Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:14 pm GMT

PDB ID	:	6QC4
EMDB ID	:	EMD-4496
Title	:	Ovine respiratory supercomplex I+III2 open class 3
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-26
Resolution	:	4.60 Å(reported)
Based on initial models	:	5LNK, 1PPJ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

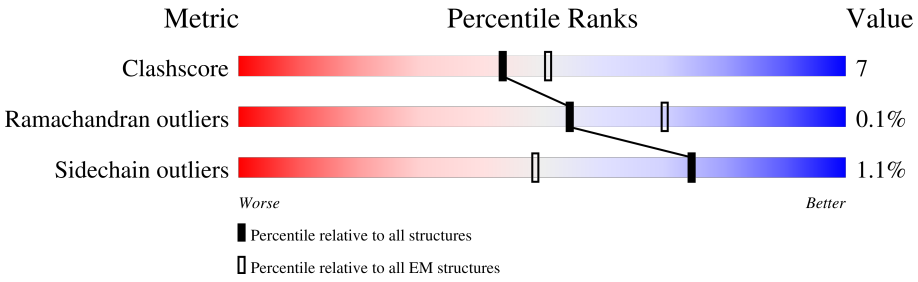
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	a1	446	26% 97%
1	a3	446	25% 98%
2	a2	439	25% 93% 6%
2	a4	439	22% 93% 6%
3	b1	379	33% 99%
3	b2	379	39% 99%
4	c1	240	26% 98%
4	c2	240	30% 98%

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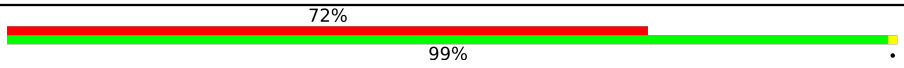
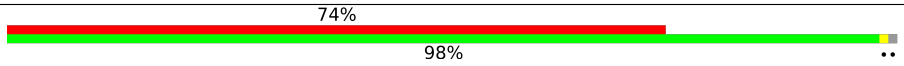
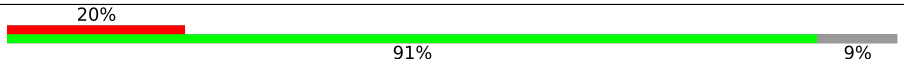
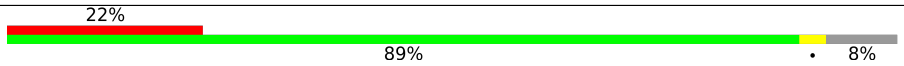
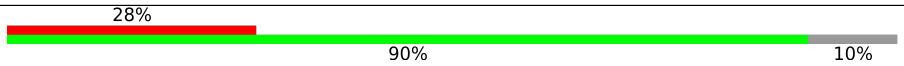
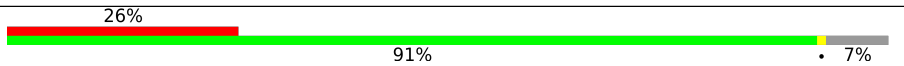
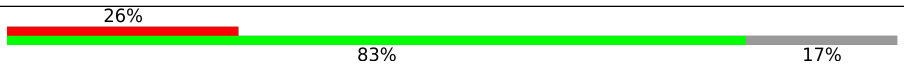
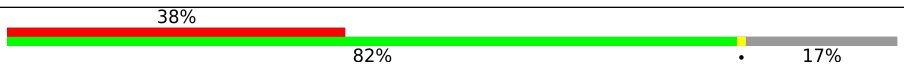
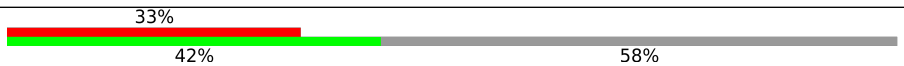
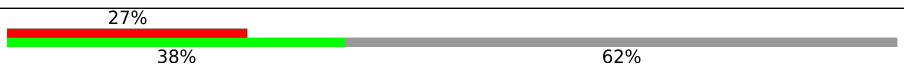
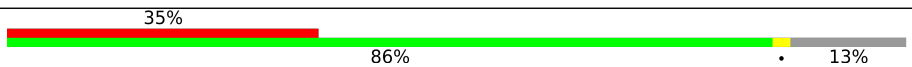
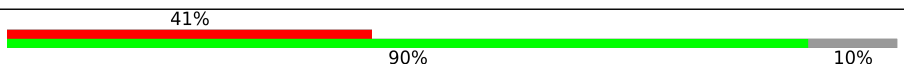
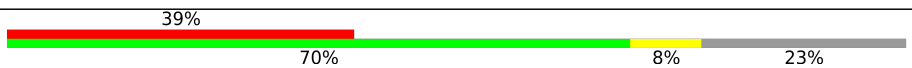
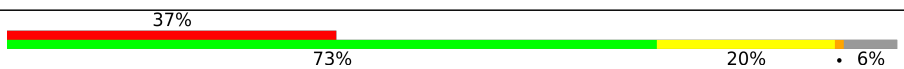
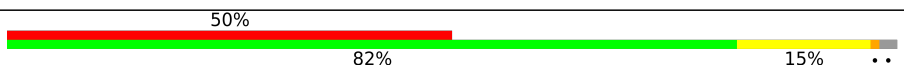
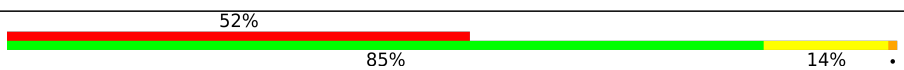
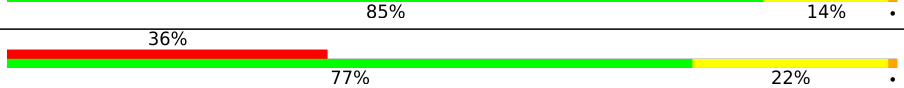
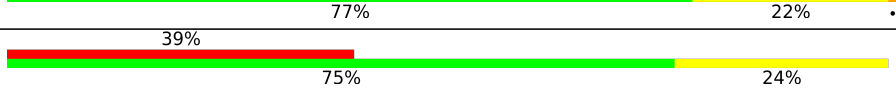
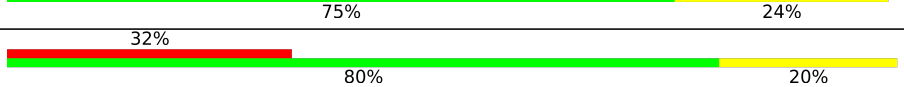
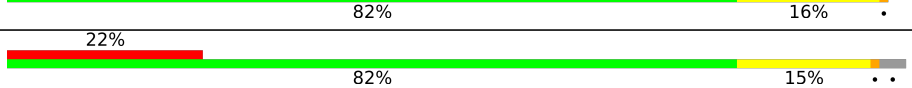
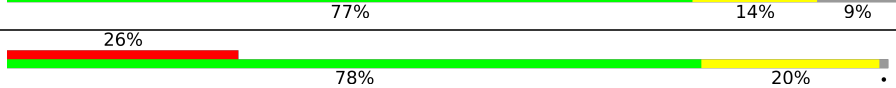
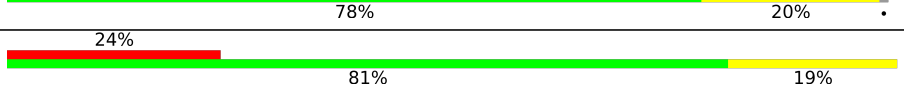
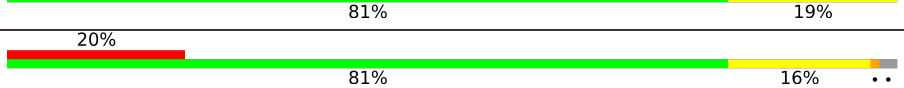
Mol	Chain	Length	Quality of chain
5	f1	196	
5	f2	196	
6	d1	110	
6	d2	110	
7	q1	81	
7	q2	81	
8	h1	78	
8	h2	78	
9	x1	78	
9	x2	78	
10	i1	63	
10	i2	63	
11	D3	115	
12	D1	318	
13	D6	175	
14	4L	98	
15	D5	606	
16	D4	459	
17	D2	347	
18	AK	140	
19	B5	143	
20	AA	88	
20	AB	88	
21	A8	171	
22	BJ	175	

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Mol	Chain	Length	Quality of chain
23	AJ	320	24% 75% 24%
24	S5	105	21% 77% 16% 6%
25	A3	83	27% 77% 12% 11%
26	B3	97	28% 61% 12% 25%
27	C2	120	28% 82% 16%
28	B4	128	29% 77% 21%
29	AM	143	27% 79% 16%
30	B6	127	19% 57% 17% 24%
31	B7	119	25% 77% 22%
32	B9	178	22% 76% 22%
33	B2	72	24% 69% 19% 10%
34	B8	158	30% 77% 21%
35	BK	125	26% 66% 15% 18%
36	C1	49	20% 80% 14% 6%
37	B1	57	25% 79% 12% 9%
38	A1	70	33% 84% 14%
39	V1	445	24% 73% 23%
40	V2	217	26% 76% 20%
41	S1	704	32% 73% 24%
42	S2	430	29% 76% 22%
43	S3	228	26% 73% 18% 9%
44	S7	179	25% 63% 24% 13%
45	S8	176	18% 76% 23%
46	V3	75	17% 35% 19% 45%
47	S6	96	35% 81% 18%

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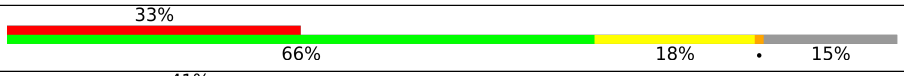
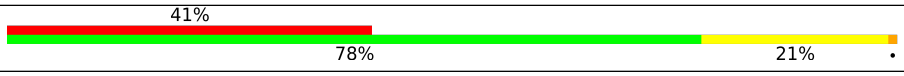
Mol	Chain	Length	Quality of chain
48	S4	133	
49	A9	338	
50	A2	98	
51	A5	115	
52	A6	127	
53	A7	112	
54	AL	145	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 96705 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 UQCRC1.

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c1	238	Total	C	N	O	S	0	0
			1902	1214	329	344	15		
4	c2	238	Total	C	N	O	S	0	0
			1903	1216	329	343	15		

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

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

- Molecule 6 is a protein called UQCRB.

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

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

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

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

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

- Molecule 9 is a protein called UQCRFS1N.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	x1	33	Total	C	N	O	0	0
			164	98	33	33		
9	x2	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i1	55	Total	C	N	O	0	0
			459	303	80	76		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	i2	57	Total 473	C 312	N 82	O 79	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D3	89	Total 719	C 495	N 101	O 118	S 5	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D1	298	Total 2372	C 1605	N 360	O 388	S 19	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D6	171	Total 1308	C 878	N 187	O 230	S 13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4L	98	Total 748	C 489	N 112	O 132	S 15	0	0

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 18 is a protein called NDUFA11.

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

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 20 is a protein called Acyl carrier protein.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 22 is a protein called NDUFB10.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 29 is a protein called NDUFA13.

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

- Molecule 30 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B6	96	Total	C	N	O	S	0	0
			809	533	136	139	1		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B2	65	Total	C	N	O	S	0	0
			560	371	93	95	1		

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

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

- Molecule 35 is a protein called NDUFB11.

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

- Molecule 36 is a protein called NDUFC1.

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

- Molecule 37 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	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 38 is a protein called NDUFA1.

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

- 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 NDUFS2.

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	288	Total	C	N	O	S	0	0
			2270	1451	409	405	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 NDUFA5.

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		

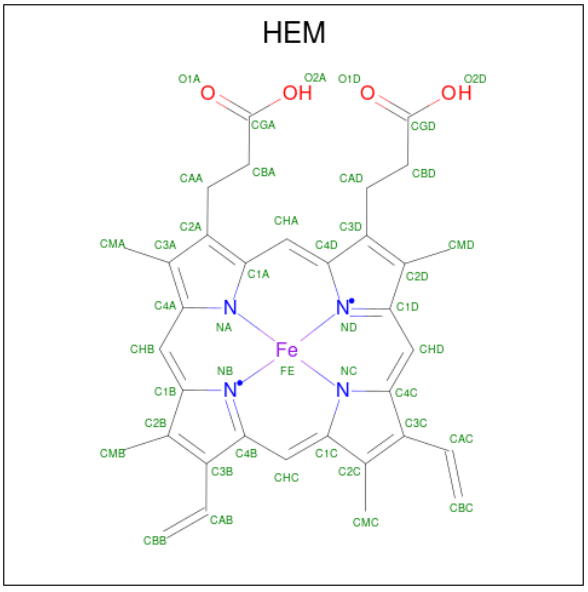
- Molecule 53 is a protein called NDUFA7.

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.

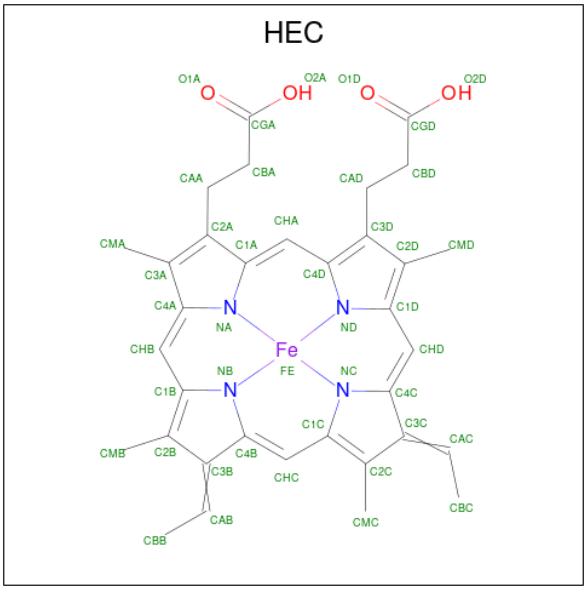
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AL	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 55 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



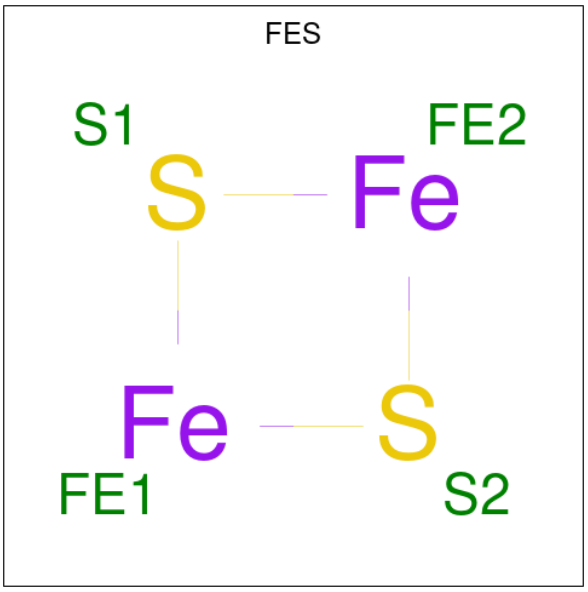
Mol	Chain	Residues	Atoms					AltConf
55	b1	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
55	b1	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
55	b2	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
55	b2	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 56 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



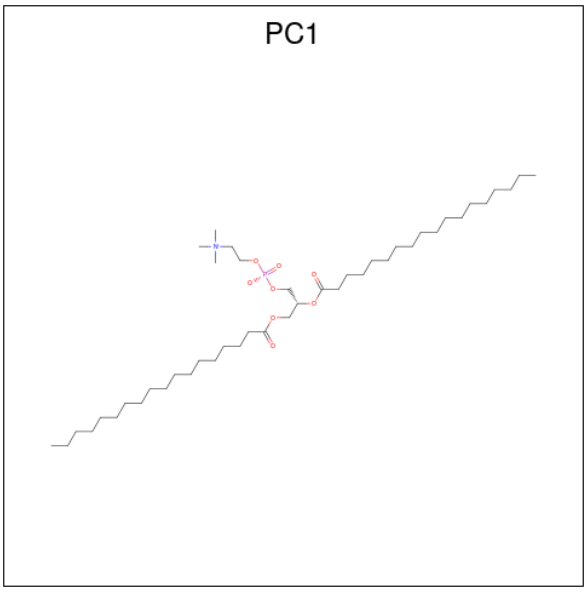
Mol	Chain	Residues	Atoms					AltConf
56	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



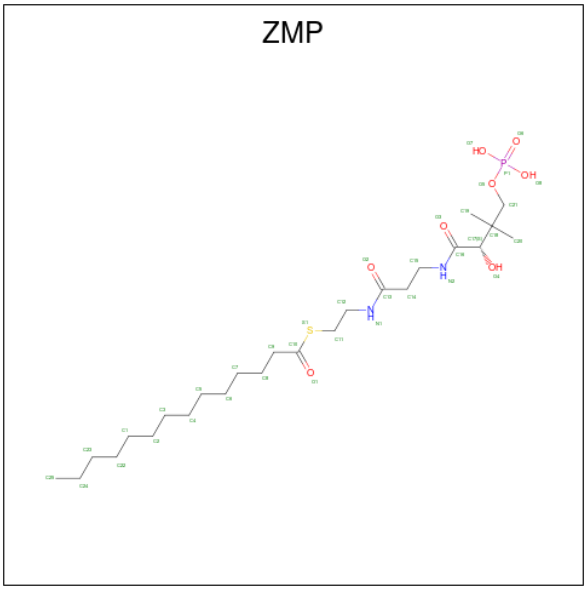
Mol	Chain	Residues	Atoms	AltConf
57	f1	1	Total Fe S 4 2 2	0
57	f2	1	Total Fe S 4 2 2	0
57	V2	1	Total Fe S 4 2 2	0
57	S1	1	Total Fe S 4 2 2	0

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



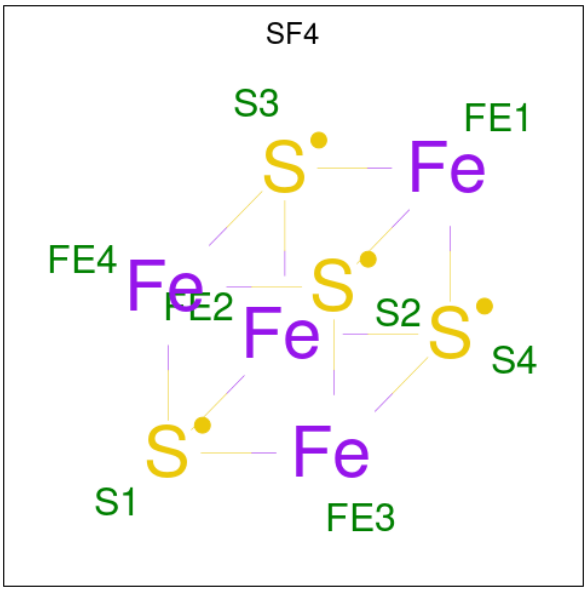
Mol	Chain	Residues	Atoms					AltConf
58	D2	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 59 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



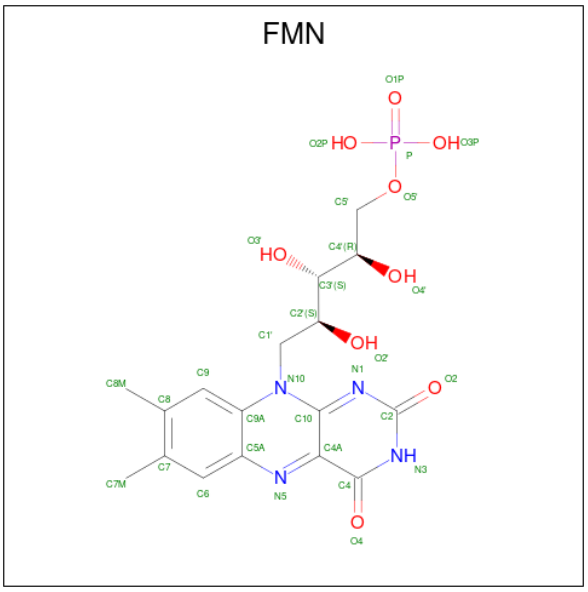
Mol	Chain	Residues	Atoms						AltConf
59	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
59	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
60	V1	1	Total Fe S 8 4 4	0
60	S1	1	Total Fe S 16 8 8	0
60	S1	1	Total Fe S 16 8 8	0
60	S7	1	Total Fe S 8 4 4	0
60	S8	1	Total Fe S 16 8 8	0
60	S8	1	Total Fe S 16 8 8	0

- Molecule 61 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

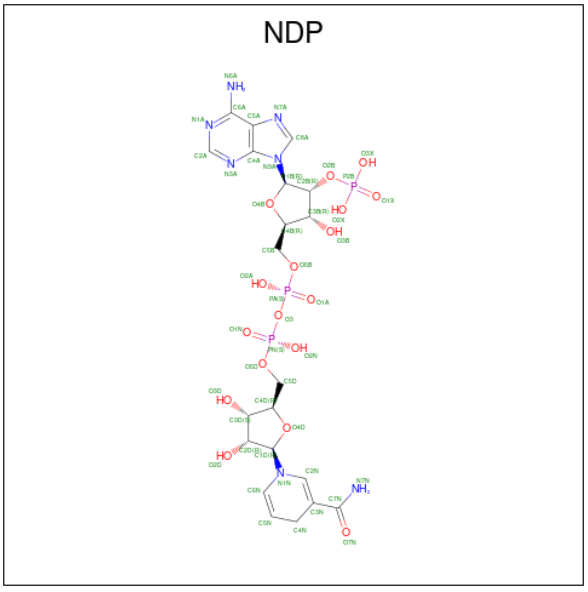


Mol	Chain	Residues	Atoms					AltConf
61	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	S6	1	Total	Zn	0
			1	1	

- Molecule 63 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



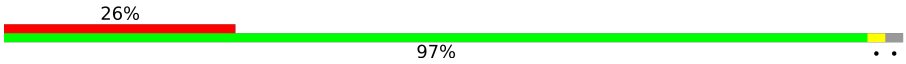
Mol	Chain	Residues	Atoms					AltConf
63	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

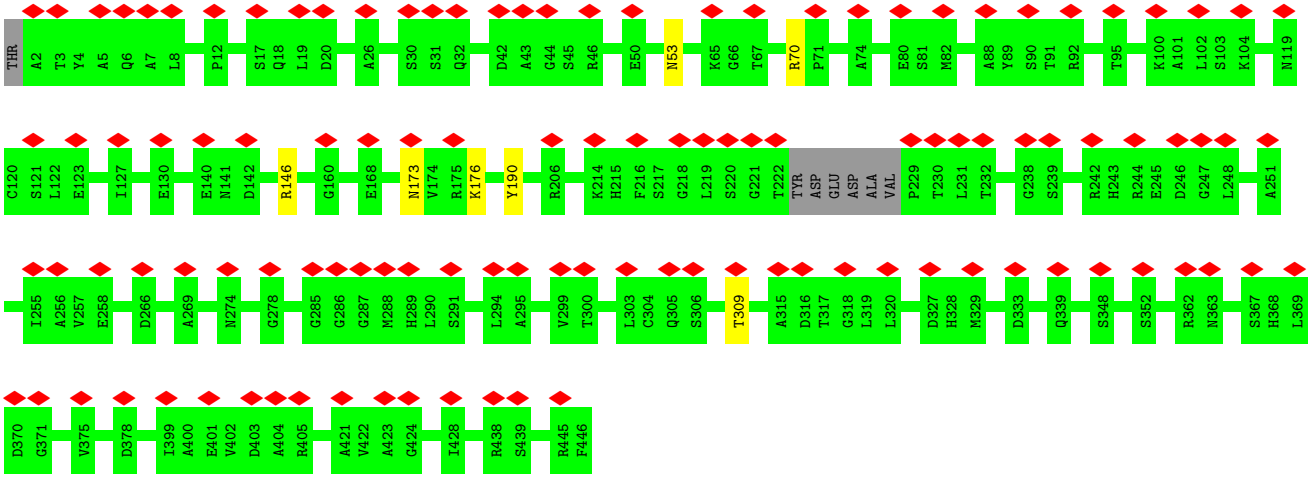
3 Residue-property plots (i)

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

• Molecule 1: UQCRC1

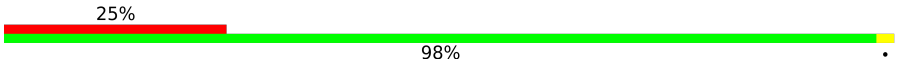
Chain a1:

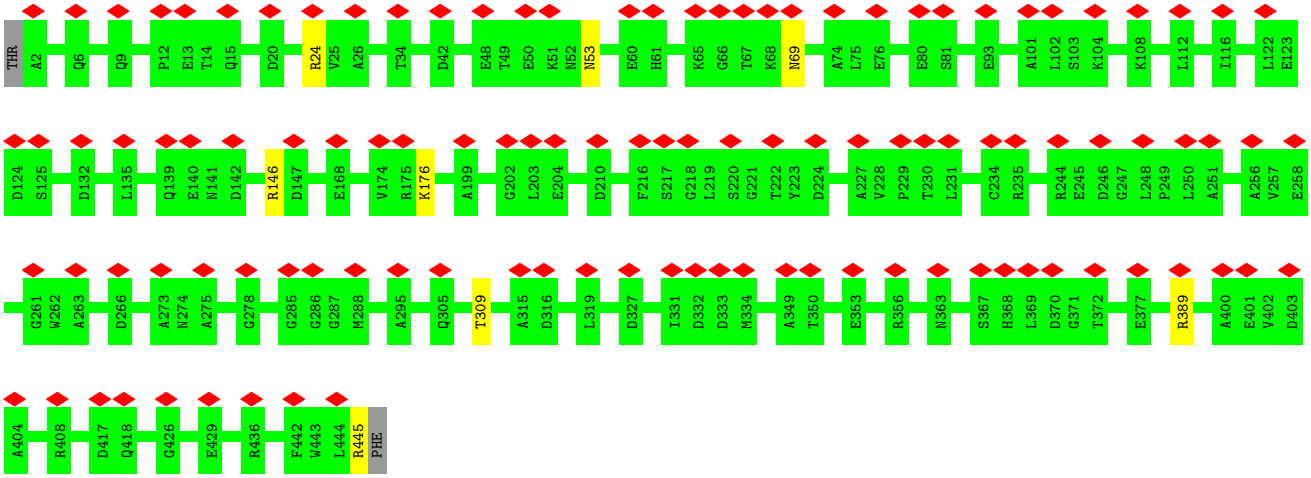




• Molecule 1: UQCRC1

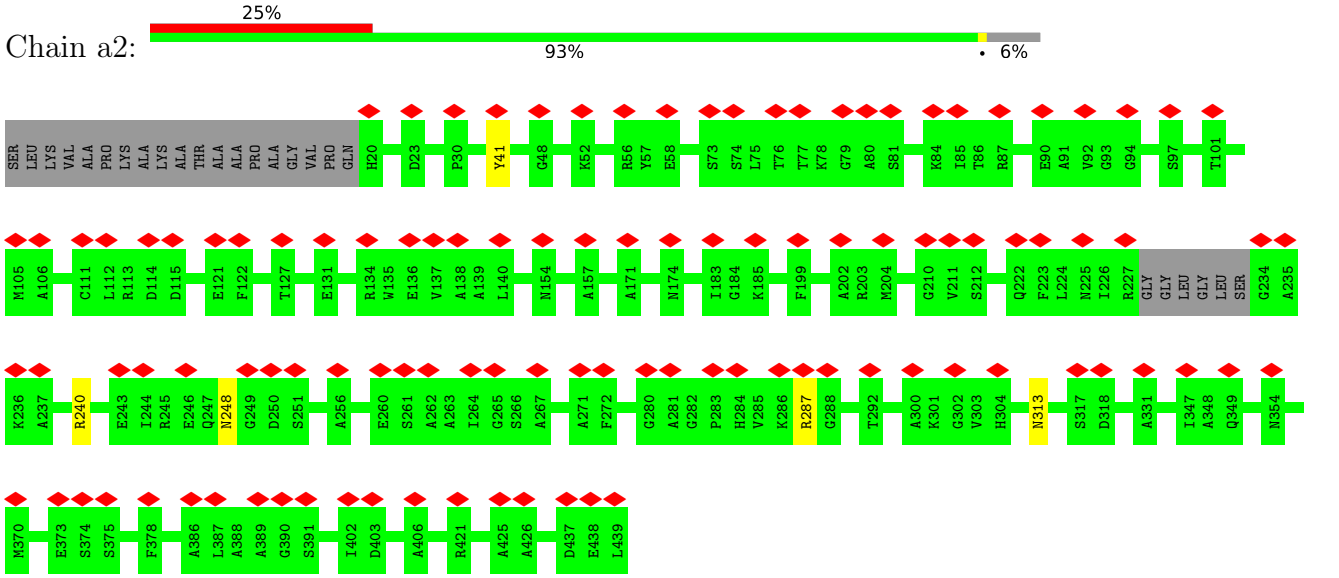
Chain a3:





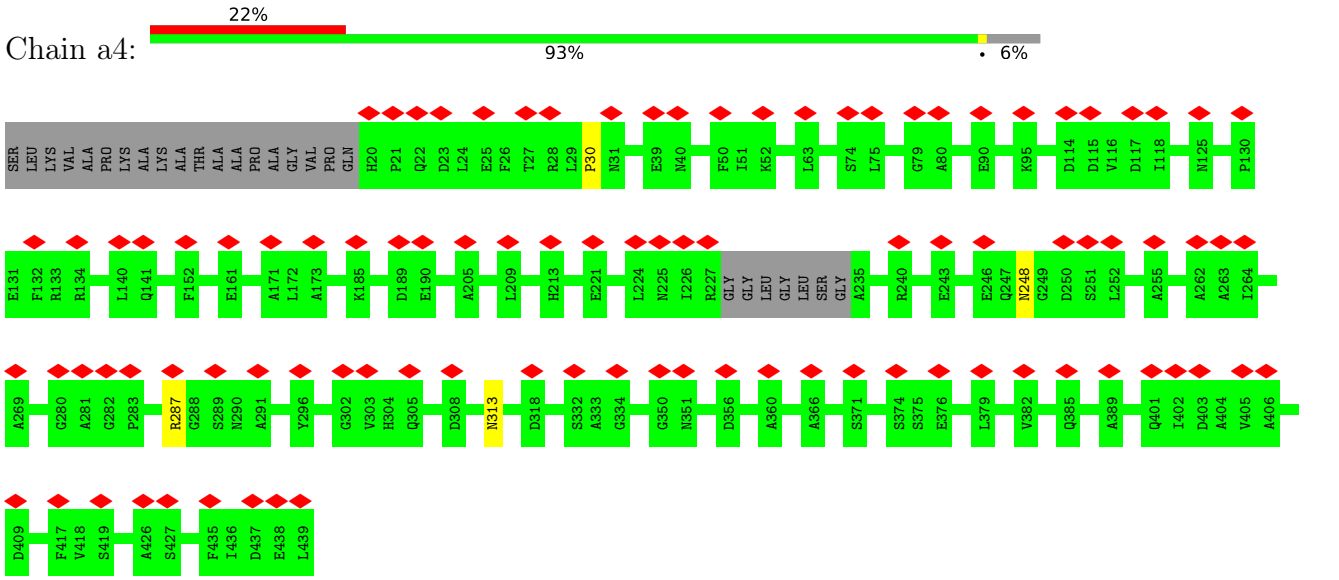
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

Chain a2:



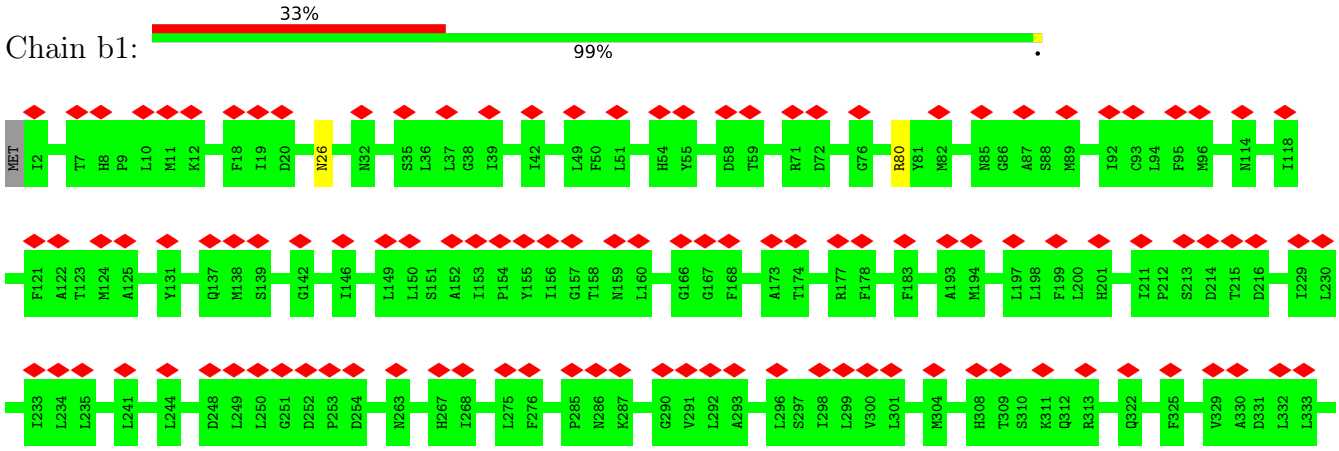
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

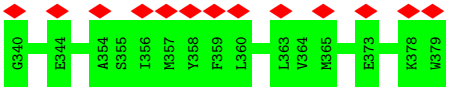
Chain a4:



• Molecule 3: Cytochrome b

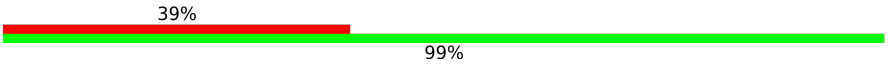
Chain b1:

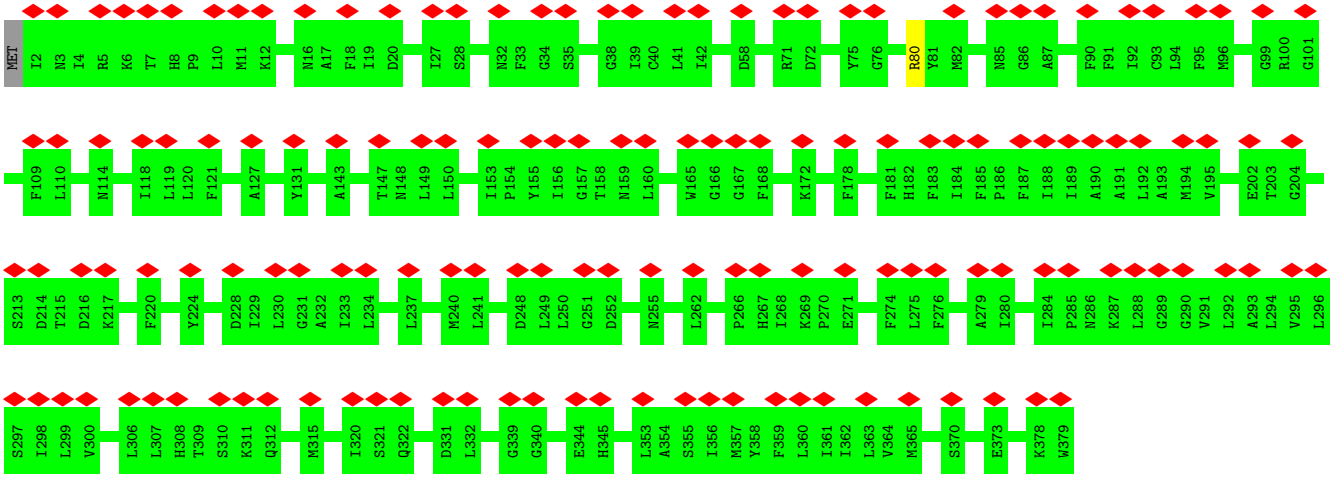




• Molecule 3: Cytochrome b

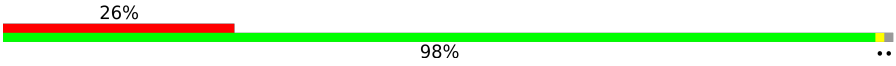
Chain b2:

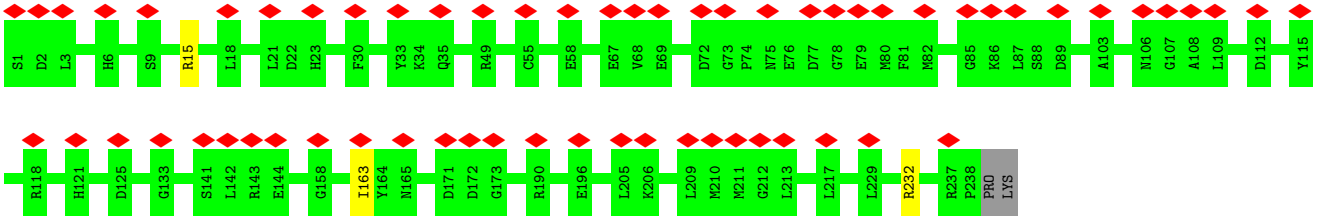




• Molecule 4: Cytochrome c1

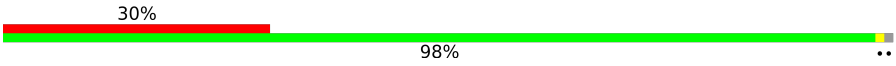
Chain c1:

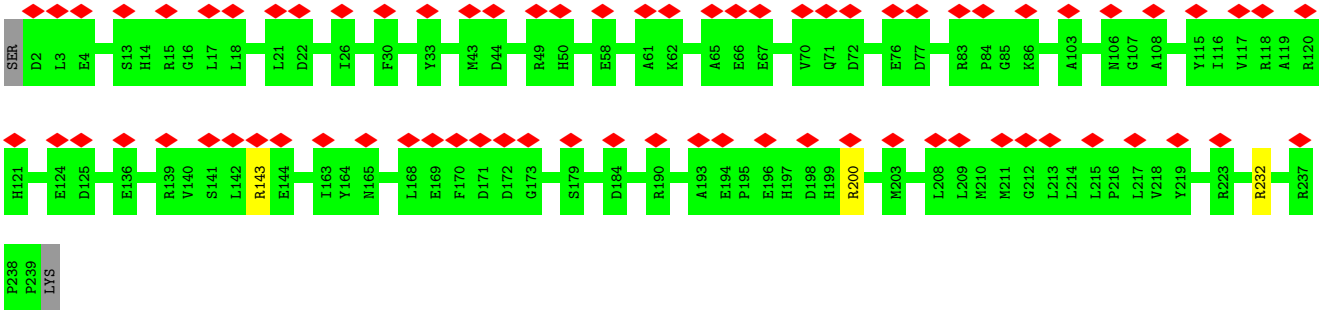




• Molecule 4: Cytochrome c1

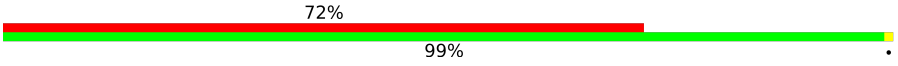
Chain c2:

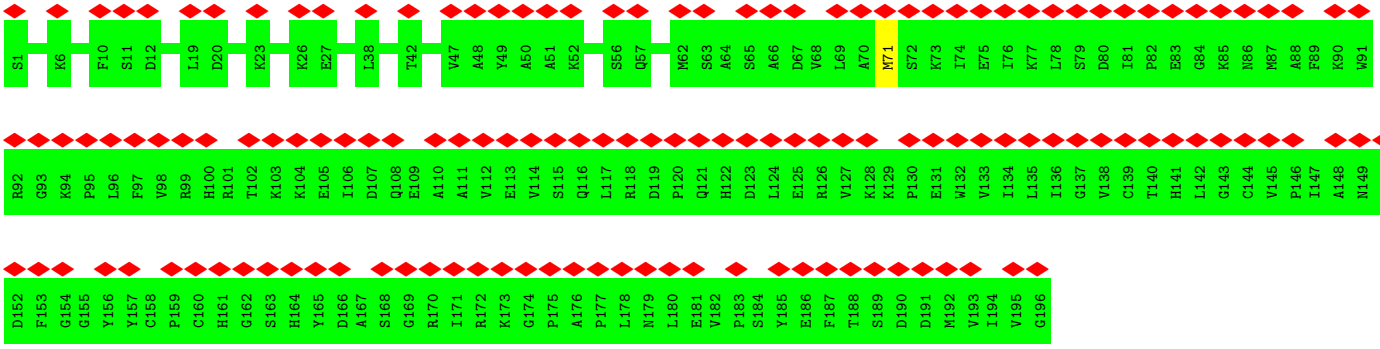




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

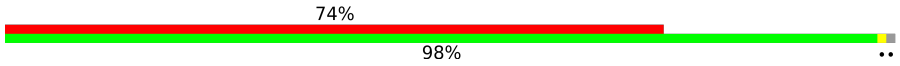
Chain f1:

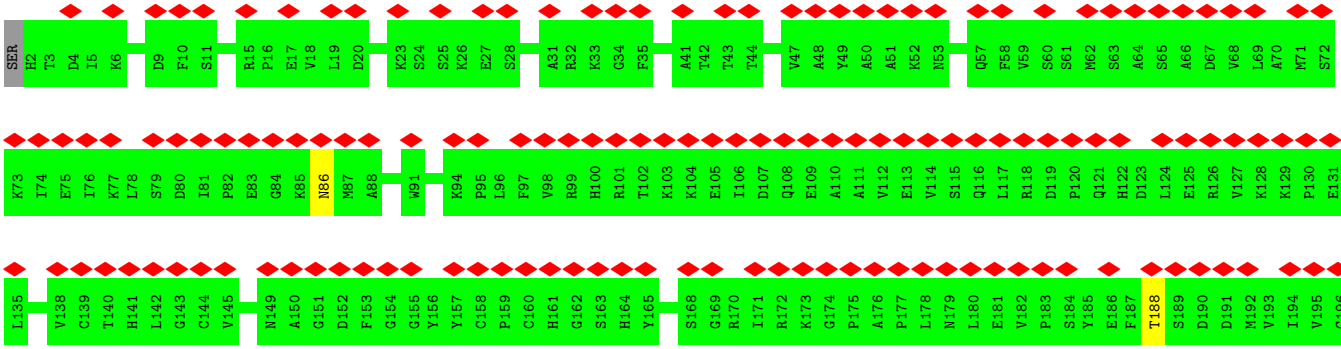




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

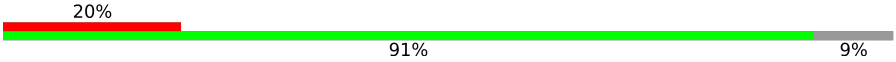
Chain f2:

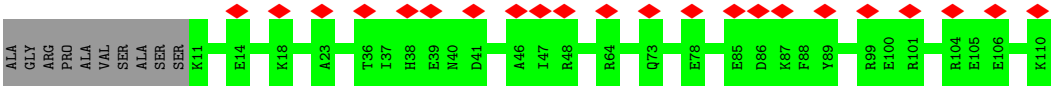




• Molecule 6: UQCRB

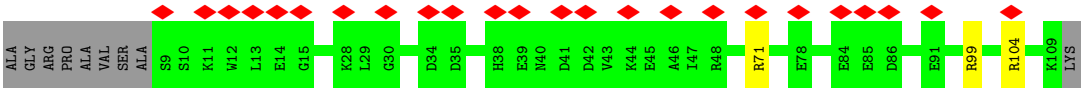
Chain d1:





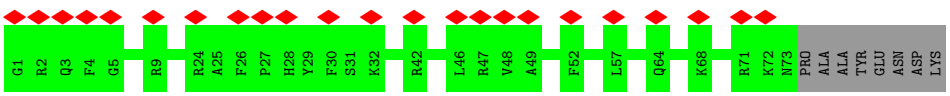
• Molecule 6: UQCRB

Chain d2:

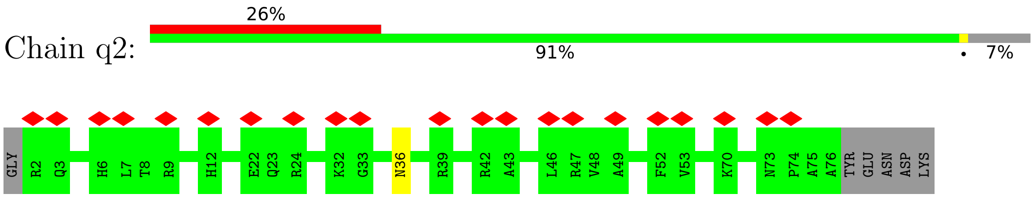


• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII

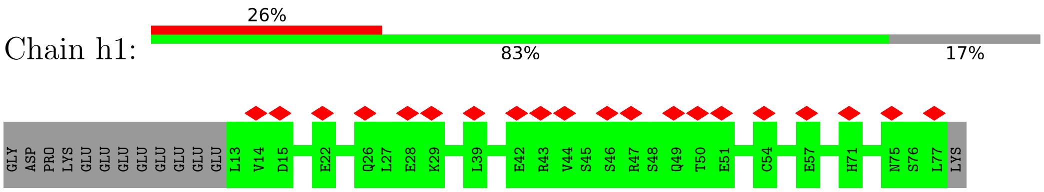
Chain q1:



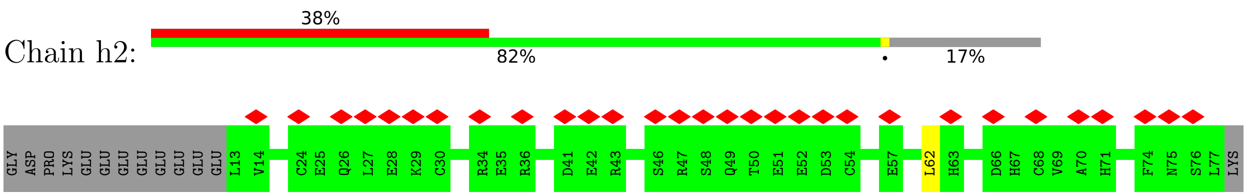
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



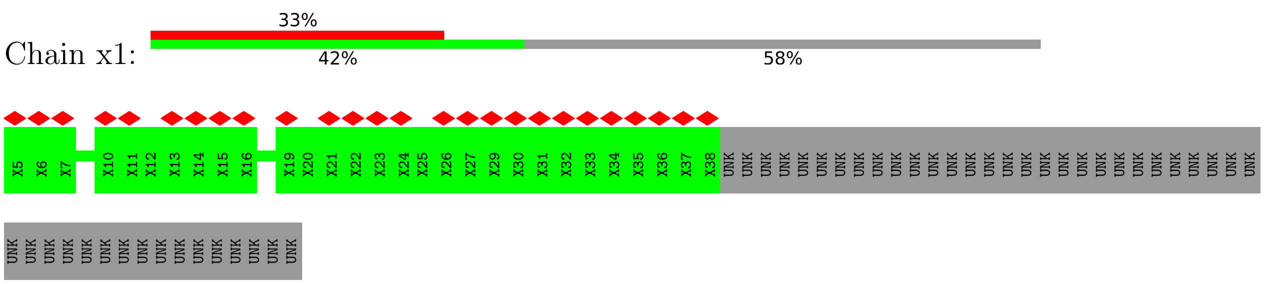
• Molecule 8: Cytochrome b-c1 complex subunit 6



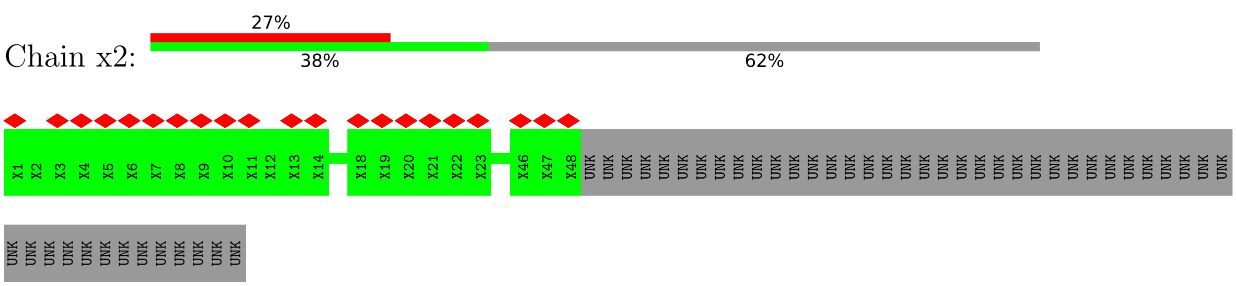
• Molecule 8: Cytochrome b-c1 complex subunit 6



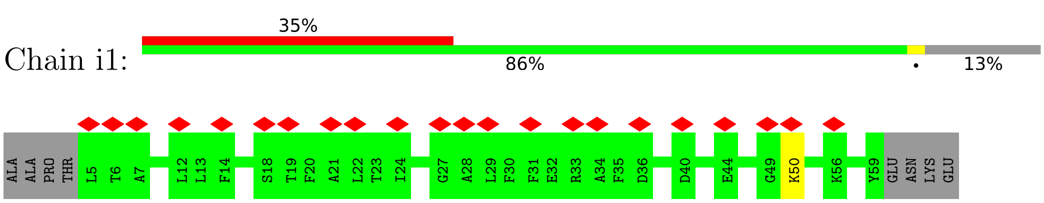
• Molecule 9: UQCRFS1N



• Molecule 9: UQCRFS1N

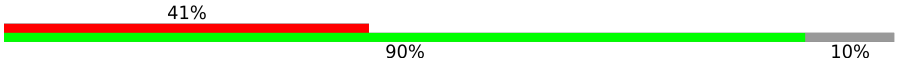


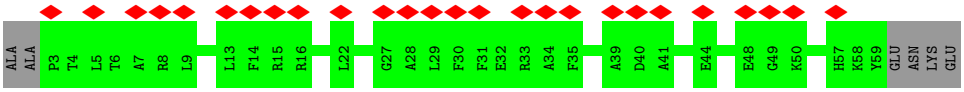
• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X



• Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

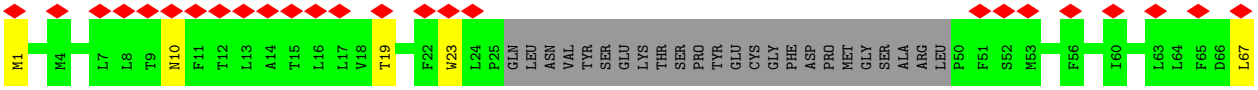
Chain i2:

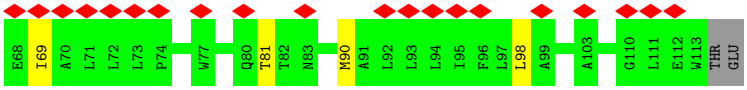




• Molecule 11: NADH-ubiquinone oxidoreductase chain 3

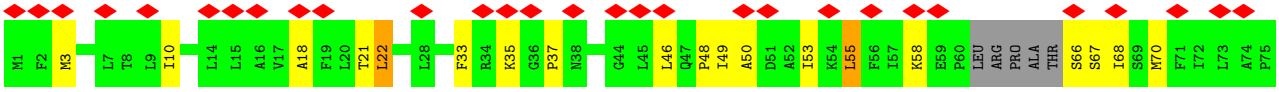
Chain D3:

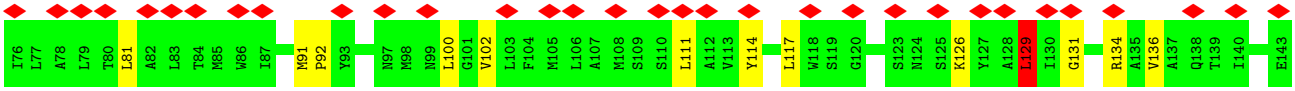


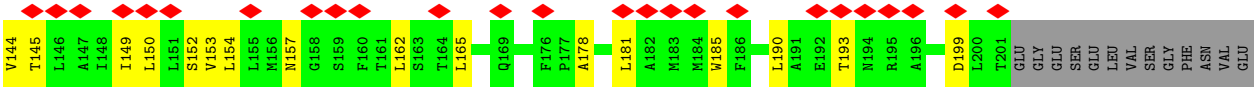


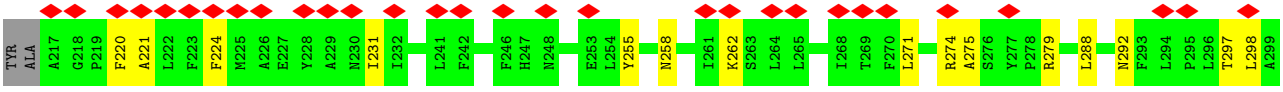
• Molecule 12: NADH-ubiquinone oxidoreductase chain 1

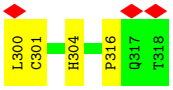
Chain D1:





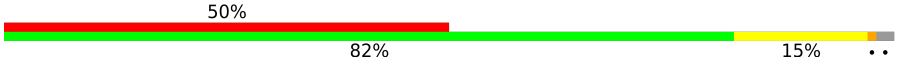


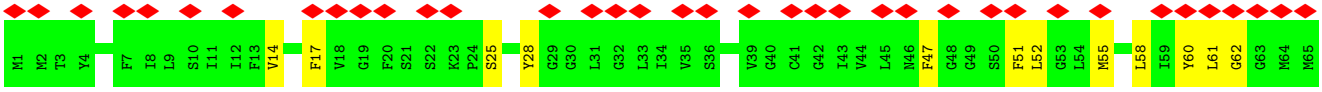


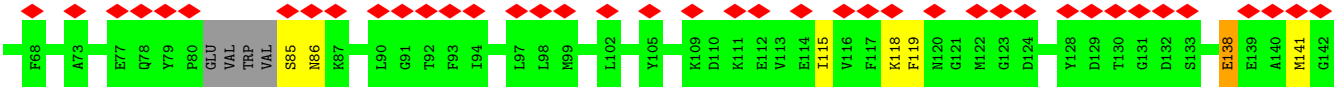


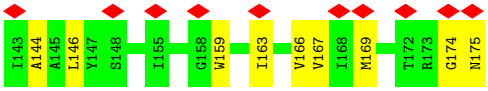
• Molecule 13: NADH-ubiquinone oxidoreductase chain 6

Chain D6:



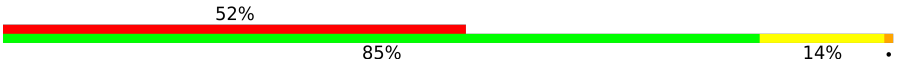


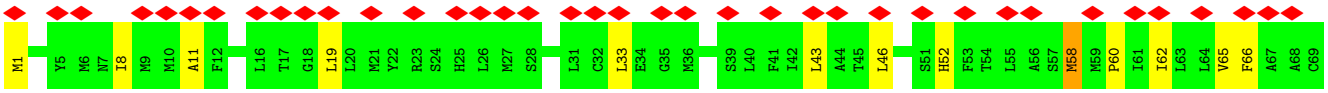


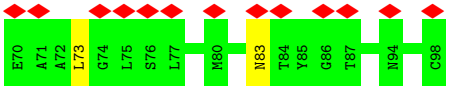


• Molecule 14: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:

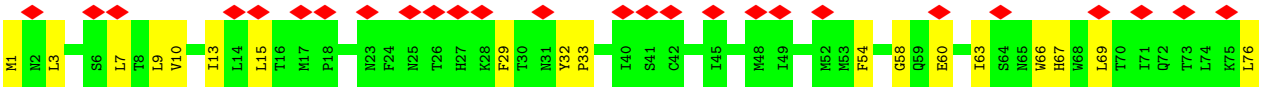


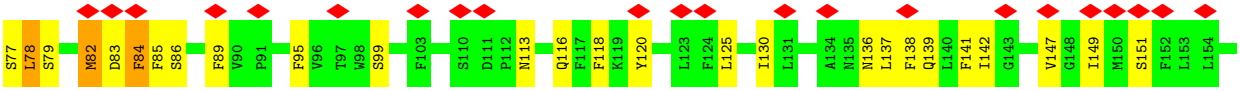


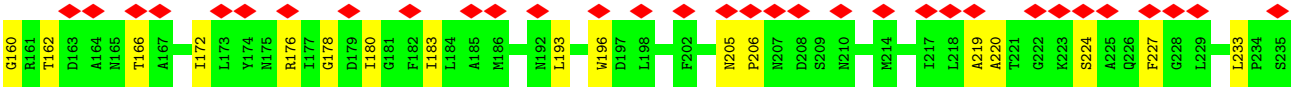


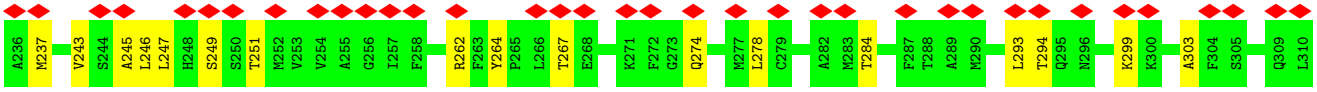
• Molecule 15: NADH-ubiquinone oxidoreductase chain 5

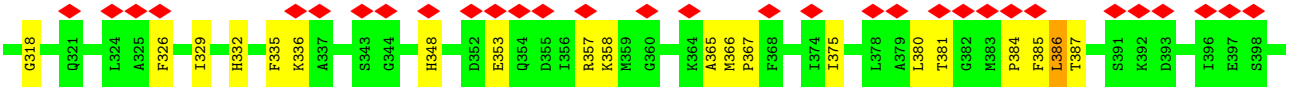
Chain D5:

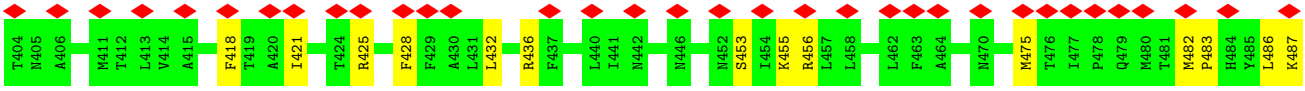


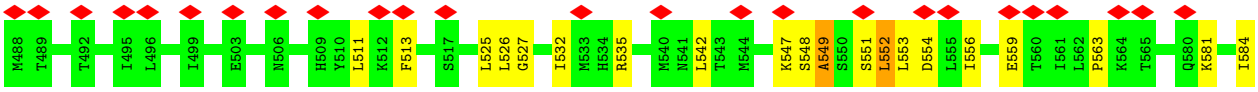


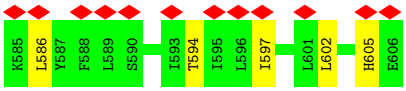






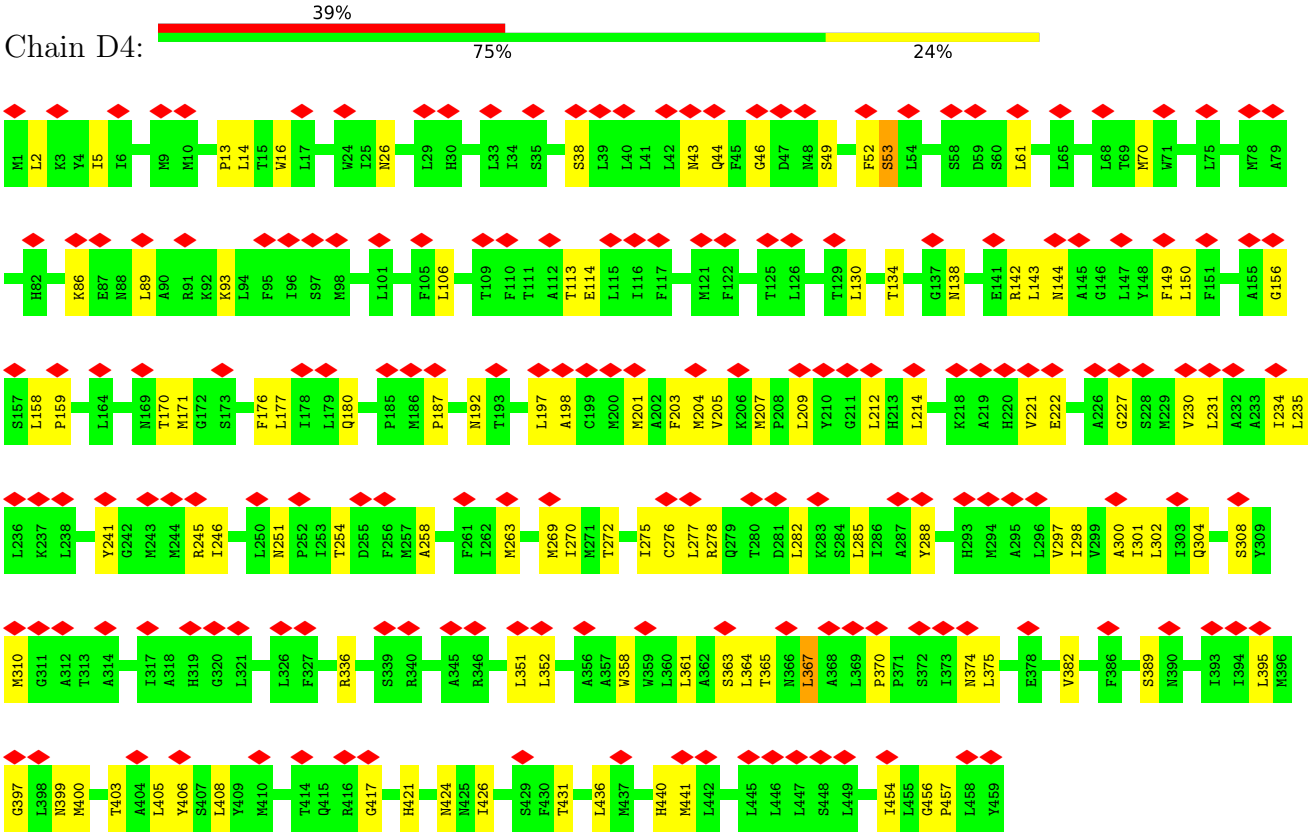






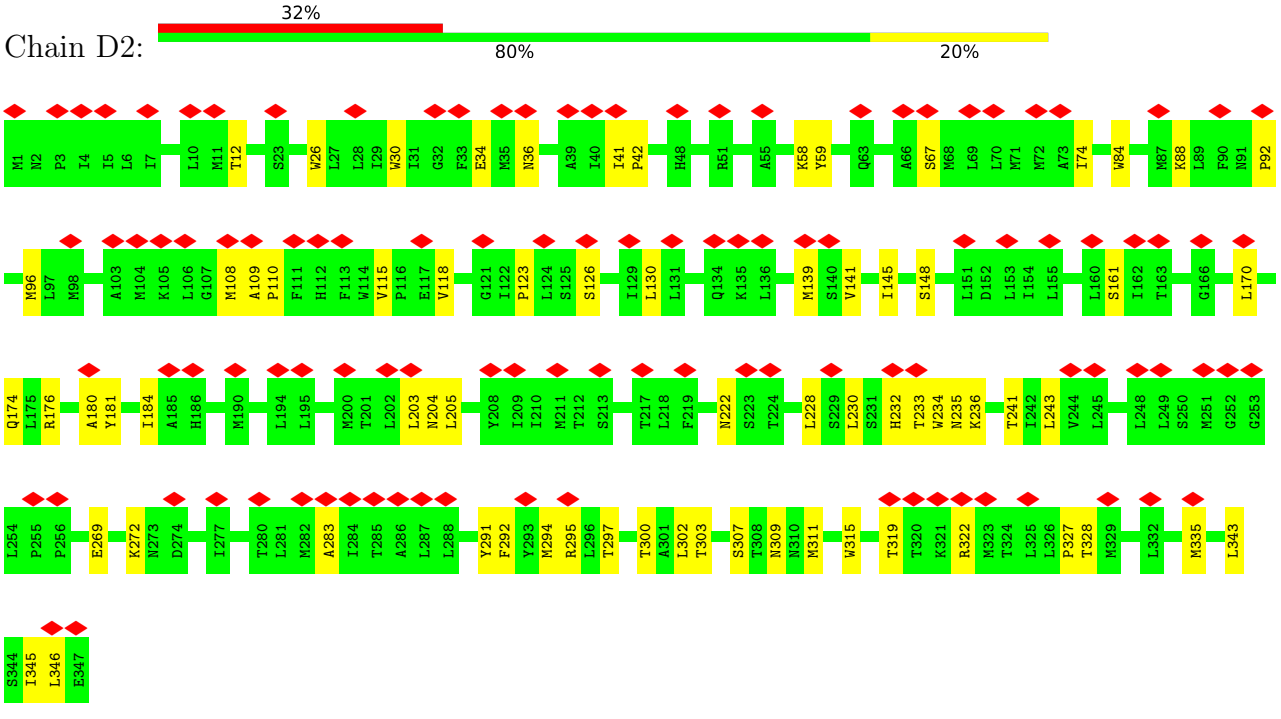
• Molecule 16: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



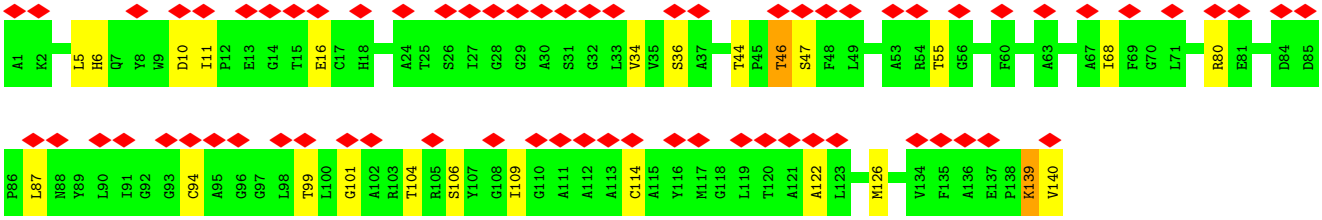
• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain D2:

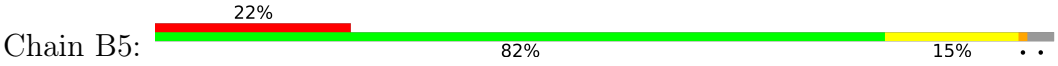


• Molecule 18: NDUFA11

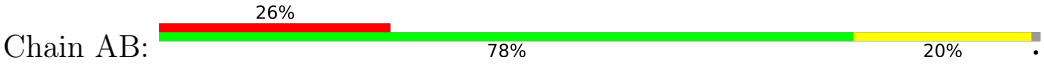
Chain AK:



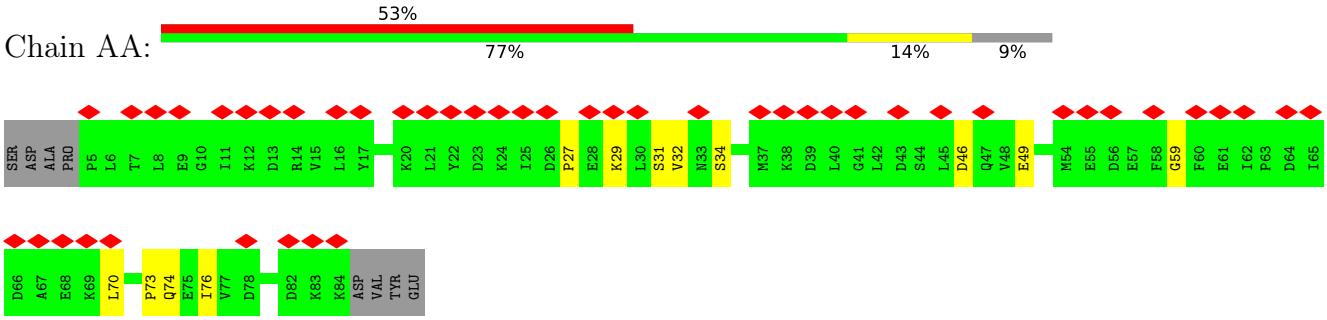
• Molecule 19: NADH:ubiquinone oxidoreductase subunit B5



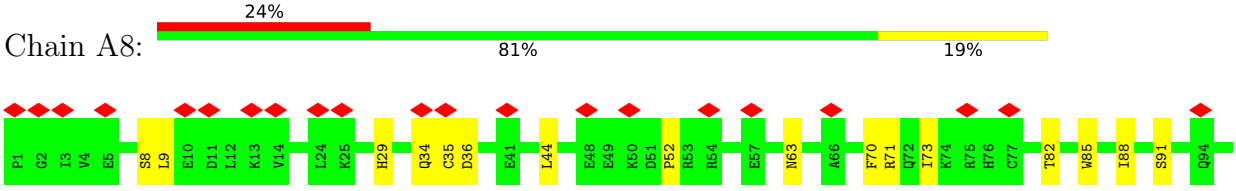
• Molecule 20: Acyl carrier protein

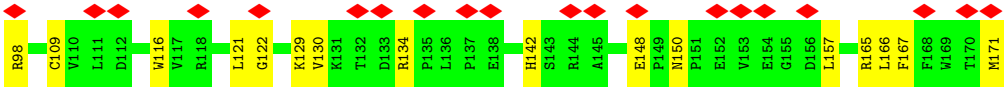


• Molecule 20: Acyl carrier protein



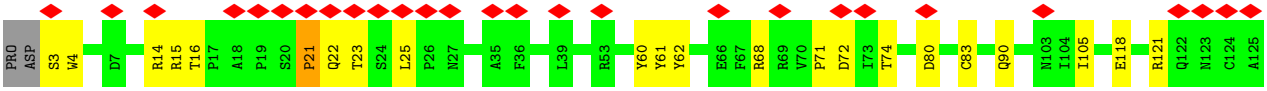
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

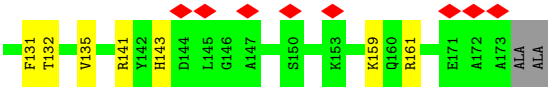




• Molecule 22: NDUFB10

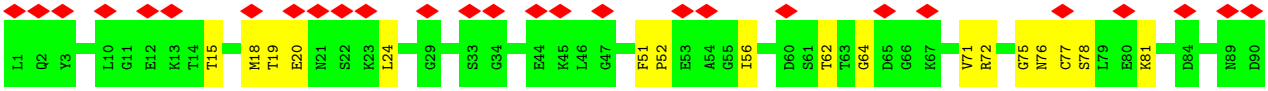
Chain BJ:

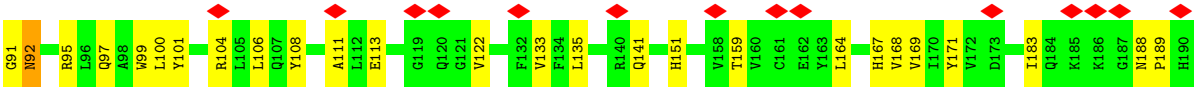


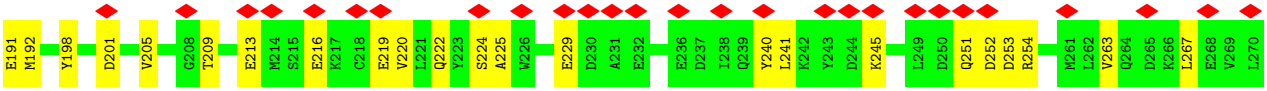


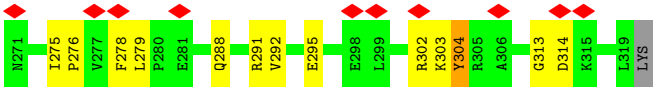
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:



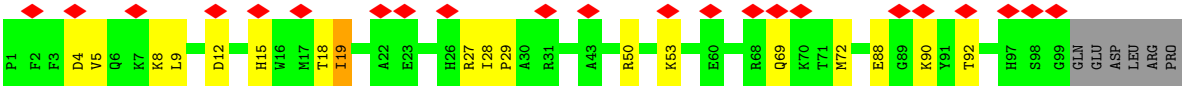






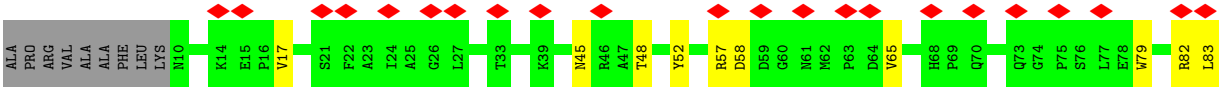
• Molecule 24: NADH:ubiquinone oxidoreductase subunit S5

Chain S5:



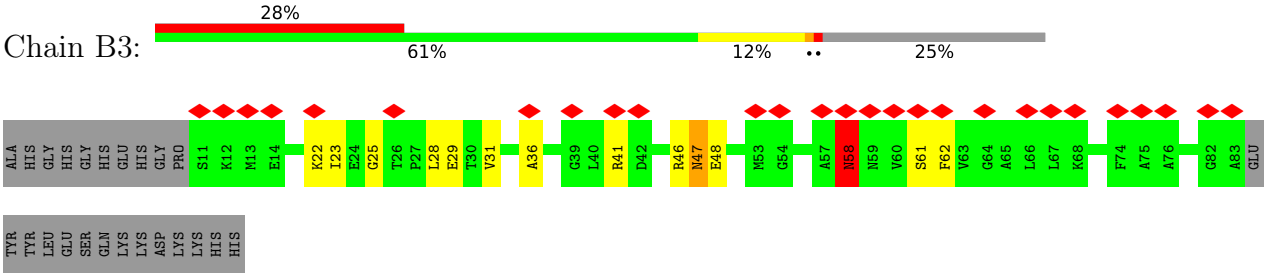
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A3

Chain A3:



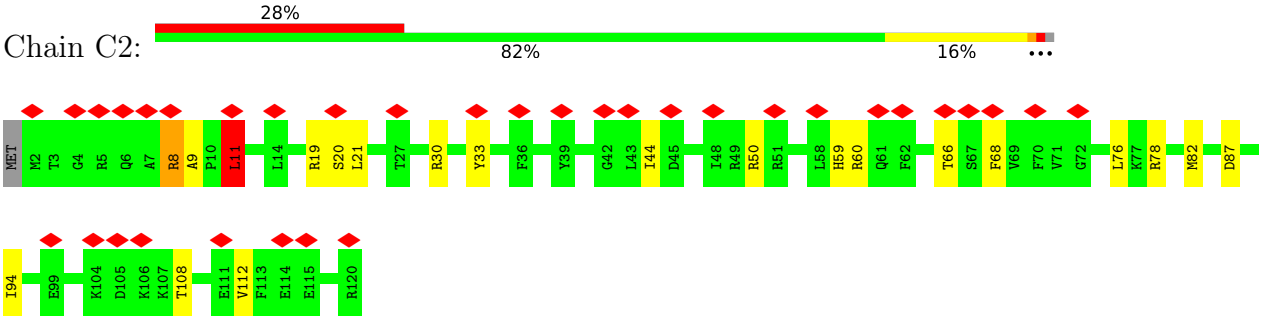
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B3

Chain B3:



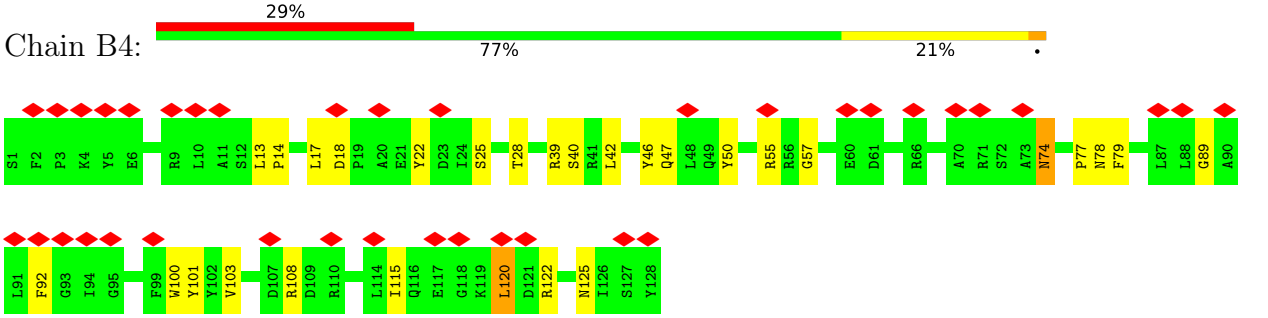
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:



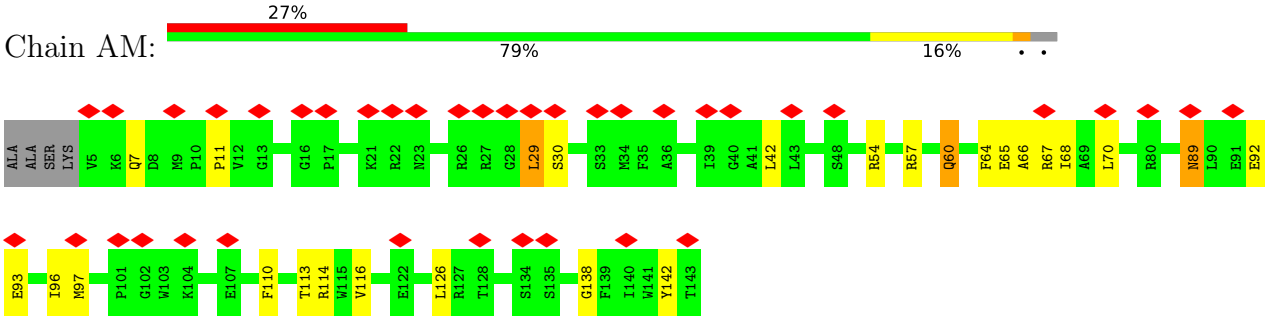
• Molecule 28: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



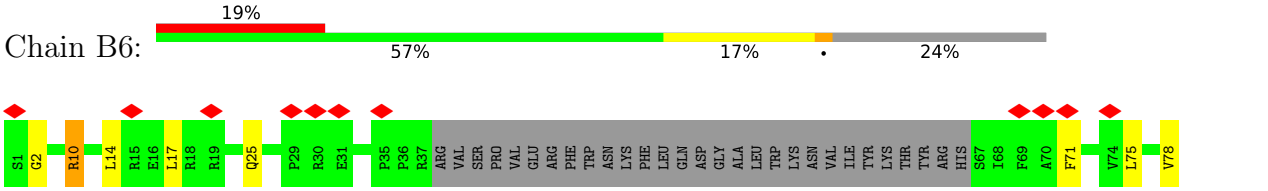
• Molecule 29: NDUFA13

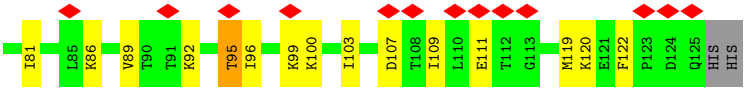
Chain AM:



• Molecule 30: NDUFB6

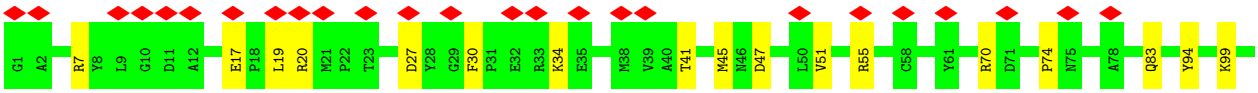
Chain B6:

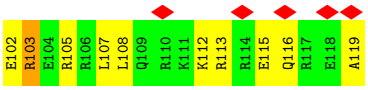




• Molecule 31: NADH:ubiquinone oxidoreductase subunit B7

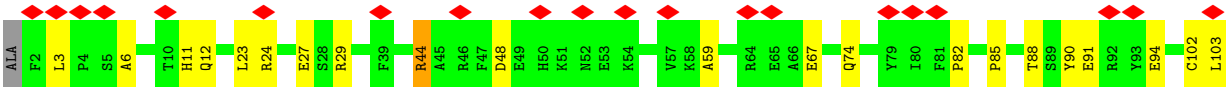
Chain B7:

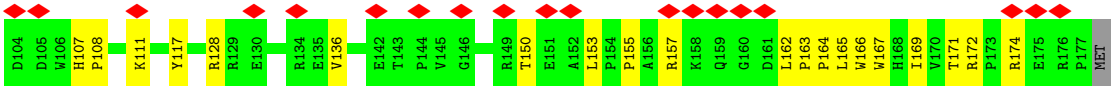




• Molecule 32: NADH:ubiquinone oxidoreductase subunit B9

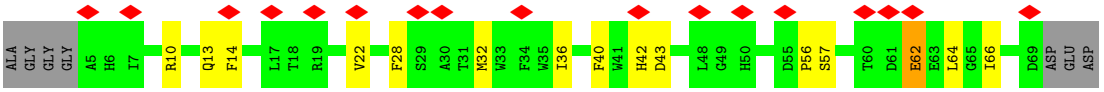
Chain B9:





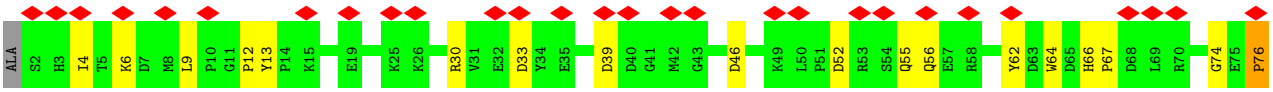
• Molecule 33: NADH:ubiquinone oxidoreductase subunit B2

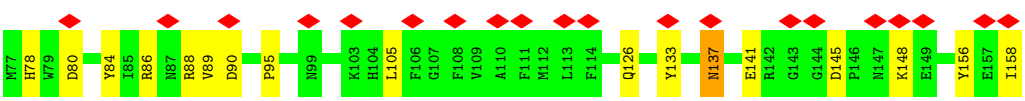
Chain B2:



• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

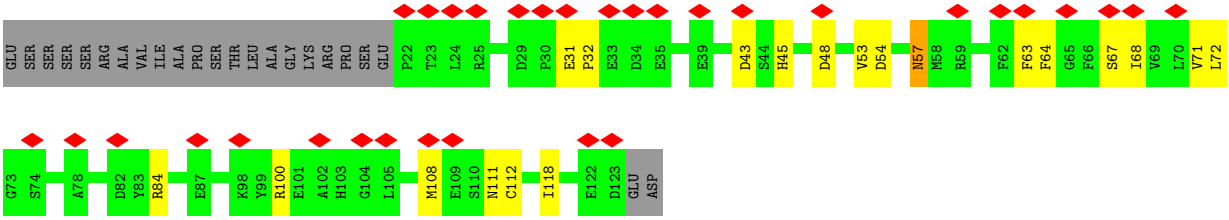
Chain B8:



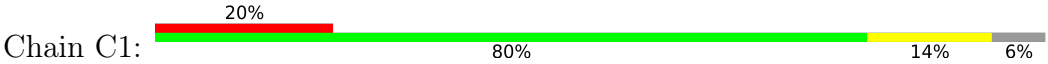


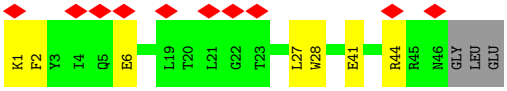
• Molecule 35: NDUFB11

Chain BK:

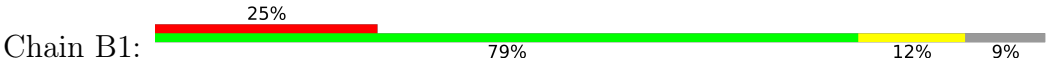


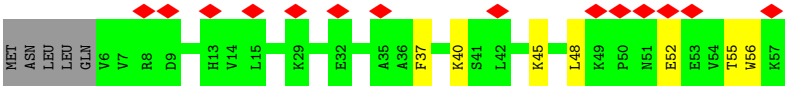
• Molecule 36: NDUFC1



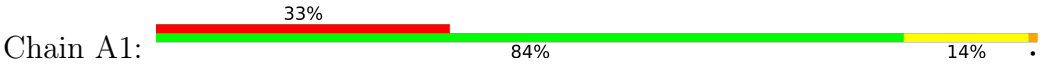


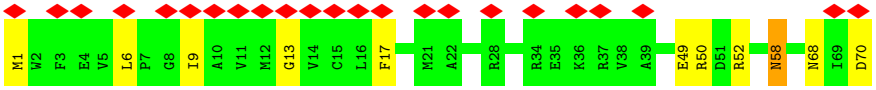
• Molecule 37: NDUFB1



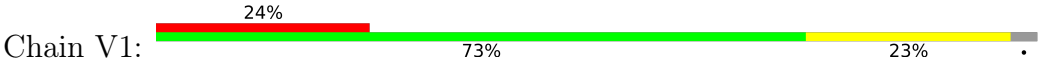


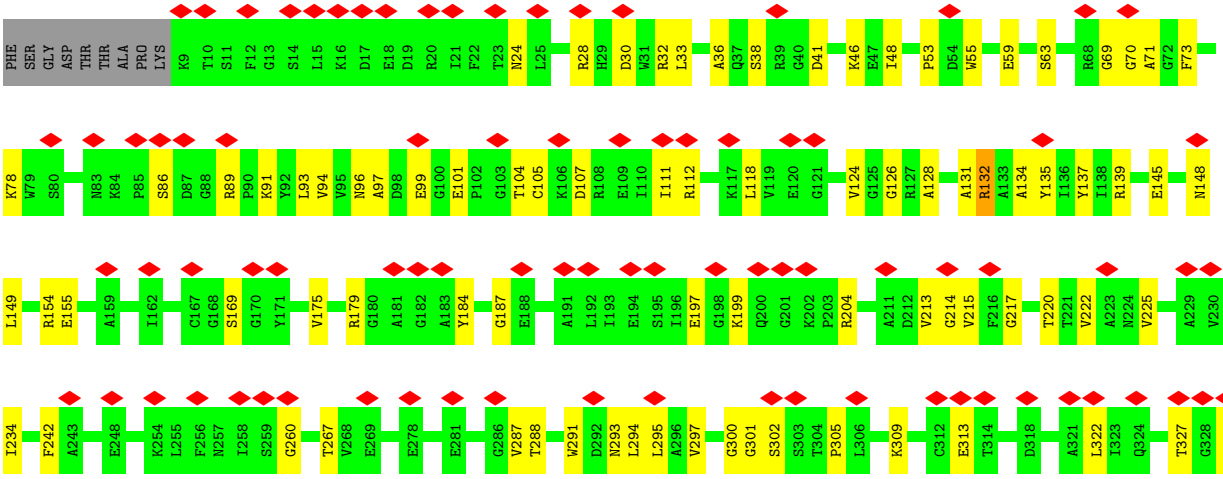
• Molecule 38: NDUFA1

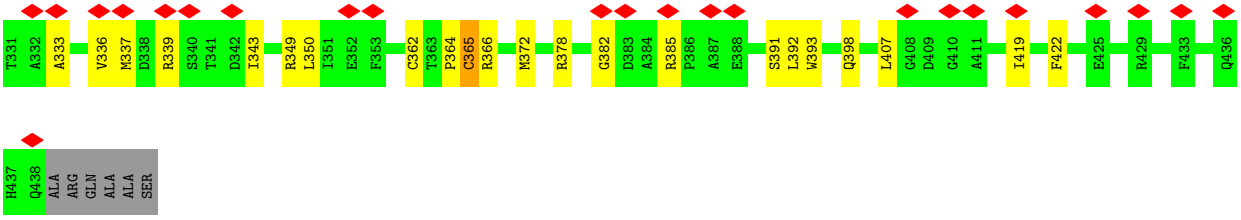




• Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

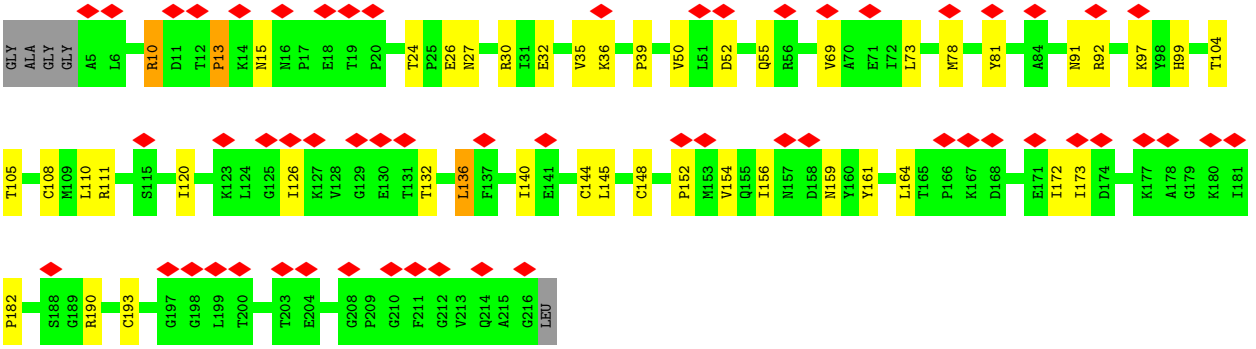






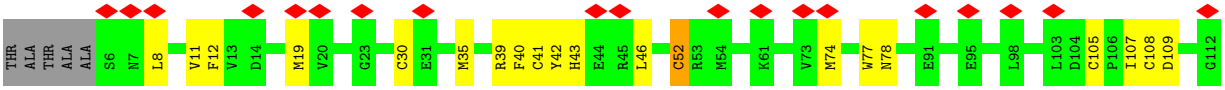
• Molecule 40: NDUFV2

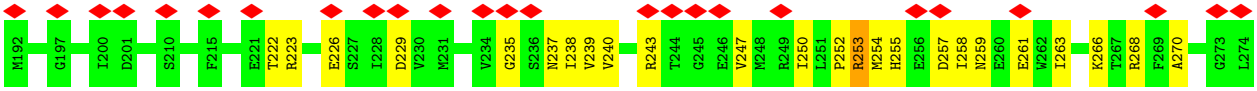
Chain V2:

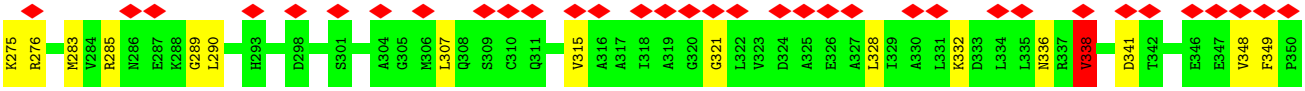


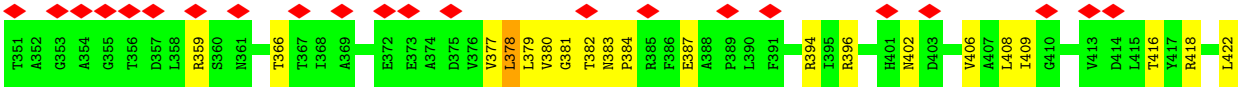
• Molecule 41: NADH:ubiquinone oxidoreductase core subunit S1

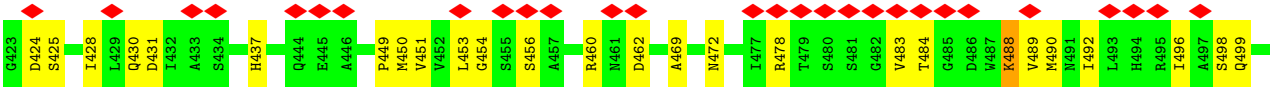
Chain S1:

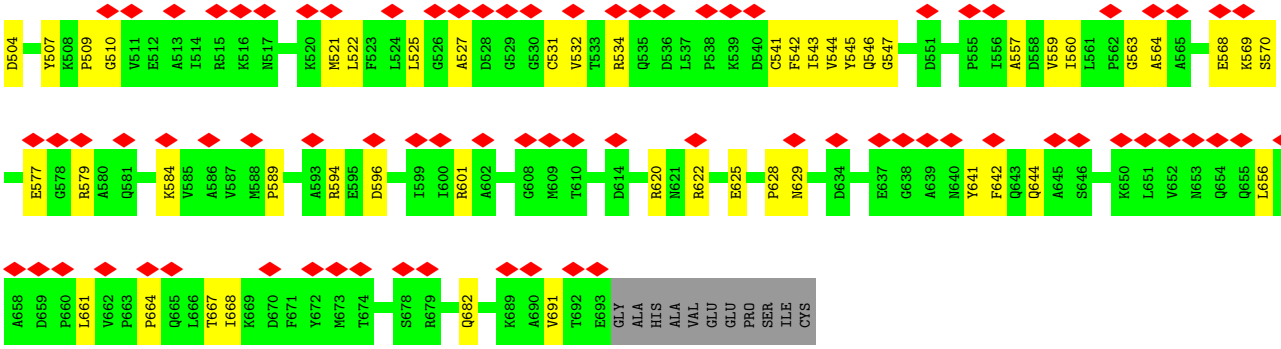






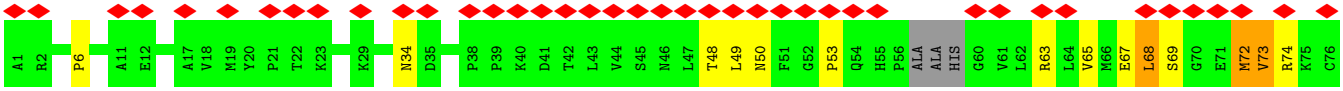






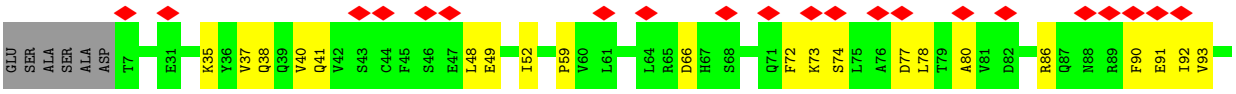
• Molecule 42: NDUFS2

Chain S2:



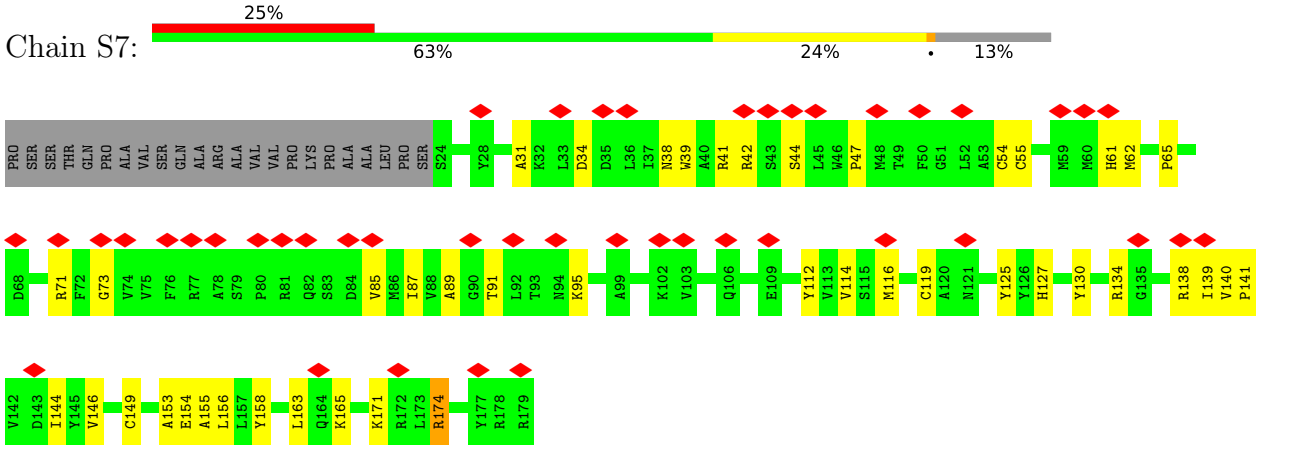
• Molecule 43: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



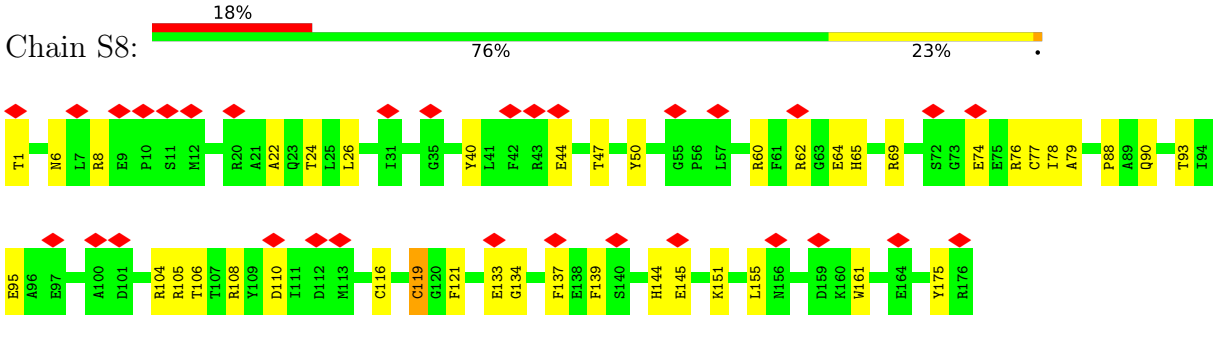
• Molecule 44: NDUFS7

Chain S7:



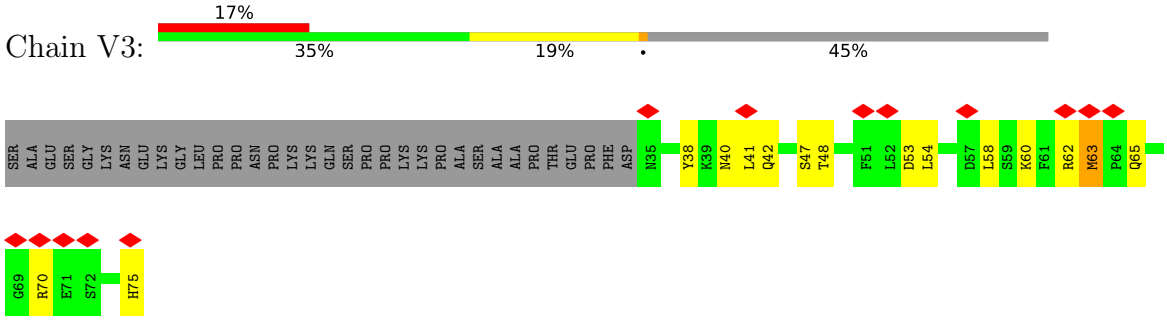
• Molecule 45: NDUFS8

Chain S8:



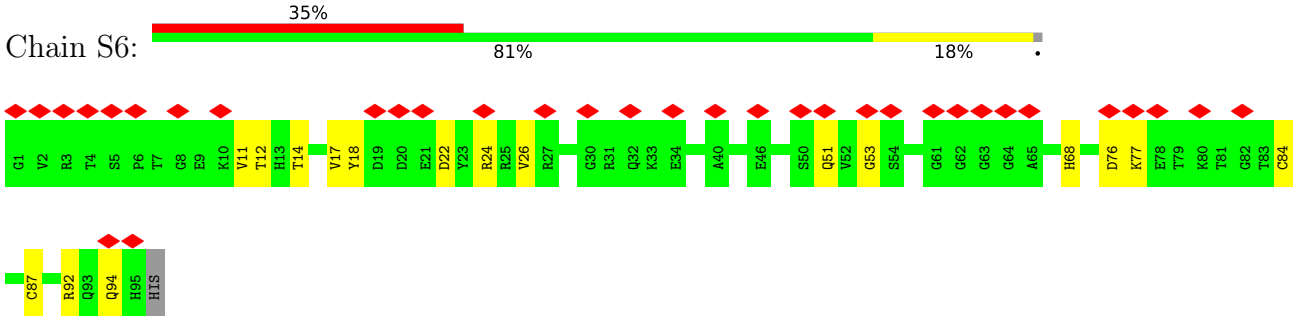
• Molecule 46: NDUFV3

Chain V3:



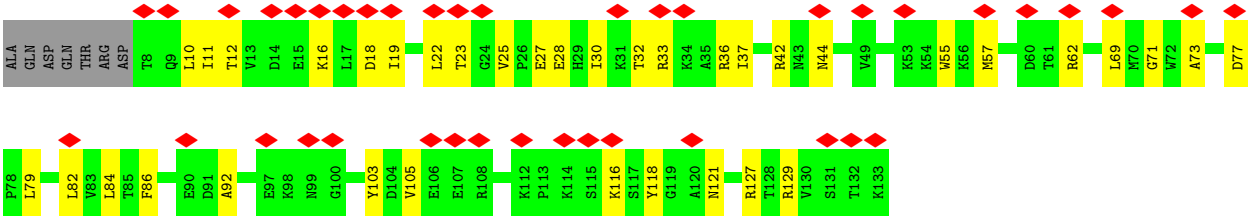
• Molecule 47: NDUFS6

Chain S6:



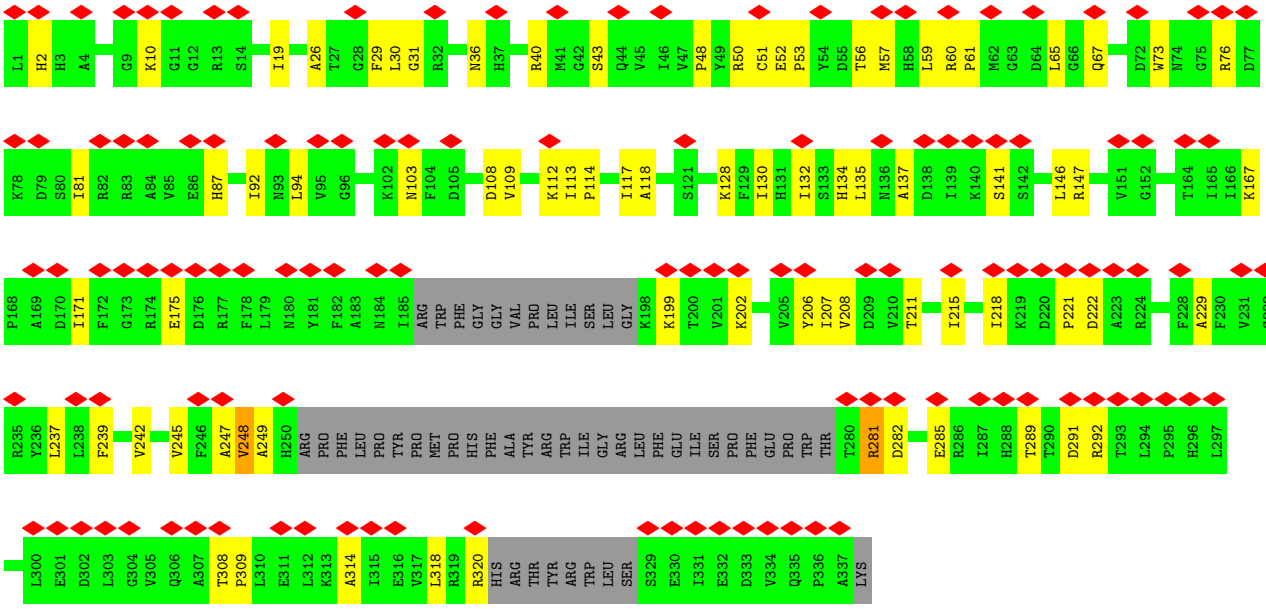
• Molecule 48: NADH:ubiquinone oxidoreductase subunit S4

Chain S4:



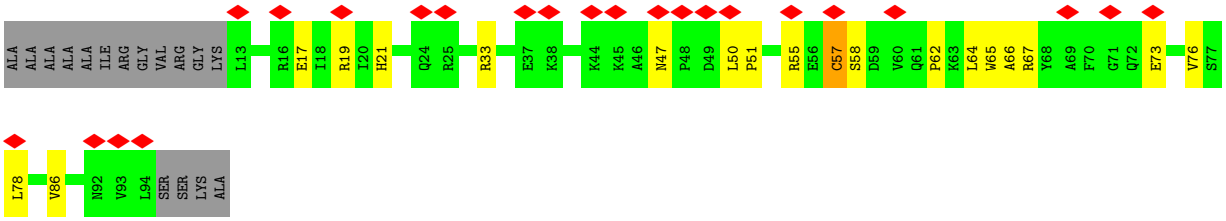
• Molecule 49: NADH:ubiquinone oxidoreductase subunit A9

Chain A9:



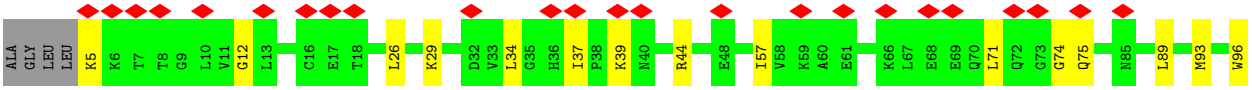
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

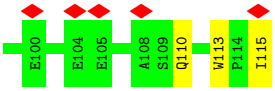
Chain A2:



• Molecule 51: NDUFA5

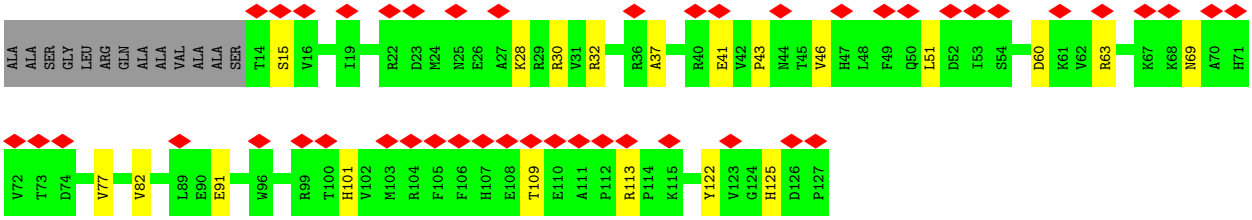
Chain A5:





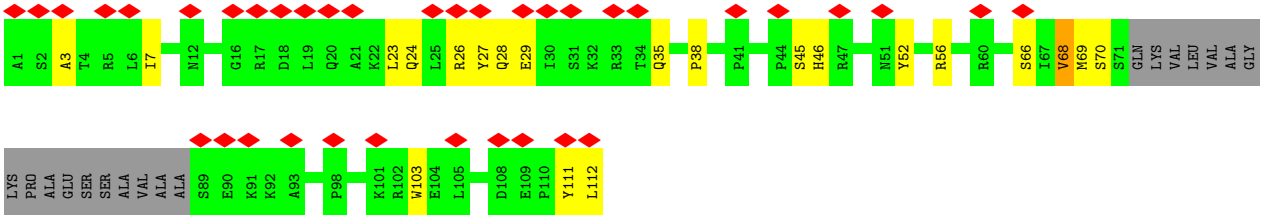
• Molecule 52: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



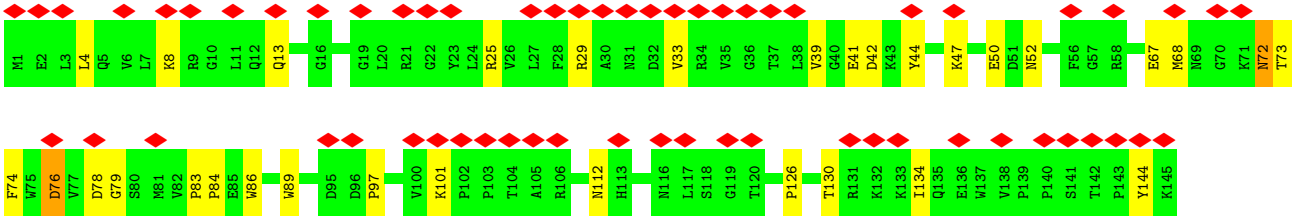
• Molecule 53: NDUFA7

Chain A7:



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

Chain AL:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14230	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 ($e^-/Å^2$)	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	0.776	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	a1	0.32	0/3479	0.55	0/4719
1	a3	0.31	0/3518	0.54	0/4776
2	a2	0.30	0/3183	0.53	1/4313 (0.0%)
2	a4	0.31	0/3179	0.52	0/4308
3	b1	0.33	0/3119	0.56	0/4268
3	b2	0.34	0/3119	0.55	0/4268
4	c1	0.32	0/1960	0.54	0/2660
4	c2	0.32	0/1962	0.55	0/2664
5	f1	0.28	0/1554	0.49	0/2101
5	f2	0.28	0/1548	0.52	0/2093
6	d1	0.30	0/906	0.52	0/1213
6	d2	0.31	0/908	0.52	0/1218
7	q1	0.31	0/638	0.51	0/862
7	q2	0.37	0/652	0.56	0/883
8	h1	0.28	0/538	0.61	0/723
8	h2	0.30	0/538	0.68	1/723 (0.1%)
10	i1	0.31	0/471	0.53	0/634
10	i2	0.30	0/486	0.50	0/655
11	D3	0.31	0/738	0.64	0/1010
12	D1	0.36	0/2442	0.69	3/3337 (0.1%)
13	D6	0.34	0/1339	0.65	0/1810
14	4L	0.32	0/758	0.69	0/1024
15	D5	0.35	0/4933	0.69	5/6710 (0.1%)
16	D4	0.36	0/3740	0.68	3/5095 (0.1%)
17	D2	0.36	0/2788	0.64	1/3795 (0.0%)
18	AK	0.33	0/1046	0.64	1/1419 (0.1%)
19	B5	0.32	0/1189	0.54	1/1607 (0.1%)
20	AA	0.30	0/655	0.65	0/881
20	AB	0.33	0/714	0.58	0/963
21	A8	0.34	0/1441	0.65	0/1942
22	BJ	0.32	0/1475	0.58	2/1989 (0.1%)
23	AJ	0.34	0/2644	0.62	3/3579 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
24	S5	0.32	0/843	0.60	1/1128 (0.1%)
25	A3	0.32	0/602	0.67	1/828 (0.1%)
26	B3	0.33	0/595	0.68	0/803
27	C2	0.33	0/1028	0.63	1/1388 (0.1%)
28	B4	0.33	0/1085	0.63	2/1467 (0.1%)
29	AM	0.33	0/1172	0.60	2/1579 (0.1%)
30	B6	0.36	0/835	0.69	0/1137
31	B7	0.33	0/1051	0.64	2/1408 (0.1%)
32	B9	0.34	0/1568	0.59	0/2123
33	B2	0.33	0/587	0.65	0/806
34	B8	0.37	0/1379	0.67	0/1884
35	BK	0.34	0/880	0.61	0/1196
36	C1	0.31	0/404	0.55	0/548
37	B1	0.31	0/462	0.62	1/624 (0.2%)
38	A1	0.32	0/592	0.63	0/795
39	V1	0.33	0/3386	0.58	0/4575
40	V2	0.33	0/1687	0.67	2/2295 (0.1%)
41	S1	0.32	0/5362	0.60	1/7266 (0.0%)
42	S2	0.36	0/3525	0.60	1/4776 (0.0%)
43	S3	0.35	0/1776	0.59	0/2417
44	S7	0.36	0/1278	0.58	0/1728
45	S8	0.40	1/1445 (0.1%)	0.59	0/1956
46	V3	0.33	0/355	0.72	1/480 (0.2%)
47	S6	0.34	0/749	0.54	0/1009
48	S4	0.31	0/1047	0.57	0/1415
49	A9	0.32	0/2317	0.64	1/3131 (0.0%)
50	A2	0.29	0/676	0.60	0/911
51	A5	0.31	0/921	0.60	1/1249 (0.1%)
52	A6	0.30	0/993	0.52	0/1336
53	A7	0.29	0/775	0.64	0/1048
54	AL	0.34	0/1250	0.60	1/1698 (0.1%)
All	All	0.33	1/98285 (0.0%)	0.60	39/133246 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a1	0	2
1	a3	0	1
2	a4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	f2	0	1
12	D1	0	2
13	D6	0	1
15	D5	0	3
16	D4	0	2
18	AK	0	1
20	AA	0	1
21	A8	0	1
23	AJ	0	2
24	S5	0	1
25	A3	0	1
26	B3	0	2
27	C2	0	2
30	B6	0	2
31	B7	0	1
33	B2	0	2
34	B8	0	2
35	BK	0	1
36	C1	0	1
37	B1	0	1
39	V1	0	1
40	V2	0	4
41	S1	0	7
42	S2	0	2
45	S8	0	1
49	A9	0	3
50	A2	0	1
51	A5	0	1
53	A7	0	2
All	All	0	56

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	S8	119	CYS	CB-SG	-5.88	1.72	1.81

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D5	69	LEU	CA-CB-CG	7.46	132.46	115.30
16	D4	367	LEU	CA-CB-CG	7.36	132.23	115.30
2	a2	41	TYR	C-N-CA	7.07	139.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	A9	222	ASP	CB-CG-OD1	7.02	124.61	118.30
31	B7	19	LEU	CA-CB-CG	6.76	130.85	115.30
28	B4	120	LEU	CA-CB-CG	6.71	130.73	115.30
15	D5	78	LEU	CA-CB-CG	6.34	129.89	115.30
23	AJ	275	ILE	C-N-CD	-6.13	107.12	120.60
29	AM	126	LEU	CA-CB-CG	6.11	129.36	115.30
28	B4	17	LEU	CA-CB-CG	6.08	129.29	115.30
40	V2	136	LEU	CA-CB-CG	5.98	129.05	115.30
22	BJ	21	PRO	C-N-CA	5.96	136.61	121.70
46	V3	41	LEU	CA-CB-CG	5.91	128.89	115.30
31	B7	27	ASP	CB-CG-OD1	5.88	123.60	118.30
8	h2	62	LEU	CA-CB-CG	5.80	128.63	115.30
15	D5	511	LEU	CA-CB-CG	5.64	128.28	115.30
29	AM	42	LEU	CA-CB-CG	5.64	128.28	115.30
23	AJ	229	GLU	C-N-CA	5.60	135.71	121.70
15	D5	386	LEU	CA-CB-CG	5.52	128.00	115.30
19	B5	30	LEU	CA-CB-CG	5.47	127.88	115.30
27	C2	11	LEU	CA-CB-CG	5.42	127.78	115.30
17	D2	130	LEU	CA-CB-CG	5.39	127.70	115.30
16	D4	214	LEU	CA-CB-CG	5.36	127.64	115.30
23	AJ	304	TYR	CA-CB-CG	5.34	123.55	113.40
15	D5	552	LEU	CA-CB-CG	5.29	127.46	115.30
24	S5	19	ILE	CG1-CB-CG2	-5.24	99.88	111.40
12	D1	22	LEU	CA-CB-CG	5.21	127.29	115.30
51	A5	89	LEU	CA-CB-CG	5.21	127.27	115.30
40	V2	110	LEU	CA-CB-CG	5.16	127.16	115.30
41	S1	378	LEU	CA-CB-CG	5.15	127.15	115.30
42	S2	72	MET	C-N-CA	5.13	134.53	121.70
18	AK	5	LEU	CA-CB-CG	5.13	127.09	115.30
54	AL	76	ASP	CB-CG-OD1	5.12	122.91	118.30
22	BJ	25	LEU	C-N-CD	-5.10	109.39	120.60
12	D1	190	LEU	CA-CB-CG	5.09	127.01	115.30
25	A3	65	VAL	CA-CB-CG1	5.07	118.50	110.90
12	D1	129	LEU	CB-CG-CD2	5.06	119.60	111.00
37	B1	48	LEU	CA-CB-CG	5.05	126.91	115.30
16	D4	230	VAL	CG1-CB-CG2	-5.02	102.86	110.90

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	A2	57	CYS	Peptide

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Mol	Chain	Res	Type	Group
25	A3	57	ARG	Peptide
51	A5	93	MET	Peptide
53	A7	68	VAL	Peptide
53	A7	69	MET	Peptide
21	A8	52	PRO	Peptide
49	A9	221	PRO	Peptide
49	A9	247	ALA	Peptide
49	A9	248	VAL	Peptide
20	AA	59	GLY	Peptide
23	AJ	241	LEU	Peptide
23	AJ	278	PHE	Peptide
18	AK	46	THR	Peptide
37	B1	52	GLU	Peptide
33	B2	56	PRO	Peptide
33	B2	62	GLU	Peptide
26	B3	22	LYS	Peptide
26	B3	58	ASN	Peptide
30	B6	122	PHE	Peptide
30	B6	86	LYS	Peptide
31	B7	30	PHE	Peptide
34	B8	56	GLN	Peptide
34	B8	76	PRO	Peptide
35	BK	48	ASP	Peptide
36	C1	6	GLU	Peptide
27	C2	11	LEU	Peptide
27	C2	8	ARG	Peptide
12	D1	275	ALA	Peptide
12	D1	91	MET	Peptide
16	D4	52	PHE	Peptide
16	D4	53	SER	Peptide
15	D5	365	ALA	Peptide
15	D5	526	LEU	Peptide
15	D5	84	PHE	Mainchain
13	D6	115	ILE	Peptide
41	S1	247	VAL	Peptide
41	S1	253	ARG	Peptide
41	S1	259	ASN	Peptide
41	S1	338	VAL	Peptide
41	S1	341	ASP	Peptide
41	S1	380	VAL	Peptide
41	S1	490	MET	Peptide
42	S2	68	LEU	Peptide

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Mol	Chain	Res	Type	Group
42	S2	73	VAL	Mainchain
24	S5	92	THR	Peptide
45	S8	106	THR	Peptide
39	V1	28	ARG	Peptide
40	V2	10	ARG	Peptide
40	V2	13	PRO	Peptide
40	V2	152	PRO	Peptide
40	V2	35	VAL	Peptide
1	a1	190	TYR	Peptide
1	a1	309	THR	Peptide
1	a3	309	THR	Peptide
2	a4	30	PRO	Peptide
5	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	a1	3409	0	3322	0	0
1	a3	3447	0	3350	0	0
2	a2	3126	0	3093	0	0
2	a4	3122	0	3090	0	0
3	b1	3019	0	3082	0	0
3	b2	3019	0	3082	0	0
4	c1	1902	0	1851	0	0
4	c2	1903	0	1850	0	0
5	f1	1520	0	1505	0	0
5	f2	1514	0	1497	0	0
6	d1	886	0	883	0	0
6	d2	888	0	880	0	0
7	q1	618	0	628	0	0
7	q2	631	0	639	0	0
8	h1	532	0	509	0	0
8	h2	532	0	509	0	0
9	x1	164	0	39	0	0
9	x2	150	0	43	0	0
10	i1	459	0	462	0	0
10	i2	473	0	477	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D3	719	0	765	6	0
12	D1	2372	0	2484	41	0
13	D6	1308	0	1329	22	0
14	4L	748	0	794	16	0
15	D5	4805	0	4950	92	0
16	D4	3646	0	3850	77	0
17	D2	2724	0	2930	47	0
18	AK	1025	0	1033	14	0
19	B5	1156	0	1177	17	0
20	AA	645	0	649	7	0
20	AB	702	0	692	12	0
21	A8	1404	0	1384	19	0
22	BJ	1441	0	1417	22	0
23	AJ	2583	0	2547	48	0
24	S5	822	0	820	16	0
25	A3	582	0	583	9	0
26	B3	578	0	570	8	0
27	C2	997	0	983	22	0
28	B4	1059	0	1062	23	0
29	AM	1143	0	1137	21	0
30	B6	809	0	826	18	0
31	B7	1026	0	995	18	0
32	B9	1515	0	1469	30	0
33	B2	560	0	507	12	0
34	B8	1324	0	1219	22	0
35	BK	853	0	800	14	0
36	C1	391	0	391	5	0
37	B1	449	0	453	3	0
38	A1	577	0	570	6	0
39	V1	3312	0	3266	68	0
40	V2	1647	0	1657	31	0
41	S1	5275	0	5300	116	0
42	S2	3435	0	3377	72	0
43	S3	1726	0	1676	41	0
44	S7	1247	0	1256	35	0
45	S8	1414	0	1370	39	0
46	V3	345	0	323	10	0
47	S6	737	0	710	11	0
48	S4	1024	0	1023	29	0
49	A9	2270	0	2273	52	0
50	A2	665	0	678	12	0
51	A5	901	0	936	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	A6	969	0	980	20	0
53	A7	757	0	771	20	0
54	AL	1209	0	1182	22	0
55	b1	86	0	60	0	0
55	b2	86	0	60	0	0
56	c1	43	0	30	0	0
56	c2	43	0	30	0	0
57	S1	4	0	0	0	0
57	V2	4	0	0	0	0
57	f1	4	0	0	0	0
57	f2	4	0	0	0	0
58	D2	28	0	30	0	0
59	AA	34	0	40	5	0
59	AB	31	0	34	2	0
60	S1	16	0	0	1	0
60	S7	8	0	0	1	0
60	S8	16	0	0	1	0
60	V1	8	0	0	1	0
61	V1	31	0	19	3	0
62	S6	1	0	0	0	0
63	A9	48	0	26	3	0
All	All	96705	0	96284	1009	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 (1009) 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	1.15	1.31
43:S3:78:LEU:HA	43:S3:93:VAL:O	1.43	1.14
43:S3:38:GLN:HA	53:A7:70:SER:O	1.50	1.10
15:D5:547:LYS:O	15:D5:552:LEU:HB2	1.60	1.01
43:S3:80:ALA:CA	43:S3:91:GLU:O	2.12	0.96
41:S1:449:PRO:O	41:S1:489:VAL:HA	1.67	0.94
49:A9:245:VAL:O	49:A9:249:ALA:HB3	1.73	0.88
42:S2:337:GLU:O	42:S2:341:SER:HB3	1.74	0.87
50:A2:21:HIS:O	50:A2:62:PRO:HA	1.79	0.83
31:B7:115:GLU:O	31:B7:119:ALA:HB3	1.81	0.81
49:A9:108:ASP:O	49:A9:112:LYS:HB3	1.81	0.80
30:B6:71:PHE:O	30:B6:75:LEU:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:266:LYS:O	41:S1:270:ALA:HB2	1.84	0.77
43:S3:74:SER:HB3	43:S3:97:LEU:O	1.84	0.76
31:B7:108:LEU:O	31:B7:112:LYS:HB2	1.86	0.76
16:D4:227:GLY:O	16:D4:231:LEU:HB2	1.85	0.76
23:AJ:169:VAL:O	23:AJ:220:VAL:HA	1.87	0.74
16:D4:363:SER:O	16:D4:367:LEU:HB2	1.89	0.73
39:V1:301:GLY:HA2	39:V1:333:ALA:HB3	1.73	0.71
15:D5:294:THR:H	15:D5:425:ARG:HH12	1.39	0.70
29:AM:138:GLY:O	29:AM:142:TYR:HB3	1.92	0.69
52:A6:37:ALA:O	52:A6:41:GLU:HB2	1.92	0.69
41:S1:377:VAL:O	41:S1:406:VAL:HA	1.93	0.68
42:S2:336:ALA:O	42:S2:339:LYS:O	2.11	0.68
12:D1:67:SER:O	12:D1:70:MET:N	2.27	0.68
35:BK:53:VAL:O	35:BK:57:ASN:HB2	1.93	0.67
50:A2:66:ALA:O	50:A2:73:GLU:HA	1.94	0.67
15:D5:160:GLY:H	16:D4:417:GLY:HA2	1.59	0.67
16:D4:231:LEU:O	16:D4:235:LEU:HB2	1.95	0.67
43:S3:41:GLN:HA	53:A7:66:SER:O	1.95	0.66
41:S1:359:ARG:HH12	41:S1:629:ASN:HD21	1.44	0.66
14:4L:58:MET:HB3	14:4L:62:ILE:HD12	1.77	0.66
49:A9:245:VAL:O	49:A9:248:VAL:O	2.14	0.66
43:S3:38:GLN:CA	53:A7:70:SER:O	2.38	0.66
50:A2:47:ASN:HB3	50:A2:50:LEU:HB2	1.78	0.66
42:S2:105:ARG:NH1	60:S7:300:SF4:S3	2.69	0.66
12:D1:35:LYS:H	45:S8:47:THR:HG21	1.60	0.66
16:D4:204:MET:HB3	16:D4:209:LEU:HD22	1.78	0.65
41:S1:117:GLN:NE2	60:S1:801:SF4:S3	2.69	0.65
15:D5:176:ARG:NH2	16:D4:400:MET:SD	2.68	0.65
41:S1:237:ASN:HB3	41:S1:253:ARG:O	1.96	0.65
13:D6:14:VAL:HG22	14:4L:11:ALA:HB2	1.79	0.65
18:AK:6:HIS:O	18:AK:10:ASP:HB2	1.97	0.64
27:C2:30:ARG:HE	27:C2:76:LEU:HD11	1.60	0.64
42:S2:175:GLU:OE2	44:S7:61:HIS:ND1	2.30	0.64
12:D1:152:SER:OG	12:D1:301:CYS:SG	2.55	0.64
15:D5:227:PHE:H	15:D5:284:THR:HG22	1.63	0.64
39:V1:124:VAL:O	39:V1:128:ALA:HB2	1.98	0.64
12:D1:55:LEU:HD11	12:D1:220:PHE:HB3	1.80	0.64
42:S2:130:PRO:HG2	42:S2:135:GLN:HE21	1.62	0.64
43:S3:40:VAL:HB	53:A7:68:VAL:HB	1.78	0.64
41:S1:240:VAL:HG12	41:S1:250:ILE:HG22	1.79	0.63
16:D4:241:TYR:OH	16:D4:245:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A9:314:ALA:O	49:A9:318:LEU:HB2	1.98	0.63
44:S7:31:ALA:HA	44:S7:174:ARG:HD2	1.81	0.63
49:A9:92:ILE:HG22	49:A9:130:ILE:HB	1.80	0.63
49:A9:281:ARG:NH1	49:A9:282:ASP:OD1	2.32	0.63
41:S1:126:ASP:HB2	42:S2:328:ALA:HB3	1.81	0.62
44:S7:154:GLU:HG3	45:S8:50:TYR:HE1	1.63	0.62
12:D1:131:GLY:HA2	12:D1:134:ARG:HE	1.64	0.62
15:D5:130:ILE:HG23	15:D5:139:GLN:HE21	1.64	0.62
39:V1:134:ALA:HB3	39:V1:175:VAL:HG12	1.81	0.62
45:S8:77:CYS:SG	45:S8:78:ILE:N	2.73	0.62
54:AL:83:PRO:HG2	54:AL:86:TRP:HD1	1.65	0.62
41:S1:456:SER:HB2	41:S1:664:PRO:HD2	1.80	0.62
23:AJ:141:GLN:NE2	23:AJ:201:ASP:OD2	2.33	0.62
51:A5:34:LEU:HD11	51:A5:44:ARG:HA	1.82	0.62
44:S7:62:MET:HG2	44:S7:156:LEU:HD23	1.82	0.61
39:V1:53:PRO:HB3	39:V1:128:ALA:HA	1.81	0.61
42:S2:300:ARG:NH2	42:S2:420:THR:O	2.33	0.61
39:V1:24:ASN:ND2	39:V1:30:ASP:O	2.33	0.61
18:AK:122:ALA:O	18:AK:126:MET:HB2	2.00	0.61
22:BJ:23:THR:HG21	31:B7:74:PRO:HD2	1.81	0.61
15:D5:233:LEU:HG	15:D5:303:ALA:HB1	1.82	0.61
41:S1:285:ARG:NH2	54:AL:144:TYR:O	2.34	0.61
13:D6:167:VAL:HG22	17:D2:42:PRO:HG2	1.82	0.61
19:B5:43:ILE:HG13	19:B5:71:ILE:HD11	1.81	0.61
29:AM:66:ALA:O	29:AM:70:LEU:HB2	2.01	0.61
42:S2:336:ALA:O	42:S2:340:THR:HB	2.00	0.61
45:S8:79:ALA:O	45:S8:104:ARG:NH2	2.34	0.61
41:S1:534:ARG:NH1	41:S1:541:CYS:SG	2.73	0.60
39:V1:297:VAL:HG22	39:V1:336:VAL:HG12	1.83	0.60
41:S1:449:PRO:HG2	41:S1:489:VAL:HG22	1.82	0.60
47:S6:53:GLY:HA2	47:S6:94:GLN:H	1.65	0.60
49:A9:109:VAL:O	49:A9:113:ILE:HB	2.01	0.60
12:D1:33:PHE:HB2	44:S7:65:PRO:HB3	1.83	0.60
13:D6:58:LEU:O	13:D6:62:GLY:HA3	2.01	0.60
43:S3:193:GLU:HB2	48:S4:73:ALA:HB3	1.84	0.60
44:S7:85:VAL:HG12	44:S7:112:TYR:HB2	1.84	0.60
16:D4:170:THR:HG23	16:D4:171:MET:HG3	1.83	0.60
23:AJ:72:ARG:NH1	23:AJ:295:GLU:OE1	2.34	0.60
22:BJ:143:HIS:NE2	28:B4:125:ASN:O	2.33	0.60
29:AM:96:ILE:HG23	29:AM:97:MET:HG2	1.84	0.60
43:S3:86:ARG:HD3	51:A5:110:GLN:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:S8:119:CYS:HB2	45:S8:121:PHE:H	1.66	0.60
22:BJ:141:ARG:HD2	35:BK:112:CYS:H	1.67	0.60
43:S3:80:ALA:HA	43:S3:91:GLU:C	2.13	0.60
15:D5:482:MET:SD	15:D5:487:LYS:NZ	2.75	0.59
40:V2:39:PRO:HA	46:V3:65:GLN:HB3	1.84	0.59
43:S3:80:ALA:HB1	43:S3:90:PHE:HB3	1.84	0.59
20:AB:31:SER:HB3	20:AB:34:SER:HB2	1.83	0.59
41:S1:163:ALA:O	41:S1:168:GLY:N	2.34	0.59
48:S4:55:TRP:HB2	48:S4:86:PHE:HB2	1.84	0.59
31:B7:103:ARG:HE	31:B7:107:LEU:HD11	1.67	0.59
16:D4:370:PRO:HA	16:D4:375:LEU:HD13	1.84	0.59
40:V2:99:HIS:HE1	40:V2:140:ILE:HG12	1.67	0.59
12:D1:153:VAL:O	12:D1:157:ASN:ND2	2.35	0.59
21:A8:142:HIS:H	29:AM:114:ARG:HD3	1.67	0.59
25:A3:83:LEU:O	29:AM:54:ARG:NH2	2.35	0.59
41:S1:568:GLU:HB3	41:S1:589:PRO:HG3	1.85	0.59
43:S3:78:LEU:CA	43:S3:93:VAL:O	2.34	0.59
52:A6:69:ASN:HB2	59:AA:101:ZMP:H11A	1.84	0.59
42:S2:425:PHE:HA	42:S2:428:VAL:HB	1.84	0.59
16:D4:389:SER:OG	28:B4:108:ARG:NH2	2.36	0.59
43:S3:72:PHE:HA	43:S3:98:SER:HA	1.84	0.59
11:D3:10:ASN:HD21	12:D1:10:ILE:HG21	1.68	0.59
13:D6:51:PHE:O	13:D6:55:MET:HB2	2.02	0.59
22:BJ:161:ARG:NH2	35:BK:111:ASN:OD1	2.35	0.59
48:S4:37:ILE:HD13	48:S4:92:ALA:HB1	1.85	0.59
49:A9:135:LEU:HA	49:A9:167:LYS:HD3	1.83	0.59
49:A9:10:LYS:HE2	52:A6:113:ARG:HH22	1.68	0.59
34:B8:12:PRO:HA	34:B8:46:ASP:HB3	1.84	0.58
15:D5:264:TYR:HA	15:D5:267:THR:HG22	1.85	0.58
33:B2:10:ARG:NH1	33:B2:14:PHE:O	2.36	0.58
41:S1:276:ARG:HH21	41:S1:682:GLN:HE21	1.52	0.58
12:D1:66:SER:O	12:D1:70:MET:HB3	2.03	0.58
15:D5:278:LEU:HB3	15:D5:318:GLY:HA3	1.84	0.58
39:V1:372:MET:HG2	39:V1:392:LEU:HD11	1.84	0.58
41:S1:283:MET:HB2	41:S1:560:ILE:HB	1.85	0.58
48:S4:18:ASP:HB2	52:A6:77:VAL:HG21	1.85	0.58
40:V2:30:ARG:NH2	46:V3:53:ASP:OD1	2.36	0.58
40:V2:172:ILE:HG23	40:V2:182:PRO:HG2	1.85	0.58
44:S7:47:PRO:HB3	44:S7:85:VAL:HG23	1.83	0.58
19:B5:138:LYS:HG3	24:S5:27:ARG:HG2	1.85	0.58
26:B3:28:LEU:HD11	26:B3:48:GLU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:40:PHE:O	41:S1:158:ARG:NH2	2.36	0.58
42:S2:111:MET:HG3	42:S2:112:MET:HG2	1.84	0.58
42:S2:231:ASN:OD1	42:S2:236:ARG:NH2	2.37	0.58
32:B9:44:ARG:NH1	32:B9:48:ASP:OD2	2.36	0.58
39:V1:362:CYS:N	60:V1:500:SF4:S2	2.76	0.58
51:A5:34:LEU:O	51:A5:44:ARG:NH1	2.36	0.58
27:C2:66:THR:OG1	36:C1:28:TRP:NE1	2.37	0.58
34:B8:13:TYR:HE1	34:B8:39:ASP:H	1.50	0.58
39:V1:46:LYS:HE3	39:V1:169:SER:HB3	1.85	0.58
20:AB:70:LEU:HD23	20:AB:76:ILE:HG12	1.85	0.58
28:B4:55:ARG:NH1	28:B4:57:GLY:O	2.37	0.58
31:B7:103:ARG:HB2	33:B2:64:LEU:HD23	1.85	0.58
32:B9:24:ARG:NH1	32:B9:27:GLU:OE1	2.37	0.58
32:B9:102:CYS:SG	32:B9:103:LEU:N	2.76	0.58
40:V2:55:GLN:NE2	40:V2:91:ASN:OD1	2.37	0.58
41:S1:261:GLU:HB3	48:S4:44:ASN:HD21	1.68	0.58
32:B9:107:HIS:NE2	35:BK:43:ASP:OD1	2.37	0.57
49:A9:171:ILE:HD13	49:A9:207:ILE:HD13	1.86	0.57
15:D5:137:LEU:HB3	15:D5:196:TRP:HD1	1.68	0.57
15:D5:267:THR:O	15:D5:274:GLN:NE2	2.37	0.57
16:D4:177:LEU:O	16:D4:180:GLN:C	2.43	0.57
41:S1:252:PRO:HB3	41:S1:263:ILE:HB	1.87	0.57
41:S1:382:THR:HB	41:S1:454:GLY:HA3	1.86	0.57
46:V3:58:LEU:O	46:V3:62:ARG:NH2	2.37	0.57
15:D5:597:ILE:HD11	18:AK:34:VAL:HG22	1.84	0.57
44:S7:165:LYS:HE2	54:AL:76:ASP:HB2	1.86	0.57
49:A9:141:SER:HA	49:A9:147:ARG:HH21	1.68	0.57
33:B2:36:ILE:O	33:B2:40:PHE:HB2	2.05	0.57
39:V1:139:ARG:NH2	40:V2:144:CYS:O	2.37	0.57
49:A9:51:CYS:SG	49:A9:52:GLU:N	2.75	0.57
42:S2:205:LEU:HB3	53:A7:35:GLN:HG2	1.87	0.57
16:D4:269:MET:SD	16:D4:399:ASN:ND2	2.78	0.56
34:B8:55:GLN:NE2	34:B8:84:TYR:O	2.38	0.56
41:S1:348:VAL:HG22	41:S1:510:GLY:HA2	1.86	0.56
49:A9:237:LEU:HG	49:A9:239:PHE:H	1.70	0.56
45:S8:1:THR:H3	53:A7:103:TRP:HB3	1.70	0.56
42:S2:269:LEU:HB2	42:S2:368:GLU:HB2	1.87	0.56
63:A9:401:NDP:N3A	63:A9:401:NDP:O3X	2.38	0.56
39:V1:32:ARG:HH11	46:V3:42:GLN:HE22	1.51	0.56
40:V2:27:ASN:OD1	40:V2:30:ARG:NH1	2.38	0.56
15:D5:180:ILE:HD12	16:D4:397:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D5:594:THR:HG21	17:D2:110:PRO:HB3	1.88	0.56
17:D2:92:PRO:O	17:D2:96:MET:HB2	2.04	0.56
32:B9:128:ARG:HA	32:B9:166:TRP:HZ2	1.70	0.56
39:V1:213:VAL:HG13	39:V1:217:GLY:HA2	1.87	0.56
43:S3:35:LYS:NZ	51:A5:96:TRP:O	2.38	0.56
48:S4:33:ARG:HG2	48:S4:62:ARG:HE	1.70	0.56
41:S1:155:GLN:NE2	41:S1:181:MET:O	2.38	0.56
16:D4:282:LEU:HD12	16:D4:285:LEU:HD12	1.87	0.56
30:B6:107:ASP:OD2	31:B7:70:ARG:NH2	2.39	0.56
32:B9:91:GLU:HB3	32:B9:94:GLU:HB2	1.88	0.56
39:V1:91:LYS:HB2	39:V1:131:ALA:HA	1.88	0.56
39:V1:393:TRP:HB2	39:V1:419:ILE:HG21	1.88	0.56
41:S1:250:ILE:HD11	41:S1:268:ARG:HA	1.86	0.56
12:D1:102:VAL:HB	12:D1:150:LEU:HD21	1.87	0.56
24:S5:12:ASP:HB3	24:S5:15:HIS:HB2	1.88	0.56
39:V1:33:LEU:HD23	39:V1:155:GLU:HB3	1.88	0.56
42:S2:105:ARG:NH1	44:S7:149:CYS:SG	2.64	0.56
16:D4:134:THR:O	16:D4:142:ARG:NH1	2.39	0.55
15:D5:138:PHE:HB2	15:D5:196:TRP:HE1	1.71	0.55
17:D2:303:THR:HB	42:S2:6:PRO:HG3	1.88	0.55
31:B7:55:ARG:NH1	34:B8:141:GLU:OE2	2.39	0.55
43:S3:41:GLN:NE2	43:S3:49:GLU:OE1	2.38	0.55
16:D4:46:GLY:HA2	35:BK:84:ARG:HD3	1.87	0.55
32:B9:169:ILE:O	32:B9:172:ARG:NH1	2.39	0.55
48:S4:12:THR:HG21	52:A6:15:SER:HA	1.88	0.55
15:D5:584:ILE:HD11	17:D2:58:LYS:HE2	1.88	0.55
41:S1:569:LYS:NZ	41:S1:596:ASP:OD2	2.40	0.55
41:S1:577:GLU:OE2	41:S1:579:ARG:NH1	2.40	0.55
17:D2:233:THR:HA	17:D2:236:LYS:HG2	1.88	0.55
19:B5:120:GLY:O	19:B5:124:GLN:NE2	2.40	0.55
26:B3:23:ILE:HB	26:B3:46:ARG:HG2	1.87	0.55
39:V1:365:CYS:SG	39:V1:366:ARG:N	2.80	0.55
49:A9:167:LYS:O	49:A9:229:ALA:HA	2.05	0.55
15:D5:54:PHE:HE1	15:D5:60:GLU:HG2	1.72	0.55
16:D4:365:THR:O	16:D4:374:ASN:ND2	2.38	0.55
34:B8:52:ASP:OD1	34:B8:78:HIS:NE2	2.39	0.55
39:V1:111:ILE:HD11	39:V1:149:LEU:HD22	1.89	0.55
41:S1:377:VAL:HG22	41:S1:450:MET:HB3	1.89	0.55
31:B7:17:GLU:OE1	31:B7:20:ARG:NH2	2.39	0.55
45:S8:64:GLU:HB3	45:S8:134:GLY:HA3	1.89	0.55
44:S7:165:LYS:NZ	54:AL:78:ASP:OD1	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D4:363:SER:O	16:D4:367:LEU:CB	2.55	0.55
19:B5:8:LEU:HB3	32:B9:174:ARG:HH12	1.72	0.55
21:A8:29:HIS:NE2	29:AM:65:GLU:OE1	2.34	0.54
41:S1:114:CYS:SG	41:S1:115:ASP:N	2.80	0.54
42:S2:48:THR:HG22	42:S2:67:GLU:HG2	1.87	0.54
14:4L:1:MET:N	24:S5:72:MET:SD	2.80	0.54
15:D5:178:GLY:HA2	15:D5:219:ALA:HA	1.89	0.54
15:D5:82:MET:SD	15:D5:82:MET:N	2.80	0.54
23:AJ:111:ALA:HB1	23:AJ:122:VAL:HG21	1.90	0.54
43:S3:195:ARG:O	45:S8:90:GLN:NE2	2.40	0.54
12:D1:92:PRO:HG3	12:D1:255:TYR:HD2	1.73	0.54
15:D5:77:SER:OG	15:D5:79:SER:OG	2.24	0.54
15:D5:475:MET:HA	31:B7:51:VAL:HG21	1.89	0.54
44:S7:62:MET:HB3	44:S7:153:ALA:HB1	1.90	0.54
45:S8:65:HIS:NE2	45:S8:116:CYS:SG	2.81	0.54
50:A2:57:CYS:SG	50:A2:58:SER:N	2.81	0.54
31:B7:99:LYS:HE3	33:B2:64:LEU:HD11	1.90	0.54
41:S1:402:ASN:O	48:S4:127:ARG:NH2	2.40	0.54
42:S2:388:ARG:NH1	42:S2:389:CYS:O	2.39	0.54
45:S8:108:ARG:NH1	54:AL:130:THR:OG1	2.41	0.54
20:AA:70:LEU:HD13	20:AA:76:ILE:HG12	1.89	0.54
17:D2:30:TRP:NE1	17:D2:67:SER:OG	2.39	0.54
42:S2:69:SER:OG	42:S2:72:MET:O	2.22	0.54
13:D6:141:MET:HA	13:D6:144:ALA:HB3	1.90	0.54
15:D5:33:PRO:HB3	15:D5:118:PHE:HE2	1.73	0.54
21:A8:148:GLU:OE1	24:S5:50:ARG:NH1	2.41	0.54
41:S1:382:THR:OG1	41:S1:387:GLU:OE1	2.26	0.54
12:D1:149:ILE:HG21	12:D1:185:TRP:HB2	1.89	0.54
42:S2:112:MET:H	42:S2:145:THR:HG21	1.73	0.54
16:D4:351:LEU:HD13	16:D4:426:ILE:HD11	1.89	0.54
41:S1:30:CYS:O	41:S1:35:MET:N	2.41	0.54
43:S3:93:VAL:HA	43:S3:107:VAL:O	2.08	0.53
49:A9:50:ARG:NE	63:A9:401:NDP:O3X	2.37	0.53
15:D5:83:ASP:O	15:D5:85:PHE:N	2.41	0.53
16:D4:38:SER:OG	16:D4:70:MET:SD	2.61	0.53
22:BJ:68:ARG:NH2	37:B1:45:LYS:O	2.41	0.53
31:B7:113:ARG:NH2	31:B7:116:GLN:OE1	2.41	0.53
40:V2:154:VAL:HB	40:V2:161:TYR:HB2	1.89	0.53
45:S8:22:ALA:O	45:S8:26:LEU:HB2	2.08	0.53
15:D5:243:VAL:O	15:D5:247:LEU:HB2	2.08	0.53
42:S2:89:LYS:NZ	43:S3:167:PRO:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D1:154:LEU:HA	12:D1:157:ASN:HD22	1.73	0.53
15:D5:205:ASN:HD22	22:BJ:121:ARG:HH22	1.57	0.53
16:D4:300:ALA:O	16:D4:308:SER:OG	2.27	0.53
19:B5:106:LYS:HD3	27:C2:94:ILE:HG13	1.91	0.53
33:B2:10:ARG:HD3	33:B2:13:GLN:HB2	1.89	0.53
36:C1:41:GLU:OE2	36:C1:44:ARG:NH2	2.42	0.53
42:S2:233:ARG:HH12	45:S8:24:THR:HG23	1.73	0.53
42:S2:324:LYS:NZ	42:S2:332:PRO:O	2.40	0.53
16:D4:231:LEU:HA	16:D4:235:LEU:HD13	1.90	0.53
39:V1:267:THR:HG1	40:V2:193:CYS:HG	1.56	0.53
43:S3:167:PRO:HA	48:S4:82:LEU:HD21	1.90	0.53
45:S8:104:ARG:O	45:S8:105:ARG:NH1	2.37	0.53
15:D5:193:LEU:HD11	15:D5:206:PRO:HG3	1.90	0.53
49:A9:26:ALA:HA	49:A9:31:GLY:HA3	1.90	0.53
41:S1:254:MET:SD	48:S4:42:ARG:NH2	2.75	0.53
42:S2:183:ARG:O	45:S8:60:ARG:NH2	2.42	0.53
42:S2:261:ARG:NH1	42:S2:267:TRP:O	2.42	0.53
13:D6:58:LEU:O	13:D6:62:GLY:CA	2.56	0.52
15:D5:116:GLN:NE2	15:D5:120:TYR:OH	2.42	0.52
23:AJ:62:THR:HG21	23:AJ:106:LEU:HD21	1.92	0.52
39:V1:89:ARG:NH1	39:V1:217:GLY:O	2.42	0.52
15:D5:547:LYS:O	15:D5:552:LEU:CB	2.45	0.52
41:S1:255:HIS:HD2	41:S1:258:ILE:H	1.57	0.52
12:D1:126:LYS:O	12:D1:129:LEU:N	2.41	0.52
19:B5:73:ARG:NH2	22:BJ:61:TYR:O	2.42	0.52
21:A8:166:LEU:HD23	21:A8:167:PHE:H	1.74	0.52
26:B3:61:SER:OG	26:B3:62:PHE:N	2.43	0.52
49:A9:43:SER:O	49:A9:67:GLN:NE2	2.42	0.52
16:D4:156:GLY:HA3	16:D4:205:VAL:HG21	1.91	0.52
23:AJ:56:ILE:O	23:AJ:99:TRP:NE1	2.34	0.52
41:S1:126:ASP:OD1	53:A7:56:ARG:NH2	2.42	0.52
41:S1:543:ILE:HD11	41:S1:557:ALA:HA	1.92	0.52
42:S2:246:THR:HG23	51:A5:12:GLY:HA3	1.90	0.52
50:A2:19:ARG:HE	50:A2:65:TRP:HE3	1.57	0.52
52:A6:32:ARG:NH2	59:AA:101:ZMP:O7	2.43	0.52
17:D2:170:LEU:HD22	17:D2:291:TYR:HD2	1.74	0.52
39:V1:93:LEU:O	39:V1:134:ALA:HA	2.10	0.52
39:V1:101:GLU:O	39:V1:104:THR:OG1	2.27	0.52
43:S3:66:ASP:OD1	43:S3:73:LYS:NZ	2.40	0.52
20:AB:46:ASP:OD1	32:B9:44:ARG:NH2	2.42	0.52
23:AJ:91:GLY:O	23:AJ:95:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:564:ALA:HB3	41:S1:569:LYS:HD3	1.90	0.52
41:S1:223:ARG:NH2	43:S3:193:GLU:OE2	2.43	0.52
44:S7:134:ARG:HB2	44:S7:138:ARG:HE	1.73	0.52
11:D3:19:THR:O	11:D3:23:TRP:HB2	2.09	0.52
16:D4:310:MET:HG2	16:D4:456:GLY:H	1.73	0.52
27:C2:19:ARG:HB3	36:C1:41:GLU:HG2	1.92	0.52
32:B9:29:ARG:NH2	32:B9:74:GLN:O	2.42	0.52
32:B9:108:PRO:HA	32:B9:111:LYS:HB2	1.92	0.52
39:V1:215:VAL:HG23	39:V1:220:THR:HG21	1.91	0.52
40:V2:10:ARG:HH21	47:S6:77:LYS:HA	1.74	0.52
41:S1:74:MET:N	41:S1:77:TRP:HE1	2.07	0.52
15:D5:86:SER:H	15:D5:262:ARG:HH22	1.58	0.52
16:D4:61:LEU:HD13	16:D4:457:PRO:HD3	1.92	0.52
21:A8:142:HIS:ND1	29:AM:113:THR:O	2.41	0.52
24:S5:18:THR:HG22	24:S5:19:ILE:HG13	1.91	0.52
40:V2:69:VAL:HG13	40:V2:73:LEU:HD13	1.92	0.52
45:S8:119:CYS:N	60:S8:201:SF4:S4	2.79	0.52
12:D1:66:SER:OG	12:D1:67:SER:N	2.42	0.52
17:D2:243:LEU:HD21	27:C2:44:ILE:HD11	1.91	0.52
42:S2:152:MET:SD	42:S2:174:ARG:NH1	2.83	0.52
49:A9:94:LEU:HG	49:A9:132:ILE:HG12	1.92	0.52
39:V1:126:GLY:HA2	39:V1:131:ALA:HB3	1.91	0.51
23:AJ:77:CYS:O	23:AJ:92:ASN:ND2	2.42	0.51
44:S7:91:THR:OG1	44:S7:119:CYS:SG	2.64	0.51
54:AL:67:GLU:HG2	54:AL:72:ASN:H	1.75	0.51
21:A8:35:CYS:SG	21:A8:36:ASP:N	2.78	0.51
23:AJ:168:VAL:HG12	23:AJ:219:GLU:HB2	1.92	0.51
12:D1:117:LEU:HD12	12:D1:136:VAL:HG11	1.92	0.51
16:D4:278:ARG:NH2	34:B8:80:ASP:OD1	2.43	0.51
23:AJ:141:GLN:HG3	23:AJ:198:TYR:HD1	1.75	0.51
41:S1:11:VAL:HG12	41:S1:77:TRP:HB2	1.92	0.51
44:S7:44:SER:HA	44:S7:73:GLY:HA3	1.92	0.51
50:A2:78:LEU:HD22	50:A2:86:VAL:HG22	1.91	0.51
30:B6:92:LYS:O	30:B6:95:THR:OG1	2.28	0.51
43:S3:150:ARG:NH2	43:S3:155:TYR:O	2.44	0.51
23:AJ:71:VAL:O	23:AJ:76:ASN:ND2	2.44	0.51
34:B8:88:ARG:HG3	34:B8:89:VAL:HG23	1.93	0.51
39:V1:99:GLU:OE2	39:V1:107:ASP:N	2.43	0.51
42:S2:385:ARG:NH2	43:S3:197:PHE:O	2.44	0.51
47:S6:18:TYR:OH	47:S6:24:ARG:NH1	2.44	0.51
16:D4:270:ILE:HG13	16:D4:395:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D2:59:TYR:HB2	17:D2:118:VAL:HG21	1.92	0.51
39:V1:349:ARG:HE	40:V2:105:THR:HA	1.74	0.51
21:A8:85:TRP:HA	21:A8:88:ILE:HG22	1.93	0.51
23:AJ:108:TYR:OH	23:AJ:164:LEU:O	2.28	0.51
39:V1:295:LEU:HB2	39:V1:339:ARG:HA	1.93	0.51
30:B6:17:LEU:HD11	32:B9:162:LEU:HD22	1.92	0.51
39:V1:48:ILE:HG23	39:V1:55:TRP:HZ3	1.76	0.51
42:S2:63:ARG:HB3	42:S2:79:HIS:HB2	1.93	0.51
17:D2:234:TRP:HD1	17:D2:241:THR:HG21	1.76	0.51
36:C1:1:LYS:HD3	36:C1:2:PHE:HB2	1.92	0.51
40:V2:92:ARG:NH1	41:S1:186:TYR:OH	2.44	0.51
47:S6:68:HIS:HE1	47:S6:87:CYS:SG	2.21	0.51
17:D2:84:TRP:HB2	24:S5:18:THR:HA	1.93	0.50
18:AK:139:LYS:HA	19:B5:115:ARG:HE	1.77	0.50
42:S2:379:VAL:HG12	42:S2:387:TYR:HB3	1.92	0.50
42:S2:406:SER:HB2	42:S2:414:VAL:HG22	1.93	0.50
12:D1:145:THR:HG23	12:D1:297:THR:HG21	1.94	0.50
18:AK:68:ILE:HD13	18:AK:99:THR:HG21	1.92	0.50
54:AL:67:GLU:H	54:AL:73:THR:HG22	1.75	0.50
23:AJ:216:GLU:OE1	23:AJ:245:LYS:NZ	2.39	0.50
12:D1:58:LYS:HZ3	44:S7:41:ARG:HH11	1.59	0.50
17:D2:115:VAL:HG12	17:D2:180:ALA:HB1	1.94	0.50
23:AJ:101:TYR:OH	23:AJ:159:THR:OG1	2.29	0.50
29:AM:11:PRO:HD3	42:S2:318:MET:HB3	1.94	0.50
33:B2:36:ILE:O	33:B2:40:PHE:CB	2.59	0.50
41:S1:285:ARG:NH2	41:S1:289:GLY:O	2.43	0.50
41:S1:449:PRO:O	41:S1:489:VAL:CA	2.52	0.50
42:S2:269:LEU:HD11	42:S2:373:GLU:HG2	1.93	0.50
44:S7:158:TYR:HE1	54:AL:79:GLY:H	1.58	0.50
15:D5:99:SER:OG	15:D5:453:SER:OG	2.24	0.50
22:BJ:159:LYS:HG2	35:BK:118:ILE:HD11	1.92	0.50
39:V1:179:ARG:NH1	40:V2:52:ASP:OD2	2.45	0.50
41:S1:8:LEU:HD22	41:S1:19:MET:HB3	1.93	0.50
41:S1:396:ARG:NH1	41:S1:416:THR:O	2.45	0.50
43:S3:173:GLU:OE2	44:S7:138:ARG:NH1	2.45	0.50
53:A7:45:SER:O	53:A7:46:HIS:ND1	2.35	0.50
12:D1:271:LEU:HD23	12:D1:274:ARG:HH21	1.77	0.50
39:V1:105:CYS:SG	40:V2:148:CYS:N	2.83	0.50
39:V1:322:LEU:HD12	39:V1:329:LEU:HD22	1.92	0.50
20:AA:73:PRO:HA	20:AA:76:ILE:HD12	1.92	0.50
12:D1:288:LEU:O	12:D1:292:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D6:52:LEU:HD21	14:4L:60:PRO:HG2	1.94	0.50
15:D5:428:PHE:HA	15:D5:432:LEU:HB2	1.94	0.50
16:D4:197:LEU:O	16:D4:201:MET:HB2	2.11	0.50
17:D2:309:ASN:HD21	23:AJ:95:ARG:HG3	1.77	0.50
19:B5:138:LYS:HB3	24:S5:29:PRO:HD3	1.94	0.50
23:AJ:15:THR:OG1	23:AJ:253:ASP:OD1	2.29	0.50
29:AM:7:GLN:HB2	53:A7:38:PRO:HA	1.92	0.50
39:V1:70:GLY:HA2	39:V1:330:GLY:HA2	1.94	0.50
45:S8:144:HIS:H	49:A9:60:ARG:HH22	1.60	0.50
15:D5:10:VAL:HA	15:D5:13:ILE:HG22	1.93	0.50
15:D5:237:MET:HG3	15:D5:303:ALA:HB2	1.94	0.50
16:D4:2:LEU:HD12	16:D4:5:ILE:HB	1.92	0.50
24:S5:4:ASP:O	24:S5:8:LYS:CB	2.60	0.50
30:B6:10:ARG:HH12	30:B6:14:LEU:HD22	1.77	0.50
43:S3:73:LYS:HB2	43:S3:99:LEU:HD23	1.93	0.50
48:S4:33:ARG:HH11	48:S4:79:LEU:HB2	1.77	0.50
49:A9:76:ARG:NH2	49:A9:103:ASN:O	2.45	0.50
43:S3:150:ARG:NH2	52:A6:91:GLU:OE1	2.45	0.50
49:A9:134:HIS:ND1	49:A9:135:LEU:O	2.45	0.50
15:D5:54:PHE:O	15:D5:58:GLY:N	2.43	0.49
16:D4:187:PRO:O	16:D4:192:ASN:ND2	2.39	0.49
23:AJ:188:ASN:HB3	23:AJ:191:GLU:HB2	1.94	0.49
45:S8:161:TRP:HB3	54:AL:84:PRO:HG2	1.94	0.49
13:D6:25:SER:HB3	13:D6:28:TYR:HD2	1.76	0.49
15:D5:7:LEU:HA	15:D5:10:VAL:HG22	1.93	0.49
19:B5:26:ARG:O	19:B5:30:LEU:HB2	2.11	0.49
41:S1:496:ILE:HG22	41:S1:499:GLN:H	1.77	0.49
46:V3:38:TYR:CZ	46:V3:40:ASN:HB2	2.47	0.49
47:S6:22:ASP:OD1	49:A9:2:HIS:NE2	2.45	0.49
17:D2:174:GLN:HE21	17:D2:176:ARG:HH21	1.59	0.49
17:D2:328:THR:HG23	27:C2:68:PHE:HZ	1.77	0.49
42:S2:139:VAL:HG21	42:S2:277:VAL:HG12	1.95	0.49
43:S3:52:ILE:O	43:S3:109:THR:HA	2.13	0.49
47:S6:12:THR:OG1	47:S6:14:THR:O	2.27	0.49
15:D5:605:HIS:HA	17:D2:92:PRO:HB2	1.93	0.49
17:D2:181:TYR:HD1	17:D2:184:ILE:HD12	1.78	0.49
17:D2:230:LEU:HB3	17:D2:300:THR:HG22	1.93	0.49
20:AB:7:THR:HG23	20:AB:10:GLY:H	1.78	0.49
21:A8:91:SER:OG	21:A8:98:ARG:NE	2.43	0.49
23:AJ:183:ILE:HD11	23:AJ:191:GLU:HB3	1.94	0.49
39:V1:197:GLU:OE2	39:V1:204:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:S7:34:ASP:OD1	44:S7:38:ASN:ND2	2.45	0.49
49:A9:202:LYS:HA	49:A9:291:ASP:HB2	1.94	0.49
11:D3:69:ILE:HD11	12:D1:144:VAL:HG13	1.93	0.49
26:B3:28:LEU:HA	26:B3:31:VAL:HG12	1.94	0.49
41:S1:222:THR:HG22	41:S1:243:ARG:HB2	1.93	0.49
50:A2:64:LEU:HB3	50:A2:76:VAL:HG23	1.93	0.49
11:D3:98:LEU:HD22	12:D1:298:LEU:HD21	1.94	0.49
12:D1:46:LEU:HA	12:D1:49:ILE:HG22	1.94	0.49
15:D5:142:ILE:HA	16:D4:370:PRO:HB2	1.93	0.49
15:D5:380:LEU:HD23	15:D5:381:THR:HG23	1.93	0.49
16:D4:364:LEU:HD23	16:D4:367:LEU:HD23	1.94	0.49
30:B6:119:MET:SD	30:B6:120:LYS:N	2.86	0.49
39:V1:391:SER:OG	41:S1:129:ARG:NH1	2.46	0.49
42:S2:405:MET:SD	42:S2:421:GLN:NE2	2.86	0.49
13:D6:118:LYS:HB2	24:S5:69:GLN:HE21	1.78	0.49
37:B1:37:PHE:HA	37:B1:40:LYS:HE2	1.94	0.49
23:AJ:24:LEU:HB2	23:AJ:167:HIS:H	1.77	0.49
27:C2:20:SER:OG	27:C2:21:LEU:N	3.22	0.49
41:S1:668:ILE:HG21	41:S1:691:VAL:HG21	1.94	0.49
43:S3:37:VAL:O	53:A7:70:SER:O	2.30	0.49
44:S7:39:TRP:HA	44:S7:42:ARG:HE	1.77	0.49
23:AJ:304:TYR:HA	27:C2:50:ARG:HE	1.78	0.49
43:S3:48:LEU:HB3	43:S3:105:ILE:HG22	1.95	0.49
45:S8:93:THR:HB	45:S8:110:ASP:HB2	1.94	0.49
16:D4:176:PHE:O	16:D4:180:GLN:HB2	2.13	0.49
18:AK:140:VAL:H	19:B5:115:ARG:HD3	1.78	0.49
23:AJ:64:GLY:HA3	23:AJ:302:ARG:HH22	1.78	0.49
28:B4:42:LEU:HD13	34:B8:74:GLY:HA3	1.94	0.48
41:S1:107:ILE:HG22	45:S8:104:ARG:HD3	1.95	0.48
41:S1:504:ASP:O	50:A2:55:ARG:NH2	2.38	0.48
48:S4:33:ARG:HH22	48:S4:77:ASP:HA	1.78	0.48
49:A9:132:ILE:HD13	63:A9:401:NDP:H1D	1.95	0.48
15:D5:149:ILE:HG12	16:D4:364:LEU:HD21	1.95	0.48
18:AK:36:SER:HB2	18:AK:55:THR:HG22	1.95	0.48
18:AK:80:ARG:HH12	18:AK:87:LEU:HB3	1.78	0.48
42:S2:242:ILE:HB	42:S2:417:ILE:HD11	1.95	0.48
49:A9:81:ILE:HG21	49:A9:117:ILE:HG22	1.95	0.48
15:D5:9:LEU:HB3	30:B6:81:ILE:HD13	1.94	0.48
31:B7:41:THR:O	31:B7:45:MET:N	2.40	0.48
34:B8:30:ARG:HB3	34:B8:33:ASP:HB2	1.95	0.48
41:S1:628:PRO:HG2	50:A2:57:CYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BJ:16:THR:HB	30:B6:111:GLU:HG3	1.95	0.48
23:AJ:78:SER:HB2	23:AJ:81:LYS:HD3	1.95	0.48
23:AJ:97:GLN:HG2	23:AJ:135:LEU:HD13	1.96	0.48
32:B9:155:PRO:HA	32:B9:163:PRO:HB3	1.94	0.48
23:AJ:209:THR:O	23:AJ:213:GLU:N	2.44	0.48
39:V1:291:TRP:HE1	39:V1:313:GLU:HG2	1.78	0.48
41:S1:460:ARG:HG3	41:S1:462:ASP:H	1.78	0.48
48:S4:69:LEU:HD21	54:AL:126:PRO:HG2	1.95	0.48
49:A9:10:LYS:HG2	52:A6:113:ARG:HH12	1.78	0.48
51:A5:37:ILE:O	51:A5:44:ARG:NH1	2.46	0.48
15:D5:85:PHE:O	15:D5:89:PHE:CB	2.61	0.48
23:AJ:224:SER:OG	23:AJ:225:ALA:N	2.47	0.48
29:AM:29:LEU:HD12	29:AM:30:SER:H	1.78	0.48
30:B6:71:PHE:HA	30:B6:75:LEU:HD13	1.95	0.48
52:A6:43:PRO:HA	52:A6:46:VAL:HG12	1.96	0.48
15:D5:147:VAL:O	15:D5:151:SER:OG	2.31	0.48
21:A8:71:ARG:NH2	38:A1:70:ASP:OD1	2.40	0.48
22:BJ:72:ASP:OD2	22:BJ:74:THR:OG1	2.30	0.48
41:S1:239:VAL:HB	41:S1:253:ARG:HD3	1.96	0.48
45:S8:69:ARG:HA	45:S8:76:ARG:HB2	1.95	0.48
15:D5:335:PHE:HD2	15:D5:336:LYS:HG3	1.79	0.48
23:AJ:288:GLN:HA	23:AJ:291:ARG:HG2	1.94	0.48
28:B4:39:ARG:NH1	34:B8:62:TYR:OH	2.46	0.48
39:V1:214:GLY:HA3	39:V1:220:THR:HG22	1.96	0.48
41:S1:261:GLU:OE2	48:S4:42:ARG:NH2	2.47	0.48
45:S8:64:GLU:HA	45:S8:139:PHE:HZ	1.78	0.48
45:S8:78:ILE:HG23	45:S8:104:ARG:HD3	1.96	0.48
23:AJ:18:MET:HB3	23:AJ:19:THR:HB	1.95	0.48
29:AM:89:ASN:ND2	29:AM:92:GLU:OE1	2.47	0.48
39:V1:378:ARG:O	39:V1:382:GLY:N	2.47	0.48
42:S2:295:ASP:OD1	45:S8:6:ASN:ND2	2.41	0.48
15:D5:525:LEU:HD21	34:B8:95:PRO:HG2	1.94	0.48
16:D4:254:THR:O	16:D4:258:ALA:CB	2.62	0.48
16:D4:421:HIS:HE1	34:B8:67:PRO:HD3	1.79	0.48
34:B8:145:ASP:HB3	34:B8:148:LYS:HB2	1.95	0.48
38:A1:1:MET:HB3	45:S8:44:GLU:HG2	1.96	0.48
40:V2:24:THR:HG22	40:V2:26:GLU:H	1.78	0.48
41:S1:531:CYS:SG	41:S1:532:VAL:N	2.86	0.48
54:AL:25:ARG:HG3	54:AL:74:PHE:HE1	1.79	0.48
14:4L:19:LEU:HD13	14:4L:33:LEU:HB2	1.96	0.47
39:V1:145:GLU:HA	39:V1:148:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D1:292:ASN:HD22	25:A3:17:VAL:HG11	1.79	0.47
15:D5:246:LEU:O	15:D5:251:THR:OG1	2.30	0.47
17:D2:319:THR:HA	23:AJ:267:LEU:HD13	1.96	0.47
39:V1:30:ASP:OD2	39:V1:38:SER:OG	2.32	0.47
41:S1:12:PHE:HB2	41:S1:78:ASN:HA	1.96	0.47
54:AL:13:GLN:NE2	54:AL:33:VAL:O	2.46	0.47
54:AL:29:ARG:NH1	54:AL:74:PHE:O	2.47	0.47
15:D5:63:ILE:HA	30:B6:96:ILE:HG22	1.95	0.47
15:D5:353:GLU:HA	32:B9:82:PRO:HG3	1.96	0.47
15:D5:428:PHE:HA	15:D5:432:LEU:HD22	1.96	0.47
17:D2:30:TRP:HE1	17:D2:67:SER:HG	1.56	0.47
43:S3:80:ALA:HB2	43:S3:92:ILE:HD13	1.97	0.47
49:A9:40:ARG:HH12	52:A6:109:THR:HG22	1.80	0.47
19:B5:87:TYR:O	19:B5:90:THR:OG1	2.29	0.47
41:S1:366:THR:HA	41:S1:488:LYS:HD3	1.97	0.47
44:S7:87:ILE:HG12	44:S7:114:VAL:HB	1.97	0.47
54:AL:44:TYR:OH	54:AL:112:ASN:OD1	2.33	0.47
17:D2:26:TRP:HB3	17:D2:74:ILE:HD13	1.97	0.47
32:B9:3:LEU:HD11	32:B9:6:ALA:HB3	1.97	0.47
61:V1:501:FMN:O5'	61:V1:501:FMN:O3'	2.32	0.47
42:S2:184:VAL:O	45:S8:60:ARG:NH2	2.42	0.47
51:A5:26:LEU:HA	51:A5:29:LYS:HZ1	1.80	0.47
15:D5:553:LEU:HD11	28:B4:92:PHE:HB3	1.96	0.47
16:D4:106:LEU:HD13	16:D4:234:ILE:HG21	1.96	0.47
16:D4:197:LEU:O	16:D4:201:MET:CB	2.63	0.47
19:B5:64:TRP:CD1	19:B5:65:GLU:HG3	2.50	0.47
22:BJ:80:ASP:HB3	22:BJ:83:CYS:HB3	1.96	0.47
13:D6:169:MET:HE1	13:D6:175:ASN:HA	1.97	0.47
15:D5:367:PRO:HG3	33:B2:22:VAL:HG23	1.97	0.47
15:D5:513:PHE:HE1	32:B9:29:ARG:HG2	1.79	0.47
16:D4:251:ASN:OD1	16:D4:251:ASN:N	2.42	0.47
35:BK:100:ARG:HH11	35:BK:108:MET:H	1.61	0.47
37:B1:55:THR:HG23	37:B1:56:TRP:HD1	1.80	0.47
39:V1:94:VAL:HB	39:V1:222:VAL:HG22	1.96	0.47
40:V2:50:VAL:HG11	40:V2:73:LEU:HD11	1.96	0.47
41:S1:74:MET:H	41:S1:77:TRP:HE1	1.63	0.47
41:S1:275:LYS:HB2	54:AL:134:ILE:HG22	1.96	0.47
41:S1:527:ALA:H	41:S1:545:TYR:HE1	1.61	0.47
41:S1:544:VAL:HG22	41:S1:559:VAL:HB	1.97	0.47
53:A7:23:LEU:HD11	53:A7:27:TYR:HE2	1.78	0.47
13:D6:60:TYR:HD2	13:D6:61:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D5:220:ALA:O	15:D5:224:SER:OG	2.32	0.47
39:V1:36:ALA:HB1	39:V1:41:ASP:HB2	1.97	0.47
39:V1:86:SER:HA	39:V1:91:LYS:HZ1	1.80	0.47
39:V1:154:ARG:HD2	46:V3:54:LEU:HD21	1.95	0.47
42:S2:50:ASN:HD22	42:S2:65:VAL:HG22	1.80	0.47
17:D2:235:ASN:ND2	17:D2:307:SER:OG	2.46	0.47
32:B9:167:TRP:O	32:B9:171:THR:OG1	2.27	0.47
48:S4:28:GLU:O	48:S4:32:THR:CB	2.63	0.47
15:D5:172:ILE:HG21	16:D4:408:LEU:HD22	1.97	0.47
15:D5:535:ARG:NE	34:B8:90:ASP:O	2.45	0.47
16:D4:158:LEU:HD21	17:D2:283:ALA:HB1	1.97	0.47
41:S1:157:THR:O	41:S1:161:ARG:NE	2.43	0.47
17:D2:345:ILE:HD12	27:C2:78:ARG:HG2	1.97	0.46
31:B7:102:GLU:OE1	33:B2:57:SER:N	2.40	0.46
41:S1:315:VAL:HA	41:S1:521:MET:O	2.15	0.46
47:S6:26:VAL:HB	49:A9:87:HIS:HB2	1.96	0.46
49:A9:215:ILE:HA	49:A9:218:ILE:HG22	1.96	0.46
52:A6:28:LYS:NZ	59:AA:101:ZMP:O4	2.48	0.46
20:AB:52:MET:SD	32:B9:24:ARG:NH2	2.88	0.46
25:A3:48:THR:HG21	29:AM:57:ARG:HH21	1.79	0.46
28:B4:22:TYR:OH	32:B9:67:GLU:OE1	2.31	0.46
39:V1:309:LYS:NZ	39:V1:313:GLU:OE2	2.40	0.46
48:S4:10:LEU:HB3	48:S4:11:ILE:H	1.58	0.46
48:S4:57:MET:HB3	48:S4:84:LEU:HB2	1.97	0.46
22:BJ:14:ARG:HH22	30:B6:100:LYS:HA	1.81	0.46
26:B3:25:GLY:O	26:B3:29:GLU:HB2	2.16	0.46
44:S7:91:THR:HA	44:S7:119:CYS:HB3	1.97	0.46
11:D3:67:LEU:HD22	14:4L:65:VAL:HG23	1.97	0.46
15:D5:76:LEU:HB2	15:D5:136:ASN:HD21	1.80	0.46
15:D5:559:GLU:HA	15:D5:563:PRO:HD2	1.97	0.46
39:V1:288:THR:O	39:V1:293:ASN:ND2	2.44	0.46
41:S1:257:ASP:O	41:S1:394:ARG:NH2	2.48	0.46
42:S2:183:ARG:HD2	42:S2:207:LEU:HD13	1.98	0.46
42:S2:224:GLU:OE1	45:S8:40:TYR:OH	2.33	0.46
42:S2:347:HIS:O	42:S2:351:LEU:CB	2.63	0.46
15:D5:237:MET:HB3	15:D5:299:LYS:HB3	1.97	0.46
42:S2:68:LEU:HA	42:S2:74:ARG:N	2.30	0.46
15:D5:183:ILE:HD13	16:D4:382:VAL:HG11	1.98	0.46
22:BJ:3:SER:OG	22:BJ:4:TRP:N	2.49	0.46
41:S1:41:CYS:SG	41:S1:52:CYS:N	2.86	0.46
41:S1:469:ALA:HA	41:S1:472:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:S7:139:ILE:HG22	44:S7:140:VAL:HG13	1.98	0.46
51:A5:5:LYS:NZ	51:A5:75:GLN:OE1	2.48	0.46
12:D1:162:LEU:HD12	12:D1:165:LEU:HD23	1.97	0.46
15:D5:348:HIS:NE2	20:AB:2:ASP:OD2	2.48	0.46
23:AJ:151:HIS:CD2	23:AJ:279:LEU:HD11	2.51	0.46
41:S1:378:LEU:HG	41:S1:451:VAL:HG22	1.97	0.46
42:S2:168:PHE:HB3	44:S7:65:PRO:HG3	1.96	0.46
52:A6:63:ARG:NH2	20:AA:46:ASP:OD1	2.39	0.46
54:AL:41:GLU:HB3	54:AL:47:LYS:HG2	1.97	0.46
20:AB:69:LYS:HA	30:B6:2:GLY:HA2	1.98	0.46
21:A8:165:ARG:NH2	27:C2:87:ASP:OD1	2.39	0.46
28:B4:47:GLN:HE21	32:B9:165:LEU:HD23	1.80	0.46
39:V1:305:PRO:HB2	39:V1:327:THR:HG22	1.97	0.46
41:S1:547:GLY:O	41:S1:563:GLY:N	2.49	0.46
42:S2:53:PRO:HD3	42:S2:63:ARG:HE	1.80	0.46
43:S3:154:ASP:OD1	52:A6:101:HIS:NE2	2.42	0.46
17:D2:292:PHE:HA	17:D2:295:ARG:HG2	1.96	0.46
59:AB:101:ZMP:H21	32:B9:12:GLN:HG3	1.98	0.46
45:S8:151:LYS:HZ3	45:S8:155:LEU:HD11	1.80	0.46
49:A9:56:THR:HA	49:A9:59:LEU:HG	1.97	0.46
16:D4:150:LEU:HD21	17:D2:294:MET:HG2	1.97	0.46
39:V1:398:GLN:NE2	53:A7:52:TYR:OH	2.49	0.46
40:V2:126:ILE:HG21	40:V2:132:THR:HA	1.98	0.46
45:S8:145:GLU:HG2	49:A9:65:LEU:HG	1.98	0.46
49:A9:29:PHE:HE1	49:A9:175:GLU:H	1.64	0.46
49:A9:30:LEU:HD22	49:A9:94:LEU:HD21	1.97	0.46
17:D2:269:GLU:HA	17:D2:272:LYS:HG2	1.98	0.45
23:AJ:303:LYS:HG2	23:AJ:304:TYR:HD1	1.81	0.45
44:S7:116:MET:HA	44:S7:146:VAL:HG23	1.98	0.45
16:D4:457:PRO:O	35:BK:84:ARG:NH2	2.49	0.45
26:B3:36:ALA:HB1	26:B3:41:ARG:HE	1.82	0.45
28:B4:115:ILE:HG22	28:B4:120:LEU:HG	1.97	0.45
39:V1:71:ALA:HB1	39:V1:73:PHE:HD2	1.80	0.45
41:S1:43:HIS:O	48:S4:116:LYS:NZ	2.49	0.45
41:S1:307:LEU:HD21	41:S1:338:VAL:HG22	1.98	0.45
41:S1:425:SER:HB3	41:S1:428:ILE:HG13	1.98	0.45
41:S1:431:ASP:HB3	41:S1:437:HIS:HE1	1.80	0.45
42:S2:366:ALA:HA	42:S2:374:PHE:O	2.16	0.45
43:S3:38:GLN:HE22	43:S3:110:TYR:HE1	1.64	0.45
44:S7:71:ARG:HH22	45:S8:50:TYR:HB2	1.81	0.45
44:S7:171:LYS:HB2	44:S7:174:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A9:53:PRO:O	49:A9:57:MET:HB2	2.16	0.45
49:A9:137:ALA:HA	49:A9:146:LEU:HB3	1.98	0.45
13:D6:17:PHE:HD2	14:4L:11:ALA:HB1	1.82	0.45
49:A9:19:ILE:O	49:A9:43:SER:OG	2.31	0.45
51:A5:39:LYS:HA	51:A5:44:ARG:HD3	1.97	0.45
15:D5:384:PRO:HA	15:D5:385:PHE:HA	1.64	0.45
21:A8:171:MET:OXT	27:C2:30:ARG:NH1	2.32	0.45
39:V1:362:CYS:HB3	39:V1:364:PRO:HD2	1.98	0.45
40:V2:120:ILE:HD13	40:V2:173:ILE:HD11	1.99	0.45
41:S1:321:GLY:O	41:S1:498:SER:OG	2.28	0.45
50:A2:17:GLU:HG2	50:A2:51:PRO:HG2	1.99	0.45
20:AA:32:VAL:HG12	20:AA:74:GLN:HE21	1.81	0.45
21:A8:34:GLN:OE1	21:A8:116:TRP:NE1	2.46	0.45
31:B7:94:TYR:OH	34:B8:126:GLN:OE1	2.29	0.45
39:V1:94:VAL:HA	39:V1:135:TYR:O	2.16	0.45
15:D5:245:ALA:O	15:D5:249:SER:CB	2.64	0.45
20:AB:20:LYS:NZ	20:AB:27:PRO:O	2.49	0.45
39:V1:101:GLU:HB3	39:V1:302:SER:H	1.81	0.45
41:S1:377:VAL:HA	41:S1:450:MET:O	2.16	0.45
42:S2:347:HIS:O	42:S2:351:LEU:HB2	2.15	0.45
47:S6:51:GLN:HG2	47:S6:92:ARG:HB2	1.99	0.45
48:S4:19:ILE:HA	48:S4:22:LEU:HD12	1.99	0.45
15:D5:67:HIS:HA	15:D5:77:SER:HA	1.99	0.45
15:D5:418:PHE:HA	15:D5:421:ILE:HG12	1.99	0.45
15:D5:455:LYS:HE3	33:B2:28:PHE:HZ	1.82	0.45
21:A8:44:LEU:HD22	21:A8:130:VAL:HG13	1.99	0.45
41:S1:40:PHE:HB2	41:S1:52:CYS:HB2	1.99	0.45
41:S1:157:THR:HG23	41:S1:160:ILE:HD12	1.99	0.45
49:A9:48:PRO:HB2	49:A9:73:TRP:CD1	2.52	0.45
49:A9:108:ASP:O	49:A9:112:LYS:CB	2.59	0.45
15:D5:66:TRP:HE3	15:D5:78:LEU:HD23	1.82	0.45
29:AM:138:GLY:O	29:AM:142:TYR:CB	2.60	0.45
35:BK:64:PHE:HA	35:BK:68:ILE:HG22	1.98	0.45
40:V2:97:LYS:H	40:V2:136:LEU:H	1.65	0.45
42:S2:110:SER:OG	42:S2:114:ASN:OD1	2.30	0.45
42:S2:422:ASP:OD1	42:S2:422:ASP:N	2.48	0.45
45:S8:74:GLU:OE1	45:S8:105:ARG:NH2	2.46	0.45
17:D2:203:LEU:HD13	17:D2:343:LEU:HD12	1.99	0.45
19:B5:139:ALA:HB3	24:S5:28:ILE:HG22	1.99	0.45
40:V2:126:ILE:HG12	40:V2:132:THR:HB	1.99	0.45
41:S1:125:SER:OG	41:S1:126:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:424:ASP:OD1	41:S1:424:ASP:N	2.49	0.45
42:S2:176:LYS:HE3	53:A7:26:ARG:HH12	1.82	0.45
42:S2:282:GLU:HB2	42:S2:313:GLN:HE22	1.80	0.45
47:S6:11:VAL:HG12	47:S6:17:VAL:HG21	1.99	0.45
12:D1:37:PRO:HA	44:S7:71:ARG:HA	1.98	0.45
30:B6:10:ARG:HH21	32:B9:153:LEU:HD21	1.81	0.45
41:S1:328:LEU:HD22	41:S1:507:TYR:HE2	1.81	0.45
12:D1:50:ALA:HA	12:D1:53:ILE:HG22	1.98	0.44
12:D1:81:LEU:HD11	12:D1:111:LEU:HB3	1.99	0.44
15:D5:586:LEU:HD21	18:AK:44:THR:HG23	1.99	0.44
17:D2:88:LYS:HG3	17:D2:148:SER:HB3	1.98	0.44
22:BJ:132:THR:HA	22:BJ:135:VAL:HG12	1.98	0.44
40:V2:78:MET:HA	40:V2:81:TYR:HD2	1.81	0.44
41:S1:379:LEU:HD23	41:S1:408:LEU:HD13	1.99	0.44
48:S4:118:TYR:HA	48:S4:121:ASN:HD22	1.81	0.44
51:A5:57:ILE:HG21	51:A5:71:LEU:HB2	1.99	0.44
12:D1:100:LEU:HD21	13:D6:51:PHE:HA	1.98	0.44
15:D5:1:MET:HG2	15:D5:3:LEU:H	1.82	0.44
15:D5:293:LEU:HD11	15:D5:421:ILE:HD11	2.00	0.44
15:D5:549:ALA:HA	15:D5:554:ASP:H	1.83	0.44
18:AK:94:CYS:HA	18:AK:114:CYS:HA	1.99	0.44
23:AJ:75:GLY:HA3	23:AJ:76:ASN:HA	1.74	0.44
39:V1:132:ARG:HH21	46:V3:63:MET:HB2	1.83	0.44
41:S1:43:HIS:HB3	41:S1:46:LEU:HB2	1.98	0.44
41:S1:226:GLU:HA	41:S1:253:ARG:HH12	1.83	0.44
42:S2:69:SER:O	42:S2:72:MET:O	2.36	0.44
47:S6:84:CYS:HB3	47:S6:87:CYS:HB2	1.98	0.44
35:BK:45:HIS:ND1	35:BK:54:ASP:OD1	2.44	0.44
41:S1:522:LEU:HD21	41:S1:543:ILE:HG22	1.98	0.44
45:S8:108:ARG:NH2	48:S4:71:GLY:O	2.50	0.44
49:A9:202:LYS:NZ	49:A9:291:ASP:OD2	2.47	0.44
13:D6:174:GLY:O	23:AJ:254:ARG:NH2	2.50	0.44
18:AK:106:SER:HB2	18:AK:109:ILE:HD12	2.00	0.44
31:B7:103:ARG:HH11	34:B8:158:ILE:HG23	1.82	0.44
49:A9:285:GLU:O	49:A9:289:THR:OG1	2.24	0.44
20:AA:31:SER:HB2	20:AA:34:SER:HB2	1.99	0.44
12:D1:316:PRO:HB3	29:AM:57:ARG:HD2	1.98	0.44
15:D5:483:PRO:HD2	15:D5:486:LEU:HD22	1.99	0.44
16:D4:361:LEU:HA	16:D4:364:LEU:HD12	1.99	0.44
41:S1:622:ARG:HA	41:S1:625:GLU:HB2	1.98	0.44
44:S7:125:TYR:HE1	45:S8:88:PRO:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D1:22:LEU:HB3	12:D1:48:PRO:HG2	1.98	0.44
16:D4:254:THR:O	16:D4:258:ALA:HB3	2.18	0.44
17:D2:228:LEU:HD23	23:AJ:276:PRO:HG2	2.00	0.44
19:B5:68:LYS:HG2	22:BJ:62:TYR:CZ	2.52	0.44
42:S2:383:SER:OG	42:S2:384:SER:N	2.50	0.44
52:A6:60:ASP:HA	52:A6:63:ARG:HG2	1.98	0.44
53:A7:26:ARG:HB2	53:A7:29:GLU:HB3	1.99	0.44
12:D1:178:ALA:HB1	12:D1:181:LEU:HB3	2.00	0.44
12:D1:258:ASN:OD1	12:D1:262:LYS:NZ	2.46	0.44
15:D5:85:PHE:O	15:D5:89:PHE:HB2	2.18	0.44
15:D5:326:PHE:HA	15:D5:329:ILE:HD12	1.99	0.44
24:S5:4:ASP:O	24:S5:8:LYS:HB3	2.18	0.44
41:S1:46:LEU:O	48:S4:116:LYS:NZ	2.44	0.44
41:S1:641:TYR:HB3	41:S1:644:GLN:HB2	2.00	0.44
42:S2:116:GLN:HG3	42:S2:138:ARG:HD3	1.98	0.44
54:AL:39:VAL:HG21	54:AL:50:GLU:HB3	2.00	0.44
12:D1:111:LEU:HA	12:D1:114:TYR:HD2	1.83	0.44
16:D4:13:PRO:HA	16:D4:16:TRP:HD1	1.83	0.44
16:D4:134:THR:HB	17:D2:302:LEU:HD23	2.00	0.44
16:D4:203:PHE:HE2	16:D4:246:ILE:HG12	1.83	0.44
23:AJ:19:THR:OG1	23:AJ:20:GLU:N	2.46	0.44
24:S5:4:ASP:HB2	27:C2:11:LEU:HD22	1.99	0.44
15:D5:358:LYS:HA	15:D5:436:ARG:HG3	1.99	0.44
16:D4:263:MET:HG3	28:B4:101:TYR:HD1	1.83	0.44
16:D4:298:ILE:HD13	16:D4:298:ILE:HA	1.70	0.44
17:D2:123:PRO:O	17:D2:126:SER:OG	2.33	0.44
29:AM:29:LEU:H	29:AM:29:LEU:HG	1.68	0.44
29:AM:93:GLU:HA	29:AM:96:ILE:HG22	1.99	0.44
41:S1:39:ARG:HD2	41:S1:42:TYR:HB3	1.99	0.44
41:S1:238:ILE:O	41:S1:253:ARG:NH1	2.51	0.44
53:A7:3:ALA:HB1	53:A7:7:ILE:HD11	2.00	0.44
54:AL:89:TRP:CD1	54:AL:97:PRO:HA	2.53	0.44
13:D6:85:SER:OG	13:D6:86:ASN:N	2.48	0.43
16:D4:403:THR:HA	16:D4:406:TYR:CE1	2.53	0.43
21:A8:121:LEU:HA	21:A8:122:GLY:HA2	1.69	0.43
22:BJ:105:ILE:HG22	22:BJ:131:PHE:HD1	1.83	0.43
28:B4:13:LEU:HD11	28:B4:18:ASP:HA	1.99	0.43
42:S2:334:LYS:O	42:S2:338:MET:HB2	2.18	0.43
49:A9:206:TYR:HD2	49:A9:208:VAL:HG22	1.83	0.43
17:D2:108:MET:SD	17:D2:161:SER:OG	2.75	0.43
22:BJ:159:LYS:NZ	27:C2:112:VAL:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B4:25:SER:HB3	28:B4:28:THR:HG23	1.99	0.43
39:V1:96:ASN:ND2	39:V1:187:GLY:O	2.50	0.43
41:S1:226:GLU:OE1	41:S1:253:ARG:NH2	2.51	0.43
49:A9:208:VAL:HA	49:A9:211:THR:HG22	1.99	0.43
52:A6:63:ARG:NH1	20:AA:49:GLU:OE2	2.51	0.43
52:A6:69:ASN:O	59:AA:101:ZMP:N1	2.42	0.43
16:D4:203:PHE:O	16:D4:207:MET:HG2	2.19	0.43
24:S5:5:VAL:HG13	24:S5:9:LEU:HD12	2.01	0.43
39:V1:302:SER:HB3	39:V1:350:LEU:HD11	1.98	0.43
40:V2:13:PRO:HA	40:V2:15:ASN:H	1.83	0.43
59:AA:101:ZMP:P1	59:AA:101:ZMP:HO4	2.41	0.43
13:D6:159:TRP:HE1	17:D2:12:THR:HG22	1.83	0.43
15:D5:375:ILE:HD12	33:B2:32:MET:HG3	2.00	0.43
16:D4:254:THR:HG21	16:D4:304:GLN:HE22	1.84	0.43
41:S1:594:ARG:NH2	52:A6:122:TYR:O	2.51	0.43
42:S2:379:VAL:HG13	51:A5:113:TRP:HZ2	1.83	0.43
17:D2:346:LEU:O	27:C2:78:ARG:NH2	2.51	0.43
23:AJ:189:PRO:HA	23:AJ:192:MET:HB2	2.01	0.43
24:S5:88:GLU:HG2	24:S5:90:LYS:HE3	2.00	0.43
28:B4:100:TRP:HA	28:B4:103:VAL:HG22	2.00	0.43
28:B4:120:LEU:HD12	28:B4:122:ARG:HB3	2.01	0.43
41:S1:108:CYS:SG	41:S1:109:ASP:N	2.91	0.43
42:S2:308:ILE:HD13	42:S2:311:ILE:HD12	2.00	0.43
43:S3:78:LEU:HD11	43:S3:130:TYR:HB3	2.00	0.43
15:D5:332:HIS:CE1	15:D5:336:LYS:HD2	2.53	0.43
17:D2:222:ASN:HD22	17:D2:233:THR:HG21	1.84	0.43
25:A3:48:THR:HB	29:AM:64:PHE:HE2	1.84	0.43
25:A3:58:ASP:OD1	25:A3:58:ASP:N	2.51	0.43
31:B7:115:GLU:O	31:B7:119:ALA:CB	2.61	0.43
39:V1:97:ALA:HB3	39:V1:137:TYR:O	2.18	0.43
41:S1:336:ASN:ND2	50:A2:67:ARG:HH11	2.17	0.43
41:S1:349:PHE:H	41:S1:509:PRO:HB2	1.84	0.43
42:S2:176:LYS:NZ	53:A7:24:GLN:OE1	2.37	0.43
42:S2:246:THR:O	42:S2:250:ALA:N	2.47	0.43
42:S2:276:ASP:N	42:S2:276:ASP:OD1	2.51	0.43
43:S3:86:ARG:HE	51:A5:115:ILE:HD12	1.84	0.43
45:S8:95:GLU:OE1	45:S8:108:ARG:NH1	2.52	0.43
14:4L:73:LEU:HD21	17:D2:41:ILE:HG13	2.01	0.43
15:D5:542:LEU:HD21	16:D4:277:LEU:HD22	2.00	0.43
17:D2:139:MET:HG3	17:D2:205:LEU:HD22	2.01	0.43
17:D2:232:HIS:CE1	23:AJ:276:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A8:82:THR:HA	21:A8:85:TRP:CD1	2.53	0.43
23:AJ:171:TYR:HD2	23:AJ:222:GLN:HG3	1.83	0.43
25:A3:79:TRP:HA	25:A3:82:ARG:HB2	2.01	0.43
33:B2:62:GLU:HA	33:B2:66:ILE:H	1.83	0.43
34:B8:64:TRP:NE1	34:B8:66:HIS:O	2.47	0.43
39:V1:69:GLY:O	61:V1:501:FMN:O2'	2.36	0.43
16:D4:14:LEU:HD21	16:D4:26:ASN:HB3	2.00	0.43
20:AB:73:PRO:HA	20:AB:76:ILE:HD12	1.99	0.43
39:V1:184:TYR:HE2	39:V1:407:LEU:HD13	1.83	0.43
41:S1:478:ARG:HD2	41:S1:642:PHE:HD2	1.83	0.43
44:S7:155:ALA:HB2	45:S8:137:PHE:HD2	1.83	0.43
52:A6:30:ARG:HB3	52:A6:82:VAL:HG11	2.01	0.43
11:D3:81:THR:O	25:A3:45:ASN:ND2	2.52	0.43
15:D5:141:PHE:HE2	16:D4:375:LEU:HD21	1.84	0.43
28:B4:25:SER:O	28:B4:28:THR:OG1	2.32	0.43
39:V1:24:ASN:ND2	39:V1:30:ASP:H	2.17	0.43
39:V1:78:LYS:NZ	61:V1:501:FMN:O1P	2.46	0.43
39:V1:139:ARG:HH21	40:V2:145:LEU:HA	1.84	0.43
46:V3:47:SER:OG	46:V3:48:THR:N	2.52	0.43
16:D4:297:VAL:O	16:D4:301:ILE:HG12	2.19	0.43
26:B3:25:GLY:O	26:B3:29:GLU:CB	2.67	0.43
35:BK:31:GLU:HA	35:BK:32:PRO:HA	1.87	0.43
41:S1:430:GLN:HE21	41:S1:656:LEU:HD13	1.84	0.43
41:S1:584:LYS:HG3	48:S4:36:ARG:HH11	1.84	0.43
43:S3:77:ASP:O	43:S3:93:VAL:O	2.37	0.43
48:S4:23:THR:HG23	48:S4:25:VAL:HG12	2.01	0.43
13:D6:138:GLU:OE1	14:4L:52:HIS:ND1	2.39	0.42
16:D4:221:VAL:HG23	16:D4:222:GLU:HG3	2.00	0.42
22:BJ:118:GLU:HG3	30:B6:99:LYS:HE3	2.00	0.42
24:S5:50:ARG:HA	24:S5:53:LYS:HB2	2.01	0.42
39:V1:118:LEU:HD12	39:V1:225:VAL:HG13	1.99	0.42
41:S1:30:CYS:HB3	41:S1:35:MET:HB2	2.01	0.42
42:S2:69:SER:O	42:S2:72:MET:C	2.57	0.42
19:B5:50:ALA:HA	22:BJ:60:TYR:HB2	2.01	0.42
21:A8:157:LEU:HD11	27:C2:21:LEU:HB3	2.00	0.42
41:S1:105:CYS:SG	41:S1:117:GLN:NE2	2.91	0.42
42:S2:417:ILE:HA	42:S2:420:THR:HG22	2.02	0.42
44:S7:141:PRO:HB3	49:A9:61:PRO:HD3	2.01	0.42
23:AJ:188:ASN:O	23:AJ:192:MET:N	2.52	0.42
40:V2:156:ILE:HD11	40:V2:159:ASN:HD22	1.84	0.42
41:S1:139:ASP:HA	41:S1:150:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:521:MET:HG3	41:S1:542:PHE:HD2	1.85	0.42
42:S2:85:ARG:HG2	44:S7:91:THR:HG21	2.02	0.42
14:4L:62:ILE:HA	14:4L:65:VAL:HG12	2.00	0.42
16:D4:130:LEU:HD12	16:D4:149:PHE:HD2	1.84	0.42
16:D4:272:THR:HA	16:D4:275:ILE:HG22	2.01	0.42
18:AK:11:ILE:HG23	18:AK:16:GLU:HB3	2.01	0.42
20:AB:21:LEU:HD21	26:B3:47:ASN:HA	1.99	0.42
23:AJ:133:VAL:HG13	23:AJ:205:VAL:HG12	2.01	0.42
28:B4:46:TYR:O	28:B4:50:TYR:CB	2.67	0.42
34:B8:4:ILE:HG22	34:B8:6:LYS:H	1.84	0.42
39:V1:59:GLU:HG3	39:V1:234:ILE:HG22	2.00	0.42
39:V1:112:ARG:NH1	46:V3:38:TYR:OH	2.51	0.42
41:S1:160:ILE:HD11	41:S1:183:VAL:HG13	2.01	0.42
16:D4:424:ASN:OD1	28:B4:55:ARG:NH1	2.52	0.42
20:AB:52:MET:HG2	32:B9:23:LEU:HD12	2.02	0.42
32:B9:136:VAL:HG13	32:B9:164:PRO:HB3	2.01	0.42
39:V1:199:LYS:HZ1	48:S4:129:ARG:HE	1.67	0.42
39:V1:343:ILE:HD13	39:V1:422:PHE:HE2	1.84	0.42
42:S2:146:ARG:HG3	42:S2:370:PRO:HG3	2.01	0.42
42:S2:284:ASP:OD1	42:S2:284:ASP:N	2.51	0.42
48:S4:28:GLU:O	48:S4:32:THR:HB	2.18	0.42
53:A7:28:GLN:NE2	54:AL:52:ASN:OD1	2.39	0.42
13:D6:119:PHE:HA	14:4L:1:MET:HG2	2.02	0.42
17:D2:335:MET:O	27:C2:33:TYR:OH	2.28	0.42
21:A8:8:SER:OG	21:A8:9:LEU:N	2.52	0.42
27:C2:82:MET:SD	27:C2:82:MET:N	4.54	0.42
41:S1:483:VAL:HA	41:S1:484:THR:HA	1.57	0.42
12:D1:300:LEU:O	12:D1:304:HIS:ND1	2.42	0.42
15:D5:95:PHE:HZ	15:D5:456:ARG:HG2	1.85	0.42
15:D5:532:ILE:HD12	34:B8:105:LEU:HD13	2.01	0.42
16:D4:159:PRO:HB2	16:D4:198:ALA:HB1	2.00	0.42
17:D2:141:VAL:O	17:D2:145:ILE:HG13	2.20	0.42
28:B4:77:PRO:HA	28:B4:78:ASN:HA	1.75	0.42
40:V2:164:LEU:HD21	40:V2:172:ILE:HD12	2.02	0.42
41:S1:381:GLY:HA3	41:S1:661:LEU:HD11	2.00	0.42
44:S7:55:CYS:HB3	44:S7:89:ALA:HB1	2.02	0.42
12:D1:193:THR:HB	12:D1:231:ILE:HG12	2.02	0.42
30:B6:25:GLN:NE2	32:B9:117:TYR:OH	2.43	0.42
41:S1:418:ARG:HG3	46:V3:75:HIS:CE1	2.54	0.42
41:S1:589:PRO:HD2	52:A6:125:HIS:HE1	1.83	0.42
43:S3:179:GLU:HG3	49:A9:36:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D6:146:LEU:HD11	14:4L:58:MET:HG3	2.02	0.42
16:D4:207:MET:HG3	16:D4:298:ILE:HD11	2.01	0.42
23:AJ:64:GLY:HA3	23:AJ:302:ARG:NH2	2.35	0.42
28:B4:13:LEU:HD22	28:B4:14:PRO:HD2	2.01	0.42
31:B7:34:LYS:HG3	34:B8:156:TYR:HD1	1.83	0.42
42:S2:80:ILE:HD12	42:S2:80:ILE:HA	1.92	0.42
16:D4:277:LEU:HD11	16:D4:405:LEU:HD22	2.01	0.42
59:AB:101:ZMP:H14	32:B9:59:ALA:HB1	2.02	0.42
41:S1:525:LEU:HD13	41:S1:546:GLN:HB3	2.01	0.42
43:S3:115:THR:HA	43:S3:116:PRO:HD3	1.84	0.42
45:S8:62:ARG:NE	45:S8:119:CYS:O	2.52	0.42
16:D4:258:ALA:HB1	16:D4:302:LEU:HD23	2.02	0.41
18:AK:101:GLY:HA2	18:AK:104:THR:HG22	2.02	0.41
29:AM:66:ALA:O	29:AM:70:LEU:CB	2.66	0.41
39:V1:287:VAL:HG11	39:V1:294:LEU:HB3	2.02	0.41
40:V2:99:HIS:CE1	40:V2:140:ILE:HG12	2.51	0.41
41:S1:570:SER:O	41:S1:620:ARG:NH2	2.53	0.41
42:S2:256:SER:HB3	42:S2:373:GLU:H	1.85	0.41
42:S2:323:ILE:HG22	42:S2:324:LYS:HG3	2.02	0.41
48:S4:28:GLU:O	48:S4:32:THR:OG1	2.37	0.41
15:D5:29:PHE:HB2	15:D5:32:TYR:HB2	2.02	0.41
15:D5:162:THR:O	15:D5:166:THR:OG1	2.29	0.41
15:D5:366:MET:SD	15:D5:366:MET:N	2.93	0.41
16:D4:177:LEU:O	16:D4:180:GLN:O	2.37	0.41
16:D4:431:THR:HG21	35:BK:45:HIS:CD2	2.55	0.41
28:B4:40:SER:OG	32:B9:150:THR:O	2.35	0.41
40:V2:104:THR:HA	40:V2:108:CYS:HB2	2.01	0.41
16:D4:336:ARG:HH21	16:D4:352:LEU:HD21	1.85	0.41
22:BJ:74:THR:O	27:C2:108:THR:OG1	2.28	0.41
43:S3:119:SER:HB2	43:S3:142:PHE:HB3	2.01	0.41
44:S7:144:ILE:HG13	44:S7:163:LEU:HB2	2.02	0.41
54:AL:4:LEU:O	54:AL:8:LYS:N	2.43	0.41
54:AL:42:ASP:OD2	54:AL:86:TRP:NE1	2.51	0.41
15:D5:556:ILE:HD11	28:B4:79:PHE:HB2	2.02	0.41
23:AJ:209:THR:HG22	23:AJ:213:GLU:HG3	2.03	0.41
27:C2:8:ARG:H	27:C2:9:ALA:HB3	1.85	0.41
32:B9:85:PRO:HA	32:B9:90:TYR:CD1	2.56	0.41
33:B2:42:HIS:ND1	33:B2:43:ASP:OD1	2.48	0.41
39:V1:63:SER:HB2	39:V1:242:PHE:HB3	2.02	0.41
40:V2:10:ARG:NH2	47:S6:76:ASP:O	2.53	0.41
41:S1:382:THR:HG23	41:S1:384:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:453:LEU:HB3	41:S1:492:ILE:HG22	2.02	0.41
48:S4:27:GLU:HA	48:S4:30:ILE:HB	2.02	0.41
19:B5:125:TYR:HA	19:B5:126:PRO:HD3	1.85	0.41
20:AB:22:TYR:HE2	20:AB:24:LYS:HG2	1.84	0.41
22:BJ:15:ARG:HH21	30:B6:109:ILE:HD11	1.86	0.41
23:AJ:313:GLY:HA3	23:AJ:314:ASP:HA	1.69	0.41
25:A3:52:TYR:HE1	29:AM:68:ILE:HG23	1.85	0.41
35:BK:71:VAL:HG13	35:BK:72:LEU:HD12	2.01	0.41
49:A9:245:VAL:O	49:A9:249:ALA:CB	2.58	0.41
52:A6:46:VAL:HG23	52:A6:51:LEU:HD12	2.02	0.41
16:D4:454:ILE:H	16:D4:454:ILE:HG13	1.74	0.41
38:A1:13:GLY:O	38:A1:17:PHE:N	2.53	0.41
41:S1:117:GLN:HG2	42:S2:346:ILE:HG23	2.02	0.41
42:S2:146:ARG:HH12	42:S2:270:ARG:HD3	1.86	0.41
13:D6:163:ILE:HA	13:D6:166:VAL:HG12	2.03	0.41
15:D5:552:LEU:HD11	28:B4:89:GLY:HA2	2.02	0.41
16:D4:436:LEU:O	16:D4:440:HIS:ND1	2.51	0.41
23:AJ:113:GLU:HB2	23:AJ:263:VAL:HG11	2.01	0.41
27:C2:59:HIS:CE1	27:C2:60:ARG:HG3	2.56	0.41
38:A1:49:GLU:HA	38:A1:52:ARG:HG2	2.03	0.41
38:A1:52:ARG:HE	38:A1:58:ASN:ND2	2.18	0.41
42:S2:82:LEU:HA	44:S7:95:LYS:HD3	2.02	0.41
49:A9:242:VAL:HA	49:A9:245:VAL:HG12	2.02	0.41
12:D1:199:ASP:HB2	12:D1:279:ARG:HD2	2.03	0.41
15:D5:137:LEU:HB3	15:D5:196:TRP:CD1	2.52	0.41
27:C2:66:THR:HG22	36:C1:27:LEU:HD23	2.02	0.41
41:S1:107:ILE:HA	45:S8:104:ARG:HH11	1.86	0.41
45:S8:62:ARG:HA	45:S8:133:GLU:HB3	2.02	0.41
45:S8:175:TYR:CZ	53:A7:38:PRO:HG3	2.56	0.41
53:A7:111:TYR:HA	53:A7:112:LEU:HA	1.83	0.41
13:D6:47:PHE:HD2	14:4L:46:LEU:HD22	1.85	0.41
15:D5:10:VAL:HG11	30:B6:78:VAL:HG22	2.03	0.41
16:D4:276:CYS:HB3	16:D4:288:TYR:HB2	2.03	0.41
17:D2:109:ALA:HB2	17:D2:161:SER:HA	2.02	0.41
17:D2:327:PRO:HB3	27:C2:44:ILE:HG23	2.03	0.41
23:AJ:51:PHE:HA	23:AJ:52:PRO:HD3	1.90	0.41
23:AJ:251:GLN:H	23:AJ:252:ASP:HA	1.86	0.41
30:B6:103:ILE:HD11	31:B7:47:ASP:HB3	2.02	0.41
32:B9:82:PRO:HB3	32:B9:88:THR:HB	2.03	0.41
32:B9:90:TYR:OH	34:B8:86:ARG:NH1	2.53	0.41
41:S1:229:ASP:HB3	41:S1:235:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S1:409:ILE:HG12	41:S1:422:LEU:HB2	2.02	0.41
43:S3:37:VAL:HG12	53:A7:70:SER:HB3	2.02	0.41
14:4L:8:ILE:HG22	14:4L:43:LEU:HD12	2.02	0.41
15:D5:602:LEU:HD22	15:D5:602:LEU:HA	1.94	0.41
39:V1:260:GLY:O	40:V2:111:ARG:NH1	2.47	0.41
40:V2:32:GLU:O	40:V2:36:LYS:HB2	2.20	0.41
41:S1:667:THR:OG1	41:S1:668:ILE:N	2.52	0.41
50:A2:19:ARG:HB2	50:A2:65:TRP:HB2	2.02	0.41
13:D6:17:PHE:CD2	14:4L:11:ALA:HB1	2.56	0.40
14:4L:66:PHE:HB3	17:D2:34:GLU:OE1	2.21	0.40
15:D5:542:LEU:HD23	15:D5:542:LEU:HA	1.90	0.40
16:D4:358:TRP:HZ3	16:D4:441:MET:HB2	1.85	0.40
21:A8:70:PHE:HA	21:A8:73:ILE:HG22	2.03	0.40
23:AJ:100:LEU:HB3	23:AJ:104:ARG:NH1	2.36	0.40
35:BK:63:PHE:HA	35:BK:67:SER:HB3	2.03	0.40
38:A1:6:LEU:HD23	38:A1:9:ILE:HD12	2.03	0.40
44:S7:127:HIS:O	44:S7:134:ARG:NE	2.54	0.40
48:S4:103:TYR:HD2	48:S4:105:VAL:HG23	1.86	0.40
49:A9:114:PRO:HA	49:A9:117:ILE:HG13	2.02	0.40
49:A9:128:LYS:NZ	49:A9:218:ILE:O	2.46	0.40
16:D4:44:GLN:HE21	16:D4:49:SER:HA	1.86	0.40
17:D2:297:THR:HG22	17:D2:302:LEU:HD13	2.03	0.40
41:S1:117:GLN:HB3	42:S2:350:LYS:HG3	2.03	0.40
49:A9:308:THR:HA	49:A9:309:PRO:HD3	1.93	0.40
12:D1:18:ALA:O	12:D1:21:THR:OG1	2.31	0.40
15:D5:15:LEU:HD21	15:D5:125:LEU:HD22	2.04	0.40
15:D5:386:LEU:HD23	15:D5:387:THR:H	1.86	0.40
16:D4:113:THR:HG22	16:D4:114:GLU:HG3	2.04	0.40
18:AK:46:THR:HA	18:AK:47:SER:HA	1.77	0.40
28:B4:74:ASN:ND2	28:B4:77:PRO:O	2.54	0.40
39:V1:300:GLY:HA2	39:V1:329:LEU:HD12	2.03	0.40
41:S1:382:THR:OG1	41:S1:383:ASN:N	2.54	0.40
43:S3:59:PRO:HG3	51:A5:96:TRP:CD2	2.56	0.40
45:S8:144:HIS:H	49:A9:60:ARG:NH2	2.19	0.40
54:AL:83:PRO:HA	54:AL:84:PRO:HD3	1.87	0.40
12:D1:220:PHE:O	12:D1:224:PHE:HB2	2.21	0.40
12:D1:316:PRO:HB2	29:AM:60:GLN:HG3	2.03	0.40
16:D4:89:LEU:HD21	16:D4:93:LYS:HE3	2.04	0.40
19:B5:136:SER:HB3	24:S5:27:ARG:HD3	2.03	0.40
21:A8:129:LYS:HE3	25:A3:58:ASP:HB2	2.03	0.40
22:BJ:21:PRO:HA	22:BJ:22:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AJ:19:THR:HG23	23:AJ:20:GLU:HG3	2.03	0.40
29:AM:110:PHE:HE2	29:AM:116:VAL:HG21	1.85	0.40
41:S1:332:LYS:HD3	41:S1:507:TYR:HE1	1.87	0.40
42:S2:49:LEU:HD13	42:S2:68:LEU:HD21	2.02	0.40
49:A9:114:PRO:O	49:A9:118:ALA:HB3	2.21	0.40
51:A5:74:GLY:HA2	51:A5:75:GLN:HA	1.66	0.40
20:AA:27:PRO:HG2	20:AA:29:LYS:HB2	2.03	0.40
12:D1:55:LEU:HD12	12:D1:221:ALA:HB2	2.03	0.40
15:D5:548:SER:O	15:D5:551:SER:N	2.47	0.40
16:D4:205:VAL:HG22	16:D4:212:LEU:HD13	2.03	0.40
17:D2:315:TRP:HZ3	23:AJ:292:VAL:HG12	1.85	0.40
34:B8:133:TYR:HB2	34:B8:137:ASN:HD22	1.87	0.40
49:A9:281:ARG:NH1	49:A9:285:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a1	435/446 (98%)	399 (92%)	36 (8%)	0	100	100
1	a3	442/446 (99%)	403 (91%)	39 (9%)	0	100	100
2	a2	410/439 (93%)	381 (93%)	29 (7%)	0	100	100
2	a4	409/439 (93%)	375 (92%)	34 (8%)	0	100	100
3	b1	376/379 (99%)	360 (96%)	16 (4%)	0	100	100
3	b2	376/379 (99%)	353 (94%)	23 (6%)	0	100	100
4	c1	236/240 (98%)	200 (85%)	36 (15%)	0	100	100
4	c2	236/240 (98%)	199 (84%)	37 (16%)	0	100	100
5	f1	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
5	f2	193/196 (98%)	173 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	d1	98/110 (89%)	90 (92%)	8 (8%)	0	100	100
6	d2	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	q1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
7	q2	73/81 (90%)	66 (90%)	7 (10%)	0	100	100
8	h1	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
8	h2	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	49 (89%)	6 (11%)	0	100	100
11	D3	85/115 (74%)	80 (94%)	5 (6%)	0	100	100
12	D1	292/318 (92%)	266 (91%)	25 (9%)	1 (0%)	41	76
13	D6	167/175 (95%)	142 (85%)	24 (14%)	1 (1%)	25	65
14	4L	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
15	D5	604/606 (100%)	538 (89%)	63 (10%)	3 (0%)	29	68
16	D4	457/459 (100%)	415 (91%)	41 (9%)	1 (0%)	47	81
17	D2	345/347 (99%)	318 (92%)	27 (8%)	0	100	100
18	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
19	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
20	AA	78/88 (89%)	65 (83%)	13 (17%)	0	100	100
20	AB	85/88 (97%)	78 (92%)	7 (8%)	0	100	100
21	A8	169/171 (99%)	140 (83%)	29 (17%)	0	100	100
22	BJ	169/175 (97%)	148 (88%)	20 (12%)	1 (1%)	25	65
23	AJ	317/320 (99%)	280 (88%)	36 (11%)	1 (0%)	41	76
24	S5	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
25	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
26	B3	71/97 (73%)	54 (76%)	16 (22%)	1 (1%)	11	47
27	C2	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
28	B4	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
29	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
30	B6	92/127 (72%)	78 (85%)	14 (15%)	0	100	100
31	B7	117/119 (98%)	93 (80%)	24 (20%)	0	100	100
32	B9	174/178 (98%)	144 (83%)	29 (17%)	1 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	B2	63/72 (88%)	56 (89%)	7 (11%)	0	100	100
34	B8	155/158 (98%)	121 (78%)	33 (21%)	1 (1%)	25	65
35	BK	100/125 (80%)	84 (84%)	16 (16%)	0	100	100
36	C1	44/49 (90%)	37 (84%)	7 (16%)	0	100	100
37	B1	50/57 (88%)	45 (90%)	5 (10%)	0	100	100
38	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
39	V1	428/445 (96%)	386 (90%)	42 (10%)	0	100	100
40	V2	210/217 (97%)	172 (82%)	38 (18%)	0	100	100
41	S1	686/704 (97%)	616 (90%)	69 (10%)	1 (0%)	51	85
42	S2	423/430 (98%)	377 (89%)	43 (10%)	3 (1%)	22	62
43	S3	206/228 (90%)	174 (84%)	32 (16%)	0	100	100
44	S7	154/179 (86%)	133 (86%)	20 (13%)	1 (1%)	25	65
45	S8	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
46	V3	39/75 (52%)	29 (74%)	10 (26%)	0	100	100
47	S6	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
48	S4	124/133 (93%)	107 (86%)	17 (14%)	0	100	100
49	A9	280/338 (83%)	241 (86%)	39 (14%)	0	100	100
50	A2	80/98 (82%)	67 (84%)	13 (16%)	0	100	100
51	A5	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
52	A6	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
53	A7	91/112 (81%)	76 (84%)	15 (16%)	0	100	100
54	AL	143/145 (99%)	121 (85%)	22 (15%)	0	100	100
All	All	11856/12556 (94%)	10556 (89%)	1284 (11%)	16 (0%)	54	85

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	D5	84	PHE
16	D4	53	SER
42	S2	293	CYS
42	S2	340	THR
44	S7	130	TYR
32	B9	11	HIS
34	B8	76	PRO

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Mol	Chain	Res	Type
42	S2	73	VAL
15	D5	527	GLY
23	AJ	240	TYR
26	B3	58	ASN
12	D1	68	ILE
13	D6	138	GLU
22	BJ	71	PRO
15	D5	549	ALA
41	S1	338	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a1	366/372 (98%)	361 (99%)	5 (1%)	67 81
1	a3	370/372 (100%)	363 (98%)	7 (2%)	57 75
2	a2	326/341 (96%)	322 (99%)	4 (1%)	71 84
2	a4	326/341 (96%)	323 (99%)	3 (1%)	78 87
3	b1	330/331 (100%)	328 (99%)	2 (1%)	86 92
3	b2	330/331 (100%)	329 (100%)	1 (0%)	92 95
4	c1	204/206 (99%)	201 (98%)	3 (2%)	65 80
4	c2	204/206 (99%)	201 (98%)	3 (2%)	65 80
5	f1	168/168 (100%)	167 (99%)	1 (1%)	86 92
5	f2	167/168 (99%)	166 (99%)	1 (1%)	86 92
6	d1	93/99 (94%)	93 (100%)	0	100 100
6	d2	94/99 (95%)	91 (97%)	3 (3%)	39 62
7	q1	66/72 (92%)	66 (100%)	0	100 100
7	q2	67/72 (93%)	66 (98%)	1 (2%)	65 80
8	h1	62/74 (84%)	62 (100%)	0	100 100
8	h2	62/74 (84%)	62 (100%)	0	100 100
10	i1	46/52 (88%)	45 (98%)	1 (2%)	52 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i2	48/52 (92%)	48 (100%)	0	100	100
11	D3	80/103 (78%)	78 (98%)	2 (2%)	47	68
12	D1	260/278 (94%)	257 (99%)	3 (1%)	71	84
13	D6	140/144 (97%)	140 (100%)	0	100	100
14	4L	87/87 (100%)	85 (98%)	2 (2%)	50	70
15	D5	539/539 (100%)	535 (99%)	4 (1%)	84	90
16	D4	412/412 (100%)	407 (99%)	5 (1%)	71	84
17	D2	315/315 (100%)	311 (99%)	4 (1%)	69	82
18	AK	101/101 (100%)	100 (99%)	1 (1%)	76	86
19	B5	122/125 (98%)	121 (99%)	1 (1%)	81	89
20	AA	74/81 (91%)	74 (100%)	0	100	100
20	AB	80/81 (99%)	78 (98%)	2 (2%)	47	68
21	A8	154/154 (100%)	150 (97%)	4 (3%)	46	67
22	BJ	155/157 (99%)	154 (99%)	1 (1%)	86	92
23	AJ	283/284 (100%)	282 (100%)	1 (0%)	91	94
24	S5	88/94 (94%)	88 (100%)	0	100	100
25	A3	65/71 (92%)	65 (100%)	0	100	100
26	B3	55/75 (73%)	53 (96%)	2 (4%)	35	59
27	C2	106/107 (99%)	106 (100%)	0	100	100
28	B4	114/114 (100%)	113 (99%)	1 (1%)	78	87
29	AM	119/121 (98%)	115 (97%)	4 (3%)	37	60
30	B6	91/121 (75%)	88 (97%)	3 (3%)	38	61
31	B7	108/108 (100%)	104 (96%)	4 (4%)	34	59
32	B9	159/160 (99%)	157 (99%)	2 (1%)	69	82
33	B2	58/62 (94%)	58 (100%)	0	100	100
34	B8	142/142 (100%)	140 (99%)	2 (1%)	67	81
35	BK	93/112 (83%)	92 (99%)	1 (1%)	73	85
36	C1	42/44 (96%)	42 (100%)	0	100	100
37	B1	48/53 (91%)	48 (100%)	0	100	100
38	A1	59/59 (100%)	56 (95%)	3 (5%)	24	50
39	V1	344/354 (97%)	340 (99%)	4 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	V2	182/183 (100%)	181 (100%)	1 (0%)	88 93
41	S1	578/588 (98%)	573 (99%)	5 (1%)	78 87
42	S2	370/371 (100%)	367 (99%)	3 (1%)	81 89
43	S3	189/204 (93%)	189 (100%)	0	100 100
44	S7	132/150 (88%)	130 (98%)	2 (2%)	65 80
45	S8	151/151 (100%)	150 (99%)	1 (1%)	84 90
46	V3	40/68 (59%)	37 (92%)	3 (8%)	13 40
47	S6	79/80 (99%)	79 (100%)	0	100 100
48	S4	113/119 (95%)	112 (99%)	1 (1%)	78 87
49	A9	239/292 (82%)	235 (98%)	4 (2%)	60 78
50	A2	73/81 (90%)	72 (99%)	1 (1%)	67 81
51	A5	99/101 (98%)	99 (100%)	0	100 100
52	A6	107/113 (95%)	107 (100%)	0	100 100
53	A7	83/94 (88%)	83 (100%)	0	100 100
54	AL	131/131 (100%)	128 (98%)	3 (2%)	50 70
All	All	10388/10814 (96%)	10273 (99%)	115 (1%)	74 85

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a1	53	ASN
1	a1	70	ARG
1	a1	146	ARG
1	a1	173	ASN
1	a1	176	LYS
2	a2	240	ARG
2	a2	248	ASN
2	a2	287	ARG
2	a2	313	ASN
3	b1	26	ASN
3	b1	80	ARG
4	c1	15	ARG
4	c1	163	ILE
4	c1	232	ARG
5	f1	71	MET
10	i1	50	LYS
1	a3	24	ARG

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Mol	Chain	Res	Type
1	a3	53	ASN
1	a3	69	ASN
1	a3	146	ARG
1	a3	176	LYS
1	a3	389	ARG
1	a3	445	ARG
2	a4	248	ASN
2	a4	287	ARG
2	a4	313	ASN
3	b2	80	ARG
4	c2	143	ARG
4	c2	200	ARG
4	c2	232	ARG
5	f2	86	ASN
6	d2	71	ARG
6	d2	99	ARG
6	d2	104	ARG
7	q2	36	ASN
11	D3	1	MET
11	D3	90	MET
12	D1	3	MET
12	D1	55	LEU
12	D1	129	LEU
14	4L	58	MET
14	4L	83	ASN
15	D5	82	MET
15	D5	113	ASN
15	D5	357	ARG
15	D5	581	LYS
16	D4	43	ASN
16	D4	86	LYS
16	D4	138	ASN
16	D4	143	LEU
16	D4	144	ASN
17	D2	36	ASN
17	D2	204	ASN
17	D2	311	MET
17	D2	322	ARG
18	AK	139	LYS
19	B5	130	LYS
20	AB	33	ASN
20	AB	54	MET

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Mol	Chain	Res	Type
21	A8	63	ASN
21	A8	109	CYS
21	A8	134	ARG
21	A8	150	ASN
22	BJ	90	GLN
23	AJ	92	ASN
26	B3	47	ASN
26	B3	58	ASN
28	B4	74	ASN
29	AM	29	LEU
29	AM	60	GLN
29	AM	67	ARG
29	AM	89	ASN
30	B6	10	ARG
30	B6	89	VAL
30	B6	95	THR
31	B7	7	ARG
31	B7	83	GLN
31	B7	103	ARG
31	B7	105	ARG
32	B9	44	ARG
32	B9	157	ARG
34	B8	9	LEU
34	B8	137	ASN
35	BK	57	ASN
38	A1	50	ARG
38	A1	58	ASN
38	A1	68	ASN
39	V1	132	ARG
39	V1	337	MET
39	V1	365	CYS
39	V1	385	ARG
40	V2	190	ARG
41	S1	52	CYS
41	S1	152	ARG
41	S1	290	LEU
41	S1	488	LYS
41	S1	601	ARG
42	S2	34	ASN
42	S2	171	PHE
42	S2	388	ARG
44	S7	54	CYS

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Mol	Chain	Res	Type
44	S7	174	ARG
45	S8	8	ARG
46	V3	60	LYS
46	V3	63	MET
46	V3	70	ARG
48	S4	16	LYS
49	A9	199	LYS
49	A9	281	ARG
49	A9	292	ARG
49	A9	320	ARG
50	A2	33	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 (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	a1	159	GLN
1	a1	301	ASN
1	a1	418	GLN
2	a2	20	HIS
2	a2	125	ASN
2	a2	248	ASN
2	a2	313	ASN
2	a2	342	ASN
2	a2	343	GLN
3	b1	26	ASN
3	b1	85	ASN
4	c1	50	HIS
5	f1	53	ASN
7	q1	23	GLN
8	h1	67	HIS
10	i1	37	GLN
1	a3	15	GLN
1	a3	21	ASN
1	a3	53	ASN
1	a3	69	ASN
1	a3	189	HIS
1	a3	289	HIS
1	a3	341	GLN
1	a3	363	ASN

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Mol	Chain	Res	Type
2	a4	22	GLN
2	a4	104	ASN
2	a4	248	ASN
2	a4	290	ASN
2	a4	342	ASN
3	b2	322	GLN
3	b2	341	GLN
3	b2	345	HIS
4	c2	50	HIS
4	c2	106	ASN
5	f2	53	ASN
5	f2	122	HIS
7	q2	12	HIS
7	q2	23	GLN
7	q2	36	ASN
8	h2	71	HIS
10	i2	54	HIS
11	D3	10	ASN
12	D1	157	ASN
12	D1	171	GLN
12	D1	235	ASN
12	D1	284	GLN
13	D6	175	ASN
14	4L	83	ASN
15	D5	113	ASN
15	D5	116	GLN
15	D5	139	GLN
15	D5	175	ASN
15	D5	205	ASN
15	D5	484	HIS
15	D5	580	GLN
16	D4	81	GLN
16	D4	82	HIS
16	D4	138	ASN
16	D4	144	ASN
16	D4	304	GLN
16	D4	319	HIS
16	D4	421	HIS
17	D2	36	ASN
17	D2	63	GLN
17	D2	174	GLN
17	D2	235	ASN

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Mol	Chain	Res	Type
17	D2	310	ASN
17	D2	316	GLN
19	B5	69	HIS
19	B5	143	ASN
20	AB	33	ASN
21	A8	63	ASN
21	A8	150	ASN
22	BJ	55	HIS
22	BJ	77	HIS
22	BJ	103	ASN
22	BJ	114	GLN
22	BJ	122	GLN
22	BJ	139	GLN
23	AJ	76	ASN
23	AJ	92	ASN
23	AJ	151	HIS
23	AJ	204	ASN
23	AJ	251	GLN
24	S5	33	HIS
24	S5	69	GLN
25	A3	45	ASN
25	A3	70	GLN
26	B3	47	ASN
26	B3	58	ASN
28	B4	47	GLN
28	B4	74	ASN
29	AM	60	GLN
29	AM	89	ASN
30	B6	25	GLN
30	B6	73	HIS
31	B7	75	ASN
32	B9	11	HIS
32	B9	32	HIS
32	B9	168	HIS
34	B8	104	HIS
34	B8	137	ASN
35	BK	27	GLN
35	BK	57	ASN
38	A1	27	HIS
38	A1	58	ASN
38	A1	68	ASN
39	V1	398	GLN

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Mol	Chain	Res	Type
39	V1	435	GLN
40	V2	67	ASN
40	V2	99	HIS
40	V2	159	ASN
41	S1	179	ASN
41	S1	336	ASN
41	S1	392	ASN
41	S1	430	GLN
41	S1	437	HIS
41	S1	459	GLN
41	S1	548	HIS
41	S1	682	GLN
42	S2	50	ASN
42	S2	135	GLN
42	S2	157	HIS
42	S2	200	HIS
46	V3	42	GLN
47	S6	13	HIS
48	S4	44	ASN
48	S4	121	ASN
49	A9	3	HIS
49	A9	36	ASN
49	A9	67	GLN
49	A9	148	ASN
49	A9	288	HIS
50	A2	47	ASN
50	A2	61	GLN
51	A5	110	GLN
52	A6	125	HIS
54	AL	72	ASN
20	AA	74	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	SF4	S8	202	45	0,12,12	-	-	-		
60	SF4	S7	300	44	0,12,12	-	-	-		
60	SF4	S1	801	41	0,12,12	-	-	-		
55	HEM	b1	401	3	41,50,50	1.33	4 (9%)	45,82,82	1.88	10 (22%)
60	SF4	V1	500	39	0,12,12	-	-	-		
59	ZMP	AA	101	20	27,33,36	0.69	1 (3%)	32,40,45	1.00	2 (6%)
58	PC1	D2	401	-	27,27,53	0.40	0	33,35,61	0.35	0
55	HEM	b2	401	3	41,50,50	1.32	4 (9%)	45,82,82	1.76	7 (15%)
57	FES	f2	501	5	0,4,4	-	-	-		
61	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.42	0
56	HEC	c2	501	4	32,50,50	2.08	4 (12%)	24,82,82	2.13	11 (45%)
57	FES	S1	803	41	0,4,4	-	-	-		
63	NDP	A9	401	-	45,52,52	0.61	1 (2%)	53,80,80	0.68	1 (1%)
57	FES	f1	501	5	0,4,4	-	-	-		
57	FES	V2	300	40	0,4,4	-	-	-		
55	HEM	b1	402	3	41,50,50	1.35	5 (12%)	45,82,82	1.82	9 (20%)
60	SF4	S8	201	45	0,12,12	-	-	-		
60	SF4	S1	802	41	0,12,12	-	-	-		
56	HEC	c1	501	4	32,50,50	2.07	4 (12%)	24,82,82	2.44	14 (58%)
59	ZMP	AB	101	20	24,30,36	0.92	1 (4%)	29,37,45	1.12	2 (6%)
55	HEM	b2	402	3	41,50,50	1.35	4 (9%)	45,82,82	1.78	9 (20%)

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	SF4	S8	202	45	-	-	0/6/5/5
60	SF4	S7	300	44	-	-	0/6/5/5
60	SF4	S1	801	41	-	-	0/6/5/5
55	HEM	b1	401	3	-	3/12/54/54	-
60	SF4	V1	500	39	-	-	0/6/5/5
59	ZMP	AA	101	20	-	13/38/40/43	-
58	PC1	D2	401	-	-	12/31/31/57	-
55	HEM	b2	401	3	-	2/12/54/54	-
57	FES	f2	501	5	-	-	0/1/1/1
61	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
56	HEC	c2	501	4	-	2/10/54/54	-
63	NDP	A9	401	-	-	8/30/77/77	0/5/5/5
57	FES	S1	803	41	-	-	0/1/1/1
57	FES	f1	501	5	-	-	0/1/1/1
57	FES	V2	300	40	-	-	0/1/1/1
55	HEM	b1	402	3	-	6/12/54/54	-
60	SF4	S8	201	45	-	-	0/6/5/5
60	SF4	S1	802	41	-	-	0/6/5/5
56	HEC	c1	501	4	-	4/10/54/54	-
59	ZMP	AB	101	20	-	13/35/37/43	-
55	HEM	b2	402	3	-	6/12/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c1	501	HEC	C3C-C2C	-6.73	1.33	1.40
56	c2	501	HEC	C3C-C2C	-6.69	1.33	1.40
56	c2	501	HEC	C2B-C3B	-6.52	1.33	1.40
56	c1	501	HEC	C2B-C3B	-6.40	1.34	1.40
55	b1	402	HEM	C4D-ND	-4.15	1.33	1.40
55	b2	401	HEM	C4D-ND	-4.07	1.33	1.40
55	b2	402	HEM	C4D-ND	-4.05	1.33	1.40
55	b1	401	HEM	C4D-ND	-3.98	1.33	1.40
55	b1	401	HEM	C1B-NB	-3.73	1.33	1.40
55	b2	402	HEM	C1B-NB	-3.64	1.34	1.40
55	b1	402	HEM	C1B-NB	-3.57	1.34	1.40
56	c2	501	HEC	CBC-CAC	-3.41	1.36	1.49
56	c1	501	HEC	CBC-CAC	-3.40	1.36	1.49
55	b2	401	HEM	C1B-NB	-3.35	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	101	ZMP	C9-C10	3.32	1.54	1.50
55	b2	402	HEM	C1D-ND	-3.16	1.32	1.38
55	b1	402	HEM	C1D-ND	-2.99	1.32	1.38
55	b1	401	HEM	C1D-ND	-2.75	1.33	1.38
55	b2	401	HEM	C1D-ND	-2.70	1.33	1.38
55	b2	401	HEM	C4B-NB	-2.49	1.33	1.38
55	b1	402	HEM	C4B-NB	-2.44	1.33	1.38
56	c2	501	HEC	CBB-CAB	-2.37	1.40	1.49
56	c1	501	HEC	CBB-CAB	-2.34	1.40	1.49
55	b1	401	HEM	C4B-NB	-2.33	1.34	1.38
55	b2	402	HEM	C4B-NB	-2.30	1.34	1.38
59	AA	101	ZMP	C9-C10	2.22	1.53	1.50
55	b1	402	HEM	C3C-C2C	-2.11	1.37	1.40
63	A9	401	NDP	P2B-O2B	2.04	1.63	1.59

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	b1	401	HEM	CHC-C4B-NB	5.14	130.02	124.43
55	b1	402	HEM	CHC-C4B-NB	5.13	130.00	124.43
55	b2	401	HEM	CHC-C4B-NB	5.01	129.87	124.43
56	c1	501	HEC	CBD-CAD-C3D	4.74	120.71	112.62
55	b2	402	HEM	CHC-C4B-NB	4.66	129.50	124.43
56	c1	501	HEC	CMD-C2D-C1D	-4.42	121.67	128.46
55	b1	401	HEM	CHB-C1B-NB	4.33	129.73	124.38
55	b2	402	HEM	CHB-C1B-NB	4.33	129.73	124.38
55	b1	402	HEM	CHB-C1B-NB	4.14	129.50	124.38
55	b2	402	HEM	C4D-ND-C1D	4.12	109.33	105.07
55	b2	401	HEM	CHB-C1B-NB	4.07	129.41	124.38
55	b1	402	HEM	C4D-ND-C1D	4.07	109.27	105.07
56	c2	501	HEC	CMD-C2D-C1D	-3.86	122.53	128.46
56	c1	501	HEC	CMB-C2B-C3B	3.51	129.94	125.82
56	c2	501	HEC	CMC-C2C-C3C	3.49	129.93	125.82
56	c1	501	HEC	CMB-C2B-C1B	-3.47	123.14	128.46
55	b1	401	HEM	C4D-ND-C1D	3.42	108.61	105.07
55	b1	402	HEM	C1B-NB-C4B	3.36	108.54	105.07
55	b2	402	HEM	C1B-NB-C4B	3.27	108.45	105.07
56	c1	501	HEC	CMC-C2C-C3C	3.27	129.66	125.82
55	b1	402	HEM	CHA-C4D-ND	3.26	128.41	124.38
55	b2	401	HEM	C4D-ND-C1D	3.21	108.39	105.07
55	b1	401	HEM	CHD-C1D-ND	3.18	127.89	124.43
56	c2	501	HEC	CMB-C2B-C1B	-3.13	123.65	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	b1	401	HEM	C1B-NB-C4B	3.07	108.25	105.07
55	b2	401	HEM	C1B-NB-C4B	3.04	108.21	105.07
59	AB	101	ZMP	O1-C10-C9	-3.00	120.45	123.99
55	b2	402	HEM	CHD-C1D-ND	2.94	127.62	124.43
55	b2	401	HEM	CHA-C4D-ND	2.88	127.94	124.38
56	c2	501	HEC	C4C-C3C-C2C	2.87	109.45	106.35
55	b2	402	HEM	CHA-C4D-ND	2.84	127.89	124.38
56	c1	501	HEC	C4C-C3C-C2C	2.81	109.39	106.35
55	b1	401	HEM	CHA-C4D-ND	2.80	127.84	124.38
55	b2	401	HEM	CHD-C1D-ND	2.77	127.44	124.43
56	c1	501	HEC	O1D-CGD-CBD	-2.77	114.19	123.08
56	c2	501	HEC	CBD-CAD-C3D	2.70	117.23	112.62
56	c2	501	HEC	O1D-CGD-CBD	-2.68	114.47	123.08
56	c2	501	HEC	CMB-C2B-C3B	2.64	128.93	125.82
55	b1	401	HEM	C4B-C3B-C2B	-2.61	105.04	107.11
55	b1	401	HEM	CBD-CAD-C3D	-2.61	105.38	112.63
56	c2	501	HEC	CMC-C2C-C1C	-2.58	124.50	128.46
56	c1	501	HEC	CMD-C2D-C3D	2.56	129.78	124.94
55	b2	402	HEM	CHB-C1B-C2B	-2.56	119.63	126.72
56	c1	501	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
56	c1	501	HEC	CMA-C3A-C2A	2.47	129.59	124.94
63	A9	401	NDP	C5A-C6A-N6A	2.46	124.08	120.35
55	b1	402	HEM	CHD-C1D-ND	2.45	127.09	124.43
59	AA	101	ZMP	C15-C14-C13	-2.45	108.28	112.36
55	b1	402	HEM	CHB-C1B-C2B	-2.42	120.02	126.72
55	b1	401	HEM	CHB-C1B-C2B	-2.40	120.08	126.72
55	b2	401	HEM	CHB-C1B-C2B	-2.38	120.15	126.72
59	AB	101	ZMP	C9-C10-S1	2.31	116.15	113.46
55	b2	402	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
56	c2	501	HEC	CMD-C2D-C3D	2.29	129.26	124.94
59	AA	101	ZMP	O1-C10-C9	-2.25	121.33	123.99
56	c1	501	HEC	C1D-C2D-C3D	2.25	108.56	107.00
55	b1	401	HEM	CHC-C4B-C3B	-2.23	121.15	124.57
56	c2	501	HEC	O1A-CGA-CBA	-2.22	115.96	123.08
56	c1	501	HEC	O1A-CGA-CBA	-2.21	115.99	123.08
56	c2	501	HEC	CMA-C3A-C2A	2.17	129.03	124.94
55	b1	402	HEM	CAD-CBD-CGD	-2.17	108.93	113.60
55	b2	402	HEM	O2D-CGD-CBD	2.15	120.95	114.03
56	c1	501	HEC	O2A-CGA-O1A	2.10	128.53	123.30
56	c1	501	HEC	C2B-C3B-C4B	2.04	108.55	106.35
55	b1	402	HEM	O2D-CGD-CBD	2.02	120.52	114.03

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	b1	401	HEM	C2B-C3B-CAB-CBB
55	b1	402	HEM	C2B-C3B-CAB-CBB
55	b1	402	HEM	C4B-C3B-CAB-CBB
55	b2	401	HEM	C2B-C3B-CAB-CBB
55	b2	401	HEM	C4B-C3B-CAB-CBB
55	b2	402	HEM	C2B-C3B-CAB-CBB
55	b2	402	HEM	C4B-C3B-CAB-CBB
58	D2	401	PC1	C11-O13-P-O12
58	D2	401	PC1	C11-O13-P-O14
58	D2	401	PC1	C1-O11-P-O12
58	D2	401	PC1	O13-C11-C12-N
59	AB	101	ZMP	C17-C18-C21-O5
59	AB	101	ZMP	S1-C11-C12-N1
59	AB	101	ZMP	C12-C11-S1-C10
59	AB	101	ZMP	C7-C8-C9-C10
59	AA	101	ZMP	C17-C18-C21-O5
59	AA	101	ZMP	O4-C17-C18-C21
59	AA	101	ZMP	C16-C17-C18-C21
59	AA	101	ZMP	O4-C17-C18-C20
59	AA	101	ZMP	C16-C17-C18-C20
59	AA	101	ZMP	C13-C14-C15-N2
59	AA	101	ZMP	C12-C11-S1-C10
61	V1	501	FMN	N10-C1'-C2'-O2'
61	V1	501	FMN	C5'-O5'-P-O2P
61	V1	501	FMN	C5'-O5'-P-O3P
63	A9	401	NDP	C5B-O5B-PA-O1A
63	A9	401	NDP	O4D-C1D-N1N-C6N
59	AB	101	ZMP	C14-C13-N1-C12
59	AA	101	ZMP	C14-C13-N1-C12
63	A9	401	NDP	C1B-C2B-O2B-P2B
59	AB	101	ZMP	O2-C13-N1-C12
59	AA	101	ZMP	O2-C13-N1-C12
56	c1	501	HEC	C3D-CAD-CBD-CGD
56	c2	501	HEC	C2A-CAA-CBA-CGA
58	D2	401	PC1	C11-O13-P-O11
58	D2	401	PC1	C1-O11-P-O13
59	AB	101	ZMP	C5-C6-C7-C8
55	b1	401	HEM	C4B-C3B-CAB-CBB
56	c1	501	HEC	C2A-CAA-CBA-CGA
59	AB	101	ZMP	O3-C16-C17-O4
59	AA	101	ZMP	C20-C18-C21-O5
61	V1	501	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
59	AA	101	ZMP	O4-C17-C18-C19
55	b1	401	HEM	C2A-CAA-CBA-CGA
59	AB	101	ZMP	N2-C16-C17-C18
58	D2	401	PC1	O11-C1-C2-O21
59	AA	101	ZMP	C19-C18-C21-O5
59	AA	101	ZMP	C16-C17-C18-C19
63	A9	401	NDP	C5B-O5B-PA-O3
63	A9	401	NDP	C2B-O2B-P2B-O3X
63	A9	401	NDP	C5B-O5B-PA-O2A
58	D2	401	PC1	O11-C1-C2-C3
58	D2	401	PC1	C12-C11-O13-P
56	c2	501	HEC	C3D-CAD-CBD-CGD
59	AB	101	ZMP	C19-C18-C21-O5
59	AB	101	ZMP	C20-C18-C21-O5
63	A9	401	NDP	C3B-C2B-O2B-P2B
59	AB	101	ZMP	O3-C16-C17-C18
63	A9	401	NDP	O4B-C4B-C5B-O5B
59	AB	101	ZMP	C6-C7-C8-C9
61	V1	501	FMN	O3'-C3'-C4'-C5'
56	c1	501	HEC	CAD-CBD-CGD-O2D
55	b2	402	HEM	CAA-CBA-CGA-O2A
58	D2	401	PC1	O31-C31-C32-C33
55	b1	402	HEM	CAA-CBA-CGA-O1A
55	b1	402	HEM	CAA-CBA-CGA-O2A
55	b2	402	HEM	CAA-CBA-CGA-O1A
56	c1	501	HEC	CAD-CBD-CGD-O1D
55	b2	402	HEM	CAD-CBD-CGD-O1D
58	D2	401	PC1	O21-C21-C22-C23
55	b2	402	HEM	CAD-CBD-CGD-O2D
58	D2	401	PC1	O32-C31-C32-C33
55	b1	402	HEM	CAD-CBD-CGD-O1D
55	b1	402	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	S7	300	SF4	1	0
60	S1	801	SF4	1	0
60	V1	500	SF4	1	0
59	AA	101	ZMP	5	0
61	V1	501	FMN	3	0

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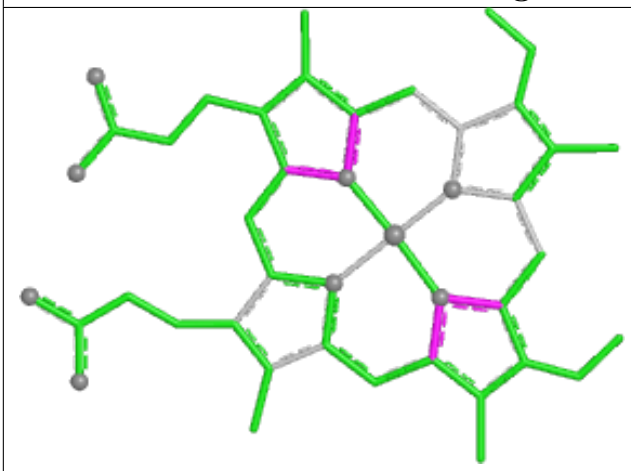
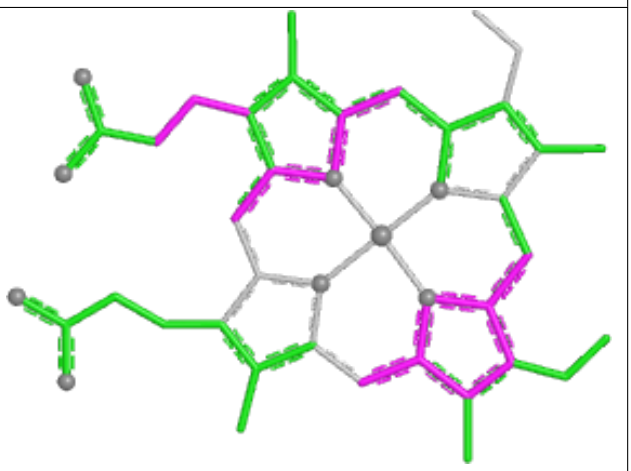
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	A9	401	NDP	3	0
60	S8	201	SF4	1	0
59	AB	101	ZMP	2	0

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

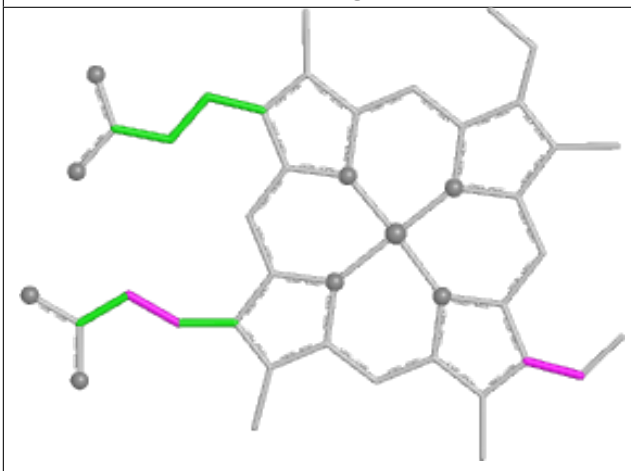
Ligand HEM b1 401



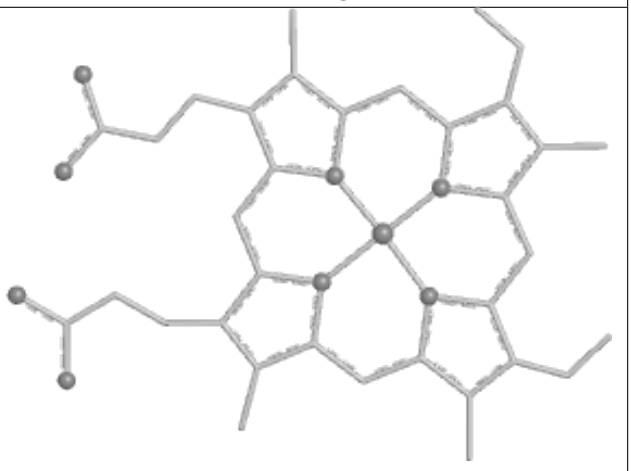
Bond lengths



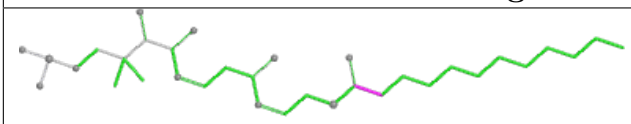
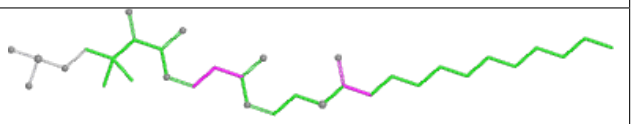
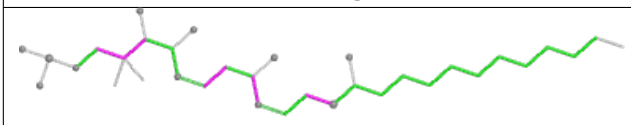
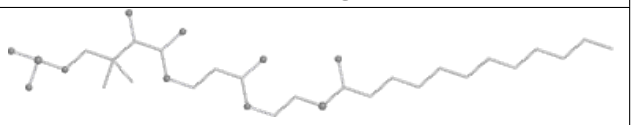
Bond angles

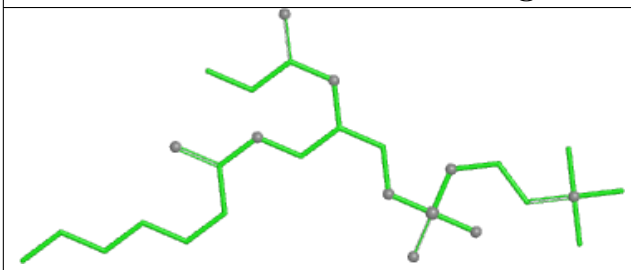
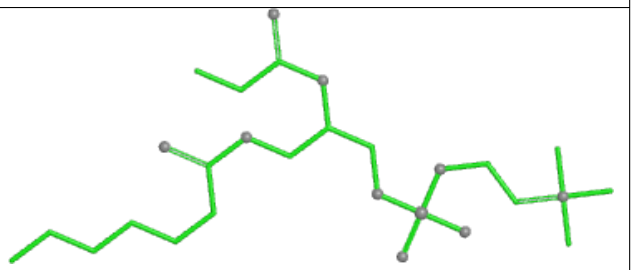
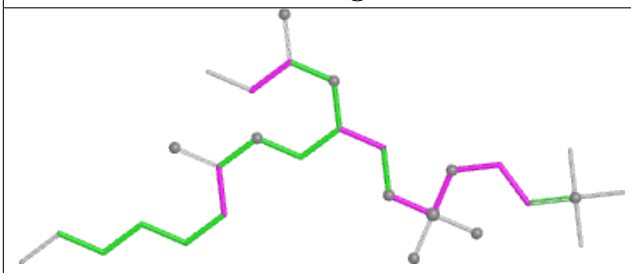
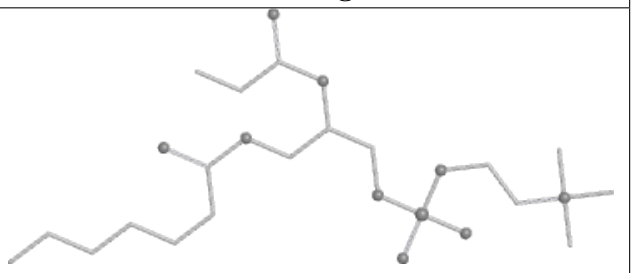


Torsions

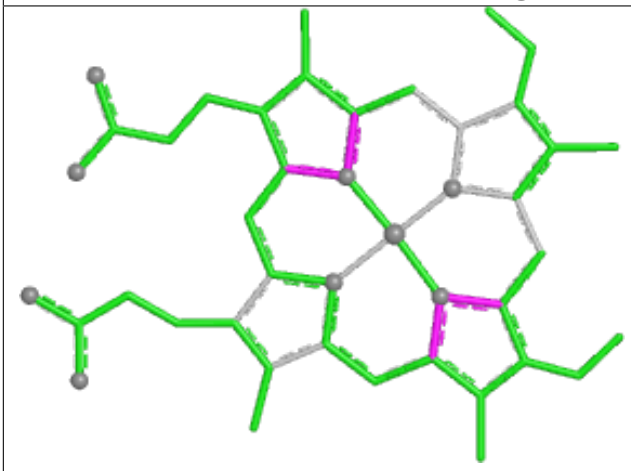


Rings

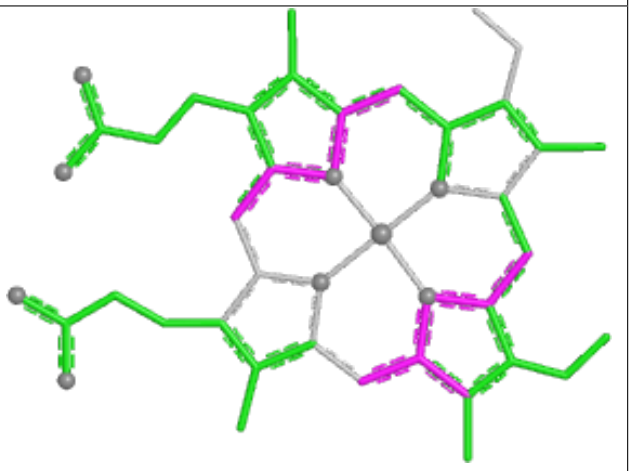
Ligand ZMP AA 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 D2 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM b2 401



Bond lengths



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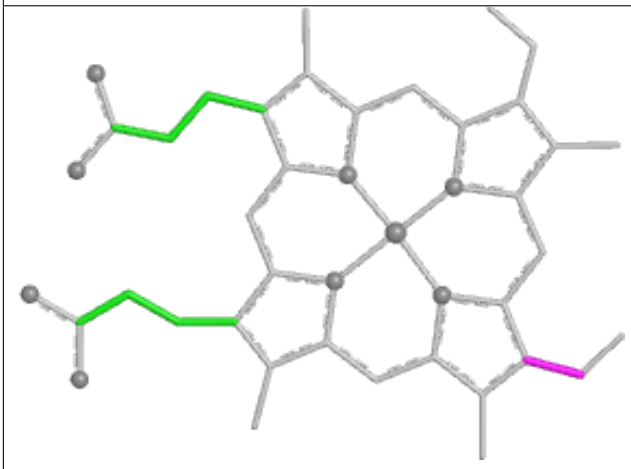
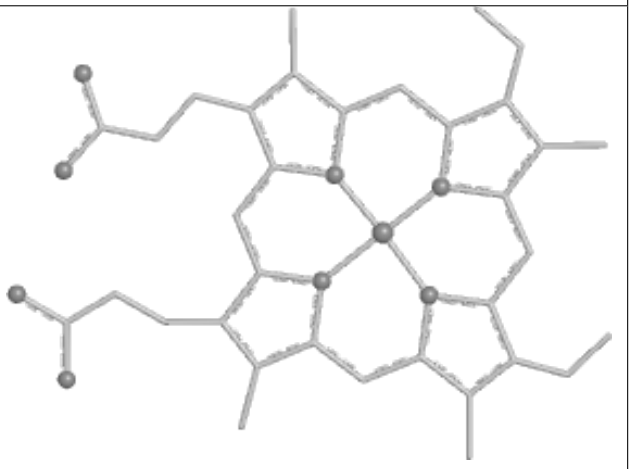
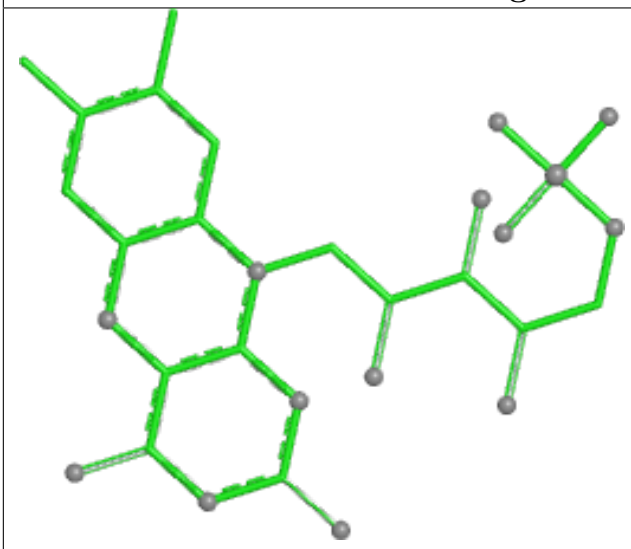


Torsions



Rings

Ligand FMN V1 501



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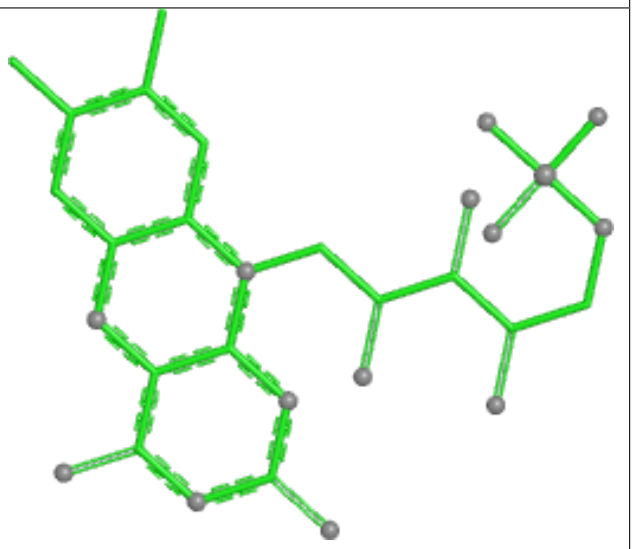

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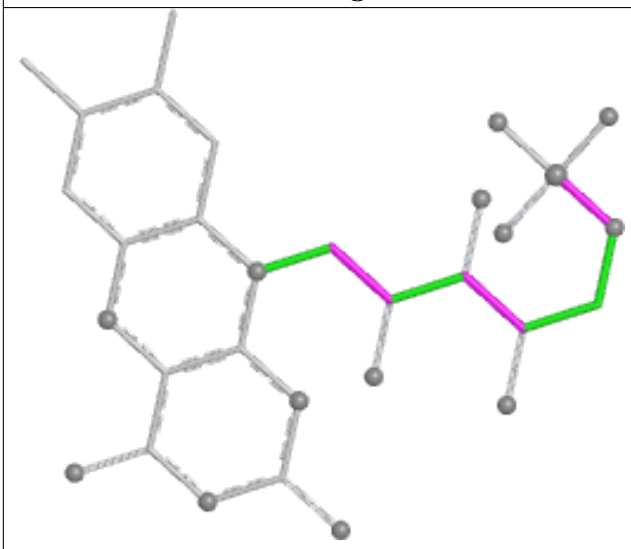

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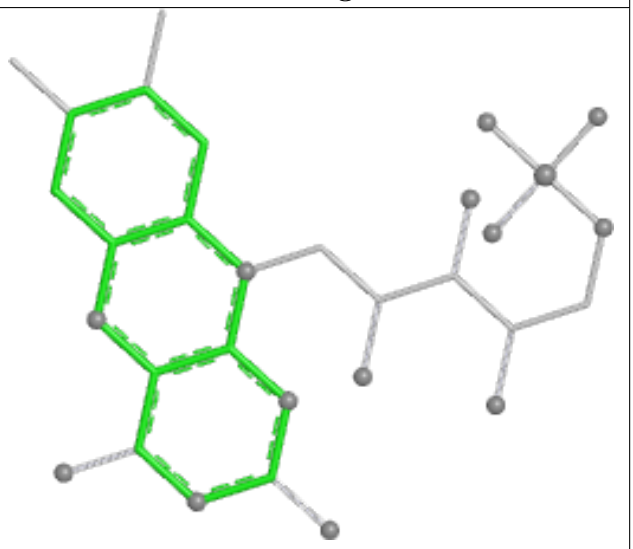
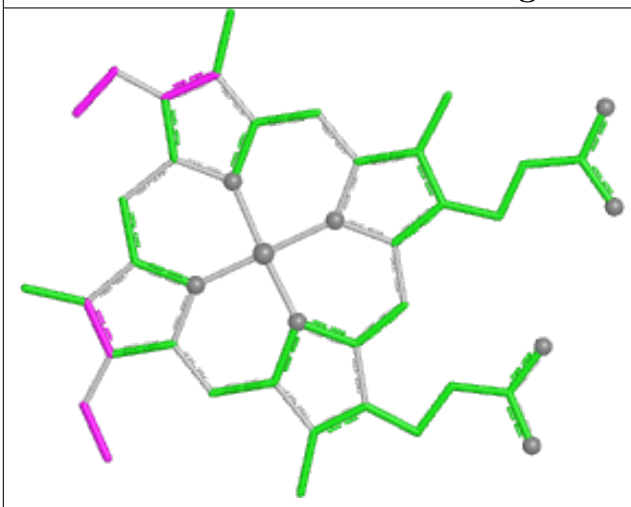


Rings

Ligand HEC c2 501



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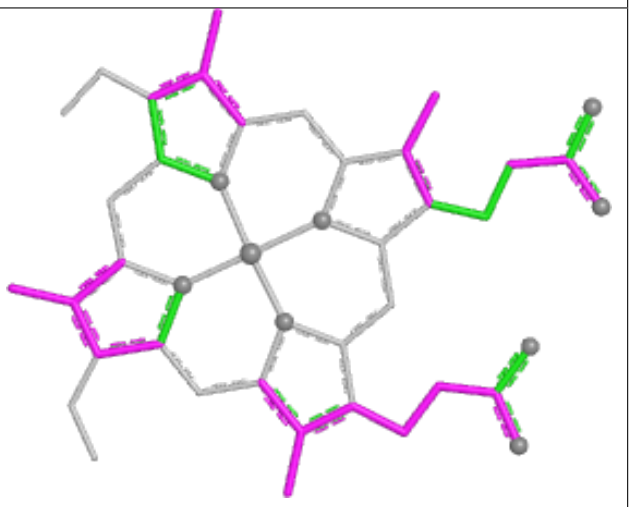

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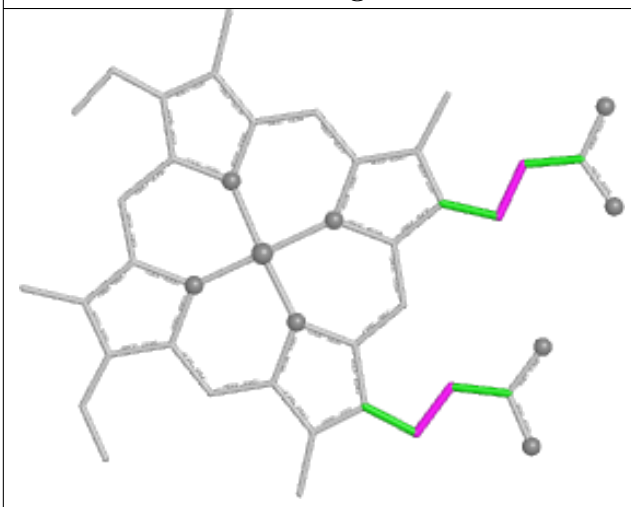

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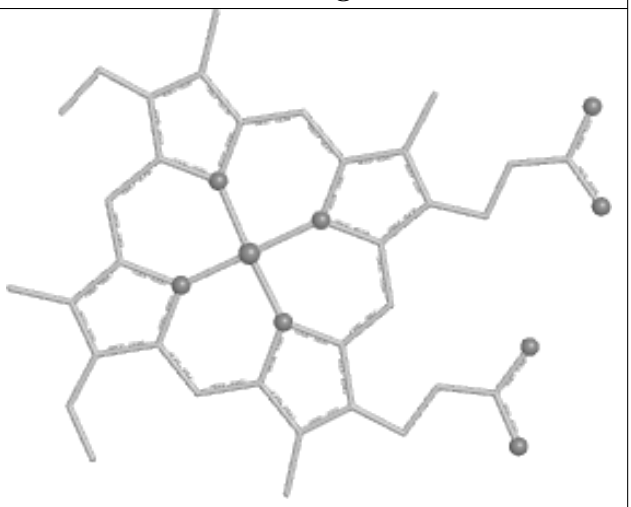
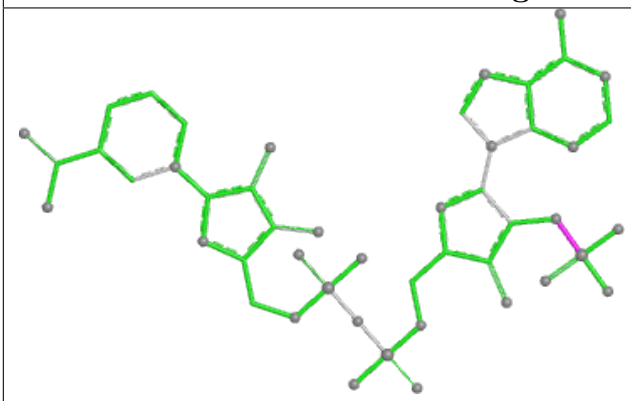
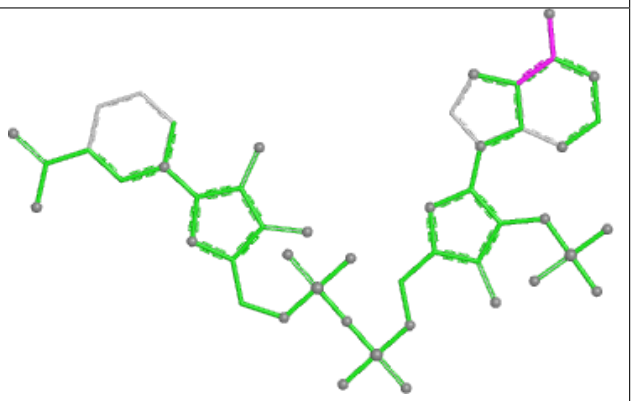
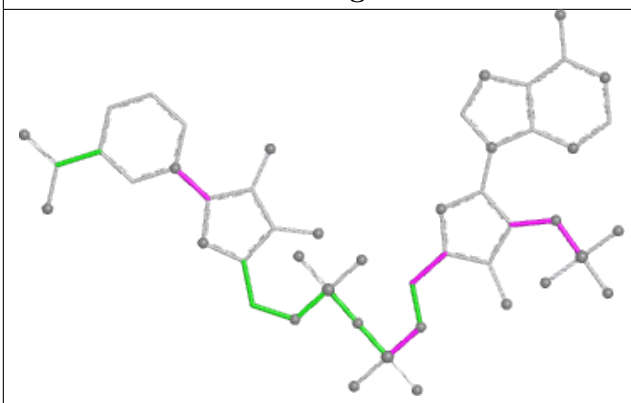
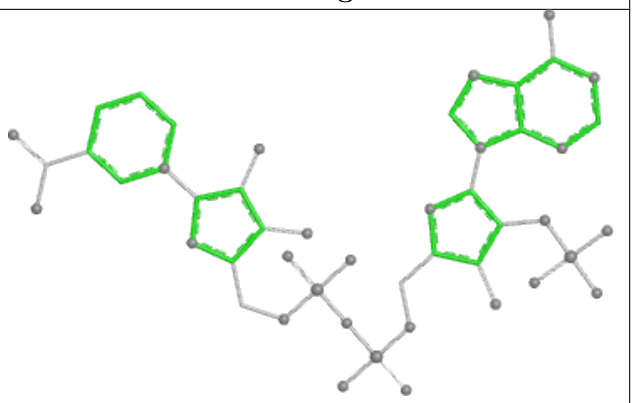


Rings

Ligand NDP A9 401	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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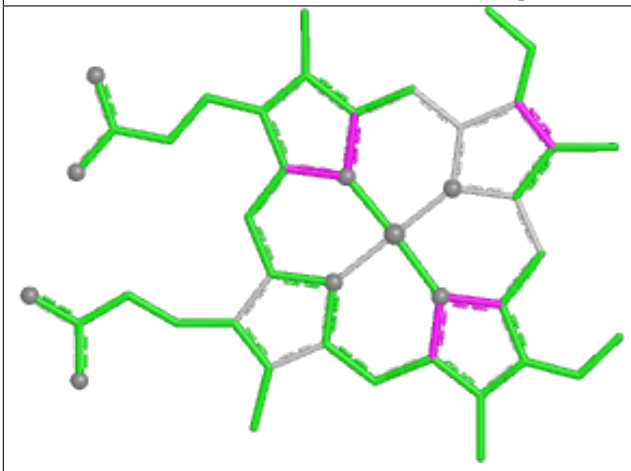	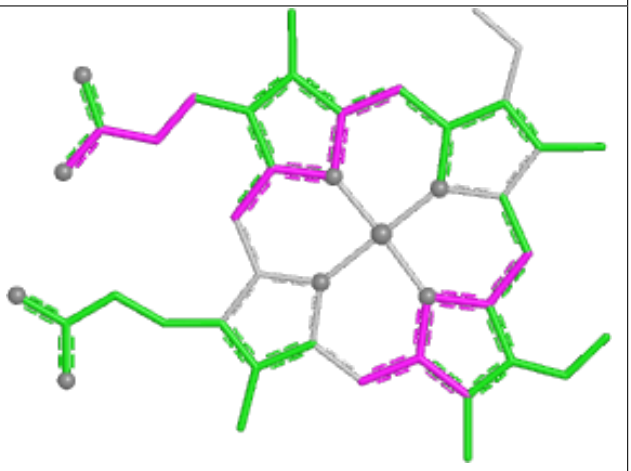
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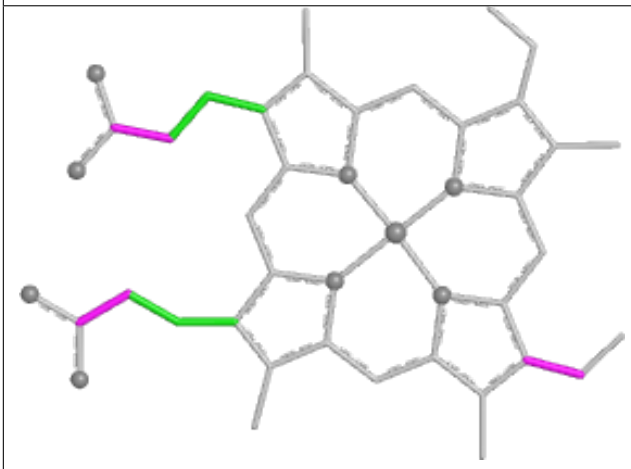	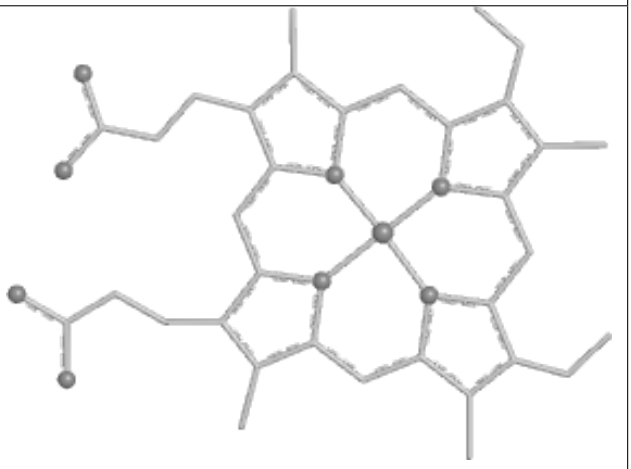
Torsions	**Rings**

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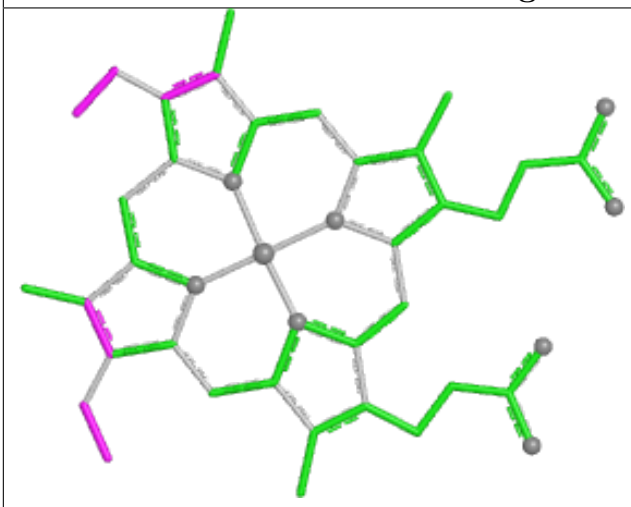
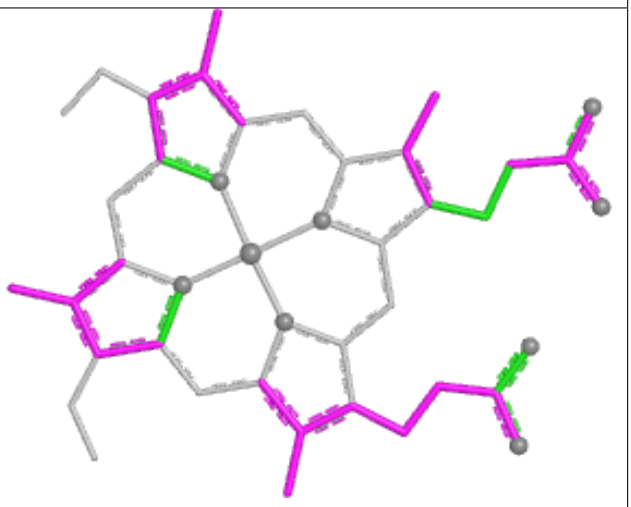
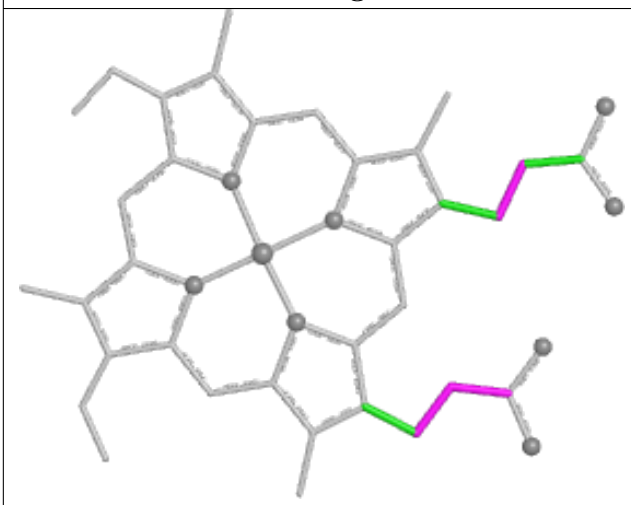
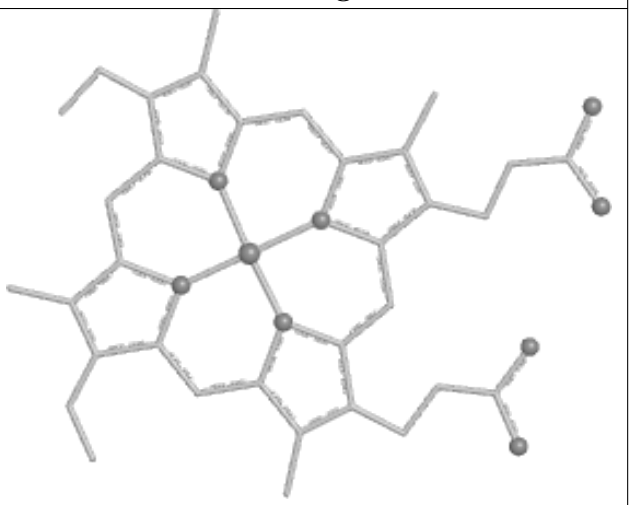
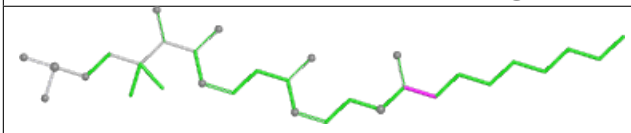
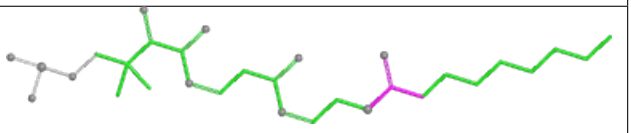
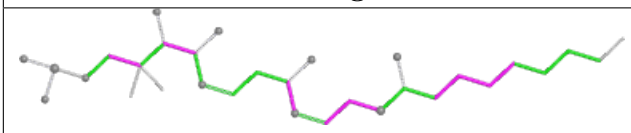
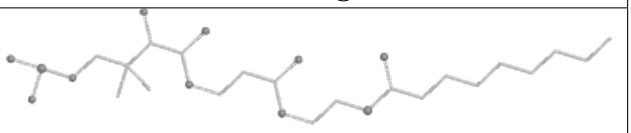
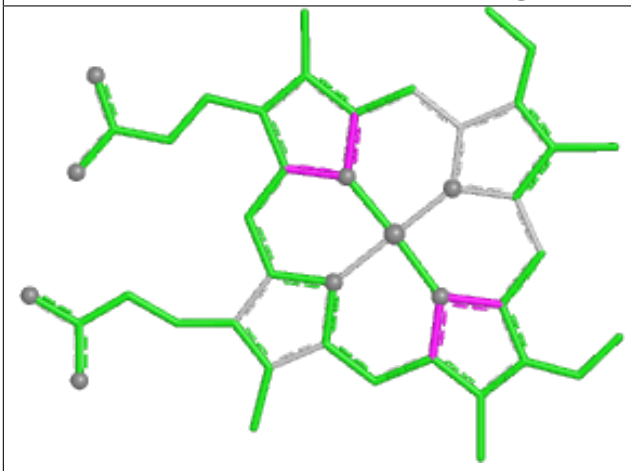
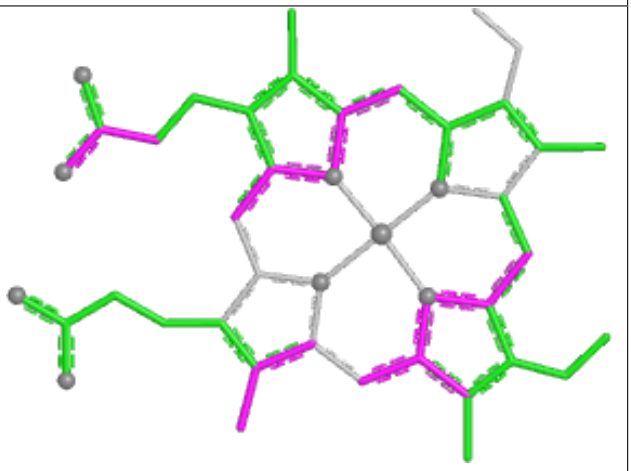
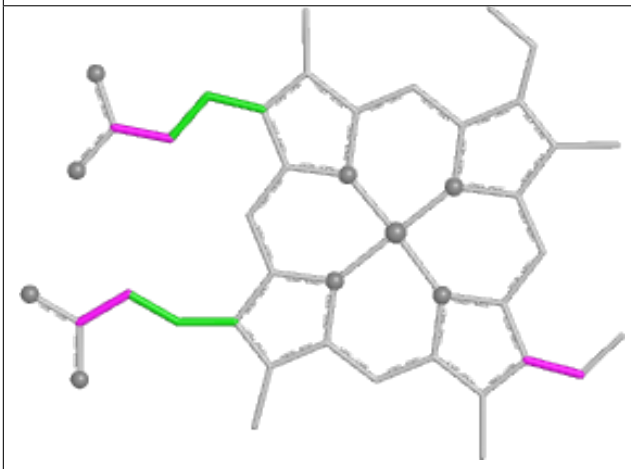
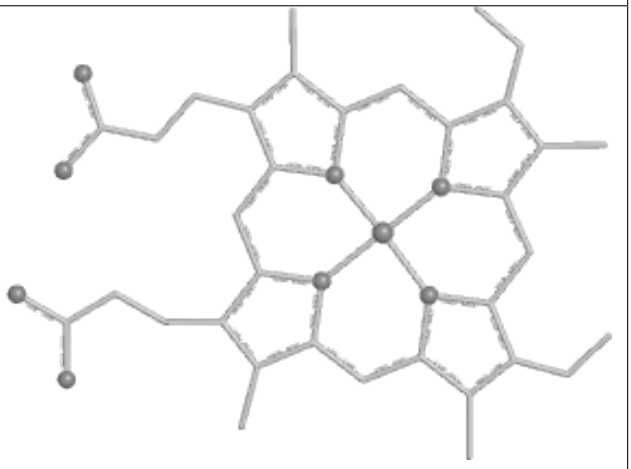
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZMP AB 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HEM b2 402	
 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
9	x2	1
9	x1	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	26.45

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x1	27:UNK	C	29:UNK	N	5.41

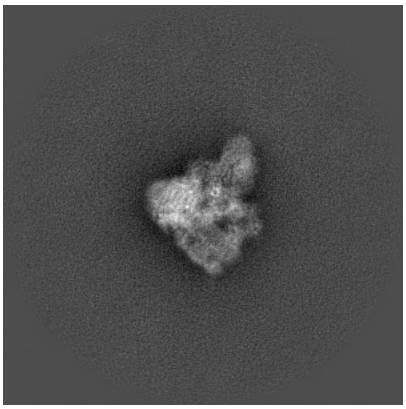
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4496. These allow visual inspection of the internal detail of the map and identification of artifacts.

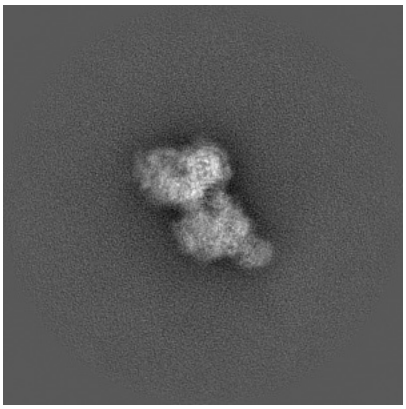
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

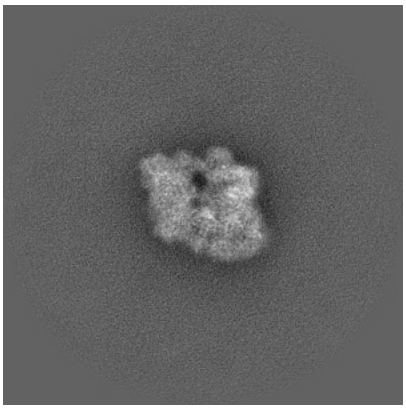
6.1.1 Primary map



X

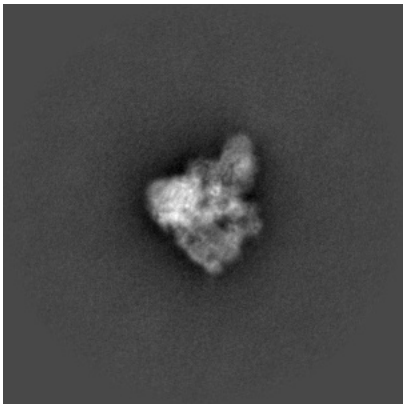


Y

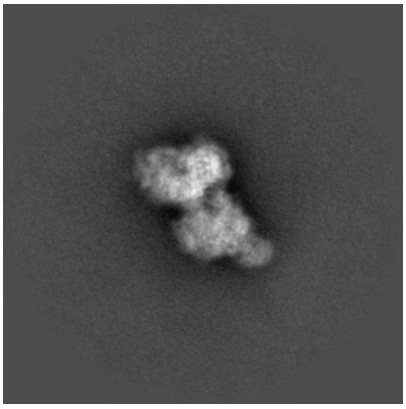


Z

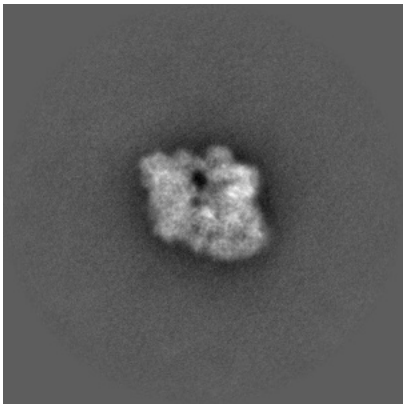
6.1.2 Raw map



X



Y

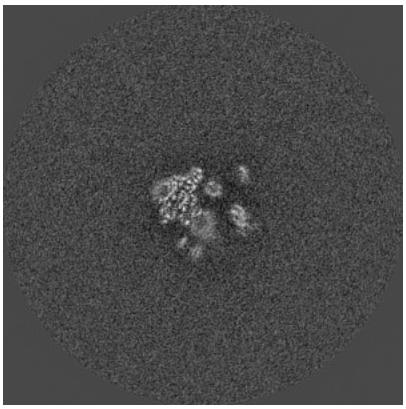


Z

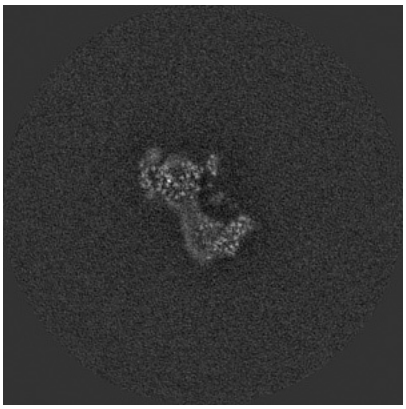
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

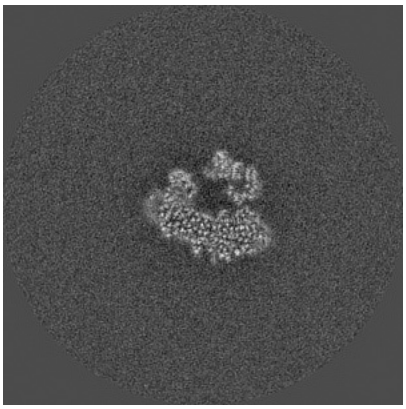
6.2.1 Primary map



X Index: 256

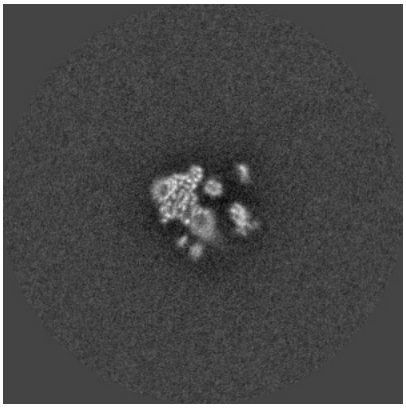


Y Index: 256

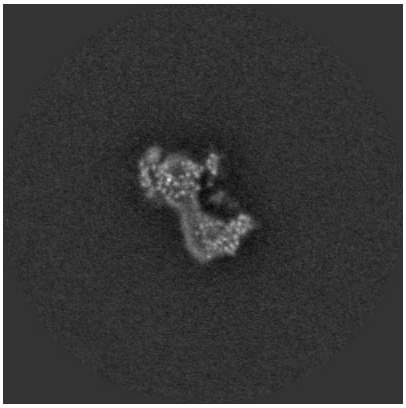


Z Index: 256

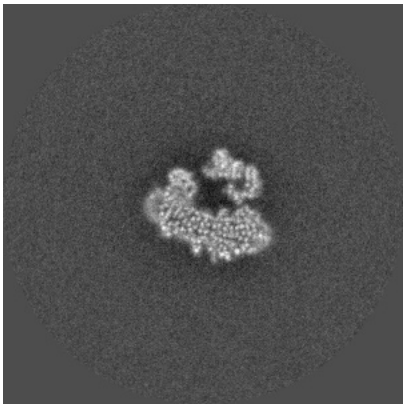
6.2.2 Raw map



X Index: 256



Y Index: 256

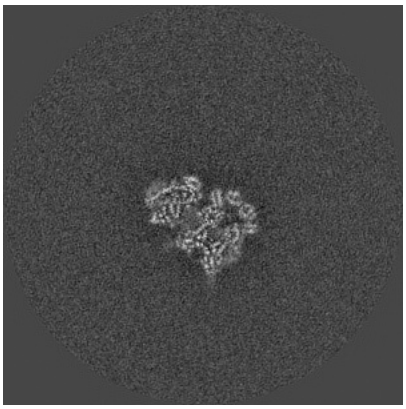


Z Index: 256

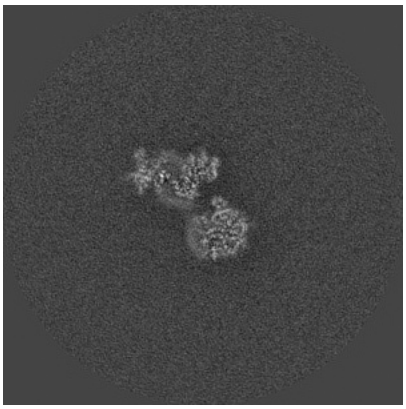
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

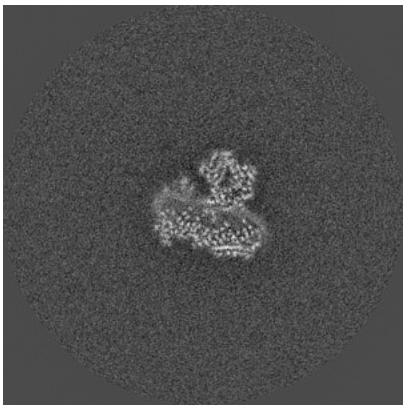
6.3.1 Primary map



X Index: 290

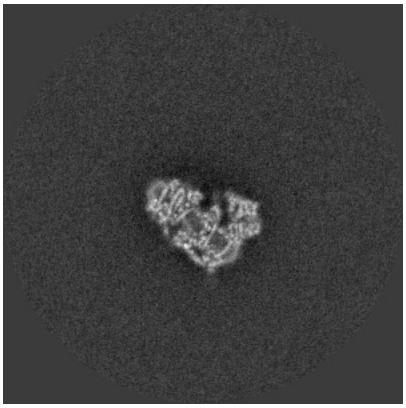


Y Index: 267

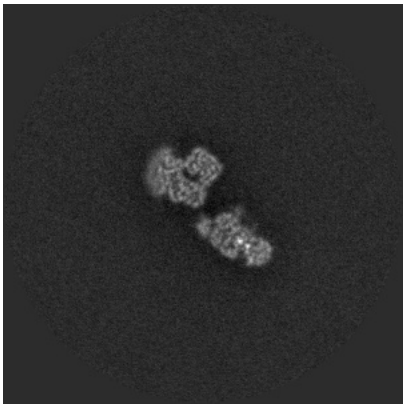


Z Index: 243

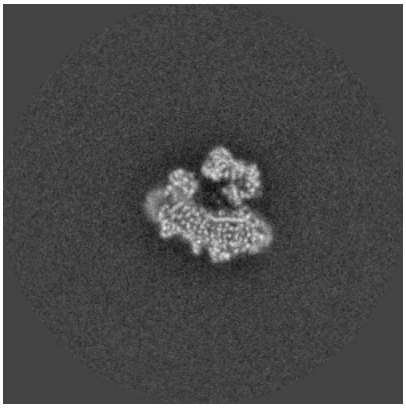
6.3.2 Raw map



X Index: 284



Y Index: 296



Z Index: 253

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

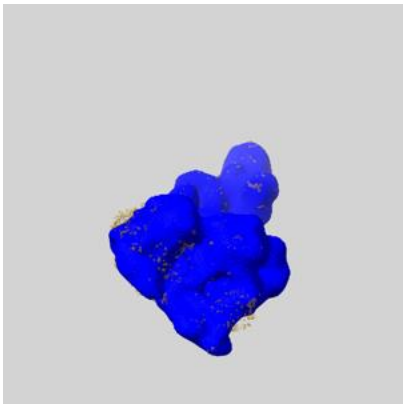
6.5 Mask visualisation (i)

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

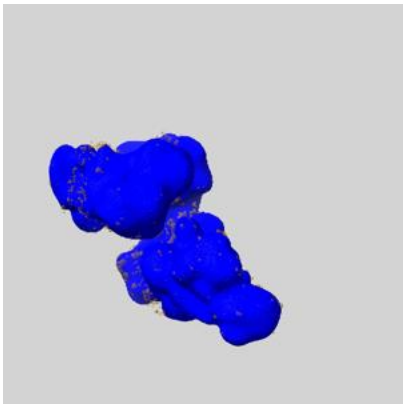
A mask typically either:

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

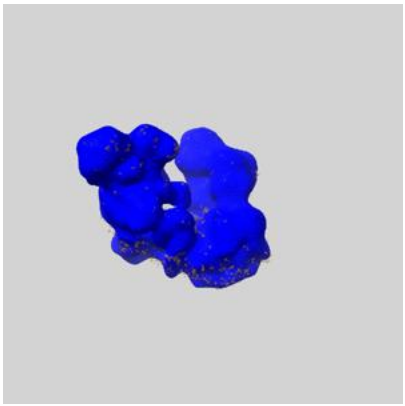
6.5.1 emd_4496_msk_1.map (i)



X



Y

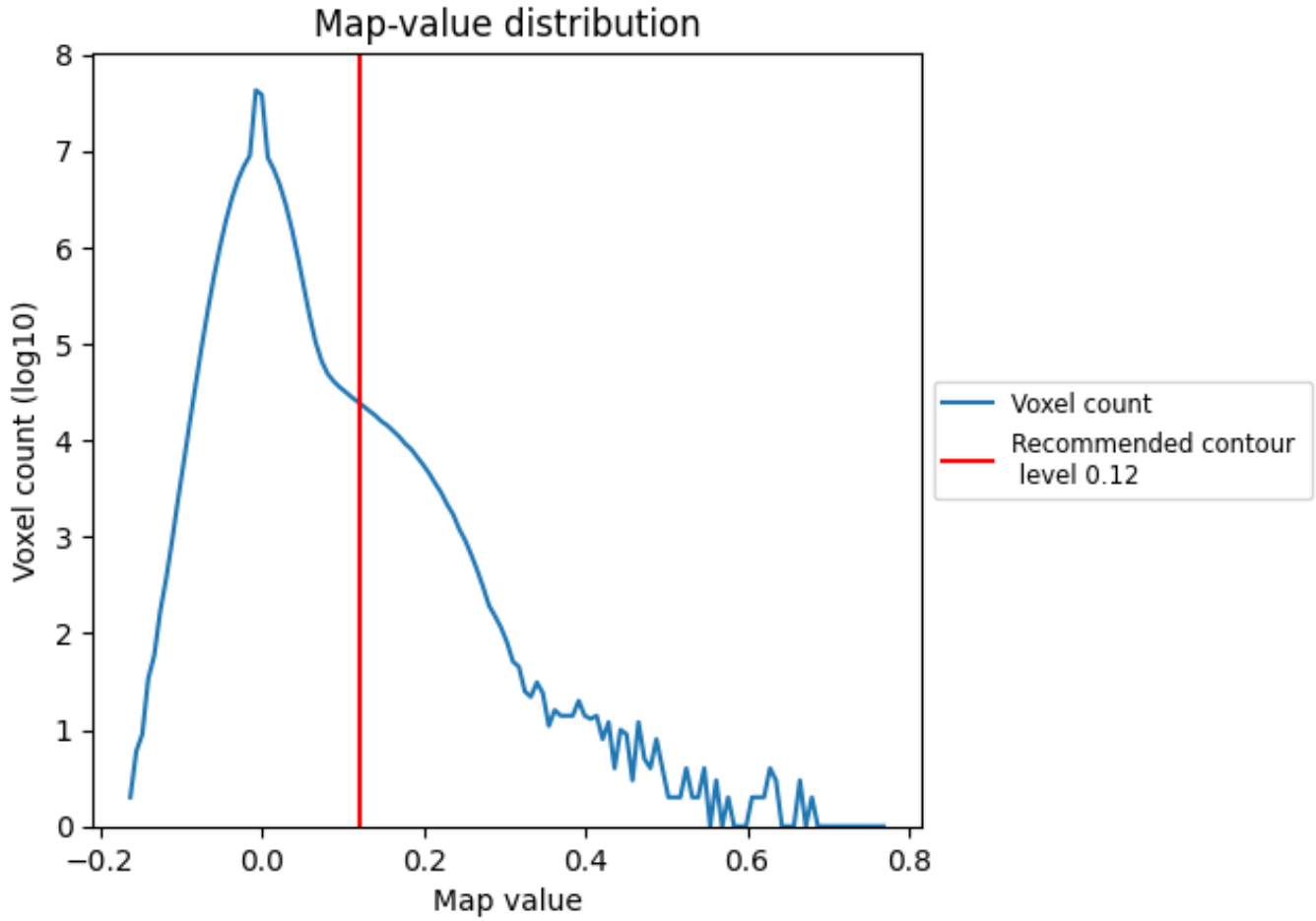


Z

7 Map analysis

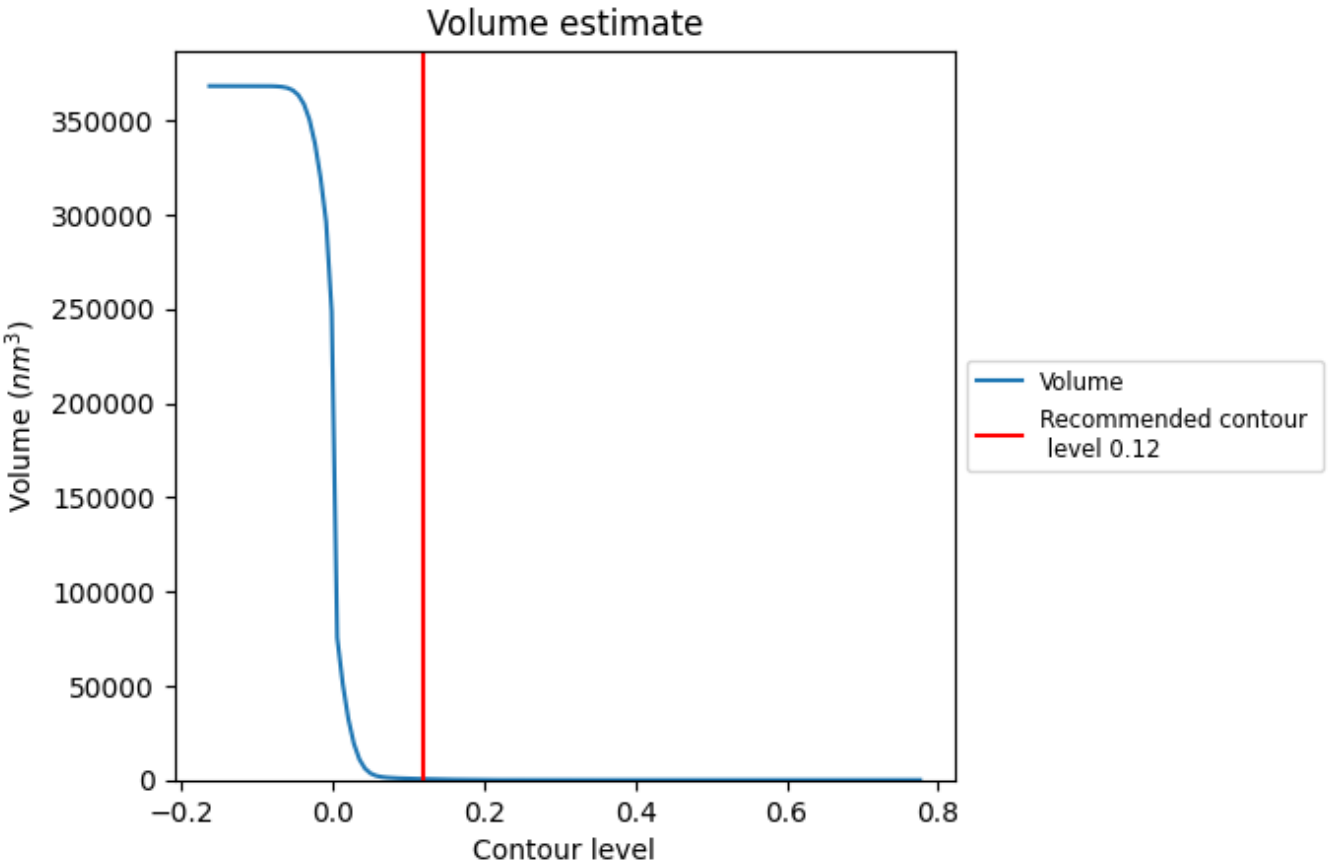
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

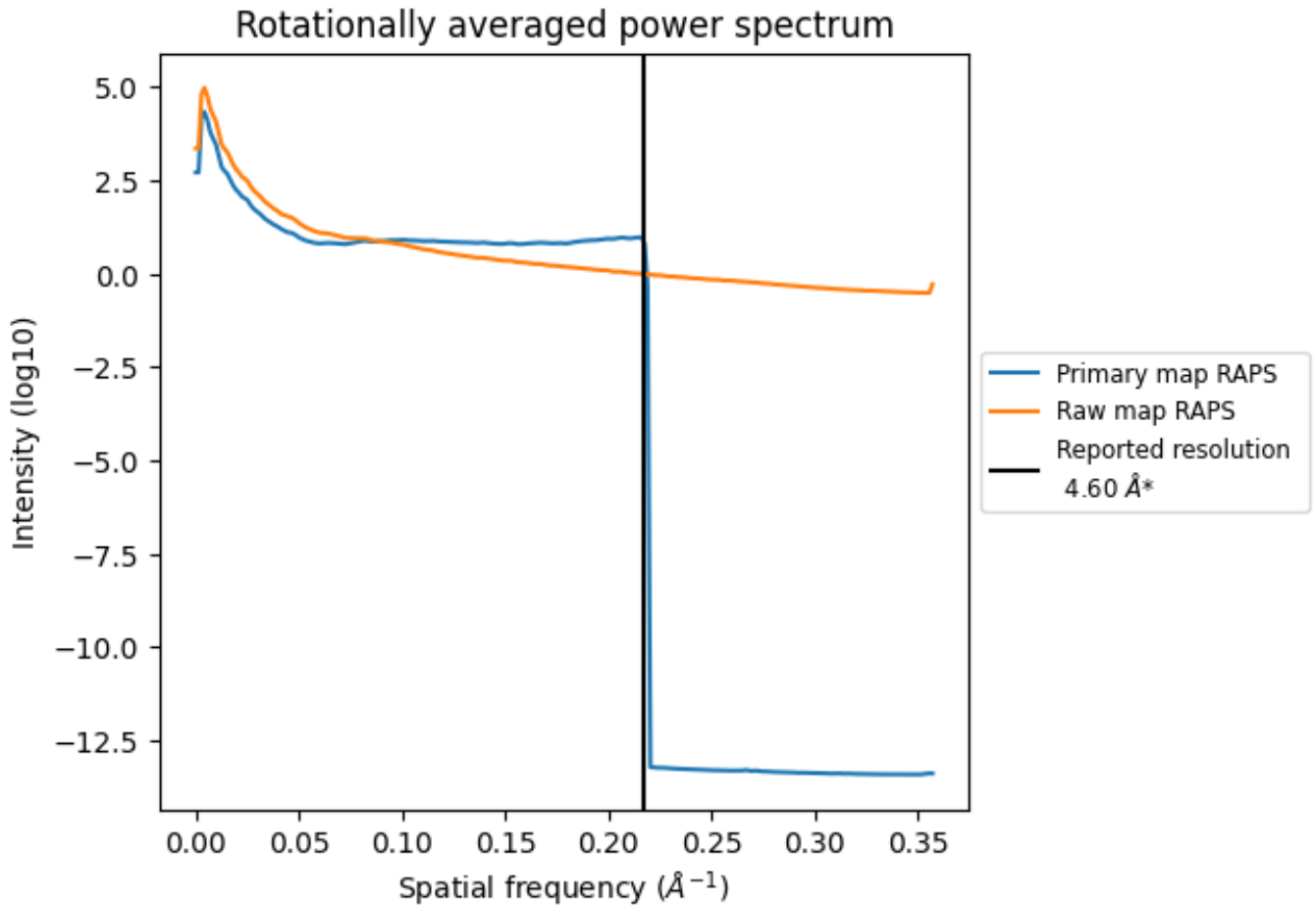
7.2 Volume estimate



The volume at the recommended contour level is 502 nm^3; this corresponds to an approximate mass of 454 kDa.

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

7.3 Rotationally averaged power spectrum (i)

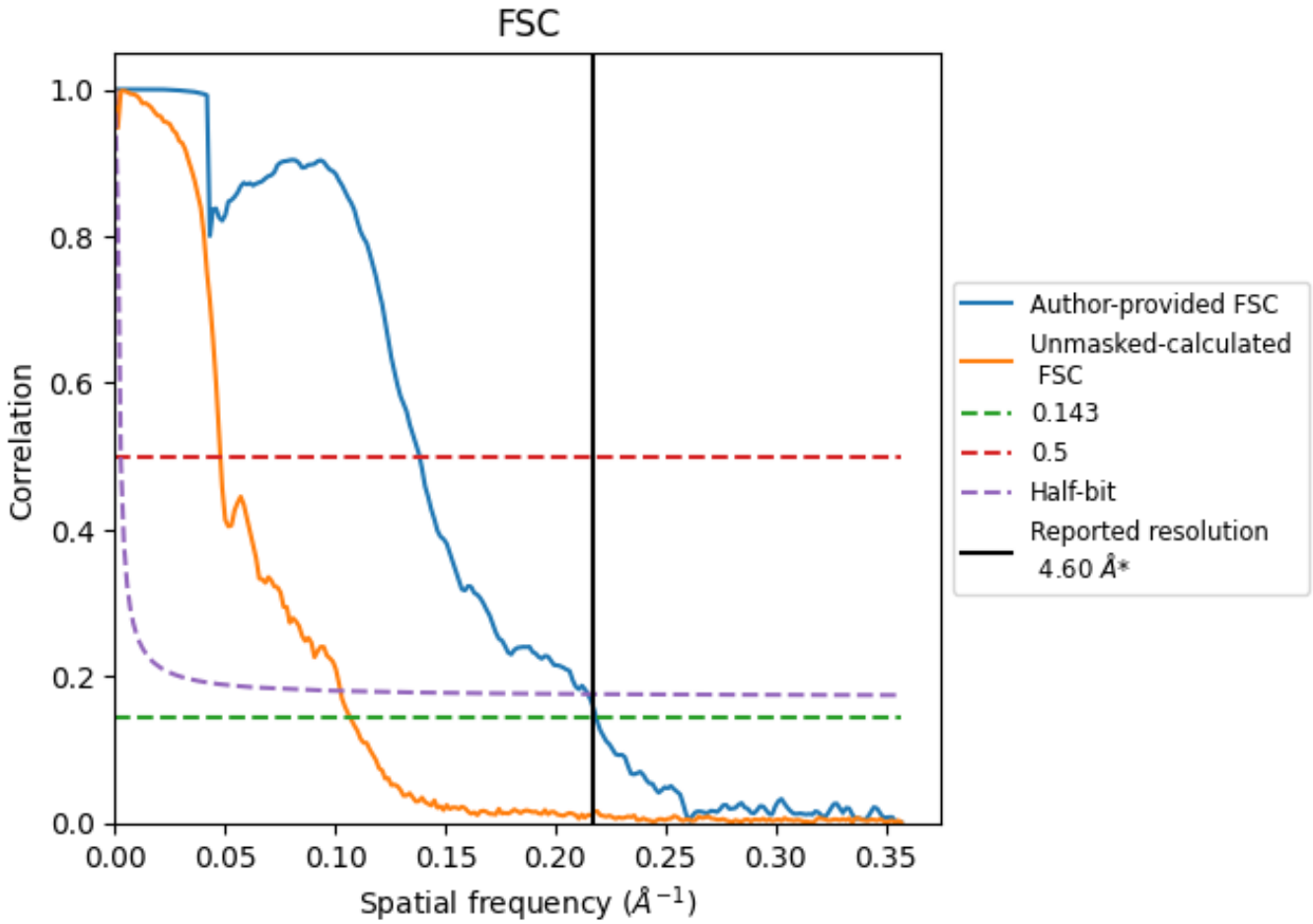


*Reported resolution corresponds to spatial frequency of 0.217 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

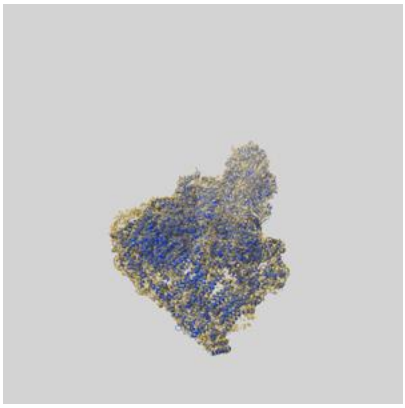
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	7.23	4.65
Unmasked-calculated*	9.35	20.83	9.76

*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 9.35 differs from the reported value 4.6 by more than 10 %

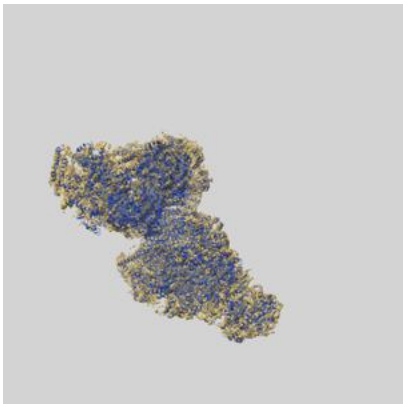
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4496 and PDB model 6QC4. Per-residue inclusion information can be found in section 3 on page 21.

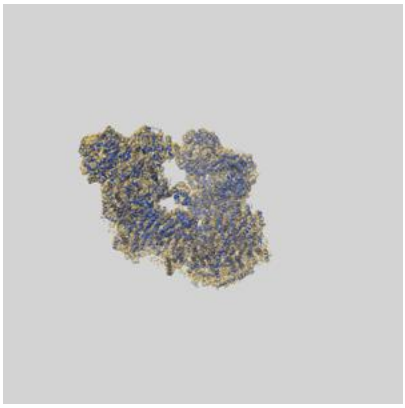
9.1 Map-model overlay



X



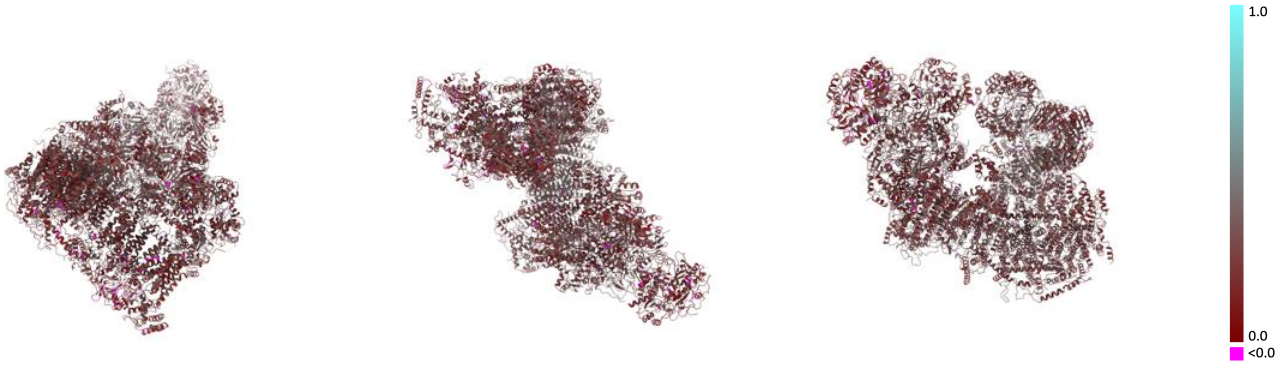
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

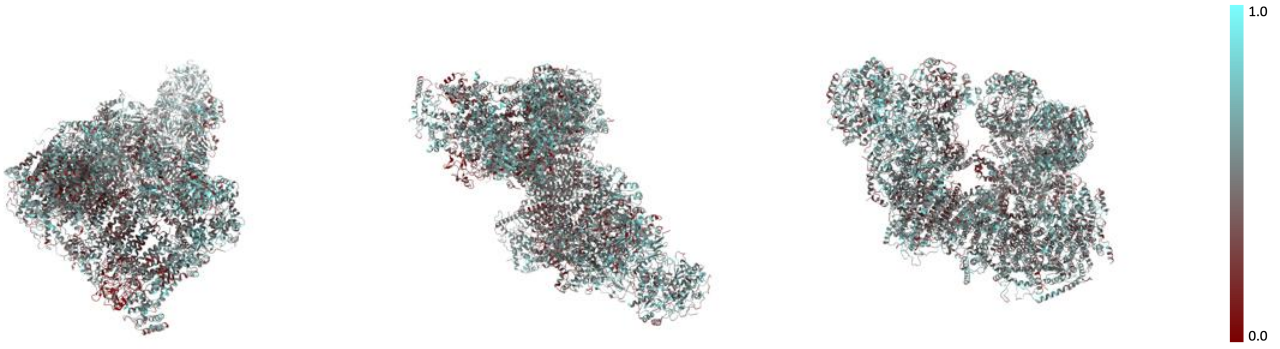
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

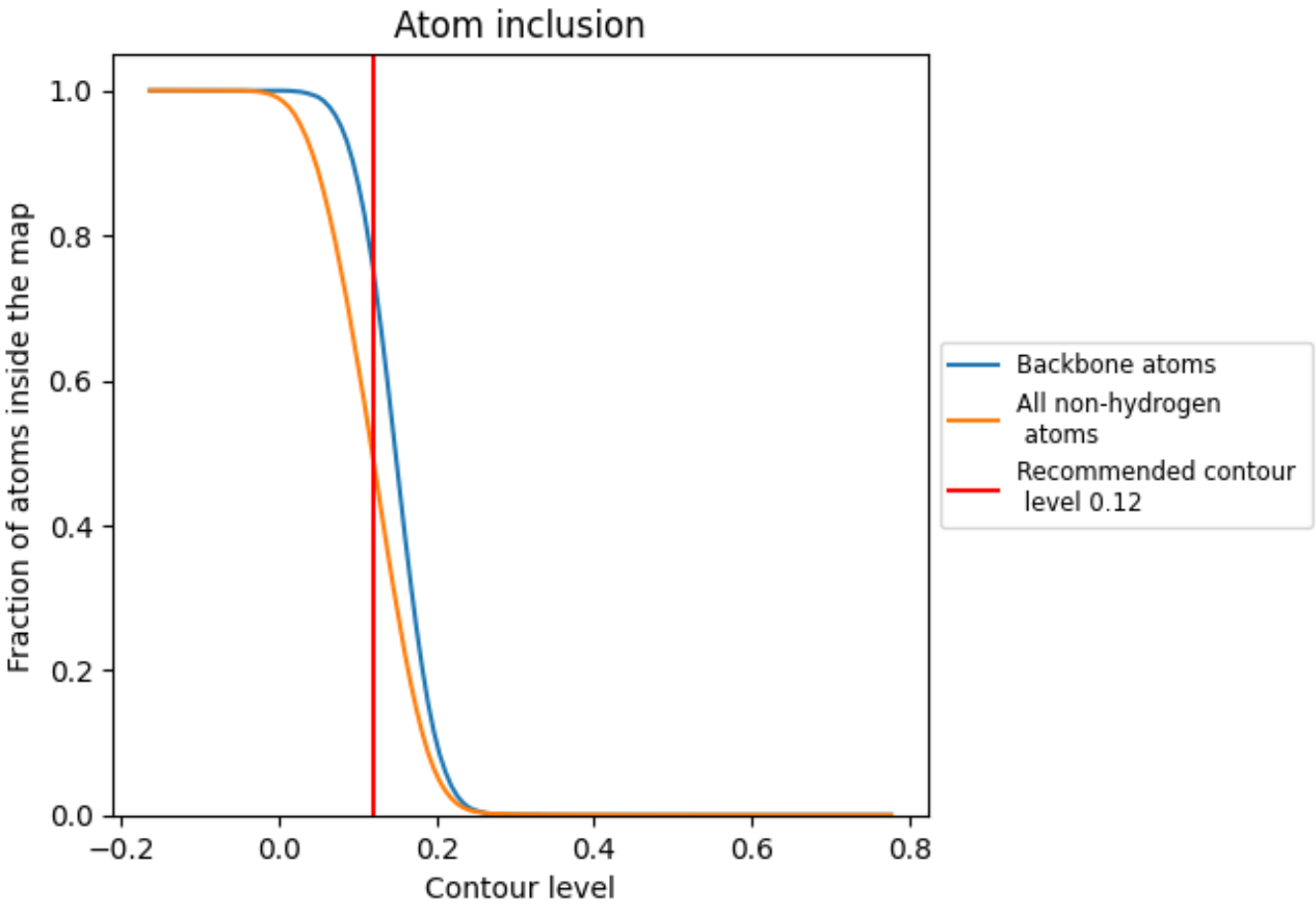
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 49% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.2820
4L	0.4084	0.2740
A1	0.5415	0.2920
A2	0.5418	0.2540
A3	0.5211	0.2880
A5	0.5034	0.2650
A6	0.4468	0.2750
A7	0.4583	0.2930
A8	0.5468	0.2970
A9	0.4352	0.2810
AA	0.3160	0.2390
AB	0.5172	0.2790
AJ	0.5284	0.2970
AK	0.4213	0.2800
AL	0.4817	0.2900
AM	0.5367	0.2720
B1	0.5275	0.3100
B2	0.5431	0.2610
B3	0.4734	0.2680
B4	0.5201	0.3010
B5	0.5404	0.2890
B6	0.5305	0.2850
B7	0.5410	0.2390
B8	0.5148	0.3120
B9	0.5568	0.2990
BJ	0.5562	0.2800
BK	0.4958	0.2990
C1	0.5524	0.3040
C2	0.5301	0.2950
D1	0.4500	0.2810
D2	0.4861	0.2950
D3	0.4006	0.2850
D4	0.4619	0.2970
D5	0.4721	0.2830
D6	0.3867	0.2760

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Chain	Atom inclusion	Q-score
S1	0.4966	0.2820
S2	0.5007	0.2940
S3	0.5241	0.3090
S4	0.5115	0.3050
S5	0.5318	0.2820
S6	0.5237	0.3320
S7	0.5153	0.2890
S8	0.5698	0.3030
V1	0.5455	0.2390
V2	0.5215	0.2530
V3	0.5179	0.2180
a1	0.5300	0.2740
a2	0.5174	0.2750
a3	0.5396	0.3170
a4	0.5402	0.2870
b1	0.4915	0.2750
b2	0.4807	0.2940
c1	0.5463	0.2870
c2	0.5264	0.3030
d1	0.5492	0.2860
d2	0.5117	0.2900
f1	0.2341	0.2070
f2	0.2263	0.2210
h1	0.5096	0.2350
h2	0.4173	0.2310
i1	0.5034	0.2500
i2	0.4512	0.2660
q1	0.5092	0.2820
q2	0.4951	0.3190
x1	0.2012	0.2850
x2	0.3400	0.3460