



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:17 PM UTC

PDB ID : 6QBX / pdb_00006qbx
EMDB ID : EMD-4493
Title : Ovine respiratory supercomplex I+III2 closed class.
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-24
Resolution : 4.20 Å(reported)
Based on initial model : 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

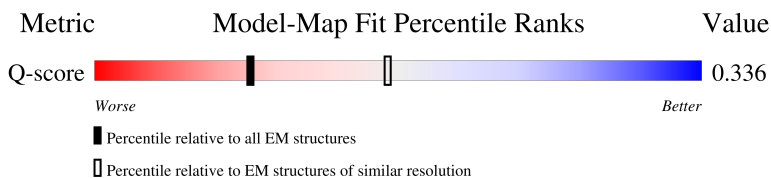
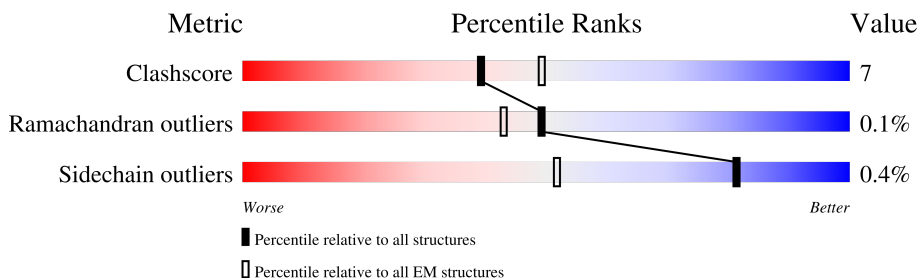
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	a1	446	
1	a3	446	
2	a2	439	
2	a4	439	

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Mol	Chain	Length	Quality of chain
3	b1	379	
3	b2	379	
4	c1	240	
4	c2	240	
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	V1	445	
12	V2	217	
13	S1	704	
14	S2	430	
15	S3	228	
16	S7	179	
17	S8	176	
18	V3	75	
19	S6	96	

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Mol	Chain	Length	Quality of chain
20	S4	133	
21	A9	338	
22	A2	98	
23	A5	115	
24	A6	127	
25	A7	112	
26	AL	145	
27	AA	88	
27	AB	88	
28	AM	143	
29	D3	115	
30	D1	318	
31	D6	175	
32	4L	98	
33	D5	606	
34	D4	459	
35	D2	347	
36	AK	140	
37	B5	143	
38	A8	171	
39	BJ	175	
40	AJ	320	
41	S5	105	
42	A3	83	
43	B3	97	

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Mol	Chain	Length	Quality of chain
44	C2	120	
45	B4	128	
46	B6	127	
47	B7	119	
48	B9	178	
49	B2	72	
50	B8	158	
51	BK	125	
52	C1	49	
53	B1	57	
54	A1	70	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 97049 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 Ubiquinol-cytochrome c reductase core protein 1.

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		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a1	241	ILE	LEU	conflict	UNP W5Q5G6
a1	242	ARG	CYS	conflict	UNP W5Q5G6
a1	244	ARG	PRO	conflict	UNP W5Q5G6
a1	245	GLU	TRP	conflict	UNP W5Q5G6
a1	246	ASP	GLY	conflict	UNP W5Q5G6
a1	?	-	ALA	deletion	UNP W5Q5G6
a1	?	-	VAL	deletion	UNP W5Q5G6
a1	?	-	PRO	deletion	UNP W5Q5G6
a1	249	PRO	GLN	conflict	UNP W5Q5G6
a1	251	ALA	TRP	conflict	UNP W5Q5G6
a1	254	ALA	PRO	conflict	UNP W5Q5G6
a1	255	ILE	PHE	conflict	UNP W5Q5G6
a1	256	ALA	GLN	conflict	UNP W5Q5G6
a1	257	VAL	ILE	conflict	UNP W5Q5G6
a1	258	GLU	ARG	conflict	UNP W5Q5G6
a1	259	GLY	HIS	conflict	UNP W5Q5G6
a3	241	ILE	LEU	conflict	UNP W5Q5G6
a3	242	ARG	CYS	conflict	UNP W5Q5G6
a3	244	ARG	PRO	conflict	UNP W5Q5G6
a3	245	GLU	TRP	conflict	UNP W5Q5G6
a3	246	ASP	GLY	conflict	UNP W5Q5G6
a3	?	-	ALA	deletion	UNP W5Q5G6
a3	?	-	VAL	deletion	UNP W5Q5G6
a3	?	-	PRO	deletion	UNP W5Q5G6
a3	249	PRO	GLN	conflict	UNP W5Q5G6
a3	251	ALA	TRP	conflict	UNP W5Q5G6

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Chain	Residue	Modelled	Actual	Comment	Reference
a3	254	ALA	PRO	conflict	UNP W5Q5G6
a3	255	ILE	PHE	conflict	UNP W5Q5G6
a3	256	ALA	GLN	conflict	UNP W5Q5G6
a3	257	VAL	ILE	conflict	UNP W5Q5G6
a3	258	GLU	ARG	conflict	UNP W5Q5G6
a3	259	GLY	HIS	conflict	UNP W5Q5G6

- 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	239	Total	C	N	O	S	0	0
			1909	1219	330	345	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 Cytochrome b-c1 complex subunit 7.

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		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d1	1	ALA	-	insertion	UNP W5P642
d1	2	GLY	SER	conflict	UNP W5P642
d1	3	ARG	ASP	conflict	UNP W5P642
d1	4	PRO	LEU	conflict	UNP W5P642
d1	5	ALA	SER	conflict	UNP W5P642
d2	1	ALA	-	insertion	UNP W5P642
d2	2	GLY	SER	conflict	UNP W5P642
d2	3	ARG	ASP	conflict	UNP W5P642
d2	4	PRO	LEU	conflict	UNP W5P642
d2	5	ALA	SER	conflict	UNP W5P642

- 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	23	Total	C	N	O	0	0
			114	68	23	23		
9	x2	26	Total	C	N	O	0	0
			130	78	26	26		

- 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		
10	i2	57	Total	C	N	O	0	0
			473	312	82	79		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

- Molecule 12 is a protein called NDUFV2.

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

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

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

- Molecule 14 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S2	430	Total	C	N	O	S	0	0
			3455	2205	594	631	25		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

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

- Molecule 16 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S7	156	Total	C	N	O	S	0	0
			1248	795	225	214	14		

- Molecule 17 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S8	176	Total	C	N	O	S	0	0
			1415	889	243	271	12		

- Molecule 18 is a protein called NDUFV3.

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

- Molecule 19 is a protein called NDUFS6.

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

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S4	126	Total	C	N	O	S	0	0
			1025	646	182	194	3		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A9	292	Total	C	N	O	S	0	0
			2344	1498	428	413	5		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 23 is a protein called NDUF5.

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

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

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

- Molecule 25 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A7	96	Total	C	N	O	S	0	0
			766	478	146	139	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AL	123	Total	C	N	O	S	0	0
			1044	676	182	182	4		

- Molecule 27 is a protein called Acyl carrier protein.

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

- Molecule 28 is a protein called NDUFA13.

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

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D3	115	Total	C	N	O	S	0	0
			923	621	133	162	7		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D1	318	Total	C	N	O	S	0	0
			2529	1704	384	422	19		

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D6	175	Total	C	N	O	S	0	0
			1345	904	192	236	13		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 36 is a protein called NDUFA11.

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

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

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

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

- Molecule 39 is a protein called NDUFB10.

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

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

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

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 43 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 46 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B6	95	Total	C	N	O	S	0	0
			804	530	135	138	1		

- Molecule 47 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B2	64	Total	C	N	O	S	0	0
			555	368	92	94	1		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 51 is a protein called NDUFB11.

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

- Molecule 52 is a protein called NDUF1.

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

- Molecule 53 is a protein called NDUFB1.

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

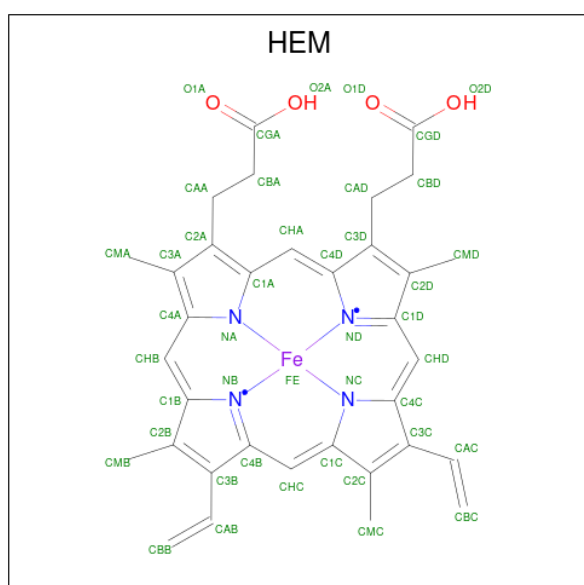
There are 3 discrepancies between the modelled and reference sequences:

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 54 is a protein called NDUFA1.

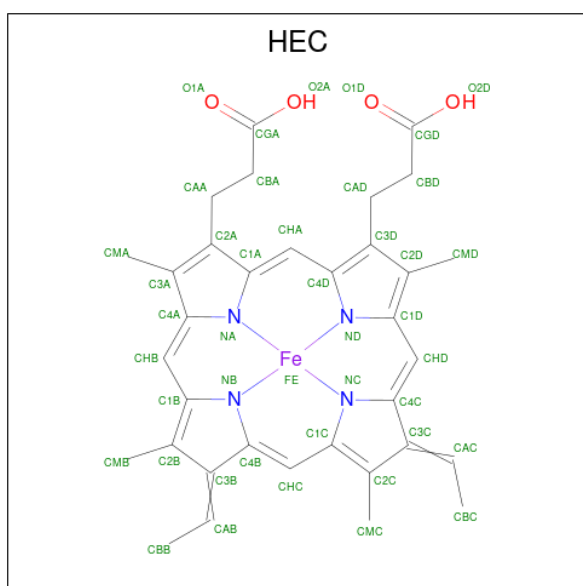
Mol	Chain	Residues	Atoms					AltConf	Trace
54	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

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



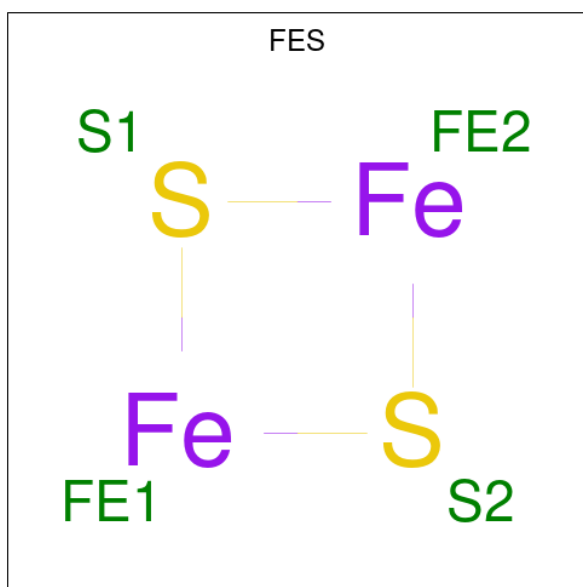
Mol	Chain	Residues	Atoms					AltConf
55	b1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
55	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 56 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



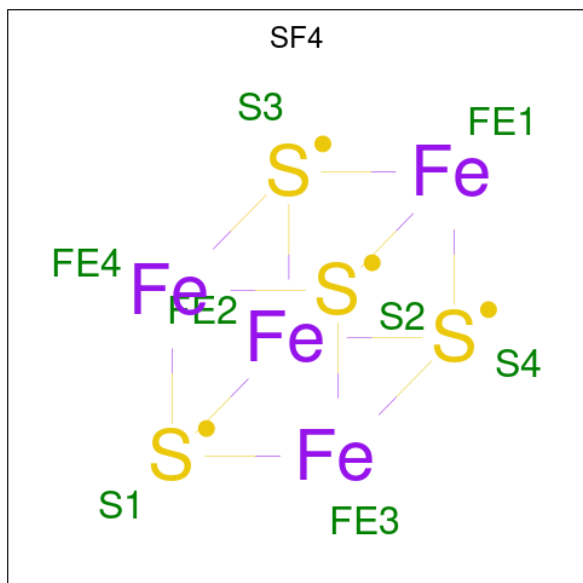
Mol	Chain	Residues	Atoms					AltConf
56	c1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	c2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



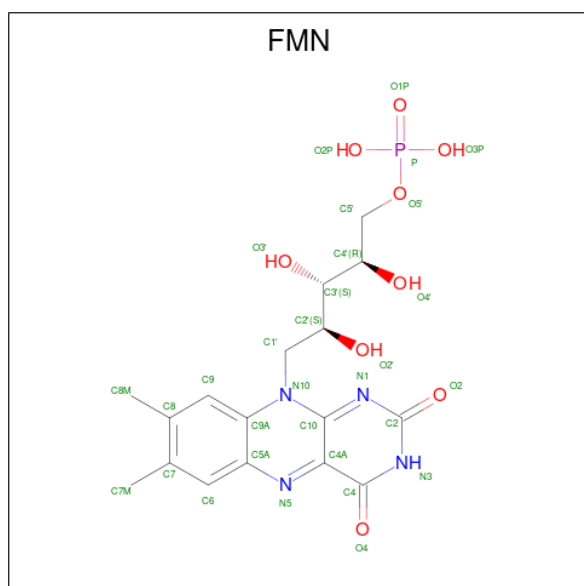
Mol	Chain	Residues	Atoms			AltConf
57	f1	1	Total	Fe	S	0
			4	2	2	
57	f2	1	Total	Fe	S	0
			4	2	2	
57	V2	1	Total	Fe	S	0
			4	2	2	
57	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



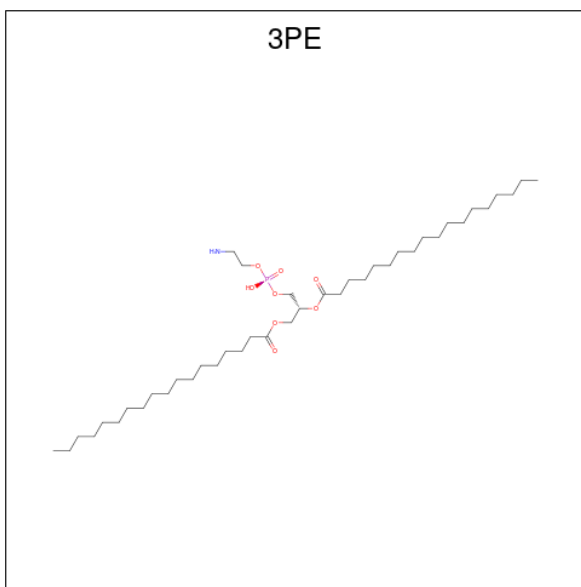
Mol	Chain	Residues	Atoms			AltConf
58	V1	1	Total	Fe	S	0
			8	4	4	
58	S1	1	Total	Fe	S	0
			8	4	4	
58	S1	1	Total	Fe	S	0
			8	4	4	
58	S7	1	Total	Fe	S	0
			8	4	4	
58	S8	1	Total	Fe	S	0
			8	4	4	
58	S8	1	Total	Fe	S	0
			8	4	4	

- Molecule 59 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 60 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).

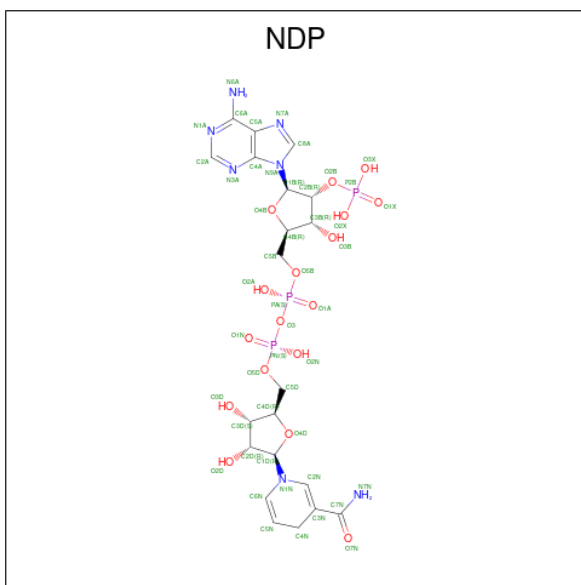


Mol	Chain	Residues	Atoms					AltConf
60	S2	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

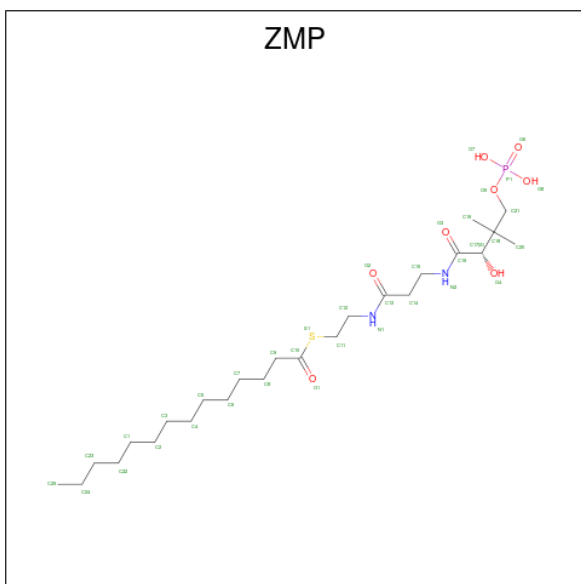
Mol	Chain	Residues	Atoms		AltConf
61	S6	1	Total	Zn	0
			1	1	

- Molecule 62 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



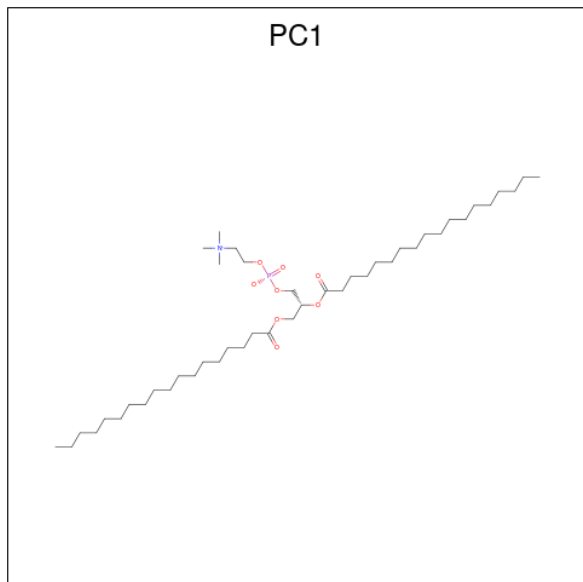
Mol	Chain	Residues	Atoms					AltConf
62	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 63 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



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

- Molecule 64 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).

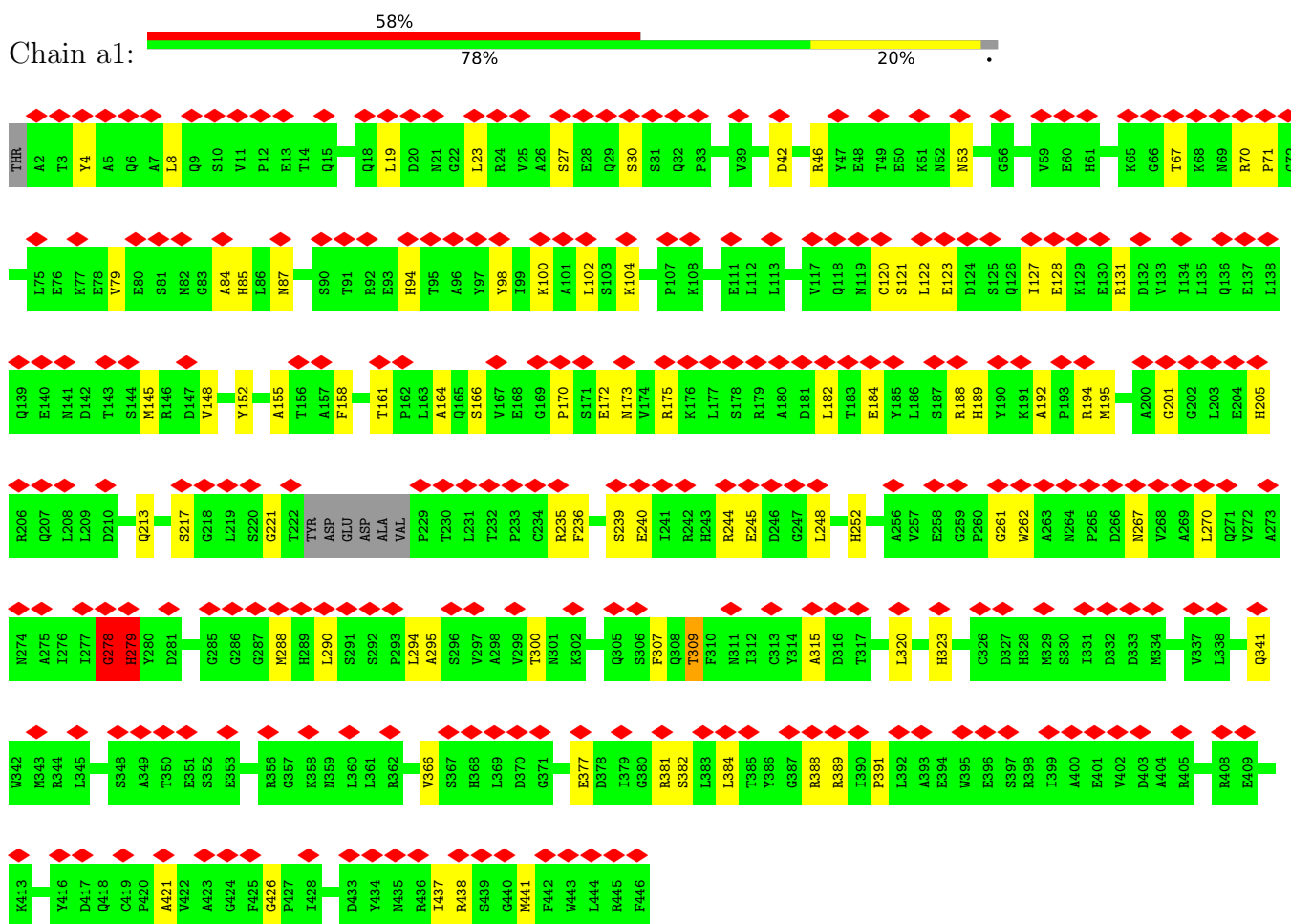


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	AK	1	28	18	1	8	1	0

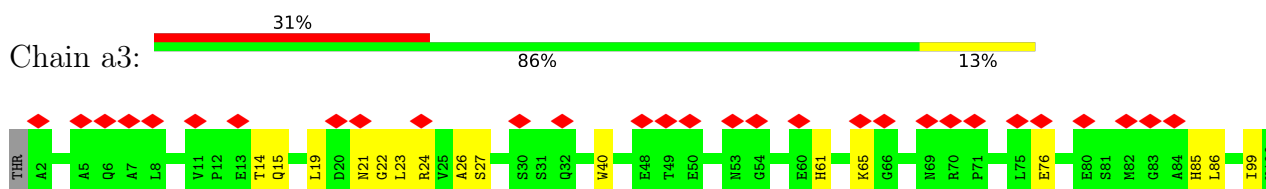
3 Residue-property plots

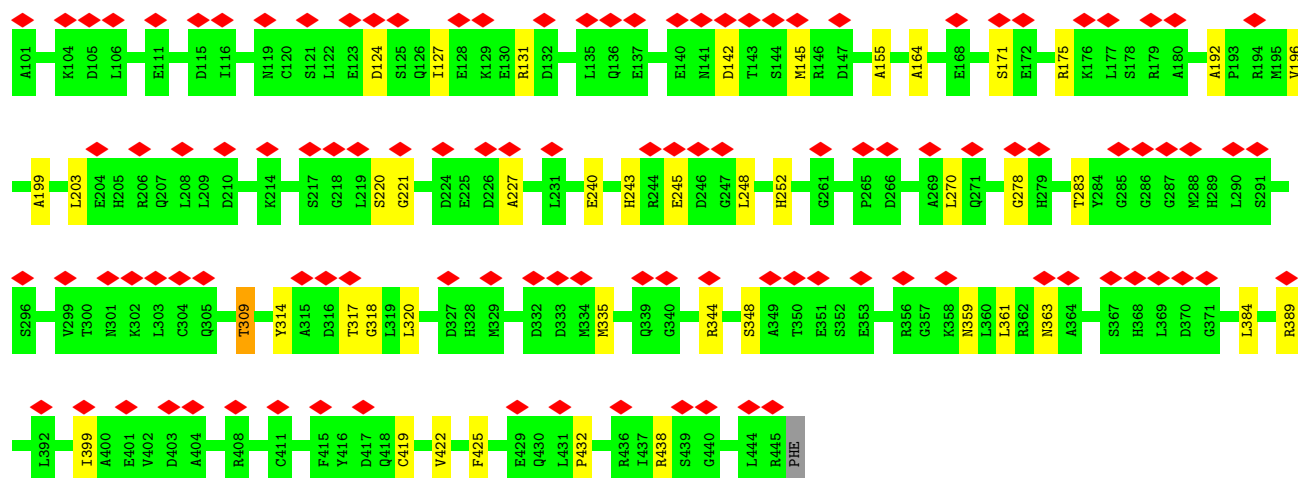
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ubiquinol-cytochrome c reductase core protein 1

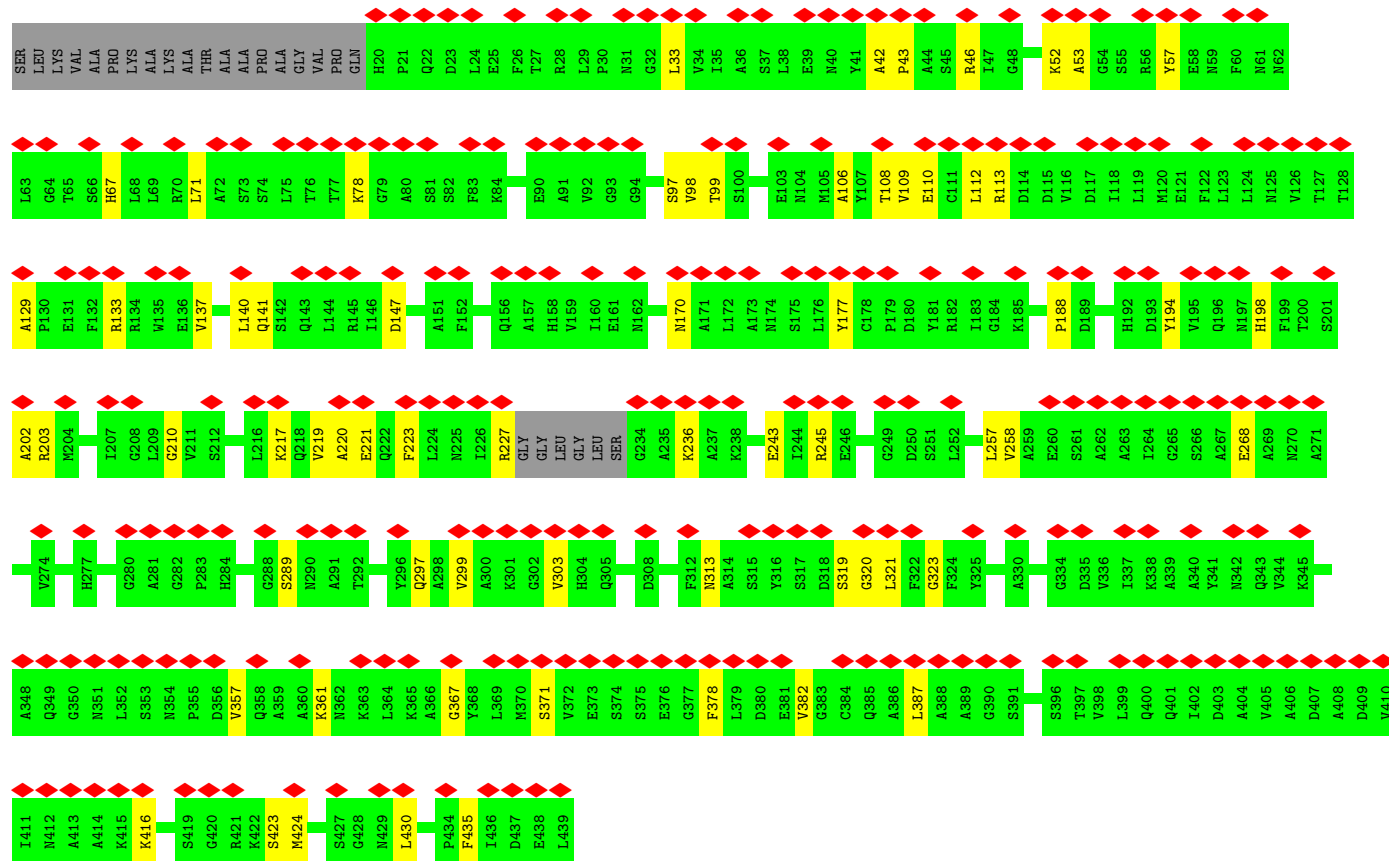
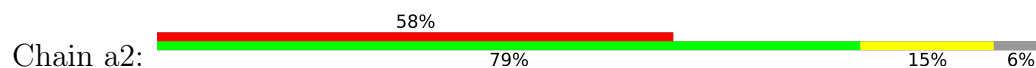


- Molecule 1: Ubiquinol-cytochrome c reductase core protein 1

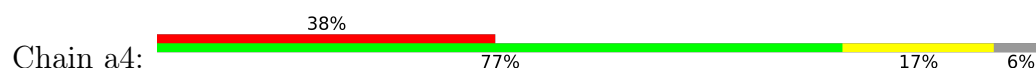


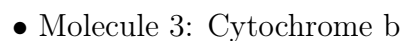


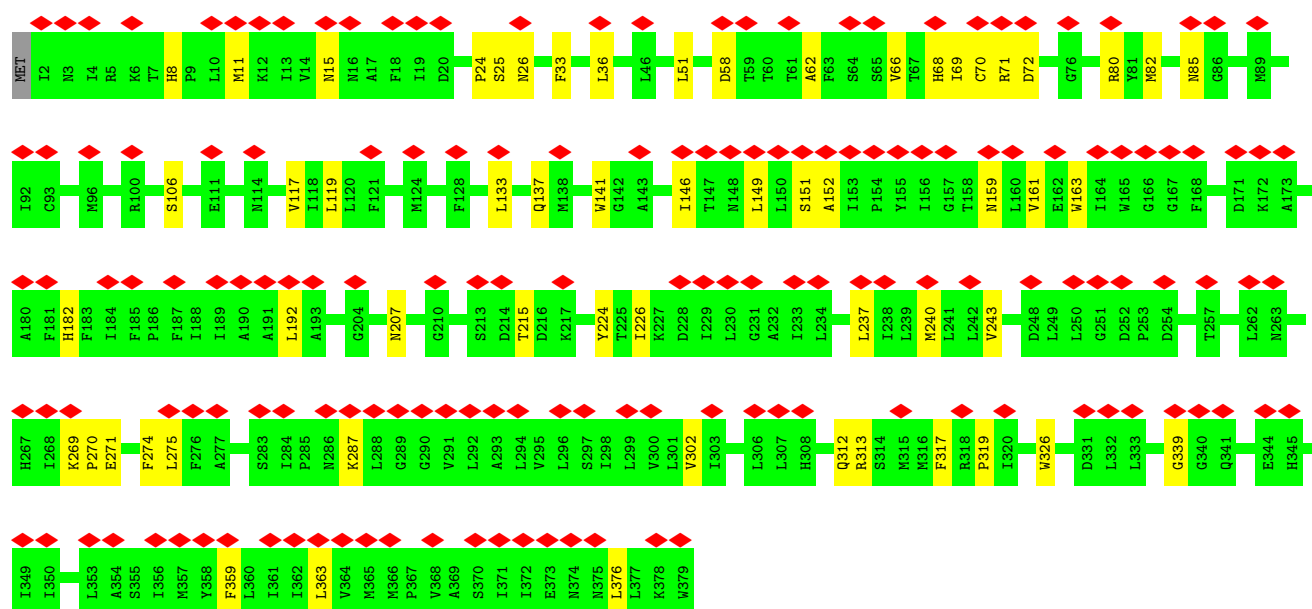
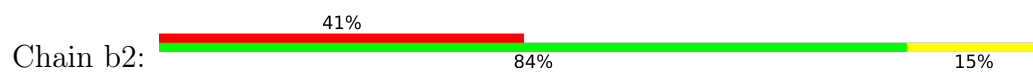
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2



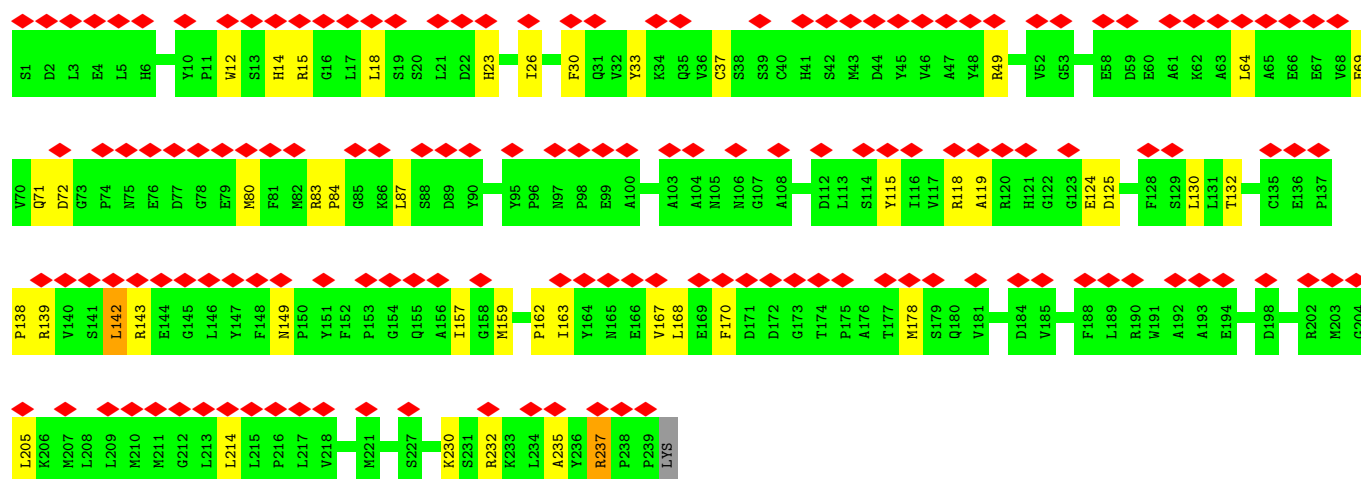
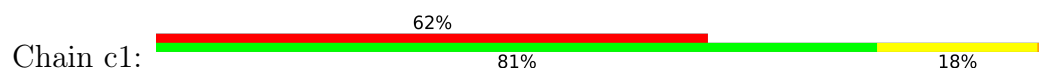
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2



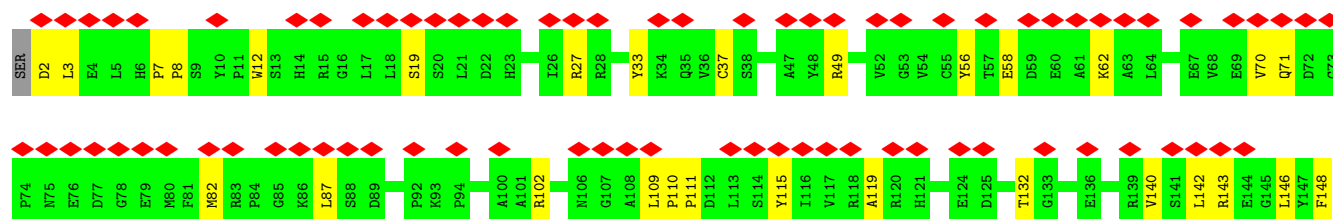
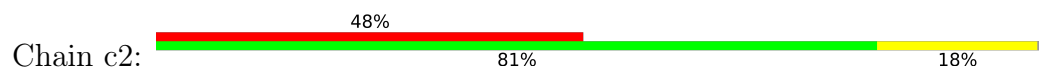


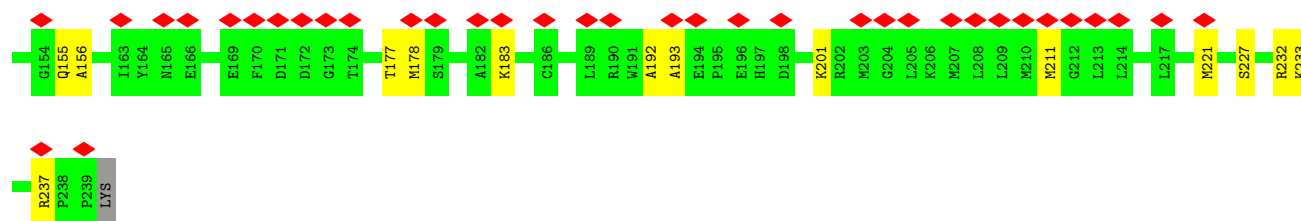


• Molecule 4: Cytochrome c1

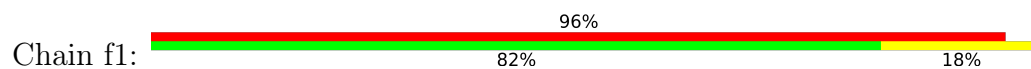


• Molecule 4: Cytochrome c1





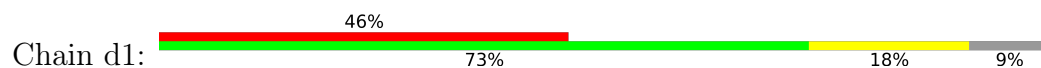
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

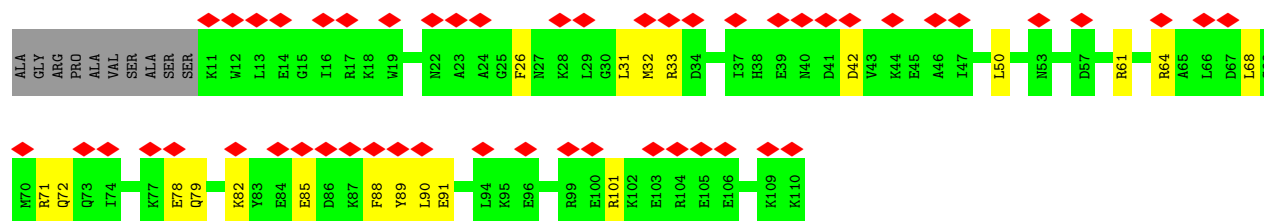


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

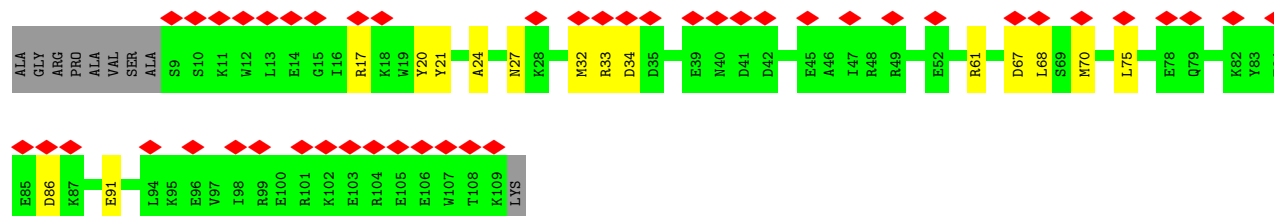
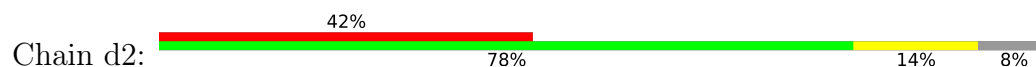


• Molecule 6: Cytochrome b-c1 complex subunit 7

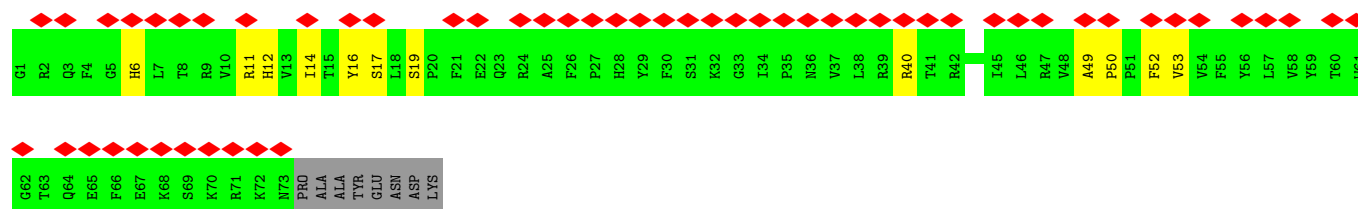
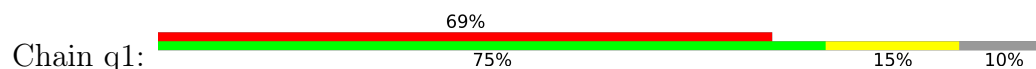




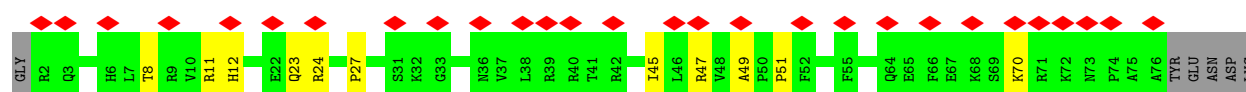
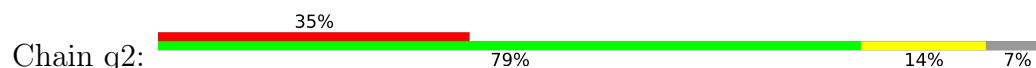
• Molecule 6: Cytochrome b-c1 complex subunit 7



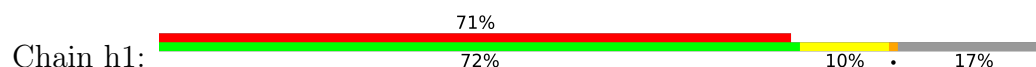
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



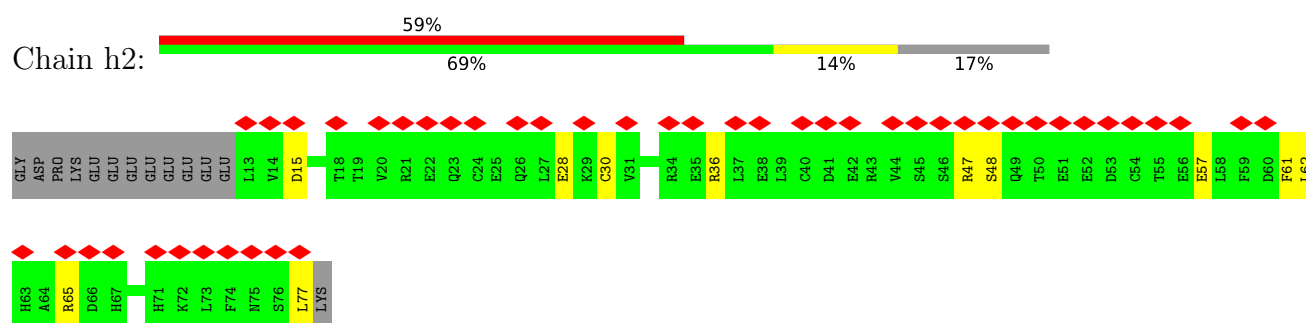
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



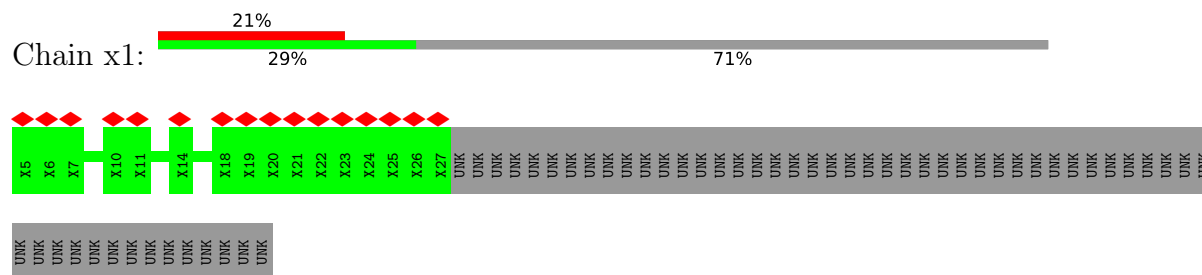
• Molecule 8: Cytochrome b-c1 complex subunit 6



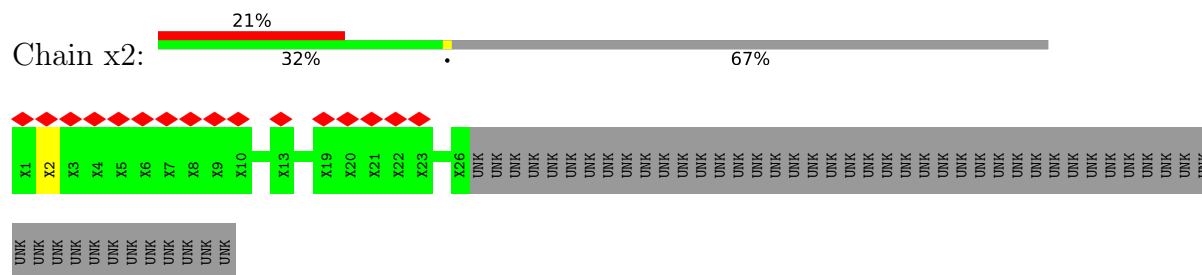
• Molecule 8: Cytochrome b-c1 complex subunit 6



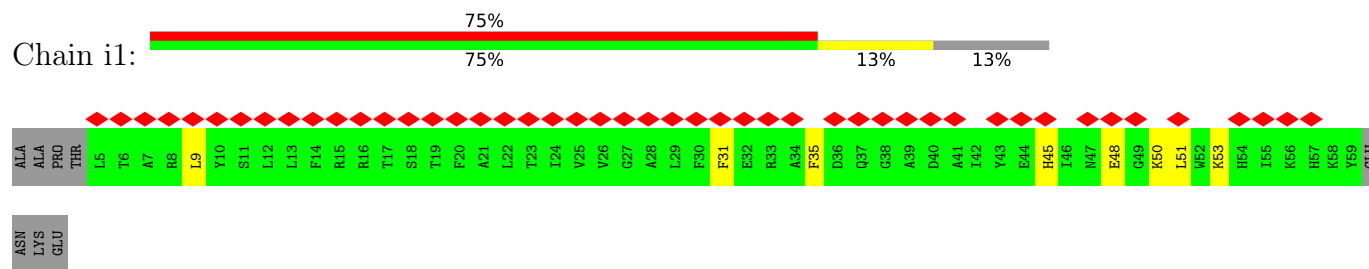
- Molecule 9: UQCRFS1N



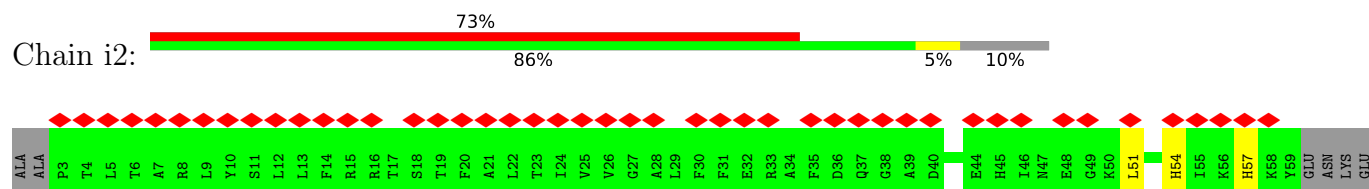
- Molecule 9: UQCRFS1N



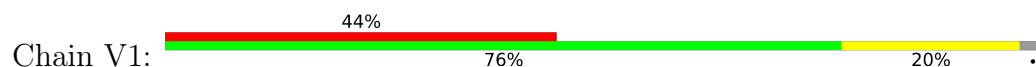
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

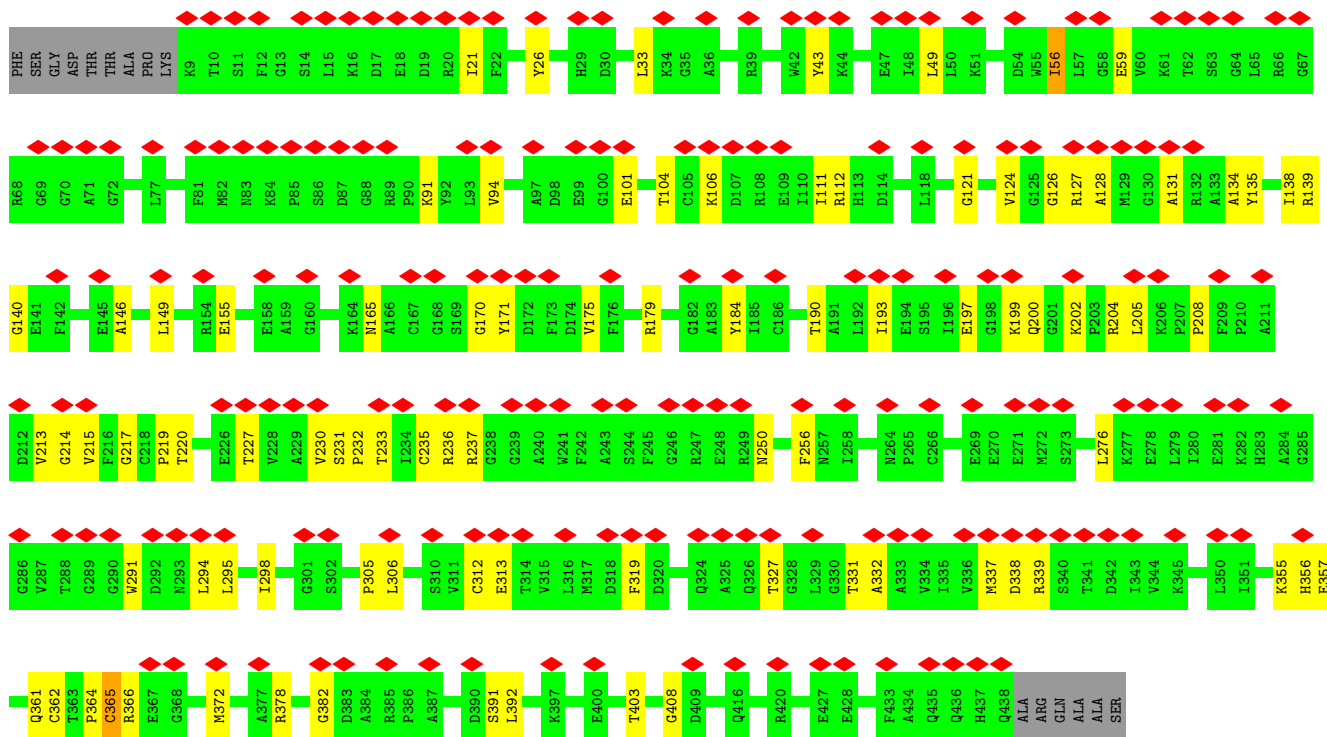


- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

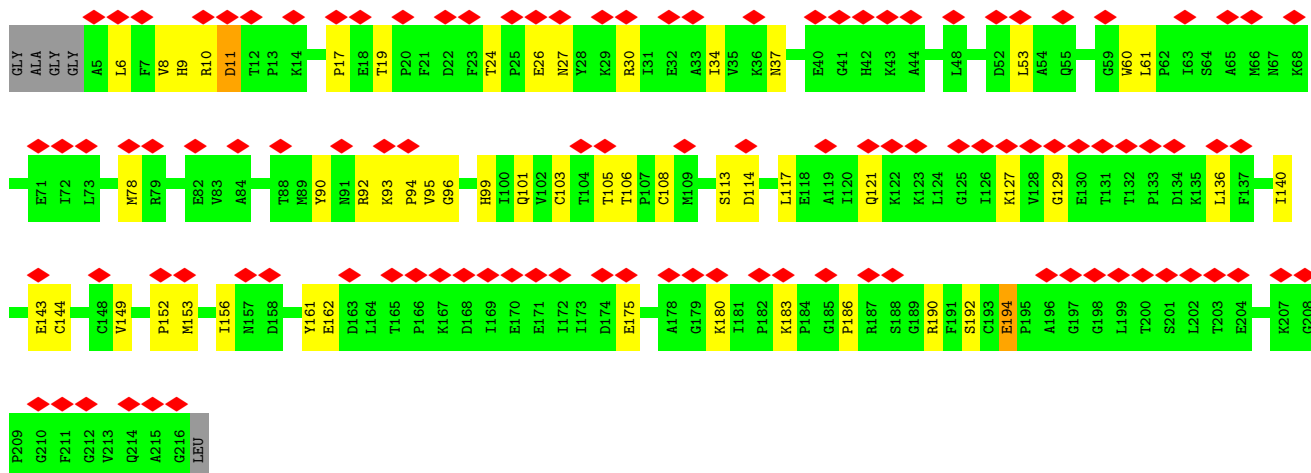
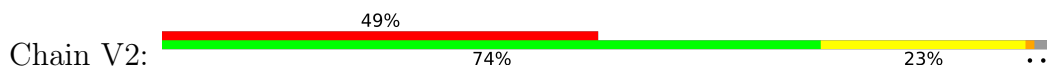


- Molecule 11: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

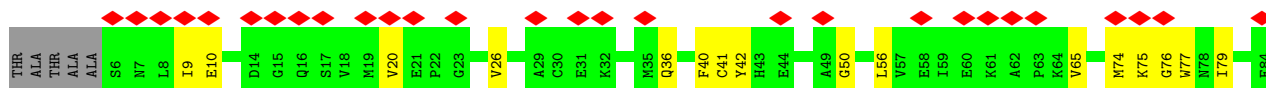


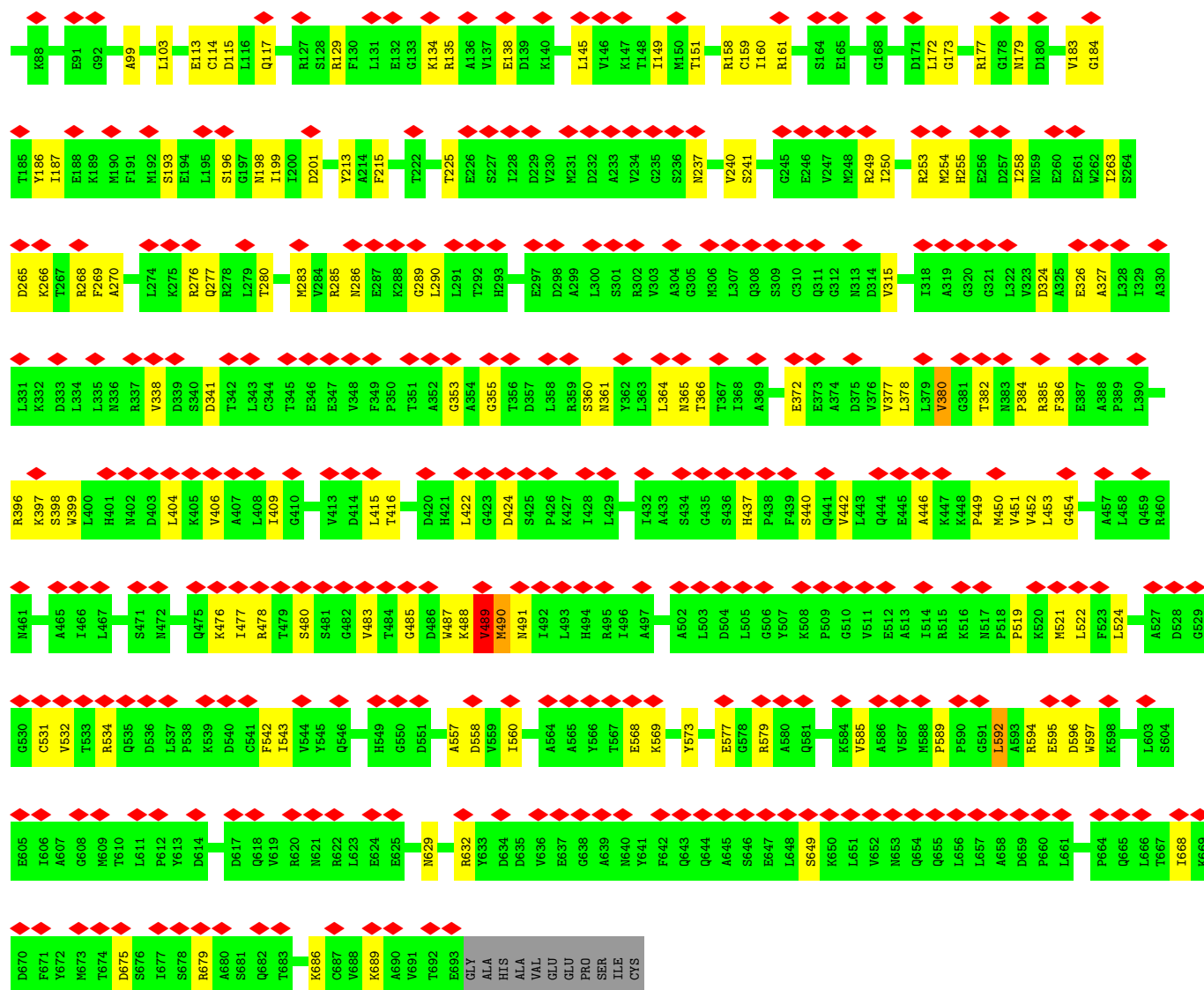


• Molecule 12: NDUFV2

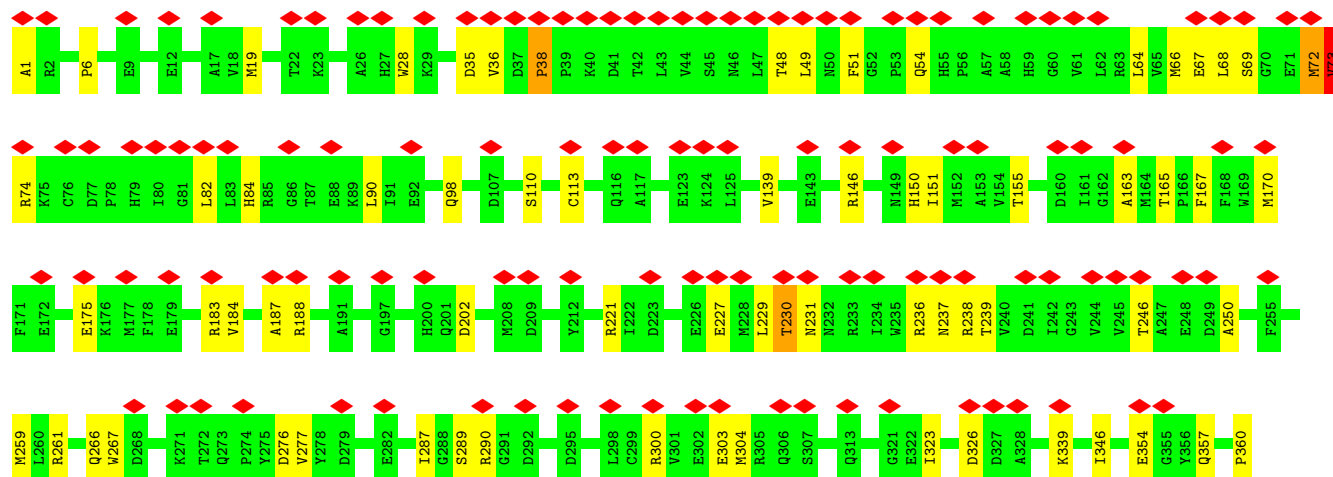
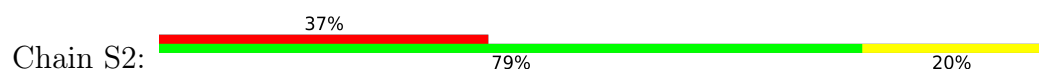


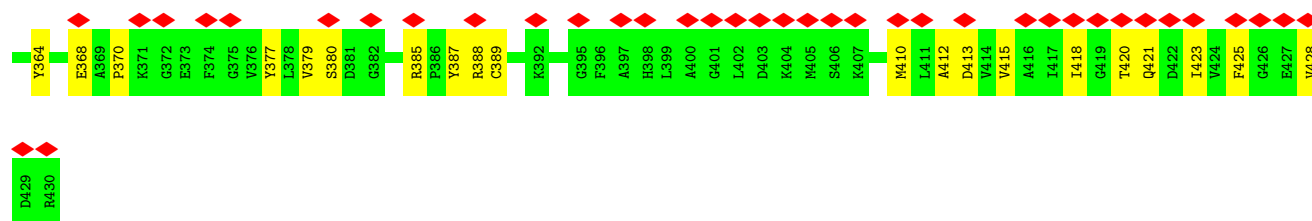
• Molecule 13: NADH:ubiquinone oxidoreductase core subunit S1



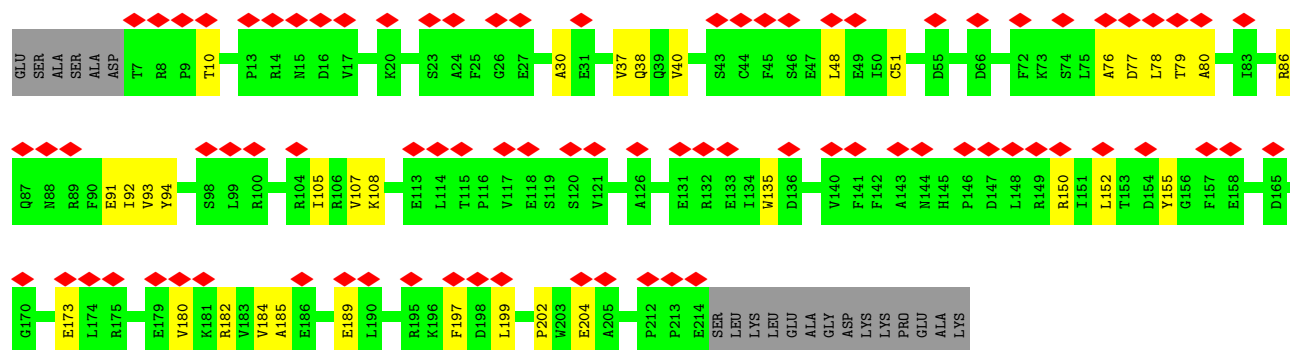
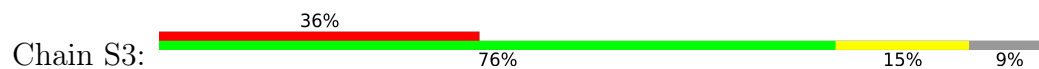


• Molecule 14: NDUFS2

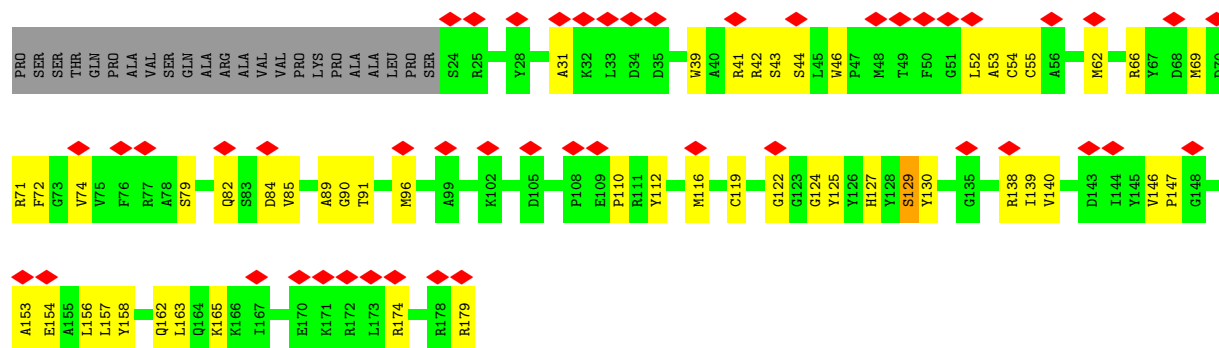




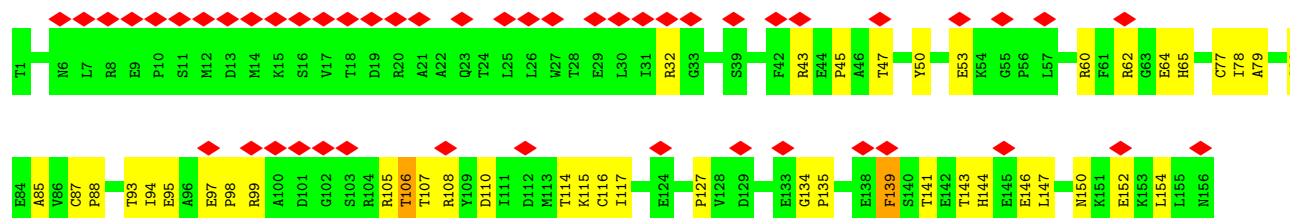
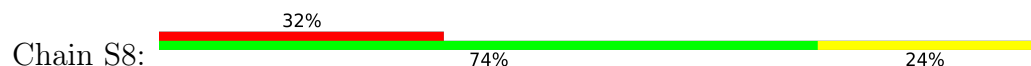
• Molecule 15: NADH:ubiquinone oxidoreductase core subunit S3

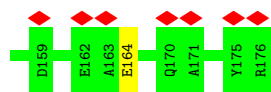


• Molecule 16: NDUFS7

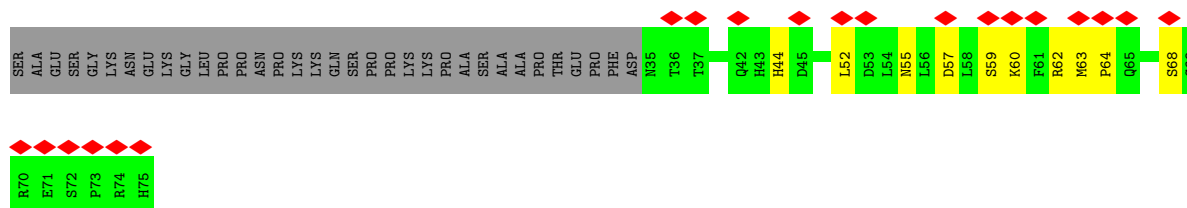
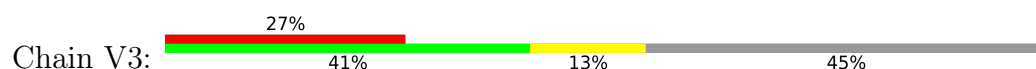


• Molecule 17: NDUFS8

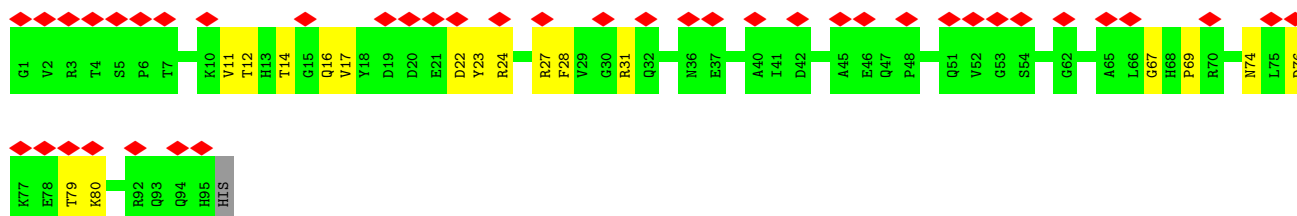
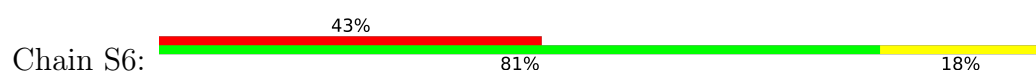




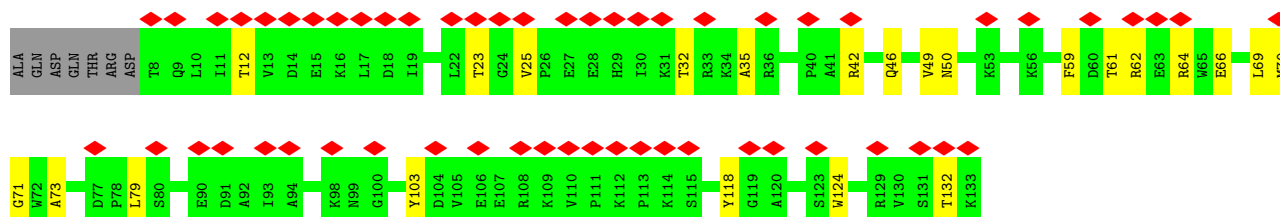
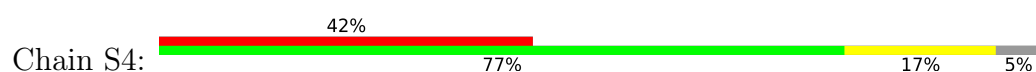
- Molecule 18: NDUFV3



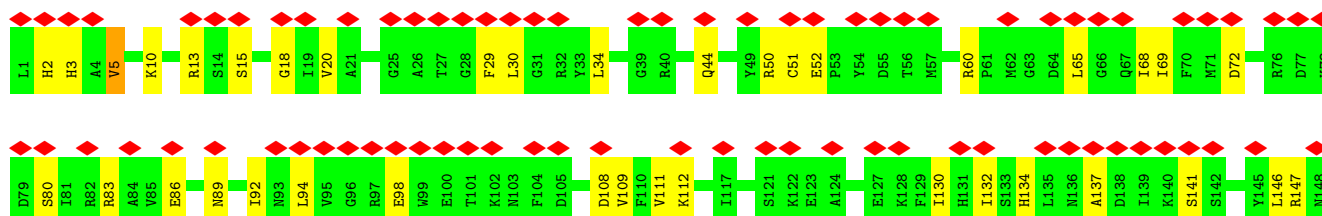
- Molecule 19: NDUFS6

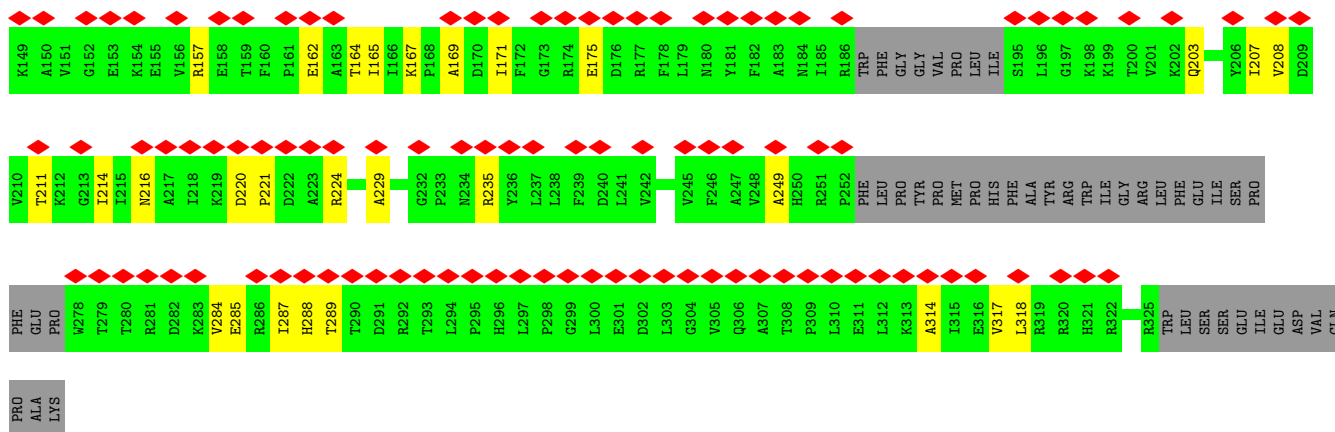


- Molecule 20: NADH:ubiquinone oxidoreductase subunit S4



- Molecule 21: NADH:ubiquinone oxidoreductase subunit A9

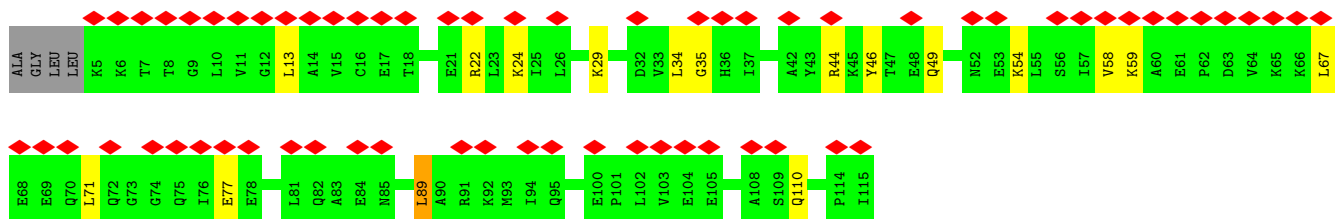
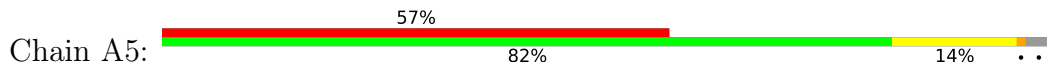




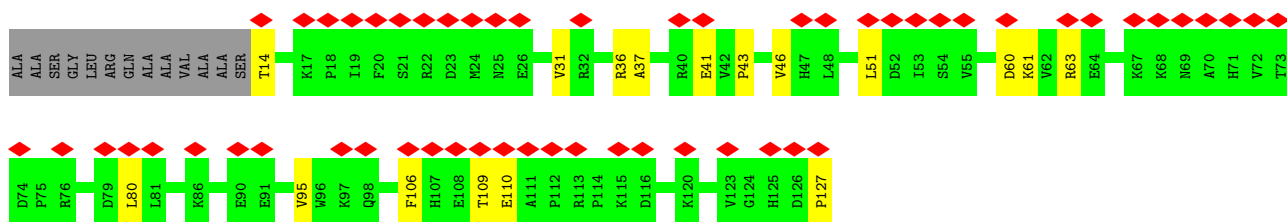
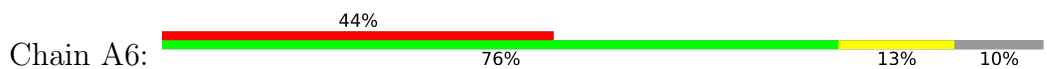
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 23: NDUFA5

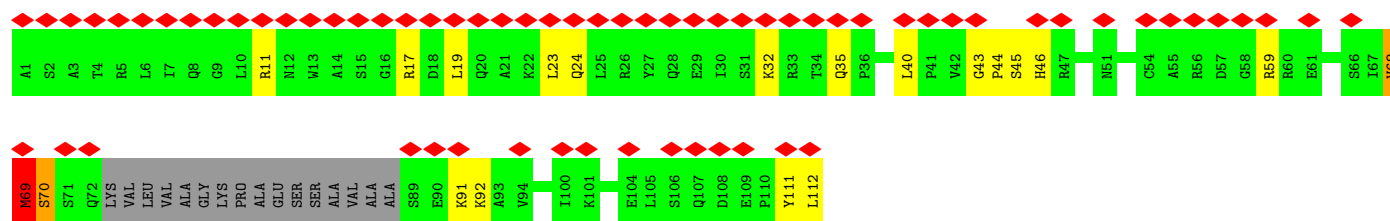


• Molecule 24: NADH:ubiquinone oxidoreductase subunit A6

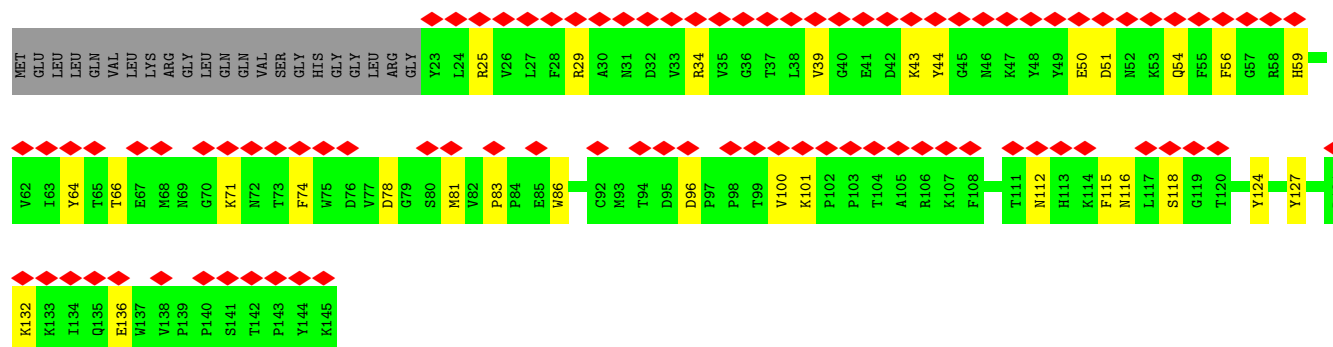


• Molecule 25: NDUFA7

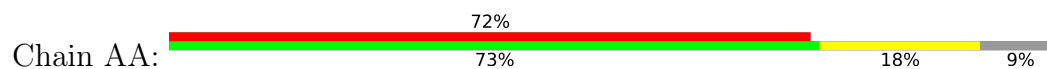




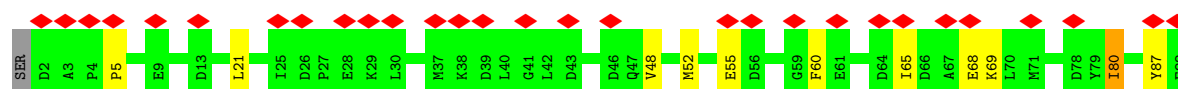
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



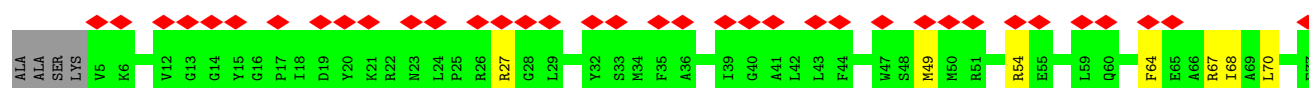
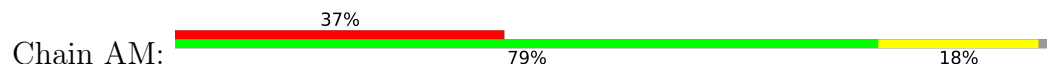
- Molecule 27: Acyl carrier protein

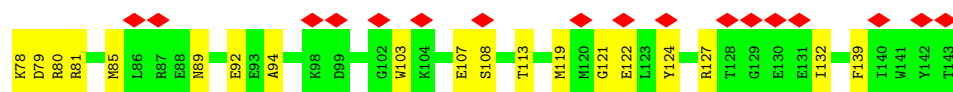


- Molecule 27: Acyl carrier protein

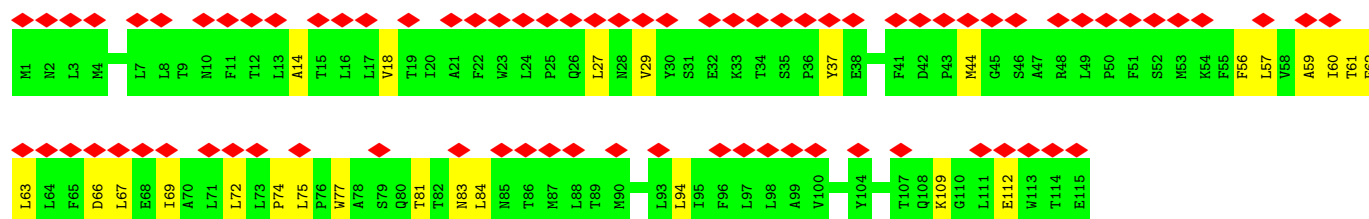
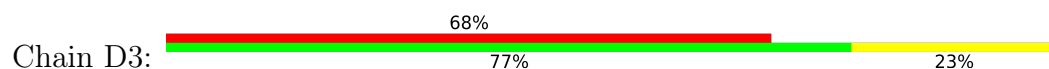


- Molecule 28: NDUFA13

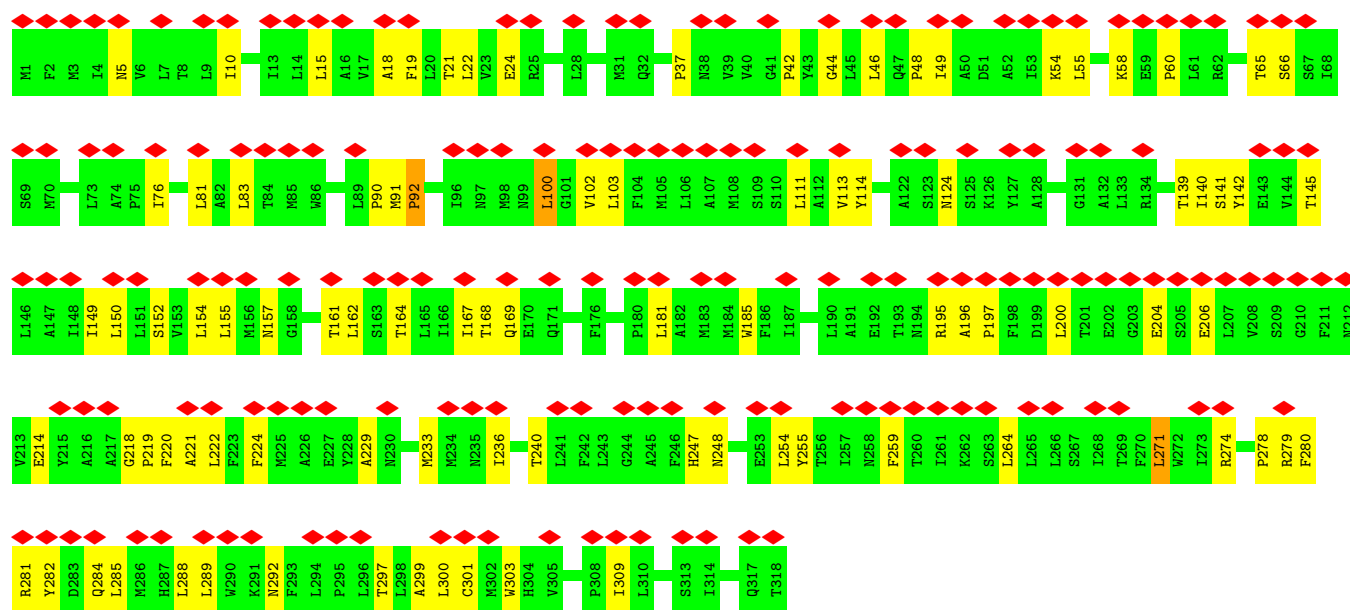
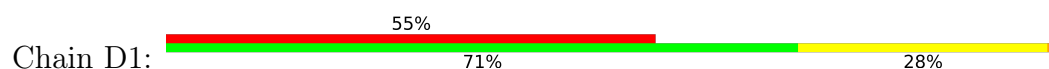




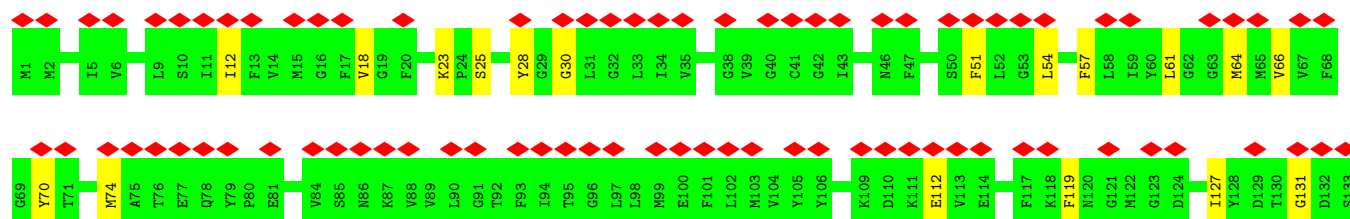
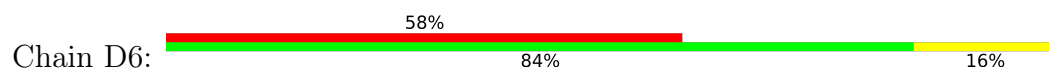
• Molecule 29: NADH-ubiquinone oxidoreductase chain 3

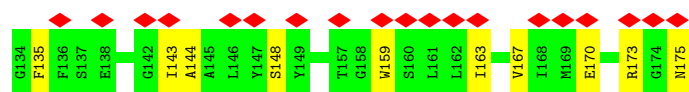


• Molecule 30: NADH-ubiquinone oxidoreductase chain 1

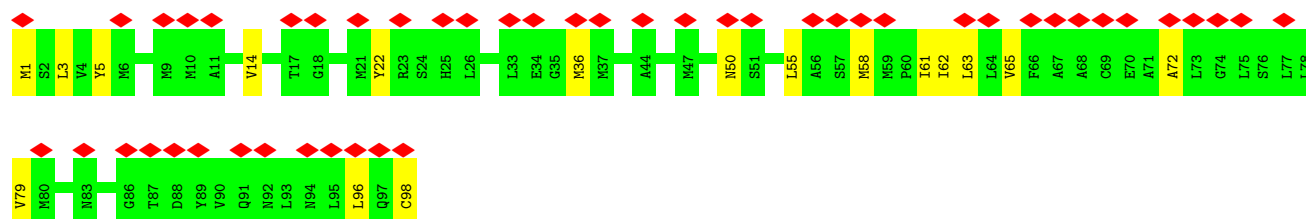
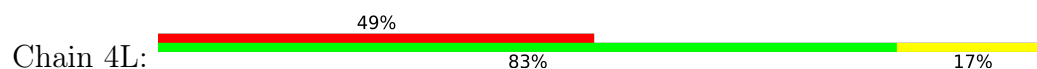


• Molecule 31: NADH-ubiquinone oxidoreductase chain 6

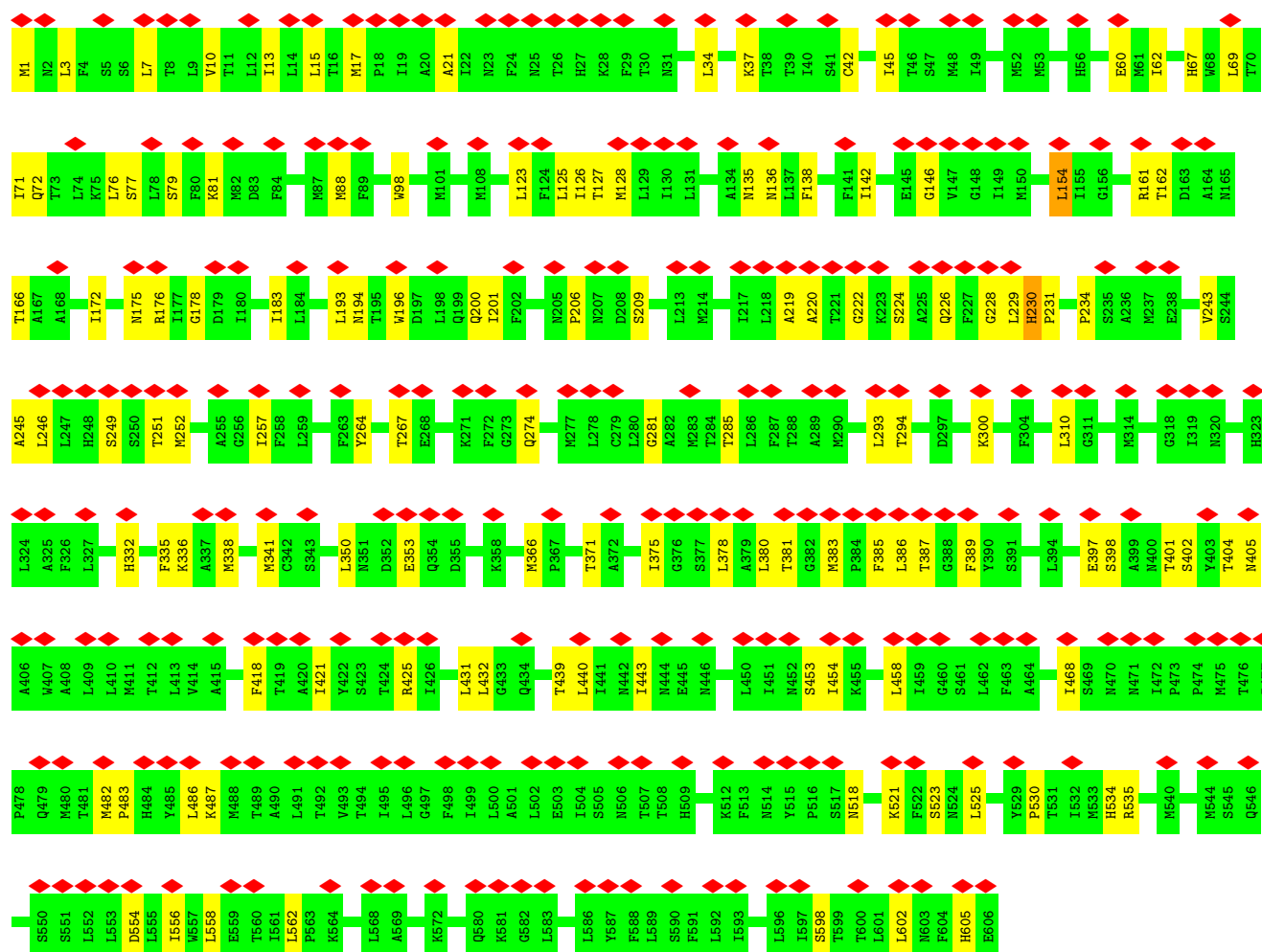
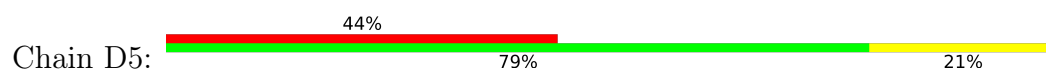




• Molecule 32: NADH-ubiquinone oxidoreductase chain 4L

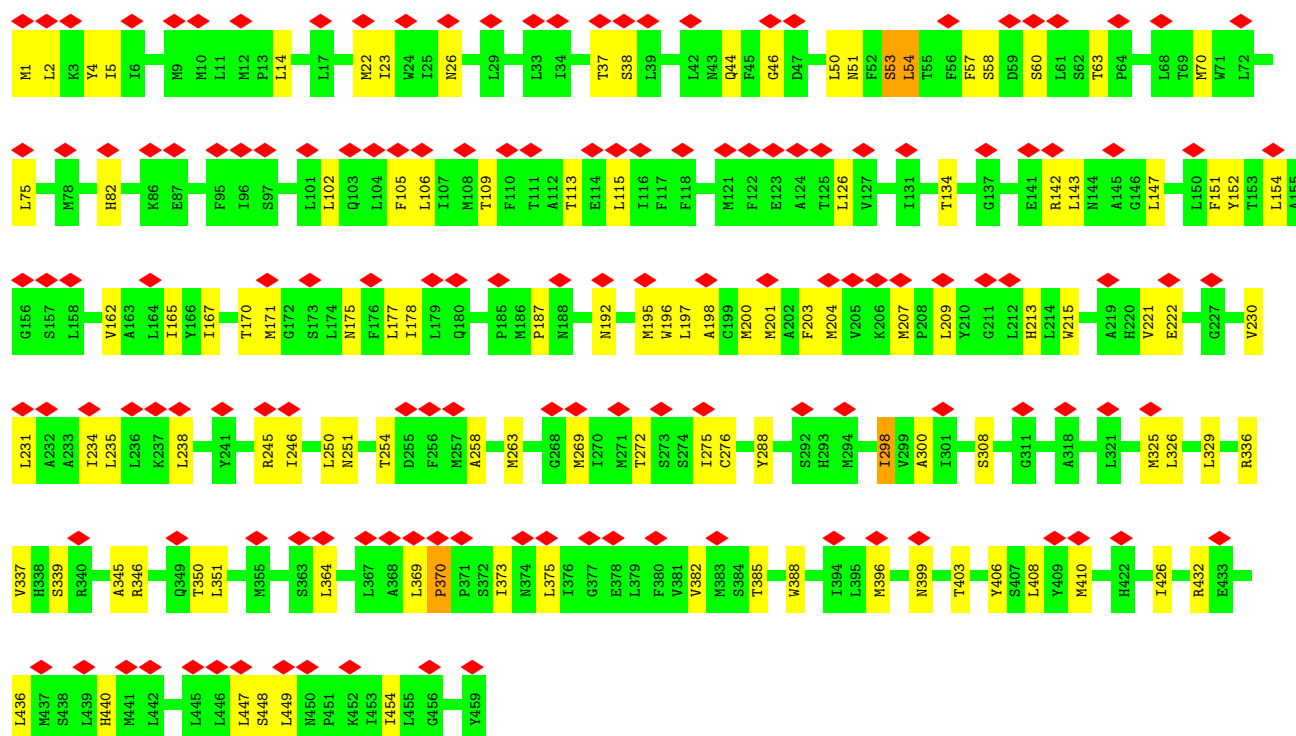


• Molecule 33: NADH-ubiquinone oxidoreductase chain 5



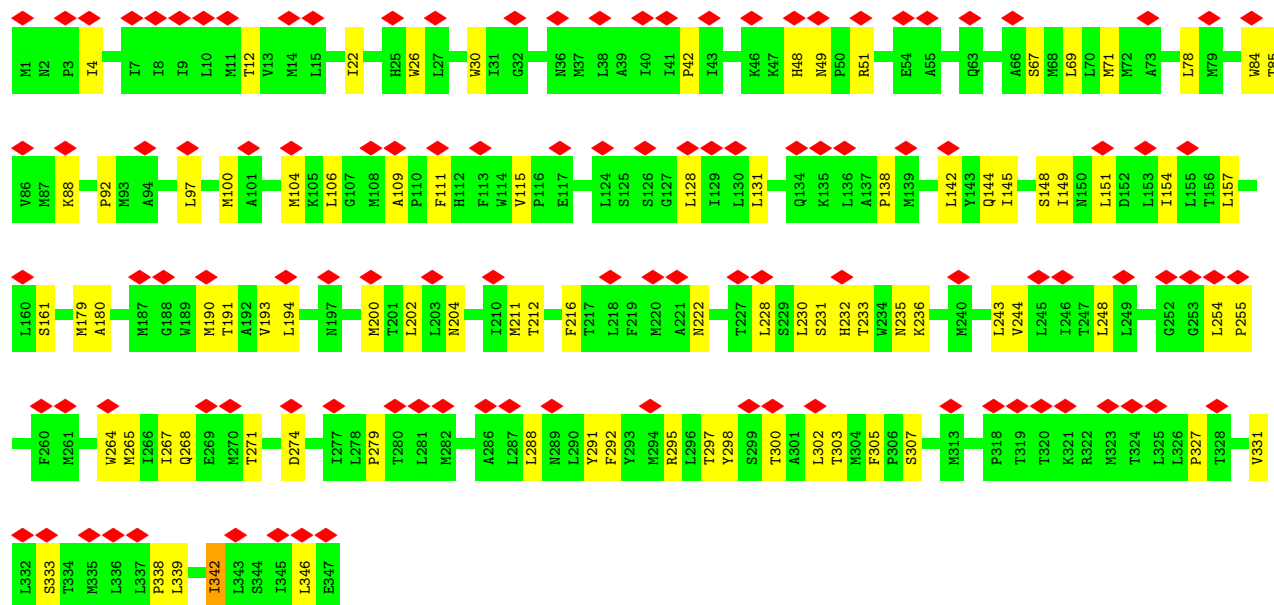
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4

Chain D4: 



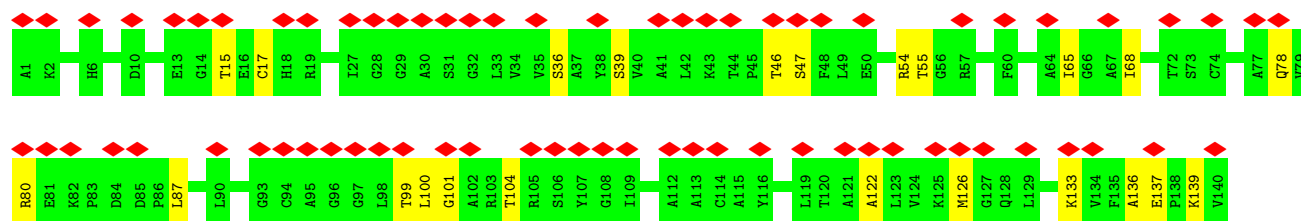
• Molecule 35: NADH-ubiquinone oxidoreductase chain 2

Chain D2: 

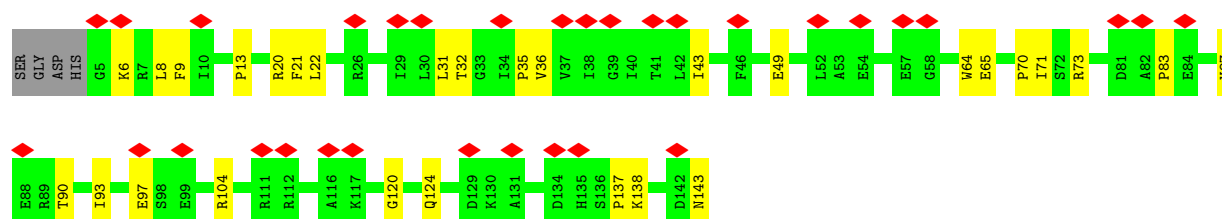
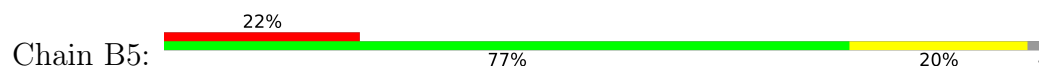


• Molecule 36: NDUF11

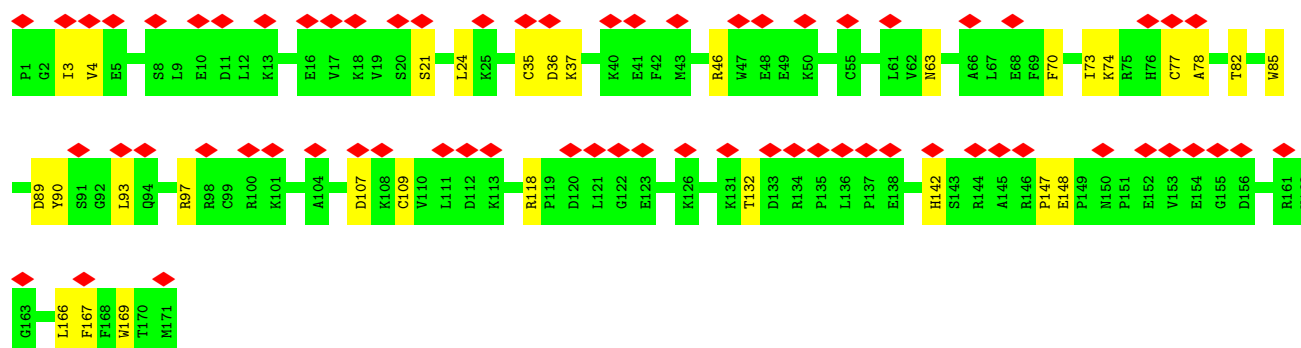
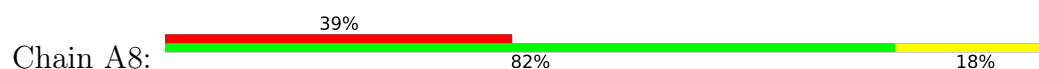
Chain AK: 



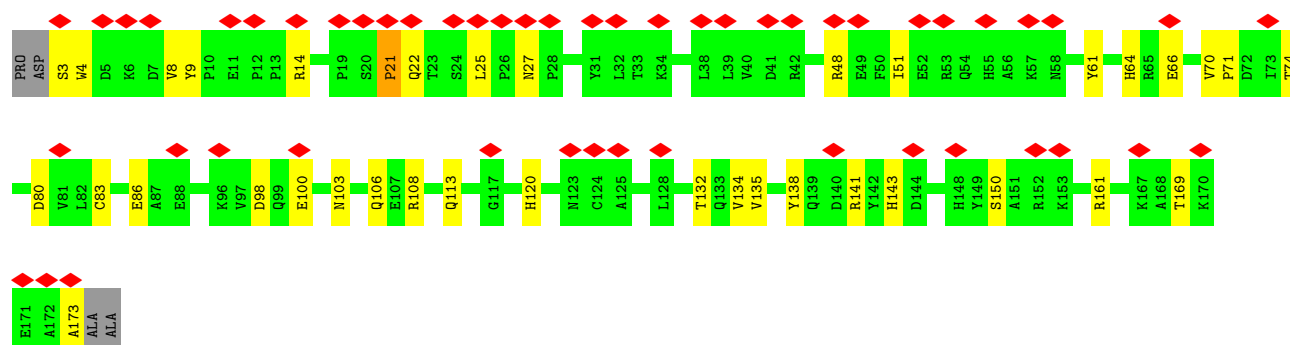
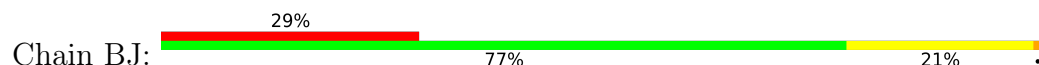
• Molecule 37: NADH:ubiquinone oxidoreductase subunit B5



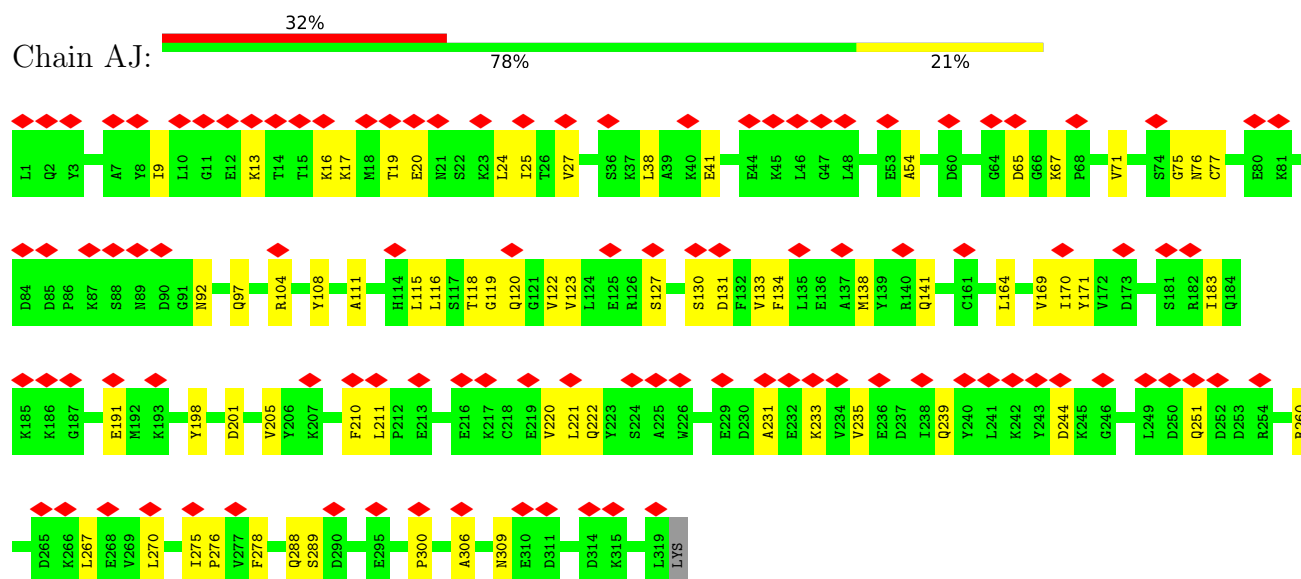
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



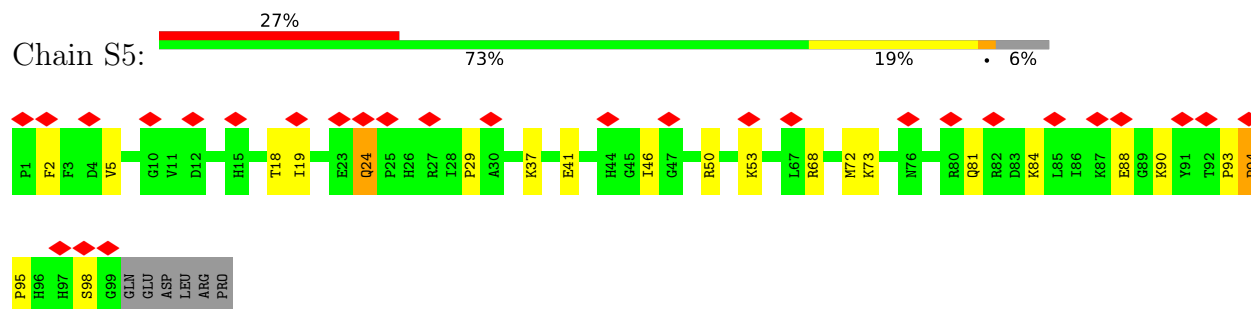
• Molecule 39: NDUFB10



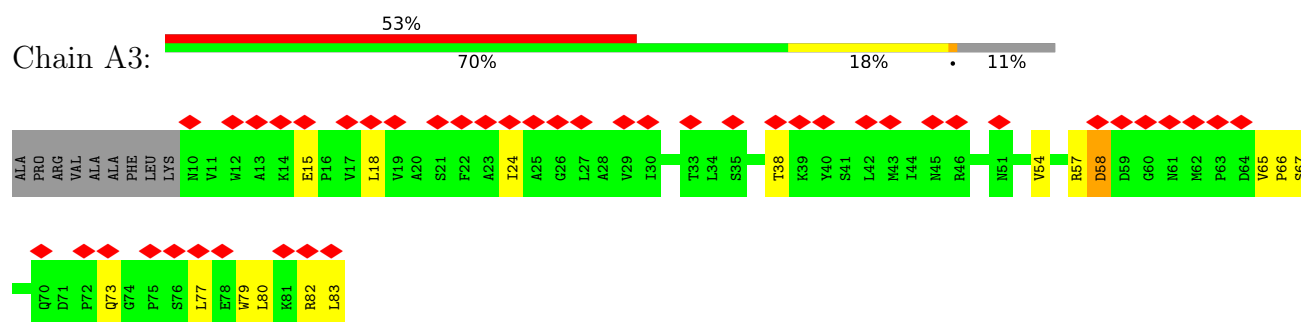
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



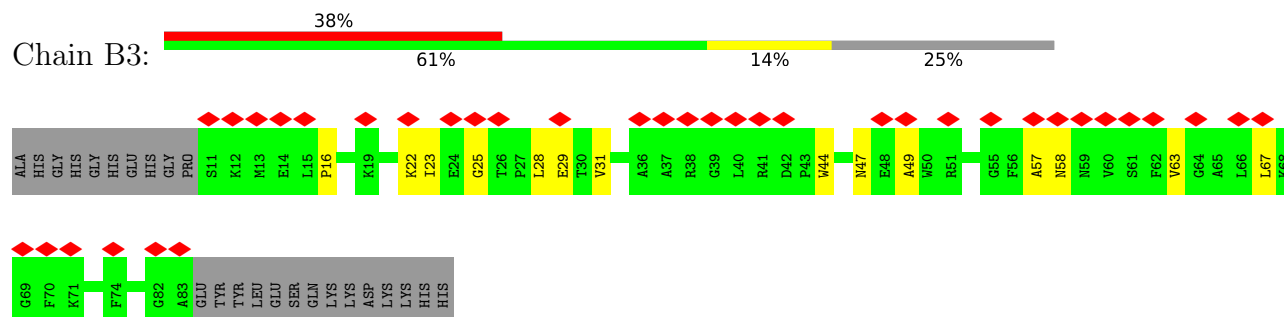
• Molecule 41: NADH:ubiquinone oxidoreductase subunit S5



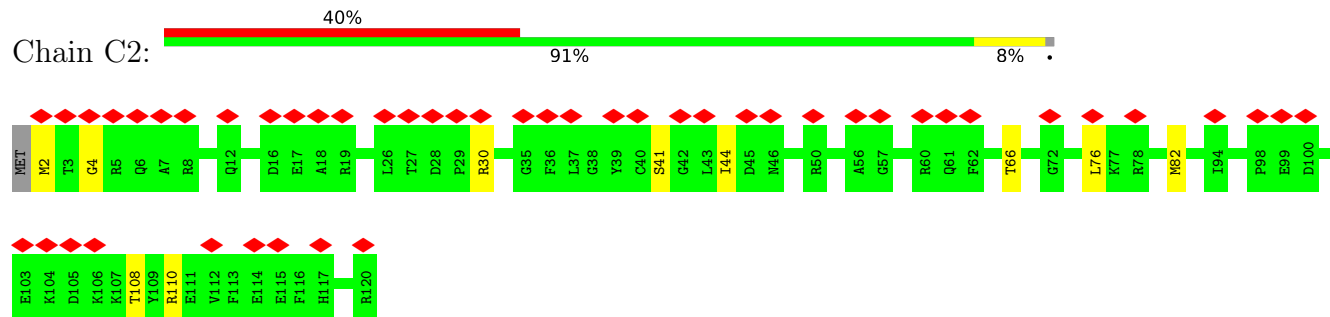
• Molecule 42: NADH:ubiquinone oxidoreductase subunit A3



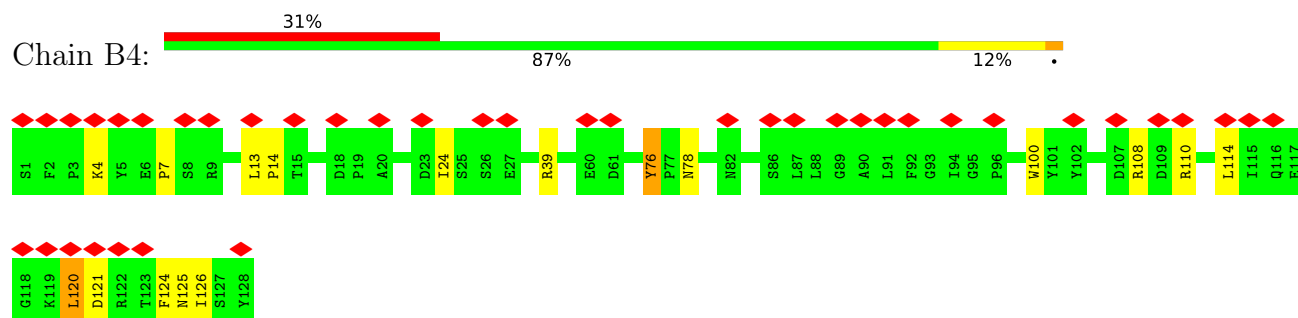
• Molecule 43: NADH:ubiquinone oxidoreductase subunit B3



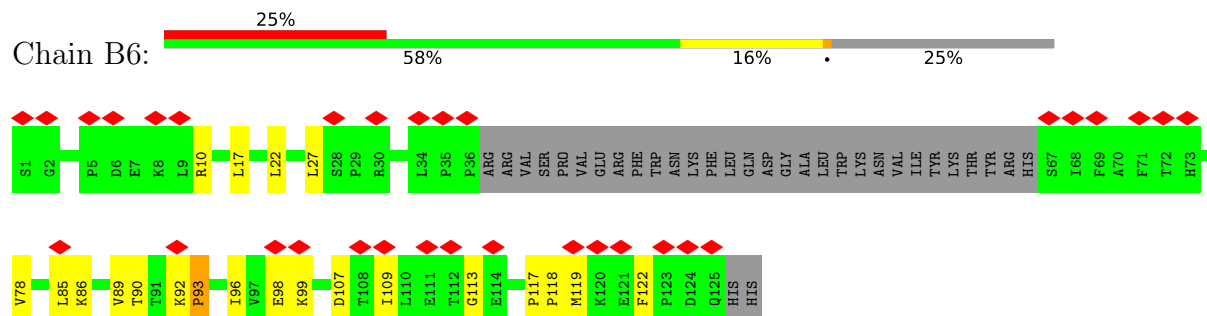
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 subunit C2



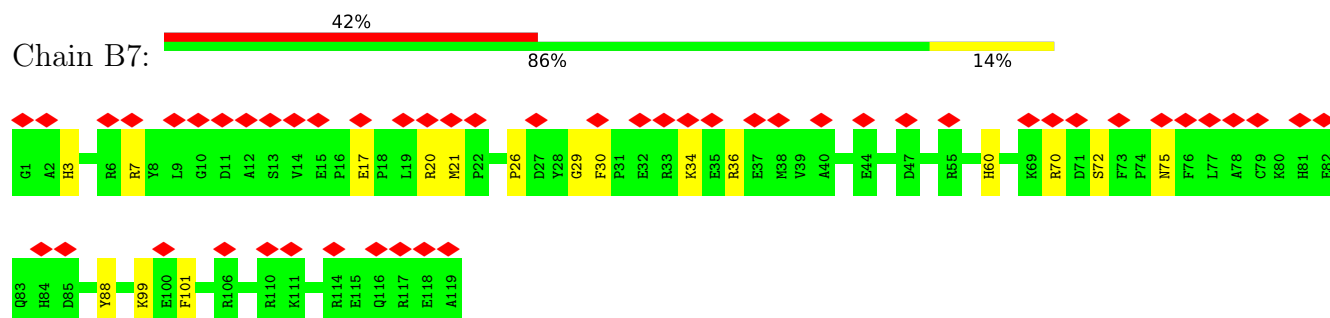
- Molecule 45: NADH:ubiquinone oxidoreductase subunit B4



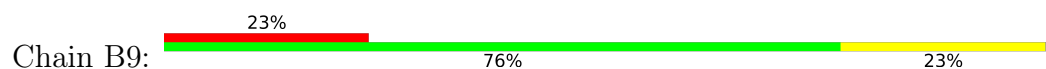
- Molecule 46: NDUFB6

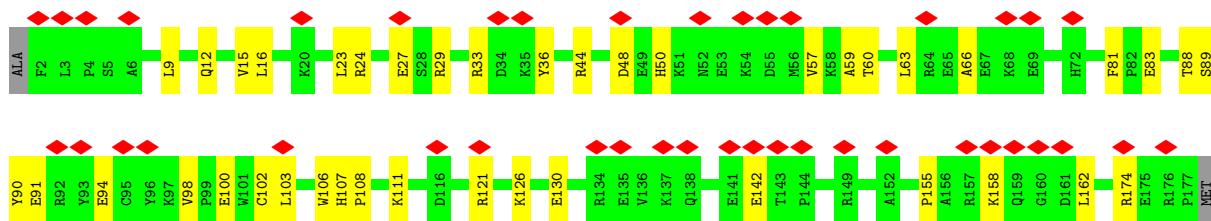


- Molecule 47: NADH:ubiquinone oxidoreductase subunit B7

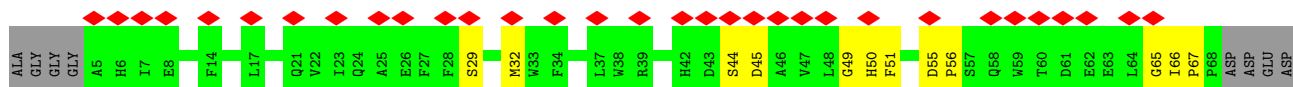
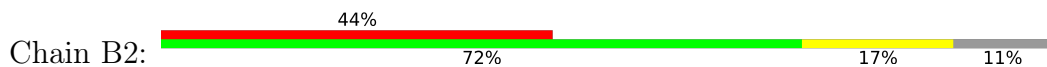


- Molecule 48: NADH:ubiquinone oxidoreductase subunit B9

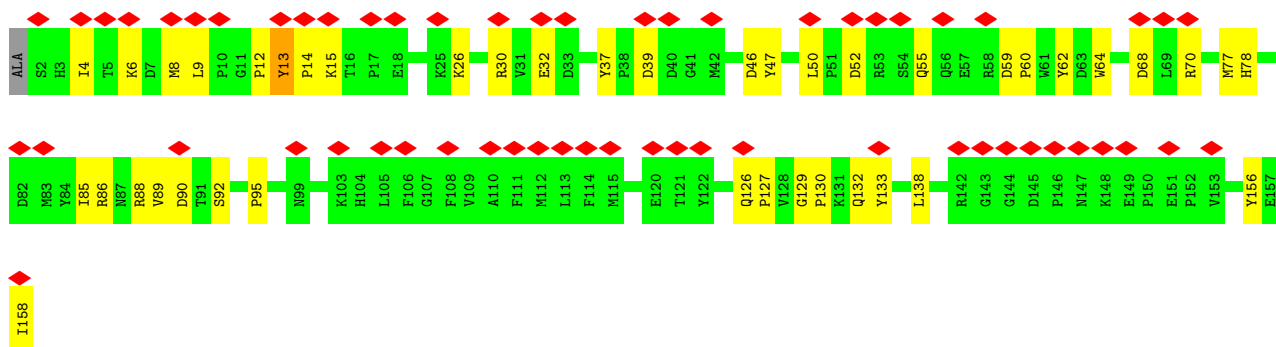
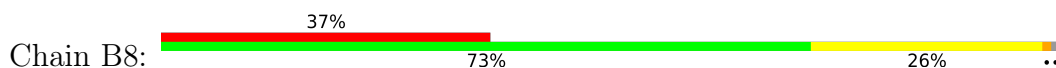




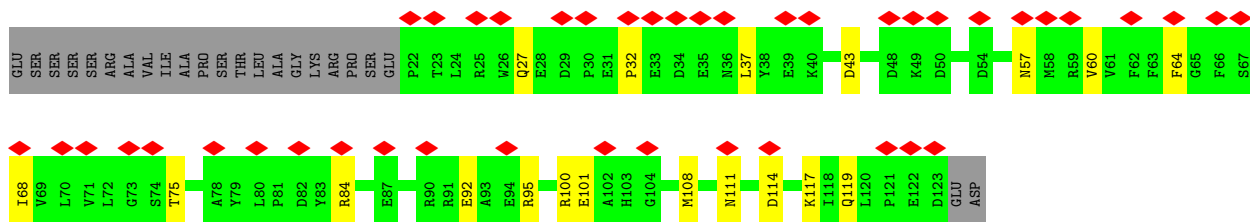
- Molecule 49: NADH:ubiquinone oxidoreductase subunit B2



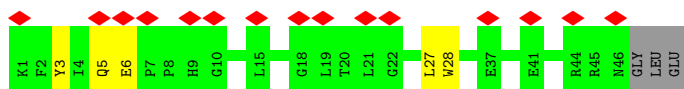
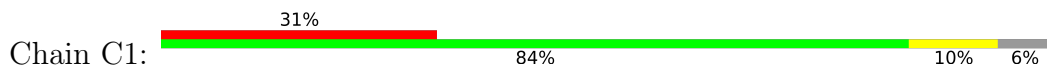
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



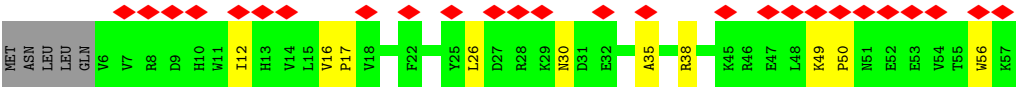
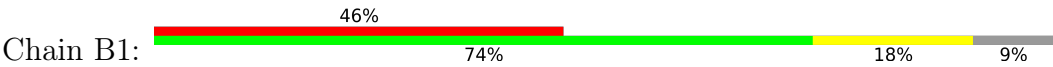
- Molecule 51: NDUFB11



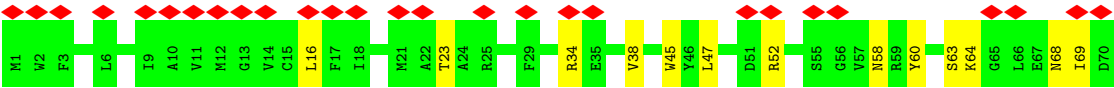
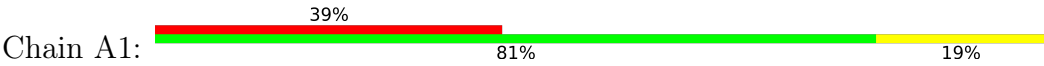
- Molecule 52: NDUFC1



- Molecule 53: NDUFB1



● Molecule 54: NDUFA1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.049	Depositor
Minimum map value	-0.332	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/3479	0.59	1/4719 (0.0%)
1	a3	0.26	0/3518	0.55	0/4776
2	a2	0.23	0/3183	0.53	0/4313
2	a4	0.24	0/3179	0.55	0/4308
3	b1	0.27	0/3119	0.57	0/4268
3	b2	0.28	0/3119	0.58	1/4268 (0.0%)
4	c1	0.23	0/1968	0.53	0/2672
4	c2	0.25	0/1962	0.58	1/2664 (0.0%)
5	f1	0.20	0/1554	0.49	0/2101
5	f2	0.21	0/1548	0.50	0/2093
6	d1	0.24	0/906	0.54	0/1213
6	d2	0.24	0/908	0.54	0/1218
7	q1	0.27	0/638	0.61	0/862
7	q2	0.30	0/652	0.67	0/883
8	h1	0.22	0/538	0.62	0/723
8	h2	0.29	0/538	0.73	0/723
10	i1	0.23	0/471	0.56	0/634
10	i2	0.23	0/486	0.59	0/655
11	V1	0.28	0/3386	0.61	0/4575
12	V2	0.28	0/1687	0.73	2/2295 (0.1%)
13	S1	0.27	0/5362	0.64	0/7266
14	S2	0.31	0/3547	0.64	5/4808 (0.1%)
15	S3	0.30	0/1776	0.71	1/2417 (0.0%)
16	S7	0.33	0/1279	0.69	2/1728 (0.1%)
17	S8	0.32	0/1446	0.64	0/1956
18	V3	0.26	0/355	0.73	0/480
19	S6	0.24	0/749	0.56	0/1009
20	S4	0.25	0/1048	0.52	0/1415
21	A9	0.27	0/2397	0.71	3/3239 (0.1%)
22	A2	0.23	0/676	0.64	0/911
23	A5	0.28	0/921	0.72	1/1249 (0.1%)
24	A6	0.26	0/993	0.65	2/1336 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	A7	0.23	0/784	0.70	0/1060
26	AL	0.27	0/1084	0.65	0/1478
27	AA	0.24	0/655	0.68	0/881
27	AB	0.24	0/714	0.58	0/963
28	AM	0.29	0/1172	0.64	0/1579
29	D3	0.32	0/948	0.74	0/1296
30	D1	0.35	0/2604	0.76	2/3561 (0.1%)
31	D6	0.31	0/1379	0.70	0/1868
32	4L	0.33	0/758	0.70	0/1024
33	D5	0.32	0/4933	0.74	2/6710 (0.0%)
34	D4	0.36	0/3740	0.76	3/5095 (0.1%)
35	D2	0.35	0/2788	0.69	1/3795 (0.0%)
36	AK	0.27	0/1046	0.74	2/1419 (0.1%)
37	B5	0.25	0/1189	0.55	0/1607
38	A8	0.28	0/1441	0.71	0/1942
39	BJ	0.30	0/1475	0.66	3/1989 (0.2%)
40	AJ	0.27	0/2644	0.64	5/3579 (0.1%)
41	S5	0.31	0/843	0.68	1/1128 (0.1%)
42	A3	0.28	0/602	0.72	0/828
43	B3	0.30	0/595	0.83	2/803 (0.2%)
44	C2	0.28	0/1028	0.65	4/1388 (0.3%)
45	B4	0.27	0/1085	0.61	0/1467
46	B6	0.30	0/830	0.79	0/1130
47	B7	0.26	0/1051	0.72	2/1408 (0.1%)
48	B9	0.28	0/1568	0.70	2/2123 (0.1%)
49	B2	0.31	0/582	0.71	2/799 (0.3%)
50	B8	0.30	0/1379	0.80	3/1884 (0.2%)
51	BK	0.28	0/880	0.67	0/1196
52	C1	0.24	0/404	0.67	0/548
53	B1	0.26	0/462	0.62	0/624
54	A1	0.28	0/592	0.66	0/795
All	All	0.28	0/98643	0.65	53/133744 (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	4
1	a3	0	1
2	a2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	c1	0	2
5	f2	0	1
7	q1	0	1
12	V2	0	1
13	S1	0	5
14	S2	0	2
15	S3	0	1
17	S8	0	2
25	A7	0	3
26	AL	0	1
30	D1	0	4
33	D5	0	1
34	D4	0	1
39	BJ	0	1
40	AJ	0	1
41	S5	0	1
42	A3	0	2
43	B3	0	3
45	B4	0	1
46	B6	0	1
48	B9	0	1
49	B2	0	1
52	C1	0	2
54	A1	0	1
All	All	0	46

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A9	5	VAL	N-CA-C	-9.09	104.62	113.53
39	BJ	21	PRO	CA-C-N	9.00	137.90	121.70
39	BJ	21	PRO	C-N-CA	9.00	137.90	121.70
14	S2	72	MET	CA-C-N	7.21	134.95	121.97
14	S2	72	MET	C-N-CA	7.21	134.95	121.97
35	D2	342	ILE	N-CA-C	-6.94	105.74	111.91
24	A6	110	GLU	CA-C-N	6.91	134.14	121.70
24	A6	110	GLU	C-N-CA	6.91	134.14	121.70
49	B2	44	SER	CA-C-N	6.50	133.40	121.70
49	B2	44	SER	C-N-CA	6.50	133.40	121.70
48	B9	9	LEU	CA-C-N	6.37	133.70	121.54
48	B9	9	LEU	C-N-CA	6.37	133.70	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S2	230	THR	CA-C-N	6.07	133.13	121.54
14	S2	230	THR	C-N-CA	6.07	133.13	121.54
36	AK	17	CYS	CA-C-N	6.01	133.01	121.54
36	AK	17	CYS	C-N-CA	6.01	133.01	121.54
44	C2	4	GLY	CA-C-N	5.81	132.16	121.70
44	C2	4	GLY	C-N-CA	5.81	132.16	121.70
3	b2	133	LEU	N-CA-C	5.77	122.56	109.81
44	C2	4	GLY	N-CA-C	5.74	118.08	111.36
40	AJ	251	GLN	CA-C-N	5.55	131.69	121.70
40	AJ	251	GLN	C-N-CA	5.55	131.69	121.70
30	D1	214	GLU	CA-C-N	-5.54	112.58	120.89
30	D1	214	GLU	C-N-CA	-5.54	112.58	120.89
44	C2	4	GLY	CA-C-O	-5.49	116.58	121.41
50	B8	13	TYR	N-CA-C	5.45	121.86	109.81
23	A5	89	LEU	CA-CB-CG	5.44	135.33	116.30
39	BJ	25	LEU	C-N-CD	-5.33	108.88	120.60
40	AJ	275	ILE	CA-C-N	5.29	139.68	127.00
40	AJ	275	ILE	C-N-CA	5.29	139.68	127.00
21	A9	221	PRO	CA-C-N	5.25	134.16	124.82
21	A9	221	PRO	C-N-CA	5.25	134.16	124.82
4	c2	70	VAL	N-CA-C	-5.22	107.74	112.96
41	S5	94	PRO	N-CA-C	5.21	117.06	110.70
50	B8	37	TYR	CA-C-N	5.21	139.50	127.00
50	B8	37	TYR	C-N-CA	5.21	139.50	127.00
12	V2	11	ASP	CA-C-N	5.18	129.96	121.57
12	V2	11	ASP	C-N-CA	5.18	129.96	121.57
16	S7	129	SER	CA-C-N	5.17	131.42	121.54
16	S7	129	SER	C-N-CA	5.17	131.42	121.54
14	S2	165	THR	N-CA-C	5.14	121.17	109.81
40	AJ	275	ILE	C-N-CD	-5.13	109.31	120.60
33	D5	230	HIS	N-CA-C	5.11	121.09	109.81
34	D4	370	PRO	N-CA-C	5.10	116.92	110.70
47	B7	26	PRO	CA-C-N	5.06	129.60	122.46
47	B7	26	PRO	C-N-CA	5.06	129.60	122.46
43	B3	57	ALA	CA-C-N	5.04	131.17	121.54
43	B3	57	ALA	C-N-CA	5.04	131.17	121.54
15	S3	77	ASP	N-CA-C	5.03	121.51	110.80
33	D5	69	LEU	CA-CB-CG	5.03	133.90	116.30
1	a1	278	GLY	N-CA-C	5.02	125.07	113.18
34	D4	339	SER	CA-C-N	5.01	131.11	121.54
34	D4	339	SER	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	A1	63	SER	Peptide
42	A3	58	ASP	Peptide
42	A3	65	VAL	Peptide
25	A7	68	VAL	Peptide
25	A7	69	MET	Peptide
25	A7	70	SER	Peptide
40	AJ	278	PHE	Peptide
26	AL	43	LYS	Peptide
49	B2	56	PRO	Peptide
43	B3	16	PRO	Peptide
43	B3	22	LYS	Peptide
43	B3	58	ASN	Peptide
45	B4	76	TYR	Peptide
46	B6	122	PHE	Peptide
48	B9	29	ARG	Peptide
39	BJ	150	SER	Peptide
52	C1	5	GLN	Peptide
52	C1	6	GLU	Peptide
30	D1	42	PRO	Peptide
30	D1	44	GLY	Peptide
30	D1	66	SER	Peptide
30	D1	91	MET	Peptide
34	D4	53	SER	Peptide
33	D5	353	GLU	Peptide
13	S1	213	TYR	Peptide
13	S1	341	ASP	Peptide
13	S1	380	VAL	Peptide
13	S1	489	VAL	Mainchain
13	S1	592	LEU	Peptide
14	S2	38	PRO	Peptide
14	S2	73	VAL	Mainchain
15	S3	76	ALA	Peptide
41	S5	24	GLN	Peptide
17	S8	106	THR	Peptide
17	S8	139	PHE	Peptide
12	V2	194	GLU	Peptide
1	a1	278	GLY	Mainchain,Peptide
1	a1	279	HIS	Peptide
1	a1	309	THR	Peptide
2	a2	133	ARG	Peptide
1	a3	309	THR	Peptide
4	c1	170	PHE	Peptide

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Mol	Chain	Res	Type	Group
4	c1	237	ARG	Peptide
5	f2	188	THR	Peptide
7	q1	6	HIS	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	54	0
1	a3	3447	0	3350	39	0
2	a2	3126	0	3093	38	0
2	a4	3122	0	3090	46	0
3	b1	3019	0	3082	33	0
3	b2	3019	0	3082	38	0
4	c1	1909	0	1858	31	0
4	c2	1903	0	1850	33	0
5	f1	1520	0	1505	23	0
5	f2	1514	0	1497	34	0
6	d1	886	0	883	13	0
6	d2	888	0	880	11	0
7	q1	618	0	628	12	0
7	q2	631	0	639	12	0
8	h1	532	0	509	5	0
8	h2	532	0	509	8	0
9	x1	114	0	29	0	0
9	x2	130	0	34	1	0
10	i1	459	0	462	6	0
10	i2	473	0	477	2	0
11	V1	3312	0	3266	60	0
12	V2	1647	0	1657	37	0
13	S1	5275	0	5300	105	0
14	S2	3455	0	3395	73	0
15	S3	1726	0	1676	32	0
16	S7	1248	0	1256	38	0
17	S8	1415	0	1371	39	0
18	V3	345	0	323	8	0
19	S6	737	0	710	17	0
20	S4	1025	0	1023	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A9	2344	0	2372	43	0
22	A2	665	0	678	18	0
23	A5	901	0	936	12	0
24	A6	969	0	980	14	0
25	A7	766	0	779	19	0
26	AL	1044	0	1001	22	0
27	AA	645	0	649	9	0
27	AB	702	0	692	11	0
28	AM	1143	0	1137	22	0
29	D3	923	0	953	22	0
30	D1	2529	0	2641	64	0
31	D6	1345	0	1364	25	0
32	4L	748	0	794	18	0
33	D5	4805	0	4950	86	0
34	D4	3646	0	3850	77	0
35	D2	2724	0	2930	66	0
36	AK	1025	0	1033	14	0
37	B5	1156	0	1177	25	0
38	A8	1404	0	1384	24	0
39	BJ	1441	0	1417	24	0
40	AJ	2583	0	2547	42	0
41	S5	822	0	820	19	0
42	A3	582	0	583	12	0
43	B3	578	0	570	7	0
44	C2	997	0	983	9	0
45	B4	1059	0	1062	14	0
46	B6	804	0	824	16	0
47	B7	1026	0	995	15	0
48	B9	1515	0	1469	30	0
49	B2	555	0	505	8	0
50	B8	1324	0	1219	31	0
51	BK	853	0	800	18	0
52	C1	391	0	391	3	0
53	B1	449	0	453	7	0
54	A1	577	0	570	11	0
55	b1	86	0	60	5	0
55	b2	86	0	60	2	0
56	c1	43	0	30	1	0
56	c2	43	0	30	0	0
57	S1	4	0	0	0	0
57	V2	4	0	0	1	0
57	f1	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	f2	4	0	0	0	0
58	S1	16	0	0	1	0
58	S7	8	0	0	0	0
58	S8	16	0	0	0	0
58	V1	8	0	0	0	0
59	V1	31	0	19	0	0
60	D5	38	0	50	1	0
60	S2	40	0	54	3	0
61	S6	1	0	0	0	0
62	A9	48	0	26	5	0
63	AA	34	0	40	1	0
63	AB	31	0	34	4	0
64	AK	28	0	30	1	0
All	All	97049	0	96697	1399	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 (1399) 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)
15:S3:38:GLN:O	25:A7:70:SER:HA	1.14	1.25
15:S3:80:ALA:HA	15:S3:91:GLU:O	1.39	1.20
4:c1:237:ARG:O	7:q1:12:HIS:HA	1.42	1.18
4:c2:237:ARG:O	7:q2:12:HIS:HA	1.45	1.16
15:S3:38:GLN:O	25:A7:70:SER:CA	2.00	1.09
1:a1:279:HIS:HA	1:a1:307:PHE:O	1.61	1.00
4:c1:237:ARG:O	7:q1:12:HIS:CA	2.15	0.95
13:S1:237:ASN:O	13:S1:253:ARG:HB2	1.70	0.91
22:A2:21:HIS:O	22:A2:62:PRO:HA	1.70	0.91
5:f1:184:SER:HB2	5:f1:196:GLY:O	1.71	0.90
4:c2:237:ARG:O	7:q2:12:HIS:CA	2.19	0.89
13:S1:442:VAL:O	13:S1:446:ALA:HB2	1.72	0.88
15:S3:80:ALA:HA	15:S3:91:GLU:C	1.98	0.86
48:B9:126:LYS:O	48:B9:130:GLU:HB2	1.77	0.85
15:S3:80:ALA:CA	15:S3:91:GLU:O	2.23	0.83
13:S1:237:ASN:HB3	13:S1:253:ARG:O	1.80	0.80
24:A6:37:ALA:O	24:A6:41:GLU:HB2	1.86	0.75
5:f2:184:SER:HB2	5:f2:196:GLY:O	1.88	0.73
33:D5:37:LYS:HG2	33:D5:98:TRP:HE1	1.53	0.73
13:S1:266:LYS:O	13:S1:270:ALA:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S2:360:PRO:HA	14:S2:380:SER:O	1.89	0.72
8:h1:20:VAL:O	8:h1:24:CYS:HB2	1.88	0.72
13:S1:198:ASN:HD21	13:S1:263:ILE:H	1.35	0.71
2:a2:219:VAL:O	2:a2:223:PHE:HB2	1.91	0.71
30:D1:229:ALA:O	30:D1:233:MET:HB2	1.90	0.71
34:D4:231:LEU:O	34:D4:235:LEU:HB2	1.91	0.71
5:f2:156:TYR:HB2	5:f2:165:TYR:HB2	1.71	0.70
13:S1:489:VAL:HG13	13:S1:490:MET:HG2	1.74	0.70
1:a1:46:ARG:HH12	1:a1:315:ALA:H	1.40	0.70
11:V1:124:VAL:O	11:V1:128:ALA:HB2	1.92	0.70
13:S1:172:LEU:HA	13:S1:184:GLY:O	1.90	0.70
35:D2:88:LYS:HG3	35:D2:148:SER:HB3	1.74	0.69
1:a1:4:TYR:O	1:a1:8:LEU:HB2	1.93	0.68
13:S1:534:ARG:HH22	13:S1:558:ASP:HB2	1.60	0.67
5:f1:89:PHE:O	5:f1:95:PRO:HA	1.95	0.67
31:D6:18:VAL:HG22	32:4L:14:VAL:HG11	1.78	0.66
23:A5:22:ARG:HH22	40:AJ:239:GLN:HB3	1.61	0.66
28:AM:124:TYR:HB3	28:AM:132:ILE:HG22	1.78	0.66
5:f2:127:VAL:HG22	5:f2:129:LYS:H	1.61	0.66
60:S2:501:3PE:H291	35:D2:288:LEU:HD23	1.77	0.65
1:a1:240:GLU:HB3	7:q1:17:SER:HB2	1.78	0.65
26:AL:25:ARG:O	26:AL:29:ARG:HB2	1.97	0.65
13:S1:283:MET:HB2	13:S1:560:ILE:HB	1.79	0.65
2:a4:370:MET:HA	2:a4:373:GLU:HG3	1.77	0.65
11:V1:355:LYS:HE2	13:S1:179:ASN:HD22	1.61	0.65
43:B3:25:GLY:O	43:B3:29:GLU:HB2	1.97	0.65
12:V2:103:CYS:HB3	12:V2:153:MET:HG2	1.78	0.65
15:S3:38:GLN:HA	25:A7:70:SER:O	1.98	0.64
33:D5:161:ARG:NH1	48:B9:88:THR:O	2.31	0.64
33:D5:267:THR:O	33:D5:274:GLN:NE2	2.31	0.64
39:BJ:169:THR:O	39:BJ:173:ALA:HB2	1.96	0.64
17:S8:141:THR:HG22	17:S8:143:THR:H	1.62	0.64
35:D2:233:THR:HA	35:D2:236:LYS:HG2	1.80	0.64
3:b1:260:ASN:HB3	3:b1:263:ASN:HB2	1.79	0.63
14:S2:36:VAL:HG22	35:D2:49:ASN:HB3	1.80	0.63
28:AM:107:GLU:HG2	38:A8:3:ILE:HG22	1.79	0.63
11:V1:21:ILE:HG21	11:V1:230:VAL:HG23	1.81	0.63
3:b1:179:PHE:O	3:b1:183:PHE:HB2	1.98	0.63
31:D6:175:ASN:HD22	35:D2:48:HIS:HE1	1.47	0.63
34:D4:51:ASN:HD22	37:B5:90:THR:HG22	1.64	0.63
12:V2:60:TRP:HB3	12:V2:95:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S2:110:SER:HB2	14:S2:113:CYS:HB2	1.81	0.63
13:S1:286:ASN:O	13:S1:289:GLY:N	2.31	0.62
3:b2:152:ALA:HA	3:b2:287:LYS:HE2	1.81	0.62
14:S2:188:ARG:HH12	16:S7:153:ALA:H	1.48	0.62
34:D4:178:ILE:HD11	37:B5:97:GLU:HB3	1.81	0.62
21:A9:157:ARG:HH21	21:A9:165:ILE:HD13	1.65	0.62
13:S1:113:GLU:HA	20:S4:46:GLN:HE21	1.65	0.62
13:S1:324:ASP:HB2	13:S1:327:ALA:H	1.64	0.62
13:S1:449:PRO:O	13:S1:489:VAL:HA	1.99	0.62
15:S3:94:TYR:HB2	15:S3:107:VAL:HB	1.81	0.62
23:A5:34:LEU:HD11	23:A5:44:ARG:HA	1.82	0.62
31:D6:159:TRP:HE1	35:D2:12:THR:HG22	1.64	0.62
37:B5:13:PRO:O	48:B9:106:TRP:NE1	2.33	0.62
30:D1:197:PRO:HA	30:D1:200:LEU:HB3	1.82	0.62
36:AK:133:LYS:HZ1	36:AK:137:GLU:HG2	1.64	0.62
2:a4:116:VAL:O	2:a4:120:MET:HB2	1.99	0.61
3:b2:85:ASN:HD22	3:b2:243:VAL:HG12	1.65	0.61
14:S2:175:GLU:HB3	16:S7:66:ARG:HH11	1.65	0.61
28:AM:113:THR:O	38:A8:142:HIS:ND1	2.33	0.61
1:a3:419:CYS:SG	1:a3:438:ARG:NH1	2.73	0.61
13:S1:117:GLN:NE2	58:S1:801:SF4:S3	2.73	0.61
13:S1:632:ARG:NH1	22:A2:57:CYS:SG	2.73	0.61
11:V1:134:ALA:HB3	11:V1:175:VAL:HG12	1.82	0.61
14:S2:51:PHE:HB3	14:S2:64:LEU:HB3	1.81	0.61
21:A9:51:CYS:SG	21:A9:52:GLU:N	2.74	0.61
14:S2:385:ARG:NH2	15:S3:197:PHE:O	2.34	0.61
2:a2:52:LYS:HE3	2:a2:387:LEU:HG	1.82	0.61
19:S6:12:THR:HG21	19:S6:16:GLN:HE21	1.66	0.61
35:D2:106:LEU:HD23	35:D2:138:PRO:HB2	1.83	0.61
41:S5:46:ILE:HG23	41:S5:50:ARG:HG3	1.82	0.61
14:S2:261:ARG:NH1	14:S2:267:TRP:O	2.34	0.61
4:c2:49:ARG:HB3	4:c2:87:LEU:HB3	1.82	0.61
13:S1:9:ILE:HB	13:S1:20:VAL:O	2.01	0.60
15:S3:38:GLN:O	25:A7:70:SER:C	2.44	0.60
34:D4:54:LEU:HA	37:B5:93:ILE:HD11	1.83	0.60
6:d2:32:MET:SD	6:d2:61:ARG:NH1	2.74	0.60
16:S7:165:LYS:NZ	26:AL:78:ASP:OD1	2.33	0.60
30:D1:114:TYR:OH	31:D6:61:LEU:O	2.19	0.60
4:c2:115:TYR:O	4:c2:119:ALA:HB3	2.01	0.60
14:S2:48:THR:HG22	14:S2:67:GLU:HG2	1.83	0.60
34:D4:22:MET:O	34:D4:26:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:382:THR:HB	13:S1:454:GLY:HA3	1.84	0.60
1:a1:245:GLU:HA	7:q1:11:ARG:HA	1.83	0.60
11:V1:101:GLU:O	11:V1:104:THR:OG1	2.20	0.60
25:A7:11:ARG:HD2	25:A7:19:LEU:HD22	1.83	0.60
13:S1:40:PHE:O	13:S1:158:ARG:NH2	2.34	0.60
13:S1:114:CYS:SG	13:S1:115:ASP:N	2.75	0.60
13:S1:449:PRO:O	13:S1:488:LYS:O	2.19	0.60
14:S2:54:GLN:NE2	29:D3:37:TYR:OH	2.34	0.60
29:D3:77:TRP:HB3	31:D6:144:ALA:HB2	1.83	0.60
5:f2:118:ARG:NH1	5:f2:176:ALA:O	2.35	0.59
4:c1:33:TYR:HA	4:c1:37:CYS:HB2	1.83	0.59
3:b2:70:CYS:SG	3:b2:80:ARG:NH1	2.75	0.59
29:D3:67:LEU:HB3	32:4L:65:VAL:HG23	1.84	0.59
2:a2:217:LYS:O	2:a2:221:GLU:HB2	2.02	0.59
15:S3:30:ALA:HA	15:S3:37:VAL:HG21	1.84	0.59
29:D3:14:ALA:HB1	30:D1:76:ILE:HD12	1.83	0.59
23:A5:24:LYS:HZ2	23:A5:59:LYS:HD3	1.67	0.59
13:S1:377:VAL:O	13:S1:406:VAL:HA	2.03	0.59
16:S7:85:VAL:HG12	16:S7:112:TYR:HB2	1.84	0.59
40:AJ:97:GLN:HE21	40:AJ:138:MET:HE2	1.68	0.59
1:a3:361:LEU:HD23	1:a3:399:ILE:HD11	1.84	0.59
23:A5:35:GLY:HA2	23:A5:44:ARG:HH12	1.68	0.59
33:D5:397:GLU:HB3	33:D5:482:MET:HE2	1.84	0.59
5:f1:121:GLN:O	5:f1:170:ARG:NH1	2.36	0.58
16:S7:46:TRP:NE1	16:S7:82:GLN:O	2.33	0.58
30:D1:60:PRO:HB3	30:D1:218:GLY:H	1.68	0.58
4:c2:177:THR:HB	8:h2:15:ASP:HB3	1.84	0.58
40:AJ:41:GLU:HB3	40:AJ:231:ALA:HB2	1.84	0.58
3:b2:319:PRO:HB3	7:q2:47:ARG:HH21	1.67	0.58
13:S1:377:VAL:HG22	13:S1:450:MET:HB3	1.84	0.58
38:A8:132:THR:OG1	42:A3:57:ARG:NH1	2.37	0.58
1:a1:128:GLU:OE1	1:a1:131:ARG:NH1	2.36	0.58
17:S8:53:GLU:OE2	26:AL:34:ARG:NH2	2.36	0.58
17:S8:65:HIS:NE2	17:S8:116:CYS:SG	2.76	0.58
21:A9:72:ASP:O	21:A9:80:SER:OG	2.22	0.58
13:S1:36:GLN:HE22	20:S4:49:VAL:H	1.51	0.58
2:a2:46:ARG:NH1	2:a2:110:GLU:OE1	2.37	0.58
1:a3:245:GLU:HA	7:q2:11:ARG:HA	1.85	0.58
48:B9:44:ARG:NH1	48:B9:48:ASP:OD2	2.37	0.58
3:b1:45:ILE:HA	55:b1:401:HEM:HAB	1.86	0.58
14:S2:237:ASN:O	30:D1:284:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AK:15:THR:HG21	36:AK:78:GLN:HE21	1.68	0.58
39:BJ:161:ARG:NH2	51:BK:111:ASN:OD1	2.36	0.58
3:b1:119:LEU:HD13	55:b1:402:HEM:HBB2	1.84	0.58
4:c1:157:ILE:HG23	4:c1:159:MET:H	1.69	0.58
2:a4:141:GLN:HE22	2:a4:186:VAL:HG13	1.68	0.58
13:S1:74:MET:H	13:S1:77:TRP:HE1	1.52	0.58
14:S2:19:MET:HG2	35:D2:295:ARG:HH12	1.69	0.58
14:S2:300:ARG:NH2	14:S2:420:THR:O	2.34	0.58
3:b1:82:MET:HG2	3:b1:240:MET:HE1	1.85	0.58
1:a3:15:GLN:O	1:a3:26:ALA:HA	2.04	0.58
15:S3:79:THR:O	15:S3:91:GLU:O	2.22	0.58
29:D3:63:LEU:HD22	32:4L:72:ALA:HB2	1.85	0.58
16:S7:71:ARG:HH22	17:S8:50:TYR:HB2	1.68	0.57
40:AJ:71:VAL:O	40:AJ:76:ASN:ND2	2.37	0.57
47:B7:17:GLU:OE1	47:B7:20:ARG:NH2	2.37	0.57
23:A5:54:LYS:HE2	23:A5:71:LEU:HD11	1.86	0.57
30:D1:65:THR:O	30:D1:124:ASN:ND2	2.33	0.57
31:D6:167:VAL:HG22	35:D2:42:PRO:HG2	1.86	0.57
34:D4:38:SER:OG	34:D4:70:MET:SD	2.56	0.57
44:C2:30:ARG:HE	44:C2:76:LEU:HD11	1.68	0.57
1:a3:40:TRP:HB3	1:a3:384:LEU:HD11	1.87	0.57
5:f2:84:GLY:N	5:f2:100:HIS:O	2.37	0.57
38:A8:93:LEU:HD23	54:A1:38:VAL:HG23	1.86	0.57
6:d1:78:GLU:HG3	6:d1:79:GLN:HG3	1.85	0.57
14:S2:231:ASN:OD1	14:S2:236:ARG:NH2	2.37	0.57
14:S2:357:GLN:O	25:A7:59:ARG:NH2	2.38	0.57
16:S7:31:ALA:HA	16:S7:174:ARG:HD2	1.86	0.57
17:S8:79:ALA:HB2	17:S8:106:THR:HG22	1.87	0.57
12:V2:6:LEU:HD12	12:V2:93:LYS:HE2	1.87	0.57
17:S8:32:ARG:NH2	28:AM:27:ARG:O	2.38	0.57
30:D1:204:GLU:HG2	30:D1:279:ARG:HD3	1.87	0.57
34:D4:269:MET:SD	34:D4:399:ASN:ND2	2.78	0.57
1:a1:437:ILE:O	1:a1:441:MET:HB2	2.03	0.57
2:a4:243:GLU:HA	2:a4:424:MET:O	2.04	0.57
11:V1:200:GLN:NE2	20:S4:132:THR:O	2.36	0.57
13:S1:135:ARG:NH2	13:S1:179:ASN:O	2.37	0.57
14:S2:238:ARG:HG3	14:S2:239:THR:HG23	1.86	0.57
3:b1:207:ASN:ND2	3:b1:211:ILE:O	2.37	0.57
21:A9:216:ASN:O	21:A9:220:ASP:HB2	2.04	0.57
30:D1:24:GLU:OE2	30:D1:195:ARG:NH2	2.33	0.57
16:S7:69:MET:HB3	16:S7:74:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D4:152:TYR:HD2	34:D4:215:TRP:HB2	1.68	0.57
34:D4:326:LEU:HD21	34:D4:410:MET:HE1	1.85	0.57
37:B5:6:LYS:HE2	27:AB:5:PRO:HB3	1.85	0.57
21:A9:20:VAL:H	21:A9:89:ASN:HB3	1.70	0.57
39:BJ:14:ARG:NH2	46:B6:98:GLU:OE2	2.38	0.57
21:A9:137:ALA:HA	21:A9:146:LEU:HB3	1.87	0.56
45:B4:39:ARG:NH1	50:B8:62:TYR:OH	2.37	0.56
1:a1:85:HIS:HB2	1:a1:100:LYS:HB2	1.87	0.56
3:b1:147:THR:HG22	3:b1:161:VAL:HG13	1.85	0.56
6:d1:61:ARG:HG2	6:d1:64:ARG:HH21	1.70	0.56
11:V1:165:ASN:HD22	11:V1:170:GLY:HA2	1.70	0.56
11:V1:215:VAL:HG23	11:V1:220:THR:HG21	1.86	0.56
4:c1:237:ARG:O	7:q1:12:HIS:CB	2.52	0.56
17:S8:146:GLU:HG3	26:AL:124:TYR:HB3	1.86	0.56
2:a4:42:ALA:O	2:a4:113:ARG:NH2	2.36	0.56
37:B5:31:LEU:HD23	37:B5:32:THR:HG23	1.88	0.56
40:AJ:141:GLN:NE2	40:AJ:201:ASP:OD2	2.38	0.56
4:c1:142:LEU:HD12	4:c1:143:ARG:H	1.71	0.56
33:D5:378:LEU:HG	33:D5:383:MET:HG3	1.86	0.56
4:c2:142:LEU:HD11	4:c2:148:PHE:HB2	1.88	0.56
13:S1:276:ARG:HG2	13:S1:277:GLN:HG3	1.86	0.56
16:S7:52:LEU:HB2	16:S7:90:GLY:HA3	1.86	0.56
37:B5:73:ARG:NH2	39:BJ:61:TYR:O	2.39	0.56
39:BJ:21:PRO:HG3	39:BJ:27:ASN:HD21	1.71	0.56
21:A9:167:LYS:O	21:A9:229:ALA:HA	2.06	0.56
5:f2:114:VAL:HG13	5:f2:170:ARG:HH12	1.70	0.55
37:B5:143:ASN:HD22	41:S5:29:PRO:HB3	1.71	0.55
48:B9:126:LYS:O	48:B9:130:GLU:CB	2.53	0.55
4:c1:12:TRP:HB2	4:c1:15:ARG:HB2	1.86	0.55
5:f1:86:ASN:ND2	5:f1:156:TYR:OH	2.39	0.55
22:A2:17:GLU:OE1	22:A2:67:ARG:NH2	2.39	0.55
28:AM:54:ARG:NH2	42:A3:83:LEU:O	2.39	0.55
36:AK:122:ALA:O	36:AK:126:MET:HB2	2.06	0.55
13:S1:10:GLU:O	13:S1:76:GLY:HA2	2.06	0.55
14:S2:415:VAL:HG11	30:D1:206:GLU:HG2	1.89	0.55
42:A3:66:PRO:HB3	42:A3:73:GLN:HB2	1.87	0.55
13:S1:159:CYS:HB2	13:S1:199:ILE:HD11	1.87	0.55
3:b1:216:ASP:OD2	4:c1:232:ARG:NH2	2.40	0.55
13:S1:592:LEU:O	13:S1:594:ARG:NH1	2.39	0.55
21:A9:108:ASP:HA	21:A9:111:VAL:HB	1.88	0.55
33:D5:60:GLU:HB2	46:B6:99:LYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a2:289:SER:O	2:a2:297:GLN:NE2	2.39	0.55
13:S1:193:SER:OG	13:S1:385:ARG:NH2	2.39	0.55
22:A2:65:TRP:NE1	22:A2:75:ASN:OD1	2.39	0.55
2:a4:92:VAL:HG21	2:a4:119:LEU:HD11	1.88	0.55
13:S1:396:ARG:NH1	13:S1:416:THR:O	2.40	0.55
40:AJ:235:VAL:O	40:AJ:239:GLN:NE2	2.40	0.55
3:b1:148:ASN:ND2	5:f2:142:LEU:O	2.40	0.55
2:a4:257:LEU:HD23	2:a4:424:MET:HE2	1.88	0.55
4:c2:71:GLN:HA	4:c2:82:MET:HA	1.88	0.55
21:A9:249:ALA:HB2	21:A9:318:LEU:HD12	1.89	0.55
26:AL:83:PRO:HG2	26:AL:86:TRP:HD1	1.72	0.55
33:D5:380:LEU:HD23	33:D5:381:THR:HG23	1.89	0.55
5:f1:163:SER:OG	57:f1:501:FES:S1	2.64	0.55
2:a4:76:THR:HG22	2:a4:82:SER:H	1.72	0.55
1:a1:87:ASN:ND2	1:a1:98:TYR:OH	2.40	0.55
2:a4:71:LEU:HD12	2:a4:144:LEU:HD23	1.89	0.55
11:V1:126:GLY:HA2	11:V1:131:ALA:HB3	1.89	0.55
12:V2:99:HIS:HE1	12:V2:101:GLN:HE21	1.53	0.55
14:S2:69:SER:OG	14:S2:72:MET:O	2.25	0.55
30:D1:90:PRO:HG3	30:D1:162:LEU:HB3	1.88	0.55
37:B5:43:ILE:HG13	37:B5:71:ILE:HD11	1.89	0.55
5:f1:99:ARG:NH2	5:f1:105:GLU:OE2	2.41	0.54
8:h2:61:PHE:HD2	8:h2:65:ARG:HE	1.55	0.54
30:D1:281:ARG:HB3	30:D1:284:GLN:HB2	1.90	0.54
32:4L:61:ILE:HG23	32:4L:62:ILE:HG13	1.89	0.54
33:D5:77:SER:OG	33:D5:79:SER:OG	2.25	0.54
16:S7:125:TYR:HE1	17:S8:88:PRO:HB2	1.72	0.54
24:A6:63:ARG:HB2	27:AA:45:LEU:HD21	1.89	0.54
33:D5:10:VAL:HG11	46:B6:78:VAL:HG22	1.87	0.54
34:D4:175:ASN:ND2	37:B5:97:GLU:OE1	2.35	0.54
3:b2:151:SER:HB3	3:b2:161:VAL:HG21	1.89	0.54
11:V1:111:ILE:HD11	11:V1:149:LEU:HD22	1.89	0.54
12:V2:53:LEU:HD12	18:V3:52:LEU:HD13	1.90	0.54
31:D6:112:GLU:OE1	41:S5:73:LYS:NZ	2.41	0.54
34:D4:447:LEU:HD11	34:D4:454:ILE:HG12	1.88	0.54
40:AJ:19:THR:HG23	40:AJ:20:GLU:HG3	1.88	0.54
50:B8:55:GLN:O	50:B8:70:ARG:NH2	2.40	0.54
2:a2:170:ASN:ND2	2:a2:236:LYS:O	2.41	0.54
11:V1:140:GLY:O	11:V1:179:ARG:NH2	2.40	0.54
15:S3:150:ARG:NH2	15:S3:155:TYR:O	2.41	0.54
34:D4:346:ARG:HH22	50:B8:68:ASP:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AK:65:ILE:HD11	36:AK:100:LEU:HD23	1.88	0.54
38:A8:148:GLU:OE1	41:S5:50:ARG:NH1	2.40	0.54
48:B9:102:CYS:SG	48:B9:103:LEU:N	2.79	0.54
10:i1:51:LEU:HD13	10:i1:53:LYS:H	1.72	0.54
4:c2:237:ARG:O	7:q2:12:HIS:CB	2.55	0.54
11:V1:365:CYS:SG	11:V1:366:ARG:N	2.81	0.54
13:S1:372:GLU:OE2	13:S1:397:LYS:NZ	2.37	0.54
16:S7:158:TYR:OH	26:AL:116:ASN:ND2	2.41	0.54
20:S4:66:GLU:HG3	20:S4:71:GLY:HA2	1.90	0.54
34:D4:373:ILE:HD11	34:D4:448:SER:HA	1.90	0.54
1:a3:363:ASN:ND2	2:a4:92:VAL:O	2.40	0.54
24:A6:31:VAL:HG21	63:AA:101:ZMP:H12A	1.90	0.54
47:B7:36:ARG:NH1	50:B8:132:GLN:OE1	2.39	0.54
5:f2:186:GLU:HB2	5:f2:194:ILE:HB	1.89	0.54
13:S1:201:ASP:OD2	13:S1:268:ARG:NH2	2.38	0.54
14:S2:6:PRO:HG3	35:D2:303:THR:HB	1.90	0.54
19:S6:27:ARG:HB3	21:A9:44:GLN:HE22	1.73	0.54
34:D4:276:CYS:HB3	34:D4:288:TYR:HB2	1.90	0.54
48:B9:24:ARG:NH1	48:B9:27:GLU:OE1	2.39	0.54
3:b2:26:ASN:HD21	3:b2:207:ASN:HB2	1.73	0.54
3:b2:215:THR:HG22	7:q2:8:THR:HG21	1.89	0.54
34:D4:170:THR:HG23	34:D4:171:MET:HG3	1.90	0.54
35:D2:30:TRP:NE1	35:D2:67:SER:OG	2.41	0.54
39:BJ:98:ASP:OD2	39:BJ:141:ARG:NH2	2.41	0.54
4:c1:30:PHE:HE2	4:c1:64:LEU:HD13	1.73	0.54
1:a3:19:LEU:O	1:a3:22:GLY:N	2.37	0.54
1:a3:155:ALA:HA	1:a3:164:ALA:HB1	1.90	0.54
14:S2:163:ALA:H	30:D1:278:PRO:HA	1.73	0.54
14:S2:420:THR:HG23	14:S2:421:GLN:HG3	1.91	0.54
29:D3:84:LEU:HD13	30:D1:309:ILE:HD11	1.90	0.54
40:AJ:169:VAL:O	40:AJ:220:VAL:HA	2.08	0.54
13:S1:9:ILE:HG23	13:S1:75:LYS:HA	1.89	0.53
13:S1:353:GLY:HA3	13:S1:649:SER:HA	1.88	0.53
13:S1:364:LEU:HG	13:S1:491:ASN:HB2	1.89	0.53
13:S1:409:ILE:HG12	13:S1:422:LEU:HB2	1.90	0.53
20:S4:12:THR:HG1	24:A6:14:THR:HG1	1.57	0.53
48:B9:100:GLU:O	48:B9:121:ARG:NH2	2.40	0.53
53:B1:35:ALA:HB1	53:B1:38:ARG:HD3	1.90	0.53
6:d1:72:GLN:OE1	7:q1:40:ARG:NH1	2.42	0.53
12:V2:92:ARG:NH1	13:S1:186:TYR:OH	2.41	0.53
12:V2:105:THR:OG1	57:V2:300:FES:S2	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D1:196:ALA:HA	30:D1:274:ARG:HG3	1.90	0.53
34:D4:197:LEU:O	34:D4:201:MET:HB2	2.08	0.53
39:BJ:108:ARG:NH2	51:BK:101:GLU:OE2	2.35	0.53
40:AJ:306:ALA:HA	40:AJ:309:ASN:HB2	1.89	0.53
2:a2:313:ASN:ND2	2:a2:321:LEU:O	2.41	0.53
8:h2:47:ARG:NH1	8:h2:48:SER:O	2.41	0.53
14:S2:1:ALA:H2	51:BK:32:PRO:HD3	1.73	0.53
33:D5:172:ILE:HG21	34:D4:408:LEU:HD23	1.89	0.53
33:D5:234:PRO:HB3	33:D5:300:LYS:HG2	1.90	0.53
27:AB:21:LEU:HD21	43:B3:47:ASN:HA	1.89	0.53
2:a2:97:SER:OG	2:a2:108:THR:OG1	2.27	0.53
2:a2:217:LYS:O	2:a2:221:GLU:CB	2.57	0.53
11:V1:43:TYR:O	11:V1:236:ARG:NH1	2.41	0.53
18:V3:57:ASP:O	18:V3:60:LYS:NZ	2.39	0.53
4:c1:230:LYS:HD3	6:d1:71:ARG:HG2	1.90	0.53
1:a3:19:LEU:HB2	1:a3:23:LEU:HB3	1.91	0.53
14:S2:339:LYS:NZ	17:S8:127:PRO:O	2.35	0.53
22:A2:68:TYR:O	22:A2:72:GLN:HB2	2.09	0.53
30:D1:152:SER:HG	30:D1:301:CYS:HG	1.49	0.53
33:D5:554:ASP:O	33:D5:558:LEU:HB2	2.07	0.53
3:b1:240:MET:HA	3:b1:243:VAL:HG22	1.89	0.53
3:b2:159:ASN:O	3:b2:163:TRP:HB2	2.09	0.53
11:V1:291:TRP:HE1	11:V1:313:GLU:HG2	1.74	0.53
14:S2:35:ASP:O	35:D2:49:ASN:ND2	2.41	0.53
14:S2:238:ARG:HH22	14:S2:412:ALA:HB1	1.73	0.53
24:A6:46:VAL:HG23	24:A6:51:LEU:HD12	1.91	0.53
29:D3:27:LEU:HD13	29:D3:29:VAL:HG23	1.91	0.53
30:D1:18:ALA:O	30:D1:21:THR:OG1	2.23	0.53
4:c2:2:ASP:OD1	4:c2:155:GLN:NE2	2.42	0.53
11:V1:250:ASN:HD22	11:V1:319:PHE:HB2	1.72	0.53
12:V2:183:LYS:HA	18:V3:44:HIS:HE1	1.74	0.53
16:S7:53:ALA:H	16:S7:90:GLY:HA3	1.74	0.53
24:A6:95:VAL:HG21	29:D3:44:MET:HB3	1.90	0.53
25:A7:45:SER:O	25:A7:46:HIS:ND1	2.42	0.53
34:D4:364:LEU:HB3	34:D4:369:LEU:HD13	1.91	0.53
1:a1:377:GLU:HG2	1:a1:381:ARG:HE	1.74	0.53
4:c2:146:LEU:HD22	4:c2:156:ALA:HB1	1.90	0.53
13:S1:366:THR:OG1	13:S1:491:ASN:ND2	2.42	0.53
23:A5:34:LEU:O	23:A5:44:ARG:NH1	2.42	0.53
34:D4:134:THR:O	34:D4:142:ARG:NH1	2.38	0.53
44:C2:66:THR:OG1	52:C1:28:TRP:NE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:585:VAL:O	20:S4:61:THR:OG1	2.27	0.53
15:S3:173:GLU:OE2	16:S7:138:ARG:NH1	2.41	0.53
16:S7:154:GLU:HG3	17:S8:50:TYR:HE1	1.74	0.53
19:S6:74:ASN:ND2	19:S6:76:ASP:OD2	2.42	0.53
5:f1:76:ILE:HG21	5:f1:98:VAL:HG21	1.90	0.52
34:D4:195:MET:HE3	34:D4:250:LEU:HD11	1.90	0.52
21:A9:92:ILE:HG22	21:A9:130:ILE:HB	1.90	0.52
1:a3:171:SER:HB2	1:a3:175:ARG:HH21	1.74	0.52
3:b2:82:MET:HE2	3:b2:240:MET:HE1	1.92	0.52
4:c2:227:SER:O	7:q2:23:GLN:NE2	2.42	0.52
30:D1:22:LEU:HB2	30:D1:48:PRO:HG2	1.91	0.52
46:B6:92:LYS:HD3	46:B6:93:PRO:HD2	1.90	0.52
1:a1:161:THR:HG21	1:a1:235:ARG:H	1.74	0.52
2:a2:57:TYR:OH	2:a2:203:ARG:NH2	2.43	0.52
5:f2:64:ALA:HB1	5:f2:68:VAL:HG21	1.92	0.52
19:S6:31:ARG:HH22	21:A9:69:ILE:HD11	1.74	0.52
35:D2:202:LEU:HB3	35:D2:346:LEU:HD11	1.92	0.52
40:AJ:111:ALA:HB1	40:AJ:122:VAL:HG21	1.91	0.52
53:B1:38:ARG:NH2	53:B1:56:TRP:O	2.43	0.52
4:c1:163:ILE:HB	4:c1:178:MET:HG3	1.91	0.52
3:b2:240:MET:HA	3:b2:243:VAL:HG22	1.91	0.52
6:d2:20:TYR:O	6:d2:24:ALA:HB2	2.10	0.52
12:V2:113:SER:HA	12:V2:152:PRO:HG3	1.90	0.52
13:S1:254:MET:SD	20:S4:42:ARG:NH2	2.83	0.52
14:S2:139:VAL:HG21	14:S2:277:VAL:HG12	1.92	0.52
33:D5:281:GLY:O	33:D5:285:THR:OG1	2.25	0.52
37:B5:20:ARG:NH1	51:BK:43:ASP:O	2.43	0.52
41:S5:88:GLU:HG2	41:S5:90:LYS:HE3	1.92	0.52
6:d1:32:MET:SD	6:d1:61:ARG:NH1	2.82	0.52
13:S1:568:GLU:HB3	13:S1:589:PRO:HG3	1.91	0.52
14:S2:187:ALA:HB2	17:S8:62:ARG:HH22	1.75	0.52
31:D6:57:PHE:O	31:D6:61:LEU:HB2	2.09	0.52
40:AJ:300:PRO:O	40:AJ:309:ASN:ND2	2.42	0.52
42:A3:79:TRP:HA	42:A3:82:ARG:HB2	1.92	0.52
45:B4:78:ASN:HD22	50:B8:12:PRO:HD3	1.75	0.52
6:d1:42:ASP:OD2	6:d1:101:ARG:NH1	2.42	0.52
2:a4:52:LYS:O	2:a4:203:ARG:NH2	2.36	0.52
4:c2:49:ARG:HH12	5:f2:66:ALA:HB1	1.74	0.52
16:S7:116:MET:HA	16:S7:146:VAL:HG23	1.91	0.52
27:AB:87:TYR:HB2	46:B6:22:LEU:HD23	1.92	0.52
14:S2:68:LEU:HA	14:S2:74:ARG:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D5:193:LEU:HD11	33:D5:206:PRO:HG3	1.92	0.52
35:D2:228:LEU:HD23	40:AJ:276:PRO:HG2	1.91	0.52
35:D2:232:HIS:CE1	40:AJ:276:PRO:HG3	2.45	0.52
4:c1:14:HIS:NE2	4:c1:124:GLU:OE2	2.36	0.52
28:AM:67:ARG:HD3	28:AM:68:ILE:HG13	1.91	0.52
44:C2:66:THR:HG22	52:C1:27:LEU:HD23	1.92	0.52
1:a1:189:HIS:O	1:a1:194:ARG:NH1	2.43	0.52
11:V1:91:LYS:HG2	11:V1:219:PRO:HG2	1.92	0.52
11:V1:94:VAL:HA	11:V1:135:TYR:O	2.08	0.52
28:AM:85:MET:O	28:AM:89:ASN:HB2	2.10	0.52
3:b1:275:LEU:HB3	3:b1:339:GLY:HA3	1.92	0.51
5:f1:75:GLU:HG2	5:f1:194:ILE:HG12	1.91	0.51
11:V1:233:THR:O	11:V1:237:ARG:HB2	2.10	0.51
14:S2:28:TRP:NE1	32:4L:98:CYS:OXT	2.43	0.51
14:S2:36:VAL:HG12	14:S2:38:PRO:HD3	1.91	0.51
33:D5:294:THR:H	33:D5:425:ARG:NH1	2.08	0.51
5:f2:28:SER:O	5:f2:32:ARG:NH1	2.44	0.51
12:V2:24:THR:HG22	12:V2:26:GLU:H	1.75	0.51
22:A2:57:CYS:SG	22:A2:58:SER:N	2.81	0.51
30:D1:149:ILE:HG21	30:D1:185:TRP:HB2	1.92	0.51
30:D1:309:ILE:HG13	42:A3:38:THR:HG22	1.92	0.51
14:S2:68:LEU:HB2	14:S2:73:VAL:HA	1.92	0.51
21:A9:162:GLU:OE1	21:A9:224:ARG:NH1	2.43	0.51
35:D2:327:PRO:HB3	44:C2:44:ILE:HG23	1.92	0.51
42:A3:15:GLU:HB3	42:A3:18:LEU:HD23	1.92	0.51
44:C2:2:MET:HE3	44:C2:82:MET:HE1	1.93	0.51
46:B6:86:LYS:O	46:B6:90:THR:OG1	2.27	0.51
14:S2:323:ILE:HD11	25:A7:40:LEU:HD12	1.93	0.51
30:D1:113:VAL:HG11	30:D1:139:THR:HG21	1.91	0.51
39:BJ:113:GLN:OE1	39:BJ:120:HIS:NE2	2.44	0.51
1:a1:53:ASN:ND2	1:a1:166:SER:O	2.43	0.51
1:a1:158:PHE:HB2	1:a1:164:ALA:HB2	1.93	0.51
3:b2:11:MET:O	3:b2:15:ASN:HB2	2.09	0.51
4:c2:102:ARG:HE	4:c2:109:LEU:HD23	1.75	0.51
11:V1:256:PHE:HA	11:V1:332:ALA:HB1	1.93	0.51
14:S2:227:GLU:OE1	25:A7:17:ARG:NH2	2.43	0.51
15:S3:86:ARG:HD3	23:A5:110:GLN:HG3	1.92	0.51
37:B5:120:GLY:O	37:B5:124:GLN:NE2	2.44	0.51
40:AJ:77:CYS:O	40:AJ:92:ASN:ND2	2.43	0.51
11:V1:214:GLY:HA3	11:V1:220:THR:HG22	1.92	0.51
13:S1:198:ASN:ND2	13:S1:263:ILE:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S7:124:GLY:HA2	17:S8:115:LYS:HA	1.92	0.51
16:S7:125:TYR:HB2	17:S8:117:ILE:HD12	1.93	0.51
30:D1:81:LEU:HD13	30:D1:111:LEU:HB3	1.91	0.51
30:D1:142:TYR:HE2	30:D1:285:LEU:HD11	1.76	0.51
1:a3:142:ASP:OD1	5:f2:2:HIS:ND1	2.39	0.51
4:c2:33:TYR:HA	4:c2:37:CYS:HB2	1.93	0.51
16:S7:62:MET:HG2	16:S7:156:LEU:HD23	1.92	0.51
30:D1:157:ASN:HB3	30:D1:168:THR:HG21	1.93	0.51
39:BJ:80:ASP:HB3	39:BJ:83:CYS:HB3	1.93	0.51
40:AJ:108:TYR:OH	40:AJ:164:LEU:O	2.29	0.51
3:b1:116:GLY:HA3	55:b1:402:HEM:HBC2	1.92	0.51
4:c2:183:LYS:HD3	8:h2:77:LEU:HD13	1.91	0.51
10:i2:54:HIS:HA	10:i2:57:HIS:CD2	2.46	0.51
11:V1:112:ARG:HH22	12:V2:192:SER:HB3	1.76	0.51
11:V1:233:THR:HA	11:V1:236:ARG:HG2	1.92	0.51
21:A9:208:VAL:HA	21:A9:211:THR:HG22	1.92	0.51
33:D5:341:MET:HE3	33:D5:454:ILE:HD13	1.92	0.51
27:AB:68:GLU:OE1	27:AB:69:LYS:NZ	2.38	0.51
54:A1:64:LYS:HE2	54:A1:68:ASN:HB2	1.93	0.51
3:b1:81:TYR:OH	4:c1:118:ARG:NH2	2.44	0.51
4:c1:23:HIS:HA	4:c1:26:ILE:HD12	1.93	0.51
21:A9:34:LEU:HD11	21:A9:214:ILE:HG21	1.92	0.51
21:A9:132:ILE:HD13	62:A9:401:NDP:H1D	1.92	0.51
33:D5:487:LYS:HE2	49:B2:49:GLY:HA3	1.93	0.51
41:S5:37:LYS:NZ	41:S5:41:GLU:OE2	2.36	0.51
2:a2:33:LEU:HD11	2:a2:220:ALA:HB1	1.91	0.51
1:a3:335:MET:HG2	1:a3:432:PRO:HG2	1.93	0.51
3:b2:359:PHE:O	3:b2:363:LEU:HB2	2.11	0.51
15:S3:202:PRO:HA	20:S4:50:ASN:HB3	1.93	0.51
30:D1:220:PHE:O	30:D1:224:PHE:HB2	2.11	0.51
33:D5:138:PHE:HB2	33:D5:196:TRP:HE1	1.75	0.51
46:B6:107:ASP:OD2	47:B7:70:ARG:NH2	2.44	0.51
10:i1:45:HIS:ND1	10:i1:48:GLU:OE2	2.44	0.50
3:b2:117:VAL:HG11	3:b2:302:VAL:HG22	1.93	0.50
13:S1:326:GLU:HB3	13:S1:597:TRP:HB3	1.92	0.50
60:S2:501:3PE:H3B1	33:D5:562:LEU:HD21	1.92	0.50
21:A9:10:LYS:O	21:A9:15:SER:OG	2.24	0.50
21:A9:141:SER:HA	21:A9:147:ARG:HH21	1.75	0.50
22:A2:19:ARG:HH21	22:A2:65:TRP:HE3	1.57	0.50
30:D1:55:LEU:HD23	30:D1:221:ALA:HB2	1.93	0.50
33:D5:154:LEU:HD13	33:D5:243:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D5:224:SER:HB2	33:D5:310:LEU:HD23	1.93	0.50
63:AB:101:ZMP:O7	48:B9:12:GLN:NE2	2.44	0.50
38:A8:37:LYS:NZ	42:A3:67:SER:O	2.43	0.50
40:AJ:306:ALA:O	52:C1:3:TYR:OH	2.23	0.50
1:a1:213:GLN:O	1:a1:217:SER:OG	2.27	0.50
4:c1:232:ARG:HA	7:q1:16:TYR:O	2.12	0.50
5:f2:23:LYS:HE3	45:B4:4:LYS:HD2	1.93	0.50
18:V3:59:SER:HA	18:V3:62:ARG:HH21	1.74	0.50
26:AL:29:ARG:NH1	26:AL:64:TYR:O	2.45	0.50
33:D5:128:MET:HE3	33:D5:251:THR:HA	1.92	0.50
34:D4:82:HIS:HB2	34:D4:432:ARG:HH12	1.76	0.50
8:h1:27:LEU:HD13	8:h1:29:LYS:H	1.77	0.50
1:a3:438:ARG:HH22	5:f2:33:LYS:HE3	1.75	0.50
14:S2:183:ARG:O	17:S8:60:ARG:NH2	2.45	0.50
15:S3:48:LEU:HB3	15:S3:105:ILE:HG22	1.92	0.50
25:A7:32:LYS:O	25:A7:35:GLN:NE2	2.44	0.50
39:BJ:74:THR:O	44:C2:108:THR:OG1	2.29	0.50
2:a2:42:ALA:O	2:a2:113:ARG:NH2	2.38	0.50
6:d1:68:LEU:O	6:d1:72:GLN:N	2.44	0.50
1:a3:21:ASN:HB3	1:a3:192:ALA:HB1	1.93	0.50
3:b2:376:LEU:O	6:d2:17:ARG:NH1	2.43	0.50
13:S1:280:THR:HG21	26:AL:136:GLU:HG2	1.92	0.50
30:D1:181:LEU:HB2	30:D1:300:LEU:HD13	1.92	0.50
33:D5:267:THR:OG1	33:D5:274:GLN:NE2	2.44	0.50
34:D4:204:MET:HB3	34:D4:209:LEU:HD22	1.93	0.50
5:f1:135:LEU:HD13	5:f1:180:LEU:HD12	1.94	0.50
7:q1:50:PRO:HA	7:q1:53:VAL:HG22	1.94	0.50
13:S1:524:LEU:HD12	13:S1:543:ILE:HD13	1.94	0.50
16:S7:84:ASP:OD1	30:D1:58:LYS:NZ	2.37	0.50
19:S6:28:PHE:HZ	26:AL:127:TYR:HB3	1.76	0.50
33:D5:15:LEU:HD21	33:D5:125:LEU:HD22	1.93	0.50
34:D4:44:GLN:OE1	34:D4:60:SER:N	2.45	0.50
2:a4:381:GLU:OE2	9:x2:2:UNK:N	2.45	0.50
13:S1:519:PRO:HG2	13:S1:522:LEU:HD22	1.93	0.50
13:S1:569:LYS:NZ	13:S1:596:ASP:OD2	2.44	0.50
16:S7:41:ARG:HA	30:D1:54:LYS:HD3	1.94	0.50
20:S4:64:ARG:HB3	20:S4:73:ALA:HB1	1.94	0.50
30:D1:248:ASN:HB2	30:D1:254:LEU:HD23	1.93	0.50
40:AJ:25:ILE:O	40:AJ:123:VAL:HA	2.12	0.50
1:a1:184:GLU:HG3	1:a1:188:ARG:HE	1.76	0.50
5:f1:73:LYS:HD3	5:f1:196:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a4:22:GLN:HG3	2:a4:41:TYR:HE2	1.77	0.50
28:AM:127:ARG:HB2	28:AM:132:ILE:HG23	1.92	0.50
30:D1:169:GLN:NE2	30:D1:240:THR:O	2.40	0.50
35:D2:154:ILE:HG23	35:D2:191:THR:HG22	1.93	0.50
2:a2:357:VAL:HG12	2:a2:361:LYS:HE2	1.94	0.50
14:S2:227:GLU:HB2	25:A7:17:ARG:HH21	1.75	0.50
15:S3:173:GLU:O	15:S3:185:ALA:HA	2.12	0.50
40:AJ:17:LYS:HG2	40:AJ:118:THR:HA	1.92	0.50
43:B3:28:LEU:HA	43:B3:31:VAL:HG12	1.93	0.50
1:a1:170:PRO:HG2	1:a1:173:ASN:HB2	1.94	0.50
3:b2:106:SER:HA	3:b2:313:ARG:HH11	1.76	0.50
32:4L:58:MET:HB3	32:4L:62:ILE:HD12	1.94	0.50
35:D2:292:PHE:HA	35:D2:295:ARG:HG2	1.94	0.50
54:A1:52:ARG:HB3	54:A1:60:TYR:HB3	1.94	0.50
1:a1:382:SER:HB3	1:a1:389:ARG:HA	1.94	0.49
3:b1:182:HIS:HE1	55:b1:401:HEM:NC	2.09	0.49
5:f2:75:GLU:OE1	5:f2:77:LYS:NZ	2.39	0.49
13:S1:483:VAL:HG22	13:S1:485:GLY:H	1.77	0.49
14:S2:339:LYS:NZ	19:S6:67:GLY:O	2.40	0.49
28:AM:79:ASP:OD2	38:A8:46:ARG:NH1	2.45	0.49
29:D3:60:ILE:HG23	32:4L:72:ALA:HB1	1.93	0.49
3:b1:152:ALA:HA	3:b1:287:LYS:HE2	1.94	0.49
7:q2:24:ARG:HD2	7:q2:27:PRO:HA	1.93	0.49
11:V1:49:LEU:HB3	11:V1:127:ARG:HG2	1.94	0.49
35:D2:69:LEU:HD11	35:D2:97:LEU:HD22	1.94	0.49
39:BJ:138:TYR:HD1	51:BK:108:MET:HE1	1.78	0.49
49:B2:45:ASP:O	49:B2:50:HIS:NE2	2.44	0.49
1:a3:145:MET:HE3	1:a3:248:LEU:HD13	1.94	0.49
5:f2:119:ASP:HB3	5:f2:179:ASN:HD21	1.75	0.49
14:S2:379:VAL:HG12	14:S2:387:TYR:HB3	1.95	0.49
36:AK:80:ARG:HH12	36:AK:87:LEU:HD12	1.76	0.49
43:B3:25:GLY:O	43:B3:29:GLU:CB	2.60	0.49
1:a1:261:GLY:O	1:a1:267:ASN:ND2	2.46	0.49
2:a2:53:ALA:O	2:a2:194:TYR:OH	2.30	0.49
3:b1:165:TRP:O	3:b1:174:THR:OG1	2.28	0.49
2:a4:29:LEU:HD22	2:a4:30:PRO:HD2	1.94	0.49
13:S1:36:GLN:N	15:S3:204:GLU:OE2	2.46	0.49
14:S2:326:ASP:HB2	15:S3:10:THR:HG21	1.93	0.49
35:D2:331:VAL:HG21	44:C2:41:SER:HB2	1.93	0.49
34:D4:388:TRP:NE1	45:B4:108:ARG:HH22	2.11	0.49
4:c1:115:TYR:O	4:c1:119:ALA:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c2:132:THR:OG1	4:c2:178:MET:SD	2.64	0.49
11:V1:213:VAL:HG13	11:V1:217:GLY:HA2	1.94	0.49
17:S8:150:ASN:HD21	20:S4:70:MET:HE1	1.76	0.49
36:AK:39:SER:HB2	36:AK:54:ARG:HH22	1.77	0.49
1:a1:120:CYS:SG	1:a1:121:SER:N	2.86	0.49
1:a1:148:VAL:O	1:a1:152:TYR:HB2	2.12	0.49
5:f1:101:ARG:NH2	5:f1:130:PRO:O	2.46	0.49
10:i1:31:PHE:O	10:i1:35:PHE:HB3	2.12	0.49
12:V2:37:ASN:OD1	18:V3:62:ARG:NH1	2.46	0.49
14:S2:364:TYR:HB2	14:S2:377:TYR:HD1	1.76	0.49
5:f1:99:ARG:NH2	5:f1:149:ASN:OD1	2.45	0.49
13:S1:452:VAL:HA	13:S1:491:ASN:O	2.12	0.49
13:S1:478:ARG:NH1	13:S1:487:TRP:O	2.45	0.49
26:AL:96:ASP:HB3	26:AL:100:VAL:HG21	1.95	0.49
3:b2:137:GLN:HE21	3:b2:141:TRP:HE1	1.61	0.49
13:S1:42:TYR:O	13:S1:158:ARG:NH2	2.46	0.49
13:S1:149:ILE:HG22	13:S1:151:THR:H	1.76	0.49
16:S7:122:GLY:HA3	17:S8:114:THR:HB	1.95	0.49
33:D5:341:MET:SD	33:D5:453:SER:OG	2.67	0.49
35:D2:222:ASN:OD1	35:D2:222:ASN:N	2.45	0.49
46:B6:119:MET:HE2	47:B7:60:HIS:HB2	1.95	0.49
48:B9:83:GLU:HA	48:B9:89:SER:HB2	1.94	0.49
1:a1:23:LEU:HD23	1:a1:195:MET:HG3	1.95	0.49
2:a2:194:TYR:O	2:a2:198:HIS:HB2	2.12	0.49
4:c1:12:TRP:NE1	4:c1:125:ASP:OD1	2.46	0.49
4:c1:235:ALA:HB3	7:q1:14:ILE:HB	1.95	0.49
2:a4:365:LYS:HG2	2:a4:399:LEU:HD22	1.95	0.49
11:V1:403:THR:HG21	11:V1:408:GLY:HA3	1.95	0.49
12:V2:78:MET:HE2	13:S1:173:GLY:H	1.78	0.49
14:S2:150:HIS:NE2	14:S2:303:GLU:OE1	2.46	0.49
26:AL:51:ASP:OD2	26:AL:54:GLN:NE2	2.44	0.49
33:D5:178:GLY:HA2	33:D5:219:ALA:HA	1.95	0.49
34:D4:147:LEU:HD21	35:D2:291:TYR:HE1	1.78	0.49
27:AB:48:VAL:HG21	48:B9:16:LEU:HD11	1.95	0.49
5:f1:165:TYR:HB3	5:f1:169:GLY:HA2	1.94	0.48
2:a4:24:LEU:HA	2:a4:38:LEU:HD23	1.95	0.48
5:f2:86:ASN:HD21	5:f2:97:PHE:HB3	1.76	0.48
8:h2:36:ARG:HG2	8:h2:57:GLU:HG2	1.95	0.48
11:V1:227:THR:O	11:V1:231:SER:HB3	2.13	0.48
17:S8:135:PRO:HG3	17:S8:164:GLU:HG2	1.95	0.48
26:AL:44:TYR:OH	26:AL:112:ASN:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D5:7:LEU:HA	33:D5:10:VAL:HG22	1.95	0.48
35:D2:22:ILE:HD11	41:S5:5:VAL:HB	1.95	0.48
27:AB:55:GLU:HB3	48:B9:81:PHE:HE2	1.78	0.48
14:S2:379:VAL:O	14:S2:387:TYR:N	2.46	0.48
33:D5:293:LEU:O	33:D5:523:SER:OG	2.29	0.48
34:D4:337:VAL:HG21	34:D4:345:ALA:HB2	1.93	0.48
37:B5:137:PRO:HG2	42:A3:54:VAL:HG11	1.95	0.48
38:A8:35:CYS:SG	38:A8:36:ASP:N	2.84	0.48
48:B9:90:TYR:OH	50:B8:86:ARG:NH1	2.46	0.48
1:a1:239:SER:O	1:a1:421:ALA:HA	2.13	0.48
11:V1:101:GLU:H	11:V1:184:TYR:HE1	1.59	0.48
13:S1:225:THR:HB	13:S1:240:VAL:HG23	1.95	0.48
13:S1:543:ILE:HD11	13:S1:557:ALA:HA	1.95	0.48
14:S2:98:GLN:NE2	17:S8:85:ALA:O	2.46	0.48
21:A9:98:GLU:OE2	62:A9:401:NDP:O2N	2.31	0.48
22:A2:41:VAL:O	22:A2:45:LYS:CB	2.61	0.48
33:D5:162:THR:O	33:D5:166:THR:OG1	2.28	0.48
35:D2:109:ALA:HB2	35:D2:161:SER:HA	1.95	0.48
2:a4:82:SER:HA	2:a4:85:ILE:HD12	1.95	0.48
2:a4:124:LEU:HD13	2:a4:223:PHE:HB2	1.94	0.48
3:b2:326:TRP:HB3	7:q2:51:PRO:HG2	1.96	0.48
14:S2:276:ASP:N	14:S2:276:ASP:OD1	2.46	0.48
15:S3:86:ARG:NH1	15:S3:91:GLU:OE2	2.36	0.48
32:4L:55:LEU:HB2	41:S5:24:GLN:HG3	1.95	0.48
33:D5:535:ARG:NH1	50:B8:90:ASP:O	2.46	0.48
34:D4:58:SER:OG	34:D4:63:THR:OG1	2.31	0.48
37:B5:138:LYS:HB3	41:S5:29:PRO:HD3	1.96	0.48
3:b1:310:SER:OG	3:b1:312:GLN:OE1	2.30	0.48
4:c2:232:ARG:HD2	6:d2:70:MET:HE1	1.95	0.48
11:V1:197:GLU:OE1	11:V1:199:LYS:NZ	2.46	0.48
17:S8:64:GLU:HB3	17:S8:134:GLY:HA3	1.94	0.48
28:AM:78:LYS:NZ	31:D6:131:GLY:O	2.40	0.48
30:D1:152:SER:OG	30:D1:301:CYS:SG	2.56	0.48
30:D1:280:PHE:HZ	30:D1:288:LEU:HD13	1.79	0.48
30:D1:299:ALA:HB1	42:A3:24:ILE:HG23	1.94	0.48
33:D5:67:HIS:HA	33:D5:77:SER:HA	1.96	0.48
47:B7:29:GLY:HA3	49:B2:65:GLY:HA3	1.95	0.48
1:a1:122:LEU:HD21	1:a1:182:LEU:HD12	1.95	0.48
12:V2:129:GLY:HA2	12:V2:140:ILE:HG22	1.95	0.48
13:S1:384:PRO:HD2	13:S1:415:LEU:HD11	1.95	0.48
27:AA:51:ILE:HD12	27:AA:70:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D1:219:PRO:HB3	30:D1:222:LEU:HD12	1.96	0.48
34:D4:254:THR:O	34:D4:258:ALA:CB	2.62	0.48
38:A8:70:PHE:HB3	54:A1:69:ILE:HD12	1.96	0.48
4:c1:132:THR:HG22	8:h1:17:LEU:HD22	1.95	0.48
8:h1:20:VAL:O	8:h1:24:CYS:CB	2.59	0.48
11:V1:276:LEU:HD23	11:V1:312:CYS:HB2	1.94	0.48
14:S2:69:SER:O	14:S2:72:MET:C	2.56	0.48
14:S2:151:ILE:HD13	14:S2:304:MET:HE1	1.94	0.48
33:D5:76:LEU:HB2	33:D5:136:ASN:HD21	1.77	0.48
33:D5:81:LYS:HD3	33:D5:135:ASN:HB3	1.95	0.48
33:D5:123:LEU:HA	33:D5:126:ILE:HD12	1.96	0.48
37:B5:64:TRP:HD1	37:B5:65:GLU:HG3	1.79	0.48
39:BJ:132:THR:HA	39:BJ:135:VAL:HG12	1.96	0.48
40:AJ:13:LYS:HD2	40:AJ:16:LYS:HE2	1.95	0.48
51:BK:57:ASN:HA	51:BK:60:VAL:HG12	1.96	0.48
13:S1:449:PRO:HB2	13:S1:489:VAL:HG23	1.95	0.48
16:S7:147:PRO:HG2	17:S8:139:PHE:HD2	1.78	0.48
21:A9:130:ILE:HG12	21:A9:164:THR:HB	1.95	0.48
33:D5:294:THR:H	33:D5:425:ARG:HH12	1.59	0.48
34:D4:2:LEU:HD23	53:B1:26:LEU:HD22	1.96	0.48
5:f1:38:LEU:HD13	10:i1:9:LEU:HD21	1.96	0.48
5:f1:155:GLY:HA3	5:f1:167:ALA:HA	1.95	0.48
34:D4:50:LEU:HG	34:D4:58:SER:HB3	1.94	0.48
34:D4:203:PHE:HE2	34:D4:246:ILE:HG12	1.78	0.48
41:S5:93:PRO:HB2	41:S5:95:PRO:HD3	1.96	0.48
3:b2:182:HIS:HE1	55:b2:401:HEM:NC	2.11	0.48
3:b2:312:GLN:NE2	3:b2:317:PHE:O	2.47	0.48
13:S1:240:VAL:HG12	13:S1:250:ILE:HG22	1.96	0.48
14:S2:229:LEU:HD23	14:S2:230:THR:H	1.78	0.48
15:S3:80:ALA:HB2	15:S3:92:ILE:HD13	1.96	0.48
17:S8:94:ILE:HA	17:S8:108:ARG:O	2.14	0.48
32:4L:62:ILE:HA	32:4L:65:VAL:HG12	1.94	0.48
34:D4:325:MET:HE2	34:D4:329:LEU:HD11	1.96	0.48
34:D4:403:THR:HA	34:D4:406:TYR:CE1	2.48	0.48
35:D2:200:MET:HE1	35:D2:265:MET:HE3	1.94	0.48
38:A8:166:LEU:HD23	38:A8:167:PHE:H	1.79	0.48
1:a1:79:VAL:HG13	1:a1:84:ALA:HB3	1.96	0.47
1:a1:192:ALA:HB2	1:a1:221:GLY:HA3	1.95	0.47
1:a3:227:ALA:HA	45:B4:24:ILE:HB	1.96	0.47
1:a3:270:LEU:HD22	1:a3:320:LEU:HD21	1.95	0.47
3:b2:275:LEU:HB3	3:b2:339:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:324:ASP:HA	13:S1:573:TYR:HE1	1.79	0.47
29:D3:109:LYS:HB2	29:D3:112:GLU:HB2	1.97	0.47
33:D5:439:THR:OG1	33:D5:440:LEU:N	2.47	0.47
51:BK:114:ASP:HB3	51:BK:117:LYS:HB2	1.96	0.47
2:a2:137:VAL:HG21	2:a2:188:PRO:HB3	1.95	0.47
2:a2:243:GLU:HA	2:a2:424:MET:O	2.14	0.47
11:V1:124:VAL:HG21	11:V1:232:PRO:HB3	1.96	0.47
13:S1:215:PHE:HB2	17:S8:98:PRO:HD3	1.95	0.47
14:S2:49:LEU:HB3	14:S2:66:MET:HG3	1.96	0.47
21:A9:60:ARG:HA	21:A9:68:ILE:HD11	1.96	0.47
22:A2:17:GLU:HG2	22:A2:51:PRO:HG2	1.96	0.47
33:D5:200:GLN:OE1	39:BJ:106:GLN:NE2	2.40	0.47
33:D5:518:ASN:HA	33:D5:521:LYS:HB2	1.96	0.47
37:B5:9:PHE:HB2	46:B6:27:LEU:HD22	1.95	0.47
40:AJ:116:LEU:O	40:AJ:260:ARG:NH2	2.47	0.47
1:a1:42:ASP:O	1:a1:194:ARG:NH2	2.48	0.47
1:a3:220:SER:OG	1:a3:221:GLY:N	2.42	0.47
1:a3:283:THR:HG21	2:a4:150:VAL:HG11	1.95	0.47
5:f2:77:LYS:HG2	5:f2:192:MET:HG3	1.96	0.47
8:h2:62:LEU:HA	8:h2:65:ARG:HG2	1.96	0.47
13:S1:577:GLU:OE2	13:S1:579:ARG:NH1	2.39	0.47
13:S1:595:GLU:OE1	13:S1:597:TRP:NE1	2.47	0.47
35:D2:179:MET:HE2	35:D2:212:THR:HG23	1.96	0.47
1:a3:61:HIS:HE1	2:a4:287:ARG:HG2	1.79	0.47
5:f2:98:VAL:HG12	5:f2:134:ILE:HG12	1.96	0.47
14:S2:184:VAL:O	17:S8:60:ARG:NH2	2.47	0.47
33:D5:127:THR:HG21	33:D5:146:GLY:HA3	1.97	0.47
33:D5:162:THR:OG1	50:B8:86:ARG:NH2	2.40	0.47
33:D5:605:HIS:HA	35:D2:92:PRO:HB2	1.96	0.47
37:B5:87:TYR:O	37:B5:90:THR:OG1	2.30	0.47
4:c1:162:PRO:HB2	56:c1:501:HEC:HBB2	1.97	0.47
40:AJ:104:ARG:NH1	40:AJ:131:ASP:OD1	2.48	0.47
1:a1:67:THR:OG1	1:a1:70:ARG:O	2.30	0.47
2:a2:71:LEU:HB3	2:a2:140:LEU:HD11	1.96	0.47
8:h2:28:GLU:HG3	8:h2:30:CYS:H	1.79	0.47
14:S2:221:ARG:HH22	25:A7:24:GLN:HB2	1.79	0.47
22:A2:41:VAL:O	22:A2:45:LYS:HB3	2.14	0.47
24:A6:60:ASP:HA	24:A6:63:ARG:HG2	1.96	0.47
34:D4:300:ALA:O	34:D4:308:SER:OG	2.28	0.47
39:BJ:70:VAL:HG11	39:BJ:86:GLU:HB3	1.96	0.47
51:BK:64:PHE:HA	51:BK:68:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:27:SER:OG	1:a1:205:HIS:ND1	2.39	0.47
1:a1:123:GLU:O	1:a1:127:ILE:N	2.47	0.47
4:c1:167:VAL:HG23	4:c1:168:LEU:HG	1.97	0.47
2:a4:71:LEU:HB3	2:a4:140:LEU:HD11	1.95	0.47
5:f2:147:ILE:O	5:f2:157:TYR:N	2.48	0.47
11:V1:378:ARG:O	11:V1:382:GLY:N	2.48	0.47
13:S1:160:ILE:HD11	13:S1:183:VAL:HG13	1.97	0.47
14:S2:266:GLN:HG2	14:S2:287:ILE:HG21	1.96	0.47
21:A9:285:GLU:O	21:A9:289:THR:OG1	2.30	0.47
28:AM:80:ARG:NH2	38:A8:63:ASN:OD1	2.47	0.47
31:D6:57:PHE:O	31:D6:61:LEU:CB	2.63	0.47
33:D5:10:VAL:HA	33:D5:13:ILE:HG22	1.97	0.47
33:D5:431:LEU:HB2	33:D5:432:LEU:HD12	1.97	0.47
34:D4:370:PRO:HA	34:D4:375:LEU:HD13	1.96	0.47
35:D2:4:ILE:HD11	40:AJ:9:ILE:HG21	1.97	0.47
35:D2:115:VAL:HG12	35:D2:180:ALA:HB1	1.96	0.47
40:AJ:19:THR:OG1	40:AJ:20:GLU:N	2.48	0.47
40:AJ:54:ALA:O	40:AJ:104:ARG:NE	2.47	0.47
47:B7:3:HIS:CE1	50:B8:127:PRO:HD3	2.49	0.47
47:B7:21:MET:HE1	47:B7:101:PHE:HA	1.97	0.47
4:c1:72:ASP:HB2	4:c1:83:ARG:HB2	1.97	0.47
3:b2:237:LEU:HB2	4:c2:211:MET:HE2	1.96	0.47
14:S2:82:LEU:HB3	16:S7:96:MET:HE2	1.97	0.47
19:S6:11:VAL:HG12	19:S6:17:VAL:HG21	1.96	0.47
20:S4:32:THR:HG21	24:A6:127:PRO:HG3	1.96	0.47
28:AM:94:ALA:HA	28:AM:103:TRP:HH2	1.78	0.47
33:D5:88:MET:HE2	33:D5:468:ILE:HG23	1.97	0.47
33:D5:398:SER:O	33:D5:402:SER:OG	2.30	0.47
35:D2:84:TRP:HB2	41:S5:18:THR:HA	1.97	0.47
48:B9:91:GLU:HB3	48:B9:94:GLU:HB2	1.97	0.47
1:a1:244:ARG:HH12	3:b1:215:THR:HA	1.80	0.47
3:b1:146:ILE:HD13	3:b1:149:LEU:HD12	1.97	0.47
6:d1:33:ARG:NH1	6:d1:91:GLU:OE1	2.47	0.47
1:a3:14:THR:OG1	1:a3:389:ARG:NH1	2.48	0.47
13:S1:386:PHE:HE1	13:S1:668:ILE:HD13	1.80	0.47
13:S1:531:CYS:SG	13:S1:532:VAL:N	2.88	0.47
17:S8:144:HIS:HD2	17:S8:147:LEU:HD12	1.79	0.47
31:D6:175:ASN:HD22	35:D2:48:HIS:CE1	2.30	0.47
11:V1:91:LYS:HB2	11:V1:131:ALA:HA	1.97	0.47
11:V1:362:CYS:HB3	11:V1:364:PRO:HD2	1.96	0.47
12:V2:61:LEU:HD21	12:V2:90:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S6:23:TYR:HE1	21:A9:5:VAL:HG22	1.80	0.47
21:A9:203:GLN:HB3	21:A9:235:ARG:H	1.79	0.47
28:AM:119:MET:HE2	28:AM:122:GLU:HG3	1.97	0.47
29:D3:62:PHE:HB2	30:D1:140:ILE:HG23	1.97	0.47
33:D5:366:MET:HE3	33:D5:443:ILE:HG22	1.97	0.47
45:B4:7:PRO:HB3	45:B4:13:LEU:HB2	1.97	0.47
2:a4:299:VAL:O	2:a4:303:VAL:N	2.38	0.46
12:V2:96:GLY:HA3	12:V2:136:LEU:HA	1.96	0.46
13:S1:380:VAL:HG23	13:S1:453:LEU:HA	1.97	0.46
30:D1:15:LEU:HD12	30:D1:19:PHE:HE2	1.80	0.46
41:S5:94:PRO:O	41:S5:98:SER:OG	2.33	0.46
2:a4:163:LEU:HD11	2:a4:258:VAL:HG21	1.98	0.46
3:b2:58:ASP:O	3:b2:62:ALA:N	2.48	0.46
4:c2:12:TRP:HZ3	4:c2:183:LYS:HG3	1.79	0.46
28:AM:81:ARG:HG2	28:AM:85:MET:HE1	1.96	0.46
33:D5:222:GLY:HA2	33:D5:229:LEU:HD22	1.96	0.46
33:D5:556:ILE:HG13	45:B4:76:TYR:HD1	1.79	0.46
35:D2:131:LEU:HD12	35:D2:216:PHE:HE2	1.80	0.46
46:B6:85:LEU:HD12	46:B6:89:VAL:HG21	1.97	0.46
1:a1:155:ALA:HA	1:a1:164:ALA:HB1	1.97	0.46
1:a1:248:LEU:HD12	1:a1:426:GLY:HA2	1.97	0.46
1:a1:278:GLY:N	1:a1:309:THR:OG1	2.48	0.46
21:A9:169:ALA:O	62:A9:401:NDP:N7N	2.32	0.46
24:A6:61:LYS:HE3	24:A6:106:PHE:HA	1.96	0.46
35:D2:244:VAL:HG11	35:D2:300:THR:HG21	1.97	0.46
46:B6:109:ILE:HB	46:B6:113:GLY:H	1.81	0.46
1:a1:279:HIS:O	1:a1:279:HIS:ND1	2.49	0.46
3:b1:137:GLN:HE21	3:b1:141:TRP:HE1	1.62	0.46
2:a4:169:ARG:HB3	2:a4:240:ARG:HB2	1.97	0.46
16:S7:41:ARG:HH12	16:S7:110:PRO:HG3	1.79	0.46
17:S8:99:ARG:HD3	17:S8:105:ARG:HD2	1.97	0.46
31:D6:25:SER:HB3	31:D6:28:TYR:HD2	1.80	0.46
35:D2:298:TYR:O	35:D2:303:THR:OG1	2.32	0.46
42:A3:58:ASP:OD1	42:A3:58:ASP:N	2.48	0.46
19:S6:24:ARG:HA	19:S6:27:ARG:HG2	1.97	0.46
27:AA:78:ASP:O	27:AA:82:ASP:HB2	2.16	0.46
33:D5:245:ALA:O	33:D5:249:SER:OG	2.29	0.46
34:D4:187:PRO:O	34:D4:192:ASN:ND2	2.44	0.46
34:D4:203:PHE:O	34:D4:207:MET:HG2	2.15	0.46
34:D4:234:ILE:O	34:D4:238:LEU:HB2	2.15	0.46
35:D2:151:LEU:HD22	36:AK:136:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q1:49:ALA:HA	7:q1:52:PHE:HD2	1.80	0.46
5:f2:107:ASP:O	5:f2:111:ALA:CB	2.64	0.46
11:V1:56:ILE:HG21	11:V1:128:ALA:HB1	1.96	0.46
14:S2:388:ARG:NH1	14:S2:389:CYS:O	2.48	0.46
17:S8:152:GLU:OE1	26:AL:127:TYR:OH	2.34	0.46
30:D1:92:PRO:HG3	30:D1:255:TYR:HD2	1.81	0.46
31:D6:127:ILE:HG21	41:S5:68:ARG:HD2	1.97	0.46
33:D5:386:LEU:HD23	33:D5:387:THR:H	1.81	0.46
34:D4:221:VAL:HG23	34:D4:222:GLU:HG3	1.97	0.46
35:D2:230:LEU:HB3	35:D2:300:THR:HG22	1.97	0.46
27:AB:65:ILE:O	27:AB:69:LYS:NZ	2.49	0.46
2:a2:99:THR:O	2:a2:106:ALA:HB3	2.16	0.46
5:f1:166:ASP:OD1	5:f1:170:ARG:N	2.38	0.46
13:S1:686:LYS:HA	13:S1:689:LYS:HE2	1.96	0.46
17:S8:141:THR:HG21	17:S8:146:GLU:HB3	1.98	0.46
31:D6:74:MET:HE3	32:4L:79:VAL:HG22	1.97	0.46
34:D4:165:ILE:HG21	35:D2:268:GLN:HA	1.96	0.46
38:A8:21:SER:HB2	54:A1:47:LEU:HG	1.97	0.46
1:a1:294:LEU:HB2	1:a1:341:GLN:HG3	1.97	0.46
2:a2:113:ARG:NH1	2:a2:210:GLY:O	2.49	0.46
2:a2:258:VAL:O	2:a2:423:SER:HB2	2.15	0.46
11:V1:298:ILE:HG22	11:V1:306:LEU:HA	1.97	0.46
16:S7:79:SER:OG	16:S7:82:GLN:NE2	2.35	0.46
24:A6:43:PRO:HA	24:A6:46:VAL:HG12	1.98	0.46
39:BJ:3:SER:OG	39:BJ:4:TRP:N	2.47	0.46
39:BJ:48:ARG:HH21	39:BJ:51:ILE:HG22	1.80	0.46
45:B4:110:ARG:O	45:B4:114:LEU:HB2	2.15	0.46
46:B6:86:LYS:O	46:B6:90:THR:CB	2.64	0.46
6:d1:82:LYS:NZ	6:d1:85:GLU:OE1	2.43	0.46
11:V1:208:PRO:HG3	20:S4:118:TYR:HD2	1.81	0.46
13:S1:476:LYS:O	13:S1:480:SER:CB	2.64	0.46
28:AM:89:ASN:ND2	28:AM:92:GLU:OE1	2.49	0.46
34:D4:57:PHE:HZ	34:D4:245:ARG:HH12	1.64	0.46
37:B5:36:VAL:HG11	51:BK:75:THR:HG21	1.97	0.46
40:AJ:170:ILE:HG12	40:AJ:221:LEU:HD12	1.97	0.46
43:B3:23:ILE:HD12	43:B3:49:ALA:HB2	1.97	0.46
2:a2:378:PHE:O	2:a2:382:VAL:HB	2.16	0.46
4:c1:18:LEU:HD11	4:c1:205:LEU:HD13	1.97	0.46
10:i1:50:LYS:H	10:i1:50:LYS:HD2	1.81	0.46
2:a4:75:LEU:HD22	2:a4:136:GLU:HB3	1.98	0.46
16:S7:139:ILE:HG22	16:S7:140:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A9:30:LEU:HD22	21:A9:94:LEU:HD21	1.97	0.46
29:D3:75:LEU:HB3	30:D1:155:LEU:HD13	1.98	0.46
32:4L:1:MET:N	41:S5:72:MET:SD	2.89	0.46
33:D5:231:PRO:HB3	33:D5:530:PRO:HG3	1.97	0.46
34:D4:350:THR:OG1	34:D4:351:LEU:N	2.49	0.46
40:AJ:127:SER:O	40:AJ:130:SER:OG	2.31	0.46
1:a1:102:LEU:HD23	1:a1:104:LYS:HE3	1.98	0.45
3:b1:307:LEU:HB3	3:b1:367:PRO:HG3	1.98	0.45
1:a3:344:ARG:O	1:a3:348:SER:OG	2.30	0.45
2:a4:382:VAL:HG22	2:a4:392:TYR:HE1	1.81	0.45
3:b2:25:SER:OG	6:d2:70:MET:SD	2.74	0.45
4:c2:233:LYS:HD2	5:f2:8:PRO:HG3	1.98	0.45
14:S2:155:THR:HG23	14:S2:167:PHE:HA	1.98	0.45
30:D1:288:LEU:O	30:D1:292:ASN:HB2	2.16	0.45
14:S2:238:ARG:HA	30:D1:284:GLN:HE22	1.81	0.45
21:A9:108:ASP:O	21:A9:112:LYS:HB2	2.15	0.45
26:AL:71:LYS:HG3	26:AL:115:PHE:HZ	1.81	0.45
33:D5:226:GLN:O	33:D5:230:HIS:N	2.48	0.45
34:D4:102:LEU:HD21	34:D4:230:VAL:HG11	1.97	0.45
6:d1:61:ARG:NH2	6:d1:89:TYR:OH	2.48	0.45
1:a3:314:TYR:HB2	1:a3:317:THR:HG23	1.99	0.45
19:S6:22:ASP:OD1	21:A9:2:HIS:NE2	2.49	0.45
23:A5:29:LYS:HG2	40:AJ:233:LYS:HE2	1.98	0.45
33:D5:142:ILE:HG12	34:D4:370:PRO:HB2	1.97	0.45
33:D5:535:ARG:HH12	50:B8:92:SER:N	2.14	0.45
34:D4:53:SER:HB2	53:B1:30:ASN:HD21	1.81	0.45
37:B5:49:GLU:HA	37:B5:70:PRO:HD3	1.99	0.45
37:B5:64:TRP:CD1	37:B5:65:GLU:HG3	2.52	0.45
10:i1:31:PHE:O	10:i1:35:PHE:CB	2.64	0.45
4:c2:58:GLU:HG2	4:c2:62:LYS:HE2	1.98	0.45
14:S2:146:ARG:HG3	14:S2:370:PRO:HG3	1.98	0.45
17:S8:43:ARG:NH1	25:A7:23:LEU:O	2.49	0.45
20:S4:69:LEU:HD13	21:A9:65:LEU:HD23	1.99	0.45
26:AL:39:VAL:HG21	26:AL:50:GLU:HB3	1.98	0.45
36:AK:137:GLU:HB3	36:AK:139:LYS:HG3	1.98	0.45
49:B2:55:ASP:OD1	49:B2:55:ASP:N	2.49	0.45
3:b1:207:ASN:ND2	3:b1:209:THR:OG1	2.49	0.45
4:c1:115:TYR:O	4:c1:119:ALA:CB	2.65	0.45
14:S2:238:ARG:NH2	30:D1:206:GLU:OE2	2.50	0.45
17:S8:93:THR:HB	17:S8:110:ASP:HB2	1.99	0.45
27:AA:73:PRO:HA	27:AA:76:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D1:161:THR:OG1	30:D1:164:THR:OG1	2.31	0.45
30:D1:236:ILE:HG23	30:D1:259:PHE:HZ	1.82	0.45
33:D5:246:LEU:O	33:D5:251:THR:OG1	2.32	0.45
35:D2:267:ILE:HD12	35:D2:279:PRO:HB3	1.97	0.45
4:c1:214:LEU:HD21	5:f1:46:GLY:HA3	1.99	0.45
38:A8:85:TRP:O	38:A8:89:ASP:HB2	2.17	0.45
39:BJ:143:HIS:NE2	45:B4:125:ASN:O	2.49	0.45
41:S5:18:THR:HG22	41:S5:19:ILE:HG13	1.97	0.45
50:B8:88:ARG:HG3	50:B8:89:VAL:HG23	1.97	0.45
1:a1:366:VAL:HG21	2:a2:112:LEU:HD21	1.99	0.45
2:a2:98:VAL:HA	2:a2:106:ALA:O	2.16	0.45
1:a3:65:LYS:NZ	1:a3:76:GLU:OE2	2.41	0.45
2:a4:56:ARG:HB2	2:a4:171:ALA:HB1	1.98	0.45
16:S7:91:THR:OG1	16:S7:119:CYS:SG	2.72	0.45
30:D1:5:ASN:HD21	54:A1:23:THR:HG23	1.82	0.45
33:D5:206:PRO:O	33:D5:209:SER:OG	2.35	0.45
27:AB:52:MET:HE3	48:B9:23:LEU:HD12	1.98	0.45
46:B6:17:LEU:HD11	48:B9:162:LEU:HD22	1.99	0.45
2:a2:268:GLU:OE2	2:a2:416:LYS:NZ	2.42	0.45
5:f1:86:ASN:HA	5:f1:99:ARG:HA	1.99	0.45
5:f1:116:GLN:HB3	5:f1:172:ARG:HE	1.82	0.45
3:b2:66:VAL:HA	3:b2:69:ILE:HD12	1.99	0.45
13:S1:266:LYS:O	13:S1:270:ALA:CB	2.62	0.45
14:S2:289:SER:OG	14:S2:290:ARG:N	2.49	0.45
14:S2:413:ASP:OD2	30:D1:281:ARG:NH2	2.50	0.45
21:A9:18:GLY:O	21:A9:89:ASN:ND2	2.50	0.45
40:AJ:267:LEU:HA	40:AJ:270:LEU:HB2	1.98	0.45
6:d2:33:ARG:NE	6:d2:34:ASP:OD1	2.44	0.45
15:S3:30:ALA:HB1	25:A7:69:MET:HB2	1.99	0.45
16:S7:43:SER:OG	16:S7:44:SER:N	2.50	0.45
16:S7:71:ARG:HA	30:D1:37:PRO:HA	1.98	0.45
34:D4:263:MET:HE1	45:B4:100:TRP:HB2	1.98	0.45
34:D4:385:THR:HG21	34:D4:396:MET:HE3	1.99	0.45
1:a1:252:HIS:HB3	1:a1:323:HIS:HE1	1.82	0.45
2:a4:168:TYR:HE2	2:a4:321:LEU:HD11	1.81	0.45
3:b2:33:PHE:HA	3:b2:36:LEU:HB2	1.98	0.45
5:f2:76:ILE:HB	5:f2:193:VAL:HG13	1.99	0.45
13:S1:399:TRP:HA	13:S1:404:LEU:H	1.82	0.45
13:S1:451:VAL:HB	13:S1:490:MET:HA	1.99	0.45
31:D6:30:GLY:HA3	31:D6:64:MET:HE2	1.99	0.45
45:B4:13:LEU:HD22	45:B4:14:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B8:52:ASP:HA	50:B8:78:HIS:CE1	2.52	0.45
3:b1:137:GLN:HE21	3:b1:141:TRP:NE1	2.15	0.44
1:a3:359:ASN:O	1:a3:363:ASN:ND2	2.50	0.44
3:b2:119:LEU:HD21	3:b2:192:LEU:HB2	1.99	0.44
6:d2:68:LEU:HD11	6:d2:75:LEU:HG	1.99	0.44
15:S3:135:TRP:HH2	24:A6:80:LEU:HD11	1.82	0.44
15:S3:189:GLU:HG3	21:A9:13:ARG:HB2	1.98	0.44
16:S7:162:GLN:NE2	26:AL:118:SER:O	2.51	0.44
17:S8:150:ASN:OD1	26:AL:124:TYR:OH	2.35	0.44
28:AM:108:SER:HB2	38:A8:4:VAL:HG13	1.99	0.44
30:D1:102:VAL:HB	30:D1:150:LEU:HD21	1.99	0.44
34:D4:1:MET:SD	34:D4:1:MET:N	2.80	0.44
34:D4:46:GLY:H	51:BK:84:ARG:HA	1.81	0.44
39:BJ:66:GLU:HG2	51:BK:95:ARG:HH22	1.81	0.44
40:AJ:183:ILE:HD11	40:AJ:191:GLU:HB3	1.99	0.44
43:B3:44:TRP:CD1	43:B3:47:ASN:HB2	2.53	0.44
47:B7:72:SER:HB2	47:B7:75:ASN:HD22	1.82	0.44
54:A1:52:ARG:HE	54:A1:58:ASN:HD21	1.65	0.44
3:b1:182:HIS:HE1	55:b1:401:HEM:C4C	2.35	0.44
6:d1:50:LEU:HD21	6:d1:90:LEU:HD23	1.99	0.44
1:a3:27:SER:HA	1:a3:199:ALA:O	2.17	0.44
13:S1:355:GLY:HA2	13:S1:361:ASN:HD21	1.83	0.44
20:S4:23:THR:HG23	20:S4:25:VAL:HG12	1.99	0.44
33:D5:17:MET:O	33:D5:21:ALA:HB2	2.17	0.44
40:AJ:75:GLY:HA3	40:AJ:76:ASN:HA	1.73	0.44
1:a3:131:ARG:HE	1:a3:175:ARG:HA	1.82	0.44
2:a4:197:ASN:OD1	2:a4:198:HIS:ND1	2.50	0.44
11:V1:106:LYS:HD3	11:V1:331:THR:HB	1.98	0.44
12:V2:190:ARG:HB2	12:V2:194:GLU:HB2	1.98	0.44
34:D4:231:LEU:HA	34:D4:235:LEU:HD13	1.99	0.44
27:AB:48:VAL:HG21	48:B9:16:LEU:HD21	2.00	0.44
39:BJ:21:PRO:HA	39:BJ:22:GLN:HB2	1.98	0.44
51:BK:100:ARG:HH11	51:BK:108:MET:H	1.63	0.44
2:a2:435:PHE:HB2	2:a4:169:ARG:HH12	1.83	0.44
1:a3:145:MET:HE2	1:a3:252:HIS:CD2	2.53	0.44
11:V1:294:LEU:HA	11:V1:338:ASP:HA	1.99	0.44
12:V2:37:ASN:ND2	18:V3:55:ASN:OD1	2.50	0.44
14:S2:339:LYS:HA	19:S6:69:PRO:HB3	1.99	0.44
16:S7:162:GLN:HE22	26:AL:118:SER:HB3	1.83	0.44
21:A9:83:ARG:HA	21:A9:86:GLU:HG3	1.99	0.44
30:D1:264:LEU:HD13	30:D1:264:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D1:264:LEU:HD21	54:A1:16:LEU:HG	1.99	0.44
40:AJ:65:ASP:OD2	40:AJ:67:LYS:NZ	2.45	0.44
48:B9:107:HIS:NE2	51:BK:43:ASP:OD1	2.43	0.44
5:f2:103:LYS:HD2	5:f2:106:ILE:HD12	1.98	0.44
19:S6:79:THR:HG23	19:S6:80:LYS:HG3	1.98	0.44
30:D1:100:LEU:HD22	31:D6:51:PHE:HB3	1.99	0.44
44:C2:110:ARG:HG2	51:BK:119:GLN:HG2	1.98	0.44
3:b2:271:GLU:HB3	3:b2:274:PHE:HD2	1.83	0.44
11:V1:139:ARG:NH2	12:V2:144:CYS:O	2.50	0.44
20:S4:62:ARG:HH12	24:A6:127:PRO:HD3	1.83	0.44
40:AJ:97:GLN:HE22	40:AJ:134:PHE:HD2	1.63	0.44
2:a4:74:SER:O	2:a4:82:SER:OG	2.33	0.44
2:a4:247:GLN:HE22	2:a4:429:ASN:HA	1.83	0.44
13:S1:241:SER:HB2	13:S1:249:ARG:HB3	2.00	0.44
17:S8:64:GLU:HA	17:S8:139:PHE:HZ	1.82	0.44
31:D6:119:PHE:HA	32:4L:1:MET:HG2	1.99	0.44
33:D5:71:ILE:HG13	33:D5:72:GLN:H	1.83	0.44
33:D5:228:GLY:H	33:D5:230:HIS:CE1	2.35	0.44
35:D2:26:TRP:NE1	35:D2:85:THR:O	2.51	0.44
48:B9:142:GLU:OE2	48:B9:158:LYS:NZ	2.48	0.44
2:a2:299:VAL:O	2:a2:303:VAL:N	2.40	0.44
4:c1:49:ARG:HB3	4:c1:87:LEU:HB3	1.99	0.44
5:f2:84:GLY:CA	5:f2:100:HIS:O	2.66	0.44
5:f2:163:SER:HA	5:f2:174:GLY:HA3	2.00	0.44
6:d2:67:ASP:HA	6:d2:70:MET:HE2	1.99	0.44
12:V2:114:ASP:HA	12:V2:117:LEU:HB2	1.99	0.44
21:A9:3:HIS:CG	26:AL:132:LYS:HE2	2.51	0.44
33:D5:62:ILE:O	46:B6:96:ILE:HA	2.18	0.44
35:D2:202:LEU:HD23	35:D2:346:LEU:HD21	1.99	0.44
35:D2:297:THR:HG22	35:D2:302:LEU:HD13	2.00	0.44
41:S5:50:ARG:HA	41:S5:53:LYS:HB2	1.99	0.44
50:B8:4:ILE:HG22	50:B8:6:LYS:H	1.82	0.44
50:B8:47:TYR:OH	50:B8:77:MET:O	2.28	0.44
1:a1:262:TRP:HD1	1:a1:315:ALA:HA	1.82	0.44
2:a4:47:ILE:HB	2:a4:109:VAL:HG13	1.99	0.44
4:c2:102:ARG:HB2	4:c2:109:LEU:HB3	2.00	0.44
11:V1:305:PRO:HD2	11:V1:327:THR:HA	2.00	0.44
12:V2:175:GLU:HB3	12:V2:180:LYS:HB2	2.00	0.44
30:D1:141:SER:HB3	30:D1:289:LEU:HG	1.99	0.44
33:D5:1:MET:HG2	33:D5:3:LEU:H	1.83	0.44
33:D5:175:ASN:HD21	33:D5:252:MET:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b2:51:LEU:HB3	55:b2:401:HEM:HMA3	2.00	0.43
12:V2:156:ILE:HG12	12:V2:161:TYR:HE2	1.83	0.43
17:S8:77:CYS:SG	17:S8:78:ILE:N	2.90	0.43
17:S8:95:GLU:OE1	17:S8:108:ARG:NH1	2.51	0.43
27:AA:63:PRO:O	27:AA:67:ALA:N	2.44	0.43
33:D5:332:HIS:CE1	33:D5:336:LYS:HD2	2.53	0.43
33:D5:401:THR:HG22	50:B8:126:GLN:HE22	1.82	0.43
35:D2:243:LEU:HD23	35:D2:243:LEU:HA	1.75	0.43
40:AJ:171:TYR:HD2	40:AJ:222:GLN:HG3	1.83	0.43
47:B7:34:LYS:HG3	50:B8:156:TYR:HA	1.98	0.43
11:V1:138:ILE:HD13	11:V1:146:ALA:HB2	2.01	0.43
12:V2:11:ASP:OD1	12:V2:11:ASP:N	2.51	0.43
13:S1:196:SER:OG	13:S1:265:ASP:OD2	2.33	0.43
21:A9:284:VAL:HG22	21:A9:288:HIS:HD2	1.82	0.43
28:AM:119:MET:HG3	28:AM:121:GLY:H	1.82	0.43
33:D5:534:HIS:CD2	60:D5:701:3PE:H221	2.53	0.43
34:D4:167:ILE:HA	34:D4:170:THR:HG22	2.00	0.43
35:D2:228:LEU:O	35:D2:231:SER:OG	2.34	0.43
37:B5:83:PRO:O	37:B5:87:TYR:HB2	2.18	0.43
1:a1:172:GLU:HA	1:a1:175:ARG:HG2	2.00	0.43
8:h1:27:LEU:HD22	8:h1:28:GLU:H	1.83	0.43
1:a3:124:ASP:HA	1:a3:127:ILE:HG22	1.99	0.43
4:c2:115:TYR:O	4:c2:119:ALA:CB	2.64	0.43
11:V1:298:ILE:HG12	11:V1:337:MET:HE1	2.00	0.43
14:S2:90:LEU:HD21	16:S7:129:SER:HB3	2.01	0.43
17:S8:83:CYS:O	17:S8:87:CYS:HB2	2.17	0.43
34:D4:57:PHE:HE1	34:D4:113:THR:HA	1.82	0.43
63:AB:101:ZMP:HN1	48:B9:50:HIS:CE1	2.37	0.43
38:A8:82:THR:HA	38:A8:85:TRP:CD1	2.54	0.43
1:a1:438:ARG:NH1	7:q1:19:SER:OG	2.51	0.43
3:b1:33:PHE:HA	3:b1:36:LEU:HB2	2.01	0.43
1:a3:85:HIS:O	1:a3:99:ILE:HA	2.19	0.43
2:a4:166:ALA:O	2:a4:240:ARG:NH1	2.51	0.43
13:S1:145:LEU:HB3	13:S1:269:PHE:HE2	1.82	0.43
27:AA:29:LYS:HE3	27:AA:40:LEU:HG	2.00	0.43
33:D5:264:TYR:HA	33:D5:267:THR:HG22	2.00	0.43
34:D4:75:LEU:HD12	34:D4:436:LEU:HG	1.99	0.43
35:D2:128:LEU:HD13	35:D2:216:PHE:HB2	1.99	0.43
41:S5:81:GLN:HA	41:S5:84:LYS:HG2	2.00	0.43
1:a3:438:ARG:HD2	1:a3:438:ARG:HA	1.85	0.43
5:f2:99:ARG:NH2	5:f2:149:ASN:OD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V1:131:ALA:O	11:V1:171:TYR:OH	2.30	0.43
12:V2:149:VAL:O	12:V2:190:ARG:NH2	2.52	0.43
13:S1:117:GLN:HG2	14:S2:346:ILE:HG23	2.01	0.43
23:A5:49:GLN:HE22	25:A7:91:LYS:HA	1.84	0.43
32:4L:5:TYR:OH	32:4L:50:ASN:ND2	2.38	0.43
33:D5:220:ALA:O	33:D5:224:SER:OG	2.31	0.43
34:D4:272:THR:HA	34:D4:275:ILE:HG22	2.00	0.43
35:D2:157:LEU:O	35:D2:161:SER:OG	2.37	0.43
27:AB:55:GLU:OE1	48:B9:24:ARG:NH2	2.51	0.43
4:c1:69:GLU:HA	4:c1:84:PRO:HA	2.00	0.43
4:c2:110:PRO:HA	4:c2:111:PRO:HD3	1.86	0.43
11:V1:202:LYS:HB3	11:V1:361:GLN:HE21	1.82	0.43
12:V2:27:ASN:OD1	12:V2:30:ARG:NH1	2.51	0.43
14:S2:84:HIS:CD2	15:S3:152:LEU:HB3	2.53	0.43
18:V3:68:SER:OG	20:S4:124:TRP:NE1	2.52	0.43
20:S4:35:ALA:O	20:S4:103:TYR:HA	2.19	0.43
20:S4:59:PHE:HD2	20:S4:79:LEU:HB3	1.84	0.43
34:D4:251:ASN:OD1	34:D4:251:ASN:N	2.43	0.43
63:AB:101:ZMP:H14	48:B9:59:ALA:HB1	2.01	0.43
42:A3:77:LEU:HD13	42:A3:80:LEU:HD23	2.01	0.43
12:V2:27:ASN:HB3	12:V2:53:LEU:HD21	2.01	0.43
13:S1:74:MET:N	13:S1:77:TRP:HE1	2.17	0.43
13:S1:629:ASN:HA	22:A2:57:CYS:HB3	2.01	0.43
27:AA:6:LEU:HD12	27:AA:11:ILE:HD11	2.01	0.43
28:AM:67:ARG:HH12	31:D6:135:PHE:HB3	1.83	0.43
29:D3:59:ALA:HB1	31:D6:66:VAL:HG13	1.99	0.43
31:D6:170:GLU:HA	31:D6:173:ARG:HB3	2.00	0.43
35:D2:338:PRO:O	38:A8:169:TRP:NE1	2.52	0.43
36:AK:68:ILE:HD13	36:AK:99:THR:HG21	2.00	0.43
40:AJ:141:GLN:HG3	40:AJ:198:TYR:HD1	1.82	0.43
2:a2:78:LYS:H	2:a2:129:ALA:HB1	1.84	0.43
1:a3:76:GLU:HG2	2:a4:285:VAL:HG21	2.01	0.43
5:f2:107:ASP:O	5:f2:111:ALA:HB2	2.18	0.43
11:V1:205:LEU:HD11	13:S1:50:GLY:H	1.84	0.43
11:V1:356:HIS:ND1	12:V2:143:GLU:OE2	2.41	0.43
16:S7:85:VAL:HG11	16:S7:163:LEU:HD21	2.01	0.43
50:B8:133:TYR:HB3	50:B8:138:LEU:HB2	2.01	0.43
1:a1:158:PHE:HE1	1:a1:236:PHE:HD1	1.67	0.43
6:d1:26:PHE:HB2	6:d1:31:LEU:HB2	2.01	0.43
3:b2:8:HIS:HB3	3:b2:11:MET:HB2	2.00	0.43
11:V1:193:ILE:HG23	11:V1:215:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D3:72:LEU:HD11	29:D3:94:LEU:HB3	1.99	0.43
36:AK:36:SER:HB2	36:AK:55:THR:HG22	2.01	0.43
40:AJ:133:VAL:HG13	40:AJ:205:VAL:HG12	2.01	0.43
47:B7:21:MET:HG3	50:B8:130:PRO:HD3	2.01	0.43
1:a1:19:LEU:HB2	1:a1:23:LEU:HD12	2.00	0.43
3:b2:159:ASN:O	3:b2:163:TRP:CB	2.66	0.43
3:b2:359:PHE:HB3	3:b2:363:LEU:HD12	2.01	0.43
11:V1:295:LEU:HD13	11:V1:339:ARG:HG3	2.01	0.43
19:S6:12:THR:OG1	19:S6:14:THR:O	2.30	0.43
21:A9:134:HIS:HD2	62:A9:401:NDP:H42N	1.84	0.43
23:A5:58:VAL:HG22	23:A5:67:LEU:HD11	2.01	0.43
40:AJ:24:LEU:HG	40:AJ:115:LEU:HD22	2.01	0.43
49:B2:66:ILE:HA	49:B2:67:PRO:HD3	1.89	0.43
50:B8:12:PRO:HA	50:B8:46:ASP:HB3	2.01	0.43
50:B8:30:ARG:NH1	50:B8:32:GLU:OE1	2.52	0.43
3:b2:71:ARG:NH2	4:c2:193:ALA:O	2.52	0.42
5:f2:128:LYS:HD3	5:f2:187:PHE:HD2	1.84	0.42
5:f2:164:HIS:N	5:f2:173:LYS:O	2.49	0.42
7:q2:45:ILE:O	7:q2:49:ALA:CB	2.67	0.42
14:S2:259:MET:SD	14:S2:421:GLN:NE2	2.81	0.42
40:AJ:210:PHE:HD2	40:AJ:211:LEU:HD22	1.84	0.42
46:B6:10:ARG:HB2	48:B9:155:PRO:HD3	2.01	0.42
50:B8:13:TYR:HE1	50:B8:39:ASP:H	1.64	0.42
1:a3:24:ARG:HB2	1:a3:196:VAL:HG22	2.00	0.42
1:a3:86:LEU:HD23	2:a4:285:VAL:HG22	2.00	0.42
2:a4:43:PRO:HA	2:a4:113:ARG:HE	1.84	0.42
2:a4:343:GLN:HA	2:a4:346:THR:HG22	2.02	0.42
5:f2:142:LEU:HD12	5:f2:161:HIS:HE1	1.84	0.42
11:V1:357:GLU:HG2	13:S1:177:ARG:HH12	1.84	0.42
24:A6:36:ARG:HG3	27:AA:52:MET:HG2	2.02	0.42
33:D5:172:ILE:O	33:D5:176:ARG:HG2	2.19	0.42
40:AJ:244:ASP:OD1	40:AJ:244:ASP:N	2.52	0.42
40:AJ:288:GLN:HE22	51:BK:27:GLN:HE22	1.67	0.42
5:f1:121:GLN:HB3	5:f1:126:ARG:HD2	2.02	0.42
12:V2:108:CYS:HB3	12:V2:152:PRO:HB3	1.99	0.42
16:S7:55:CYS:HB3	16:S7:89:ALA:HB1	2.01	0.42
22:A2:13:LEU:HB2	22:A2:69:ALA:HA	2.02	0.42
38:A8:90:TYR:HD1	54:A1:34:ARG:HH11	1.66	0.42
6:d1:33:ARG:CZ	6:d1:88:PHE:HB2	2.50	0.42
2:a4:375:SER:O	2:a4:379:LEU:HB2	2.19	0.42
12:V2:105:THR:OG1	12:V2:106:THR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S2:69:SER:O	14:S2:72:MET:O	2.37	0.42
22:A2:86:VAL:O	22:A2:90:LEU:HB2	2.20	0.42
26:AL:78:ASP:HB2	26:AL:81:MET:HE3	2.02	0.42
37:B5:104:ARG:NH2	38:A8:166:LEU:O	2.52	0.42
38:A8:74:LYS:HD2	54:A1:69:ILE:HG13	2.02	0.42
39:BJ:8:VAL:O	39:BJ:108:ARG:NH2	2.38	0.42
50:B8:50:LEU:HB2	50:B8:78:HIS:CD2	2.55	0.42
4:c1:71:GLN:HE21	4:c1:80:MET:HB3	1.84	0.42
12:V2:10:ARG:NH2	19:S6:76:ASP:HB3	2.34	0.42
21:A9:284:VAL:HA	21:A9:287:ILE:HG13	2.01	0.42
29:D3:81:THR:HG21	31:D6:148:SER:HB3	2.02	0.42
30:D1:24:GLU:HG2	30:D1:271:LEU:HD21	2.01	0.42
45:B4:124:PHE:HB2	45:B4:126:ILE:HD11	2.00	0.42
2:a2:245:ARG:HB3	2:a2:430:LEU:HD11	2.01	0.42
2:a4:242:GLY:O	2:a4:423:SER:HA	2.20	0.42
3:b2:146:ILE:HG12	3:b2:149:LEU:HD12	2.02	0.42
13:S1:360:SER:O	13:S1:365:ASN:ND2	2.47	0.42
22:A2:33:ARG:HA	22:A2:36:ILE:HG22	2.00	0.42
33:D5:385:PHE:HB2	33:D5:389:PHE:CG	2.55	0.42
33:D5:483:PRO:HD2	33:D5:486:LEU:HD22	2.00	0.42
34:D4:298:ILE:HD13	34:D4:298:ILE:HA	1.66	0.42
27:AB:60:PHE:HZ	27:AB:80:ILE:HG13	1.84	0.42
48:B9:33:ARG:HA	48:B9:36:TYR:HB3	2.01	0.42
13:S1:285:ARG:NH2	13:S1:289:GLY:O	2.38	0.42
13:S1:675:ASP:O	13:S1:679:ARG:HB2	2.20	0.42
14:S2:202:ASP:HB3	14:S2:323:ILE:HG23	2.02	0.42
14:S2:354:GLU:HA	15:S3:199:LEU:HD22	2.02	0.42
15:S3:40:VAL:HB	25:A7:68:VAL:HG23	2.01	0.42
16:S7:179:ARG:HG3	21:A9:50:ARG:HH22	1.84	0.42
23:A5:46:TYR:HE1	25:A7:92:LYS:HB2	1.85	0.42
33:D5:371:THR:HG23	49:B2:29:SER:HB2	2.02	0.42
38:A8:70:PHE:HA	38:A8:73:ILE:HG22	2.01	0.42
8:h2:28:GLU:HB3	8:h2:30:CYS:HB2	2.01	0.42
11:V1:124:VAL:O	11:V1:128:ALA:CB	2.63	0.42
11:V1:295:LEU:HB2	11:V1:339:ARG:HA	2.01	0.42
11:V1:372:MET:HG2	11:V1:392:LEU:HD11	2.02	0.42
13:S1:315:VAL:HA	13:S1:521:MET:O	2.19	0.42
14:S2:238:ARG:HH11	30:D1:281:ARG:HB2	1.85	0.42
16:S7:39:TRP:HA	16:S7:42:ARG:HG2	2.02	0.42
28:AM:139:PHE:HB2	54:A1:45:TRP:CD1	2.55	0.42
33:D5:183:ILE:HD13	34:D4:382:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D5:257:ILE:H	33:D5:257:ILE:HG13	1.71	0.42
34:D4:165:ILE:HD11	35:D2:264:TRP:HE1	1.84	0.42
35:D2:104:MET:HA	35:D2:111:PHE:HB3	2.02	0.42
63:AB:101:ZMP:H9	48:B9:66:ALA:HB2	2.01	0.42
40:AJ:27:VAL:HG11	40:AJ:38:LEU:HD22	2.01	0.42
46:B6:117:PRO:HA	46:B6:118:PRO:HD3	1.90	0.42
47:B7:21:MET:HE2	50:B8:129:GLY:HA2	2.01	0.42
50:B8:8:MET:O	50:B8:26:LYS:NZ	2.45	0.42
50:B8:62:TYR:HD2	50:B8:64:TRP:HE3	1.68	0.42
2:a2:67:HIS:NE2	2:a2:147:ASP:OD2	2.52	0.42
2:a2:202:ALA:N	2:a2:227:ARG:O	2.46	0.42
35:D2:190:MET:HG2	35:D2:204:ASN:HB3	2.02	0.42
36:AK:68:ILE:HG21	36:AK:99:THR:HG21	2.02	0.42
48:B9:108:PRO:HA	48:B9:111:LYS:HB2	2.02	0.42
2:a2:319:SER:OG	2:a2:320:GLY:N	2.53	0.42
3:b1:31:TRP:HA	3:b1:100:ARG:NH1	2.35	0.42
3:b1:365:MET:O	3:b1:369:ALA:CB	2.68	0.42
7:q2:45:ILE:O	7:q2:49:ALA:HB3	2.20	0.42
14:S2:425:PHE:HA	14:S2:428:VAL:HB	2.01	0.42
22:A2:23:CYS:HB2	22:A2:59:ASP:HA	2.02	0.42
26:AL:56:PHE:HA	26:AL:59:HIS:CD2	2.55	0.42
33:D5:418:PHE:HA	33:D5:421:ILE:HG12	2.02	0.42
34:D4:449:LEU:HD23	34:D4:449:LEU:HA	1.92	0.42
1:a1:278:GLY:N	1:a1:309:THR:HG1	2.18	0.41
2:a4:246:GLU:O	2:a4:427:SER:HA	2.19	0.41
13:S1:632:ARG:NH2	22:A2:59:ASP:O	2.53	0.41
31:D6:163:ILE:HG13	35:D2:12:THR:HG21	2.01	0.41
34:D4:106:LEU:HD13	34:D4:234:ILE:HG21	2.01	0.41
35:D2:244:VAL:O	35:D2:248:LEU:HB2	2.20	0.41
39:BJ:4:TRP:CD1	39:BJ:9:TYR:HB2	2.56	0.41
51:BK:60:VAL:O	51:BK:64:PHE:HB2	2.20	0.41
53:B1:49:LYS:HA	53:B1:50:PRO:HA	1.82	0.41
3:b1:300:VAL:HA	3:b1:303:ILE:HB	2.02	0.41
11:V1:121:GLY:HA2	11:V1:232:PRO:HD3	2.01	0.41
13:S1:476:LYS:O	13:S1:480:SER:HB2	2.19	0.41
34:D4:105:PHE:O	34:D4:109:THR:OG1	2.32	0.41
34:D4:196:TRP:CE2	34:D4:200:MET:HG3	2.54	0.41
35:D2:235:ASN:ND2	35:D2:307:SER:OG	2.47	0.41
47:B7:99:LYS:HE2	50:B8:158:ILE:HG22	2.00	0.41
1:a1:30:SER:N	1:a1:201:GLY:O	2.53	0.41
4:c2:19:SER:O	4:c2:201:LYS:NZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V3:63:MET:HA	18:V3:64:PRO:HD3	1.91	0.41
21:A9:314:ALA:HA	21:A9:317:VAL:HG12	2.01	0.41
22:A2:64:LEU:HB3	22:A2:76:VAL:HG23	2.01	0.41
32:4L:63:LEU:HD23	35:D2:71:MET:HE3	2.01	0.41
33:D5:598:SER:HB2	35:D2:100:MET:HE1	2.02	0.41
1:a1:94:HIS:CE1	1:a1:384:LEU:HD13	2.55	0.41
1:a1:388:ARG:HH22	1:a1:391:PRO:HD3	1.85	0.41
3:b2:24:PRO:O	3:b2:224:TYR:OH	2.28	0.41
3:b2:269:LYS:HA	3:b2:270:PRO:HD3	1.94	0.41
11:V1:227:THR:HA	11:V1:230:VAL:HG12	2.03	0.41
12:V2:162:GLU:HB2	12:V2:186:PRO:HA	2.01	0.41
25:A7:43:GLY:HA3	25:A7:44:PRO:HD3	1.91	0.41
29:D3:81:THR:HG23	29:D3:83:ASN:H	1.85	0.41
30:D1:300:LEU:HD23	30:D1:300:LEU:HA	1.94	0.41
34:D4:14:LEU:HD11	53:B1:12:ILE:HG23	2.01	0.41
35:D2:145:ILE:HD12	35:D2:149:ILE:HD11	2.02	0.41
50:B8:14:PRO:HA	50:B8:15:LYS:HA	1.72	0.41
1:a1:270:LEU:HD13	1:a1:320:LEU:HD22	2.02	0.41
3:b1:161:VAL:HA	3:b1:164:ILE:HG12	2.02	0.41
5:f2:78:LEU:HD13	5:f2:98:VAL:HB	2.03	0.41
11:V1:204:ARG:HB3	20:S4:118:TYR:HE2	1.85	0.41
12:V2:9:HIS:HB2	13:S1:187:ILE:HA	2.02	0.41
12:V2:121:GLN:HE22	12:V2:127:LYS:HA	1.83	0.41
33:D5:404:THR:HG22	33:D5:405:ASN:H	1.85	0.41
34:D4:2:LEU:HD12	34:D4:5:ILE:HB	2.02	0.41
34:D4:197:LEU:O	34:D4:201:MET:CB	2.68	0.41
34:D4:336:ARG:HD2	34:D4:426:ILE:HG22	2.03	0.41
35:D2:142:LEU:HB3	35:D2:194:LEU:HD21	2.03	0.41
1:a1:288:MET:HE1	1:a1:300:THR:HG23	2.01	0.41
2:a2:67:HIS:HB2	2:a2:177:TYR:HA	2.03	0.41
2:a4:309:VAL:HG22	2:a4:326:THR:HG22	2.03	0.41
4:c2:27:ARG:HG3	4:c2:56:TYR:CZ	2.56	0.41
11:V1:391:SER:OG	13:S1:129:ARG:NH1	2.50	0.41
13:S1:255:HIS:CD2	13:S1:258:ILE:HG12	2.56	0.41
14:S2:146:ARG:NH2	14:S2:368:GLU:O	2.52	0.41
15:S3:51:CYS:HA	15:S3:108:LYS:O	2.20	0.41
15:S3:184:VAL:HG11	24:A6:109:THR:HG21	2.01	0.41
16:S7:127:HIS:CG	17:S8:115:LYS:HE3	2.56	0.41
29:D3:18:VAL:HG23	30:D1:76:ILE:HD11	2.02	0.41
29:D3:67:LEU:HD22	32:4L:65:VAL:HA	2.01	0.41
31:D6:23:LYS:HZ2	32:4L:22:TYR:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4L:96:LEU:HD12	35:D2:51:ARG:HD2	2.02	0.41
33:D5:194:ASN:CG	45:B4:126:ILE:HD13	2.46	0.41
33:D5:338:MET:HE3	33:D5:458:LEU:HB3	2.03	0.41
34:D4:75:LEU:HD21	34:D4:440:HIS:CD2	2.56	0.41
35:D2:254:LEU:HA	35:D2:255:PRO:HD3	1.87	0.41
37:B5:21:PHE:HD2	37:B5:22:LEU:HD12	1.84	0.41
48:B9:15:VAL:HG22	48:B9:63:LEU:HD13	2.02	0.41
53:B1:16:VAL:HG23	53:B1:17:PRO:HD3	2.03	0.41
1:a3:278:GLY:N	1:a3:309:THR:OG1	2.53	0.41
2:a4:364:LEU:HD23	2:a4:402:ILE:HG23	2.02	0.41
3:b2:226:ILE:HD11	4:c2:221:MET:HG3	2.01	0.41
4:c2:3:LEU:HD23	7:q2:70:LYS:HE2	2.02	0.41
6:d2:86:ASP:N	6:d2:86:ASP:OD1	2.51	0.41
13:S1:10:GLU:O	13:S1:76:GLY:CA	2.69	0.41
14:S2:151:ILE:HD12	14:S2:151:ILE:HA	1.88	0.41
15:S3:93:VAL:HG22	15:S3:108:LYS:HG2	2.02	0.41
15:S3:180:VAL:HG23	15:S3:182:ARG:HG2	2.03	0.41
33:D5:34:LEU:HD12	33:D5:37:LYS:HE3	2.03	0.41
34:D4:4:TYR:CE1	34:D4:37:THR:HG22	2.56	0.41
36:AK:101:GLY:HA2	36:AK:104:THR:HG22	2.03	0.41
41:S5:19:ILE:HD13	41:S5:19:ILE:HG21	1.92	0.41
47:B7:88:TYR:HD1	49:B2:51:PHE:HE1	1.69	0.41
2:a2:257:LEU:O	2:a2:323:GLY:HA3	2.21	0.41
3:b1:39:ILE:HA	3:b1:42:ILE:HG12	2.01	0.41
4:c1:130:LEU:HD11	4:c1:149:ASN:HD21	1.86	0.41
4:c2:140:VAL:HG23	4:c2:142:LEU:HG	2.02	0.41
4:c2:143:ARG:H	4:c2:146:LEU:HD12	1.86	0.41
5:f2:128:LYS:H	5:f2:187:PHE:HE2	1.68	0.41
6:d2:21:TYR:CZ	6:d2:27:ASN:HB3	2.56	0.41
11:V1:26:TYR:HB2	12:V2:192:SER:HB2	2.02	0.41
11:V1:33:LEU:HD23	11:V1:155:GLU:HB3	2.01	0.41
60:S2:501:3PE:H281	60:S2:501:3PE:H371	2.03	0.41
17:S8:45:PRO:HB2	17:S8:47:THR:HG23	2.03	0.41
48:B9:57:VAL:HA	48:B9:60:THR:HG22	2.02	0.41
50:B8:59:ASP:HA	50:B8:60:PRO:HD3	1.85	0.41
1:a1:145:MET:HE3	1:a1:248:LEU:HD13	2.01	0.41
3:b1:85:ASN:HD22	3:b1:243:VAL:HG12	1.86	0.41
3:b1:132:VAL:HA	3:b1:139:SER:HB3	2.02	0.41
1:a3:240:GLU:HA	1:a3:422:VAL:O	2.20	0.41
5:f2:131:GLU:HG2	5:f2:132:TRP:CD1	2.56	0.41
12:V2:17:PRO:HA	12:V2:19:THR:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:26:VAL:HG13	13:S1:79:ILE:HD13	2.03	0.41
13:S1:56:LEU:HD22	13:S1:65:VAL:HG12	2.03	0.41
13:S1:437:HIS:H	13:S1:440:SER:HB2	1.86	0.41
14:S2:246:THR:O	14:S2:250:ALA:N	2.52	0.41
25:A7:111:TYR:HA	25:A7:112:LEU:HA	1.86	0.41
28:AM:49:MET:HG2	30:D1:157:ASN:HD21	1.85	0.41
28:AM:64:PHE:HA	28:AM:67:ARG:HG3	2.03	0.41
33:D5:335:PHE:CD2	33:D5:336:LYS:HG3	2.56	0.41
33:D5:554:ASP:OD1	34:D4:213:HIS:NE2	2.48	0.41
34:D4:51:ASN:HD21	34:D4:177:LEU:HD21	1.85	0.41
34:D4:162:VAL:HG13	35:D2:271:THR:HG21	2.03	0.41
35:D2:235:ASN:HD21	40:AJ:289:SER:HB2	1.86	0.41
36:AK:46:THR:HA	36:AK:47:SER:HA	1.73	0.41
47:B7:30:PHE:HE2	50:B8:156:TYR:HB3	1.86	0.41
1:a1:19:LEU:HB2	1:a1:23:LEU:HB3	2.02	0.41
1:a1:70:ARG:HA	1:a1:71:PRO:HD3	1.92	0.41
2:a2:367:GLY:O	2:a2:371:SER:CB	2.69	0.41
4:c1:138:PRO:HB2	4:c1:139:ARG:HG2	2.03	0.41
4:c1:237:ARG:O	7:q1:12:HIS:HB3	2.19	0.41
1:a3:317:THR:OG1	1:a3:318:GLY:N	2.54	0.41
2:a4:375:SER:HA	2:a4:378:PHE:HB3	2.02	0.41
3:b2:71:ARG:NH2	4:c2:192:ALA:O	2.47	0.41
13:S1:41:CYS:O	13:S1:161:ARG:NH2	2.41	0.41
13:S1:103:LEU:HD13	19:S6:69:PRO:HB2	2.03	0.41
13:S1:477:ILE:HA	13:S1:480:SER:HB3	2.03	0.41
13:S1:521:MET:HG3	13:S1:542:PHE:HD2	1.85	0.41
14:S2:151:ILE:HD11	14:S2:170:MET:HG3	2.03	0.41
17:S8:87:CYS:HA	17:S8:88:PRO:HD3	1.87	0.41
21:A9:94:LEU:HD23	62:A9:401:NDP:H4D	2.02	0.41
29:D3:56:PHE:O	31:D6:70:TYR:OH	2.39	0.41
33:D5:193:LEU:HD22	33:D5:201:ILE:HG12	2.02	0.41
35:D2:243:LEU:HD21	44:C2:44:ILE:HD11	2.03	0.41
39:BJ:134:VAL:HG23	51:BK:108:MET:HB3	2.03	0.41
47:B7:7:ARG:NH2	47:B7:17:GLU:OE2	2.54	0.41
2:a2:137:VAL:O	2:a2:141:GLN:HG2	2.21	0.40
2:a2:367:GLY:O	2:a2:371:SER:HB3	2.21	0.40
1:a3:199:ALA:HB1	1:a3:203:LEU:HD21	2.03	0.40
2:a4:319:SER:OG	2:a4:320:GLY:N	2.54	0.40
12:V2:8:VAL:HG12	12:V2:9:HIS:H	1.86	0.40
13:S1:372:GLU:HG2	13:S1:398:SER:HB2	2.02	0.40
29:D3:74:PRO:HG3	31:D6:143:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D1:303:TRP:CD2	42:A3:24:ILE:HD11	2.56	0.40
33:D5:525:LEU:HD21	50:B8:95:PRO:HD2	2.01	0.40
34:D4:350:THR:HB	48:B9:98:VAL:HG22	2.03	0.40
35:D2:144:GLN:HE21	41:S5:2:PHE:HA	1.85	0.40
35:D2:339:LEU:HD23	35:D2:342:ILE:HG13	2.02	0.40
38:A8:77:CYS:HA	38:A8:78:ALA:HA	1.84	0.40
40:AJ:119:GLY:HA3	40:AJ:120:GLN:HA	1.86	0.40
43:B3:63:VAL:O	43:B3:67:LEU:HB2	2.21	0.40
1:a1:290:LEU:HD12	1:a1:295:ALA:HB1	2.03	0.40
2:a2:43:PRO:HA	2:a2:113:ARG:HE	1.86	0.40
6:d2:33:ARG:HH22	6:d2:91:GLU:HB2	1.85	0.40
10:i2:51:LEU:H	10:i2:54:HIS:HE1	1.69	0.40
12:V2:60:TRP:CG	12:V2:94:PRO:HA	2.56	0.40
15:S3:79:THR:O	15:S3:93:VAL:N	2.55	0.40
16:S7:72:PHE:HD2	16:S7:157:LEU:HD11	1.86	0.40
23:A5:13:LEU:HG	23:A5:77:GLU:HB3	2.02	0.40
26:AL:66:THR:HG22	26:AL:74:PHE:HB2	2.04	0.40
29:D3:66:ASP:HA	29:D3:69:ILE:HD12	2.04	0.40
30:D1:167:ILE:HG23	38:A8:97:ARG:HH21	1.86	0.40
35:D2:274:ASP:H	36:AK:137:GLU:HG3	1.86	0.40
38:A8:107:ASP:OD2	38:A8:118:ARG:NH1	2.54	0.40
45:B4:120:LEU:HD22	45:B4:121:ASP:H	1.86	0.40
50:B8:30:ARG:NH2	50:B8:32:GLU:OE2	2.54	0.40
5:f1:89:PHE:HB2	5:f1:96:LEU:HB3	2.03	0.40
5:f1:144:CYS:HB2	5:f1:158:CYS:SG	2.61	0.40
2:a4:282:GLY:HA2	2:a4:283:PRO:HD3	1.83	0.40
11:V1:190:THR:HG21	11:V1:204:ARG:HB2	2.03	0.40
13:S1:99:ALA:O	13:S1:134:LYS:NZ	2.38	0.40
13:S1:378:LEU:HD13	13:S1:409:ILE:HD12	2.02	0.40
13:S1:380:VAL:HG12	13:S1:409:ILE:HB	2.03	0.40
17:S8:97:GLU:HB2	17:S8:107:THR:HG23	2.02	0.40
21:A9:29:PHE:HE1	21:A9:175:GLU:H	1.68	0.40
21:A9:30:LEU:HG	21:A9:207:ILE:HD11	2.03	0.40
30:D1:10:ILE:HG22	30:D1:83:LEU:HD11	2.03	0.40
30:D1:145:THR:HG23	30:D1:297:THR:HG21	2.04	0.40
32:4L:36:MET:HE2	32:4L:36:MET:HB3	1.87	0.40
33:D5:558:LEU:HD13	33:D5:558:LEU:HA	1.89	0.40
34:D4:369:LEU:HG	34:D4:370:PRO:HD2	2.02	0.40
37:B5:32:THR:HA	37:B5:35:PRO:HD2	2.04	0.40
5:f1:142:LEU:HD12	5:f1:161:HIS:CE1	2.56	0.40
1:a3:243:HIS:HB3	1:a3:425:PHE:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A9:211:THR:HA	21:A9:214:ILE:HD12	2.04	0.40
22:A2:61:GLN:HB2	22:A2:63:LYS:HE3	2.03	0.40
30:D1:150:LEU:HG	30:D1:154:LEU:HD23	2.03	0.40
30:D1:247:HIS:HB2	30:D1:255:TYR:HB2	2.04	0.40
34:D4:126:LEU:HD11	34:D4:154:LEU:HD12	2.02	0.40
39:BJ:64:HIS:NE2	51:BK:92:GLU:OE1	2.40	0.40
39:BJ:100:GLU:HA	39:BJ:103:ASN:HD22	1.86	0.40
3:b1:117:VAL:HG21	3:b1:302:VAL:HG22	2.03	0.40
3:b2:68:HIS:O	3:b2:72:ASP:HB2	2.21	0.40
4:c2:7:PRO:HA	4:c2:8:PRO:HD3	1.91	0.40
11:V1:59:GLU:HG2	11:V1:235:CYS:HA	2.04	0.40
13:S1:138:GLU:N	19:S6:74:ASN:HD22	2.19	0.40
14:S2:410:MET:HE1	30:D1:282:TYR:HB3	2.03	0.40
17:S8:154:LEU:HA	17:S8:154:LEU:HD23	1.90	0.40
19:S6:27:ARG:NH2	21:A9:44:GLN:OE1	2.54	0.40
27:AA:42:LEU:HD13	27:AA:42:LEU:HA	1.97	0.40
28:AM:70:LEU:HD11	38:A8:24:LEU:HG	2.03	0.40
29:D3:57:LEU:O	29:D3:61:THR:OG1	2.33	0.40
33:D5:42:CYS:HA	33:D5:45:ILE:HG22	2.03	0.40
33:D5:375:ILE:HD12	49:B2:32:MET:HG3	2.02	0.40
34:D4:115:LEU:HD13	34:D4:246:ILE:HG22	2.03	0.40
34:D4:198:ALA:HB2	64:AK:201:PC1:H351	2.03	0.40
34:D4:203:PHE:CE2	34:D4:246:ILE:HG12	2.55	0.40
35:D2:211:MET:SD	35:D2:333:SER:HB2	2.60	0.40
35:D2:231:SER:HB2	35:D2:305:PHE:HB2	2.04	0.40
37:B5:8:LEU:HB3	48:B9:174:ARG:HH12	1.86	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%)	397 (91%)	37 (8%)	1 (0%)	43	77
1	a3	442/446 (99%)	407 (92%)	35 (8%)	0	100	100
2	a2	410/439 (93%)	373 (91%)	37 (9%)	0	100	100
2	a4	409/439 (93%)	376 (92%)	33 (8%)	0	100	100
3	b1	376/379 (99%)	355 (94%)	21 (6%)	0	100	100
3	b2	376/379 (99%)	352 (94%)	24 (6%)	0	100	100
4	c1	237/240 (99%)	206 (87%)	31 (13%)	0	100	100
4	c2	236/240 (98%)	203 (86%)	33 (14%)	0	100	100
5	f1	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
5	f2	193/196 (98%)	180 (93%)	13 (7%)	0	100	100
6	d1	98/110 (89%)	95 (97%)	3 (3%)	0	100	100
6	d2	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
7	q1	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
7	q2	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
8	h1	63/78 (81%)	57 (90%)	6 (10%)	0	100	100
8	h2	63/78 (81%)	59 (94%)	4 (6%)	0	100	100
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	51 (93%)	4 (7%)	0	100	100
11	V1	428/445 (96%)	383 (90%)	45 (10%)	0	100	100
12	V2	210/217 (97%)	174 (83%)	36 (17%)	0	100	100
13	S1	686/704 (97%)	595 (87%)	87 (13%)	4 (1%)	21	58
14	S2	428/430 (100%)	374 (87%)	53 (12%)	1 (0%)	43	77
15	S3	206/228 (90%)	169 (82%)	36 (18%)	1 (0%)	24	62
16	S7	154/179 (86%)	133 (86%)	20 (13%)	1 (1%)	21	58
17	S8	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
18	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
19	S6	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
21	A9	286/338 (85%)	245 (86%)	41 (14%)	0	100	100
22	A2	80/98 (82%)	67 (84%)	13 (16%)	0	100	100
23	A5	109/115 (95%)	100 (92%)	9 (8%)	0	100	100
24	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	A7	92/112 (82%)	71 (77%)	20 (22%)	1 (1%)	11	45
26	AL	121/145 (83%)	100 (83%)	21 (17%)	0	100	100
27	AA	78/88 (89%)	64 (82%)	14 (18%)	0	100	100
27	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100	100
28	AM	137/143 (96%)	123 (90%)	14 (10%)	0	100	100
29	D3	113/115 (98%)	91 (80%)	22 (20%)	0	100	100
30	D1	316/318 (99%)	274 (87%)	41 (13%)	1 (0%)	36	71
31	D6	173/175 (99%)	151 (87%)	22 (13%)	0	100	100
32	4L	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	12	47
33	D5	604/606 (100%)	532 (88%)	72 (12%)	0	100	100
34	D4	457/459 (100%)	423 (93%)	33 (7%)	1 (0%)	43	77
35	D2	345/347 (99%)	314 (91%)	31 (9%)	0	100	100
36	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
37	B5	137/143 (96%)	123 (90%)	14 (10%)	0	100	100
38	A8	169/171 (99%)	137 (81%)	31 (18%)	1 (1%)	21	58
39	BJ	169/175 (97%)	153 (90%)	15 (9%)	1 (1%)	21	58
40	AJ	317/320 (99%)	271 (86%)	46 (14%)	0	100	100
41	S5	97/105 (92%)	83 (86%)	14 (14%)	0	100	100
42	A3	72/83 (87%)	61 (85%)	11 (15%)	0	100	100
43	B3	71/97 (73%)	55 (78%)	16 (22%)	0	100	100
44	C2	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
45	B4	126/128 (98%)	107 (85%)	19 (15%)	0	100	100
46	B6	91/127 (72%)	79 (87%)	11 (12%)	1 (1%)	11	45
47	B7	117/119 (98%)	102 (87%)	15 (13%)	0	100	100
48	B9	174/178 (98%)	147 (84%)	27 (16%)	0	100	100
49	B2	62/72 (86%)	58 (94%)	4 (6%)	0	100	100
50	B8	155/158 (98%)	110 (71%)	45 (29%)	0	100	100
51	BK	100/125 (80%)	83 (83%)	17 (17%)	0	100	100
52	C1	44/49 (90%)	41 (93%)	3 (7%)	0	100	100
53	B1	50/57 (88%)	45 (90%)	5 (10%)	0	100	100
54	A1	68/70 (97%)	60 (88%)	8 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11903/12556 (95%)	10550 (89%)	1338 (11%)	15 (0%)	49	82

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a1	279	HIS
13	S1	490	MET
16	S7	130	TYR
34	D4	54	LEU
32	4L	3	LEU
13	S1	424	ASP
15	S3	78	LEU
14	S2	73	VAL
25	A7	69	MET
39	BJ	71	PRO
13	S1	489	VAL
30	D1	92	PRO
46	B6	93	PRO
38	A8	147	PRO
13	S1	338	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	366/372 (98%)	366 (100%)	0	100	100
1	a3	370/372 (100%)	370 (100%)	0	100	100
2	a2	326/341 (96%)	325 (100%)	1 (0%)	86	84
2	a4	326/341 (96%)	325 (100%)	1 (0%)	86	84
3	b1	330/331 (100%)	329 (100%)	1 (0%)	86	84
3	b2	330/331 (100%)	330 (100%)	0	100	100
4	c1	205/206 (100%)	204 (100%)	1 (0%)	81	81
4	c2	204/206 (99%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	f1	168/168 (100%)	168 (100%)	0	100	100
5	f2	167/168 (99%)	167 (100%)	0	100	100
6	d1	93/99 (94%)	93 (100%)	0	100	100
6	d2	94/99 (95%)	94 (100%)	0	100	100
7	q1	66/72 (92%)	66 (100%)	0	100	100
7	q2	67/72 (93%)	67 (100%)	0	100	100
8	h1	62/74 (84%)	58 (94%)	4 (6%)	15	38
8	h2	62/74 (84%)	62 (100%)	0	100	100
10	i1	46/52 (88%)	46 (100%)	0	100	100
10	i2	48/52 (92%)	48 (100%)	0	100	100
11	V1	344/354 (97%)	342 (99%)	2 (1%)	78	80
12	V2	182/183 (100%)	181 (100%)	1 (0%)	81	81
13	S1	578/588 (98%)	577 (100%)	1 (0%)	87	85
14	S2	371/371 (100%)	369 (100%)	2 (0%)	81	81
15	S3	189/204 (93%)	189 (100%)	0	100	100
16	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
17	S8	151/151 (100%)	151 (100%)	0	100	100
18	V3	40/68 (59%)	40 (100%)	0	100	100
19	S6	79/80 (99%)	79 (100%)	0	100	100
20	S4	113/119 (95%)	113 (100%)	0	100	100
21	A9	251/292 (86%)	249 (99%)	2 (1%)	73	77
22	A2	73/81 (90%)	73 (100%)	0	100	100
23	A5	99/101 (98%)	98 (99%)	1 (1%)	68	75
24	A6	107/113 (95%)	107 (100%)	0	100	100
25	A7	84/94 (89%)	84 (100%)	0	100	100
26	AL	114/131 (87%)	113 (99%)	1 (1%)	70	75
27	AA	74/81 (91%)	73 (99%)	1 (1%)	59	70
27	AB	80/81 (99%)	79 (99%)	1 (1%)	61	71
28	AM	119/121 (98%)	119 (100%)	0	100	100
29	D3	103/103 (100%)	103 (100%)	0	100	100
30	D1	278/278 (100%)	273 (98%)	5 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D6	144/144 (100%)	142 (99%)	2 (1%)	59	70
32	4L	87/87 (100%)	87 (100%)	0	100	100
33	D5	539/539 (100%)	536 (99%)	3 (1%)	78	80
34	D4	412/412 (100%)	408 (99%)	4 (1%)	68	75
35	D2	315/315 (100%)	313 (99%)	2 (1%)	78	80
36	AK	101/101 (100%)	101 (100%)	0	100	100
37	B5	122/125 (98%)	122 (100%)	0	100	100
38	A8	154/154 (100%)	153 (99%)	1 (1%)	78	80
39	BJ	155/157 (99%)	155 (100%)	0	100	100
40	AJ	283/284 (100%)	283 (100%)	0	100	100
41	S5	88/94 (94%)	88 (100%)	0	100	100
42	A3	65/71 (92%)	65 (100%)	0	100	100
43	B3	55/75 (73%)	55 (100%)	0	100	100
44	C2	106/107 (99%)	106 (100%)	0	100	100
45	B4	114/114 (100%)	113 (99%)	1 (1%)	70	75
46	B6	91/121 (75%)	91 (100%)	0	100	100
47	B7	108/108 (100%)	108 (100%)	0	100	100
48	B9	159/160 (99%)	159 (100%)	0	100	100
49	B2	58/62 (94%)	58 (100%)	0	100	100
50	B8	142/142 (100%)	140 (99%)	2 (1%)	59	70
51	BK	93/112 (83%)	92 (99%)	1 (1%)	65	73
52	C1	42/44 (96%)	42 (100%)	0	100	100
53	B1	48/53 (91%)	48 (100%)	0	100	100
54	A1	59/59 (100%)	59 (100%)	0	100	100
All	All	10431/10814 (96%)	10389 (100%)	42 (0%)	81	82

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a2	109	VAL
3	b1	298	ILE
4	c1	142	LEU
8	h1	27	LEU
8	h1	37	LEU

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Mol	Chain	Res	Type
8	h1	72	LYS
8	h1	77	LEU
2	a4	109	VAL
11	V1	56	ILE
11	V1	365	CYS
12	V2	34	ILE
13	S1	290	LEU
14	S2	418	ILE
14	S2	423	ILE
16	S7	54	CYS
21	A9	109	VAL
21	A9	171	ILE
23	A5	89	LEU
26	AL	101	LYS
27	AA	80	ILE
30	D1	46	LEU
30	D1	49	ILE
30	D1	100	LEU
30	D1	103	LEU
30	D1	271	LEU
31	D6	12	ILE
31	D6	54	LEU
33	D5	154	LEU
33	D5	350	LEU
33	D5	602	LEU
34	D4	23	ILE
34	D4	143	LEU
34	D4	151	PHE
34	D4	298	ILE
35	D2	78	LEU
35	D2	193	VAL
27	AB	80	ILE
38	A8	109	CYS
45	B4	120	LEU
50	B8	9	LEU
50	B8	85	ILE
51	BK	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (192) such sidechains are listed below:

Mol	Chain	Res	Type
1	a1	53	ASN

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Mol	Chain	Res	Type
1	a1	85	HIS
1	a1	87	ASN
1	a1	165	GLN
1	a1	173	ASN
1	a1	215	HIS
1	a1	252	HIS
1	a1	267	ASN
1	a1	271	GLN
1	a1	359	ASN
1	a1	418	GLN
2	a2	22	GLN
2	a2	104	ASN
2	a2	125	ASN
2	a2	143	GLN
2	a2	162	ASN
2	a2	248	ASN
2	a2	284	HIS
2	a2	305	GLN
2	a2	313	ASN
2	a2	342	ASN
2	a2	343	GLN
2	a2	351	ASN
2	a2	362	ASN
3	b1	8	HIS
3	b1	26	ASN
3	b1	32	ASN
3	b1	221	HIS
3	b1	322	GLN
3	b1	345	HIS
4	c1	6	HIS
4	c1	50	HIS
4	c1	71	GLN
4	c1	121	HIS
5	f1	53	ASN
5	f1	86	ASN
5	f1	161	HIS
6	d1	73	GLN
8	h1	67	HIS
8	h1	75	ASN
1	a3	32	GLN
1	a3	53	ASN
1	a3	69	ASN

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Mol	Chain	Res	Type
1	a3	136	GLN
1	a3	141	ASN
1	a3	289	HIS
1	a3	323	HIS
1	a3	328	HIS
2	a4	67	HIS
2	a4	141	GLN
2	a4	143	GLN
2	a4	162	ASN
2	a4	248	ASN
2	a4	270	ASN
2	a4	297	GLN
2	a4	313	ASN
2	a4	329	GLN
2	a4	351	ASN
3	b2	85	ASN
3	b2	114	ASN
3	b2	137	GLN
3	b2	308	HIS
3	b2	322	GLN
3	b2	341	GLN
3	b2	345	HIS
4	c2	23	HIS
4	c2	197	HIS
4	c2	224	HIS
5	f2	53	ASN
5	f2	86	ASN
5	f2	116	GLN
5	f2	122	HIS
5	f2	161	HIS
5	f2	179	ASN
6	d2	22	ASN
7	q2	6	HIS
7	q2	23	GLN
8	h2	63	HIS
10	i2	54	HIS
11	V1	37	GLN
11	V1	165	ASN
11	V1	257	ASN
11	V1	283	HIS
11	V1	421	HIS
12	V2	55	GLN

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Mol	Chain	Res	Type
12	V2	99	HIS
12	V2	121	GLN
13	S1	36	GLN
13	S1	43	HIS
13	S1	179	ASN
13	S1	365	ASN
13	S1	421	HIS
14	S2	13	GLN
14	S2	34	ASN
14	S2	54	GLN
14	S2	84	HIS
14	S2	157	HIS
14	S2	217	ASN
14	S2	347	HIS
14	S2	409	HIS
15	S3	53	HIS
15	S3	88	ASN
16	S7	106	GLN
16	S7	162	GLN
17	S8	150	ASN
17	S8	157	ASN
17	S8	168	ASN
18	V3	44	HIS
19	S6	16	GLN
19	S6	47	GLN
20	S4	46	GLN
21	A9	89	ASN
21	A9	234	ASN
21	A9	288	HIS
21	A9	321	HIS
23	A5	49	GLN
23	A5	72	GLN
24	A6	125	HIS
25	A7	20	GLN
25	A7	24	GLN
26	AL	31	ASN
26	AL	72	ASN
26	AL	91	HIS
27	AA	74	GLN
28	AM	89	ASN
30	D1	5	ASN
30	D1	157	ASN

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Mol	Chain	Res	Type
30	D1	284	GLN
30	D1	317	GLN
31	D6	175	ASN
32	4L	83	ASN
32	4L	97	GLN
33	D5	136	ASN
33	D5	139	GLN
33	D5	274	GLN
33	D5	295	GLN
33	D5	323	HIS
33	D5	479	GLN
33	D5	484	HIS
33	D5	506	ASN
33	D5	546	GLN
33	D5	580	GLN
34	D4	51	ASN
34	D4	138	ASN
34	D4	220	HIS
34	D4	279	GLN
34	D4	319	HIS
34	D4	374	ASN
34	D4	399	ASN
35	D2	36	ASN
35	D2	204	ASN
35	D2	235	ASN
37	B5	143	ASN
27	AB	33	ASN
27	AB	35	HIS
27	AB	47	GLN
38	A8	30	HIS
38	A8	63	ASN
38	A8	150	ASN
39	BJ	27	ASN
39	BJ	90	GLN
39	BJ	103	ASN
39	BJ	113	GLN
40	AJ	92	ASN
40	AJ	97	GLN
40	AJ	151	HIS
40	AJ	239	GLN
40	AJ	251	GLN
40	AJ	294	GLN

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Mol	Chain	Res	Type
41	S5	15	HIS
41	S5	20	GLN
41	S5	44	HIS
42	A3	45	ASN
42	A3	70	GLN
43	B3	58	ASN
45	B4	74	ASN
45	B4	78	ASN
46	B6	13	GLN
47	B7	43	GLN
47	B7	83	GLN
48	B9	32	HIS
49	B2	16	GLN
49	B2	21	GLN
50	B8	78	HIS
50	B8	126	GLN
50	B8	136	ASN
50	B8	137	ASN
51	BK	27	GLN
51	BK	45	HIS
51	BK	103	HIS
52	C1	34	GLN
54	A1	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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$
57	FES	f1	501	5	0,4,4	-	-	-		
63	ZMP	AA	101	27	28,33,36	0.69	1 (3%)	32,40,45	0.95	1 (3%)
57	FES	V2	300	12	0,4,4	-	-	-		
64	PC1	AK	201	-	27,27,53	0.40	0	33,35,61	0.39	0
58	SF4	S7	300	16	0,12,12	-	-	-		
55	HEM	b1	401	3	50,50,50	1.36	5 (10%)	67,82,82	1.69	14 (20%)
55	HEM	b2	401	3	50,50,50	1.35	6 (12%)	67,82,82	1.60	12 (17%)
60	3PE	S2	501	-	39,39,50	0.34	0	42,44,55	0.37	0
57	FES	S1	803	13	0,4,4	-	-	-		
59	FMN	V1	501	-	33,33,33	0.24	0	48,50,50	0.35	0
56	HEC	c2	501	4	46,50,50	1.94	8 (17%)	58,82,82	1.86	6 (10%)
55	HEM	b2	402	3	50,50,50	1.42	7 (14%)	67,82,82	1.76	14 (20%)
57	FES	f2	501	5	0,4,4	-	-	-		
58	SF4	S8	201	17	0,12,12	-	-	-		
58	SF4	S1	802	13	0,12,12	-	-	-		
55	HEM	b1	402	3	50,50,50	1.36	6 (12%)	67,82,82	1.65	14 (20%)
58	SF4	V1	500	11	0,12,12	-	-	-		
60	3PE	D5	701	-	37,37,50	0.34	0	40,42,55	0.31	0
62	NDP	A9	401	-	51,52,52	0.43	0	71,80,80	0.49	0
58	SF4	S8	202	17	0,12,12	-	-	-		
63	ZMP	AB	101	27	25,30,36	0.68	0	29,37,45	1.02	2 (6%)
58	SF4	S1	801	13	0,12,12	-	-	-		
56	HEC	c1	501	4	46,50,50	1.96	8 (17%)	58,82,82	1.73	10 (17%)

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
57	FES	f1	501	5	-	-	0/1/1/1
63	ZMP	AA	101	27	-	12/38/40/43	-
64	PC1	AK	201	-	-	4/31/31/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	FES	V2	300	12	-	-	0/1/1/1
58	SF4	S7	300	16	-	-	0/6/5/5
55	HEM	b1	401	3	-	7/14/54/54	-
55	HEM	b2	401	3	-	5/14/54/54	-
60	3PE	S2	501	-	-	8/43/43/54	-
57	FES	S1	803	13	-	-	0/1/1/1
59	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
56	HEC	c2	501	4	-	2/14/54/54	-
55	HEM	b2	402	3	-	9/14/54/54	-
57	FES	f2	501	5	-	-	0/1/1/1
58	SF4	S8	201	17	-	-	0/6/5/5
58	SF4	S1	802	13	-	-	0/6/5/5
55	HEM	b1	402	3	-	7/14/54/54	-
58	SF4	V1	500	11	-	-	0/6/5/5
60	3PE	D5	701	-	-	15/41/41/54	-
62	NDP	A9	401	-	-	11/34/77/77	0/5/5/5
58	SF4	S8	202	17	-	-	0/6/5/5
63	ZMP	AB	101	27	-	12/35/37/43	-
58	SF4	S1	801	13	-	-	0/6/5/5
56	HEC	c1	501	4	-	8/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c1	501	HEC	CAC-C3C	7.26	1.58	1.35
56	c2	501	HEC	CAC-C3C	7.08	1.58	1.35
56	c1	501	HEC	CAB-C3B	7.04	1.57	1.35
56	c2	501	HEC	CAB-C3B	6.59	1.56	1.35
55	b2	402	HEM	C4D-ND	-4.02	1.33	1.40
55	b1	402	HEM	C4D-ND	-3.96	1.33	1.40
55	b1	401	HEM	C4D-ND	-3.72	1.33	1.40
55	b2	402	HEM	C1B-NB	-3.64	1.34	1.40
55	b2	401	HEM	C4D-ND	-3.58	1.34	1.40
55	b1	401	HEM	C1B-NB	-3.53	1.34	1.40
55	b1	402	HEM	C1B-NB	-3.51	1.34	1.40
56	c2	501	HEC	CBC-CAC	-3.48	1.36	1.49
55	b2	401	HEM	C1B-NB	-3.44	1.34	1.40
56	c1	501	HEC	CBC-CAC	-3.37	1.37	1.49
55	b2	402	HEM	C1D-ND	-3.21	1.32	1.38
55	b1	401	HEM	C1D-ND	-3.07	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	b1	402	HEM	C1C-C2C	-3.07	1.39	1.45
55	b2	401	HEM	C1C-C2C	-3.06	1.39	1.45
55	b1	402	HEM	C1D-ND	-3.05	1.32	1.38
55	b2	402	HEM	C1C-C2C	-3.04	1.39	1.45
55	b2	401	HEM	C1D-ND	-2.94	1.33	1.38
55	b1	401	HEM	C1C-C2C	-2.79	1.39	1.45
55	b2	401	HEM	C4B-NB	-2.46	1.34	1.38
63	AA	101	ZMP	C9-C10	2.45	1.53	1.50
56	c2	501	HEC	CBB-CAB	-2.44	1.40	1.49
55	b1	402	HEM	C4B-NB	-2.44	1.34	1.38
56	c2	501	HEC	C3D-C2D	-2.42	1.32	1.38
55	b2	402	HEM	C4B-NB	-2.40	1.34	1.38
56	c1	501	HEC	C3D-C2D	-2.36	1.32	1.38
55	b1	401	HEM	C4B-NB	-2.35	1.34	1.38
55	b2	402	HEM	C3C-C4C	-2.32	1.42	1.46
56	c1	501	HEC	CBB-CAB	-2.29	1.41	1.49
56	c1	501	HEC	CMB-C2B	2.27	1.55	1.50
56	c2	501	HEC	C3C-C2C	-2.25	1.33	1.41
56	c2	501	HEC	C3B-C2B	-2.19	1.33	1.41
56	c1	501	HEC	CMA-C3A	2.16	1.55	1.50
56	c1	501	HEC	CMD-C2D	2.10	1.55	1.50
55	b2	401	HEM	FE-NB	2.06	2.01	1.94
55	b1	402	HEM	FE-NB	2.02	2.01	1.94
56	c2	501	HEC	CMD-C2D	2.01	1.54	1.50
55	b2	402	HEM	FE-NB	2.01	2.01	1.94

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	c2	501	HEC	CBB-CAB-C3B	-8.80	109.85	127.43
56	c2	501	HEC	CBC-CAC-C3C	-6.96	113.52	127.43
56	c1	501	HEC	CBB-CAB-C3B	-6.23	114.98	127.43
56	c1	501	HEC	CBC-CAC-C3C	-6.22	115.00	127.43
55	b2	402	HEM	CHC-C4B-NB	5.35	130.18	124.42
55	b1	402	HEM	CHC-C4B-NB	5.23	130.05	124.42
55	b1	401	HEM	CHC-C4B-NB	5.05	129.85	124.42
55	b2	402	HEM	CHD-C4C-NC	4.91	129.79	124.45
55	b2	401	HEM	CHC-C4B-NB	4.87	129.66	124.42
55	b1	401	HEM	CHB-C1B-NB	4.35	129.75	124.37
55	b2	402	HEM	CHB-C1B-NB	4.32	129.71	124.37
55	b2	401	HEM	CHB-C1B-NB	4.08	129.41	124.37
55	b1	402	HEM	C4D-ND-C1D	3.83	109.74	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	b2	401	HEM	CHD-C4C-NC	3.81	128.61	124.45
55	b1	401	HEM	CHD-C4C-NC	3.63	128.41	124.45
55	b1	402	HEM	CHB-C1B-NB	3.53	128.73	124.37
55	b1	402	HEM	CHD-C4C-NC	3.33	128.08	124.45
56	c1	501	HEC	CMB-C2B-C1B	-3.14	120.63	125.42
55	b2	401	HEM	CHA-C4D-ND	3.10	128.20	124.37
55	b2	402	HEM	CHA-C4D-ND	3.02	128.10	124.37
55	b2	401	HEM	C4D-ND-C1D	3.01	108.77	105.21
55	b2	401	HEM	CHD-C1D-ND	2.98	127.63	124.42
55	b2	402	HEM	C4D-ND-C1D	2.95	108.70	105.21
55	b1	401	HEM	CBD-CAD-C3D	-2.93	104.43	112.53
55	b2	402	HEM	CHD-C1D-ND	2.91	127.55	124.42
55	b1	401	HEM	CHD-C1D-ND	2.90	127.55	124.42
55	b1	401	HEM	C1B-NB-C4B	2.85	108.58	105.21
55	b1	402	HEM	CHD-C1D-ND	2.84	127.48	124.42
55	b1	401	HEM	CHA-C1A-NA	2.83	128.98	123.86
56	c2	501	HEC	CBD-CAD-C3D	2.81	120.29	112.53
56	c2	501	HEC	O1D-CGD-CBD	-2.78	114.27	123.09
55	b1	401	HEM	C4D-ND-C1D	2.76	108.48	105.21
56	c1	501	HEC	O1D-CGD-CBD	-2.71	114.49	123.09
55	b2	402	HEM	CHB-C1B-C2B	-2.70	119.28	126.95
56	c1	501	HEC	CBD-CAD-C3D	2.67	119.92	112.53
55	b1	402	HEM	C1C-CHC-C4B	-2.66	120.36	126.02
55	b1	402	HEM	CHA-C4D-ND	2.65	127.65	124.37
55	b2	402	HEM	C1C-CHC-C4B	-2.64	120.40	126.02
55	b2	401	HEM	CHA-C1A-NA	2.64	128.64	123.86
55	b2	402	HEM	CHA-C1A-NA	2.64	128.64	123.86
55	b2	401	HEM	CHB-C1B-C2B	-2.62	119.50	126.95
55	b1	402	HEM	C2A-C1A-NA	-2.62	107.25	110.15
55	b1	402	HEM	C1B-NB-C4B	2.62	108.31	105.21
55	b2	401	HEM	CBD-CAD-C3D	-2.59	105.38	112.53
55	b1	402	HEM	C4A-CHB-C1B	-2.55	120.25	126.25
56	c1	501	HEC	O1A-CGA-CBA	-2.50	115.15	123.09
56	c1	501	HEC	CMB-C2B-C3B	2.46	132.33	126.55
63	AB	101	ZMP	O1-C10-C9	-2.44	121.17	123.98
55	b1	401	HEM	CHA-C4D-ND	2.42	127.36	124.37
63	AB	101	ZMP	C11-C12-N1	-2.38	107.44	112.41
55	b1	401	HEM	CHB-C1B-C2B	-2.37	120.21	126.95
56	c1	501	HEC	CMD-C2D-C1D	-2.36	121.82	125.42
55	b1	401	HEM	C4A-CHB-C1B	-2.35	120.73	126.25
55	b2	402	HEM	CBD-CAD-C3D	-2.33	106.09	112.53
55	b1	401	HEM	C1C-CHC-C4B	-2.33	121.08	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	c1	501	HEC	CAA-CBA-CGA	-2.31	107.55	113.67
63	AA	101	ZMP	O1-C10-C9	-2.29	121.34	123.98
55	b2	402	HEM	C1B-NB-C4B	2.28	107.90	105.21
55	b2	401	HEM	C4A-CHB-C1B	-2.24	120.99	126.25
55	b2	402	HEM	C4A-CHB-C1B	-2.22	121.02	126.25
55	b1	401	HEM	CAA-CBA-CGA	-2.22	107.78	113.67
55	b2	401	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
56	c2	501	HEC	O1A-CGA-CBA	-2.19	116.14	123.09
55	b2	402	HEM	CBC-CAC-C3C	-2.18	116.63	127.53
55	b1	402	HEM	CHB-C1B-C2B	-2.17	120.78	126.95
55	b2	401	HEM	C1B-NB-C4B	2.17	107.78	105.21
56	c2	501	HEC	CMD-C2D-C1D	-2.12	122.19	125.42
56	c1	501	HEC	O2A-CGA-O1A	2.09	128.71	123.33
55	b2	402	HEM	O2A-CGA-CBA	2.09	120.59	114.00
55	b1	402	HEM	C4C-CHD-C1D	-2.08	121.59	126.02
55	b1	401	HEM	O2D-CGD-CBD	2.07	120.55	114.00
55	b1	402	HEM	CHA-C1A-NA	2.05	127.58	123.86
55	b1	402	HEM	O2D-CGD-CBD	2.00	120.33	114.00

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	b1	401	HEM	C2B-C3B-CAB-CBB
55	b1	401	HEM	C4B-C3B-CAB-CBB
55	b1	401	HEM	C2C-C3C-CAC-CBC
55	b1	401	HEM	C4C-C3C-CAC-CBC
55	b1	402	HEM	C2B-C3B-CAB-CBB
55	b1	402	HEM	C4B-C3B-CAB-CBB
55	b1	402	HEM	C2C-C3C-CAC-CBC
55	b1	402	HEM	C4C-C3C-CAC-CBC
55	b2	401	HEM	C2B-C3B-CAB-CBB
55	b2	402	HEM	C2B-C3B-CAB-CBB
55	b2	402	HEM	C4B-C3B-CAB-CBB
55	b2	402	HEM	C2C-C3C-CAC-CBC
55	b2	402	HEM	C4C-C3C-CAC-CBC
56	c1	501	HEC	C2B-C3B-CAB-CBB
56	c1	501	HEC	C4B-C3B-CAB-CBB
59	V1	501	FMN	C5'-O5'-P-O1P
59	V1	501	FMN	C5'-O5'-P-O2P
59	V1	501	FMN	C5'-O5'-P-O3P
60	S2	501	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
60	S2	501	3PE	C11-O13-P-O12
60	S2	501	3PE	C11-O13-P-O14
60	S2	501	3PE	O13-C11-C12-N
60	D5	701	3PE	C1-O11-P-O12
60	D5	701	3PE	C1-O11-P-O13
60	D5	701	3PE	C1-O11-P-O14
60	D5	701	3PE	C11-O13-P-O11
60	D5	701	3PE	C11-O13-P-O12
60	D5	701	3PE	C11-O13-P-O14
60	D5	701	3PE	O13-C11-C12-N
60	D5	701	3PE	O21-C2-C3-O31
62	A9	401	NDP	C5D-O5D-PN-O3
62	A9	401	NDP	C2D-C1D-N1N-C6N
62	A9	401	NDP	C2N-C3N-C7N-O7N
62	A9	401	NDP	C2N-C3N-C7N-N7N
63	AA	101	ZMP	N2-C16-C17-O4
63	AB	101	ZMP	C12-C11-S1-C10
63	AB	101	ZMP	O1-C10-S1-C11
63	AB	101	ZMP	C9-C10-S1-C11
63	AA	101	ZMP	C14-C13-N1-C12
63	AB	101	ZMP	C14-C13-N1-C12
62	A9	401	NDP	C2D-C1D-N1N-C2N
56	c1	501	HEC	C3D-CAD-CBD-CGD
63	AA	101	ZMP	O2-C13-N1-C12
63	AB	101	ZMP	O2-C13-N1-C12
60	D5	701	3PE	C22-C23-C24-C25
60	S2	501	3PE	C35-C36-C37-C38
55	b2	401	HEM	C2C-C3C-CAC-CBC
55	b2	401	HEM	C4B-C3B-CAB-CBB
55	b2	401	HEM	C2A-CAA-CBA-CGA
55	b2	402	HEM	C2A-CAA-CBA-CGA
64	AK	201	PC1	C31-C32-C33-C34
60	D5	701	3PE	C1-C2-C3-O31
60	D5	701	3PE	C25-C26-C27-C28
59	V1	501	FMN	C4'-C5'-O5'-P
60	D5	701	3PE	O11-C1-C2-C3
63	AA	101	ZMP	C2-C3-C4-C5
60	D5	701	3PE	O11-C1-C2-O21
64	AK	201	PC1	O11-C1-C2-O21
55	b2	401	HEM	C4C-C3C-CAC-CBC
63	AA	101	ZMP	C16-C17-C18-C19
64	AK	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
55	b1	402	HEM	C2A-CAA-CBA-CGA
63	AA	101	ZMP	O3-C16-C17-O4
63	AB	101	ZMP	O3-C16-C17-O4
64	AK	201	PC1	O11-C1-C2-C3
59	V1	501	FMN	N10-C1'-C2'-O2'
63	AA	101	ZMP	C19-C18-C21-O5
63	AA	101	ZMP	C16-C17-C18-C21
56	c1	501	HEC	C4C-C3C-CAC-CBC
56	c2	501	HEC	C4C-C3C-CAC-CBC
63	AB	101	ZMP	C6-C7-C8-C9
56	c1	501	HEC	C2C-C3C-CAC-CBC
62	A9	401	NDP	C5D-O5D-PN-O1N
62	A9	401	NDP	C5D-O5D-PN-O2N
60	S2	501	3PE	C34-C35-C36-C37
60	D5	701	3PE	C21-C22-C23-C24
63	AA	101	ZMP	O4-C17-C18-C20
63	AB	101	ZMP	O4-C17-C18-C20
62	A9	401	NDP	PN-O3-PA-O2A
62	A9	401	NDP	O4D-C1D-N1N-C6N
60	S2	501	3PE	C2-C1-O11-P
55	b1	401	HEM	C2A-CAA-CBA-CGA
55	b1	401	HEM	CAD-CBD-CGD-O1D
55	b1	401	HEM	CAD-CBD-CGD-O2D
55	b2	402	HEM	CAA-CBA-CGA-O1A
55	b2	402	HEM	CAD-CBD-CGD-O2D
55	b2	402	HEM	CAA-CBA-CGA-O2A
55	b1	402	HEM	CAA-CBA-CGA-O1A
55	b1	402	HEM	CAA-CBA-CGA-O2A
55	b2	402	HEM	CAD-CBD-CGD-O1D
63	AA	101	ZMP	C7-C8-C9-C10
60	D5	701	3PE	C23-C24-C25-C26
63	AA	101	ZMP	C16-C17-C18-C20
63	AB	101	ZMP	C16-C17-C18-C19
63	AB	101	ZMP	C16-C17-C18-C20
60	S2	501	3PE	C25-C26-C27-C28
56	c1	501	HEC	CAA-CBA-CGA-O2A
63	AA	101	ZMP	C20-C18-C21-O5
63	AB	101	ZMP	C16-C17-C18-C21
62	A9	401	NDP	O4D-C1D-N1N-C2N
56	c2	501	HEC	C4B-C3B-CAB-CBB
63	AB	101	ZMP	N2-C16-C17-O4
56	c1	501	HEC	CAA-CBA-CGA-O1A

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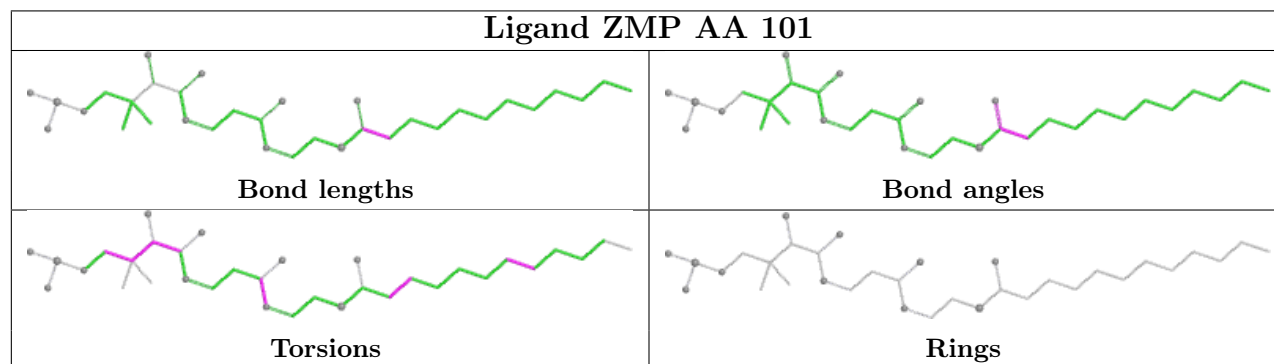
Mol	Chain	Res	Type	Atoms
56	c1	501	HEC	CAD-CBD-CGD-O2D
62	A9	401	NDP	PN-O3-PA-O1A

There are no ring outliers.

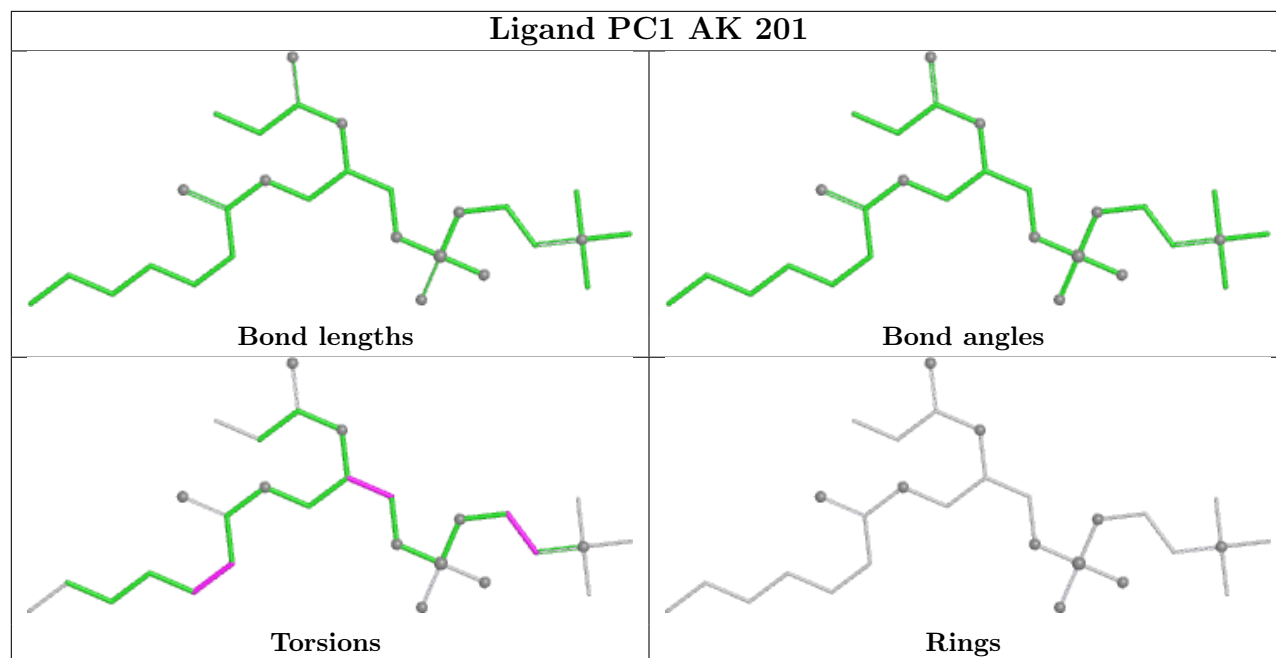
13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	f1	501	FES	1	0
63	AA	101	ZMP	1	0
57	V2	300	FES	1	0
64	AK	201	PC1	1	0
55	b1	401	HEM	3	0
55	b2	401	HEM	2	0
60	S2	501	3PE	3	0
55	b1	402	HEM	2	0
60	D5	701	3PE	1	0
62	A9	401	NDP	5	0
63	AB	101	ZMP	4	0
58	S1	801	SF4	1	0
56	c1	501	HEC	1	0

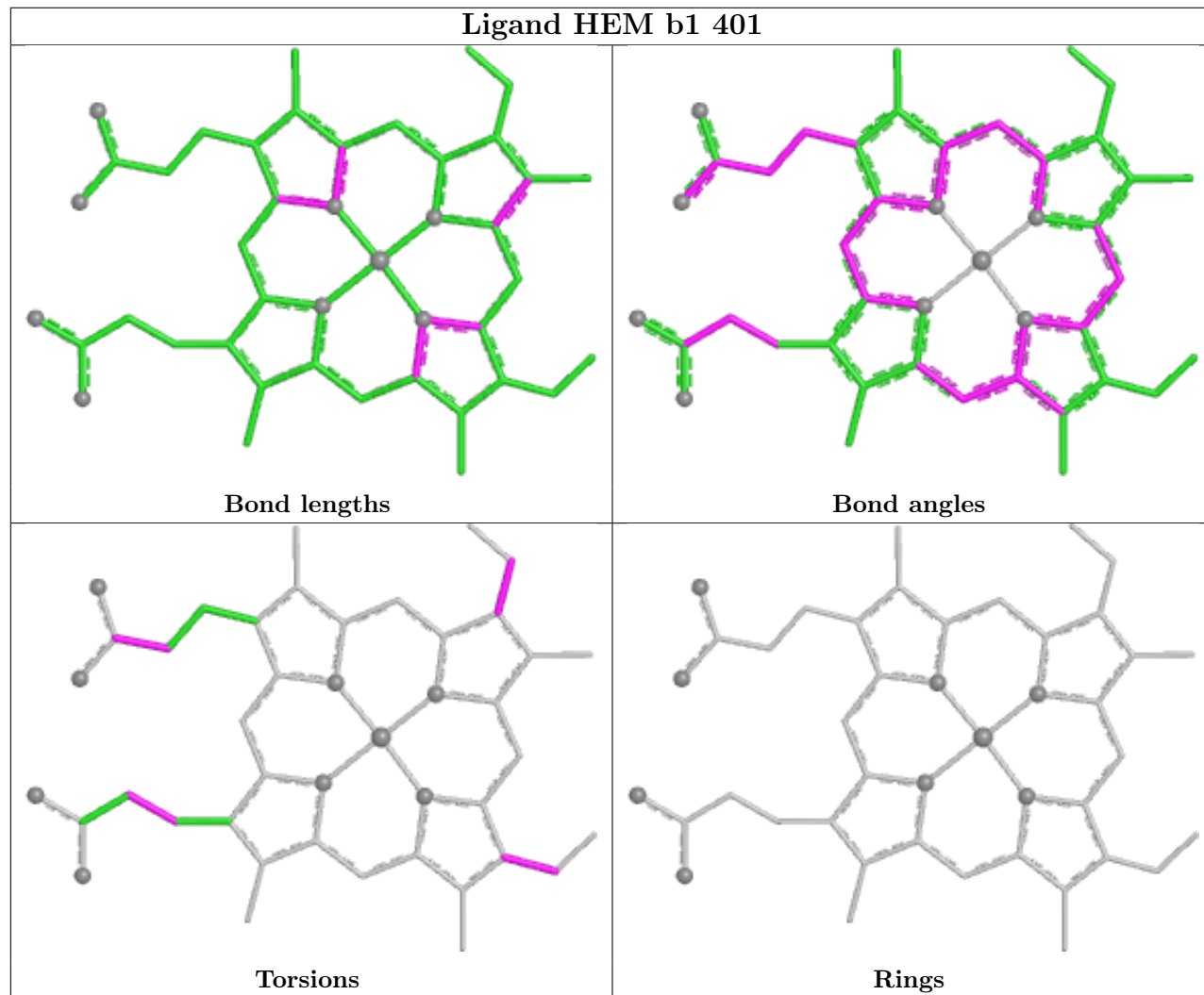
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

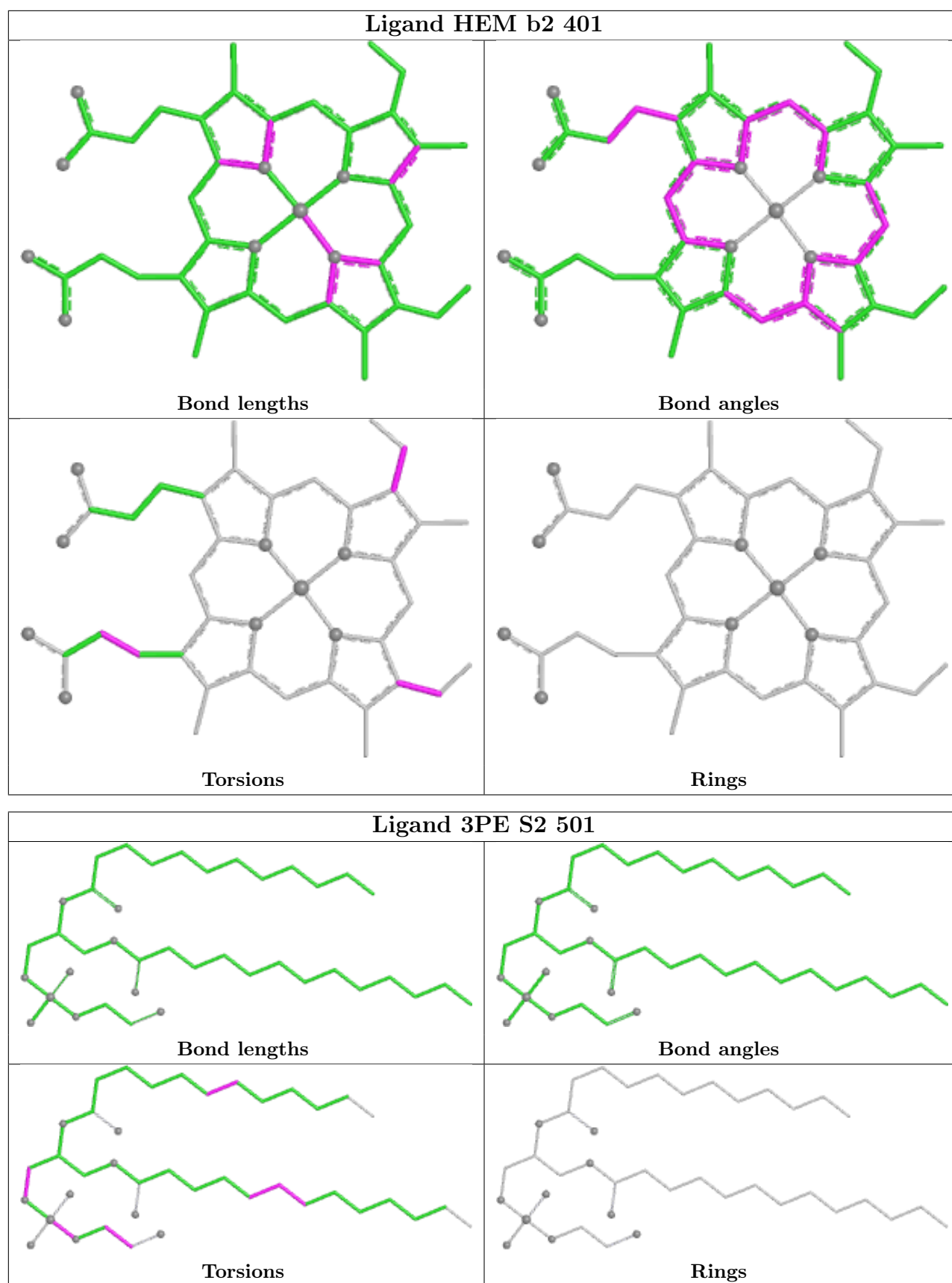


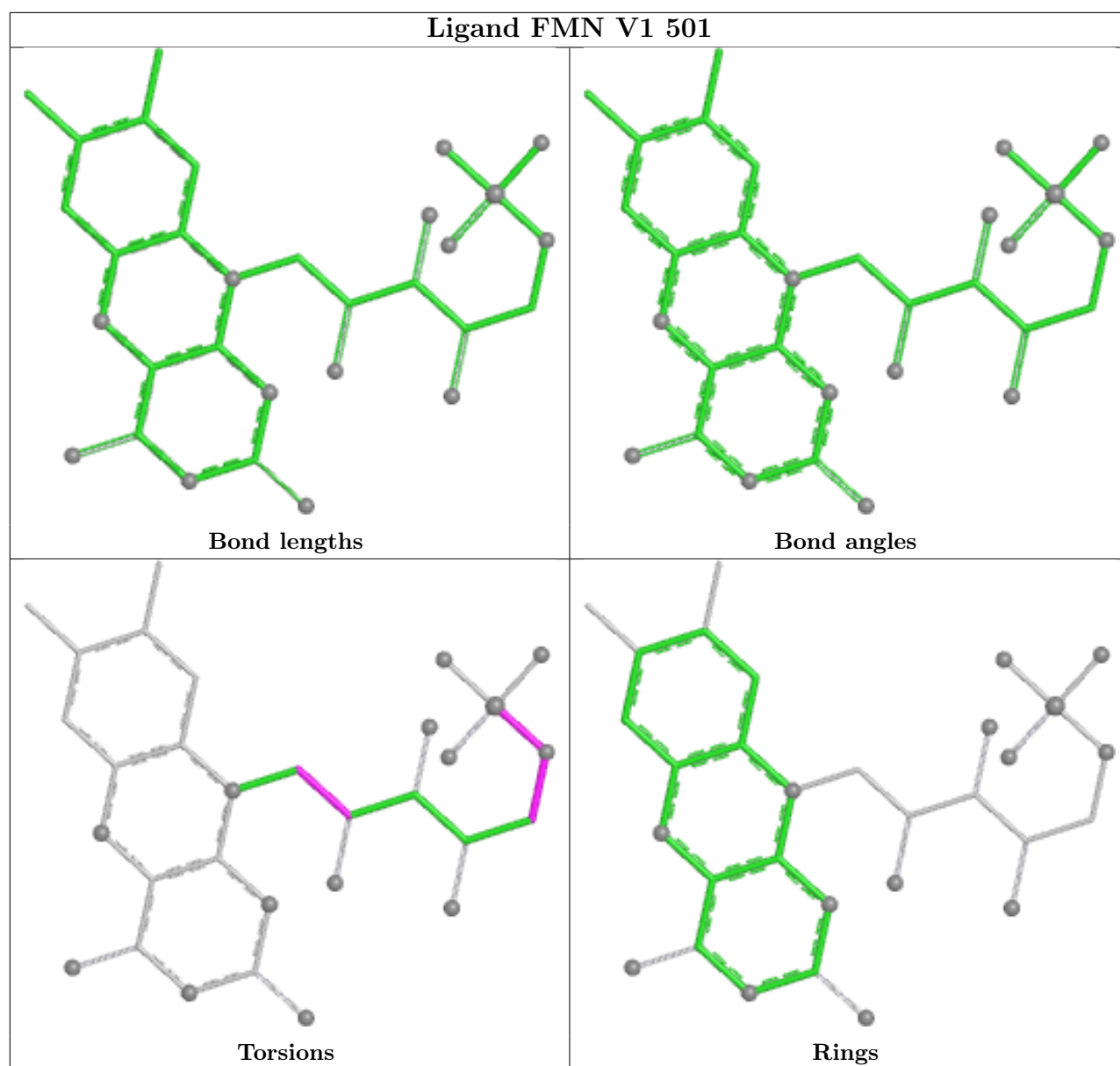
Ligand PC1 AK 201

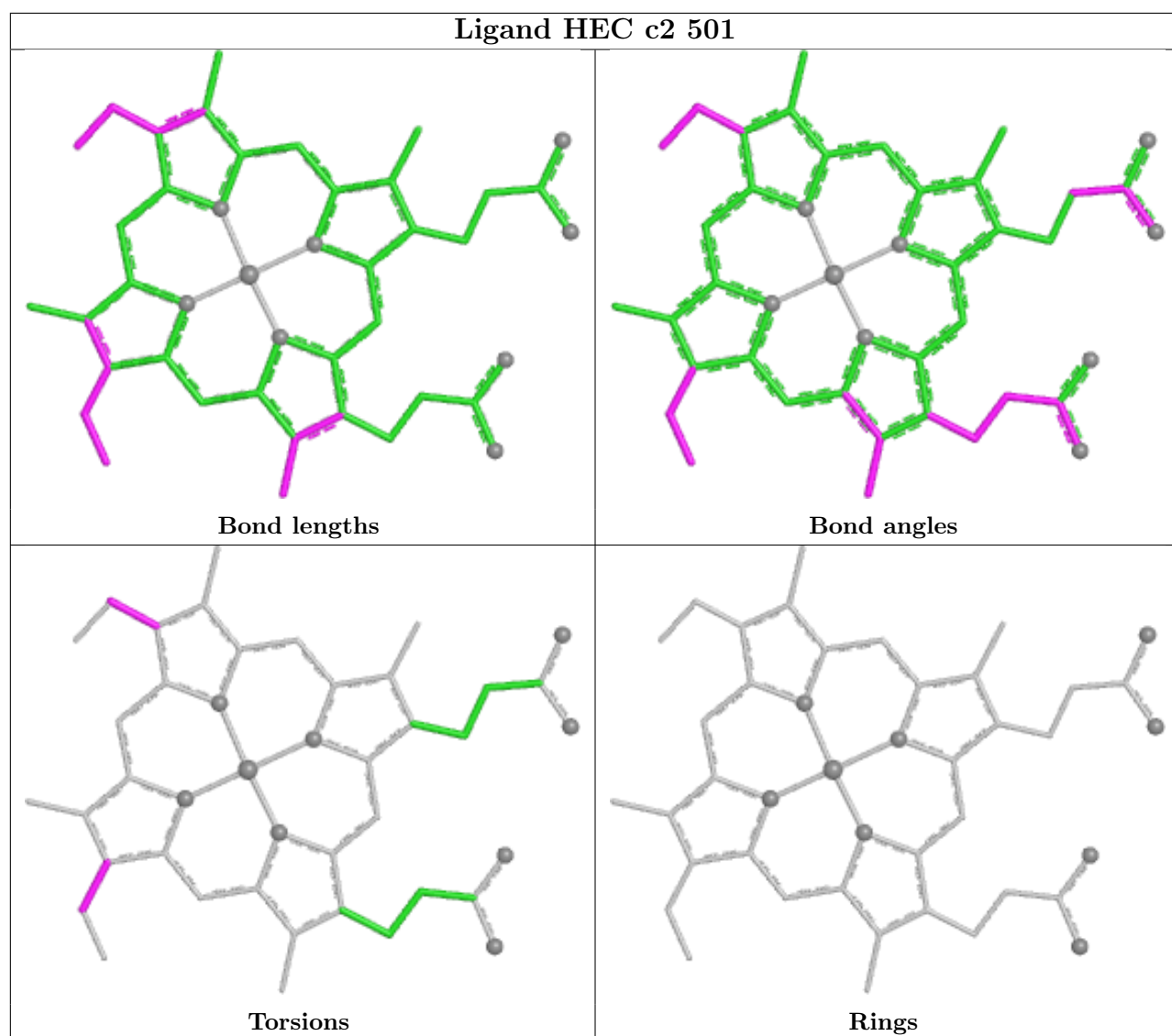


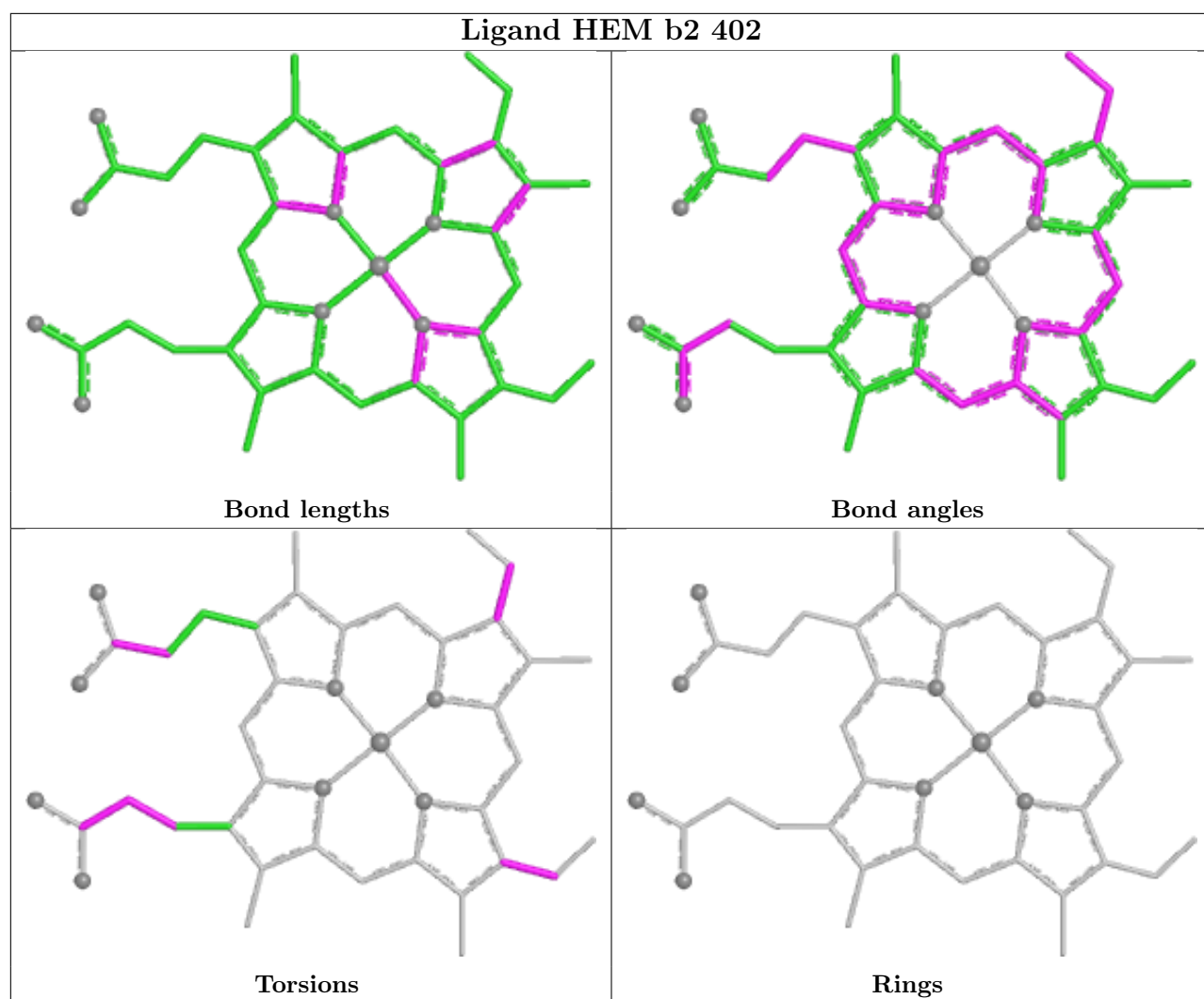
Ligand HEM b1 401

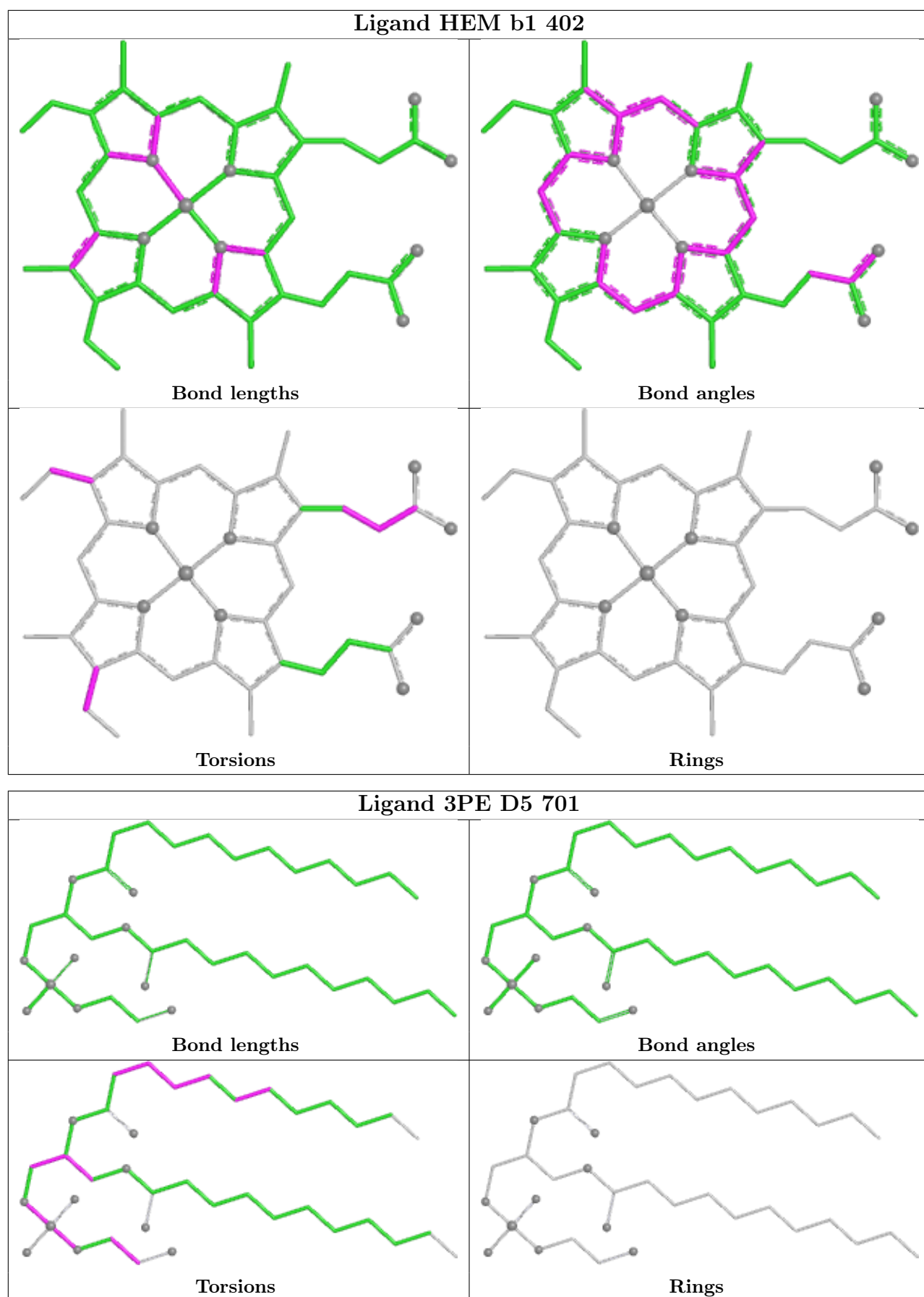


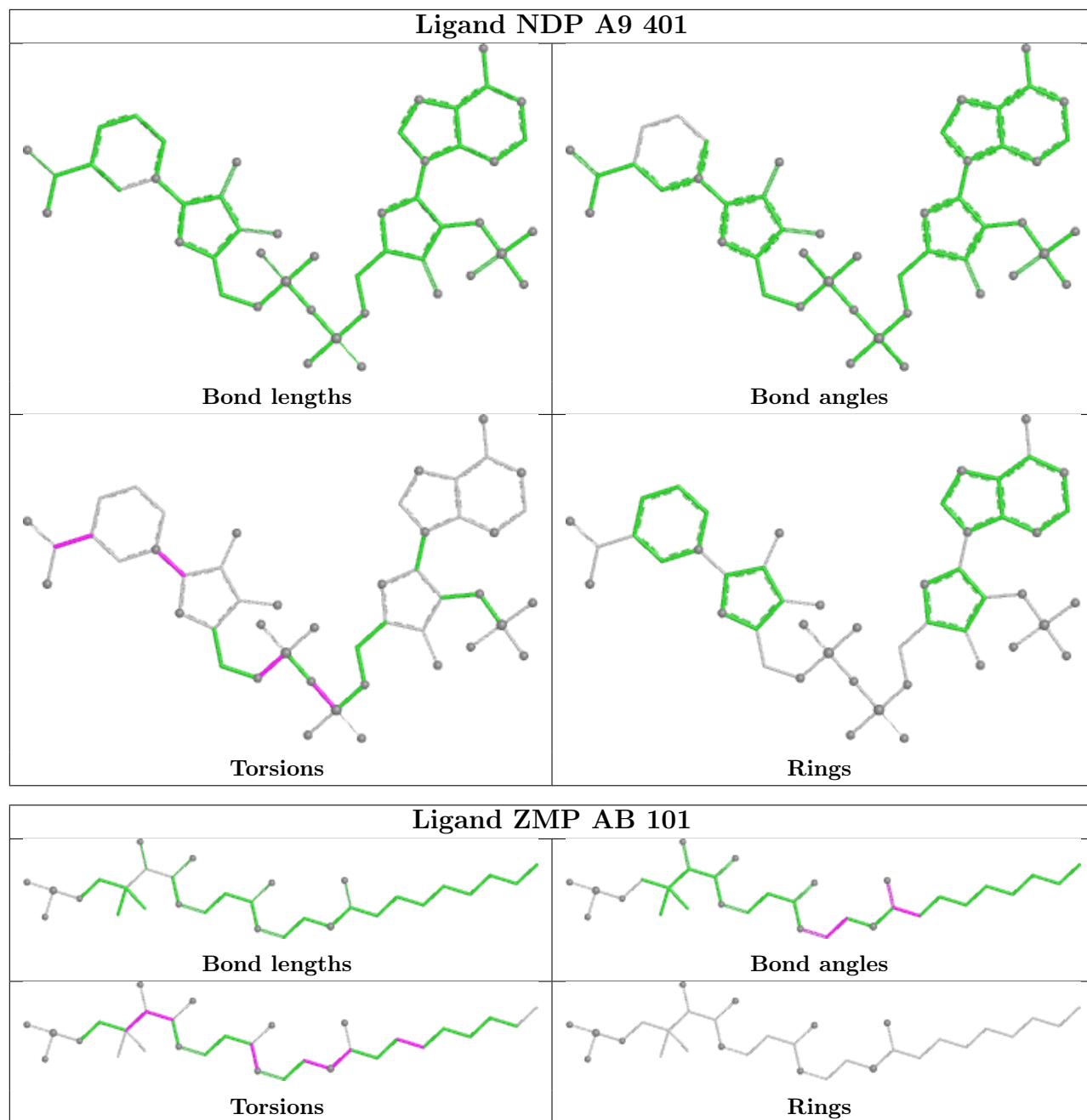


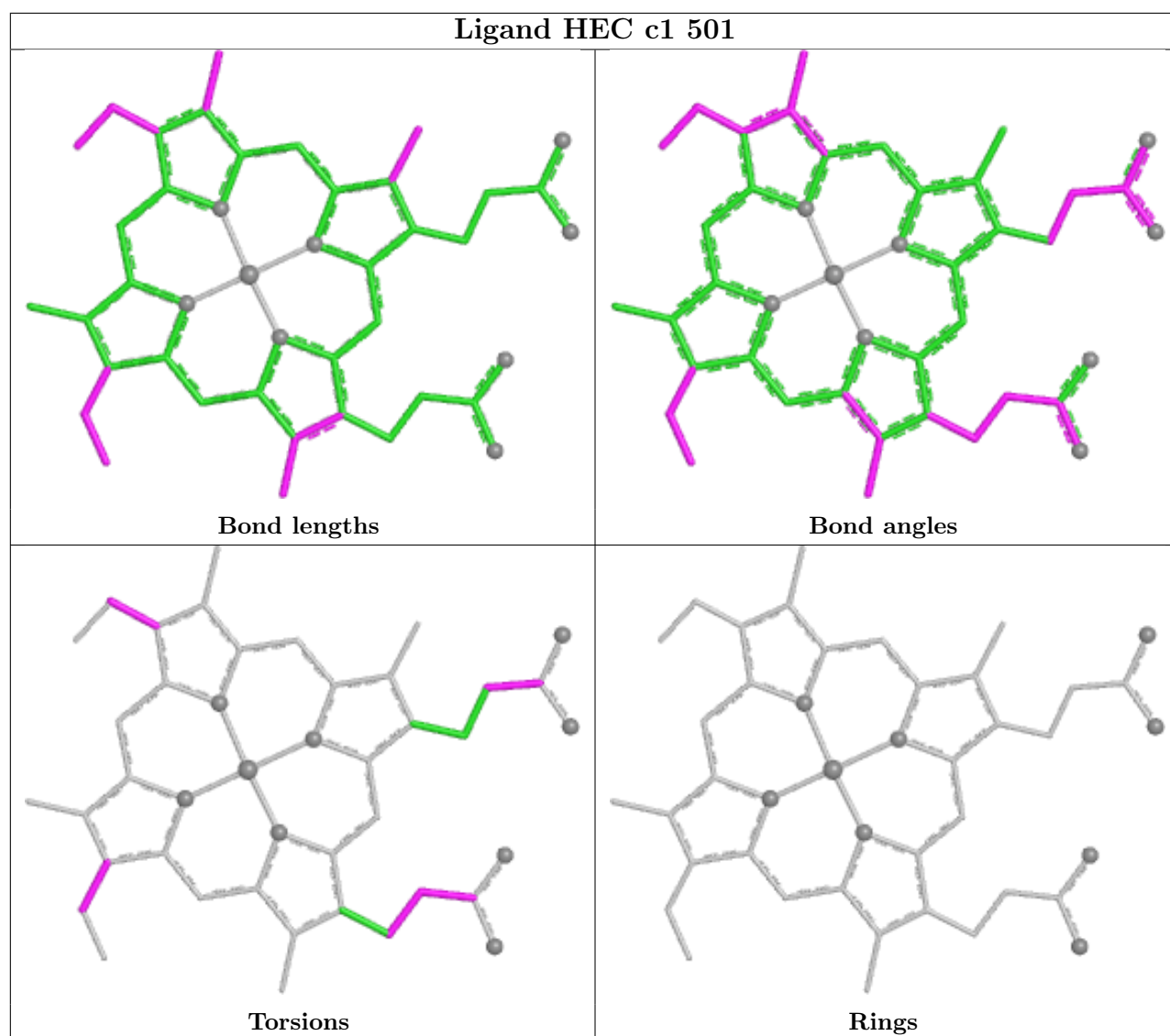












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

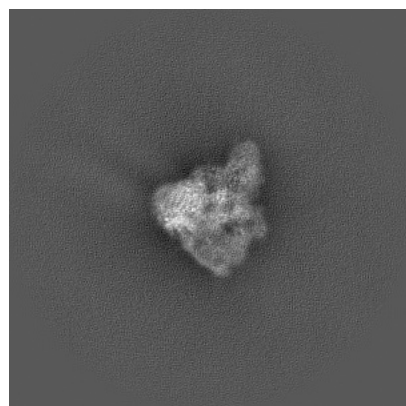
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4493. These allow visual inspection of the internal detail of the map and identification of artifacts.

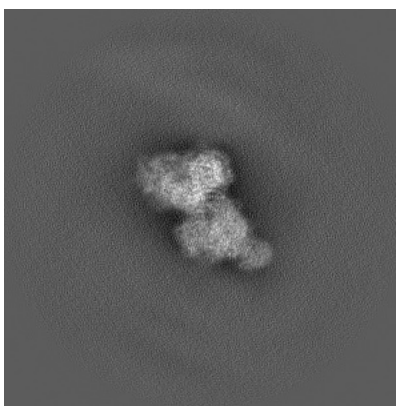
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

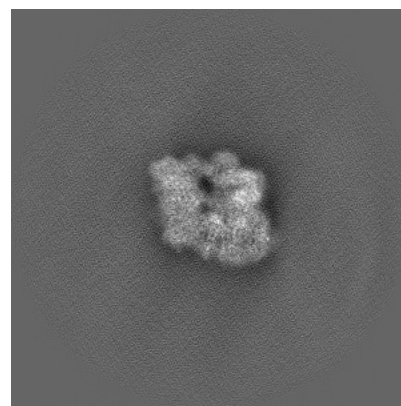
6.1.1 Primary map



X

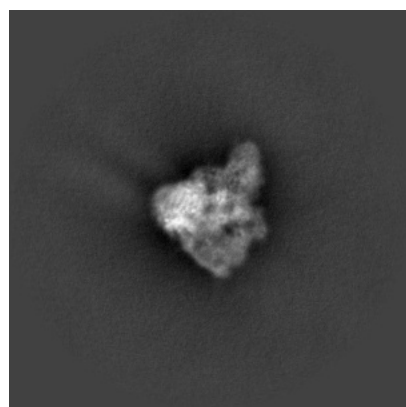


Y

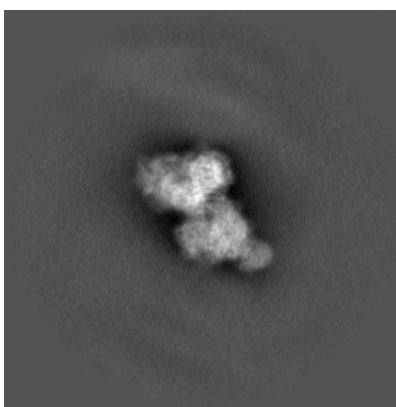


Z

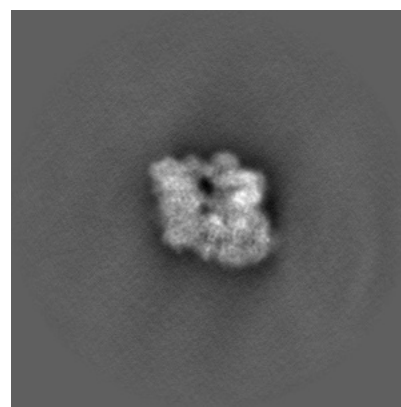
6.1.2 Raw map



X



Y

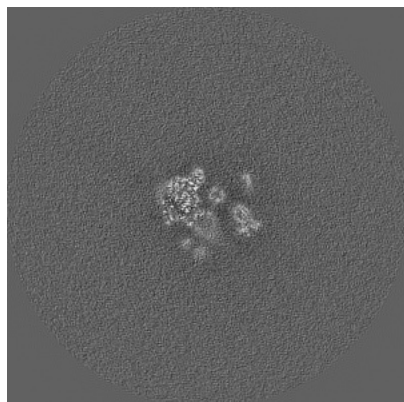


Z

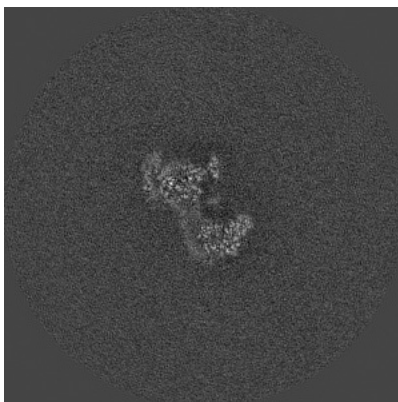
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

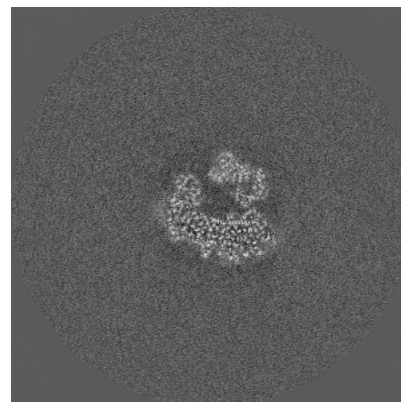
6.2.1 Primary map



X Index: 256

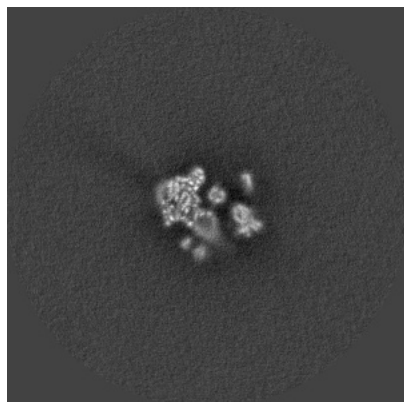


Y Index: 256

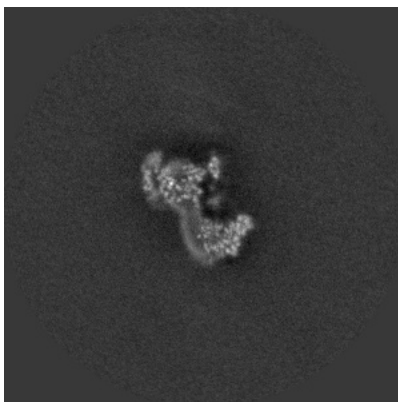


Z Index: 256

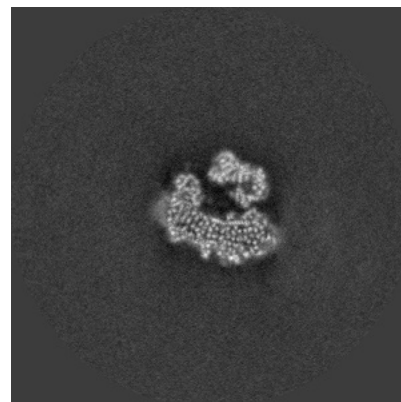
6.2.2 Raw map



X Index: 256



Y Index: 256

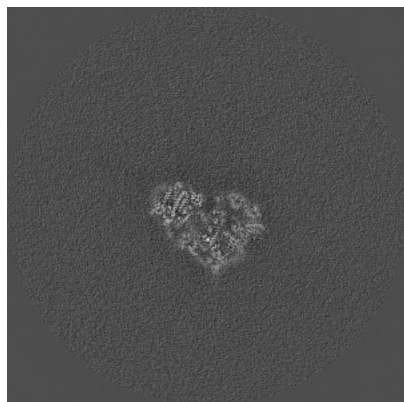


Z Index: 256

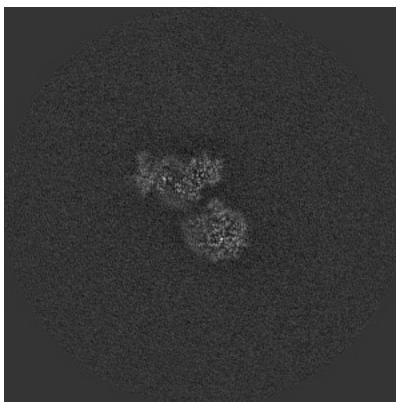
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

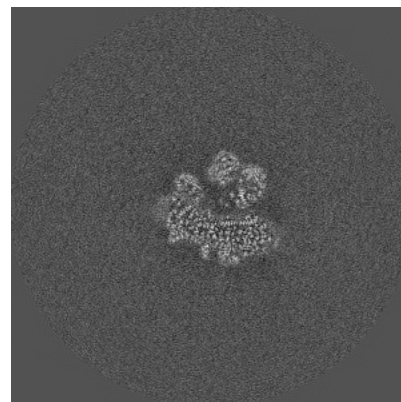
6.3.1 Primary map



X Index: 285

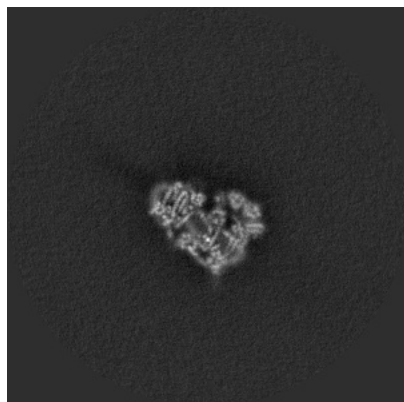


Y Index: 268

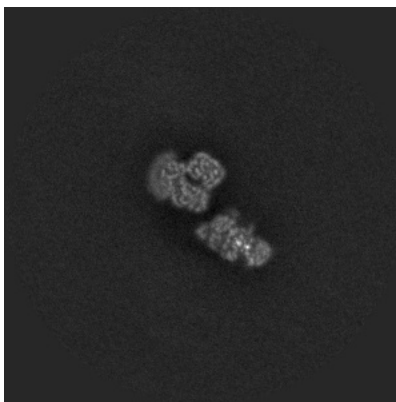


Z Index: 253

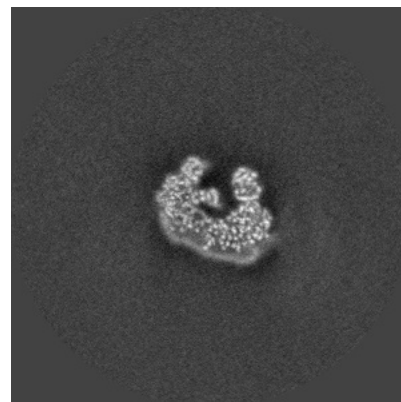
6.3.2 Raw map



X Index: 285



Y Index: 296

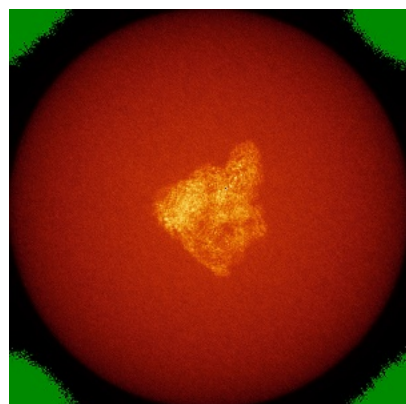


Z Index: 272

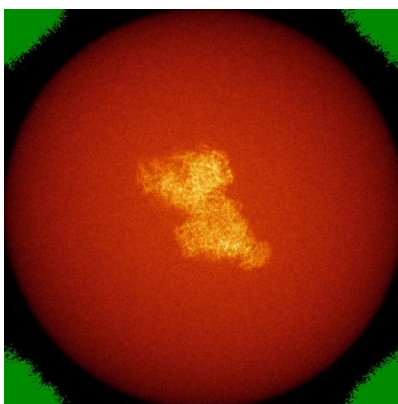
The images above show the largest variance slices of the map in three orthogonal directions.

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

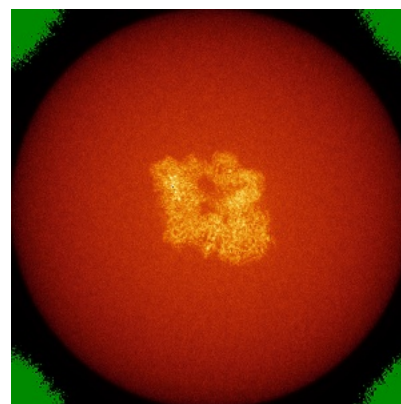
6.4.1 Primary map



X

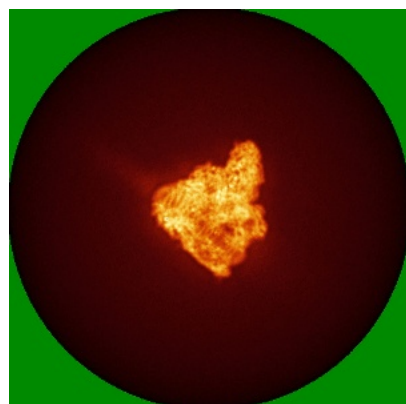


Y

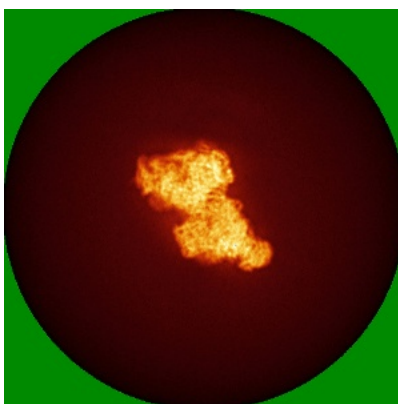


Z

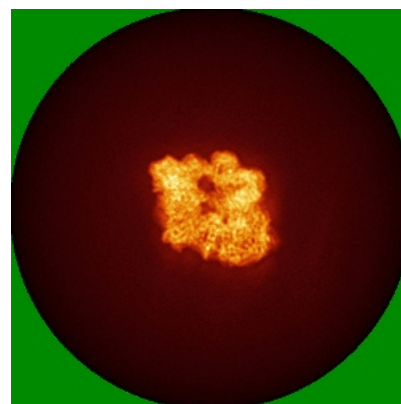
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



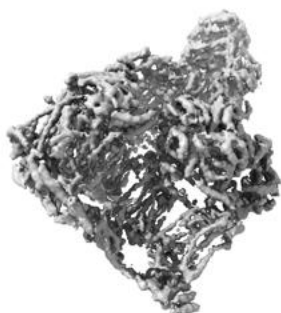
Y



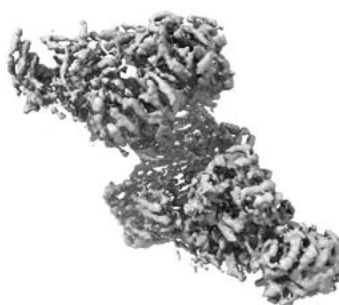
Z

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

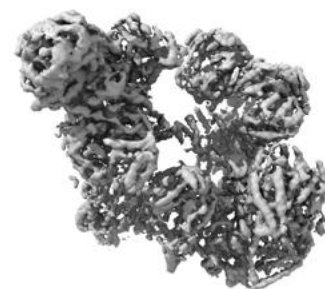
6.5.2 Raw map



X



Y



Z

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

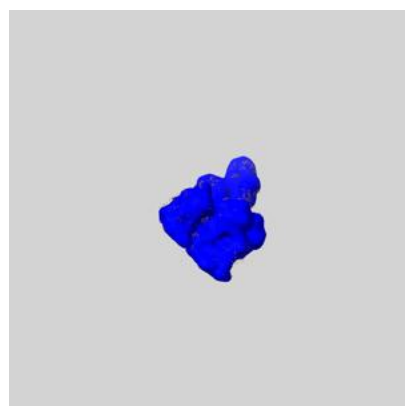
6.6 Mask visualisation [i](#)

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

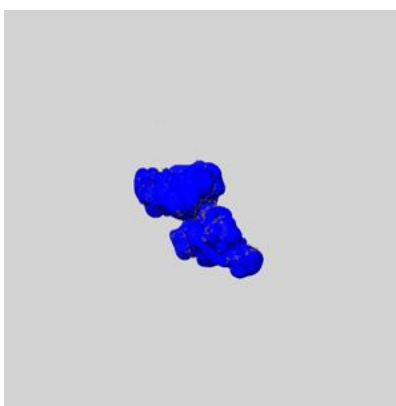
A mask typically either:

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

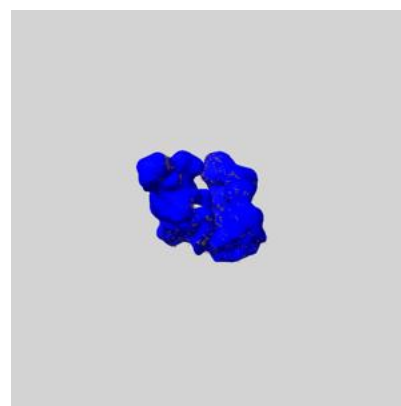
6.6.1 emd_4493_msk_1.map [i](#)



X



Y

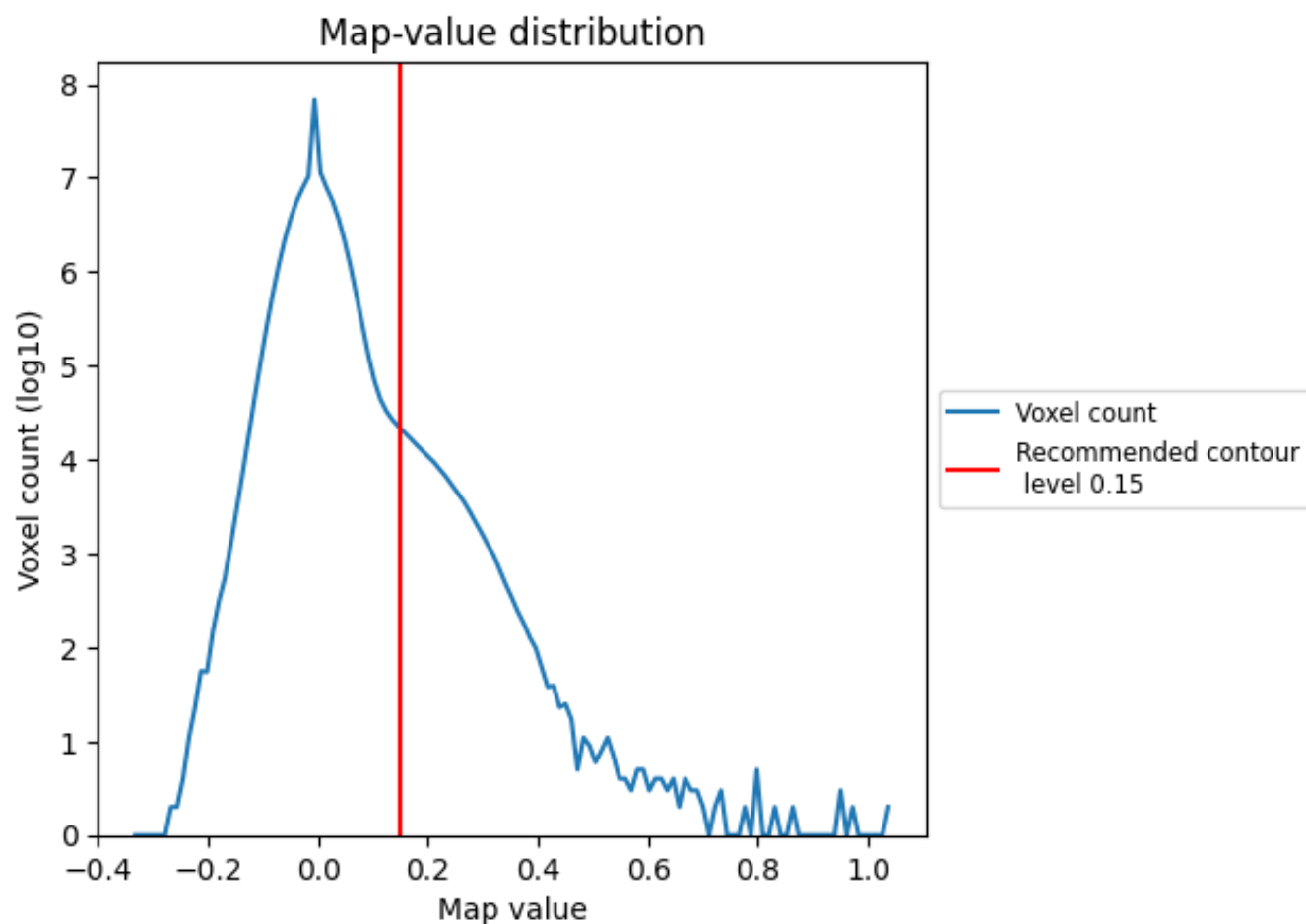


Z

7 Map analysis [i](#)

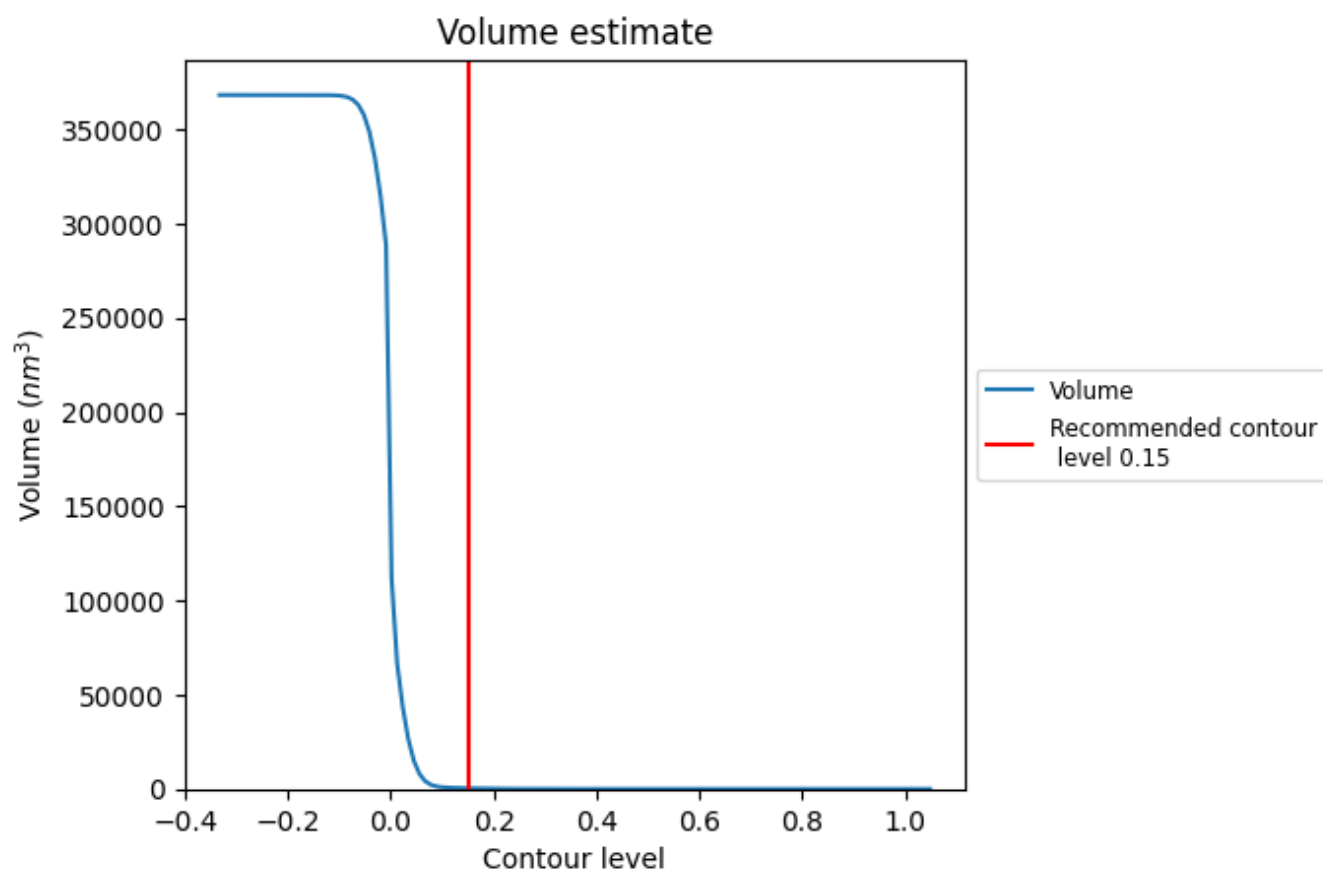
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

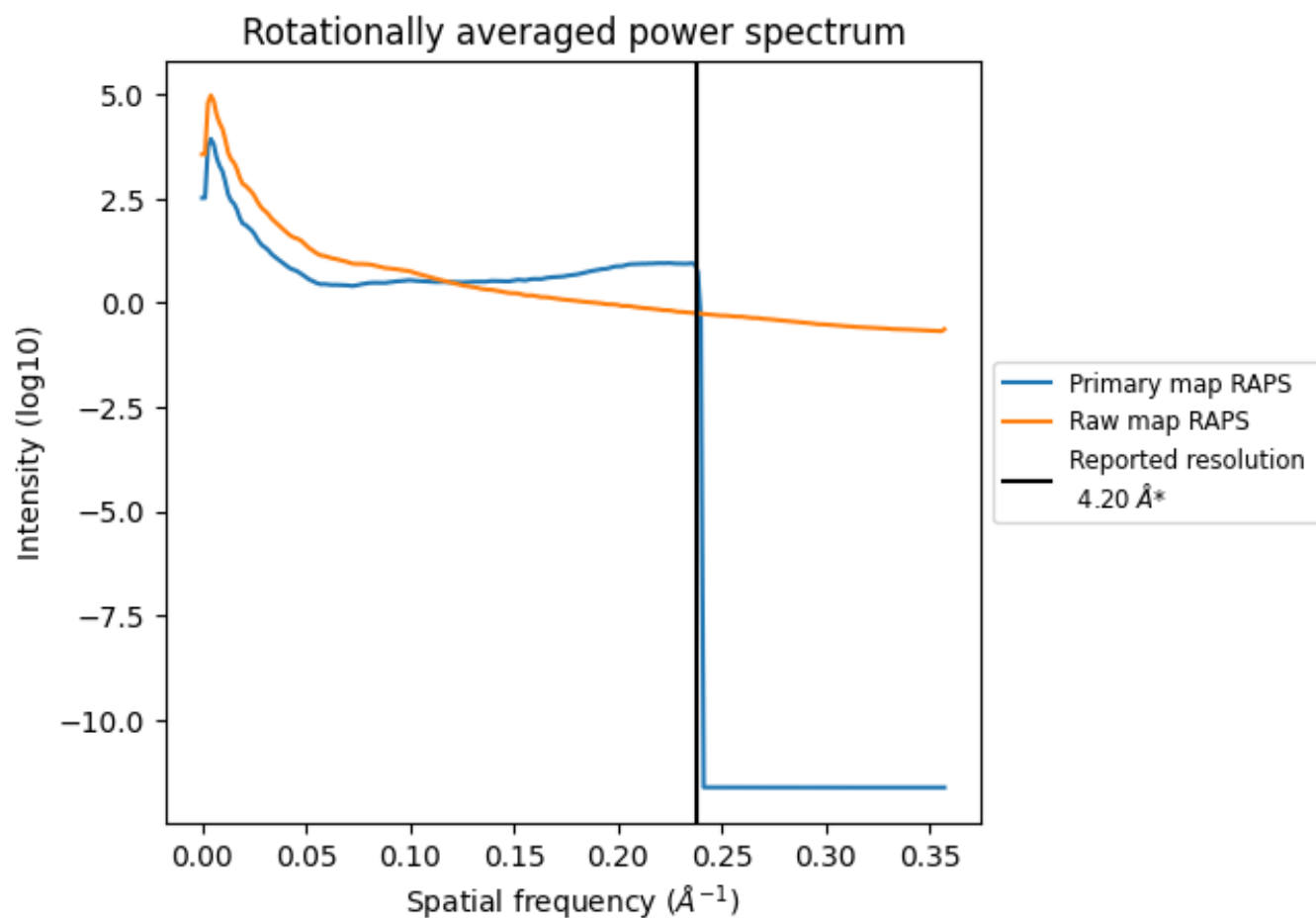
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm^3 ; this corresponds to an approximate mass of 339 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

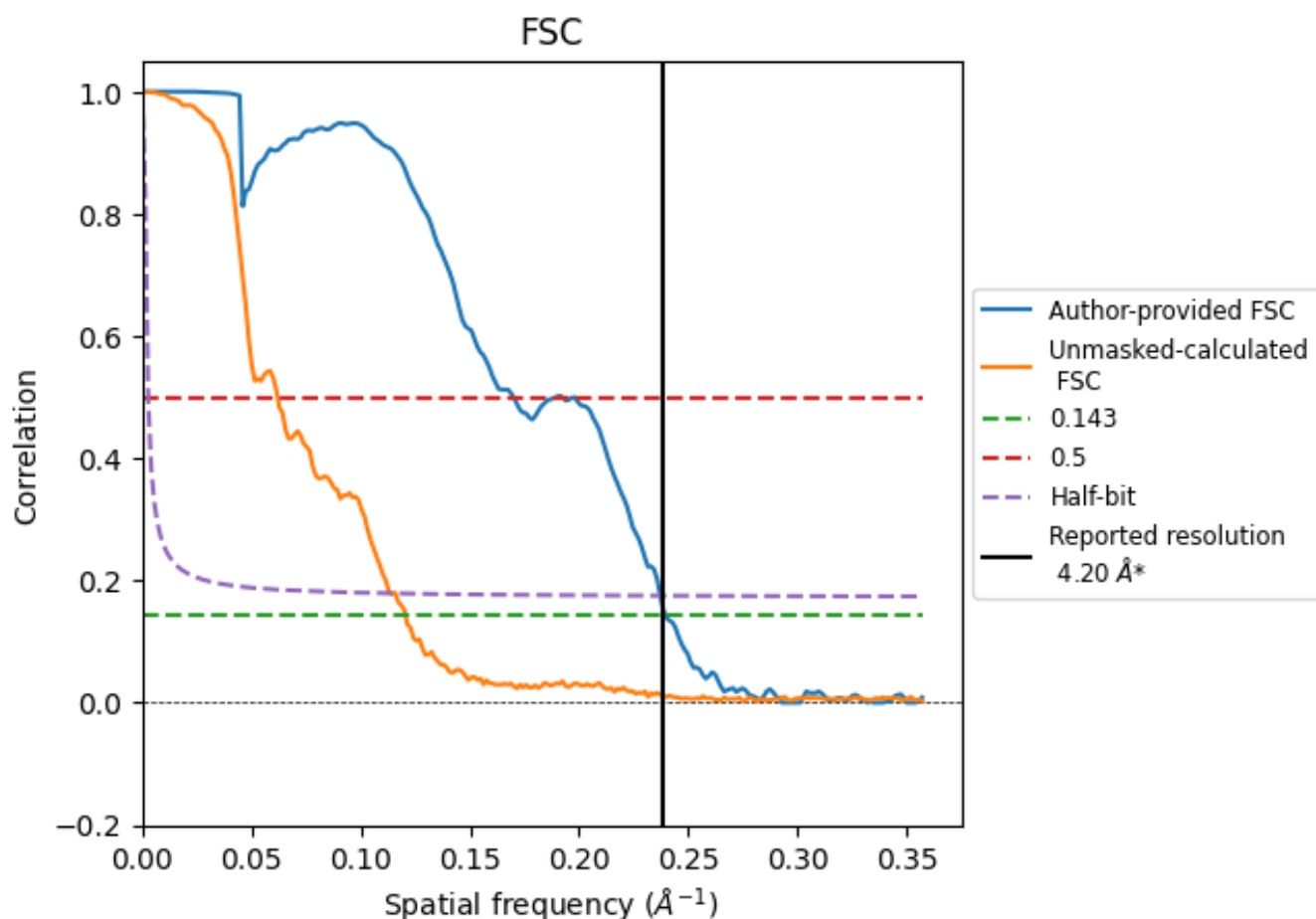


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

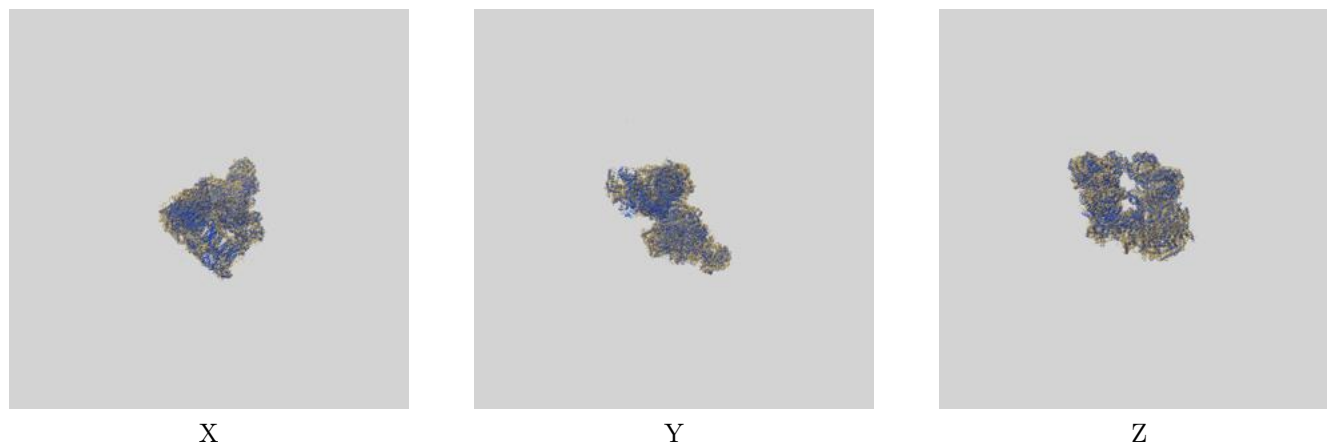
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	5.88	4.22
Unmasked-calculated*	8.30	16.13	8.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.30 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

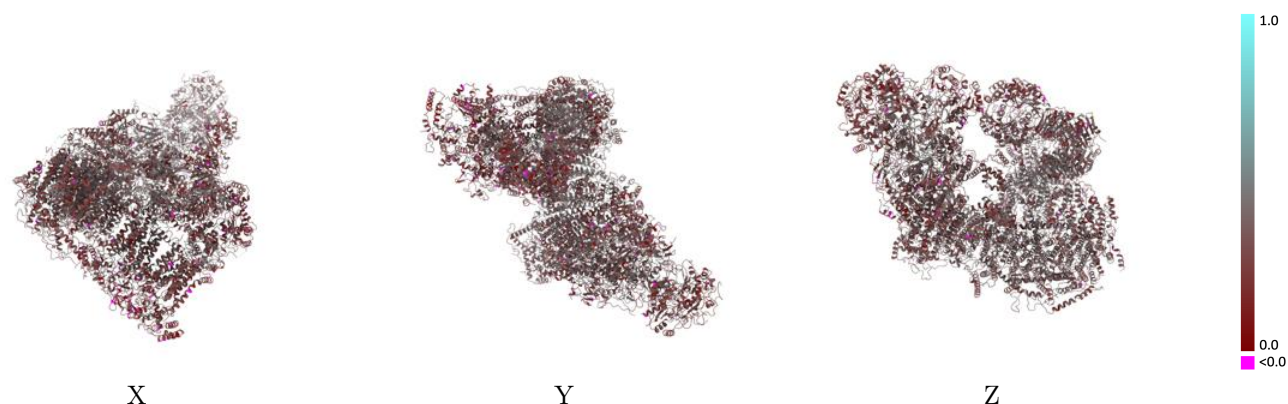
This section contains information regarding the fit between EMDB map EMD-4493 and PDB model 6QBX. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



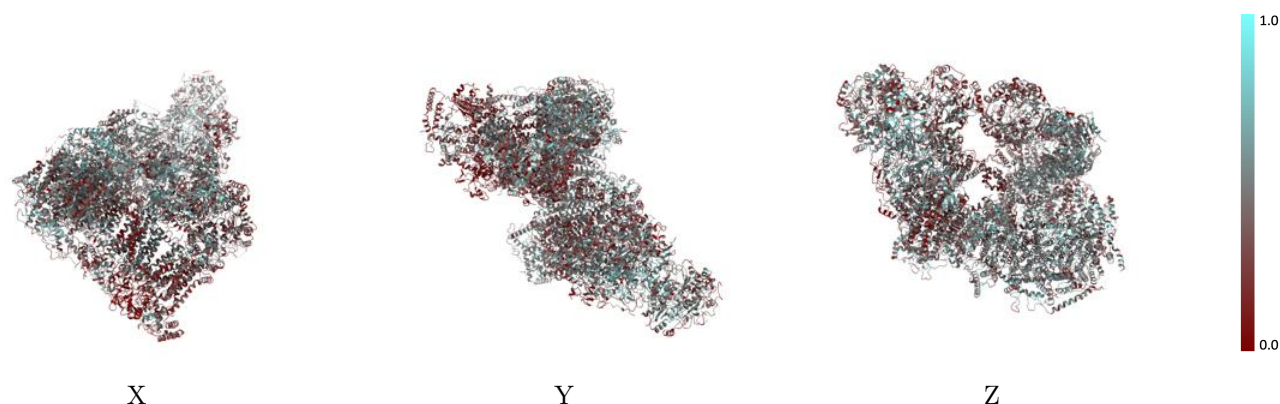
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



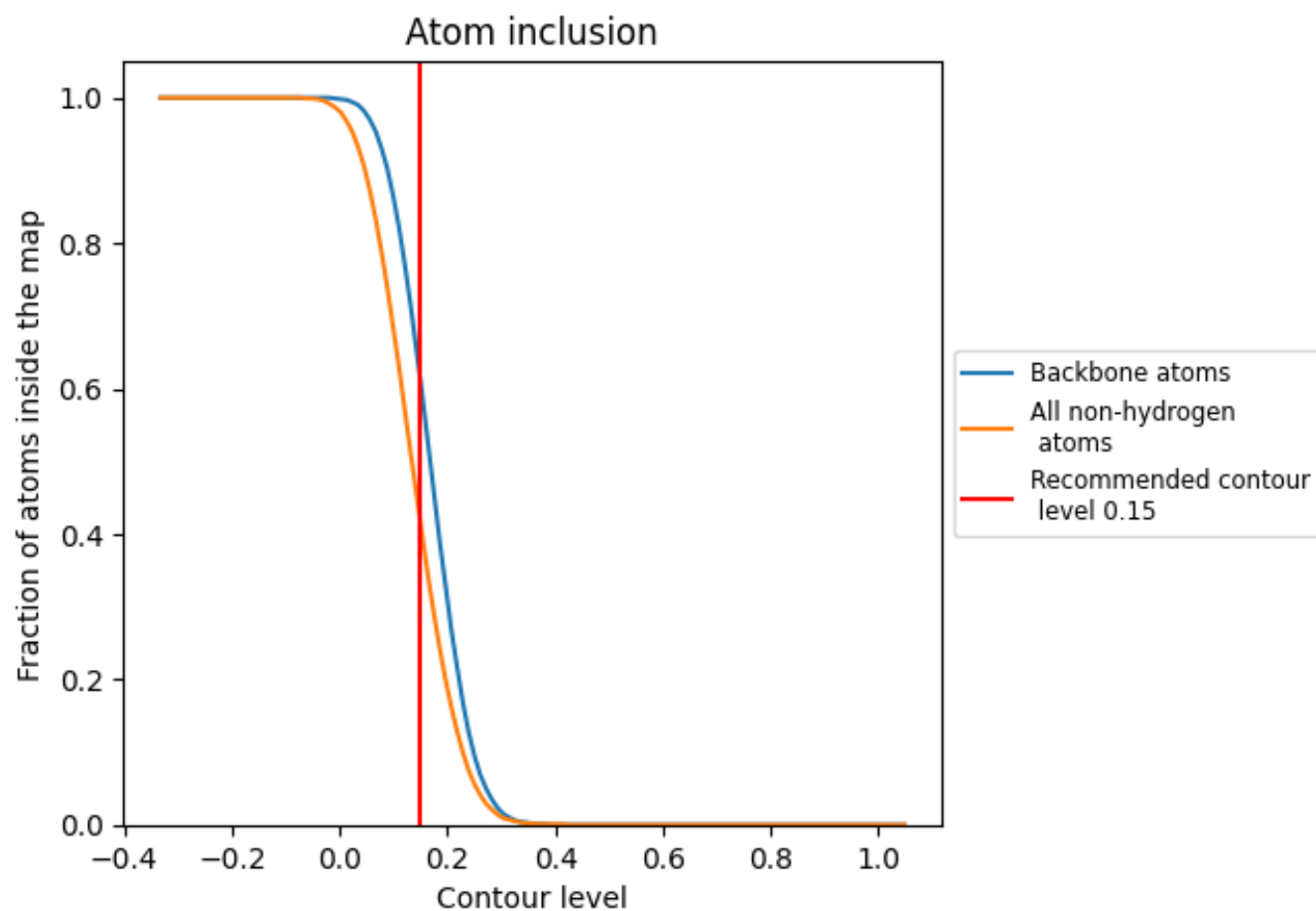
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.4150	 0.3360
4L	 0.3940	 0.3590
A1	 0.4710	 0.3330
A2	 0.3130	 0.2780
A3	 0.3460	 0.3120
A5	 0.3690	 0.3210
A6	 0.3800	 0.3320
A7	 0.2700	 0.3190
A8	 0.4650	 0.3360
A9	 0.3600	 0.3290
AA	 0.2200	 0.3030
AB	 0.4910	 0.3530
AJ	 0.4870	 0.3520
AK	 0.3740	 0.3480
AL	 0.2680	 0.3110
AM	 0.4490	 0.3210
B1	 0.3990	 0.3530
B2	 0.4180	 0.3390
B3	 0.4310	 0.3280
B4	 0.5210	 0.3750
B5	 0.5340	 0.3630
B6	 0.4670	 0.3570
B7	 0.4600	 0.3100
B8	 0.4700	 0.3630
B9	 0.5570	 0.3660
BJ	 0.5110	 0.3510
BK	 0.4740	 0.3550
C1	 0.4790	 0.3430
C2	 0.4760	 0.3740
D1	 0.3900	 0.3420
D2	 0.4760	 0.3750
D3	 0.3000	 0.3330
D4	 0.4820	 0.3790
D5	 0.4310	 0.3550
D6	 0.3590	 0.3490



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Chain	Atom inclusion	Q-score
S1	 0.4230	 0.3290
S2	 0.4700	 0.3640
S3	 0.4570	 0.3600
S4	 0.4310	 0.3760
S5	 0.4810	 0.3670
S6	 0.4420	 0.3660
S7	 0.5160	 0.3850
S8	 0.5120	 0.3620
V1	 0.4370	 0.3020
V2	 0.4110	 0.3010
V3	 0.4260	 0.3080
a1	 0.3600	 0.2930
a2	 0.3340	 0.2930
a3	 0.5000	 0.3690
a4	 0.4570	 0.3370
b1	 0.3720	 0.3270
b2	 0.4570	 0.3590
c1	 0.3530	 0.2920
c2	 0.4200	 0.3360
d1	 0.4090	 0.3150
d2	 0.4110	 0.3570
f1	 0.0740	 0.2430
f2	 0.1120	 0.2470
h1	 0.2310	 0.2220
h2	 0.3020	 0.2410
i1	 0.2240	 0.2760
i2	 0.2520	 0.2980
q1	 0.2820	 0.2790
q2	 0.4590	 0.4030
x1	 0.3250	 0.3620
x2	 0.3460	 0.4180