0.40
13:AJ:58:TYR:O	13:AJ:62:THR:HB	2.21	0.40
18:B4:29:ARG:NH1	18:B4:32:GLN:OE1	2.50	0.40
22:B9:167:TRP:O	22:B9:171:THR:OG1	2.26	0.40
43:S3:67:HIS:HB2	51:A5:89:LEU:HD21	2.03	0.40
44:S7:176:TRP:HD1	44:S7:179:ARG:HH12	1.68	0.40
4:4L:30:LEU:HD11	4:4L:74:GLY:HA3	2.04	0.40
5:D5:245:ALA:O	5:D5:249:SER:HB3	2.22	0.40
7:D2:26:TRP:HB3	7:D2:74:ILE:HD13	2.02	0.40
7:D2:154:ILE:HG23	7:D2:191:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AK:137:GLU:HB3	8:AK:139:LYS:HG3	2.02	0.40
9:B5:83:PRO:O	9:B5:87:TYR:HB2	2.22	0.40
12:BJ:48:ARG:NH1	12:BJ:52:GLU:OE2	2.54	0.40
19:AM:64:PHE:HD1	19:AM:64:PHE:HA	1.75	0.40
23:B2:37:LEU:HD23	23:B2:37:LEU:HA	2.06	0.40
24:B8:64:TRP:CZ2	24:B8:70:ARG:HG3	2.57	0.40
40:V2:104:THR:HA	40:V2:108:CYS:HB2	2.02	0.40
42:S2:120:LEU:HD23	42:S2:120:LEU:HA	1.92	0.40
42:S2:202:ASP:HB3	42:S2:323:ILE:HG23	2.04	0.40
48:S4:94:ALA:O	48:S4:98:LYS:HB2	2.22	0.40
57:AA:101:ZMP:H22	57:AA:101:ZMP:H3A	1.78	0.40
5:D5:69:LEU:HD23	6:D4:451:PRO:HG2	2.04	0.40
5:D5:226:GLN:O	5:D5:230:HIS:N	2.54	0.40
9:B5:56:PRO:HG2	9:B5:59:TYR:HB3	2.04	0.40
9:B5:85:LYS:NZ	9:B5:89:ARG:HH22	2.19	0.40
39:V1:27:GLY:H	39:V1:113:HIS:HE1	1.68	0.40
40:V2:78:MET:HE1	41:S1:186:TYR:H	1.86	0.40
42:S2:80:ILE:HD12	42:S2:80:ILE:HA	1.95	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	D3	86/115 (75%)	80 (93%)	6 (7%)	0	100	100
2	D1	290/318 (91%)	264 (91%)	23 (8%)	3 (1%)	13	48
3	D6	164/175 (94%)	140 (85%)	24 (15%)	0	100	100
4	4L	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
5	D5	604/606 (100%)	533 (88%)	71 (12%)	0	100	100
6	D4	457/459 (100%)	424 (93%)	32 (7%)	1 (0%)	44	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
8	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
9	B5	137/143 (96%)	117 (85%)	19 (14%)	1 (1%)	19	56
10	AA	78/88 (89%)	69 (88%)	9 (12%)	0	100	100
10	AB	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
11	A8	169/171 (99%)	142 (84%)	26 (15%)	1 (1%)	22	59
12	BJ	169/175 (97%)	153 (90%)	15 (9%)	1 (1%)	22	59
13	AJ	317/320 (99%)	270 (85%)	47 (15%)	0	100	100
14	S5	97/105 (92%)	78 (80%)	19 (20%)	0	100	100
15	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
16	B3	71/97 (73%)	52 (73%)	19 (27%)	0	100	100
17	C2	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	14	50
18	B4	126/128 (98%)	105 (83%)	21 (17%)	0	100	100
19	AM	137/143 (96%)	121 (88%)	16 (12%)	0	100	100
20	B6	90/127 (71%)	74 (82%)	16 (18%)	0	100	100
21	B7	117/119 (98%)	99 (85%)	18 (15%)	0	100	100
22	B9	174/178 (98%)	144 (83%)	30 (17%)	0	100	100
23	B2	63/72 (88%)	51 (81%)	12 (19%)	0	100	100
24	B8	155/158 (98%)	118 (76%)	37 (24%)	0	100	100
25	BK	100/125 (80%)	79 (79%)	21 (21%)	0	100	100
26	C1	44/49 (90%)	40 (91%)	4 (9%)	0	100	100
27	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
28	A1	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
29	a1	435/446 (98%)	393 (90%)	42 (10%)	0	100	100
29	a3	442/446 (99%)	405 (92%)	37 (8%)	0	100	100
30	a2	410/439 (93%)	383 (93%)	27 (7%)	0	100	100
30	a4	409/439 (93%)	367 (90%)	42 (10%)	0	100	100
31	b1	376/379 (99%)	350 (93%)	26 (7%)	0	100	100
31	b2	376/379 (99%)	349 (93%)	27 (7%)	0	100	100
32	c1	237/240 (99%)	201 (85%)	36 (15%)	0	100	100
32	c2	236/240 (98%)	200 (85%)	36 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	f1	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
33	f2	193/196 (98%)	170 (88%)	23 (12%)	0	100	100
34	d1	98/110 (89%)	94 (96%)	4 (4%)	0	100	100
34	d2	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
35	q1	71/81 (88%)	64 (90%)	7 (10%)	0	100	100
35	q2	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
36	h1	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
36	h2	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
38	i1	53/63 (84%)	48 (91%)	5 (9%)	0	100	100
38	i2	55/63 (87%)	50 (91%)	5 (9%)	0	100	100
39	V1	428/445 (96%)	379 (89%)	49 (11%)	0	100	100
40	V2	210/217 (97%)	171 (81%)	39 (19%)	0	100	100
41	S1	686/704 (97%)	611 (89%)	74 (11%)	1 (0%)	48	82
42	S2	423/430 (98%)	378 (89%)	45 (11%)	0	100	100
43	S3	206/228 (90%)	183 (89%)	23 (11%)	0	100	100
44	S7	154/179 (86%)	137 (89%)	17 (11%)	0	100	100
45	S8	174/176 (99%)	152 (87%)	22 (13%)	0	100	100
46	V3	39/75 (52%)	29 (74%)	10 (26%)	0	100	100
47	S6	93/96 (97%)	82 (88%)	11 (12%)	0	100	100
48	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
49	A9	283/338 (84%)	237 (84%)	46 (16%)	0	100	100
50	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
51	A5	109/115 (95%)	97 (89%)	12 (11%)	0	100	100
52	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
53	A7	91/112 (81%)	74 (81%)	16 (18%)	1 (1%)	12	46
54	AL	137/145 (94%)	111 (81%)	26 (19%)	0	100	100
All	All	11848/12556 (94%)	10487 (88%)	1351 (11%)	10 (0%)	50	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D4	54	LEU
2	D1	32	GLN

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Mol	Chain	Res	Type
53	A7	69	MET
17	C2	10	PRO
2	D1	68	ILE
11	A8	147	PRO
12	BJ	71	PRO
41	S1	338	VAL
2	D1	92	PRO
9	B5	13	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	D3	81/103 (79%)	80 (99%)	1 (1%)	67	78
2	D1	260/278 (94%)	259 (100%)	1 (0%)	89	91
3	D6	137/144 (95%)	137 (100%)	0	100	100
4	4L	87/87 (100%)	83 (95%)	4 (5%)	23	46
5	D5	539/539 (100%)	533 (99%)	6 (1%)	70	79
6	D4	412/412 (100%)	404 (98%)	8 (2%)	52	69
7	D2	315/315 (100%)	309 (98%)	6 (2%)	52	69
8	AK	101/101 (100%)	98 (97%)	3 (3%)	36	57
9	B5	122/125 (98%)	121 (99%)	1 (1%)	79	84
10	AA	74/81 (91%)	74 (100%)	0	100	100
10	AB	80/81 (99%)	78 (98%)	2 (2%)	42	62
11	A8	154/154 (100%)	149 (97%)	5 (3%)	34	55
12	BJ	155/157 (99%)	154 (99%)	1 (1%)	84	88
13	AJ	283/284 (100%)	282 (100%)	1 (0%)	89	91
14	S5	88/94 (94%)	88 (100%)	0	100	100
15	A3	65/71 (92%)	65 (100%)	0	100	100
16	B3	55/75 (73%)	52 (94%)	3 (6%)	18	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C2	106/107 (99%)	106 (100%)	0	100	100
18	B4	114/114 (100%)	113 (99%)	1 (1%)	75	83
19	AM	119/121 (98%)	116 (98%)	3 (2%)	42	62
20	B6	90/121 (74%)	86 (96%)	4 (4%)	24	47
21	B7	108/108 (100%)	105 (97%)	3 (3%)	38	59
22	B9	159/160 (99%)	156 (98%)	3 (2%)	52	69
23	B2	59/62 (95%)	59 (100%)	0	100	100
24	B8	142/142 (100%)	140 (99%)	2 (1%)	62	75
25	BK	93/112 (83%)	91 (98%)	2 (2%)	47	65
26	C1	42/44 (96%)	42 (100%)	0	100	100
27	B1	48/53 (91%)	48 (100%)	0	100	100
28	A1	59/59 (100%)	56 (95%)	3 (5%)	20	44
29	a1	366/372 (98%)	361 (99%)	5 (1%)	62	75
29	a3	370/372 (100%)	364 (98%)	6 (2%)	58	73
30	a2	326/341 (96%)	322 (99%)	4 (1%)	67	78
30	a4	326/341 (96%)	324 (99%)	2 (1%)	84	88
31	b1	330/331 (100%)	327 (99%)	3 (1%)	75	83
31	b2	330/331 (100%)	328 (99%)	2 (1%)	84	88
32	c1	205/206 (100%)	203 (99%)	2 (1%)	73	81
32	c2	204/206 (99%)	202 (99%)	2 (1%)	73	81
33	f1	168/168 (100%)	167 (99%)	1 (1%)	84	88
33	f2	167/168 (99%)	166 (99%)	1 (1%)	84	88
34	d1	93/99 (94%)	92 (99%)	1 (1%)	70	79
34	d2	94/99 (95%)	91 (97%)	3 (3%)	34	55
35	q1	66/72 (92%)	66 (100%)	0	100	100
35	q2	67/72 (93%)	66 (98%)	1 (2%)	60	74
36	h1	62/74 (84%)	61 (98%)	1 (2%)	58	73
36	h2	62/74 (84%)	61 (98%)	1 (2%)	58	73
38	i1	46/52 (88%)	45 (98%)	1 (2%)	47	65
38	i2	48/52 (92%)	48 (100%)	0	100	100
39	V1	344/354 (97%)	340 (99%)	4 (1%)	67	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	V2	182/183 (100%)	181 (100%)	1 (0%)	86	90
41	S1	578/588 (98%)	574 (99%)	4 (1%)	81	86
42	S2	370/371 (100%)	366 (99%)	4 (1%)	70	79
43	S3	189/204 (93%)	189 (100%)	0	100	100
44	S7	132/150 (88%)	130 (98%)	2 (2%)	60	74
45	S8	151/151 (100%)	149 (99%)	2 (1%)	65	76
46	V3	40/68 (59%)	36 (90%)	4 (10%)	6	23
47	S6	79/80 (99%)	78 (99%)	1 (1%)	65	76
48	S4	113/119 (95%)	112 (99%)	1 (1%)	75	83
49	A9	242/292 (83%)	238 (98%)	4 (2%)	56	72
50	A2	73/81 (90%)	72 (99%)	1 (1%)	62	75
51	A5	99/101 (98%)	99 (100%)	0	100	100
52	A6	107/113 (95%)	106 (99%)	1 (1%)	75	83
53	A7	83/94 (88%)	83 (100%)	0	100	100
54	AL	125/131 (95%)	121 (97%)	4 (3%)	34	55
All	All	10384/10814 (96%)	10252 (99%)	132 (1%)	64	76

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D3	1	MET
2	D1	3	MET
4	4L	43	LEU
4	4L	58	MET
4	4L	64	LEU
4	4L	83	ASN
5	D5	59	GLN
5	D5	82	MET
5	D5	113	ASN
5	D5	357	ARG
5	D5	366	MET
5	D5	581	LYS
6	D4	43	ASN
6	D4	86	LYS
6	D4	138	ASN
6	D4	143	LEU
6	D4	144	ASN

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Mol	Chain	Res	Type
6	D4	150	LEU
6	D4	152	TYR
6	D4	251	ASN
7	D2	36	ASN
7	D2	78	LEU
7	D2	106	LEU
7	D2	204	ASN
7	D2	311	MET
7	D2	322	ARG
8	AK	4	LEU
8	AK	114	CYS
8	AK	139	LYS
9	B5	130	LYS
10	AB	33	ASN
10	AB	54	MET
11	A8	63	ASN
11	A8	109	CYS
11	A8	114	LEU
11	A8	134	ARG
11	A8	150	ASN
12	BJ	90	GLN
13	AJ	92	ASN
16	B3	47	ASN
16	B3	58	ASN
16	B3	74	PHE
18	B4	74	ASN
19	AM	60	GLN
19	AM	67	ARG
19	AM	89	ASN
20	B6	10	ARG
20	B6	89	VAL
20	B6	90	THR
20	B6	94	TYR
21	B7	7	ARG
21	B7	103	ARG
21	B7	105	ARG
22	B9	44	ARG
22	B9	157	ARG
22	B9	174	ARG
24	B8	9	LEU
24	B8	137	ASN
25	BK	27	GLN

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Mol	Chain	Res	Type
25	BK	57	ASN
28	A1	50	ARG
28	A1	58	ASN
28	A1	68	ASN
29	a1	53	ASN
29	a1	70	ARG
29	a1	146	ARG
29	a1	173	ASN
29	a1	176	LYS
30	a2	240	ARG
30	a2	248	ASN
30	a2	287	ARG
30	a2	313	ASN
31	b1	26	ASN
31	b1	80	ARG
31	b1	185	PHE
32	c1	15	ARG
32	c1	232	ARG
33	f1	71	MET
34	d1	110	LYS
36	h1	37	LEU
38	i1	50	LYS
29	a3	24	ARG
29	a3	53	ASN
29	a3	69	ASN
29	a3	146	ARG
29	a3	176	LYS
29	a3	389	ARG
30	a4	248	ASN
30	a4	313	ASN
31	b2	78	ILE
31	b2	80	ARG
32	c2	200	ARG
32	c2	232	ARG
33	f2	86	ASN
34	d2	71	ARG
34	d2	99	ARG
34	d2	104	ARG
35	q2	36	ASN
36	h2	68	CYS
39	V1	132	ARG
39	V1	365	CYS

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Mol	Chain	Res	Type
39	V1	385	ARG
39	V1	405	CYS
40	V2	190	ARG
41	S1	52	CYS
41	S1	152	ARG
41	S1	488	LYS
41	S1	601	ARG
42	S2	34	ASN
42	S2	229	LEU
42	S2	388	ARG
42	S2	418	ILE
44	S7	54	CYS
44	S7	174	ARG
45	S8	8	ARG
45	S8	119	CYS
46	V3	41	LEU
46	V3	60	LYS
46	V3	63	MET
46	V3	70	ARG
47	S6	26	VAL
48	S4	16	LYS
49	A9	281	ARG
49	A9	284	VAL
49	A9	292	ARG
49	A9	320	ARG
50	A2	33	ARG
52	A6	32	ARG
54	AL	9	ARG
54	AL	68	MET
54	AL	72	ASN
54	AL	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	D3	10	ASN
2	D1	5	ASN
2	D1	47	GLN
2	D1	194	ASN
2	D1	287	HIS
3	D6	46	ASN
4	4L	83	ASN

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Mol	Chain	Res	Type
4	4L	97	GLN
5	D5	65	ASN
5	D5	72	GLN
5	D5	113	ASN
5	D5	115	ASN
5	D5	354	GLN
5	D5	434	GLN
5	D5	509	HIS
6	D4	82	HIS
6	D4	138	ASN
6	D4	319	HIS
6	D4	399	ASN
7	D2	36	ASN
7	D2	134	GLN
7	D2	174	GLN
7	D2	204	ASN
7	D2	235	ASN
7	D2	316	GLN
9	B5	124	GLN
9	B5	143	ASN
10	AB	33	ASN
11	A8	29	HIS
11	A8	63	ASN
11	A8	150	ASN
12	BJ	54	GLN
12	BJ	55	HIS
12	BJ	99	GLN
12	BJ	103	ASN
12	BJ	120	HIS
13	AJ	76	ASN
13	AJ	114	HIS
13	AJ	151	HIS
13	AJ	257	HIS
14	S5	33	HIS
15	A3	45	ASN
15	A3	68	HIS
16	B3	47	ASN
16	B3	58	ASN
17	C2	79	GLN
17	C2	88	HIS
18	B4	51	ASN
19	AM	60	GLN

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Mol	Chain	Res	Type
19	AM	75	GLN
19	AM	89	ASN
20	B6	73	HIS
21	B7	46	ASN
21	B7	49	GLN
22	B9	17	GLN
22	B9	32	HIS
22	B9	168	HIS
24	B8	104	HIS
24	B8	137	ASN
25	BK	36	ASN
25	BK	45	HIS
25	BK	57	ASN
26	C1	9	HIS
28	A1	27	HIS
28	A1	58	ASN
28	A1	68	ASN
29	a1	53	ASN
29	a1	159	GLN
29	a1	173	ASN
29	a1	264	ASN
30	a2	248	ASN
30	a2	297	GLN
30	a2	313	ASN
30	a2	385	GLN
31	b1	8	HIS
31	b1	26	ASN
31	b1	68	HIS
31	b1	85	ASN
31	b1	148	ASN
32	c1	50	HIS
33	f1	53	ASN
33	f1	164	HIS
34	d1	56	ASN
35	q1	12	HIS
35	q1	23	GLN
35	q1	73	ASN
29	a3	21	ASN
29	a3	53	ASN
29	a3	61	HIS
29	a3	69	ASN
29	a3	85	HIS

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Mol	Chain	Res	Type
29	a3	173	ASN
29	a3	289	HIS
29	a3	339	GLN
30	a4	22	GLN
30	a4	104	ASN
30	a4	248	ASN
30	a4	305	GLN
30	a4	313	ASN
31	b2	85	ASN
31	b2	345	HIS
33	f2	161	HIS
35	q2	36	ASN
35	q2	64	GLN
36	h2	71	HIS
39	V1	293	ASN
40	V2	9	HIS
40	V2	42	HIS
40	V2	150	ASN
41	S1	43	HIS
41	S1	472	ASN
41	S1	517	ASN
41	S1	548	HIS
41	S1	549	HIS
41	S1	665	GLN
42	S2	34	ASN
42	S2	50	ASN
42	S2	84	HIS
42	S2	157	HIS
42	S2	316	ASN
42	S2	347	HIS
43	S3	39	GLN
43	S3	88	ASN
44	S7	82	GLN
46	V3	75	HIS
49	A9	36	ASN
49	A9	136	ASN
49	A9	288	HIS
50	A2	80	ASN
51	A5	72	GLN
51	A5	82	GLN
53	A7	20	GLN
54	AL	17	HIS

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Mol	Chain	Res	Type
54	AL	31	ASN
54	AL	46	ASN
54	AL	72	ASN
10	AA	47	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	$\# Z  > 2$
60	FES	V2	300	40	0,4,4	-	-	-		
57	ZMP	AB	101	10	24,30,36	0.72	1 (4%)	29,37,45	1.01	1 (3%)
55	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.36	0
55	3PE	f2	201	-	22,22,50	0.44	0	25,27,55	0.48	0
60	FES	f2	202	33	0,4,4	-	-	-		
55	3PE	b2	404	-	28,28,50	0.40	0	31,33,55	0.39	0
58	HEM	b1	402	31	41,50,50	1.49	5 (12%)	45,82,82	1.85	10 (22%)
62	SF4	S8	201	45	0,12,12	-	-	-		
65	NDP	A9	401	-	45,52,52	0.65	0	53,80,80	0.71	1 (1%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	HEM	b1	401	31	41,50,50	1.43	5 (12%)	45,82,82	2.11	13 (28%)
59	HEC	c1	501	32	32,50,50	2.20	4 (12%)	24,82,82	2.60	15 (62%)
62	SF4	S7	300	44	0,12,12	-	-	-	-	-
59	HEC	c2	501	32	32,50,50	2.11	4 (12%)	24,82,82	2.81	13 (54%)
62	SF4	S1	802	41	0,12,12	-	-	-	-	-
56	PC1	D4	502	-	27,27,53	0.40	0	33,35,61	0.44	0
61	CDL	b2	401	-	37,37,99	0.45	0	43,49,111	0.41	0
55	3PE	D5	701	-	37,37,50	0.35	0	40,42,55	0.39	0
61	CDL	c2	502	-	40,40,99	0.42	0	46,52,111	0.63	1 (2%)
60	FES	S1	803	41	0,4,4	-	-	-	-	-
61	CDL	b2	405	-	40,40,99	0.47	0	46,52,111	0.59	1 (2%)
55	3PE	D1	501	-	31,31,50	0.38	0	34,36,55	0.46	0
58	HEM	b2	402	31	41,50,50	1.42	4 (9%)	45,82,82	1.83	10 (22%)
60	FES	f1	501	33	0,4,4	-	-	-	-	-
62	SF4	V1	500	39	0,12,12	-	-	-	-	-
57	ZMP	AA	101	10	27,33,36	0.69	1 (3%)	32,40,45	1.07	1 (3%)
58	HEM	b2	403	31	41,50,50	1.55	6 (14%)	45,82,82	1.94	11 (24%)
62	SF4	S8	202	45	0,12,12	-	-	-	-	-
62	SF4	S1	801	41	0,12,12	-	-	-	-	-
63	FMN	V1	501	-	33,33,33	0.36	0	48,50,50	0.43	0

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
60	FES	V2	300	40	-	-	0/1/1/1
57	ZMP	AB	101	10	-	13/35/37/43	-
55	3PE	D4	501	-	-	9/43/43/54	-
55	3PE	f2	201	-	-	5/26/26/54	-
60	FES	f2	202	33	-	-	0/1/1/1
55	3PE	b2	404	-	-	10/32/32/54	-
58	HEM	b1	402	31	-	6/12/54/54	-
62	SF4	S8	201	45	-	-	0/6/5/5
65	NDP	A9	401	-	-	15/30/77/77	0/5/5/5
58	HEM	b1	401	31	-	3/12/54/54	-
59	HEC	c1	501	32	-	5/10/54/54	-
62	SF4	S7	300	44	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	HEC	c2	501	32	-	4/10/54/54	-
62	SF4	S1	802	41	-	-	0/6/5/5
56	PC1	D4	502	-	-	11/31/31/57	-
61	CDL	b2	401	-	-	17/46/46/110	-
55	3PE	D5	701	-	-	13/41/41/54	-
61	CDL	c2	502	-	-	14/48/48/110	-
60	FES	S1	803	41	-	-	0/1/1/1
61	CDL	b2	405	-	-	17/51/51/110	-
55	3PE	D1	501	-	-	9/35/35/54	-
58	HEM	b2	402	31	-	5/12/54/54	-
60	FES	f1	501	33	-	-	0/1/1/1
62	SF4	V1	500	39	-	-	0/6/5/5
57	ZMP	AA	101	10	-	12/38/40/43	-
58	HEM	b2	403	31	-	4/12/54/54	-
62	SF4	S8	202	45	-	-	0/6/5/5
62	SF4	S1	801	41	-	-	0/6/5/5
63	FMN	V1	501	-	-	5/18/18/18	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	501	HEC	C2B-C3B	-7.27	1.33	1.40
59	c1	501	HEC	C3C-C2C	-7.08	1.33	1.40
59	c2	501	HEC	C3C-C2C	-7.03	1.33	1.40
59	c2	501	HEC	C2B-C3B	-6.63	1.33	1.40
58	b1	401	HEM	C4D-ND	-4.42	1.32	1.40
58	b2	403	HEM	C4D-ND	-4.37	1.32	1.40
58	b2	402	HEM	C4D-ND	-4.36	1.32	1.40
58	b1	402	HEM	C4D-ND	-4.30	1.32	1.40
58	b2	403	HEM	C1B-NB	-3.91	1.33	1.40
58	b1	402	HEM	C1B-NB	-3.91	1.33	1.40
58	b2	403	HEM	C1D-ND	-3.59	1.31	1.38
58	b2	402	HEM	C1B-NB	-3.56	1.34	1.40
58	b1	401	HEM	C1B-NB	-3.48	1.34	1.40
59	c2	501	HEC	CBC-CAC	-3.44	1.36	1.49
59	c1	501	HEC	CBC-CAC	-3.43	1.36	1.49
58	b2	403	HEM	C3C-C2C	-3.20	1.35	1.40
58	b2	402	HEM	C1D-ND	-3.19	1.32	1.38
58	b1	402	HEM	C1D-ND	-3.15	1.32	1.38
58	b1	401	HEM	C1D-ND	-3.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	b1	402	HEM	C3C-C2C	-2.96	1.36	1.40
58	b2	403	HEM	C4B-NB	-2.87	1.32	1.38
58	b2	402	HEM	C4B-NB	-2.74	1.33	1.38
58	b1	402	HEM	C4B-NB	-2.59	1.33	1.38
58	b1	401	HEM	C4B-NB	-2.52	1.33	1.38
58	b1	401	HEM	C3C-C2C	-2.51	1.36	1.40
57	AA	101	ZMP	C9-C10	2.50	1.53	1.50
59	c1	501	HEC	CBB-CAB	-2.48	1.40	1.49
57	AB	101	ZMP	C9-C10	2.43	1.53	1.50
59	c2	501	HEC	CBB-CAB	-2.35	1.40	1.49
58	b2	403	HEM	C1B-C2B	-2.16	1.40	1.44

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c2	501	HEC	CBA-CAA-C2A	6.42	123.43	112.60
58	b2	403	HEM	CHC-C4B-NB	5.87	130.81	124.43
58	b1	401	HEM	CHC-C4B-NB	5.60	130.52	124.43
58	b1	402	HEM	CHC-C4B-NB	5.25	130.14	124.43
58	b2	402	HEM	CHC-C4B-NB	5.07	129.94	124.43
59	c1	501	HEC	CBA-CAA-C2A	4.78	120.65	112.60
59	c2	501	HEC	CMD-C2D-C1D	-4.47	121.59	128.46
59	c1	501	HEC	CMB-C2B-C3B	4.40	131.00	125.82
58	b2	403	HEM	CHB-C1B-NB	4.28	129.67	124.38
58	b1	401	HEM	CAD-CBD-CGD	-4.27	104.41	113.60
58	b2	402	HEM	CHB-C1B-NB	4.05	129.38	124.38
58	b1	402	HEM	CHB-C1B-NB	4.04	129.38	124.38
59	c2	501	HEC	CMB-C2B-C3B	4.02	130.54	125.82
59	c2	501	HEC	CMB-C2B-C1B	-3.99	122.34	128.46
59	c1	501	HEC	CMB-C2B-C1B	-3.96	122.38	128.46
58	b1	401	HEM	CHB-C1B-NB	3.88	129.18	124.38
59	c1	501	HEC	CMD-C2D-C1D	-3.80	122.63	128.46
59	c2	501	HEC	CMA-C3A-C2A	3.79	132.09	124.94
58	b1	401	HEM	CMB-C2B-C1B	3.75	130.75	125.04
59	c1	501	HEC	CMC-C2C-C3C	3.74	130.21	125.82
58	b1	402	HEM	C4D-ND-C1D	3.70	108.89	105.07
58	b2	403	HEM	C4D-ND-C1D	3.67	108.86	105.07
58	b2	403	HEM	C1B-NB-C4B	3.62	108.82	105.07
58	b1	401	HEM	CHD-C1D-ND	3.52	128.26	124.43
59	c2	501	HEC	CMC-C2C-C3C	3.39	129.80	125.82
58	b1	401	HEM	C4D-ND-C1D	3.36	108.54	105.07
59	c1	501	HEC	C4C-C3C-C2C	3.36	109.97	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	b2	402	HEM	C1B-NB-C4B	3.34	108.52	105.07
58	b2	402	HEM	CBA-CAA-C2A	-3.31	106.96	112.62
58	b2	403	HEM	CHD-C1D-ND	3.17	127.87	124.43
59	c2	501	HEC	C4C-C3C-C2C	3.09	109.69	106.35
58	b1	402	HEM	CAA-CBA-CGA	-3.09	105.10	113.76
58	b2	402	HEM	CBD-CAD-C3D	-3.05	104.15	112.63
58	b1	402	HEM	CHD-C1D-ND	3.01	127.70	124.43
58	b2	402	HEM	CHD-C1D-ND	2.96	127.65	124.43
57	AB	101	ZMP	O1-C10-C9	-2.93	120.53	123.99
59	c2	501	HEC	CAA-C2A-C3A	2.93	135.65	127.25
58	b1	401	HEM	CAD-C3D-C4D	2.90	129.72	124.66
58	b1	401	HEM	C1B-NB-C4B	2.89	108.06	105.07
58	b1	401	HEM	CBA-CAA-C2A	-2.88	107.70	112.62
59	c2	501	HEC	O1D-CGD-CBD	-2.82	114.01	123.08
58	b2	402	HEM	C4D-ND-C1D	2.82	107.99	105.07
59	c1	501	HEC	CBD-CAD-C3D	2.81	117.42	112.62
58	b1	401	HEM	CMB-C2B-C3B	-2.81	121.43	128.30
58	b1	402	HEM	C1B-NB-C4B	2.77	107.93	105.07
58	b2	402	HEM	CHA-C4D-ND	2.77	127.80	124.38
59	c1	501	HEC	O1D-CGD-CBD	-2.76	114.22	123.08
58	b2	403	HEM	CMA-C3A-C4A	-2.75	124.24	128.46
59	c1	501	HEC	CMC-C2C-C1C	-2.71	124.30	128.46
58	b1	402	HEM	CMA-C3A-C4A	-2.64	124.41	128.46
58	b2	403	HEM	CHA-C4D-ND	2.59	127.58	124.38
57	AA	101	ZMP	O1-C10-C9	-2.59	120.94	123.99
59	c2	501	HEC	CMD-C2D-C3D	2.58	129.81	124.94
58	b2	403	HEM	CHB-C1B-C2B	-2.54	119.71	126.72
58	b1	402	HEM	CHA-C4D-ND	2.53	127.50	124.38
58	b1	402	HEM	CHB-C1B-C2B	-2.47	119.89	126.72
58	b1	401	HEM	CHC-C4B-C3B	-2.46	120.80	124.57
59	c2	501	HEC	CMC-C2C-C1C	-2.43	124.73	128.46
59	c1	501	HEC	CAA-CBA-CGA	-2.39	107.07	113.76
59	c2	501	HEC	O1A-CGA-CBA	-2.35	115.53	123.08
61	b2	405	CDL	CA4-OA6-CA5	2.35	123.58	117.79
59	c2	501	HEC	C1D-C2D-C3D	2.31	108.60	107.00
59	c1	501	HEC	O1A-CGA-CBA	-2.28	115.76	123.08
58	b2	403	HEM	CAD-CBD-CGD	-2.25	108.77	113.60
65	A9	401	NDP	C5A-C6A-N6A	2.22	123.73	120.35
61	c2	502	CDL	CB4-OB6-CB5	2.22	123.25	117.79
59	c1	501	HEC	C2B-C3B-C4B	2.17	108.70	106.35
59	c1	501	HEC	CMA-C3A-C2A	2.17	129.03	124.94
58	b1	401	HEM	CAA-CBA-CGA	-2.16	107.71	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c1	501	HEC	CMD-C2D-C3D	2.15	129.00	124.94
58	b2	402	HEM	CHB-C1B-C2B	-2.15	120.78	126.72
58	b1	402	HEM	O2D-CGD-CBD	2.11	120.81	114.03
58	b1	401	HEM	CAD-C3D-C2D	-2.10	123.97	127.88
58	b2	402	HEM	O2A-CGA-CBA	2.04	120.57	114.03
59	c1	501	HEC	O2A-CGA-O1A	2.03	128.37	123.30
58	b2	403	HEM	CBB-CAB-C3B	-2.02	117.57	127.62
58	b2	403	HEM	O2A-CGA-CBA	2.00	120.47	114.03

There are no chirality outliers.

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	D1	501	3PE	C1-O11-P-O12
55	D1	501	3PE	C1-O11-P-O13
55	D1	501	3PE	C1-O11-P-O14
55	D5	701	3PE	C1-O11-P-O12
55	D5	701	3PE	C1-O11-P-O14
55	D5	701	3PE	C11-O13-P-O12
55	D5	701	3PE	O21-C2-C3-O31
55	D4	501	3PE	C1-O11-P-O12
55	D4	501	3PE	C1-O11-P-O13
55	D4	501	3PE	C1-O11-P-O14
55	D4	501	3PE	O13-C11-C12-N
55	b2	404	3PE	C1-O11-P-O12
55	b2	404	3PE	C1-O11-P-O14
55	b2	404	3PE	C11-O13-P-O14
55	f2	201	3PE	O13-C11-C12-N
56	D4	502	PC1	C1-O11-P-O13
56	D4	502	PC1	O13-C11-C12-N
57	AB	101	ZMP	C12-C11-S1-C10
57	AB	101	ZMP	O1-C10-S1-C11
57	AB	101	ZMP	C9-C10-S1-C11
57	AB	101	ZMP	S1-C10-C9-C8
57	AB	101	ZMP	C7-C8-C9-C10
57	AA	101	ZMP	C13-C14-C15-N2
57	AA	101	ZMP	C12-C11-S1-C10
57	AA	101	ZMP	O1-C10-S1-C11
57	AA	101	ZMP	C9-C10-S1-C11
58	b1	401	HEM	C2B-C3B-CAB-CBB
58	b1	401	HEM	C4B-C3B-CAB-CBB
58	b1	402	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
58	b1	402	HEM	C4B-C3B-CAB-CBB
58	b2	402	HEM	C2A-CAA-CBA-CGA
58	b2	402	HEM	C2B-C3B-CAB-CBB
58	b2	402	HEM	C4B-C3B-CAB-CBB
58	b2	403	HEM	C2B-C3B-CAB-CBB
58	b2	403	HEM	C4B-C3B-CAB-CBB
59	c2	501	HEC	C1A-C2A-CAA-CBA
59	c2	501	HEC	C3A-C2A-CAA-CBA
61	b2	401	CDL	CA2-OA2-PA1-OA3
61	b2	401	CDL	CB2-OB2-PB2-OB3
61	b2	401	CDL	CB2-OB2-PB2-OB5
61	b2	405	CDL	O1-C1-CA2-OA2
61	b2	405	CDL	CB2-OB2-PB2-OB3
61	b2	405	CDL	CB2-OB2-PB2-OB4
61	b2	405	CDL	CB2-OB2-PB2-OB5
61	c2	502	CDL	CA3-OA5-PA1-OA2
61	c2	502	CDL	CA3-OA5-PA1-OA3
61	c2	502	CDL	CA3-OA5-PA1-OA4
61	c2	502	CDL	CB3-OB5-PB2-OB3
63	V1	501	FMN	N10-C1'-C2'-O2'
63	V1	501	FMN	N10-C1'-C2'-C3'
65	A9	401	NDP	C5B-O5B-PA-O2A
65	A9	401	NDP	C5B-O5B-PA-O3
65	A9	401	NDP	C3B-C2B-O2B-P2B
65	A9	401	NDP	C1B-C2B-O2B-P2B
65	A9	401	NDP	C5D-O5D-PN-O1N
65	A9	401	NDP	C5D-O5D-PN-O2N
65	A9	401	NDP	C2D-C1D-N1N-C2N
57	AB	101	ZMP	C14-C13-N1-C12
57	AA	101	ZMP	C14-C13-N1-C12
57	AB	101	ZMP	O2-C13-N1-C12
57	AA	101	ZMP	O2-C13-N1-C12
65	A9	401	NDP	C2D-C1D-N1N-C6N
58	b1	401	HEM	C2A-CAA-CBA-CGA
59	c1	501	HEC	C3D-CAD-CBD-CGD
55	D1	501	3PE	C21-C22-C23-C24
55	D5	701	3PE	C21-C22-C23-C24
56	D4	502	PC1	C31-C32-C33-C34
55	D5	701	3PE	C1-O11-P-O13
55	D5	701	3PE	C11-O13-P-O11
55	D4	501	3PE	C11-O13-P-O11
55	b2	404	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
55	b2	404	3PE	C11-O13-P-O11
61	b2	401	CDL	CA2-OA2-PA1-OA5
61	b2	401	CDL	CA3-OA5-PA1-OA2
61	b2	401	CDL	CB3-OB5-PB2-OB2
61	b2	405	CDL	CA3-OA5-PA1-OA2
61	c2	502	CDL	CA2-OA2-PA1-OA5
61	b2	405	CDL	CB2-C1-CA2-OA2
57	AB	101	ZMP	C5-C6-C7-C8
57	AA	101	ZMP	C2-C3-C4-C5
55	D4	501	3PE	C33-C34-C35-C36
57	AB	101	ZMP	C13-C14-C15-N2
55	D5	701	3PE	C27-C28-C29-C2A
57	AB	101	ZMP	C4-C5-C6-C7
55	D5	701	3PE	C1-C2-C3-O31
55	f2	201	3PE	O11-C1-C2-O21
55	b2	404	3PE	C21-C22-C23-C24
61	b2	401	CDL	OB5-CB3-CB4-CB6
61	c2	502	CDL	OB5-CB3-CB4-CB6
55	D1	501	3PE	O13-C11-C12-N
55	D1	501	3PE	C1-C2-C3-O31
57	AB	101	ZMP	C6-C7-C8-C9
57	AA	101	ZMP	C1-C2-C3-C4
57	AB	101	ZMP	C3-C4-C5-C6
61	c2	502	CDL	CB3-OB5-PB2-OB2
61	b2	405	CDL	OA6-CA4-CA6-OA8
55	D4	501	3PE	C34-C35-C36-C37
61	b2	405	CDL	CA4-CA3-OA5-PA1
55	D5	701	3PE	C22-C23-C24-C25
57	AB	101	ZMP	O1-C10-C9-C8
65	A9	401	NDP	PN-O3-PA-O5B
65	A9	401	NDP	PA-O3-PN-O5D
55	D1	501	3PE	C2-C1-O11-P
61	b2	401	CDL	OB5-CB3-CB4-OB6
61	b2	405	CDL	OB5-CB3-CB4-OB6
55	D1	501	3PE	O21-C21-C22-C23
55	D4	501	3PE	C11-O13-P-O14
55	b2	404	3PE	C11-O13-P-O12
56	D4	502	PC1	C1-O11-P-O12
61	b2	401	CDL	CA2-OA2-PA1-OA4
61	b2	401	CDL	CA3-OA5-PA1-OA3
61	b2	401	CDL	CA3-OA5-PA1-OA4
61	b2	401	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
61	b2	401	CDL	CB3-OB5-PB2-OB4
61	b2	405	CDL	CA3-OA5-PA1-OA3
61	b2	405	CDL	CA3-OA5-PA1-OA4
61	c2	502	CDL	CA2-OA2-PA1-OA3
61	c2	502	CDL	CB3-OB5-PB2-OB4
61	b2	405	CDL	OB5-CB3-CB4-CB6
63	V1	501	FMN	C1'-C2'-C3'-O3'
56	D4	502	PC1	O11-C1-C2-O21
59	c2	501	HEC	C2A-CAA-CBA-CGA
59	c2	501	HEC	C3D-CAD-CBD-CGD
61	c2	502	CDL	OB5-CB3-CB4-OB6
57	AA	101	ZMP	C17-C18-C21-O5
55	D1	501	3PE	O21-C2-C3-O31
61	b2	401	CDL	CB4-CB3-OB5-PB2
57	AA	101	ZMP	C20-C18-C21-O5
56	D4	502	PC1	O22-C21-C22-C23
55	f2	201	3PE	O11-C1-C2-C3
56	D4	502	PC1	O11-C1-C2-C3
56	D4	502	PC1	C2-C1-O11-P
65	A9	401	NDP	O4D-C1D-N1N-C2N
61	b2	405	CDL	CA2-OA2-PA1-OA5
61	b2	401	CDL	C1-CB2-OB2-PB2
61	b2	405	CDL	C1-CA2-OA2-PA1
61	c2	502	CDL	C1-CA2-OA2-PA1
61	b2	405	CDL	CB3-CB4-CB6-OB8
57	AA	101	ZMP	C19-C18-C21-O5
55	D5	701	3PE	C23-C24-C25-C26
56	D4	502	PC1	O21-C21-C22-C23
61	b2	401	CDL	C32-C31-CA7-OA8
55	D5	701	3PE	O11-C1-C2-C3
59	c1	501	HEC	CAA-CBA-CGA-O2A
59	c1	501	HEC	CAA-CBA-CGA-O1A
61	b2	405	CDL	OB6-CB4-CB6-OB8
58	b1	402	HEM	CAA-CBA-CGA-O2A
55	D4	501	3PE	C22-C23-C24-C25
55	b2	404	3PE	O31-C31-C32-C33
58	b1	402	HEM	CAA-CBA-CGA-O1A
55	D5	701	3PE	C32-C33-C34-C35
63	V1	501	FMN	O2'-C2'-C3'-O3'
55	b2	404	3PE	O11-C1-C2-O21
55	f2	201	3PE	O21-C21-C22-C23
58	b1	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
56	D4	502	PC1	O31-C31-C32-C33
57	AA	101	ZMP	C6-C7-C8-C9
58	b1	402	HEM	CAD-CBD-CGD-O2D
65	A9	401	NDP	C5D-O5D-PN-O3
61	c2	502	CDL	CA4-CA3-OA5-PA1
59	c1	501	HEC	CAD-CBD-CGD-O1D
65	A9	401	NDP	O4B-C4B-C5B-O5B
58	b2	402	HEM	CAD-CBD-CGD-O2D
55	f2	201	3PE	O22-C21-C22-C23
65	A9	401	NDP	PA-O3-PN-O1N
58	b2	402	HEM	CAD-CBD-CGD-O1D
63	V1	501	FMN	O3'-C3'-C4'-C5'
56	D4	502	PC1	O32-C31-C32-C33
58	b2	403	HEM	CAD-CBD-CGD-O2D
61	b2	405	CDL	CA6-CA4-OA6-CA5
61	c2	502	CDL	CB6-CB4-OB6-CB5
65	A9	401	NDP	O4D-C1D-N1N-C6N
59	c1	501	HEC	CAD-CBD-CGD-O2D
61	b2	401	CDL	C32-C31-CA7-OA9
58	b2	403	HEM	CAD-CBD-CGD-O1D
55	b2	404	3PE	C32-C33-C34-C35
61	c2	502	CDL	C51-C52-C53-C54

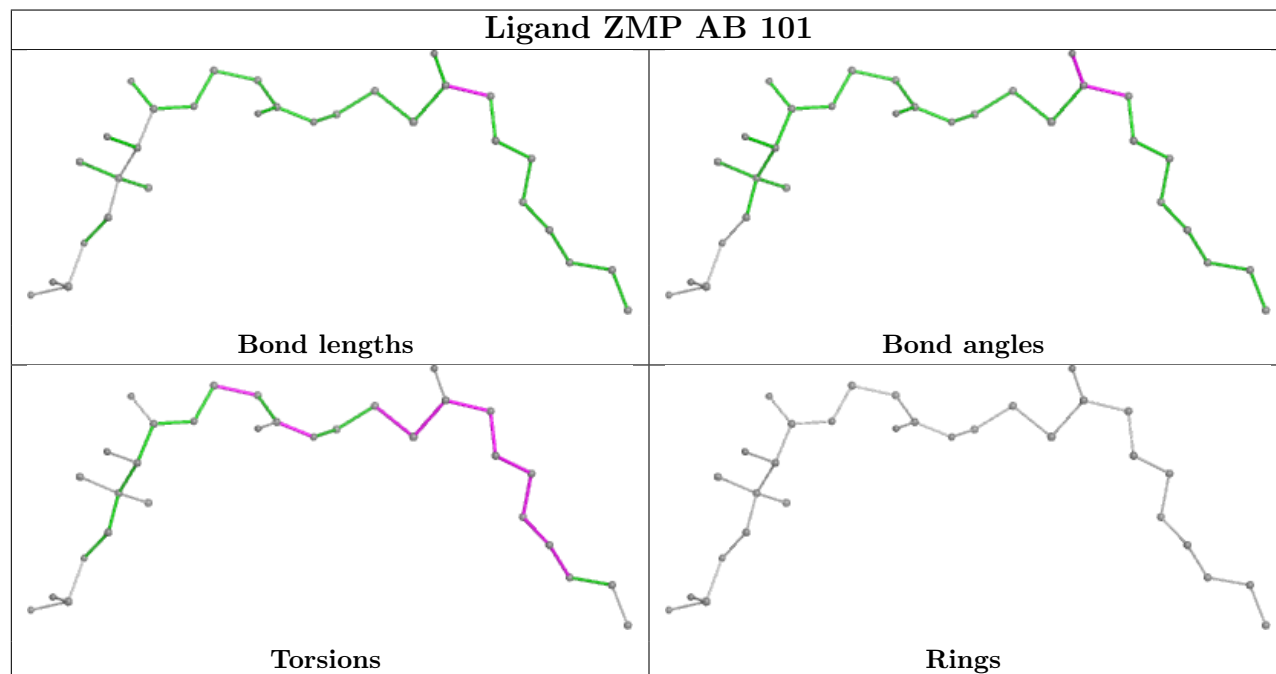
There are no ring outliers.

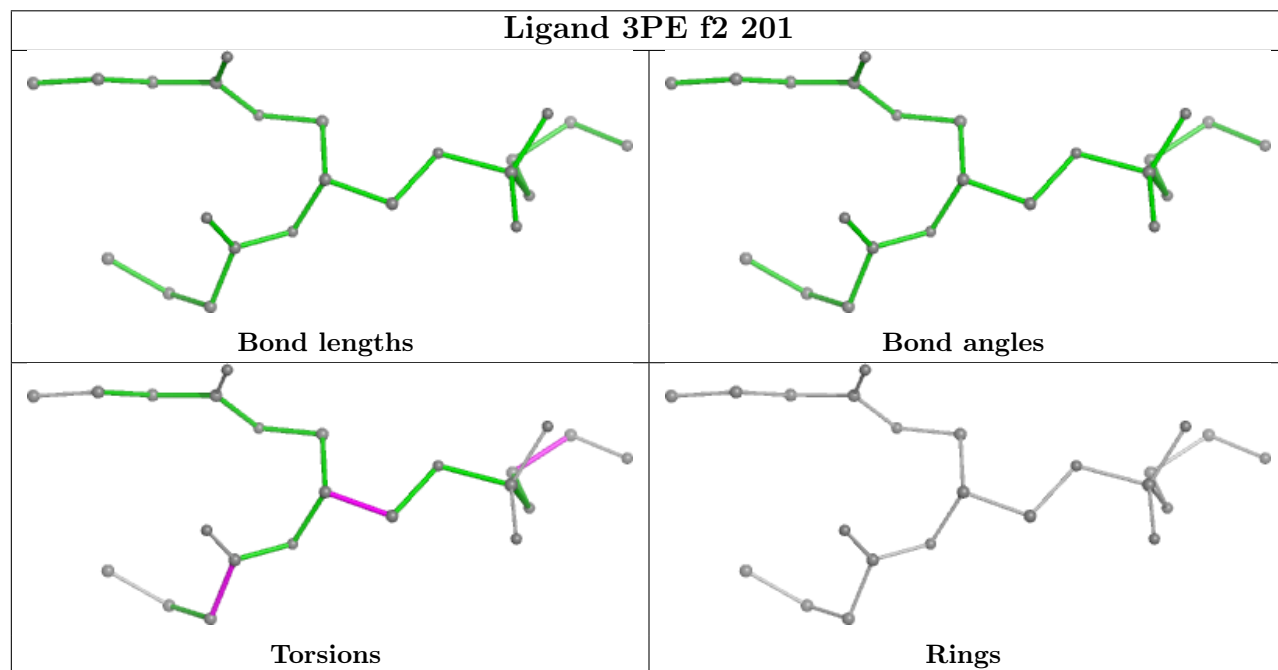
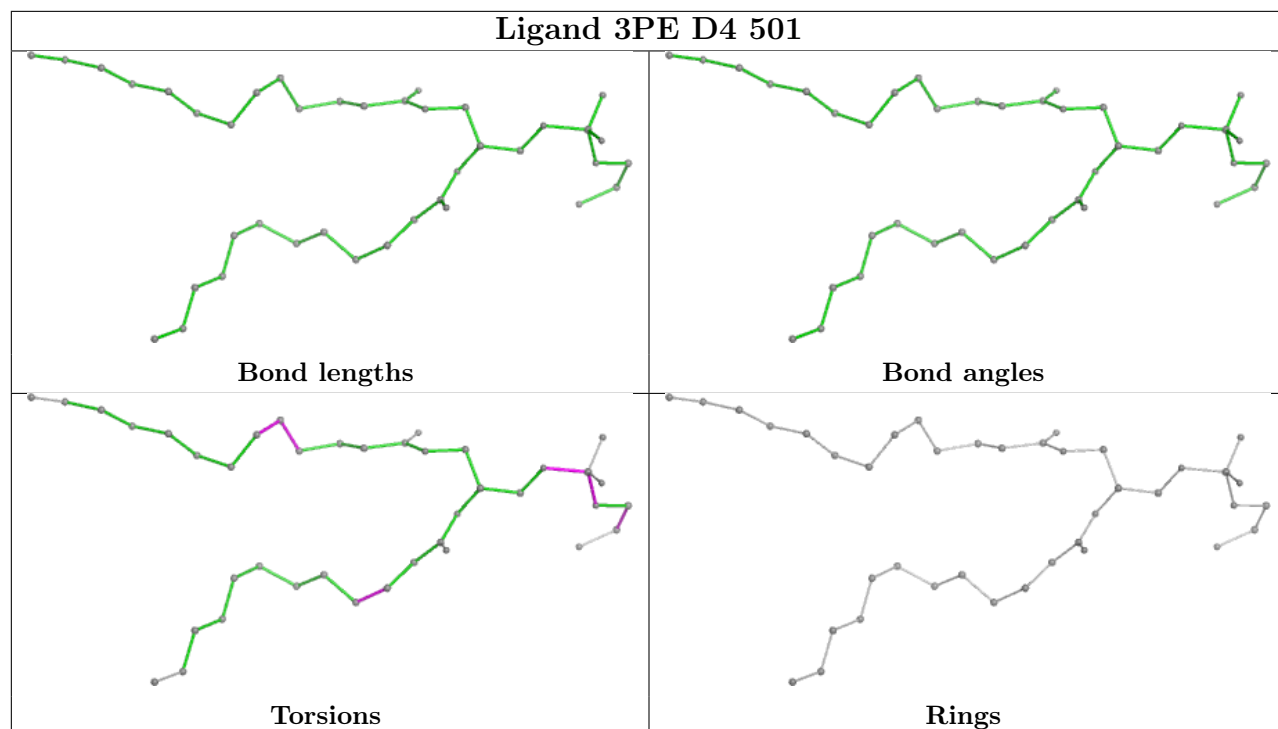
12 monomers are involved in 28 short contacts:

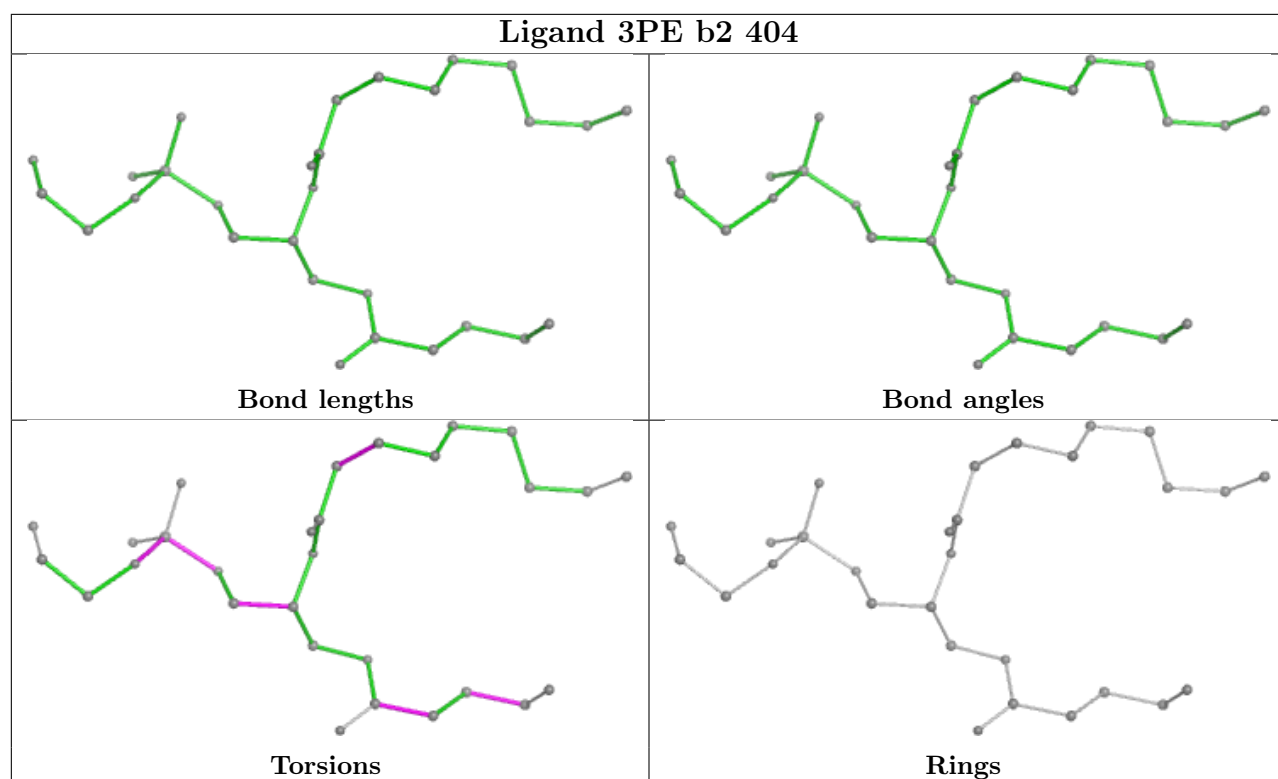
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AB	101	ZMP	6	0
55	D4	501	3PE	3	0
65	A9	401	NDP	4	0
62	S1	802	SF4	1	0
55	D5	701	3PE	1	0
60	S1	803	FES	1	0
55	D1	501	3PE	1	0
62	V1	500	SF4	3	0
57	AA	101	ZMP	4	0
62	S8	202	SF4	2	0
62	S1	801	SF4	1	0
63	V1	501	FMN	1	0

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

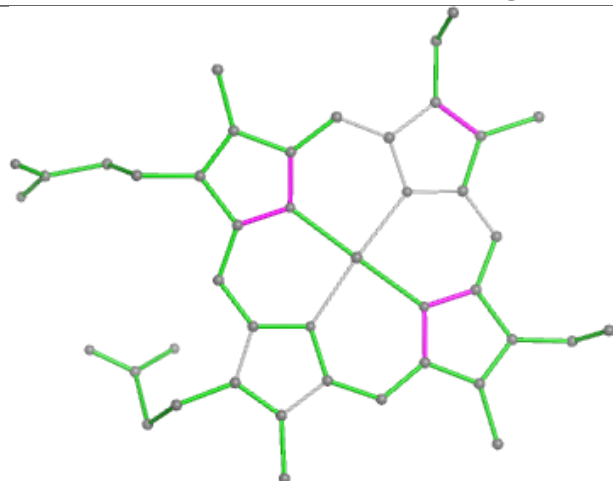
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



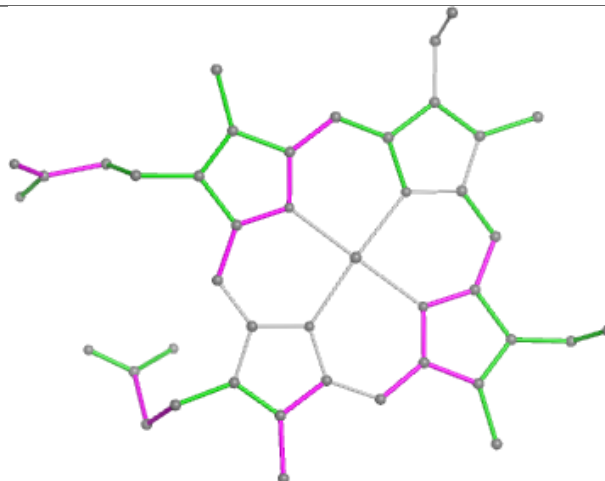




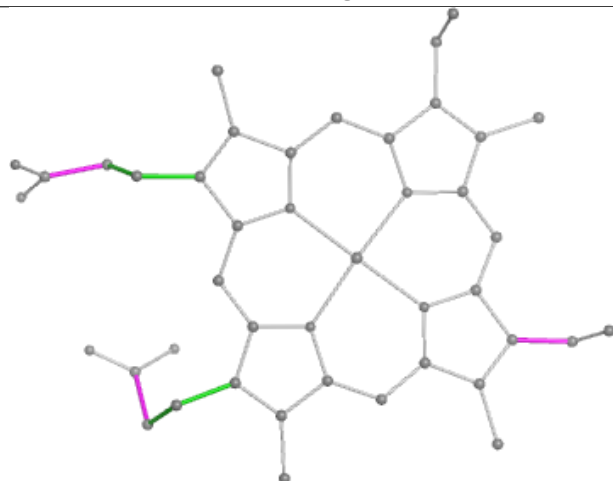
## Ligand HEM b1 402



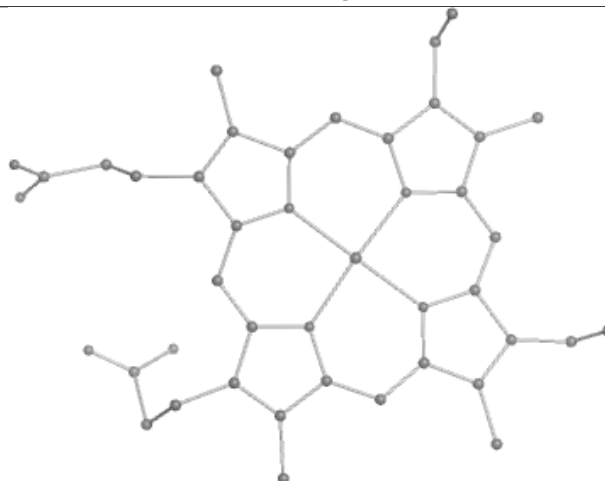
Bond lengths



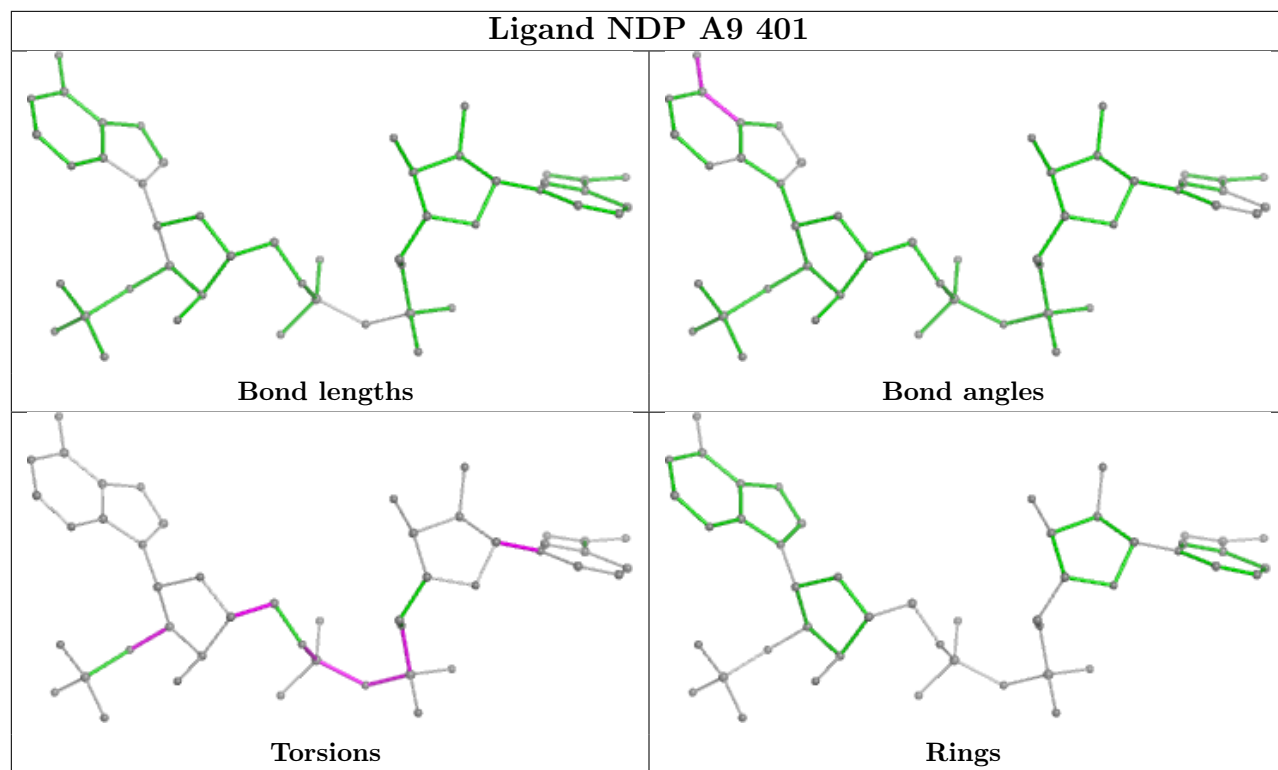
Bond angles



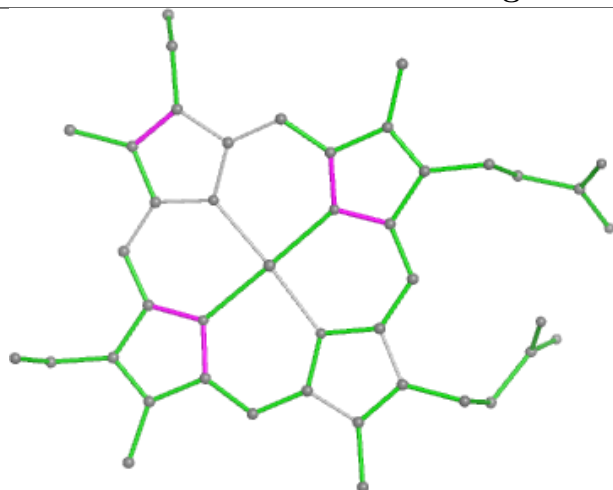
Torsions



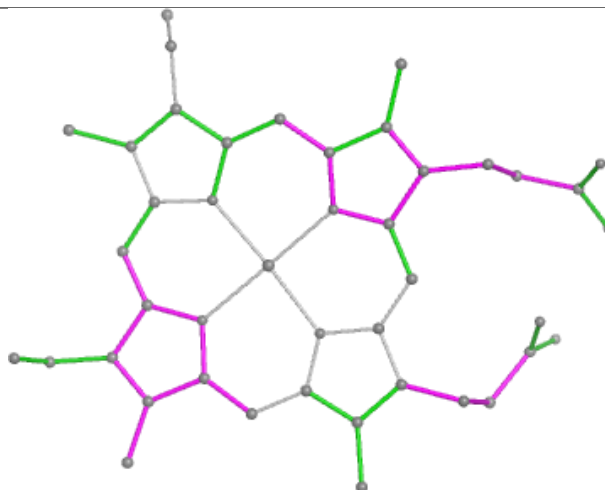
Rings



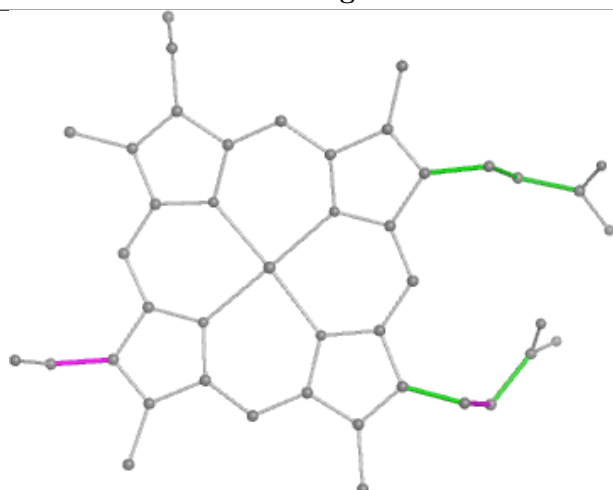
## Ligand HEM b1 401



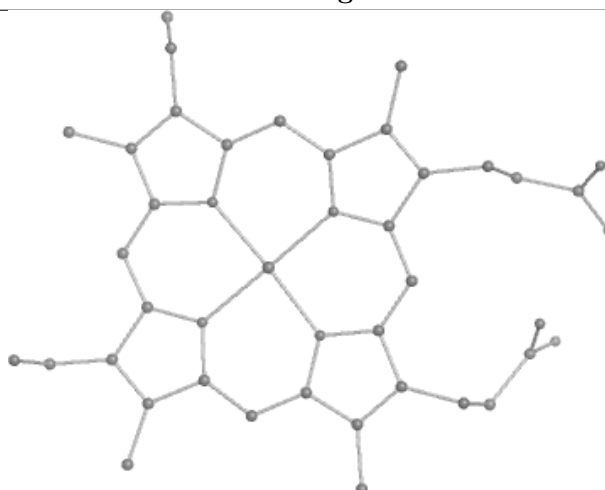
Bond lengths



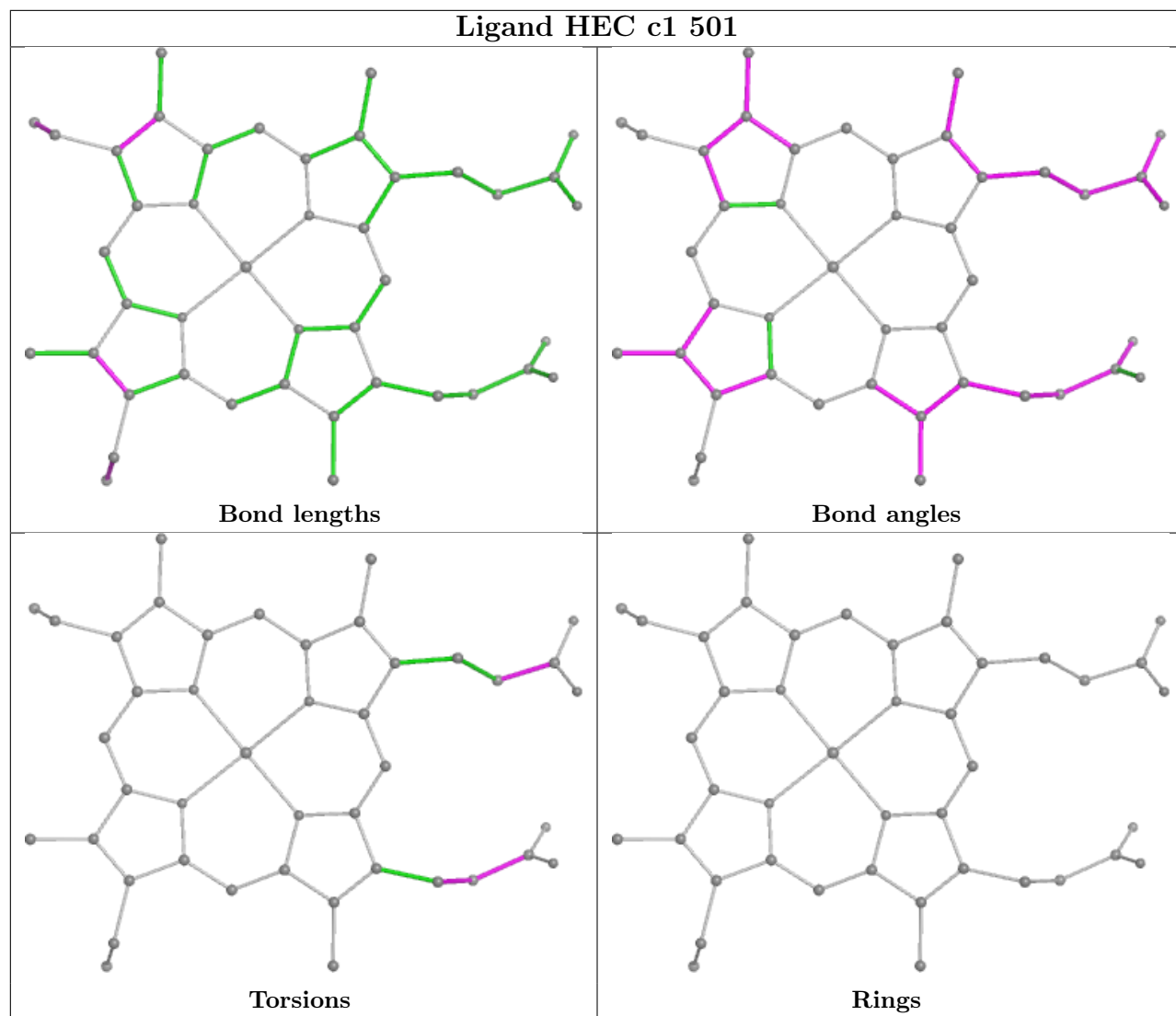
Bond angles



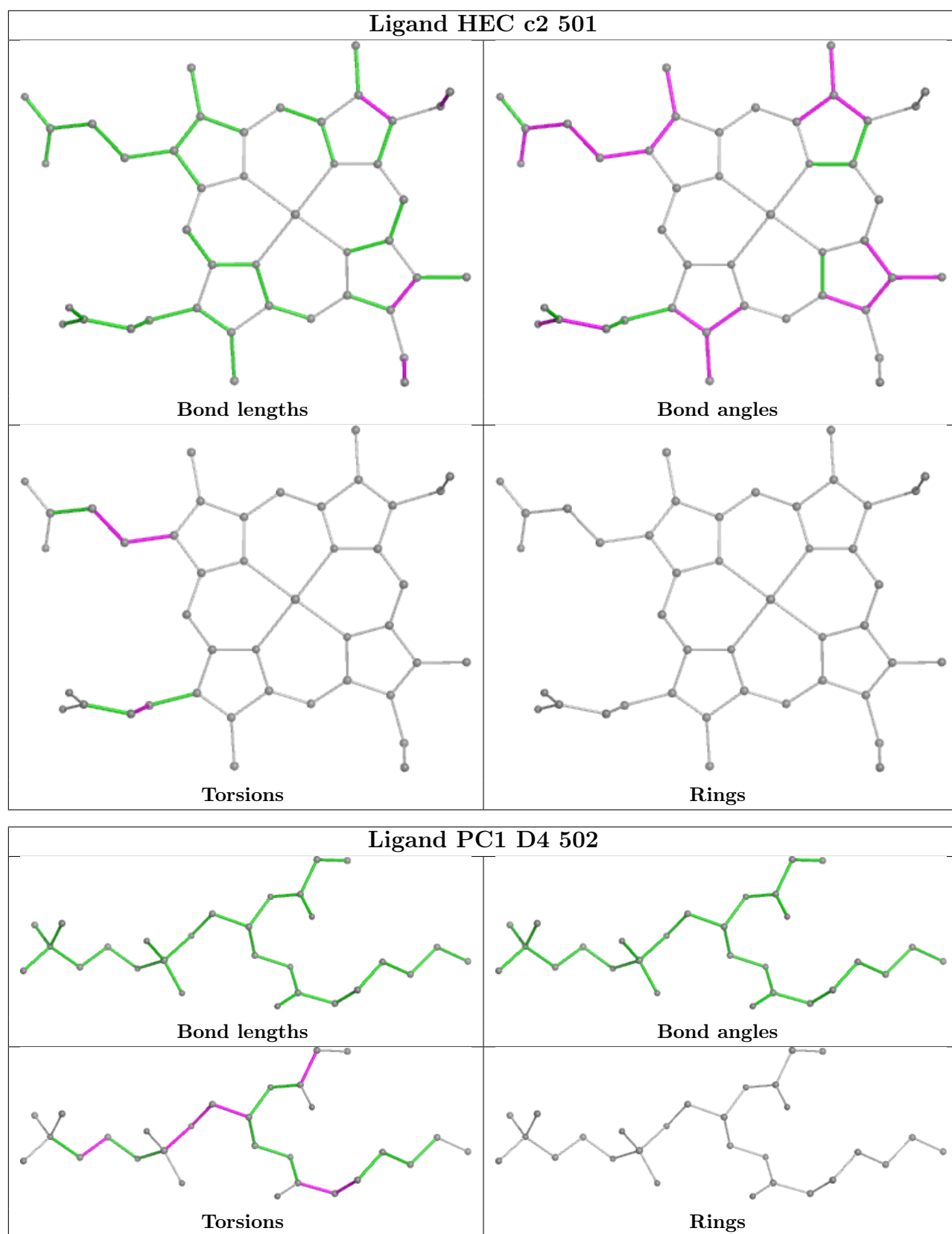
Torsions

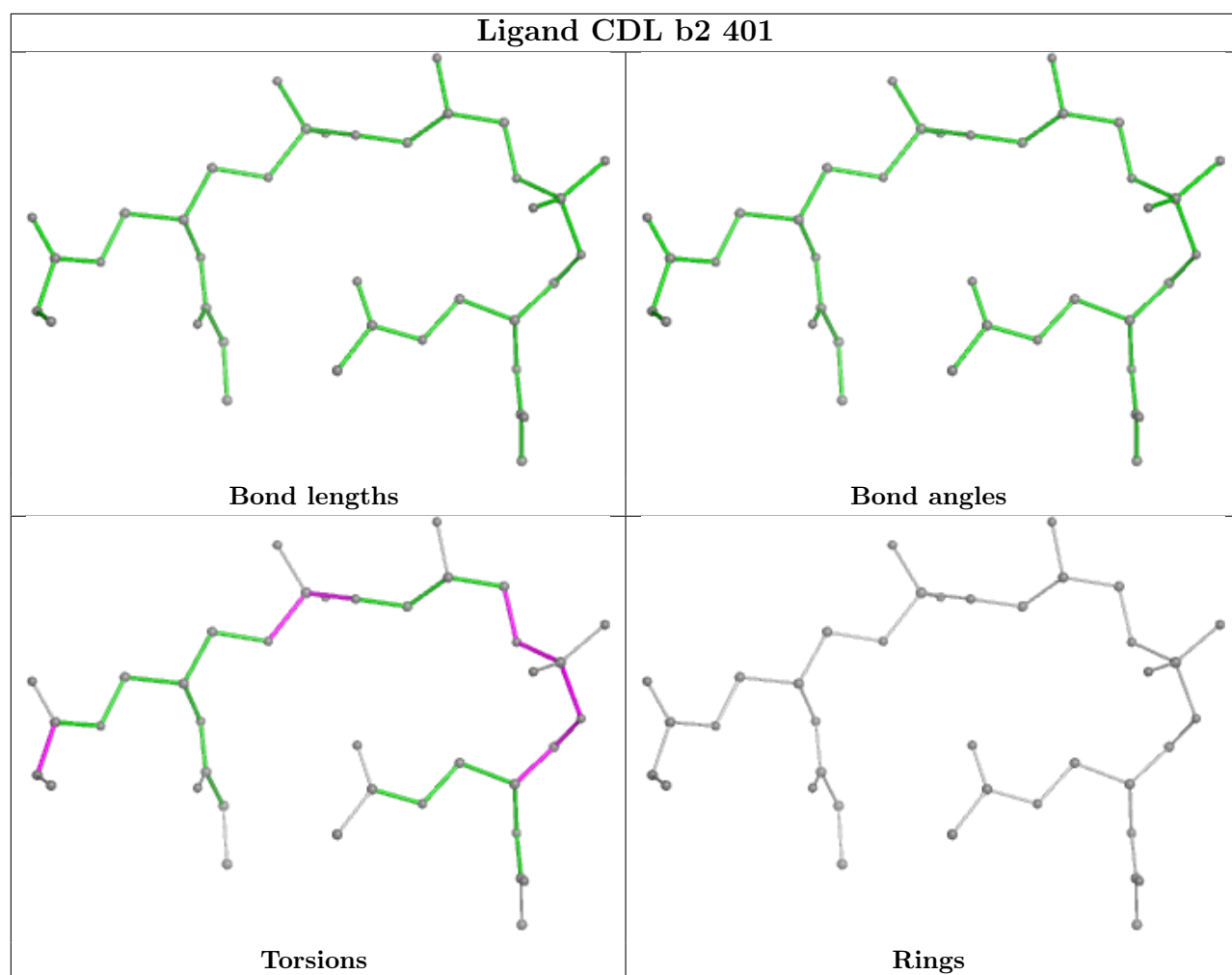


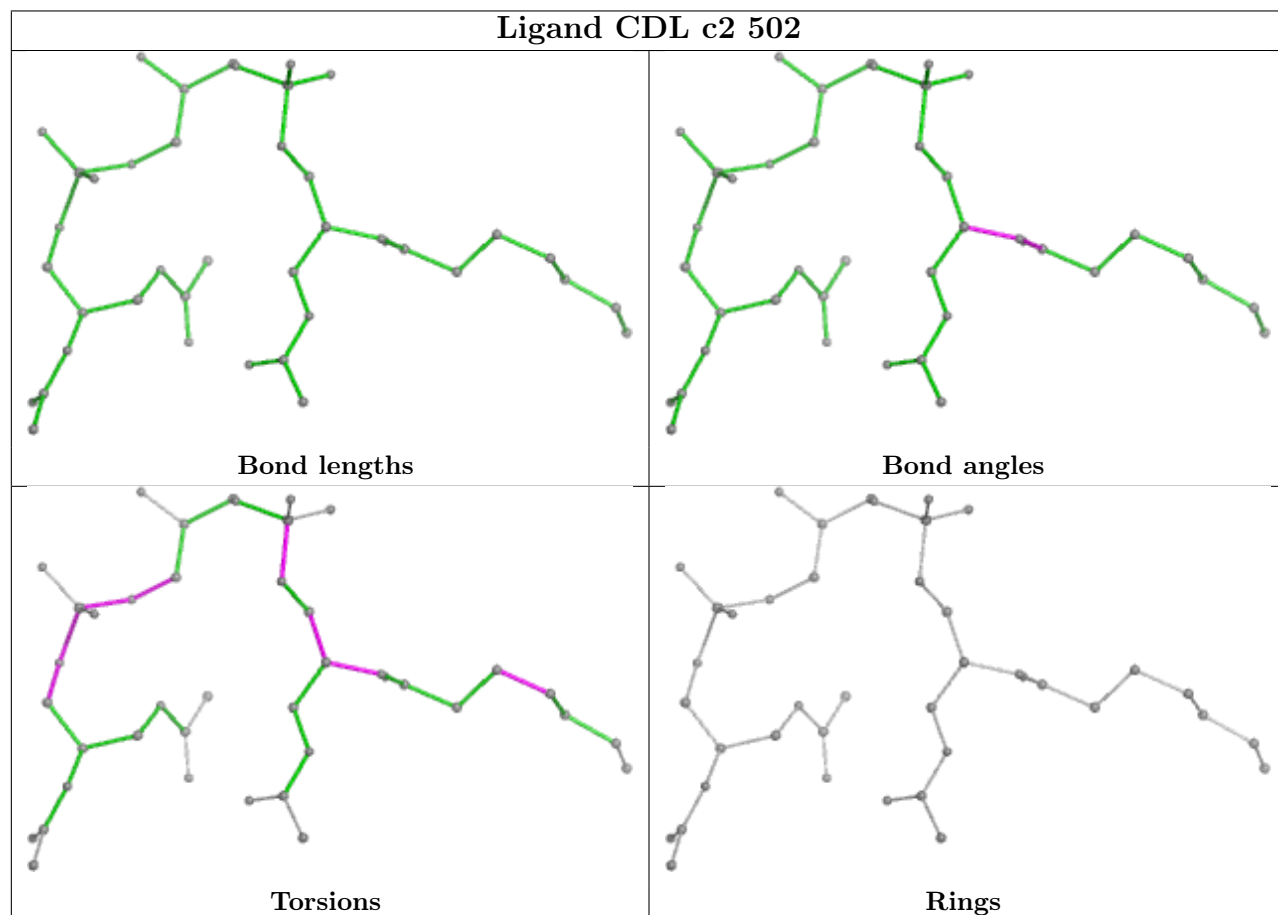
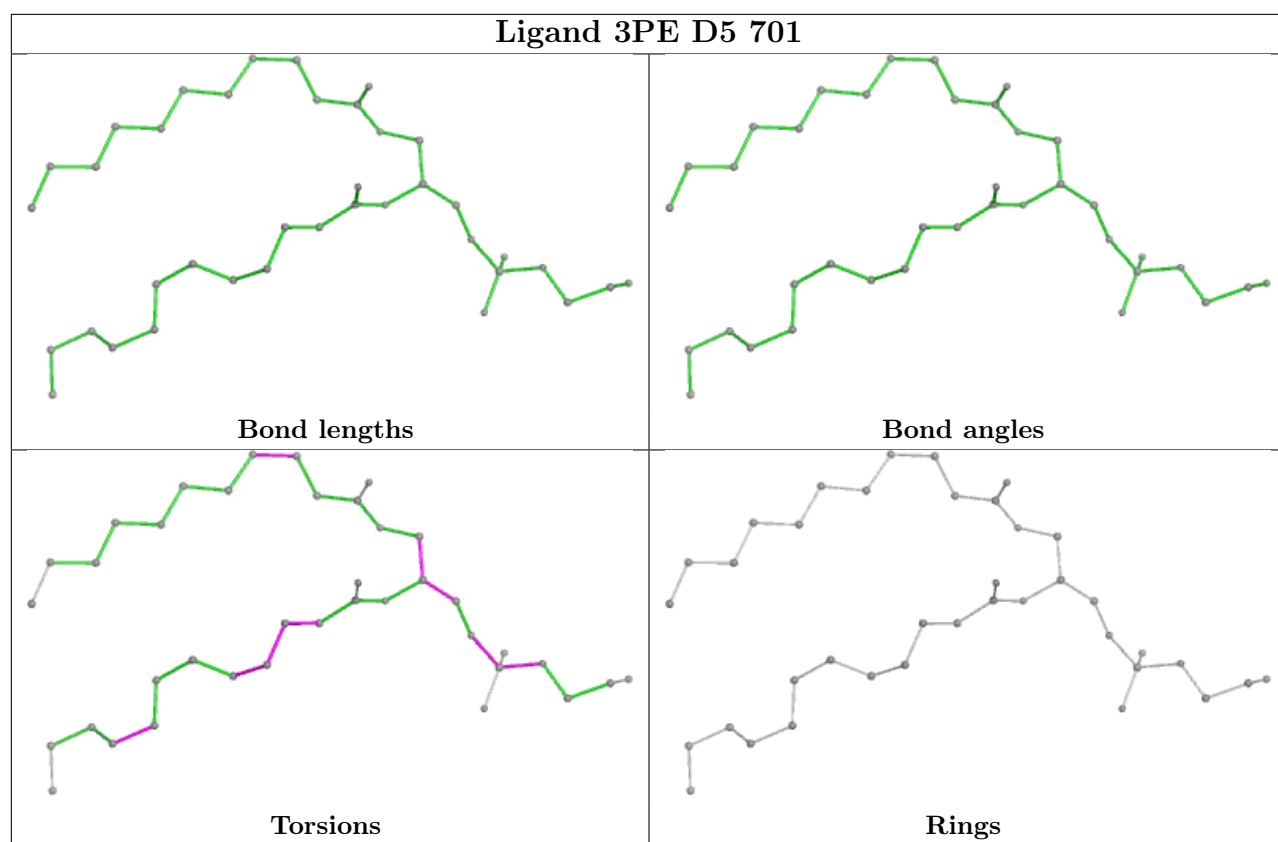
Rings

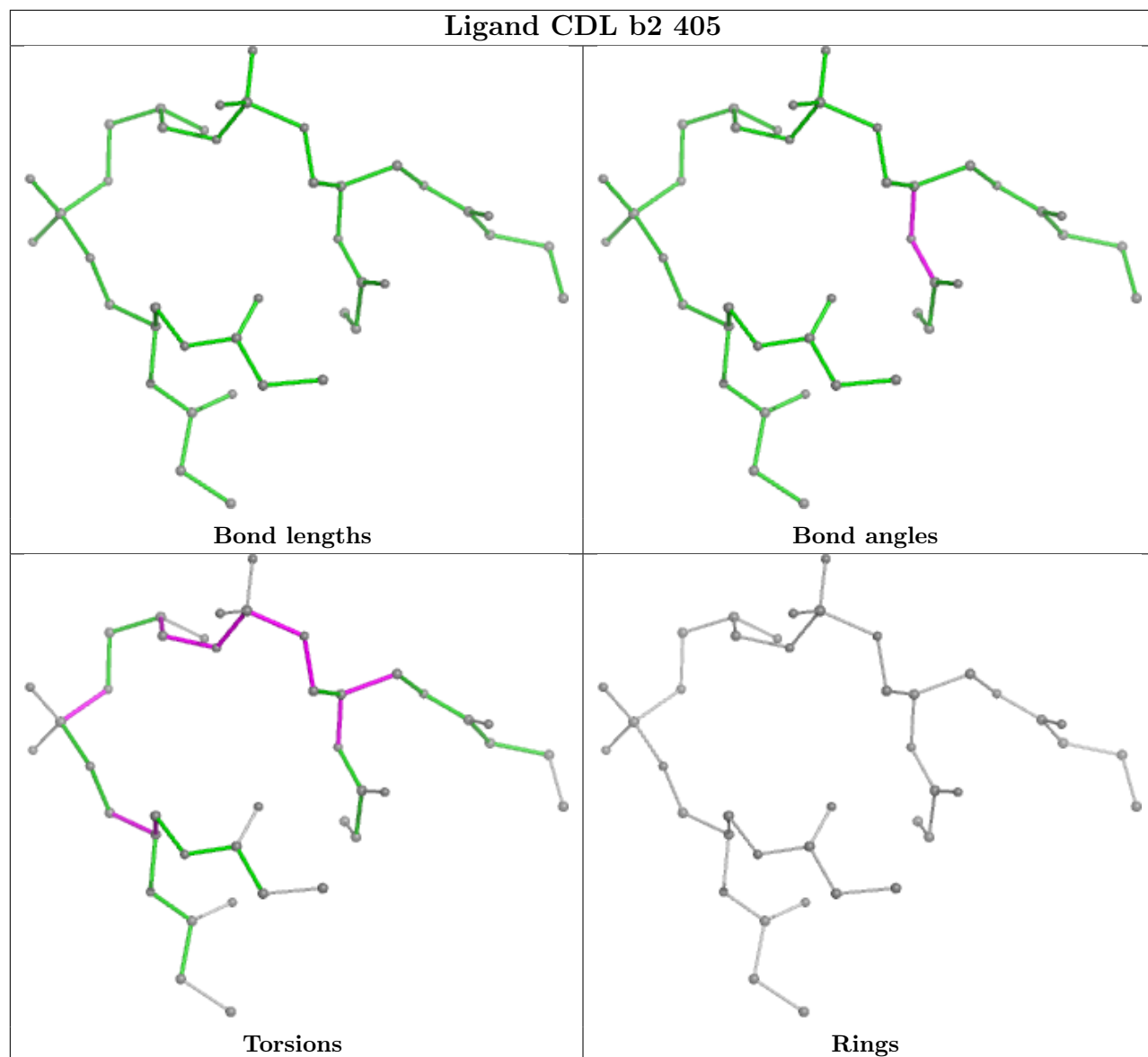


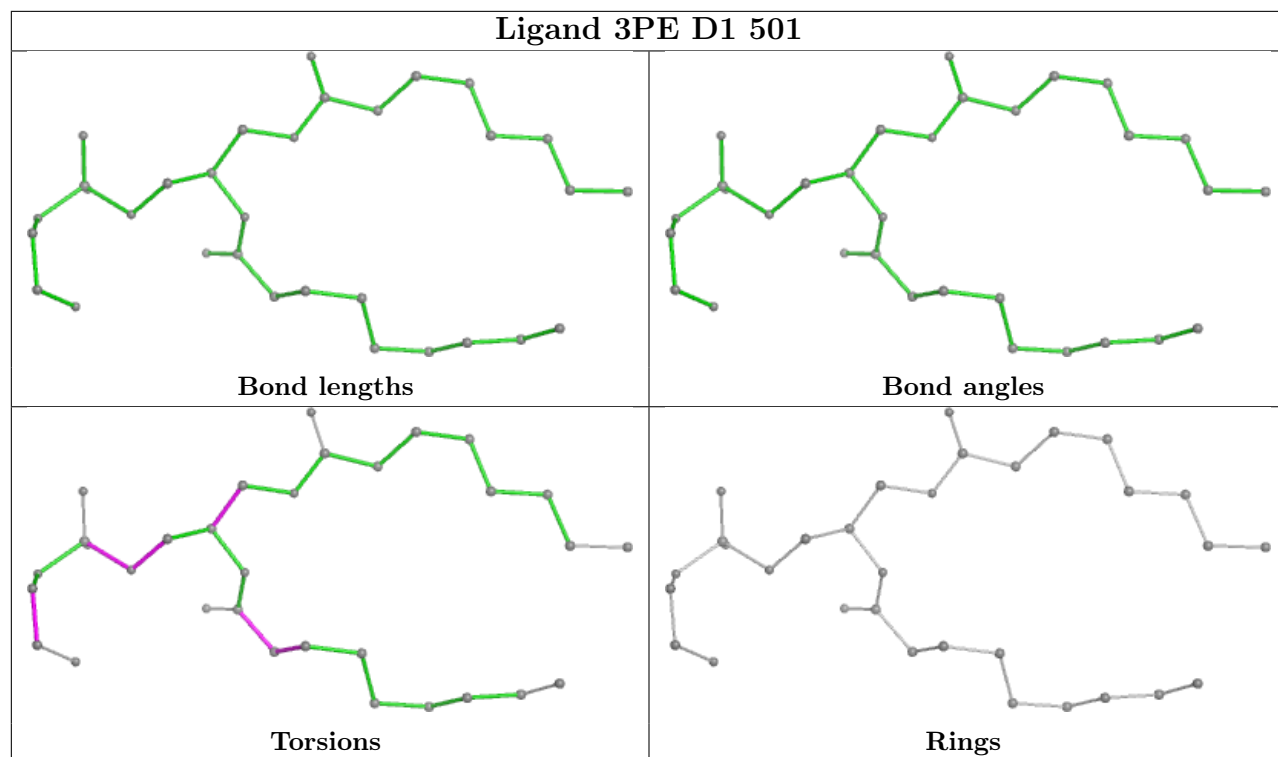




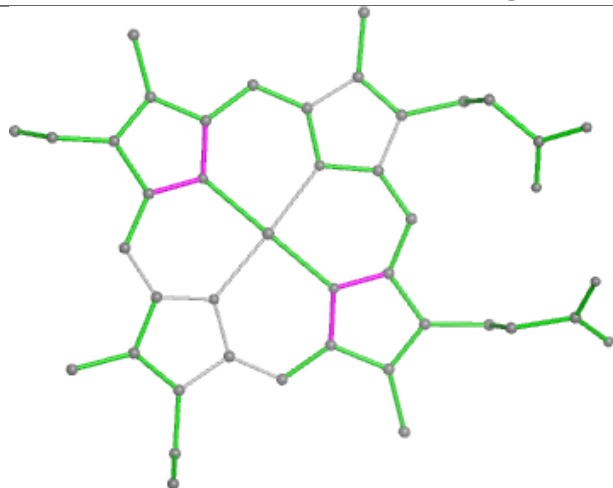




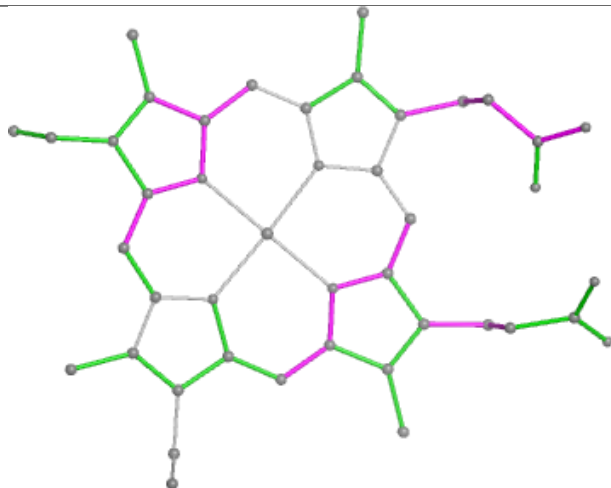




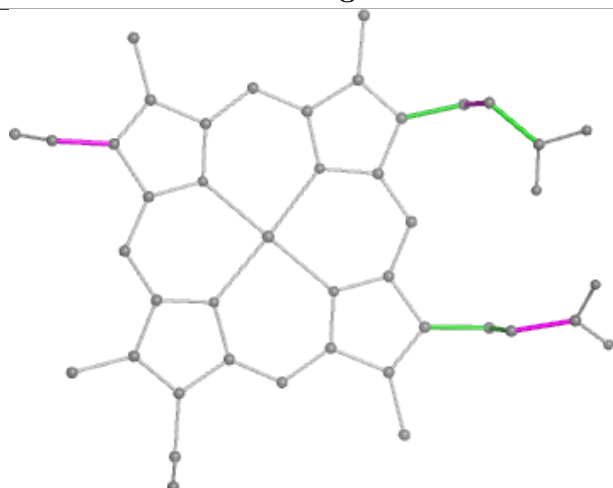
## Ligand HEM b2 402



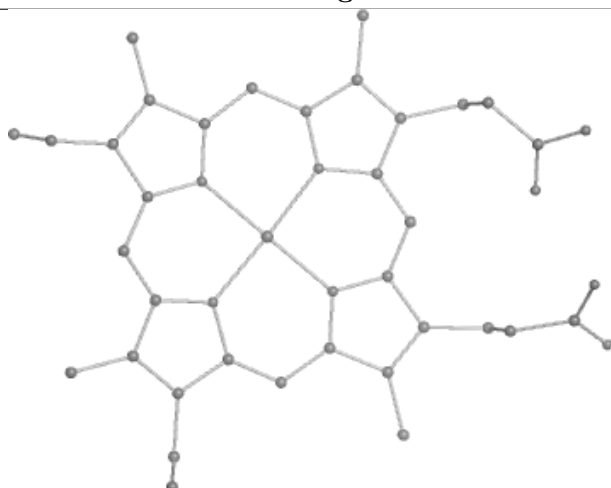
Bond lengths



Bond angles

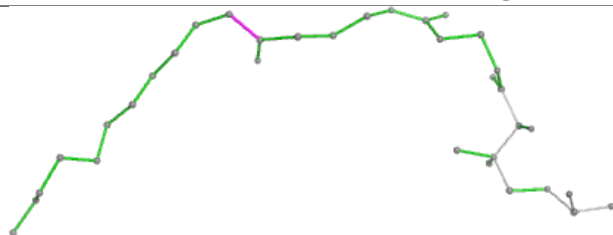


Torsions

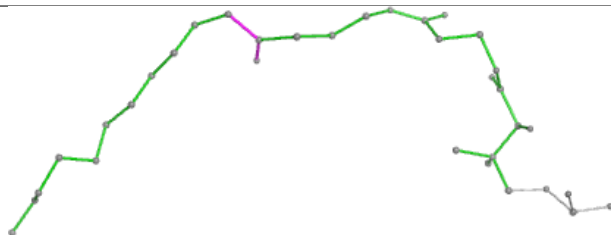


Rings

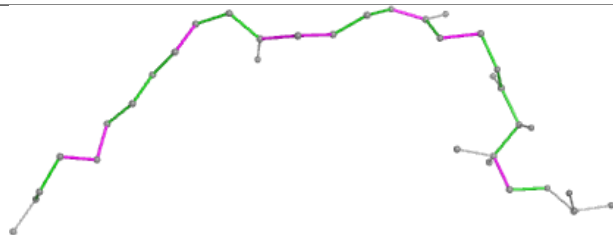
## Ligand ZMP AA 101



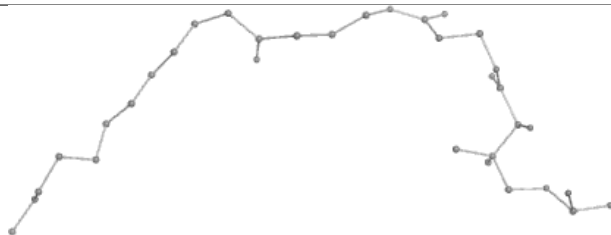
Bond lengths



Bond angles

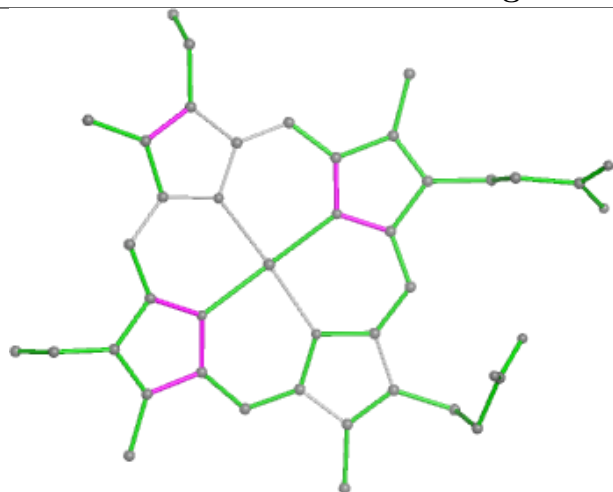


Torsions

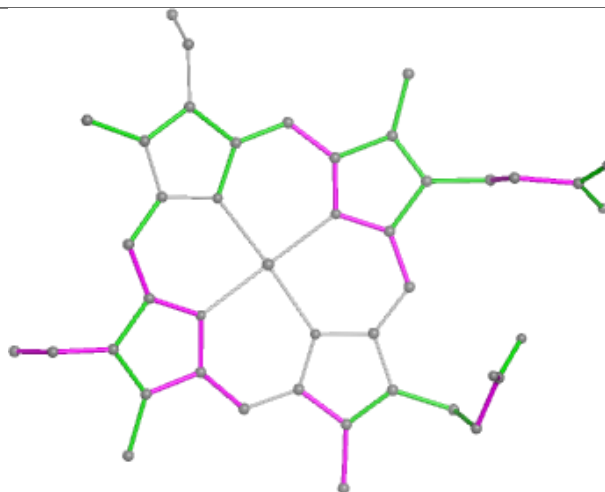


Rings

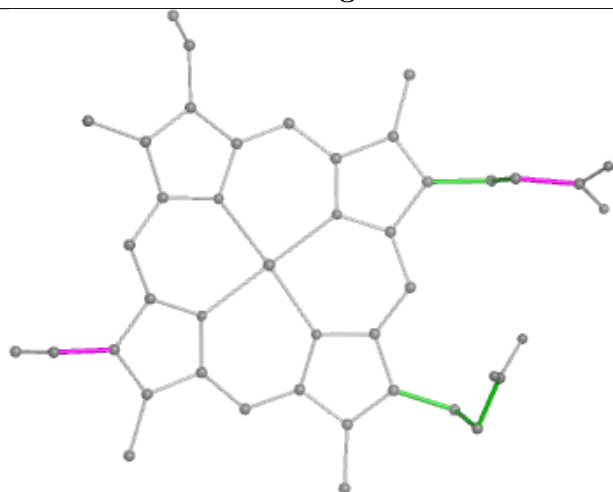
## Ligand HEM b2 403



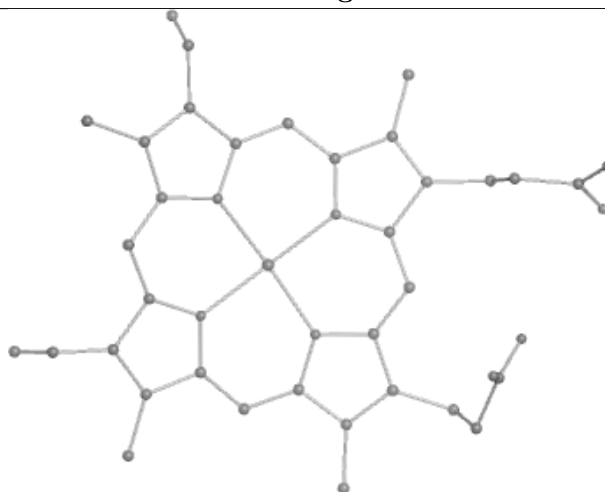
Bond lengths



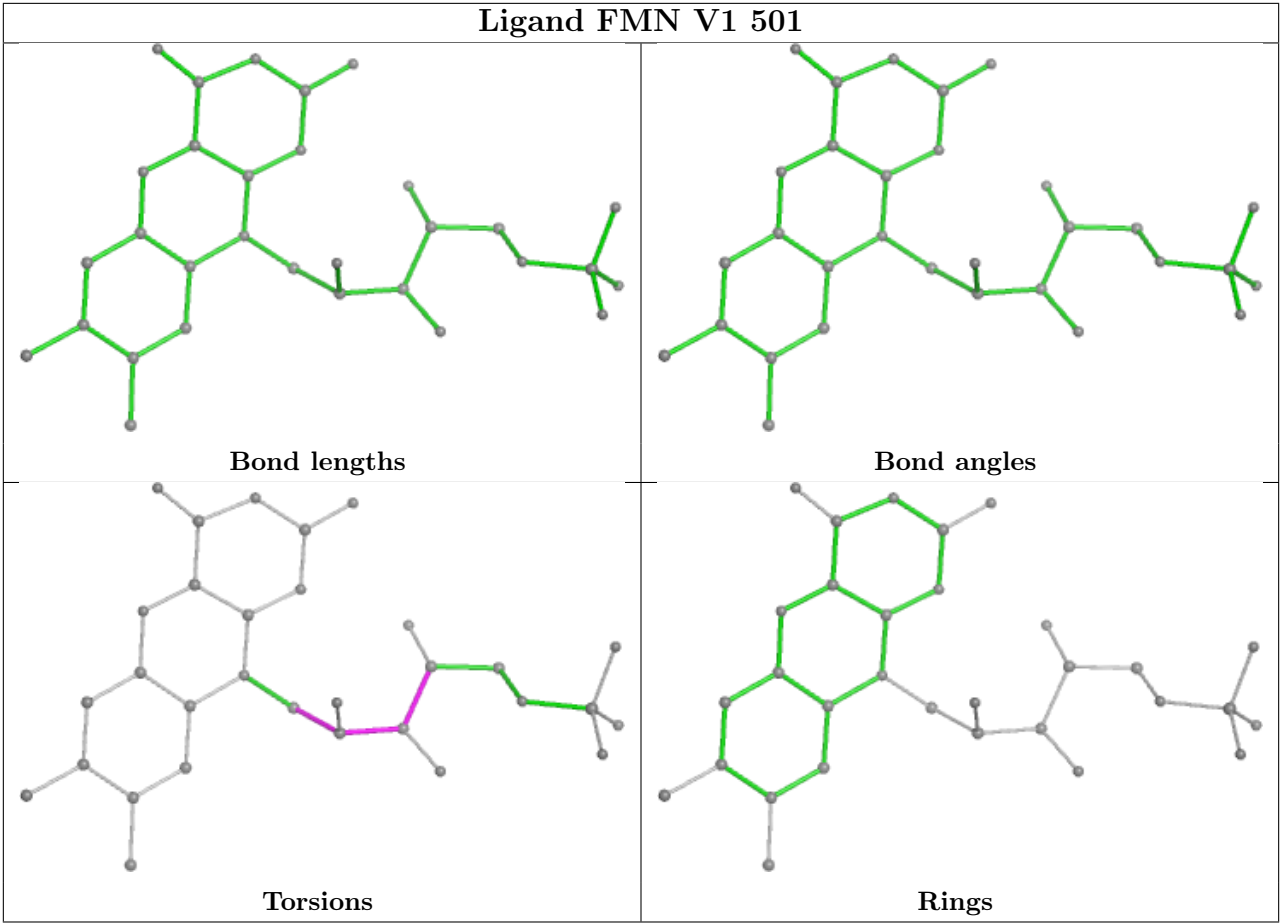
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	x2	1
37	x1	1
24	B8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x2	26:UNK	C	45:UNK	N	27.65
1	x1	27:UNK	C	29:UNK	N	5.59
1	B8	46:ASP	C	47:TYR	N	1.20



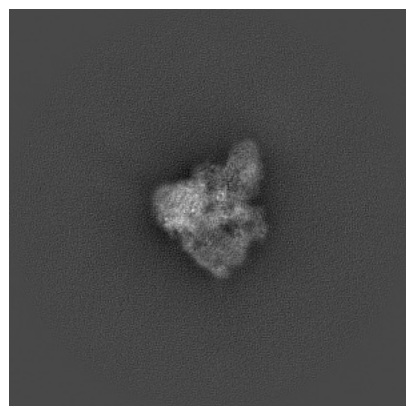
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4494. These allow visual inspection of the internal detail of the map and identification of artifacts.

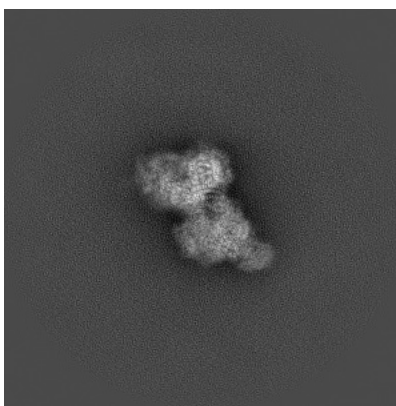
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

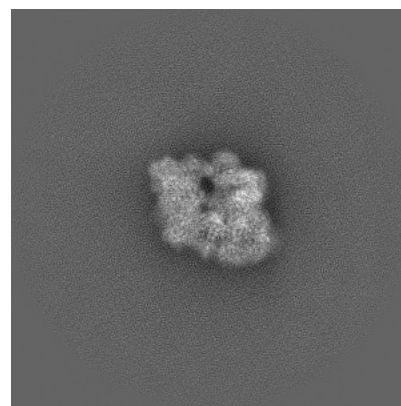
#### 6.1.1 Primary map



X

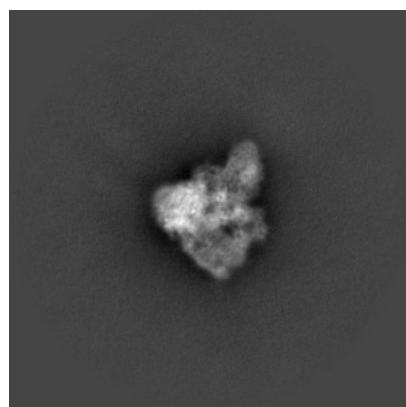


Y

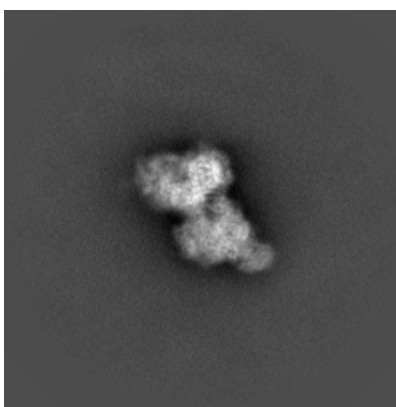


Z

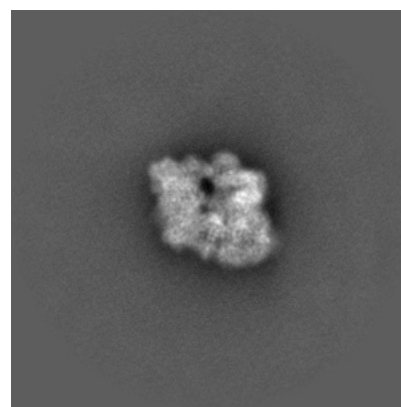
#### 6.1.2 Raw map



X



Y

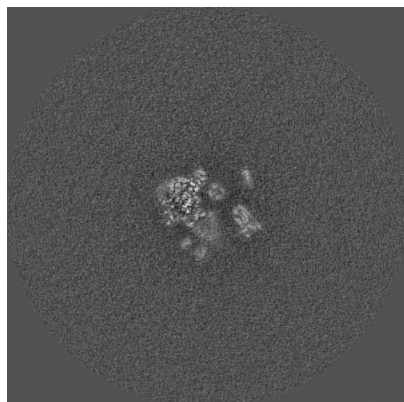


Z

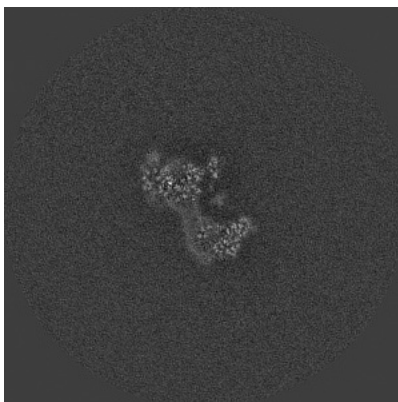
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

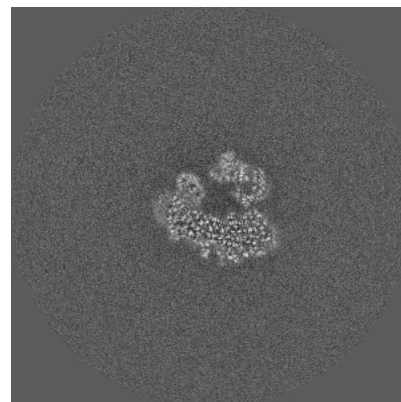
### 6.2.1 Primary map



X Index: 256

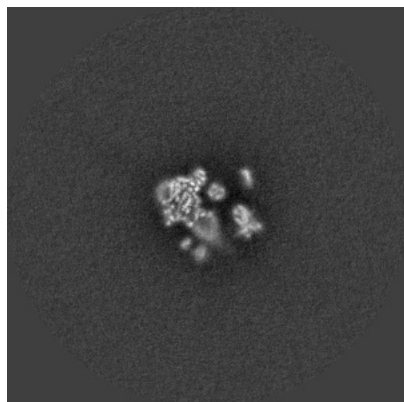


Y Index: 256

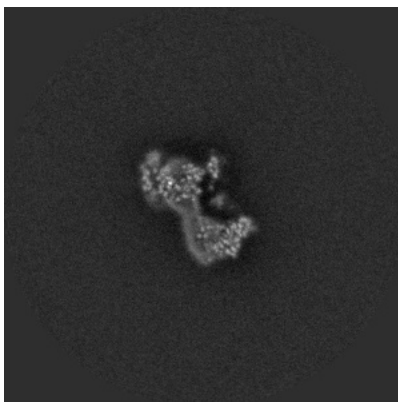


Z Index: 256

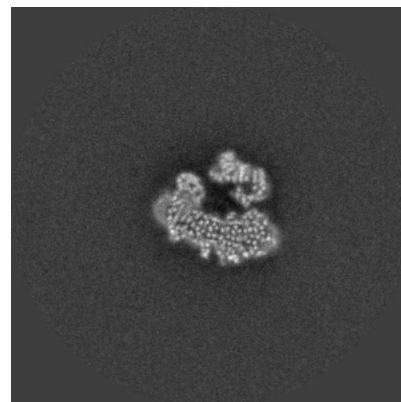
### 6.2.2 Raw map



X Index: 256



Y Index: 256

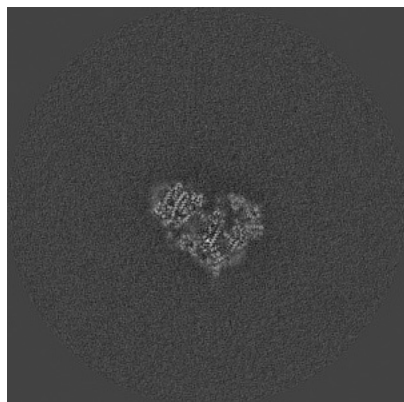


Z Index: 256

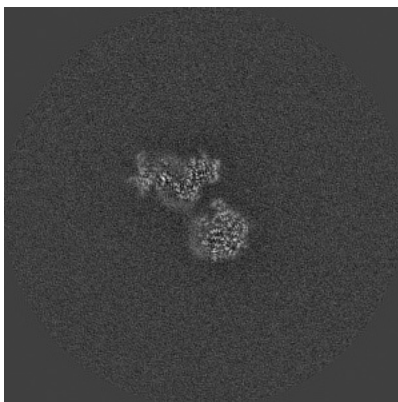
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

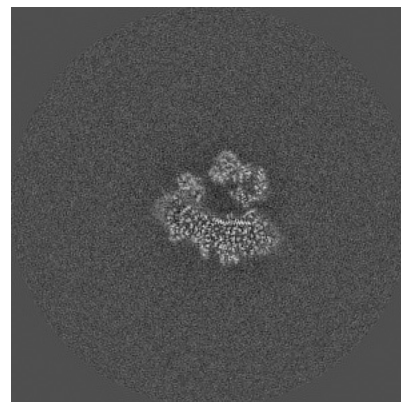
### 6.3.1 Primary map



X Index: 285

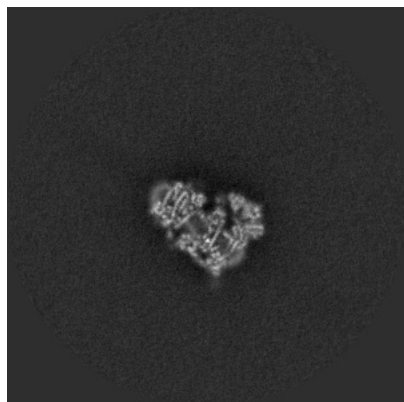


Y Index: 267

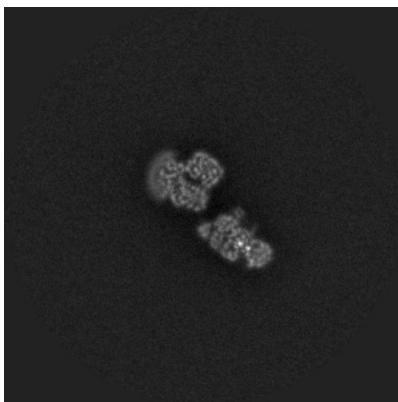


Z Index: 254

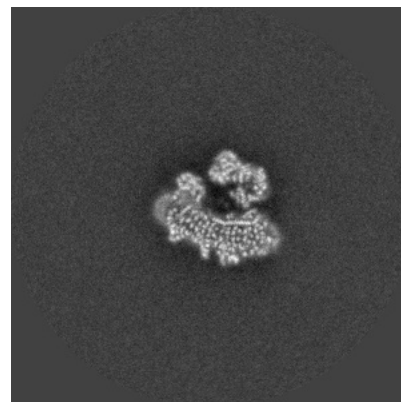
### 6.3.2 Raw map



X Index: 285



Y Index: 296

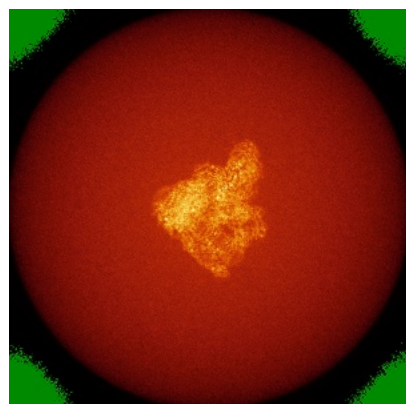


Z Index: 254

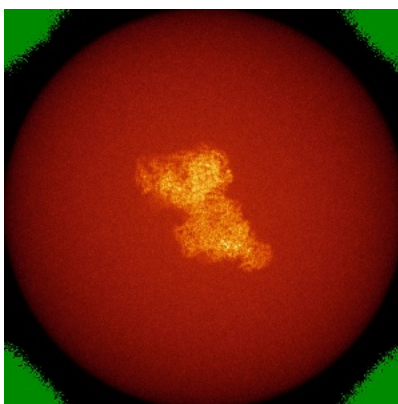
The images above show the largest variance slices of the map in three orthogonal directions.

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

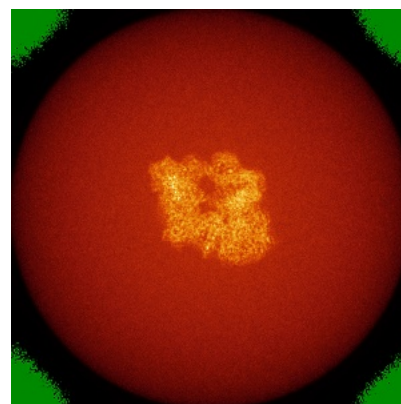
### 6.4.1 Primary map



X

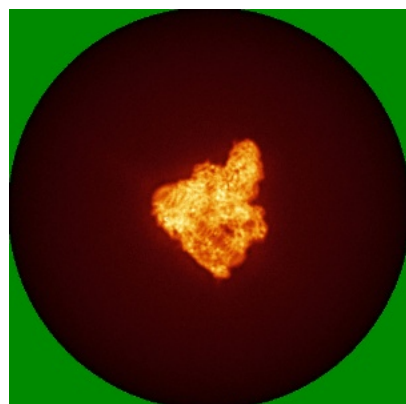


Y

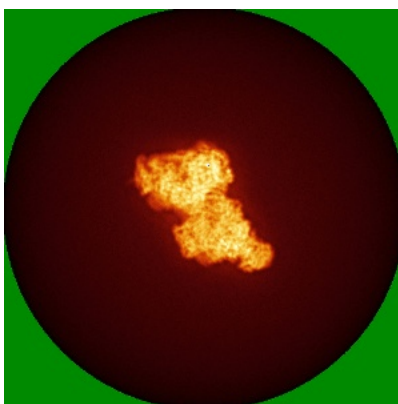


Z

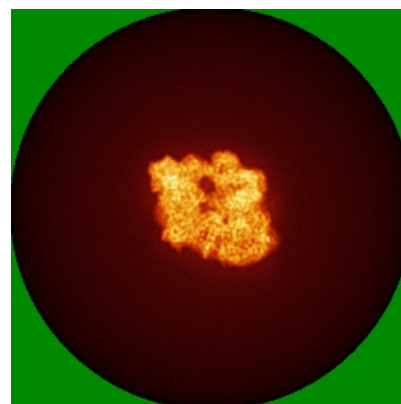
### 6.4.2 Raw map



X



Y



Z

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

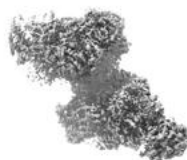


## 6.5 Orthogonal surface views [i](#)

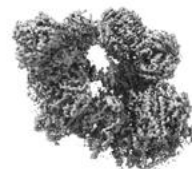
### 6.5.1 Primary map



X



Y



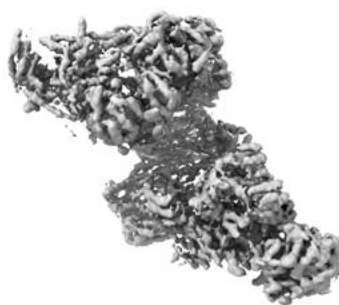
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

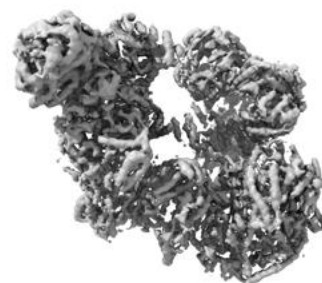
### 6.5.2 Raw map



X



Y



Z

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

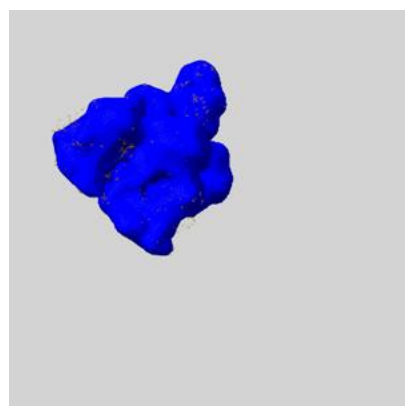
## 6.6 Mask visualisation [i](#)

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

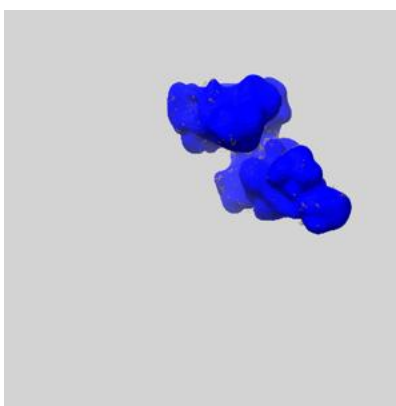
A mask typically either:

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

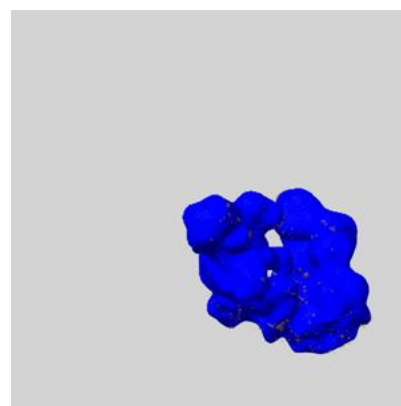
### 6.6.1 emd\_4494\_msk\_1.map [i](#)



X



Y

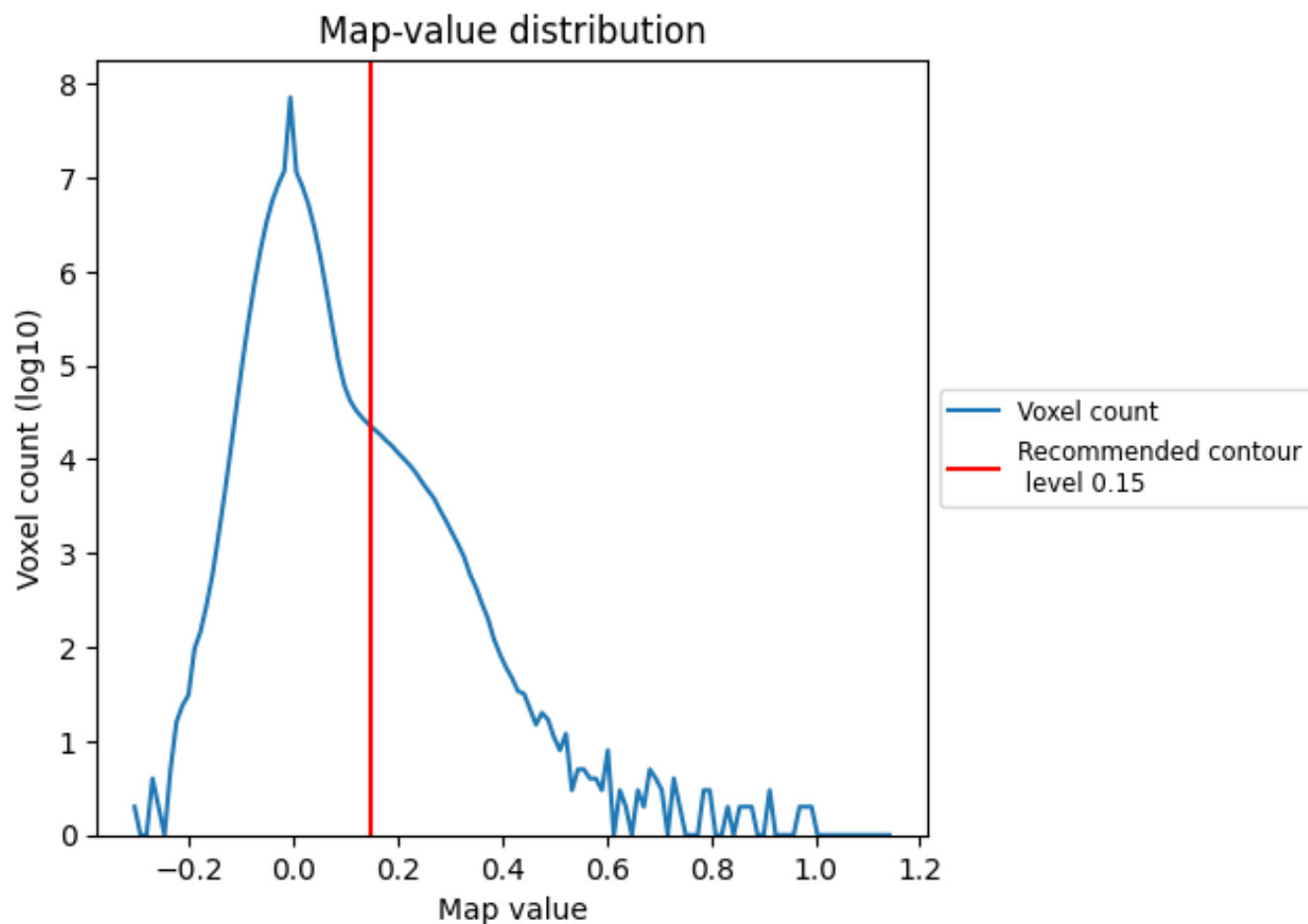


Z

## 7 Map analysis [i](#)

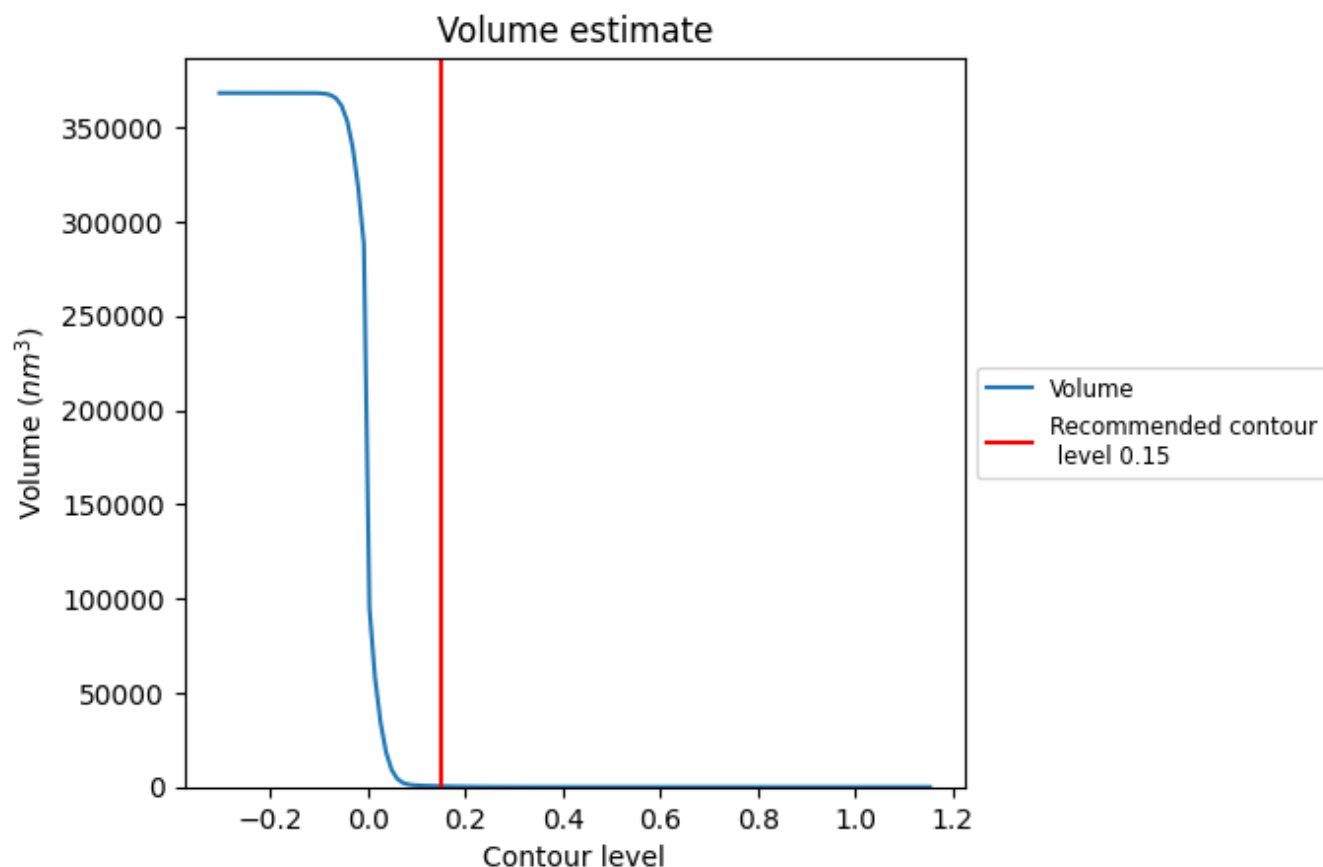
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

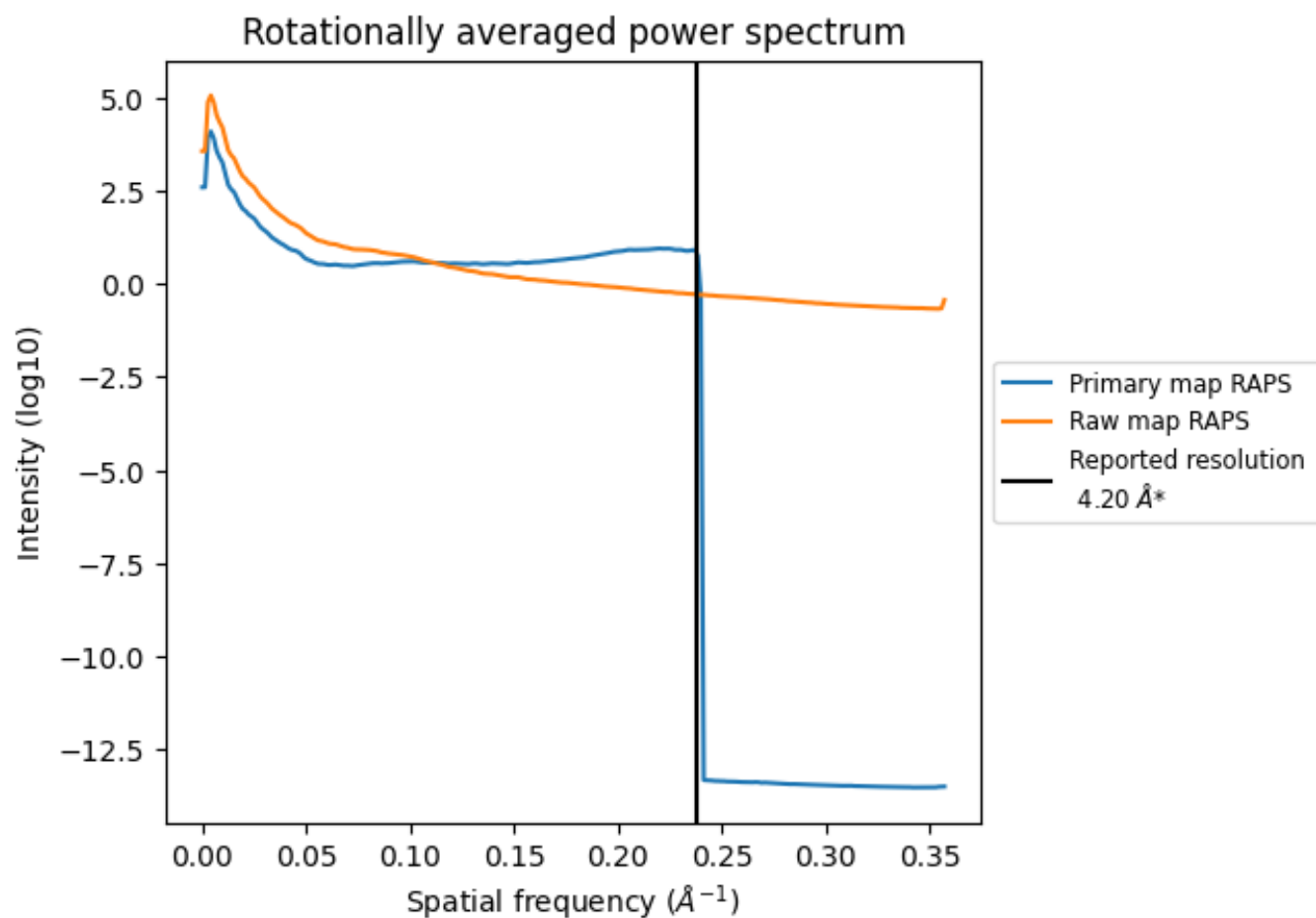


The volume at the recommended contour level is 389  $\text{nm}^3$ ; this corresponds to an approximate mass of 351 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

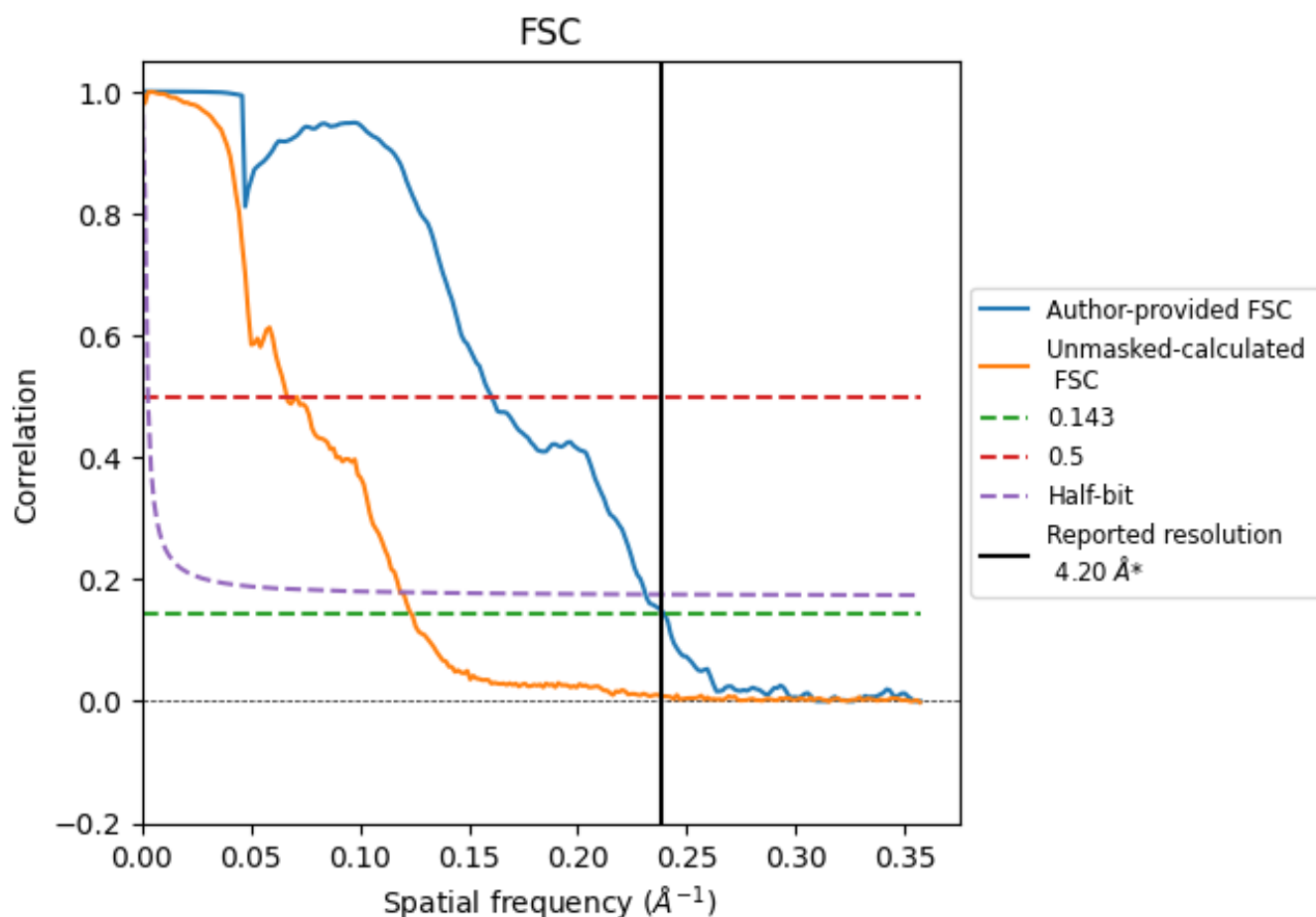


\*Reported resolution corresponds to spatial frequency of 0.238  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.238 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

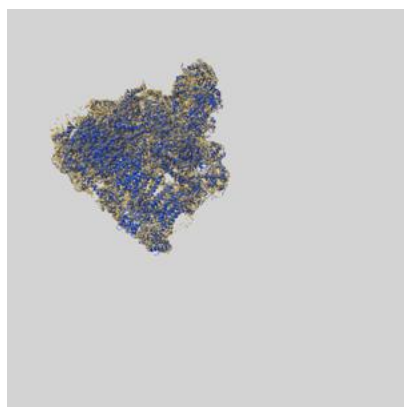
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.17	6.23	4.33
Unmasked-calculated*	8.09	15.06	8.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.09 differs from the reported value 4.2 by more than 10 %

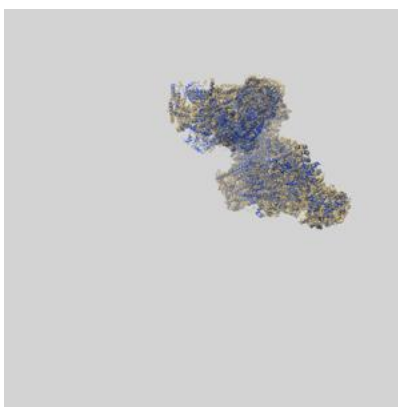
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4494 and PDB model 6QC2. Per-residue inclusion information can be found in section [3](#) on page [22](#).

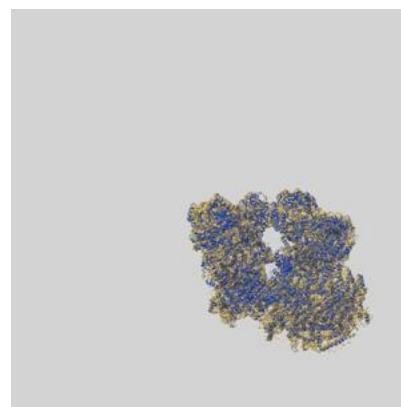
### 9.1 Map-model overlay [i](#)



X



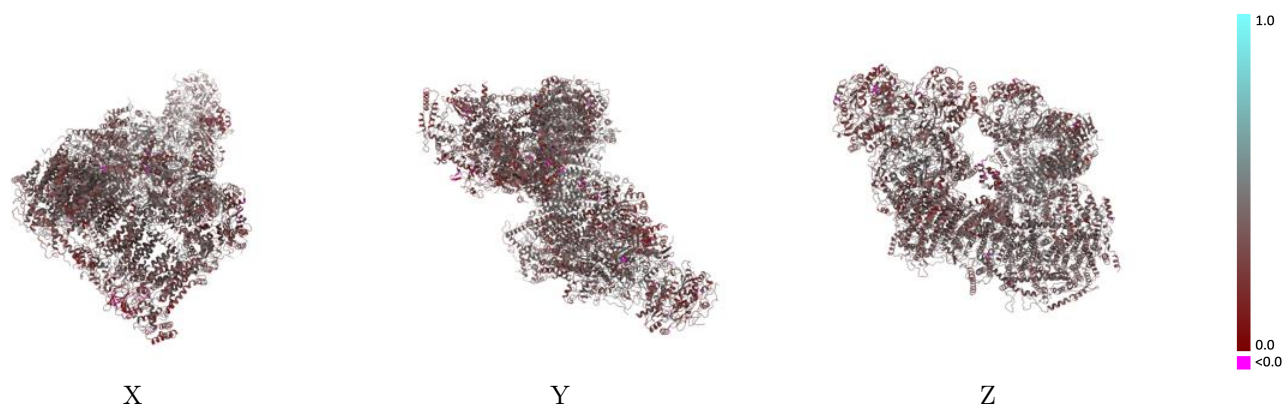
Y



Z

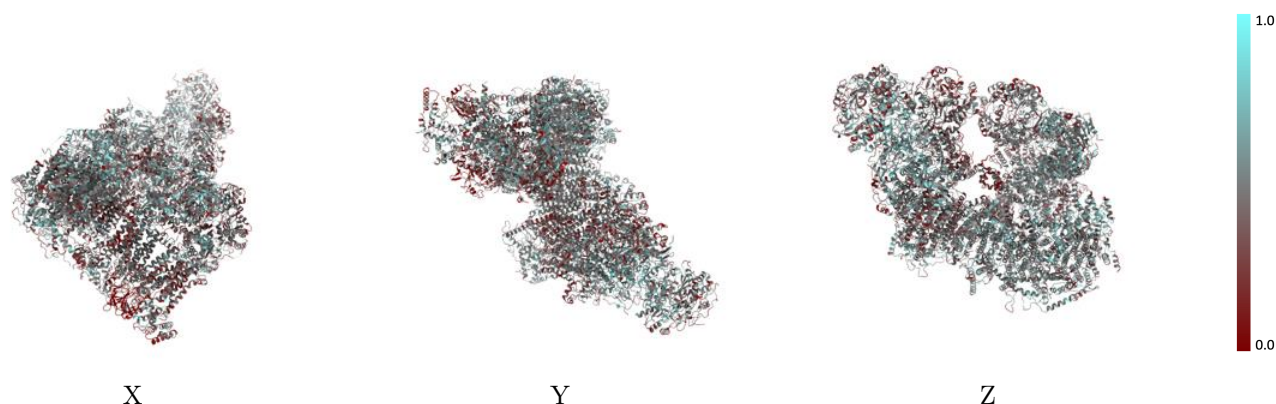
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



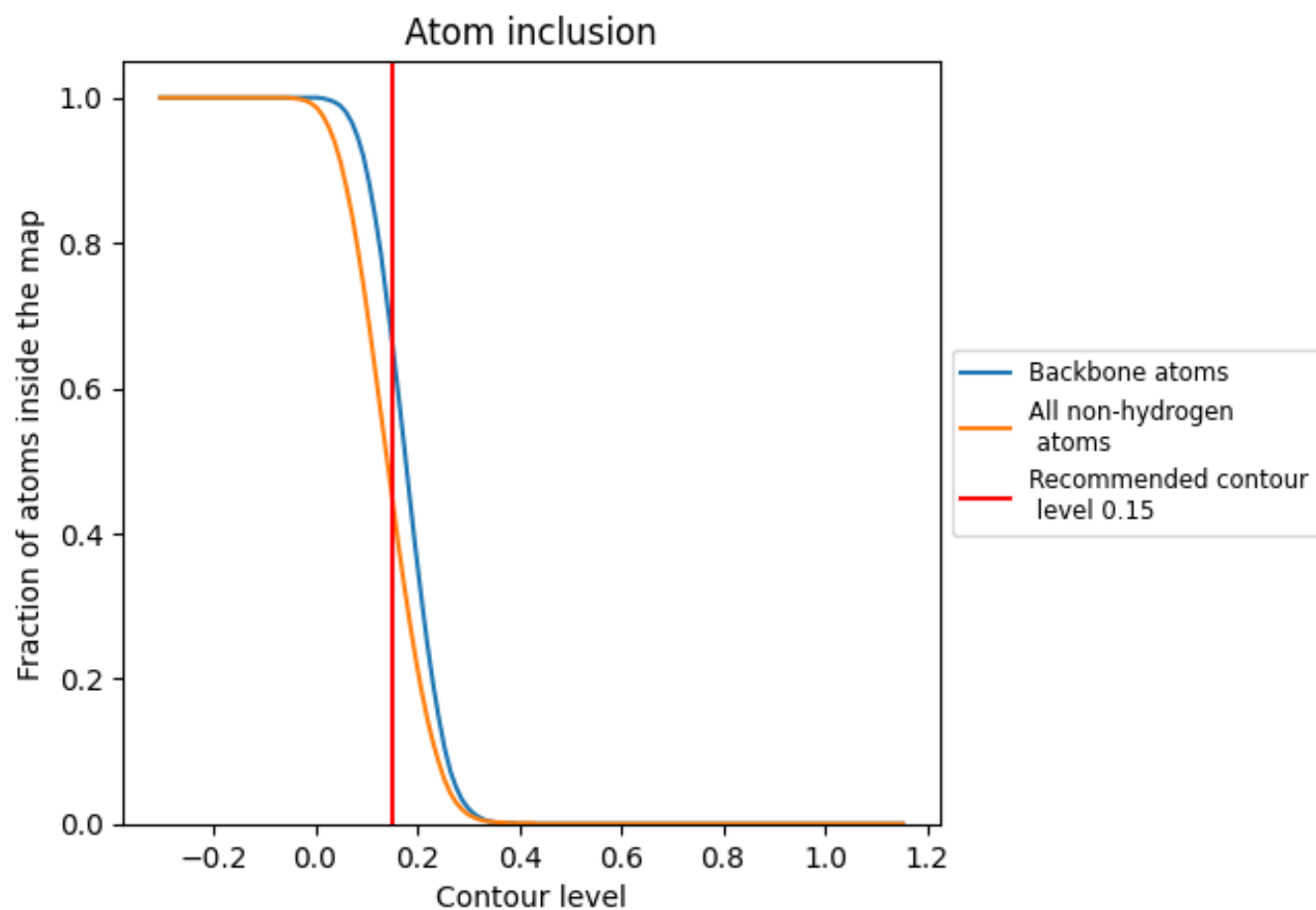
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 67% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ































































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4530	0.3600
4L	0.4300	0.3770
A1	0.4910	0.3620
A2	0.4100	0.3080
A3	0.4390	0.3380
A5	0.4390	0.3260
A6	0.3780	0.3480
A7	0.3460	0.3720
A8	0.5110	0.3660
A9	0.3500	0.3480
AA	0.2110	0.2710
AB	0.5030	0.3740
AJ	0.4960	0.3740
AK	0.4010	0.3630
AL	0.4010	0.3690
AM	0.5190	0.3570
B1	0.4610	0.3890
B2	0.4820	0.3600
B3	0.4800	0.3520
B4	0.4950	0.3840
B5	0.5450	0.3910
B6	0.4940	0.3620
B7	0.4640	0.3030
B8	0.4890	0.3790
B9	0.5790	0.3880
BJ	0.5210	0.3600
BK	0.4630	0.3570
C1	0.4970	0.3620
C2	0.5180	0.3840
D1	0.4390	0.3660
D2	0.5070	0.4000
D3	0.3800	0.3470
D4	0.4990	0.4000
D5	0.4720	0.3790
D6	0.3590	0.3540



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
S1	 0.4440	 0.3450
S2	 0.5020	 0.3910
S3	 0.5150	 0.3880
S4	 0.4390	 0.3810
S5	 0.5060	 0.3610
S6	 0.4890	 0.3840
S7	 0.5320	 0.3870
S8	 0.5710	 0.3950
V1	 0.4700	 0.3270
V2	 0.4550	 0.3260
V3	 0.4550	 0.3090
a1	 0.4380	 0.3370
a2	 0.3920	 0.3360
a3	 0.5230	 0.3900
a4	 0.4900	 0.3670
b1	 0.4550	 0.3710
b2	 0.4750	 0.3810
c1	 0.4470	 0.3510
c2	 0.4730	 0.3720
d1	 0.4860	 0.3670
d2	 0.4650	 0.3710
f1	 0.1300	 0.2700
f2	 0.1360	 0.2640
h1	 0.3060	 0.2590
h2	 0.3400	 0.2690
i1	 0.3220	 0.2930
i2	 0.3300	 0.3570
q1	 0.3970	 0.3240
q2	 0.4610	 0.3880
x1	 0.1950	 0.3380
x2	 0.3000	 0.3960