



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:25 PM UTC

PDB ID : 6QC3 / pdb_00006qc3
EMDB ID : EMD-4495
Title : Ovine respiratory supercomplex I+III2 open class 1
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-26
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:

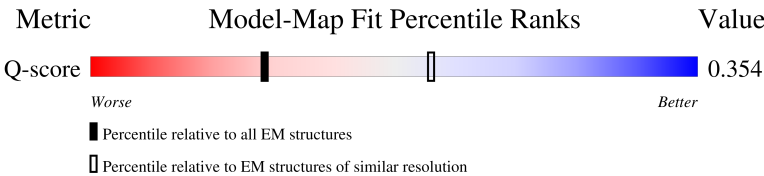
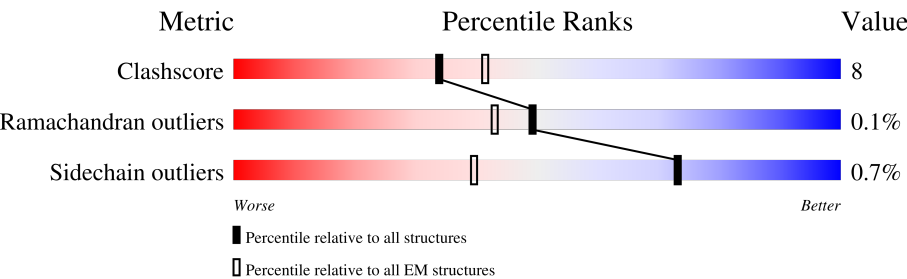
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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	52% 79% 19% ..
1	a3	446	29% 83% 17%
2	a2	439	53% 78% 16% 6%
2	a4	439	36% 71% 22% 6%

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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	26	
9	x2	26	
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	D3	115	
29	D1	318	
30	D6	175	
31	4L	98	
32	D5	606	
33	D4	459	
34	D2	347	
35	AK	140	
36	B5	143	
37	A8	171	
38	BJ	175	
39	AJ	320	
40	S5	105	
41	A3	83	
42	B3	97	
43	C2	120	

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Mol	Chain	Length	Quality of chain
44	B4	128	
45	AM	143	
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 65 unique types of molecules in this entry. The entry contains 96897 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called UQCRC1.

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c1	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 UQCRB.

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

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

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

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

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

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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 NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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 NDUF11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S2	424	Total	C	N	O	S	0	0
			3414	2180	584	625	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 NDUF1.

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

- Molecule 17 is a protein called NDUF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	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 NDUFB6.

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
			1024	646	182	193	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A9	287	Total	C	N	O	S	0	0
			2293	1464	419	405	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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AL	144	Total	C	N	O	S	0	0
			1201	773	215	209	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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D3	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D1	303	Total	C	N	O	S	0	0
			2415	1633	368	395	19		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 36 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 38 is a protein called MT-ND5.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 40 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 45 is a protein called MT-ND1.

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

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B6	96	Total	C	N	O	S	0	0
			815	536	139	139	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	65	Total	C	N	O	S	0	0
			563	372	93	97	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

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

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

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

- # HEM

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

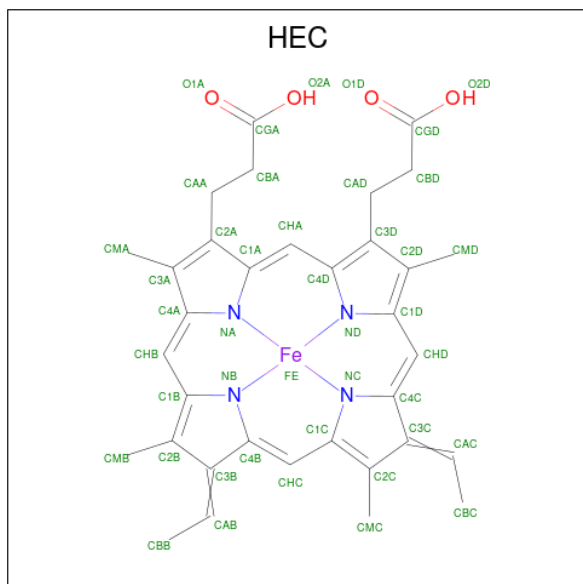


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PROTEIN DATA BANK

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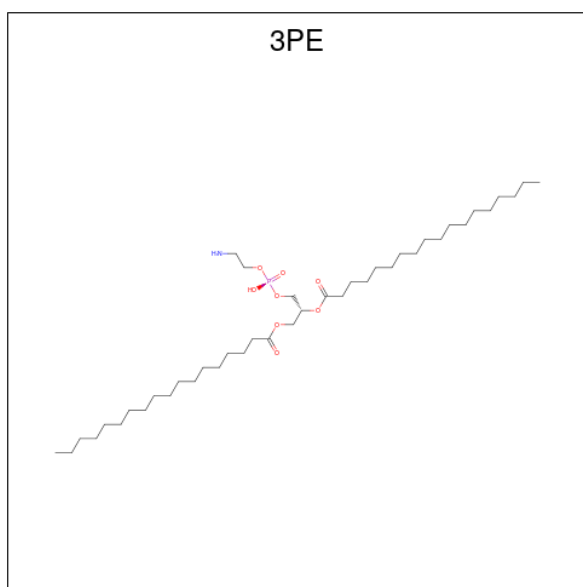
Mol	Chain	Residues	Atoms					AltConf
55	b2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 56 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



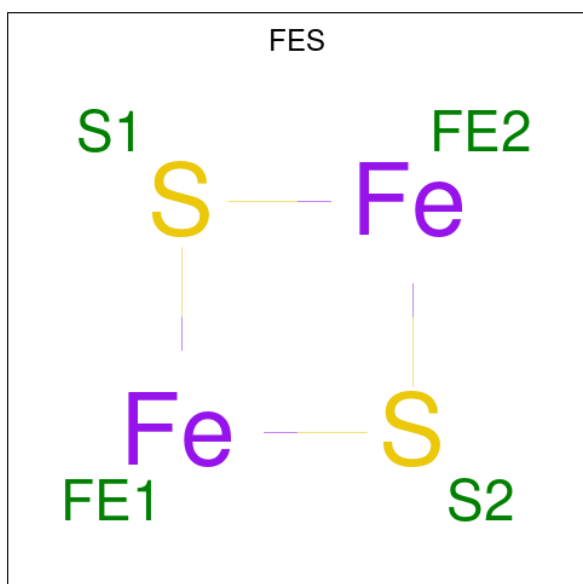
Mol	Chain	Residues	Atoms					AltConf
56	c1	1	Total 43	C 34	Fe 1	N 4	O 4	0
56	c2	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 57 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



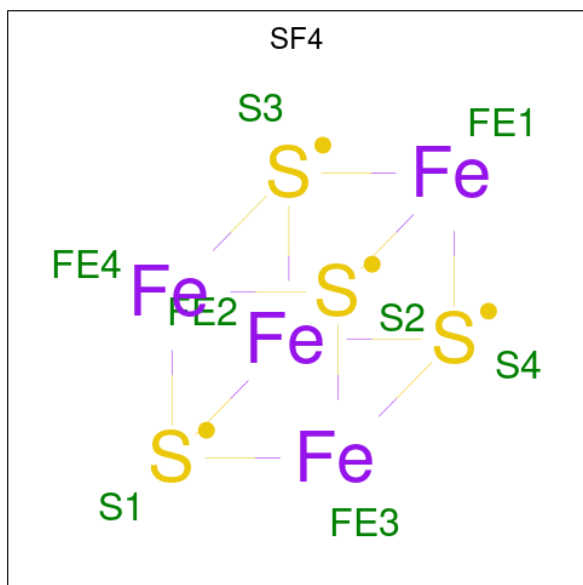
Mol	Chain	Residues	Atoms					AltConf
57	c1	1	Total	C	N	O	P	0
			13	5	1	6	1	
57	f2	1	Total	C	N	O	P	0
			23	13	1	8	1	
57	D1	1	Total	C	N	O	P	0
			26	16	1	8	1	
57	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
57	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 58 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



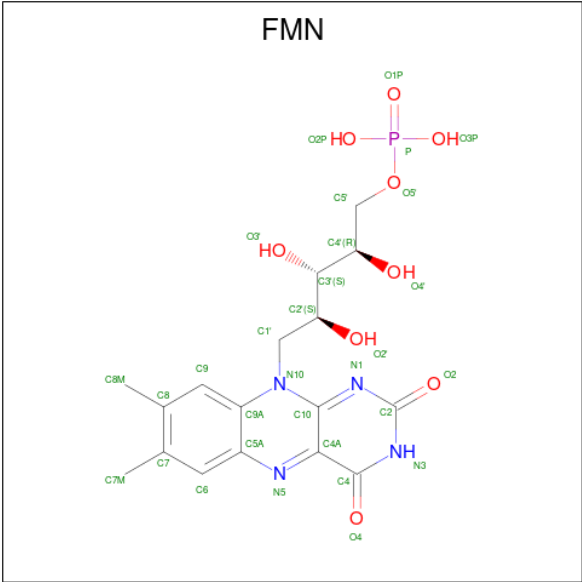
Mol	Chain	Residues	Atoms			AltConf
58	f1	1	Total	Fe	S	0
			4	2	2	
58	f2	1	Total	Fe	S	0
			4	2	2	
58	V2	1	Total	Fe	S	0
			4	2	2	
58	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

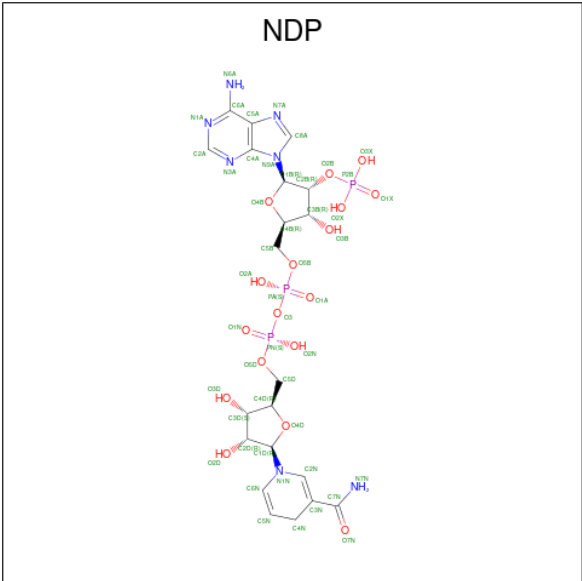


Mol	Chain	Residues	Atoms					AltConf
60	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

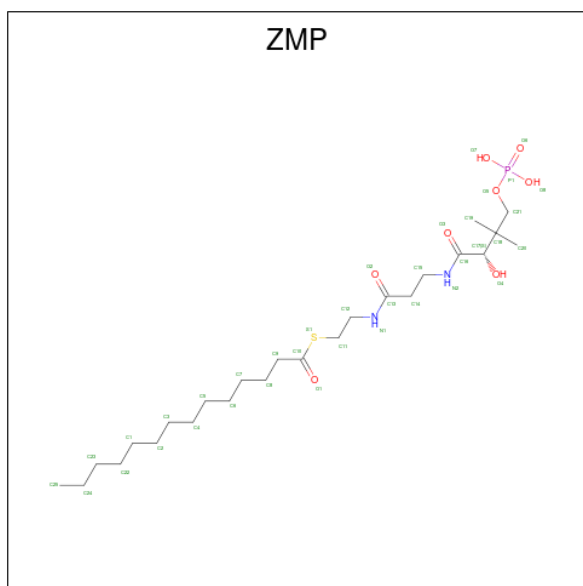
Mol	Chain	Residues	Atoms		AltConf
61	S6	1	Total	Zn	0
			1	1	

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



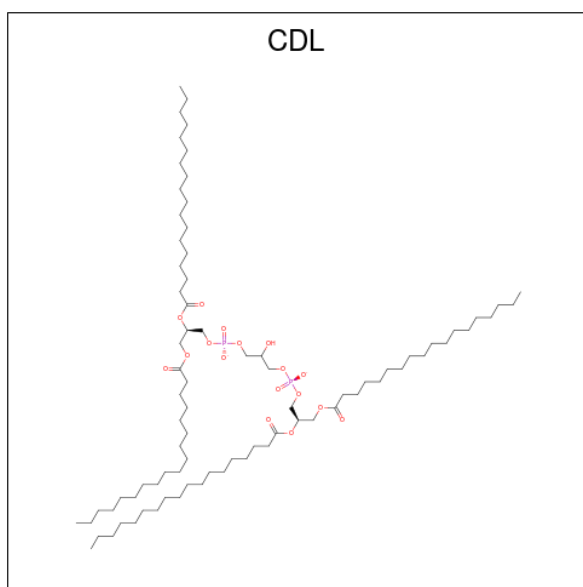
Mol	Chain	Residues	Atoms					AltConf
62	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 63 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



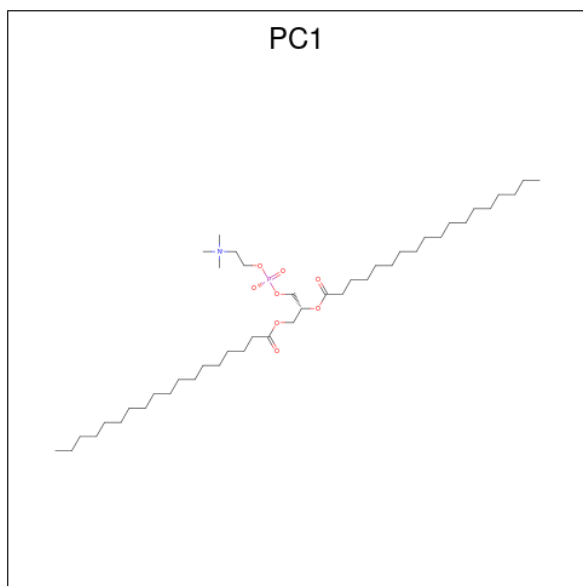
Mol	Chain	Residues	Atoms						AltConf
63	AA	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
63	AB	1	Total 31	C 20	N 2	O 7	P 1	S 1	0

- Molecule 64 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
64	D5	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 65 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).

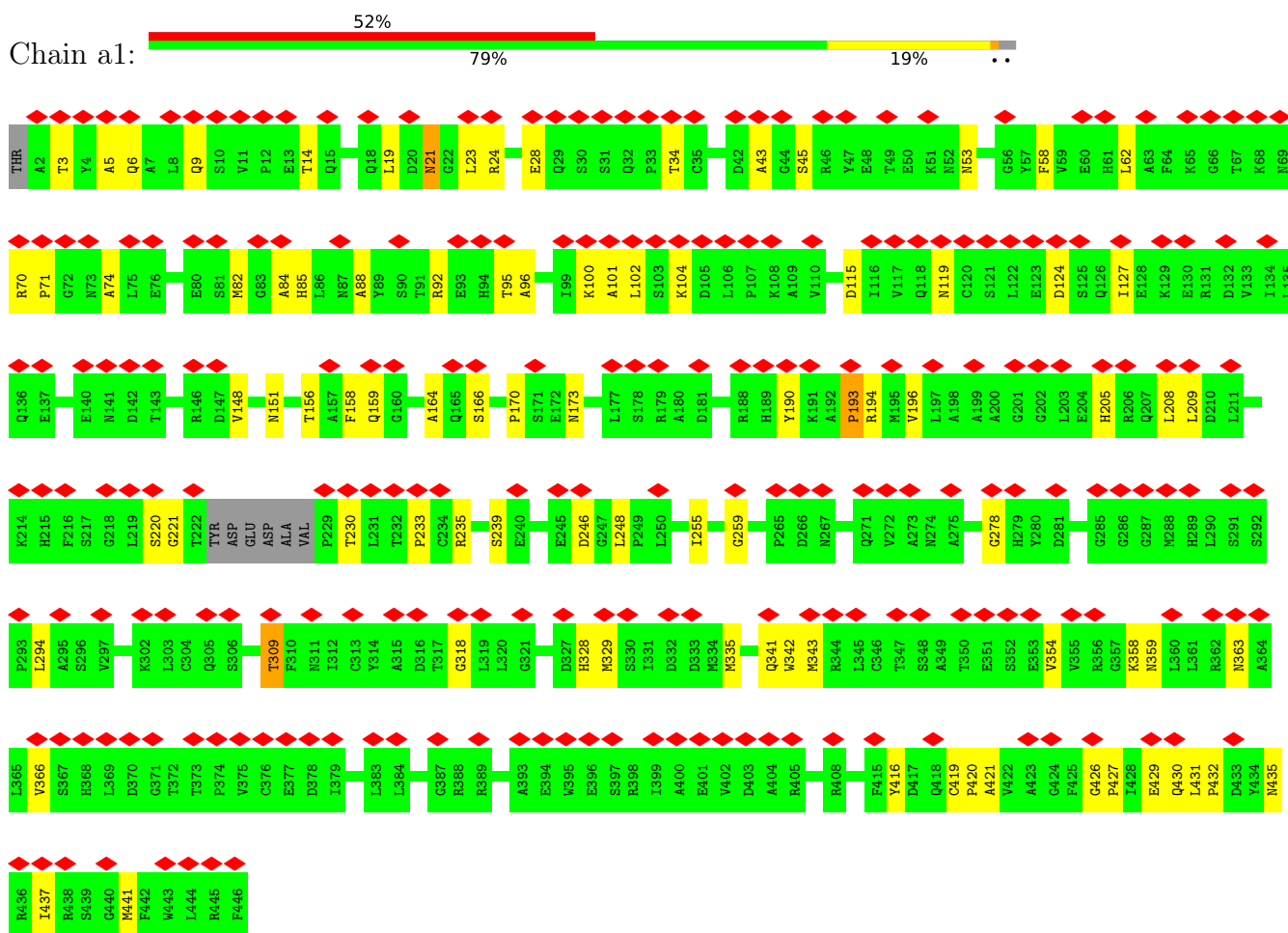


Mol	Chain	Residues	Atoms					AltConf
65	AK	1	Total	C	N	O	P	0
			28	18	1	8	1	

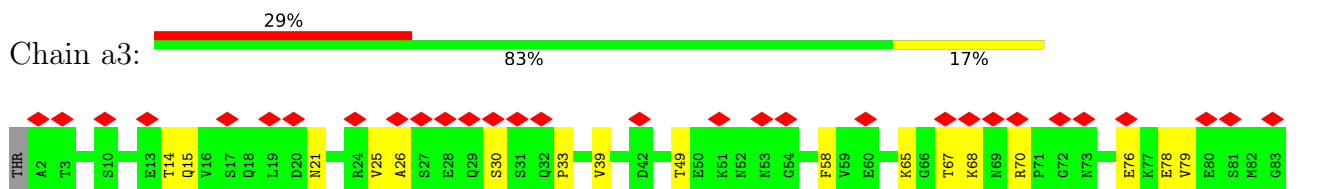
3 Residue-property plots

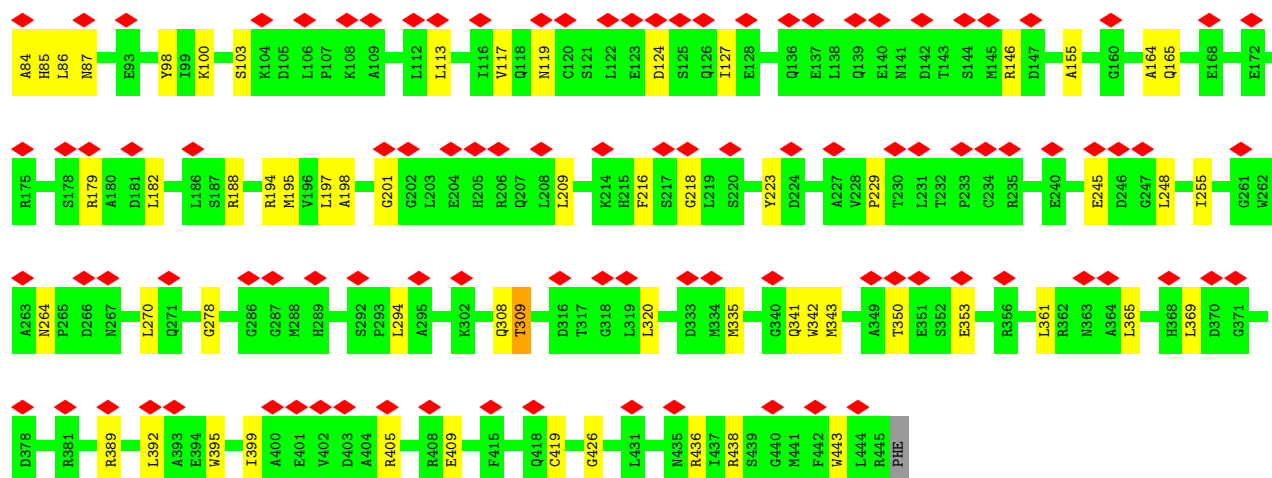
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: UQCRC1

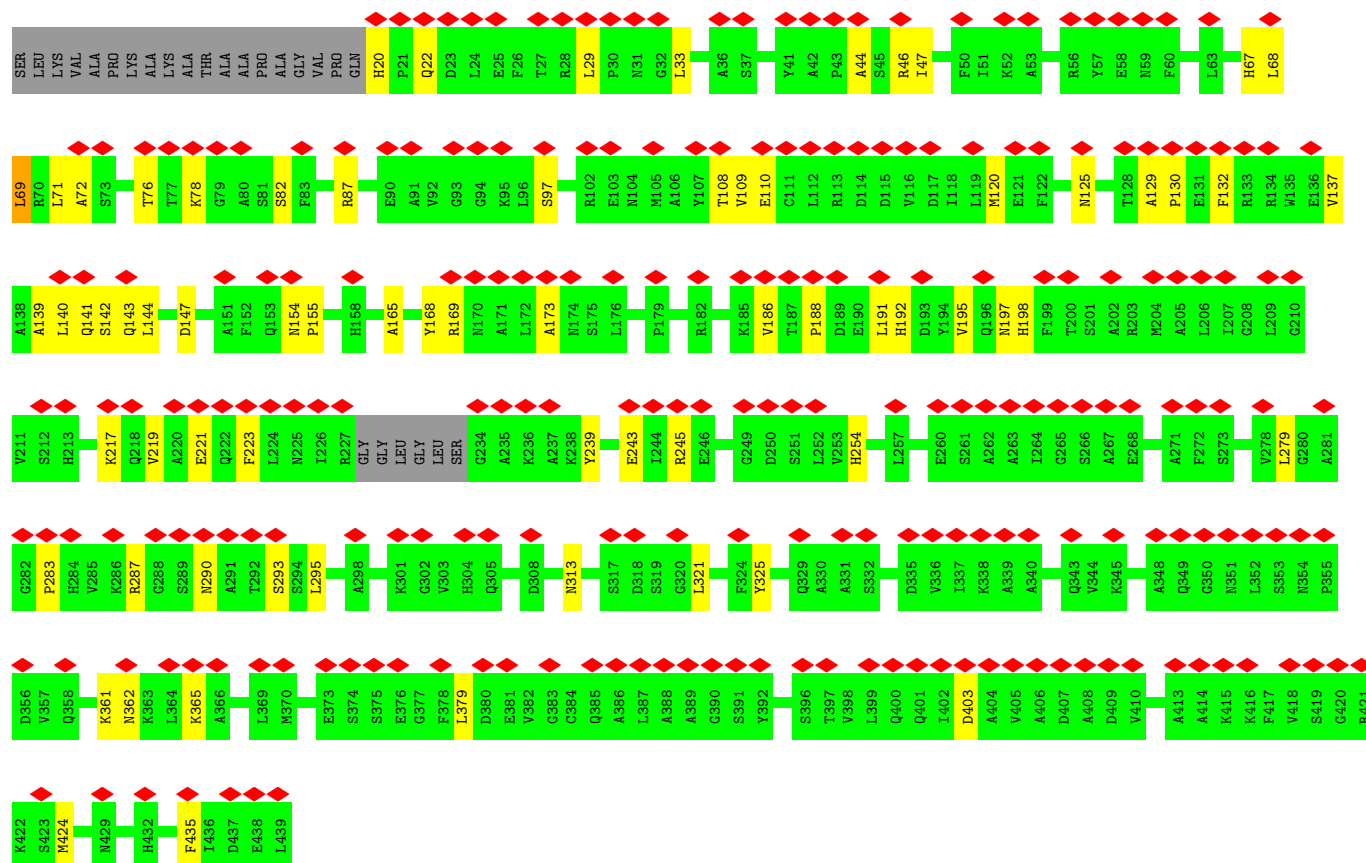
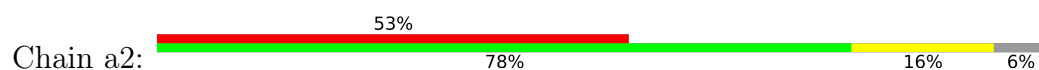


• Molecule 1: UQCRC1

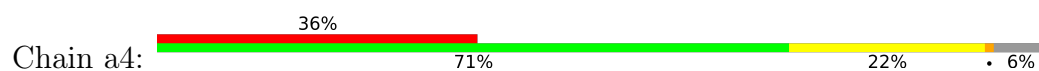


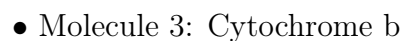


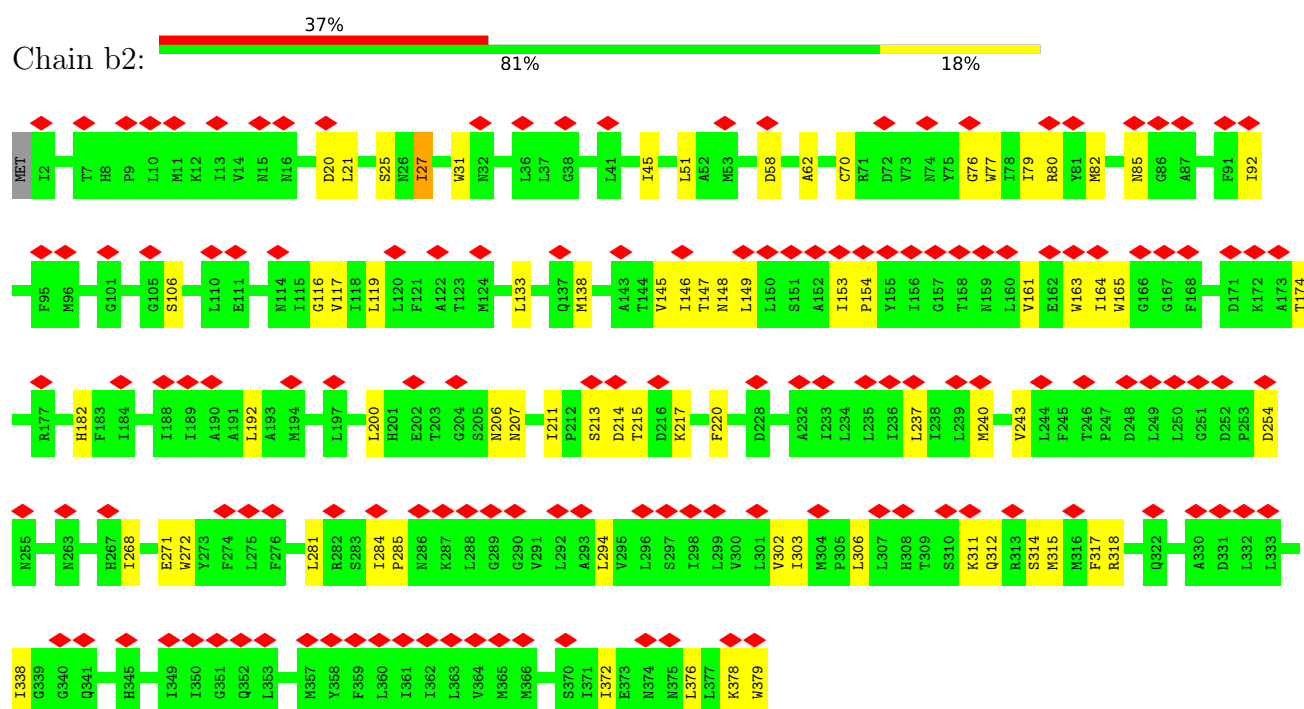
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2



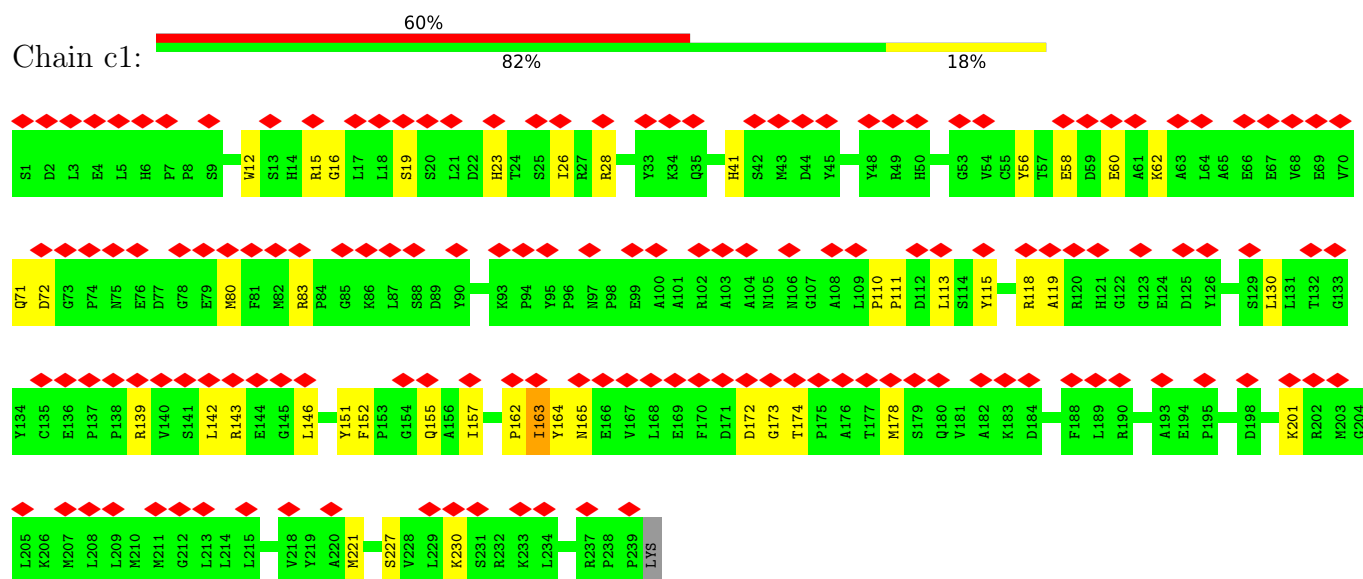
• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2



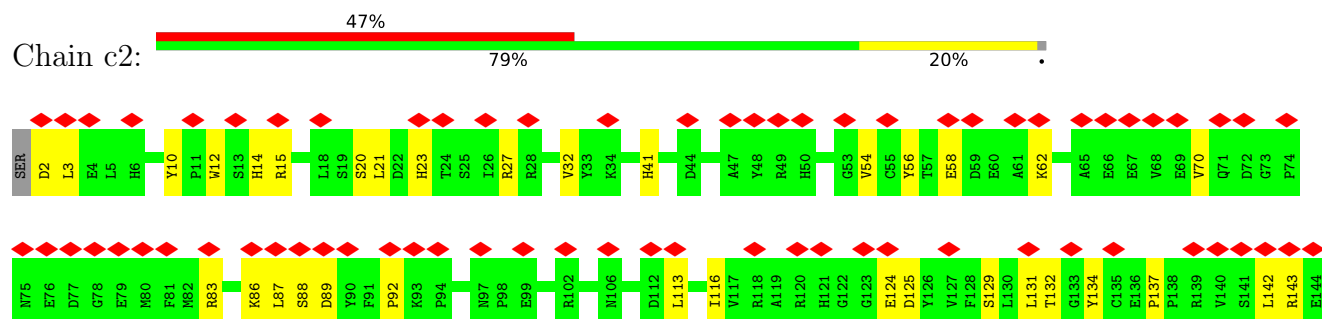


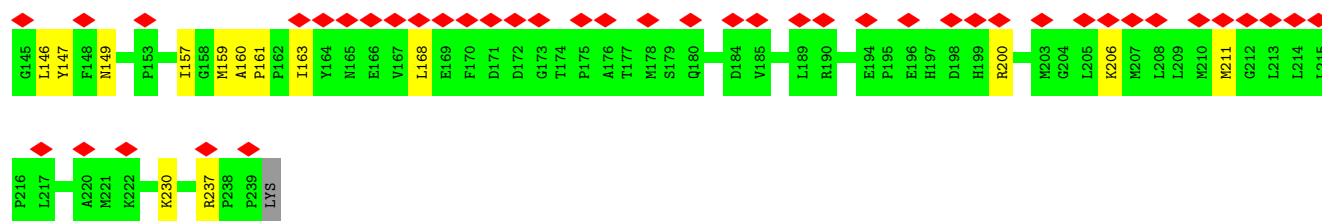


• Molecule 4: Cytochrome c1

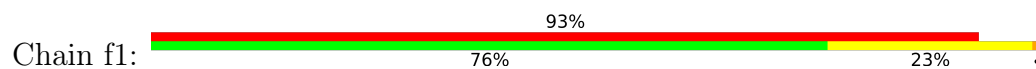


• Molecule 4: Cytochrome c1

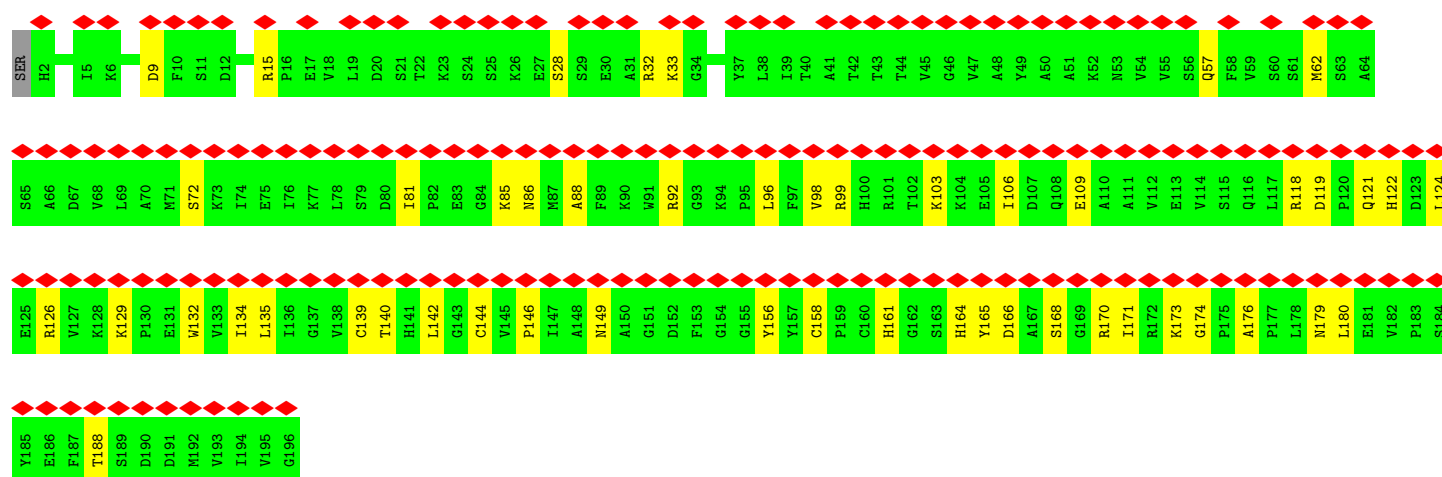
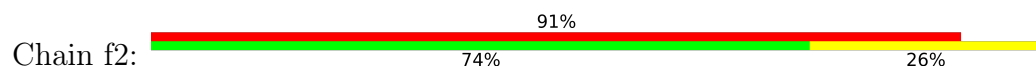




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

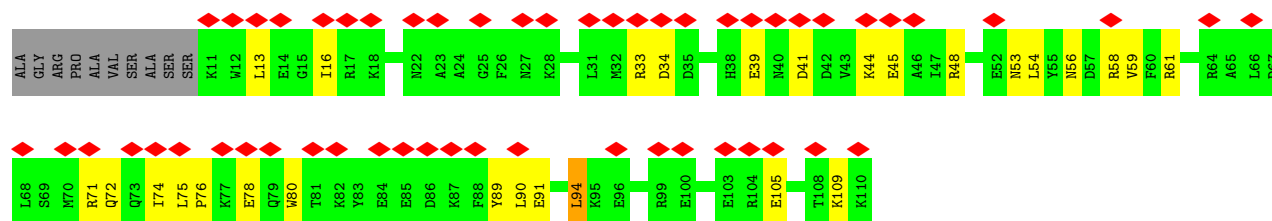


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

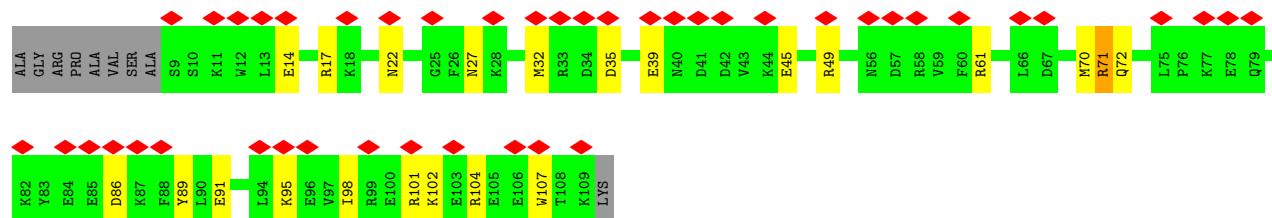
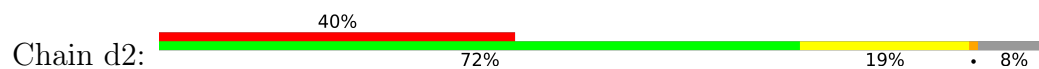


• Molecule 6: UQCRB

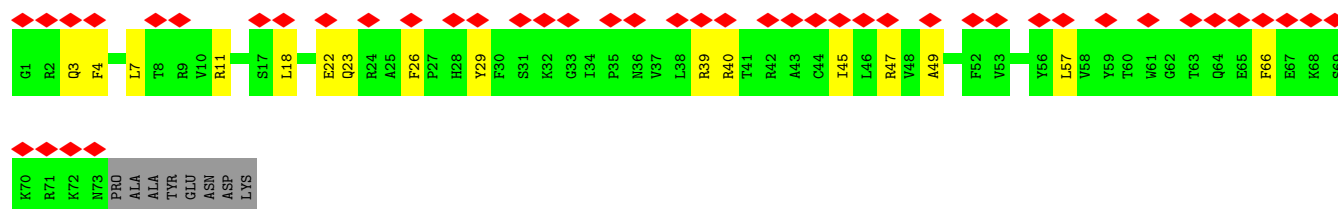
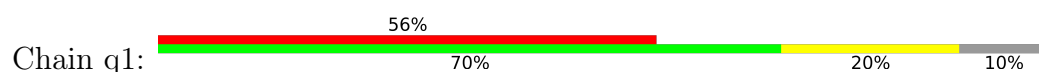




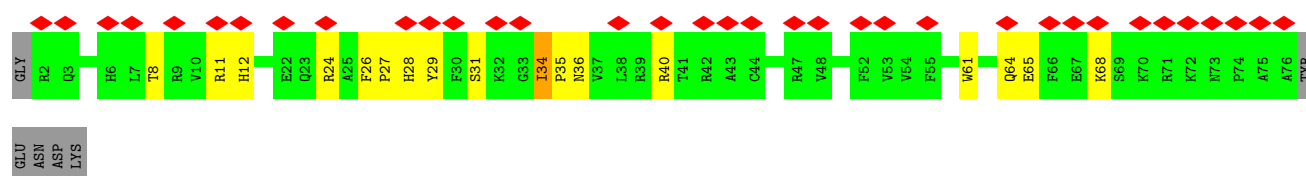
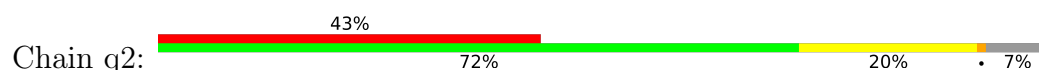
• Molecule 6: UQCRB



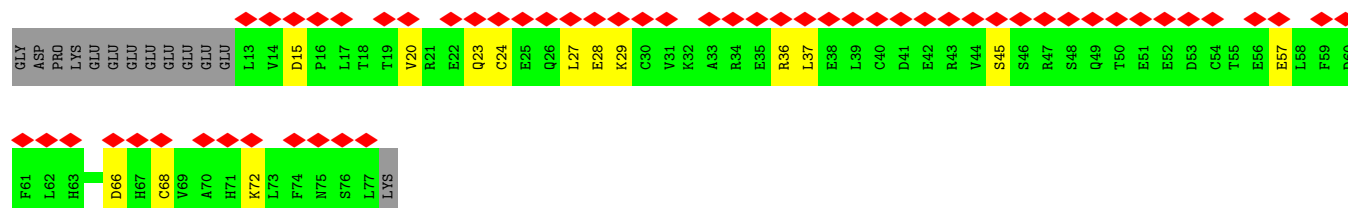
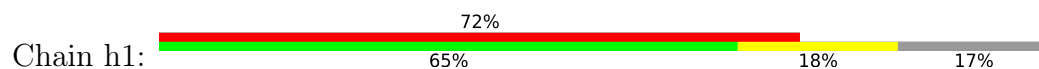
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



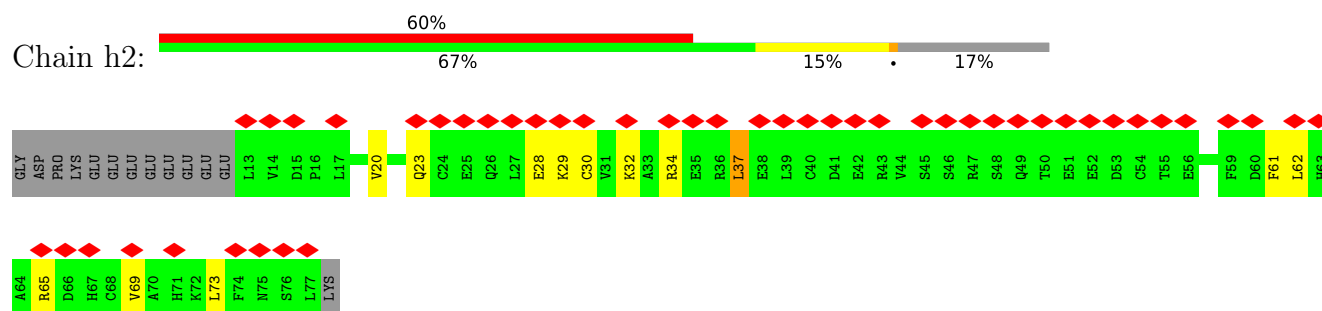
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



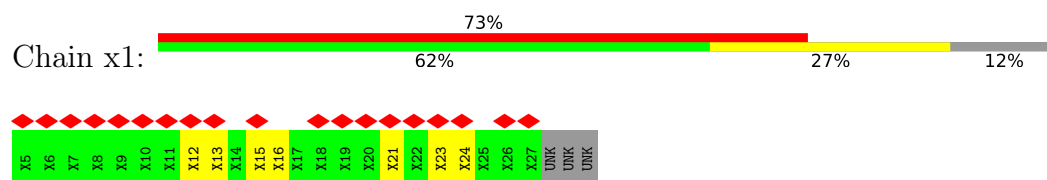
• Molecule 8: Cytochrome b-c1 complex subunit 6



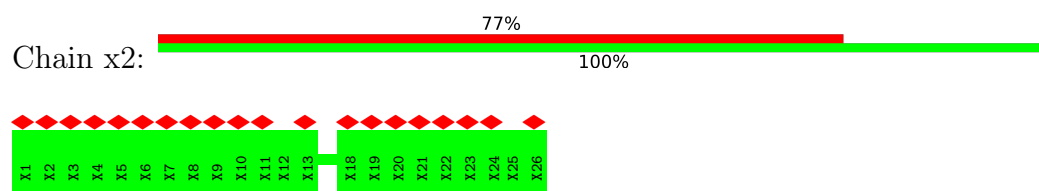
- Molecule 8: Cytochrome b-c1 complex subunit 6



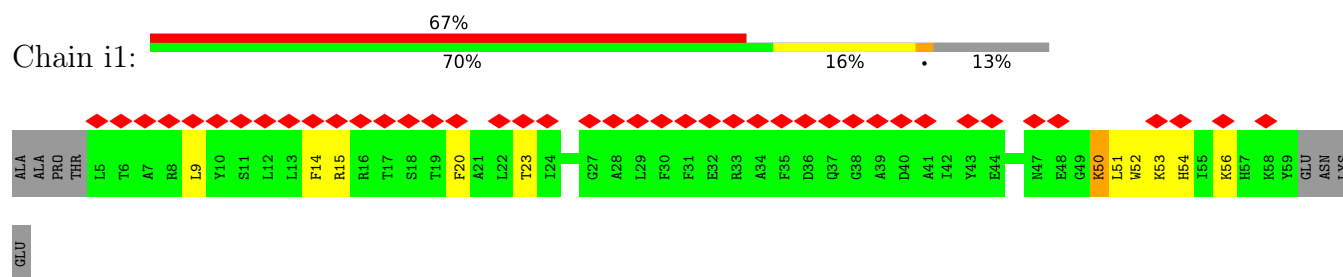
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



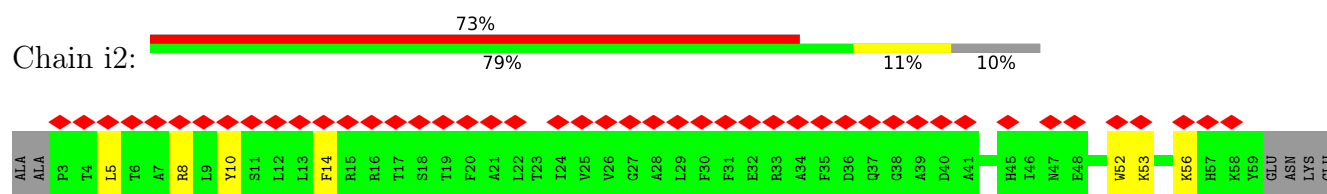
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



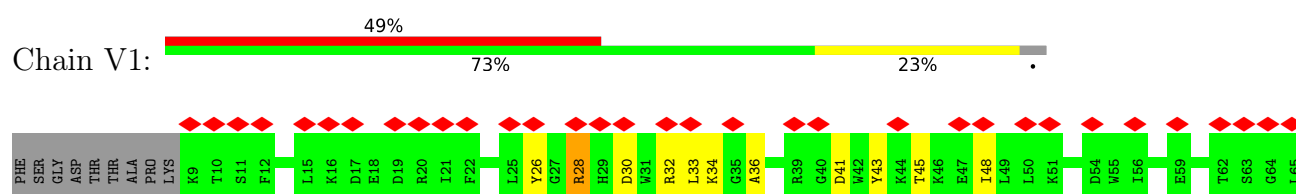
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

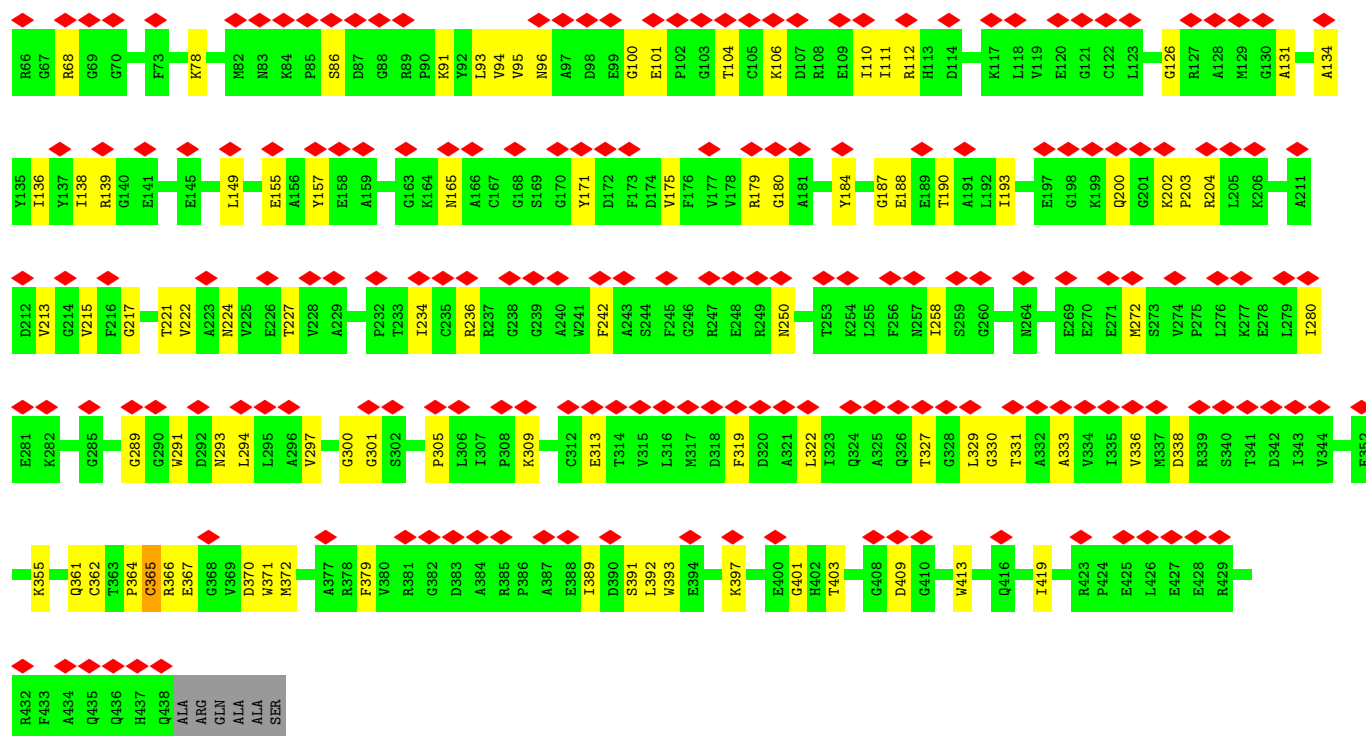


- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

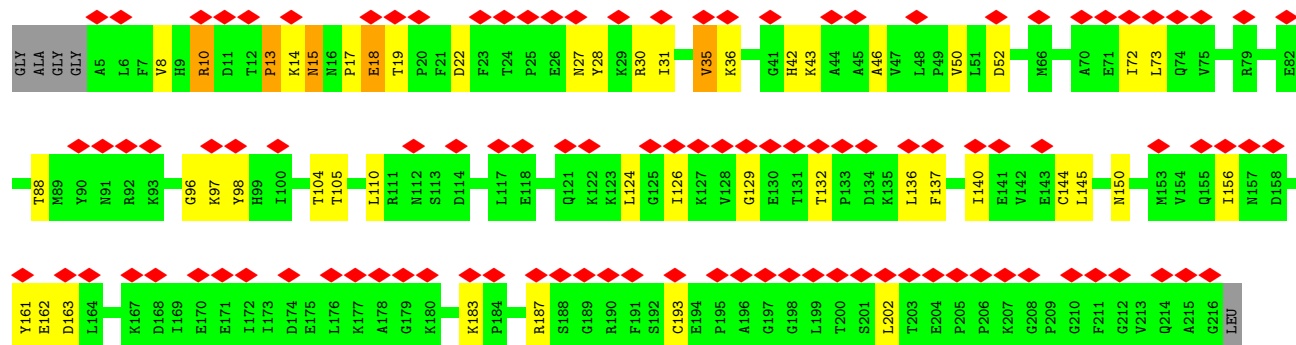
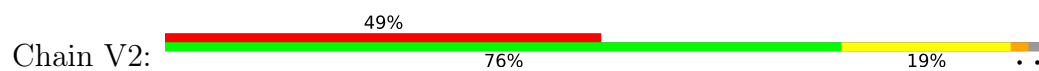


- Molecule 11: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

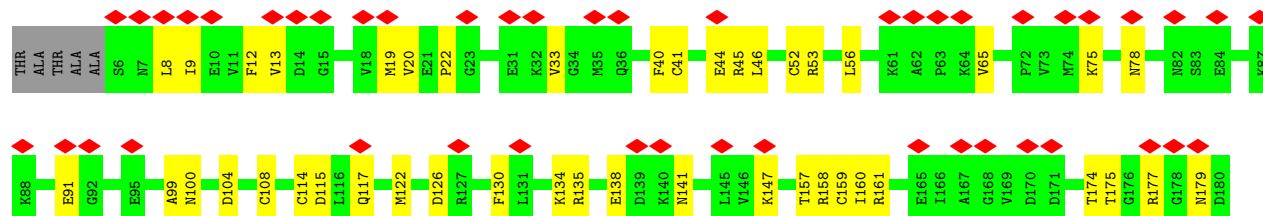
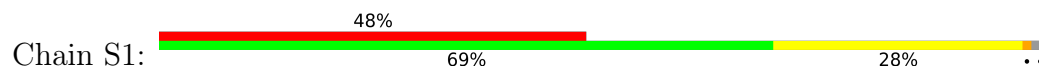


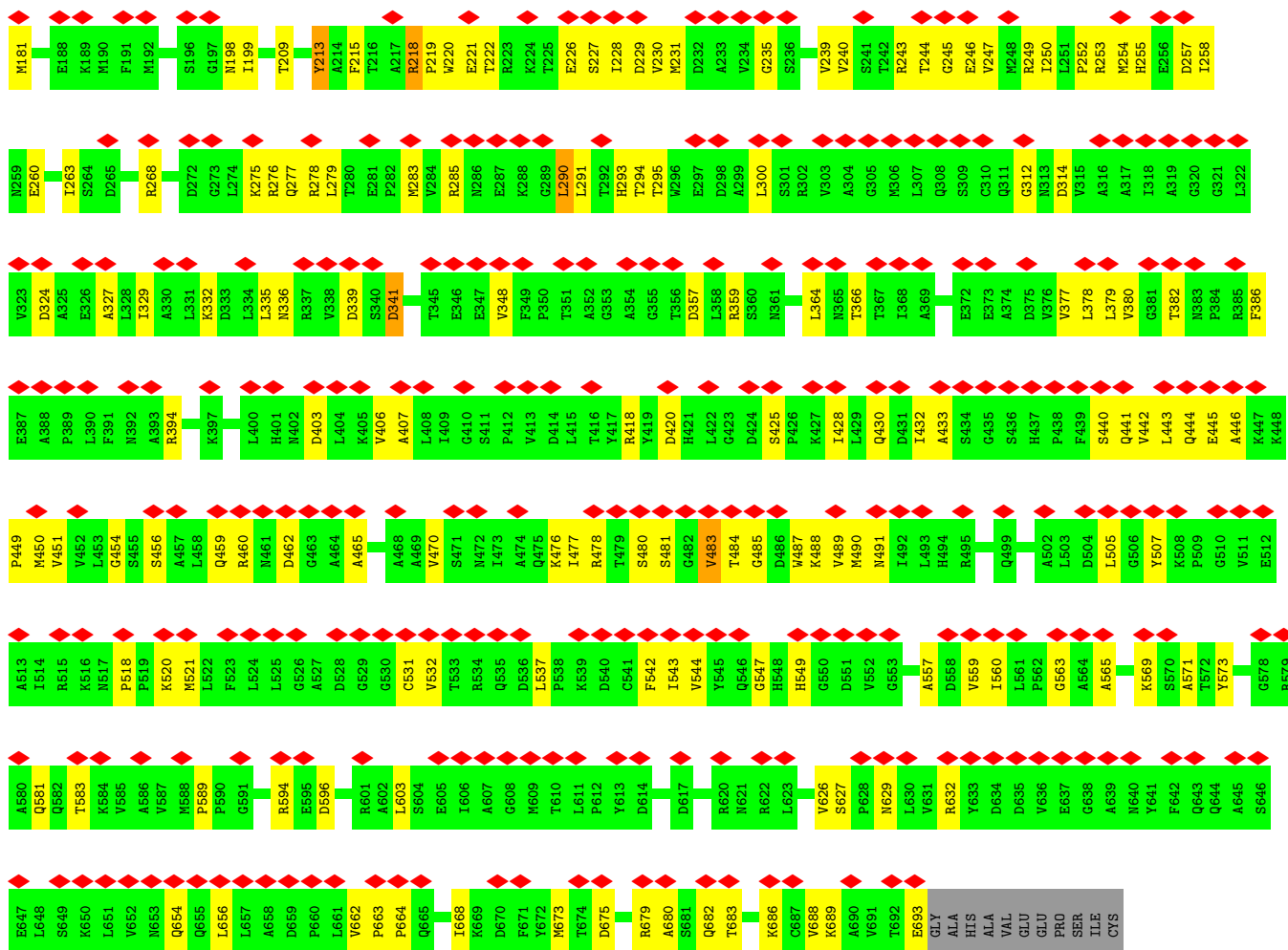


- Molecule 12: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

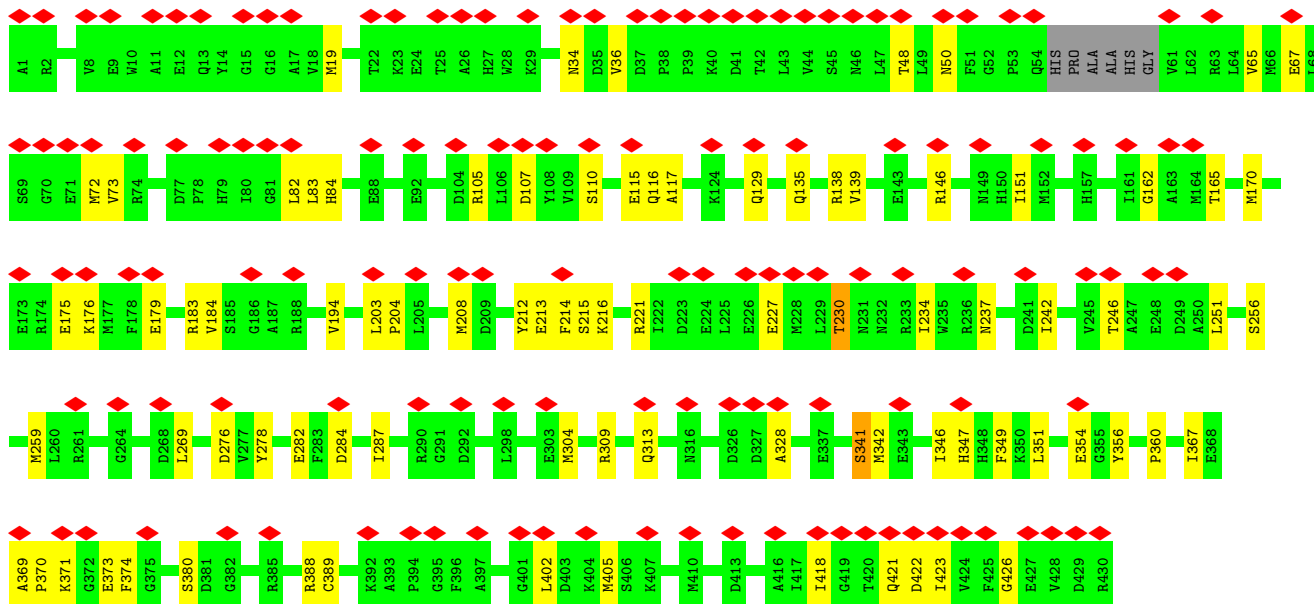
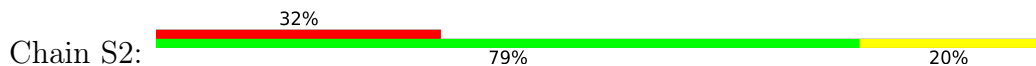


- Molecule 13: NADH:ubiquinone oxidoreductase core subunit S1

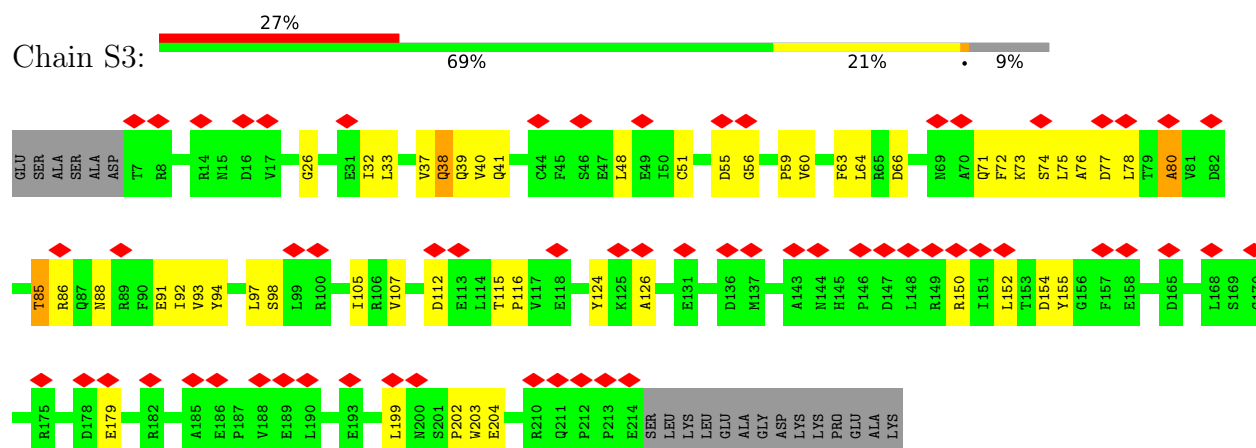




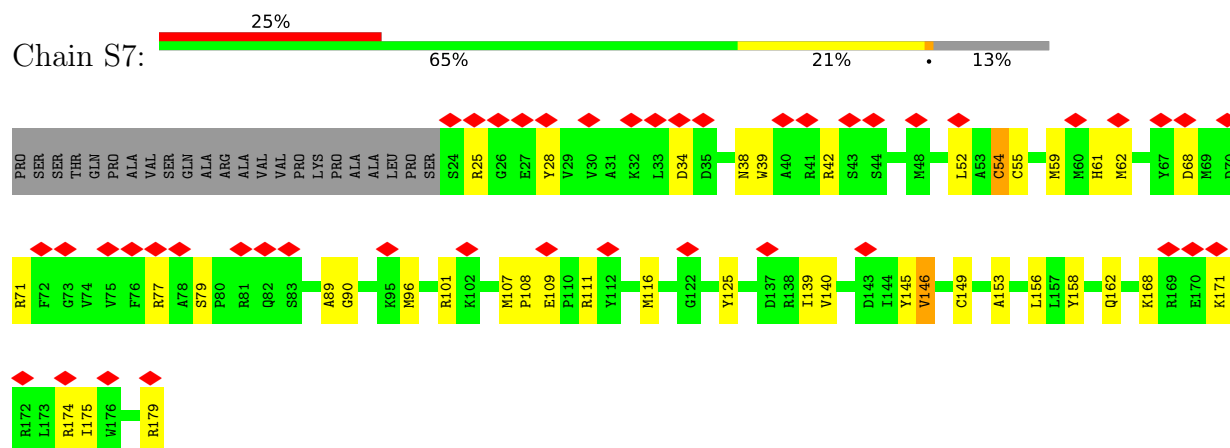
• Molecule 14: NDUFB11



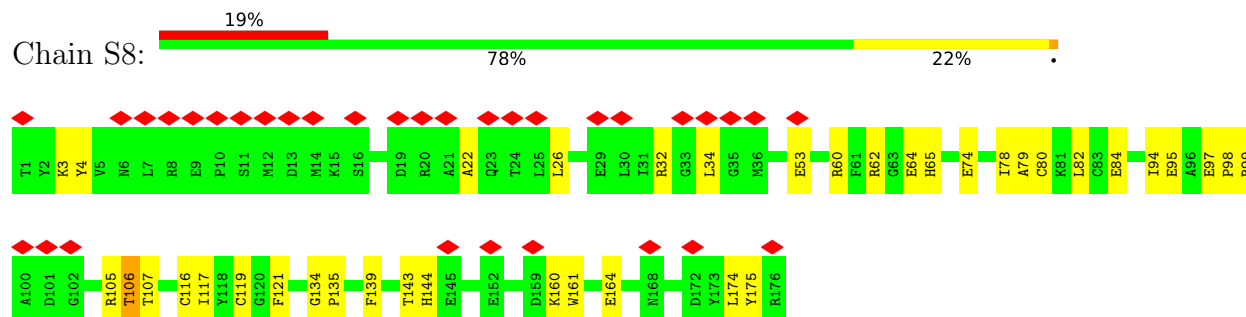
- Molecule 15: NADH:ubiquinone oxidoreductase core subunit S3



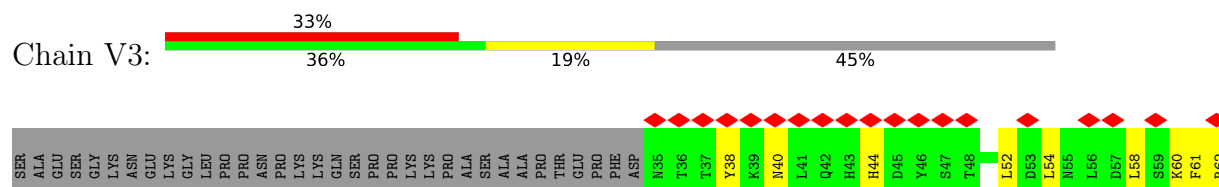
- Molecule 16: NDUFB1

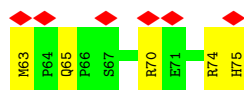


- Molecule 17: NDUFA1

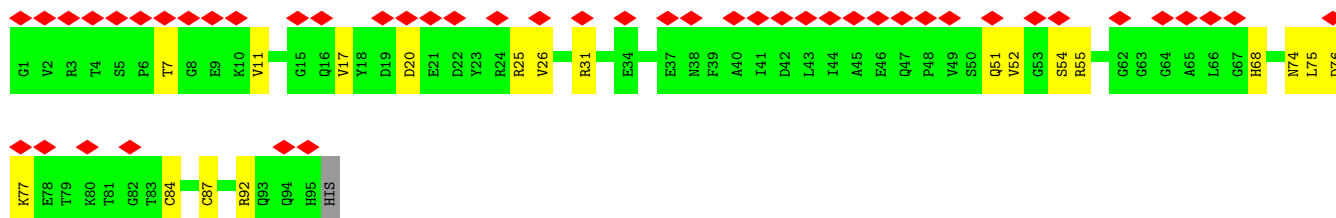
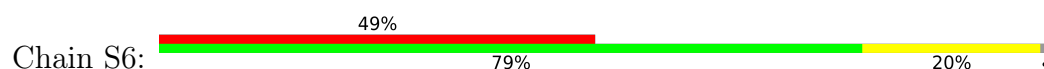


- Molecule 18: NDUFV3

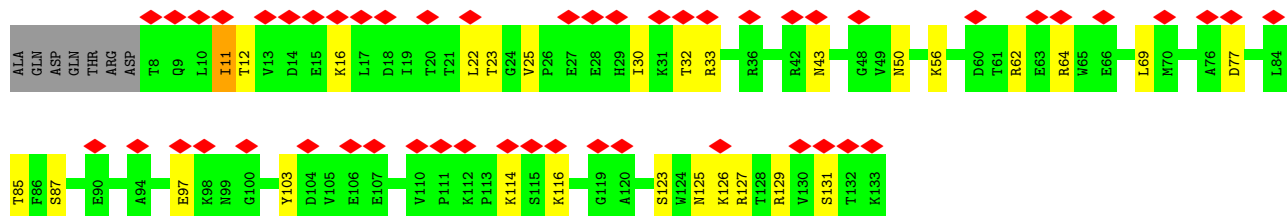
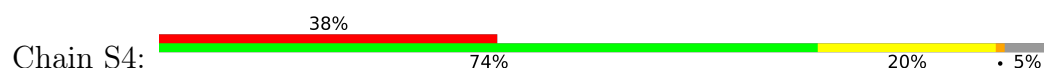




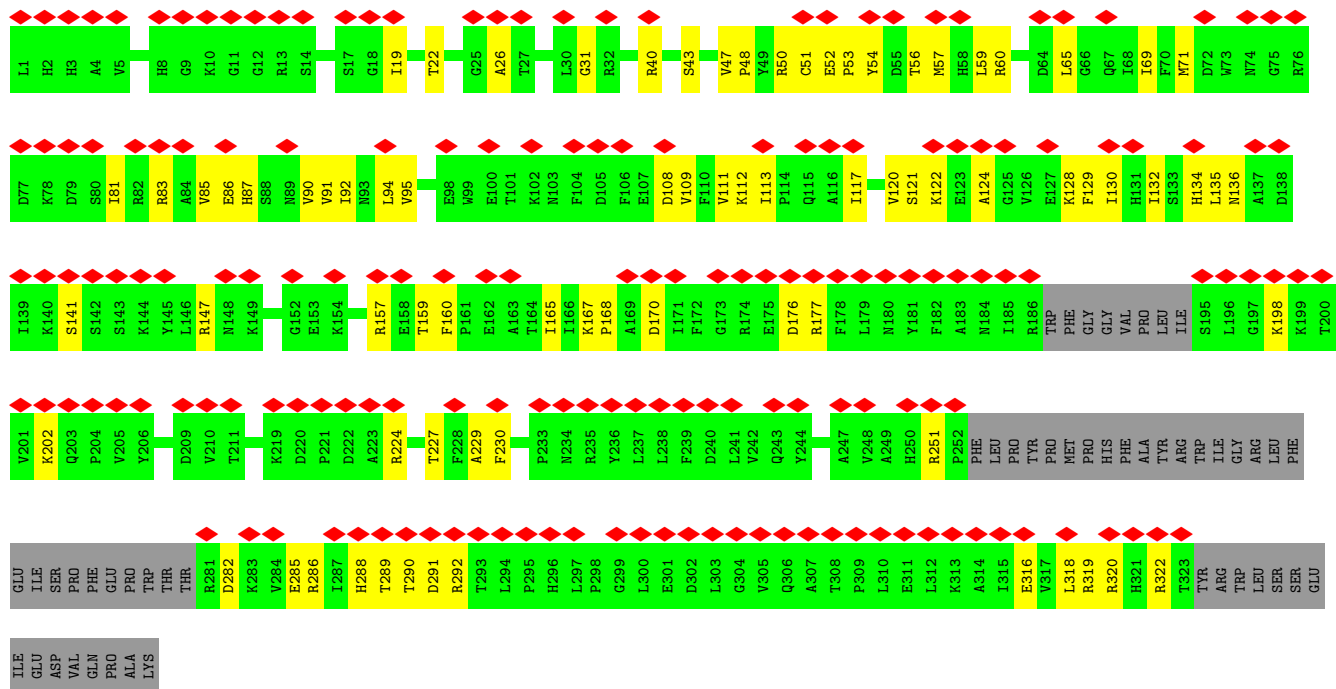
• Molecule 19: NDUFB6



• Molecule 20: NADH:ubiquinone oxidoreductase subunit S4

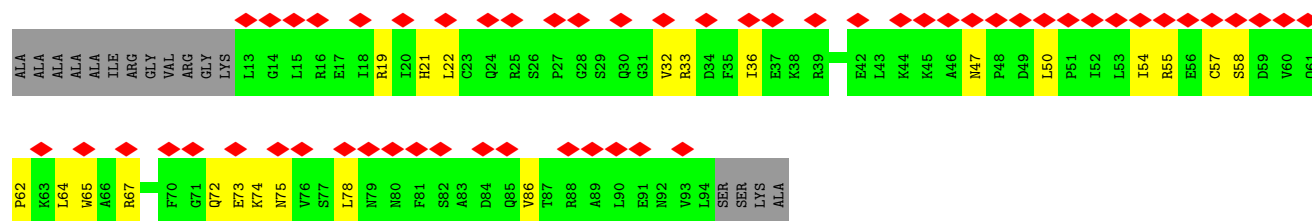


• Molecule 21: NADH:ubiquinone oxidoreductase subunit A9

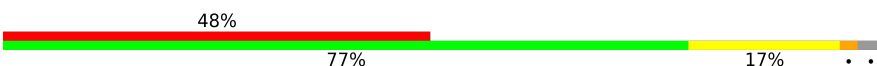


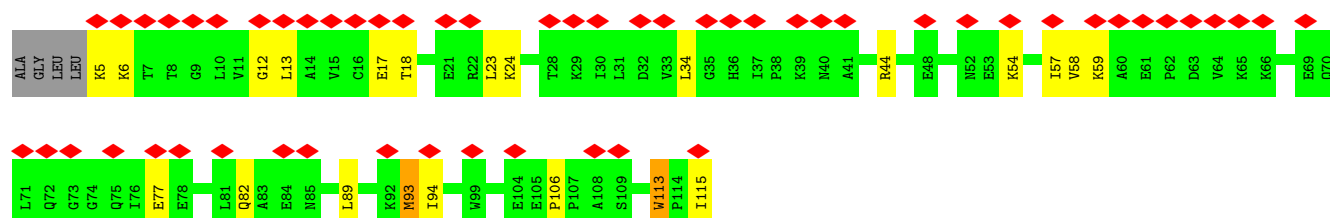
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2: 



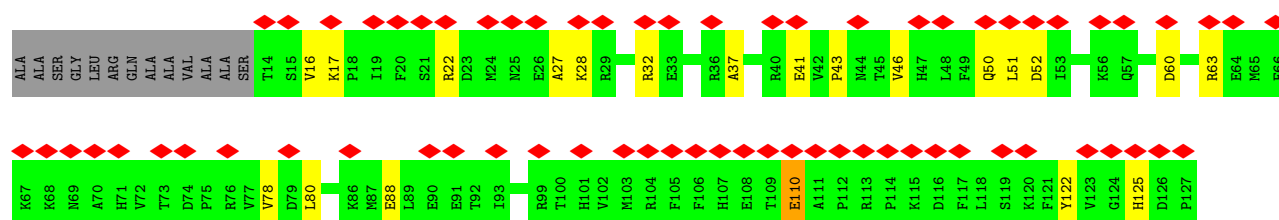
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5: 



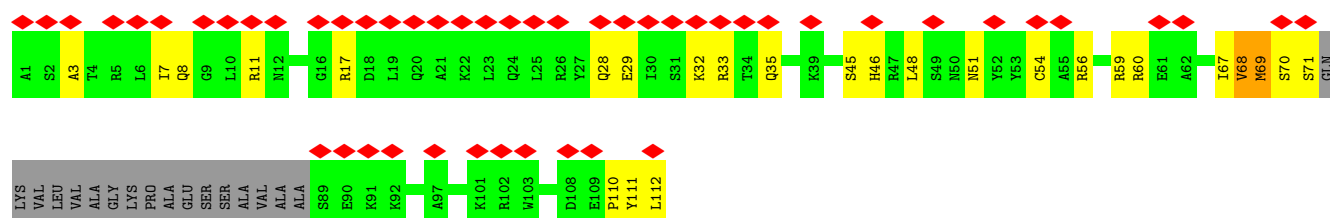
- Molecule 24: NADH:ubiquinone oxidoreductase subunit A6

Chain A6: 



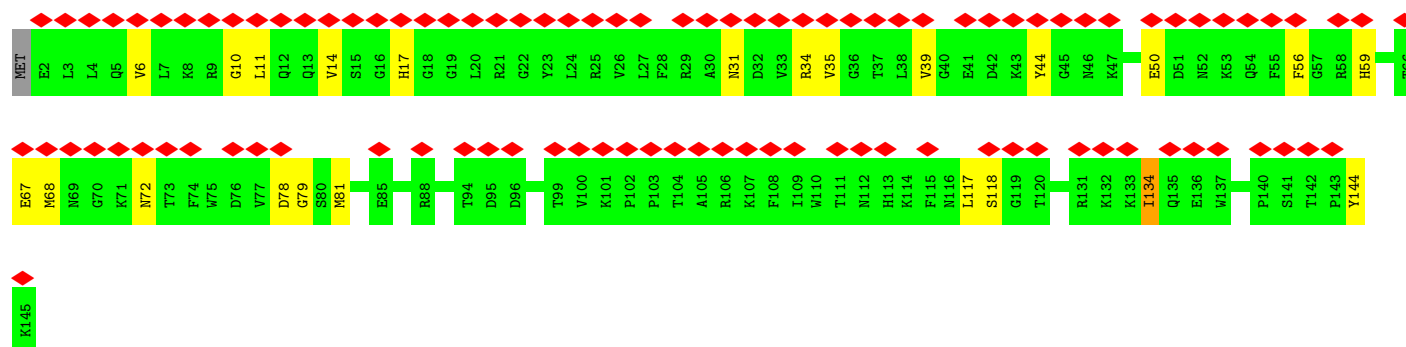
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7: 

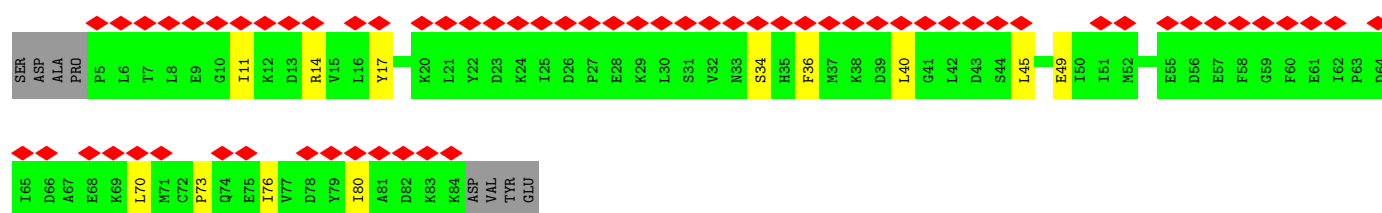
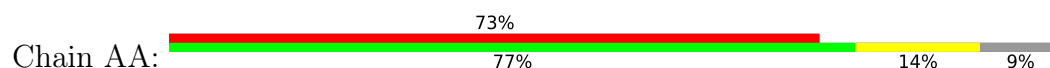


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

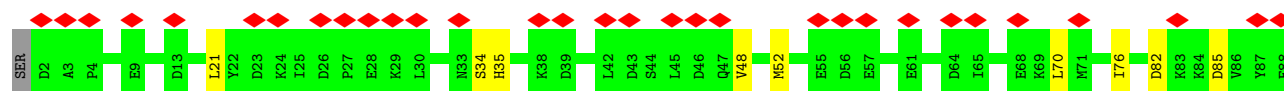
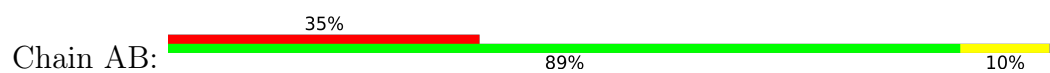
Chain AL: 



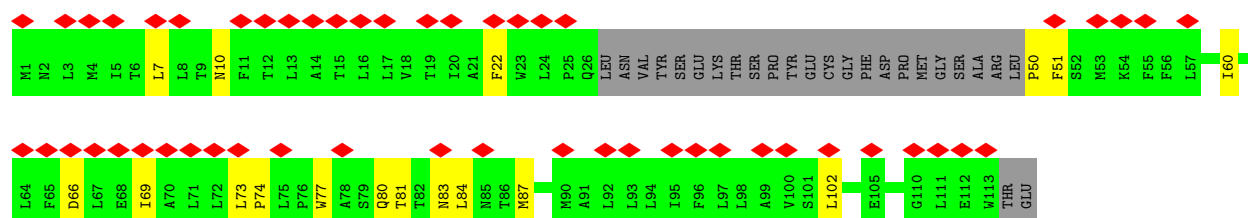
- Molecule 27: Acyl carrier protein



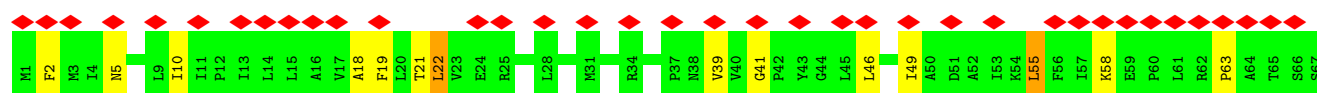
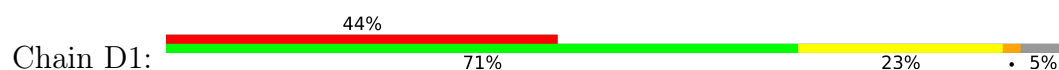
- Molecule 27: Acyl carrier protein

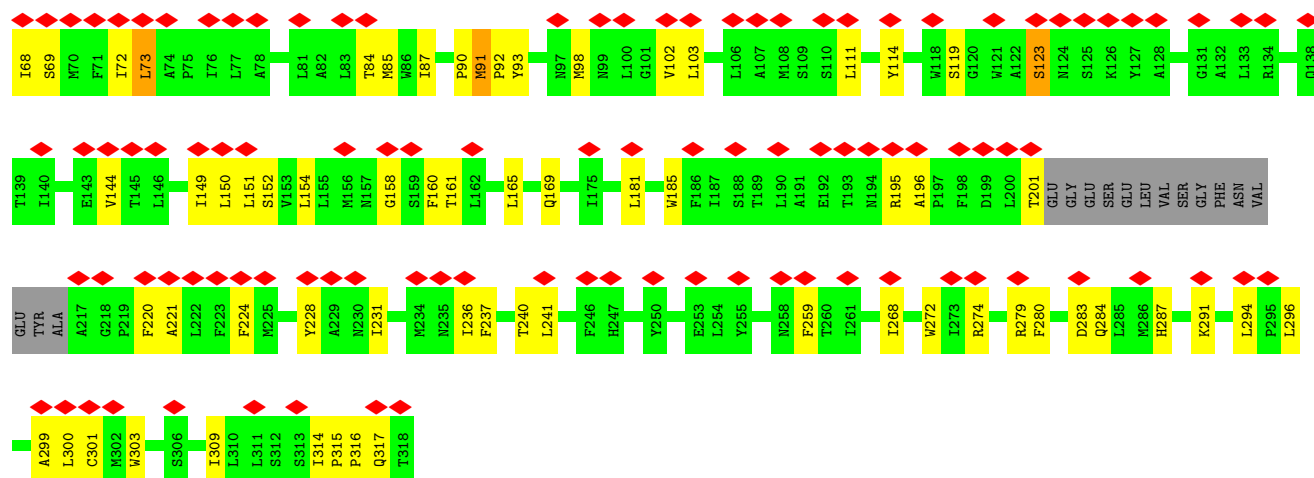


- Molecule 28: NADH-ubiquinone oxidoreductase chain 3



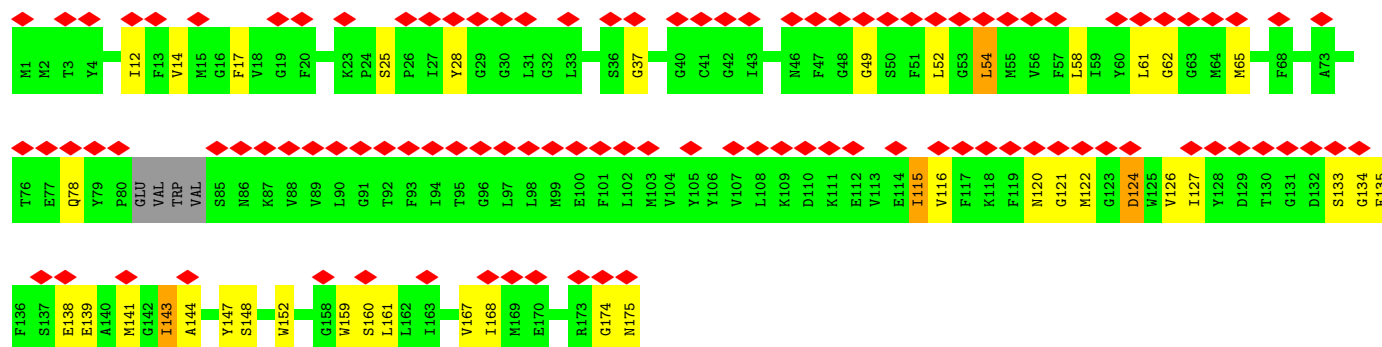
- Molecule 29: NADH-ubiquinone oxidoreductase chain 1





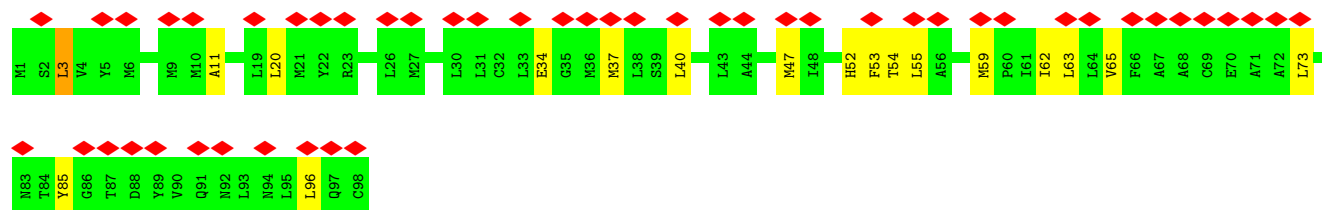
• Molecule 30: NADH-ubiquinone oxidoreductase chain 6

Chain D6:



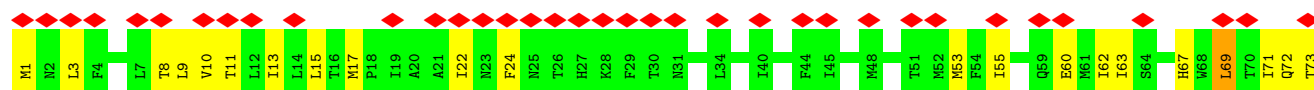
• Molecule 31: NADH-ubiquinone oxidoreductase chain 4L

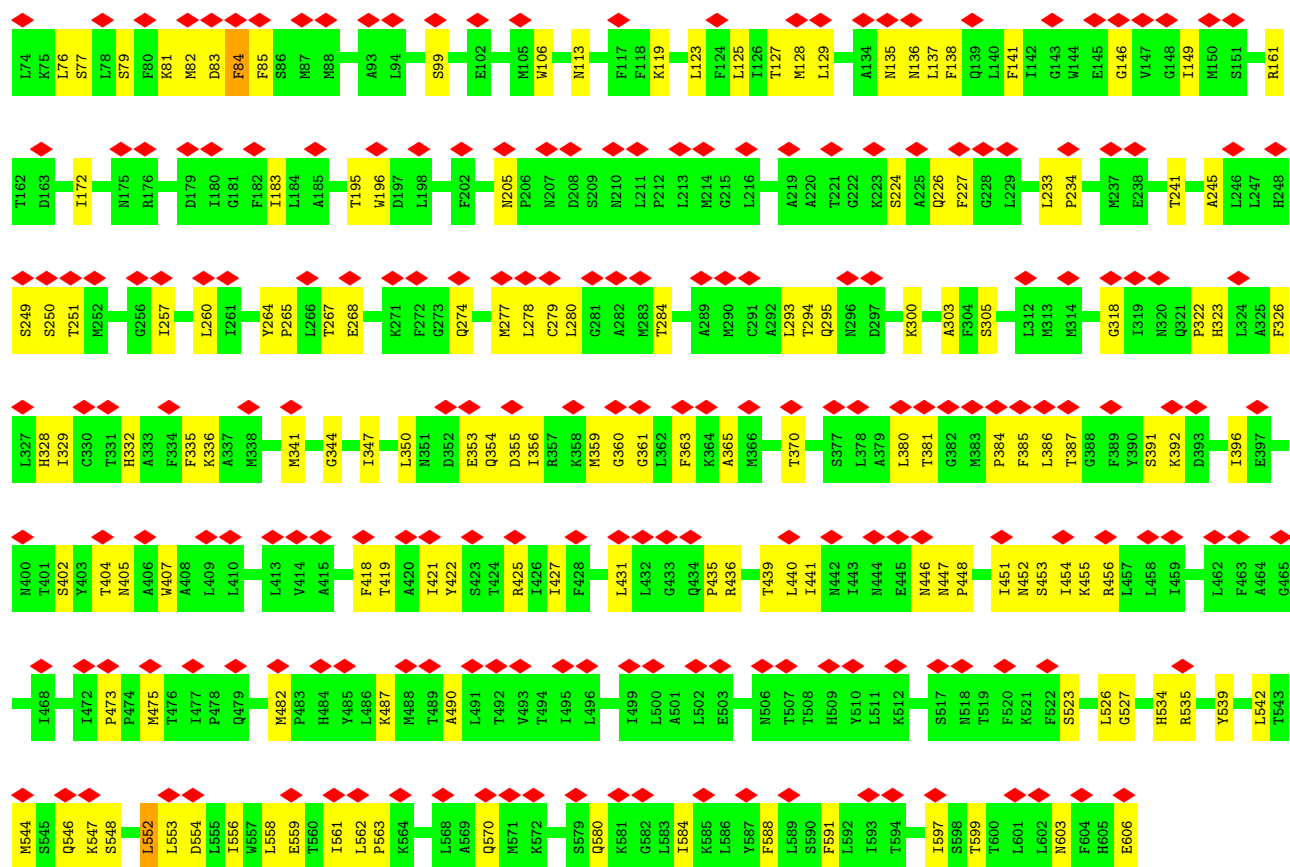
Chain 4L:



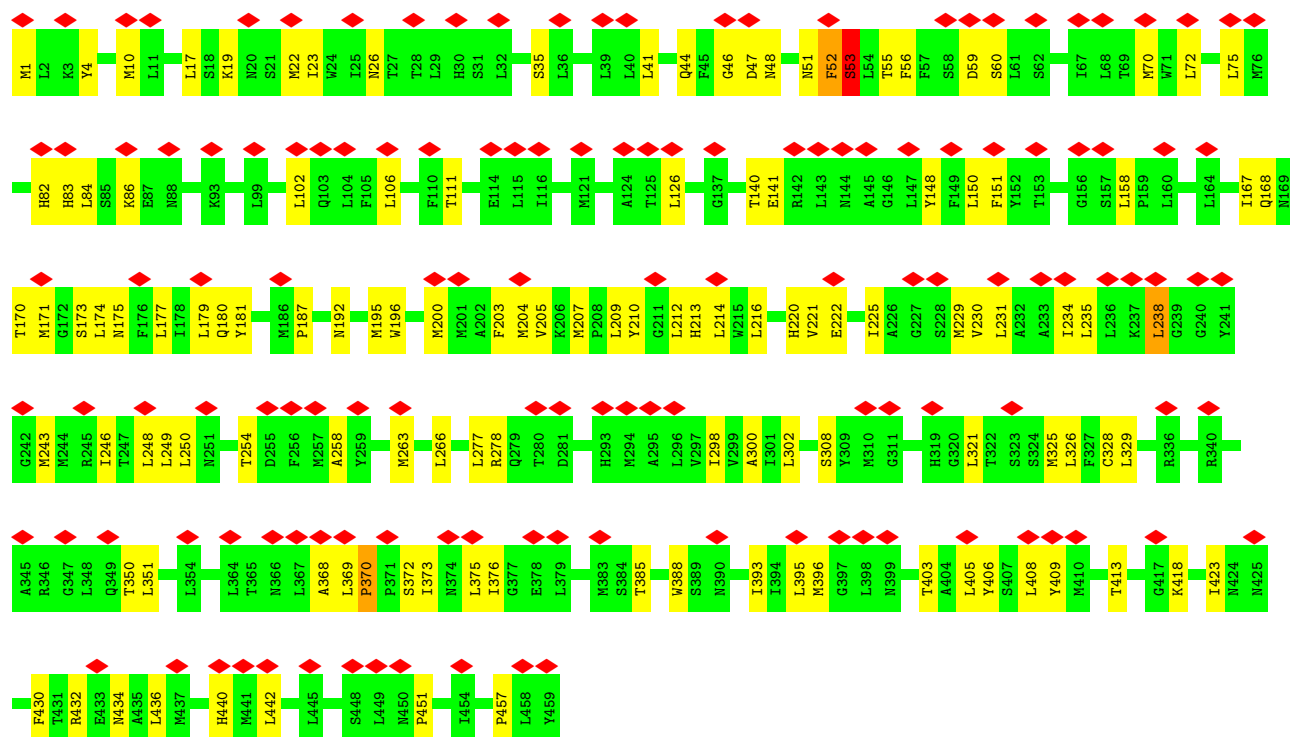
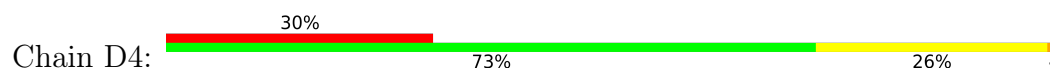
• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

Chain D5:

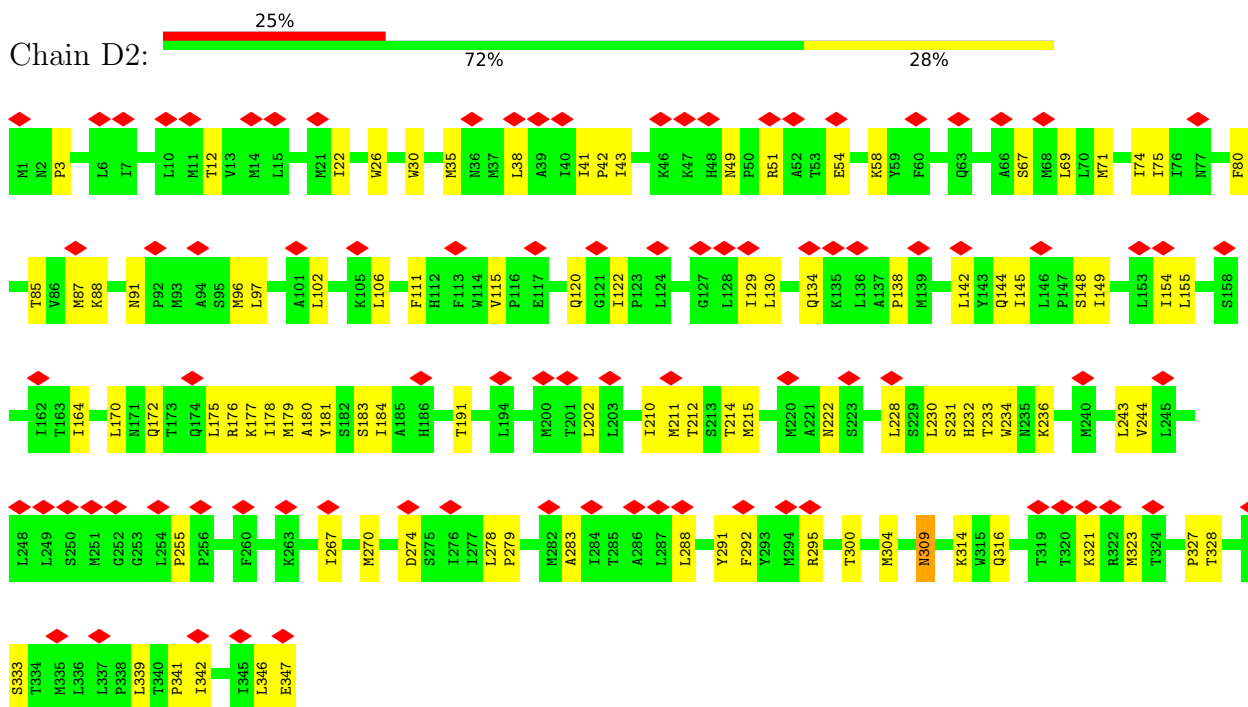




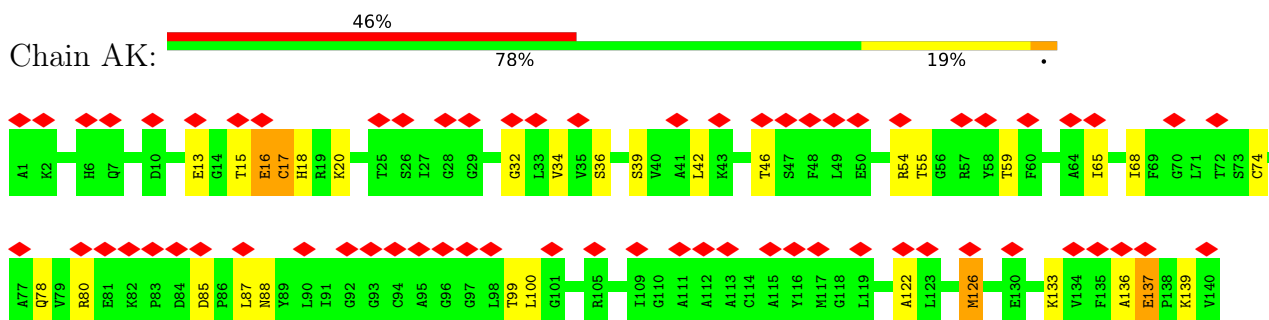
• Molecule 33: NADH-ubiquinone oxidoreductase chain 4



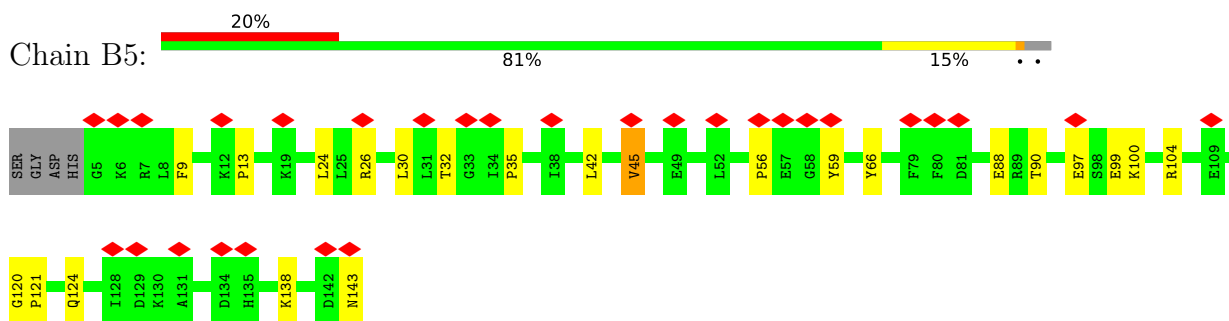
- Molecule 34: NADH-ubiquinone oxidoreductase chain 2



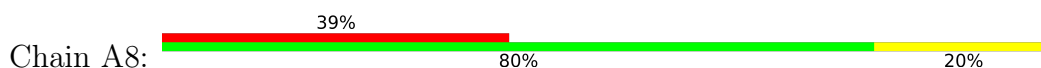
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

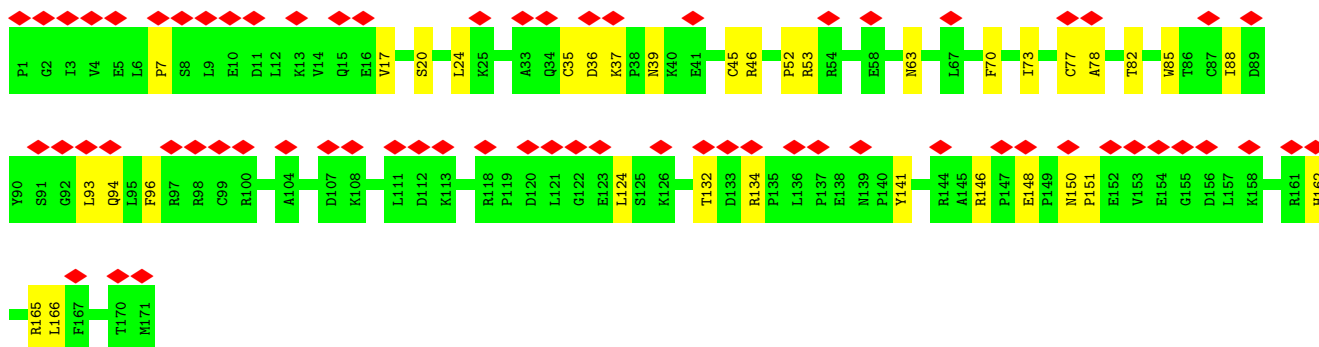


- Molecule 36: NADH:ubiquinone oxidoreductase subunit B5

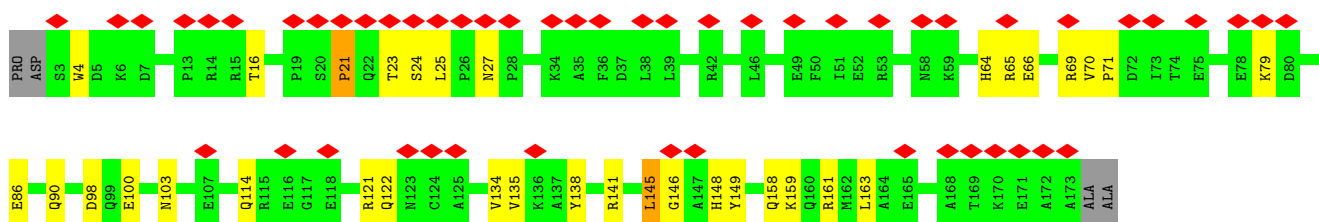
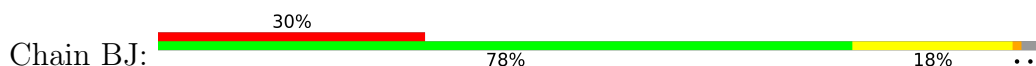


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

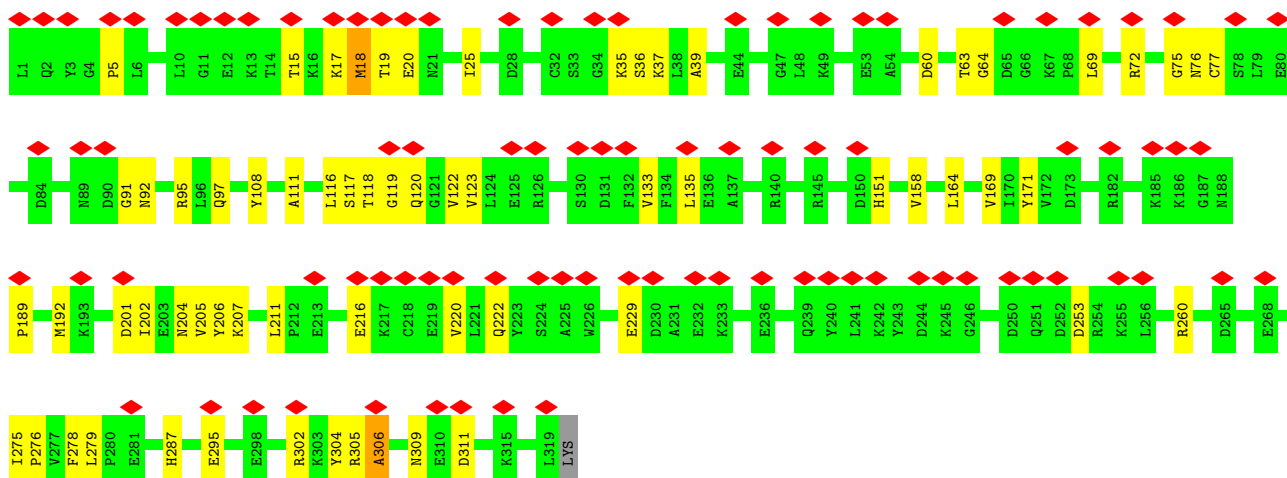
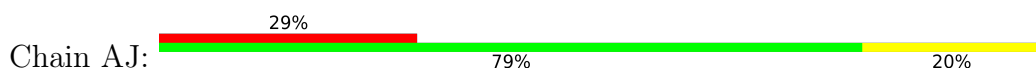




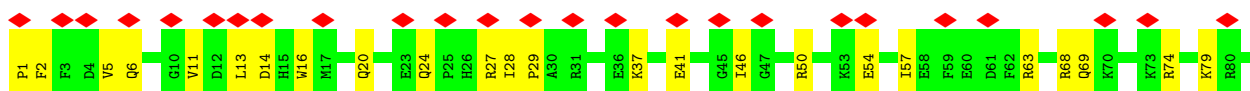
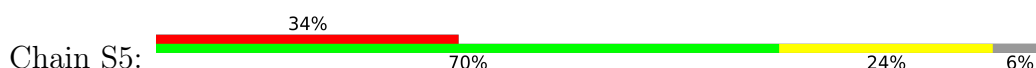
• Molecule 38: MT-ND5

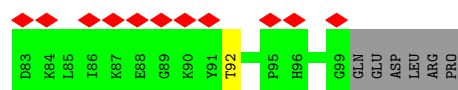


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

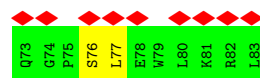
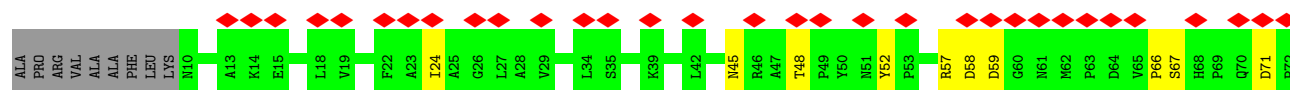
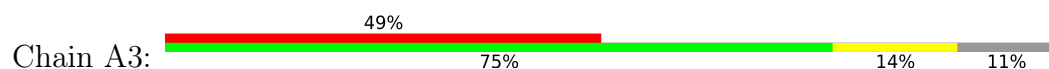


• Molecule 40: NADH:ubiquinone oxidoreductase subunit S5

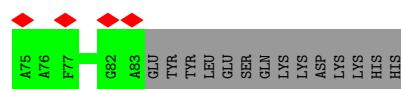
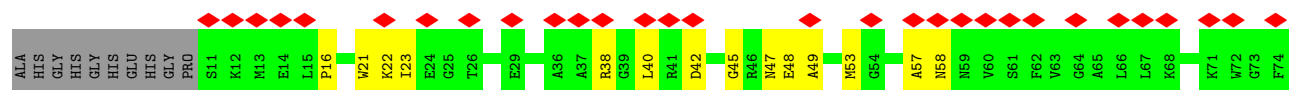




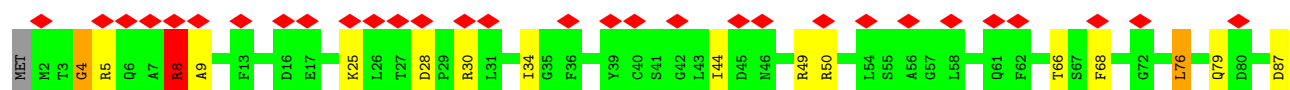
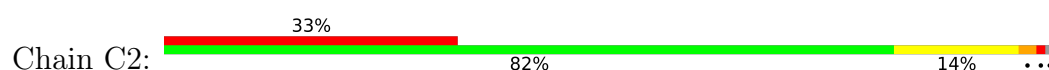
- Molecule 41: NADH:ubiquinone oxidoreductase subunit A3



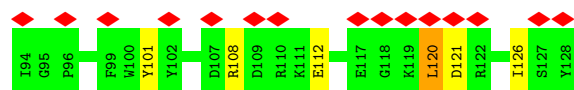
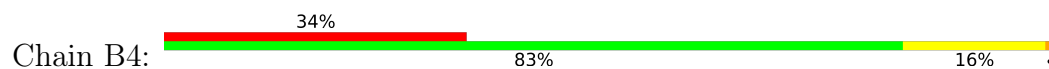
- Molecule 42: NADH:ubiquinone oxidoreductase subunit B3



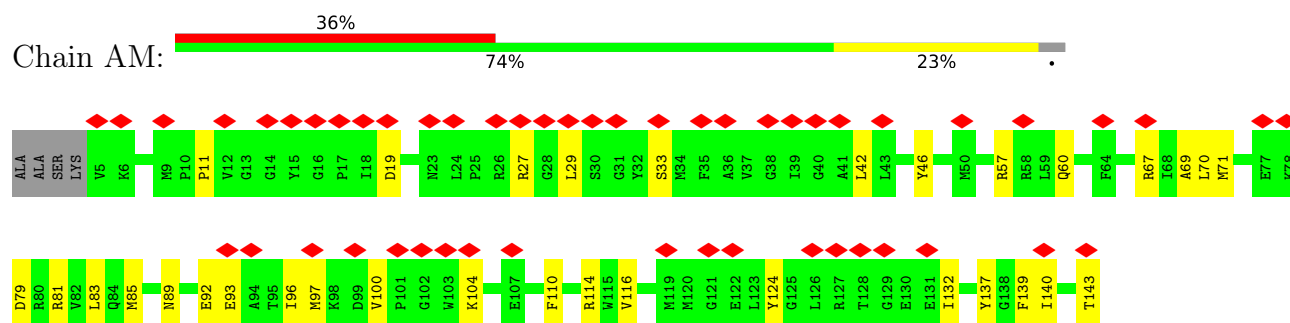
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 subunit C2



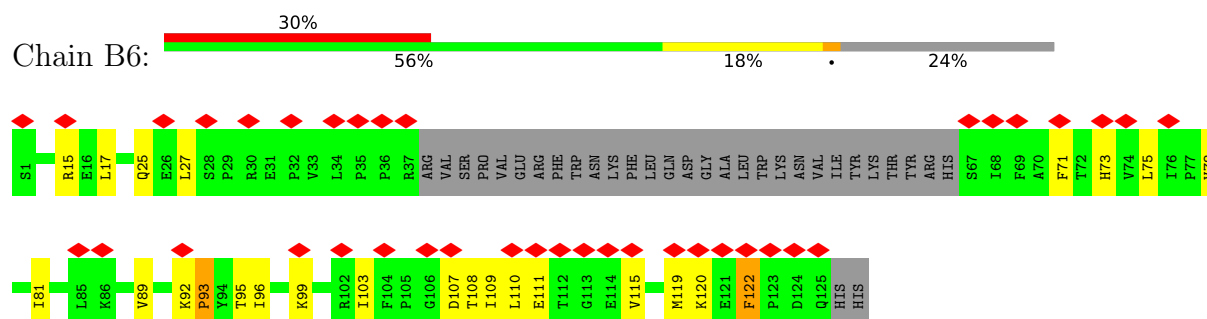
- Molecule 44: NADH:ubiquinone oxidoreductase subunit B4



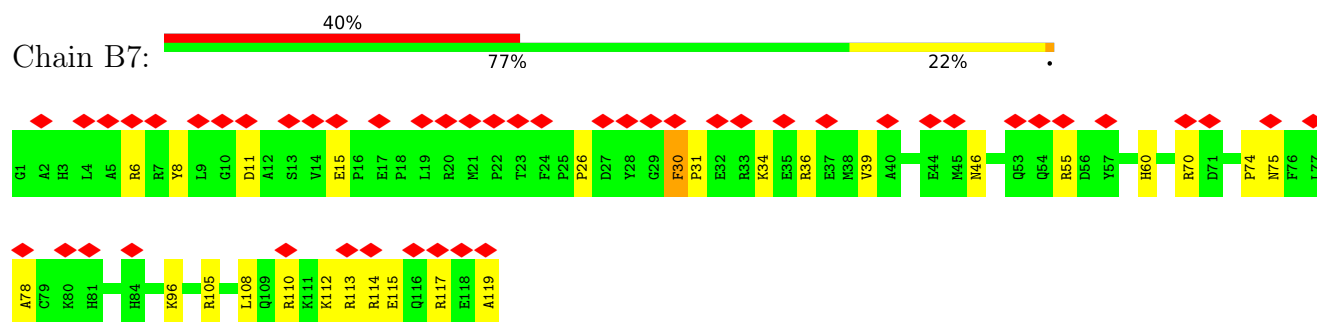
- Molecule 45: MT-ND1



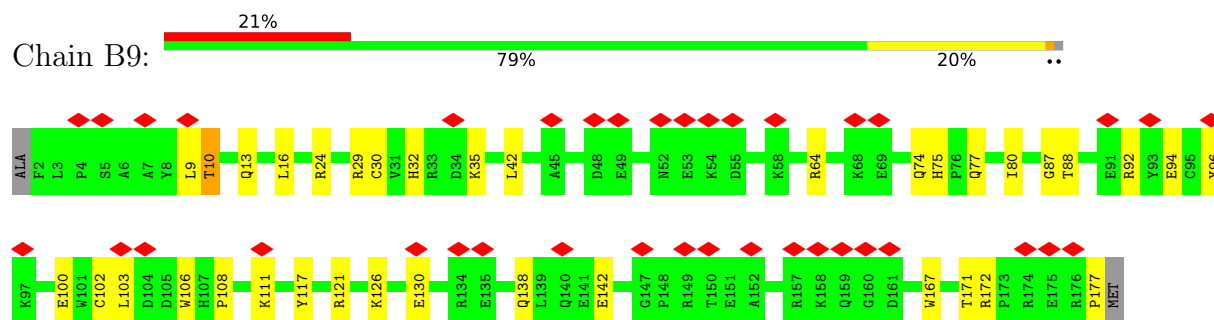
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



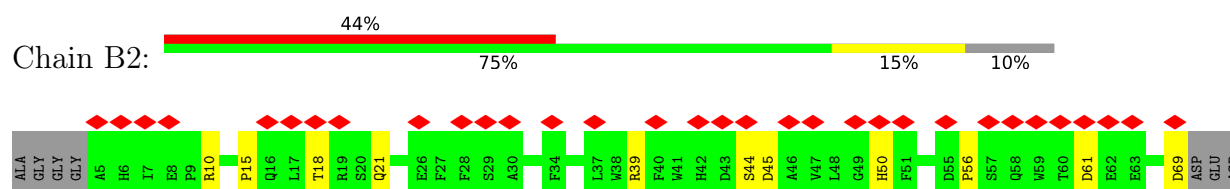
- Molecule 47: NADH:ubiquinone oxidoreductase subunit B7



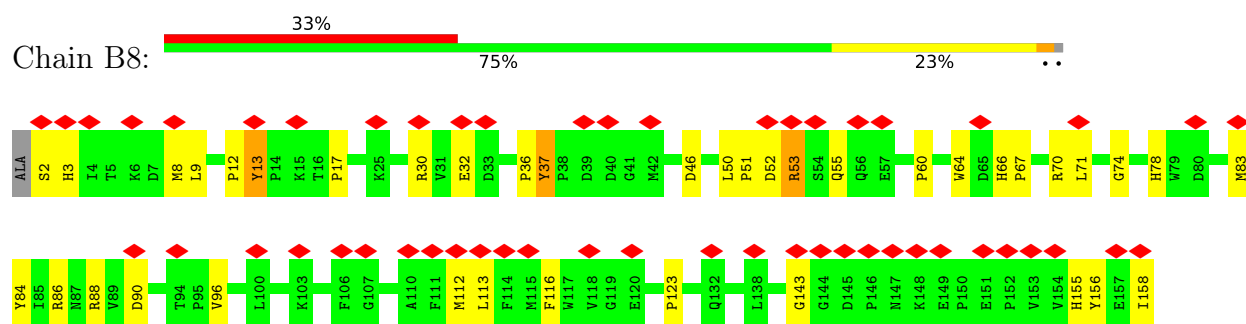
- Molecule 48: NADH:ubiquinone oxidoreductase subunit B9



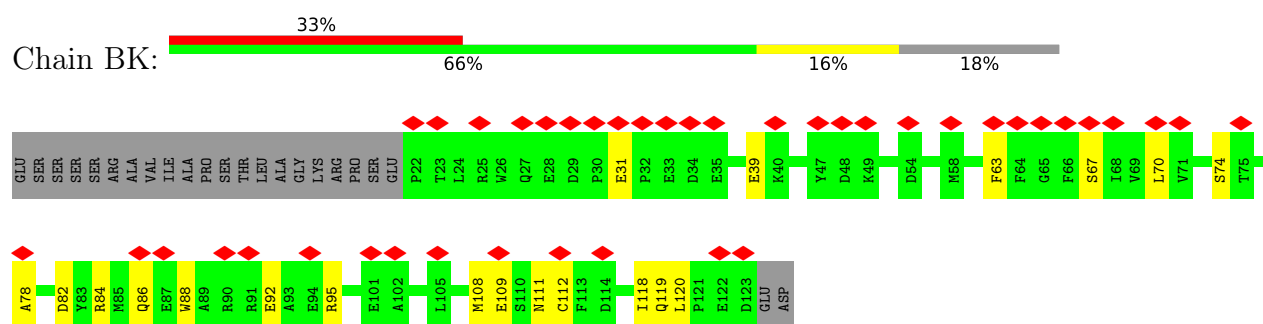
- Molecule 49: NADH:ubiquinone oxidoreductase subunit B2



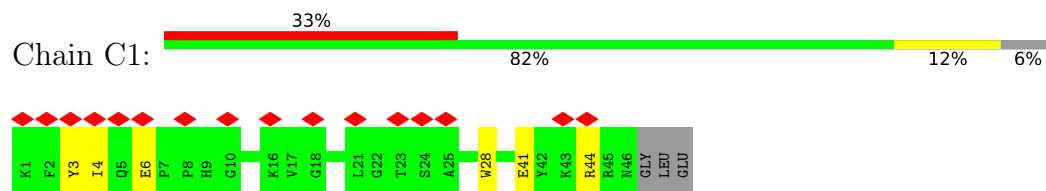
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



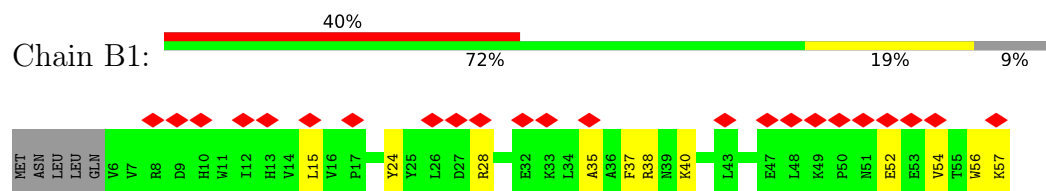
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



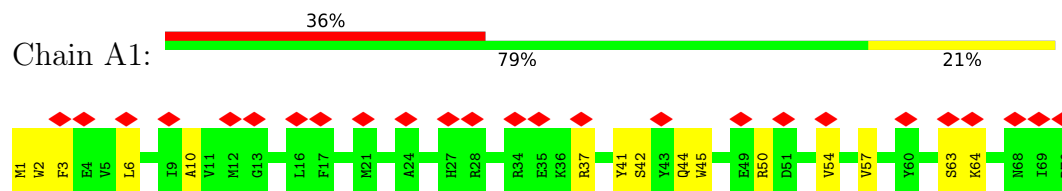
- Molecule 52: NDUFB4



- Molecule 53: NDUFA13



- Molecule 54: NDUFA1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35640	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	1.179	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	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: ZN, FMN, SF4, NDP, HEC, 3PE, PC1, ZMP, FES, CDL, HEM

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	0.36	0/3479	0.66	1/4719 (0.0%)
1	a3	0.43	0/3518	0.69	2/4776 (0.0%)
2	a2	0.34	0/3183	0.60	0/4313
2	a4	0.38	0/3179	0.63	0/4308
3	b1	0.41	0/3119	0.64	0/4268
3	b2	0.46	0/3119	0.68	1/4268 (0.0%)
4	c1	0.34	0/1968	0.65	0/2672
4	c2	0.38	0/1962	0.68	0/2664
5	f1	0.27	0/1554	0.55	1/2101 (0.0%)
5	f2	0.29	0/1548	0.56	0/2093
6	d1	0.36	0/906	0.62	0/1213
6	d2	0.40	0/908	0.64	0/1218
7	q1	0.35	0/638	0.65	0/862
7	q2	0.45	0/652	0.73	0/883
8	h1	0.29	0/538	0.67	0/723
8	h2	0.35	0/538	0.78	0/723
10	i1	0.29	0/471	0.62	0/634
10	i2	0.32	0/486	0.64	0/655
11	V1	0.39	0/3386	0.71	0/4575
12	V2	0.39	0/1687	0.85	3/2295 (0.1%)
13	S1	0.43	0/5362	0.73	0/7266
14	S2	0.52	0/3502	0.78	4/4744 (0.1%)
15	S3	0.49	0/1776	0.78	3/2417 (0.1%)
16	S7	0.52	0/1278	0.81	0/1728
17	S8	0.59	0/1445	0.78	0/1956
18	V3	0.33	0/355	0.76	0/480
19	S6	0.37	0/749	0.63	0/1009
20	S4	0.41	0/1047	0.72	0/1415
21	A9	0.37	0/2343	0.74	1/3164 (0.0%)
22	A2	0.32	0/676	0.72	0/911
23	A5	0.36	0/921	0.75	0/1249
24	A6	0.38	0/993	0.71	2/1336 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	A7	0.38	0/775	0.75	0/1048
26	AL	0.37	0/1242	0.73	0/1688
27	AA	0.31	0/655	0.75	0/881
27	AB	0.43	0/714	0.69	0/963
28	D3	0.45	0/747	0.73	1/1022 (0.1%)
29	D1	0.52	0/2487	0.86	6/3401 (0.2%)
30	D6	0.41	0/1339	0.78	0/1810
31	4L	0.50	0/758	0.80	0/1024
32	D5	0.49	0/4933	0.85	2/6710 (0.0%)
33	D4	0.55	0/3740	0.86	1/5095 (0.0%)
34	D2	0.54	0/2788	0.79	1/3795 (0.0%)
35	AK	0.40	0/1046	0.81	6/1419 (0.4%)
36	B5	0.44	0/1189	0.66	0/1607
37	A8	0.40	0/1441	0.75	0/1942
38	BJ	0.44	0/1475	0.75	3/1989 (0.2%)
39	AJ	0.44	0/2644	0.77	8/3579 (0.2%)
40	S5	0.45	0/843	0.77	0/1128
41	A3	0.37	0/602	0.76	0/828
42	B3	0.44	0/595	0.88	1/803 (0.1%)
43	C2	0.44	0/1028	0.79	4/1388 (0.3%)
44	B4	0.44	0/1085	0.73	0/1467
45	AM	0.40	0/1172	0.75	0/1579
46	B6	0.44	0/841	0.88	1/1144 (0.1%)
47	B7	0.39	0/1051	0.73	2/1408 (0.1%)
48	B9	0.49	0/1568	0.75	2/2123 (0.1%)
49	B2	0.41	0/590	0.83	4/810 (0.5%)
50	B8	0.48	0/1379	0.92	6/1884 (0.3%)
51	BK	0.44	0/880	0.76	0/1196
52	C1	0.35	0/404	0.71	2/548 (0.4%)
53	B1	0.37	0/462	0.69	0/624
54	A1	0.38	0/592	0.70	1/795 (0.1%)
All	All	0.43	0/98351	0.74	69/133336 (0.1%)

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	3
1	a3	0	1
2	a4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	b2	0	1
4	c1	0	1
4	c2	0	2
5	f2	0	1
6	d1	0	1
6	d2	0	1
11	V1	0	2
12	V2	0	4
13	S1	0	6
14	S2	0	4
15	S3	0	3
17	S8	0	1
18	V3	0	2
20	S4	0	2
22	A2	0	1
23	A5	0	2
25	A7	0	2
29	D1	0	3
30	D6	0	2
32	D5	0	4
33	D4	0	4
34	D2	0	1
35	AK	0	3
37	A8	0	2
38	BJ	0	2
39	AJ	0	3
40	S5	0	1
41	A3	0	1
42	B3	0	3
43	C2	0	1
44	B4	0	1
46	B6	0	1
47	B7	0	1
49	B2	0	1
50	B8	0	3
51	BK	0	1
52	C1	0	1
53	B1	0	1
54	A1	0	1
All	All	0	82

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BJ	21	PRO	CA-C-N	7.70	135.56	121.70
38	BJ	21	PRO	C-N-CA	7.70	135.56	121.70
39	AJ	229	GLU	CA-C-N	7.50	135.21	121.70
39	AJ	229	GLU	C-N-CA	7.50	135.21	121.70
49	B2	44	SER	CA-C-N	7.38	134.99	121.70
49	B2	44	SER	C-N-CA	7.38	134.99	121.70
15	S3	38	GLN	N-CA-C	-7.36	103.39	113.18
29	D1	63	PRO	CA-C-N	7.28	134.81	121.70
29	D1	63	PRO	C-N-CA	7.28	134.81	121.70
24	A6	110	GLU	CA-C-N	6.95	134.22	121.70
24	A6	110	GLU	C-N-CA	6.95	134.22	121.70
35	AK	17	CYS	CA-C-N	6.93	134.77	121.54
35	AK	17	CYS	C-N-CA	6.93	134.77	121.54
54	A1	57	VAL	N-CA-C	-6.73	106.17	112.83
43	C2	8	ARG	CA-C-N	6.64	133.65	121.70
43	C2	8	ARG	C-N-CA	6.64	133.65	121.70
42	B3	45	GLY	N-CA-C	6.11	117.57	111.21
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
50	B8	37	TYR	N-CA-C	6.03	123.13	109.81
3	b2	133	LEU	N-CA-C	5.95	122.96	109.81
12	V2	15	ASN	N-CA-C	-5.88	98.27	110.80
12	V2	14	LYS	CA-C-N	5.84	132.70	121.54
12	V2	14	LYS	C-N-CA	5.84	132.70	121.54
38	BJ	25	LEU	C-N-CD	-5.80	107.84	120.60
35	AK	137	GLU	CA-C-N	5.78	140.88	127.00
35	AK	137	GLU	C-N-CA	5.78	140.88	127.00
43	C2	4	GLY	CA-C-N	5.77	132.08	121.70
43	C2	4	GLY	C-N-CA	5.77	132.08	121.70
50	B8	37	TYR	CA-C-N	5.75	140.81	127.00
50	B8	37	TYR	C-N-CA	5.75	140.81	127.00
49	B2	61	ASP	CA-C-N	5.72	132.46	121.54
49	B2	61	ASP	C-N-CA	5.72	132.46	121.54
35	AK	137	GLU	C-N-CD	-5.66	108.15	120.60
5	f1	18	VAL	N-CA-C	-5.64	106.89	111.91
39	AJ	304	TYR	CA-CB-CG	5.64	124.06	113.90
48	B9	9	LEU	CA-C-N	5.61	132.26	121.54
48	B9	9	LEU	C-N-CA	5.61	132.26	121.54
14	S2	72	MET	N-CA-C	-5.58	98.92	110.80
33	D4	370	PRO	N-CA-C	5.56	117.48	110.70
21	A9	320	ARG	CA-CB-CG	5.53	125.16	114.10
32	D5	335	PHE	N-CA-CB	-5.52	101.16	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a3	320	LEU	CA-C-N	-5.47	112.83	121.37
1	a3	320	LEU	C-N-CA	-5.47	112.83	121.37
29	D1	161	THR	CA-C-N	5.47	131.99	121.54
29	D1	161	THR	C-N-CA	5.47	131.99	121.54
52	C1	4	ILE	CA-C-N	5.45	131.95	121.54
52	C1	4	ILE	C-N-CA	5.45	131.95	121.54
50	B8	8	MET	CA-C-N	-5.43	117.50	122.28
50	B8	8	MET	C-N-CA	-5.43	117.50	122.28
46	B6	122	PHE	N-CA-C	5.33	121.58	109.81
35	AK	126	MET	CB-CG-SD	-5.30	96.81	112.70
47	B7	26	PRO	CA-C-N	5.27	131.60	121.54
47	B7	26	PRO	C-N-CA	5.27	131.60	121.54
28	D3	73	LEU	N-CA-C	5.26	121.43	109.81
39	AJ	275	ILE	C-N-CD	-5.21	109.14	120.60
50	B8	13	TYR	N-CA-C	5.17	121.23	109.81
32	D5	69	LEU	CA-CB-CG	5.13	134.25	116.30
14	S2	165	THR	N-CA-C	5.11	121.10	109.81
15	S3	38	GLN	CA-C-N	-5.11	113.59	122.37
15	S3	38	GLN	C-N-CA	-5.11	113.59	122.37
1	a1	21	ASN	N-CA-C	-5.08	106.22	114.09
39	AJ	18	MET	CA-C-N	5.07	130.83	121.70
39	AJ	18	MET	C-N-CA	5.07	130.83	121.70
29	D1	87	ILE	CA-C-N	-5.02	116.58	121.65
29	D1	87	ILE	C-N-CA	-5.02	116.58	121.65
34	D2	255	PRO	N-CA-C	5.02	116.83	110.70
39	AJ	275	ILE	CA-C-N	5.01	139.03	127.00
39	AJ	275	ILE	C-N-CA	5.01	139.03	127.00

There are no chirality outliers.

All (82) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	A1	63	SER	Peptide
22	A2	74	LYS	Peptide
41	A3	59	ASP	Peptide
23	A5	113	TRP	Peptide
23	A5	93	MET	Peptide
25	A7	29	GLU	Peptide
25	A7	68	VAL	Peptide
37	A8	146	ARG	Peptide
37	A8	52	PRO	Peptide
39	AJ	216	GLU	Peptide

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Mol	Chain	Res	Type	Group
39	AJ	278	PHE	Peptide
39	AJ	311	ASP	Peptide
35	AK	136	ALA	Peptide
35	AK	16	GLU	Peptide
35	AK	46	THR	Peptide
53	B1	52	GLU	Peptide
49	B2	56	PRO	Peptide
42	B3	16	PRO	Peptide
42	B3	22	LYS	Peptide
42	B3	58	ASN	Peptide
44	B4	76	TYR	Peptide
46	B6	122	PHE	Peptide
47	B7	30	PHE	Peptide
50	B8	51	PRO	Peptide
50	B8	53	ARG	Peptide
50	B8	86	ARG	Peptide
38	BJ	24	SER	Peptide
38	BJ	79	LYS	Peptide
51	BK	39	GLU	Peptide
52	C1	6	GLU	Peptide
43	C2	8	ARG	Peptide
29	D1	123	SER	Peptide
29	D1	90	PRO	Peptide
29	D1	91	MET	Peptide
34	D2	309	ASN	Peptide
33	D4	17	LEU	Peptide
33	D4	214	LEU	Peptide
33	D4	52	PHE	Peptide
33	D4	53	SER	Peptide
32	D5	353	GLU	Peptide
32	D5	365	ALA	Peptide
32	D5	526	LEU	Peptide
32	D5	84	PHE	Mainchain
30	D6	115	ILE	Peptide
30	D6	124	ASP	Peptide
13	S1	213	TYR	Peptide
13	S1	218	ARG	Peptide
13	S1	247	VAL	Peptide
13	S1	254	MET	Peptide
13	S1	341	ASP	Peptide
13	S1	380	VAL	Peptide
14	S2	162	GLY	Peptide

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Mol	Chain	Res	Type	Group
14	S2	230	THR	Peptide
14	S2	341	SER	Peptide
14	S2	73	VAL	Peptide
15	S3	203	TRP	Peptide
15	S3	76	ALA	Peptide
15	S3	80	ALA	Mainchain
20	S4	11	ILE	Peptide
20	S4	43	ASN	Peptide
40	S5	92	THR	Peptide
17	S8	106	THR	Peptide
11	V1	28	ARG	Peptide
11	V1	331	THR	Peptide
12	V2	10	ARG	Peptide
12	V2	13	PRO	Peptide
12	V2	18	GLU	Peptide
12	V2	35	VAL	Peptide
18	V3	63	MET	Peptide
18	V3	65	GLN	Peptide
1	a1	190	TYR	Peptide
1	a1	193	PRO	Peptide
1	a1	309	THR	Peptide
1	a3	309	THR	Peptide
2	a4	30	PRO	Peptide
3	b2	271	GLU	Peptide
4	c1	173	GLY	Peptide
4	c2	88	SER	Peptide
4	c2	92	PRO	Peptide
6	d1	39	GLU	Peptide
6	d2	39	GLU	Peptide
5	f2	188	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a1	3409	0	3322	53	0
1	a3	3447	0	3350	49	0
2	a2	3126	0	3093	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a4	3122	0	3090	61	0
3	b1	3019	0	3082	48	0
3	b2	3019	0	3082	49	0
4	c1	1909	0	1858	29	0
4	c2	1903	0	1850	33	0
5	f1	1520	0	1505	34	0
5	f2	1514	0	1497	36	0
6	d1	886	0	883	16	0
6	d2	888	0	880	15	0
7	q1	618	0	628	15	0
7	q2	631	0	639	14	0
8	h1	532	0	509	9	0
8	h2	532	0	509	7	0
9	x1	114	0	28	4	0
9	x2	130	0	33	0	0
10	i1	459	0	462	8	0
10	i2	473	0	477	4	0
11	V1	3312	0	3266	67	0
12	V2	1647	0	1657	33	0
13	S1	5275	0	5300	141	0
14	S2	3414	0	3360	60	0
15	S3	1726	0	1676	40	0
16	S7	1247	0	1256	29	0
17	S8	1414	0	1370	33	0
18	V3	345	0	323	9	0
19	S6	737	0	710	14	0
20	S4	1024	0	1023	25	0
21	A9	2293	0	2326	55	0
22	A2	665	0	678	16	0
23	A5	901	0	936	13	0
24	A6	969	0	980	20	0
25	A7	757	0	771	22	0
26	AL	1201	0	1170	14	0
27	AA	645	0	649	7	0
27	AB	702	0	692	8	0
28	D3	728	0	773	17	0
29	D1	2415	0	2542	55	0
30	D6	1308	0	1329	35	0
31	4L	748	0	794	20	0
32	D5	4805	0	4950	116	0
33	D4	3646	0	3850	87	0
34	D2	2724	0	2930	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	AK	1025	0	1033	20	0
36	B5	1156	0	1177	20	0
37	A8	1404	0	1384	26	0
38	BJ	1441	0	1417	25	0
39	AJ	2583	0	2547	38	0
40	S5	822	0	820	23	0
41	A3	582	0	583	9	0
42	B3	578	0	570	8	0
43	C2	997	0	983	19	0
44	B4	1059	0	1062	19	0
45	AM	1143	0	1137	28	0
46	B6	815	0	837	22	0
47	B7	1026	0	995	23	0
48	B9	1515	0	1469	26	0
49	B2	563	0	509	9	0
50	B8	1324	0	1219	27	0
51	BK	853	0	800	20	0
52	C1	391	0	391	4	0
53	B1	449	0	453	6	0
54	A1	577	0	570	11	0
55	b1	86	0	60	7	0
55	b2	86	0	60	5	0
56	c1	43	0	30	3	0
56	c2	43	0	30	2	0
57	D1	26	0	26	2	0
57	D4	40	0	54	3	0
57	D5	38	0	50	2	0
57	c1	13	0	12	1	0
57	f2	23	0	20	2	0
58	S1	4	0	0	0	0
58	V2	4	0	0	1	0
58	f1	4	0	0	0	0
58	f2	4	0	0	0	0
59	S1	16	0	0	1	0
59	S7	8	0	0	1	0
59	S8	16	0	0	1	0
59	V1	8	0	0	1	0
60	V1	31	0	19	3	0
61	S6	1	0	0	0	0
62	A9	48	0	26	3	0
63	AA	34	0	40	0	0
63	AB	31	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	D5	60	0	64	4	0
65	AK	28	0	30	0	0
All	All	96897	0	96599	1593	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1593) 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:S3:80:ALA:HA	15:S3:91:GLU:O	1.15	1.24
4:c2:237:ARG:O	7:q2:12:HIS:HA	1.51	1.10
13:S1:449:PRO:O	13:S1:489:VAL:HA	1.60	1.02
15:S3:80:ALA:CA	15:S3:91:GLU:O	2.11	0.98
15:S3:38:GLN:HA	25:A7:70:SER:O	1.64	0.97
4:c2:237:ARG:O	7:q2:12:HIS:CA	2.22	0.87
33:D4:52:PHE:O	33:D4:56:PHE:HB2	1.73	0.87
5:f1:184:SER:HB2	5:f1:196:GLY:O	1.74	0.86
13:S1:689:LYS:O	13:S1:693:GLU:HB2	1.80	0.81
32:D5:547:LYS:O	32:D5:552:LEU:HB2	1.80	0.80
13:S1:442:VAL:O	13:S1:446:ALA:HB2	1.82	0.79
15:S3:78:LEU:HA	15:S3:93:VAL:O	1.82	0.79
32:D5:227:PHE:H	32:D5:284:THR:HG22	1.48	0.78
1:a1:437:ILE:O	1:a1:441:MET:HB2	1.84	0.77
13:S1:675:ASP:O	13:S1:679:ARG:HB2	1.85	0.76
34:D2:130:LEU:O	34:D2:134:GLN:HB2	1.86	0.75
2:a2:219:VAL:O	2:a2:223:PHE:HB2	1.86	0.75
14:S2:256:SER:HB3	14:S2:373:GLU:H	1.52	0.72
29:D1:41:GLY:HA3	29:D1:46:LEU:HD21	1.72	0.72
48:B9:138:GLN:O	48:B9:142:GLU:HB2	1.91	0.71
15:S3:80:ALA:HA	15:S3:91:GLU:C	2.12	0.71
47:B7:36:ARG:HH22	47:B7:96:LYS:HD3	1.54	0.71
14:S2:105:ARG:NH1	16:S7:149:CYS:SG	2.59	0.71
13:S1:227:SER:H	13:S1:253:ARG:HH22	1.37	0.70
7:q1:45:ILE:O	7:q1:49:ALA:HB3	1.90	0.70
21:A9:108:ASP:O	21:A9:112:LYS:HB3	1.91	0.70
38:BJ:23:THR:HG21	47:B7:74:PRO:HD2	1.74	0.70
13:S1:444:GLN:HG3	13:S1:477:ILE:HG12	1.73	0.70
33:D4:177:LEU:O	33:D4:180:GLN:C	2.35	0.70
13:S1:276:ARG:HH21	13:S1:682:GLN:HE21	1.38	0.69
4:c1:142:LEU:HD11	4:c1:146:LEU:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A8:45:CYS:SG	37:A8:134:ARG:NH2	2.65	0.69
11:V1:126:GLY:HA2	11:V1:131:ALA:HB3	1.75	0.69
14:S2:204:PRO:HD3	17:S8:60:ARG:HH22	1.57	0.69
32:D5:138:PHE:HB2	32:D5:196:TRP:HE1	1.58	0.69
33:D4:46:GLY:H	51:BK:84:ARG:HA	1.57	0.68
30:D6:133:SER:OG	45:AM:67:ARG:NH2	2.26	0.68
3:b2:70:CYS:SG	3:b2:80:ARG:NH1	2.67	0.68
13:S1:243:ARG:HG2	13:S1:244:THR:HG23	1.75	0.67
11:V1:96:ASN:ND2	11:V1:187:GLY:O	2.28	0.67
21:A9:52:GLU:HG2	21:A9:54:TYR:H	1.60	0.66
30:D6:58:LEU:O	30:D6:62:GLY:HA3	1.95	0.66
28:D3:81:THR:HG23	28:D3:83:ASN:H	1.59	0.66
16:S7:62:MET:HB3	16:S7:153:ALA:HB1	1.78	0.66
21:A9:51:CYS:SG	21:A9:52:GLU:N	2.69	0.66
13:S1:255:HIS:HD2	13:S1:258:ILE:H	1.44	0.66
13:S1:377:VAL:HG22	13:S1:450:MET:HB3	1.77	0.65
21:A9:135:LEU:HA	21:A9:167:LYS:HD3	1.78	0.65
5:f1:84:GLY:N	5:f1:100:HIS:O	2.30	0.65
33:D4:204:MET:HB3	33:D4:209:LEU:HD22	1.79	0.65
2:a2:78:LYS:H	2:a2:129:ALA:HB1	1.60	0.65
13:S1:470:VAL:HG12	13:S1:490:MET:HE1	1.79	0.65
48:B9:102:CYS:SG	48:B9:103:LEU:N	2.70	0.65
15:S3:48:LEU:HB3	15:S3:105:ILE:HG22	1.76	0.65
1:a1:3:THR:H	1:a1:6:GLN:HB2	1.62	0.64
21:A9:50:ARG:HG2	62:A9:401:NDP:H2A	1.80	0.64
29:D1:196:ALA:HB3	29:D1:274:ARG:HG3	1.77	0.64
47:B7:115:GLU:O	47:B7:119:ALA:HB3	1.97	0.64
2:a2:313:ASN:ND2	2:a2:321:LEU:O	2.30	0.64
3:b2:116:GLY:HA3	55:b2:402:HEM:HBC2	1.79	0.64
4:c2:27:ARG:HH21	4:c2:56:TYR:HA	1.63	0.64
11:V1:134:ALA:HB3	11:V1:175:VAL:HG12	1.78	0.64
37:A8:165:ARG:NH1	43:C2:87:ASP:OD1	2.32	0.63
17:S8:53:GLU:OE2	26:AL:34:ARG:NH2	2.32	0.63
25:A7:51:ASN:HB2	25:A7:56:ARG:HH22	1.63	0.63
13:S1:117:GLN:NE2	59:S1:801:SF4:S3	2.72	0.63
34:D2:102:LEU:HD22	34:D2:138:PRO:HB3	1.80	0.63
1:a3:245:GLU:HA	7:q2:11:ARG:HA	1.81	0.63
38:BJ:122:GLN:HG3	47:B7:46:ASN:HD21	1.64	0.63
3:b1:53:MET:HE1	5:f1:62:MET:HG2	1.80	0.63
1:a3:21:ASN:ND2	1:a3:216:PHE:O	2.32	0.63
7:q2:64:GLN:HE22	35:AK:16:GLU:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:114:CYS:SG	13:S1:115:ASP:N	2.71	0.63
13:S1:518:PRO:HB3	13:S1:537:LEU:HA	1.79	0.63
21:A9:316:GLU:HG2	24:A6:52:ASP:HB3	1.79	0.63
5:f1:142:LEU:O	3:b2:148:ASN:ND2	2.30	0.62
13:S1:229:ASP:HB3	13:S1:235:GLY:HA2	1.81	0.62
21:A9:157:ARG:HE	21:A9:165:ILE:HD13	1.64	0.62
36:B5:26:ARG:O	36:B5:30:LEU:HB2	1.99	0.62
11:V1:93:LEU:O	11:V1:134:ALA:HA	1.99	0.62
13:S1:215:PHE:HB2	17:S8:98:PRO:HD3	1.81	0.62
14:S2:347:HIS:O	14:S2:351:LEU:HB2	1.99	0.62
25:A7:28:GLN:O	25:A7:32:LYS:NZ	2.33	0.62
1:a1:159:GLN:OE1	5:f1:14:ARG:NH2	2.33	0.62
3:b1:44:GLN:HG3	55:b1:401:HEM:HBC2	1.81	0.62
13:S1:283:MET:HB2	13:S1:560:ILE:HB	1.79	0.62
14:S2:388:ARG:NH1	14:S2:389:CYS:O	2.33	0.62
32:D5:81:LYS:HG2	32:D5:135:ASN:HB3	1.81	0.62
32:D5:542:LEU:HD21	33:D4:277:LEU:HD22	1.80	0.62
32:D5:554:ASP:O	32:D5:558:LEU:HB3	1.99	0.62
5:f1:75:GLU:HG2	5:f1:194:ILE:HG12	1.81	0.62
32:D5:278:LEU:HB3	32:D5:318:GLY:HA3	1.82	0.62
39:AJ:287:HIS:ND1	51:BK:31:GLU:OE2	2.32	0.62
48:B9:100:GLU:O	48:B9:121:ARG:NH2	2.32	0.62
17:S8:22:ALA:O	17:S8:26:LEU:HB2	1.99	0.62
1:a1:328:HIS:HB3	1:a1:427:PRO:HB2	1.81	0.62
39:AJ:116:LEU:O	39:AJ:260:ARG:NH2	2.33	0.62
3:b1:252:ASP:HB2	3:b1:255:ASN:HB2	1.82	0.61
13:S1:9:ILE:HB	13:S1:20:VAL:HB	1.81	0.61
5:f1:138:VAL:HG13	5:f1:143:GLY:HA2	1.81	0.61
5:f2:121:GLN:O	5:f2:170:ARG:NH1	2.33	0.61
13:S1:285:ARG:NH1	13:S1:557:ALA:O	2.33	0.61
17:S8:79:ALA:HB2	17:S8:106:THR:HG22	1.82	0.61
43:C2:30:ARG:HE	43:C2:76:LEU:HD11	1.66	0.61
3:b1:146:ILE:HG12	3:b1:149:LEU:HD12	1.83	0.61
29:D1:119:SER:O	29:D1:123:SER:OG	2.16	0.61
32:D5:407:TRP:HE1	50:B8:112:MET:HE1	1.65	0.61
48:B9:88:THR:HG22	48:B9:92:ARG:HH22	1.65	0.61
50:B8:46:ASP:OD1	50:B8:46:ASP:N	2.33	0.61
3:b2:117:VAL:HG11	3:b2:302:VAL:HG22	1.81	0.61
5:f2:57:GLN:HE22	57:f2:201:3PE:H222	1.66	0.61
13:S1:40:PHE:O	13:S1:158:ARG:NH2	2.30	0.61
14:S2:183:ARG:HH21	25:A7:33:ARG:HH22	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A3:48:THR:HG21	45:AM:57:ARG:HH21	1.65	0.61
3:b1:182:HIS:HE1	55:b1:401:HEM:NC	1.97	0.61
36:B5:124:GLN:NE2	37:A8:150:ASN:OD1	2.34	0.61
13:S1:594:ARG:NH2	24:A6:122:TYR:O	2.34	0.61
17:S8:3:LYS:HG3	25:A7:110:PRO:HA	1.83	0.61
4:c1:163:ILE:HD12	4:c1:164:TYR:H	1.64	0.61
40:S5:50:ARG:O	40:S5:54:GLU:HB2	2.01	0.61
11:V1:294:LEU:HA	11:V1:338:ASP:HA	1.82	0.61
33:D4:179:LEU:HD11	33:D4:249:LEU:HD23	1.83	0.61
2:a2:169:ARG:NH2	2:a2:239:TYR:O	2.34	0.60
6:d2:91:GLU:O	6:d2:95:LYS:HB2	2.01	0.60
13:S1:449:PRO:HG2	13:S1:489:VAL:HG22	1.83	0.60
36:B5:120:GLY:O	36:B5:124:GLN:NE2	2.35	0.60
1:a1:235:ARG:HD2	5:f1:18:VAL:HG12	1.83	0.60
1:a1:248:LEU:HD12	1:a1:426:GLY:HA2	1.83	0.60
13:S1:257:ASP:O	13:S1:394:ARG:NH2	2.34	0.60
29:D1:201:THR:OG1	29:D1:279:ARG:NH1	2.34	0.60
32:D5:547:LYS:O	32:D5:552:LEU:CB	2.49	0.60
27:AB:70:LEU:HD23	27:AB:76:ILE:HG12	1.82	0.60
21:A9:289:THR:HG22	21:A9:290:THR:HG23	1.82	0.60
14:S2:19:MET:SD	34:D2:295:ARG:NH2	2.74	0.60
13:S1:543:ILE:HD11	13:S1:557:ALA:HA	1.84	0.60
17:S8:65:HIS:NE2	17:S8:116:CYS:SG	2.74	0.60
33:D4:177:LEU:O	33:D4:180:GLN:O	2.20	0.60
36:B5:88:GLU:OE1	53:B1:56:TRP:NE1	2.31	0.60
54:A1:54:VAL:O	54:A1:64:LYS:NZ	2.35	0.60
17:S8:119:CYS:HB2	17:S8:121:PHE:H	1.67	0.60
54:A1:1:MET:HG3	54:A1:3:PHE:H	1.67	0.60
6:d1:45:GLU:OE1	6:d1:48:ARG:NH1	2.35	0.59
3:b2:25:SER:OG	6:d2:70:MET:SD	2.60	0.59
6:d2:22:ASN:HA	6:d2:27:ASN:HD21	1.67	0.59
38:BJ:161:ARG:NH2	51:BK:111:ASN:OD1	2.34	0.59
3:b1:82:MET:HG2	3:b1:240:MET:HE1	1.83	0.59
10:i1:51:LEU:HD13	10:i1:53:LYS:H	1.66	0.59
30:D6:167:VAL:HG22	34:D2:42:PRO:HG2	1.85	0.59
13:S1:240:VAL:HG12	13:S1:250:ILE:HG22	1.84	0.59
1:a3:419:CYS:SG	1:a3:438:ARG:NH1	2.73	0.59
2:a4:290:ASN:O	2:a4:297:GLN:NE2	2.36	0.59
28:D3:102:LEU:HD13	29:D1:294:LEU:HD23	1.84	0.59
29:D1:111:LEU:HD13	29:D1:114:TYR:HD2	1.68	0.59
2:a4:76:THR:HG22	2:a4:82:SER:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b1:161:VAL:HA	3:b1:164:ILE:HG12	1.85	0.59
16:S7:77:ARG:HG3	16:S7:79:SER:H	1.67	0.59
32:D5:22:ILE:HD11	32:D5:119:LYS:HD3	1.82	0.59
32:D5:137:LEU:HB3	32:D5:196:TRP:HD1	1.68	0.59
32:D5:603:ASN:ND2	32:D5:606:GLU:OE1	2.35	0.59
35:AK:39:SER:HB2	35:AK:54:ARG:HH22	1.68	0.59
46:B6:109:ILE:HG22	46:B6:111:GLU:H	1.68	0.59
14:S2:116:GLN:HG3	14:S2:138:ARG:HD3	1.84	0.59
15:S3:77:ASP:O	15:S3:93:VAL:O	2.21	0.59
22:A2:19:ARG:HB2	22:A2:65:TRP:HB2	1.85	0.59
26:AL:6:VAL:O	26:AL:10:GLY:N	2.34	0.59
30:D6:120:ASN:HD21	40:S5:69:GLN:HG3	1.68	0.59
2:a4:97:SER:HG	2:a4:108:THR:HG1	1.51	0.59
26:AL:78:ASP:HB2	26:AL:81:MET:HE3	1.85	0.59
32:D5:279:CYS:SG	32:D5:405:ASN:ND2	2.76	0.59
33:D4:300:ALA:O	33:D4:308:SER:OG	2.21	0.59
34:D2:122:ILE:O	34:D2:176:ARG:NH1	2.35	0.59
21:A9:48:PRO:HA	21:A9:71:MET:O	2.03	0.58
29:D1:152:SER:HG	29:D1:301:CYS:HG	1.48	0.58
5:f1:101:ARG:NH2	5:f1:130:PRO:O	2.36	0.58
10:i1:51:LEU:HB3	10:i1:54:HIS:HD2	1.68	0.58
11:V1:32:ARG:HG3	11:V1:34:LYS:H	1.68	0.58
22:A2:21:HIS:O	22:A2:62:PRO:HA	2.03	0.58
1:a1:92:ARG:NH2	1:a1:151:ASN:OD1	2.36	0.58
1:a1:239:SER:O	1:a1:421:ALA:HA	2.03	0.58
9:x1:13:UNK:HA	9:x1:23:UNK:HA	1.85	0.58
32:D5:128:MET:HE3	32:D5:251:THR:HA	1.85	0.58
57:D4:501:3PE:H291	34:D2:288:LEU:HD23	1.84	0.58
3:b2:378:LYS:HG3	6:d2:17:ARG:HH22	1.68	0.58
34:D2:30:TRP:NE1	34:D2:67:SER:OG	2.36	0.58
39:AJ:91:GLY:O	39:AJ:95:ARG:NH2	2.35	0.58
11:V1:362:CYS:N	59:V1:500:SF4:S2	2.73	0.58
11:V1:391:SER:HB2	25:A7:48:LEU:HD23	1.86	0.58
29:D1:195:ARG:HE	29:D1:274:ARG:HD2	1.67	0.58
11:V1:364:PRO:HG2	11:V1:403:THR:HG22	1.85	0.58
30:D6:25:SER:HB3	30:D6:28:TYR:HD2	1.68	0.58
2:a4:365:LYS:HG2	2:a4:399:LEU:HD22	1.84	0.58
4:c2:237:ARG:O	7:q2:12:HIS:CB	2.51	0.58
53:B1:24:TYR:OH	53:B1:28:ARG:NH2	2.32	0.58
5:f2:109:GLU:HG3	5:f2:170:ARG:HH21	1.69	0.58
27:AB:52:MET:SD	48:B9:24:ARG:NH2	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c2:23:HIS:ND1	4:c2:54:VAL:O	2.37	0.58
28:D3:80:GLN:HA	41:A3:45:ASN:HD21	1.68	0.58
37:A8:36:ASP:OD1	37:A8:39:ASN:ND2	2.35	0.58
50:B8:13:TYR:HB3	50:B8:36:PRO:HG3	1.85	0.58
3:b2:85:ASN:HD22	3:b2:243:VAL:HG12	1.68	0.58
11:V1:213:VAL:HG13	11:V1:217:GLY:HA2	1.86	0.58
15:S3:179:GLU:OE1	21:A9:40:ARG:NH2	2.36	0.58
16:S7:175:ILE:O	16:S7:179:ARG:HB2	2.04	0.58
32:D5:294:THR:H	32:D5:425:ARG:HH12	1.51	0.58
13:S1:285:ARG:HH22	26:AL:144:TYR:HB3	1.67	0.57
33:D4:388:TRP:O	44:B4:108:ARG:NH2	2.33	0.57
33:D4:254:THR:O	33:D4:258:ALA:HB2	2.04	0.57
33:D4:385:THR:HG21	33:D4:396:MET:HE3	1.85	0.57
38:BJ:141:ARG:NH1	51:BK:109:GLU:O	2.37	0.57
4:c2:70:VAL:HG21	4:c2:83:ARG:HE	1.69	0.57
11:V1:106:LYS:HE3	11:V1:224:ASN:HD21	1.69	0.57
13:S1:332:LYS:HD3	13:S1:507:TYR:HE1	1.70	0.57
28:D3:10:ASN:HD21	29:D1:10:ILE:HG21	1.70	0.57
38:BJ:145:LEU:HD13	38:BJ:149:TYR:HB3	1.87	0.57
3:b1:207:ASN:ND2	3:b1:211:ILE:O	2.37	0.57
32:D5:380:LEU:HD23	32:D5:381:THR:HG23	1.86	0.57
32:D5:482:MET:SD	32:D5:487:LYS:NZ	2.77	0.57
33:D4:225:ILE:HG13	33:D4:229:MET:HE2	1.87	0.57
36:B5:121:PRO:HB2	43:C2:5:ARG:HD3	1.85	0.57
17:S8:64:GLU:HB3	17:S8:134:GLY:HA3	1.85	0.57
22:A2:57:CYS:SG	22:A2:58:SER:N	2.75	0.57
30:D6:65:MET:HE1	31:4L:34:GLU:HG2	1.86	0.57
39:AJ:64:GLY:HA3	39:AJ:302:ARG:HH22	1.70	0.57
53:B1:35:ALA:HB1	53:B1:38:ARG:HD3	1.87	0.57
53:B1:37:PHE:HA	53:B1:40:LYS:HE2	1.85	0.57
3:b2:138:MET:HB2	3:b2:254:ASP:HB3	1.87	0.57
3:b2:214:ASP:HA	3:b2:217:LYS:HE2	1.87	0.57
31:4L:55:LEU:HB2	40:S5:24:GLN:HG3	1.85	0.57
32:D5:76:LEU:HB2	32:D5:136:ASN:HD21	1.69	0.57
11:V1:200:GLN:NE2	13:S1:174:THR:OG1	2.34	0.57
19:S6:68:HIS:HE1	19:S6:87:CYS:SG	2.16	0.57
30:D6:160:SER:HB2	34:D2:35:MET:HE2	1.87	0.57
32:D5:233:LEU:HG	32:D5:303:ALA:HB1	1.85	0.57
5:f1:89:PHE:O	5:f1:96:LEU:HB3	2.04	0.57
33:D4:423:ILE:HA	44:B4:58:VAL:HG12	1.86	0.57
33:D4:22:MET:O	33:D4:26:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A8:141:TYR:HA	45:AM:114:ARG:HD3	1.86	0.57
11:V1:111:ILE:HD11	11:V1:149:LEU:HD22	1.86	0.57
14:S2:208:MET:HE1	45:AM:11:PRO:HD3	1.87	0.57
16:S7:52:LEU:HB2	16:S7:90:GLY:HA3	1.87	0.57
45:AM:137:TYR:HA	45:AM:140:ILE:HD12	1.86	0.57
3:b2:182:HIS:HE1	55:b2:401:HEM:NC	2.00	0.56
38:BJ:66:GLU:OE2	51:BK:95:ARG:NH1	2.38	0.56
11:V1:355:LYS:HE2	13:S1:179:ASN:HD22	1.69	0.56
13:S1:276:ARG:NH1	13:S1:680:ALA:O	2.38	0.56
32:D5:234:PRO:HB3	32:D5:300:LYS:HG2	1.87	0.56
34:D2:175:LEU:HD23	34:D2:178:ILE:HD12	1.87	0.56
3:b1:344:GLU:HG3	7:q1:66:PHE:HE1	1.71	0.56
3:b2:146:ILE:HA	3:b2:149:LEU:HD12	1.87	0.56
4:c2:147:TYR:HE2	4:c2:160:ALA:HA	1.71	0.56
5:f2:28:SER:O	5:f2:32:ARG:NH1	2.38	0.56
6:d2:72:GLN:OE1	7:q2:40:ARG:NH2	2.38	0.56
14:S2:269:LEU:HD11	14:S2:373:GLU:HG2	1.86	0.56
15:S3:39:GLN:HB3	15:S3:51:CYS:HB2	1.86	0.56
15:S3:39:GLN:HE21	25:A7:67:ILE:HG22	1.71	0.56
16:S7:107:MET:O	16:S7:111:ARG:NH2	2.33	0.56
16:S7:109:GLU:O	21:A9:54:TYR:OH	2.22	0.56
21:A9:83:ARG:HA	21:A9:86:GLU:HG3	1.87	0.56
34:D2:309:ASN:HD21	39:AJ:95:ARG:HG3	1.70	0.56
35:AK:88:ASN:OD1	35:AK:88:ASN:N	2.37	0.56
40:S5:11:VAL:HG12	40:S5:13:LEU:HB3	1.87	0.56
3:b1:119:LEU:HD13	55:b1:402:HEM:HBB2	1.87	0.56
3:b2:21:LEU:HB3	3:b2:220:PHE:HB2	1.88	0.56
18:V3:70:ARG:NH2	20:S4:125:ASN:O	2.37	0.56
4:c2:230:LYS:O	6:d2:71:ARG:NH1	2.38	0.56
13:S1:627:SER:OG	13:S1:629:ASN:OD1	2.22	0.56
29:D1:152:SER:OG	29:D1:301:CYS:SG	2.62	0.56
32:D5:436:ARG:HH12	48:B9:32:HIS:H	1.54	0.56
33:D4:140:THR:HG23	33:D4:141:GLU:HG3	1.88	0.56
33:D4:205:VAL:HG22	33:D4:212:LEU:HD13	1.86	0.56
32:D5:360:GLY:H	32:D5:436:ARG:HD2	1.70	0.56
1:a1:58:PHE:HZ	1:a1:127:ILE:HG13	1.71	0.56
4:c2:206:LYS:NZ	57:f2:201:3PE:O12	2.39	0.56
11:V1:112:ARG:HH22	12:V2:193:CYS:H	1.53	0.56
12:V2:150:ASN:ND2	12:V2:162:GLU:OE1	2.33	0.56
34:D2:339:LEU:HD21	43:C2:34:ILE:HD11	1.88	0.56
50:B8:66:HIS:HB2	50:B8:71:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:5:ALA:O	1:a1:9:GLN:HB2	2.06	0.56
1:a1:294:LEU:HB2	1:a1:341:GLN:HG3	1.88	0.56
2:a4:309:VAL:HG22	2:a4:326:THR:HG22	1.86	0.56
5:f2:156:TYR:HB2	5:f2:165:TYR:HB2	1.88	0.56
7:q2:26:PHE:HB3	7:q2:29:TYR:HB2	1.87	0.56
29:D1:236:ILE:HG23	29:D1:259:PHE:HZ	1.70	0.56
34:D2:115:VAL:HG12	34:D2:180:ALA:HB1	1.87	0.56
33:D4:35:SER:OG	33:D4:70:MET:O	2.24	0.56
2:a4:385:GLN:NE2	2:a4:391:SER:O	2.39	0.56
21:A9:120:VAL:O	21:A9:124:ALA:HB2	2.05	0.56
32:D5:260:LEU:HD22	32:D5:277:MET:HE1	1.88	0.56
7:q2:28:HIS:HB3	7:q2:31:SER:HB2	1.88	0.55
13:S1:478:ARG:NH1	13:S1:487:TRP:O	2.38	0.55
6:d1:33:ARG:NH2	6:d1:91:GLU:OE1	2.39	0.55
6:d1:75:LEU:O	6:d1:80:TRP:NE1	2.39	0.55
14:S2:251:LEU:HD13	15:S3:73:LYS:HG3	1.89	0.55
33:D4:266:LEU:HB3	33:D4:395:LEU:HD13	1.89	0.55
50:B8:55:GLN:O	50:B8:70:ARG:NH2	2.38	0.55
3:b1:85:ASN:HD22	3:b1:243:VAL:HG12	1.71	0.55
5:f2:118:ARG:HG2	5:f2:171:ILE:HG21	1.87	0.55
34:D2:323:MET:SD	34:D2:323:MET:N	2.79	0.55
1:a1:21:ASN:HD21	1:a1:220:SER:H	1.52	0.55
4:c1:165:ASN:ND2	8:h1:15:ASP:OD2	2.39	0.55
11:V1:101:GLU:H	11:V1:184:TYR:HE1	1.54	0.55
13:S1:159:CYS:HB2	13:S1:199:ILE:HD11	1.88	0.55
16:S7:158:TYR:HE1	26:AL:79:GLY:H	1.53	0.55
22:A2:19:ARG:HE	22:A2:65:TRP:HE3	1.55	0.55
23:A5:24:LYS:HZ2	23:A5:59:LYS:HD3	1.71	0.55
29:D1:55:LEU:HD12	29:D1:221:ALA:HB2	1.88	0.55
47:B7:6:ARG:HH12	47:B7:105:ARG:HH21	1.55	0.55
3:b1:148:ASN:ND2	5:f2:142:LEU:O	2.39	0.55
10:i1:52:TRP:O	10:i1:56:LYS:HB2	2.06	0.55
14:S2:107:ASP:OD2	14:S2:110:SER:OG	2.25	0.55
17:S8:32:ARG:NH2	45:AM:27:ARG:O	2.40	0.55
36:B5:9:PHE:HB2	46:B6:27:LEU:HD22	1.89	0.55
2:a2:165:ALA:HA	2:a2:173:ALA:HB1	1.88	0.55
3:b1:207:ASN:ND2	3:b1:209:THR:OG1	2.40	0.55
13:S1:41:CYS:HB3	13:S1:52:CYS:HB3	1.87	0.55
29:D1:102:VAL:HB	29:D1:150:LEU:HD21	1.88	0.55
3:b2:240:MET:HA	3:b2:243:VAL:HG22	1.89	0.55
3:b2:281:LEU:HD22	3:b2:294:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:i2:52:TRP:O	10:i2:56:LYS:HB3	2.07	0.55
14:S2:129:GLN:HE21	14:S2:135:GLN:HE22	1.55	0.55
31:4L:73:LEU:HD22	34:D2:38:LEU:HD23	1.89	0.55
32:D5:396:ILE:HD11	32:D5:490:ALA:HB2	1.89	0.55
37:A8:46:ARG:NH1	45:AM:79:ASP:OD2	2.39	0.55
5:f2:81:ILE:HG23	5:f2:85:LYS:HE3	1.87	0.55
32:D5:17:MET:HG2	46:B6:73:HIS:HE1	1.72	0.55
34:D2:106:LEU:HD23	34:D2:138:PRO:HB2	1.88	0.55
39:AJ:202:ILE:O	39:AJ:206:TYR:HB2	2.07	0.55
47:B7:34:LYS:HE3	47:B7:36:ARG:HB2	1.89	0.55
3:b1:66:VAL:HA	3:b1:69:ILE:HD12	1.88	0.55
1:a3:438:ARG:HH22	5:f2:33:LYS:HE3	1.70	0.55
8:h2:28:GLU:HG3	8:h2:30:CYS:H	1.72	0.55
14:S2:115:GLU:HB3	14:S2:194:VAL:HB	1.88	0.54
33:D4:187:PRO:O	33:D4:192:ASN:ND2	2.39	0.54
36:B5:56:PRO:HG2	36:B5:59:TYR:HB3	1.89	0.54
39:AJ:19:THR:OG1	39:AJ:20:GLU:N	2.39	0.54
39:AJ:72:ARG:NH1	39:AJ:295:GLU:OE1	2.40	0.54
3:b2:237:LEU:HB2	4:c2:211:MET:HE2	1.90	0.54
14:S2:341:SER:OG	14:S2:342:MET:N	2.40	0.54
26:AL:67:GLU:HG2	26:AL:72:ASN:H	1.72	0.54
27:AB:21:LEU:HD21	42:B3:47:ASN:HA	1.88	0.54
39:AJ:25:ILE:O	39:AJ:123:VAL:HA	2.07	0.54
21:A9:168:PRO:HA	21:A9:230:PHE:HB2	1.88	0.54
29:D1:220:PHE:O	29:D1:224:PHE:HB2	2.08	0.54
35:AK:80:ARG:NH2	35:AK:85:ASP:OD2	2.41	0.54
3:b1:8:HIS:HB3	3:b1:11:MET:HB2	1.90	0.54
3:b2:119:LEU:HD13	55:b2:402:HEM:HBB2	1.89	0.54
3:b2:312:GLN:NE2	3:b2:317:PHE:O	2.40	0.54
31:4L:40:LEU:HD22	34:D2:75:ILE:HD12	1.89	0.54
37:A8:132:THR:OG1	41:A3:57:ARG:NH1	2.41	0.54
11:V1:289:GLY:HA3	11:V1:293:ASN:HD22	1.72	0.54
12:V2:27:ASN:OD1	12:V2:30:ARG:NH1	2.40	0.54
13:S1:379:LEU:HB3	13:S1:407:ALA:O	2.06	0.54
14:S2:184:VAL:O	17:S8:60:ARG:NH2	2.32	0.54
31:4L:54:THR:HG23	40:S5:24:GLN:HG2	1.88	0.54
43:C2:25:LYS:N	43:C2:28:ASP:OD2	2.41	0.54
4:c1:172:ASP:OD1	4:c1:172:ASP:N	2.41	0.54
2:a4:148:LYS:NZ	2:a4:180:ASP:OD1	2.39	0.54
21:A9:92:ILE:HG22	21:A9:130:ILE:HB	1.89	0.54
21:A9:94:LEU:HG	21:A9:132:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D5:3:LEU:HD22	32:D5:53:MET:HE1	1.88	0.54
33:D4:207:MET:HG3	33:D4:298:ILE:HD11	1.90	0.54
50:B8:2:SER:OG	50:B8:3:HIS:N	2.41	0.54
11:V1:33:LEU:HD23	11:V1:155:GLU:HB3	1.89	0.54
20:S4:11:ILE:HD11	24:A6:22:ARG:HG3	1.90	0.54
32:D5:205:ASN:HD22	38:BJ:121:ARG:HH22	1.55	0.54
32:D5:441:ILE:HD13	49:B2:15:PRO:HB3	1.90	0.54
1:a1:115:ASP:HA	1:a1:119:ASN:HB2	1.90	0.54
3:b1:214:ASP:HA	3:b1:217:LYS:HE2	1.88	0.54
13:S1:8:LEU:HD22	13:S1:19:MET:HB3	1.90	0.54
32:D5:341:MET:HE3	32:D5:454:ILE:HD13	1.90	0.54
32:D5:441:ILE:HD11	49:B2:10:ARG:HG2	1.88	0.54
4:c2:20:SER:OG	4:c2:21:LEU:N	2.40	0.54
5:f2:98:VAL:HG12	5:f2:134:ILE:HG12	1.90	0.54
15:S3:37:VAL:HG12	25:A7:69:MET:HG2	1.88	0.54
17:S8:74:GLU:OE1	17:S8:99:ARG:NH2	2.37	0.54
17:S8:135:PRO:HG3	17:S8:164:GLU:HG2	1.90	0.54
21:A9:165:ILE:O	21:A9:227:THR:HA	2.08	0.54
22:A2:78:LEU:HD22	22:A2:86:VAL:HG22	1.89	0.54
27:AA:36:PHE:HA	27:AA:40:LEU:HD13	1.89	0.54
32:D5:439:THR:OG1	32:D5:440:LEU:N	2.41	0.54
5:f2:86:ASN:OD1	5:f2:156:TYR:OH	2.26	0.53
11:V1:300:GLY:HA2	11:V1:330:GLY:H	1.74	0.53
13:S1:382:THR:HB	13:S1:454:GLY:HA3	1.89	0.53
15:S3:40:VAL:HB	25:A7:68:VAL:O	2.09	0.53
31:4L:20:LEU:HG	32:D5:588:PHE:HD1	1.73	0.53
63:AB:101:ZMP:O2	63:AB:101:ZMP:N2	2.37	0.53
45:AM:85:MET:O	45:AM:89:ASN:HB2	2.08	0.53
1:a1:354:VAL:HG12	1:a1:358:LYS:HE2	1.91	0.53
4:c1:142:LEU:HD12	4:c1:143:ARG:HG2	1.89	0.53
38:BJ:69:ARG:NH1	38:BJ:90:GLN:OE1	2.41	0.53
29:D1:91:MET:SD	29:D1:91:MET:N	2.81	0.53
32:D5:427:ILE:HG23	32:D5:431:LEU:HD12	1.89	0.53
32:D5:60:GLU:O	46:B6:99:LYS:HB3	2.09	0.53
40:S5:46:ILE:HG23	40:S5:50:ARG:HG3	1.91	0.53
45:AM:93:GLU:HA	45:AM:96:ILE:HG22	1.91	0.53
48:B9:29:ARG:NH2	48:B9:74:GLN:O	2.41	0.53
49:B2:45:ASP:O	49:B2:50:HIS:NE2	2.41	0.53
1:a1:102:LEU:HD23	1:a1:104:LYS:HE3	1.89	0.53
2:a2:46:ARG:HH21	2:a2:379:LEU:HD23	1.73	0.53
11:V1:365:CYS:SG	11:V1:366:ARG:N	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A6:46:VAL:HA	24:A6:51:LEU:HD12	1.90	0.53
33:D4:60:SER:OG	51:BK:84:ARG:NH2	2.41	0.53
34:D2:327:PRO:HB3	43:C2:44:ILE:HG23	1.91	0.53
1:a1:70:ARG:HB3	1:a1:74:ALA:HB3	1.89	0.53
13:S1:378:LEU:HG	13:S1:451:VAL:HG22	1.90	0.53
27:AA:70:LEU:HD13	27:AA:76:ILE:HG12	1.89	0.53
6:d1:41:ASP:HA	6:d1:44:LYS:HD3	1.90	0.53
4:c2:131:LEU:HG	4:c2:163:ILE:HD13	1.91	0.53
30:D6:58:LEU:O	30:D6:62:GLY:CA	2.57	0.53
32:D5:584:ILE:HD11	34:D2:58:LYS:HE2	1.90	0.53
33:D4:350:THR:OG1	33:D4:351:LEU:N	2.41	0.53
1:a3:25:VAL:HA	1:a3:197:LEU:O	2.09	0.53
1:a3:392:LEU:HA	1:a3:395:TRP:HD1	1.74	0.53
14:S2:284:ASP:OD1	14:S2:284:ASP:N	2.41	0.53
33:D4:195:MET:HE3	33:D4:250:LEU:HD11	1.91	0.53
35:AK:133:LYS:HZ1	35:AK:137:GLU:HG2	1.73	0.53
39:AJ:117:SER:HA	39:AJ:260:ARG:HH22	1.72	0.53
3:b1:29:SER:HA	3:b1:227:LYS:HZ1	1.74	0.53
1:a3:117:VAL:HG11	1:a3:195:MET:HE1	1.91	0.53
4:c2:32:VAL:HG22	4:c2:168:LEU:HD21	1.90	0.53
13:S1:126:ASP:HB2	14:S2:328:ALA:HB3	1.91	0.53
21:A9:109:VAL:O	21:A9:113:ILE:HB	2.09	0.53
23:A5:17:GLU:HG2	23:A5:18:THR:HG23	1.90	0.53
1:a3:49:THR:O	1:a3:165:GLN:NE2	2.40	0.53
5:f2:129:LYS:HE3	5:f2:132:TRP:HD1	1.74	0.53
13:S1:245:GLY:HA2	20:S4:64:ARG:HD2	1.91	0.53
13:S1:348:VAL:O	13:S1:459:GLN:NE2	2.39	0.53
13:S1:407:ALA:HA	13:S1:420:ASP:O	2.09	0.53
32:D5:123:LEU:HD21	64:D5:901:CDL:H731	1.91	0.53
57:D5:902:3PE:H351	33:D4:405:LEU:HD13	1.91	0.53
2:a2:243:GLU:HA	2:a2:424:MET:O	2.09	0.52
7:q1:26:PHE:HB3	7:q1:29:TYR:HB2	1.90	0.52
13:S1:117:GLN:HG2	14:S2:346:ILE:HG23	1.91	0.52
14:S2:356:TYR:HB2	25:A7:59:ARG:HH12	1.75	0.52
21:A9:136:ASN:HD22	21:A9:292:ARG:HD2	1.74	0.52
29:D1:69:SER:O	29:D1:73:LEU:HB2	2.08	0.52
34:D2:321:LYS:O	43:C2:49:ARG:NH2	2.42	0.52
2:a2:97:SER:OG	2:a2:108:THR:OG1	2.23	0.52
5:f2:103:LYS:HD2	5:f2:106:ILE:HD12	1.91	0.52
11:V1:372:MET:HG2	11:V1:392:LEU:HD11	1.91	0.52
13:S1:377:VAL:HA	13:S1:450:MET:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d1:34:ASP:OD2	6:d1:89:TYR:N	2.34	0.52
5:f2:118:ARG:NH1	5:f2:174:GLY:O	2.42	0.52
11:V1:370:ASP:OD1	13:S1:179:ASN:ND2	2.43	0.52
12:V2:50:VAL:HG21	12:V2:73:LEU:HD11	1.92	0.52
13:S1:99:ALA:O	13:S1:134:LYS:NZ	2.41	0.52
13:S1:430:GLN:HE21	13:S1:656:LEU:HD22	1.73	0.52
32:D5:597:ILE:HD11	35:AK:34:VAL:HG22	1.92	0.52
34:D2:106:LEU:HB3	34:D2:138:PRO:HG2	1.92	0.52
5:f1:83:GLU:HG2	5:f1:102:THR:HG22	1.91	0.52
8:h1:24:CYS:SG	8:h1:72:LYS:NZ	2.82	0.52
2:a4:279:LEU:HB3	2:a4:295:LEU:HD11	1.91	0.52
3:b2:215:THR:HG22	7:q2:8:THR:HG21	1.90	0.52
13:S1:324:ASP:HA	13:S1:573:TYR:HE1	1.75	0.52
13:S1:433:ALA:O	13:S1:476:LYS:NZ	2.43	0.52
32:D5:77:SER:O	32:D5:136:ASN:ND2	2.34	0.52
32:D5:127:THR:HG21	32:D5:146:GLY:HA3	1.92	0.52
32:D5:580:GLN:HE21	35:AK:42:LEU:HD12	1.75	0.52
34:D2:26:TRP:HB3	34:D2:74:ILE:HD13	1.90	0.52
46:B6:25:GLN:NE2	48:B9:117:TYR:OH	2.35	0.52
1:a1:193:PRO:HD2	1:a1:194:ARG:HG3	1.90	0.52
2:a2:69:LEU:HD23	2:a2:191:LEU:HD22	1.90	0.52
3:b1:324:MET:HB3	3:b1:366:MET:HE1	1.92	0.52
1:a3:26:ALA:O	1:a3:198:ALA:HA	2.10	0.52
6:d2:32:MET:SD	6:d2:61:ARG:NH1	2.82	0.52
11:V1:301:GLY:HA2	11:V1:333:ALA:HB3	1.91	0.52
21:A9:167:LYS:O	21:A9:229:ALA:HA	2.10	0.52
42:B3:53:MET:HA	42:B3:57:ALA:HB2	1.92	0.52
46:B6:119:MET:SD	46:B6:120:LYS:N	2.82	0.52
1:a1:43:ALA:O	1:a1:95:THR:OG1	2.25	0.52
2:a2:47:ILE:HG21	2:a2:120:MET:HE1	1.92	0.52
2:a2:197:ASN:OD1	2:a2:198:HIS:ND1	2.43	0.52
1:a3:85:HIS:HB2	1:a3:100:LYS:HB2	1.92	0.52
13:S1:324:ASP:HB2	13:S1:327:ALA:H	1.74	0.52
16:S7:108:PRO:HB2	29:D1:58:LYS:HE2	1.92	0.52
30:D6:159:TRP:HE1	34:D2:12:THR:HG22	1.74	0.52
2:a2:290:ASN:HB3	2:a2:293:SER:HB3	1.92	0.52
20:S4:56:LYS:HG2	20:S4:85:THR:HG22	1.92	0.52
21:A9:251:ARG:HE	21:A9:322:ARG:HG3	1.74	0.52
30:D6:14:VAL:HG22	31:4L:11:ALA:HB2	1.91	0.52
44:B4:22:TYR:HD2	48:B9:64:ARG:HH11	1.57	0.52
3:b1:282:ARG:NH2	3:b1:341:GLN:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b2:182:HIS:HE1	55:b2:401:HEM:C4C	2.28	0.52
6:d2:35:ASP:OD1	6:d2:89:TYR:OH	2.28	0.52
13:S1:122:MET:O	25:A7:60:ARG:NH2	2.43	0.52
33:D4:102:LEU:HD21	33:D4:230:VAL:HG11	1.91	0.52
33:D4:196:TRP:CE2	33:D4:200:MET:HG3	2.44	0.52
5:f1:14:ARG:HG2	7:q1:22:GLU:HG3	1.92	0.52
5:f2:164:HIS:N	5:f2:173:LYS:O	2.42	0.52
11:V1:367:GLU:OE1	13:S1:100:ASN:ND2	2.43	0.52
13:S1:544:VAL:HG22	13:S1:559:VAL:HB	1.91	0.52
15:S3:74:SER:HB3	15:S3:97:LEU:HB3	1.91	0.52
19:S6:51:GLN:HG2	19:S6:92:ARG:HB2	1.91	0.52
20:S4:33:ARG:NH2	20:S4:77:ASP:OD1	2.43	0.52
21:A9:319:ARG:NH2	24:A6:52:ASP:OD1	2.43	0.52
2:a4:143:GLN:HA	2:a4:146:ILE:HD12	1.92	0.52
7:q2:61:TRP:NE1	7:q2:65:GLU:OE2	2.43	0.52
11:V1:157:TYR:HD2	18:V3:58:LEU:HD12	1.75	0.52
14:S2:369:ALA:HB2	14:S2:374:PHE:HB2	1.92	0.52
15:S3:66:ASP:HB2	23:A5:89:LEU:HD23	1.91	0.52
22:A2:54:ILE:O	22:A2:55:ARG:NH1	2.39	0.52
22:A2:64:LEU:HD22	22:A2:78:LEU:HD11	1.92	0.52
24:A6:63:ARG:NH1	27:AA:49:GLU:OE2	2.43	0.52
28:D3:77:TRP:HA	29:D1:317:GLN:HE22	1.74	0.52
36:B5:104:ARG:NH2	37:A8:166:LEU:O	2.43	0.52
1:a1:246:ASP:H	7:q1:11:ARG:HG2	1.75	0.51
6:d2:14:GLU:HA	6:d2:17:ARG:HD3	1.92	0.51
11:V1:78:LYS:NZ	60:V1:501:FMN:O2P	2.36	0.51
13:S1:378:LEU:HD23	13:S1:443:LEU:HD11	1.91	0.51
32:D5:24:PHE:HE1	64:D5:901:CDL:H331	1.74	0.51
45:AM:89:ASN:ND2	45:AM:92:GLU:OE1	2.43	0.51
48:B9:108:PRO:HA	48:B9:111:LYS:HB2	1.92	0.51
54:A1:6:LEU:O	54:A1:10:ALA:HB2	2.10	0.51
4:c1:230:LYS:HD3	6:d1:71:ARG:HG2	1.93	0.51
4:c2:143:ARG:HB2	4:c2:146:LEU:HD12	1.92	0.51
15:S3:63:PHE:HD2	15:S3:64:LEU:HD12	1.74	0.51
34:D2:267:ILE:HD12	34:D2:279:PRO:HB3	1.93	0.51
45:AM:81:ARG:HG2	45:AM:85:MET:HE1	1.92	0.51
3:b1:159:ASN:ND2	3:b1:162:GLU:OE1	2.44	0.51
2:a4:314:ALA:HB3	2:a4:321:LEU:HB2	1.92	0.51
3:b2:45:ILE:HA	55:b2:401:HEM:HAB	1.92	0.51
12:V2:88:THR:HG22	13:S1:177:ARG:HH22	1.76	0.51
33:D4:409:TYR:O	33:D4:413:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AJ:77:CYS:O	39:AJ:92:ASN:ND2	2.38	0.51
4:c1:71:GLN:NE2	4:c1:80:MET:SD	2.80	0.51
1:a3:255:ILE:HD12	1:a3:335:MET:HE1	1.92	0.51
13:S1:283:MET:HA	13:S1:293:HIS:HA	1.92	0.51
13:S1:460:ARG:HG3	13:S1:462:ASP:H	1.76	0.51
33:D4:11:MET:HE3	33:D4:111:THR:HG21	1.92	0.51
34:D2:328:THR:HG23	43:C2:68:PHE:HZ	1.75	0.51
35:AK:137:GLU:HB3	35:AK:139:LYS:HG3	1.92	0.51
2:a2:71:LEU:HD13	2:a2:143:GLN:HG3	1.93	0.51
13:S1:230:VAL:HG23	13:S1:231:MET:HG3	1.92	0.51
13:S1:386:PHE:HE1	13:S1:668:ILE:HD13	1.75	0.51
32:D5:241:THR:HG21	32:D5:344:GLY:HA3	1.93	0.51
3:b1:240:MET:HA	3:b1:243:VAL:HG22	1.91	0.51
4:c1:12:TRP:HB2	4:c1:15:ARG:HB2	1.93	0.51
8:h1:20:VAL:HA	8:h1:23:GLN:HG2	1.92	0.51
1:a3:294:LEU:HB2	1:a3:341:GLN:HG3	1.93	0.51
16:S7:55:CYS:HB3	16:S7:89:ALA:HB1	1.93	0.51
50:B8:53:ARG:NH2	50:B8:84:TYR:OH	2.35	0.51
53:B1:54:VAL:HG21	53:B1:57:LYS:HE2	1.92	0.51
1:a3:264:ASN:N	1:a3:264:ASN:OD1	2.42	0.51
3:b2:92:ILE:HD11	3:b2:272:TRP:HH2	1.76	0.51
11:V1:101:GLU:O	11:V1:104:THR:OG1	2.29	0.51
13:S1:222:THR:HG22	13:S1:243:ARG:HB2	1.92	0.51
15:S3:38:GLN:CA	25:A7:70:SER:O	2.48	0.51
20:S4:12:THR:HB	24:A6:16:VAL:H	1.76	0.51
32:D5:332:HIS:CE1	32:D5:336:LYS:HD2	2.46	0.51
32:D5:363:PHE:HA	32:D5:370:THR:HG21	1.93	0.51
2:a4:29:LEU:HD22	2:a4:30:PRO:HD2	1.91	0.51
2:a4:78:LYS:HE3	2:a4:129:ALA:HB1	1.92	0.51
34:D2:88:LYS:HG3	34:D2:148:SER:HB3	1.92	0.51
3:b1:45:ILE:HA	55:b1:401:HEM:HAB	1.93	0.51
1:a3:124:ASP:HA	1:a3:127:ILE:HG22	1.92	0.51
19:S6:7:THR:O	19:S6:25:ARG:NH2	2.44	0.51
22:A2:65:TRP:NE1	22:A2:75:ASN:OD1	2.44	0.51
24:A6:63:ARG:HB2	27:AA:45:LEU:HD21	1.91	0.51
2:a4:169:ARG:NE	2:a4:239:TYR:O	2.39	0.51
23:A5:23:LEU:HD22	23:A5:58:VAL:HG11	1.93	0.51
32:D5:83:ASP:O	32:D5:85:PHE:N	2.43	0.51
34:D2:49:ASN:N	34:D2:49:ASN:OD1	2.43	0.51
42:B3:38:ARG:HG3	42:B3:40:LEU:HD13	1.93	0.51
45:AM:124:TYR:HB3	45:AM:132:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b1:177:ARG:NH2	5:f2:62:MET:O	2.41	0.50
5:f1:99:ARG:NH2	5:f1:105:GLU:OE1	2.44	0.50
11:V1:138:ILE:O	11:V1:180:GLY:N	2.44	0.50
31:4L:62:ILE:HA	31:4L:65:VAL:HG12	1.92	0.50
33:D4:204:MET:HE2	33:D4:243:MET:HE1	1.93	0.50
1:a1:21:ASN:OD1	1:a1:221:GLY:N	2.44	0.50
1:a3:86:LEU:HD23	2:a4:285:VAL:HG13	1.94	0.50
4:c2:58:GLU:HG2	4:c2:62:LYS:HE2	1.93	0.50
14:S2:287:ILE:HB	17:S8:4:TYR:HB3	1.93	0.50
28:D3:69:ILE:HD11	29:D1:144:VAL:HG13	1.92	0.50
33:D4:82:HIS:HB2	33:D4:432:ARG:HH12	1.75	0.50
44:B4:13:LEU:HD22	44:B4:14:PRO:HD2	1.91	0.50
48:B9:10:THR:HG23	48:B9:13:GLN:H	1.76	0.50
1:a1:255:ILE:HG21	1:a1:335:MET:HE1	1.93	0.50
2:a2:76:THR:HG22	2:a2:82:SER:H	1.76	0.50
3:b1:377:LEU:O	6:d1:33:ARG:NH1	2.44	0.50
1:a3:14:THR:OG1	1:a3:389:ARG:NH1	2.43	0.50
4:c2:12:TRP:HB2	4:c2:15:ARG:HB2	1.93	0.50
12:V2:35:VAL:HG11	12:V2:43:LYS:HG3	1.93	0.50
20:S4:125:ASN:OD1	20:S4:125:ASN:N	2.44	0.50
27:AB:82:ASP:OD1	46:B6:15:ARG:NH2	2.44	0.50
5:f1:9:ASP:OD2	5:f1:14:ARG:NH1	2.41	0.50
5:f2:166:ASP:OD1	5:f2:170:ARG:N	2.44	0.50
8:h2:34:ARG:HD2	8:h2:65:ARG:HH22	1.75	0.50
11:V1:362:CYS:HB3	11:V1:364:PRO:HD2	1.93	0.50
34:D2:202:LEU:HD11	40:S5:1:PRO:HD3	1.94	0.50
1:a1:359:ASN:O	1:a1:363:ASN:ND2	2.45	0.50
29:D1:169:GLN:NE2	29:D1:240:THR:O	2.44	0.50
42:B3:21:TRP:HB3	42:B3:49:ALA:HB3	1.94	0.50
2:a4:31:ASN:ND2	2:a4:225:ASN:OD1	2.45	0.50
24:A6:27:ALA:HB1	24:A6:78:VAL:HG11	1.94	0.50
28:D3:80:GLN:NE2	29:D1:317:GLN:O	2.34	0.50
34:D2:230:LEU:HB3	34:D2:300:THR:HG22	1.93	0.50
34:D2:244:VAL:HG11	34:D2:300:THR:HG21	1.94	0.50
1:a1:53:ASN:ND2	1:a1:166:SER:O	2.42	0.50
12:V2:97:LYS:HB3	12:V2:136:LEU:HB3	1.93	0.50
16:S7:25:ARG:HA	16:S7:28:TYR:HB3	1.93	0.50
17:S8:34:LEU:HD12	29:D1:272:TRP:CE2	2.46	0.50
33:D4:254:THR:O	33:D4:258:ALA:CB	2.60	0.50
4:c1:56:TYR:HD1	4:c1:60:GLU:HB3	1.77	0.50
3:b2:311:LYS:HD3	3:b2:379:TRP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V1:86:SER:OG	11:V1:91:LYS:NZ	2.45	0.50
13:S1:444:GLN:HA	13:S1:477:ILE:HG23	1.93	0.50
29:D1:154:LEU:HD13	29:D1:160:PHE:HE1	1.77	0.50
30:D6:49:GLY:N	30:D6:139:GLU:OE2	2.33	0.50
2:a2:361:LYS:HD3	2:a2:403:ASP:HA	1.94	0.50
2:a4:261:SER:HB3	2:a4:322:PHE:HB2	1.93	0.50
17:S8:74:GLU:OE2	17:S8:105:ARG:NH2	2.45	0.50
21:A9:117:ILE:O	21:A9:121:SER:OG	2.25	0.50
32:D5:452:ASN:HB3	32:D5:456:ARG:HH22	1.76	0.50
2:a2:46:ARG:NH1	2:a2:110:GLU:OE1	2.45	0.49
2:a2:254:HIS:ND1	2:a2:325:TYR:OH	2.43	0.49
4:c2:14:HIS:NE2	4:c2:124:GLU:OE2	2.42	0.49
14:S2:354:GLU:HA	15:S3:199:LEU:HD22	1.94	0.49
24:A6:60:ASP:HA	24:A6:63:ARG:HG2	1.93	0.49
32:D5:305:SER:C	32:D5:336:LYS:HZ3	2.20	0.49
38:BJ:98:ASP:OD2	38:BJ:141:ARG:NH2	2.44	0.49
13:S1:300:LEU:HD22	13:S1:603:LEU:HD23	1.93	0.49
14:S2:227:GLU:OE1	25:A7:17:ARG:NH2	2.46	0.49
17:S8:160:LYS:HD2	17:S8:161:TRP:HZ3	1.78	0.49
27:AB:34:SER:OG	27:AB:35:HIS:N	2.44	0.49
3:b1:179:PHE:O	3:b1:183:PHE:HB2	2.12	0.49
12:V2:144:CYS:SG	12:V2:145:LEU:N	2.85	0.49
13:S1:279:LEU:H	13:S1:549:HIS:H	1.59	0.49
15:S3:80:ALA:HB2	15:S3:92:ILE:HD13	1.93	0.49
21:A9:91:VAL:HG13	21:A9:129:PHE:HD1	1.77	0.49
26:AL:39:VAL:HG21	26:AL:50:GLU:HB3	1.94	0.49
39:AJ:17:LYS:HG2	39:AJ:118:THR:HA	1.94	0.49
2:a4:197:ASN:OD1	2:a4:198:HIS:ND1	2.45	0.49
21:A9:319:ARG:NH2	24:A6:50:GLN:O	2.44	0.49
29:D1:151:LEU:HD12	29:D1:154:LEU:HD11	1.94	0.49
30:D6:122:MET:SD	40:S5:79:LYS:NZ	2.77	0.49
32:D5:544:MET:O	32:D5:548:SER:OG	2.24	0.49
33:D4:403:THR:HA	33:D4:406:TYR:CE1	2.48	0.49
34:D2:211:MET:O	34:D2:214:THR:OG1	2.26	0.49
38:BJ:146:GLY:HA3	43:C2:119:VAL:HG23	1.93	0.49
39:AJ:151:HIS:CG	39:AJ:279:LEU:HD11	2.48	0.49
1:a1:85:HIS:HB2	1:a1:100:LYS:HB2	1.94	0.49
2:a2:168:TYR:HB2	2:a2:173:ALA:HB2	1.95	0.49
18:V3:74:ARG:NH2	20:S4:131:SER:OG	2.43	0.49
2:a2:362:ASN:HD22	2:a2:365:LYS:HD3	1.78	0.49
3:b1:116:GLY:HA3	55:b1:402:HEM:HBC2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D4:82:HIS:O	33:D4:86:LYS:NZ	2.45	0.49
42:B3:47:ASN:HB3	42:B3:48:GLU:HG3	1.95	0.49
11:V1:179:ARG:NH1	12:V2:52:ASP:OD2	2.44	0.49
11:V1:305:PRO:HG3	11:V1:413:TRP:HB3	1.94	0.49
21:A9:134:HIS:NE2	21:A9:170:ASP:OD1	2.45	0.49
32:D5:10:VAL:HA	32:D5:13:ILE:HG22	1.95	0.49
32:D5:448:PRO:O	32:D5:452:ASN:ND2	2.46	0.49
33:D4:106:LEU:HD13	33:D4:234:ILE:HG21	1.94	0.49
5:f1:9:ASP:OD2	5:f1:11:SER:OG	2.24	0.49
13:S1:449:PRO:HD2	13:S1:483:VAL:HG21	1.94	0.49
14:S2:84:HIS:HD2	15:S3:152:LEU:HB3	1.78	0.49
14:S2:282:GLU:HB2	14:S2:313:GLN:HE22	1.77	0.49
15:S3:94:TYR:HB2	15:S3:107:VAL:HB	1.94	0.49
33:D4:231:LEU:O	33:D4:235:LEU:HB2	2.13	0.49
47:B7:34:LYS:HG3	50:B8:156:TYR:HA	1.95	0.49
9:x1:15:UNK:HA	9:x1:21:UNK:HA	1.95	0.49
10:i1:51:LEU:HB3	10:i1:54:HIS:CD2	2.46	0.49
8:h2:29:LYS:HA	8:h2:32:LYS:HB2	1.95	0.49
11:V1:309:LYS:NZ	11:V1:313:GLU:OE2	2.43	0.49
15:S3:86:ARG:NH1	15:S3:91:GLU:OE2	2.41	0.49
32:D5:295:GLN:H	32:D5:425:ARG:HH22	1.59	0.49
1:a3:100:LYS:HE3	2:a4:370:MET:HE3	1.95	0.49
33:D4:370:PRO:HA	33:D4:375:LEU:HD13	1.95	0.49
33:D4:372:SER:OG	33:D4:373:ILE:N	2.43	0.49
12:V2:156:ILE:HG12	12:V2:161:TYR:HE2	1.78	0.48
14:S2:405:MET:SD	14:S2:421:GLN:NE2	2.85	0.48
16:S7:139:ILE:HG22	16:S7:140:VAL:HG13	1.93	0.48
32:D5:341:MET:SD	32:D5:453:SER:OG	2.70	0.48
34:D2:69:LEU:HD11	34:D2:97:LEU:HD22	1.94	0.48
4:c1:130:LEU:HD21	56:c1:501:HEC:HBA1	1.95	0.48
3:b2:312:GLN:HE21	3:b2:318:ARG:HG3	1.78	0.48
5:f2:139:CYS:N	5:f2:144:CYS:O	2.36	0.48
13:S1:45:ARG:HD3	20:S4:114:LYS:HZ1	1.77	0.48
13:S1:465:ALA:HB2	13:S1:654:GLN:HB2	1.94	0.48
22:A2:47:ASN:HB3	22:A2:50:LEU:HD13	1.95	0.48
28:D3:60:ILE:HG21	30:D6:168:ILE:HG21	1.95	0.48
35:AK:68:ILE:HD13	35:AK:99:THR:HG21	1.95	0.48
38:BJ:159:LYS:NZ	43:C2:112:VAL:O	2.46	0.48
47:B7:108:LEU:O	47:B7:112:LYS:HB2	2.13	0.48
1:a1:233:PRO:HD2	5:f1:22:THR:HG23	1.95	0.48
4:c1:115:TYR:O	4:c1:119:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c2:86:LYS:N	4:c2:89:ASP:OD2	2.46	0.48
6:d2:91:GLU:O	6:d2:95:LYS:CB	2.62	0.48
11:V1:393:TRP:HB2	11:V1:419:ILE:HD13	1.95	0.48
12:V2:22:ASP:OD1	12:V2:28:TYR:OH	2.31	0.48
17:S8:143:THR:HA	21:A9:60:ARG:HH22	1.77	0.48
29:D1:165:LEU:HD21	29:D1:241:LEU:HA	1.95	0.48
37:A8:93:LEU:HD22	54:A1:44:GLN:HE22	1.78	0.48
50:B8:50:LEU:HB2	50:B8:78:HIS:HD2	1.78	0.48
2:a2:130:PRO:HG2	2:a2:195:VAL:HG11	1.94	0.48
4:c1:41:HIS:HB3	4:c1:113:LEU:HD13	1.95	0.48
5:f2:122:HIS:HD2	5:f2:124:LEU:HB2	1.78	0.48
13:S1:91:GLU:OE2	25:A7:54:CYS:N	2.47	0.48
14:S2:175:GLU:OE2	16:S7:61:HIS:ND1	2.47	0.48
15:S3:204:GLU:H	20:S4:50:ASN:HD22	1.60	0.48
28:D3:83:ASN:HD22	30:D6:148:SER:HB2	1.77	0.48
30:D6:127:ILE:HG21	40:S5:68:ARG:HD2	1.95	0.48
32:D5:15:LEU:HD21	32:D5:125:LEU:HD22	1.95	0.48
32:D5:71:ILE:HG13	32:D5:72:GLN:H	1.78	0.48
32:D5:106:TRP:CD1	32:D5:447:ASN:HD21	2.32	0.48
35:AK:17:CYS:SG	35:AK:18:HIS:N	2.85	0.48
38:BJ:158:GLN:HE22	51:BK:111:ASN:HA	1.78	0.48
45:AM:29:LEU:O	45:AM:33:SER:OG	2.32	0.48
1:a1:156:THR:OG1	1:a1:239:SER:OG	2.31	0.48
13:S1:366:THR:OG1	13:S1:491:ASN:ND2	2.45	0.48
16:S7:171:LYS:HA	16:S7:174:ARG:HE	1.77	0.48
19:S6:31:ARG:HH22	21:A9:69:ILE:HD11	1.78	0.48
32:D5:60:GLU:HB2	46:B6:99:LYS:HB3	1.95	0.48
27:AB:48:VAL:HG21	48:B9:16:LEU:HD11	1.96	0.48
50:B8:60:PRO:HA	50:B8:64:TRP:HH2	1.77	0.48
3:b1:36:LEU:HD22	3:b1:235:LEU:HD13	1.96	0.48
3:b1:242:LEU:HD21	3:b1:250:LEU:HD12	1.95	0.48
11:V1:224:ASN:O	11:V1:227:THR:OG1	2.28	0.48
13:S1:40:PHE:HE1	13:S1:115:ASP:HB3	1.77	0.48
14:S2:276:ASP:N	14:S2:276:ASP:OD1	2.46	0.48
25:A7:32:LYS:O	25:A7:35:GLN:NE2	2.47	0.48
32:D5:361:GLY:H	32:D5:435:PRO:HA	1.79	0.48
34:D2:80:PHE:HB3	40:S5:63:ARG:HH12	1.78	0.48
37:A8:24:LEU:HG	45:AM:70:LEU:HD11	1.96	0.48
4:c1:162:PRO:HG2	56:c1:501:HEC:HBB2	1.95	0.48
10:i1:9:LEU:HG	10:i1:14:PHE:HE2	1.78	0.48
2:a4:257:LEU:HD23	2:a4:424:MET:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:314:ASP:HB3	13:S1:520:LYS:H	1.79	0.48
16:S7:101:ARG:NH1	16:S7:139:ILE:O	2.47	0.48
21:A9:202:LYS:NZ	21:A9:291:ASP:OD2	2.34	0.48
24:A6:43:PRO:HA	24:A6:46:VAL:HG12	1.94	0.48
32:D5:570:GLN:HG3	57:D4:501:3PE:H241	1.94	0.48
33:D4:457:PRO:O	51:BK:84:ARG:NH1	2.29	0.48
3:b1:165:TRP:O	3:b1:174:THR:OG1	2.31	0.48
6:d1:74:ILE:HD12	7:q1:39:ARG:HH12	1.79	0.48
2:a4:319:SER:OG	2:a4:320:GLY:N	2.46	0.48
2:a4:416:LYS:O	2:a4:420:GLY:N	2.47	0.48
11:V1:401:GLY:N	11:V1:409:ASP:OD1	2.37	0.48
14:S2:83:LEU:HD23	14:S2:426:GLY:HA2	1.96	0.48
14:S2:151:ILE:HD13	14:S2:304:MET:HE1	1.95	0.48
14:S2:347:HIS:O	14:S2:351:LEU:CB	2.62	0.48
16:S7:116:MET:HA	16:S7:146:VAL:HG23	1.94	0.48
33:D4:72:LEU:HD12	33:D4:75:LEU:HD23	1.94	0.48
2:a4:165:ALA:HA	2:a4:173:ALA:HB1	1.95	0.48
3:b2:147:THR:HG22	3:b2:161:VAL:HG13	1.94	0.48
14:S2:246:THR:HG23	23:A5:12:GLY:HA3	1.95	0.48
23:A5:13:LEU:HD21	23:A5:77:GLU:HB3	1.95	0.48
33:D4:388:TRP:CD1	44:B4:108:ARG:HH22	2.32	0.48
43:C2:120:ARG:HH22	44:B4:112:GLU:HG2	1.78	0.48
7:q2:34:ILE:HG23	7:q2:35:PRO:HD3	1.96	0.48
14:S2:371:LYS:NZ	14:S2:422:ASP:O	2.45	0.48
15:S3:32:ILE:HG13	15:S3:33:LEU:HD12	1.96	0.48
20:S4:16:LYS:H	20:S4:16:LYS:HD3	1.79	0.48
32:D5:1:MET:HG2	32:D5:3:LEU:H	1.78	0.48
48:B9:138:GLN:O	48:B9:142:GLU:CB	2.61	0.48
4:c1:28:ARG:HE	4:c1:174:THR:HG21	1.79	0.47
2:a4:27:THR:HG21	2:a4:217:LYS:HE2	1.96	0.47
29:D1:149:ILE:HG21	29:D1:185:TRP:HB2	1.96	0.47
2:a4:424:MET:HE3	2:a4:436:ILE:HG12	1.96	0.47
5:f2:146:PRO:HG3	5:f2:158:CYS:HB2	1.96	0.47
11:V1:94:VAL:HB	11:V1:222:VAL:HG22	1.97	0.47
14:S2:36:VAL:HG22	34:D2:49:ASN:HB3	1.96	0.47
16:S7:59:MET:HE2	16:S7:59:MET:HB3	1.73	0.47
22:A2:67:ARG:HA	22:A2:72:GLN:O	2.14	0.47
25:A7:3:ALA:HB1	25:A7:7:ILE:HD11	1.95	0.47
33:D4:158:LEU:HD21	34:D2:283:ALA:HB1	1.97	0.47
4:c1:163:ILE:HD13	4:c1:178:MET:HG3	1.96	0.47
28:D3:87:MET:HE2	30:D6:147:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D5:82:MET:SD	32:D5:82:MET:N	2.87	0.47
41:A3:58:ASP:OD1	41:A3:58:ASP:N	2.47	0.47
47:B7:8:TYR:OH	50:B8:123:PRO:O	2.28	0.47
5:f1:15:ARG:HD3	5:f1:32:ARG:HD2	1.97	0.47
5:f1:63:SER:HA	3:b2:163:TRP:HD1	1.79	0.47
5:f1:146:PRO:HA	5:f1:158:CYS:HA	1.95	0.47
1:a3:33:PRO:O	1:a3:103:SER:OG	2.31	0.47
13:S1:278:ARG:HH12	13:S1:565:ALA:HB2	1.78	0.47
15:S3:75:LEU:HD22	15:S3:124:TYR:HB3	1.97	0.47
15:S3:202:PRO:HA	20:S4:50:ASN:HB3	1.96	0.47
34:D2:85:THR:OG1	34:D2:87:MET:SD	2.73	0.47
47:B7:6:ARG:NH1	47:B7:15:GLU:OE2	2.47	0.47
15:S3:26:GLY:HA3	15:S3:40:VAL:HG11	1.96	0.47
30:D6:25:SER:HB2	30:D6:78:GLN:HG2	1.96	0.47
32:D5:10:VAL:HG11	46:B6:78:VAL:HG22	1.95	0.47
32:D5:328:HIS:O	32:D5:332:HIS:HB3	2.14	0.47
36:B5:143:ASN:HD22	40:S5:29:PRO:HG3	1.80	0.47
45:AM:97:MET:HE3	45:AM:100:VAL:HG11	1.96	0.47
2:a4:411:ILE:O	2:a4:415:LYS:HB2	2.15	0.47
11:V1:322:LEU:HD12	11:V1:329:LEU:HB2	1.95	0.47
34:D2:243:LEU:HD21	43:C2:44:ILE:HD11	1.96	0.47
1:a3:65:LYS:NZ	2:a4:287:ARG:O	2.36	0.47
1:a3:76:GLU:OE1	2:a4:289:SER:OG	2.27	0.47
1:a3:179:ARG:HA	1:a3:182:LEU:HD12	1.95	0.47
2:a4:299:VAL:HG11	2:a4:336:VAL:HG13	1.96	0.47
13:S1:147:LYS:HB3	13:S1:209:THR:HG23	1.96	0.47
15:S3:150:ARG:HH22	24:A6:88:GLU:HG2	1.79	0.47
21:A9:81:ILE:HG21	21:A9:117:ILE:HG22	1.97	0.47
30:D6:121:GLY:HA2	31:4L:3:LEU:HD13	1.96	0.47
30:D6:138:GLU:OE1	31:4L:52:HIS:ND1	2.45	0.47
32:D5:172:ILE:HG21	33:D4:408:LEU:HD22	1.97	0.47
33:D4:210:TYR:O	33:D4:213:HIS:ND1	2.39	0.47
34:D2:270:MET:HG2	34:D2:279:PRO:HG3	1.97	0.47
34:D2:292:PHE:HA	34:D2:295:ARG:HG2	1.95	0.47
37:A8:148:GLU:OE1	40:S5:50:ARG:NH1	2.45	0.47
41:A3:76:SER:OG	41:A3:77:LEU:N	2.47	0.47
1:a3:87:ASN:ND2	1:a3:98:TYR:OH	2.48	0.47
2:a4:145:ARG:HB2	2:a4:183:ILE:HG21	1.97	0.47
4:c2:157:ILE:HG22	4:c2:159:MET:H	1.79	0.47
11:V1:203:PRO:O	11:V1:361:GLN:NE2	2.28	0.47
12:V2:27:ASN:HA	12:V2:30:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V2:105:THR:OG1	58:V2:300:FES:S2	2.72	0.47
12:V2:124:LEU:HD21	12:V2:137:PHE:HB3	1.97	0.47
14:S2:179:GLU:OE2	14:S2:183:ARG:NH2	2.48	0.47
30:D6:134:GLY:H	54:A1:42:SER:HB3	1.79	0.47
32:D5:293:LEU:O	32:D5:523:SER:OG	2.31	0.47
43:C2:8:ARG:H	43:C2:9:ALA:HB3	1.80	0.47
44:B4:42:LEU:HD13	50:B8:74:GLY:HA3	1.97	0.47
13:S1:141:ASN:OD1	13:S1:141:ASN:N	2.48	0.47
15:S3:71:GLN:HE21	23:A5:82:GLN:HE22	1.62	0.47
17:S8:64:GLU:HA	17:S8:139:PHE:HZ	1.79	0.47
21:A9:134:HIS:ND1	21:A9:135:LEU:O	2.37	0.47
24:A6:28:LYS:HB3	24:A6:32:ARG:HH21	1.80	0.47
35:AK:15:THR:HG23	35:AK:17:CYS:HB2	1.97	0.47
5:f1:14:ARG:HA	7:q1:23:GLN:HA	1.96	0.47
5:f1:175:PRO:HB3	3:b2:285:PRO:HA	1.97	0.47
4:c2:12:TRP:NE1	4:c2:125:ASP:OD1	2.42	0.47
13:S1:104:ASP:O	13:S1:108:CYS:N	2.41	0.47
13:S1:531:CYS:SG	13:S1:532:VAL:N	2.88	0.47
21:A9:22:THR:HG21	21:A9:85:VAL:HG12	1.96	0.47
32:D5:591:PHE:CE1	34:D2:111:PHE:HA	2.50	0.47
4:c1:23:HIS:HA	4:c1:26:ILE:HD12	1.97	0.46
1:a3:30:SER:N	1:a3:201:GLY:O	2.42	0.46
13:S1:198:ASN:OD1	13:S1:268:ARG:NH2	2.39	0.46
25:A7:8:GLN:HA	25:A7:11:ARG:HE	1.80	0.46
39:AJ:306:ALA:HB1	52:C1:3:TYR:HE1	1.80	0.46
12:V2:183:LYS:HA	18:V3:44:HIS:HE1	1.79	0.46
14:S2:176:LYS:HZ1	14:S2:214:PHE:HA	1.80	0.46
30:D6:115:ILE:HG13	30:D6:116:VAL:H	1.81	0.46
34:D2:120:GLN:O	34:D2:176:ARG:NH2	2.48	0.46
46:B6:107:ASP:OD2	47:B7:70:ARG:NH2	2.44	0.46
3:b1:33:PHE:HA	3:b1:36:LEU:HB2	1.96	0.46
2:a4:242:GLY:O	2:a4:423:SER:HA	2.16	0.46
2:a4:243:GLU:HA	2:a4:424:MET:O	2.15	0.46
4:c2:129:SER:HA	4:c2:132:THR:HG22	1.97	0.46
5:f2:122:HIS:CD2	5:f2:124:LEU:H	2.33	0.46
11:V1:36:ALA:O	11:V1:41:ASP:N	2.47	0.46
12:V2:129:GLY:HA2	12:V2:140:ILE:HG22	1.98	0.46
13:S1:44:GLU:O	20:S4:114:LYS:NZ	2.48	0.46
16:S7:34:ASP:OD1	16:S7:38:ASN:ND2	2.47	0.46
21:A9:285:GLU:O	21:A9:289:THR:OG1	2.23	0.46
37:A8:124:LEU:HD13	45:AM:69:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A3:52:TYR:HB2	45:AM:71:MET:HE1	1.97	0.46
1:a3:70:ARG:NH1	1:a3:78:GLU:OE1	2.49	0.46
2:a4:45:SER:O	2:a4:110:GLU:HA	2.15	0.46
3:b2:161:VAL:HA	3:b2:164:ILE:HG12	1.98	0.46
4:c2:41:HIS:CD2	56:c2:501:HEC:NB	2.84	0.46
8:h2:62:LEU:HA	8:h2:65:ARG:HG2	1.98	0.46
13:S1:283:MET:HB3	13:S1:291:LEU:HD11	1.98	0.46
14:S2:50:ASN:HD22	14:S2:65:VAL:HG22	1.80	0.46
29:D1:228:TYR:HD1	29:D1:231:ILE:HD12	1.81	0.46
30:D6:17:PHE:HD2	31:4L:11:ALA:HB1	1.80	0.46
33:D4:170:THR:HG23	33:D4:171:MET:HG3	1.97	0.46
36:B5:32:THR:HA	36:B5:35:PRO:HD2	1.97	0.46
36:B5:42:LEU:HA	36:B5:45:VAL:HG12	1.98	0.46
37:A8:70:PHE:HA	37:A8:73:ILE:HG22	1.97	0.46
44:B4:120:LEU:HD22	44:B4:121:ASP:H	1.80	0.46
48:B9:75:HIS:HD2	48:B9:77:GLN:H	1.63	0.46
2:a2:279:LEU:HD22	2:a2:295:LEU:HD21	1.98	0.46
1:a3:350:THR:N	1:a3:353:GLU:OE2	2.35	0.46
2:a4:97:SER:OG	2:a4:108:THR:OG1	2.26	0.46
13:S1:329:ILE:HD11	13:S1:505:LEU:HD22	1.97	0.46
13:S1:357:ASP:OD1	13:S1:357:ASP:N	2.48	0.46
50:B8:113:LEU:HD23	50:B8:116:PHE:HD2	1.81	0.46
4:c1:16:GLY:O	4:c1:201:LYS:NZ	2.45	0.46
13:S1:228:ILE:HB	13:S1:583:THR:HG22	1.97	0.46
32:D5:161:ARG:NH1	48:B9:88:THR:O	2.49	0.46
64:D5:901:CDL:H721	33:D4:369:LEU:HD11	1.98	0.46
34:D2:22:ILE:HD11	40:S5:5:VAL:H	1.80	0.46
34:D2:339:LEU:HD23	34:D2:342:ILE:HG13	1.97	0.46
43:C2:110:ARG:HG2	51:BK:119:GLN:HG2	1.98	0.46
44:B4:77:PRO:HA	44:B4:78:ASN:HA	1.67	0.46
46:B6:71:PHE:O	46:B6:75:LEU:HB2	2.15	0.46
5:f1:74:ILE:HG22	5:f1:195:VAL:HB	1.98	0.46
2:a4:51:ILE:HG12	2:a4:204:MET:HG2	1.97	0.46
11:V1:202:LYS:HB3	11:V1:361:GLN:NE2	2.31	0.46
13:S1:46:LEU:O	20:S4:116:LYS:NZ	2.41	0.46
13:S1:440:SER:OG	13:S1:444:GLN:OE1	2.34	0.46
32:D5:535:ARG:NE	50:B8:90:ASP:O	2.48	0.46
47:B7:114:ARG:NE	49:B2:69:ASP:O	2.49	0.46
1:a1:124:ASP:HA	1:a1:127:ILE:HG22	1.98	0.46
1:a1:158:PHE:HB2	1:a1:164:ALA:HB2	1.98	0.46
4:c2:27:ARG:HG3	4:c2:56:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f2:99:ARG:NH2	5:f2:149:ASN:OD1	2.49	0.46
19:S6:52:VAL:HG12	19:S6:54:SER:H	1.81	0.46
20:S4:25:VAL:HG13	20:S4:30:ILE:HD11	1.98	0.46
30:D6:135:PHE:HA	54:A1:41:TYR:HB3	1.97	0.46
35:AK:13:GLU:CD	35:AK:20:LYS:HZ1	2.23	0.46
46:B6:92:LYS:O	46:B6:95:THR:OG1	2.28	0.46
3:b1:136:GLY:H	3:b1:139:SER:HB2	1.80	0.46
8:h2:20:VAL:HA	8:h2:23:GLN:HB3	1.97	0.46
11:V1:45:THR:HA	11:V1:48:ILE:HD12	1.98	0.46
11:V1:297:VAL:HG22	11:V1:336:VAL:HG12	1.97	0.46
13:S1:276:ARG:HG2	13:S1:277:GLN:HG3	1.96	0.46
19:S6:11:VAL:HG12	19:S6:17:VAL:HG21	1.98	0.46
32:D5:268:GLU:O	32:D5:274:GLN:NE2	2.48	0.46
32:D5:322:PRO:HG2	32:D5:323:HIS:CD2	2.51	0.46
33:D4:48:ASN:HD21	36:B5:90:THR:HG21	1.81	0.46
33:D4:216:LEU:HD11	33:D4:220:HIS:CE1	2.51	0.46
38:BJ:64:HIS:NE2	51:BK:92:GLU:OE1	2.39	0.46
38:BJ:100:GLU:HA	38:BJ:103:ASN:HD22	1.81	0.46
38:BJ:141:ARG:HD2	51:BK:112:CYS:H	1.80	0.46
44:B4:42:LEU:HD23	44:B4:42:LEU:HA	1.80	0.46
3:b1:117:VAL:HG11	3:b1:302:VAL:HG22	1.98	0.46
3:b1:127:ALA:HB2	55:b1:401:HEM:HAC	1.96	0.46
14:S2:82:LEU:HB3	16:S7:96:MET:HE1	1.97	0.46
15:S3:59:PRO:HB3	23:A5:93:MET:HE1	1.98	0.46
32:D5:326:PHE:HA	32:D5:329:ILE:HD12	1.98	0.46
33:D4:47:ASP:OD1	33:D4:47:ASP:N	2.49	0.46
39:AJ:171:TYR:HD2	39:AJ:222:GLN:HG3	1.81	0.46
48:B9:80:ILE:HD12	48:B9:87:GLY:HA2	1.98	0.46
2:a4:264:ILE:HG22	2:a4:317:SER:HA	1.98	0.45
3:b2:207:ASN:ND2	3:b2:211:ILE:O	2.49	0.45
4:c2:137:PRO:HG3	4:c2:142:LEU:HD21	1.98	0.45
60:V1:501:FMN:O5'	60:V1:501:FMN:O3'	2.29	0.45
12:V2:28:TYR:HD1	12:V2:31:ILE:HD12	1.81	0.45
26:AL:44:TYR:HB3	26:AL:68:MET:HB2	1.98	0.45
31:4L:47:MET:HE2	31:4L:47:MET:HB3	1.73	0.45
31:4L:54:THR:HG21	40:S5:28:ILE:HD11	1.98	0.45
32:D5:73:THR:HG21	44:B4:126:ILE:HG21	1.97	0.45
34:D2:180:ALA:O	34:D2:183:SER:OG	2.25	0.45
34:D2:202:LEU:HB3	34:D2:346:LEU:HD21	1.98	0.45
36:B5:138:LYS:HA	40:S5:27:ARG:HG2	1.97	0.45
1:a1:429:GLU:OE2	7:q1:7:LEU:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a2:283:PRO:HG3	2:a2:290:ASN:HD21	1.81	0.45
4:c1:19:SER:O	4:c1:201:LYS:NZ	2.46	0.45
5:f2:140:THR:HG23	5:f2:176:ALA:HB1	1.98	0.45
13:S1:341:ASP:OD1	13:S1:341:ASP:N	2.48	0.45
16:S7:162:GLN:HE22	26:AL:118:SER:HB3	1.81	0.45
26:AL:31:ASN:HD21	29:D1:39:VAL:HG22	1.82	0.45
34:D2:222:ASN:OD1	34:D2:222:ASN:N	2.46	0.45
35:AK:74:CYS:SG	35:AK:78:GLN:NE2	2.89	0.45
38:BJ:134:VAL:HG23	51:BK:108:MET:HB3	1.98	0.45
39:AJ:305:ARG:HB2	43:C2:50:ARG:HB2	1.97	0.45
10:i1:50:LYS:H	10:i1:50:LYS:HD2	1.80	0.45
2:a4:47:ILE:HB	2:a4:109:VAL:HG13	1.98	0.45
15:S3:75:LEU:HD23	15:S3:126:ALA:HB3	1.98	0.45
23:A5:113:TRP:O	23:A5:115:ILE:N	2.50	0.45
28:D3:22:PHE:HE2	29:D1:72:ILE:HD12	1.80	0.45
32:D5:418:PHE:HA	32:D5:421:ILE:HG12	1.98	0.45
32:D5:451:ILE:O	32:D5:455:LYS:HB2	2.17	0.45
45:AM:139:PHE:HB2	54:A1:45:TRP:CG	2.51	0.45
48:B9:96:TYR:HB2	48:B9:177:PRO:HG2	1.97	0.45
52:C1:41:GLU:OE2	52:C1:44:ARG:NH2	2.50	0.45
2:a2:141:GLN:HE22	2:a2:186:VAL:HG13	1.81	0.45
2:a4:48:GLY:HA3	2:a4:379:LEU:HD11	1.97	0.45
2:a4:96:LEU:HA	2:a4:108:THR:O	2.15	0.45
11:V1:26:TYR:O	11:V1:28:ARG:NH1	2.49	0.45
13:S1:521:MET:HG3	13:S1:542:PHE:HD2	1.81	0.45
23:A5:106:PRO:HD2	25:A7:71:SER:HB3	1.97	0.45
31:4L:85:TYR:OH	34:D2:54:GLU:OE2	2.31	0.45
33:D4:173:SER:OG	33:D4:174:LEU:N	2.50	0.45
40:S5:74:ARG:NH2	45:AM:104:LYS:O	2.47	0.45
47:B7:46:ASN:OD1	47:B7:55:ARG:NH2	2.43	0.45
1:a1:435:ASN:ND2	3:b1:223:TYR:OH	2.44	0.45
6:d1:76:PRO:HB2	6:d1:78:GLU:HG2	1.98	0.45
8:h1:20:VAL:O	8:h1:24:CYS:HB2	2.17	0.45
2:a4:139:ALA:O	2:a4:142:SER:OG	2.31	0.45
2:a4:286:LYS:HG2	2:a4:287:ARG:HD3	1.98	0.45
11:V1:393:TRP:CH2	11:V1:397:LYS:HD3	2.52	0.45
13:S1:403:ASP:HA	20:S4:127:ARG:HH22	1.81	0.45
14:S2:105:ARG:NH1	59:S7:300:SF4:S3	2.88	0.45
35:AK:32:GLY:HA3	35:AK:59:THR:HA	1.97	0.45
35:AK:122:ALA:O	35:AK:126:MET:HB2	2.17	0.45
2:a4:102:ARG:NH2	2:a4:161:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f2:103:LYS:HA	5:f2:106:ILE:HB	1.99	0.45
11:V1:95:VAL:HB	11:V1:136:ILE:HG12	1.98	0.45
13:S1:483:VAL:HA	13:S1:484:THR:HA	1.68	0.45
23:A5:34:LEU:HD11	23:A5:44:ARG:HA	1.99	0.45
33:D4:373:ILE:HA	33:D4:376:ILE:HD12	1.98	0.45
39:AJ:189:PRO:HA	39:AJ:192:MET:HB2	1.98	0.45
1:a3:58:PHE:HZ	1:a3:127:ILE:HG13	1.82	0.45
11:V1:371:TRP:CZ2	13:S1:130:PHE:HB2	2.52	0.45
12:V2:15:ASN:O	12:V2:19:THR:OG1	2.34	0.45
13:S1:336:ASN:ND2	22:A2:67:ARG:HH11	2.15	0.45
21:A9:198:LYS:HB2	21:A9:288:HIS:CE1	2.51	0.45
33:D4:430:PHE:O	33:D4:434:ASN:ND2	2.50	0.45
39:AJ:111:ALA:HB1	39:AJ:122:VAL:HG21	1.98	0.45
1:a1:14:THR:HG23	1:a1:28:GLU:HB2	1.98	0.45
1:a1:24:ARG:O	1:a1:196:VAL:HA	2.16	0.45
1:a1:88:ALA:HB3	2:a2:287:ARG:HH22	1.82	0.45
3:b1:81:TYR:OH	4:c1:118:ARG:NH2	2.50	0.45
5:f1:121:GLN:HB3	5:f1:126:ARG:HD2	1.99	0.45
5:f2:126:ARG:NE	5:f2:168:SER:OG	2.50	0.45
12:V2:98:TYR:H	12:V2:136:LEU:HA	1.82	0.45
13:S1:9:ILE:HD11	13:S1:22:PRO:HA	1.97	0.45
13:S1:425:SER:HB3	13:S1:428:ILE:HG13	1.98	0.45
15:S3:72:PHE:HA	15:S3:98:SER:HA	1.99	0.45
32:D5:8:THR:O	32:D5:11:THR:OG1	2.30	0.45
33:D4:4:TYR:HE2	33:D4:41:LEU:HD12	1.82	0.45
34:D2:144:GLN:HE21	40:S5:2:PHE:HB2	1.82	0.45
39:AJ:64:GLY:HA2	52:C1:3:TYR:HA	1.99	0.45
39:AJ:133:VAL:HG13	39:AJ:205:VAL:HG12	1.98	0.45
1:a1:34:THR:OG1	1:a1:101:ALA:O	2.34	0.45
1:a1:205:HIS:O	1:a1:209:LEU:HB2	2.17	0.45
1:a1:419:CYS:HA	1:a1:420:PRO:HD3	1.84	0.45
4:c1:221:MET:HE3	5:f1:40:THR:HG22	1.99	0.45
1:a3:343:MET:HB3	1:a3:443:TRP:NE1	2.32	0.45
13:S1:213:TYR:CZ	13:S1:249:ARG:HD3	2.52	0.45
14:S2:34:ASN:HB2	39:AJ:158:VAL:HG13	1.99	0.45
33:D4:53:SER:HB2	33:D4:55:THR:H	1.81	0.45
34:D2:154:ILE:HG23	34:D2:191:THR:HG22	1.99	0.45
1:a3:58:PHE:CZ	1:a3:127:ILE:HG13	2.52	0.45
3:b2:58:ASP:O	3:b2:62:ALA:N	2.50	0.45
3:b2:82:MET:HE2	3:b2:240:MET:HE1	1.99	0.45
11:V1:68:ARG:HH21	11:V1:272:MET:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V1:100:GLY:O	11:V1:104:THR:OG1	2.25	0.45
13:S1:312:GLY:N	13:S1:339:ASP:OD2	2.50	0.45
15:S3:56:GLY:O	15:S3:60:VAL:HB	2.16	0.45
8:h1:36:ARG:HB3	8:h1:57:GLU:HG2	1.99	0.44
2:a4:56:ARG:NH1	2:a4:103:GLU:OE2	2.50	0.44
11:V1:305:PRO:HB2	11:V1:327:THR:HG22	1.98	0.44
19:S6:74:ASN:ND2	19:S6:76:ASP:OD2	2.49	0.44
64:D5:901:CDL:H161	64:D5:901:CDL:H362	1.99	0.44
33:D4:368:ALA:HB1	33:D4:375:LEU:HB2	1.99	0.44
37:A8:17:VAL:HG22	37:A8:63:ASN:HD21	1.82	0.44
43:C2:66:THR:OG1	52:C1:28:TRP:NE1	2.50	0.44
2:a2:29:LEU:HB2	2:a2:33:LEU:HG	1.98	0.44
4:c1:130:LEU:HD11	4:c1:157:ILE:HD12	1.99	0.44
4:c2:41:HIS:HB3	4:c2:113:LEU:HD13	2.00	0.44
15:S3:39:GLN:NE2	15:S3:41:GLN:OE1	2.50	0.44
31:4L:96:LEU:HD12	34:D2:51:ARG:HD2	1.98	0.44
32:D5:347:ILE:HG12	32:D5:354:GLN:HA	1.99	0.44
34:D2:179:MET:HE2	34:D2:212:THR:HG23	2.00	0.44
40:S5:37:LYS:NZ	40:S5:41:GLU:OE2	2.40	0.44
41:A3:66:PRO:HB2	41:A3:71:ASP:HB3	2.00	0.44
44:B4:52:ASP:HB2	44:B4:55:ARG:HB2	1.98	0.44
2:a2:139:ALA:O	2:a2:142:SER:OG	2.33	0.44
8:h1:27:LEU:HD22	8:h1:28:GLU:H	1.83	0.44
13:S1:377:VAL:O	13:S1:406:VAL:HA	2.16	0.44
25:A7:45:SER:O	25:A7:46:HIS:ND1	2.42	0.44
32:D5:257:ILE:H	32:D5:257:ILE:HG13	1.61	0.44
37:A8:35:CYS:SG	37:A8:36:ASP:N	2.78	0.44
1:a1:366:VAL:HG12	2:a2:44:ALA:HB2	1.99	0.44
2:a2:72:ALA:HB2	2:a2:140:LEU:HD21	1.99	0.44
2:a4:74:SER:O	2:a4:82:SER:OG	2.30	0.44
14:S2:259:MET:HE2	14:S2:421:GLN:HE21	1.82	0.44
16:S7:68:ASP:HB2	16:S7:71:ARG:HE	1.81	0.44
21:A9:176:ASP:OD1	21:A9:177:ARG:N	2.49	0.44
34:D2:181:TYR:HD1	34:D2:184:ILE:HD12	1.83	0.44
51:BK:74:SER:O	51:BK:78:ALA:HB2	2.17	0.44
3:b2:106:SER:OG	3:b2:206:ASN:ND2	2.41	0.44
13:S1:252:PRO:HB3	13:S1:263:ILE:HB	2.00	0.44
13:S1:275:LYS:HB2	26:AL:134:ILE:HG22	1.99	0.44
29:D1:114:TYR:OH	30:D6:65:MET:HB2	2.18	0.44
34:D2:80:PHE:HD2	34:D2:91:ASN:HB2	1.83	0.44
38:BJ:114:GLN:HE21	46:B6:99:LYS:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a3:79:VAL:HG13	1:a3:84:ALA:HB3	2.00	0.44
1:a3:278:GLY:N	1:a3:309:THR:OG1	2.51	0.44
13:S1:290:LEU:HD13	13:S1:291:LEU:H	1.83	0.44
13:S1:329:ILE:HD12	13:S1:626:VAL:HG21	1.99	0.44
13:S1:364:LEU:HG	13:S1:491:ASN:HB2	1.98	0.44
13:S1:547:GLY:O	13:S1:563:GLY:N	2.50	0.44
21:A9:141:SER:HA	21:A9:147:ARG:HH21	1.83	0.44
26:AL:56:PHE:HA	26:AL:59:HIS:CD2	2.52	0.44
28:D3:7:LEU:HD12	29:D1:84:THR:HG21	2.00	0.44
32:D5:542:LEU:HD23	32:D5:542:LEU:HA	1.80	0.44
38:BJ:65:ARG:HB3	51:BK:88:TRP:CD1	2.52	0.44
47:B7:75:ASN:HB3	47:B7:78:ALA:HB2	1.99	0.44
2:a2:217:LYS:O	2:a2:221:GLU:HB2	2.18	0.44
2:a2:245:ARG:HH21	2:a2:435:PHE:HA	1.82	0.44
5:f1:169:GLY:HA2	5:f1:180:LEU:HD12	1.99	0.44
2:a4:77:THR:HG21	2:a4:126:VAL:HA	2.00	0.44
12:V2:17:PRO:HA	12:V2:18:GLU:HA	1.61	0.44
13:S1:227:SER:N	13:S1:253:ARG:HH22	2.12	0.44
21:A9:19:ILE:O	21:A9:43:SER:OG	2.28	0.44
21:A9:128:LYS:HG2	21:A9:224:ARG:HD3	1.99	0.44
32:D5:599:THR:HA	34:D2:96:MET:HE1	2.00	0.44
34:D2:3:PRO:HB3	39:AJ:5:PRO:HB3	2.00	0.44
47:B7:30:PHE:HZ	50:B8:158:ILE:HG23	1.81	0.44
2:a2:67:HIS:NE2	2:a2:147:ASP:OD2	2.51	0.44
2:a2:97:SER:HA	9:x1:16:UNK:HA	1.99	0.44
5:f1:91:TRP:CE2	5:f1:92:ARG:HG3	2.52	0.44
13:S1:157:THR:HG23	13:S1:160:ILE:HD12	2.00	0.44
14:S2:117:ALA:HB2	14:S2:367:ILE:HG12	2.00	0.44
16:S7:145:TYR:CZ	17:S8:144:HIS:HB2	2.53	0.44
21:A9:26:ALA:HA	21:A9:31:GLY:HA3	2.00	0.44
21:A9:120:VAL:O	21:A9:124:ALA:CB	2.66	0.44
24:A6:37:ALA:O	24:A6:41:GLU:HB2	2.18	0.44
29:D1:283:ASP:O	29:D1:287:HIS:HB3	2.18	0.44
32:D5:77:SER:OG	32:D5:79:SER:OG	2.34	0.44
32:D5:385:PHE:CZ	49:B2:39:ARG:HG3	2.52	0.44
34:D2:145:ILE:HD12	34:D2:149:ILE:HD11	1.99	0.44
27:AB:48:VAL:HG21	48:B9:16:LEU:HD21	1.99	0.44
46:B6:119:MET:HE2	47:B7:60:HIS:HB2	1.99	0.44
2:a2:125:ASN:O	2:a2:129:ALA:HB3	2.18	0.44
3:b1:8:HIS:HA	3:b1:9:PRO:HD3	1.89	0.44
5:f1:142:LEU:HD13	3:b2:145:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:i2:5:LEU:HA	10:i2:8:ARG:HG2	2.00	0.44
13:S1:442:VAL:O	13:S1:446:ALA:CB	2.60	0.44
15:S3:154:ASP:OD1	15:S3:155:TYR:N	2.51	0.44
27:AA:11:ILE:HD13	27:AA:14:ARG:HD3	2.00	0.44
34:D2:155:LEU:HD11	34:D2:278:LEU:HD21	2.00	0.44
3:b2:77:TRP:CD1	3:b2:77:TRP:H	2.36	0.43
3:b2:119:LEU:HD21	3:b2:192:LEU:HB2	2.00	0.43
13:S1:219:PRO:HB3	13:S1:249:ARG:HH21	1.83	0.43
13:S1:243:ARG:O	13:S1:246:GLU:C	2.61	0.43
13:S1:441:GLN:O	13:S1:445:GLU:HB2	2.18	0.43
14:S2:360:PRO:HA	14:S2:380:SER:O	2.18	0.43
29:D1:314:ILE:HA	29:D1:315:PRO:HD3	1.82	0.43
34:D2:234:TRP:CZ2	34:D2:304:MET:HG2	2.53	0.43
3:b1:152:ALA:HA	3:b1:287:LYS:HE2	2.00	0.43
3:b1:328:LEU:HD23	3:b1:361:ILE:HG21	1.99	0.43
56:c1:501:HEC:O2D	56:c1:501:HEC:HHA	2.18	0.43
2:a4:176:LEU:HD13	2:a4:176:LEU:HA	1.88	0.43
3:b2:200:LEU:HD12	3:b2:200:LEU:HA	1.85	0.43
4:c2:10:TYR:HB2	4:c2:12:TRP:NE1	2.33	0.43
11:V1:43:TYR:H	11:V1:236:ARG:HH12	1.66	0.43
12:V2:43:LYS:HE2	12:V2:73:LEU:HA	2.01	0.43
21:A9:90:VAL:HG12	21:A9:128:LYS:HB2	2.00	0.43
30:D6:152:TRP:HB2	40:S5:13:LEU:HD12	2.00	0.43
32:D5:129:LEU:HD12	32:D5:129:LEU:HA	1.86	0.43
33:D4:75:LEU:HD21	33:D4:440:HIS:CE1	2.53	0.43
35:AK:65:ILE:HD11	35:AK:100:LEU:HD23	1.99	0.43
36:B5:99:GLU:OE1	37:A8:162:HIS:NE2	2.46	0.43
2:a2:132:PHE:HB2	2:a2:192:HIS:NE2	2.33	0.43
12:V2:36:LYS:HB3	18:V3:62:ARG:HH11	1.83	0.43
13:S1:158:ARG:HG3	13:S1:161:ARG:HH21	1.82	0.43
22:A2:19:ARG:HH22	22:A2:73:GLU:HB3	1.82	0.43
31:4L:53:PHE:HD1	40:S5:20:GLN:HG2	1.84	0.43
32:D5:99:SER:HG	32:D5:453:SER:HG	1.53	0.43
7:q1:18:LEU:HD11	7:q1:22:GLU:HG2	2.00	0.43
11:V1:126:GLY:O	11:V1:171:TYR:OH	2.36	0.43
11:V1:291:TRP:HE1	11:V1:313:GLU:HG2	1.82	0.43
13:S1:9:ILE:HG23	13:S1:75:LYS:HA	1.98	0.43
13:S1:243:ARG:N	13:S1:246:GLU:O	2.47	0.43
16:S7:62:MET:HG2	16:S7:156:LEU:HD23	2.00	0.43
29:D1:18:ALA:O	29:D1:21:THR:OG1	2.30	0.43
33:D4:388:TRP:NE1	44:B4:108:ARG:HH12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:D2:41:ILE:HD13	34:D2:41:ILE:HA	1.91	0.43
34:D2:155:LEU:HD12	34:D2:155:LEU:HA	1.83	0.43
34:D2:172:GLN:HE21	34:D2:177:LYS:HD2	1.83	0.43
39:AJ:151:HIS:CD2	39:AJ:279:LEU:HD11	2.54	0.43
45:AM:46:TYR:HD1	45:AM:46:TYR:HA	1.72	0.43
1:a3:194:ARG:NH2	1:a3:223:TYR:OH	2.49	0.43
11:V1:104:THR:HG22	11:V1:106:LYS:H	1.83	0.43
13:S1:589:PRO:HD2	24:A6:125:HIS:CE1	2.53	0.43
14:S2:83:LEU:HD12	14:S2:83:LEU:HA	1.81	0.43
20:S4:123:SER:HB2	20:S4:126:LYS:HB2	2.00	0.43
30:D6:124:ASP:O	45:AM:137:TYR:OH	2.35	0.43
48:B9:126:LYS:O	48:B9:130:GLU:HB2	2.18	0.43
4:c1:110:PRO:HA	4:c1:111:PRO:HD3	1.86	0.43
5:f1:29:SER:HB2	5:f1:33:LYS:NZ	2.34	0.43
4:c2:237:ARG:O	7:q2:12:HIS:HB3	2.19	0.43
10:i2:10:TYR:HA	10:i2:14:PHE:HB2	2.00	0.43
11:V1:165:ASN:HA	11:V1:171:TYR:H	1.82	0.43
11:V1:322:LEU:HD23	11:V1:322:LEU:HA	1.88	0.43
13:S1:258:ILE:HD11	13:S1:581:GLN:HE22	1.83	0.43
13:S1:450:MET:HA	13:S1:489:VAL:O	2.18	0.43
14:S2:146:ARG:HA	14:S2:370:PRO:HG3	2.01	0.43
14:S2:234:ILE:HG12	29:D1:280:PHE:CE1	2.53	0.43
25:A7:7:ILE:HD12	54:A1:2:TRP:HH2	1.83	0.43
32:D5:62:ILE:O	46:B6:96:ILE:HA	2.19	0.43
32:D5:332:HIS:HE1	32:D5:336:LYS:HD2	1.84	0.43
32:D5:558:LEU:HA	32:D5:561:ILE:HG22	2.00	0.43
34:D2:215:MET:HE2	34:D2:215:MET:HB2	1.86	0.43
34:D2:341:PRO:O	43:C2:79:GLN:NE2	2.52	0.43
35:AK:85:ASP:HB3	35:AK:87:LEU:H	1.83	0.43
1:a1:431:LEU:HA	1:a1:432:PRO:HD3	1.89	0.43
4:c1:152:PHE:HB3	4:c1:155:GLN:HA	2.00	0.43
2:a4:75:LEU:HD22	2:a4:136:GLU:HB3	2.01	0.43
5:f2:88:ALA:HA	5:f2:96:LEU:O	2.18	0.43
11:V1:188:GLU:HG2	60:V1:501:FMN:C8	2.49	0.43
11:V1:258:ILE:HD11	11:V1:280:ILE:HA	2.01	0.43
14:S2:242:ILE:H	14:S2:242:ILE:HG13	1.68	0.43
21:A9:108:ASP:HA	21:A9:111:VAL:HB	2.00	0.43
21:A9:318:LEU:HA	21:A9:318:LEU:HD13	1.87	0.43
33:D4:325:MET:HE2	33:D4:329:LEU:HD11	1.99	0.43
37:A8:82:THR:HA	37:A8:85:TRP:CD1	2.54	0.43
54:A1:6:LEU:O	54:A1:10:ALA:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:19:LEU:HB2	1:a1:23:LEU:HB3	2.01	0.43
3:b2:76:GLY:HA2	3:b2:79:ILE:HD12	2.01	0.43
13:S1:175:THR:O	13:S1:181:MET:HA	2.19	0.43
13:S1:418:ARG:NE	18:V3:75:HIS:O	2.48	0.43
13:S1:673:MET:HE3	13:S1:688:VAL:HG21	2.01	0.43
14:S2:139:VAL:HG13	14:S2:278:TYR:HE1	1.83	0.43
17:S8:82:LEU:HA	17:S8:82:LEU:HD23	1.81	0.43
20:S4:69:LEU:HD13	21:A9:65:LEU:HD23	2.01	0.43
23:A5:54:LYS:HA	23:A5:57:ILE:HD12	2.01	0.43
28:D3:84:LEU:HB3	29:D1:309:ILE:HD11	2.00	0.43
32:D5:280:LEU:O	32:D5:284:THR:HG23	2.19	0.43
32:D5:546:GLN:OE1	33:D4:278:ARG:NH1	2.52	0.43
32:D5:556:ILE:HD11	44:B4:79:PHE:HB2	1.99	0.43
33:D4:266:LEU:HD23	33:D4:266:LEU:HA	1.81	0.43
36:B5:26:ARG:O	36:B5:30:LEU:CB	2.66	0.43
2:a2:435:PHE:CE2	2:a4:169:ARG:HB2	2.54	0.43
2:a4:343:GLN:HE21	2:a4:347:ILE:HD11	1.84	0.43
10:i2:53:LYS:O	10:i2:56:LYS:HG2	2.19	0.43
11:V1:193:ILE:HG23	11:V1:215:VAL:HG22	2.01	0.43
19:S6:26:VAL:HB	21:A9:87:HIS:CD2	2.54	0.43
33:D4:388:TRP:CG	44:B4:108:ARG:HH22	2.37	0.43
39:AJ:97:GLN:HG2	39:AJ:135:LEU:HD22	2.01	0.43
50:B8:50:LEU:HB2	50:B8:78:HIS:CD2	2.54	0.43
2:a2:154:ASN:HA	2:a2:155:PRO:HD3	1.87	0.43
6:d1:72:GLN:OE1	7:q1:40:ARG:NH1	2.50	0.43
1:a3:436:ARG:NH1	3:b2:20:ASP:OD1	2.47	0.43
3:b2:303:ILE:HG23	3:b2:306:LEU:HD12	2.00	0.43
5:f2:135:LEU:HD13	5:f2:180:LEU:HD12	2.01	0.43
11:V1:139:ARG:NE	12:V2:145:LEU:O	2.52	0.43
12:V2:98:TYR:HD2	12:V2:136:LEU:HB2	1.84	0.43
13:S1:683:THR:HA	13:S1:686:LYS:HD2	2.00	0.43
14:S2:221:ARG:HA	14:S2:221:ARG:HD3	1.76	0.43
17:S8:174:LEU:HA	17:S8:174:LEU:HD23	1.81	0.43
32:D5:278:LEU:HD11	32:D5:405:ASN:HB2	2.01	0.43
35:AK:36:SER:HB2	35:AK:55:THR:HG22	2.01	0.43
1:a1:82:MET:HE3	1:a1:84:ALA:HB3	2.00	0.42
3:b1:287:LYS:HE3	5:f2:142:LEU:HD23	2.00	0.42
1:a3:361:LEU:HD23	1:a3:399:ILE:HD11	2.00	0.42
4:c2:113:LEU:HA	4:c2:116:ILE:HG12	2.00	0.42
13:S1:157:THR:O	13:S1:161:ARG:NE	2.52	0.42
14:S2:151:ILE:HD11	14:S2:170:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S7:42:ARG:HH12	16:S7:168:LYS:HD2	1.84	0.42
19:S6:26:VAL:HB	21:A9:87:HIS:HD2	1.84	0.42
22:A2:22:LEU:HD11	22:A2:32:VAL:HG12	2.01	0.42
31:4L:34:GLU:HA	31:4L:37:MET:HE3	2.00	0.42
32:D5:9:LEU:HB3	46:B6:81:ILE:HD13	2.01	0.42
32:D5:183:ILE:HD12	33:D4:393:ILE:HD11	2.01	0.42
34:D2:43:ILE:HG21	34:D2:129:ILE:HG21	2.01	0.42
34:D2:142:LEU:HD23	34:D2:142:LEU:HA	1.89	0.42
34:D2:210:ILE:HG22	34:D2:333:SER:HB3	2.01	0.42
39:AJ:75:GLY:HA3	39:AJ:76:ASN:HA	1.70	0.42
39:AJ:169:VAL:HB	39:AJ:220:VAL:HG12	2.00	0.42
39:AJ:306:ALA:HA	39:AJ:309:ASN:HB2	2.01	0.42
47:B7:15:GLU:OE2	47:B7:105:ARG:NH2	2.51	0.42
4:c1:227:SER:O	7:q1:23:GLN:NE2	2.46	0.42
13:S1:135:ARG:HE	13:S1:179:ASN:HB3	1.83	0.42
13:S1:632:ARG:NH1	22:A2:57:CYS:SG	2.92	0.42
19:S6:84:CYS:HB3	19:S6:87:CYS:HB2	2.01	0.42
45:AM:83:LEU:HD13	45:AM:83:LEU:HA	1.81	0.42
2:a2:20:HIS:CE1	2:a2:22:GLN:HB2	2.54	0.42
5:f2:164:HIS:HD2	5:f2:173:LYS:HB3	1.85	0.42
13:S1:221:GLU:OE1	13:S1:243:ARG:NE	2.40	0.42
28:D3:50:PRO:HB2	28:D3:51:PHE:H	1.61	0.42
29:D1:2:PHE:HA	29:D1:5:ASN:HD22	1.83	0.42
32:D5:539:TYR:OH	44:B4:9:ARG:NH2	2.53	0.42
33:D4:19:LYS:HG2	33:D4:22:MET:SD	2.60	0.42
33:D4:258:ALA:HB1	33:D4:302:LEU:HD23	2.02	0.42
37:A8:94:GLN:HE22	54:A1:37:ARG:CZ	2.32	0.42
47:B7:34:LYS:NZ	50:B8:155:HIS:O	2.39	0.42
1:a1:88:ALA:HA	1:a1:96:ALA:O	2.19	0.42
2:a2:68:LEU:HD13	2:a2:144:LEU:HD11	2.01	0.42
3:b1:37:LEU:HD11	3:b1:94:LEU:HA	1.99	0.42
8:h1:27:LEU:HD13	8:h1:29:LYS:H	1.84	0.42
1:a3:39:VAL:HG23	1:a3:113:LEU:HD21	2.01	0.42
1:a3:342:TRP:HB3	1:a3:343:MET:HE2	2.02	0.42
2:a4:249:GLY:HA2	2:a4:429:ASN:HB2	2.01	0.42
3:b2:372:ILE:O	3:b2:376:LEU:HB2	2.19	0.42
4:c2:159:MET:HB2	56:c2:501:HEC:C1D	2.49	0.42
6:d2:86:ASP:N	6:d2:86:ASP:OD1	2.48	0.42
32:D5:63:ILE:HA	46:B6:96:ILE:HG22	2.02	0.42
33:D4:221:VAL:HG23	33:D4:222:GLU:HG3	1.99	0.42
34:D2:243:LEU:HD23	34:D2:243:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B5:13:PRO:O	48:B9:106:TRP:NE1	2.46	0.42
37:A8:77:CYS:HA	37:A8:78:ALA:HA	1.77	0.42
39:AJ:201:ASP:HA	39:AJ:204:ASN:HD22	1.84	0.42
1:a1:58:PHE:O	1:a1:62:LEU:HB2	2.20	0.42
1:a1:170:PRO:HG2	1:a1:173:ASN:HB2	2.01	0.42
2:a2:87:ARG:HB3	6:d2:107:TRP:CZ2	2.55	0.42
1:a3:146:ARG:NH2	1:a3:308:GLN:HE22	2.18	0.42
12:V2:163:ASP:HB2	12:V2:187:ARG:HB2	2.00	0.42
13:S1:227:SER:O	13:S1:253:ARG:NH2	2.53	0.42
16:S7:125:TYR:CG	17:S8:117:ILE:HD12	2.54	0.42
28:D3:77:TRP:HB3	30:D6:144:ALA:HB2	2.01	0.42
29:D1:149:ILE:HG23	29:D1:181:LEU:HG	2.02	0.42
32:D5:141:PHE:CE2	33:D4:375:LEU:HD11	2.54	0.42
32:D5:224:SER:OG	32:D5:226:GLN:NE2	2.52	0.42
32:D5:534:HIS:ND1	57:D5:902:3PE:O14	2.46	0.42
38:BJ:4:TRP:CD2	46:B6:93:PRO:HB3	2.54	0.42
39:AJ:119:GLY:HA3	39:AJ:120:GLN:HA	1.82	0.42
3:b1:147:THR:HG23	3:b1:164:ILE:HD11	2.01	0.42
1:a3:405:ARG:NH1	1:a3:409:GLU:OE2	2.52	0.42
2:a4:299:VAL:O	2:a4:303:VAL:N	2.37	0.42
5:f2:119:ASP:OD2	5:f2:179:ASN:N	2.52	0.42
12:V2:8:VAL:HB	12:V2:10:ARG:NH1	2.34	0.42
13:S1:403:ASP:HA	20:S4:127:ARG:NH2	2.34	0.42
23:A5:5:LYS:HB3	23:A5:6:LYS:H	1.43	0.42
26:AL:11:LEU:HD12	26:AL:14:VAL:HB	2.02	0.42
30:D6:174:GLY:HA2	30:D6:175:ASN:HA	1.76	0.42
36:B5:97:GLU:HA	36:B5:100:LYS:HD3	2.02	0.42
47:B7:113:ARG:O	47:B7:117:ARG:HB2	2.20	0.42
50:B8:37:TYR:HD1	50:B8:37:TYR:HA	1.68	0.42
51:BK:82:ASP:HB2	51:BK:86:GLN:H	1.84	0.42
3:b1:58:ASP:O	3:b1:62:ALA:N	2.52	0.42
3:b1:314:SER:OG	3:b1:315:MET:N	2.52	0.42
6:d1:90:LEU:HD13	6:d1:94:LEU:HB2	2.00	0.42
4:c2:134:TYR:CE2	4:c2:161:PRO:HB3	2.54	0.42
12:V2:30:ARG:HG2	18:V3:52:LEU:HB3	2.01	0.42
12:V2:35:VAL:HG22	12:V2:46:ALA:HB3	2.01	0.42
12:V2:42:HIS:CD2	20:S4:129:ARG:HH12	2.38	0.42
14:S2:212:TYR:O	14:S2:215:SER:OG	2.29	0.42
17:S8:62:ARG:NE	17:S8:119:CYS:O	2.52	0.42
18:V3:38:TYR:CZ	18:V3:40:ASN:HB2	2.54	0.42
19:S6:54:SER:OG	19:S6:55:ARG:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D1:303:TRP:HH2	45:AM:42:LEU:HD11	1.83	0.42
33:D4:10:MET:HE3	53:B1:15:LEU:HD21	2.01	0.42
33:D4:203:PHE:HE2	33:D4:246:ILE:HG12	1.84	0.42
33:D4:220:HIS:CD2	33:D4:231:LEU:HD23	2.54	0.42
45:AM:110:PHE:HE2	45:AM:116:VAL:HG21	1.85	0.42
46:B6:17:LEU:HD23	46:B6:17:LEU:HA	1.82	0.42
1:a1:430:GLN:HA	7:q1:4:PHE:HB3	2.01	0.42
4:c1:163:ILE:H	4:c1:163:ILE:HG13	1.76	0.42
6:d1:58:ARG:HA	6:d1:61:ARG:HH21	1.84	0.42
1:a3:438:ARG:HD2	1:a3:438:ARG:HA	1.82	0.42
2:a4:253:VAL:HG22	2:a4:430:LEU:HD23	2.01	0.42
12:V2:72:ILE:HG22	12:V2:73:LEU:HD12	2.02	0.42
13:S1:294:THR:OG1	13:S1:295:THR:N	2.52	0.42
14:S2:349:PHE:CE1	17:S8:82:LEU:HD21	2.55	0.42
20:S4:23:THR:HG23	20:S4:25:VAL:HG12	2.01	0.42
26:AL:17:HIS:HD2	26:AL:35:VAL:HG21	1.85	0.42
30:D6:126:VAL:HA	30:D6:127:ILE:HA	1.61	0.42
33:D4:83:HIS:CE1	33:D4:84:LEU:HD23	2.55	0.42
33:D4:298:ILE:HD13	33:D4:298:ILE:HA	1.68	0.42
34:D2:232:HIS:HE1	39:AJ:276:PRO:HG3	1.84	0.42
37:A8:150:ASN:HD22	37:A8:151:PRO:HD2	1.85	0.42
38:BJ:70:VAL:HG21	38:BJ:86:GLU:HB3	2.00	0.42
39:AJ:15:THR:OG1	39:AJ:253:ASP:OD1	2.32	0.42
39:AJ:108:TYR:OH	39:AJ:164:LEU:O	2.38	0.42
50:B8:52:ASP:OD1	50:B8:78:HIS:NE2	2.50	0.42
50:B8:60:PRO:HA	50:B8:64:TRP:CH2	2.54	0.42
3:b1:322:GLN:OE1	7:q1:47:ARG:NH1	2.52	0.42
2:a4:257:LEU:HD23	2:a4:424:MET:HE2	2.01	0.42
3:b2:338:ILE:HD13	3:b2:338:ILE:HA	1.88	0.42
11:V1:30:ASP:OD1	11:V1:30:ASP:N	2.53	0.42
13:S1:218:ARG:HD2	13:S1:220:TRP:CH2	2.55	0.42
15:S3:88:ASN:HD22	15:S3:112:ASP:HB3	1.85	0.42
15:S3:150:ARG:NH2	15:S3:155:TYR:O	2.53	0.42
17:S8:160:LYS:HD2	17:S8:161:TRP:CZ3	2.55	0.42
32:D5:264:TYR:HA	32:D5:267:THR:HG22	2.01	0.42
32:D5:356:ILE:HD13	32:D5:356:ILE:HA	1.83	0.42
32:D5:391:SER:OG	32:D5:392:LYS:N	2.52	0.42
33:D4:167:ILE:HA	33:D4:170:THR:HG22	2.02	0.42
48:B9:167:TRP:O	48:B9:171:THR:OG1	2.34	0.42
4:c2:149:ASN:HB3	4:c2:157:ILE:HD12	2.01	0.42
12:V2:96:GLY:HA3	12:V2:136:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S1:480:SER:OG	13:S1:481:SER:N	2.51	0.42
13:S1:569:LYS:NZ	13:S1:596:ASP:OD2	2.52	0.42
14:S2:284:ASP:OD1	14:S2:309:ARG:NH1	2.52	0.42
20:S4:32:THR:HG22	20:S4:62:ARG:HH22	1.84	0.42
21:A9:56:THR:HA	21:A9:59:LEU:HG	2.02	0.42
21:A9:95:VAL:O	62:A9:401:NDP:O3D	2.31	0.42
29:D1:154:LEU:O	29:D1:158:GLY:N	2.45	0.42
30:D6:52:LEU:HD21	30:D6:143:ILE:HD13	2.02	0.42
32:D5:195:THR:OG1	32:D5:196:TRP:N	2.53	0.42
32:D5:419:THR:HA	32:D5:422:TYR:CE1	2.55	0.42
38:BJ:163:LEU:HB2	51:BK:120:LEU:HD22	2.02	0.42
39:AJ:18:MET:HB3	39:AJ:19:THR:HB	2.02	0.42
50:B8:64:TRP:CH2	50:B8:70:ARG:HG3	2.55	0.42
1:a1:278:GLY:N	1:a1:309:THR:OG1	2.53	0.41
1:a3:21:ASN:HD21	1:a3:218:GLY:H	1.66	0.41
5:f2:81:ILE:HD12	5:f2:132:TRP:HZ3	1.85	0.41
5:f2:142:LEU:HD12	5:f2:161:HIS:HE1	1.84	0.41
29:D1:98:MET:HE3	57:D1:501:3PE:H32	2.02	0.41
57:D1:501:3PE:N	45:AM:143:THR:OXT	2.46	0.41
47:B7:114:ARG:HG2	49:B2:69:ASP:HB3	2.01	0.41
50:B8:64:TRP:HE1	50:B8:67:PRO:HA	1.84	0.41
2:a2:137:VAL:HG11	2:a2:188:PRO:HD3	2.02	0.41
3:b1:146:ILE:HA	3:b1:149:LEU:HB2	2.01	0.41
2:a4:159:VAL:HG11	2:a4:325:TYR:HE1	1.85	0.41
14:S2:208:MET:HE2	14:S2:208:MET:HB3	1.93	0.41
19:S6:20:ASP:HA	19:S6:25:ARG:HH11	1.85	0.41
32:D5:245:ALA:O	32:D5:249:SER:HB3	2.20	0.41
32:D5:446:ASN:ND2	49:B2:18:THR:OG1	2.49	0.41
34:D2:274:ASP:H	35:AK:137:GLU:HG3	1.84	0.41
39:AJ:60:ASP:HB3	39:AJ:69:LEU:HD13	2.01	0.41
42:B3:42:ASP:OD1	42:B3:42:ASP:N	2.53	0.41
3:b1:62:ALA:O	3:b1:65:SER:OG	2.34	0.41
13:S1:53:ARG:HH11	13:S1:56:LEU:HD21	1.86	0.41
14:S2:237:ASN:O	29:D1:284:GLN:NE2	2.44	0.41
18:V3:60:LYS:HG2	18:V3:61:PHE:CD1	2.55	0.41
27:AA:34:SER:HB3	27:AA:73:PRO:HG2	2.01	0.41
29:D1:85:MET:HE3	29:D1:85:MET:HB3	1.88	0.41
29:D1:91:MET:O	29:D1:93:TYR:N	2.53	0.41
29:D1:300:LEU:HD23	29:D1:300:LEU:HA	1.88	0.41
32:D5:355:ASP:O	32:D5:359:MET:HB2	2.20	0.41
36:B5:24:LEU:HD23	36:B5:24:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A8:124:LEU:HD23	37:A8:124:LEU:HA	1.90	0.41
1:a1:70:ARG:HA	1:a1:71:PRO:HD3	1.90	0.41
4:c1:139:ARG:NH2	8:h1:45:SER:OG	2.53	0.41
57:c1:502:3PE:O12	5:f1:57:GLN:NE2	2.47	0.41
7:q2:64:GLN:HG2	7:q2:68:LYS:HE2	2.01	0.41
11:V1:234:ILE:HD12	11:V1:242:PHE:HB2	2.02	0.41
13:S1:13:VAL:HG11	13:S1:33:VAL:HG21	2.02	0.41
21:A9:40:ARG:NH1	24:A6:110:GLU:O	2.53	0.41
32:D5:386:LEU:HD23	32:D5:387:THR:H	1.85	0.41
37:A8:37:LYS:NZ	41:A3:67:SER:O	2.53	0.41
44:B4:25:SER:OG	44:B4:26:SER:N	2.52	0.41
47:B7:36:ARG:NH2	47:B7:96:LYS:HD3	2.28	0.41
50:B8:83:MET:HA	50:B8:88:ARG:HG2	2.02	0.41
1:a1:21:ASN:HD21	1:a1:220:SER:N	2.18	0.41
4:c1:58:GLU:HG2	4:c1:62:LYS:HE2	2.02	0.41
6:d1:56:ASN:HA	6:d1:59:VAL:HG22	2.01	0.41
10:i1:20:PHE:HA	10:i1:23:THR:HG22	2.00	0.41
1:a3:67:THR:HG23	1:a3:70:ARG:H	1.86	0.41
1:a3:67:THR:OG1	1:a3:119:ASN:O	2.23	0.41
2:a4:254:HIS:ND1	2:a4:327:ILE:HG12	2.36	0.41
2:a4:282:GLY:HA2	2:a4:283:PRO:HD3	1.91	0.41
4:c2:62:LYS:HD3	4:c2:87:LEU:HD11	2.02	0.41
6:d2:45:GLU:OE2	6:d2:49:ARG:NE	2.53	0.41
12:V2:126:ILE:HG21	12:V2:132:THR:HA	2.01	0.41
15:S3:55:ASP:OD2	24:A6:17:LYS:NZ	2.53	0.41
16:S7:96:MET:HB2	16:S7:96:MET:HE2	1.80	0.41
16:S7:107:MET:HE2	16:S7:111:ARG:HB2	2.03	0.41
17:S8:95:GLU:O	17:S8:107:THR:N	2.46	0.41
28:D3:74:PRO:HA	28:D3:77:TRP:HD1	1.85	0.41
29:D1:19:PHE:HA	29:D1:22:LEU:HD23	2.02	0.41
29:D1:268:ILE:HD13	29:D1:268:ILE:HA	1.92	0.41
32:D5:67:HIS:HA	32:D5:77:SER:HA	2.03	0.41
33:D4:328:CYS:SG	33:D4:436:LEU:HD23	2.60	0.41
33:D4:442:LEU:HD23	33:D4:442:LEU:HA	1.90	0.41
37:A8:20:SER:HB3	54:A1:64:LYS:HB3	2.02	0.41
37:A8:88:ILE:HD11	37:A8:96:PHE:HA	2.02	0.41
40:S5:16:TRP:CD1	40:S5:16:TRP:H	2.39	0.41
47:B7:110:ARG:HG3	49:B2:69:ASP:HB2	2.03	0.41
1:a1:342:TRP:HB3	1:a1:343:MET:HE2	2.02	0.41
2:a2:137:VAL:HG21	2:a2:188:PRO:HB3	2.02	0.41
9:x1:12:UNK:O	9:x1:24:UNK:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f2:15:ARG:HH11	5:f2:32:ARG:HG3	1.85	0.41
11:V1:190:THR:HG21	11:V1:204:ARG:HB2	2.02	0.41
13:S1:456:SER:HB2	13:S1:664:PRO:HD2	2.01	0.41
14:S2:48:THR:HG22	14:S2:67:GLU:HG2	2.02	0.41
14:S2:213:GLU:HA	14:S2:216:LYS:HZ2	1.86	0.41
22:A2:32:VAL:HG22	22:A2:86:VAL:HG11	2.02	0.41
29:D1:68:ILE:O	29:D1:72:ILE:HG12	2.21	0.41
30:D6:161:LEU:HD13	30:D6:161:LEU:HA	1.93	0.41
32:D5:559:GLU:HA	32:D5:563:PRO:HD2	2.03	0.41
33:D4:248:LEU:HA	38:BJ:148:HIS:CD2	2.55	0.41
33:D4:263:MET:HG3	44:B4:101:TYR:HA	2.01	0.41
48:B9:30:CYS:SG	48:B9:35:LYS:HG3	2.61	0.41
27:AA:14:ARG:HA	27:AA:17:TYR:CD1	2.56	0.41
28:D3:66:ASP:HA	28:D3:69:ILE:HD12	2.02	0.41
29:D1:296:LEU:HA	29:D1:296:LEU:HD12	1.87	0.41
32:D5:265:PRO:HA	32:D5:268:GLU:HG3	2.02	0.41
33:D4:44:GLN:HE22	33:D4:59:ASP:HA	1.85	0.41
33:D4:457:PRO:HA	51:BK:84:ARG:HH22	1.86	0.41
46:B6:108:THR:HB	46:B6:115:VAL:HG12	2.03	0.41
6:d1:105:GLU:O	6:d1:109:LYS:HG2	2.20	0.41
2:a4:163:LEU:O	2:a4:167:ALA:N	2.53	0.41
12:V2:13:PRO:HA	12:V2:15:ASN:H	1.86	0.41
15:S3:115:THR:HA	15:S3:116:PRO:HD3	1.96	0.41
16:S7:179:ARG:HG3	21:A9:50:ARG:HH22	1.85	0.41
19:S6:74:ASN:OD1	19:S6:75:LEU:N	2.54	0.41
20:S4:97:GLU:OE2	20:S4:103:TYR:OH	2.33	0.41
21:A9:53:PRO:O	21:A9:57:MET:HB2	2.21	0.41
32:D5:402:SER:O	32:D5:404:THR:OG1	2.38	0.41
32:D5:473:PRO:HB2	32:D5:475:MET:HE2	2.02	0.41
32:D5:561:ILE:HG23	32:D5:562:LEU:HG	2.02	0.41
57:D4:501:3PE:H342	57:D4:501:3PE:H272	2.03	0.41
38:BJ:16:THR:O	46:B6:110:LEU:N	2.40	0.41
39:AJ:35:LYS:HG3	39:AJ:37:LYS:H	1.86	0.41
1:a1:148:VAL:HG22	5:f1:2:HIS:CG	2.55	0.41
3:b1:97:HIS:HE1	55:b1:402:HEM:NA	2.16	0.41
4:c1:72:ASP:HB2	4:c1:83:ARG:HB2	2.03	0.41
5:f1:160:CYS:HA	3:b2:268:ILE:HG21	2.02	0.41
1:a3:15:GLN:O	1:a3:26:ALA:HA	2.21	0.41
1:a3:155:ALA:HA	1:a3:164:ALA:HB1	2.03	0.41
1:a3:270:LEU:HD23	1:a3:270:LEU:HA	1.91	0.41
1:a3:365:LEU:HD12	1:a3:365:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b2:147:THR:HG23	3:b2:164:ILE:HD11	2.02	0.41
3:b2:314:SER:OG	3:b2:315:MET:N	2.54	0.41
11:V1:250:ASN:HD22	11:V1:319:PHE:HD2	1.69	0.41
13:S1:226:GLU:HA	13:S1:253:ARG:NH1	2.36	0.41
13:S1:571:ALA:O	13:S1:583:THR:N	2.44	0.41
14:S2:105:ARG:CZ	17:S8:117:ILE:HD11	2.51	0.41
17:S8:97:GLU:O	17:S8:105:ARG:O	2.39	0.41
20:S4:22:LEU:HD13	24:A6:80:LEU:HD23	2.03	0.41
21:A9:129:PHE:HB3	21:A9:160:PHE:CE2	2.56	0.41
30:D6:17:PHE:HD1	30:D6:17:PHE:HA	1.71	0.41
33:D4:51:ASN:ND2	36:B5:90:THR:HG22	2.35	0.41
33:D4:175:ASN:HD21	33:D4:177:LEU:HD12	1.85	0.41
34:D2:164:ILE:HD13	34:D2:164:ILE:HA	1.96	0.41
34:D2:170:LEU:HD22	34:D2:291:TYR:HD2	1.84	0.41
34:D2:202:LEU:HD12	34:D2:202:LEU:HA	1.90	0.41
35:AK:80:ARG:HH12	35:AK:87:LEU:HB3	1.84	0.41
38:BJ:21:PRO:HG3	38:BJ:27:ASN:HD21	1.86	0.41
43:C2:68:PHE:HD1	43:C2:68:PHE:HA	1.75	0.41
50:B8:113:LEU:HD23	50:B8:113:LEU:HA	1.90	0.41
51:BK:63:PHE:HA	51:BK:67:SER:HB3	2.02	0.41
51:BK:118:ILE:HD12	51:BK:118:ILE:HA	1.86	0.41
1:a1:329:MET:HE1	7:q1:3:GLN:HE21	1.85	0.41
1:a1:416:TYR:OH	10:i1:15:ARG:O	2.34	0.41
1:a3:67:THR:OG1	1:a3:68:LYS:N	2.54	0.41
2:a4:152:PHE:HB3	2:a4:158:HIS:NE2	2.36	0.41
11:V1:379:PHE:CZ	11:V1:389:ILE:HG22	2.56	0.41
13:S1:218:ARG:HH21	17:S8:80:CYS:HA	1.86	0.41
13:S1:544:VAL:HA	13:S1:559:VAL:O	2.21	0.41
17:S8:80:CYS:N	59:S8:202:SF4:S1	2.94	0.41
22:A2:33:ARG:HA	22:A2:36:ILE:HG22	2.03	0.41
25:A7:69:MET:HG3	25:A7:70:SER:H	1.86	0.41
29:D1:299:ALA:HB1	41:A3:24:ILE:HG23	2.02	0.41
29:D1:316:PRO:HB2	45:AM:60:GLN:HG3	2.03	0.41
33:D4:321:LEU:HD23	33:D4:321:LEU:HA	1.83	0.41
33:D4:326:LEU:HA	33:D4:326:LEU:HD12	1.77	0.41
37:A8:7:PRO:HD3	37:A8:53:ARG:HB2	2.02	0.41
39:AJ:207:LYS:HA	39:AJ:211:LEU:HD23	2.02	0.41
1:a1:259:GLY:N	1:a1:318:GLY:O	2.46	0.40
5:f1:126:ARG:HH21	5:f1:182:VAL:HG23	1.85	0.40
7:q1:57:LEU:HD13	7:q1:57:LEU:HA	1.90	0.40
1:a3:248:LEU:HD12	1:a3:426:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a4:31:ASN:HD22	2:a4:225:ASN:HA	1.86	0.40
3:b2:153:ILE:HA	3:b2:154:PRO:HD3	1.91	0.40
3:b2:165:TRP:O	3:b2:174:THR:OG1	2.33	0.40
4:c2:2:ASP:HB3	4:c2:3:LEU:H	1.64	0.40
5:f2:9:ASP:OD1	5:f2:9:ASP:N	2.52	0.40
5:f2:72:SER:O	5:f2:92:ARG:NE	2.53	0.40
13:S1:12:PHE:O	13:S1:78:ASN:HA	2.22	0.40
13:S1:260:GLU:HG3	13:S1:394:ARG:HH22	1.85	0.40
13:S1:662:VAL:HA	13:S1:663:PRO:HD3	1.96	0.40
25:A7:111:TYR:HA	25:A7:112:LEU:HA	1.58	0.40
33:D4:151:PHE:HD1	33:D4:151:PHE:HA	1.74	0.40
34:D2:228:LEU:O	34:D2:231:SER:OG	2.30	0.40
42:B3:23:ILE:HD12	42:B3:49:ALA:HB2	2.03	0.40
45:AM:96:ILE:HG23	45:AM:97:MET:HG2	2.02	0.40
49:B2:18:THR:H	49:B2:21:GLN:HE21	1.68	0.40
5:f1:135:LEU:HD12	5:f1:156:TYR:HE2	1.86	0.40
6:d1:53:ASN:OD1	6:d1:54:LEU:N	2.53	0.40
1:a3:369:LEU:HD12	1:a3:392:LEU:HD21	2.03	0.40
2:a4:57:TYR:HB3	2:a4:198:HIS:NE2	2.36	0.40
3:b2:149:LEU:HD13	3:b2:281:LEU:HD21	2.03	0.40
6:d2:98:ILE:HG22	6:d2:102:LYS:HE2	2.04	0.40
13:S1:335:LEU:HD12	13:S1:335:LEU:HA	1.88	0.40
13:S1:484:THR:H	13:S1:485:GLY:HA2	1.86	0.40
14:S2:204:PRO:HA	17:S8:175:TYR:CZ	2.56	0.40
29:D1:46:LEU:HA	29:D1:49:ILE:HB	2.03	0.40
30:D6:37:GLY:HA3	30:D6:61:LEU:HD11	2.04	0.40
31:4L:63:LEU:HD21	34:D2:71:MET:HG2	2.02	0.40
32:D5:384:PRO:HA	32:D5:385:PHE:HA	1.52	0.40
34:D2:316:GLN:HB3	39:AJ:63:THR:HG21	2.01	0.40
38:BJ:138:TYR:HD1	51:BK:108:MET:HE1	1.86	0.40
46:B6:92:LYS:HA	46:B6:93:PRO:HD3	1.87	0.40
5:f1:73:LYS:HD3	5:f1:196:GLY:HA3	2.03	0.40
6:d1:13:LEU:HA	6:d1:16:ILE:HD12	2.01	0.40
3:b2:284:ILE:HA	3:b2:285:PRO:HD3	1.90	0.40
5:f2:142:LEU:HD12	5:f2:161:HIS:CE1	2.57	0.40
6:d2:101:ARG:HA	6:d2:104:ARG:HH21	1.86	0.40
7:q2:24:ARG:HD2	7:q2:27:PRO:HA	2.03	0.40
11:V1:221:THR:OG1	11:V1:222:VAL:N	2.53	0.40
13:S1:138:GLU:HG2	19:S6:77:LYS:HG2	2.04	0.40
29:D1:237:PHE:O	29:D1:241:LEU:HB2	2.21	0.40
31:4L:53:PHE:CD1	40:S5:20:GLN:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4L:59:MET:HE3	31:4L:59:MET:HB3	1.96	0.40
34:D2:233:THR:HA	34:D2:236:LYS:HG2	2.02	0.40
27:AB:85:ASP:OD1	48:B9:172:ARG:NH2	2.54	0.40
44:B4:83:THR:O	44:B4:87:LEU:HB2	2.21	0.40
47:B7:11:ASP:OD1	47:B7:11:ASP:N	2.54	0.40
50:B8:12:PRO:HB2	50:B8:13:TYR:CD1	2.56	0.40
1:a1:45:SER:N	1:a1:92:ARG:O	2.54	0.40
3:b1:91:PHE:HD1	3:b1:91:PHE:HA	1.75	0.40
1:a3:188:ARG:CZ	1:a3:229:PRO:HG3	2.51	0.40
2:a4:71:LEU:HB3	2:a4:140:LEU:HD11	2.03	0.40
2:a4:279:LEU:HD22	2:a4:295:LEU:HD21	2.03	0.40
3:b2:27:ILE:HG23	3:b2:31:TRP:HB2	2.03	0.40
3:b2:207:ASN:ND2	3:b2:213:SER:HB3	2.36	0.40
8:h2:69:VAL:HG12	8:h2:73:LEU:HD12	2.03	0.40
11:V1:389:ILE:HG21	11:V1:389:ILE:HD13	1.87	0.40
13:S1:56:LEU:HB3	13:S1:65:VAL:HG12	2.03	0.40
15:S3:85:THR:HG21	20:S4:87:SER:HB2	2.04	0.40
21:A9:122:LYS:NZ	21:A9:159:THR:OG1	2.36	0.40
21:A9:282:ASP:HB3	21:A9:286:ARG:HH21	1.85	0.40
24:A6:80:LEU:HD12	24:A6:80:LEU:HA	1.93	0.40
29:D1:46:LEU:HD23	29:D1:46:LEU:H	1.87	0.40
29:D1:287:HIS:CE1	29:D1:291:LYS:HD2	2.56	0.40
30:D6:54:LEU:HA	30:D6:54:LEU:HD22	1.84	0.40
30:D6:141:MET:HA	30:D6:144:ALA:HB3	2.03	0.40
32:D5:69:LEU:HD23	33:D4:451:PRO:HG2	2.03	0.40
32:D5:149:ILE:HD12	32:D5:149:ILE:HA	1.87	0.40
32:D5:249:SER:OG	32:D5:250:SER:N	2.51	0.40
33:D4:86:LYS:HB3	33:D4:86:LYS:HE3	1.94	0.40
33:D4:234:ILE:O	33:D4:238:LEU:HB2	2.21	0.40
39:AJ:36:SER:HA	39:AJ:39:ALA:HB3	2.03	0.40
40:S5:6:GLN:NE2	40:S5:14:ASP:OD2	2.55	0.40
45:AM:19:ASP:OD1	45:AM:19:ASP:N	2.53	0.40
4:c1:151:TYR:OH	8:h1:66:ASP:OD2	2.35	0.40
8:h2:37:LEU:HD13	8:h2:61:PHE:HE1	1.86	0.40
16:S7:39:TRP:HA	16:S7:42:ARG:HG2	2.03	0.40
17:S8:84:GLU:OE1	17:S8:94:ILE:N	2.46	0.40
21:A9:50:ARG:NE	62:A9:401:NDP:O3X	2.49	0.40
32:D5:436:ARG:NH1	48:B9:32:HIS:H	2.19	0.40
33:D4:168:GLN:OE1	36:B5:104:ARG:NH1	2.52	0.40
33:D4:418:LYS:HD3	48:B9:94:GLU:OE2	2.21	0.40
34:D2:347:GLU:OE2	43:C2:4:GLY:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A8:73:ILE:HD12	37:A8:73:ILE:HA	1.94	0.40
42:B3:38:ARG:NH1	48:B9:42:LEU:HD11	2.36	0.40
50:B8:30:ARG:NH2	50:B8:32:GLU:OE2	2.54	0.40
50:B8:64:TRP:CZ2	50:B8:70:ARG:HG3	2.57	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%)	391 (90%)	44 (10%)	0	100	100
1	a3	442/446 (99%)	400 (90%)	42 (10%)	0	100	100
2	a2	410/439 (93%)	367 (90%)	43 (10%)	0	100	100
2	a4	409/439 (93%)	369 (90%)	40 (10%)	0	100	100
3	b1	376/379 (99%)	351 (93%)	25 (7%)	0	100	100
3	b2	376/379 (99%)	349 (93%)	27 (7%)	0	100	100
4	c1	237/240 (99%)	195 (82%)	42 (18%)	0	100	100
4	c2	236/240 (98%)	202 (86%)	34 (14%)	0	100	100
5	f1	194/196 (99%)	179 (92%)	15 (8%)	0	100	100
5	f2	193/196 (98%)	168 (87%)	25 (13%)	0	100	100
6	d1	98/110 (89%)	93 (95%)	5 (5%)	0	100	100
6	d2	99/110 (90%)	96 (97%)	3 (3%)	0	100	100
7	q1	71/81 (88%)	68 (96%)	3 (4%)	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%)	56 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	i1	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	i2	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
11	V1	428/445 (96%)	380 (89%)	48 (11%)	0	100	100
12	V2	210/217 (97%)	165 (79%)	45 (21%)	0	100	100
13	S1	686/704 (97%)	595 (87%)	90 (13%)	1 (0%)	48	82
14	S2	420/430 (98%)	373 (89%)	47 (11%)	0	100	100
15	S3	206/228 (90%)	176 (85%)	30 (15%)	0	100	100
16	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	21	58
17	S8	174/176 (99%)	155 (89%)	19 (11%)	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	281/338 (83%)	245 (87%)	36 (13%)	0	100	100
22	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
23	A5	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
24	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
25	A7	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	11	45
26	AL	142/145 (98%)	111 (78%)	31 (22%)	0	100	100
27	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
27	AB	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
28	D3	86/115 (75%)	83 (96%)	3 (4%)	0	100	100
29	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	36	71
30	D6	167/175 (95%)	144 (86%)	23 (14%)	0	100	100
31	4L	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	47
32	D5	604/606 (100%)	524 (87%)	78 (13%)	2 (0%)	36	71
33	D4	457/459 (100%)	411 (90%)	44 (10%)	2 (0%)	30	66
34	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
35	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
36	B5	137/143 (96%)	120 (88%)	17 (12%)	0	100	100
37	A8	169/171 (99%)	138 (82%)	31 (18%)	0	100	100
38	BJ	169/175 (97%)	150 (89%)	18 (11%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AJ	317/320 (99%)	270 (85%)	46 (14%)	1 (0%)	36	71
40	S5	97/105 (92%)	82 (84%)	15 (16%)	0	100	100
41	A3	72/83 (87%)	58 (81%)	14 (19%)	0	100	100
42	B3	71/97 (73%)	59 (83%)	12 (17%)	0	100	100
43	C2	117/120 (98%)	100 (86%)	17 (14%)	0	100	100
44	B4	126/128 (98%)	112 (89%)	14 (11%)	0	100	100
45	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
46	B6	92/127 (72%)	79 (86%)	12 (13%)	1 (1%)	11	45
47	B7	117/119 (98%)	97 (83%)	19 (16%)	1 (1%)	14	49
48	B9	174/178 (98%)	144 (83%)	29 (17%)	1 (1%)	21	58
49	B2	63/72 (88%)	51 (81%)	12 (19%)	0	100	100
50	B8	155/158 (98%)	115 (74%)	38 (24%)	2 (1%)	9	41
51	BK	100/125 (80%)	83 (83%)	17 (17%)	0	100	100
52	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
53	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
54	A1	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
All	All	11862/12556 (94%)	10455 (88%)	1391 (12%)	16 (0%)	49	82

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	D5	84	PHE
33	D4	53	SER
16	S7	54	CYS
25	A7	69	MET
32	D5	527	GLY
50	B8	143	GLY
31	4L	3	LEU
48	B9	10	THR
13	S1	359	ARG
33	D4	181	TYR
38	BJ	71	PRO
39	AJ	306	ALA
50	B8	17	PRO
46	B6	93	PRO
29	D1	92	PRO

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Mol	Chain	Res	Type
47	B7	31	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	366/372 (98%)	364 (100%)	2 (0%)	81	81
1	a3	370/372 (100%)	369 (100%)	1 (0%)	86	84
2	a2	326/341 (96%)	324 (99%)	2 (1%)	78	80
2	a4	326/341 (96%)	323 (99%)	3 (1%)	70	75
3	b1	330/331 (100%)	328 (99%)	2 (1%)	78	80
3	b2	330/331 (100%)	328 (99%)	2 (1%)	78	80
4	c1	205/206 (100%)	204 (100%)	1 (0%)	81	81
4	c2	204/206 (99%)	203 (100%)	1 (0%)	81	81
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%)	92 (99%)	1 (1%)	65	73
6	d2	94/99 (95%)	93 (99%)	1 (1%)	65	73
7	q1	66/72 (92%)	66 (100%)	0	100	100
7	q2	67/72 (93%)	65 (97%)	2 (3%)	36	57
8	h1	62/74 (84%)	60 (97%)	2 (3%)	34	56
8	h2	62/74 (84%)	61 (98%)	1 (2%)	55	69
10	i1	46/52 (88%)	45 (98%)	1 (2%)	45	64
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%)	179 (98%)	3 (2%)	55	69
13	S1	578/588 (98%)	573 (99%)	5 (1%)	70	75
14	S2	368/371 (99%)	364 (99%)	4 (1%)	65	73
15	S3	189/204 (93%)	188 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	S7	132/150 (88%)	130 (98%)	2 (2%)	57	70
17	S8	151/151 (100%)	150 (99%)	1 (1%)	76	78
18	V3	40/68 (59%)	39 (98%)	1 (2%)	42	62
19	S6	79/80 (99%)	79 (100%)	0	100	100
20	S4	113/119 (95%)	113 (100%)	0	100	100
21	A9	246/292 (84%)	245 (100%)	1 (0%)	84	82
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	83/94 (88%)	83 (100%)	0	100	100
26	AL	130/131 (99%)	128 (98%)	2 (2%)	57	70
27	AA	74/81 (91%)	73 (99%)	1 (1%)	59	70
27	AB	80/81 (99%)	80 (100%)	0	100	100
28	D3	81/103 (79%)	81 (100%)	0	100	100
29	D1	266/278 (96%)	262 (98%)	4 (2%)	57	70
30	D6	140/144 (97%)	137 (98%)	3 (2%)	47	65
31	4L	87/87 (100%)	87 (100%)	0	100	100
32	D5	539/539 (100%)	534 (99%)	5 (1%)	70	75
33	D4	412/412 (100%)	407 (99%)	5 (1%)	63	73
34	D2	315/315 (100%)	314 (100%)	1 (0%)	86	84
35	AK	101/101 (100%)	101 (100%)	0	100	100
36	B5	122/125 (98%)	120 (98%)	2 (2%)	55	69
37	A8	154/154 (100%)	154 (100%)	0	100	100
38	BJ	155/157 (99%)	153 (99%)	2 (1%)	61	71
39	AJ	283/284 (100%)	283 (100%)	0	100	100
40	S5	88/94 (94%)	87 (99%)	1 (1%)	65	73
41	A3	65/71 (92%)	65 (100%)	0	100	100
42	B3	55/75 (73%)	55 (100%)	0	100	100
43	C2	106/107 (99%)	105 (99%)	1 (1%)	70	75
44	B4	114/114 (100%)	113 (99%)	1 (1%)	70	75
45	AM	119/121 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	B6	92/121 (76%)	90 (98%)	2 (2%)	45	64
47	B7	108/108 (100%)	107 (99%)	1 (1%)	70	75
48	B9	159/160 (99%)	159 (100%)	0	100	100
49	B2	59/62 (95%)	59 (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%)	58 (98%)	1 (2%)	53	67
All	All	10402/10814 (96%)	10324 (99%)	78 (1%)	73	78

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a1	208	LEU
1	a1	230	THR
2	a2	69	LEU
2	a2	109	VAL
3	b1	328	LEU
3	b1	376	LEU
4	c1	163	ILE
6	d1	94	LEU
8	h1	37	LEU
8	h1	68	CYS
10	i1	50	LYS
1	a3	209	LEU
2	a4	69	LEU
2	a4	109	VAL
2	a4	176	LEU
3	b2	27	ILE
3	b2	51	LEU
4	c2	200	ARG
6	d2	71	ARG
7	q2	34	ILE
7	q2	36	ASN
8	h2	37	LEU
11	V1	110	ILE
11	V1	365	CYS
12	V2	104	THR

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Mol	Chain	Res	Type
12	V2	110	LEU
12	V2	202	LEU
13	S1	239	VAL
13	S1	290	LEU
13	S1	432	ILE
13	S1	483	VAL
13	S1	488	LYS
14	S2	203	LEU
14	S2	402	LEU
14	S2	418	ILE
14	S2	423	ILE
15	S3	85	THR
16	S7	54	CYS
16	S7	146	VAL
17	S8	78	ILE
18	V3	54	LEU
21	A9	47	VAL
23	A5	94	ILE
26	AL	117	LEU
26	AL	134	ILE
27	AA	80	ILE
29	D1	22	LEU
29	D1	55	LEU
29	D1	73	LEU
29	D1	103	LEU
30	D6	12	ILE
30	D6	54	LEU
30	D6	143	ILE
32	D5	55	ILE
32	D5	113	ASN
32	D5	350	LEU
32	D5	552	LEU
32	D5	553	LEU
33	D4	23	ILE
33	D4	126	LEU
33	D4	148	TYR
33	D4	150	LEU
33	D4	238	LEU
34	D2	314	LYS
36	B5	45	VAL
36	B5	66	TYR
38	BJ	135	VAL

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Mol	Chain	Res	Type
38	BJ	145	LEU
40	S5	57	ILE
43	C2	76	LEU
44	B4	120	LEU
46	B6	89	VAL
46	B6	103	ILE
47	B7	39	VAL
50	B8	9	LEU
50	B8	96	VAL
51	BK	70	LEU
54	A1	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	a1	6	GLN
1	a1	53	ASN
1	a1	85	HIS
1	a1	141	ASN
1	a1	215	HIS
1	a1	252	HIS
1	a1	271	GLN
1	a1	323	HIS
1	a1	328	HIS
1	a1	359	ASN
1	a1	363	ASN
2	a2	20	HIS
2	a2	143	GLN
2	a2	162	ASN
2	a2	174	ASN
2	a2	247	GLN
2	a2	248	ASN
2	a2	290	ASN
2	a2	304	HIS
2	a2	313	ASN
2	a2	343	GLN
2	a2	362	ASN
2	a2	412	ASN
3	b1	8	HIS
3	b1	26	ASN
3	b1	85	ASN
3	b1	201	HIS

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Mol	Chain	Res	Type
3	b1	345	HIS
4	c1	97	ASN
4	c1	121	HIS
4	c1	165	ASN
4	c1	180	GLN
4	c1	197	HIS
5	f1	164	HIS
6	d1	38	HIS
7	q1	23	GLN
8	h1	63	HIS
10	i1	54	HIS
1	a3	6	GLN
1	a3	21	ASN
1	a3	53	ASN
1	a3	69	ASN
1	a3	85	HIS
1	a3	151	ASN
1	a3	213	GLN
1	a3	215	HIS
1	a3	308	GLN
1	a3	323	HIS
1	a3	328	HIS
1	a3	359	ASN
2	a4	31	ASN
2	a4	143	GLN
2	a4	162	ASN
2	a4	174	ASN
2	a4	225	ASN
2	a4	248	ASN
2	a4	305	GLN
2	a4	313	ASN
2	a4	342	ASN
2	a4	362	ASN
2	a4	385	GLN
2	a4	432	HIS
3	b2	8	HIS
3	b2	44	GLN
3	b2	85	ASN
3	b2	312	GLN
3	b2	341	GLN
3	b2	345	HIS
4	c2	50	HIS

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Mol	Chain	Res	Type
4	c2	155	GLN
4	c2	165	ASN
4	c2	199	HIS
4	c2	224	HIS
5	f2	57	GLN
5	f2	86	ASN
5	f2	122	HIS
5	f2	161	HIS
5	f2	164	HIS
6	d2	22	ASN
7	q2	12	HIS
7	q2	23	GLN
7	q2	64	GLN
8	h2	71	HIS
8	h2	75	ASN
11	V1	24	ASN
11	V1	37	GLN
11	V1	148	ASN
11	V1	165	ASN
11	V1	293	ASN
11	V1	431	GLN
12	V2	9	HIS
12	V2	16	ASN
12	V2	42	HIS
12	V2	74	GLN
13	S1	36	GLN
13	S1	51	ASN
13	S1	117	GLN
13	S1	179	ASN
13	S1	308	GLN
13	S1	430	GLN
13	S1	437	HIS
13	S1	548	HIS
13	S1	665	GLN
13	S1	682	GLN
14	S2	5	GLN
14	S2	34	ASN
14	S2	50	ASN
14	S2	98	GLN
14	S2	129	GLN
14	S2	149	ASN
14	S2	157	HIS

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Mol	Chain	Res	Type
14	S2	190	HIS
15	S3	19	HIS
15	S3	39	GLN
15	S3	88	ASN
16	S7	127	HIS
16	S7	162	GLN
18	V3	43	HIS
18	V3	44	HIS
19	S6	16	GLN
19	S6	47	GLN
19	S6	93	GLN
20	S4	46	GLN
20	S4	50	ASN
21	A9	8	HIS
21	A9	67	GLN
21	A9	87	HIS
21	A9	288	HIS
23	A5	52	ASN
23	A5	72	GLN
23	A5	82	GLN
23	A5	95	GLN
24	A6	94	ASN
25	A7	20	GLN
25	A7	24	GLN
26	AL	17	HIS
26	AL	31	ASN
26	AL	59	HIS
26	AL	72	ASN
26	AL	135	GLN
27	AA	74	GLN
28	D3	10	ASN
28	D3	83	ASN
29	D1	5	ASN
29	D1	194	ASN
29	D1	235	ASN
29	D1	247	HIS
29	D1	292	ASN
29	D1	317	GLN
30	D6	120	ASN
31	4L	25	HIS
31	4L	83	ASN
32	D5	113	ASN

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Mol	Chain	Res	Type
32	D5	205	ASN
32	D5	226	GLN
32	D5	332	HIS
32	D5	479	GLN
32	D5	506	ASN
32	D5	509	HIS
32	D5	514	ASN
32	D5	580	GLN
33	D4	26	ASN
33	D4	44	GLN
33	D4	83	HIS
33	D4	138	ASN
33	D4	144	ASN
33	D4	220	HIS
33	D4	279	GLN
33	D4	319	HIS
33	D4	440	HIS
34	D2	174	GLN
34	D2	186	HIS
34	D2	316	GLN
36	B5	95	GLN
36	B5	124	GLN
36	B5	143	ASN
27	AB	33	ASN
27	AB	74	GLN
37	A8	29	HIS
37	A8	63	ASN
37	A8	76	HIS
37	A8	150	ASN
38	BJ	27	ASN
38	BJ	103	ASN
38	BJ	114	GLN
38	BJ	122	GLN
39	AJ	92	ASN
39	AJ	151	HIS
39	AJ	200	GLN
39	AJ	204	ASN
39	AJ	251	GLN
39	AJ	257	HIS
40	S5	15	HIS
40	S5	44	HIS
41	A3	10	ASN

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Mol	Chain	Res	Type
41	A3	45	ASN
41	A3	68	HIS
41	A3	70	GLN
42	B3	58	ASN
43	C2	59	HIS
43	C2	61	GLN
43	C2	79	GLN
44	B4	47	GLN
44	B4	74	ASN
45	AM	89	ASN
46	B6	25	GLN
46	B6	73	HIS
46	B6	82	HIS
47	B7	43	GLN
47	B7	83	GLN
48	B9	13	GLN
48	B9	32	HIS
48	B9	140	GLN
48	B9	159	GLN
48	B9	168	HIS
49	B2	21	GLN
49	B2	58	GLN
50	B8	137	ASN
51	BK	27	GLN
51	BK	45	HIS
51	BK	57	ASN
53	B1	51	ASN
54	A1	27	HIS
54	A1	44	GLN
54	A1	58	ASN
54	A1	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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
58	FES	f1	501	5	0,4,4	-	-	-		
56	HEC	c1	501	4	46,50,50	2.00	9 (19%)	58,82,82	1.88	9 (15%)
58	FES	f2	202	5	0,4,4	-	-	-		
59	SF4	V1	500	11	0,12,12	-	-	-		
55	HEM	b2	402	3	50,50,50	1.66	9 (18%)	67,82,82	1.77	15 (22%)
58	FES	S1	803	13	0,4,4	-	-	-		
59	SF4	S8	201	17	0,12,12	-	-	-		
59	SF4	S8	202	17	0,12,12	-	-	-		
57	3PE	D1	501	-	25,25,50	0.40	0	28,30,55	0.46	0
56	HEC	c2	501	4	46,50,50	2.00	9 (19%)	58,82,82	2.06	7 (12%)
57	3PE	c1	502	-	12,12,50	0.63	0	13,15,55	0.66	0
63	ZMP	AB	101	27	25,30,36	0.67	0	29,37,45	1.47	4 (13%)
59	SF4	S1	801	13	0,12,12	-	-	-		
57	3PE	f2	201	-	22,22,50	0.44	0	25,27,55	0.47	0
63	ZMP	AA	101	27	28,33,36	0.57	0	32,40,45	1.08	2 (6%)
60	FMN	V1	501	-	33,33,33	0.45	0	48,50,50	0.39	0
62	NDP	A9	401	-	51,52,52	0.50	1 (1%)	71,80,80	0.64	1 (1%)
55	HEM	b1	402	3	50,50,50	1.55	7 (14%)	67,82,82	1.87	15 (22%)
57	3PE	D5	902	-	37,37,50	0.36	0	40,42,55	0.41	0
59	SF4	S7	300	16	0,12,12	-	-	-		
55	HEM	b1	401	3	50,50,50	1.51	7 (14%)	67,82,82	1.76	14 (20%)
65	PC1	AK	201	-	27,27,53	0.41	0	33,35,61	0.41	0
64	CDL	D5	901	-	59,59,99	0.40	0	65,71,111	0.57	1 (1%)
59	SF4	S1	802	13	0,12,12	-	-	-		
57	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	HEM	b2	401	3	50,50,50	1.54	9 (18%)	67,82,82	1.79	18 (26%)
58	FES	V2	300	12	0,4,4	-	-	-		

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
58	FES	f1	501	5	-	-	0/1/1/1
56	HEC	c1	501	4	-	8/14/54/54	-
58	FES	f2	202	5	-	-	0/1/1/1
59	SF4	V1	500	11	-	-	0/6/5/5
55	HEM	b2	402	3	-	6/14/54/54	-
58	FES	S1	803	13	-	-	0/1/1/1
59	SF4	S8	201	17	-	-	0/6/5/5
59	SF4	S8	202	17	-	-	0/6/5/5
57	3PE	D1	501	-	-	12/28/28/54	-
56	HEC	c2	501	4	-	7/14/54/54	-
57	3PE	c1	502	-	-	7/13/13/54	-
63	ZMP	AB	101	27	-	17/35/37/43	-
59	SF4	S1	801	13	-	-	0/6/5/5
57	3PE	f2	201	-	-	7/26/26/54	-
63	ZMP	AA	101	27	-	16/38/40/43	-
60	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
62	NDP	A9	401	-	-	9/34/77/77	0/5/5/5
55	HEM	b1	402	3	-	9/14/54/54	-
57	3PE	D5	902	-	-	12/41/41/54	-
59	SF4	S7	300	16	-	-	0/6/5/5
55	HEM	b1	401	3	-	9/14/54/54	-
65	PC1	AK	201	-	-	8/31/31/57	-
64	CDL	D5	901	-	-	12/70/70/110	-
59	SF4	S1	802	13	-	-	0/6/5/5
57	3PE	D4	501	-	-	7/43/43/54	-
55	HEM	b2	401	3	-	5/14/54/54	-
58	FES	V2	300	12	-	-	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	c1	501	HEC	CAC-C3C	7.10	1.58	1.35
56	c2	501	HEC	CAC-C3C	6.64	1.56	1.35
56	c1	501	HEC	CAB-C3B	6.48	1.56	1.35
56	c2	501	HEC	CAB-C3B	6.33	1.55	1.35
55	b1	401	HEM	C4D-ND	-4.51	1.32	1.40
55	b1	402	HEM	C4D-ND	-4.47	1.32	1.40
55	b2	401	HEM	C4D-ND	-4.34	1.32	1.40
55	b2	402	HEM	C4D-ND	-4.31	1.32	1.40
55	b1	402	HEM	C1B-NB	-4.14	1.33	1.40
55	b2	402	HEM	C1B-NB	-3.89	1.33	1.40
55	b1	401	HEM	C1B-NB	-3.78	1.33	1.40
55	b2	402	HEM	C1D-ND	-3.77	1.31	1.38
55	b2	401	HEM	C1B-NB	-3.61	1.34	1.40
55	b2	402	HEM	C1C-C2C	-3.52	1.38	1.45
55	b1	402	HEM	C1C-C2C	-3.50	1.38	1.45
55	b1	402	HEM	C1D-ND	-3.43	1.32	1.38
55	b1	401	HEM	C1D-ND	-3.41	1.32	1.38
55	b1	401	HEM	C1C-C2C	-3.39	1.38	1.45
56	c2	501	HEC	CBC-CAC	-3.38	1.37	1.49
56	c1	501	HEC	CBC-CAC	-3.37	1.37	1.49
55	b2	401	HEM	C1C-C2C	-3.32	1.38	1.45
55	b2	401	HEM	C1D-ND	-3.30	1.32	1.38
55	b2	402	HEM	C4B-NB	-3.04	1.32	1.38
55	b1	402	HEM	C4B-NB	-3.00	1.32	1.38
55	b2	401	HEM	C4B-NB	-3.00	1.33	1.38
56	c2	501	HEC	C3B-C4B	-2.90	1.41	1.46
56	c2	501	HEC	C3D-C2D	-2.84	1.31	1.38
55	b2	401	HEM	C1A-C2A	-2.71	1.39	1.44
55	b2	402	HEM	C3C-C4C	-2.62	1.41	1.46
55	b1	401	HEM	C4B-NB	-2.60	1.33	1.38
56	c2	501	HEC	C3C-C4C	-2.57	1.41	1.46
55	b2	402	HEM	C1A-C2A	-2.54	1.39	1.44
55	b2	401	HEM	C3C-C4C	-2.53	1.41	1.46
56	c2	501	HEC	CBB-CAB	-2.52	1.40	1.49
56	c2	501	HEC	C3C-C2C	-2.52	1.32	1.41
55	b1	401	HEM	C3C-C4C	-2.48	1.41	1.46
56	c1	501	HEC	C3B-C4B	-2.42	1.41	1.46
56	c1	501	HEC	CBB-CAB	-2.40	1.40	1.49
55	b2	402	HEM	C1B-C2B	-2.33	1.39	1.44
56	c2	501	HEC	C3B-C2B	-2.30	1.33	1.41
56	c1	501	HEC	C3C-C2C	-2.27	1.33	1.41
56	c1	501	HEC	C3D-C2D	-2.27	1.33	1.38
55	b1	402	HEM	C3C-C4C	-2.23	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	b2	402	HEM	C4A-NA	-2.19	1.35	1.39
56	c1	501	HEC	C3B-C2B	-2.19	1.33	1.41
62	A9	401	NDP	P2B-O2B	2.17	1.63	1.59
56	c1	501	HEC	CMD-C2D	2.15	1.55	1.50
55	b2	401	HEM	C1C-NC	-2.13	1.35	1.39
55	b2	401	HEM	C4A-NA	-2.12	1.35	1.39
55	b1	401	HEM	C4A-NA	-2.06	1.35	1.39
55	b1	402	HEM	C4A-NA	-2.03	1.35	1.39

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	c2	501	HEC	CBC-CAC-C3C	-9.20	109.04	127.43
56	c2	501	HEC	CBB-CAB-C3B	-8.64	110.17	127.43
56	c1	501	HEC	CBB-CAB-C3B	-7.77	111.90	127.43
55	b1	402	HEM	CHC-C4B-NB	6.38	131.28	124.42
55	b1	401	HEM	CHC-C4B-NB	6.26	131.16	124.42
56	c1	501	HEC	CBC-CAC-C3C	-6.25	114.94	127.43
55	b2	401	HEM	CHC-C4B-NB	6.14	131.03	124.42
55	b2	402	HEM	CHC-C4B-NB	5.50	130.34	124.42
55	b2	402	HEM	CHD-C4C-NC	5.14	130.05	124.45
55	b2	402	HEM	CHB-C1B-NB	5.11	130.68	124.37
55	b1	402	HEM	CHB-C1B-NB	5.01	130.57	124.37
55	b1	402	HEM	CHD-C4C-NC	4.66	129.53	124.45
55	b1	401	HEM	CHD-C4C-NC	4.50	129.35	124.45
55	b1	401	HEM	CHB-C1B-NB	4.26	129.64	124.37
55	b2	401	HEM	CHD-C1D-ND	3.91	128.64	124.42
55	b2	401	HEM	CHD-C4C-NC	3.91	128.71	124.45
55	b1	402	HEM	C4D-ND-C1D	3.60	109.47	105.21
55	b2	401	HEM	CHB-C1B-NB	3.42	128.59	124.37
56	c1	501	HEC	CMD-C2D-C1D	-3.31	120.38	125.42
63	AB	101	ZMP	O1-C10-C9	-3.29	120.18	123.98
55	b1	402	HEM	CHA-C4D-ND	3.26	128.40	124.37
55	b2	401	HEM	CHA-C1A-NA	3.22	129.70	123.86
63	AB	101	ZMP	C15-C14-C13	-3.14	107.17	112.39
63	AB	101	ZMP	C11-C12-N1	-3.13	105.87	112.41
55	b1	401	HEM	CHD-C1D-ND	3.12	127.78	124.42
55	b1	402	HEM	CHD-C1D-ND	3.12	127.78	124.42
55	b2	402	HEM	CHB-C1B-C2B	-2.98	118.48	126.95
56	c1	501	HEC	O1D-CGD-CBD	-2.92	113.82	123.09
55	b1	401	HEM	C1C-CHC-C4B	-2.88	119.90	126.02
55	b2	402	HEM	CHA-C1A-NA	2.88	129.07	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	b1	402	HEM	CHB-C1B-C2B	-2.86	118.82	126.95
55	b1	401	HEM	C1B-NB-C4B	2.84	108.57	105.21
55	b2	402	HEM	C4A-CHB-C1B	-2.83	119.58	126.25
55	b1	401	HEM	CHA-C1A-NA	2.83	128.99	123.86
55	b1	401	HEM	C4D-ND-C1D	2.81	108.53	105.21
63	AA	101	ZMP	O1-C10-C9	-2.80	120.75	123.98
55	b2	401	HEM	C1B-NB-C4B	2.79	108.51	105.21
56	c1	501	HEC	O1A-CGA-CBA	-2.78	114.28	123.09
56	c1	501	HEC	CMD-C2D-C3D	2.78	131.51	125.62
56	c2	501	HEC	O1D-CGD-CBD	-2.76	114.32	123.09
55	b1	402	HEM	C1C-CHC-C4B	-2.76	120.16	126.02
56	c1	501	HEC	CHC-C4B-NB	2.69	127.39	124.45
55	b1	402	HEM	C4A-CHB-C1B	-2.63	120.05	126.25
56	c2	501	HEC	CHC-C4B-NB	2.63	127.32	124.45
55	b2	402	HEM	C4D-ND-C1D	2.61	108.30	105.21
55	b1	402	HEM	C1B-NB-C4B	2.59	108.28	105.21
55	b2	401	HEM	CBD-CAD-C3D	-2.57	105.42	112.53
55	b2	402	HEM	C1B-NB-C4B	2.57	108.25	105.21
55	b1	401	HEM	CHA-C4D-ND	2.55	127.52	124.37
63	AA	101	ZMP	C15-C14-C13	-2.52	108.20	112.39
62	A9	401	NDP	P2B-O2B-C2B	2.51	130.12	123.43
55	b2	401	HEM	C4D-ND-C1D	2.49	108.15	105.21
56	c1	501	HEC	O2A-CGA-O1A	2.49	129.72	123.33
55	b2	401	HEM	C4C-CHD-C1D	-2.48	120.74	126.02
55	b2	402	HEM	C1C-CHC-C4B	-2.47	120.78	126.02
55	b2	401	HEM	C4A-CHB-C1B	-2.45	120.49	126.25
55	b2	402	HEM	C3B-C4B-NB	-2.43	107.72	109.47
64	D5	901	CDL	CB4-OB6-CB5	2.42	123.58	117.80
55	b1	401	HEM	O2A-CGA-CBA	2.34	121.40	114.00
55	b2	401	HEM	CMB-C2B-C1B	2.34	128.69	125.03
55	b1	401	HEM	CHC-C4B-C3B	-2.34	120.41	125.07
55	b1	402	HEM	CHC-C4B-C3B	-2.32	120.44	125.07
55	b2	402	HEM	CAD-C3D-C4D	2.30	128.70	124.70
55	b1	401	HEM	C4A-CHB-C1B	-2.24	120.98	126.25
55	b2	402	HEM	CHA-C4D-ND	2.24	127.13	124.37
55	b1	401	HEM	CHB-C1B-C2B	-2.23	120.62	126.95
56	c2	501	HEC	CBA-CAA-C2A	2.21	118.64	112.53
55	b2	402	HEM	CHD-C1D-ND	2.20	126.80	124.42
56	c1	501	HEC	CBD-CAD-C3D	2.20	118.62	112.53
55	b2	402	HEM	O2D-CGD-CBD	2.20	120.95	114.00
55	b2	401	HEM	C1C-CHC-C4B	-2.20	121.35	126.02
55	b2	401	HEM	CHD-C1D-C2D	-2.20	121.56	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	b2	401	HEM	CHC-C4B-C3B	-2.18	120.73	125.07
55	b2	402	HEM	CBA-CAA-C2A	-2.18	106.52	112.53
55	b2	401	HEM	CHA-C4D-ND	2.17	127.05	124.37
55	b2	401	HEM	O2A-CGA-CBA	2.16	120.82	114.00
55	b2	401	HEM	CAA-CBA-CGA	-2.14	108.00	113.67
56	c2	501	HEC	CBD-CAD-C3D	2.12	118.40	112.53
56	c2	501	HEC	C3D-C4D-ND	-2.11	107.81	110.15
55	b1	402	HEM	O2D-CGD-CBD	2.10	120.65	114.00
55	b1	401	HEM	O2A-CGA-O1A	-2.08	117.99	123.33
55	b1	402	HEM	O2A-CGA-CBA	2.07	120.56	114.00
55	b1	402	HEM	CHA-C1A-NA	2.05	127.58	123.86
63	AB	101	ZMP	C12-N1-C13	2.05	126.64	122.82
55	b2	401	HEM	CHB-C1B-C2B	-2.02	121.20	126.95
55	b1	402	HEM	C4C-CHD-C1D	-2.01	121.74	126.02

There are no chirality outliers.

All (158) 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	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	401	HEM	C4B-C3B-CAB-CBB
55	b2	401	HEM	C2C-C3C-CAC-CBC
55	b2	401	HEM	C4C-C3C-CAC-CBC
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
57	c1	502	3PE	C1-O11-P-O12
57	c1	502	3PE	C11-O13-P-O11
57	c1	502	3PE	C11-O13-P-O12
57	f2	201	3PE	C11-O13-P-O11
57	f2	201	3PE	C11-O13-P-O12
57	f2	201	3PE	O21-C2-C3-O31
57	D1	501	3PE	C1-O11-P-O12
57	D1	501	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
57	D1	501	3PE	C1-O11-P-O14
57	D1	501	3PE	C11-O13-P-O11
57	D1	501	3PE	C11-O13-P-O12
57	D1	501	3PE	C11-O13-P-O14
57	D5	902	3PE	C1-O11-P-O12
57	D5	902	3PE	C1-O11-P-O13
57	D5	902	3PE	C11-O13-P-O11
57	D5	902	3PE	C11-O13-P-O12
57	D5	902	3PE	O13-C11-C12-N
57	D5	902	3PE	O21-C2-C3-O31
57	D4	501	3PE	C1-O11-P-O14
57	D4	501	3PE	C11-O13-P-O11
57	D4	501	3PE	C11-O13-P-O12
57	D4	501	3PE	C11-O13-P-O14
60	V1	501	FMN	O3'-C3'-C4'-C5'
60	V1	501	FMN	C5'-O5'-P-O2P
60	V1	501	FMN	C5'-O5'-P-O3P
62	A9	401	NDP	C5B-O5B-PA-O1A
62	A9	401	NDP	C5B-O5B-PA-O2A
62	A9	401	NDP	C5B-O5B-PA-O3
62	A9	401	NDP	C1B-C2B-O2B-P2B
63	AA	101	ZMP	O4-C17-C18-C21
63	AA	101	ZMP	O1-C10-S1-C11
63	AA	101	ZMP	C9-C10-S1-C11
63	AA	101	ZMP	C7-C8-C9-C10
63	AB	101	ZMP	C17-C18-C21-O5
63	AB	101	ZMP	C12-C11-S1-C10
63	AB	101	ZMP	O1-C10-S1-C11
63	AB	101	ZMP	C9-C10-S1-C11
64	D5	901	CDL	CB2-OB2-PB2-OB4
64	D5	901	CDL	CB2-OB2-PB2-OB5
65	AK	201	PC1	C11-O13-P-O12
65	AK	201	PC1	C11-O13-P-O14
65	AK	201	PC1	C11-O13-P-O11
63	AA	101	ZMP	C14-C13-N1-C12
63	AB	101	ZMP	C14-C13-N1-C12
60	V1	501	FMN	C2'-C3'-C4'-O4'
60	V1	501	FMN	C2'-C3'-C4'-C5'
55	b2	401	HEM	C2A-CAA-CBA-CGA
63	AA	101	ZMP	O2-C13-N1-C12
63	AB	101	ZMP	O2-C13-N1-C12
60	V1	501	FMN	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
55	b1	401	HEM	C2A-CAA-CBA-CGA
63	AB	101	ZMP	C5-C6-C7-C8
63	AB	101	ZMP	S1-C11-C12-N1
57	D5	902	3PE	C21-C22-C23-C24
57	D4	501	3PE	C35-C36-C37-C38
57	D1	501	3PE	C22-C23-C24-C25
57	D5	902	3PE	C26-C27-C28-C29
63	AB	101	ZMP	C6-C7-C8-C9
63	AB	101	ZMP	C3-C4-C5-C6
55	b1	401	HEM	C4C-C3C-CAC-CBC
64	D5	901	CDL	OB6-CB4-CB6-OB8
56	c1	501	HEC	C3D-CAD-CBD-CGD
63	AB	101	ZMP	O3-C16-C17-O4
60	V1	501	FMN	C5'-O5'-P-O1P
64	D5	901	CDL	OB5-CB3-CB4-OB6
63	AA	101	ZMP	O4-C17-C18-C19
63	AA	101	ZMP	C2-C1-C22-C23
57	D1	501	3PE	C1-C2-C3-O31
65	AK	201	PC1	C1-C2-C3-O31
63	AA	101	ZMP	C4-C5-C6-C7
57	D1	501	3PE	O21-C2-C3-O31
62	A9	401	NDP	PN-O3-PA-O5B
64	D5	901	CDL	OB5-CB3-CB4-CB6
56	c2	501	HEC	C3D-CAD-CBD-CGD
57	f2	201	3PE	C1-C2-C3-O31
57	D5	902	3PE	C1-C2-C3-O31
57	c1	502	3PE	C12-C11-O13-P
63	AA	101	ZMP	C16-C17-C18-C20
65	AK	201	PC1	C12-C11-O13-P
65	AK	201	PC1	O13-C11-C12-N
57	D5	902	3PE	C34-C35-C36-C37
65	AK	201	PC1	O11-C1-C2-C3
64	D5	901	CDL	C52-C53-C54-C55
63	AA	101	ZMP	C16-C17-C18-C21
63	AB	101	ZMP	C19-C18-C21-O5
63	AB	101	ZMP	C20-C18-C21-O5
56	c1	501	HEC	C4B-C3B-CAB-CBB
56	c1	501	HEC	C4C-C3C-CAC-CBC
56	c2	501	HEC	C4B-C3B-CAB-CBB
65	AK	201	PC1	O11-C1-C2-O21
64	D5	901	CDL	CB3-CB4-CB6-OB8
56	c1	501	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
56	c1	501	HEC	C2C-C3C-CAC-CBC
56	c2	501	HEC	C2B-C3B-CAB-CBB
56	c2	501	HEC	C2C-C3C-CAC-CBC
57	c1	502	3PE	C1-O11-P-O13
57	c1	502	3PE	C1-O11-P-O14
57	c1	502	3PE	O13-C11-C12-N
57	f2	201	3PE	C11-O13-P-O14
57	D5	902	3PE	C1-O11-P-O14
57	D4	501	3PE	O13-C11-C12-N
57	D5	902	3PE	C22-C23-C24-C25
63	AB	101	ZMP	O3-C16-C17-C18
63	AA	101	ZMP	S1-C11-C12-N1
57	D1	501	3PE	C24-C25-C26-C27
63	AA	101	ZMP	C1-C2-C3-C4
63	AB	101	ZMP	N2-C16-C17-C18
62	A9	401	NDP	C4B-C5B-O5B-PA
63	AB	101	ZMP	C4-C5-C6-C7
57	D4	501	3PE	C33-C34-C35-C36
55	b2	402	HEM	CAD-CBD-CGD-O2D
62	A9	401	NDP	O4D-C1D-N1N-C6N
55	b1	402	HEM	CAD-CBD-CGD-O1D
55	b1	402	HEM	CAA-CBA-CGA-O2A
55	b2	402	HEM	CAD-CBD-CGD-O1D
55	b1	402	HEM	CAA-CBA-CGA-O1A
55	b1	402	HEM	CAD-CBD-CGD-O2D
55	b1	402	HEM	C3D-CAD-CBD-CGD
56	c1	501	HEC	C2A-CAA-CBA-CGA
56	c1	501	HEC	CAA-CBA-CGA-O2A
64	D5	901	CDL	C1-CB2-OB2-PB2
62	A9	401	NDP	C2D-C1D-N1N-C6N
64	D5	901	CDL	C51-C52-C53-C54
55	b1	401	HEM	CAD-CBD-CGD-O2D
55	b1	401	HEM	CAA-CBA-CGA-O2A
55	b1	401	HEM	CAD-CBD-CGD-O1D
57	D1	501	3PE	C2-C1-O11-P
56	c1	501	HEC	CAA-CBA-CGA-O1A
63	AA	101	ZMP	C11-C12-N1-C13
55	b1	401	HEM	CAA-CBA-CGA-O1A
63	AA	101	ZMP	C16-C17-C18-C19
57	D1	501	3PE	C26-C27-C28-C29
64	D5	901	CDL	C12-C11-CA5-OA6
63	AA	101	ZMP	O4-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
62	A9	401	NDP	PA-O3-PN-O2N
56	c2	501	HEC	CAA-CBA-CGA-O2A
57	f2	201	3PE	O21-C21-C22-C23
64	D5	901	CDL	CB6-CB4-OB6-CB5
56	c2	501	HEC	C4C-C3C-CAC-CBC
56	c2	501	HEC	CAA-CBA-CGA-O1A
64	D5	901	CDL	C12-C11-CA5-OA7
63	AB	101	ZMP	N2-C16-C17-O4
57	f2	201	3PE	O22-C21-C22-C23

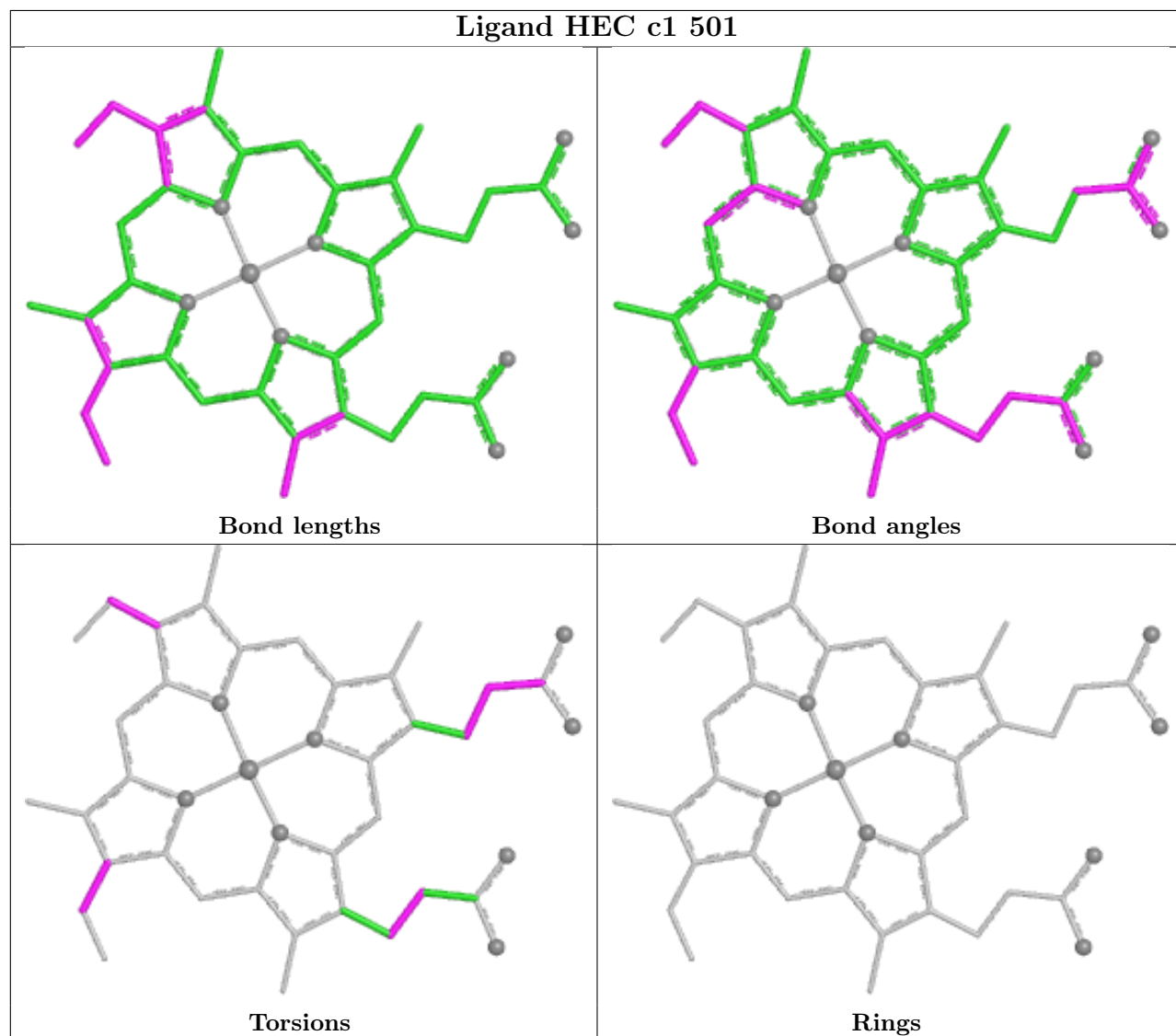
There are no ring outliers.

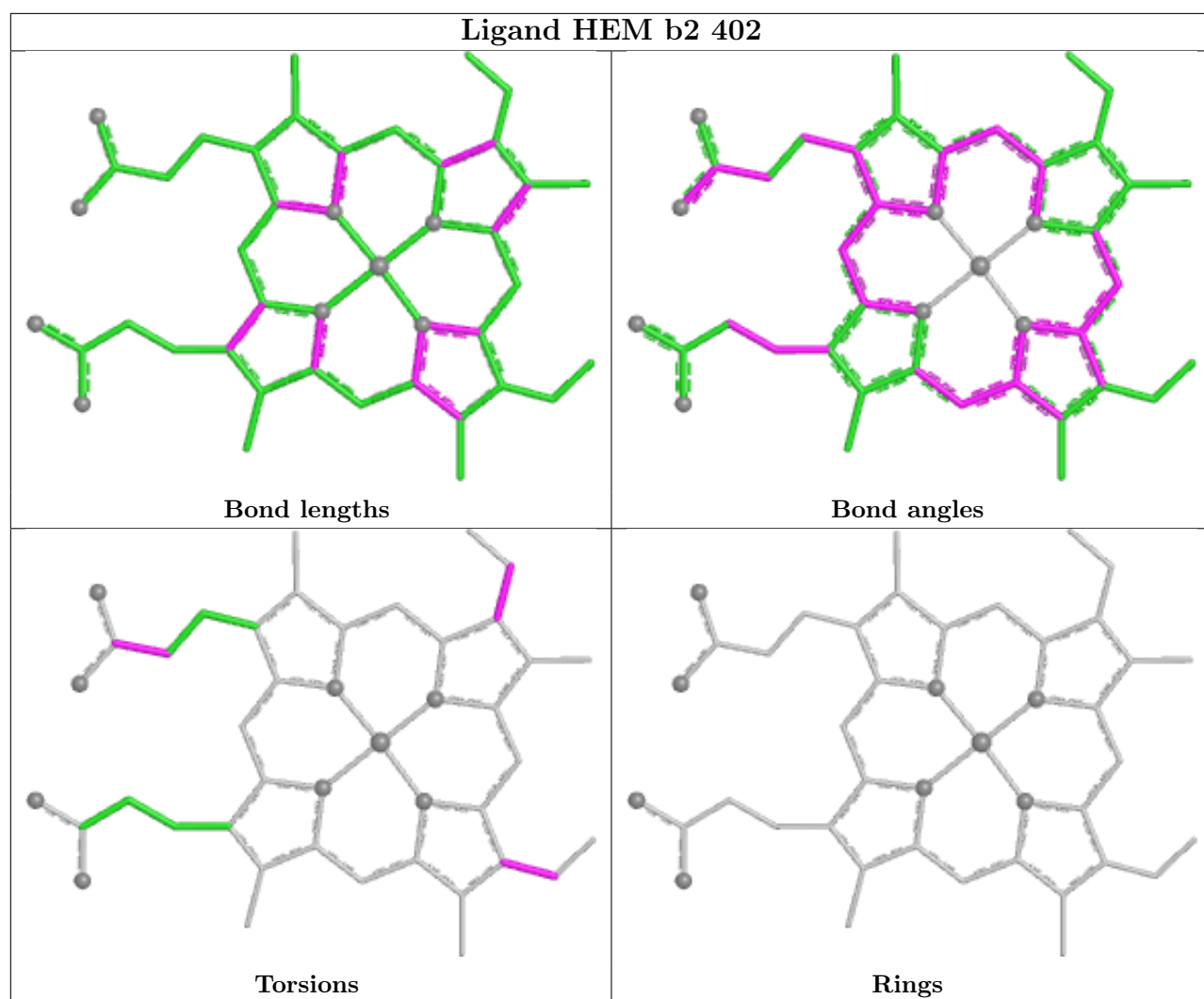
20 monomers are involved in 43 short contacts:

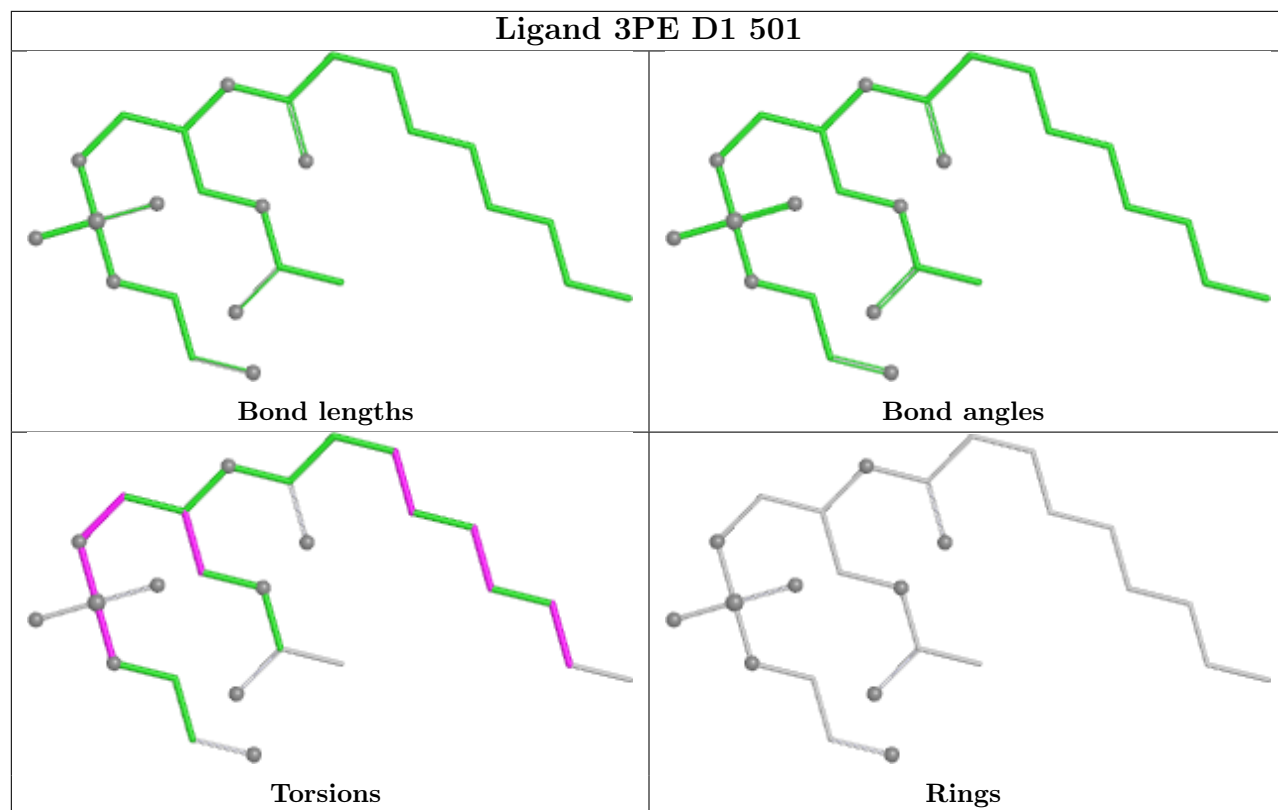
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	c1	501	HEC	3	0
59	V1	500	SF4	1	0
55	b2	402	HEM	2	0
59	S8	202	SF4	1	0
57	D1	501	3PE	2	0
56	c2	501	HEC	2	0
57	c1	502	3PE	1	0
63	AB	101	ZMP	1	0
59	S1	801	SF4	1	0
57	f2	201	3PE	2	0
60	V1	501	FMN	3	0
62	A9	401	NDP	3	0
55	b1	402	HEM	3	0
57	D5	902	3PE	2	0
59	S7	300	SF4	1	0
55	b1	401	HEM	4	0
64	D5	901	CDL	4	0
57	D4	501	3PE	3	0
55	b2	401	HEM	3	0
58	V2	300	FES	1	0

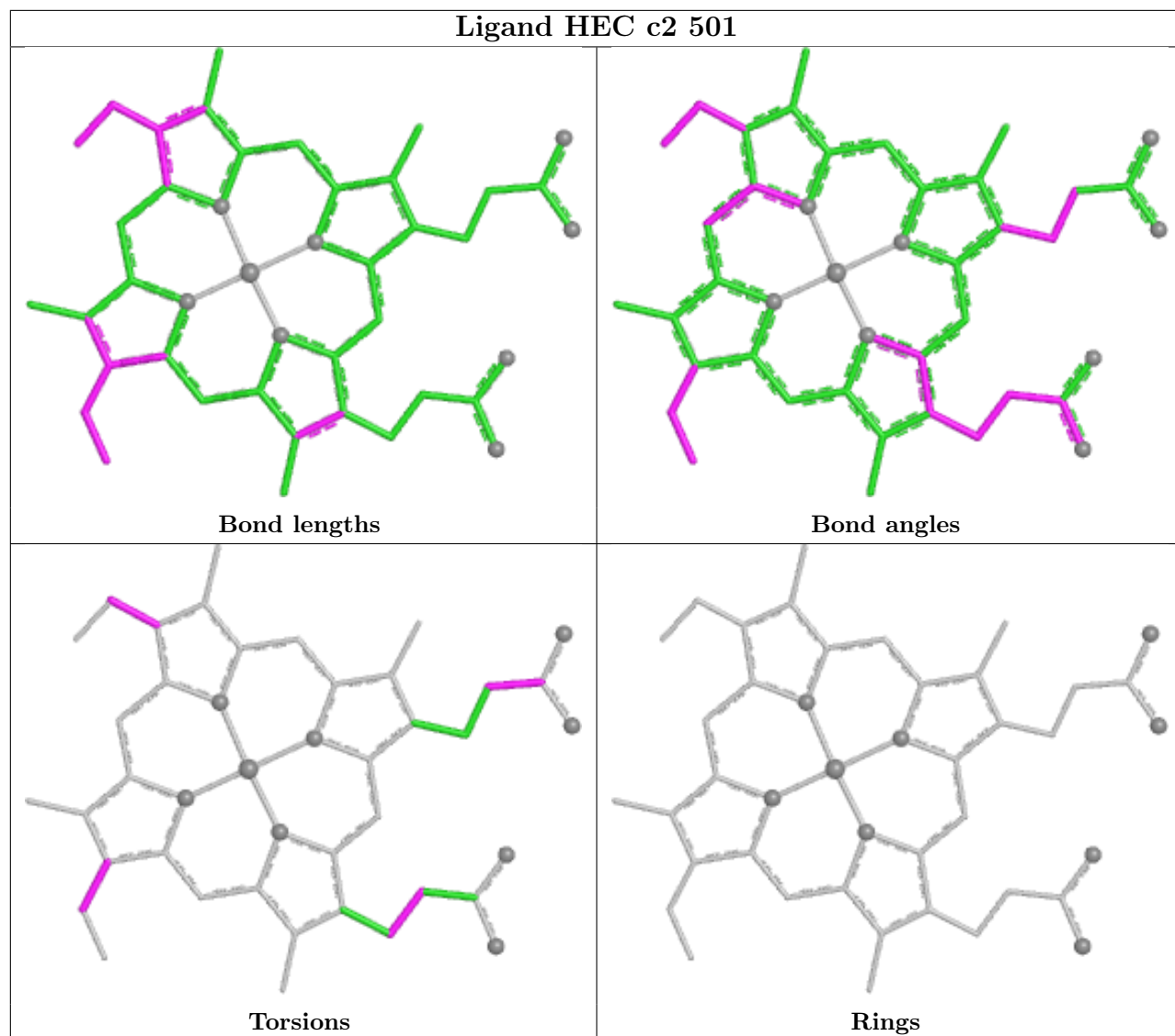
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

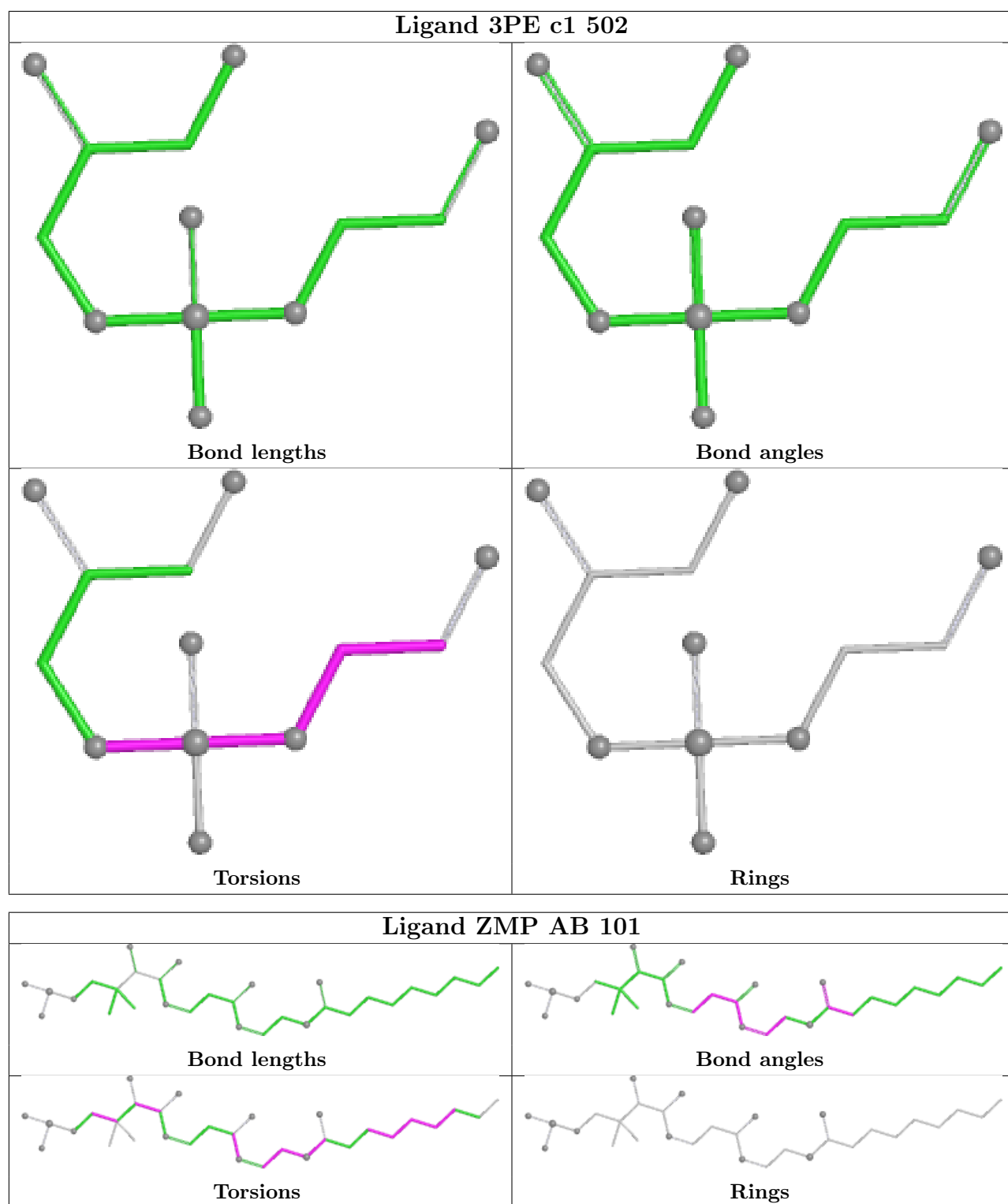
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

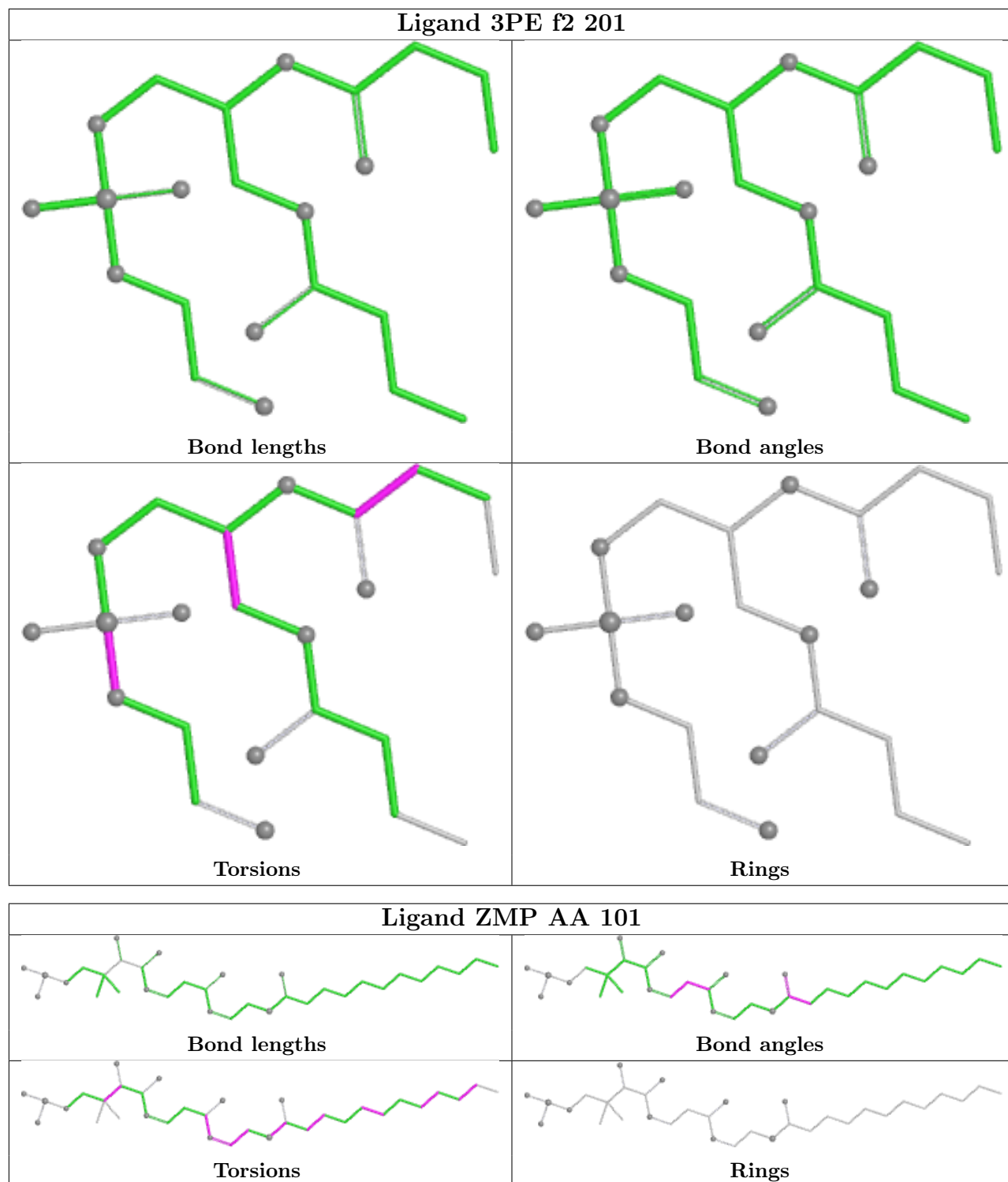


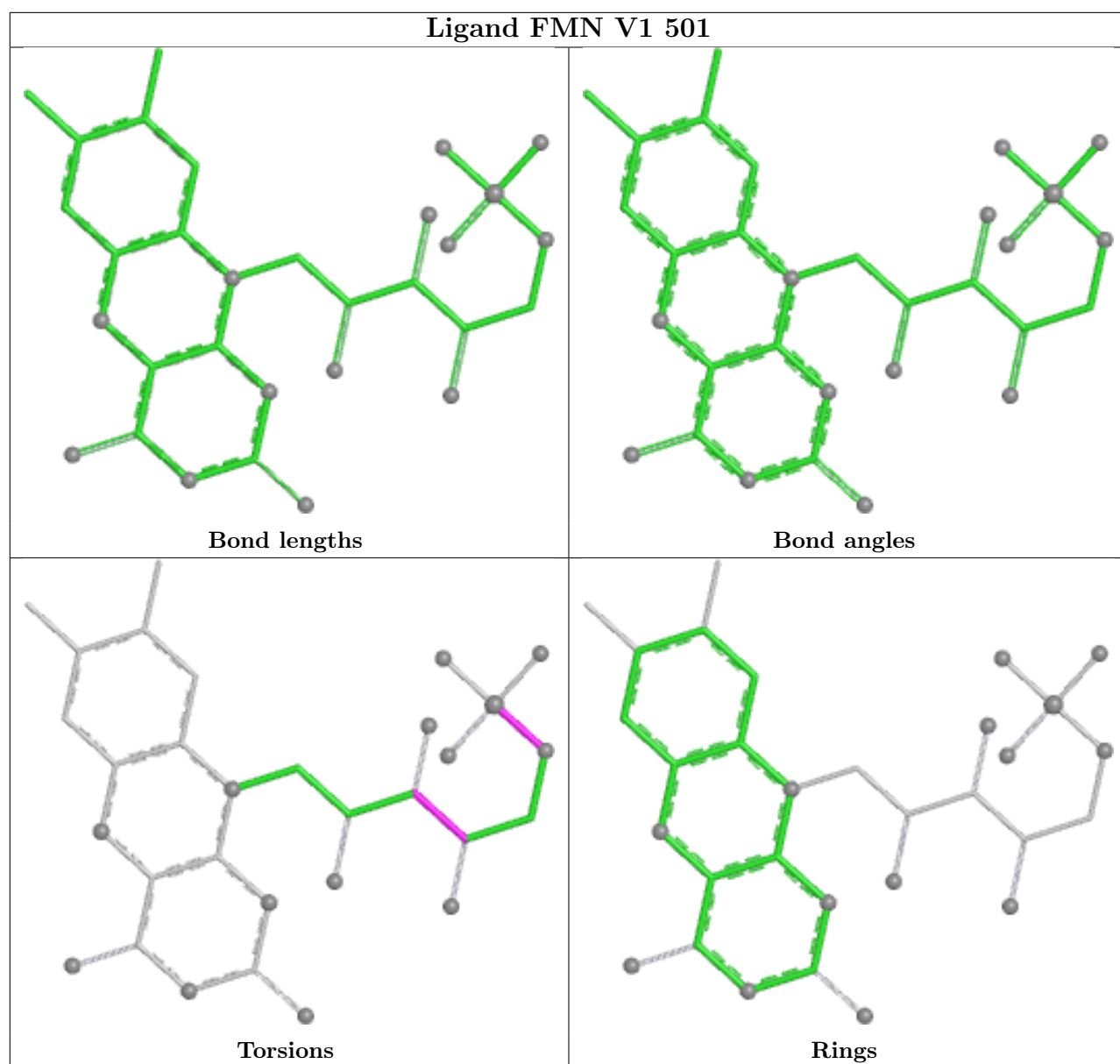


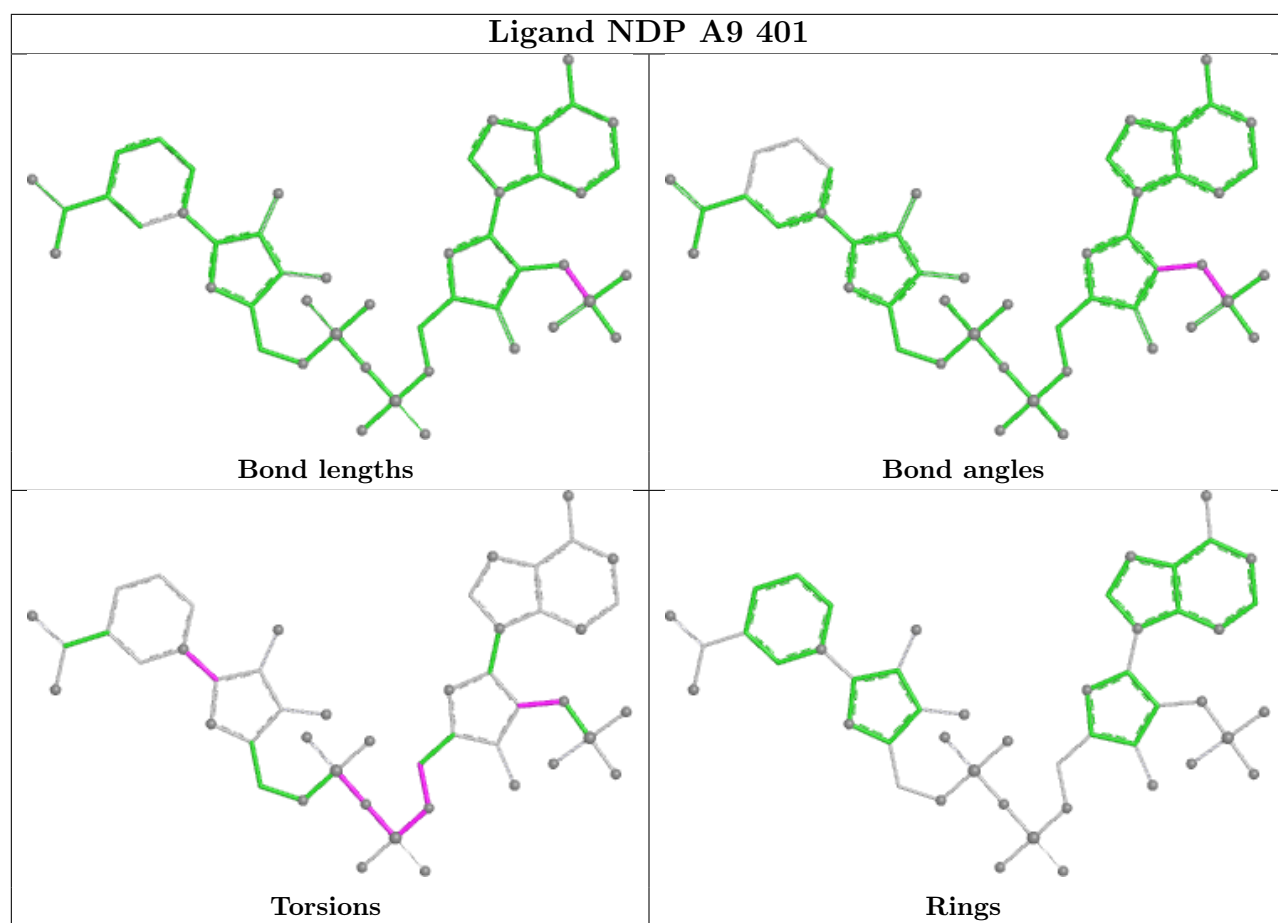


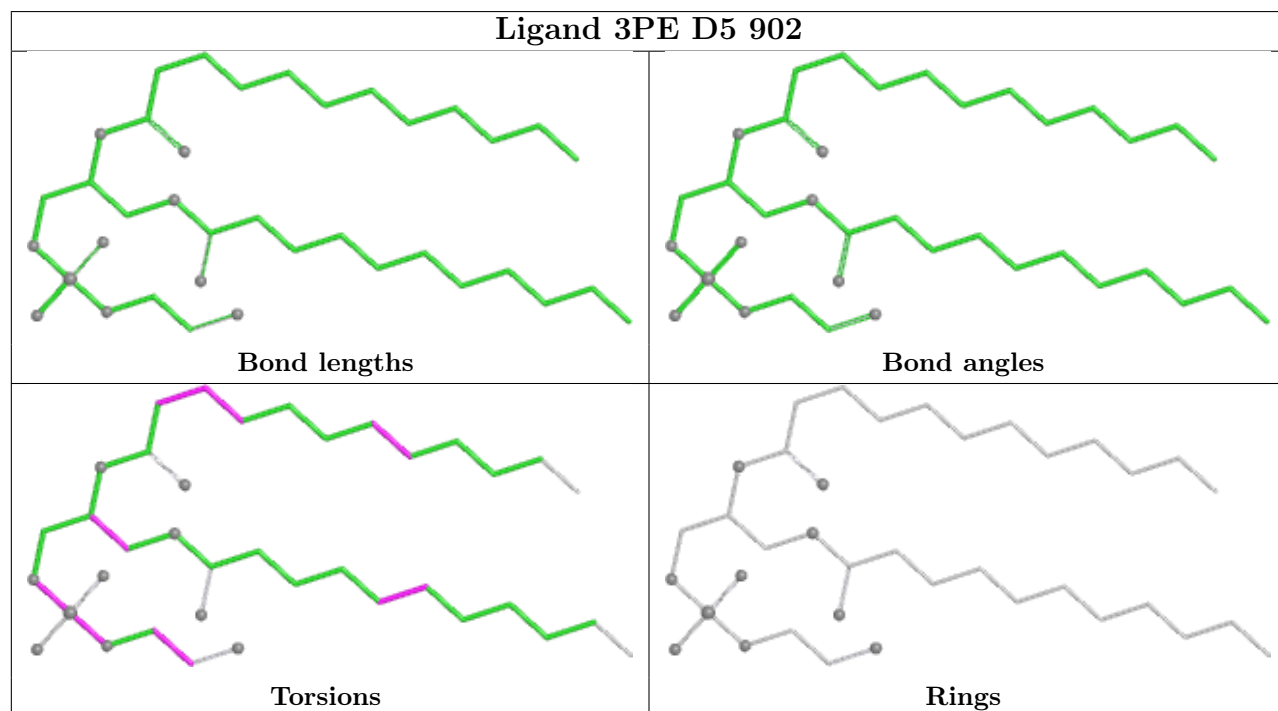
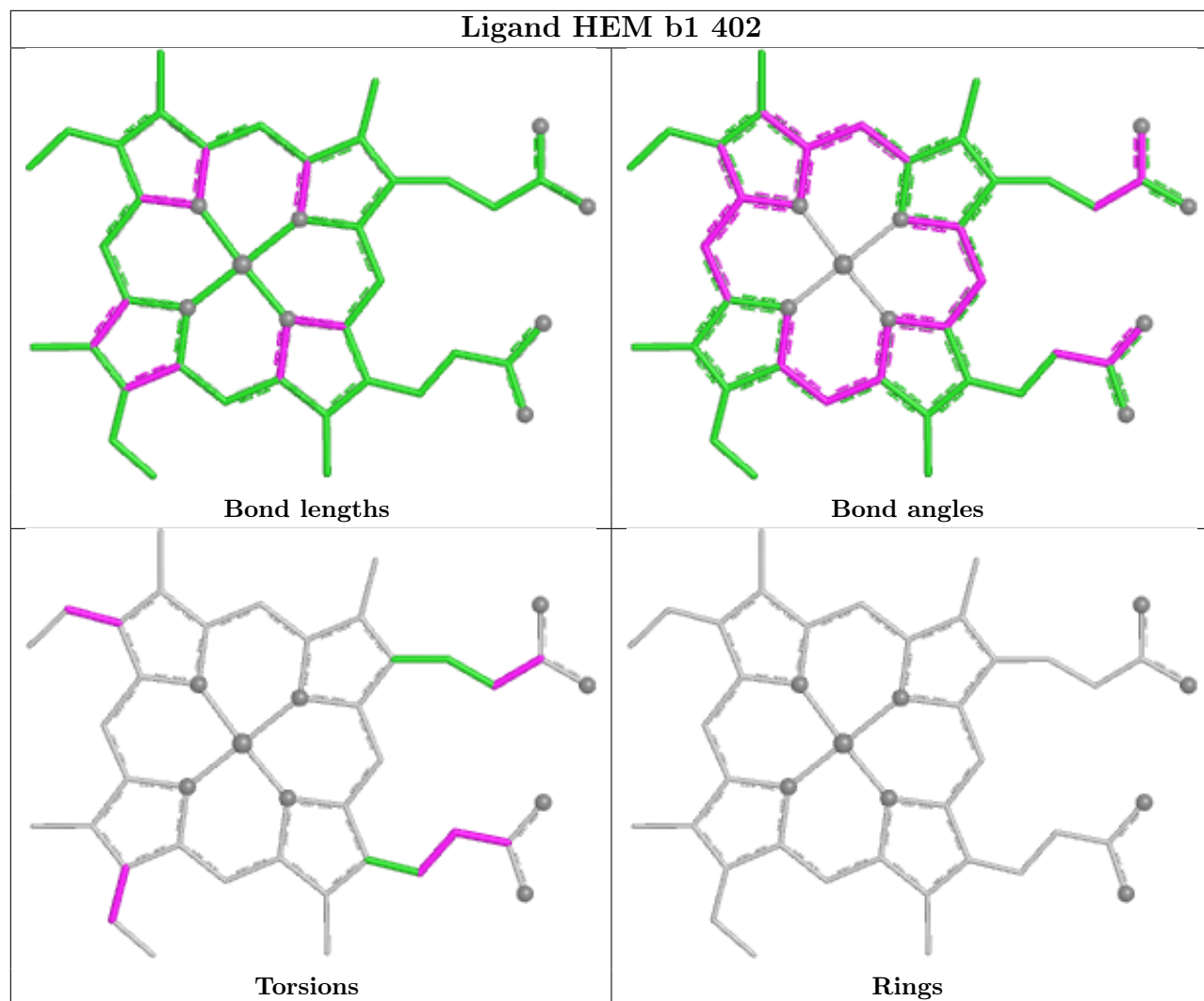


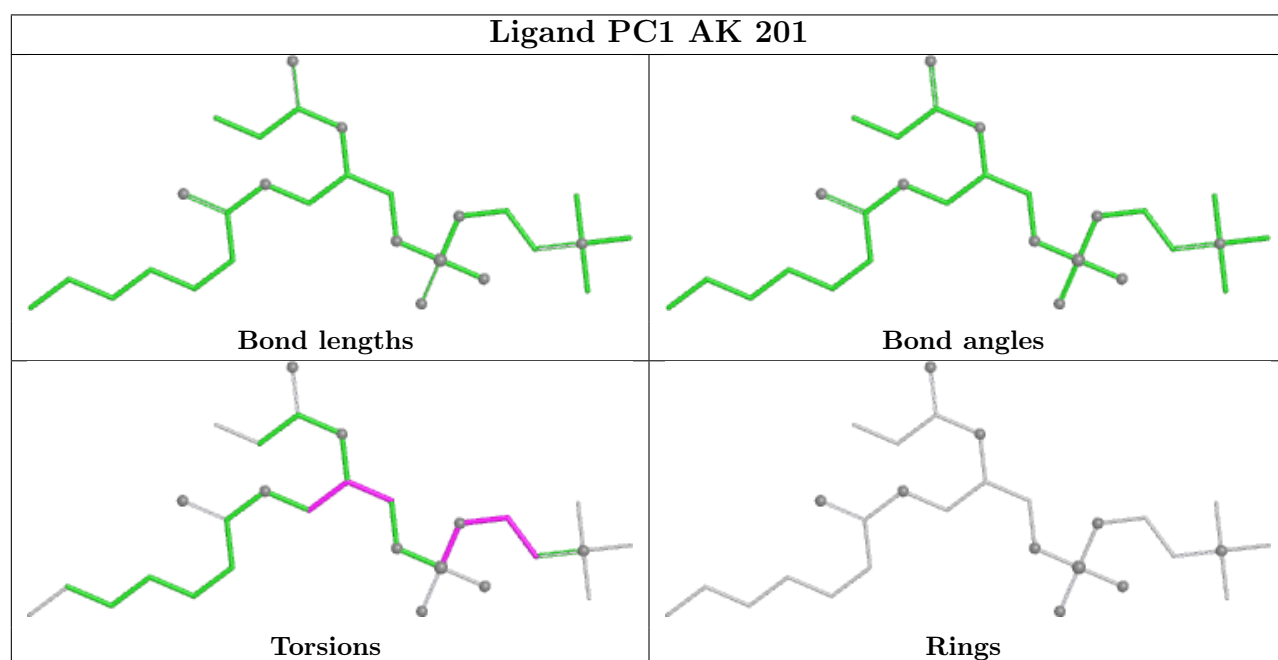
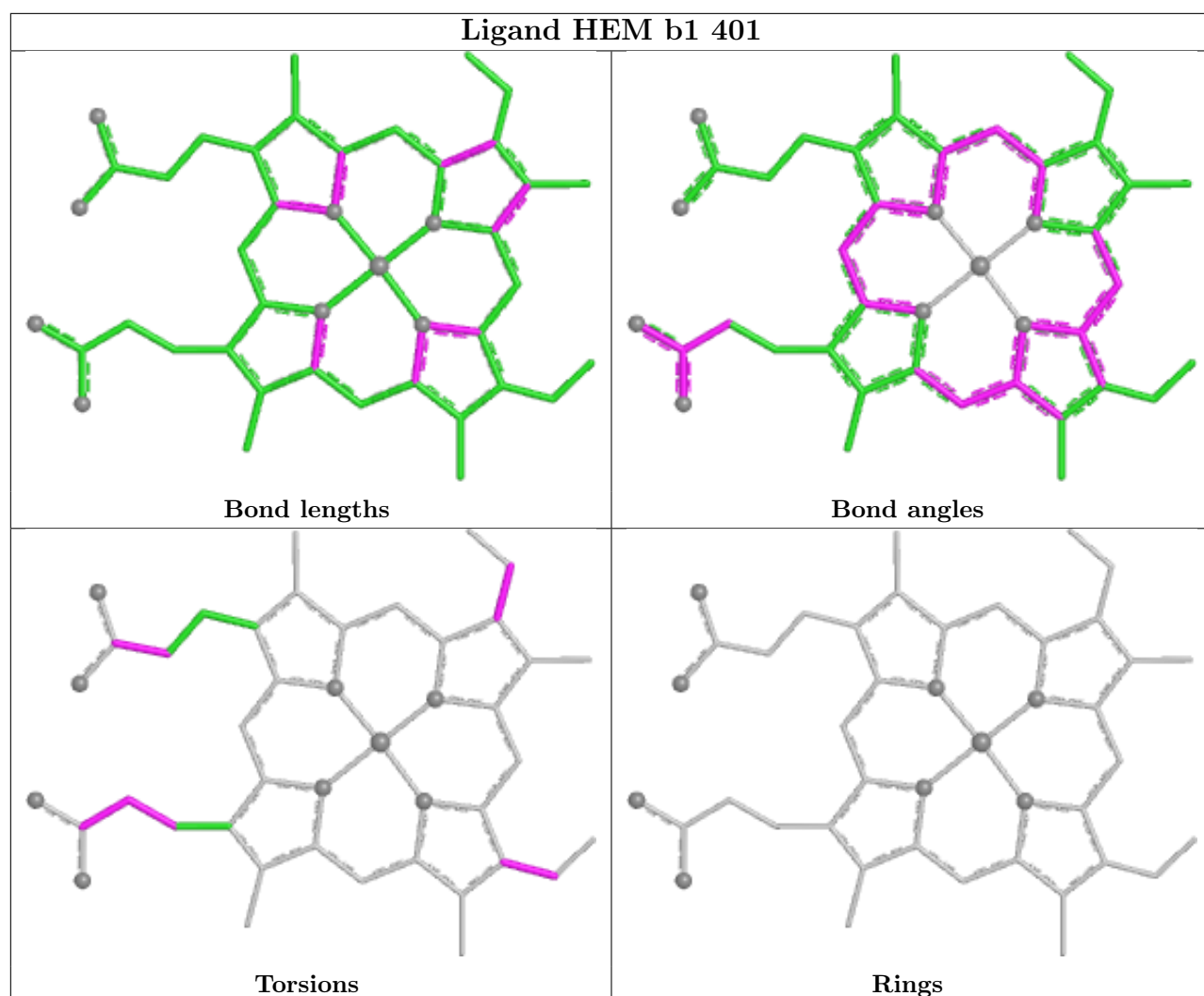


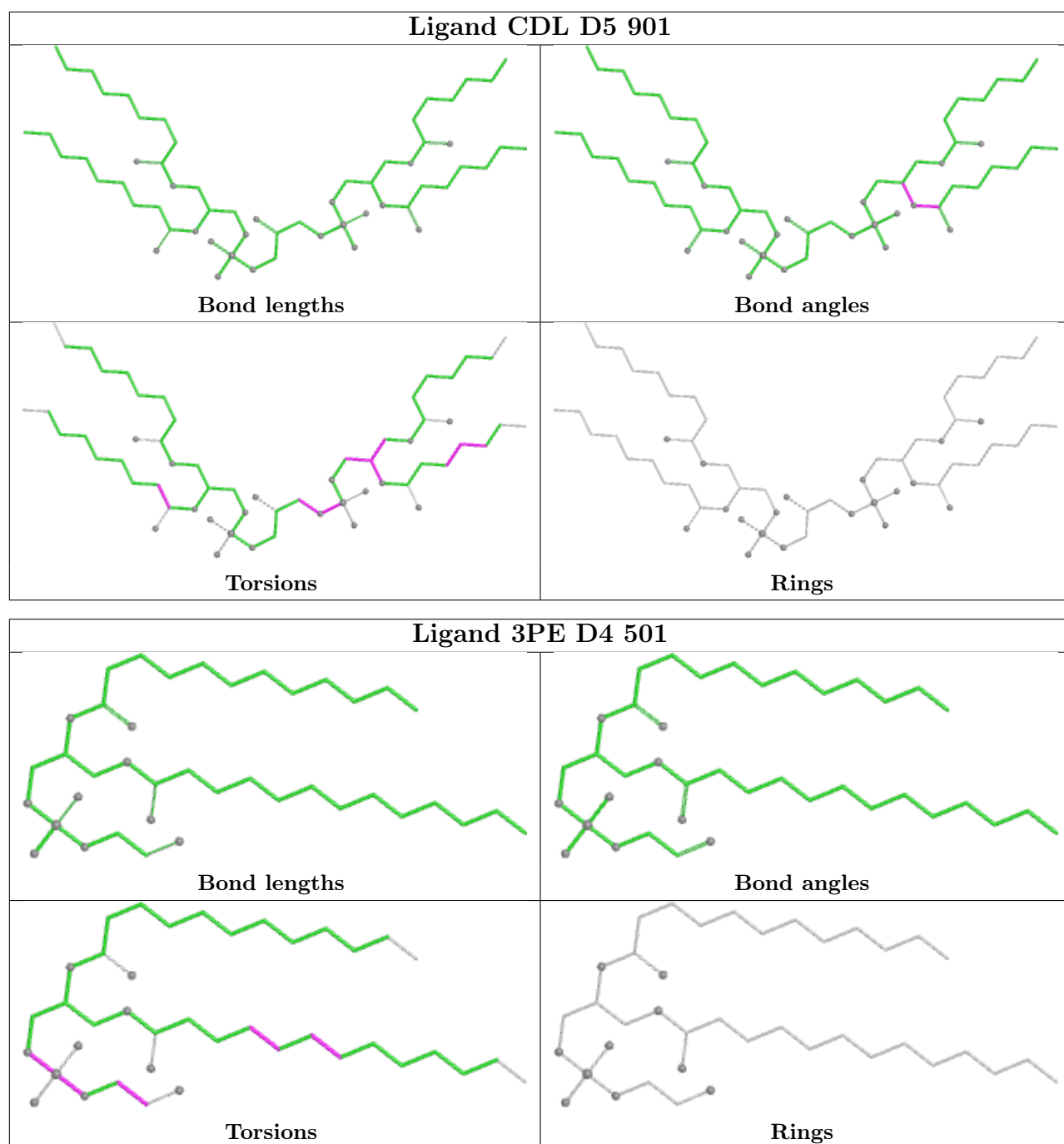


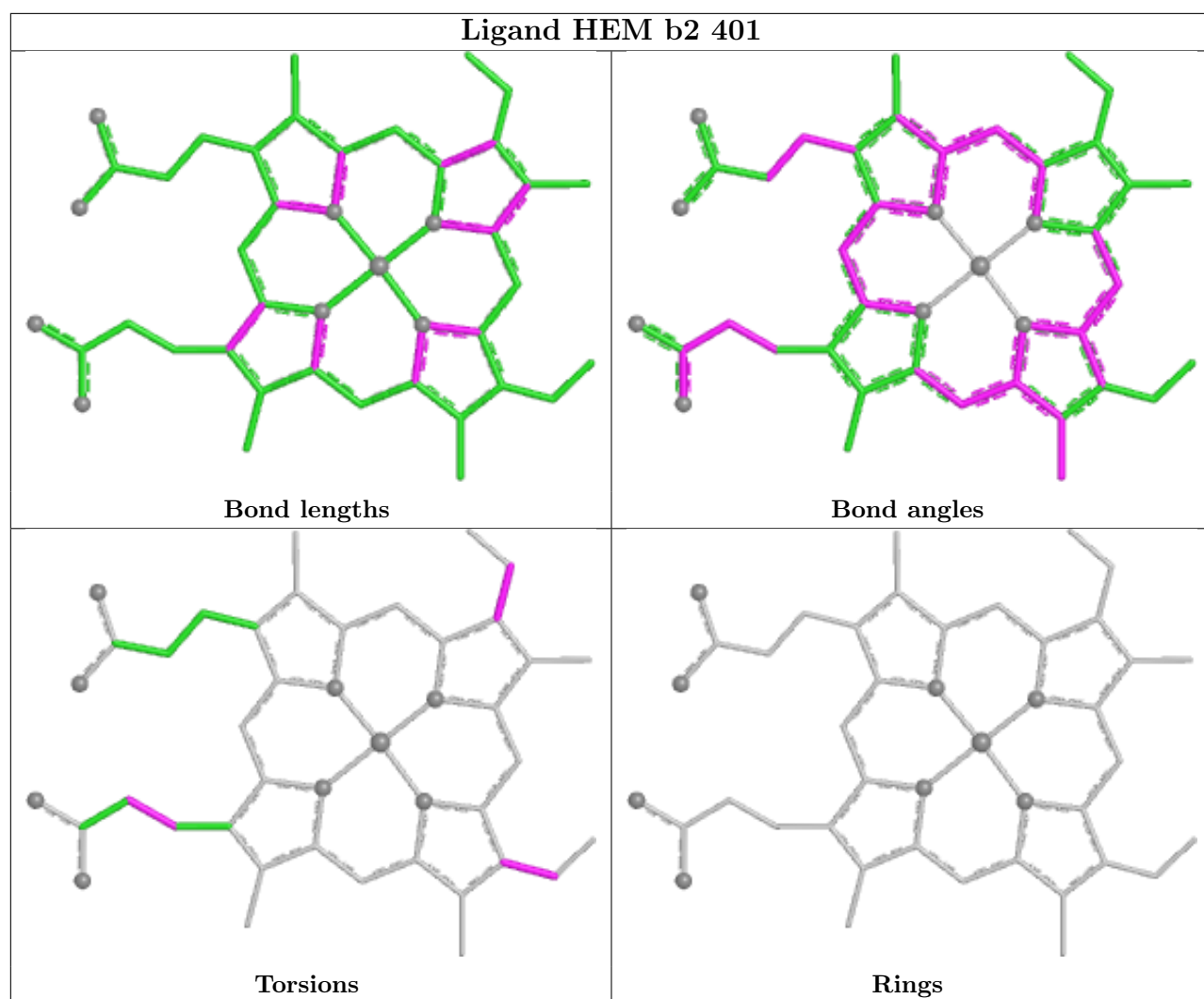












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

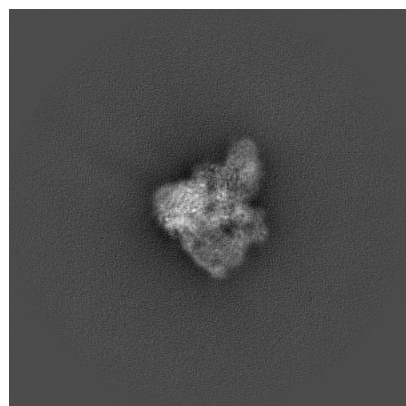
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4495. These allow visual inspection of the internal detail of the map and identification of artifacts.

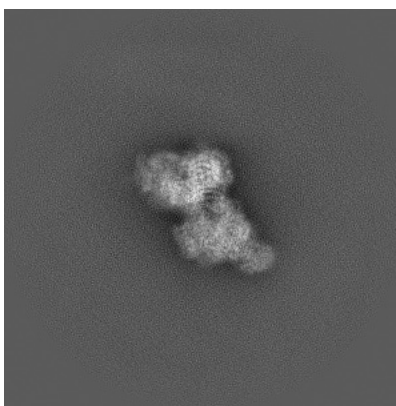
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

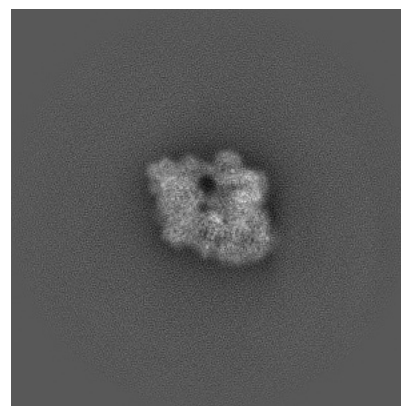
6.1.1 Primary map



X

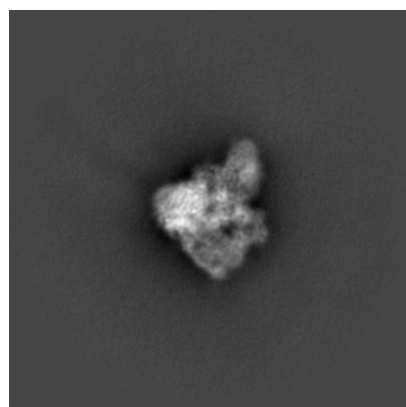


Y

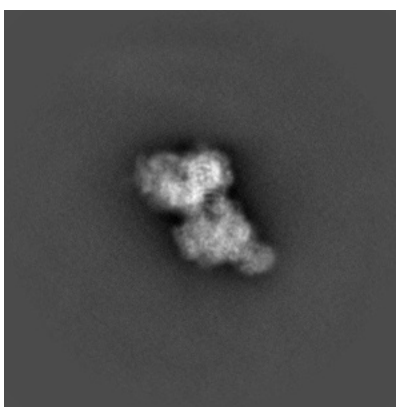


Z

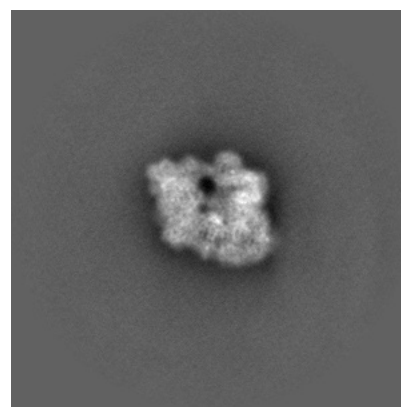
6.1.2 Raw map



X



Y

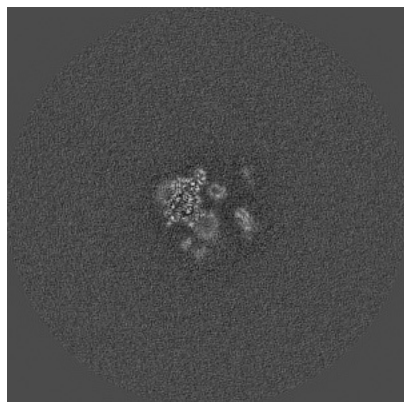


Z

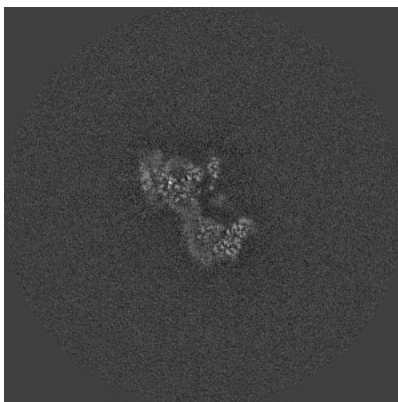
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

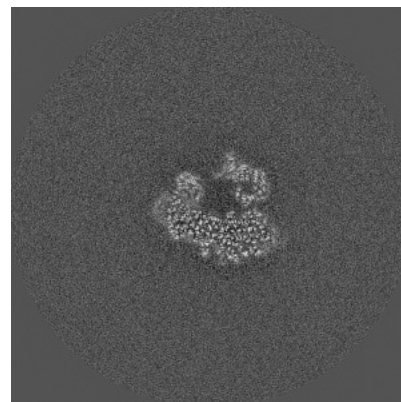
6.2.1 Primary map



X Index: 256

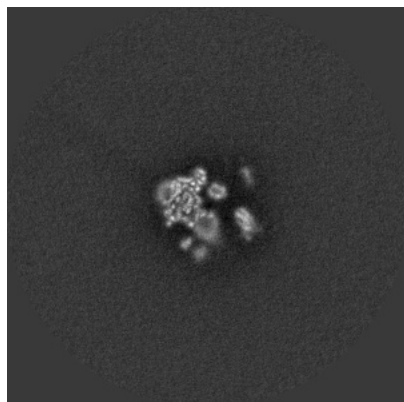


Y Index: 256

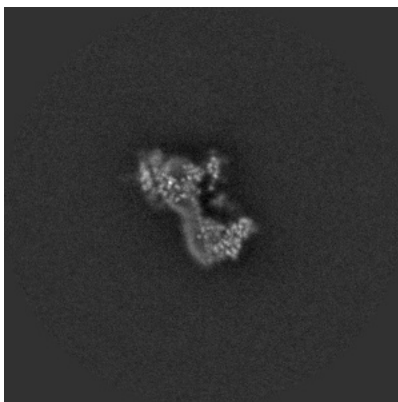


Z Index: 256

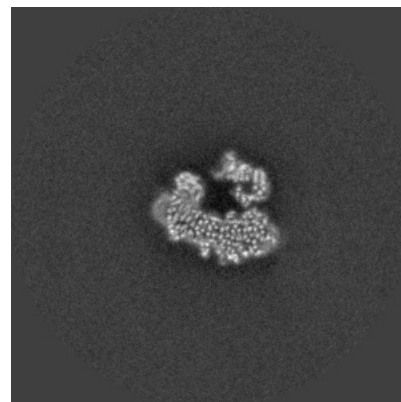
6.2.2 Raw map



X Index: 256



Y Index: 256

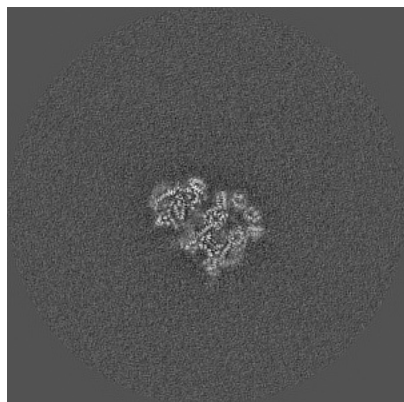


Z Index: 256

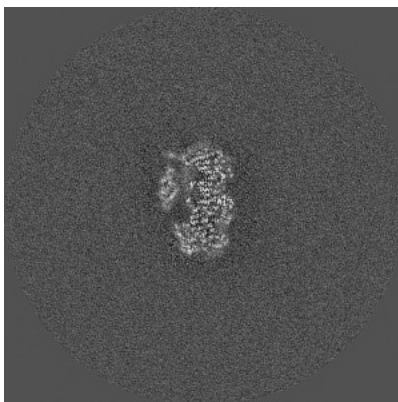
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

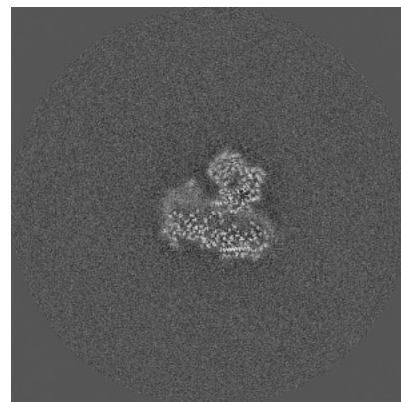
6.3.1 Primary map



X Index: 290

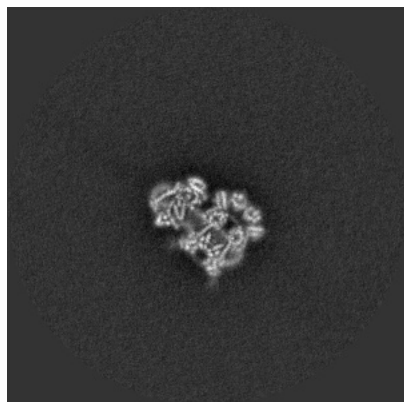


Y Index: 229

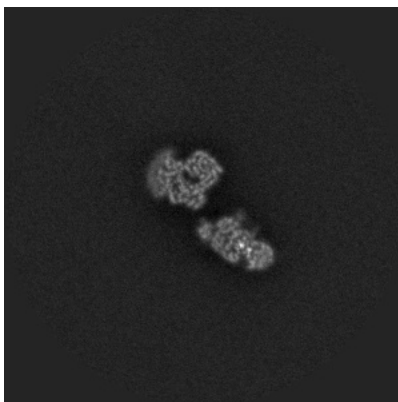


Z Index: 243

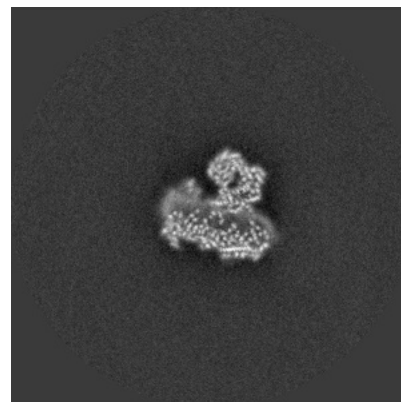
6.3.2 Raw map



X Index: 290



Y Index: 295

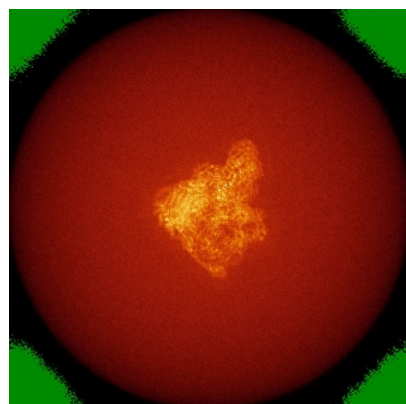


Z Index: 243

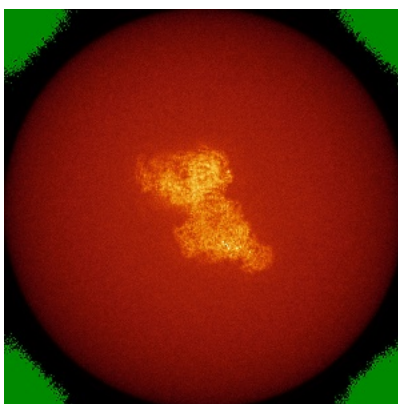
The images above show the largest variance slices of the map in three orthogonal directions.

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

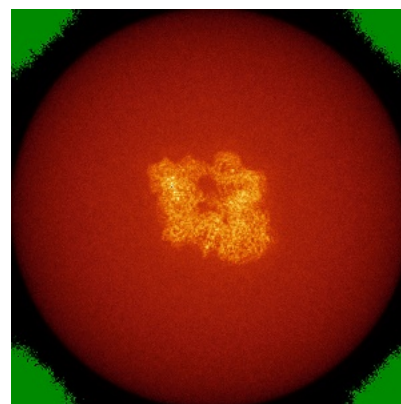
6.4.1 Primary map



X

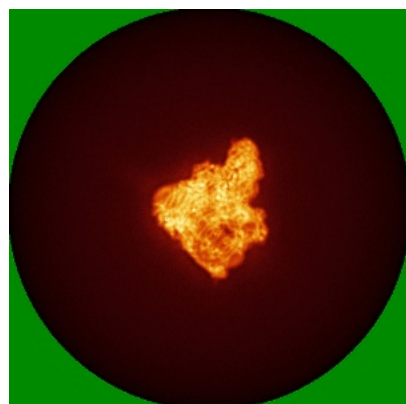


Y

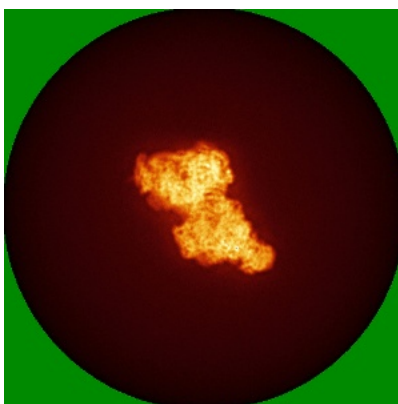


Z

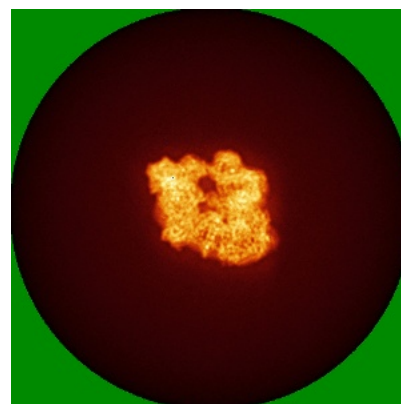
6.4.2 Raw map



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](#)

This section was not generated.

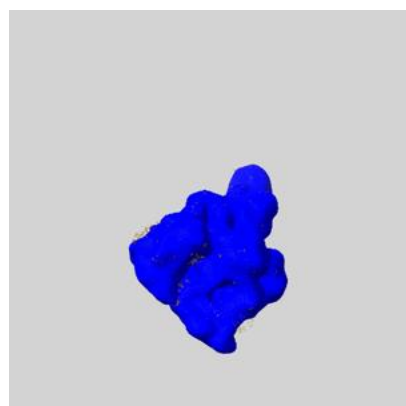
6.6 Mask visualisation [i](#)

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

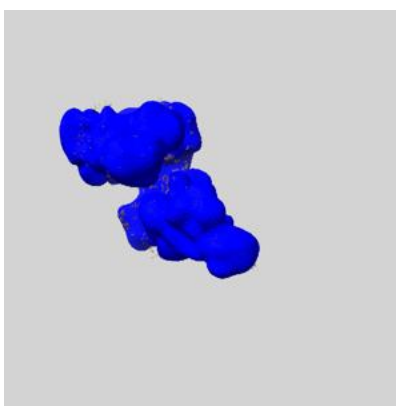
A mask typically either:

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

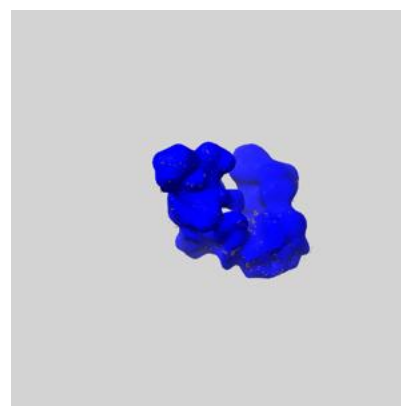
6.6.1 emd_4495_msk_1.map [i](#)



X



Y

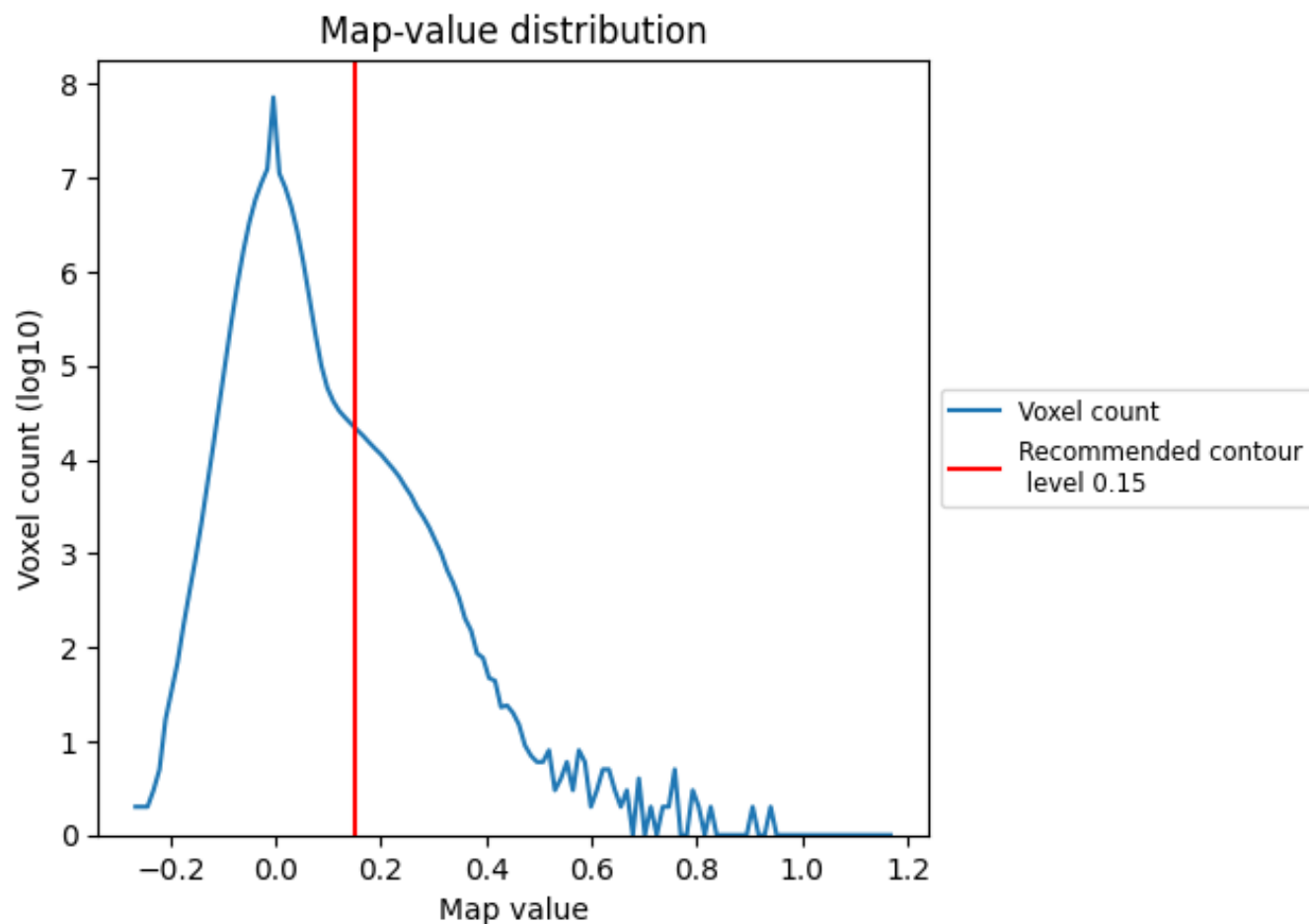


Z

7 Map analysis [i](#)

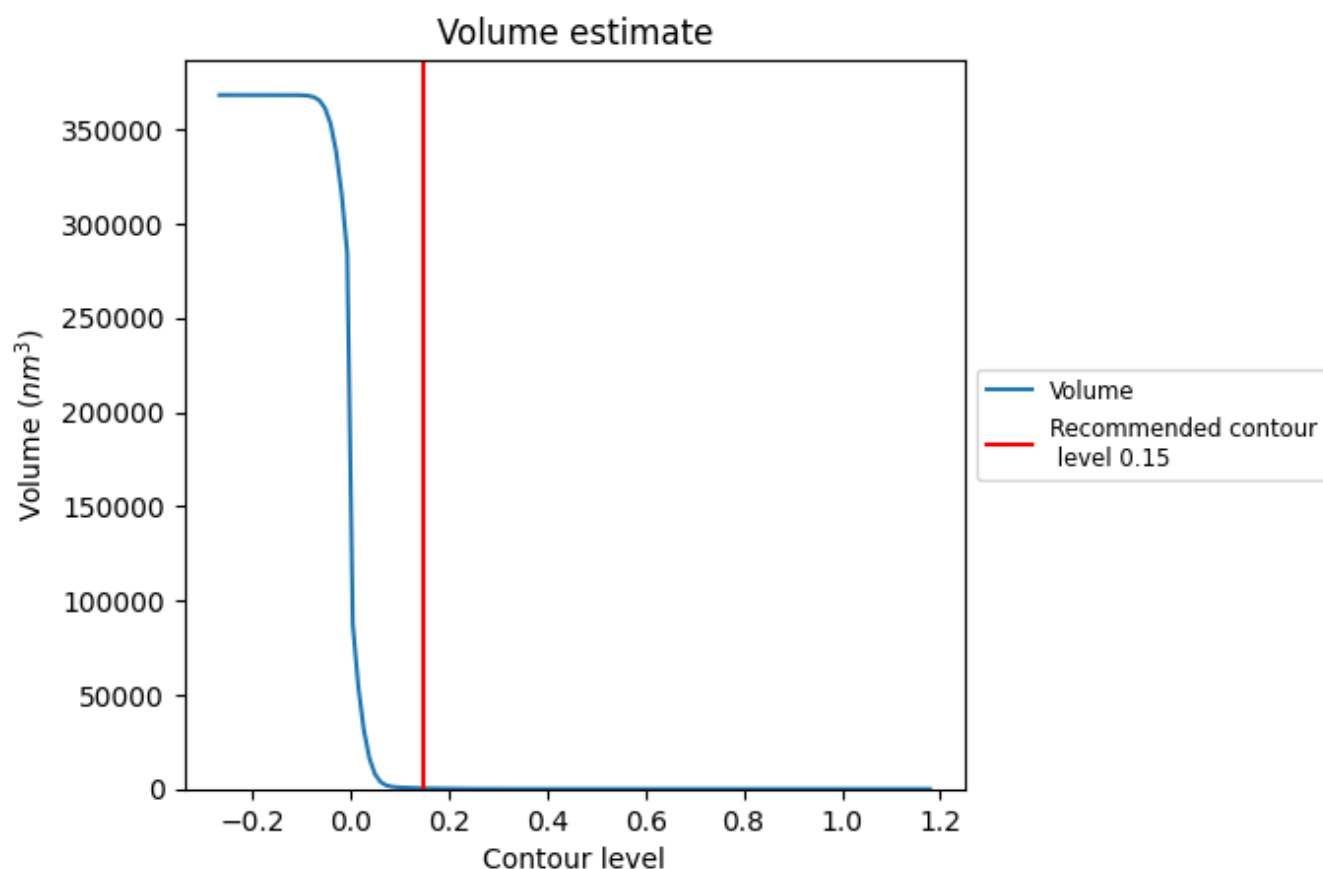
This section contains the results of statistical analysis of the map.

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.

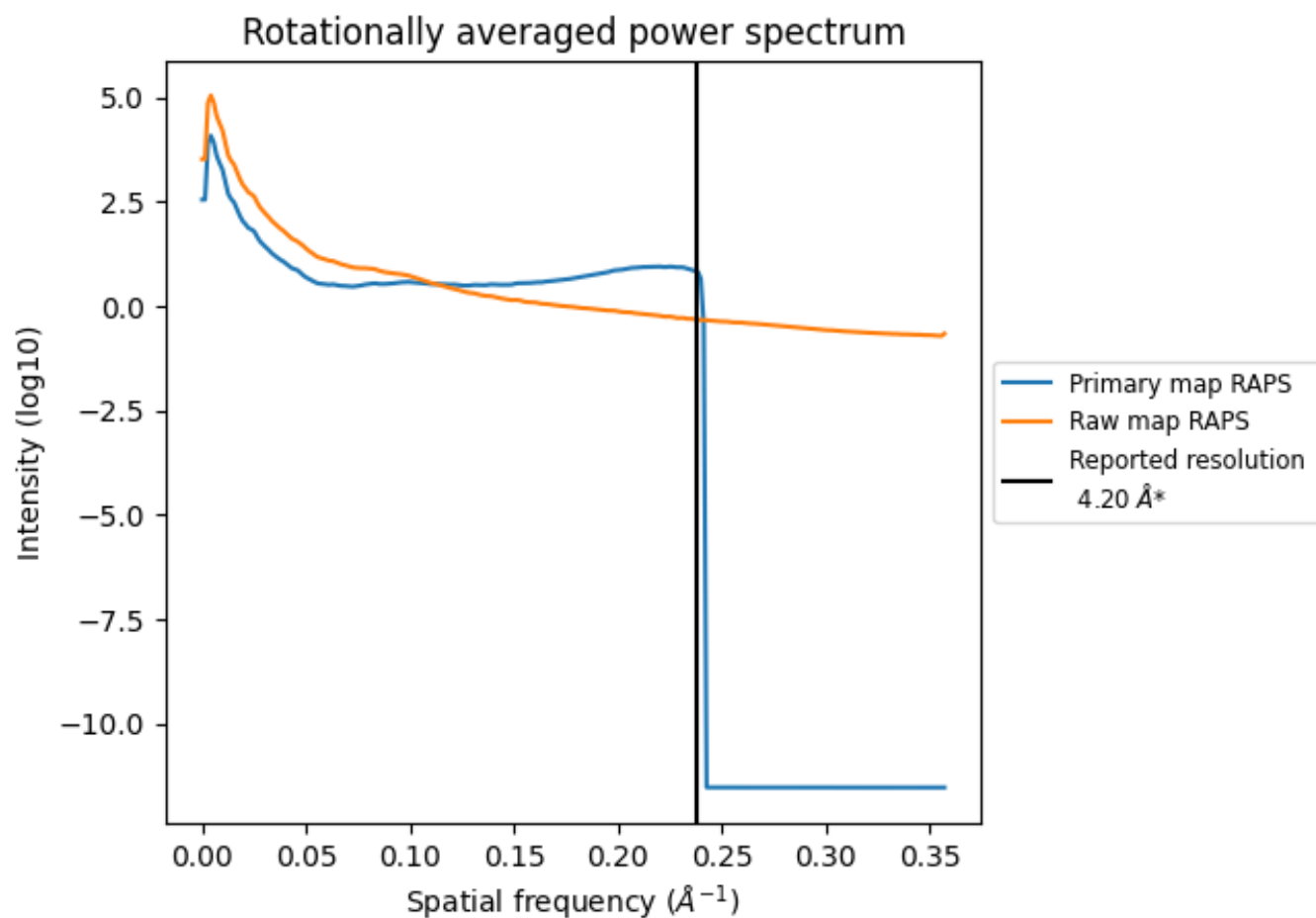
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; this corresponds to an approximate mass of 330 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 ⓘ

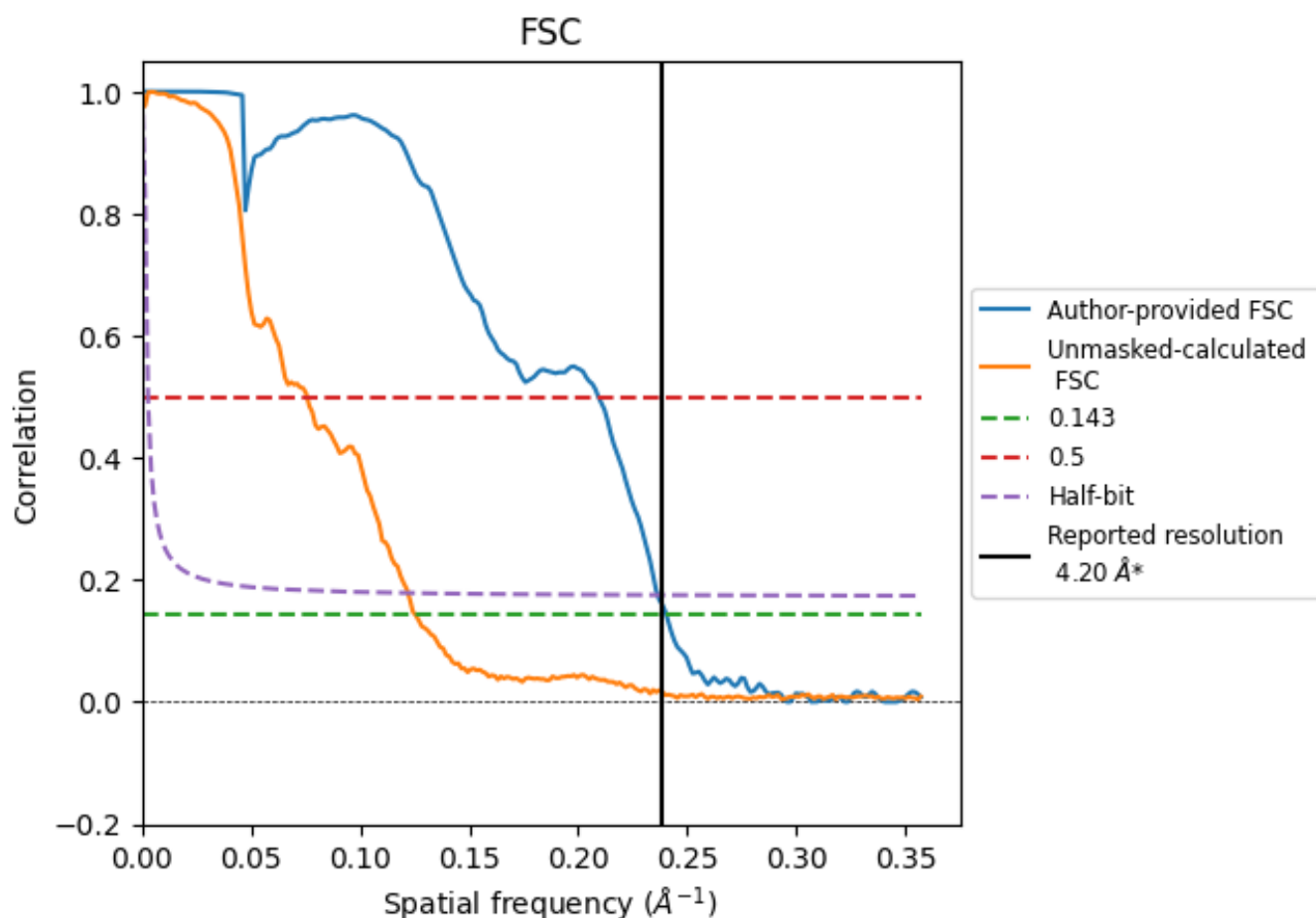


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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](#)

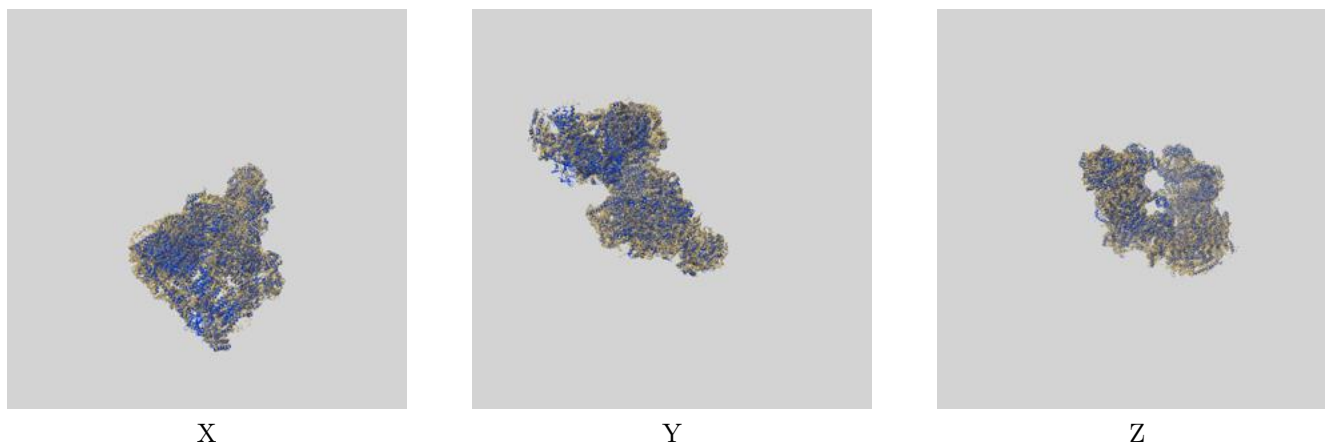
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	4.78	4.23
Unmasked-calculated*	7.99	13.21	8.20

*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 7.99 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

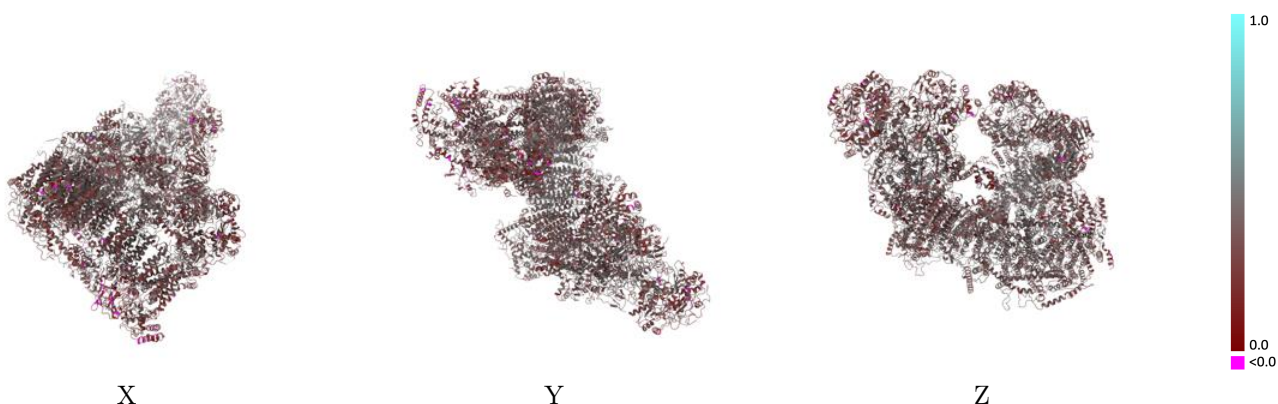
This section contains information regarding the fit between EMDB map EMD-4495 and PDB model 6QC3. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



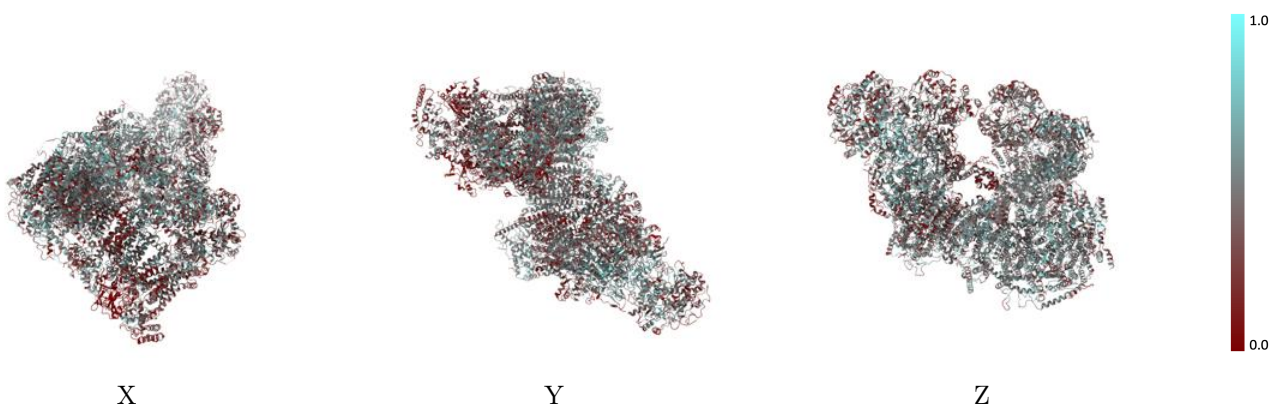
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



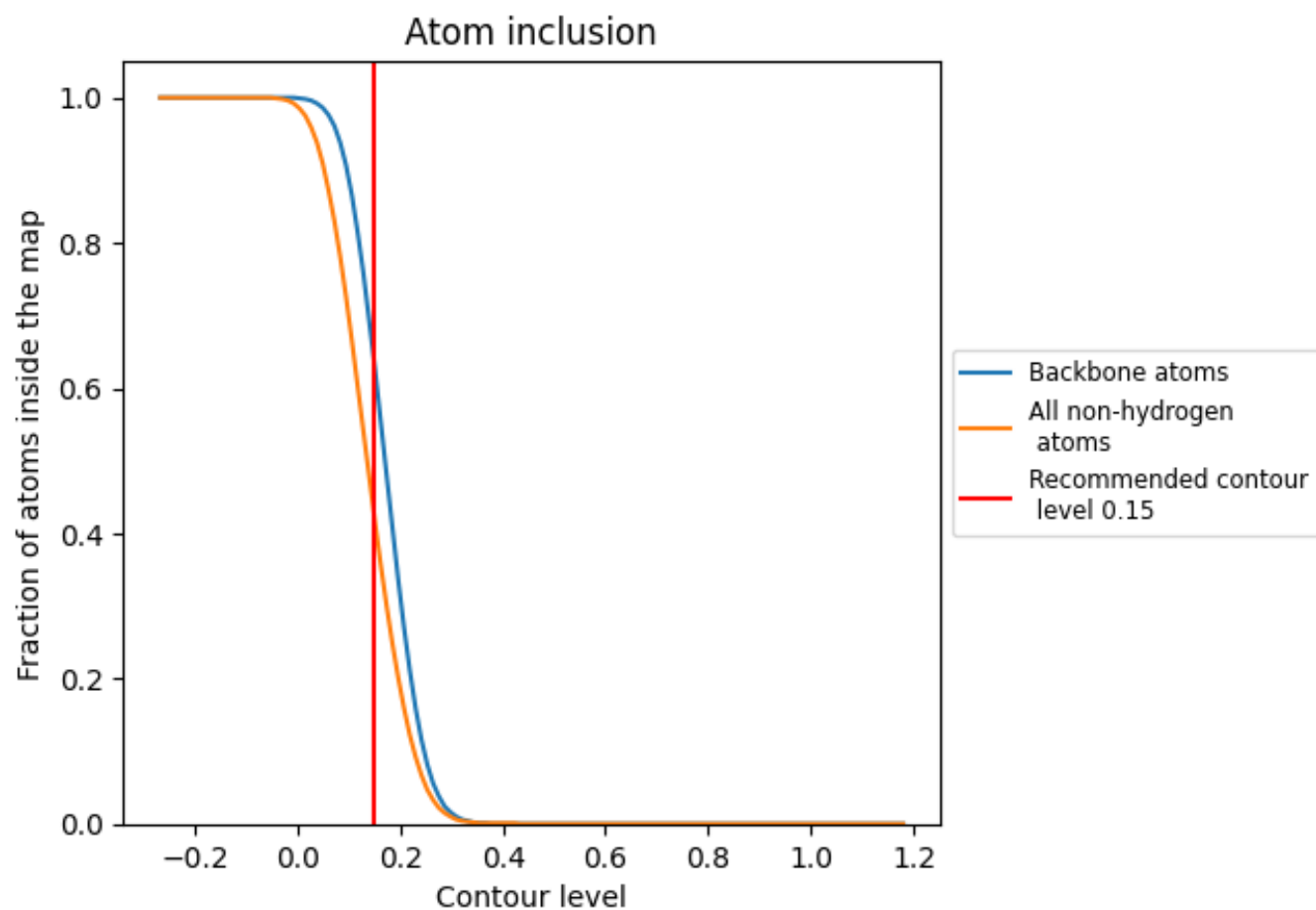
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% 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	 0.4230	 0.3540
4L	 0.4160	 0.3700
A1	 0.4660	 0.3710
A2	 0.3140	 0.2760
A3	 0.4170	 0.3490
A5	 0.4010	 0.3400
A6	 0.3640	 0.3520
A7	 0.3320	 0.3480
A8	 0.4610	 0.3420
A9	 0.3330	 0.3300
AA	 0.1990	 0.2840
AB	 0.4620	 0.3350
AJ	 0.4950	 0.3710
AK	 0.4050	 0.3780
AL	 0.3000	 0.3580
AM	 0.4660	 0.3500
B1	 0.4060	 0.3760
B2	 0.4230	 0.3280
B3	 0.4400	 0.3180
B4	 0.4940	 0.3850
B5	 0.5330	 0.3720
B6	 0.4530	 0.3460
B7	 0.4400	 0.3040
B8	 0.5030	 0.3840
B9	 0.5660	 0.3800
BJ	 0.5100	 0.3570
BK	 0.4560	 0.3700
C1	 0.4580	 0.3520
C2	 0.4930	 0.3920
D1	 0.4210	 0.3780
D2	 0.4970	 0.3980
D3	 0.3680	 0.3780
D4	 0.4860	 0.3970
D5	 0.4420	 0.3640
D6	 0.3330	 0.3560



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Chain	Atom inclusion	Q-score
S1	 0.4170	 0.3430
S2	 0.4960	 0.3800
S3	 0.5020	 0.3990
S4	 0.4440	 0.3890
S5	 0.4780	 0.3540
S6	 0.4160	 0.3720
S7	 0.5130	 0.3790
S8	 0.5730	 0.3970
V1	 0.4180	 0.3130
V2	 0.3950	 0.3090
V3	 0.3420	 0.3270
a1	 0.3890	 0.3280
a2	 0.3650	 0.3260
a3	 0.5050	 0.3810
a4	 0.4610	 0.3530
b1	 0.3900	 0.3570
b2	 0.4720	 0.3910
c1	 0.3560	 0.3280
c2	 0.4320	 0.3670
d1	 0.4020	 0.3300
d2	 0.4360	 0.3630
f1	 0.0800	 0.2870
f2	 0.0910	 0.2590
h1	 0.2130	 0.2530
h2	 0.2900	 0.2710
i1	 0.2600	 0.2770
i2	 0.2410	 0.2970
q1	 0.3400	 0.3290
q2	 0.4310	 0.3880
x1	 0.2720	 0.3730
x2	 0.2770	 0.4020