



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:19 PM UTC

PDB ID : 8BQ6 / pdb_00008bq6
EMDB ID : EMD-16172
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (Complete conformation 2 composition)
Authors : Klusch, N.; Kuehlbrandt, W.
Deposited on : 2022-11-18
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

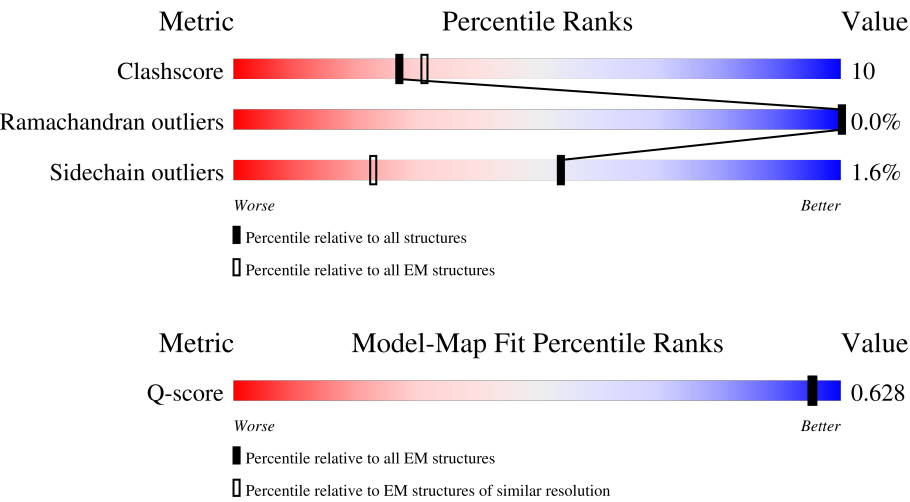
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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	11806 (2.30 - 3.30)

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	A	119	
2	B	218	
3	C	190	
4	D	394	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Y	159	
26	Z	143	
27	a	65	
28	b	65	
29	c	88	

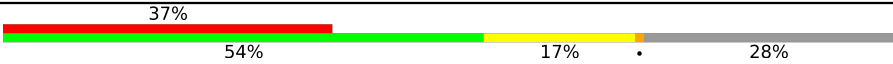
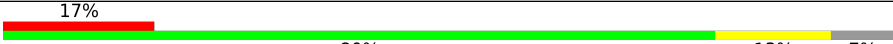
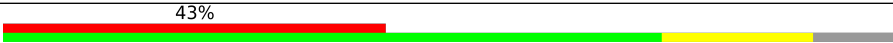
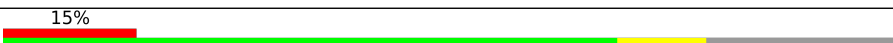
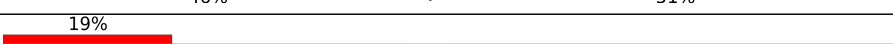
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	d	81	
31	e	83	
32	f	106	
33	g	114	
34	i	98	
35	j	69	
36	k	72	
37	l	125	
38	m	71	
39	n	117	
40	o	103	
41	p	106	
42	q	159	
43	u	63	
44	v	113	
45	x	256	
46	y	278	
47	z	275	
48	AA	503	
48	BA	503	
49	AB	531	
49	BB	531	
50	AC	393	
50	BC	393	
51	AD	272	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	BD	272	
52	AE	307	
52	BE	307	
53	AF	122	
53	BF	122	
54	AG	72	
54	BG	72	
55	AH	69	
55	BH	69	
56	AI	72	
56	BI	72	
57	AJ	57	
57	BJ	57	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	SF4	F	501	-	-	X	-
58	SF4	I	500	-	-	X	-
59	FES	BD	301	-	-	X	-
66	COO	y	301	X	-	-	-

2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 96522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	94	Total	C	N	O	S	0	0
			802	565	110	123	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total	C	N	O	S	0	0
			1545	997	266	276	6		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3079	1957	542	556	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5243	3285	919	1000	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1349	849	229	261	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1399	949	213	228	9		

- Molecule 11 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			784	525	121	131	7		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	665	Total	C	N	O	S	0	0
			5222	3474	808	901	39		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	494	Total	C	N	O	S	0	0
			3946	2664	610	647	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	1	0
			3832	2582	578	644	28		

- Molecule 15 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			963	603	170	186	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	316	Total	C	N	O	S	0	0
			2453	1580	414	444	15		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	105	Total	C	N	O	S	0	0
			837	536	144	156	1		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	73	Total	C	N	O	S	0	0
			571	359	101	105	6		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			659	417	104	135	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	87	Total	C	N	O	S	0	0
			677	427	110	139	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	98	Total	C	N	O	S	0	0
			776	486	134	144	12		

- Molecule 25 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	125	Total	C	N	O	S	0	0
			928	596	162	167	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 28 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	43	Total	C	N	O	S	0	0
			315	206	51	55	3		

- Molecule 29 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 30 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	65	Total	C	N	O	S	0	0
			554	343	103	100	8		

- Molecule 32 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 33 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	79	Total	C	N	O	S	0	0
			641	412	111	115	3		

- Molecule 34 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	48	Total	C	N	O	S	0	0
			382	244	72	63	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	74	Total	C	N	O	S	0	0
			562	367	91	103	1		

- Molecule 38 is a protein called B15 – 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	90	Total	C	N	O	S	0	0
			757	479	141	133	4		

- Molecule 42 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	80	Total	C	N	O	S	1	0
			669	427	120	120	2		

- Molecule 43 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	55	Total	C	N	O	S	0	0
			463	298	84	78	3		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	29	Total	C	N	O		0	0
			219	142	38	39			

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	210	Total	C	N	O	S	0	0
			1629	1043	280	301	5		

- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	265	Total	C	N	O	S	0	0
			2013	1258	359	388	8		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 48 is a protein called Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	420	Total	C	N	O	S	0	0
			3201	2034	530	621	16		
48	BA	420	Total	C	N	O	S	0	0
			3202	2035	530	621	16		

- Molecule 49 is a protein called Probable mitochondrial-processing peptidase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

- Molecule 50 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
50	BC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AD	196	Total	C	N	O	S	0	0
			1528	978	264	281	5		
51	BD	195	Total	C	N	O	S	0	0
			1519	973	263	278	5		

- Molecule 52 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
52	BE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		
53	BF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	69	Total	C	N	O	S	0	0
			581	387	95	98	1		
54	BG	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AH	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
55	BH	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

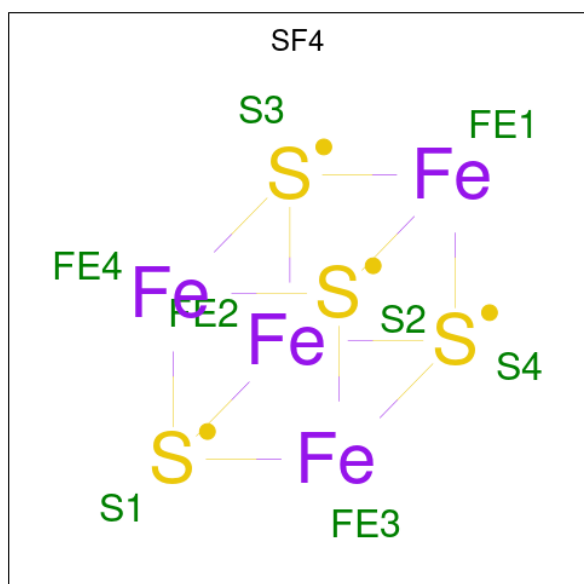
- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
56	BI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

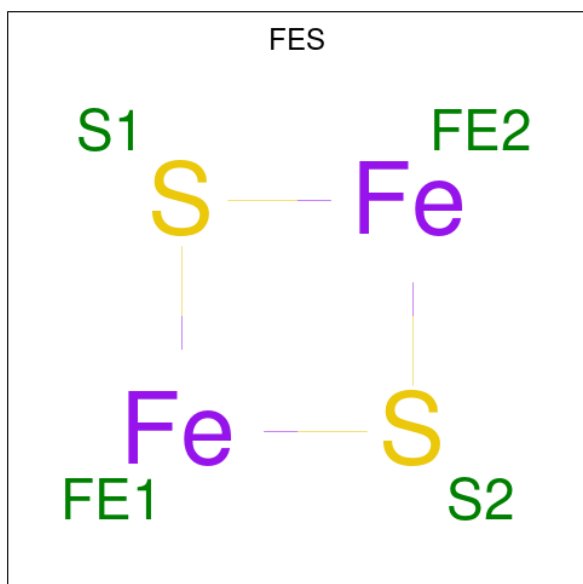
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		
57	BJ	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



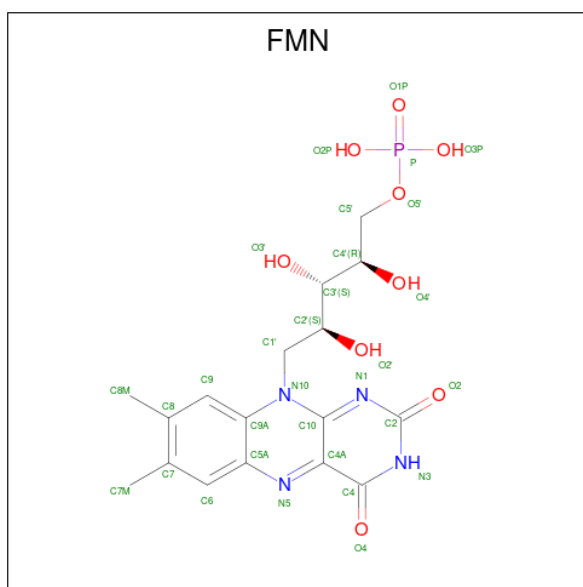
Mol	Chain	Residues	Atoms			AltConf
58	B	1	Total	Fe	S	0
			8	4	4	
58	F	1	Total	Fe	S	0
			8	4	4	
58	G	1	Total	Fe	S	0
			8	4	4	
58	G	1	Total	Fe	S	0
			8	4	4	
58	I	1	Total	Fe	S	0
			8	4	4	
58	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



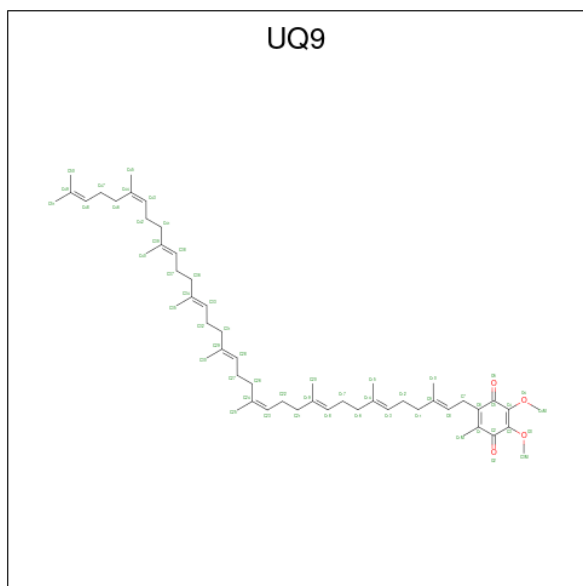
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	
59	AD	1	Total	Fe	S	0
			4	2	2	
59	BD	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 61 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).

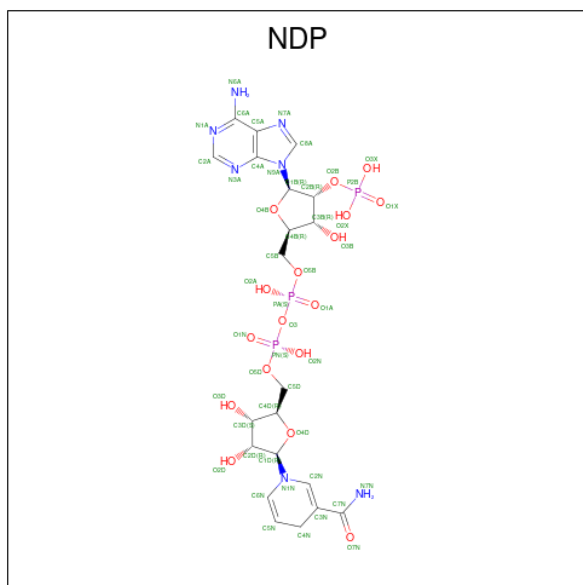


Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
62	O	1	Total	Fe	0
			1	1	

- Molecule 63 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

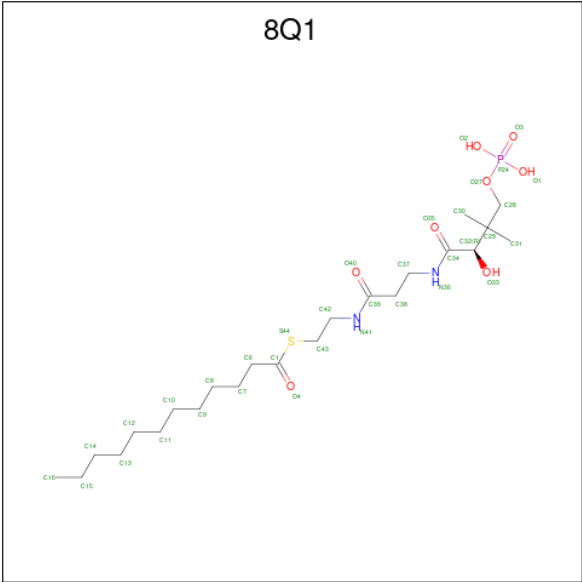


Mol	Chain	Residues	Atoms					AltConf
63	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

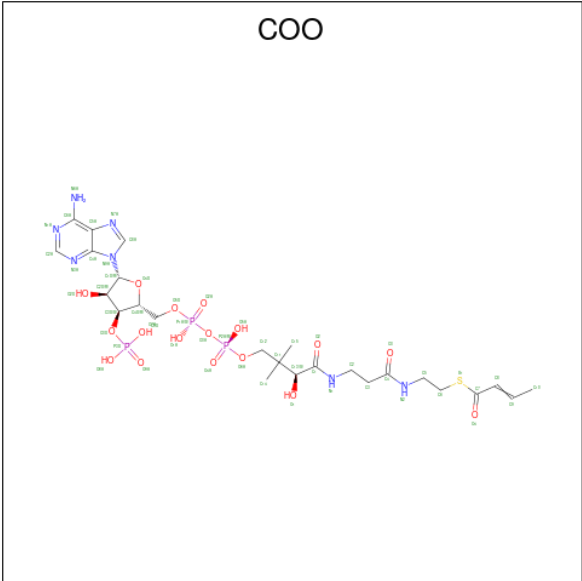
Mol	Chain	Residues	Atoms		AltConf
64	R	1	Total	Zn	0
			1	1	
64	y	1	Total	Zn	0
			1	1	
64	AB	1	Total	Zn	0
			1	1	
64	BB	1	Total	Zn	0
			1	1	

- Molecule 65 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
65	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
65	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

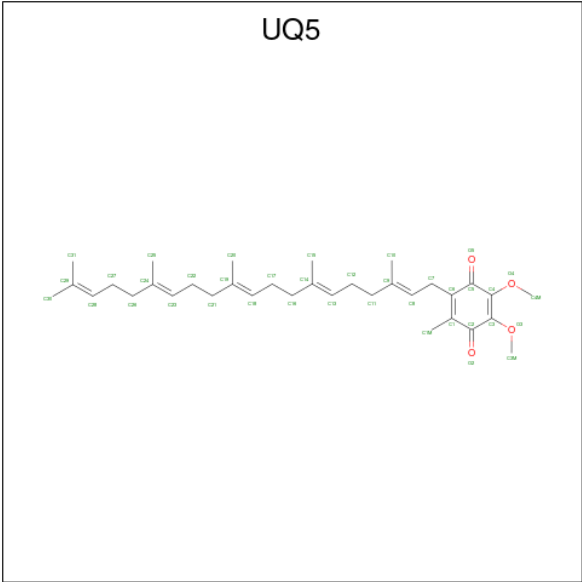
- Molecule 66 is CROTONYL COENZYME A (CCD ID: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
66	y	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

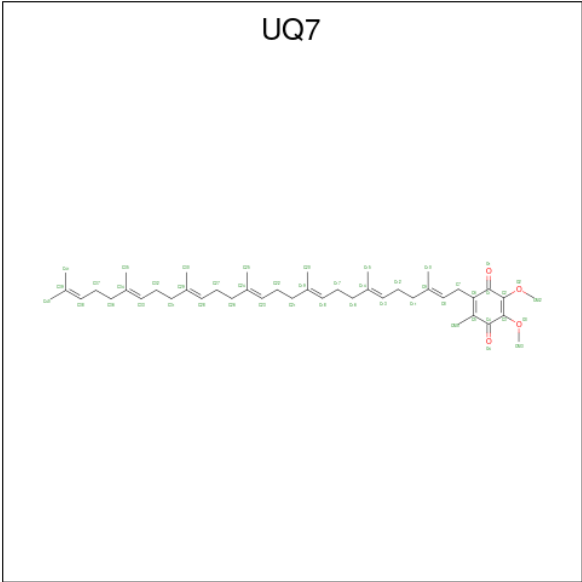
-
- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme label.

- Molecule 68 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			38	34	4	
68	AC	1	Total	C	O	0
			38	34	4	
68	BC	1	Total	C	O	0
			38	34	4	

- Molecule 69 is UBIQUINONE-7 (CCD ID: UQ7) (formula: C₄₄H₆₆O₄) (labeled as "Ligand of Interest" by depositor).



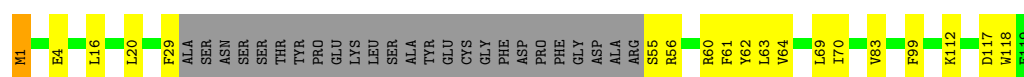
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
69	BC	1	48	44	4	0

3 Residue-property plots [i](#)

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

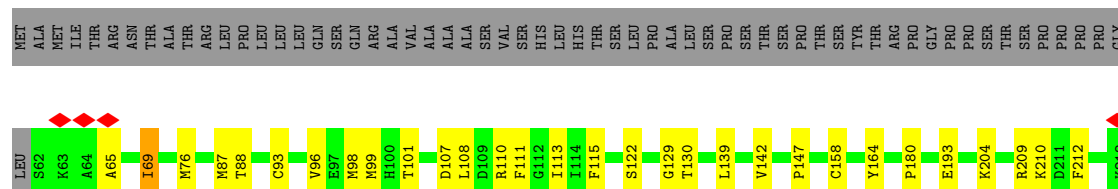
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



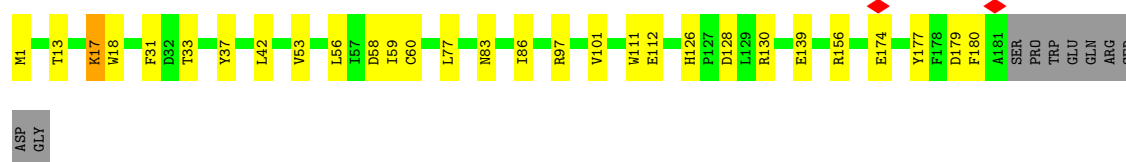
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



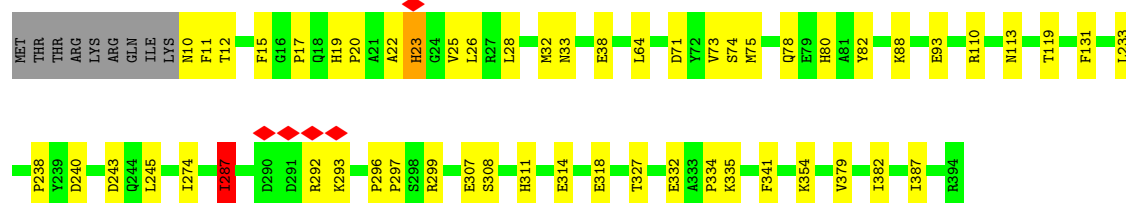
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

Chain C: 

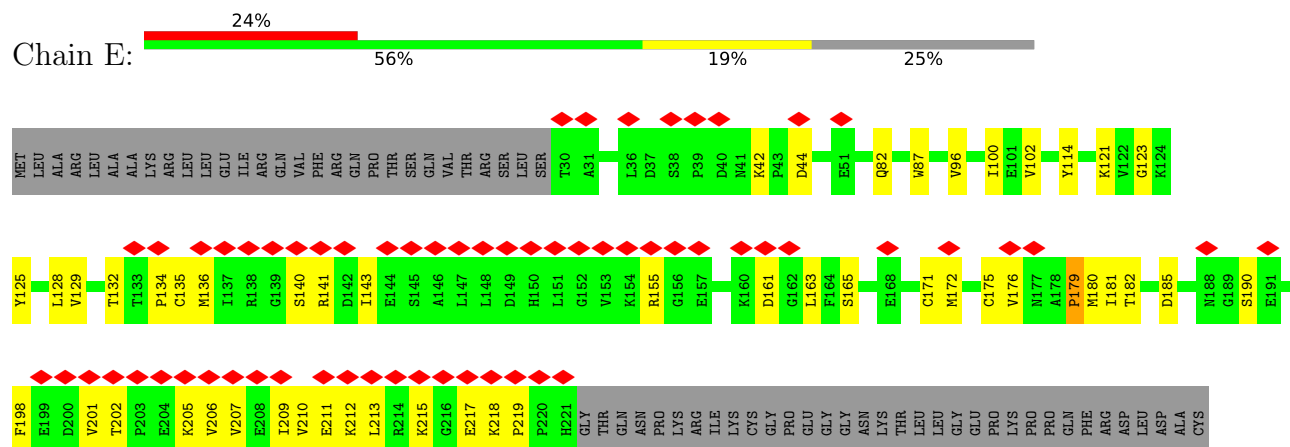


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

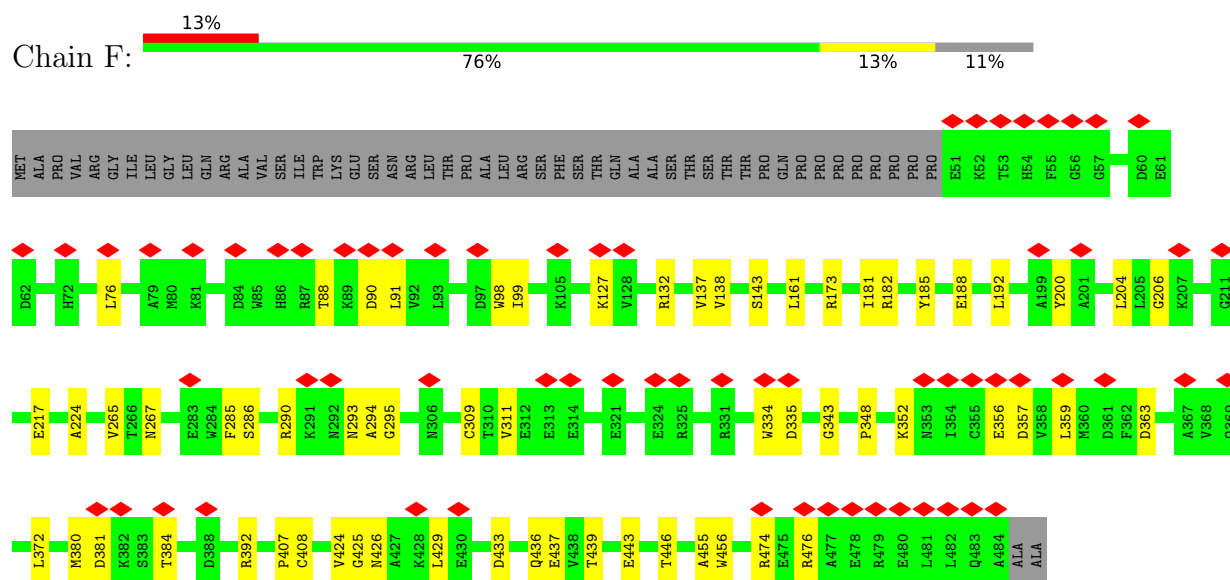
Chain D: 



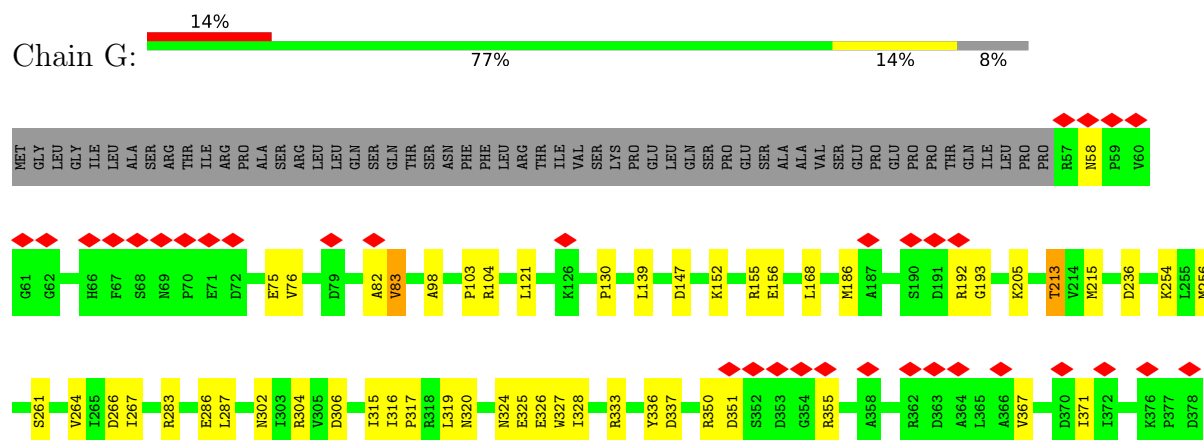
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

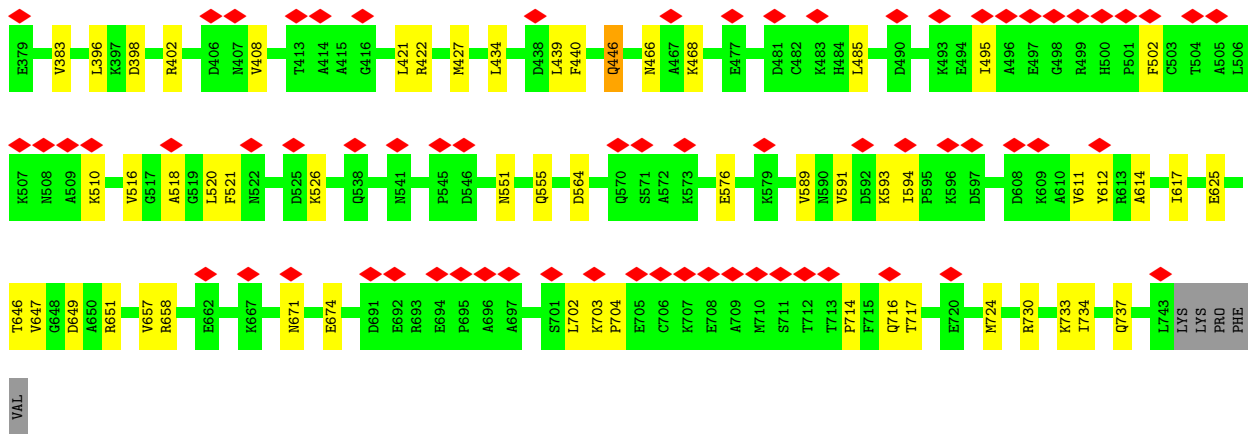


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

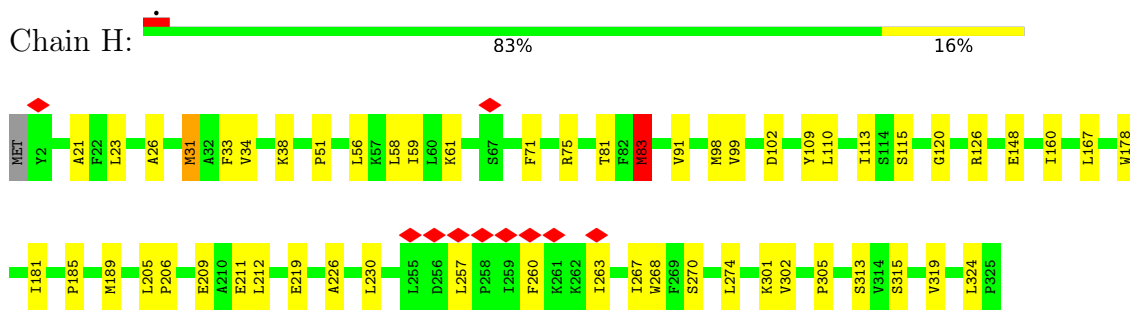


• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

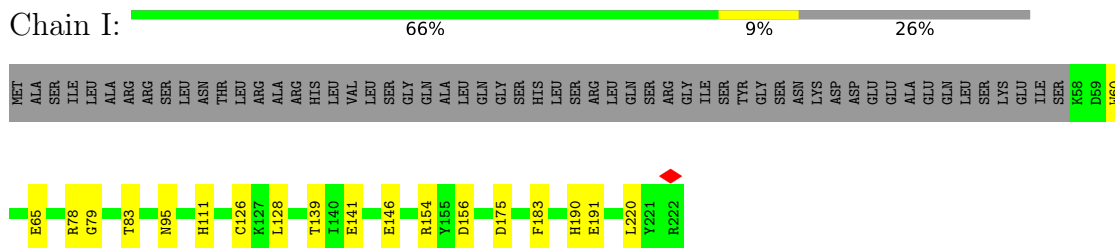




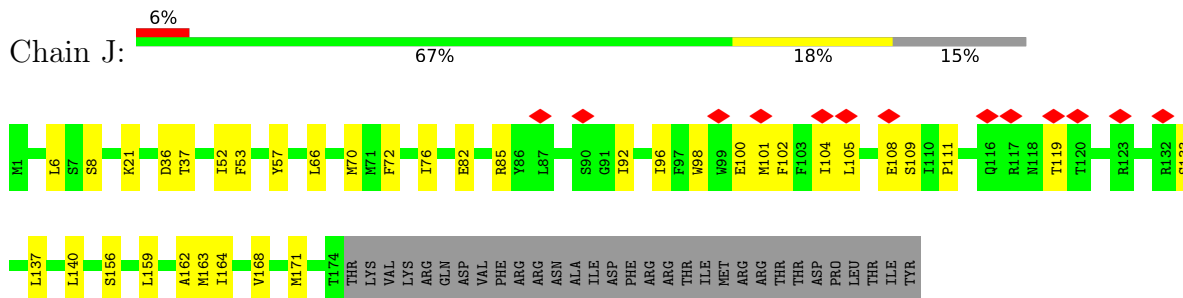
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial



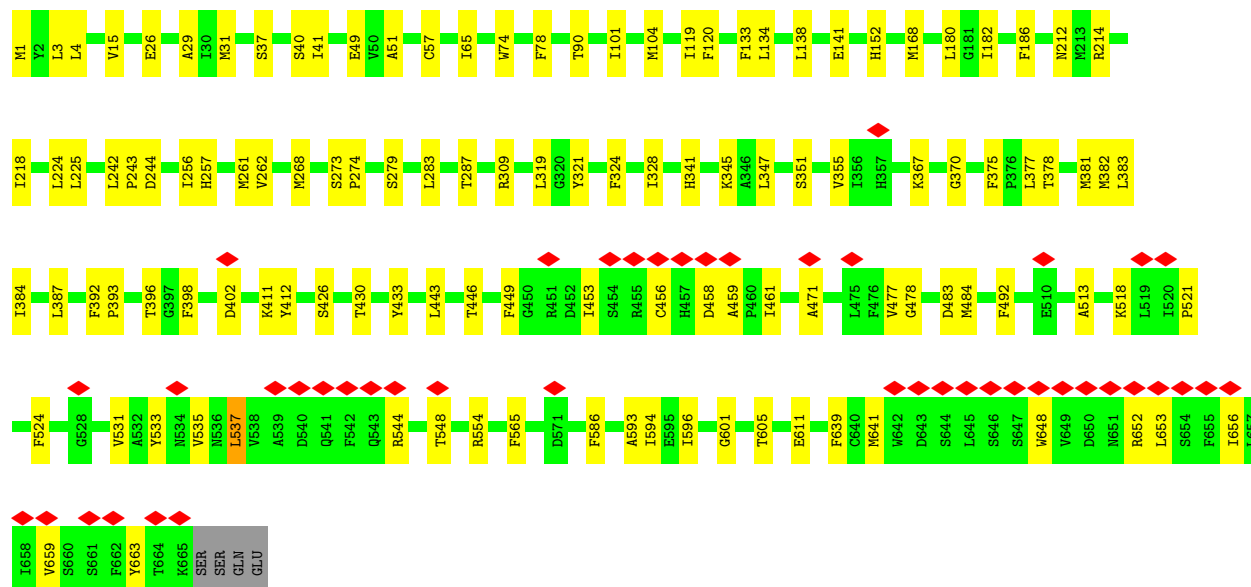
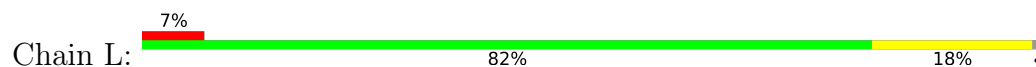
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



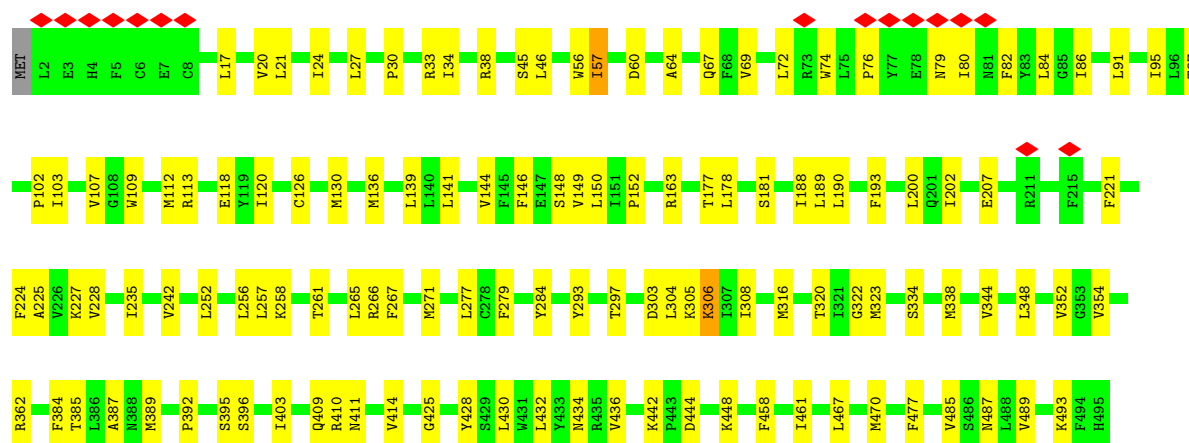
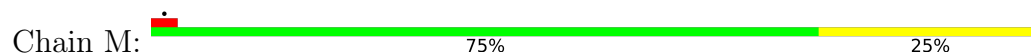
- Molecule 11: NADH dehydrogenase subunit 4L



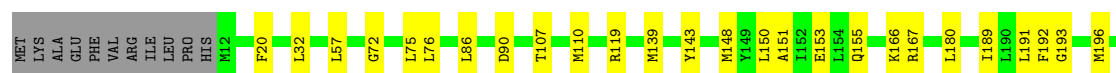
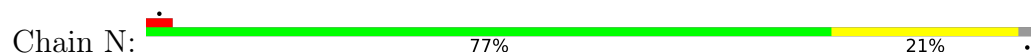
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

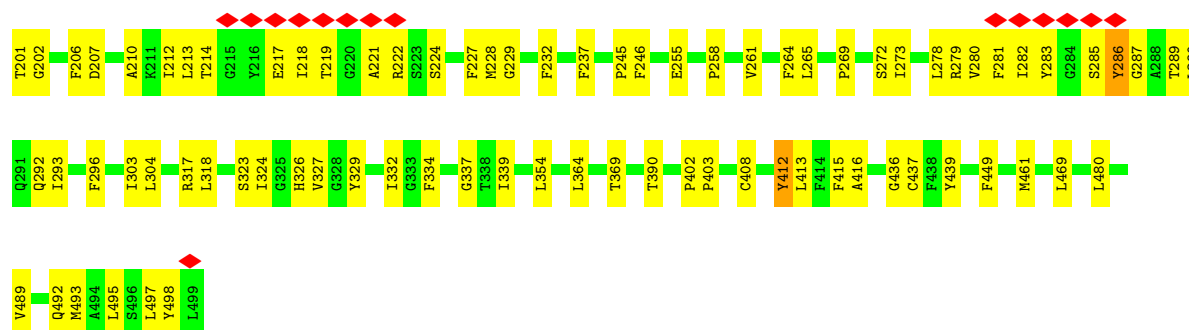


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



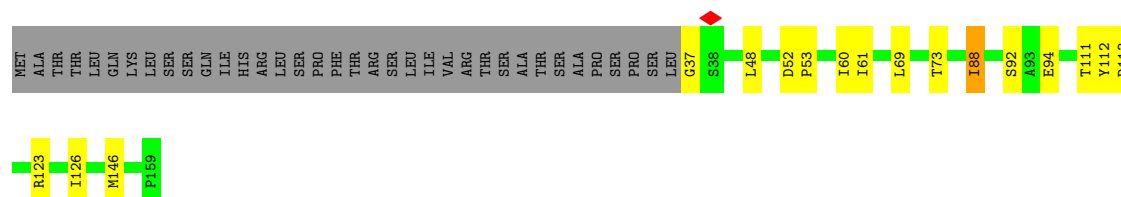
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2





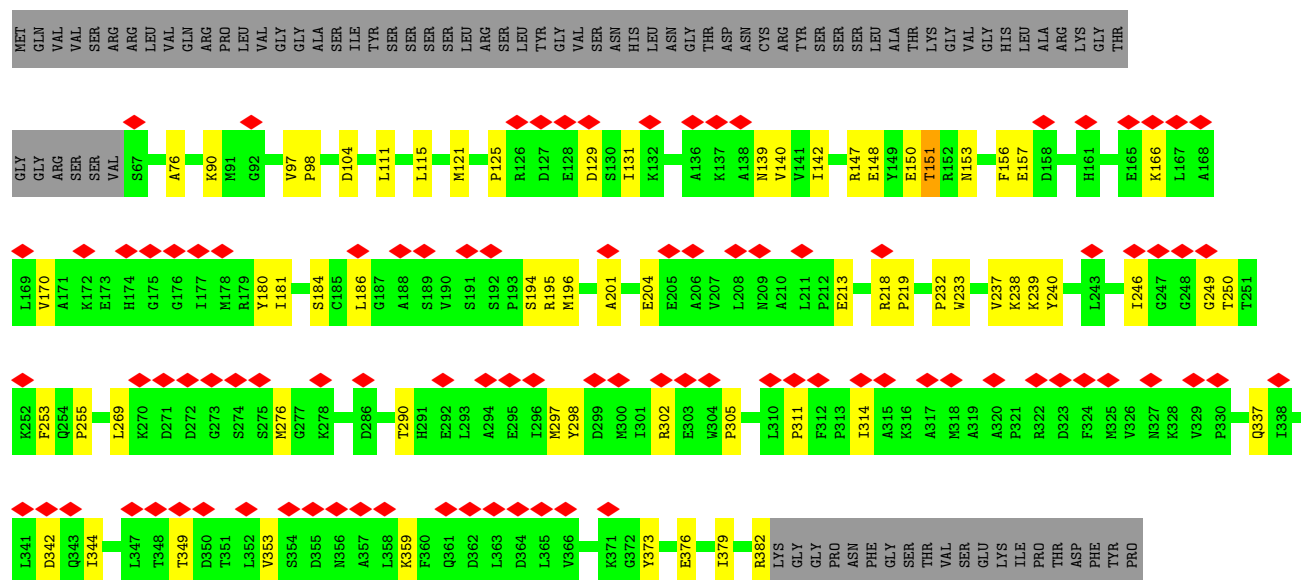
- Molecule 15: AT3G07480.1

Chain O: 67% 10% 23%



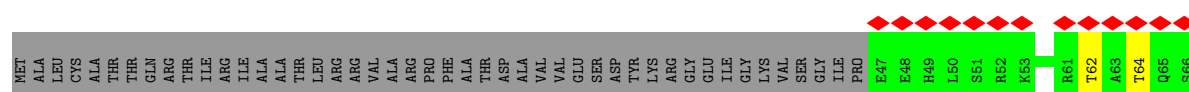
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

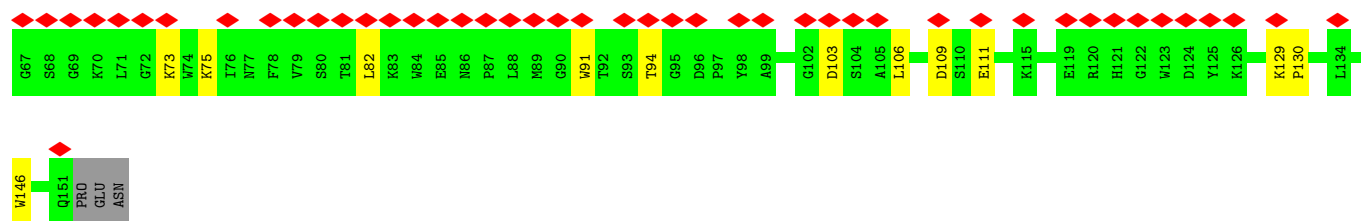
Chain P: 23% 62% 16% 21%



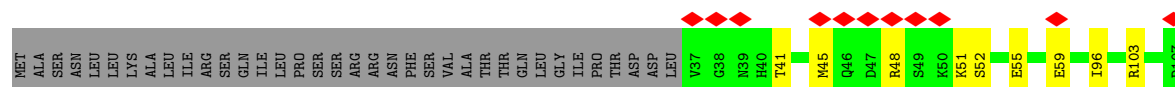
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 38% 59% 9% 32%

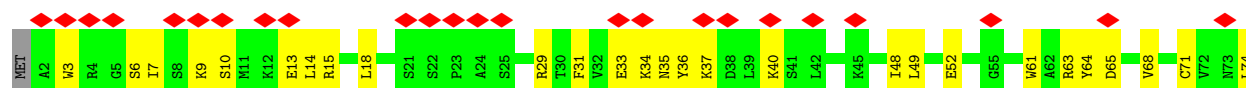




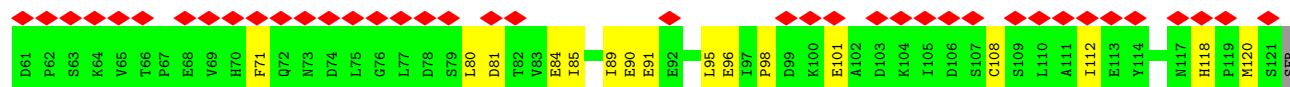
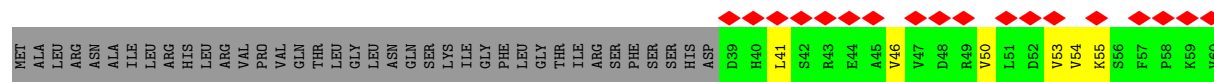
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



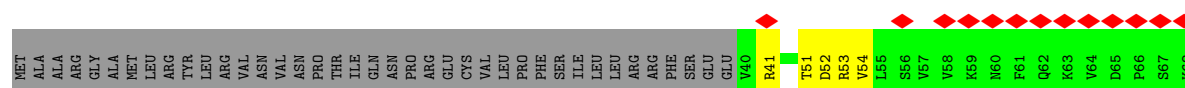
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

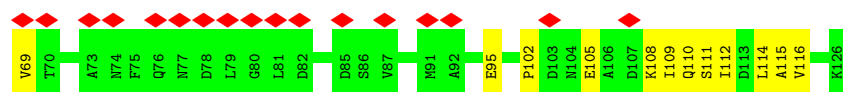


- Molecule 20: Acyl carrier protein 1, mitochondrial

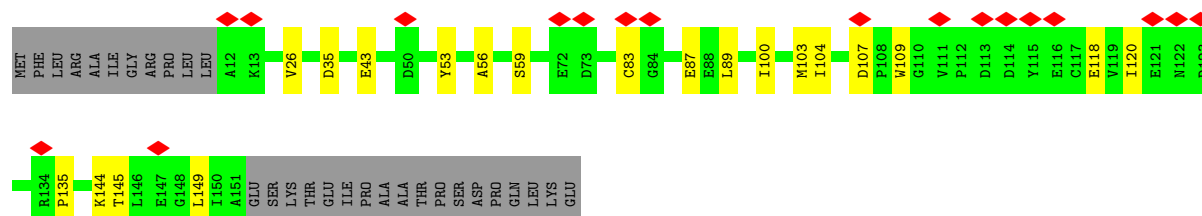


- Molecule 21: Acyl carrier protein 2, mitochondrial

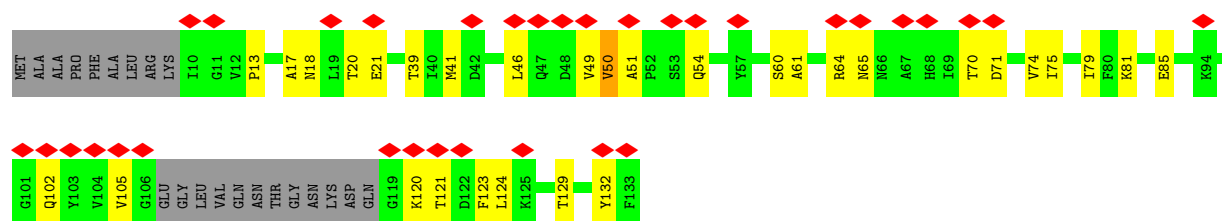




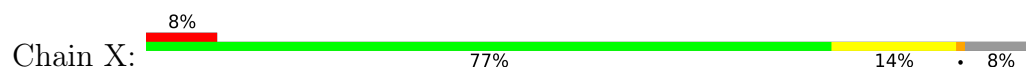
- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



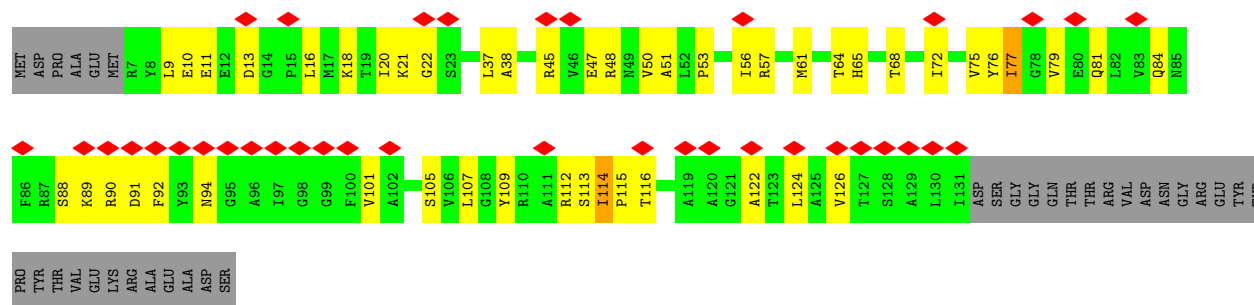
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



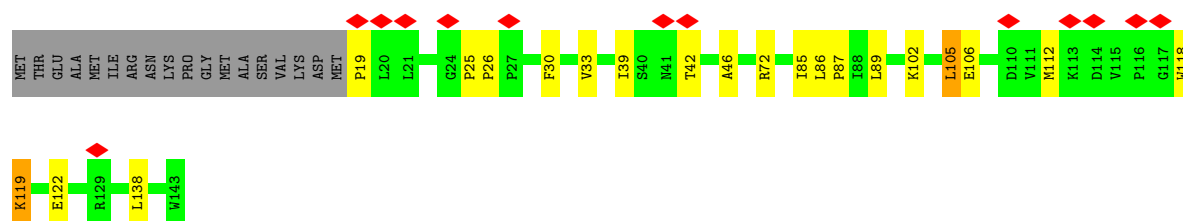
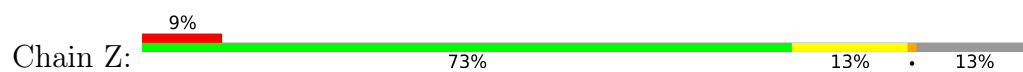
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



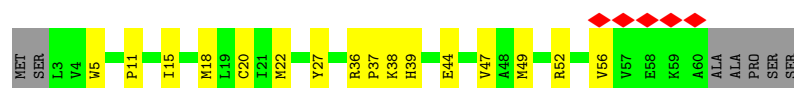
- Molecule 25: Outer envelope pore protein 16-3, chloroplastic/mitochondrial



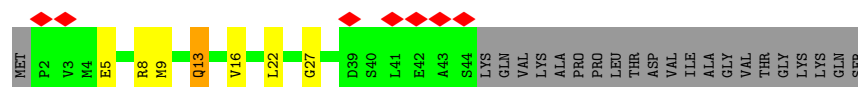
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



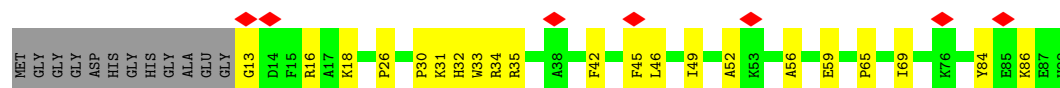
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



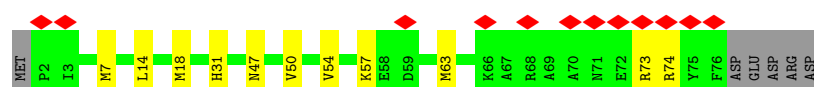
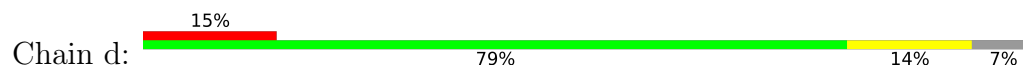
- Molecule 28: At2g46540/F11C10.23



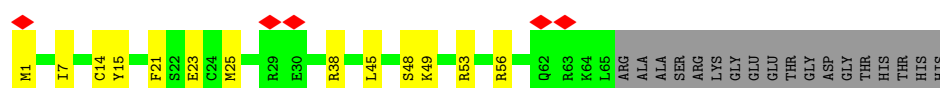
- Molecule 29: Transmembrane protein



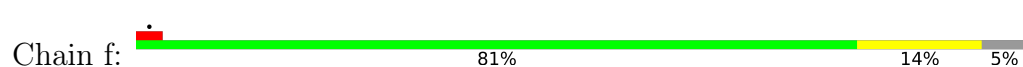
- Molecule 30: Excitatory amino acid transporter

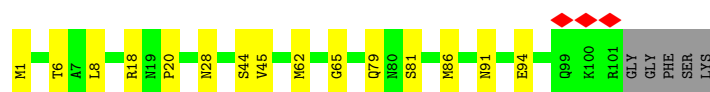


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B

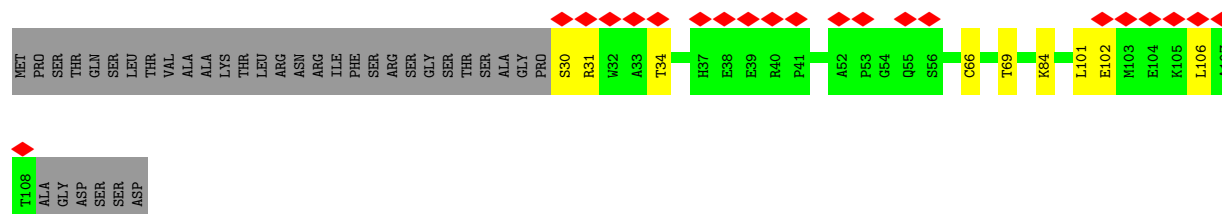


- Molecule 32: At4g16450

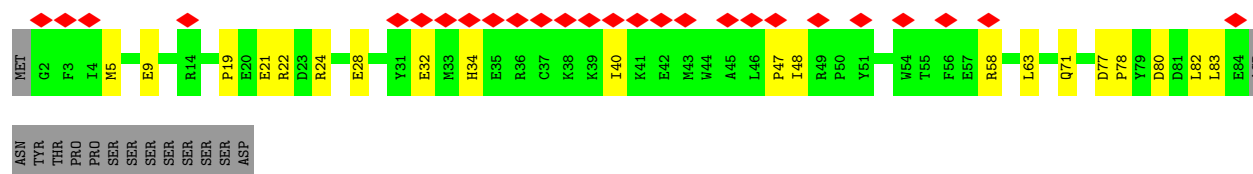




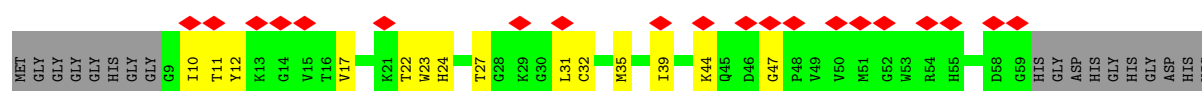
- Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



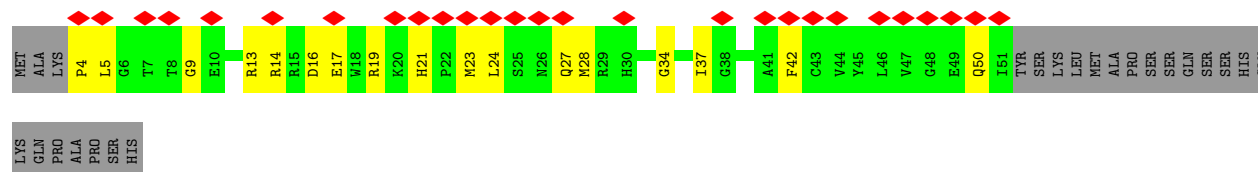
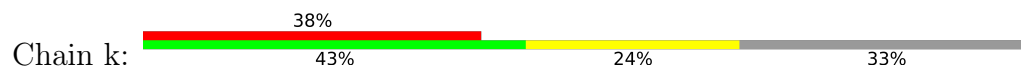
- Molecule 34: P1



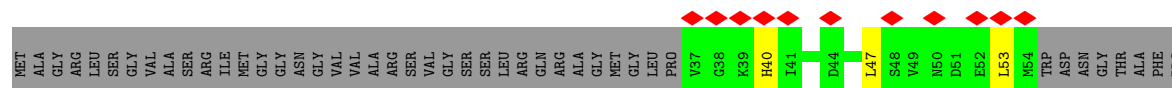
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

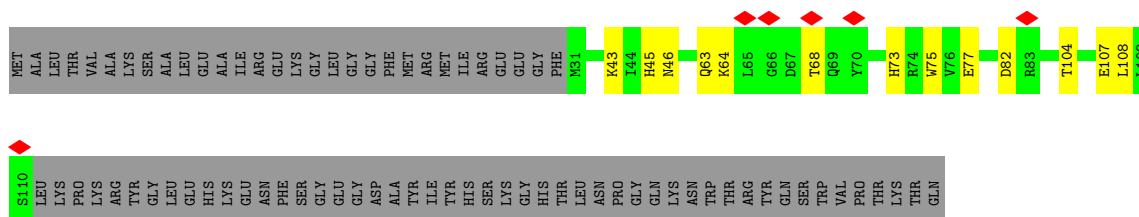


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A

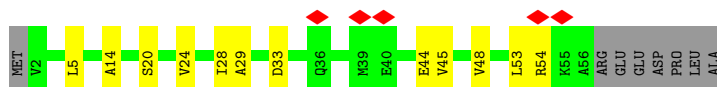


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





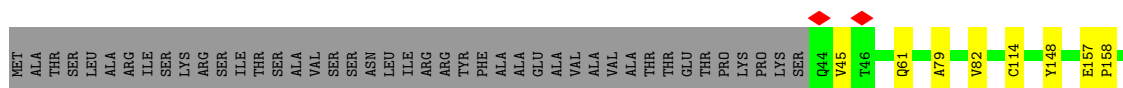
- Molecule 43: Uncharacterized protein At1g67785



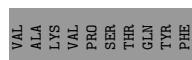
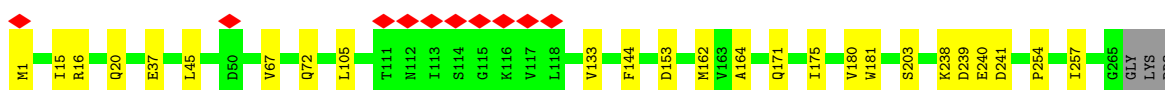
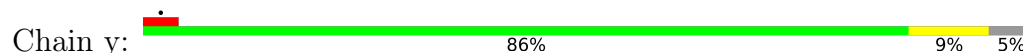
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial



- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial

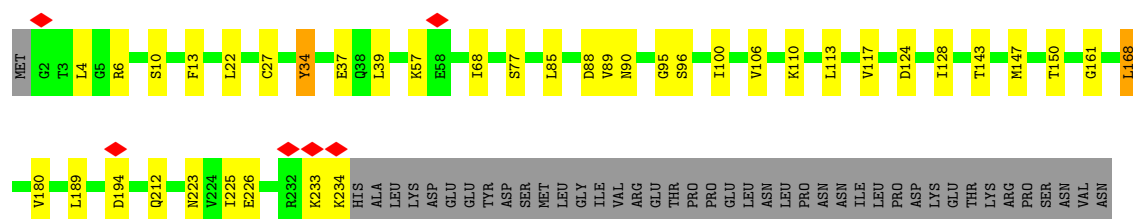


- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial



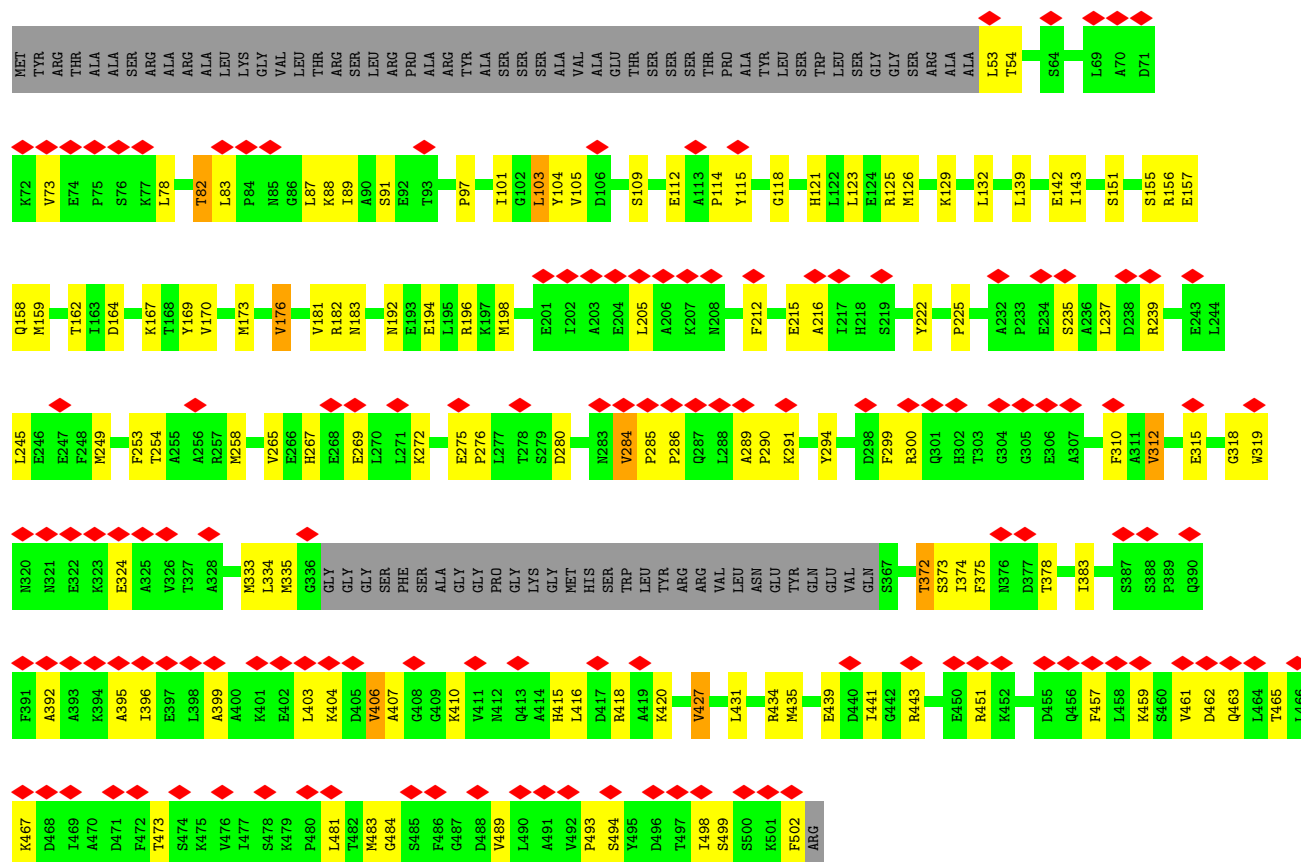
- Molecule 47: Gamma carbonic anhydrase 1, mitochondrial





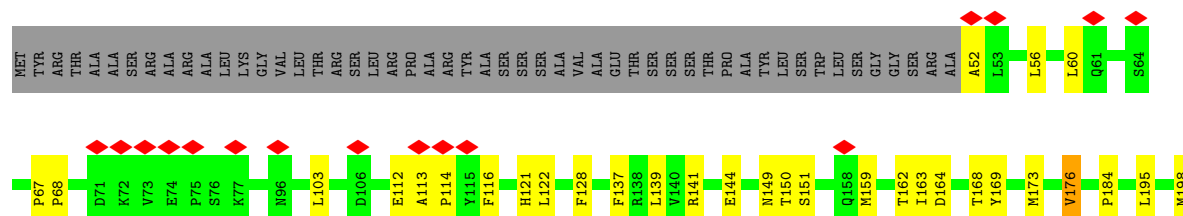
- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

Chain AA: 26% 57% 25% 17%

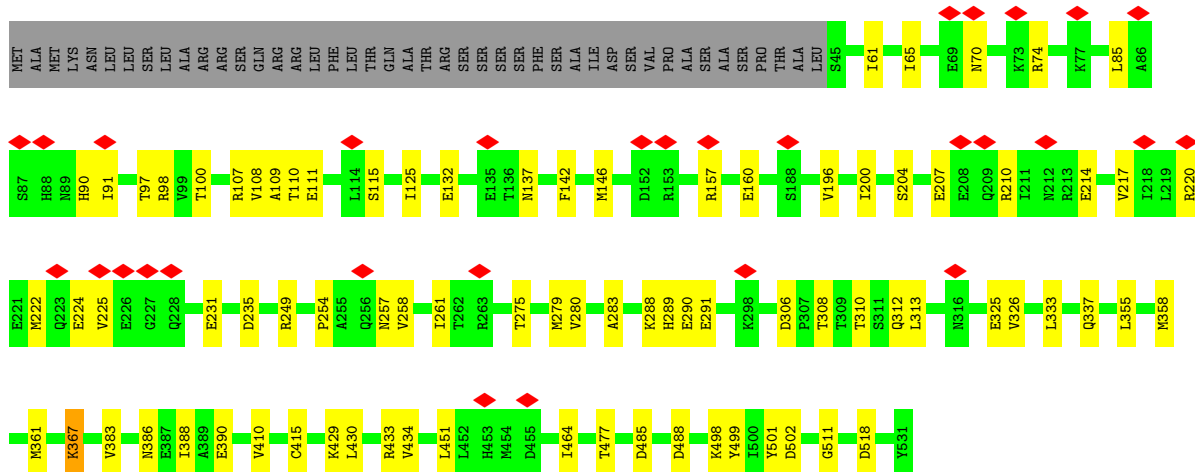
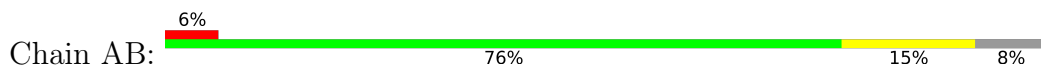


- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

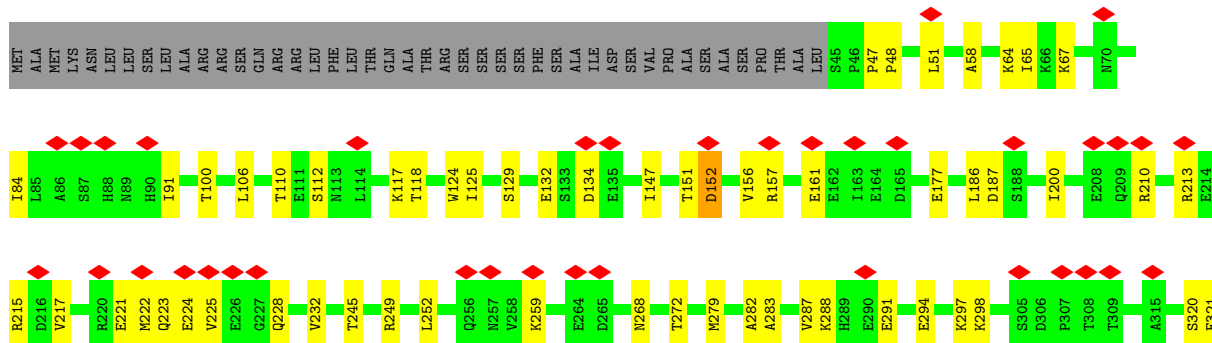
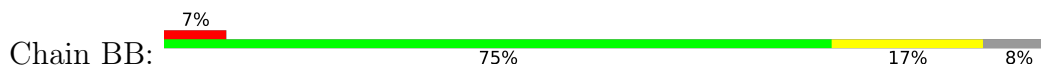
Chain BA: 24% 64% 20% 17%

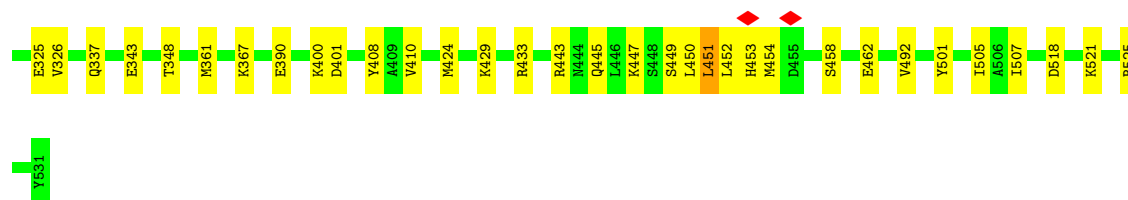


- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

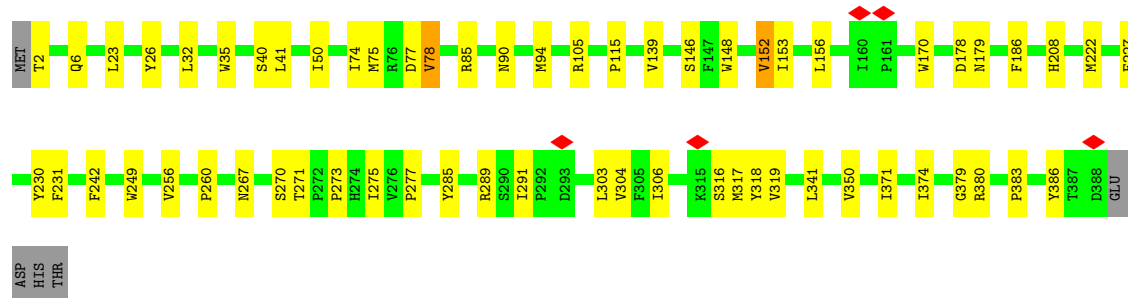
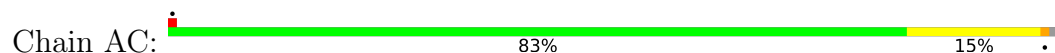


- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

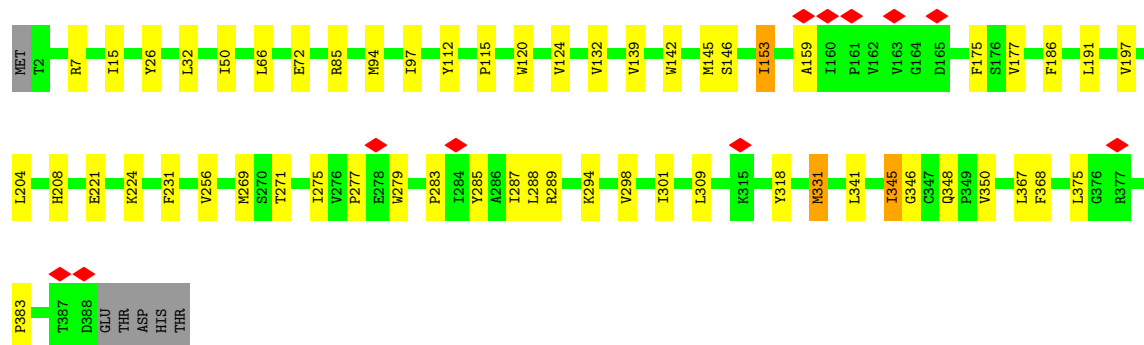
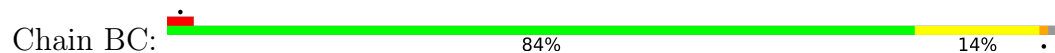




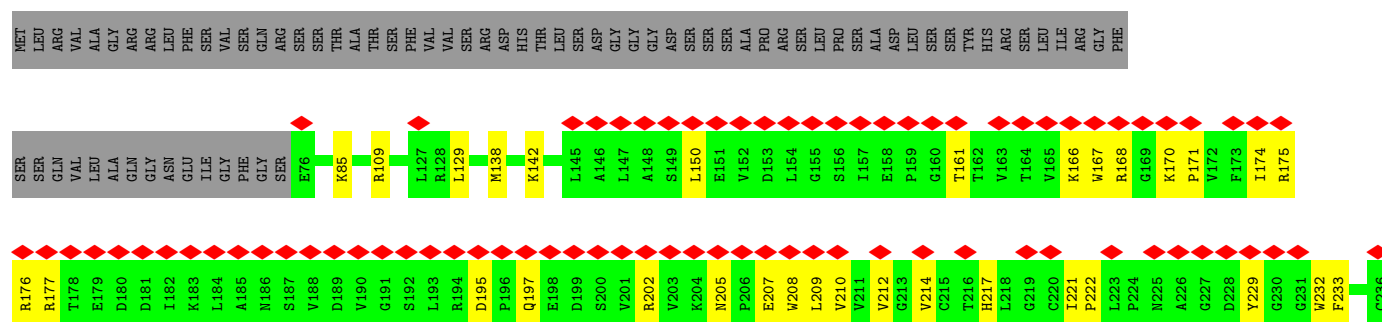
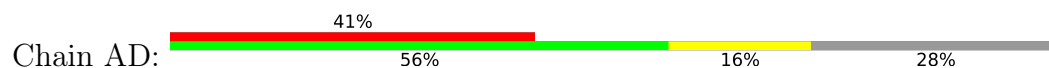
• Molecule 50: Cytochrome b

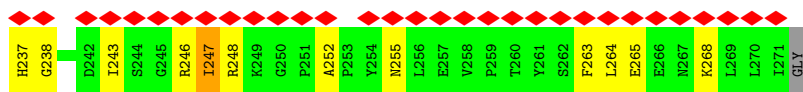


• Molecule 50: Cytochrome b

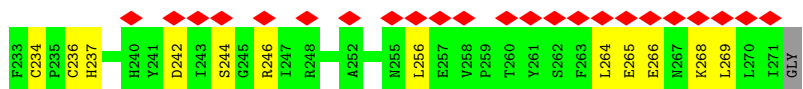
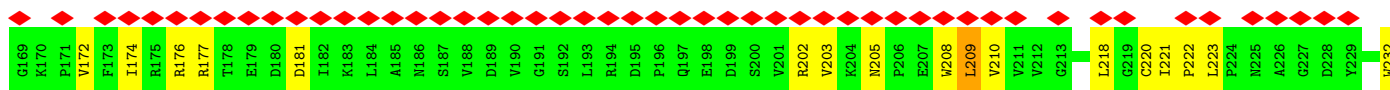
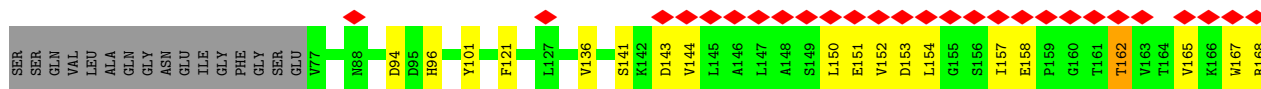
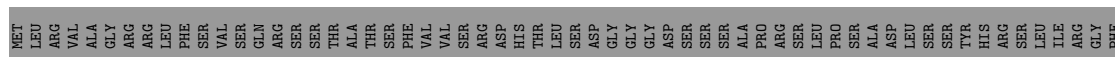
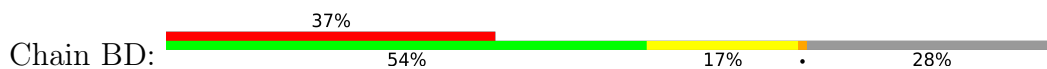


• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

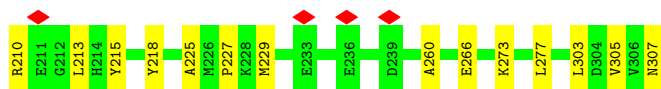
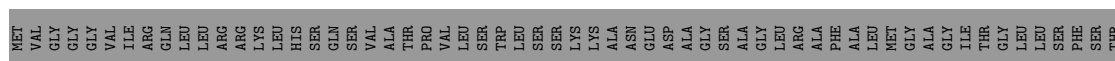




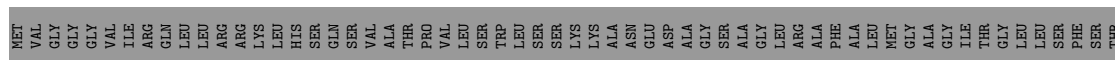
- Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



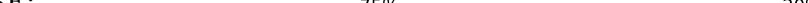
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

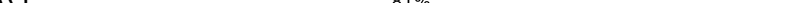


- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial



- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

- Chain BF: 

- Chain AG:  81% 15% .

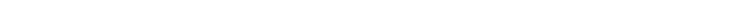
MET	GLY	LYS	Q4	P5	V6	K7	L8	A14	H36	E40	Y61	Q65	E69	F72
-----	-----	-----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----

- Chain BG: 

Diagram illustrating the structure of the 12S oxygen binding domain of hemoglobin, showing residues and their corresponding colors (green, yellow, grey) and positions (P5, V6, K7, K21, I22, M23, T24, W27, L30, E40, E64, Q65, K66, K67, L68, E69, H70, R71, F72). Red diamonds indicate specific residues or positions.

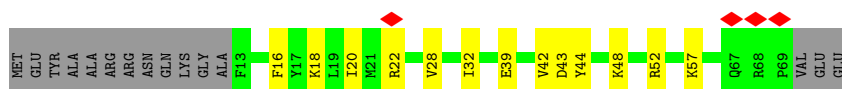
- Chain AH: 

Figure 1: Schematic representation of the 16S rRNA gene. The gene is shown as a horizontal bar divided into segments representing different regions. The segments are labeled with their corresponding nucleotide positions: MET (1-13), ALA (14-21), ASP (22-29), GLU (30-37), V6 (38-45), V7 (46-53), D8 (54-61), K11 (62-69), Y12 (70-77), L13 (78-85), K23 (86-93), P24 (94-101), L25 (102-109), L26 (110-117), Q36 (118-125), G37 (126-133), D38 (134-141), D39 (142-149), S40 (150-157), G41 (158-165), H42 (166-173), Y52 (174-181), D57 (182-189), K63 (190-197), and K69 (198-205). Red diamonds above the bar indicate specific sites of interest: V6, V7, D8, K11, K23, G37, D38, D39, S40, G41, H42, Y52, D57, K63, and K69.

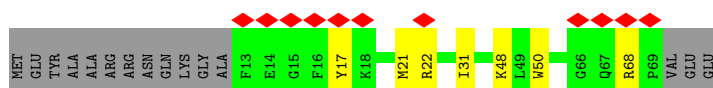
- Chain BH:  43% 74% 17% 9%

[illegible]

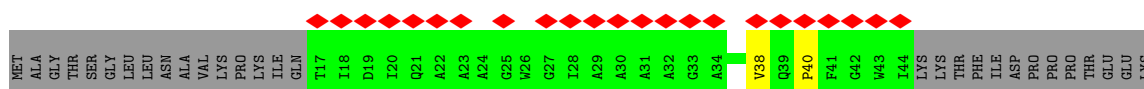
- 



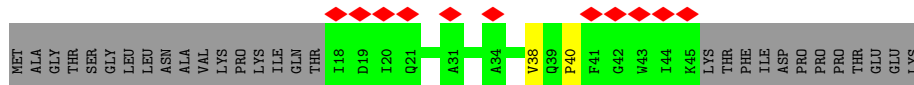
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50886	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	429.75, 429.75, 429.75	wwPDB
Map dimensions	750, 750, 750	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, NDP, UQ5, SF4, FME, FES, 8Q1, HEM, COO, UQ7, UQ9, FMN, ZN

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	A	0.48	0/820	0.68	0/1113
2	B	0.38	0/1279	0.56	0/1734
3	C	0.39	0/1590	0.53	0/2152
4	D	0.48	0/3149	0.71	3/4259 (0.1%)
5	E	0.29	0/1535	0.53	1/2084 (0.0%)
6	F	0.25	0/3441	0.41	0/4641
7	G	0.41	0/5338	0.57	0/7231
8	H	0.49	1/2609 (0.0%)	0.70	0/3553
9	I	0.28	0/1378	0.43	0/1862
10	J	0.36	0/1435	0.56	0/1957
11	K	0.47	0/785	0.69	0/1062
12	L	0.38	0/5368	0.58	0/7291
13	M	0.42	0/4057	0.62	0/5513
14	N	0.43	0/3937	0.69	2/5345 (0.0%)
15	O	0.31	0/979	0.46	0/1326
16	P	0.48	0/2509	0.65	0/3401
17	Q	0.18	0/862	0.35	0/1166
18	R	0.21	0/585	0.37	0/793
19	S	0.29	0/739	0.41	0/996
20	T	0.70	0/671	0.92	0/911
21	U	0.94	0/687	1.20	2/929 (0.2%)
22	V	0.21	0/1146	0.38	0/1555
23	W	0.55	0/923	0.74	0/1249
24	X	0.49	0/790	0.72	0/1060
25	Y	0.28	0/944	0.60	1/1277 (0.1%)
26	Z	0.31	0/1027	0.51	2/1392 (0.1%)
27	a	0.22	0/481	0.38	0/646
28	b	0.31	0/320	0.48	0/434
29	c	0.42	0/637	0.58	0/860
30	d	0.58	0/605	0.83	2/815 (0.2%)
31	e	0.35	0/567	0.50	0/755
32	f	0.24	0/771	0.38	0/1042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.24	0/661	0.44	0/899
34	i	0.37	0/741	0.59	0/997
35	j	0.50	0/433	0.69	1/592 (0.2%)
36	k	0.30	0/392	0.47	0/526
37	l	0.45	0/575	0.64	0/781
38	m	0.43	0/592	0.60	0/793
39	n	0.45	0/938	0.60	0/1273
40	o	0.38	1/666 (0.2%)	0.58	0/886
41	p	0.45	0/777	0.68	0/1043
42	q	0.20	0/690	0.38	0/936
43	u	0.50	0/472	0.75	0/632
44	v	0.27	0/222	0.42	0/300
45	x	0.24	0/1669	0.44	0/2279
46	y	0.28	0/2046	0.44	0/2772
47	z	0.39	0/1804	0.62	0/2441
48	AA	0.36	1/3265 (0.0%)	0.56	0/4431
48	BA	0.31	0/3266	0.54	0/4433
49	AB	0.25	0/3908	0.45	0/5305
49	BB	0.23	0/3908	0.41	0/5305
50	AC	0.30	0/3208	0.47	0/4395
50	BC	0.27	0/3208	0.45	0/4395
51	AD	0.31	0/1567	0.48	0/2135
51	BD	0.29	0/1558	0.46	0/2123
52	AE	0.35	0/1968	0.51	1/2672 (0.0%)
52	BE	0.24	0/1968	0.38	0/2672
53	AF	0.25	0/993	0.46	1/1336 (0.1%)
53	BF	0.27	0/993	0.38	0/1336
54	AG	0.18	0/600	0.39	0/815
54	BG	0.17	0/591	0.37	0/802
55	AH	0.53	0/531	0.71	0/713
55	BH	0.17	0/524	0.35	0/703
56	AI	0.49	0/488	0.73	0/655
56	BI	0.36	0/488	0.52	0/655
57	AJ	0.19	0/210	0.37	0/290
57	BJ	0.18	0/212	0.35	0/291
All	All	0.37	3/98096 (0.0%)	0.56	16/133016 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	83	MET	SD-CE	-7.41	1.61	1.79
40	o	75	LYS	C-O	-5.11	1.18	1.24
48	AA	284	VAL	N-CA	5.03	1.49	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	179	PRO	N-CA-C	-10.29	93.65	110.74
14	N	287	GLY	N-CA-C	6.97	120.02	111.45
4	D	73	VAL	N-CA-C	-6.60	105.70	113.42
4	D	25	VAL	N-CA-C	-5.86	106.61	112.17
53	AF	40	ASP	CA-CB-CG	5.86	118.46	112.60
14	N	286	TYR	CB-CA-C	5.72	119.26	109.24
4	D	287	ILE	N-CA-C	-5.68	107.45	112.90
26	Z	46	ALA	CB-CA-C	-5.59	109.63	117.23
21	U	110	GLN	N-CA-C	-5.51	106.92	113.97
21	U	102	PRO	CB-CA-C	-5.49	103.75	110.95
30	d	31	HIS	CA-C-N	5.26	125.07	119.28
30	d	31	HIS	C-N-CA	5.26	125.07	119.28
52	AE	120	VAL	N-CA-C	-5.26	107.46	111.62
26	Z	25	PRO	CA-N-CD	-5.16	104.78	112.00
25	Y	92	PHE	N-CA-C	-5.04	106.97	113.23
35	j	47	GLY	O-C-N	-5.02	116.75	121.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	412[B]	TYR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	817	32	0
2	B	1244	0	1231	32	0
3	C	1545	0	1501	31	0
4	D	3079	0	3049	70	0
5	E	1500	0	1473	39	0
6	F	3368	0	3354	48	0
7	G	5243	0	5228	99	0
8	H	2536	0	2641	56	0
9	I	1349	0	1293	33	0
10	J	1399	0	1472	46	0
11	K	784	0	843	31	0
12	L	5222	0	5253	101	0
13	M	3946	0	4086	139	0
14	N	3832	0	3934	107	0
15	O	963	0	975	14	0
16	P	2453	0	2493	45	0
17	Q	837	0	818	18	0
18	R	571	0	559	6	0
19	S	727	0	759	26	0
20	T	659	0	644	26	0
21	U	677	0	665	11	0
22	V	1123	0	1112	13	0
23	W	904	0	901	23	0
24	X	776	0	777	16	0
25	Y	928	0	960	43	0
26	Z	997	0	979	15	0
27	a	469	0	472	18	0
28	b	315	0	338	11	0
29	c	617	0	619	23	0
30	d	592	0	610	18	0
31	e	554	0	522	14	0
32	f	765	0	766	8	0
33	g	641	0	632	10	0
34	i	721	0	695	18	0
35	j	415	0	406	25	0
36	k	382	0	380	18	0
37	l	562	0	567	10	0
38	m	577	0	564	36	0
39	n	911	0	879	32	0
40	o	657	0	669	23	0
41	p	757	0	743	18	0
42	q	669	0	630	9	0
43	u	463	0	471	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	v	219	0	227	3	0
45	x	1629	0	1636	18	0
46	y	2013	0	2024	33	0
47	z	1772	0	1771	37	0
48	AA	3201	0	3201	125	0
48	BA	3202	0	3203	92	0
49	AB	3834	0	3797	65	0
49	BB	3834	0	3797	70	0
50	AC	3093	0	3074	67	0
50	BC	3093	0	3074	51	0
51	AD	1528	0	1529	63	0
51	BD	1519	0	1524	42	0
52	AE	1917	0	1844	34	0
52	BE	1917	0	1844	34	0
53	AF	976	0	1001	30	0
53	BF	976	0	1001	18	0
54	AG	581	0	589	25	0
54	BG	572	0	582	7	0
55	AH	518	0	518	9	0
55	BH	511	0	511	9	0
56	AI	476	0	469	12	0
56	BI	476	0	469	8	0
57	AJ	203	0	197	1	0
57	BJ	205	0	203	1	0
58	B	8	0	0	1	0
58	F	8	0	0	2	0
58	G	16	0	0	0	0
58	I	16	0	0	2	0
59	AD	4	0	0	1	0
59	BD	4	0	0	2	0
59	E	4	0	0	1	0
59	G	4	0	0	0	0
60	F	31	0	19	1	0
61	H	35	0	43	6	0
62	O	1	0	0	0	0
63	P	48	0	26	2	0
64	AB	1	0	0	0	0
64	BB	1	0	0	0	0
64	R	1	0	0	0	0
64	y	1	0	0	0	0
65	W	35	0	0	0	0
65	n	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	y	53	0	35	14	0
67	AC	86	0	60	4	0
67	AE	43	0	30	4	0
67	BC	86	0	60	3	0
67	BE	43	0	30	10	0
68	AC	76	0	100	13	0
68	BC	38	0	50	6	0
69	BC	48	0	66	7	0
All	All	96522	0	96384	1896	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 10.

All (1896) 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)
50:AC:222:MET:SD	54:AG:6:VAL:HG11	1.43	1.55
13:M:279:PHE:CE1	38:m:71:LEU:CD2	1.96	1.49
20:T:95:LEU:CD2	20:T:118:HIS:CD2	2.05	1.40
13:M:279:PHE:CE1	38:m:71:LEU:HD22	1.57	1.39
50:AC:222:MET:SD	54:AG:6:VAL:CG1	2.07	1.39
50:AC:222:MET:SD	54:AG:6:VAL:HG21	1.63	1.38
12:L:384:ILE:CD1	35:j:31:LEU:CD2	2.05	1.33
12:L:384:ILE:HD11	35:j:31:LEU:CD2	1.60	1.30
51:AD:264:LEU:CD1	51:AD:268:LYS:HE2	1.62	1.29
13:M:279:PHE:CZ	38:m:71:LEU:HD22	1.66	1.28
50:AC:222:MET:SD	54:AG:6:VAL:CG2	2.22	1.28
13:M:189:LEU:O	13:M:193:PHE:CD2	1.90	1.25
43:u:53:LEU:HD22	43:u:54:ARG:NH1	1.49	1.25
5:E:172:MET:SD	6:F:185:TYR:HE1	1.59	1.24
7:G:302:ASN:ND2	7:G:320:ASN:HD22	1.37	1.23
7:G:236:ASP:CB	7:G:254:LYS:HZ3	1.51	1.22
7:G:236:ASP:HB2	7:G:254:LYS:NZ	1.57	1.19
20:T:95:LEU:HD22	20:T:118:HIS:CD2	1.66	1.19
7:G:337:ASP:OD2	7:G:734:ILE:HD12	1.43	1.19
9:I:154:ARG:HH22	17:Q:91:TRP:NE1	1.42	1.18
46:y:162:MET:HE1	66:y:301:COO:C15	1.72	1.18
50:AC:222:MET:CE	54:AG:8:LEU:HD12	1.71	1.17
4:D:292:ARG:NH2	4:D:307:GLU:CB	2.07	1.17
46:y:162:MET:HE1	66:y:301:COO:H151	1.19	1.17
4:D:292:ARG:HH21	4:D:307:GLU:C	1.53	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:95:LEU:HD21	20:T:118:HIS:CD2	1.72	1.16
7:G:576:GLU:OE1	7:G:593:LYS:HD3	1.46	1.16
9:I:139:THR:CG2	9:I:154:ARG:HH12	1.57	1.16
50:AC:222:MET:HE3	54:AG:8:LEU:CD1	1.75	1.16
19:S:13:GLU:OE2	19:S:49:LEU:HD11	1.46	1.15
43:u:53:LEU:CD2	43:u:54:ARG:NH1	2.09	1.14
46:y:162:MET:CE	66:y:301:COO:H151	1.76	1.14
7:G:302:ASN:HD22	7:G:320:ASN:HB2	0.98	1.14
7:G:302:ASN:HD21	7:G:320:ASN:ND2	1.44	1.14
7:G:704:PRO:HA	19:S:37:LYS:HE3	1.24	1.14
4:D:292:ARG:NH1	7:G:192:ARG:HA	1.64	1.12
48:AA:164:ASP:CG	48:AA:435:MET:HE1	1.74	1.12
20:T:95:LEU:HD22	20:T:118:HIS:NE2	1.63	1.12
43:u:53:LEU:CD2	43:u:54:ARG:HH12	1.62	1.11
2:B:87:MET:HE1	2:B:142:VAL:HG12	1.32	1.11
7:G:236:ASP:HB2	7:G:254:LYS:HZ3	1.03	1.11
5:E:172:MET:SD	6:F:185:TYR:CE1	2.44	1.10
49:BB:450:LEU:HA	49:BB:453:HIS:NE2	1.66	1.10
4:D:292:ARG:NH2	4:D:307:GLU:HB3	1.60	1.09
21:U:111:SER:OG	21:U:114:LEU:HD13	1.52	1.09
12:L:384:ILE:HD13	35:j:31:LEU:HD21	1.26	1.09
46:y:162:MET:CE	66:y:301:COO:C15	2.28	1.09
48:AA:269:GLU:CB	48:AA:272:LYS:HE2	1.81	1.09
13:M:279:PHE:CE1	38:m:71:LEU:HD23	1.85	1.08
49:BB:449:SER:O	49:BB:453:HIS:HD2	1.36	1.08
9:I:154:ARG:NH2	9:I:156:ASP:OD2	1.86	1.08
10:J:101:MET:CE	14:N:192:PHE:CE1	2.36	1.07
4:D:292:ARG:HH11	7:G:192:ARG:HA	1.17	1.07
12:L:384:ILE:CD1	35:j:31:LEU:HD22	1.85	1.07
51:AD:264:LEU:HD12	51:AD:268:LYS:HE2	1.26	1.07
20:T:95:LEU:CD2	20:T:118:HIS:NE2	2.15	1.06
4:D:292:ARG:NH2	4:D:307:GLU:C	2.14	1.05
4:D:292:ARG:HH22	4:D:307:GLU:CB	1.67	1.05
50:AC:222:MET:HE1	54:AG:8:LEU:HB2	1.31	1.05
43:u:53:LEU:HD22	43:u:54:ARG:HH12	0.89	1.04
48:AA:164:ASP:OD1	48:AA:435:MET:CE	2.05	1.04
48:AA:198:MET:HE2	48:AA:237:LEU:HD21	1.36	1.04
7:G:302:ASN:ND2	7:G:320:ASN:HB2	1.72	1.03
10:J:101:MET:HE1	14:N:192:PHE:CE1	1.93	1.03
24:X:29:CYS:SG	24:X:59:CYS:HB3	1.97	1.03
9:I:154:ARG:NH2	17:Q:91:TRP:HE1	1.57	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:164:ASP:OD1	48:AA:435:MET:HE1	1.57	1.02
12:L:384:ILE:HD11	35:j:31:LEU:HD23	1.37	1.01
9:I:139:THR:CG2	9:I:154:ARG:NH1	2.21	1.00
48:AA:164:ASP:OD1	48:AA:435:MET:SD	2.19	1.00
51:BD:94:ASP:OD2	53:BF:75:LYS:NZ	1.93	1.00
13:M:448:LYS:HZ1	38:m:4:GLY:H	1.03	1.00
43:u:53:LEU:HD23	43:u:54:ARG:CZ	1.89	1.00
20:T:98:PRO:HB2	20:T:101:GLU:OE1	1.60	1.00
3:C:56:LEU:HD13	3:C:77:LEU:HD21	1.44	1.00
43:u:53:LEU:HD23	43:u:54:ARG:NH2	1.74	0.99
43:u:53:LEU:CD2	43:u:54:ARG:CZ	2.41	0.98
9:I:154:ARG:CZ	9:I:156:ASP:OD2	2.11	0.98
50:AC:222:MET:SD	54:AG:6:VAL:CB	2.51	0.98
14:N:408:CYS:SG	14:N:480:LEU:HD21	2.04	0.98
4:D:292:ARG:HH22	4:D:307:GLU:HB2	1.26	0.98
9:I:154:ARG:NH2	17:Q:91:TRP:NE1	2.11	0.98
49:BB:449:SER:O	49:BB:453:HIS:CD2	2.15	0.97
35:j:10:ILE:CD1	36:k:23:MET:HE1	1.94	0.97
43:u:53:LEU:CD2	43:u:54:ARG:NH2	2.27	0.97
13:M:17:LEU:O	13:M:20:VAL:HG22	1.65	0.97
1:A:56:ARG:HH12	4:D:11:PHE:H	0.97	0.96
2:B:107:ASP:O	2:B:110:ARG:HG2	1.66	0.96
51:AD:264:LEU:HD13	51:AD:268:LYS:HE2	1.45	0.96
20:T:95:LEU:HD21	20:T:118:HIS:HD2	1.17	0.95
53:AF:97:MET:HE2	49:BB:65:ILE:HD11	1.49	0.95
48:BA:416:LEU:HD22	48:BA:466:LEU:HD23	1.47	0.95
13:M:448:LYS:HZ1	38:m:4:GLY:N	1.65	0.94
19:S:13:GLU:OE2	19:S:49:LEU:CD1	2.15	0.94
12:L:384:ILE:CD1	35:j:31:LEU:HD21	1.85	0.94
15:O:48:LEU:HD12	15:O:146:MET:O	1.67	0.94
48:BA:300:ARG:NH2	48:BA:494:SER:HA	1.83	0.94
48:AA:420:LYS:HG3	48:AA:461:VAL:HG12	1.50	0.93
13:M:487:ASN:HD22	41:p:34:ARG:HE	1.15	0.93
10:J:53:PHE:HZ	11:K:43:ASN:ND2	1.67	0.93
7:G:704:PRO:HA	19:S:37:LYS:CE	1.99	0.92
51:AD:170:LYS:HG2	51:AD:212:VAL:CG1	2.00	0.92
39:n:53:ASN:O	39:n:56:GLN:HG2	1.68	0.92
1:A:16:LEU:HD13	8:H:83:MET:HE1	1.49	0.92
52:BE:124:GLU:O	52:BE:128:LYS:HG3	1.70	0.92
10:J:101:MET:HE3	14:N:192:PHE:HE1	1.34	0.91
13:M:279:PHE:HE1	38:m:71:LEU:CD2	1.62	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:PHE:CZ	11:K:43:ASN:ND2	2.38	0.91
49:BB:450:LEU:HA	49:BB:453:HIS:CD2	2.05	0.90
3:C:17:LYS:HE2	3:C:37:TYR:CZ	2.07	0.90
40:o:9:LYS:C	40:o:29:MET:HE1	1.96	0.90
9:I:139:THR:HG22	9:I:154:ARG:NH1	1.85	0.90
48:BA:163:ILE:HG23	48:BA:173:MET:HE2	1.53	0.90
12:L:351:SER:CB	12:L:382:MET:SD	2.59	0.90
14:N:218:ILE:HD11	14:N:286:TYR:OH	1.71	0.90
43:u:53:LEU:CD2	43:u:54:ARG:HH22	1.85	0.90
48:AA:269:GLU:HB3	48:AA:272:LYS:HE2	1.50	0.90
25:Y:45:ARG:NH1	25:Y:48:ARG:NH2	2.21	0.89
48:BA:150:THR:HG22	48:BA:163:ILE:HD13	1.53	0.89
7:G:302:ASN:ND2	7:G:320:ASN:ND2	2.11	0.89
16:P:131:ILE:HD12	16:P:166:LYS:HE2	1.51	0.89
35:j:23:TRP:O	35:j:27:THR:HG22	1.72	0.89
4:D:71:ASP:HB3	4:D:78:GLN:NE2	1.88	0.89
12:L:351:SER:HB2	12:L:382:MET:SD	2.12	0.88
1:A:56:ARG:HH11	4:D:11:PHE:HB3	1.36	0.88
12:L:381:MET:HE1	35:j:31:LEU:HD13	1.53	0.88
12:L:426:SER:O	12:L:430:THR:HG23	1.74	0.88
13:M:76:PRO:HB2	30:d:57:LYS:NZ	1.89	0.88
51:AD:176:ARG:NE	51:AD:207:GLU:OE2	2.05	0.88
51:AD:264:LEU:CD1	51:AD:268:LYS:CE	2.49	0.87
51:AD:264:LEU:HD12	51:AD:268:LYS:CE	2.04	0.87
10:J:101:MET:CE	14:N:192:PHE:CZ	2.57	0.87
7:G:302:ASN:HD22	7:G:320:ASN:CB	1.86	0.87
48:AA:420:LYS:CG	48:AA:461:VAL:HG12	2.04	0.87
51:BD:234:CYS:HG	59:BD:301:FES:FE1	0.60	0.87
1:A:56:ARG:HH12	4:D:11:PHE:N	1.71	0.86
7:G:518:ALA:HB3	7:G:555:GLN:OE1	1.75	0.86
12:L:214:ARG:NH1	38:m:62:ASP:OD1	2.08	0.86
51:AD:237:HIS:HD2	50:BC:289:ARG:HG2	1.38	0.86
13:M:189:LEU:O	13:M:193:PHE:CE2	2.29	0.86
25:Y:10:GLU:O	25:Y:11:GLU:HG3	1.77	0.85
50:AC:222:MET:CE	54:AG:8:LEU:HB2	2.07	0.85
47:z:6:ARG:NH1	47:z:10:SER:OG	2.09	0.85
3:C:56:LEU:HD13	3:C:77:LEU:CD2	2.06	0.85
4:D:292:ARG:NH2	4:D:308:SER:N	2.25	0.85
13:M:395:SER:HB2	13:M:470:MET:HE2	1.57	0.85
7:G:367:VAL:O	7:G:371:ILE:HD12	1.76	0.85
2:B:87:MET:CE	2:B:142:VAL:HG12	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:162:MET:CE	66:y:301:COO:H152	2.06	0.84
49:AB:70:ASN:OD1	49:AB:70:ASN:O	1.95	0.84
41:p:28:VAL:O	41:p:32:GLU:HG2	1.77	0.84
49:AB:220:ARG:CD	49:AB:224:GLU:OE1	2.26	0.84
20:T:118:HIS:NE2	20:T:120:MET:HB2	1.92	0.84
29:c:16:ARG:HE	29:c:26:PRO:HG3	1.41	0.84
46:y:164:ALA:HB1	66:y:301:COO:N6A	1.92	0.84
43:u:53:LEU:HD21	43:u:54:ARG:HH22	1.42	0.84
6:F:380:MET:HB3	6:F:384:THR:HG21	1.57	0.84
7:G:724:MET:HE3	7:G:730:ARG:HG2	1.60	0.84
13:M:189:LEU:O	13:M:193:PHE:HD2	1.56	0.84
15:O:126:ILE:HG21	21:U:41:ARG:HG3	1.60	0.83
35:j:10:ILE:HD12	36:k:23:MET:HE1	1.61	0.83
10:J:101:MET:HE3	14:N:192:PHE:CE1	2.10	0.83
46:y:162:MET:HE3	66:y:301:COO:C15	2.08	0.83
24:X:88:GLU:OE2	27:a:39:HIS:NE2	2.11	0.83
48:BA:150:THR:CG2	48:BA:163:ILE:HD13	2.07	0.83
25:Y:45:ARG:NH1	25:Y:48:ARG:HH22	1.77	0.83
16:P:194:SER:OG	16:P:342:ASP:OD2	1.96	0.83
46:y:162:MET:HE3	66:y:301:COO:H152	1.60	0.82
35:j:10:ILE:HD13	36:k:23:MET:HE1	1.60	0.82
16:P:353:VAL:CG1	16:P:359:LYS:HE2	2.09	0.82
5:E:143:ILE:HD12	5:E:201:VAL:HG23	1.58	0.82
9:I:139:THR:CB	9:I:154:ARG:HH12	1.92	0.82
4:D:292:ARG:CZ	4:D:307:GLU:HB3	2.07	0.82
25:Y:90:ARG:HA	25:Y:94:ASN:HD21	1.42	0.82
49:BB:501:TYR:HD2	56:BI:22:ARG:NH1	1.77	0.82
13:M:76:PRO:HB2	30:d:57:LYS:HZ1	1.43	0.81
51:AD:170:LYS:CG	51:AD:212:VAL:HG11	2.09	0.81
49:BB:501:TYR:HD2	56:BI:22:ARG:HH11	1.25	0.81
1:A:56:ARG:NH1	4:D:11:PHE:H	1.77	0.81
7:G:302:ASN:ND2	7:G:320:ASN:CB	2.42	0.81
48:BA:416:LEU:HD22	48:BA:466:LEU:CD2	2.11	0.81
1:A:16:LEU:HA	8:H:83:MET:HE3	1.63	0.80
4:D:292:ARG:HH21	4:D:308:SER:N	1.79	0.80
13:M:17:LEU:O	13:M:20:VAL:CG2	2.29	0.80
51:AD:264:LEU:HB2	51:AD:268:LYS:HD3	1.64	0.80
2:B:87:MET:HG2	4:D:19:HIS:CE1	2.17	0.80
7:G:337:ASP:OD2	7:G:734:ILE:CD1	2.27	0.80
51:BD:209:LEU:HD21	51:BD:244:SER:HA	1.63	0.80
12:L:351:SER:HB3	12:L:382:MET:SD	2.21	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BA:330:VAL:O	48:BA:334:LEU:HD13	1.83	0.79
25:Y:113:SER:OG	25:Y:116:THR:OG1	2.01	0.79
52:AE:190:GLN:OE1	52:AE:190:GLN:N	2.14	0.79
1:A:56:ARG:NH1	4:D:11:PHE:HB3	1.97	0.79
13:M:163:ARG:NH2	38:m:21:GLU:OE1	2.15	0.79
25:Y:84:GLN:HE21	25:Y:90:ARG:HG2	1.46	0.79
7:G:304:ARG:NH2	7:G:316:ILE:HD11	1.98	0.79
14:N:492:GLN:O	30:d:63:MET:HE1	1.83	0.79
12:L:370:GLY:HA2	36:k:27:GLN:HG3	1.64	0.79
7:G:724:MET:HE1	7:G:730:ARG:HA	1.63	0.79
9:I:139:THR:HG21	9:I:154:ARG:HH12	1.46	0.79
13:M:279:PHE:CZ	38:m:71:LEU:CD2	2.45	0.78
39:n:58:VAL:HG13	39:n:63:ARG:HH21	1.49	0.78
48:AA:269:GLU:CG	48:AA:272:LYS:NZ	2.47	0.78
48:AA:494:SER:O	48:AA:498:ILE:HD12	1.83	0.78
16:P:180:TYR:C	16:P:181:ILE:HD12	2.09	0.78
19:S:31:PHE:CD1	19:S:35:ASN:OD1	2.36	0.78
24:X:32:GLU:CD	24:X:59:CYS:SG	2.66	0.78
49:BB:223:GLN:NE2	49:BB:224:GLU:OE2	2.17	0.78
1:A:56:ARG:NH1	4:D:11:PHE:CD1	2.51	0.78
16:P:148:GLU:HA	16:P:196:MET:SD	2.24	0.78
52:BE:106:CYS:SG	67:BE:400:HEM:C3C	2.77	0.78
49:BB:450:LEU:CA	49:BB:453:HIS:NE2	2.46	0.78
6:F:309:CYS:SG	6:F:311:VAL:HG13	2.24	0.77
2:B:87:MET:HE1	2:B:142:VAL:CG1	2.12	0.77
48:AA:91:SER:HG	48:AA:267:HIS:HD1	1.31	0.77
48:BA:310:PHE:CZ	48:BA:396:ILE:HG23	2.19	0.77
12:L:1:MET:HA	12:L:4:LEU:HD12	1.66	0.77
49:AB:288:LYS:HD2	49:AB:289:HIS:H	1.50	0.77
48:AA:269:GLU:CA	48:AA:272:LYS:HE2	2.13	0.77
1:A:16:LEU:O	1:A:20:LEU:HD22	1.84	0.77
7:G:304:ARG:HH12	17:Q:62:THR:HG23	1.48	0.77
43:u:44:GLU:OE1	55:AH:26:LEU:HD13	1.84	0.77
48:AA:83:LEU:HD12	48:AA:87:LEU:HB3	1.67	0.77
10:J:101:MET:CE	11:K:11:MET:HE1	2.13	0.77
14:N:207:ASP:OD2	14:N:283:TYR:OH	2.03	0.76
48:BA:459:LYS:HB3	48:BA:463:GLN:HE22	1.50	0.76
14:N:281:PHE:CG	14:N:290:LEU:HD11	2.20	0.76
16:P:353:VAL:HG12	16:P:359:LYS:HE2	1.66	0.76
7:G:714:PRO:O	7:G:716:GLN:NE2	2.18	0.76
49:AB:288:LYS:HD2	49:AB:289:HIS:N	2.01	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:1:MET:HG2	31:e:14:CYS:H	1.51	0.76
48:BA:164:ASP:OD2	48:BA:434:ARG:NH1	2.18	0.76
12:L:384:ILE:HD11	35:j:31:LEU:HD22	1.53	0.76
13:M:448:LYS:HD2	38:m:5:MET:CG	2.15	0.76
48:AA:143:ILE:HD11	48:AA:176:VAL:HG11	1.68	0.76
51:AD:170:LYS:CG	51:AD:212:VAL:CG1	2.63	0.76
7:G:304:ARG:CZ	7:G:316:ILE:HD11	2.17	0.75
3:C:180:PHE:HB3	4:D:318:GLU:HG3	1.69	0.75
7:G:337:ASP:CG	7:G:734:ILE:HD12	2.11	0.75
48:AA:170:VAL:HG11	48:AA:265:VAL:HG21	1.69	0.75
48:BA:396:ILE:HD12	48:BA:396:ILE:H	1.51	0.75
49:AB:220:ARG:HD2	49:AB:224:GLU:OE1	1.86	0.75
52:BE:78:TRP:HB2	52:BE:81:GLU:HG3	1.69	0.75
7:G:236:ASP:CB	7:G:254:LYS:NZ	2.30	0.74
48:AA:269:GLU:CG	48:AA:272:LYS:HE2	2.16	0.74
26:Z:112:MET:HE2	26:Z:118:TRP:CD2	2.22	0.74
48:AA:103:LEU:HD21	48:AA:258:MET:HE3	1.69	0.74
48:AA:269:GLU:HG2	48:AA:272:LYS:NZ	2.02	0.74
8:H:59:ILE:HD13	61:H:500:UQ9:H21A	1.68	0.74
9:I:154:ARG:NH2	17:Q:91:TRP:CD1	2.56	0.74
13:M:448:LYS:HD2	38:m:5:MET:HG3	1.68	0.74
47:z:27:CYS:HG	47:z:34:TYR:HH	1.33	0.74
13:M:193:PHE:CZ	14:N:415:PHE:CD1	2.75	0.73
48:AA:269:GLU:HA	48:AA:272:LYS:HG2	1.69	0.73
25:Y:89:LYS:O	25:Y:94:ASN:ND2	2.21	0.73
32:f:8:LEU:HD22	34:i:58:ARG:HH11	1.52	0.73
48:AA:269:GLU:O	48:AA:272:LYS:HG2	1.87	0.73
50:AC:222:MET:HE3	54:AG:8:LEU:HD12	0.83	0.73
7:G:510:LYS:H	7:G:510:LYS:HD2	1.53	0.73
9:I:139:THR:HG21	9:I:154:ARG:NH1	2.03	0.73
50:AC:222:MET:HE1	54:AG:8:LEU:CB	2.15	0.73
51:AD:170:LYS:CD	51:AD:212:VAL:HG11	2.17	0.73
8:H:219:GLU:OE1	8:H:219:GLU:O	2.07	0.73
7:G:674:GLU:CD	7:G:674:GLU:H	1.97	0.73
53:AF:67:MET:SD	54:AG:8:LEU:HD11	2.27	0.73
50:BC:132:VAL:HG22	69:BC:503:UQ7:H172	1.71	0.73
51:AD:264:LEU:HD13	51:AD:268:LYS:CE	2.14	0.73
25:Y:22:GLY:HA3	25:Y:77:ILE:HD11	1.70	0.72
51:BD:234:CYS:SG	59:BD:301:FES:FE1	1.77	0.72
8:H:126:ARG:HG2	8:H:126:ARG:HH11	1.53	0.72
20:T:118:HIS:CE1	20:T:120:MET:HB2	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:45:ARG:HG3	25:Y:48:ARG:HH21	1.54	0.72
53:AF:56:ARG:HH22	54:AG:7:LYS:NZ	1.86	0.72
49:BB:215:ARG:HD3	49:BB:259:LYS:HA	1.70	0.72
7:G:724:MET:CE	7:G:730:ARG:HA	2.19	0.71
10:J:101:MET:CE	14:N:192:PHE:HE1	1.88	0.71
14:N:292:GLN:O	14:N:296:PHE:HD2	1.73	0.71
35:j:10:ILE:HD13	36:k:23:MET:CE	2.20	0.71
48:AA:269:GLU:CG	48:AA:272:LYS:CE	2.67	0.71
2:B:88:THR:HG23	2:B:115:PHE:CD1	2.26	0.71
5:E:143:ILE:CD1	5:E:201:VAL:HG23	2.21	0.71
9:I:154:ARG:HH22	17:Q:91:TRP:HE1	0.78	0.71
41:p:22:ASN:O	41:p:22:ASN:OD1	2.09	0.71
48:AA:198:MET:HE2	48:AA:237:LEU:CD2	2.15	0.71
2:B:69:ILE:HD12	2:B:212:PHE:CD2	2.25	0.71
15:O:126:ILE:CG2	21:U:41:ARG:HG3	2.21	0.71
51:AD:170:LYS:HG2	51:AD:212:VAL:HG13	1.71	0.71
48:BA:330:VAL:O	48:BA:334:LEU:CD1	2.38	0.71
52:BE:66:GLU:OE2	54:BG:67:LYS:HG3	1.91	0.71
47:z:6:ARG:NH1	47:z:10:SER:HG	1.88	0.70
50:AC:139:VAL:HA	50:AC:146:SER:HB3	1.73	0.70
14:N:143:TYR:OH	14:N:283:TYR:CZ	2.41	0.70
20:T:71:PHE:HE1	20:T:108:CYS:HG	1.35	0.70
50:AC:222:MET:SD	54:AG:6:VAL:HG13	2.29	0.70
2:B:87:MET:CE	2:B:142:VAL:CG1	2.68	0.70
5:E:129:VAL:HG12	5:E:181:ILE:HG22	1.74	0.70
17:Q:75:LYS:HE3	17:Q:103:ASP:HA	1.72	0.70
51:BD:265:GLU:HG2	51:BD:266:GLU:H	1.57	0.70
48:AA:78:LEU:CD2	48:AA:451:ARG:HD3	2.20	0.70
48:AA:420:LYS:HD3	48:AA:462:ASP:HA	1.73	0.70
51:AD:205:ASN:HB2	51:AD:263:PHE:CE1	2.27	0.70
52:AE:74:PRO:HG3	55:AH:57:ASP:HB3	1.72	0.70
48:BA:428:LEU:CD2	49:BB:117:LYS:HD2	2.22	0.70
48:AA:294:TYR:HB3	48:AA:315:GLU:OE1	1.92	0.69
14:N:143:TYR:OH	14:N:283:TYR:OH	1.67	0.69
3:C:56:LEU:HA	3:C:77:LEU:HD23	1.74	0.69
7:G:317:PRO:HG3	7:G:328:ILE:HG12	1.74	0.69
7:G:625:GLU:HB3	7:G:646:THR:HG22	1.75	0.69
48:AA:73:VAL:O	49:AB:115:SER:OG	2.09	0.69
1:A:56:ARG:NH1	4:D:11:PHE:CB	2.56	0.69
4:D:292:ARG:HD2	7:G:192:ARG:HD3	1.74	0.69
48:AA:205:LEU:HG	48:AA:212:PHE:HD1	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AB:291:GLU:N	49:AB:291:GLU:OE2	2.26	0.69
49:BB:450:LEU:CA	49:BB:453:HIS:CD2	2.76	0.69
1:A:56:ARG:HH12	4:D:11:PHE:HD1	1.41	0.69
14:N:281:PHE:CD1	14:N:290:LEU:HD11	2.28	0.69
24:X:41:LYS:HD2	34:i:83:LEU:HD12	1.74	0.69
5:E:181:ILE:HG12	5:E:201:VAL:HG11	1.75	0.69
7:G:576:GLU:HG3	7:G:593:LYS:HG2	1.74	0.69
4:D:292:ARG:NH2	4:D:307:GLU:CA	2.56	0.68
48:BA:150:THR:HG22	48:BA:163:ILE:CD1	2.24	0.68
13:M:279:PHE:CE1	38:m:71:LEU:HD21	2.25	0.68
52:BE:103:CYS:SG	67:BE:400:HEM:CAB	2.81	0.68
13:M:448:LYS:NZ	38:m:4:GLY:CA	2.57	0.68
2:B:209:ARG:NH1	16:P:104:ASP:OD2	2.26	0.68
29:c:56:ALA:HA	29:c:59:GLU:OE1	1.94	0.68
40:o:10:MET:N	40:o:29:MET:HE1	2.08	0.68
51:BD:153:ASP:O	51:BD:154:LEU:HD13	1.93	0.68
4:D:292:ARG:HB2	7:G:192:ARG:NH1	2.08	0.68
10:J:101:MET:HE1	14:N:192:PHE:CZ	2.23	0.68
13:M:411:ASN:HB3	13:M:414:VAL:HG12	1.74	0.68
32:f:6:THR:OG1	32:f:18:ARG:NH2	2.26	0.68
48:AA:372:THR:HG23	48:AA:374:ILE:HD13	1.74	0.68
48:AA:481:LEU:CD1	48:AA:483:MET:HG2	2.23	0.68
48:BA:300:ARG:HH21	48:BA:494:SER:HA	1.58	0.68
5:E:181:ILE:HG23	5:E:201:VAL:HG21	1.75	0.68
44:v:80:LYS:HD3	46:y:1:MET:H3	1.58	0.68
48:AA:434:ARG:HH21	48:AA:435:MET:HE2	1.57	0.68
9:I:139:THR:HB	9:I:154:ARG:HH12	1.59	0.67
27:a:44:GLU:H	27:a:44:GLU:CD	2.02	0.67
21:U:111:SER:HG	21:U:114:LEU:HD13	1.58	0.67
6:F:381:ASP:O	6:F:384:THR:HG22	1.95	0.67
13:M:76:PRO:CB	30:d:57:LYS:HZ1	2.07	0.67
52:AE:96:HIS:NE2	52:AE:130:MET:HE1	2.09	0.67
52:AE:273:LYS:HE2	56:AI:43:ASP:OD1	1.95	0.67
5:E:132:THR:HG23	5:E:134:PRO:HD2	1.77	0.67
13:M:334:SER:HA	13:M:403:ILE:HD11	1.76	0.67
13:M:344:VAL:HG22	13:M:467:LEU:HD21	1.76	0.67
51:BD:203:VAL:HG12	51:BD:209:LEU:HD13	1.75	0.67
1:A:56:ARG:NH1	4:D:11:PHE:N	2.38	0.67
33:g:102:GLU:OE1	33:g:106:LEU:HG	1.94	0.67
50:AC:6:GLN:NE2	53:BF:115:PRO:O	2.28	0.67
51:AD:237:HIS:CD2	50:BC:289:ARG:HG2	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:SER:O	4:D:78:GLN:OE1	2.12	0.67
41:p:14:ALA:HB1	41:p:33:MET:HE1	1.77	0.67
49:AB:518:ASP:OD2	50:AC:230:TYR:OH	2.13	0.67
29:c:32:HIS:CD2	29:c:35:ARG:HE	2.13	0.67
7:G:236:ASP:CA	7:G:254:LYS:HZ3	2.06	0.67
13:M:17:LEU:C	13:M:20:VAL:HG22	2.19	0.67
51:AD:248:ARG:HH11	51:AD:248:ARG:HG3	1.59	0.66
49:BB:110:THR:HG22	49:BB:283:ALA:HB3	1.76	0.66
51:BD:152:VAL:HG12	51:BD:153:ASP:N	2.09	0.66
25:Y:113:SER:OG	25:Y:116:THR:CB	2.43	0.66
29:c:32:HIS:HB3	29:c:35:ARG:NE	2.11	0.66
39:n:58:VAL:HG13	39:n:63:ARG:NH2	2.09	0.66
52:AE:273:LYS:NZ	56:AI:39:GLU:OE2	2.25	0.66
13:M:261:THR:OG1	13:M:338:MET:HE3	1.95	0.66
14:N:218:ILE:CD1	14:N:286:TYR:OH	2.43	0.66
28:b:9:MET:HG2	28:b:13:GLN:OE1	1.96	0.66
48:AA:289:ALA:O	48:AA:291:LYS:NZ	2.29	0.66
50:BC:221:GLU:HA	50:BC:224:LYS:HD2	1.77	0.66
6:F:334:TRP:O	6:F:352:LYS:NZ	2.28	0.66
51:AD:170:LYS:HD2	51:AD:212:VAL:HG11	1.78	0.66
48:BA:150:THR:CG2	48:BA:163:ILE:CD1	2.73	0.66
12:L:243:PRO:O	12:L:309:ARG:NH1	2.29	0.66
26:Z:112:MET:HE2	26:Z:118:TRP:CE2	2.30	0.66
48:BA:234:GLU:HA	48:BA:237:LEU:HD12	1.78	0.66
53:AF:56:ARG:HH22	54:AG:7:LYS:CE	2.09	0.65
48:BA:367:SER:N	48:BA:386:CYS:HG	1.95	0.65
13:M:304:LEU:HD23	13:M:432:LEU:HD11	1.78	0.65
48:BA:334:LEU:HD12	48:BA:419:ALA:HB1	1.78	0.65
9:I:154:ARG:HH22	17:Q:91:TRP:CD1	2.12	0.65
13:M:76:PRO:CB	30:d:57:LYS:NZ	2.60	0.65
47:z:223:ASN:HD22	47:z:226:GLU:HG2	1.59	0.65
53:BF:98:LEU:HG	53:BF:102:LYS:HE2	1.77	0.65
14:N:227:PHE:CD2	14:N:286:TYR:CZ	2.85	0.65
43:u:44:GLU:OE2	43:u:48:VAL:CG2	2.45	0.65
9:I:79:GLY:O	9:I:83:THR:OG1	2.15	0.65
31:e:1:MET:HB3	31:e:14:CYS:HB2	1.79	0.65
55:BH:35:ILE:HG22	55:BH:43:LYS:HD2	1.78	0.65
12:L:168:MET:HE3	13:M:430:LEU:HD11	1.78	0.65
39:n:58:VAL:CG1	39:n:63:ARG:HE	2.09	0.65
4:D:314:GLU:HG3	7:G:186:MET:HG3	1.78	0.64
21:U:108:LYS:O	21:U:114:LEU:HD23	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:43:GLU:OE1	22:V:43:GLU:HA	1.97	0.64
8:H:71:PHE:HE1	8:H:75:ARG:NH2	1.95	0.64
51:AD:237:HIS:HD2	50:BC:289:ARG:CG	2.10	0.64
52:BE:210:ARG:NH1	52:BE:211:GLU:O	2.30	0.64
13:M:60:ASP:OD2	34:i:22:ARG:NH2	2.30	0.64
48:BA:312:VAL:HG22	48:BA:481:LEU:HD21	1.79	0.64
13:M:487:ASN:ND2	41:p:34:ARG:HE	1.92	0.64
20:T:71:PHE:CE1	20:T:108:CYS:SG	2.89	0.64
48:AA:91:SER:OG	48:AA:267:HIS:ND1	2.22	0.64
48:AA:158:GLN:HE22	48:AA:443:ARG:HA	1.63	0.64
49:AB:355:LEU:HD23	49:AB:358:MET:HE2	1.79	0.64
48:BA:149:ASN:O	48:BA:163:ILE:HD12	1.97	0.64
48:BA:121:HIS:ND1	48:BA:198:MET:HE2	2.13	0.64
3:C:56:LEU:CD1	3:C:77:LEU:CD2	2.75	0.64
48:AA:269:GLU:HA	48:AA:272:LYS:CD	2.27	0.64
50:BC:72:GLU:HG2	52:BE:111:LEU:HD13	1.80	0.64
50:BC:269:MET:HE2	50:BC:269:MET:HA	1.79	0.64
49:BB:112:SER:OG	49:BB:287:VAL:O	2.13	0.64
4:D:311:HIS:HD2	7:G:186:MET:HE1	1.62	0.64
48:BA:240:LEU:HD23	48:BA:244:LEU:HD22	1.79	0.64
49:BB:134:ASP:OD1	49:BB:249:ARG:NH1	2.31	0.64
25:Y:9:LEU:HD23	25:Y:9:LEU:H	1.63	0.64
40:o:9:LYS:CA	40:o:29:MET:HE1	2.28	0.64
51:AD:248:ARG:HG3	51:AD:248:ARG:NH1	2.12	0.64
13:M:34:ILE:HD11	13:M:112:MET:HB3	1.81	0.63
13:M:64:ALA:HB3	41:p:35:GLU:OE2	1.97	0.63
14:N:436:GLY:HA2	14:N:439:TYR:CE2	2.33	0.63
23:W:18:ASN:OD1	23:W:20:THR:OG1	2.16	0.63
50:BC:26:TYR:HD2	68:BC:502:UQ5:H3M1	1.62	0.63
16:P:353:VAL:HG11	16:P:359:LYS:HG2	1.79	0.63
48:AA:269:GLU:HG3	48:AA:272:LYS:HZ3	1.63	0.63
55:AH:39:ASP:O	55:AH:42:HIS:CE1	2.51	0.63
48:BA:122:LEU:HG	48:BA:245:LEU:HD11	1.80	0.63
51:BD:150:LEU:HD12	51:BD:151:GLU:H	1.64	0.63
9:I:78:ARG:NH1	26:Z:42:THR:O	2.31	0.63
20:T:50:VAL:HG11	20:T:112:ILE:HG12	1.79	0.63
29:c:16:ARG:NH1	39:n:101:PRO:HG3	2.13	0.63
13:M:146:PHE:CE2	13:M:227:LYS:HE2	2.33	0.63
20:T:71:PHE:HE1	20:T:108:CYS:SG	2.20	0.63
48:BA:334:LEU:HD12	48:BA:419:ALA:CB	2.29	0.63
7:G:350:ARG:NH2	7:G:612:TYR:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:LEU:HD13	14:N:150:LEU:HD11	1.81	0.63
13:M:279:PHE:HE1	38:m:71:LEU:HD23	1.39	0.63
48:AA:481:LEU:HD21	48:AA:499:SER:HA	1.81	0.63
5:E:128:LEU:HB2	5:E:182:THR:HB	1.81	0.63
29:c:42:PHE:O	29:c:46:LEU:HD23	1.98	0.63
48:AA:269:GLU:HG3	48:AA:272:LYS:CE	2.29	0.63
49:BB:325:GLU:HB2	49:BB:507:ILE:HB	1.80	0.63
50:BC:145:MET:HE1	50:BC:275:ILE:HA	1.81	0.63
3:C:139:GLU:HG3	23:W:102:GLN:NE2	2.13	0.63
13:M:150:LEU:HD11	13:M:177:THR:HG21	1.81	0.63
19:S:88:ASN:O	19:S:92:SER:OG	2.16	0.62
52:AE:227:PRO:HG2	52:AE:229:MET:SD	2.39	0.62
19:S:10:SER:HB2	19:S:94:ALA:HB1	1.80	0.62
10:J:101:MET:HE2	11:K:11:MET:HE1	1.82	0.62
51:BD:205:ASN:HD22	51:BD:208:TRP:HD1	1.47	0.62
8:H:324:LEU:O	26:Z:72:ARG:NH2	2.32	0.62
48:AA:139:LEU:HA	48:AA:142:GLU:OE2	1.99	0.62
48:AA:269:GLU:HA	48:AA:272:LYS:CG	2.30	0.62
10:J:133:SER:OG	27:a:44:GLU:OE1	2.04	0.62
40:o:9:LYS:C	40:o:29:MET:CE	2.72	0.62
14:N:210:ALA:O	14:N:214:THR:HG23	1.99	0.62
15:O:48:LEU:HD23	15:O:60:ILE:HD11	1.82	0.62
52:AE:99:TYR:HA	52:AE:103:CYS:SG	2.40	0.62
2:B:88:THR:HG22	2:B:98:MET:HE3	1.82	0.62
4:D:299:ARG:NH2	9:I:175:ASP:OD2	2.33	0.62
7:G:674:GLU:OE2	7:G:674:GLU:N	2.23	0.62
67:BE:400:HEM:HMC1	67:BE:400:HEM:HBC2	1.81	0.62
18:R:52:SER:OG	18:R:55:GLU:HG3	1.99	0.62
6:F:425:GLY:C	6:F:476:ARG:HD3	2.25	0.62
23:W:41:MET:HA	23:W:46:LEU:HD12	1.82	0.62
8:H:126:ARG:HG2	8:H:126:ARG:NH1	2.13	0.61
8:H:185:PRO:O	8:H:189:MET:HG3	1.99	0.61
12:L:544:ARG:HH22	39:n:43:ARG:NE	1.98	0.61
1:A:16:LEU:HD13	8:H:83:MET:CE	2.26	0.61
13:M:448:LYS:HZ1	38:m:4:GLY:CA	2.14	0.61
29:c:42:PHE:CE1	29:c:46:LEU:HD21	2.35	0.61
49:AB:288:LYS:HG3	49:AB:291:GLU:OE2	2.00	0.61
6:F:90:ASP:OD2	6:F:91:LEU:HD22	2.00	0.61
52:BE:73:CYS:SG	52:BE:188:ASN:ND2	2.74	0.61
29:c:32:HIS:HB3	29:c:35:ARG:HE	1.64	0.61
43:u:44:GLU:OE1	55:AH:26:LEU:CD1	2.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:101:ILE:HD11	48:AA:170:VAL:HG13	1.81	0.61
48:AA:269:GLU:C	48:AA:272:LYS:HG2	2.25	0.61
51:AD:238:GLY:HA3	50:BC:350:VAL:HG11	1.83	0.61
56:AI:44:TYR:O	56:AI:48:LYS:HG2	1.99	0.61
5:E:212:LYS:HE2	5:E:219:PRO:HA	1.83	0.61
48:AA:78:LEU:HD22	48:AA:451:ARG:HD3	1.81	0.61
2:B:69:ILE:HD12	2:B:212:PHE:HD2	1.64	0.61
12:L:15:VAL:HB	12:L:31:MET:HE2	1.80	0.61
14:N:227:PHE:HD2	14:N:286:TYR:CZ	2.19	0.61
18:R:96:ILE:HG13	18:R:103:ARG:HG2	1.81	0.61
49:AB:310:THR:HA	49:AB:313:LEU:HD12	1.81	0.61
1:A:56:ARG:NH1	4:D:11:PHE:HD1	1.95	0.61
10:J:101:MET:HE2	11:K:11:MET:SD	2.40	0.61
48:AA:103:LEU:HD13	48:AA:181:VAL:HG21	1.82	0.61
49:BB:505:ILE:CD1	49:BB:507:ILE:HG13	2.31	0.61
68:BC:502:UQ5:H4M2	68:BC:502:UQ5:H3M3	1.82	0.61
51:BD:96:HIS:HB3	53:BF:77:GLU:OE2	2.01	0.61
4:D:292:ARG:O	4:D:292:ARG:HG2	2.01	0.61
12:L:262:VAL:HG22	12:L:319:LEU:HD11	1.83	0.61
23:W:17:ALA:N	23:W:21:GLU:OE1	2.30	0.61
49:BB:222:MET:HG2	49:BB:252:LEU:HD23	1.83	0.61
25:Y:101:VAL:O	25:Y:105:SER:OG	2.16	0.61
27:a:18:MET:O	27:a:22:MET:HG3	2.00	0.61
48:BA:163:ILE:HG21	48:BA:173:MET:HB3	1.81	0.61
5:E:201:VAL:HA	5:E:205:LYS:HD2	1.83	0.60
6:F:334:TRP:NE1	6:F:356:GLU:OE2	2.34	0.60
25:Y:10:GLU:O	25:Y:11:GLU:CG	2.49	0.60
26:Z:102:LYS:O	26:Z:106:GLU:HG3	2.01	0.60
28:b:9:MET:CG	28:b:13:GLN:OE1	2.49	0.60
50:AC:267:ASN:OD1	50:AC:270:SER:OG	2.19	0.60
51:BD:174:ILE:HD11	51:BD:208:TRP:HE3	1.66	0.60
12:L:392:PHE:CE2	35:j:39:ILE:HD13	2.36	0.60
13:M:385:THR:O	13:M:389:MET:HG3	2.01	0.60
56:AI:52:ARG:HH11	56:AI:52:ARG:HG3	1.65	0.60
48:AA:420:LYS:HG2	48:AA:461:VAL:HG12	1.83	0.60
22:V:56:ALA:HB2	22:V:149:LEU:HD11	1.83	0.60
44:v:80:LYS:HD3	46:y:1:MET:N	2.17	0.60
48:AA:383:ILE:HD11	48:AA:399:ALA:HB1	1.84	0.60
54:AG:4:GLN:NE2	54:AG:5:PRO:O	2.33	0.60
8:H:267:ILE:HD13	27:a:20:CYS:SG	2.41	0.60
10:J:101:MET:HE2	11:K:11:MET:CE	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:105:LEU:HB3	10:J:109:SER:OG	2.01	0.60
6:F:425:GLY:O	6:F:476:ARG:HD3	2.01	0.60
67:AC:500:HEM:HMC2	67:AC:500:HEM:HBC2	1.84	0.60
4:D:292:ARG:HH12	7:G:193:GLY:H	1.48	0.60
28:b:5:GLU:OE1	28:b:8:ARG:HD2	2.02	0.60
49:AB:207:GLU:HB2	49:AB:210:ARG:HG3	1.84	0.60
54:AG:65:GLN:O	54:AG:69:GLU:HG2	2.02	0.60
25:Y:122:ALA:O	25:Y:126:VAL:HG23	2.01	0.60
34:i:21:GLU:OE2	34:i:24:ARG:NE	2.20	0.60
7:G:350:ARG:NH2	7:G:614:ALA:O	2.35	0.60
14:N:292:GLN:O	14:N:296:PHE:CD2	2.54	0.60
23:W:121:THR:HG23	23:W:123:PHE:H	1.65	0.60
25:Y:91:ASP:H	25:Y:94:ASN:ND2	2.00	0.60
48:AA:269:GLU:HG2	48:AA:272:LYS:HZ1	1.62	0.60
48:AA:156:ARG:HH22	48:AA:215:GLU:HG2	1.66	0.60
48:BA:310:PHE:HE1	48:BA:483:MET:SD	2.24	0.60
10:J:100:GLU:CD	14:N:228:MET:HE1	2.27	0.59
3:C:17:LYS:HE2	3:C:37:TYR:OH	2.02	0.59
19:S:6:SER:HB3	19:S:9:LYS:HE3	1.84	0.59
41:p:7:LEU:HG	41:p:8:PRO:HD2	1.84	0.59
51:AD:237:HIS:HA	50:BC:289:ARG:HD3	1.85	0.59
53:AF:41:PRO:HB3	53:AF:48:LYS:HB2	1.85	0.59
3:C:56:LEU:CD1	3:C:77:LEU:HD23	2.33	0.59
7:G:658:ARG:NH2	7:G:671:ASN:OD1	2.27	0.59
49:AB:355:LEU:HD23	49:AB:358:MET:CE	2.33	0.59
51:BD:167:TRP:CG	51:BD:168:ARG:H	2.20	0.59
8:H:75:ARG:HG2	8:H:75:ARG:HH11	1.68	0.59
13:M:308:ILE:HD13	13:M:348:LEU:HB3	1.84	0.59
46:y:203:SER:HA	66:y:301:COO:H103	1.85	0.59
48:AA:415:HIS:HD2	48:AA:418:ARG:HH21	1.49	0.59
49:BB:501:TYR:CD2	56:BI:22:ARG:NH1	2.56	0.59
51:BD:202:ARG:NH1	51:BD:244:SER:O	2.34	0.59
12:L:384:ILE:HD13	35:j:31:LEU:CD2	1.90	0.59
14:N:326:HIS:HA	14:N:329:TYR:HD1	1.67	0.59
55:BH:10:LYS:HG3	55:BH:64:LEU:HD22	1.85	0.59
1:A:16:LEU:CA	8:H:83:MET:HE3	2.32	0.59
7:G:383:VAL:HG11	7:G:589:VAL:HG21	1.85	0.59
46:y:133:VAL:HG11	47:z:147:MET:CE	2.33	0.59
49:AB:97:THR:HB	49:AB:111:GLU:OE2	2.03	0.59
52:BE:106:CYS:SG	67:BE:400:HEM:C2C	2.96	0.59
7:G:422:ARG:NH1	7:G:564:ASP:OD2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:113:SER:OG	25:Y:116:THR:HB	2.02	0.59
29:c:13:GLY:HA3	39:n:101:PRO:HG2	1.85	0.59
49:AB:275:THR:HG21	49:AB:306:ASP:HB3	1.83	0.59
50:AC:50:ILE:HA	67:AC:501:HEM:HAB	1.85	0.59
54:AG:61:TYR:O	54:AG:65:GLN:HG2	2.03	0.58
67:BC:500:HEM:HMC2	67:BC:500:HEM:HBC2	1.85	0.58
51:BD:174:ILE:HD13	51:BD:210:VAL:HG22	1.84	0.58
48:AA:126:MET:HE3	48:AA:129:LYS:HG3	1.84	0.58
48:AA:269:GLU:CG	48:AA:272:LYS:HZ3	2.14	0.58
49:AB:337:GLN:HG2	49:AB:410:VAL:HG22	1.86	0.58
48:BA:139:LEU:HD11	48:BA:176:VAL:HG13	1.85	0.58
19:S:64:TYR:HB2	19:S:68:VAL:HG13	1.85	0.58
48:AA:269:GLU:CA	48:AA:272:LYS:HG2	2.33	0.58
48:AA:269:GLU:HG3	48:AA:272:LYS:NZ	2.14	0.58
13:M:144:VAL:HG13	14:N:402:PRO:HB2	1.83	0.58
24:X:37:LEU:HD13	34:i:82:LEU:HB3	1.84	0.58
25:Y:13:ASP:HA	25:Y:18:LYS:HE2	1.86	0.58
45:x:227:LEU:HD23	47:z:110:LYS:HG2	1.84	0.58
56:BI:17:TYR:CZ	56:BI:21:MET:HE1	2.38	0.58
1:A:117:ASP:OD2	8:H:301:LYS:NZ	2.36	0.58
7:G:521:PHE:O	7:G:526:LYS:HD3	2.03	0.58
25:Y:90:ARG:HA	25:Y:94:ASN:ND2	2.17	0.58
41:p:34:ARG:NH2	41:p:35:GLU:OE1	2.35	0.58
13:M:410:ARG:HB3	13:M:410:ARG:NH1	2.19	0.58
40:o:79:GLU:OE1	40:o:79:GLU:N	2.36	0.58
48:BA:210:MET:SD	48:BA:367:SER:OG	2.55	0.58
50:BC:50:ILE:HA	67:BC:501:HEM:HAB	1.85	0.58
14:N:412[A]:TYR:CZ	14:N:416:ALA:HB2	2.38	0.58
15:O:126:ILE:HG21	21:U:41:ARG:CG	2.33	0.58
13:M:448:LYS:HD2	38:m:5:MET:HG2	1.84	0.58
40:o:49:TRP:CD1	40:o:50:LYS:HZ2	2.21	0.58
47:z:150:THR:HB	47:z:168:LEU:HD22	1.86	0.58
48:BA:52:ALA:HB3	48:BA:60:LEU:HD11	1.86	0.58
12:L:594:ILE:HG22	13:M:235:ILE:HD13	1.86	0.57
34:i:77:ASP:OD1	34:i:78:PRO:HD2	2.04	0.57
50:AC:186:PHE:HE2	50:BC:186:PHE:HE2	1.51	0.57
13:M:305:LYS:HG3	13:M:352:VAL:HG11	1.86	0.57
20:T:84:GLU:OE1	39:n:49:ARG:NH1	2.37	0.57
48:AA:300:ARG:NH2	48:AA:493:PRO:O	2.37	0.57
48:BA:198:MET:SD	48:BA:237:LEU:CD2	2.92	0.57
7:G:510:LYS:HD2	7:G:510:LYS:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:MET:SD	5:E:140:SER:OG	2.58	0.57
29:c:34:ARG:HH22	33:g:34:THR:C	2.12	0.57
42:q:64:LYS:HB2	42:q:73:HIS:HB3	1.86	0.57
39:n:58:VAL:HG13	39:n:63:ARG:HE	1.69	0.57
2:B:88:THR:CG2	2:B:98:MET:HE3	2.34	0.57
10:J:108:GLU:O	31:e:48:SER:OG	2.22	0.57
31:e:56:ARG:NE	43:u:33:ASP:OD1	2.38	0.57
43:u:44:GLU:OE2	43:u:48:VAL:HG21	2.04	0.57
46:y:133:VAL:CG1	47:z:147:MET:HE1	2.35	0.57
52:AE:229:MET:HA	52:AE:229:MET:HE3	1.86	0.57
4:D:17:PRO:HB3	4:D:22:ALA:HB3	1.86	0.57
4:D:311:HIS:CD2	7:G:186:MET:HE1	2.40	0.57
14:N:269:PRO:O	14:N:273:ILE:HG22	2.05	0.57
49:AB:110:THR:OG1	49:AB:289:HIS:ND1	2.35	0.57
52:BE:198:THR:OG1	55:BH:10:LYS:NZ	2.35	0.57
12:L:648:TRP:HA	25:Y:21:LYS:HD3	1.86	0.56
50:AC:285:TYR:OH	51:BD:236:CYS:O	2.18	0.56
7:G:264:VAL:HA	7:G:267:ILE:HG12	1.87	0.56
10:J:100:GLU:CG	14:N:228:MET:HE1	2.34	0.56
10:J:162:ALA:HA	11:K:75:ILE:HD11	1.86	0.56
20:T:53:VAL:HG11	20:T:89:ILE:HG13	1.87	0.56
52:AE:225:ALA:HB3	67:AE:400:HEM:HBD2	1.87	0.56
52:BE:87:TYR:HB3	52:BE:92:ILE:HD11	1.86	0.56
14:N:201:THR:HB	14:N:212:ILE:HD13	1.87	0.56
52:BE:204:PRO:HG2	52:BE:207:ILE:HG13	1.87	0.56
10:J:57:TYR:CE1	11:K:66:LEU:HD11	2.40	0.56
12:L:430:THR:HA	12:L:433:TYR:CE2	2.41	0.56
13:M:265:LEU:HG	13:M:323:MET:HE2	1.88	0.56
16:P:249:GLY:HA2	16:P:290:THR:HB	1.86	0.56
48:AA:78:LEU:CD2	48:AA:451:ARG:CD	2.84	0.56
49:BB:288:LYS:HB2	49:BB:291:GLU:HG3	1.87	0.56
13:M:113:ARG:NH1	47:z:113:LEU:HD23	2.21	0.56
49:AB:220:ARG:HD3	49:AB:224:GLU:OE1	2.02	0.56
7:G:302:ASN:ND2	7:G:320:ASN:CG	2.64	0.56
48:AA:269:GLU:HA	48:AA:272:LYS:HE2	1.86	0.56
7:G:576:GLU:OE1	7:G:593:LYS:CD	2.37	0.56
13:M:316:MET:HE2	13:M:316:MET:HA	1.86	0.56
20:T:81:ASP:HA	20:T:84:GLU:OE2	2.05	0.56
50:AC:317:MET:HG3	50:AC:319:VAL:H	1.71	0.56
48:BA:300:ARG:NH2	48:BA:493:PRO:O	2.24	0.56
51:BD:152:VAL:CG1	51:BD:153:ASP:N	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BD:202:ARG:NH2	51:BD:256:LEU:O	2.38	0.56
67:BE:400:HEM:HBB2	67:BE:400:HEM:HMB1	1.86	0.56
4:D:64:LEU:HD23	4:D:82:TYR:HD2	1.71	0.56
12:L:611:GLU:OE2	15:O:112:TYR:OH	2.20	0.56
52:BE:103:CYS:HG	67:BE:400:HEM:CAB	2.19	0.56
7:G:466:ASN:OD1	7:G:466:ASN:O	2.24	0.55
12:L:586:PHE:CE2	38:m:20:ARG:HD2	2.41	0.55
10:J:111:PRO:HG2	43:u:29:ALA:HB2	1.88	0.55
49:BB:157:ARG:O	49:BB:161:GLU:HG3	2.06	0.55
51:AD:247:ILE:HD13	51:AD:252:ALA:O	2.06	0.55
55:AH:24:PRO:HB2	55:AH:52:TYR:HA	1.89	0.55
2:B:65:ALA:O	2:B:69:ILE:HG12	2.05	0.55
48:AA:415:HIS:CD2	48:AA:418:ARG:HH21	2.24	0.55
49:AB:125:ILE:HG23	49:AB:279:MET:HG2	1.87	0.55
4:D:379:VAL:HG11	8:H:211:GLU:HG3	1.89	0.55
7:G:236:ASP:HB2	7:G:254:LYS:HZ2	1.67	0.55
49:BB:450:LEU:O	49:BB:453:HIS:NE2	2.40	0.55
1:A:4:GLU:OE2	8:H:102:ASP:HB3	2.06	0.55
13:M:76:PRO:HG2	30:d:57:LYS:NZ	2.22	0.55
40:o:17:MET:HA	40:o:22:ILE:HD12	1.89	0.55
49:BB:268:ASN:O	49:BB:272:THR:HG22	2.06	0.55
50:BC:197:VAL:HG22	68:BC:502:UQ5:H202	1.89	0.55
51:BD:162:THR:OG1	51:BD:174:ILE:O	2.14	0.55
51:BD:242:ASP:OD1	51:BD:246:ARG:N	2.35	0.55
13:M:448:LYS:HE3	38:m:4:GLY:O	2.06	0.55
15:O:52:ASP:HB2	15:O:53:PRO:HD2	1.88	0.55
16:P:376:GLU:HG2	16:P:379:ILE:HD12	1.88	0.55
29:c:42:PHE:CZ	29:c:46:LEU:HD21	2.42	0.55
51:AD:170:LYS:HG2	51:AD:212:VAL:HG11	1.70	0.55
51:AD:264:LEU:HD12	51:AD:268:LYS:HG2	1.88	0.55
55:AH:13:LEU:HD22	55:AH:63:LYS:CD	2.37	0.55
3:C:128:ASP:OD2	3:C:130:ARG:NH1	2.39	0.55
8:H:257:LEU:HB2	8:H:260:PHE:HD2	1.72	0.55
14:N:206:PHE:HB3	14:N:283:TYR:HE2	1.72	0.55
50:BC:139:VAL:HA	50:BC:146:SER:HB3	1.87	0.55
53:BF:57:GLU:H	53:BF:57:GLU:CD	2.15	0.55
47:z:34:TYR:H	47:z:34:TYR:HD2	1.54	0.55
47:z:88:ASP:OD1	47:z:89:VAL:HG23	2.06	0.55
47:z:100:ILE:HD13	47:z:128:ILE:HG13	1.89	0.55
49:AB:85:LEU:HD21	49:AB:485:ASP:HB2	1.89	0.55
51:AD:174:ILE:HG12	51:AD:210:VAL:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:ASP:HB3	4:D:78:GLN:HE21	1.67	0.55
13:M:148:SER:OG	14:N:403:PRO:HD3	2.06	0.55
13:M:190:LEU:HA	13:M:193:PHE:HD2	1.72	0.55
47:z:233:LYS:HD3	47:z:234:LYS:N	2.21	0.55
48:AA:169:TYR:O	48:AA:173:MET:HG3	2.06	0.55
48:BA:459:LYS:HB3	48:BA:459:LYS:HZ2	1.72	0.55
2:B:87:MET:CG	4:D:19:HIS:CE1	2.89	0.54
49:AB:361:MET:HE1	49:AB:434:VAL:HG13	1.89	0.54
48:BA:198:MET:SD	48:BA:237:LEU:HD22	2.47	0.54
7:G:704:PRO:CA	19:S:37:LYS:HE3	2.18	0.54
12:L:384:ILE:HD12	35:j:31:LEU:HD22	1.82	0.54
16:P:302:ARG:CZ	16:P:382:ARG:NH1	2.69	0.54
39:n:26:ARG:HD2	39:n:75:TYR:CZ	2.42	0.54
47:z:212:GLN:OE1	47:z:212:GLN:HA	2.05	0.54
49:AB:146:MET:HE1	49:AB:214:GLU:HB2	1.89	0.54
7:G:75:GLU:OE2	7:G:82:ALA:HB1	2.07	0.54
49:BB:294:GLU:O	49:BB:298:LYS:HG3	2.07	0.54
25:Y:47:GLU:OE1	25:Y:57:ARG:NH1	2.41	0.54
51:AD:168:ARG:HD2	50:BC:175:PHE:CE1	2.42	0.54
53:AF:44:ASP:OD2	53:AF:46:ASP:HB2	2.07	0.54
51:BD:218:LEU:HD12	51:BD:237:HIS:CE1	2.41	0.54
5:E:179:PRO:O	5:E:201:VAL:HG22	2.08	0.54
10:J:37:THR:HG23	11:K:44:LEU:HD21	1.88	0.54
14:N:110:MET:HE3	14:N:364:LEU:HD12	1.89	0.54
26:Z:85:ILE:HD12	26:Z:89:LEU:HD11	1.90	0.54
47:z:96:SER:N	47:z:124:ASP:OD2	2.40	0.54
50:AC:318:TYR:OH	50:AC:380:ARG:NH1	2.40	0.54
13:M:322:GLY:HA3	13:M:403:ILE:HG12	1.89	0.54
25:Y:91:ASP:H	25:Y:94:ASN:HD21	1.55	0.54
32:f:45:VAL:HG13	32:f:62:MET:HG2	1.90	0.54
55:AH:13:LEU:HD22	55:AH:63:LYS:HD2	1.90	0.54
48:BA:306:GLU:HA	48:BA:389:PRO:HG3	1.88	0.54
52:BE:78:TRP:NE1	52:BE:191:ASN:OD1	2.34	0.54
6:F:424:VAL:O	6:F:476:ARG:HD2	2.08	0.54
16:P:237:VAL:HG21	16:P:297:MET:HE1	1.90	0.54
24:X:23:LYS:O	24:X:27:MET:HG2	2.06	0.54
39:n:68:ILE:O	39:n:72:GLU:HG3	2.08	0.54
40:o:70:MET:O	40:o:74:LYS:HG3	2.08	0.54
12:L:392:PHE:HE2	35:j:39:ILE:HD13	1.71	0.54
37:l:120:GLU:HG2	40:o:27:ARG:HH11	1.73	0.54
40:o:10:MET:HE3	40:o:11:ILE:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:300:ARG:HH22	48:AA:494:SER:HA	1.73	0.54
49:BB:177:GLU:OE1	49:BB:400:LYS:HG3	2.07	0.54
6:F:348:PRO:HG3	6:F:456:TRP:HB3	1.90	0.54
13:M:193:PHE:CE1	14:N:415:PHE:CE1	2.96	0.54
13:M:470:MET:HG3	13:M:477:PHE:CE2	2.43	0.54
34:i:28:GLU:O	34:i:32:GLU:HG2	2.07	0.54
39:n:73:ALA:O	39:n:77:LYS:HG3	2.07	0.54
51:AD:264:LEU:HD12	51:AD:268:LYS:CD	2.37	0.54
5:E:143:ILE:HG23	5:E:206:VAL:HG11	1.90	0.54
12:L:533:TYR:O	12:L:537:LEU:HB2	2.07	0.54
17:Q:111:GLU:H	17:Q:111:GLU:CD	2.13	0.54
23:W:51:ALA:HB3	23:W:54:GLN:HG3	1.88	0.54
46:y:203:SER:HB3	66:y:301:COO:H8	1.90	0.54
48:AA:404:LYS:HE2	48:AA:502:PHE:HA	1.90	0.54
51:AD:233:PHE:HE1	51:AD:238:GLY:HA2	1.73	0.54
54:AG:36:HIS:O	54:AG:40:GLU:HG3	2.08	0.54
48:BA:169:TYR:O	48:BA:173:MET:HG3	2.07	0.54
48:BA:335:MET:HE2	48:BA:406:VAL:HG21	1.90	0.54
52:BE:93:ARG:HB2	52:BE:121:ALA:HB1	1.90	0.54
7:G:674:GLU:CD	7:G:674:GLU:N	2.66	0.53
48:AA:155:SER:OG	48:AA:156:ARG:N	2.41	0.53
50:AC:153:ILE:HD11	68:AC:503:UQ5:C1	2.38	0.53
49:BB:458:SER:O	49:BB:462:GLU:HG3	2.08	0.53
50:BC:142:TRP:HH2	50:BC:177:VAL:HG12	1.73	0.53
14:N:369:THR:O	14:N:369:THR:HG22	2.09	0.53
22:V:100:ILE:O	22:V:104:ILE:HG12	2.08	0.53
37:l:124:GLU:HG3	41:p:71:ARG:NH2	2.23	0.53
48:AA:333:MET:HE2	48:AA:333:MET:HA	1.90	0.53
51:BD:157:ILE:HG13	51:BD:158:GLU:H	1.73	0.53
3:C:17:LYS:CE	3:C:37:TYR:CZ	2.88	0.53
7:G:236:ASP:CA	7:G:254:LYS:NZ	2.70	0.53
24:X:19:THR:HG21	24:X:87:ASN:HB3	1.90	0.53
33:g:102:GLU:OE1	33:g:106:LEU:CD1	2.56	0.53
4:D:93:GLU:H	4:D:93:GLU:CD	2.16	0.53
13:M:76:PRO:CG	30:d:57:LYS:HZ1	2.21	0.53
20:T:80:LEU:O	20:T:84:GLU:OE2	2.25	0.53
48:AA:78:LEU:HD23	48:AA:451:ARG:HD3	1.89	0.53
67:AE:400:HEM:HBB2	67:AE:400:HEM:HMB1	1.89	0.53
53:AF:119:ARG:O	50:BC:7:ARG:NH1	2.34	0.53
68:BC:502:UQ5:H251	68:BC:502:UQ5:H313	1.90	0.53
4:D:28:LEU:HD11	4:D:382:ILE:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:407:PRO:HG2	6:F:446:THR:HG22	1.90	0.53
13:M:425:GLY:HA2	13:M:428:TYR:CE2	2.44	0.53
39:n:26:ARG:HD2	39:n:75:TYR:OH	2.08	0.53
50:AC:227:PHE:CD2	68:AC:502:UQ5:H3M2	2.43	0.53
48:BA:470:ALA:O	48:BA:474:SER:OG	2.23	0.53
46:y:153:ASP:O	46:y:171:GLN:HG2	2.09	0.53
48:AA:406:VAL:HG22	48:AA:473:THR:HG21	1.90	0.53
50:BC:271:THR:HG23	50:BC:275:ILE:HD11	1.91	0.53
6:F:143:SER:HA	6:F:182:ARG:NH1	2.24	0.53
8:H:313:SER:HA	28:b:27:GLY:HA3	1.91	0.53
12:L:387:LEU:HD12	35:j:35:MET:HE1	1.89	0.53
47:z:194:ASP:OD1	47:z:194:ASP:N	2.41	0.53
52:AE:218:TYR:OH	55:AH:57:ASP:OD2	2.23	0.53
8:H:230:LEU:HD11	61:H:500:UQ9:H10	1.91	0.53
17:Q:129:LYS:HG2	17:Q:130:PRO:HD2	1.91	0.53
48:AA:483:MET:HE3	48:AA:484:GLY:H	1.73	0.53
4:D:17:PRO:CB	4:D:22:ALA:HB3	2.38	0.53
14:N:290:LEU:HD21	14:N:334:PHE:HZ	1.73	0.53
17:Q:62:THR:HG22	17:Q:64:THR:H	1.74	0.53
49:AB:132:GLU:O	49:AB:249:ARG:NH2	2.42	0.53
56:AI:16:PHE:CZ	56:AI:20:ILE:HD12	2.44	0.53
25:Y:77:ILE:O	25:Y:81:GLN:HG2	2.08	0.53
29:c:32:HIS:CB	29:c:35:ARG:HE	2.21	0.53
51:AD:175:ARG:HE	51:AD:177:ARG:HG3	1.72	0.53
12:L:347:LEU:HD11	12:L:381:MET:HB3	1.91	0.52
13:M:193:PHE:CZ	14:N:415:PHE:CE1	2.97	0.52
19:S:13:GLU:OE1	19:S:63:ARG:NH2	2.31	0.52
24:X:32:GLU:CG	24:X:59:CYS:SG	2.97	0.52
45:x:231:TYR:HE2	47:z:68:ILE:HG21	1.74	0.52
51:AD:161:THR:O	51:AD:175:ARG:HG2	2.09	0.52
53:AF:15:PHE:O	53:AF:19:MET:HG3	2.07	0.52
53:AF:58:ILE:HD12	49:BB:58:ALA:HB2	1.92	0.52
48:BA:428:LEU:HD22	49:BB:117:LYS:HD2	1.90	0.52
51:BD:101:TYR:CZ	54:BG:21:LYS:HG2	2.44	0.52
6:F:290:ARG:NH1	6:F:359:LEU:HD12	2.24	0.52
11:K:43:ASN:OD1	11:K:62:ALA:HB1	2.10	0.52
12:L:586:PHE:HE2	38:m:20:ARG:HD2	1.73	0.52
45:x:79:ALA:HB3	45:x:82:VAL:HG23	1.90	0.52
50:AC:383:PRO:HG3	53:AF:35:TYR:CE2	2.44	0.52
2:B:69:ILE:HD12	2:B:212:PHE:CE2	2.44	0.52
8:H:26:ALA:HB2	27:a:11:PRO:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:495:LEU:HB3	30:d:63:MET:HE2	1.90	0.52
19:S:31:PHE:CE1	19:S:35:ASN:OD1	2.62	0.52
52:AE:99:TYR:CD1	52:AE:103:CYS:HB2	2.44	0.52
50:BC:283:PRO:O	50:BC:287:ILE:HG13	2.09	0.52
4:D:15:PHE:HB3	8:H:212:LEU:HD22	1.92	0.52
5:E:136:MET:HE1	5:E:141:ARG:HB2	1.90	0.52
7:G:266:ASP:OD2	7:G:333:ARG:NH2	2.39	0.52
16:P:76:ALA:HB3	16:P:97:VAL:HG13	1.90	0.52
47:z:223:ASN:ND2	47:z:226:GLU:HG2	2.24	0.52
49:AB:110:THR:HG22	49:AB:283:ALA:HB3	1.90	0.52
51:AD:176:ARG:HE	51:AD:207:GLU:CD	2.17	0.52
6:F:293:ASN:ND2	6:F:363:ASP:OD2	2.34	0.52
6:F:309:CYS:SG	6:F:311:VAL:CG1	2.96	0.52
9:I:139:THR:HG22	9:I:154:ARG:HH11	1.70	0.52
14:N:292:GLN:HB3	14:N:296:PHE:HE2	1.74	0.52
2:B:108:LEU:HD22	2:B:113:ILE:HD13	1.92	0.52
14:N:167:ARG:HG2	46:y:241:ASP:OD2	2.10	0.52
50:AC:318:TYR:CD2	53:AF:47:ILE:HD11	2.45	0.52
52:BE:130:MET:HE2	56:BI:68:ARG:HD2	1.91	0.52
10:J:140:LEU:HD21	11:K:63:LEU:HD22	1.92	0.52
45:x:158:PRO:O	45:x:176:THR:OG1	2.24	0.52
48:AA:483:MET:HE3	48:AA:484:GLY:N	2.25	0.52
12:L:355:VAL:HG22	12:L:378:THR:HG21	1.92	0.52
50:AC:152:VAL:HG21	68:AC:503:UQ5:O3	2.10	0.52
48:BA:266:GLU:OE2	48:BA:269:GLU:HB2	2.10	0.52
51:BD:121:PHE:HE1	56:BI:31:ILE:HA	1.75	0.52
7:G:304:ARG:NH2	7:G:316:ILE:CD1	2.72	0.52
13:M:189:LEU:C	13:M:193:PHE:CD2	2.81	0.52
36:k:16:ASP:OD1	36:k:19:ARG:NE	2.36	0.52
48:AA:254:THR:HG21	48:AA:284:VAL:HB	1.90	0.52
4:D:23:HIS:NE2	4:D:387:ILE:HB	2.25	0.51
4:D:245:LEU:HD13	4:D:274:ILE:HG23	1.91	0.51
6:F:90:ASP:OD2	6:F:91:LEU:N	2.42	0.51
11:K:54:ASP:O	31:e:1:MET:SD	2.67	0.51
17:Q:73:LYS:NZ	17:Q:109:ASP:OD2	2.43	0.51
50:AC:316:SER:HG	53:AF:43:TYR:HH	1.58	0.51
56:AI:52:ARG:HG3	56:AI:52:ARG:NH1	2.25	0.51
5:E:212:LYS:HE3	5:E:217:GLU:HB2	1.93	0.51
29:c:32:HIS:CG	29:c:35:ARG:HE	2.28	0.51
51:AD:217:HIS:HD2	50:BC:294:LYS:HB2	1.75	0.51
6:F:357:ASP:OD2	6:F:357:ASP:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:PRO:HB2	30:d:57:LYS:HZ3	1.74	0.51
13:M:442:LYS:HB3	37:l:40:HIS:CE1	2.45	0.51
14:N:139:MET:HG3	14:N:151:ALA:HB1	1.91	0.51
25:Y:79:VAL:HG11	25:Y:101:VAL:HG11	1.91	0.51
49:AB:306:ASP:OD1	49:AB:308:THR:OG1	2.22	0.51
49:BB:450:LEU:C	49:BB:453:HIS:NE2	2.69	0.51
49:BB:505:ILE:HD12	49:BB:507:ILE:HG13	1.92	0.51
50:BC:289:ARG:NH2	50:BC:348:GLN:O	2.38	0.51
50:BC:331:MET:HE1	50:BC:368:PHE:CD1	2.46	0.51
14:N:495:LEU:CB	30:d:63:MET:HE2	2.40	0.51
16:P:201:ALA:HA	16:P:204:GLU:HG3	1.91	0.51
49:BB:453:HIS:CE1	49:BB:454:MET:HE2	2.45	0.51
12:L:653:LEU:HD23	25:Y:76:TYR:HD1	1.75	0.51
13:M:410:ARG:HB3	13:M:410:ARG:HH11	1.75	0.51
14:N:408:CYS:HG	14:N:480:LEU:HD21	1.75	0.51
16:P:166:LYS:O	16:P:170:VAL:HG23	2.10	0.51
50:AC:148:TRP:CH2	51:BD:221:ILE:HD13	2.45	0.51
5:E:198:PHE:CZ	5:E:219:PRO:HG2	2.45	0.51
6:F:335:ASP:OD2	6:F:335:ASP:N	2.44	0.51
13:M:178:LEU:HD21	14:N:437:CYS:SG	2.50	0.51
48:AA:83:LEU:HD11	48:AA:89:ILE:HD11	1.93	0.51
52:BE:84:LEU:HD23	56:BI:50:TRP:HE3	1.76	0.51
39:n:94:LYS:HZ3	39:n:97:ARG:HD2	1.76	0.51
5:E:206:VAL:O	5:E:210:VAL:HG23	2.10	0.51
13:M:86:ILE:HD12	13:M:91:LEU:HD23	1.93	0.51
29:c:18:LYS:HE3	39:n:107:ILE:HB	1.92	0.51
46:y:203:SER:HA	66:y:301:COO:C10	2.41	0.51
49:AB:312:GLN:OE1	49:AB:312:GLN:N	2.44	0.51
51:AD:233:PHE:CE1	51:AD:238:GLY:HA2	2.46	0.51
49:BB:518:ASP:OD1	49:BB:521:LYS:HG2	2.10	0.51
21:U:69:VAL:O	21:U:69:VAL:HG22	2.10	0.51
1:A:16:LEU:HB2	8:H:83:MET:CE	2.40	0.51
3:C:83:ASN:HB3	22:V:135:PRO:HB3	1.93	0.51
14:N:219:THR:O	14:N:219:THR:HG22	2.11	0.51
46:y:144:PHE:CZ	66:y:301:COO:H61	2.46	0.51
48:AA:410:LYS:HG2	48:AA:410:LYS:O	2.09	0.51
50:AC:74:ILE:HA	50:AC:78:VAL:HG13	1.93	0.51
51:BD:264:LEU:HB2	51:BD:268:LYS:HB2	1.93	0.51
7:G:434:LEU:HD22	7:G:440:PHE:HE1	1.76	0.50
10:J:101:MET:CE	11:K:11:MET:CE	2.87	0.50
10:J:159:LEU:O	10:J:163:MET:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:51:ALA:HB1	12:L:492:PHE:CE1	2.46	0.50
12:L:383:LEU:HD23	35:j:32:CYS:SG	2.51	0.50
13:M:76:PRO:CG	30:d:57:LYS:NZ	2.74	0.50
48:AA:407:ALA:HB2	48:AA:473:THR:HG22	1.91	0.50
50:AC:26:TYR:HB3	68:AC:502:UQ5:H3M1	1.93	0.50
52:AE:273:LYS:CE	56:AI:43:ASP:OD1	2.58	0.50
16:P:181:ILE:HD12	16:P:181:ILE:N	2.26	0.50
29:c:65:PRO:HG3	29:c:69:ILE:HG12	1.92	0.50
32:f:20:PRO:HD2	32:f:86:MET:HE3	1.91	0.50
48:AA:78:LEU:HD22	48:AA:451:ARG:CD	2.41	0.50
23:W:71:ASP:OD1	23:W:74:VAL:HG23	2.11	0.50
25:Y:53:PRO:HA	25:Y:56:ILE:HD12	1.94	0.50
48:AA:87:LEU:HD12	48:AA:258:MET:HB2	1.91	0.50
51:AD:246:ARG:HA	51:AD:255:ASN:HB3	1.94	0.50
3:C:13:THR:HG23	22:V:53:TYR:HA	1.92	0.50
7:G:427:MET:HG2	7:G:551:ASN:HB3	1.93	0.50
14:N:139:MET:HE2	14:N:272:SER:HB2	1.93	0.50
35:j:44:LYS:HG3	36:k:42:PHE:HZ	1.76	0.50
53:BF:71:ASP:OD1	53:BF:75:LYS:HD2	2.11	0.50
4:D:233:LEU:HB2	4:D:332:GLU:HB2	1.93	0.50
8:H:21:ALA:HA	61:H:500:UQ9:H10B	1.92	0.50
8:H:51:PRO:HA	61:H:500:UQ9:H1MB	1.94	0.50
12:L:180:LEU:HB3	12:L:224:LEU:HD13	1.93	0.50
19:S:18:LEU:HD13	19:S:29:ARG:HG2	1.93	0.50
23:W:81:LYS:O	23:W:85:GLU:HG3	2.11	0.50
45:x:45:VAL:HG21	46:y:72:GLN:HE21	1.77	0.50
48:AA:222:TYR:CE2	48:AA:378:THR:HG21	2.46	0.50
6:F:267:ASN:ND2	60:F:500:FMN:O2	2.37	0.50
9:I:111:HIS:CE1	58:I:500:SF4:S4	3.05	0.50
13:M:279:PHE:HE1	38:m:71:LEU:HD21	1.66	0.50
15:O:48:LEU:CD2	15:O:60:ILE:HD11	2.42	0.50
16:P:253:PHE:HD2	16:P:255:PRO:HD3	1.75	0.50
19:S:6:SER:CB	19:S:9:LYS:HE3	2.42	0.50
39:n:49:ARG:HD2	39:n:49:ARG:O	2.11	0.50
50:AC:277:PRO:HB3	68:AC:503:UQ5:C5	2.42	0.50
7:G:147:ASP:OD1	7:G:147:ASP:N	2.44	0.50
8:H:23:LEU:HA	27:a:15:ILE:HD11	1.93	0.50
10:J:85:ARG:NH2	25:Y:38:ALA:O	2.45	0.50
13:M:189:LEU:C	13:M:193:PHE:CE2	2.89	0.50
14:N:323:SER:O	14:N:327:VAL:HG13	2.11	0.50
46:y:45:LEU:HD22	46:y:67:VAL:HB	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:HIS:NE2	58:I:500:SF4:S4	2.84	0.50
14:N:219:THR:O	14:N:221:ALA:N	2.45	0.50
1:A:1:FME:HE3	27:a:47:VAL:HG21	1.93	0.50
13:M:242:VAL:HG21	13:M:306:LYS:HG2	1.94	0.50
16:P:98:PRO:HA	16:P:121:MET:O	2.12	0.50
40:o:8:LYS:HZ1	40:o:64:GLU:HB3	1.77	0.50
45:x:241:ILE:HD11	46:y:37:GLU:HB3	1.94	0.50
51:AD:176:ARG:HG3	51:AD:207:GLU:OE2	2.12	0.50
48:BA:150:THR:HG23	48:BA:163:ILE:CD1	2.40	0.50
48:BA:310:PHE:CE2	48:BA:396:ILE:HG23	2.46	0.50
52:BE:66:GLU:OE2	54:BG:67:LYS:CG	2.57	0.50
3:C:56:LEU:HD12	3:C:77:LEU:HD23	1.92	0.49
4:D:292:ARG:HH12	7:G:192:ARG:HA	1.68	0.49
7:G:256:MET:HE3	7:G:261:SER:HB2	1.93	0.49
13:M:46:LEU:HD22	33:g:69:THR:HG21	1.93	0.49
14:N:492:GLN:HG3	30:d:63:MET:SD	2.51	0.49
20:T:54:VAL:HG12	20:T:85:ILE:HG21	1.94	0.49
46:y:133:VAL:HG11	47:z:147:MET:HE1	1.94	0.49
49:AB:100:THR:HG22	49:AB:108:VAL:HB	1.94	0.49
50:AC:178:ASP:OD1	50:AC:179:ASN:N	2.35	0.49
13:M:17:LEU:HA	13:M:20:VAL:CG2	2.42	0.49
13:M:118:GLU:CD	13:M:118:GLU:H	2.20	0.49
13:M:193:PHE:CZ	14:N:415:PHE:HD1	2.26	0.49
39:n:58:VAL:HG11	39:n:63:ARG:HE	1.77	0.49
49:BB:337:GLN:HG2	49:BB:410:VAL:HG13	1.93	0.49
12:L:393:PRO:HA	12:L:398:PHE:CD1	2.47	0.49
13:M:305:LYS:HB2	13:M:362:ARG:HD2	1.95	0.49
19:S:14:LEU:HD23	19:S:48:ILE:HG23	1.94	0.49
34:i:24:ARG:NH1	34:i:28:GLU:OE2	2.45	0.49
41:p:31:VAL:O	41:p:35:GLU:HG2	2.11	0.49
49:AB:160:GLU:N	49:AB:160:GLU:OE1	2.44	0.49
49:AB:288:LYS:HE3	49:AB:290:GLU:HB2	1.93	0.49
51:BD:141:SER:OG	51:BD:143:ASP:OD1	2.30	0.49
52:BE:197:LEU:HD21	67:BE:400:HEM:HMB1	1.94	0.49
33:g:102:GLU:OE1	33:g:106:LEU:CG	2.59	0.49
48:AA:494:SER:O	48:AA:498:ILE:CD1	2.58	0.49
49:AB:132:GLU:OE2	49:AB:137:ASN:HA	2.12	0.49
49:AB:488:ASP:OD2	49:AB:488:ASP:N	2.41	0.49
49:BB:64:LYS:O	49:BB:67:LYS:HG2	2.11	0.49
7:G:702:LEU:HD21	19:S:33:GLU:HA	1.94	0.49
39:n:58:VAL:HG13	39:n:63:ARG:NE	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:156:VAL:HG13	49:BB:157:ARG:N	2.26	0.49
50:BC:26:TYR:CD2	68:BC:502:UQ5:H3M1	2.45	0.49
1:A:62:TYR:OH	11:K:78:ALA:HB2	2.13	0.49
7:G:287:LEU:HD13	7:G:306:ASP:HB3	1.93	0.49
7:G:593:LYS:HG2	7:G:593:LYS:O	2.12	0.49
19:S:65:ASP:O	19:S:68:VAL:HG12	2.11	0.49
48:BA:481:LEU:HD22	48:BA:482:THR:H	1.78	0.49
2:B:111:PHE:HB2	2:B:113:ILE:HD12	1.94	0.49
6:F:137:VAL:HB	6:F:265:VAL:HG22	1.94	0.49
14:N:324:ILE:O	14:N:327:VAL:HG22	2.13	0.49
34:i:19:PRO:HG3	41:p:3:ARG:NH2	2.28	0.49
39:n:39:HIS:HA	39:n:42:TYR:CD2	2.47	0.49
48:BA:300:ARG:NH2	48:BA:494:SER:CA	2.66	0.49
48:BA:428:LEU:CD2	49:BB:117:LYS:CD	2.90	0.49
51:BD:154:LEU:HD22	51:BD:269:LEU:O	2.12	0.49
52:BE:305:VAL:HG21	53:BF:65:ARG:HG3	1.95	0.49
1:A:70:ILE:HG13	10:J:163:MET:HG2	1.93	0.49
4:D:292:ARG:NH1	7:G:192:ARG:CA	2.57	0.49
8:H:71:PHE:HE1	8:H:75:ARG:CZ	2.25	0.49
12:L:225:LEU:HB3	12:L:268:MET:HE1	1.93	0.49
13:M:200:LEU:HD21	13:M:266:ARG:HD2	1.94	0.49
24:X:32:GLU:HG2	24:X:59:CYS:SG	2.53	0.49
49:AB:383:VAL:HA	49:AB:388:ILE:HG12	1.94	0.49
50:AC:222:MET:CE	54:AG:8:LEU:CD1	2.58	0.49
51:AD:167:TRP:CE2	51:AD:168:ARG:HG2	2.47	0.49
49:BB:129:SER:HA	49:BB:132:GLU:HG3	1.94	0.49
51:BD:222:PRO:HB2	51:BD:232:TRP:HB3	1.94	0.49
53:BF:37:ASP:OD1	53:BF:93:TYR:OH	2.31	0.49
4:D:26:LEU:HD21	4:D:382:ILE:HD13	1.95	0.49
13:M:293:TYR:OH	38:m:44:LEU:HD22	2.13	0.49
20:T:54:VAL:HG11	20:T:71:PHE:CE1	2.48	0.49
40:o:8:LYS:O	40:o:9:LYS:HD3	2.12	0.49
45:x:157:GLU:HG3	45:x:175:GLU:HA	1.94	0.49
52:AE:210:ARG:HB3	52:AE:213:LEU:HD12	1.93	0.49
13:M:458:PHE:HA	13:M:461:ILE:HD12	1.95	0.49
39:n:110:ASN:HB3	39:n:113:LEU:HD11	1.94	0.49
50:AC:152:VAL:O	50:AC:156:LEU:HD13	2.13	0.49
52:AE:124:GLU:OE1	52:AE:128:LYS:HD2	2.13	0.49
49:BB:125:ILE:HG23	49:BB:279:MET:HG2	1.94	0.49
7:G:205:LYS:H	7:G:213:THR:HG21	1.77	0.48
11:K:9:PHE:O	11:K:12:ILE:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:449:PHE:CE1	20:T:91:GLU:HG3	2.48	0.48
13:M:444:ASP:HB2	37:l:40:HIS:NE2	2.27	0.48
29:c:30:PRO:HG2	29:c:33:TRP:HB3	1.95	0.48
30:d:7:MET:HE2	30:d:7:MET:HA	1.95	0.48
39:n:37:HIS:HB2	39:n:40:ILE:HG13	1.95	0.48
6:F:181:ILE:HD11	6:F:192:LEU:HD23	1.95	0.48
10:J:98:TRP:HA	10:J:102:PHE:CD1	2.47	0.48
13:M:261:THR:HG1	13:M:338:MET:HE3	1.78	0.48
14:N:255:GLU:OE1	14:N:317:ARG:CG	2.62	0.48
21:U:52:ASP:OD1	21:U:53:ARG:N	2.46	0.48
36:k:21:HIS:HB3	36:k:24:LEU:HB2	1.94	0.48
45:x:161:ILE:HD12	45:x:217:ILE:HG12	1.95	0.48
48:AA:235:SER:OG	48:BA:304:GLY:HA3	2.13	0.48
1:A:56:ARG:NH1	4:D:11:PHE:CG	2.81	0.48
11:K:61:PHE:CZ	14:N:191:LEU:HD11	2.48	0.48
23:W:50:VAL:CG2	23:W:54:GLN:OE1	2.61	0.48
25:Y:109:TYR:O	25:Y:112:ARG:NH1	2.46	0.48
48:AA:109:SER:HA	48:AA:112:GLU:HG3	1.95	0.48
67:BC:500:HEM:HBB2	67:BC:500:HEM:HMB1	1.94	0.48
1:A:60:ARG:HB3	1:A:118:TRP:CZ2	2.48	0.48
3:C:174:GLU:OE2	17:Q:94:THR:HB	2.13	0.48
48:AA:269:GLU:HA	48:AA:272:LYS:CE	2.43	0.48
49:AB:142:PHE:HE2	49:AB:258:VAL:HG23	1.79	0.48
3:C:18:TRP:O	3:C:33:THR:OG1	2.30	0.48
8:H:21:ALA:HB1	8:H:51:PRO:HB3	1.95	0.48
11:K:7:PHE:HZ	14:N:196:MET:HE1	1.78	0.48
12:L:471:ALA:HB3	35:j:31:LEU:HD11	1.94	0.48
12:L:652:ARG:O	12:L:656:ILE:HG12	2.13	0.48
13:M:448:LYS:HZ2	38:m:4:GLY:CA	2.24	0.48
14:N:90:ASP:OD1	14:N:279:ARG:NH2	2.46	0.48
52:AE:277:LEU:HD21	56:AI:42:VAL:HG21	1.95	0.48
49:BB:118:THR:HG22	49:BB:186:LEU:HD23	1.96	0.48
2:B:129:GLY:HA2	58:B:500:SF4:S3	2.54	0.48
7:G:398:ASP:O	7:G:402:ARG:HG2	2.14	0.48
8:H:178:TRP:HB2	8:H:181:ILE:HD12	1.94	0.48
10:J:57:TYR:CZ	11:K:66:LEU:HD11	2.49	0.48
26:Z:122:GLU:H	31:e:53:ARG:NH2	2.12	0.48
48:AA:276:PRO:O	49:AB:74:ARG:NH1	2.47	0.48
3:C:17:LYS:CE	3:C:37:TYR:OH	2.61	0.48
7:G:485:LEU:HD23	7:G:495:ILE:HD11	1.95	0.48
11:K:56:MET:SD	31:e:7:ILE:HA	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:286:TYR:HE2	14:N:289:THR:HB	1.79	0.48
16:P:186:LEU:HA	16:P:218:ARG:HB3	1.95	0.48
16:P:246:ILE:HG21	16:P:344:ILE:HG12	1.95	0.48
22:V:26:VAL:HG23	22:V:87:GLU:HG3	1.96	0.48
28:b:5:GLU:HA	28:b:8:ARG:HB2	1.94	0.48
29:c:45:PHE:CD1	29:c:46:LEU:HD22	2.49	0.48
38:m:60:ASP:OD2	38:m:65:ARG:NH1	2.46	0.48
42:q:46:ASN:ND2	42:q:77:GLU:OE1	2.46	0.48
53:AF:8:LEU:O	53:AF:8:LEU:HD23	2.14	0.48
48:BA:144:GLU:OE2	49:BB:445:GLN:NE2	2.46	0.48
50:BC:285:TYR:HE2	50:BC:346:GLY:O	1.97	0.48
51:BD:265:GLU:HG2	51:BD:266:GLU:N	2.26	0.48
52:BE:291:LEU:HA	54:BG:22:ILE:HD12	1.96	0.48
7:G:439:LEU:HD12	7:G:468:LYS:HE2	1.96	0.48
12:L:186:PHE:HE2	13:M:409:GLN:NE2	2.12	0.48
14:N:227:PHE:CE2	14:N:286:TYR:CE2	3.02	0.48
51:AD:176:ARG:CG	51:AD:207:GLU:OE2	2.62	0.48
51:BD:152:VAL:CG1	51:BD:153:ASP:H	2.27	0.48
3:C:42:LEU:HD22	3:C:77:LEU:HD11	1.95	0.48
12:L:26:GLU:HG3	33:g:31:ARG:HE	1.78	0.48
12:L:120:PHE:CZ	12:L:256:ILE:HG13	2.49	0.48
13:M:56:TRP:HB2	13:M:95:ILE:HD11	1.96	0.48
16:P:131:ILE:HD12	16:P:166:LYS:CE	2.33	0.48
36:k:14:ARG:HA	36:k:17:GLU:OE2	2.13	0.48
50:AC:386:TYR:CG	53:AF:21:MET:HG3	2.49	0.48
50:BC:153:ILE:HD11	69:BC:503:UQ7:C5	2.44	0.48
13:M:60:ASP:O	13:M:67:GLN:NE2	2.46	0.48
13:M:72:LEU:HD11	13:M:84:LEU:HD11	1.96	0.48
14:N:390:THR:HG21	14:N:469:LEU:HG	1.95	0.48
20:T:41:LEU:HD23	20:T:41:LEU:H	1.79	0.48
42:q:68:THR:HB	42:q:73:HIS:CE1	2.49	0.48
51:BD:220:CYS:HB2	51:BD:234:CYS:SG	2.53	0.48
52:BE:102:VAL:HG12	67:BE:400:HEM:HAB	1.95	0.48
3:C:31:PHE:CE1	3:C:86:ILE:HD11	2.48	0.47
8:H:115:SER:HA	8:H:148:GLU:OE1	2.14	0.47
12:L:262:VAL:CG2	12:L:319:LEU:HD11	2.43	0.47
13:M:76:PRO:HG2	30:d:57:LYS:HZ2	1.79	0.47
14:N:278:LEU:HD13	14:N:497:LEU:HD11	1.96	0.47
21:U:109:ILE:HG23	21:U:115:ALA:HB2	1.96	0.47
22:V:118:GLU:OE1	22:V:120:ILE:HD11	2.14	0.47
25:Y:45:ARG:HH11	25:Y:48:ARG:NH2	2.06	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:61:MET:HE3	25:Y:65:HIS:HE1	1.79	0.47
46:y:144:PHE:HZ	66:y:301:COO:H61	1.79	0.47
50:AC:35:TRP:HB3	50:AC:105:ARG:HG3	1.95	0.47
48:BA:330:VAL:C	48:BA:334:LEU:HD13	2.38	0.47
3:C:58:ASP:HB2	3:C:111:TRP:NE1	2.28	0.47
13:M:84:LEU:HD22	13:M:136:MET:HE1	1.95	0.47
13:M:103:ILE:O	13:M:107:VAL:HG23	2.15	0.47
23:W:50:VAL:HG22	23:W:54:GLN:OE1	2.14	0.47
35:j:17:VAL:HG11	36:k:23:MET:SD	2.54	0.47
49:AB:429:LYS:HE2	49:AB:433:ARG:NH1	2.28	0.47
48:BA:168:THR:HG23	49:BB:91:ILE:HD13	1.96	0.47
9:I:190:HIS:HB3	16:P:115:LEU:HD11	1.95	0.47
13:M:320:THR:HA	13:M:323:MET:HG2	1.96	0.47
14:N:461:MET:HE1	14:N:469:LEU:HD23	1.96	0.47
51:AD:197:GLN:HG2	51:AD:202:ARG:HD2	1.96	0.47
48:BA:195:LEU:O	48:BA:199:LYS:HG2	2.14	0.47
2:B:147:PRO:O	8:H:61:LYS:NZ	2.46	0.47
5:E:44:ASP:OD2	5:E:44:ASP:N	2.46	0.47
8:H:31:MET:HE2	8:H:31:MET:HB3	1.75	0.47
8:H:126:ARG:CD	10:J:70:MET:HG2	2.45	0.47
19:S:74:LEU:HD22	19:S:82:ILE:HG12	1.95	0.47
26:Z:89:LEU:HD13	27:a:49:MET:HE1	1.96	0.47
27:a:52:ARG:O	27:a:56:VAL:HG23	2.14	0.47
38:m:70:PHE:O	38:m:71:LEU:C	2.58	0.47
47:z:223:ASN:HD21	47:z:225:ILE:HB	1.79	0.47
69:BC:503:UQ7:HM33	69:BC:503:UQ7:HM22	1.95	0.47
52:BE:135:GLU:HG3	52:BE:148:THR:HB	1.96	0.47
5:E:123:GLY:N	5:E:165:SER:OG	2.46	0.47
7:G:421:LEU:HD12	7:G:703:LYS:HD3	1.95	0.47
8:H:109:TYR:CZ	8:H:113:ILE:HD11	2.50	0.47
14:N:218:ILE:HG12	14:N:222:ARG:HD3	1.97	0.47
30:d:14:LEU:HG	30:d:18:MET:HE2	1.95	0.47
50:AC:222:MET:SD	54:AG:6:VAL:HG22	2.42	0.47
48:BA:310:PHE:CZ	48:BA:396:ILE:CG2	2.95	0.47
51:BD:176:ARG:HD2	51:BD:208:TRP:CH2	2.50	0.47
6:F:185:TYR:HB3	6:F:188:GLU:HB2	1.96	0.47
25:Y:50:VAL:HG22	25:Y:53:PRO:HD2	1.96	0.47
33:g:30:SER:O	33:g:34:THR:OG1	2.31	0.47
49:AB:146:MET:HE1	49:AB:214:GLU:CB	2.45	0.47
48:BA:308:THR:OG1	48:BA:488:ASP:O	2.32	0.47
50:BC:294:LYS:O	50:BC:298:VAL:HG23	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BC:383:PRO:HG3	53:BF:35:TYR:CE2	2.48	0.47
2:B:87:MET:HG2	4:D:19:HIS:HE1	1.72	0.47
6:F:132:ARG:HG2	17:Q:146:TRP:CE3	2.50	0.47
8:H:319:VAL:HG22	8:H:324:LEU:HD11	1.97	0.47
10:J:82:GLU:OE2	25:Y:51:ALA:HB2	2.15	0.47
12:L:120:PHE:CZ	12:L:261:MET:HB2	2.50	0.47
12:L:601:GLY:O	12:L:605:THR:HG22	2.15	0.47
13:M:84:LEU:HD22	13:M:136:MET:CE	2.44	0.47
13:M:178:LEU:CD2	14:N:437:CYS:SG	3.03	0.47
16:P:195:ARG:N	16:P:342:ASP:OD1	2.47	0.47
28:b:5:GLU:CD	28:b:8:ARG:HD2	2.40	0.47
41:p:52:ARG:HB2	41:p:77:TYR:CE1	2.50	0.47
48:AA:97:PRO:HB2	49:AB:91:ILE:HD12	1.97	0.47
51:AD:171:PRO:HG3	50:BC:269:MET:CE	2.45	0.47
51:AD:212:VAL:HG12	51:AD:214:VAL:HG22	1.97	0.47
53:AF:56:ARG:HH22	54:AG:7:LYS:HE3	1.79	0.47
56:AI:28:VAL:O	56:AI:32:ILE:HG12	2.14	0.47
48:BA:300:ARG:HH22	48:BA:494:SER:HA	1.76	0.47
48:BA:459:LYS:HB3	48:BA:463:GLN:NE2	2.26	0.47
9:I:220:LEU:HD12	26:Z:19:PRO:HD3	1.97	0.47
13:M:448:LYS:HZ2	38:m:4:GLY:HA2	1.80	0.47
14:N:290:LEU:HD21	14:N:334:PHE:CZ	2.49	0.47
45:x:202:PRO:HG3	66:y:301:COO:O2X	2.13	0.47
47:z:77:SER:OG	47:z:95:GLY:O	2.32	0.47
48:BA:483:MET:HE1	48:BA:485:SER:HB3	1.96	0.47
1:A:99:PHE:CD1	10:J:156:SER:HB3	2.50	0.47
13:M:224:PHE:O	13:M:228:VAL:HG23	2.15	0.47
23:W:121:THR:HG23	23:W:123:PHE:N	2.30	0.47
48:AA:82:THR:HG23	48:AA:88:LYS:HG2	1.97	0.47
51:AD:168:ARG:HD2	50:BC:175:PHE:CD1	2.49	0.47
52:AE:107:HIS:HE1	52:AE:177:PRO:HD2	1.80	0.47
53:AF:98:LEU:O	53:AF:102:LYS:HG3	2.14	0.47
48:BA:265:VAL:HG21	48:BA:270:LEU:HG	1.96	0.47
12:L:544:ARG:O	12:L:548:THR:HG22	2.15	0.47
13:M:17:LEU:HA	13:M:20:VAL:HG22	1.97	0.47
16:P:302:ARG:NH2	16:P:382:ARG:NH1	2.62	0.47
31:e:23:GLU:HG2	34:i:63:LEU:HD22	1.96	0.47
48:AA:216:ALA:HB1	48:AA:299:PHE:CG	2.50	0.47
53:AF:28:LEU:HD21	53:AF:38:LEU:HD11	1.97	0.47
11:K:53:LEU:HD13	14:N:202:GLY:HA2	1.96	0.46
22:V:59:SER:HB3	22:V:145:THR:HG23	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:392:ALA:O	48:AA:396:ILE:HG12	2.14	0.46
48:BA:271:LEU:HD22	48:BA:275:GLU:OE1	2.14	0.46
48:BA:300:ARG:HH22	48:BA:493:PRO:C	2.17	0.46
48:BA:383:ILE:CD1	48:BA:403:LEU:HD21	2.45	0.46
6:F:425:GLY:C	6:F:476:ARG:CD	2.87	0.46
12:L:4:LEU:HD11	29:c:52:ALA:HB2	1.96	0.46
12:L:212:ASN:HB3	38:m:54:LYS:NZ	2.30	0.46
13:M:139:LEU:HB3	13:M:188:ILE:HG12	1.96	0.46
13:M:444:ASP:HB2	37:l:40:HIS:CE1	2.49	0.46
14:N:339:ILE:HD11	14:N:498:TYR:HE1	1.79	0.46
48:BA:323:LYS:C	48:BA:325:ALA:H	2.21	0.46
50:BC:94:MET:HE2	50:BC:97:ILE:HD12	1.96	0.46
1:A:69:LEU:HD11	11:K:70:ALA:HB1	1.96	0.46
7:G:302:ASN:HD21	7:G:320:ASN:HD22	0.61	0.46
7:G:518:ALA:HB3	7:G:555:GLN:CD	2.38	0.46
8:H:126:ARG:HD3	10:J:70:MET:HG2	1.96	0.46
11:K:76:GLY:HA2	14:N:180:LEU:HG	1.96	0.46
12:L:244:ASP:HA	12:L:309:ARG:HH12	1.81	0.46
13:M:38:ARG:HB3	13:M:109:TRP:CH2	2.50	0.46
49:BB:453:HIS:HE1	49:BB:454:MET:HE2	1.80	0.46
52:BE:229:MET:HE3	52:BE:229:MET:HB3	1.77	0.46
5:E:132:THR:HG22	5:E:171:CYS:SG	2.55	0.46
6:F:286:SER:HA	6:F:294:ALA:HB1	1.97	0.46
7:G:446:GLN:HE21	7:G:717:THR:HG22	1.81	0.46
11:K:53:LEU:HD22	31:e:45:LEU:HD22	1.98	0.46
14:N:212:ILE:HG22	14:N:213:LEU:HD23	1.98	0.46
16:P:157:GLU:H	16:P:157:GLU:CD	2.23	0.46
32:f:91:ASN:HB2	32:f:94:GLU:HB2	1.98	0.46
46:y:133:VAL:HG11	47:z:147:MET:HE2	1.96	0.46
48:AA:164:ASP:CB	48:AA:435:MET:HE1	2.42	0.46
50:AC:32:LEU:HB2	50:AC:231:PHE:CE1	2.51	0.46
52:AE:73:CYS:SG	52:AE:192:TYR:HA	2.56	0.46
53:BF:55:PRO:HD2	53:BF:58:ILE:HD12	1.97	0.46
2:B:88:THR:HG23	2:B:115:PHE:HD1	1.75	0.46
8:H:126:ARG:HD3	10:J:70:MET:HE2	1.97	0.46
8:H:302:VAL:HA	28:b:16:VAL:HG11	1.98	0.46
12:L:375:PHE:CE1	12:L:456:CYS:HB3	2.50	0.46
14:N:206:PHE:HB3	14:N:283:TYR:CE2	2.50	0.46
47:z:27:CYS:SG	47:z:34:TYR:OH	2.48	0.46
48:AA:151:SER:OG	48:AA:162:THR:OG1	2.34	0.46
49:BB:367:LYS:HE2	49:BB:390:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:133:PHE:HB3	12:L:182:ILE:HD13	1.96	0.46
36:k:4:PRO:HA	36:k:9:GLY:HA3	1.97	0.46
46:y:15:ILE:HG23	47:z:22:LEU:HD22	1.98	0.46
67:AC:500:HEM:HAA2	68:AC:502:UQ5:H4M2	1.96	0.46
48:BA:212:PHE:CE2	48:BA:486:PHE:HD1	2.33	0.46
2:B:180:PRO:HD3	16:P:111:LEU:HD11	1.98	0.46
8:H:58:LEU:HD13	8:H:226:ALA:HB2	1.97	0.46
14:N:489:VAL:O	14:N:493:MET:HG3	2.16	0.46
16:P:184:SER:O	16:P:219:PRO:HD2	2.16	0.46
16:P:238:LYS:HE3	16:P:238:LYS:HB3	1.60	0.46
37:l:73:VAL:HG23	37:l:77:GLU:HG2	1.97	0.46
39:n:55:ASN:HB3	39:n:67:LEU:HD13	1.97	0.46
46:y:254:PRO:HA	46:y:257:ILE:HD12	1.97	0.46
47:z:88:ASP:OD1	47:z:89:VAL:N	2.48	0.46
49:AB:157:ARG:HG3	49:AB:157:ARG:O	2.15	0.46
49:AB:502:ASP:O	51:AD:109:ARG:NH1	2.49	0.46
51:AD:237:HIS:HB2	59:AD:301:FES:S2	2.56	0.46
48:BA:184:PRO:HG2	48:BA:249:MET:SD	2.56	0.46
49:BB:297:LYS:HE2	49:BB:297:LYS:HB3	1.74	0.46
3:C:56:LEU:HD21	3:C:59:ILE:HD11	1.98	0.46
8:H:81:THR:OG1	8:H:120:GLY:HA3	2.16	0.46
12:L:458:ASP:OD1	12:L:459:ALA:N	2.35	0.46
12:L:513:ALA:HB3	12:L:518:LYS:NZ	2.30	0.46
12:L:639:PHE:CE1	14:N:293:ILE:HD13	2.51	0.46
18:R:51:LYS:NZ	18:R:59:GLU:OE2	2.49	0.46
25:Y:68:THR:O	25:Y:72:ILE:HG13	2.15	0.46
48:AA:105:VAL:HG21	48:AA:253:PHE:CE2	2.50	0.46
48:AA:312:VAL:HB	48:AA:483:MET:SD	2.55	0.46
48:AA:465:THR:HB	48:AA:467:LYS:HG2	1.98	0.46
53:AF:111:LEU:HD12	48:BA:137:PHE:CE2	2.51	0.46
5:E:207:VAL:O	5:E:211:GLU:HG2	2.15	0.46
7:G:325:GLU:O	7:G:326:GLU:HG2	2.16	0.46
12:L:242:LEU:HD11	12:L:257:HIS:HB3	1.97	0.46
22:V:103:MET:HE3	22:V:109:TRP:CH2	2.50	0.46
43:u:45:VAL:HG11	55:AH:23:LYS:HE2	1.97	0.46
46:y:238:LYS:HD2	46:y:240:GLU:CG	2.46	0.46
6:F:200:TYR:OH	6:F:217:GLU:OE1	2.25	0.46
13:M:74:TRP:HB2	13:M:82:PHE:HE1	1.81	0.46
24:X:38:LYS:HE2	24:X:38:LYS:HB2	1.75	0.46
67:AC:500:HEM:HBB2	67:AC:500:HEM:HMB1	1.96	0.46
50:BC:277:PRO:HG3	69:BC:503:UQ7:C1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:593:ALA:HB2	38:m:37:ILE:HD13	1.97	0.45
13:M:69:VAL:HA	13:M:84:LEU:O	2.17	0.45
13:M:267:PHE:O	13:M:271:MET:HB2	2.15	0.45
48:AA:335:MET:HE3	48:AA:335:MET:HB3	1.84	0.45
50:AC:285:TYR:CE2	50:AC:289:ARG:HD2	2.51	0.45
48:BA:56:LEU:HB2	49:BB:348:THR:HA	1.97	0.45
50:BC:288:LEU:HB2	50:BC:301:ILE:HD11	1.98	0.45
1:A:16:LEU:CD1	8:H:83:MET:CE	2.94	0.45
5:E:175:CYS:SG	5:E:180:MET:HE3	2.56	0.45
7:G:121:LEU:HD13	7:G:130:PRO:HB2	1.98	0.45
52:AE:110:SER:O	52:AE:156:ARG:HD2	2.16	0.45
6:F:88:THR:HA	6:F:91:LEU:HD23	1.97	0.45
8:H:98:MET:HG2	27:a:27:TYR:CD2	2.52	0.45
8:H:263:ILE:HD11	8:H:268:TRP:CZ2	2.50	0.45
10:J:101:MET:HE2	14:N:192:PHE:CZ	2.45	0.45
13:M:21:LEU:HD12	13:M:21:LEU:HA	1.77	0.45
13:M:113:ARG:HH11	47:z:113:LEU:HD23	1.81	0.45
25:Y:10:GLU:C	25:Y:11:GLU:HG3	2.39	0.45
32:f:44:SER:HB3	32:f:65:GLY:O	2.16	0.45
36:k:13:ARG:HG3	39:n:42:TYR:CE2	2.51	0.45
48:AA:78:LEU:HD21	48:AA:441:ILE:HG23	1.97	0.45
48:AA:192:ASN:O	48:AA:196:ARG:HG3	2.15	0.45
50:AC:90:ASN:O	50:AC:94:MET:HG2	2.17	0.45
49:BB:321:PHE:CG	49:BB:343:GLU:HB2	2.52	0.45
50:BC:124:VAL:HG11	50:BC:309:LEU:HG	1.99	0.45
2:B:88:THR:HB	4:D:20:PRO:HD2	1.99	0.45
2:B:110:ARG:NH2	9:I:95:ASN:OD1	2.50	0.45
5:E:135:CYS:HB2	59:E:500:FES:S2	2.52	0.45
5:E:209:ILE:HG23	5:E:219:PRO:HG3	1.99	0.45
13:M:242:VAL:HG22	13:M:305:LYS:HB3	1.97	0.45
13:M:304:LEU:HD21	13:M:436:VAL:HG21	1.99	0.45
23:W:41:MET:HE2	23:W:41:MET:HB2	1.72	0.45
27:a:44:GLU:CD	27:a:44:GLU:N	2.72	0.45
38:m:23:LEU:HD12	38:m:23:LEU:HA	1.78	0.45
42:q:63:GLN:HA	42:q:73:HIS:O	2.16	0.45
48:AA:159:MET:HE3	48:AA:253:PHE:HZ	1.82	0.45
50:AC:285:TYR:CD2	50:AC:289:ARG:HD2	2.52	0.45
50:BC:289:ARG:NH2	50:BC:346:GLY:O	2.50	0.45
50:BC:318:TYR:CD2	53:BF:47:ILE:HD11	2.51	0.45
52:BE:74:PRO:HG2	52:BE:76:TYR:CE2	2.50	0.45
10:J:171:MET:HA	10:J:171:MET:HE3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:353:VAL:HG11	16:P:359:LYS:HE2	1.93	0.45
31:e:1:MET:HE3	31:e:15:TYR:HB2	1.98	0.45
45:x:114:CYS:O	45:x:114:CYS:SG	2.75	0.45
45:x:242:TYR:HD2	47:z:34:TYR:CE1	2.35	0.45
50:AC:23:LEU:HA	68:AC:502:UQ5:O2	2.16	0.45
51:AD:205:ASN:HB2	51:AD:263:PHE:HE1	1.79	0.45
50:BC:375:LEU:HD23	50:BC:375:LEU:HA	1.81	0.45
52:BE:224:ILE:HG12	52:BE:226:MET:H	1.82	0.45
4:D:238:PRO:CB	4:D:243:ASP:OD1	2.64	0.45
5:E:82:GLN:HB3	5:E:190:SER:HA	1.98	0.45
48:AA:239:ARG:HB2	48:AA:239:ARG:HH11	1.82	0.45
49:AB:61:ILE:O	49:AB:65:ILE:HG13	2.16	0.45
52:AE:153:LEU:HD23	52:AE:153:LEU:HA	1.84	0.45
48:BA:448:TYR:CD2	48:BA:452:LYS:HE2	2.51	0.45
5:E:87:TRP:CE2	5:E:121:LYS:HG2	2.52	0.45
6:F:290:ARG:HH11	6:F:359:LEU:HD12	1.82	0.45
8:H:99:VAL:O	27:a:38:LYS:HE3	2.16	0.45
12:L:328:ILE:HB	12:L:411:LYS:HD3	1.99	0.45
49:AB:386:ASN:HD21	50:AC:6:GLN:HG3	1.82	0.45
49:BB:147:ILE:HD12	49:BB:147:ILE:HA	1.84	0.45
4:D:88:LYS:HD3	4:D:327:THR:HG21	1.99	0.45
5:E:215:LYS:HA	5:E:215:LYS:HD3	1.64	0.45
8:H:21:ALA:HB2	61:H:500:UQ9:H12	1.99	0.45
9:I:146:GLU:OE1	9:I:146:GLU:N	2.42	0.45
17:Q:73:LYS:HD2	17:Q:73:LYS:HA	1.66	0.45
34:i:5:MET:O	34:i:9:GLU:HG2	2.17	0.45
48:AA:157:GLU:OE2	48:AA:375:PHE:HB3	2.17	0.45
48:AA:415:HIS:HD2	48:AA:418:ARG:NH2	2.13	0.45
68:AC:502:UQ5:H101	68:AC:502:UQ5:H121	1.37	0.45
48:BA:459:LYS:HB3	48:BA:459:LYS:NZ	2.32	0.45
51:BD:177:ARG:HB3	51:BD:181:ASP:CG	2.42	0.45
12:L:283:LEU:O	12:L:287:THR:OG1	2.35	0.45
12:L:321:TYR:HA	12:L:324:PHE:CE2	2.52	0.45
12:L:446:THR:HG21	36:k:24:LEU:HB3	1.99	0.45
16:P:233:TRP:O	16:P:237:VAL:HG23	2.17	0.45
19:S:15:ARG:HB2	19:S:61:TRP:HB2	1.99	0.45
21:U:51:THR:O	21:U:54:VAL:HG22	2.17	0.45
23:W:61:ALA:O	23:W:65:ASN:OD1	2.35	0.45
34:i:34:HIS:CD2	41:p:27:PRO:HG2	2.52	0.45
40:o:10:MET:HE3	40:o:11:ILE:N	2.32	0.45
50:AC:222:MET:CE	54:AG:8:LEU:CB	2.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AD:171:PRO:HG2	51:AD:221:ILE:HD13	1.98	0.45
52:AE:115:ARG:HG2	52:AE:153:LEU:O	2.16	0.45
48:BA:401:LYS:HD3	48:BA:401:LYS:HA	1.63	0.45
51:BD:205:ASN:HD22	51:BD:208:TRP:CD1	2.31	0.45
2:B:96:VAL:HA	2:B:99:MET:HE2	1.98	0.45
10:J:104:ILE:HG13	14:N:224:SER:OG	2.17	0.45
14:N:206:PHE:CZ	14:N:280:VAL:HG22	2.52	0.45
16:P:139:ASN:OD1	16:P:140:VAL:HG23	2.16	0.45
19:S:88:ASN:OD1	19:S:89:LEU:N	2.50	0.45
46:y:105:LEU:HD12	46:y:133:VAL:HG13	1.99	0.45
50:AC:371:ILE:HA	50:AC:374:ILE:HD12	1.99	0.45
51:AD:171:PRO:HG3	50:BC:269:MET:HE2	1.99	0.45
49:BB:401:ASP:N	49:BB:401:ASP:OD1	2.49	0.45
50:BC:159:ALA:HA	50:BC:294:LYS:HD3	1.98	0.45
4:D:110:ARG:HA	4:D:334:PRO:HG3	1.99	0.44
6:F:98:TRP:HE3	6:F:99:ILE:HG13	1.82	0.44
6:F:439:THR:HB	6:F:455:ALA:HB1	1.99	0.44
10:J:8:SER:HB2	43:u:14:ALA:HB3	1.98	0.44
11:K:68:VAL:HG11	14:N:153:GLU:HG3	1.99	0.44
12:L:49:GLU:HG2	29:c:69:ILE:HB	2.00	0.44
13:M:284:TYR:HB3	38:m:52:ILE:HD13	1.99	0.44
14:N:72:GLY:O	14:N:76:LEU:HG	2.18	0.44
14:N:281:PHE:CB	14:N:290:LEU:HD11	2.47	0.44
14:N:303:ILE:HG23	14:N:304:LEU:N	2.32	0.44
23:W:17:ALA:HB3	23:W:21:GLU:OE1	2.17	0.44
25:Y:124:LEU:HD23	25:Y:124:LEU:HA	1.70	0.44
29:c:45:PHE:HD1	29:c:46:LEU:HD22	1.81	0.44
48:AA:129:LYS:HE2	48:AA:194:GLU:OE2	2.16	0.44
48:AA:167:LYS:O	48:AA:170:VAL:HG23	2.17	0.44
48:AA:275:GLU:HB3	48:AA:276:PRO:HD3	1.99	0.44
51:AD:222:PRO:HB2	51:AD:232:TRP:HB3	1.99	0.44
51:AD:264:LEU:HD12	51:AD:268:LYS:CG	2.47	0.44
48:BA:383:ILE:HD13	48:BA:403:LEU:HD21	1.98	0.44
49:BB:47:PRO:HB3	49:BB:51:LEU:HD23	1.99	0.44
50:BC:115:PRO:HA	53:BF:119:ARG:HH21	1.82	0.44
51:BD:143:ASP:OD1	51:BD:144:VAL:N	2.50	0.44
52:BE:299:ARG:O	53:BF:75:LYS:NZ	2.50	0.44
53:BF:80:PRO:HD2	53:BF:83:LEU:HD12	1.99	0.44
7:G:76:VAL:HG12	7:G:139:LEU:O	2.16	0.44
12:L:402:ASP:OD2	12:L:521:PRO:HG2	2.17	0.44
17:Q:111:GLU:OE1	17:Q:111:GLU:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:54:VAL:HG12	20:T:85:ILE:CG2	2.47	0.44
40:o:71:LEU:HA	40:o:74:LYS:HD2	1.98	0.44
47:z:90:ASN:ND2	47:z:117:VAL:O	2.44	0.44
48:AA:427:VAL:HG21	48:AA:457:PHE:CE2	2.53	0.44
48:BA:330:VAL:O	48:BA:334:LEU:HD12	2.16	0.44
48:BA:396:ILE:H	48:BA:396:ILE:CD1	2.26	0.44
48:BA:459:LYS:O	48:BA:463:GLN:NE2	2.50	0.44
49:BB:151:THR:HG22	49:BB:152:ASP:N	2.33	0.44
4:D:11:PHE:CE1	4:D:32:MET:HB2	2.51	0.44
7:G:283:ARG:O	7:G:286:GLU:HG2	2.17	0.44
12:L:29:ALA:HB1	12:L:101:ILE:HG12	1.98	0.44
12:L:367:LYS:HG3	39:n:84:TYR:CE1	2.51	0.44
14:N:107:THR:HG21	14:N:264:PHE:HB2	2.00	0.44
14:N:166:LYS:HG3	14:N:258:PRO:HG3	1.99	0.44
24:X:40:LYS:HD2	24:X:40:LYS:HA	1.67	0.44
48:AA:225:PRO:HG2	48:AA:290:PRO:HB2	2.00	0.44
53:AF:76:HIS:ND1	53:AF:76:HIS:O	2.50	0.44
3:C:97:ARG:NH1	23:W:13:PRO:O	2.49	0.44
4:D:10:ASN:OD1	4:D:33:ASN:OD1	2.35	0.44
13:M:252:LEU:HD23	13:M:256:LEU:HD12	2.00	0.44
16:P:142:ILE:HD11	16:P:269:LEU:HD21	1.98	0.44
16:P:298:TYR:CE1	16:P:305:PRO:HA	2.52	0.44
20:T:120:MET:HE2	39:n:88:TRP:CD1	2.52	0.44
31:e:21:PHE:CE1	31:e:38:ARG:HB2	2.53	0.44
37:l:53:LEU:C	37:l:53:LEU:HD12	2.42	0.44
48:AA:126:MET:CE	48:AA:129:LYS:HG3	2.48	0.44
48:AA:269:GLU:O	48:AA:272:LYS:CG	2.62	0.44
48:AA:310:PHE:CZ	48:AA:395:ALA:HB1	2.53	0.44
48:AA:481:LEU:HD13	48:AA:483:MET:HG2	1.96	0.44
49:AB:308:THR:CG2	49:AB:313:LEU:HD21	2.48	0.44
4:D:292:ARG:O	4:D:292:ARG:CG	2.66	0.44
7:G:702:LEU:HB3	19:S:36:TYR:CD2	2.51	0.44
8:H:38:LYS:HD2	8:H:38:LYS:HA	1.87	0.44
12:L:15:VAL:CB	12:L:31:MET:HE2	2.47	0.44
12:L:120:PHE:HZ	12:L:261:MET:HB2	1.83	0.44
16:P:213:GLU:HG3	16:P:276:MET:HB3	1.99	0.44
50:AC:153:ILE:O	50:AC:156:LEU:HB2	2.17	0.44
53:BF:28:LEU:HD21	53:BF:38:LEU:HD11	1.99	0.44
4:D:17:PRO:HG2	4:D:26:LEU:HD23	2.00	0.44
5:E:125:TYR:CE1	5:E:213:LEU:HD22	2.52	0.44
12:L:119:ILE:HD12	12:L:119:ILE:HA	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:74:TRP:HB2	13:M:82:PHE:CE1	2.53	0.44
14:N:227:PHE:CE2	14:N:286:TYR:CZ	3.06	0.44
16:P:298:TYR:CZ	16:P:305:PRO:HA	2.53	0.44
45:x:175:GLU:OE2	45:x:191:ARG:HD2	2.18	0.44
47:z:4:LEU:HD23	47:z:4:LEU:HA	1.83	0.44
47:z:57:LYS:HD2	47:z:57:LYS:HA	1.79	0.44
49:AB:415:CYS:SG	50:AC:2:THR:HG22	2.58	0.44
4:D:119:THR:HB	4:D:131:PHE:HA	2.00	0.44
5:E:114:TYR:HB3	6:F:224:ALA:O	2.18	0.44
10:J:96:ILE:HG23	12:L:641:MET:HE1	1.99	0.44
12:L:57:CYS:HB3	12:L:78:PHE:HB2	2.00	0.44
13:M:45:SER:HB2	13:M:102:PRO:HG3	1.99	0.44
13:M:146:PHE:O	13:M:149:VAL:HG22	2.17	0.44
16:P:151:THR:HG23	16:P:153:ASN:H	1.83	0.44
23:W:120:LYS:HG3	23:W:124:LEU:HD23	1.99	0.44
50:AC:341:LEU:HD23	50:AC:341:LEU:HA	1.86	0.44
49:BB:450:LEU:C	49:BB:453:HIS:CD2	2.96	0.44
50:BC:318:TYR:HD2	53:BF:47:ILE:HD11	1.83	0.44
4:D:287:ILE:H	4:D:287:ILE:HG13	1.70	0.44
8:H:75:ARG:HH11	8:H:75:ARG:CG	2.29	0.44
14:N:148:MET:HE2	14:N:148:MET:HB3	1.92	0.44
20:T:90:GLU:OE1	39:n:25:ARG:NH2	2.45	0.44
25:Y:79:VAL:HG21	25:Y:101:VAL:HG11	1.99	0.44
28:b:9:MET:HG3	28:b:13:GLN:OE1	2.17	0.44
48:AA:123:LEU:HD12	48:AA:245:LEU:HD22	2.00	0.44
49:AB:337:GLN:HG2	49:AB:410:VAL:HG13	1.98	0.44
51:AD:221:ILE:HB	50:BC:271:THR:OG1	2.18	0.44
55:BH:24:PRO:HB2	55:BH:52:TYR:HA	1.99	0.44
3:C:42:LEU:HD12	3:C:101:VAL:HG11	1.99	0.44
6:F:408:CYS:HB3	58:F:501:SF4:S4	2.57	0.44
12:L:218:ILE:HG22	12:L:279:SER:HB2	1.99	0.44
13:M:57:ILE:O	33:g:84:LYS:HE3	2.18	0.44
20:T:96:GLU:OE1	39:n:86:VAL:HG23	2.18	0.44
21:U:54:VAL:HG21	21:U:116:VAL:HG22	2.00	0.44
43:u:53:LEU:HD23	43:u:53:LEU:O	2.17	0.44
53:AF:11:PRO:O	53:AF:18:ARG:NH1	2.51	0.44
50:BC:32:LEU:HB2	50:BC:231:PHE:CE1	2.53	0.44
9:I:60:TRP:CE2	28:b:8:ARG:HG3	2.52	0.43
13:M:458:PHE:CZ	33:g:66:CYS:HB3	2.53	0.43
47:z:85:LEU:HA	47:z:106:VAL:O	2.18	0.43
48:AA:53:LEU:HB3	48:AA:54:THR:H	1.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:427:VAL:O	48:AA:431:LEU:HD23	2.18	0.43
49:AB:367:LYS:HE3	49:AB:390:GLU:CD	2.42	0.43
51:AD:150:LEU:HD23	51:AD:150:LEU:HA	1.80	0.43
51:BD:174:ILE:HD11	51:BD:208:TRP:CE3	2.49	0.43
5:E:155:ARG:HG2	5:E:155:ARG:HH11	1.83	0.43
13:M:126:CYS:SG	13:M:152:PRO:HB2	2.58	0.43
15:O:111:THR:HG22	15:O:113:ASP:H	1.82	0.43
49:AB:358:MET:HG3	49:AB:430:LEU:HD13	1.99	0.43
56:BI:48:LYS:HD3	56:BI:48:LYS:HA	1.78	0.43
57:BJ:38:VAL:O	57:BJ:40:PRO:HD3	2.18	0.43
1:A:83:VAL:HG21	10:J:137:LEU:HG	1.99	0.43
4:D:80:HIS:NE2	4:D:240:ASP:OD2	2.50	0.43
12:L:3:LEU:HD23	12:L:3:LEU:HA	1.77	0.43
14:N:318:LEU:HD11	14:N:439:TYR:CD1	2.53	0.43
22:V:107:ASP:O	22:V:107:ASP:OD2	2.35	0.43
25:Y:114:ILE:N	25:Y:115:PRO:HD2	2.33	0.43
26:Z:86:LEU:HB3	26:Z:87:PRO:HD3	2.00	0.43
40:o:62:GLU:O	40:o:66:VAL:HG23	2.18	0.43
41:p:46:GLU:HA	41:p:49:LYS:HD3	2.01	0.43
45:x:248:PHE:O	45:x:252:LEU:HD13	2.18	0.43
50:AC:40:SER:HB3	68:AC:502:UQ5:H71	1.99	0.43
50:AC:249:TRP:HZ3	50:AC:256:VAL:HG21	1.83	0.43
53:AF:66:LEU:O	53:AF:70:MET:HG3	2.18	0.43
48:BA:369:THR:H	48:BA:384:TYR:HB2	1.84	0.43
53:BF:48:LYS:HB2	53:BF:48:LYS:HE3	1.76	0.43
2:B:130:THR:OG1	2:B:158:CYS:SG	2.77	0.43
2:B:193:GLU:HB3	9:I:183:PHE:CE2	2.54	0.43
6:F:206:GLY:HA2	6:F:217:GLU:OE2	2.19	0.43
6:F:433:ASP:O	6:F:437:GLU:HG2	2.18	0.43
7:G:351:ASP:N	7:G:355:ARG:O	2.46	0.43
13:M:258:LYS:HA	13:M:258:LYS:HD3	1.91	0.43
14:N:193:GLY:HA2	14:N:229:GLY:HA2	2.00	0.43
47:z:34:TYR:N	47:z:34:TYR:CD2	2.86	0.43
47:z:180:VAL:HG12	47:z:189:LEU:HD12	1.99	0.43
48:BA:128:PHE:CE2	48:BA:150:THR:HB	2.53	0.43
48:BA:446:LEU:HD23	48:BA:446:LEU:HA	1.90	0.43
48:BA:471:ASP:OD1	48:BA:472:PHE:N	2.51	0.43
2:B:87:MET:HB2	2:B:122:SER:OG	2.18	0.43
12:L:225:LEU:HB3	12:L:268:MET:CE	2.49	0.43
13:M:112:MET:HE2	13:M:120:ILE:HD11	2.01	0.43
14:N:245:PRO:HD2	14:N:246:PHE:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:u:44:GLU:OE2	43:u:48:VAL:HG23	2.19	0.43
49:AB:288:LYS:HE3	49:AB:290:GLU:H	1.83	0.43
48:BA:428:LEU:HD22	49:BB:117:LYS:CD	2.47	0.43
49:BB:156:VAL:HB	49:BB:210:ARG:HH12	1.83	0.43
49:BB:337:GLN:OE1	49:BB:408:TYR:OH	2.36	0.43
50:BC:97:ILE:HG13	50:BC:279:TRP:HH2	1.84	0.43
54:BG:27:TRP:HA	54:BG:30:LEU:HD13	2.00	0.43
6:F:127:LYS:HG2	6:F:173:ARG:HH21	1.84	0.43
13:M:434:ASN:HD22	13:M:434:ASN:HA	1.58	0.43
45:x:45:VAL:CG2	46:y:72:GLN:HE21	2.32	0.43
48:AA:132:LEU:HD12	48:AA:183:ASN:HB3	2.00	0.43
52:AE:103:CYS:SG	67:AE:400:HEM:CAB	3.07	0.43
52:AE:152:LYS:HE2	52:AE:152:LYS:HB2	1.76	0.43
52:AE:303:LEU:HD22	53:AF:64:GLN:HG2	2.01	0.43
55:BH:23:LYS:HB2	55:BH:24:PRO:HD3	2.00	0.43
2:B:101:THR:HG22	2:B:108:LEU:HG	2.00	0.43
5:E:161:ASP:OD2	5:E:163:LEU:HD12	2.18	0.43
6:F:343:GLY:HA3	6:F:372:LEU:O	2.19	0.43
13:M:411:ASN:HD21	38:m:55:ASP:HB3	1.84	0.43
14:N:32:LEU:HD21	14:N:57:LEU:HB3	2.00	0.43
48:BA:151:SER:OG	48:BA:162:THR:OG1	2.32	0.43
52:BE:226:MET:HB2	67:BE:400:HEM:C1D	2.53	0.43
7:G:83:VAL:HG11	7:G:98:ALA:HB2	1.99	0.43
10:J:21:LYS:HB3	10:J:76:ILE:HD11	2.00	0.43
16:P:150:GLU:OE1	16:P:156:PHE:N	2.49	0.43
39:n:58:VAL:HG13	39:n:63:ARG:CZ	2.48	0.43
50:AC:273:PRO:HA	51:BD:223:LEU:HD11	2.01	0.43
8:H:302:VAL:C	8:H:305:PRO:HD2	2.44	0.43
14:N:214:THR:HG22	14:N:285:SER:OG	2.18	0.43
16:P:239:LYS:HD3	16:P:240:TYR:CZ	2.54	0.43
26:Z:119:LYS:HA	26:Z:119:LYS:HD2	1.58	0.43
42:q:104:THR:HG23	42:q:107:GLU:OE2	2.18	0.43
46:y:175:ILE:HG23	46:y:181:TRP:CD1	2.54	0.43
48:AA:112:GLU:OE1	48:AA:118:GLY:N	2.48	0.43
48:AA:182:ARG:HH12	48:AA:280:ASP:HB2	1.83	0.43
49:AB:142:PHE:CE2	49:AB:258:VAL:HG23	2.54	0.43
50:BC:341:LEU:HD12	50:BC:341:LEU:HA	1.86	0.43
53:BF:97:MET:CE	53:BF:100:LEU:HD22	2.49	0.43
55:BH:26:LEU:HD23	55:BH:26:LEU:HA	1.71	0.43
8:H:59:ILE:CD1	61:H:500:UQ9:H21A	2.44	0.43
48:AA:114:PRO:HG2	48:AA:115:TYR:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:158:GLN:NE2	48:AA:443:ARG:HA	2.33	0.43
49:AB:98:ARG:O	49:AB:109:ALA:HA	2.19	0.43
49:AB:107:ARG:HB2	49:AB:280:VAL:HG22	2.01	0.43
49:AB:225:VAL:HB	51:AD:85:LYS:HG3	2.01	0.43
49:AB:231:GLU:O	49:AB:235:ASP:OD2	2.36	0.43
50:AC:318:TYR:N	50:AC:318:TYR:CD1	2.87	0.43
68:AC:503:UQ5:H151	68:AC:503:UQ5:H171	1.74	0.43
53:AF:11:PRO:HG3	53:AF:21:MET:HE2	1.99	0.43
48:BA:314:PHE:CE2	48:BA:481:LEU:HD23	2.54	0.43
49:BB:84:ILE:HD12	49:BB:84:ILE:N	2.34	0.43
50:BC:26:TYR:OH	50:BC:208:HIS:O	2.27	0.43
4:D:113:ASN:OD1	4:D:335:LYS:NZ	2.52	0.42
5:E:206:VAL:HA	5:E:209:ILE:HD12	2.01	0.42
6:F:436:GLN:O	6:F:439:THR:OG1	2.36	0.42
9:I:141:GLU:HB2	9:I:154:ARG:HB3	2.00	0.42
18:R:45:MET:O	18:R:48:ARG:NH1	2.52	0.42
52:AE:143:GLU:N	52:AE:143:GLU:OE2	2.52	0.42
49:BB:47:PRO:CB	49:BB:51:LEU:HD23	2.49	0.42
51:BD:154:LEU:HB2	51:BD:269:LEU:HB2	2.00	0.42
1:A:29:PHE:CZ	2:B:76:MET:HE1	2.54	0.42
3:C:53:VAL:CG1	3:C:77:LEU:HB3	2.49	0.42
4:D:296:PRO:HA	4:D:297:PRO:HD3	1.96	0.42
7:G:103:PRO:HG3	7:G:155:ARG:CD	2.49	0.42
8:H:56:LEU:HA	8:H:59:ILE:HG12	2.01	0.42
12:L:40:SER:HA	12:L:90:THR:HB	2.01	0.42
12:L:214:ARG:NH2	38:m:58:MET:HG2	2.34	0.42
12:L:471:ALA:CB	35:j:31:LEU:HD11	2.49	0.42
13:M:79:ASN:CG	34:i:40:ILE:HG13	2.44	0.42
13:M:202:ILE:HG23	34:i:34:HIS:CE1	2.55	0.42
14:N:227:PHE:HE2	14:N:286:TYR:CE2	2.36	0.42
14:N:337:GLY:O	34:i:48:ILE:HG21	2.19	0.42
16:P:232:PRO:HB3	16:P:337:GLN:HB3	2.00	0.42
22:V:35:ASP:OD2	22:V:35:ASP:C	2.62	0.42
29:c:31:LYS:HE3	29:c:32:HIS:HE1	1.84	0.42
48:AA:97:PRO:HG2	49:AB:451:LEU:HD13	2.01	0.42
51:AD:171:PRO:HG2	51:AD:221:ILE:CD1	2.49	0.42
52:AE:141:ASN:OD1	52:AE:145:GLU:O	2.36	0.42
52:AE:184:LYS:HG3	52:AE:260:ALA:HB1	2.01	0.42
53:AF:70:MET:HE2	53:AF:70:MET:HB3	1.92	0.42
52:BE:96:HIS:HE1	52:BE:130:MET:SD	2.43	0.42
8:H:270:SER:O	8:H:274:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:66:LEU:HD12	11:K:66:LEU:HA	1.67	0.42
12:L:412:TYR:CD2	37:I:101:LYS:HG2	2.54	0.42
12:L:653:LEU:HD23	25:Y:76:TYR:CD1	2.53	0.42
12:L:663:TYR:HB2	25:Y:107:LEU:HD22	2.01	0.42
14:N:75:LEU:HD12	32:f:79:GLN:HG2	2.02	0.42
15:O:37:GLY:HA2	45:x:204:ARG:HH12	1.83	0.42
35:j:12:TYR:HB3	36:k:21:HIS:CD2	2.54	0.42
40:o:44:GLU:O	40:o:47:LEU:HD23	2.19	0.42
48:AA:249:MET:HE3	48:AA:253:PHE:CD2	2.53	0.42
48:AA:254:THR:O	48:AA:258:MET:HG3	2.19	0.42
50:AC:77:ASP:O	51:AD:142:LYS:HG3	2.20	0.42
9:I:60:TRP:NE1	28:b:8:ARG:HE	2.17	0.42
10:J:164:ILE:O	10:J:168:VAL:HG23	2.20	0.42
13:M:80:ILE:N	13:M:80:ILE:HD12	2.34	0.42
13:M:448:LYS:NZ	38:m:4:GLY:C	2.77	0.42
18:R:45:MET:HE1	18:R:52:SER:HB3	2.00	0.42
48:AA:104:TYR:OH	48:AA:439:GLU:HA	2.19	0.42
50:AC:271:THR:HG21	51:BD:221:ILE:H	1.84	0.42
52:AE:190:GLN:H	52:AE:190:GLN:CD	2.16	0.42
69:BC:503:UQ7:H322	69:BC:503:UQ7:H28	1.66	0.42
4:D:293:LYS:HD3	4:D:293:LYS:HA	1.60	0.42
8:H:91:VAL:O	8:H:167:LEU:HD12	2.20	0.42
12:L:375:PHE:HE1	12:L:456:CYS:HB3	1.84	0.42
12:L:396:THR:HG23	12:L:478:GLY:N	2.35	0.42
12:L:483:ASP:OD2	40:o:41:ARG:HD3	2.20	0.42
14:N:119:ARG:O	46:y:239:ASP:HB2	2.20	0.42
14:N:279:ARG:O	14:N:283:TYR:HB3	2.19	0.42
14:N:354:LEU:HD23	14:N:354:LEU:HA	1.94	0.42
16:P:311:PRO:O	16:P:314:ILE:HG22	2.19	0.42
23:W:120:LYS:HA	23:W:120:LYS:HD3	1.61	0.42
48:AA:300:ARG:HH22	48:AA:494:SER:CA	2.32	0.42
49:AB:498:LYS:HD3	49:AB:499:TYR:CE2	2.54	0.42
51:AD:229:TYR:CE2	51:AD:248:ARG:HB2	2.54	0.42
48:BA:448:TYR:CG	48:BA:452:LYS:HE2	2.54	0.42
49:BB:424:MET:HB3	49:BB:525:ARG:HB3	2.01	0.42
3:C:112:GLU:OE1	3:C:126:HIS:HD2	2.03	0.42
7:G:649:ASP:OD1	7:G:651:ARG:NH1	2.49	0.42
8:H:110:LEU:HD11	8:H:167:LEU:HD11	2.00	0.42
8:H:206:PRO:O	8:H:209:GLU:OE1	2.38	0.42
11:K:52:SER:HB2	26:Z:138:LEU:HD21	2.01	0.42
12:L:453:ILE:HG21	36:k:24:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:448:LYS:NZ	38:m:4:GLY:HA2	2.32	0.42
16:P:125:PRO:HG3	63:P:500:NDP:H2A	2.00	0.42
22:V:83:CYS:HB2	22:V:89:LEU:HD21	2.02	0.42
26:Z:105:LEU:HD12	26:Z:105:LEU:HA	1.77	0.42
34:i:77:ASP:HB3	34:i:80:ASP:OD2	2.20	0.42
45:x:61:GLN:NE2	45:x:79:ALA:O	2.52	0.42
48:AA:318:GLY:HA2	48:AA:374:ILE:HG23	2.02	0.42
50:AC:170:TRP:CH2	68:AC:503:UQ5:H28	2.54	0.42
51:AD:176:ARG:HD2	51:AD:208:TRP:CH2	2.55	0.42
51:AD:248:ARG:HA	51:AD:248:ARG:HD2	1.90	0.42
48:BA:141:ARG:HA	48:BA:141:ARG:HD3	1.79	0.42
5:E:202:THR:H	5:E:205:LYS:HB3	1.85	0.42
12:L:484:MET:HE2	12:L:484:MET:HB3	1.82	0.42
14:N:408:CYS:SG	14:N:480:LEU:CD2	2.91	0.42
51:AD:175:ARG:NH2	51:AD:243:ILE:HG23	2.35	0.42
51:AD:209:LEU:HD12	51:AD:210:VAL:N	2.34	0.42
48:BA:212:PHE:CE2	48:BA:486:PHE:CD1	3.08	0.42
48:BA:473:THR:O	48:BA:477:ILE:HG23	2.19	0.42
49:BB:124:TRP:CZ3	49:BB:282:ALA:HB3	2.55	0.42
49:BB:213:ARG:O	49:BB:217:VAL:HG23	2.19	0.42
49:BB:245:THR:HG21	49:BB:320:SER:H	1.84	0.42
52:BE:182:VAL:HG21	67:BE:400:HEM:HMA1	2.00	0.42
3:C:139:GLU:HG3	23:W:102:GLN:HE22	1.83	0.42
24:X:33:ASN:CG	26:Z:87:PRO:HG2	2.45	0.42
40:o:33:LEU:C	40:o:36:PRO:HD2	2.45	0.42
40:o:33:LEU:O	40:o:36:PRO:HD2	2.20	0.42
50:AC:41:LEU:HD23	50:AC:41:LEU:HA	1.85	0.42
49:BB:361:MET:HE1	49:BB:492:VAL:HG11	2.01	0.42
7:G:103:PRO:HG3	7:G:155:ARG:HD3	2.00	0.42
12:L:74:TRP:CH2	12:L:138:LEU:HD13	2.55	0.42
12:L:586:PHE:HB2	13:M:297:THR:HG23	2.01	0.42
13:M:279:PHE:CD1	38:m:71:LEU:HD23	2.47	0.42
14:N:227:PHE:CE2	14:N:286:TYR:OH	2.72	0.42
42:q:45:HIS:CD2	42:q:75[A]:TRP:CH2	3.08	0.42
49:AB:200:ILE:O	49:AB:204:SER:OG	2.35	0.42
50:AC:318:TYR:HD2	53:AF:47:ILE:HD11	1.84	0.42
50:BC:345:ILE:HD13	50:BC:345:ILE:HA	1.80	0.42
7:G:213:THR:HG23	7:G:215:MET:SD	2.60	0.42
7:G:611:VAL:HG13	7:G:617:ILE:HD11	2.01	0.42
9:I:154:ARG:NE	9:I:156:ASP:OD2	2.47	0.42
15:O:69:LEU:O	15:O:73:THR:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:13:ARG:O	39:n:17:LYS:HG2	2.20	0.42
45:x:157:GLU:HG3	45:x:174:VAL:O	2.20	0.42
48:AA:459:LYS:O	48:AA:463:GLN:HG3	2.20	0.42
49:AB:111:GLU:HB2	49:AB:464:ILE:HD11	2.02	0.42
50:AC:289:ARG:NH2	50:AC:350:VAL:HG22	2.35	0.42
52:AE:204:PRO:HD3	52:AE:215:TYR:CZ	2.54	0.42
53:AF:41:PRO:HG3	53:AF:51:LEU:HD22	2.01	0.42
51:BD:165:VAL:HG23	51:BD:172:VAL:HB	2.02	0.42
54:BG:24:THR:HA	54:BG:27:TRP:CZ2	2.55	0.42
7:G:439:LEU:HD21	7:G:502:PHE:CZ	2.55	0.41
8:H:205:LEU:N	8:H:206:PRO:HD2	2.34	0.41
13:M:17:LEU:O	13:M:20:VAL:HG23	2.19	0.41
13:M:24:ILE:O	13:M:27:LEU:HB2	2.19	0.41
18:R:41:THR:HG21	18:R:52:SER:HB2	2.01	0.41
25:Y:16:LEU:O	25:Y:20:ILE:HD12	2.19	0.41
25:Y:94:ASN:O	25:Y:94:ASN:OD1	2.37	0.41
32:f:28:ASN:HB3	32:f:81:SER:OG	2.19	0.41
41:p:54:LYS:HB3	41:p:73:LEU:HD13	2.02	0.41
42:q:43:LYS:HD2	42:q:43:LYS:HA	1.82	0.41
48:AA:87:LEU:CD1	48:AA:258:MET:HB2	2.49	0.41
48:AA:319:TRP:HA	48:AA:319:TRP:CE3	2.55	0.41
49:BB:147:ILE:HG13	49:BB:200:ILE:CD1	2.49	0.41
13:M:207:GLU:HB3	41:p:24:TYR:CG	2.55	0.41
20:T:46:VAL:O	20:T:50:VAL:HG12	2.20	0.41
37:l:121:LEU:HD23	37:l:121:LEU:HA	1.92	0.41
50:AC:75:MET:HE3	50:AC:75:MET:HB3	1.75	0.41
51:AD:138:MET:HE1	69:BC:503:UQ7:H271	2.02	0.41
52:AE:305:VAL:HG21	53:AF:65:ARG:HG3	2.00	0.41
57:AJ:38:VAL:O	57:AJ:40:PRO:HD3	2.20	0.41
48:BA:113:ALA:HA	48:BA:114:PRO:HA	1.88	0.41
49:BB:429:LYS:HE2	49:BB:433:ARG:NH1	2.35	0.41
7:G:702:LEU:HB3	19:S:36:TYR:HD2	1.86	0.41
11:K:39:LEU:HD12	11:K:39:LEU:HA	1.80	0.41
12:L:242:LEU:HD12	12:L:242:LEU:HA	1.84	0.41
12:L:377:LEU:HD22	35:j:24:HIS:CD2	2.56	0.41
14:N:339:ILE:CD1	14:N:498:TYR:HE1	2.34	0.41
19:S:3:TRP:NE1	19:S:87:GLU:OE2	2.54	0.41
24:X:28:ARG:HG2	24:X:63:LEU:HD22	2.02	0.41
48:AA:291:LYS:HA	48:AA:291:LYS:HD3	1.93	0.41
49:AB:451:LEU:HD21	49:AB:477:THR:HG21	2.02	0.41
48:BA:268:GLU:HB3	48:BA:269:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:187:ASP:OD2	49:BB:187:ASP:C	2.63	0.41
52:BE:201:ARG:NH2	52:BE:218:TYR:OH	2.53	0.41
3:C:60:CYS:HB3	4:D:354:LYS:HG2	2.02	0.41
5:E:185:ASP:OD2	5:E:218:LYS:NZ	2.47	0.41
10:J:52:ILE:HD13	10:J:52:ILE:HA	1.80	0.41
13:M:303:ASP:C	13:M:303:ASP:OD2	2.63	0.41
14:N:480:LEU:HD23	14:N:480:LEU:HA	1.86	0.41
19:S:40:LYS:HA	19:S:40:LYS:HD2	1.90	0.41
19:S:61:TRP:CE2	19:S:71:CYS:HB3	2.54	0.41
36:k:14:ARG:HD3	36:k:17:GLU:OE2	2.20	0.41
50:AC:317:MET:HE2	50:AC:379:GLY:HA3	2.02	0.41
1:A:112:LYS:HA	1:A:112:LYS:HD2	1.86	0.41
3:C:1:MET:HE2	3:C:1:MET:HB2	1.91	0.41
6:F:76:LEU:HD11	6:F:204:LEU:HD11	2.03	0.41
6:F:426:ASN:HB2	6:F:476:ARG:CZ	2.50	0.41
7:G:315:ILE:HD12	7:G:336:TYR:HB3	2.03	0.41
7:G:396:LEU:HA	7:G:657:VAL:HG11	2.01	0.41
8:H:160:ILE:HD13	8:H:315:SER:HB3	2.03	0.41
12:L:341:HIS:NE2	12:L:345:LYS:HG3	2.36	0.41
15:O:92:SER:HB2	15:O:94:GLU:OE2	2.20	0.41
23:W:124:LEU:HD12	23:W:124:LEU:HA	1.92	0.41
24:X:74:GLU:CD	24:X:74:GLU:H	2.28	0.41
24:X:88:GLU:CD	27:a:39:HIS:HE2	2.27	0.41
25:Y:64:THR:O	25:Y:68:THR:HG22	2.20	0.41
25:Y:84:GLN:O	25:Y:88:SER:HA	2.20	0.41
26:Z:26:PRO:HD3	26:Z:30:PHE:CZ	2.56	0.41
50:BC:331:MET:CE	50:BC:368:PHE:CD1	3.02	0.41
1:A:61:PHE:HA	1:A:64:VAL:HG12	2.03	0.41
4:D:64:LEU:HD23	4:D:82:TYR:CD2	2.51	0.41
6:F:446:THR:HB	58:F:501:SF4:S3	2.60	0.41
12:L:531:VAL:O	12:L:535:VAL:HG22	2.21	0.41
13:M:257:LEU:HD23	13:M:257:LEU:HA	1.78	0.41
13:M:493:LYS:HB3	13:M:493:LYS:HE2	1.85	0.41
15:O:123:ARG:HG2	15:O:123:ARG:HH11	1.85	0.41
16:P:239:LYS:HD3	16:P:240:TYR:CE1	2.55	0.41
16:P:373:TYR:OH	23:W:49:VAL:HG11	2.21	0.41
23:W:75:ILE:O	23:W:79:ILE:HG13	2.21	0.41
30:d:74:ARG:HH22	34:i:47:PRO:HG3	1.84	0.41
37:l:47:LEU:HB2	38:m:16:TRP:HB2	2.03	0.41
41:p:69:LYS:HA	41:p:69:LYS:HD2	1.82	0.41
48:AA:285:PRO:HA	48:AA:286:PRO:HD2	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AB:308:THR:H	49:AB:308:THR:HG1	1.57	0.41
49:BB:106:LEU:HD11	49:BB:279:MET:HE2	2.02	0.41
9:I:60:TRP:CZ2	28:b:8:ARG:HG3	2.56	0.41
12:L:37:SER:O	12:L:41:ILE:HG13	2.19	0.41
14:N:332:ILE:HG21	14:N:413:LEU:HD22	2.01	0.41
63:P:500:NDP:H2N	63:P:500:NDP:H2D	1.82	0.41
29:c:84:TYR:C	29:c:86:LYS:H	2.29	0.41
31:e:49:LYS:HB2	31:e:49:LYS:HE2	1.73	0.41
39:n:28:LEU:HD12	39:n:28:LEU:HA	1.93	0.41
50:AC:275:ILE:HG21	51:BD:236:CYS:SG	2.61	0.41
48:BA:396:ILE:HD12	48:BA:396:ILE:N	2.27	0.41
52:BE:65:ASP:OD1	52:BE:65:ASP:N	2.52	0.41
3:C:177:TYR:OH	3:C:179:ASP:OD1	2.30	0.41
5:E:96:VAL:O	5:E:100:ILE:HG12	2.21	0.41
6:F:138:VAL:HG11	6:F:161:LEU:HD11	2.03	0.41
6:F:429:LEU:HD11	6:F:474:ARG:HH21	1.85	0.41
7:G:516:VAL:HG13	7:G:520:LEU:HD12	2.02	0.41
10:J:53:PHE:O	10:J:57:TYR:HB2	2.21	0.41
13:M:30:PRO:HG2	13:M:33:ARG:HG2	2.03	0.41
13:M:384:PHE:CE1	13:M:467:LEU:HD22	2.56	0.41
16:P:181:ILE:CD1	16:P:269:LEU:HD11	2.50	0.41
30:d:50:VAL:O	30:d:54:VAL:HG23	2.21	0.41
31:e:25:MET:HE3	31:e:25:MET:HB3	1.98	0.41
42:q:45:HIS:HD2	42:q:75[A]:TRP:CZ2	2.39	0.41
43:u:20:SER:O	43:u:24:VAL:HG23	2.21	0.41
44:v:75:LYS:HG3	44:v:76:VAL:HG12	2.03	0.41
45:x:244:GLU:OE1	45:x:247:LYS:HE2	2.21	0.41
48:AA:457:PHE:O	48:AA:461:VAL:HG23	2.21	0.41
49:AB:70:ASN:O	49:AB:70:ASN:CG	2.59	0.41
50:AC:208:HIS:NE2	68:AC:502:UQ5:H4M3	2.35	0.41
51:AD:166:LYS:HE3	51:AD:166:LYS:HB3	1.73	0.41
51:AD:265:GLU:HG2	51:AD:268:LYS:HB3	2.03	0.41
52:AE:141:ASN:OD1	52:AE:141:ASN:N	2.41	0.41
53:AF:121:ILE:HG22	50:BC:15:ILE:HB	2.03	0.41
1:A:63:LEU:HA	1:A:63:LEU:HD23	1.83	0.41
2:B:210:LYS:HE3	2:B:210:LYS:HB2	1.70	0.41
5:E:132:THR:HA	6:F:392:ARG:HH21	1.85	0.41
7:G:152:LYS:O	7:G:156:GLU:HG3	2.21	0.41
8:H:33:PHE:CE2	27:a:5:TRP:HA	2.56	0.41
9:I:126:CYS:SG	9:I:128:LEU:HB2	2.61	0.41
10:J:66:LEU:HD12	10:J:66:LEU:HA	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:443:LEU:HB3	36:k:28:MET:CE	2.51	0.41
13:M:79:ASN:ND2	34:i:40:ILE:HG13	2.36	0.41
13:M:221:PHE:CE1	13:M:225:ALA:HB2	2.56	0.41
14:N:189:ILE:HG23	14:N:232:PHE:CD2	2.56	0.41
14:N:261:VAL:O	14:N:265:LEU:HG	2.21	0.41
23:W:60:SER:O	23:W:64:ARG:HG3	2.20	0.41
24:X:88:GLU:OE2	27:a:39:HIS:CD2	2.71	0.41
25:Y:45:ARG:HH12	25:Y:48:ARG:HH22	1.63	0.41
31:e:1:MET:HG3	31:e:1:MET:O	2.20	0.41
36:k:34:GLY:HA2	36:k:37:ILE:HD12	2.02	0.41
39:n:58:VAL:CG1	39:n:63:ARG:HH21	2.26	0.41
39:n:70:HIS:O	39:n:74:GLU:HG2	2.21	0.41
46:y:133:VAL:CG1	47:z:147:MET:CE	2.96	0.41
49:AB:254:PRO:HD2	49:AB:257:ASN:HD22	1.86	0.41
49:AB:333:LEU:HD12	49:AB:511:GLY:HA2	2.01	0.41
50:AC:94:MET:HB3	50:AC:242:PHE:HE1	1.85	0.41
52:AE:307:ASN:OD1	52:AE:307:ASN:N	2.53	0.41
52:BE:80:HIS:HB2	52:BE:264:MET:HE2	2.03	0.41
52:BE:99:TYR:CD1	52:BE:103:CYS:HB2	2.55	0.41
4:D:292:ARG:HB2	7:G:192:ARG:CZ	2.51	0.41
7:G:591:VAL:HA	7:G:594:ILE:HD12	2.02	0.41
11:K:90:ILE:HD12	11:K:90:ILE:HA	1.83	0.41
13:M:97:THR:HG23	13:M:130:MET:HE3	2.02	0.41
14:N:191:LEU:HD12	14:N:191:LEU:HA	1.89	0.41
17:Q:82:LEU:HD13	23:W:132:TYR:CE1	2.56	0.41
22:V:144:LYS:C	22:V:144:LYS:HD3	2.46	0.41
30:d:73:ARG:HD2	30:d:73:ARG:HA	1.86	0.41
50:AC:277:PRO:HB3	68:AC:503:UQ5:O5	2.21	0.41
53:AF:56:ARG:HH22	54:AG:7:LYS:HZ1	1.66	0.41
56:AI:18:LYS:O	56:AI:22:ARG:NH2	2.54	0.41
48:BA:159:MET:HE2	48:BA:159:MET:HB3	1.94	0.41
48:BA:420:LYS:HE2	48:BA:464:LEU:HB2	2.02	0.41
49:BB:228:GLN:O	49:BB:232:VAL:HG23	2.21	0.41
6:F:426:ASN:HA	6:F:476:ARG:NE	2.36	0.40
7:G:733:LYS:O	7:G:737:GLN:HG3	2.21	0.40
12:L:141:GLU:HG3	13:M:392:PRO:HG2	2.03	0.40
14:N:237:PHE:CD1	14:N:273:ILE:HD11	2.56	0.40
14:N:449:PHE:N	14:N:449:PHE:CD1	2.88	0.40
33:g:84:LYS:HE2	33:g:84:LYS:HB2	1.89	0.40
40:o:78:GLU:C	40:o:79:GLU:OE1	2.64	0.40
49:AB:222:MET:HE2	49:AB:222:MET:HB3	1.72	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BA:112:GLU:O	48:BA:116:PHE:HB2	2.20	0.40
48:BA:330:VAL:HG12	48:BA:334:LEU:HD11	2.03	0.40
49:BB:221:GLU:O	49:BB:225:VAL:HG12	2.20	0.40
49:BB:443:ARG:O	49:BB:447:LYS:HG3	2.21	0.40
55:BH:15:GLU:HA	55:BH:18:LYS:CD	2.51	0.40
4:D:341:PHE:HB3	4:D:354:LYS:HB3	2.03	0.40
6:F:443:GLU:OE2	6:F:456:TRP:NE1	2.49	0.40
12:L:104:MET:HE3	12:L:104:MET:HB3	1.98	0.40
12:L:273:SER:OG	12:L:274:PRO:HD3	2.22	0.40
13:M:387:ALA:O	13:M:396:SER:OG	2.29	0.40
14:N:218:ILE:CG1	14:N:286:TYR:OH	2.70	0.40
40:o:9:LYS:HA	40:o:29:MET:HE1	2.01	0.40
47:z:37:GLU:HG2	47:z:39:LEU:HG	2.02	0.40
47:z:143:THR:HG22	47:z:161:GLY:H	1.86	0.40
48:AA:121:HIS:CE1	48:AA:198:MET:HG2	2.56	0.40
50:AC:115:PRO:HG3	53:AF:42:LEU:HB3	2.03	0.40
50:AC:303:LEU:HA	50:AC:306:ILE:HD12	2.02	0.40
52:AE:192:TYR:OH	67:AE:400:HEM:O1A	2.27	0.40
3:C:31:PHE:HE1	3:C:86:ILE:HD11	1.85	0.40
3:C:156:ARG:NH2	16:P:90:LYS:HE3	2.36	0.40
5:E:42:LYS:HG3	5:E:44:ASP:OD2	2.21	0.40
6:F:285:PHE:CZ	6:F:295:GLY:HA3	2.57	0.40
10:J:6:LEU:O	10:J:36:ASP:OD1	2.39	0.40
11:K:7:PHE:CZ	14:N:196:MET:HE1	2.56	0.40
11:K:42:VAL:HG11	14:N:191:LEU:HG	2.04	0.40
12:L:524:PHE:HD1	12:L:524:PHE:HA	1.71	0.40
13:M:17:LEU:CA	13:M:20:VAL:HG22	2.50	0.40
13:M:113:ARG:HH11	47:z:113:LEU:CD2	2.34	0.40
13:M:485:VAL:O	13:M:489:VAL:HG23	2.22	0.40
14:N:280:VAL:HG12	14:N:281:PHE:CD1	2.56	0.40
17:Q:106:LEU:HD12	17:Q:106:LEU:HA	1.89	0.40
19:S:34:LYS:NZ	19:S:34:LYS:HB2	2.36	0.40
27:a:36:ARG:HB2	27:a:37:PRO:HD2	2.04	0.40
40:o:45:PHE:HB2	40:o:47:LEU:CD2	2.50	0.40
42:q:82:ASP:OD1	42:q:82:ASP:C	2.64	0.40
49:AB:501:TYR:OH	56:AI:22:ARG:O	2.29	0.40
48:BA:122:LEU:N	48:BA:198:MET:HE1	2.37	0.40
49:BB:451:LEU:HA	49:BB:451:LEU:HD12	1.88	0.40
50:BC:367:LEU:HD23	50:BC:367:LEU:HA	1.89	0.40
69:BC:503:UQ7:H122	69:BC:503:UQ7:H162	1.89	0.40
2:B:204:LYS:HB3	2:B:204:LYS:HE3	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ILE:HG13	5:E:102:VAL:HG22	2.03	0.40
9:I:191:GLU:H	9:I:191:GLU:CD	2.30	0.40
12:L:537:LEU:HD13	12:L:537:LEU:HA	1.96	0.40
12:L:554:ARG:HD2	12:L:554:ARG:HA	1.91	0.40
27:a:49:MET:HA	27:a:49:MET:HE2	2.03	0.40
46:y:16:ARG:O	46:y:20:GLN:HG3	2.21	0.40
49:AB:325:GLU:HG3	54:AG:14:ALA:HB3	2.03	0.40
50:AC:260:PRO:HB2	52:AE:185:ALA:C	2.46	0.40
52:AE:273:LYS:NZ	56:AI:43:ASP:OD1	2.54	0.40
48:BA:67:PRO:HA	48:BA:68:PRO:HD3	1.97	0.40
68:BC:502:UQ5:C13	68:BC:502:UQ5:H101	2.51	0.40
54:BG:69:GLU:OE1	54:BG:70:HIS:ND1	2.54	0.40
55:BH:16:SER:O	55:BH:19:PRO:HD2	2.21	0.40
55:BH:23:LYS:HB2	55:BH:23:LYS:HE2	1.68	0.40
1:A:55:SER:O	1:A:56:ARG:HD2	2.21	0.40
4:D:292:ARG:HH12	7:G:193:GLY:N	2.17	0.40
7:G:324:ASN:HB2	7:G:327:TRP:O	2.22	0.40
15:O:88:ILE:O	15:O:88:ILE:HG13	2.22	0.40
29:c:32:HIS:CB	29:c:35:ARG:NE	2.80	0.40
40:o:22:ILE:O	41:p:64:VAL:HG11	2.21	0.40
48:AA:125:ARG:HD2	48:AA:198:MET:HG3	2.03	0.40
49:AB:261:ILE:HD13	49:AB:261:ILE:HA	1.93	0.40
51:AD:195:ASP:HB3	51:AD:255:ASN:HD21	1.86	0.40
48:BA:230:LEU:HD12	48:BA:230:LEU:HA	1.91	0.40
49:BB:48:PRO:HD2	49:BB:51:LEU:HD22	2.04	0.40
50:BC:112:TYR:HB3	50:BC:120:TRP:CD2	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	A	90/119 (76%)	88 (98%)	2 (2%)	0	100	100
2	B	24/218 (11%)	24 (100%)	0	0	100	100
3	C	5/190 (3%)	5 (100%)	0	0	100	100
4	D	378/394 (96%)	362 (96%)	15 (4%)	1 (0%)	36	66
5	E	190/255 (74%)	181 (95%)	9 (5%)	0	100	100
6	F	432/486 (89%)	420 (97%)	12 (3%)	0	100	100
7	G	685/748 (92%)	665 (97%)	20 (3%)	0	100	100
8	H	322/325 (99%)	316 (98%)	6 (2%)	0	100	100
9	I	163/222 (73%)	162 (99%)	1 (1%)	0	100	100
10	J	172/205 (84%)	170 (99%)	2 (1%)	0	100	100
11	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
12	L	405/669 (60%)	393 (97%)	12 (3%)	0	100	100
18	R	15/110 (14%)	14 (93%)	1 (7%)	0	100	100
19	S	91/97 (94%)	90 (99%)	1 (1%)	0	100	100
20	T	54/122 (44%)	51 (94%)	3 (6%)	0	100	100
21	U	19/126 (15%)	19 (100%)	0	0	100	100
22	V	1/169 (1%)	1 (100%)	0	0	100	100
23	W	93/133 (70%)	88 (95%)	5 (5%)	0	100	100
24	X	96/106 (91%)	94 (98%)	2 (2%)	0	100	100
25	Y	108/159 (68%)	104 (96%)	4 (4%)	0	100	100
26	Z	84/143 (59%)	80 (95%)	4 (5%)	0	100	100
27	a	56/65 (86%)	56 (100%)	0	0	100	100
28	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
29	c	74/88 (84%)	71 (96%)	3 (4%)	0	100	100
30	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
31	e	63/83 (76%)	62 (98%)	1 (2%)	0	100	100
32	f	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
33	g	77/114 (68%)	76 (99%)	1 (1%)	0	100	100
34	i	81/98 (83%)	79 (98%)	2 (2%)	0	100	100
35	j	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
36	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100
37	l	70/125 (56%)	68 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
39	n	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
40	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
41	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
42	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
43	u	53/63 (84%)	50 (94%)	3 (6%)	0	100	100
44	v	27/113 (24%)	26 (96%)	1 (4%)	0	100	100
45	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
46	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
47	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
48	AA	296/503 (59%)	287 (97%)	9 (3%)	0	100	100
48	BA	416/503 (83%)	402 (97%)	14 (3%)	0	100	100
49	AB	485/531 (91%)	473 (98%)	12 (2%)	0	100	100
49	BB	485/531 (91%)	478 (99%)	7 (1%)	0	100	100
50	AC	385/393 (98%)	378 (98%)	7 (2%)	0	100	100
50	BC	385/393 (98%)	377 (98%)	8 (2%)	0	100	100
51	AD	194/272 (71%)	181 (93%)	13 (7%)	0	100	100
51	BD	193/272 (71%)	182 (94%)	11 (6%)	0	100	100
52	AE	242/307 (79%)	239 (99%)	3 (1%)	0	100	100
52	BE	242/307 (79%)	240 (99%)	2 (1%)	0	100	100
53	AF	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
53	BF	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
54	AG	67/72 (93%)	67 (100%)	0	0	100	100
54	BG	66/72 (92%)	66 (100%)	0	0	100	100
55	AH	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
55	BH	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
56	AI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
56	BI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
57	AJ	26/57 (46%)	26 (100%)	0	0	100	100
57	BJ	26/57 (46%)	24 (92%)	2 (8%)	0	100	100
All	All	9425/12399 (76%)	9184 (97%)	240 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	23	HIS

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	A	85/105 (81%)	85 (100%)	0	100	100
2	B	132/184 (72%)	128 (97%)	4 (3%)	36	72
3	C	171/179 (96%)	170 (99%)	1 (1%)	78	92
4	D	331/340 (97%)	327 (99%)	4 (1%)	63	87
5	E	166/220 (76%)	165 (99%)	1 (1%)	78	92
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	570/625 (91%)	561 (98%)	9 (2%)	55	83
8	H	271/272 (100%)	268 (99%)	3 (1%)	65	87
9	I	147/195 (75%)	146 (99%)	1 (1%)	76	91
10	J	156/186 (84%)	153 (98%)	3 (2%)	50	81
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	77
12	L	564/568 (99%)	555 (98%)	9 (2%)	55	83
13	M	433/434 (100%)	427 (99%)	6 (1%)	59	85
14	N	407/416 (98%)	402 (99%)	5 (1%)	63	87
15	O	108/141 (77%)	106 (98%)	2 (2%)	50	81
16	P	263/334 (79%)	258 (98%)	5 (2%)	50	81
17	Q	89/128 (70%)	89 (100%)	0	100	100
18	R	64/97 (66%)	64 (100%)	0	100	100
19	S	82/85 (96%)	80 (98%)	2 (2%)	43	77
20	T	78/112 (70%)	77 (99%)	1 (1%)	61	86
21	U	78/113 (69%)	75 (96%)	3 (4%)	29	64
22	V	123/148 (83%)	123 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	98/114 (86%)	93 (95%)	5 (5%)	21	54
24	X	88/94 (94%)	87 (99%)	1 (1%)	65	87
25	Y	92/120 (77%)	88 (96%)	4 (4%)	26	60
26	Z	100/115 (87%)	96 (96%)	4 (4%)	28	63
27	a	48/53 (91%)	48 (100%)	0	100	100
28	b	35/53 (66%)	33 (94%)	2 (6%)	18	49
29	c	66/71 (93%)	65 (98%)	1 (2%)	57	84
30	d	60/66 (91%)	59 (98%)	1 (2%)	53	83
31	e	60/73 (82%)	60 (100%)	0	100	100
32	f	80/83 (96%)	80 (100%)	0	100	100
33	g	68/96 (71%)	67 (98%)	1 (2%)	57	84
34	i	75/90 (83%)	74 (99%)	1 (1%)	61	86
35	j	42/51 (82%)	40 (95%)	2 (5%)	23	56
36	k	39/60 (65%)	37 (95%)	2 (5%)	21	54
37	l	60/97 (62%)	59 (98%)	1 (2%)	53	83
38	m	58/59 (98%)	57 (98%)	1 (2%)	53	83
39	n	92/99 (93%)	90 (98%)	2 (2%)	45	78
40	o	70/87 (80%)	69 (99%)	1 (1%)	59	85
41	p	80/93 (86%)	77 (96%)	3 (4%)	29	64
42	q	69/133 (52%)	68 (99%)	1 (1%)	59	85
43	u	47/54 (87%)	45 (96%)	2 (4%)	26	60
44	v	22/84 (26%)	22 (100%)	0	100	100
45	x	179/216 (83%)	178 (99%)	1 (1%)	78	92
46	y	221/232 (95%)	220 (100%)	1 (0%)	81	93
47	z	188/228 (82%)	185 (98%)	3 (2%)	55	83
48	AA	347/408 (85%)	334 (96%)	13 (4%)	30	65
48	BA	347/408 (85%)	341 (98%)	6 (2%)	53	83
49	AB	415/452 (92%)	410 (99%)	5 (1%)	63	87
49	BB	415/452 (92%)	410 (99%)	5 (1%)	63	87
50	AC	330/336 (98%)	325 (98%)	5 (2%)	57	84
50	BC	330/336 (98%)	322 (98%)	8 (2%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	AD	170/232 (73%)	168 (99%)	2 (1%)	63	87
51	BD	169/232 (73%)	166 (98%)	3 (2%)	51	82
52	AE	200/247 (81%)	197 (98%)	3 (2%)	57	84
52	BE	200/247 (81%)	197 (98%)	3 (2%)	57	84
53	AF	105/110 (96%)	103 (98%)	2 (2%)	50	81
53	BF	105/110 (96%)	102 (97%)	3 (3%)	37	73
54	AG	63/65 (97%)	63 (100%)	0	100	100
54	BG	62/65 (95%)	62 (100%)	0	100	100
55	AH	58/62 (94%)	58 (100%)	0	100	100
55	BH	57/62 (92%)	57 (100%)	0	100	100
56	AI	48/59 (81%)	47 (98%)	1 (2%)	47	79
56	BI	48/59 (81%)	48 (100%)	0	100	100
57	AJ	16/41 (39%)	16 (100%)	0	100	100
57	BJ	16/41 (39%)	16 (100%)	0	100	100
All	All	10294/11908 (86%)	10134 (98%)	160 (2%)	54	83

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	ILE
2	B	93	CYS
2	B	139	LEU
2	B	164	TYR
3	C	17	LYS
4	D	12	THR
4	D	38	GLU
4	D	75	MET
4	D	287	ILE
5	E	176	VAL
7	G	58	ASN
7	G	83	VAL
7	G	104	ARG
7	G	168	LEU
7	G	213	THR
7	G	319	LEU
7	G	408	VAL
7	G	446	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	647	VAL
8	H	31	MET
8	H	34	VAL
8	H	83	MET
9	I	65	GLU
10	J	72	PHE
10	J	92	ILE
10	J	119	THR
11	K	15	ILE
11	K	90	ILE
12	L	65	ILE
12	L	134	LEU
12	L	152	HIS
12	L	461	ILE
12	L	477	VAL
12	L	537	LEU
12	L	565	PHE
12	L	596	ILE
12	L	659	VAL
13	M	57	ILE
13	M	141	LEU
13	M	181	SER
13	M	277	LEU
13	M	306	LYS
13	M	354	VAL
14	N	20	PHE
14	N	86	LEU
14	N	155	GLN
14	N	217	GLU
14	N	282	ILE
15	O	61	ILE
15	O	88	ILE
16	P	129	ASP
16	P	147	ARG
16	P	151	THR
16	P	250	THR
16	P	349	THR
19	S	7	ILE
19	S	52	GLU
20	T	55	LYS
21	U	95	GLU
21	U	105	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	U	112	ILE
23	W	39	THR
23	W	50	VAL
23	W	70	THR
23	W	105	VAL
23	W	129	THR
24	X	74	GLU
25	Y	37	LEU
25	Y	75	VAL
25	Y	77	ILE
25	Y	114	ILE
26	Z	33	VAL
26	Z	39	ILE
26	Z	105	LEU
26	Z	119	LYS
28	b	13	GLN
28	b	22	LEU
29	c	49	ILE
30	d	47	ASN
33	g	101	LEU
34	i	71	GLN
35	j	11	THR
35	j	22	THR
36	k	5	LEU
36	k	50	GLN
37	l	105	VAL
38	m	71	LEU
39	n	54	VAL
39	n	59	GLU
40	o	16	GLU
41	p	21	GLU
41	p	53	GLU
41	p	70	CYS
42	q	108	LEU
43	u	5	LEU
43	u	28	ILE
45	x	148	TYR
46	y	180	VAL
47	z	13	PHE
47	z	34	TYR
47	z	168	LEU
48	AA	82	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	AA	103	LEU
48	AA	176	VAL
48	AA	312	VAL
48	AA	324	GLU
48	AA	334	LEU
48	AA	372	THR
48	AA	373	SER
48	AA	403	LEU
48	AA	406	VAL
48	AA	416	LEU
48	AA	427	VAL
48	AA	489	VAL
49	AB	90	HIS
49	AB	196	VAL
49	AB	217	VAL
49	AB	326	VAL
49	AB	367	LYS
50	AC	78	VAL
50	AC	85	ARG
50	AC	152	VAL
50	AC	291	ILE
50	AC	304	VAL
51	AD	129	LEU
51	AD	247	ILE
52	AE	110	SER
52	AE	137	VAL
52	AE	266	GLU
53	AF	103	ARG
53	AF	105	ARG
56	AI	57	LYS
48	BA	103	LEU
48	BA	176	VAL
48	BA	293	GLN
48	BA	327	THR
48	BA	436	ILE
48	BA	476	VAL
49	BB	100	THR
49	BB	152	ASP
49	BB	326	VAL
49	BB	451	LEU
49	BB	452	LEU
50	BC	66	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	BC	85	ARG
50	BC	153	ILE
50	BC	191	LEU
50	BC	204	LEU
50	BC	256	VAL
50	BC	331	MET
50	BC	345	ILE
51	BD	136	VAL
51	BD	162	THR
51	BD	209	LEU
52	BE	75	ASN
52	BE	164	GLU
52	BE	289	ARG
53	BF	8	LEU
53	BF	45	LEU
53	BF	67	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	GLN
2	B	203	GLN
3	C	40	GLN
3	C	173	GLN
4	D	91	ASN
4	D	165	GLN
4	D	212	GLN
4	D	281	GLN
4	D	311	HIS
6	F	86	HIS
6	F	101	ASN
6	F	156	HIS
6	F	464	HIS
7	G	184	GLN
7	G	206	ASN
7	G	284	ASN
7	G	302	ASN
7	G	455	ASN
8	H	50	GLN
8	H	176	GLN
10	J	80	HIS
12	L	318	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	341	HIS
13	M	388	ASN
13	M	411	ASN
13	M	434	ASN
13	M	487	ASN
13	M	495	HIS
14	N	291	GLN
14	N	491	HIS
16	P	327	ASN
16	P	343	GLN
17	Q	65	GLN
18	R	40	HIS
18	R	109	HIS
19	S	59	GLN
23	W	66	ASN
23	W	102	GLN
25	Y	84	GLN
25	Y	94	ASN
26	Z	126	ASN
27	a	34	HIS
29	c	27	ASN
29	c	32	HIS
31	e	10	ASN
34	i	10	ASN
34	i	68	GLN
34	i	71	GLN
35	j	18	HIS
40	o	32	HIS
41	p	22	ASN
41	p	66	HIS
42	q	45	HIS
43	u	32	GLN
46	y	42	HIS
46	y	72	GLN
47	z	101	GLN
47	z	107	HIS
47	z	223	ASN
48	AA	320	ASN
48	AA	415	HIS
49	AB	88	HIS
49	AB	268	ASN
49	AB	368	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	AB	396	ASN
50	AC	6	GLN
50	AC	348	GLN
51	AD	96	HIS
51	AD	197	GLN
51	AD	237	HIS
52	AE	100	GLN
52	AE	101	GLN
54	AG	60	GLN
55	AH	42	HIS
48	BA	301	GLN
48	BA	320	ASN
48	BA	463	GLN
49	BB	63	ASN
49	BB	113	ASN
49	BB	169	HIS
49	BB	337	GLN
49	BB	445	GLN
49	BB	453	HIS
49	BB	497	ASN
50	BC	5	ASN
50	BC	59	HIS
51	BD	205	ASN
52	BE	101	GLN
52	BE	247	GLN
53	BF	84	GLN
54	BG	19	GLN
54	BG	20	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	FME	f	1	32	8,9,10	0.80	1 (12%)	8,9,11	1.71	1 (12%)
11	FME	K	1	11	8,9,10	0.99	0	8,9,11	1.10	0
1	FME	A	1	1	8,9,10	1.78	1 (12%)	8,9,11	1.98	3 (37%)

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
32	FME	f	1	32	-	5/7/9/11	-
11	FME	K	1	11	-	6/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	FME	O-C	4.34	1.36	1.20
32	f	1	FME	O-C	2.13	1.28	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	1	FME	O-C-CA	-4.35	113.59	124.77
1	A	1	FME	O-C-CA	-4.16	114.07	124.77
1	A	1	FME	C-CA-N	2.62	114.56	109.50
1	A	1	FME	CA-N-CN	2.23	126.25	122.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	O-C-CA-CB
32	f	1	FME	O1-CN-N-CA
32	f	1	FME	CB-CA-N-CN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	f	1	FME	N-CA-CB-CG
32	f	1	FME	C-CA-CB-CG
32	f	1	FME	CA-CB-CG-SD
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 5 are monoatomic - leaving 26 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	$\# Z > 2$
67	HEM	AE	400	52	50,50,50	1.34	7 (14%)	67,82,82	1.16	5 (7%)
60	FMN	F	500	-	33,33,33	1.04	2 (6%)	48,50,50	1.24	6 (12%)
59	FES	BD	301	51	0,4,4	-	-	-	-	-
67	HEM	BC	501	50	50,50,50	1.66	10 (20%)	67,82,82	1.60	14 (20%)
68	UQ5	BC	502	-	38,38,38	0.46	0	48,49,49	0.69	1 (2%)
68	UQ5	AC	503	-	38,38,38	0.47	0	48,49,49	0.93	1 (2%)
58	SF4	G	802	7	0,12,12	-	-	-	-	-
65	8Q1	W	200	-	32,34,34	0.33	0	39,43,43	0.50	0
58	SF4	I	501	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	HEM	AC	501	50	50,50,50	1.67	8 (16%)	67,82,82	1.57	12 (17%)
67	HEM	AC	500	50	50,50,50	1.36	6 (12%)	67,82,82	1.07	3 (4%)
59	FES	G	801	7	0,4,4	-	-	-	-	-
69	UQ7	BC	503	-	48,48,48	0.45	0	60,61,61	0.59	0
63	NDP	P	500	-	51,52,52	0.52	0	71,80,80	0.67	1 (1%)
59	FES	E	500	5	0,4,4	-	-	-	-	-
66	COO	y	301	-	51,55,55	4.39	19 (37%)	73,81,81	4.16	21 (28%)
58	SF4	F	501	6	0,12,12	-	-	-	-	-
65	8Q1	n	200	-	32,34,34	0.30	0	39,43,43	0.64	1 (2%)
58	SF4	G	803	7	0,12,12	-	-	-	-	-
58	SF4	B	500	2	0,12,12	-	-	-	-	-
58	SF4	I	500	9	0,12,12	-	-	-	-	-
59	FES	AD	301	51	0,4,4	-	-	-	-	-
68	UQ5	AC	502	-	38,38,38	0.52	0	48,49,49	0.74	0
67	HEM	BC	500	50	50,50,50	1.32	7 (14%)	67,82,82	1.08	6 (8%)
67	HEM	BE	400	52	50,50,50	1.29	6 (12%)	67,82,82	1.13	5 (7%)
61	UQ9	H	500	-	35,35,58	0.79	2 (5%)	43,45,73	1.01	6 (13%)

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
67	HEM	AE	400	52	-	2/14/54/54	-
60	FMN	F	500	-	-	5/18/18/18	0/3/3/3
59	FES	BD	301	51	-	-	0/1/1/1
67	HEM	BC	501	50	-	9/14/54/54	-
68	UQ5	BC	502	-	-	8/33/57/57	0/1/1/1
68	UQ5	AC	503	-	-	12/33/57/57	0/1/1/1
58	SF4	G	802	7	-	-	0/6/5/5
65	8Q1	W	200	-	-	22/41/41/41	-
58	SF4	I	501	9	-	-	0/6/5/5
67	HEM	AC	501	50	-	9/14/54/54	-
67	HEM	AC	500	50	-	4/14/54/54	-
59	FES	G	801	7	-	-	0/1/1/1
69	UQ7	BC	503	-	-	8/45/69/69	0/1/1/1
63	NDP	P	500	-	-	6/34/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FES	E	500	5	-	-	0/1/1/1
66	COO	y	301	-	1/1/12/16	23/54/70/70	0/3/3/3
65	8Q1	n	200	-	-	21/41/41/41	-
61	UQ9	H	500	-	-	19/30/54/81	0/1/1/1
58	SF4	G	803	7	-	-	0/6/5/5
58	SF4	B	500	2	-	-	0/6/5/5
58	SF4	I	500	9	-	-	0/6/5/5
59	FES	AD	301	51	-	-	0/1/1/1
68	UQ5	AC	502	-	-	7/33/57/57	0/1/1/1
67	HEM	BC	500	50	-	2/14/54/54	-
67	HEM	BE	400	52	-	2/14/54/54	-
58	SF4	F	501	6	-	-	0/6/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	y	301	COO	C2A-N1A	-16.62	1.04	1.33
66	y	301	COO	C5A-C4A	12.91	1.62	1.39
66	y	301	COO	C2A-N3A	-9.20	1.17	1.33
66	y	301	COO	C6A-N1A	-8.32	1.12	1.35
66	y	301	COO	C5A-N7A	-7.65	1.25	1.39
66	y	301	COO	P1A-O3A	7.13	1.67	1.59
66	y	301	COO	C1-N1	7.11	1.50	1.33
66	y	301	COO	P2A-O3A	6.32	1.66	1.59
66	y	301	COO	C4-N2	6.28	1.48	1.33
67	AC	501	HEM	FE-NB	5.61	2.12	1.94
67	BC	501	HEM	FE-NB	5.42	2.11	1.94
66	y	301	COO	C4A-N3A	4.74	1.43	1.34
67	AC	501	HEM	FE-NC	4.58	2.10	1.95
67	BC	501	HEM	FE-NC	4.43	2.09	1.95
66	y	301	COO	C6A-N6A	4.28	1.45	1.34
67	AC	501	HEM	C1B-NB	-3.77	1.33	1.40
67	BC	501	HEM	C1B-NB	-3.75	1.33	1.40
67	AC	500	HEM	FE-ND	3.49	2.05	1.94
66	y	301	COO	P3X-O3X	3.48	1.65	1.59
67	BC	501	HEM	C4D-ND	-3.38	1.34	1.40
60	F	500	FMN	C4A-N5	3.33	1.38	1.30
67	AC	501	HEM	C4D-ND	-3.33	1.34	1.40
66	y	301	COO	O4X-C1X	3.28	1.49	1.42
67	AE	400	HEM	FE-NA	3.18	2.05	1.95
67	BE	400	HEM	CAC-C3C	3.00	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AC	500	HEM	CAC-C3C	2.95	1.55	1.47
66	y	301	COO	C12-C11	2.94	1.57	1.52
67	BC	500	HEM	FE-NC	2.93	2.04	1.95
67	BC	500	HEM	CAB-C3B	2.92	1.55	1.47
67	AC	500	HEM	CAB-C3B	2.90	1.55	1.47
67	AE	400	HEM	FE-ND	2.88	2.03	1.94
67	BC	500	HEM	CAC-C3C	2.88	1.55	1.47
67	AE	400	HEM	CAC-C3C	2.83	1.54	1.47
67	BC	500	HEM	FE-ND	2.83	2.03	1.94
67	AC	500	HEM	FE-NC	2.80	2.04	1.95
67	BE	400	HEM	CAB-C3B	2.74	1.54	1.47
67	AE	400	HEM	CAB-C3B	2.70	1.54	1.47
61	H	500	UQ9	C4-C5	-2.67	1.41	1.48
66	y	301	COO	C3-C4	2.58	1.56	1.51
67	BE	400	HEM	FE-ND	2.55	2.02	1.94
67	AC	500	HEM	FE-NB	2.52	2.02	1.94
67	BE	400	HEM	FE-NC	2.49	2.03	1.95
67	AC	501	HEM	C1C-C2C	-2.49	1.40	1.45
67	AE	400	HEM	FE-NB	2.49	2.02	1.94
67	BC	501	HEM	C1C-C2C	-2.48	1.40	1.45
66	y	301	COO	C2X-C3X	-2.45	1.47	1.53
66	y	301	COO	O3-C4	-2.37	1.18	1.23
67	BC	501	HEM	C1D-ND	-2.35	1.34	1.38
66	y	301	COO	P1A-O5X	2.35	1.68	1.59
67	AC	500	HEM	FE-NA	2.34	2.02	1.95
67	BE	400	HEM	FE-NB	2.34	2.02	1.94
67	BC	500	HEM	FE-NA	2.25	2.02	1.95
67	BC	501	HEM	C4B-NB	-2.23	1.34	1.38
67	AC	501	HEM	FE-ND	-2.23	1.88	1.94
60	F	500	FMN	C10-N1	2.21	1.37	1.33
67	AC	501	HEM	C4B-NB	-2.19	1.34	1.38
67	AE	400	HEM	C2A-C3A	-2.19	1.33	1.38
67	BC	501	HEM	FE-ND	-2.19	1.88	1.94
67	AC	501	HEM	C1D-ND	-2.19	1.34	1.38
61	H	500	UQ9	C3-C2	-2.17	1.42	1.48
67	AE	400	HEM	FE-NC	2.14	2.02	1.95
67	BC	500	HEM	FE-NB	2.10	2.01	1.94
66	y	301	COO	O2-C1	-2.05	1.19	1.23
67	BC	501	HEM	C3B-C4B	2.02	1.48	1.44
67	BC	501	HEM	C3C-C4C	-2.02	1.42	1.46
67	BC	500	HEM	C2A-C3A	-2.01	1.33	1.38
67	BE	400	HEM	C2A-C3A	-2.01	1.33	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	y	301	COO	C5A-C4A-N3A	-14.87	106.24	126.72
66	y	301	COO	C6A-C5A-N7A	14.18	159.43	132.09
66	y	301	COO	C4A-C5A-N7A	-13.83	94.77	110.58
66	y	301	COO	C4A-N9A-C8A	-11.92	93.22	105.74
66	y	301	COO	C5A-C4A-N9A	8.93	115.54	105.81
66	y	301	COO	C6A-C5A-C4A	-8.34	105.79	117.18
66	y	301	COO	C6-S1-C7	7.86	109.12	99.85
66	y	301	COO	C5A-N7A-C8A	6.61	113.84	103.45
66	y	301	COO	N3A-C4A-N9A	6.49	138.21	127.17
66	y	301	COO	C2A-N3A-C4A	5.99	126.46	111.83
66	y	301	COO	C4A-N9A-C1X	-5.10	114.70	126.63
66	y	301	COO	C1X-N9A-C8A	-4.67	116.74	127.09
68	AC	503	UQ5	C7-C6-C5	-4.57	113.21	118.52
66	y	301	COO	C2A-N1A-C6A	4.46	126.06	118.73
67	BC	501	HEM	CHD-C1D-ND	4.43	129.19	124.42
67	AC	501	HEM	CHD-C1D-ND	4.39	129.15	124.42
67	AC	501	HEM	CHC-C4B-NB	4.34	129.09	124.42
67	BC	501	HEM	CHC-C4B-NB	4.31	129.06	124.42
66	y	301	COO	C5A-C6A-N1A	4.10	127.92	117.51
67	BC	501	HEM	CHA-C4D-ND	3.83	129.10	124.37
67	AC	501	HEM	CHA-C4D-ND	3.74	129.00	124.37
67	BC	501	HEM	CHB-C1B-NB	3.67	128.91	124.37
67	AC	501	HEM	CHB-C1B-NB	3.63	128.86	124.37
67	AC	501	HEM	C1B-NB-C4B	3.58	109.44	105.21
60	F	500	FMN	C4-N3-C2	-3.37	119.66	125.64
67	BC	501	HEM	C1B-NB-C4B	3.36	109.19	105.21
63	P	500	NDP	P2B-O2B-C2B	-3.27	114.70	123.43
60	F	500	FMN	C4A-C10-N10	3.08	120.89	116.48
66	y	301	COO	C5A-C6A-N6A	-3.00	115.85	123.29
67	AE	400	HEM	CAA-CBA-CGA	-2.91	105.96	113.67
61	H	500	UQ9	C7-C6-C5	2.84	121.81	118.52
66	y	301	COO	C2X-C1X-N9A	-2.81	106.33	113.30
66	y	301	COO	C3X-C2X-C1X	2.78	106.00	99.89
66	y	301	COO	C2-C3-C4	-2.74	107.83	112.39
67	BE	400	HEM	CAA-CBA-CGA	-2.71	106.47	113.67
61	H	500	UQ9	C1-C6-C5	-2.68	117.01	119.62
67	AC	501	HEM	C3B-C4B-NB	-2.68	107.55	109.47
60	F	500	FMN	C4A-C4-N3	2.64	119.96	113.25
67	BC	500	HEM	CBD-CAD-C3D	-2.55	105.47	112.53
61	H	500	UQ9	C4-C3-C2	-2.54	116.02	120.69
67	AE	400	HEM	C2A-C1A-NA	-2.54	107.34	110.15
60	F	500	FMN	C10-C4A-N5	-2.50	119.70	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	BC	501	HEM	C4D-ND-C1D	2.48	108.15	105.21
67	AC	501	HEM	CHD-C1D-C2D	-2.47	121.13	125.03
67	AE	400	HEM	C4D-ND-C1D	2.44	108.09	105.21
66	y	301	COO	C10-C9-C8	-2.42	120.41	125.28
61	H	500	UQ9	C7-C6-C1	-2.36	120.84	124.89
60	F	500	FMN	O4-C4-C4A	-2.33	120.38	126.53
67	BC	501	HEM	CHD-C1D-C2D	-2.29	121.41	125.03
67	AC	500	HEM	C1B-NB-C4B	2.29	107.91	105.21
67	AE	400	HEM	CHC-C1C-NC	2.28	126.94	124.45
67	BC	501	HEM	C4B-C3B-C2B	-2.26	105.21	107.28
66	y	301	COO	C3-C4-N2	2.26	120.45	116.34
67	BC	501	HEM	CHD-C4C-NC	2.23	126.89	124.45
67	AC	501	HEM	C4D-ND-C1D	2.23	107.84	105.21
67	BC	501	HEM	C3B-C4B-NB	-2.22	107.87	109.47
67	AC	501	HEM	CHD-C4C-NC	2.21	126.86	124.45
67	BC	500	HEM	C4D-ND-C1D	2.20	107.81	105.21
67	BC	500	HEM	C3D-C4D-ND	-2.18	107.78	110.17
61	H	500	UQ9	C3-C4-C5	-2.17	116.71	120.69
67	AC	500	HEM	C4D-ND-C1D	2.16	107.77	105.21
67	BE	400	HEM	C4D-ND-C1D	2.15	107.75	105.21
66	y	301	COO	C6-C5-N2	-2.14	107.94	112.41
67	BC	501	HEM	CHB-C1B-C2B	-2.14	120.88	126.95
67	AC	501	HEM	C4B-C3B-C2B	-2.13	105.32	107.28
67	AC	500	HEM	CBD-CAD-C3D	-2.12	106.67	112.53
67	BC	500	HEM	C1B-NB-C4B	2.11	107.71	105.21
67	BE	400	HEM	C3D-C4D-ND	-2.11	107.86	110.17
67	BC	500	HEM	C2A-C1A-NA	-2.10	107.82	110.15
67	AC	501	HEM	CHA-C4D-C3D	-2.10	121.36	125.23
67	BE	400	HEM	CHC-C1C-NC	2.09	126.73	124.45
67	AE	400	HEM	C3D-C4D-ND	-2.09	107.88	110.17
61	H	500	UQ9	C6-C1-C2	-2.08	117.53	119.17
67	BC	501	HEM	CHA-C4D-C3D	-2.08	121.38	125.23
68	BC	502	UQ5	C7-C6-C5	-2.08	116.10	118.52
67	BC	501	HEM	O2A-CGA-CBA	2.07	120.54	114.00
67	AC	501	HEM	CHB-C1B-C2B	-2.05	121.11	126.95
67	BC	501	HEM	CAA-CBA-CGA	-2.05	108.23	113.67
67	BC	500	HEM	C3B-C2B-C1B	2.03	107.94	106.41
60	F	500	FMN	C4A-C10-N1	-2.01	119.66	124.59
67	BE	400	HEM	CAD-CBD-CGD	-2.01	108.33	113.67
65	n	200	8Q1	C37-C38-C39	2.01	115.73	112.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
66	y	301	COO	C13

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	F	500	FMN	N10-C1'-C2'-O2'
60	F	500	FMN	N10-C1'-C2'-C3'
60	F	500	FMN	C5'-O5'-P-O2P
60	F	500	FMN	C5'-O5'-P-O3P
61	H	500	UQ9	C17-C18-C19-C21
61	H	500	UQ9	C17-C18-C19-C20
61	H	500	UQ9	C12-C11-C9-C10
61	H	500	UQ9	C12-C11-C9-C8
61	H	500	UQ9	C7-C8-C9-C11
61	H	500	UQ9	C7-C8-C9-C10
65	W	200	8Q1	O27-C28-C29-C30
65	W	200	8Q1	O27-C28-C29-C31
65	W	200	8Q1	O27-C28-C29-C32
65	W	200	8Q1	C29-C28-O27-P24
65	W	200	8Q1	C28-C29-C32-C34
65	W	200	8Q1	C28-C29-C32-O33
65	W	200	8Q1	C30-C29-C32-C34
65	W	200	8Q1	C30-C29-C32-O33
65	W	200	8Q1	C31-C29-C32-C34
65	W	200	8Q1	C31-C29-C32-O33
65	W	200	8Q1	C28-O27-P24-O2
65	W	200	8Q1	C28-O27-P24-O1
65	n	200	8Q1	O4-C1-S44-C43
65	n	200	8Q1	C6-C1-S44-C43
65	n	200	8Q1	O27-C28-C29-C31
65	n	200	8Q1	C29-C32-C34-N36
65	n	200	8Q1	C29-C32-C34-O35
65	n	200	8Q1	O33-C32-C34-N36
65	n	200	8Q1	O33-C32-C34-O35
65	n	200	8Q1	C32-C34-N36-C37
65	n	200	8Q1	N36-C37-C38-C39
66	y	301	COO	C13-C11-C12-O6A
66	y	301	COO	C14-C11-C12-O6A
66	y	301	COO	C15-C11-C12-O6A
66	y	301	COO	C5X-O5X-P1A-O3A
66	y	301	COO	C5X-O5X-P1A-O2A
66	y	301	COO	C5X-O5X-P1A-O1A
66	y	301	COO	O4X-C4X-C5X-O5X

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
66	y	301	COO	C5-C6-S1-C7
66	y	301	COO	O4-C7-S1-C6
66	y	301	COO	C8-C7-S1-C6
66	y	301	COO	S1-C7-C8-C9
67	BC	501	HEM	C2C-C3C-CAC-CBC
68	BC	502	UQ5	C12-C11-C9-C10
69	BC	503	UQ7	C25-C24-C26-C27
68	BC	502	UQ5	C12-C11-C9-C8
69	BC	503	UQ7	C23-C24-C26-C27
65	n	200	8Q1	O35-C34-N36-C37
61	H	500	UQ9	C22-C23-C24-C25
61	H	500	UQ9	C12-C13-C14-C15
61	H	500	UQ9	C22-C23-C24-C26
61	H	500	UQ9	C12-C13-C14-C16
68	AC	502	UQ5	C12-C11-C9-C10
68	AC	502	UQ5	C12-C11-C9-C8
68	BC	502	UQ5	C23-C24-C26-C27
61	H	500	UQ9	C19-C21-C22-C23
61	H	500	UQ9	C14-C16-C17-C18
68	AC	502	UQ5	C9-C11-C12-C13
68	AC	503	UQ5	C14-C16-C17-C18
68	AC	503	UQ5	C19-C21-C22-C23
68	BC	502	UQ5	C19-C21-C22-C23
69	BC	503	UQ7	C9-C11-C12-C13
69	BC	503	UQ7	C14-C16-C17-C18
69	BC	503	UQ7	C19-C21-C22-C23
69	BC	503	UQ7	C29-C31-C32-C33
61	H	500	UQ9	C24-C26-C27-C28
66	y	301	COO	C2X-C3X-O3X-P3X
68	BC	502	UQ5	C25-C24-C26-C27
65	W	200	8Q1	O40-C39-N41-C42
65	W	200	8Q1	C38-C39-N41-C42
63	P	500	NDP	C2D-C1D-N1N-C2N
63	P	500	NDP	C2D-C1D-N1N-C6N
68	AC	503	UQ5	C24-C26-C27-C28
66	y	301	COO	C4X-C3X-O3X-P3X
61	H	500	UQ9	C16-C17-C18-C19
68	AC	503	UQ5	C15-C14-C16-C17
68	BC	502	UQ5	C9-C11-C12-C13
65	W	200	8Q1	C6-C7-C8-C9
66	y	301	COO	C3X-C4X-C5X-O5X
65	W	200	8Q1	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
65	n	200	8Q1	C7-C8-C9-C10
68	AC	503	UQ5	C13-C14-C16-C17
68	AC	502	UQ5	C6-C7-C8-C9
65	n	200	8Q1	C9-C10-C11-C12
67	BC	501	HEM	C4C-C3C-CAC-CBC
65	n	200	8Q1	C10-C11-C12-C13
66	y	301	COO	O4-C7-C8-C9
61	H	500	UQ9	C13-C14-C16-C17
61	H	500	UQ9	C15-C14-C16-C17
68	AC	503	UQ5	C18-C19-C21-C22
67	BC	501	HEM	C2A-CAA-CBA-CGA
60	F	500	FMN	C5'-O5'-P-O1P
68	AC	503	UQ5	C20-C19-C21-C22
65	W	200	8Q1	C13-C14-C15-C16
68	AC	503	UQ5	C12-C11-C9-C10
65	W	200	8Q1	O4-C1-S44-C43
67	AC	501	HEM	C2A-CAA-CBA-CGA
65	W	200	8Q1	C1-C6-C7-C8
67	AC	501	HEM	C2B-C3B-CAB-CBB
67	AC	501	HEM	C2C-C3C-CAC-CBC
67	BC	501	HEM	C2B-C3B-CAB-CBB
68	AC	503	UQ5	C2-C3-O3-C3M
65	W	200	8Q1	C7-C8-C9-C10
68	BC	502	UQ5	C24-C26-C27-C28
68	AC	503	UQ5	C12-C11-C9-C8
66	y	301	COO	P1A-O3A-P2A-O5A
65	n	200	8Q1	O27-C28-C29-C30
61	H	500	UQ9	C20-C19-C21-C22
68	BC	502	UQ5	C14-C16-C17-C18
65	n	200	8Q1	O27-C28-C29-C32
66	y	301	COO	C12-O6A-P2A-O4A
66	y	301	COO	C12-O6A-P2A-O3A
63	P	500	NDP	O4D-C1D-N1N-C2N
63	P	500	NDP	O4D-C1D-N1N-C6N
65	n	200	8Q1	C11-C10-C9-C8
66	y	301	COO	C3X-O3X-P3X-O7A
68	AC	502	UQ5	C15-C14-C16-C17
67	BC	501	HEM	C4B-C3B-CAB-CBB
68	AC	503	UQ5	C5-C6-C7-C8
61	H	500	UQ9	C18-C19-C21-C22
68	AC	502	UQ5	C2-C3-O3-C3M
65	W	200	8Q1	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
68	AC	503	UQ5	C4-C3-O3-C3M
67	AE	400	HEM	CAA-CBA-CGA-O1A
67	BE	400	HEM	CAA-CBA-CGA-O2A
68	AC	502	UQ5	C13-C14-C16-C17
63	P	500	NDP	C2N-C3N-C7N-N7N
67	AC	501	HEM	CAD-CBD-CGD-O2D
67	BE	400	HEM	CAA-CBA-CGA-O1A
67	AC	501	HEM	CAD-CBD-CGD-O1D
67	AE	400	HEM	CAA-CBA-CGA-O2A
67	AC	500	HEM	CAA-CBA-CGA-O2A
63	P	500	NDP	O4B-C4B-C5B-O5B
65	W	200	8Q1	C6-C1-S44-C43
67	BC	500	HEM	CAA-CBA-CGA-O2A
67	BC	501	HEM	CAA-CBA-CGA-O2A
65	n	200	8Q1	C28-O27-P24-O2
67	BC	500	HEM	CAA-CBA-CGA-O1A
67	BC	501	HEM	CAD-CBD-CGD-O2D
67	AC	500	HEM	CAA-CBA-CGA-O1A
67	BC	501	HEM	CAD-CBD-CGD-O1D
67	AC	501	HEM	C4B-C3B-CAB-CBB
67	AC	501	HEM	C4C-C3C-CAC-CBC
67	BC	501	HEM	CAA-CBA-CGA-O1A
65	n	200	8Q1	C31-C29-C32-C34
67	AC	501	HEM	CAA-CBA-CGA-O2A
66	y	301	COO	P1A-O3A-P2A-O4A
69	BC	503	UQ7	C28-C29-C31-C32
61	H	500	UQ9	C2-C3-O3-C3M
69	BC	503	UQ7	C30-C29-C31-C32
65	n	200	8Q1	C28-C29-C32-C34
65	n	200	8Q1	C42-C43-S44-C1
66	y	301	COO	C3X-O3X-P3X-O9A
67	AC	501	HEM	CAA-CBA-CGA-O1A
67	AC	500	HEM	CAD-CBD-CGD-O2D
66	y	301	COO	N1-C1-C13-O1
67	AC	500	HEM	CAD-CBD-CGD-O1D
66	y	301	COO	P2A-O3A-P1A-O1A
65	n	200	8Q1	C12-C13-C14-C15

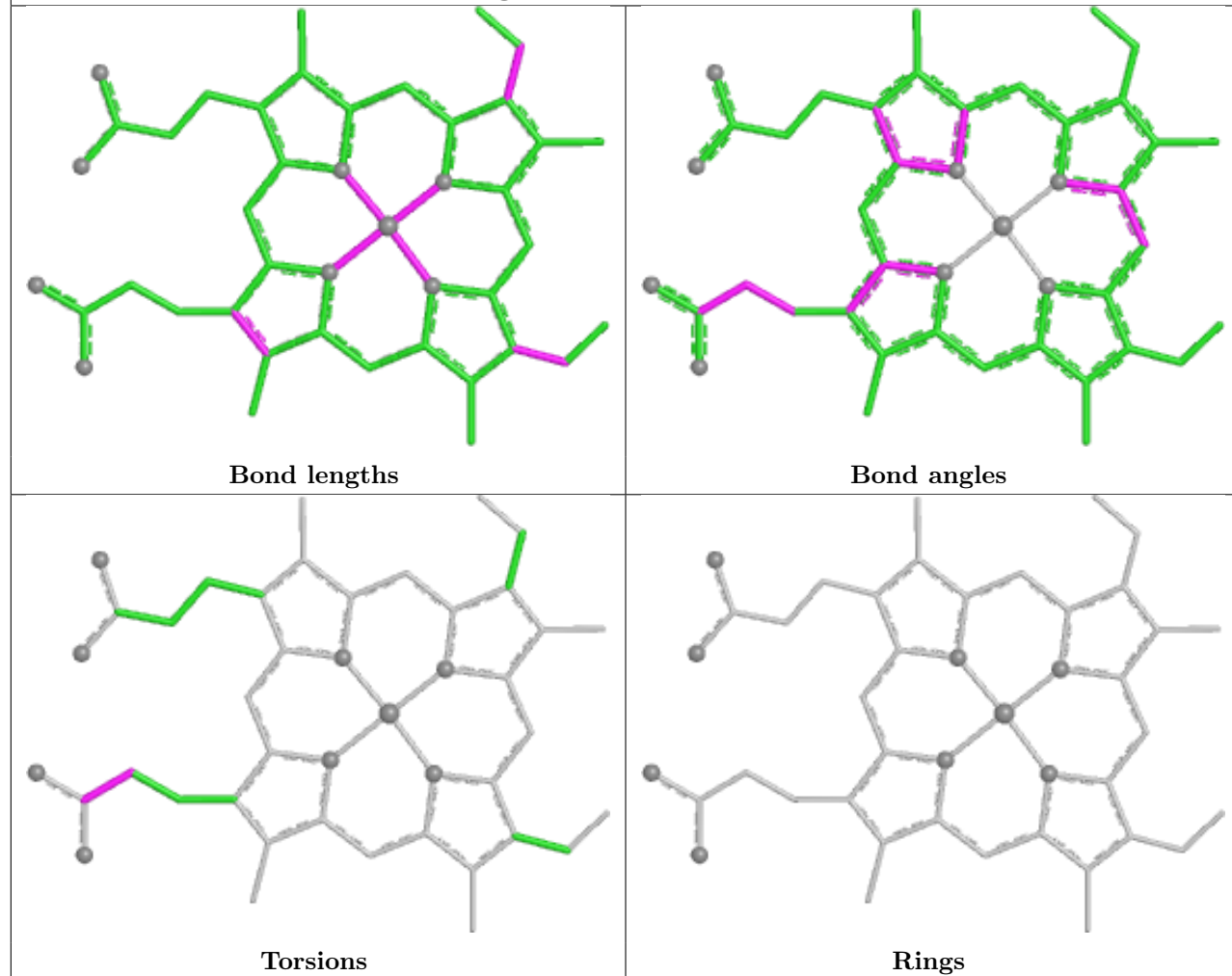
There are no ring outliers.

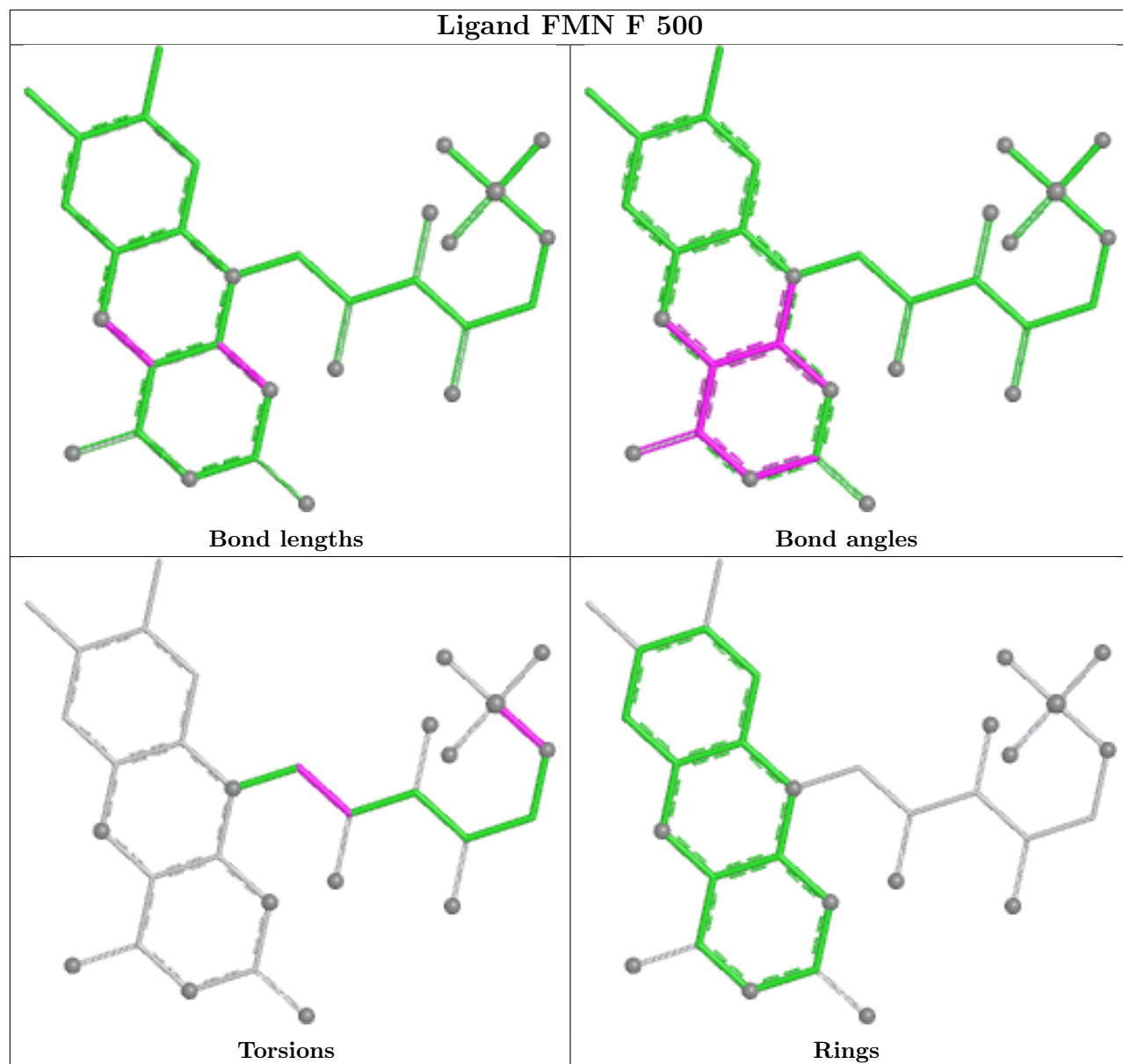
20 monomers are involved in 78 short contacts:

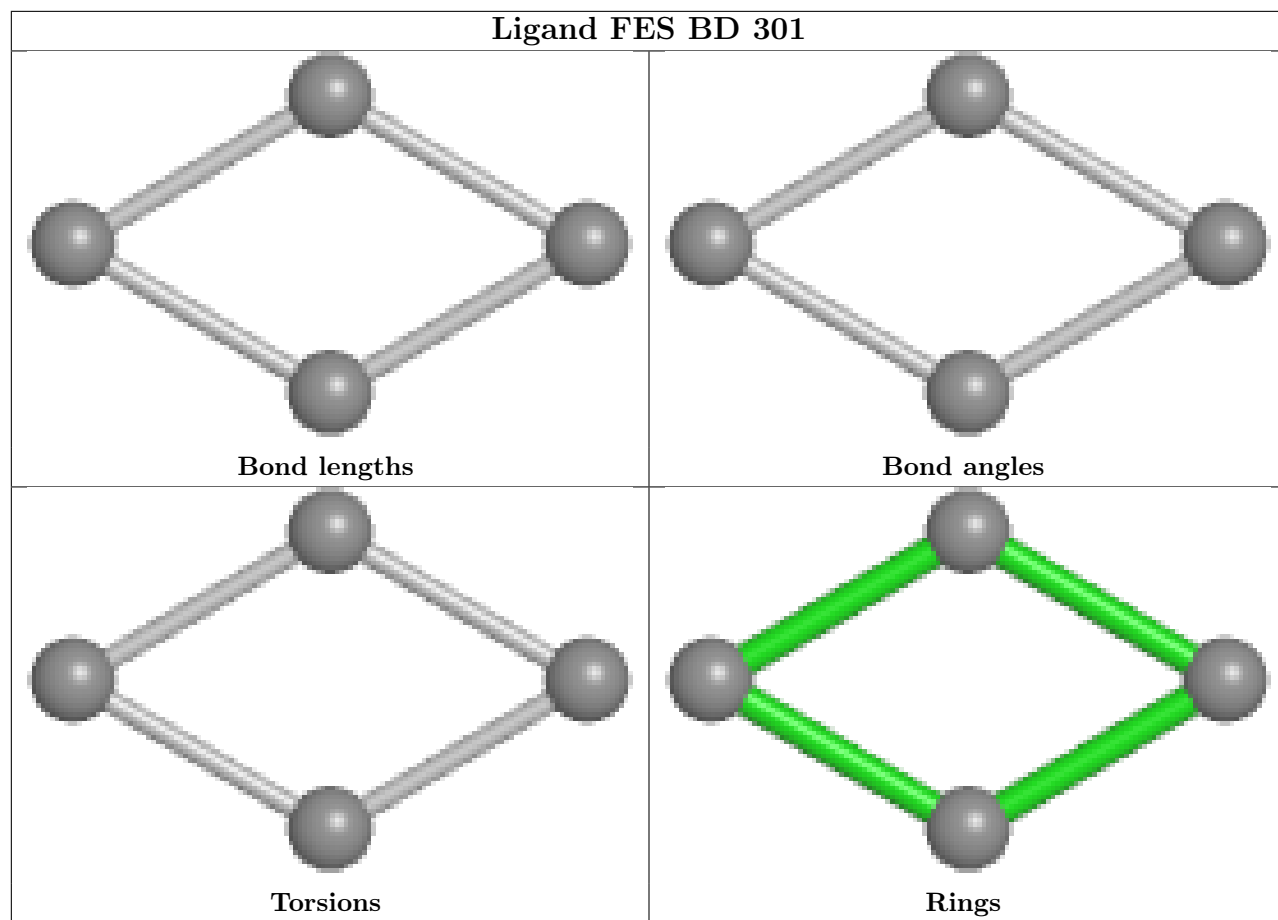
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	AE	400	HEM	4	0
60	F	500	FMN	1	0
59	BD	301	FES	2	0
67	BC	501	HEM	1	0
68	BC	502	UQ5	6	0
68	AC	503	UQ5	6	0
67	AC	501	HEM	1	0
67	AC	500	HEM	3	0
69	BC	503	UQ7	7	0
63	P	500	NDP	2	0
59	E	500	FES	1	0
66	y	301	COO	14	0
58	F	501	SF4	2	0
58	B	500	SF4	1	0
58	I	500	SF4	2	0
59	AD	301	FES	1	0
68	AC	502	UQ5	7	0
67	BC	500	HEM	2	0
67	BE	400	HEM	10	0
61	H	500	UQ9	6	0

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

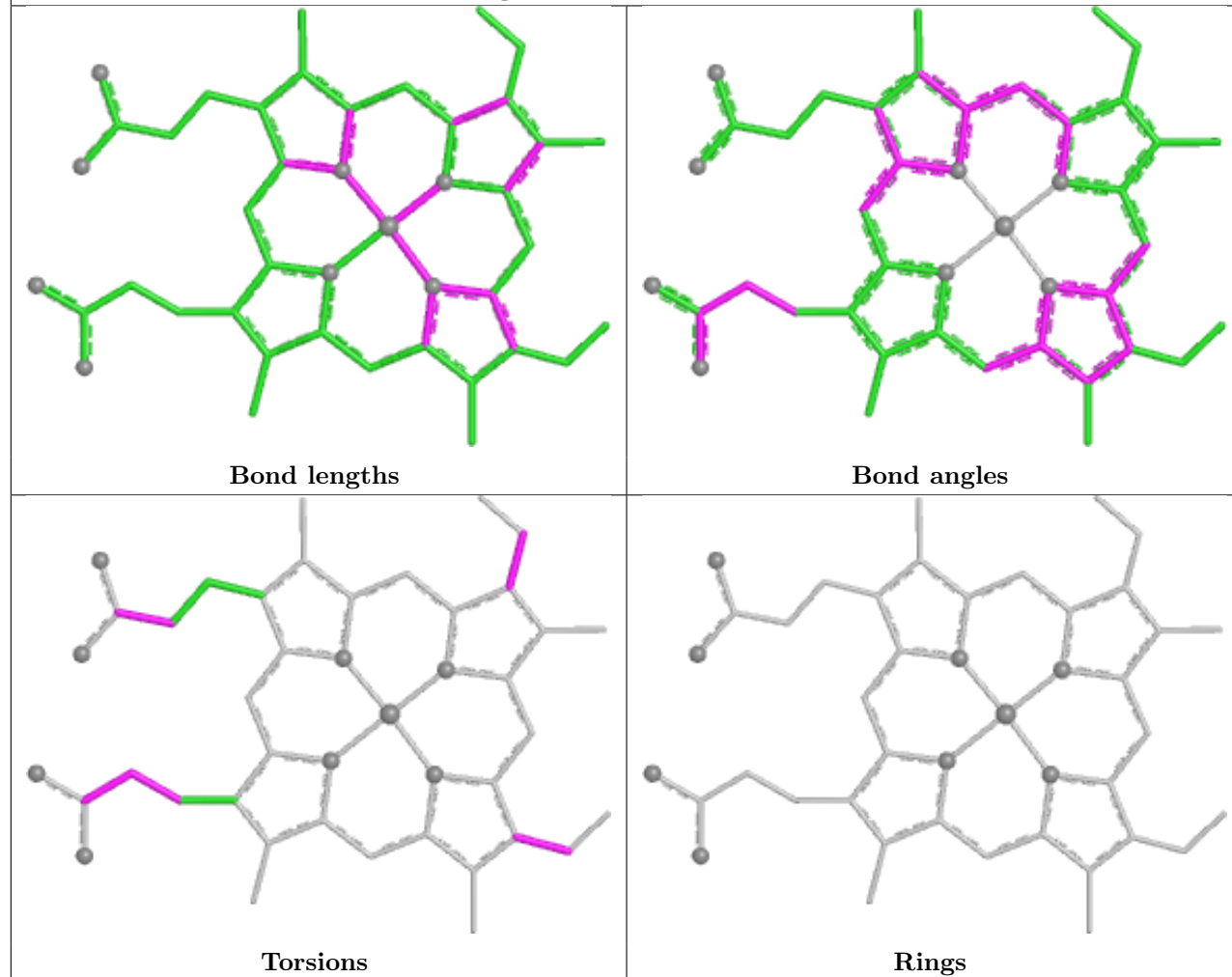
Ligand HEM AE 400



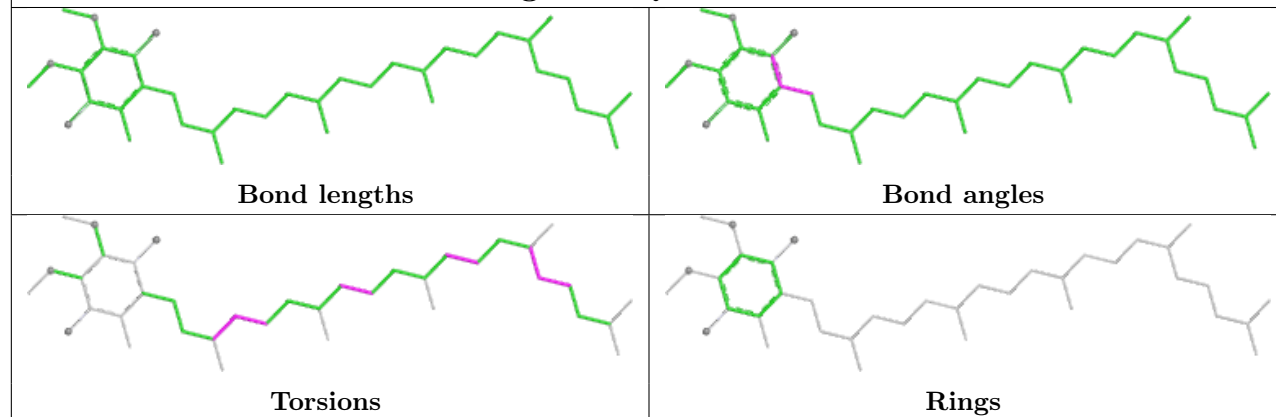


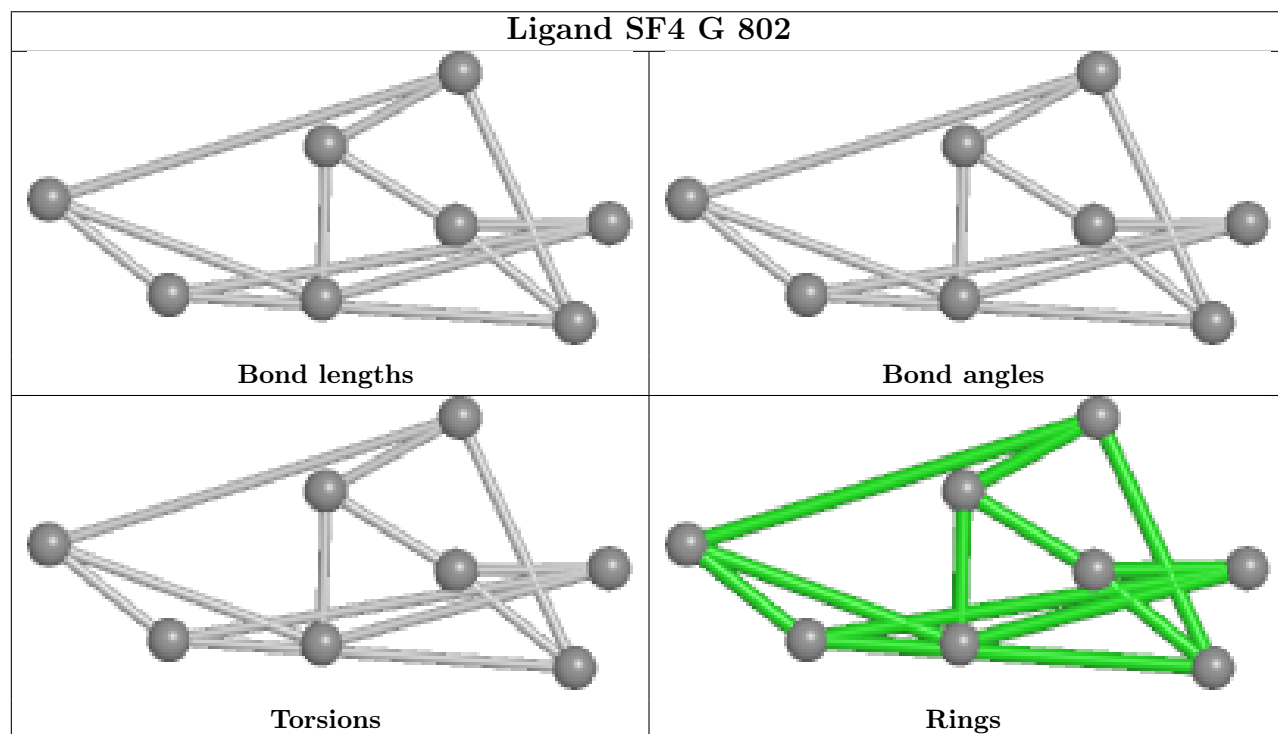
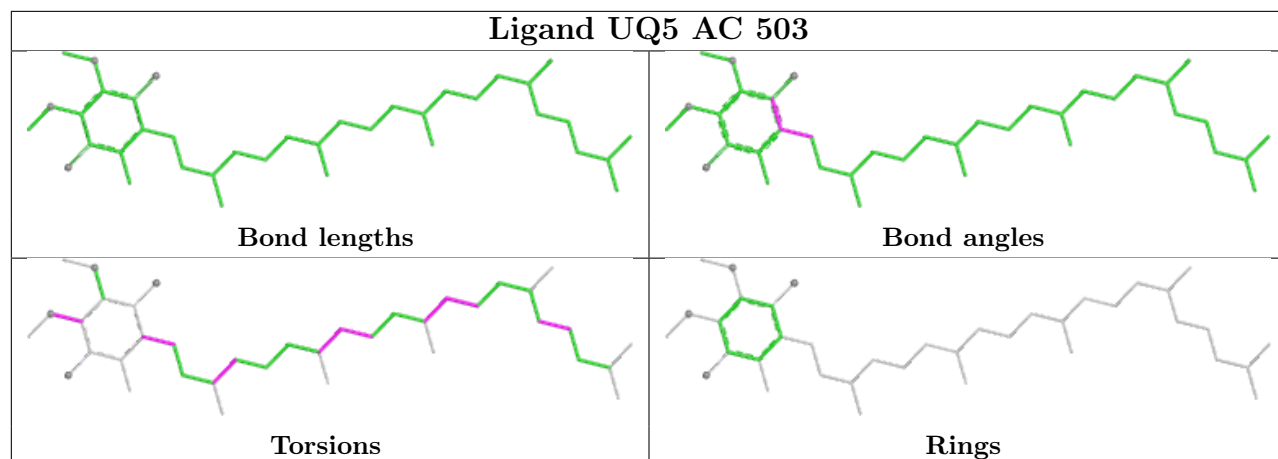


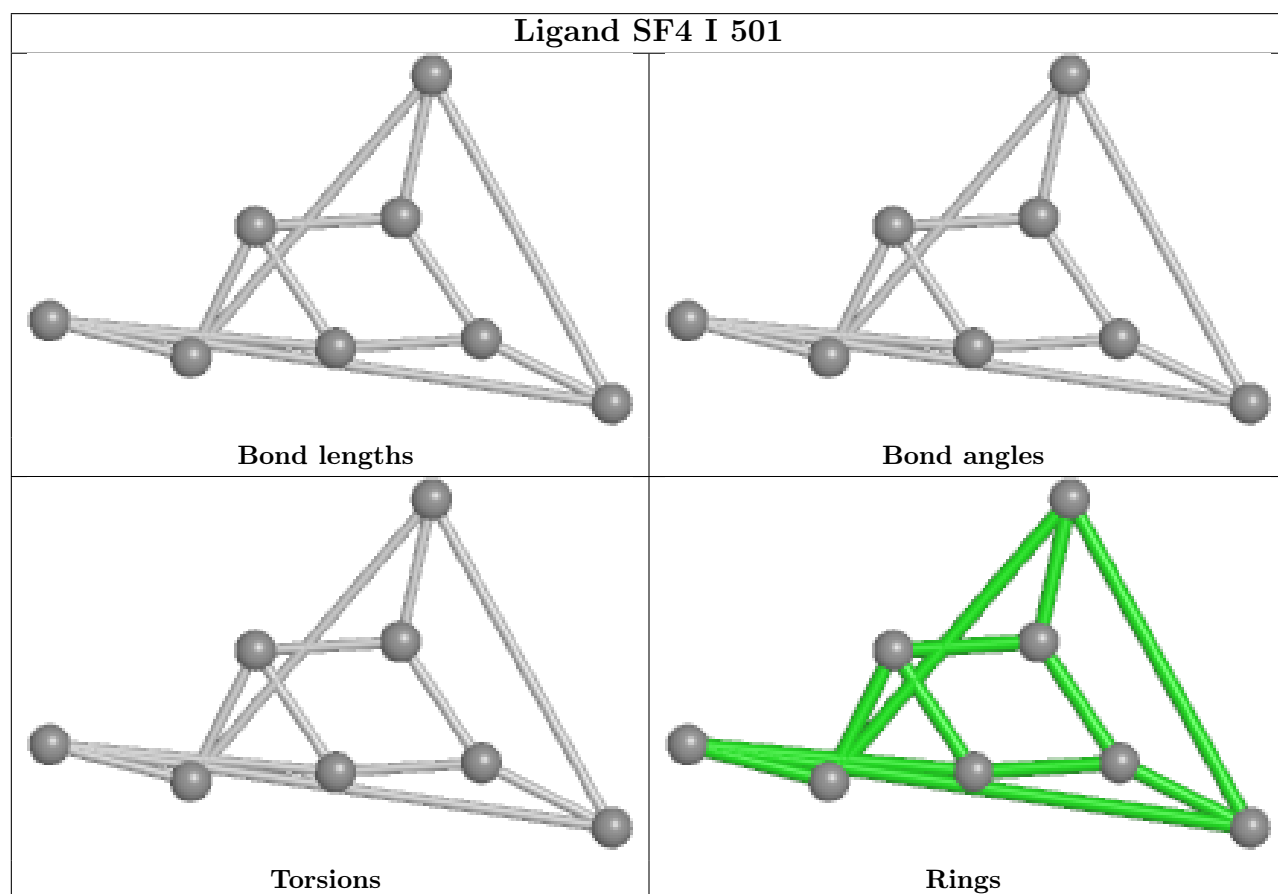
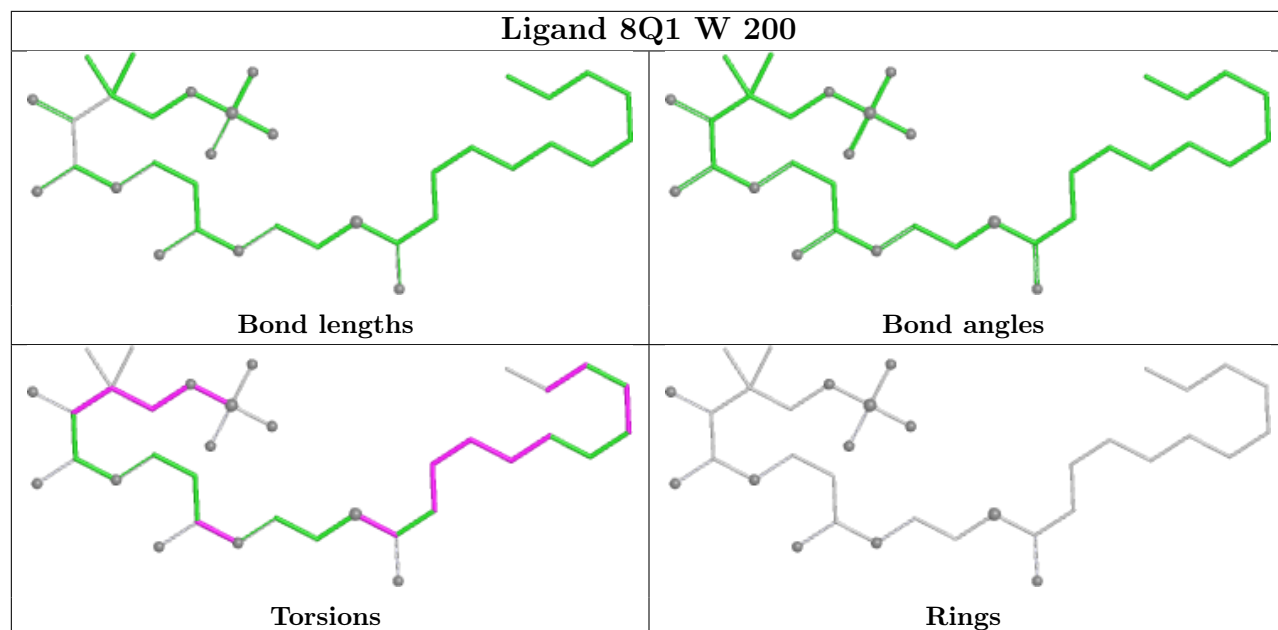
Ligand HEM BC 501

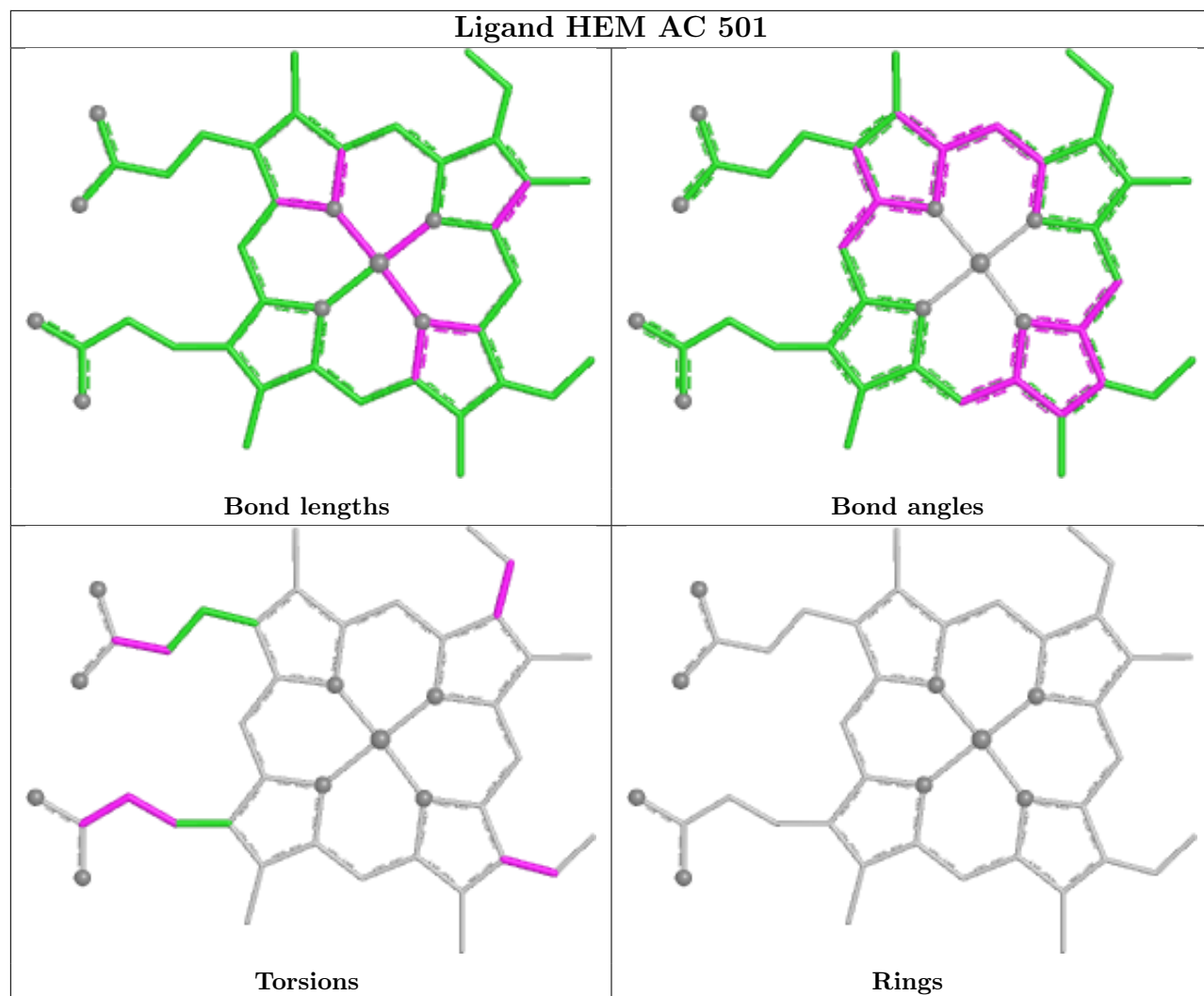


Ligand UQ5 BC 502

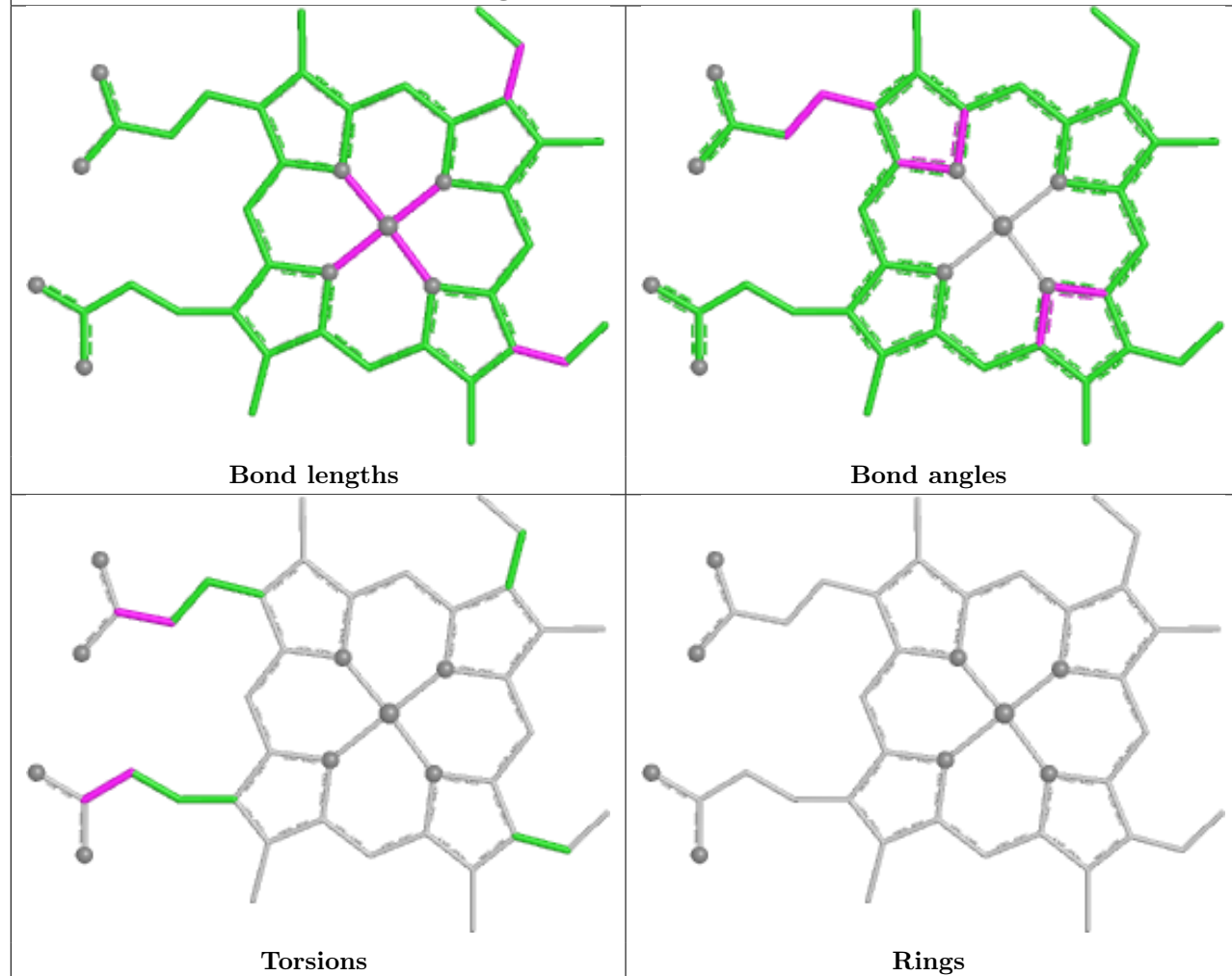


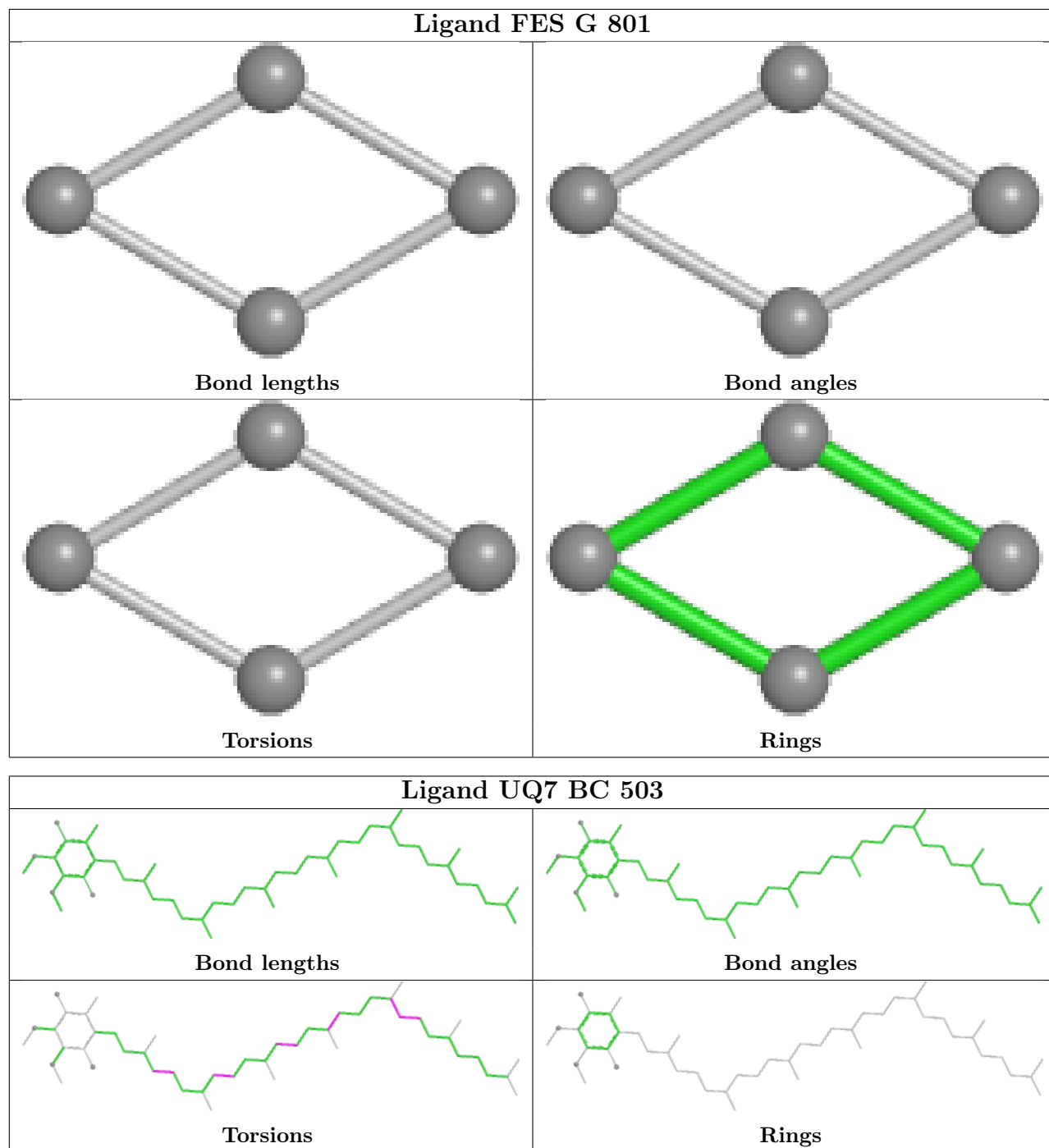


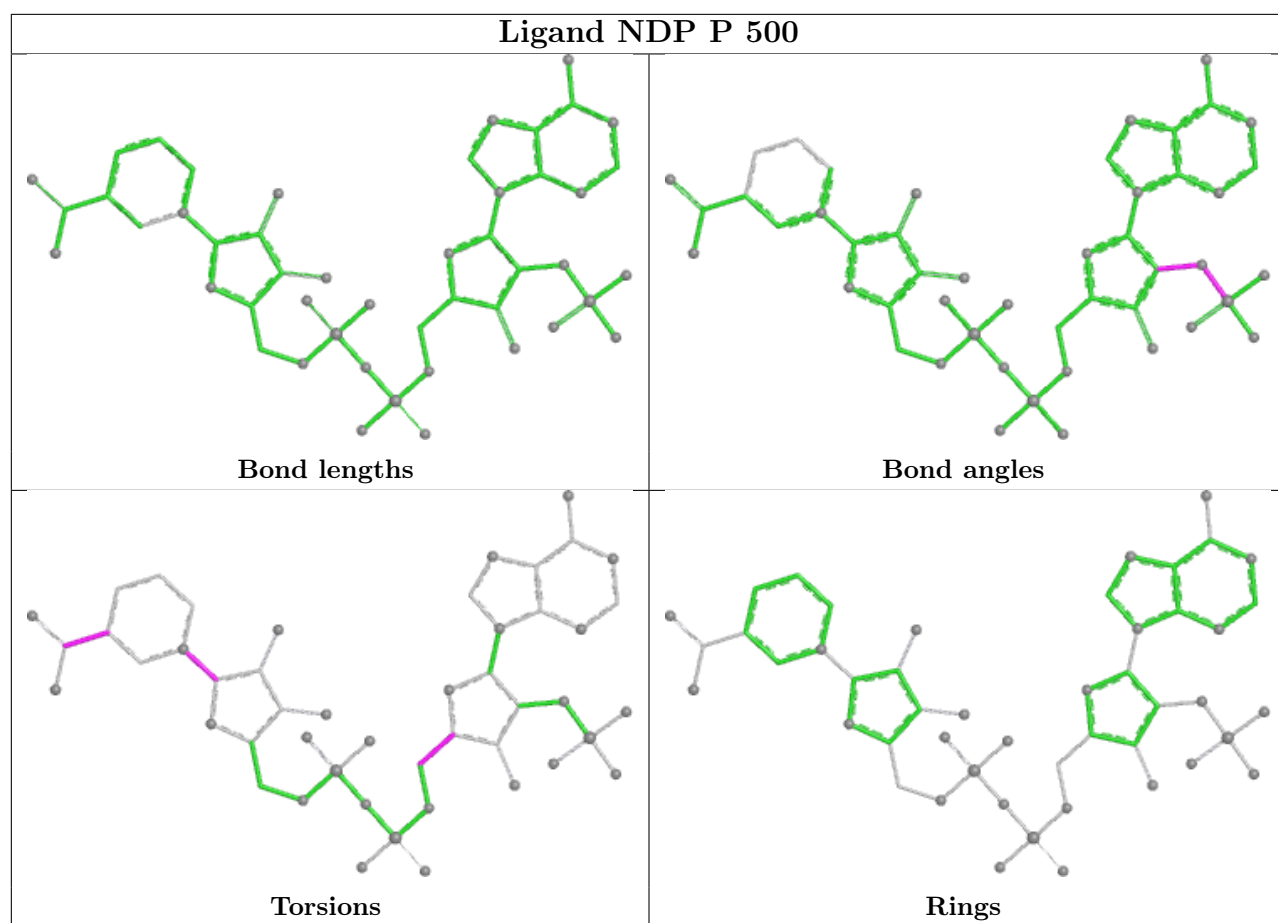


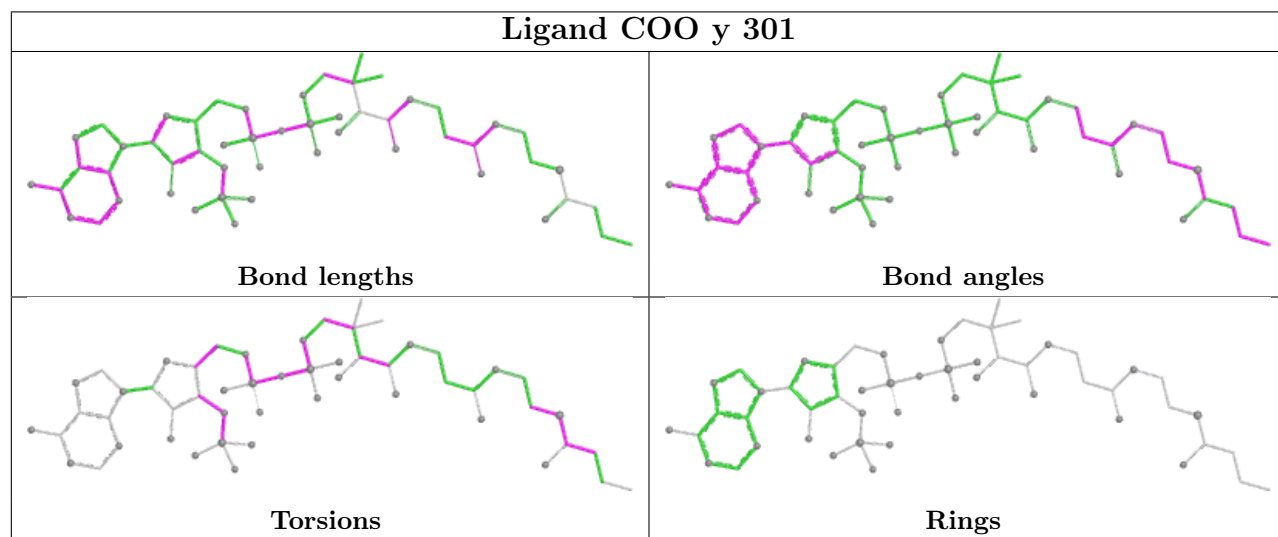
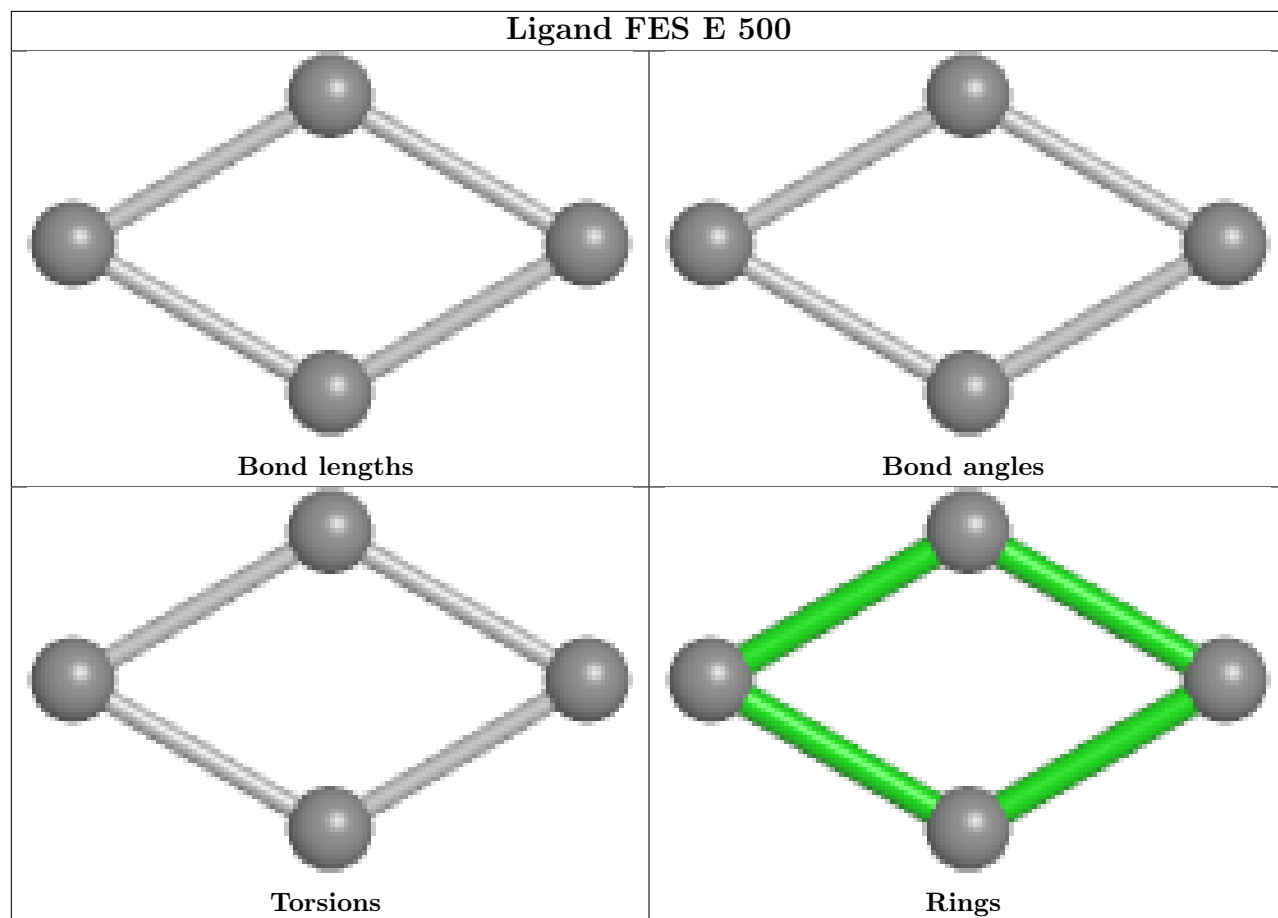


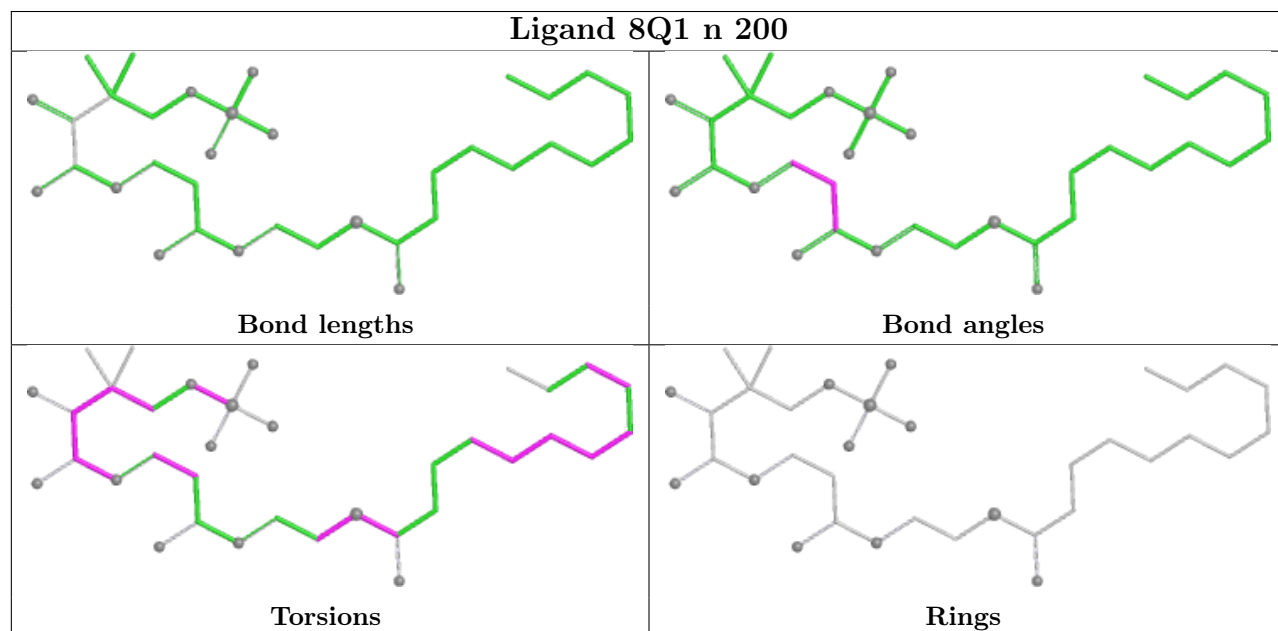
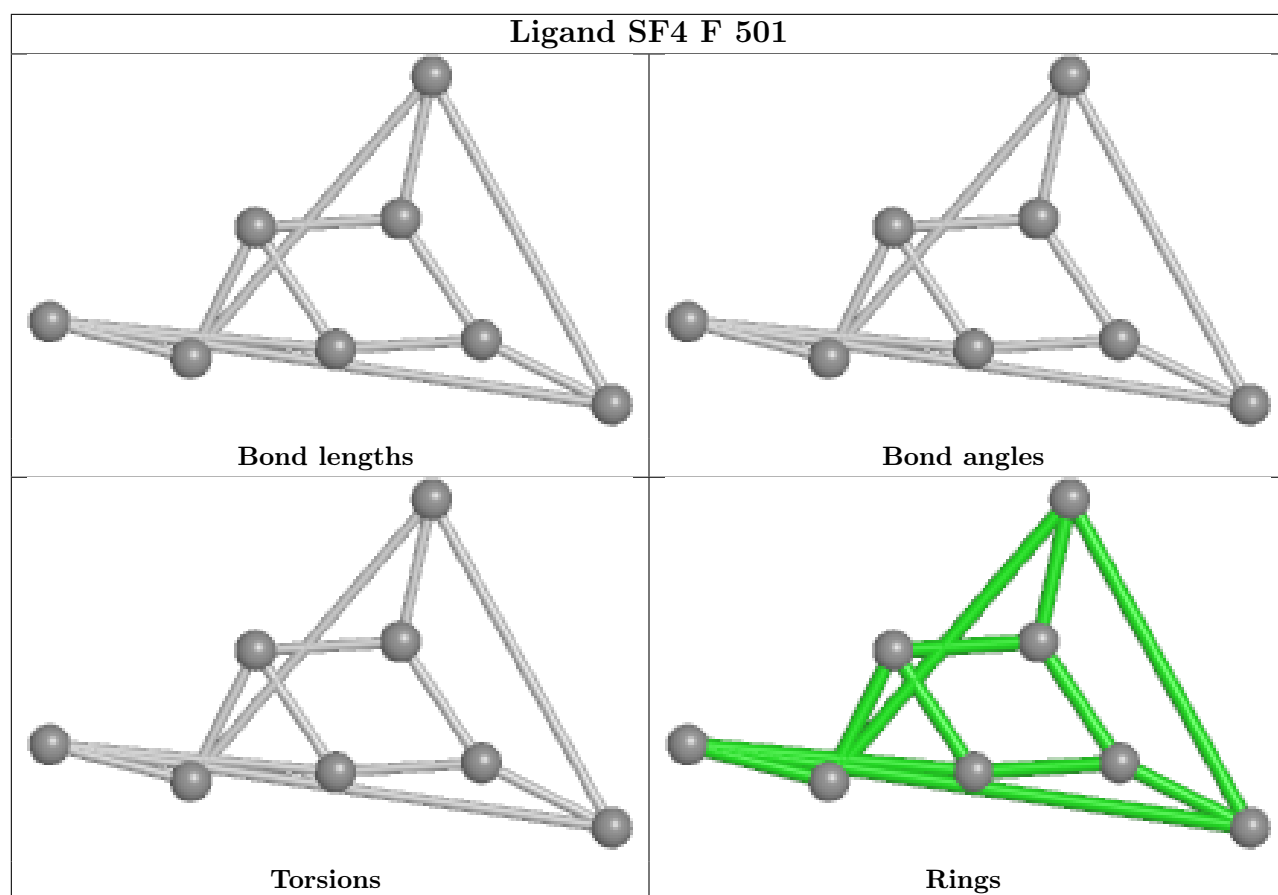
Ligand HEM AC 500



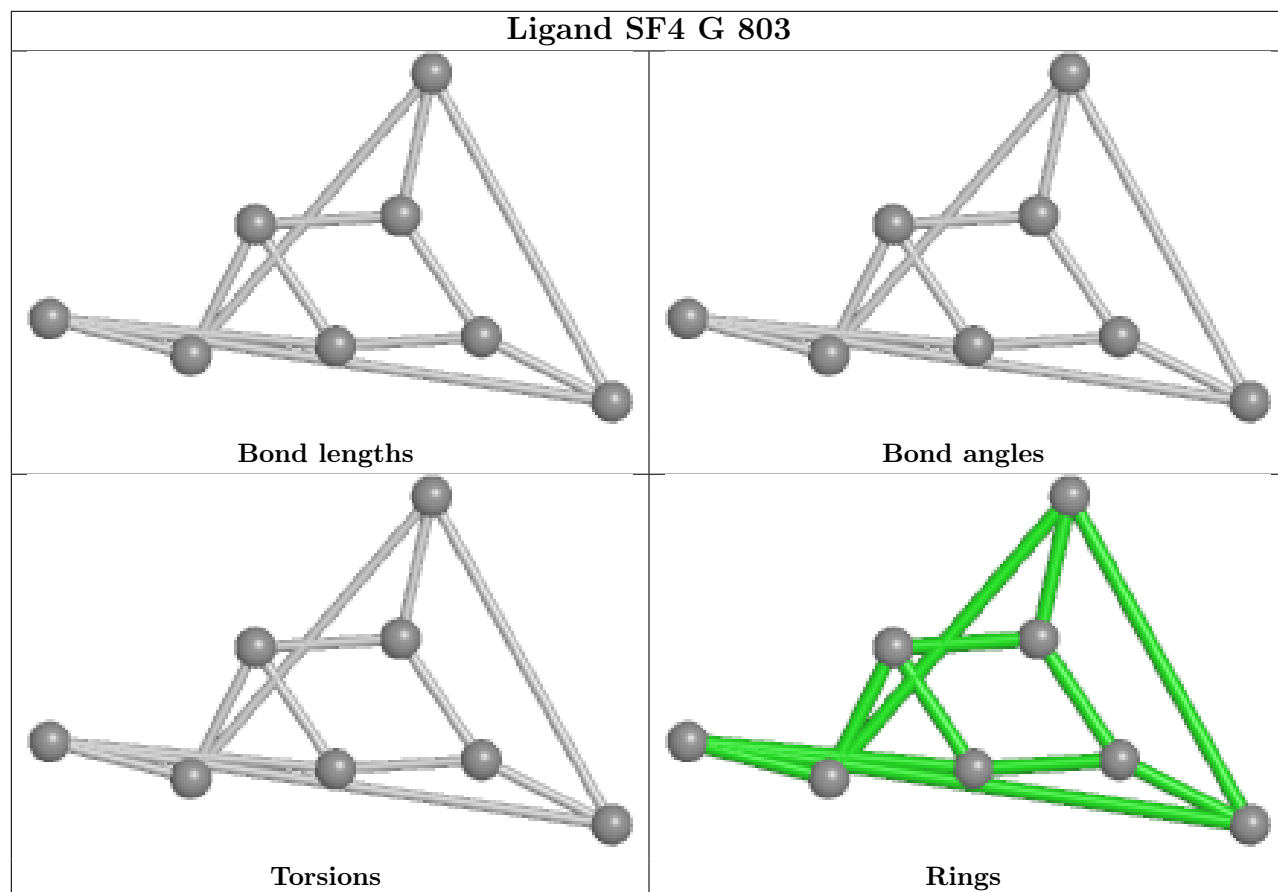




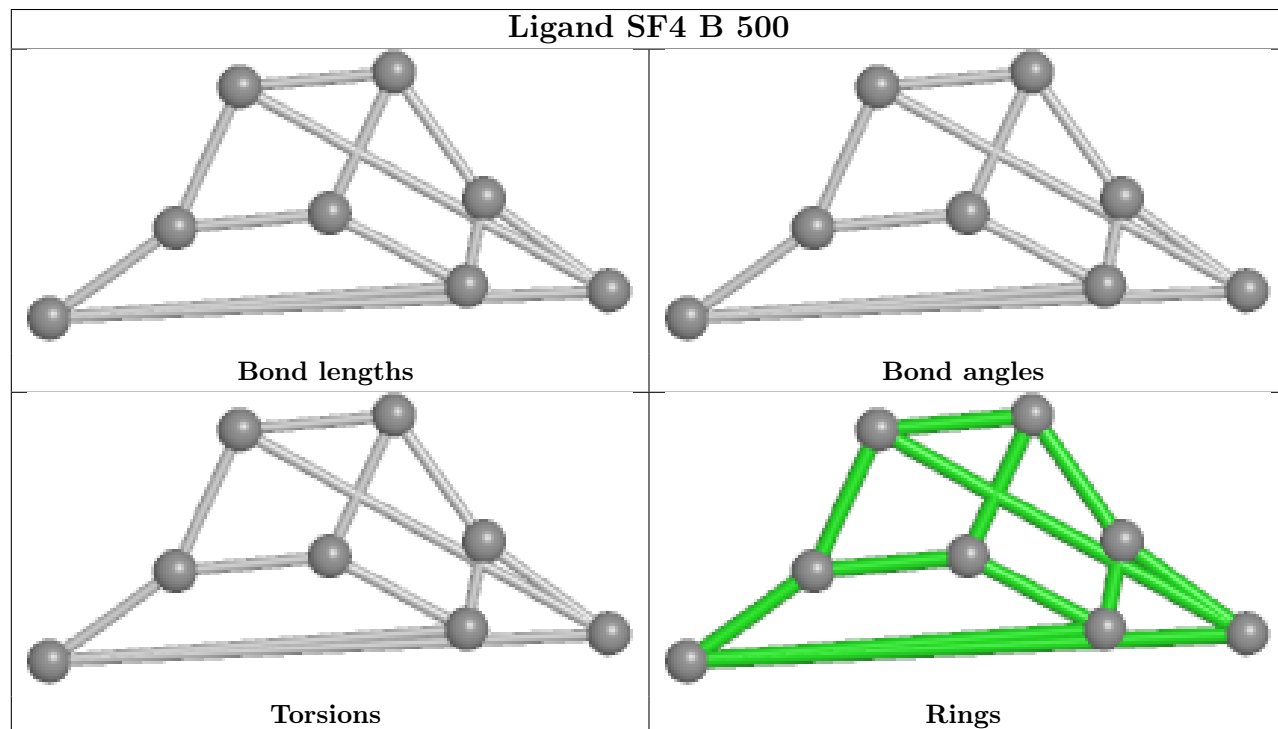


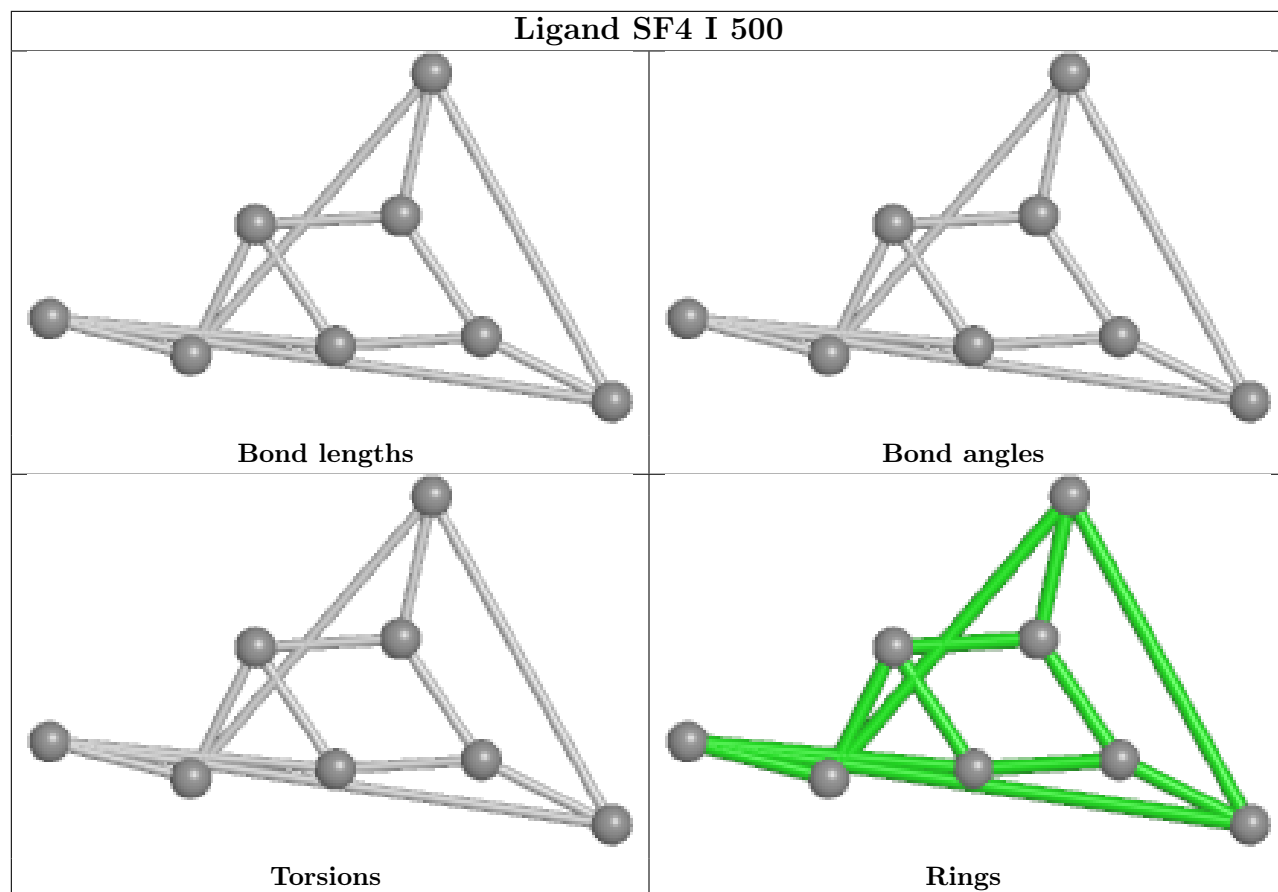


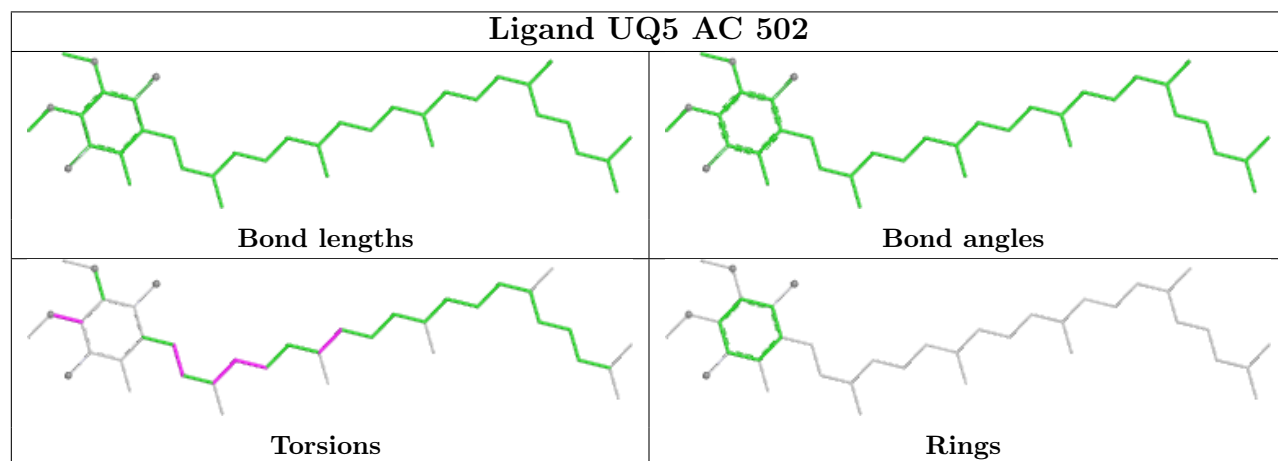
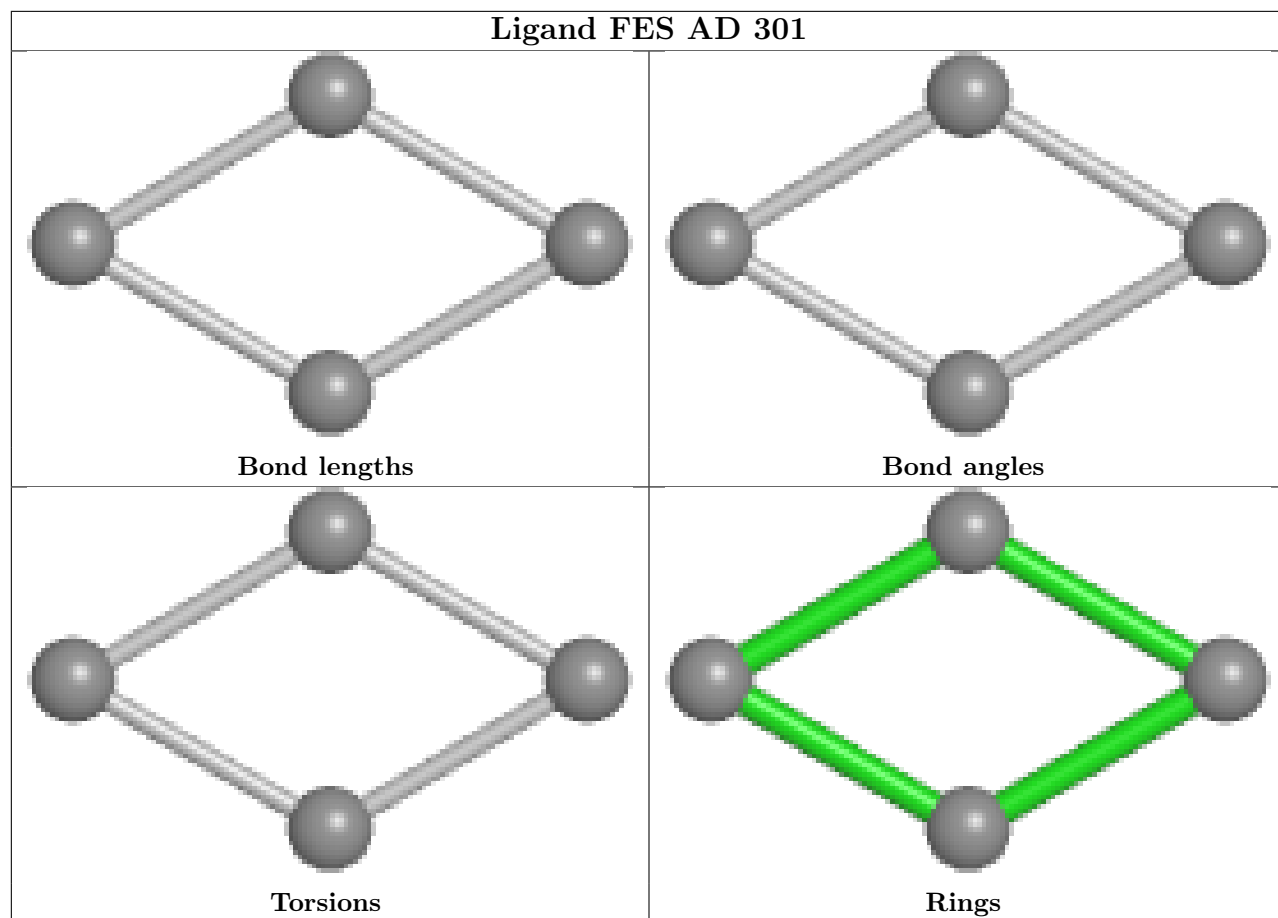
Ligand SF4 G 803

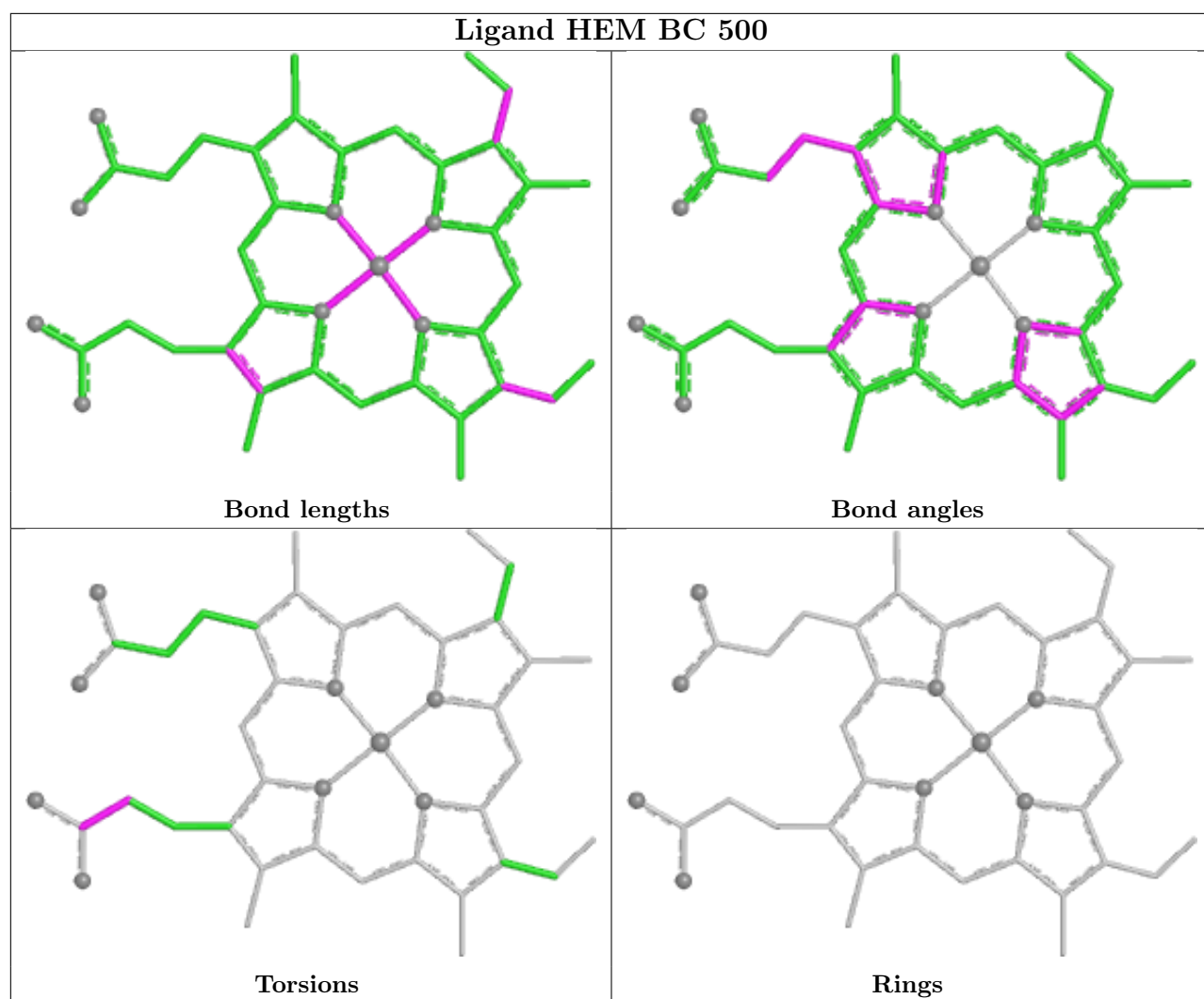


Ligand SF4 B 500

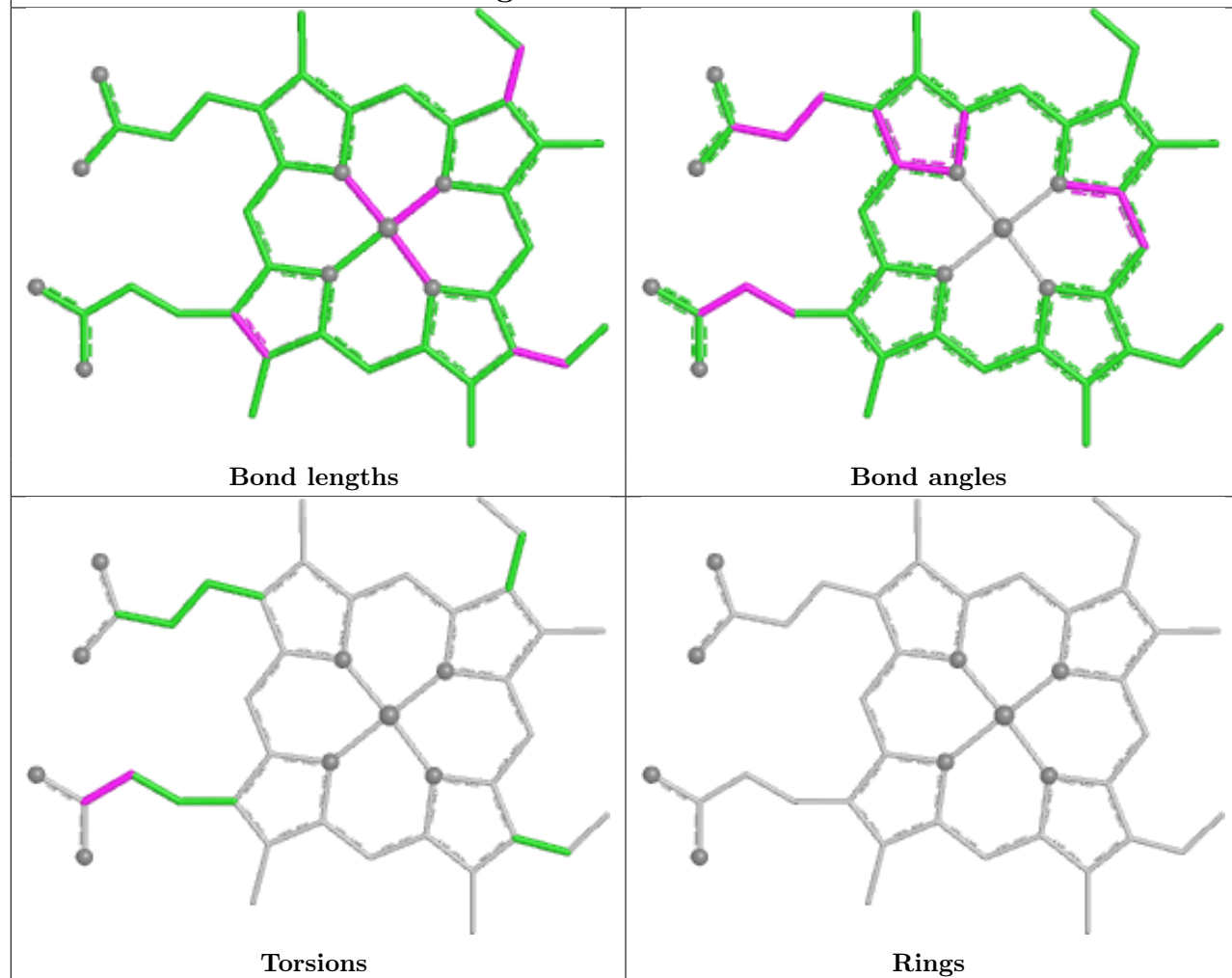




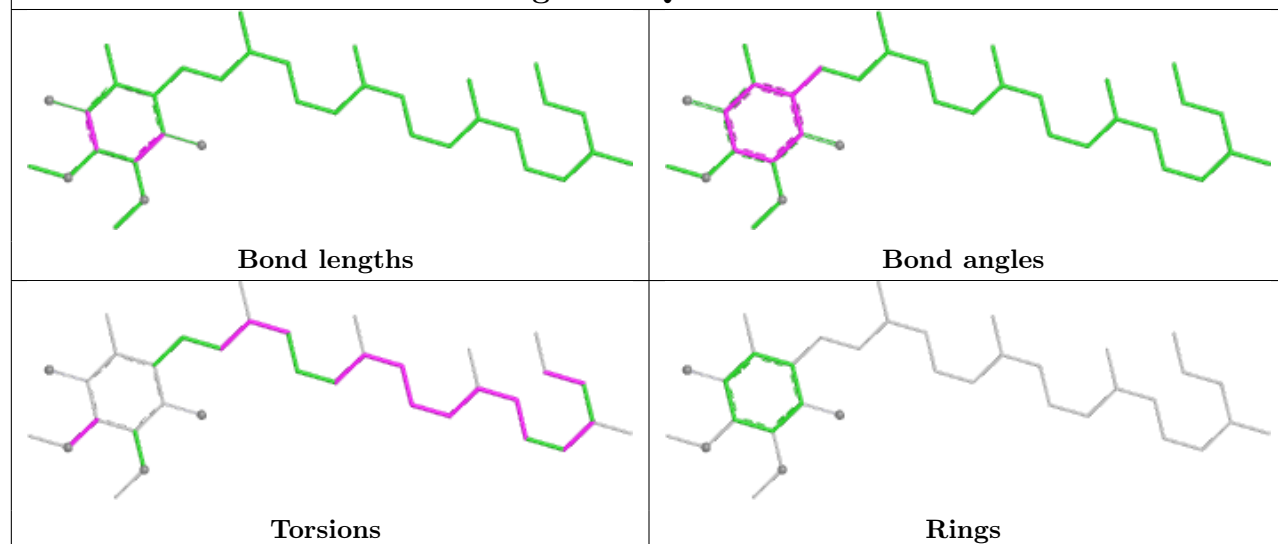




Ligand HEM BE 400



Ligand UQ9 H 500



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.

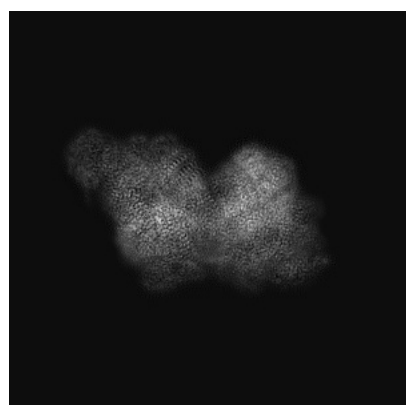
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16172. These allow visual inspection of the internal detail of the map and identification of artifacts.

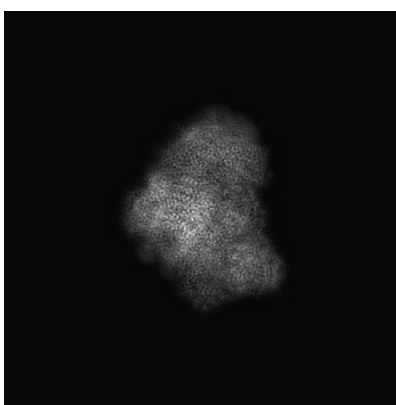
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

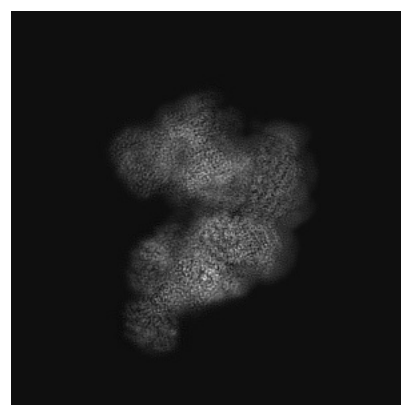
6.1.1 Primary map



X



Y

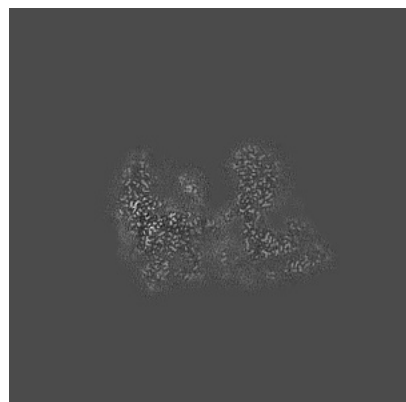


Z

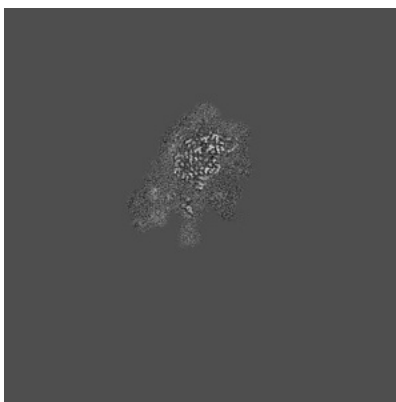
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

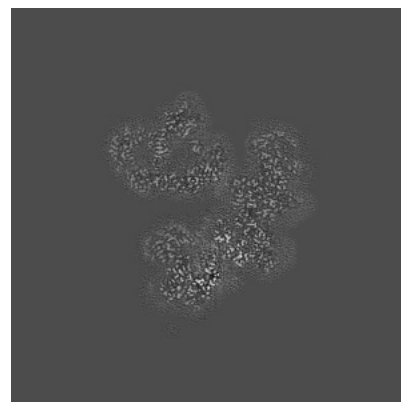
6.2.1 Primary map



X Index: 375



Y Index: 375

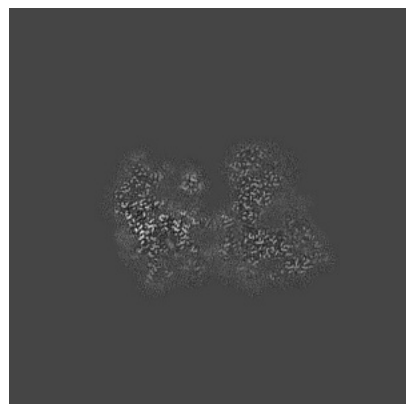


Z Index: 375

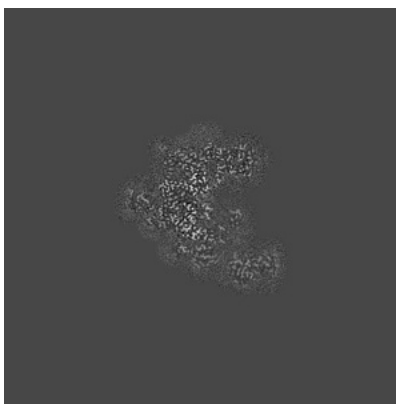
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

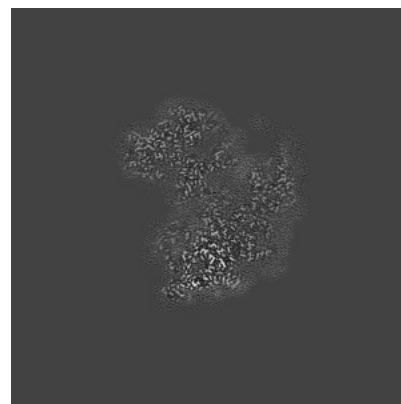
6.3.1 Primary map



X Index: 366



Y Index: 283

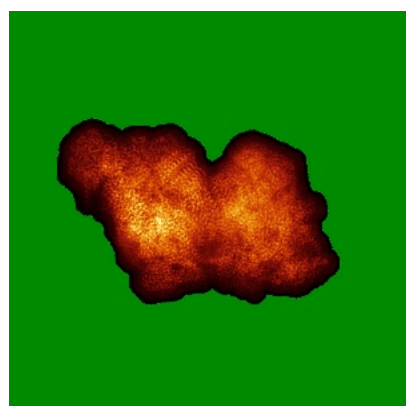


Z Index: 345

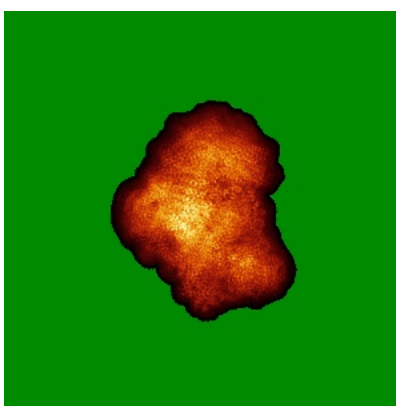
The images above show the largest variance slices of the map in three orthogonal directions.

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

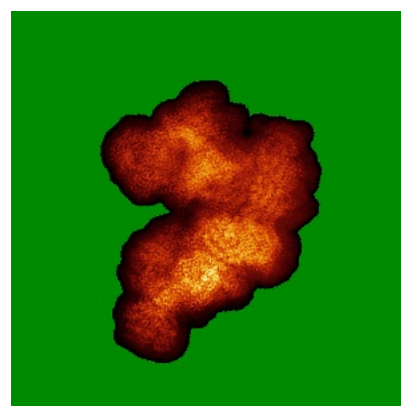
6.4.1 Primary map



X



Y

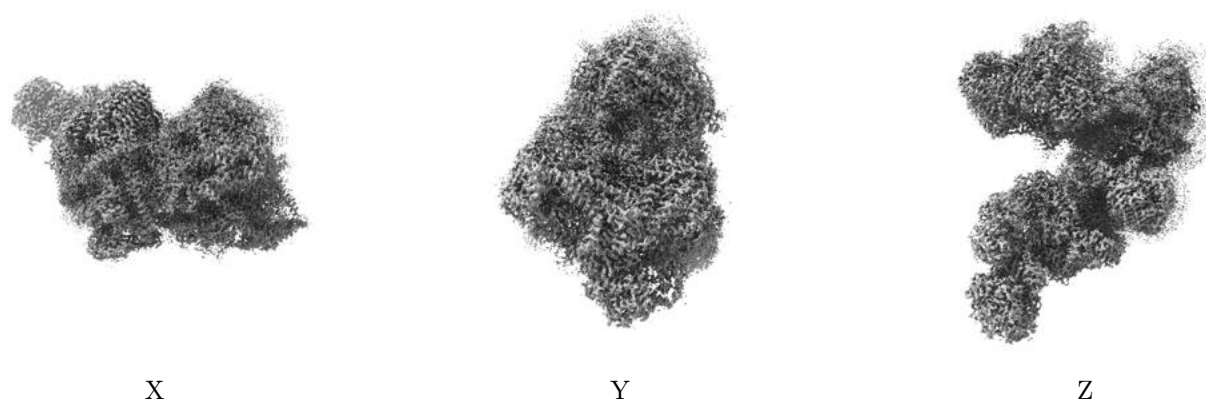


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

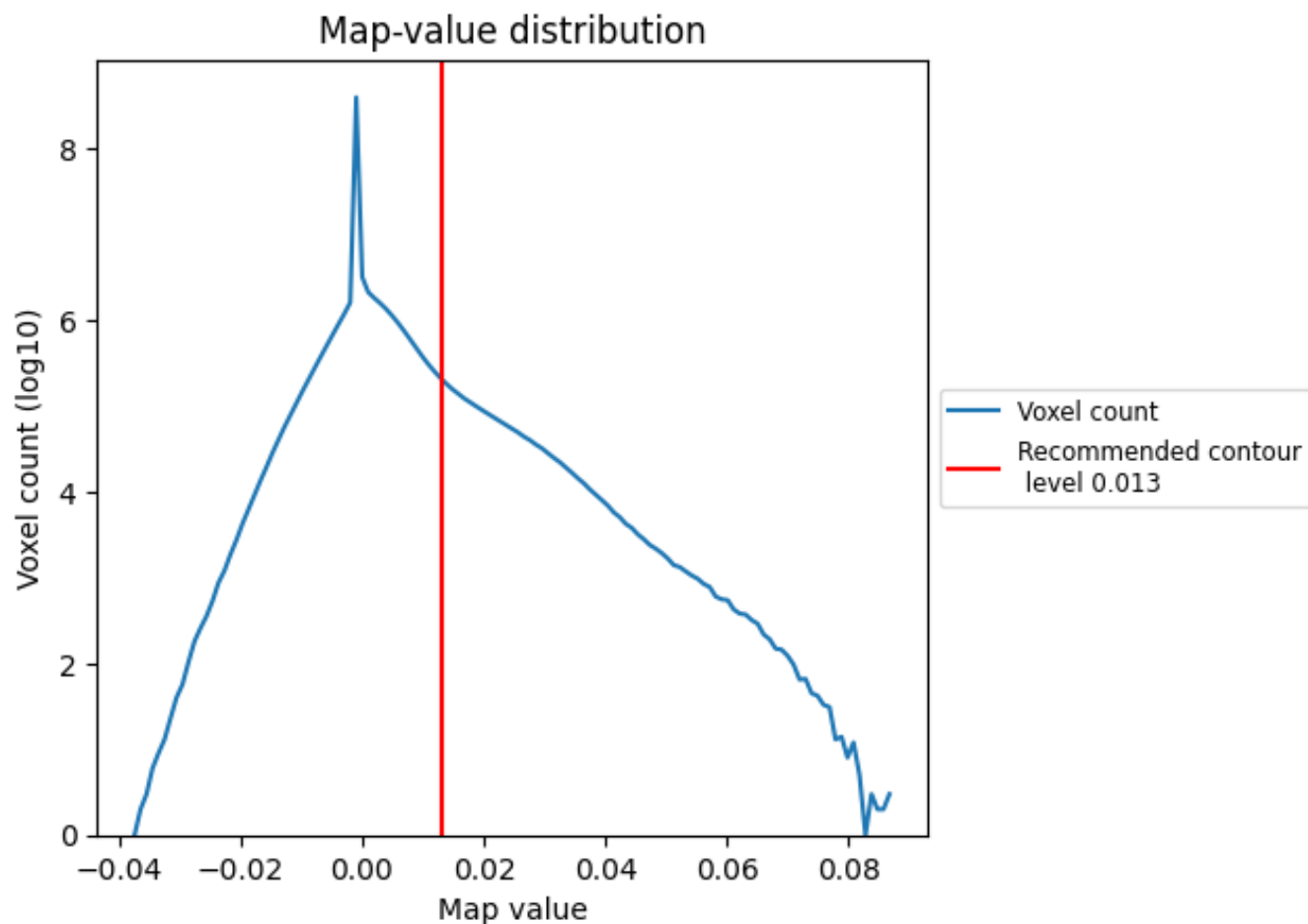
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

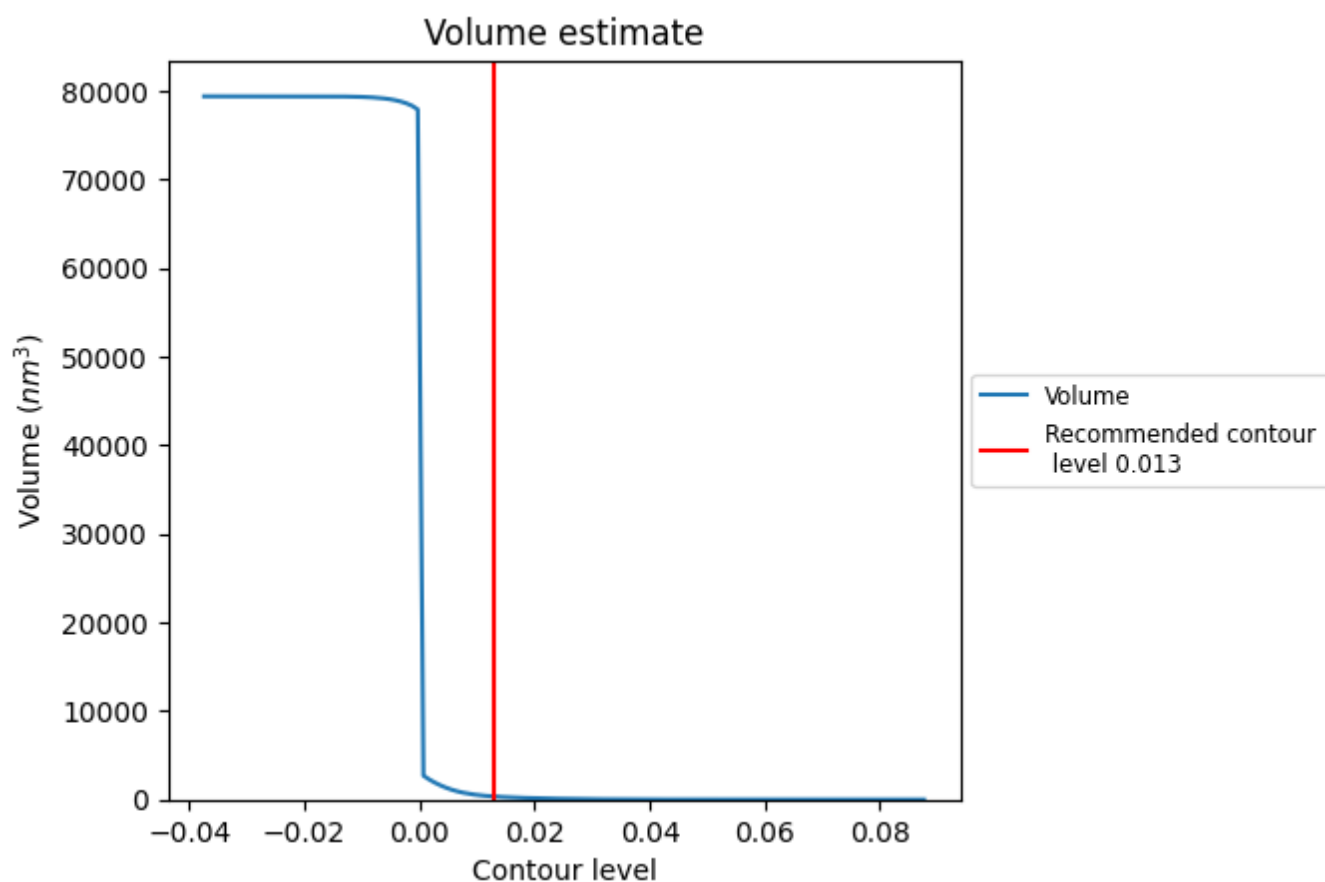
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

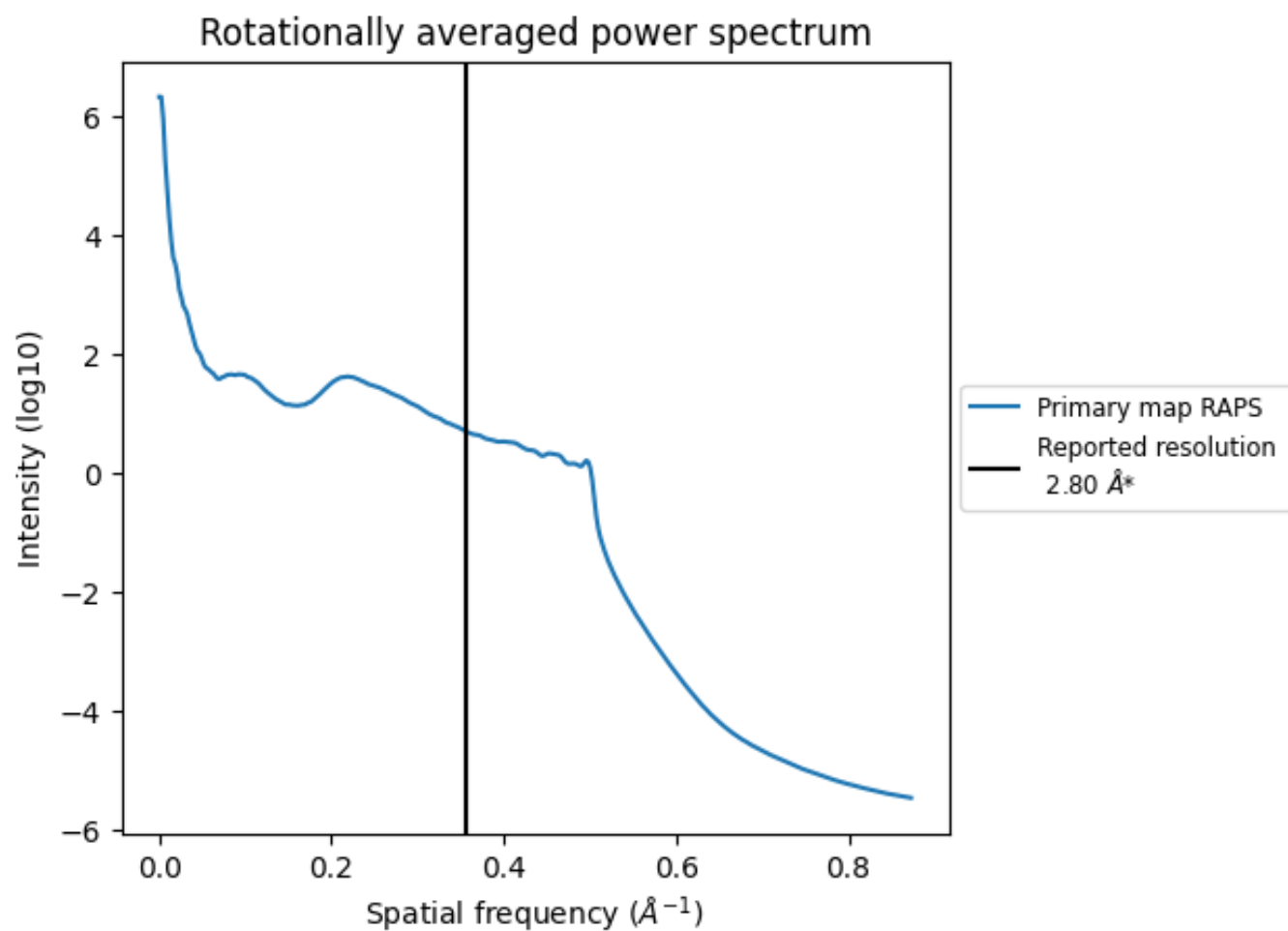
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 348 nm^3 ; this corresponds to an approximate mass of 314 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

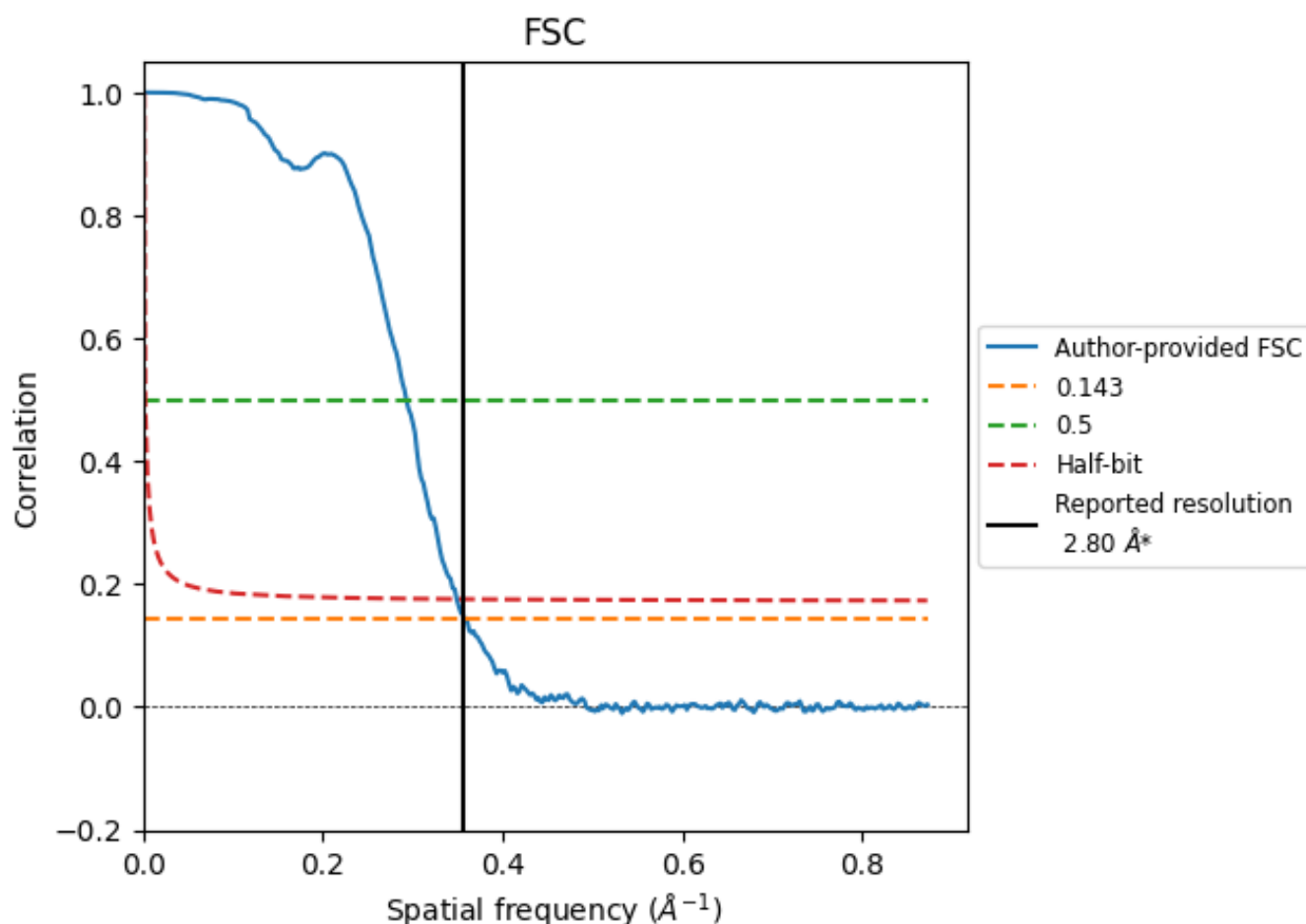


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

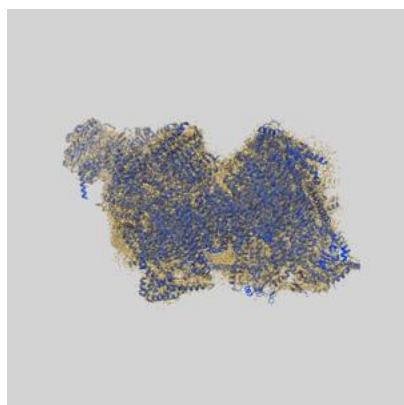
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.42	2.87
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

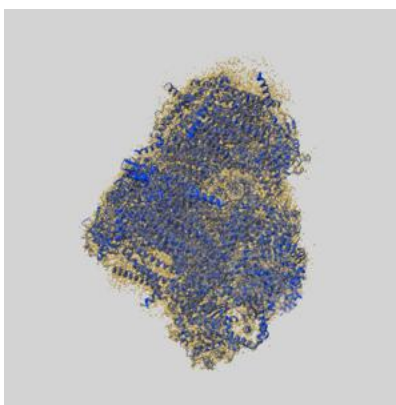
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16172 and PDB model 8BQ6. Per-residue inclusion information can be found in section [3](#) on page [23](#).

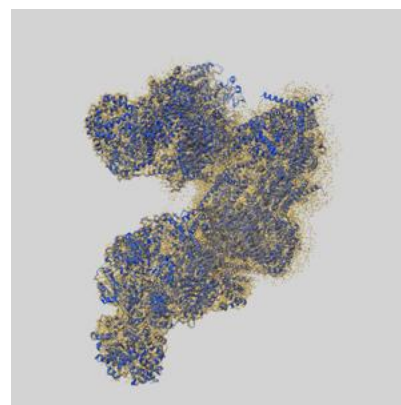
9.1 Map-model overlay [i](#)



X



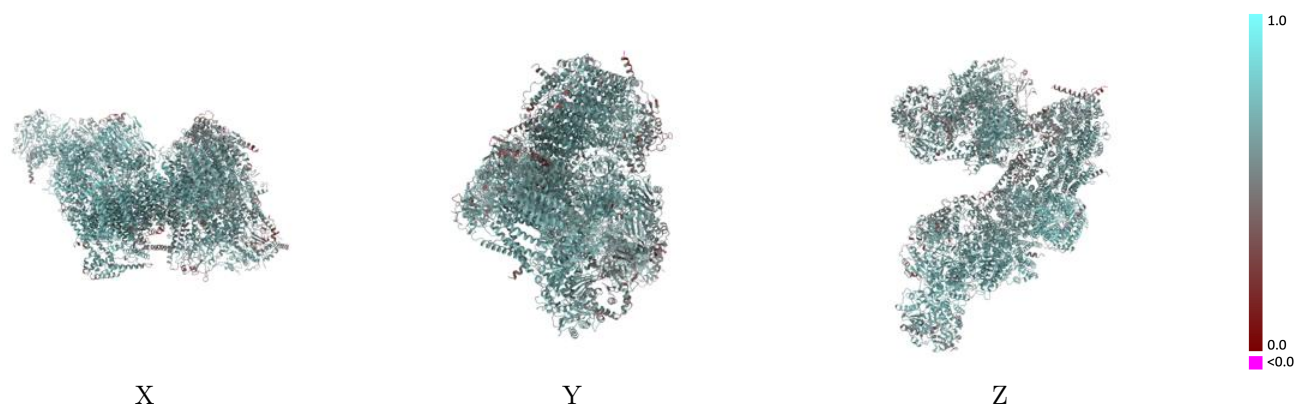
Y



Z

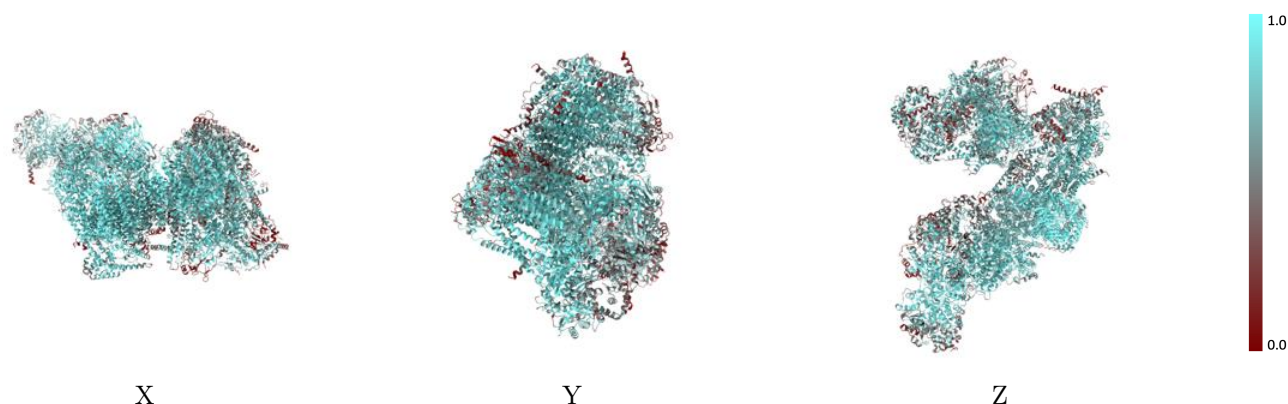
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



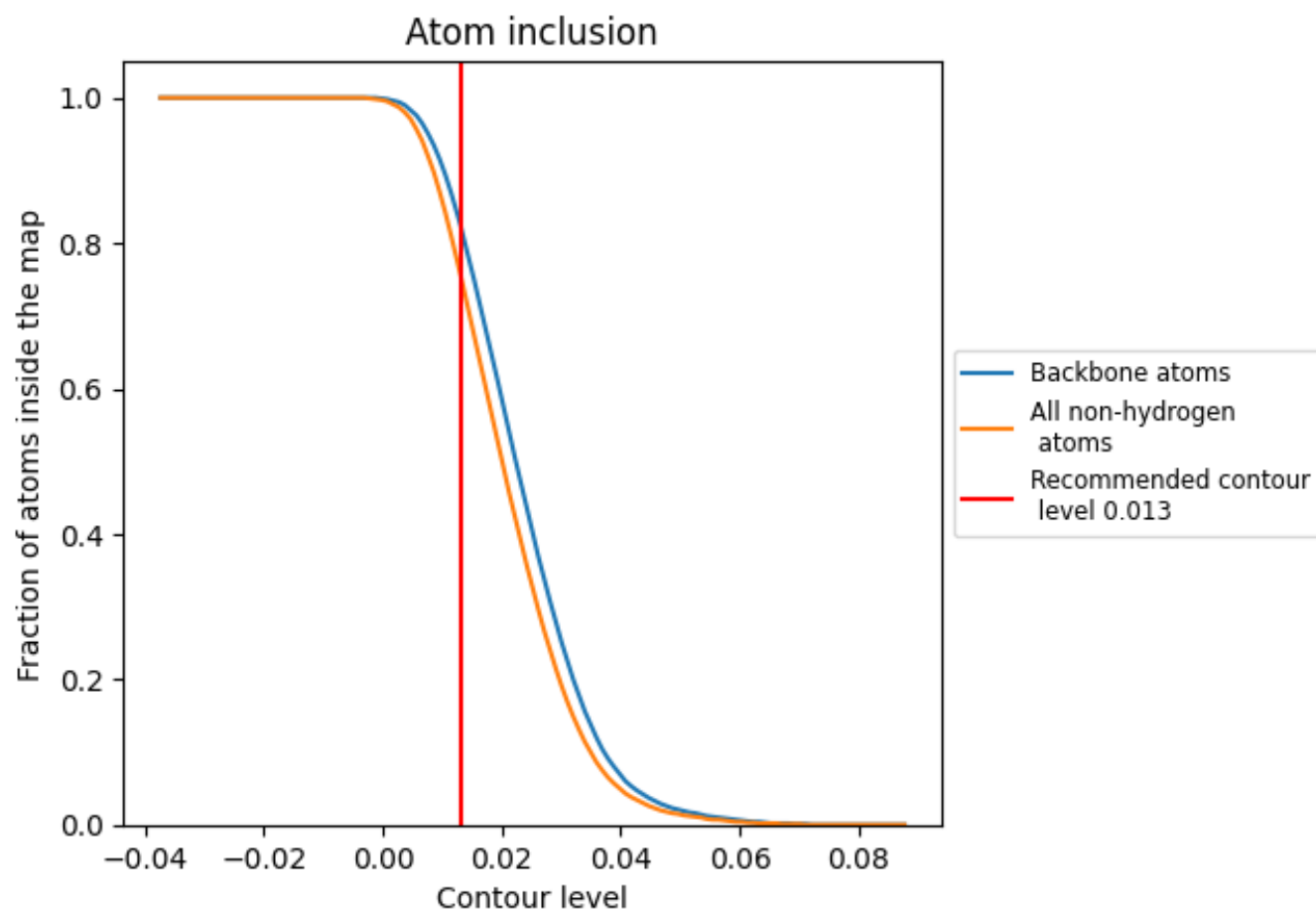
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.6280
A	 0.9520	 0.6900
AA	 0.5340	 0.5470
AB	 0.7810	 0.6360
AC	 0.8840	 0.6700
AD	 0.4040	 0.5070
AE	 0.8620	 0.6630
AF	 0.8600	 0.6720
AG	 0.8150	 0.6300
AH	 0.7460	 0.5890
AI	 0.7580	 0.6320
AJ	 0.3000	 0.4920
B	 0.9500	 0.7180
BA	 0.5760	 0.5650
BB	 0.7830	 0.6290
BC	 0.8420	 0.6490
BD	 0.4270	 0.5060
BE	 0.7980	 0.6330
BF	 0.8160	 0.6390
BG	 0.6800	 0.6010
BH	 0.4760	 0.5230
BI	 0.6510	 0.5710
BJ	 0.5450	 0.5330
C	 0.8700	 0.7030
D	 0.9430	 0.7160
E	 0.6000	 0.5770
F	 0.6970	 0.6260
G	 0.7340	 0.6390
H	 0.9370	 0.6930
I	 0.9470	 0.7170
J	 0.8790	 0.6680
K	 0.9390	 0.7030
L	 0.8040	 0.6340
M	 0.8840	 0.6630
N	 0.9120	 0.6930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.9420	 0.6630
P	 0.5970	 0.5790
Q	 0.4090	 0.5980
R	 0.7530	 0.6680
S	 0.4770	 0.5330
T	 0.3030	 0.4250
U	 0.5600	 0.4830
V	 0.6930	 0.6390
W	 0.5540	 0.5930
X	 0.7130	 0.5920
Y	 0.5750	 0.4950
Z	 0.7760	 0.6180
a	 0.8520	 0.6460
b	 0.7680	 0.5950
c	 0.6990	 0.5860
d	 0.7310	 0.5990
e	 0.8340	 0.6500
f	 0.8870	 0.6750
g	 0.6300	 0.5600
i	 0.5660	 0.5190
j	 0.4430	 0.4690
k	 0.3950	 0.4610
l	 0.5870	 0.5510
m	 0.7310	 0.6100
n	 0.7370	 0.5620
o	 0.5320	 0.5230
p	 0.6880	 0.5690
q	 0.8280	 0.6690
u	 0.7270	 0.5670
v	 0.8550	 0.6630
x	 0.9380	 0.7090
y	 0.8800	 0.6720
z	 0.8710	 0.6690