Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:56 AM UTC

PDB ID	:	5GPN / pdb_00005gpn
EMDB ID	:	EMD-9534
Title	:	Architecture of mammalian respirasome
Authors	:	Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on	:	2016-08-03
Resolution	:	5.40 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:

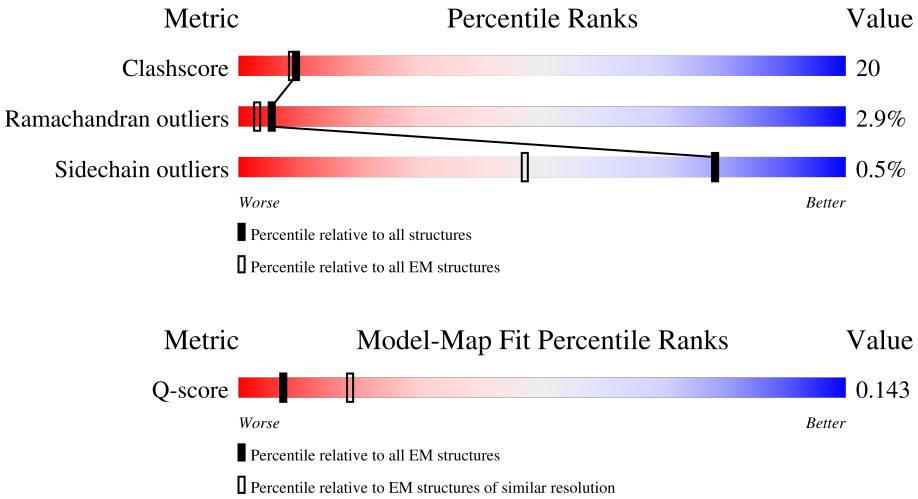
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 5.40 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	538 (4.90 - 5.90)

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

Mol	Chain	Length	Quality of chain
1	A	446	16% 57% 35% 8%
1	M	446	15% 58% 35% 7%
2	B	439	22% 63% 28% • 5%
2	N	439	8% 61% 32% • 5%

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Mol	Chain	Length	Quality of chain
3	C	379	13% 56% 36% 7%
3	O	379	33% 60% 36%
4	D	241	15% 69% 26% 5%
4	P	241	20% 63% 31% 5%
5	E	274	13% 60% 10% 28%
5	Q	274	24% 47% 19% 6% 28%
6	F	110	10% 66% 22% 8%
6	R	110	33% 78% 14% 5%
7	G	81	15% 49% 40% 11%
7	S	81	28% 73% 17% 5%
8	H	78	10% 64% 18% 18%
8	T	78	21% 68% 13% 18%
9	I	78	19% 27% 13% 58%
9	U	78	23% 19% 18% 58%
10	J	62	21% 61% 27% 11%
10	L	62	37% 60% 34% 6%
11	K	56	25% 62% 12% 23%
11	V	56	18% 55% 11% 34%
12	W	264	8% 28% 34% 36%
13	Y	727	9% 42% 46% 8%
14	Z	463	40% 38% 19%
15	a	216	31% 33% 32%
16	b	212	44% 24% 30%
17	c	464	8% 42% 42% 12%
18	d	249	9% 31% 35% 32%

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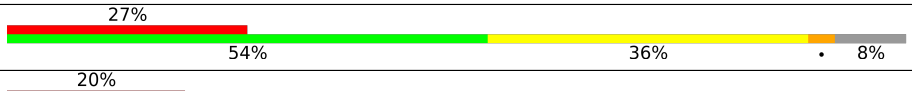
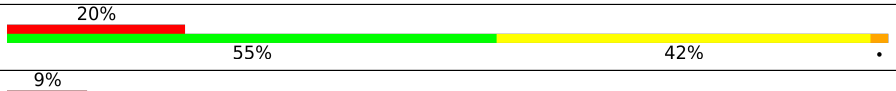
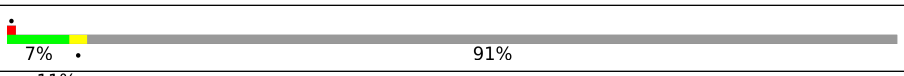
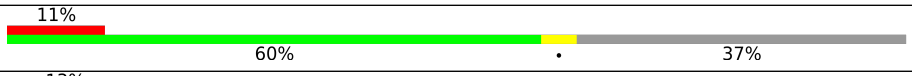
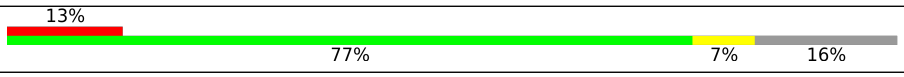
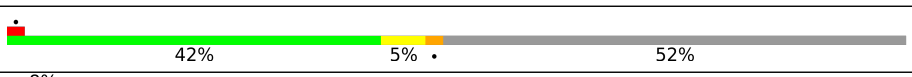
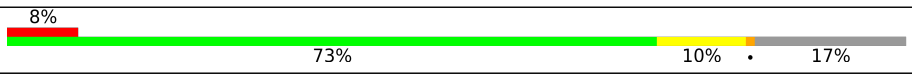
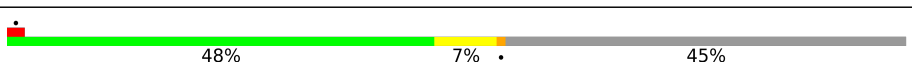
Mol	Chain	Length	Quality of chain
19	e	318	
20	f	347	
21	g	115	
22	h	459	
23	i	98	
24	j	606	
25	k	175	
25	l	175	
26	m	84	
27	n	99	
28	o	106	
29	p	377	
30	q	357	
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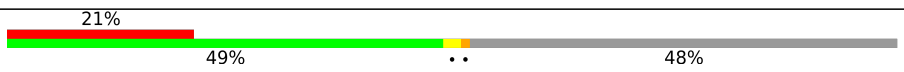
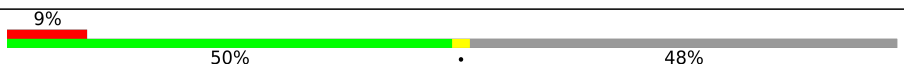
31	r	144	
32	Aa	156	
32	t	156	
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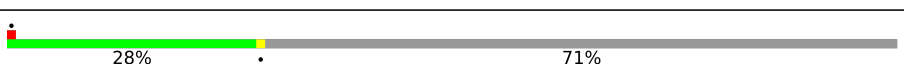
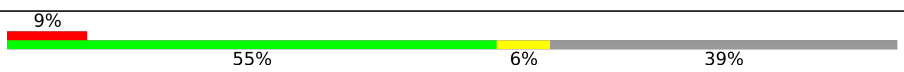
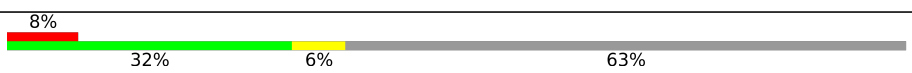
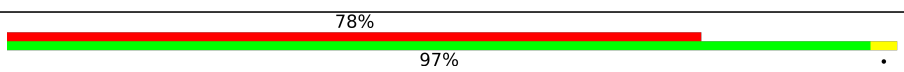
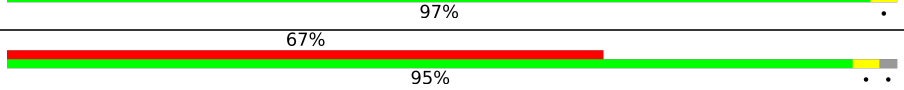
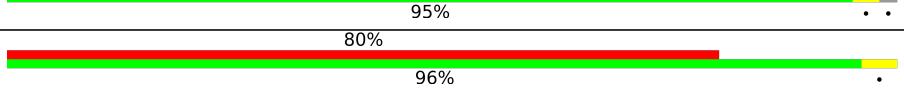
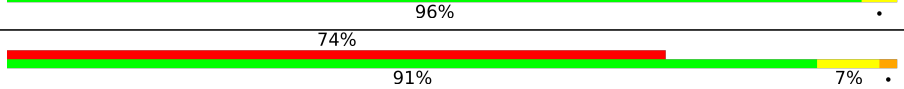
33	u	189	
34	w	175	
35	x	123	
36	0	261	
37	1	147	
38	2	109	
39	3	98	

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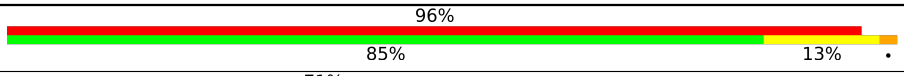
Mol	Chain	Length	Quality of chain
40	4	84	
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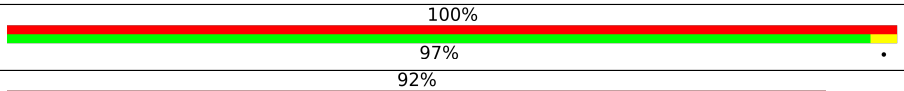
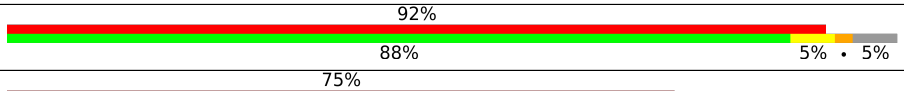
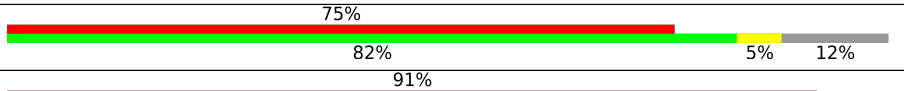
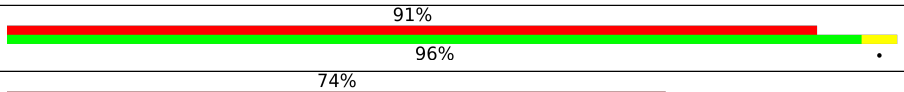
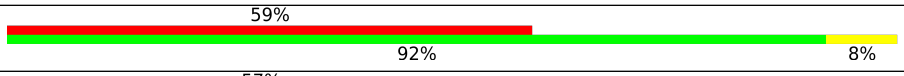
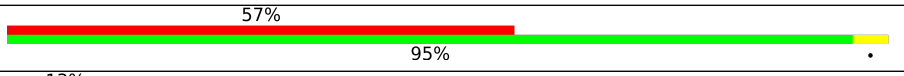
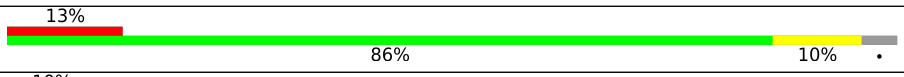
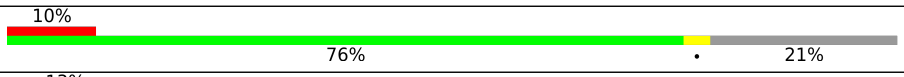
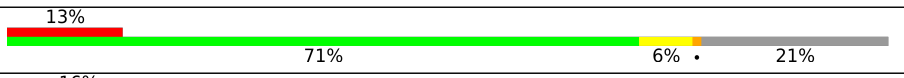
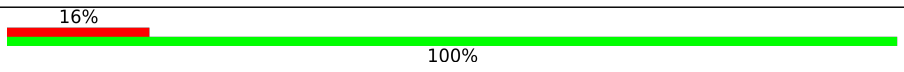
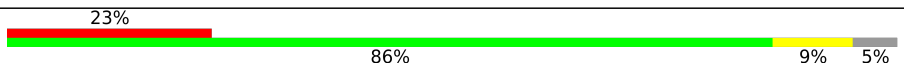
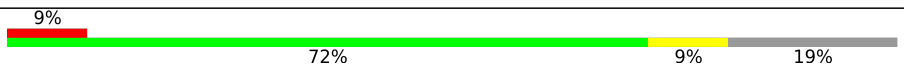
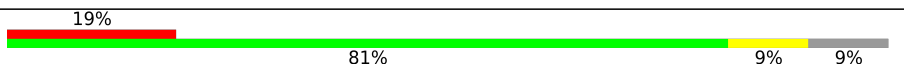
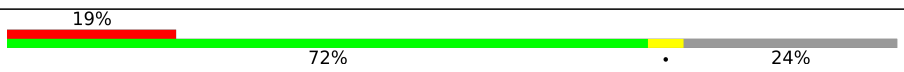
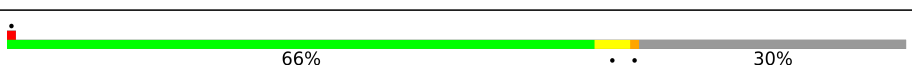
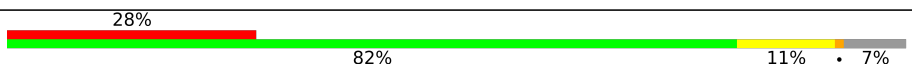
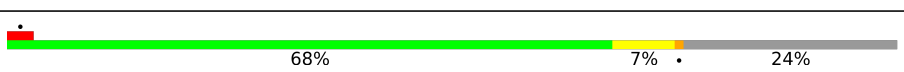
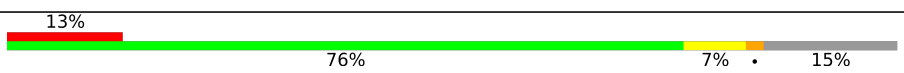
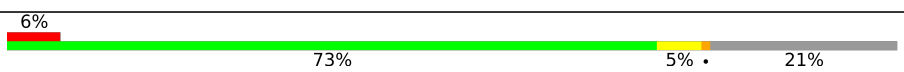
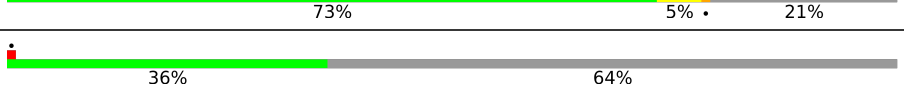
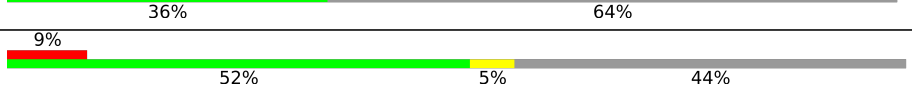
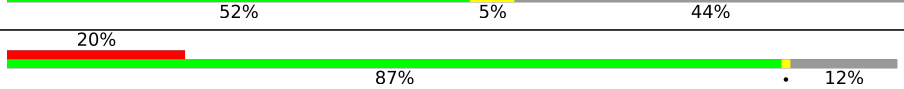
42	6	73	
43	7	59	
44	8	56	
45	9	47	
46	s	46	
47	y	514	
48	z	227	
49	Ab	134	
49	Ah	134	
50	Ac	70	
51	Ad	43	
51	Ao	43	
51	Ap	43	
51	Av	43	
52	Ae	116	
53	Af	128	
54	Ag	141	
55	Aj	176	
56	Ak	178	
57	Al	122	
58	Am	76	
59	An	172	
60	Aq	76	

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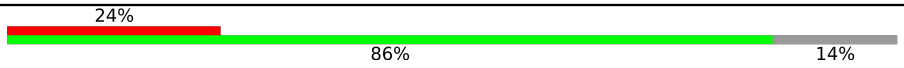
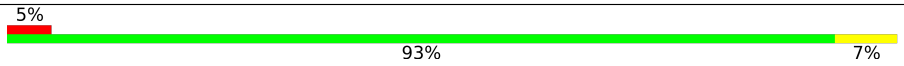
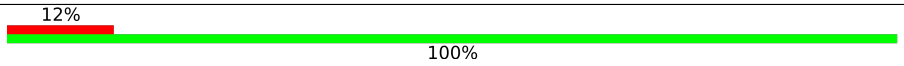
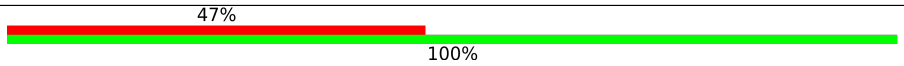
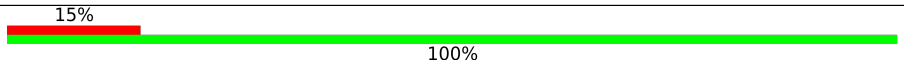
Mol	Chain	Length	Quality of chain
60	As	76	
60	Aw	76	
61	Ar	34	
62	At	17	
63	Au	13	

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
64	HEM	C	402	-	-	X	-
67	SF4	Y	801	-	-	X	-
67	SF4	b	301	-	-	X	-
67	SF4	c	501	-	-	X	-
68	FMN	c	502	-	-	X	-
69	NDP	p	401	-	-	X	-

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 75545 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	446	Total 2198	C 1306	N 446	O 446	0	0
1	M	446	Total 2198	C 1306	N 446	O 446	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	419	Total 2061	C 1223	N 419	O 419	0	0
2	N	419	Total 2061	C 1223	N 419	O 419	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	379	Total 1870	C 1112	N 379	O 379	0	0
3	O	379	Total 1870	C 1112	N 379	O 379	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	241	Total 1188	C 706	N 241	O 241	0	0
4	P	241	Total 1188	C 706	N 241	O 241	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	196	Total 967	C 575	N 196	O 196	0	0
5	Q	196	Total 966	C 574	N 196	O 196	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	106	Total 527	C 315	N 106	O 106	0	0
6	R	106	Total 527	C 315	N 106	O 106	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	81	Total 401	C 239	N 81	O 81	0	0
7	S	78	Total 386	C 230	N 78	O 78	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	64	Total 320	C 192	N 64	O 64	0	0
8	T	64	Total 320	C 192	N 64	O 64	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	33	Total 163	C 97	N 33	O 33	0	0
9	U	33	Total 163	C 97	N 33	O 33	0	0

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	62	Total 307	C 183	N 62	O 62	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	62	Total 307	C 183	N 62	O 62	0	0

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	43	Total 211	C 125	N 43	O 43	0	0
11	V	37	Total 182	C 108	N 37	O 37	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	169	Total 1366	C 884	N 234	O 246	S 2	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	672	Total 4998	C 3128	N 874	O 958	S 38	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	375	Total 3003	C 1917	N 515	O 548	S 23	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	147	Total 1146	C 730	N 204	O 198	S 14	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	149	Total 1189	C 746	N 205	O 228	S 10	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	410	Total	C	N	O	S	0	0
			3125	1974	558	573	20		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	169	Total	C	N	O	S	0	0
			1324	852	218	245	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	315	Total	C	N	O	S	0	0
			2486	1665	381	419	21		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	346	Total	C	N	O	S	0	0
			2698	1774	418	461	45		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	106	Total	C	N	O	S	0	0
			829	559	120	144	6		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	457	Total	C	N	O	S	0	0
			3610	2396	570	606	38		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	90	Total	C	N	O	S	0	0
			677	448	101	115	13		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	594	Total	C	N	O	S	0	0
			4705	3120	729	807	49		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	142	Total	C	N	O	S	0	0
			1059	712	152	183	12		
25	l	15	Total	C	N	O		0	0
			73	43	15	15			

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	m	53	Total	C	N	O	0	0
			263	157	53	53		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	n	83	Total	C	N	O	0	0
			411	245	83	83		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	o	51	Total	C	N	O	0	0
			251	149	51	51		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	p	314	Total	C	N	O	0	0
			1546	918	314	314		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	q	196	Total 967	C 575	N 196	O 196	0	0
30	v	51	Total 252	C 150	N 51	O 51	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	r	63	Total 311	C 185	N 63	O 63	0	0

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	t	81	Total 403	C 241	N 81	O 81	0	0
32	Aa	81	Total 403	C 241	N 81	O 81	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	u	54	Total 267	C 159	N 54	O 54	0	0
33	Ai	34	Total 167	C 99	N 34	O 34	0	0

- Molecule 34 is a protein called Mitochondrial NADH dehydrogenase Fe-S protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	w	107	Total 530	C 316	N 107	O 107	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	46	Total 221	C 129	N 46	O 46	0	0

- Molecule 36 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	0	261	Total	C	N	O	0	0
			1284	762	261	261		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	1	144	Total	C	N	O	0	0
			716	428	144	144		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2	109	Total	C	N	O	0	0
			539	321	109	109		

- Molecule 39 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	3	98	Total	C	N	O	0	0
			481	285	98	98		

- Molecule 40 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	4	84	Total	C	N	O	0	0
			411	243	84	84		

- Molecule 41 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	5	75	Total	C	N	O	0	0
			371	221	75	75		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	6	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	7	56	Total	C	N	O	0	0
			274	162	56	56		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	8	49	Total	C	N	O	0	0
			241	143	49	49		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	9	47	Total	C	N	O	0	0
			231	137	47	47		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	s	43	Total	C	N	O	0	0
			213	127	43	43		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	y	514	Total	C	N	O	0	0
			2523	1495	514	514		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	227	Total	C	N	O	0	0
			1127	673	227	227		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Ab	129	Total	C	N	O	0	0
			637	379	129	129		
49	Ah	106	Total	C	N	O	0	0
			526	314	106	106		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Ac	55	Total 271	C 161	N 55	O 55	0	0

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ad	43	Total 211	C 125	N 43	O 43	0	0
51	Ao	41	Total 205	C 123	N 41	O 41	0	0
51	Ap	35	Total 173	C 103	N 35	O 35	0	0
51	Av	39	Total 193	C 115	N 39	O 39	0	0

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Ae	88	Total 435	C 259	N 88	O 88	0	0

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Af	90	Total 448	C 268	N 90	O 90	0	0

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Ag	131	Total 637	C 375	N 131	O 131	0	0

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Aj	133	Total 663	C 397	N 133	O 133	0	0

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Ak	151	Total 750	C 448	N 151	O 151	0	0

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Al	96	Total 473	C 281	N 96	O 96	0	0

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Am	27	Total 134	C 80	N 27	O 27	0	0

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	An	97	Total 482	C 288	N 97	O 97	0	0

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	Aq	67	Total 335	C 201	N 67	O 67	0	0
60	As	65	Total 322	C 192	N 65	O 65	0	0
60	Aw	76	Total 376	C 224	N 76	O 76	0	0

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	Ar	34	Total	C	N	O	0	0
			169	101	34	34		

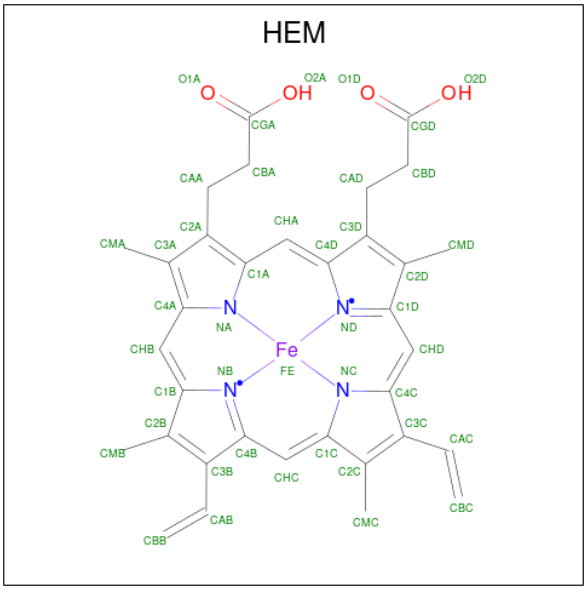
- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	At	17	Total	C	N	O	0	0
			84	50	17	17		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	Au	13	Total	C	N	O	0	0
			62	36	13	13		

- Molecule 64 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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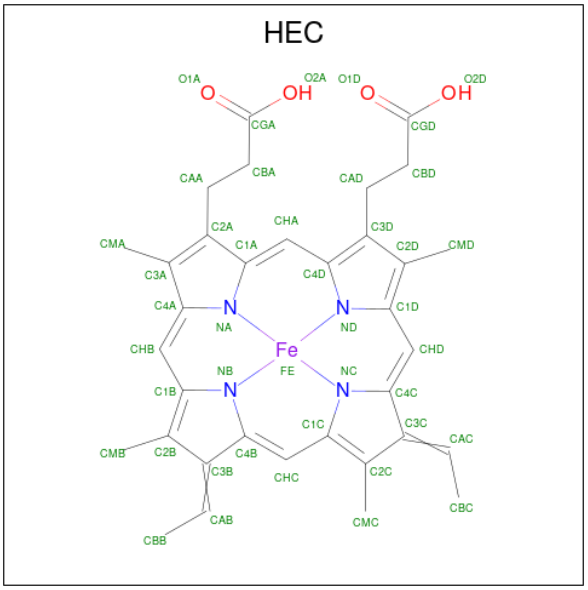
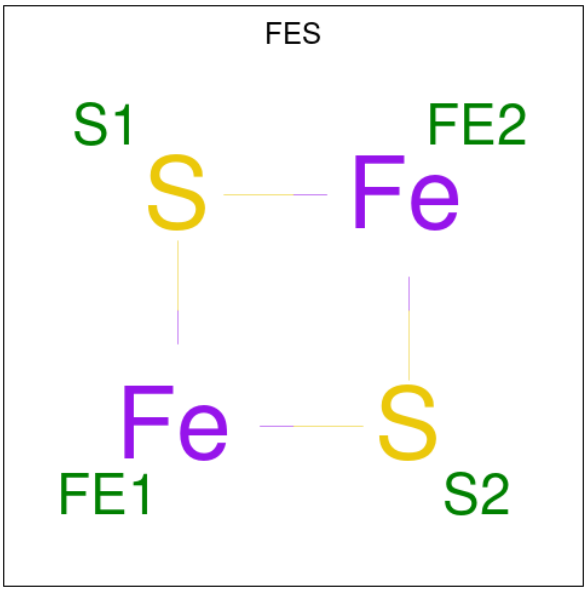
Mol	Chain	Residues	Atoms					AltConf
64	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 65 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



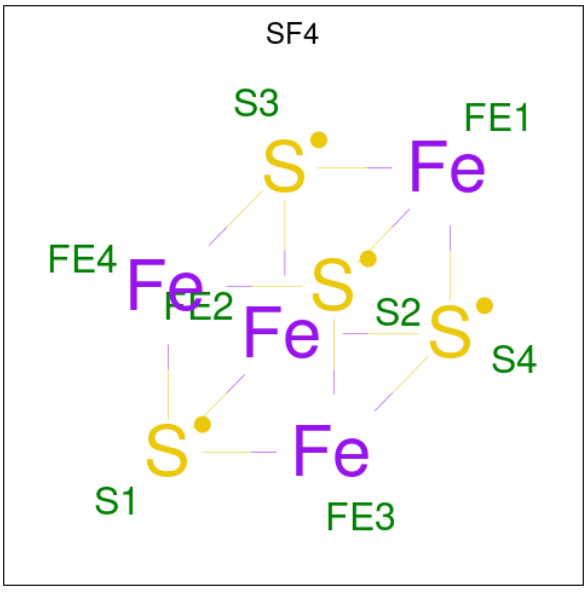
Mol	Chain	Residues	Atoms					AltConf
65	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
65	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 66 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



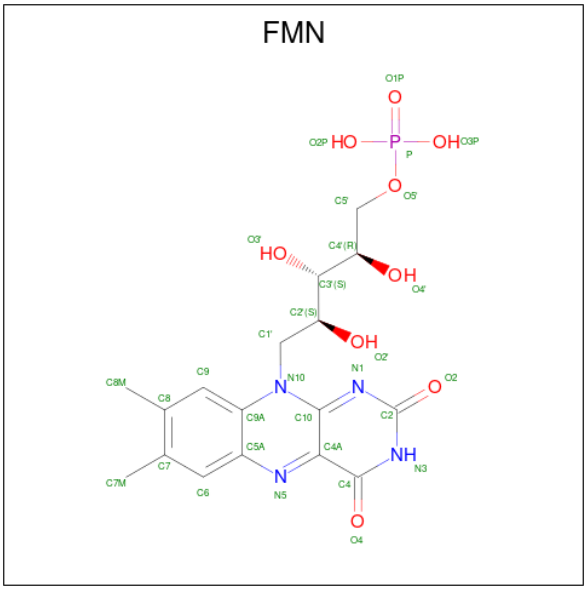
Mol	Chain	Residues	Atoms	AltConf
66	E	1	Total Fe S 4 2 2	0
66	Q	1	Total Fe S 4 2 2	0
66	Y	1	Total Fe S 4 2 2	0
66	d	1	Total Fe S 4 2 2	0

- Molecule 67 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



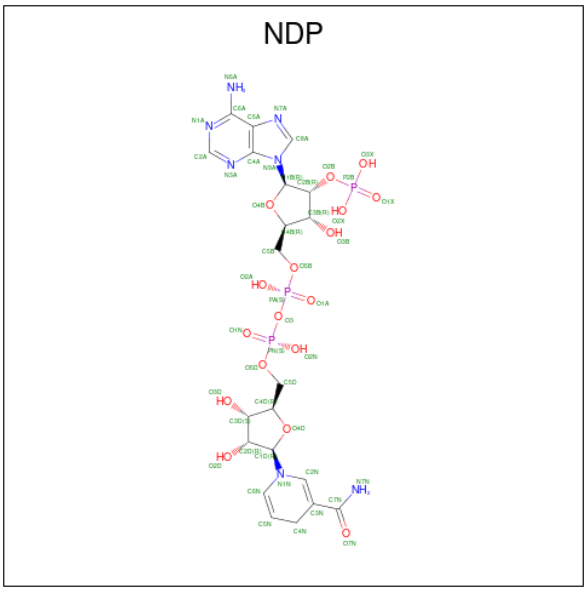
Mol	Chain	Residues	Atoms	AltConf
67	Y	1	Total Fe S 8 4 4	0
67	Y	1	Total Fe S 8 4 4	0
67	a	1	Total Fe S 8 4 4	0
67	b	1	Total Fe S 8 4 4	0
67	b	1	Total Fe S 8 4 4	0
67	c	1	Total Fe S 8 4 4	0

- Molecule 68 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 69 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

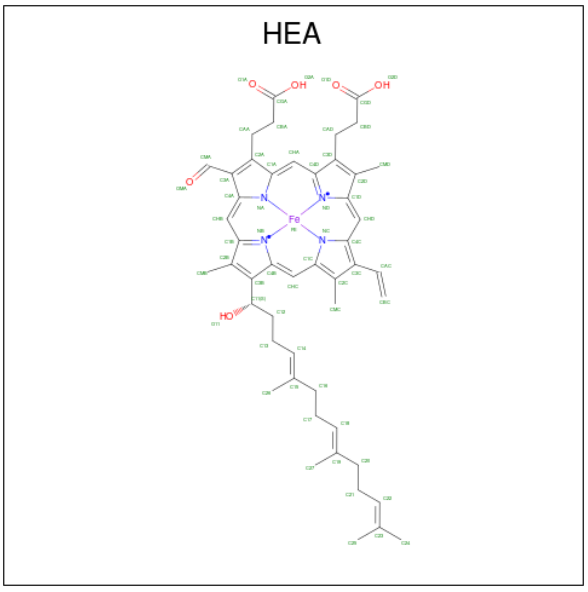


Mol	Chain	Residues	Atoms					AltConf
69	p	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
70	3	1	Total	Zn	0
			1	1	

- Molecule 71 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
71	y	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
71	y	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 72 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
72	y	1	Total	Cu	0
			1	1	
72	z	2	Total	Cu	0
			2	2	

- Molecule 73 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

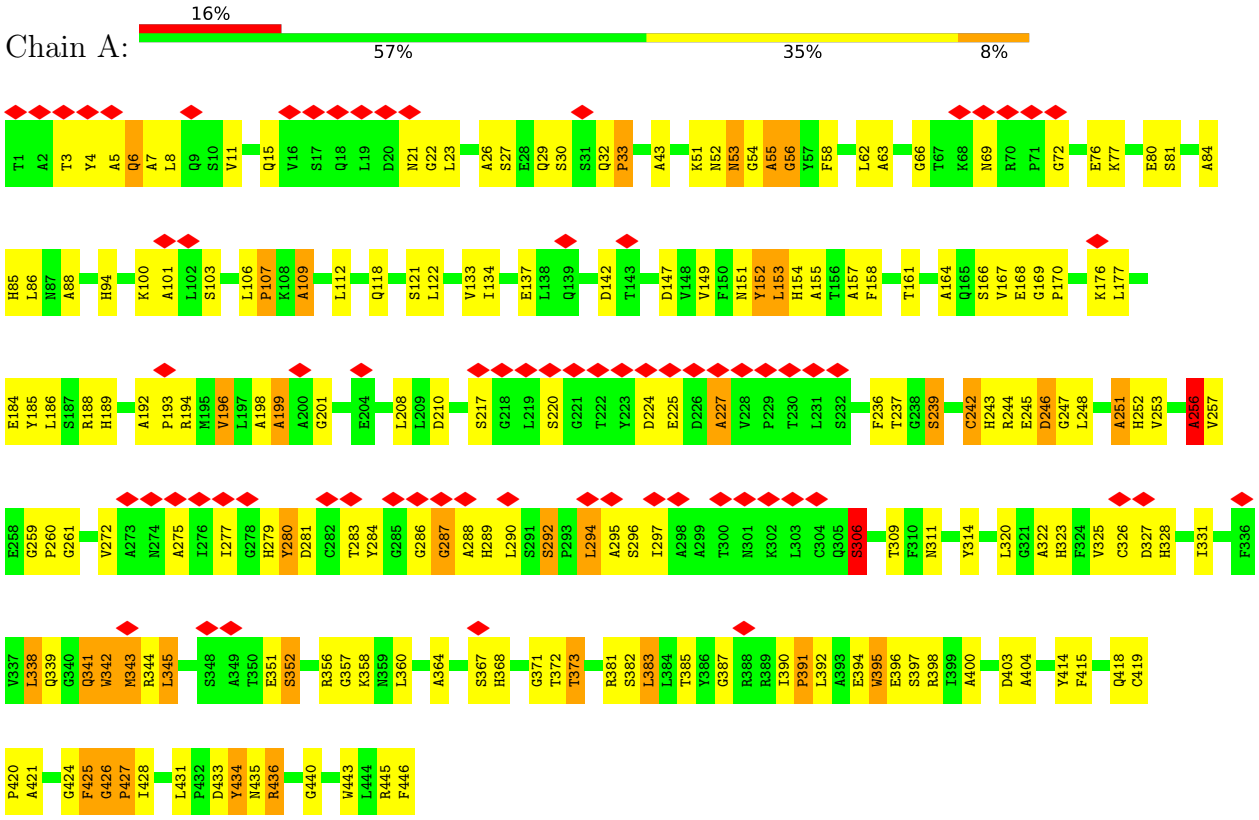
Mol	Chain	Residues	Atoms		AltConf
73	y	1	Total	Mg	0
			1	1	

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.

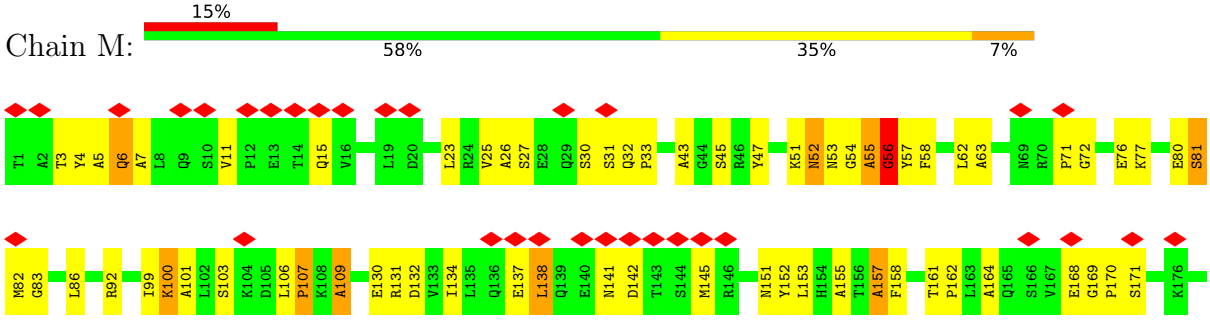
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

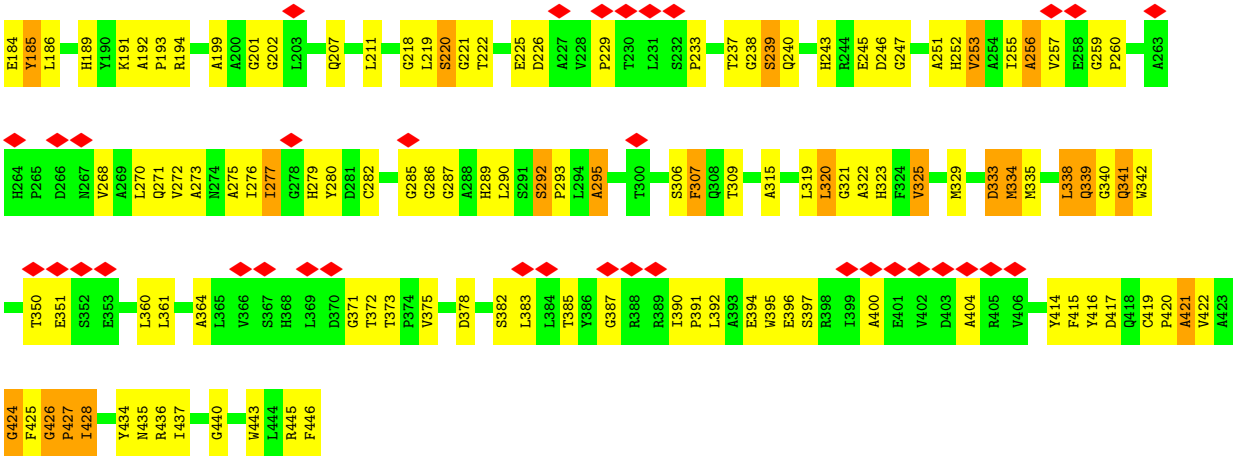
Chain A:



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

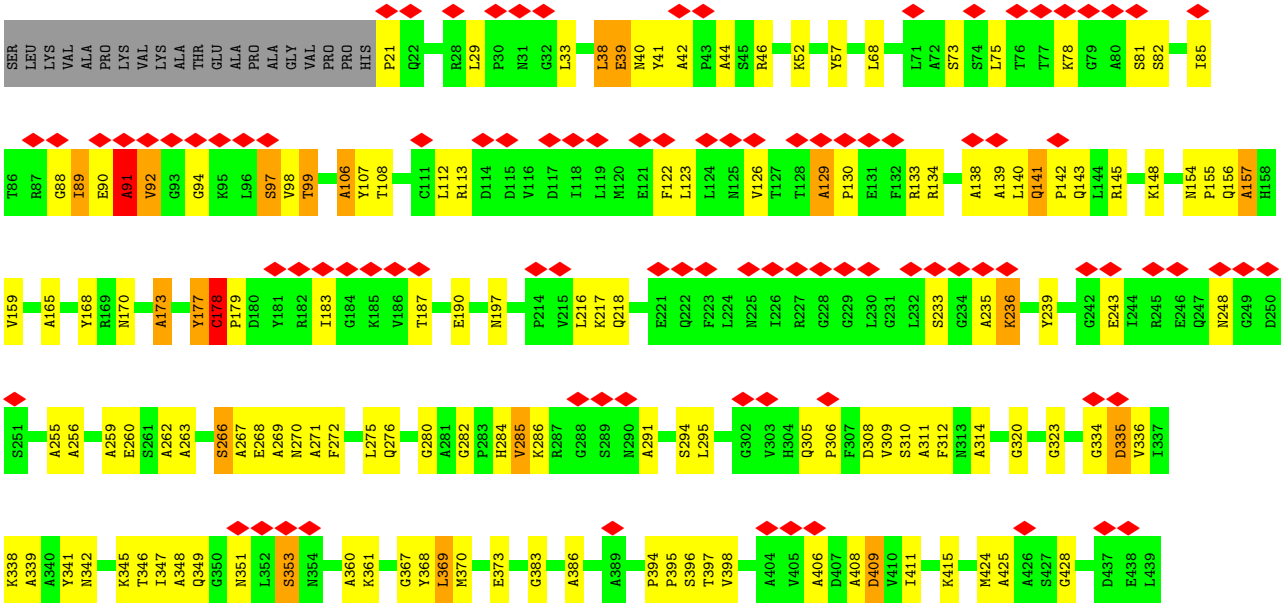
Chain M:





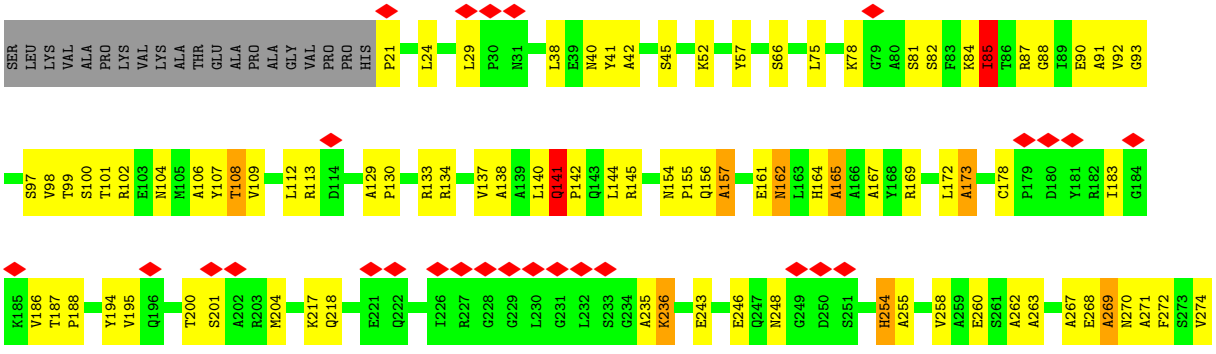
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

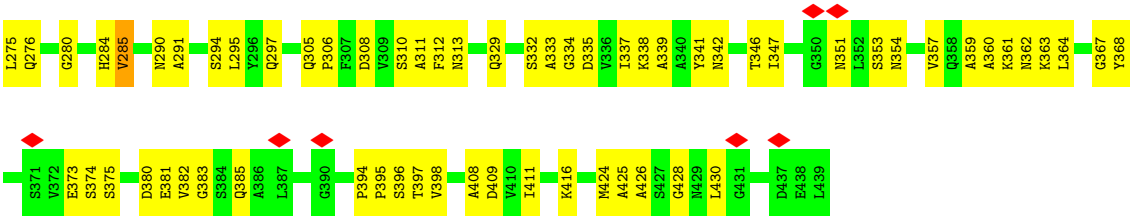
Chain B:



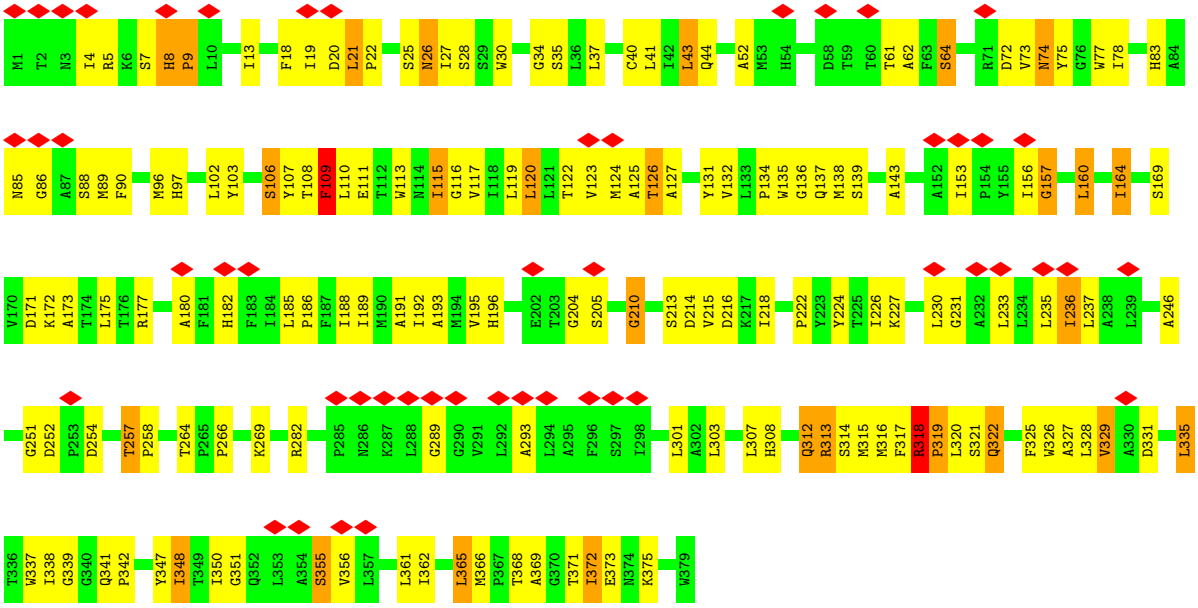
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain N:

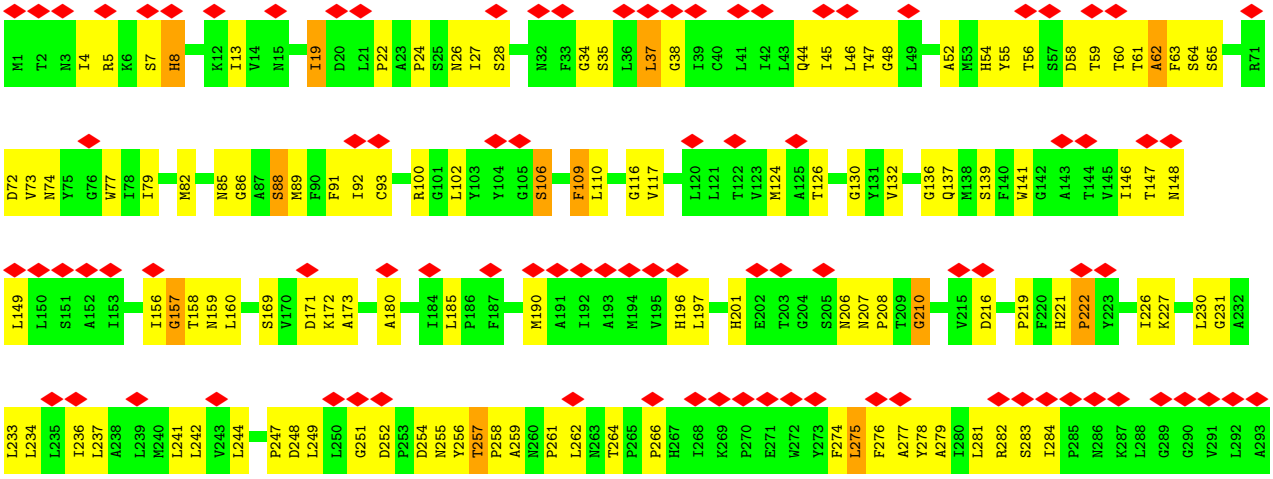


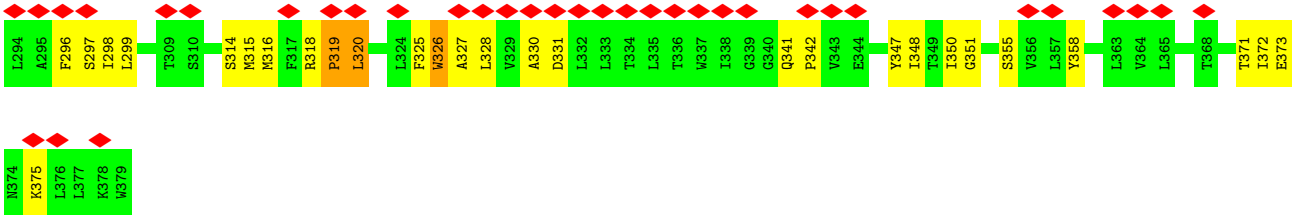


• Molecule 3: Cytochrome b



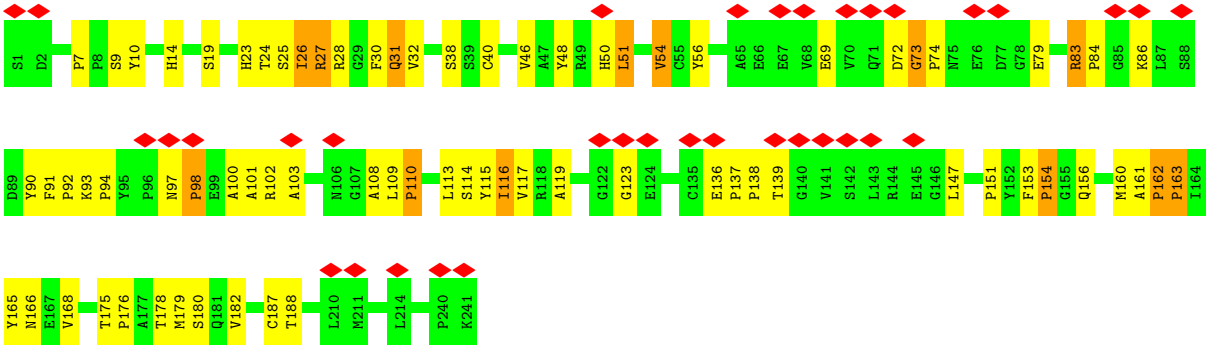
• Molecule 3: Cytochrome b





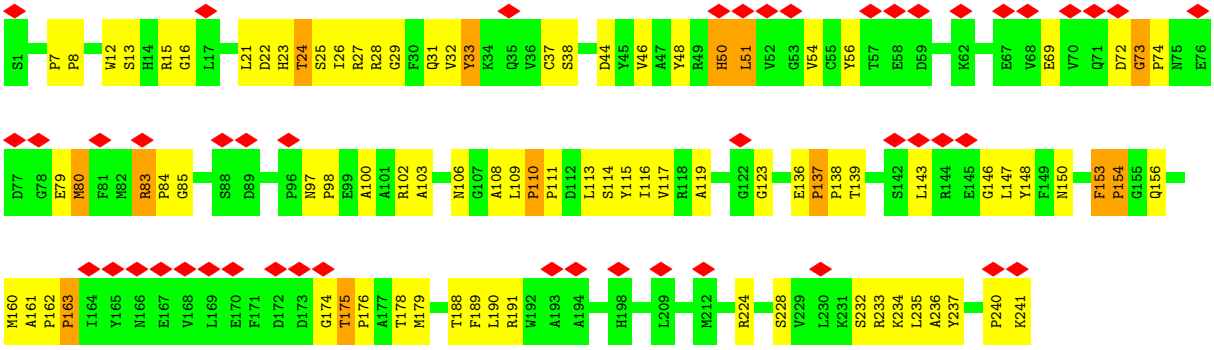
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



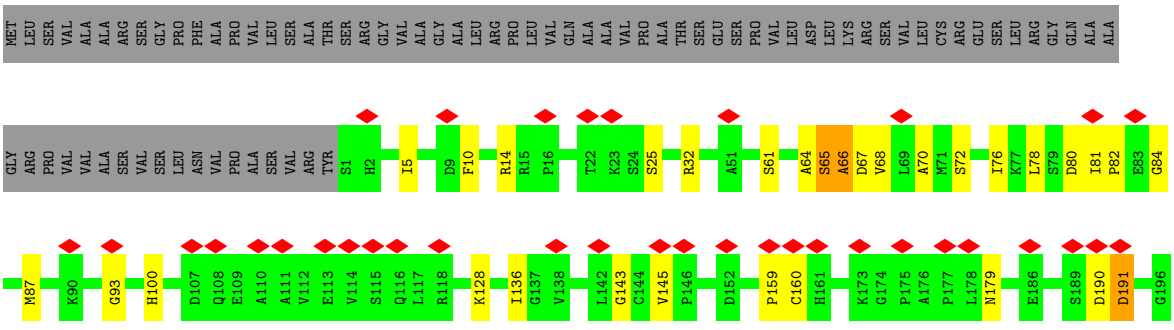
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain P:



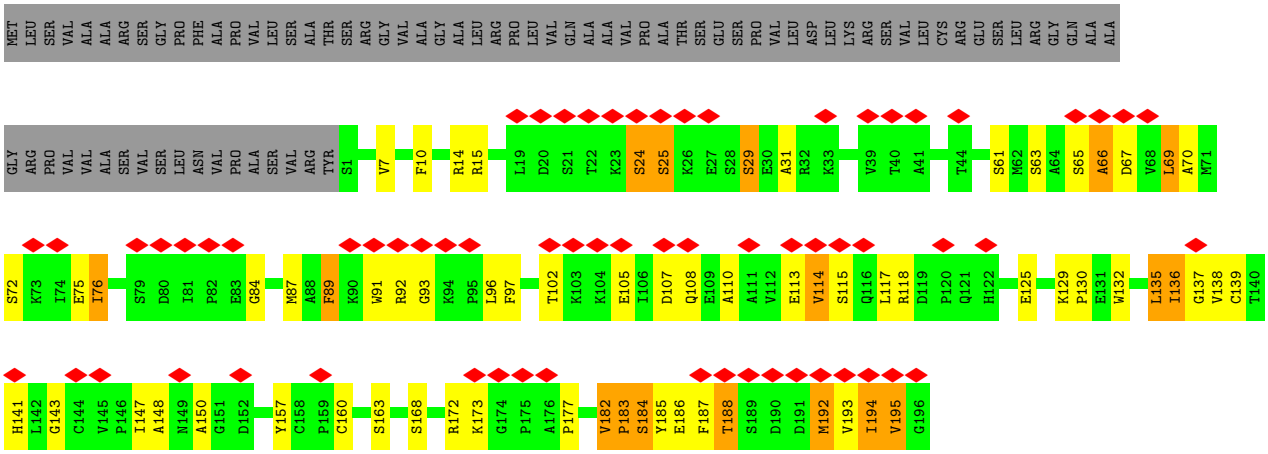
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



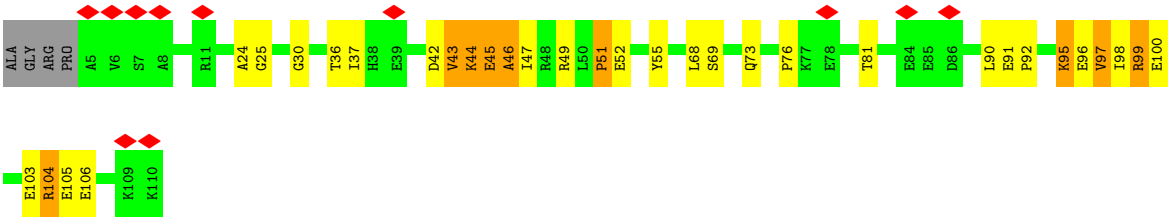
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Q:



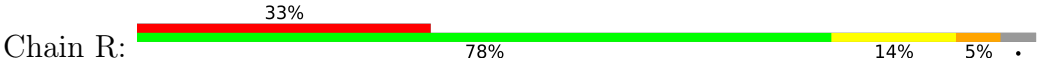
• Molecule 6: Cytochrome b-c1 complex subunit 7

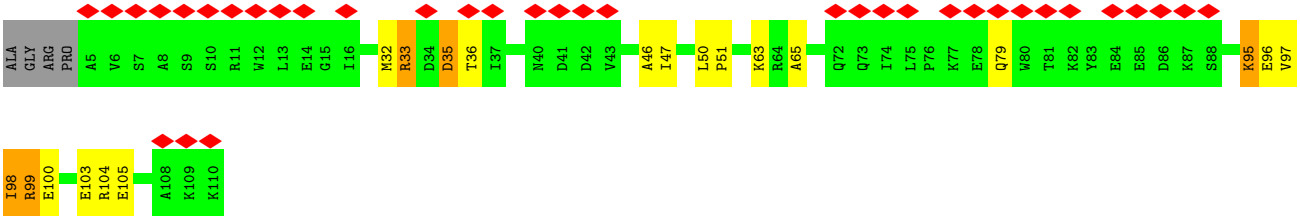
Chain F:



• Molecule 6: Cytochrome b-c1 complex subunit 7

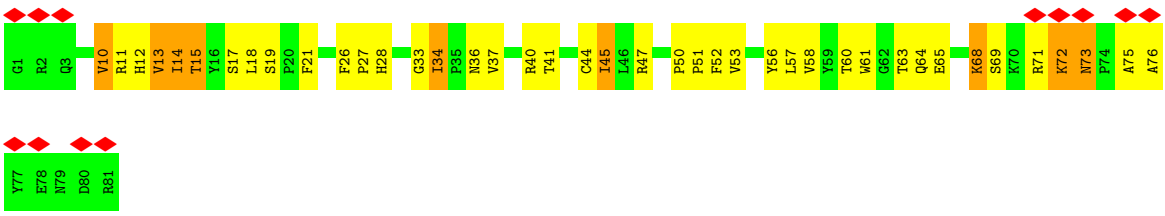
Chain R:





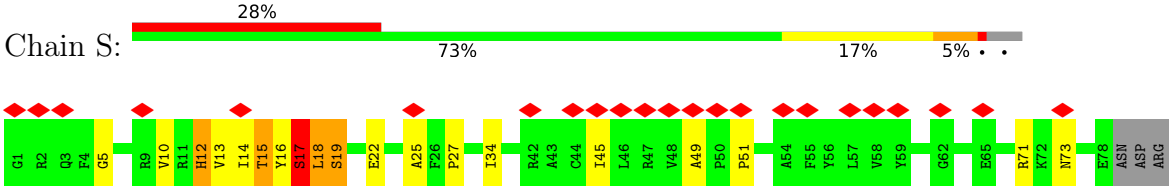
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G:



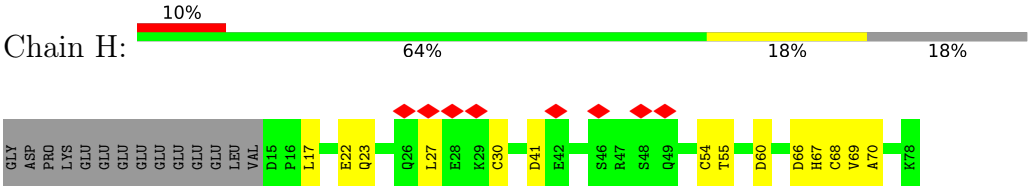
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain S:



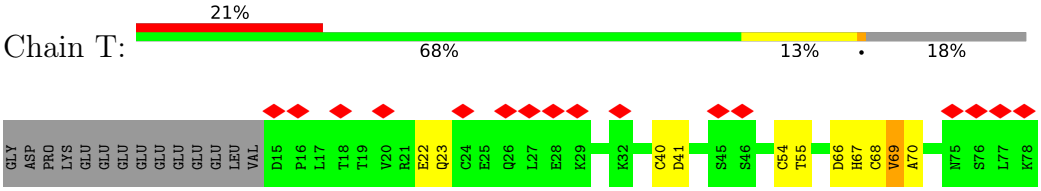
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



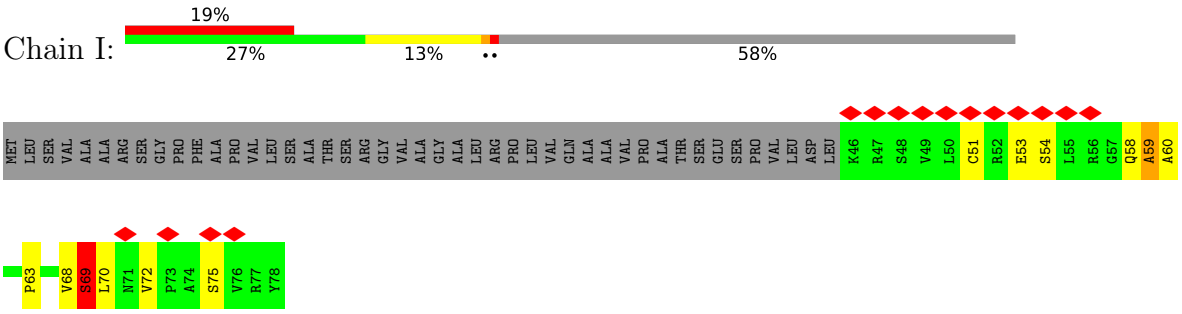
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain T:



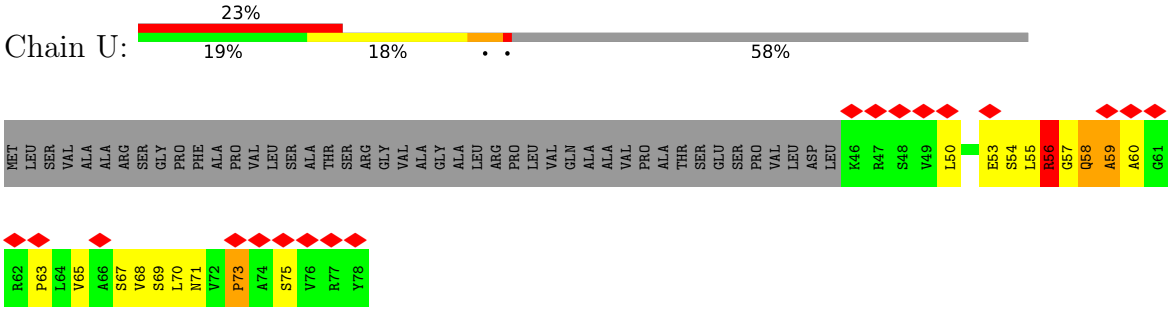
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



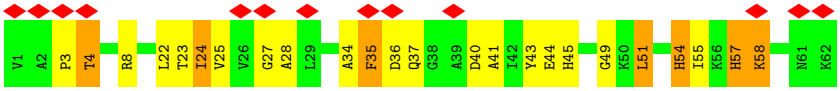
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain U:



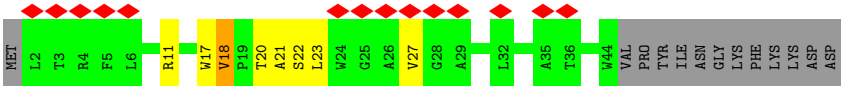
• Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:

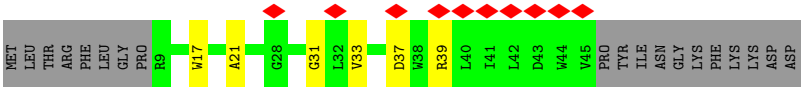


• Molecule 10: Cytochrome b-c1 complex subunit 9

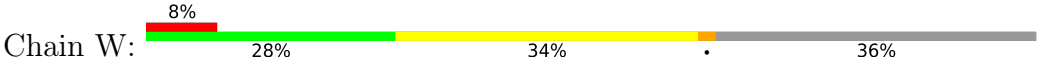
• Molecule 11: Cytochrome b-c1 complex subunit 10

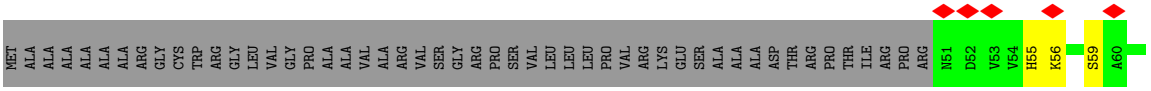


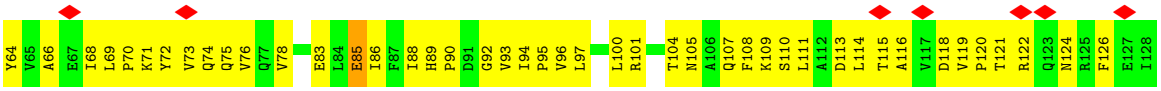
• Molecule 11: Cytochrome b-c1 complex subunit 10

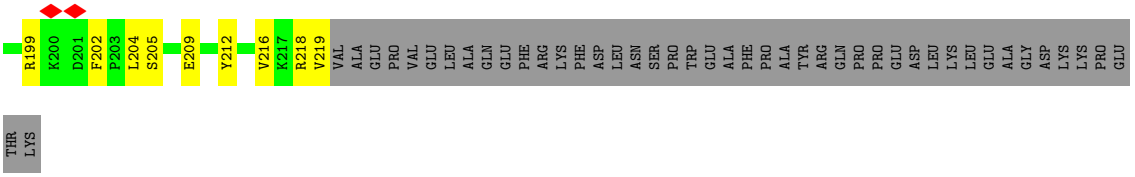


• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

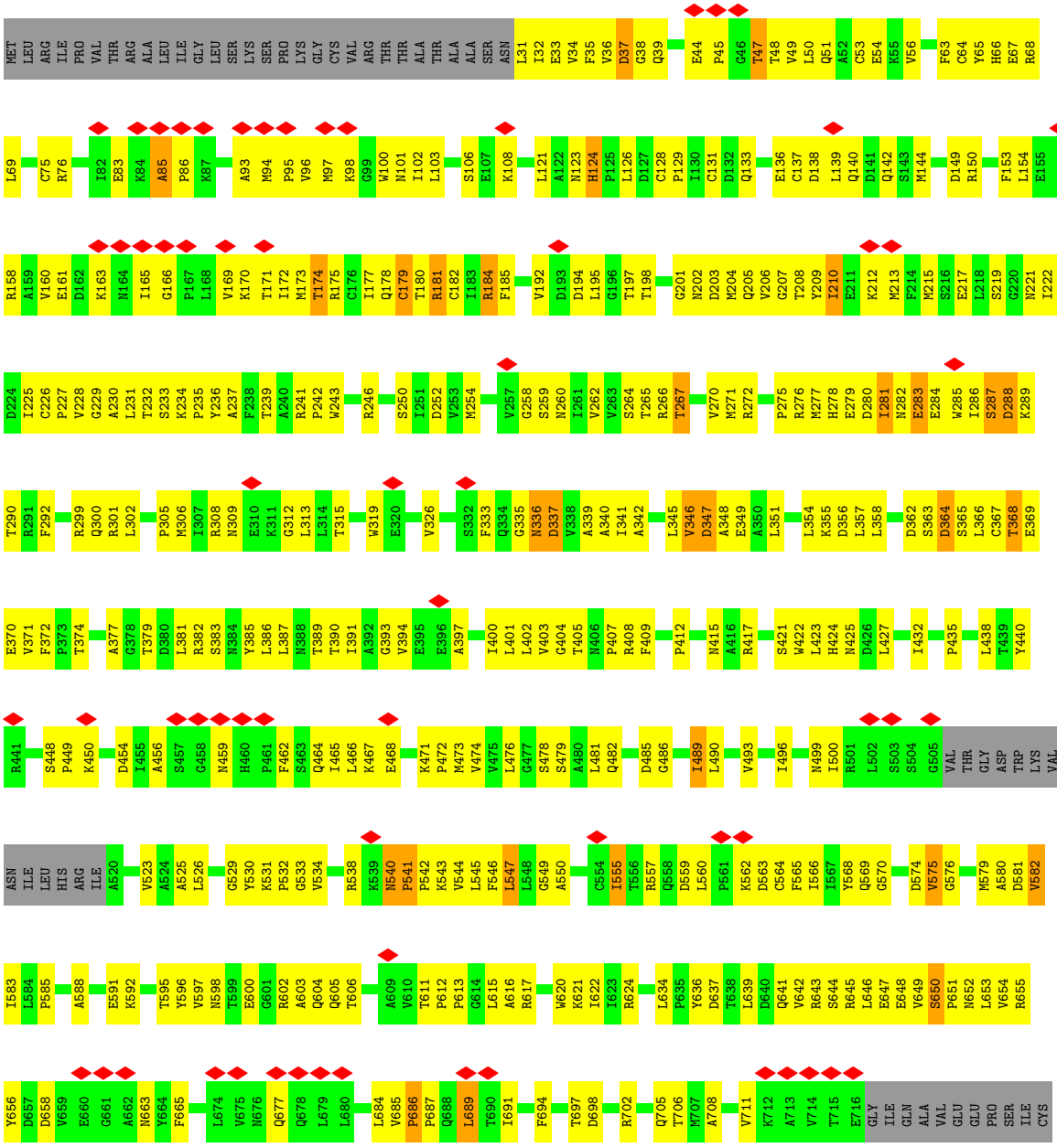






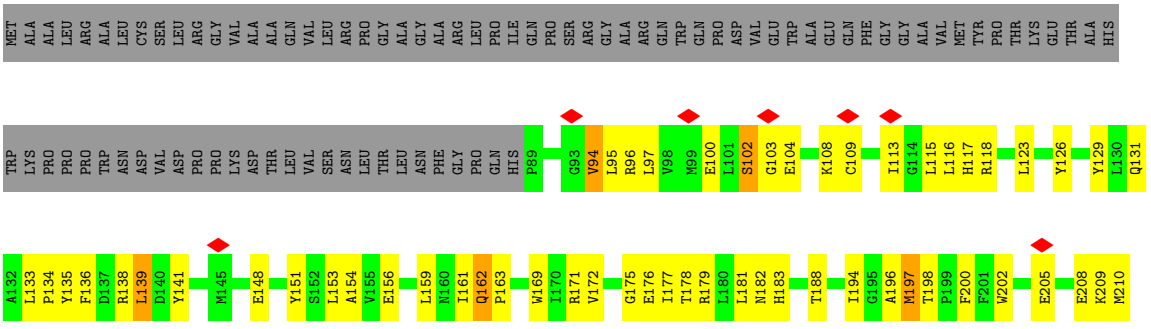


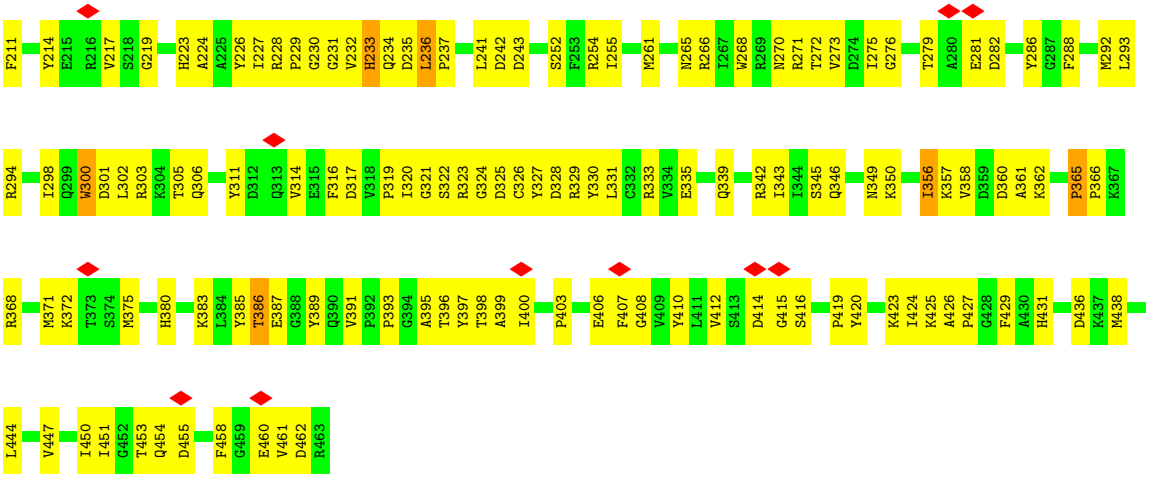
• Molecule 13: NADH-ubiquinone oxidoreductase 75 kDa subunit



• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

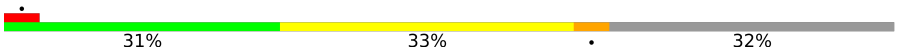
Chain Z:

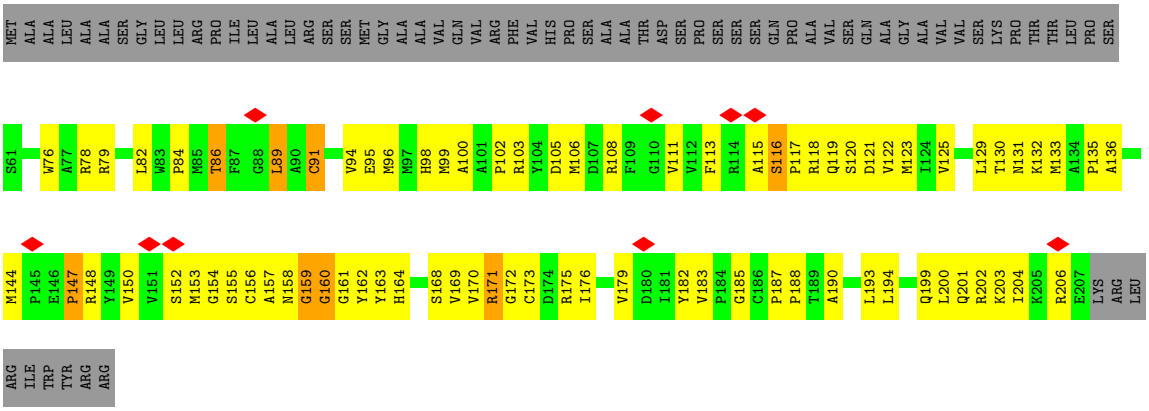




• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7

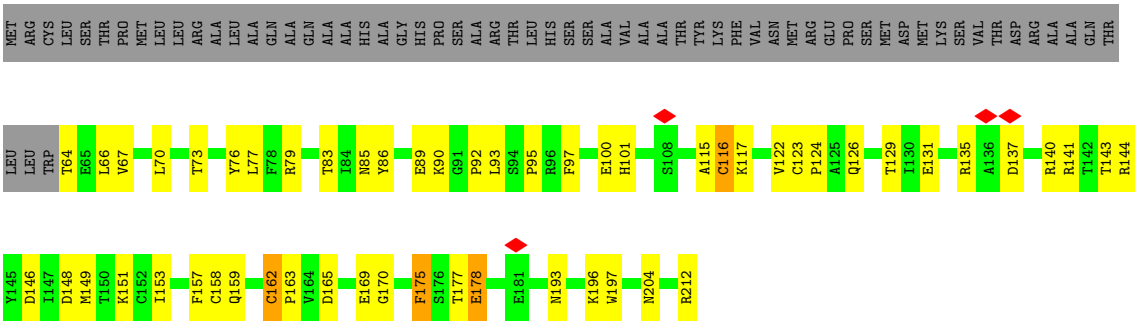
Chain a:





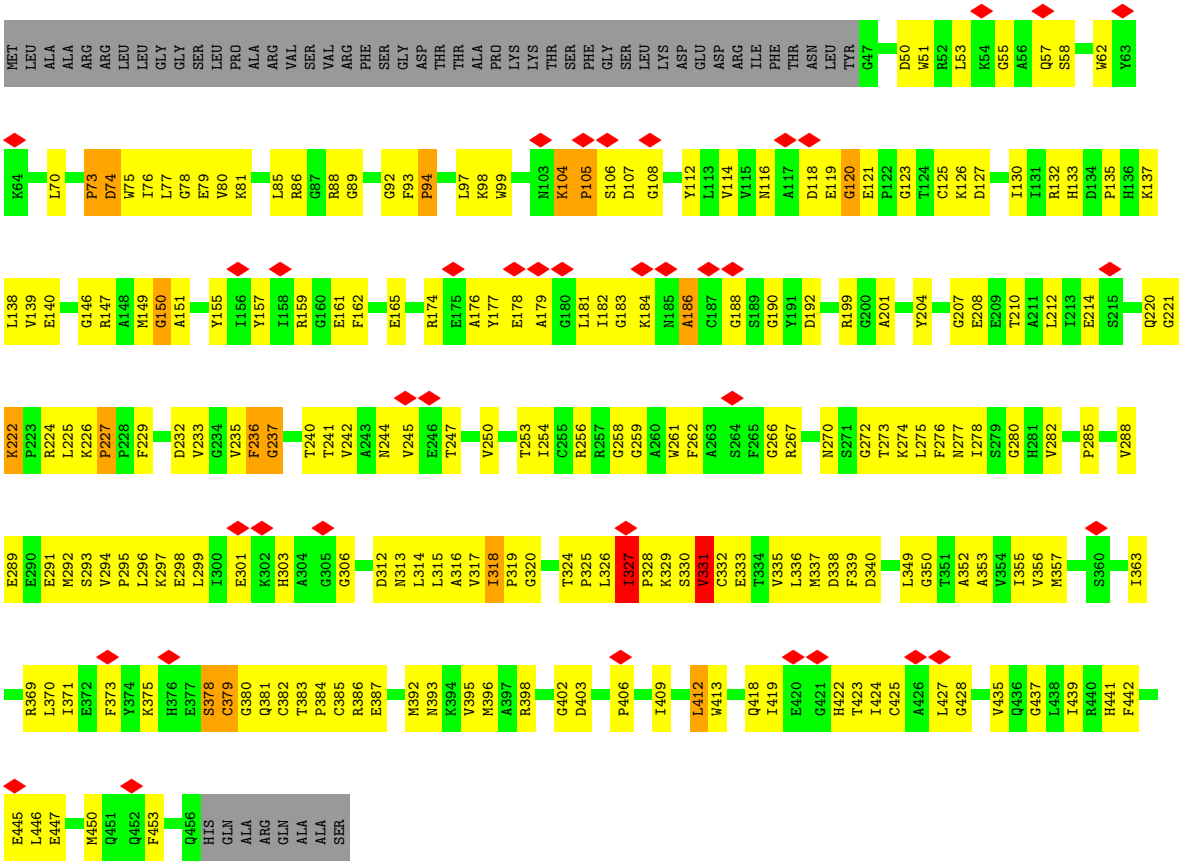
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8

Chain b:



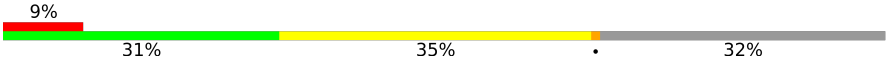
• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

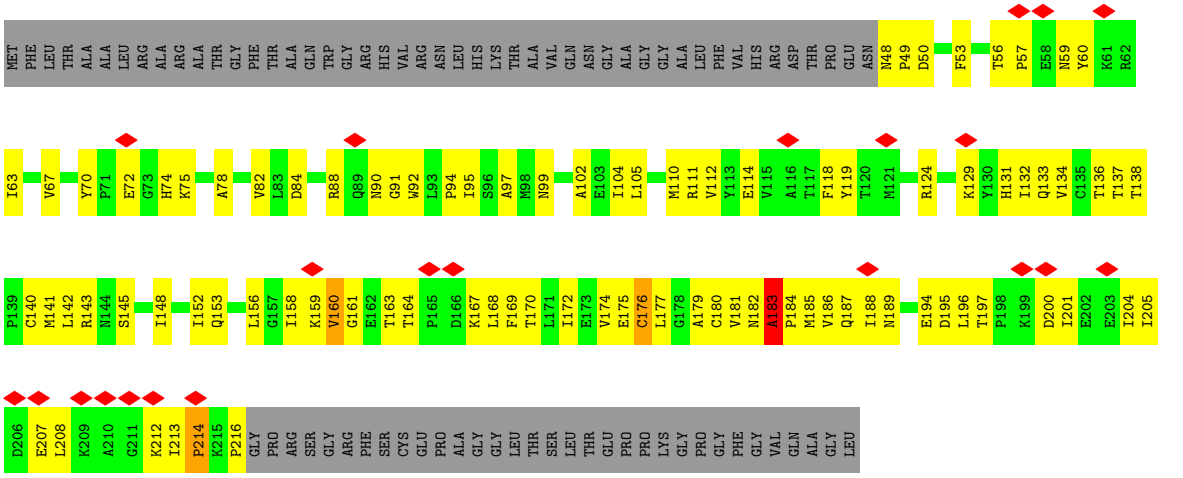
Chain c:



• Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

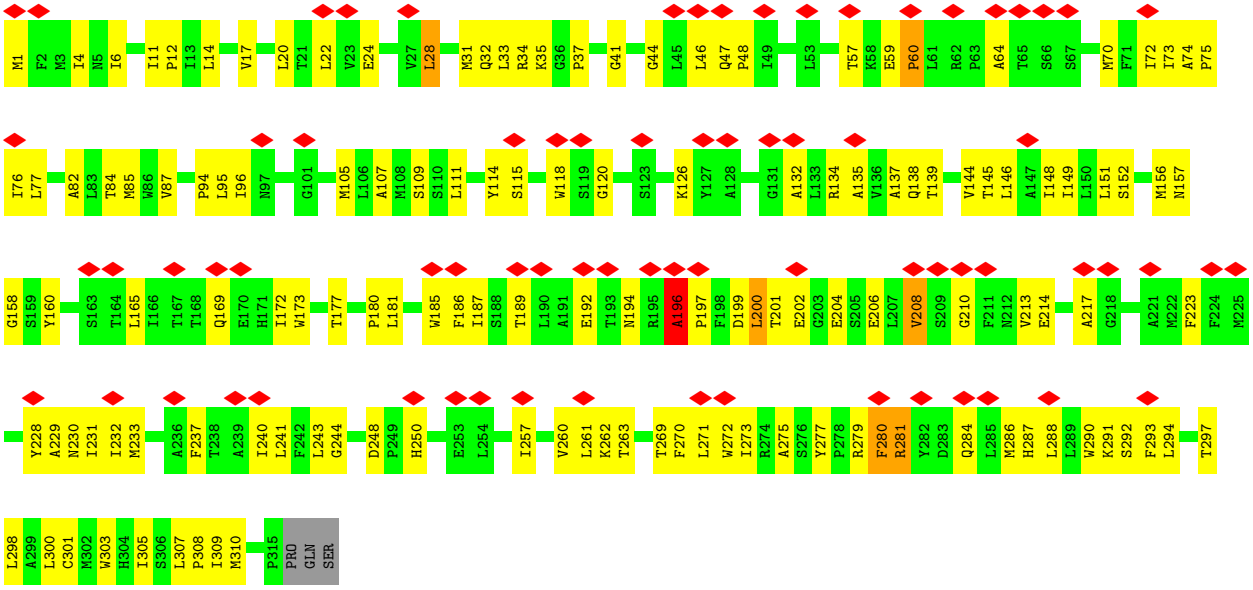
Chain d:





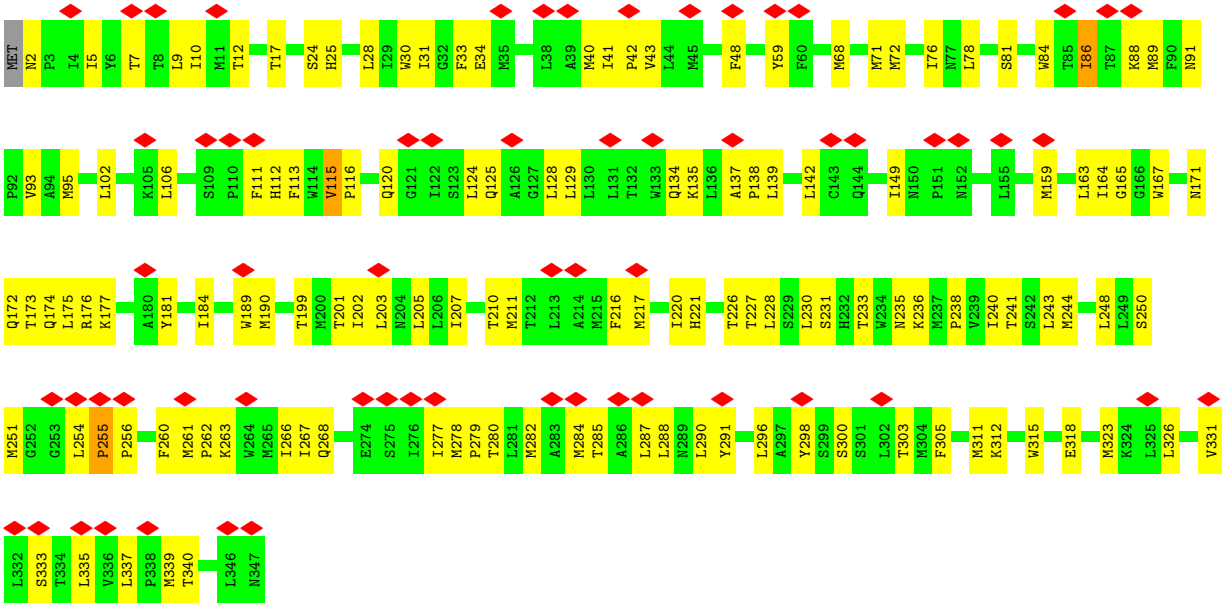
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain e:



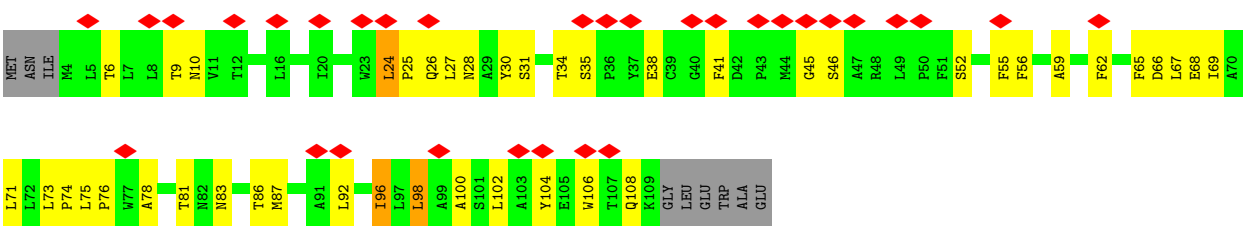
• Molecule 20: NADH-ubiquinone oxidoreductase chain 2

Chain f:



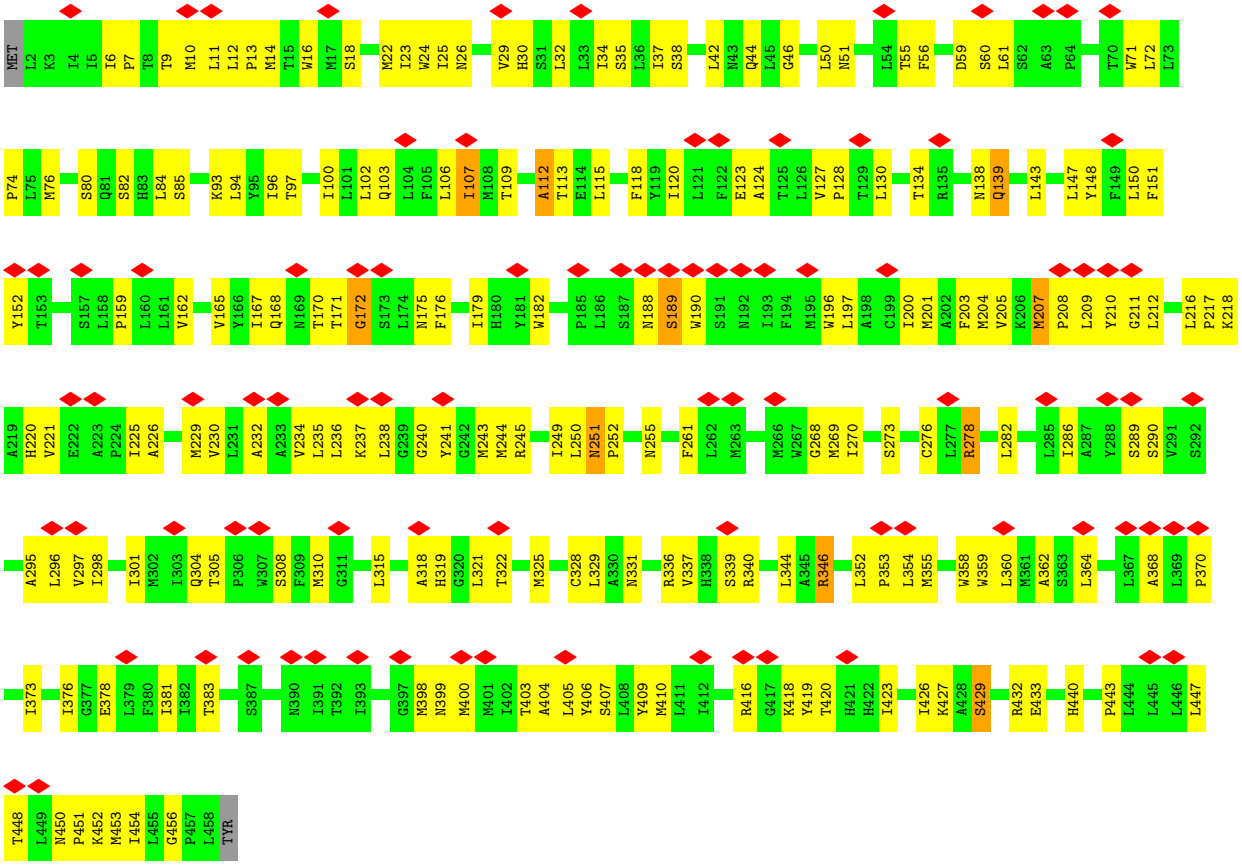
• Molecule 21: NADH-ubiquinone oxidoreductase chain 3

Chain g:



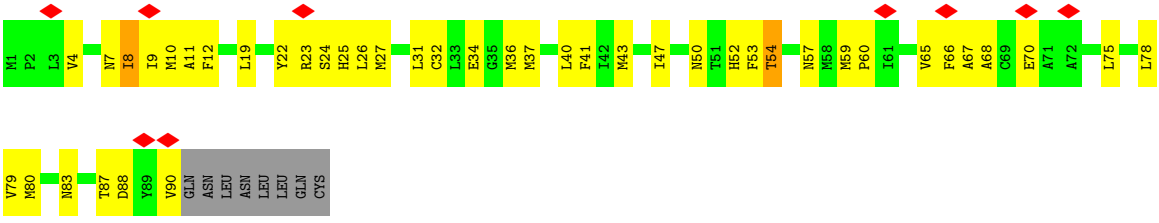
• Molecule 22: NADH-ubiquinone oxidoreductase chain 4

Chain h:



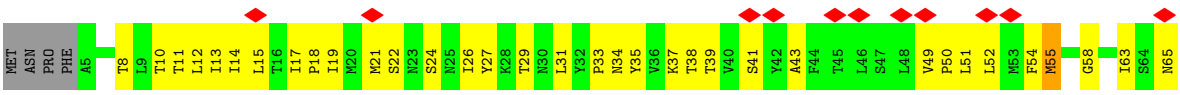
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4L

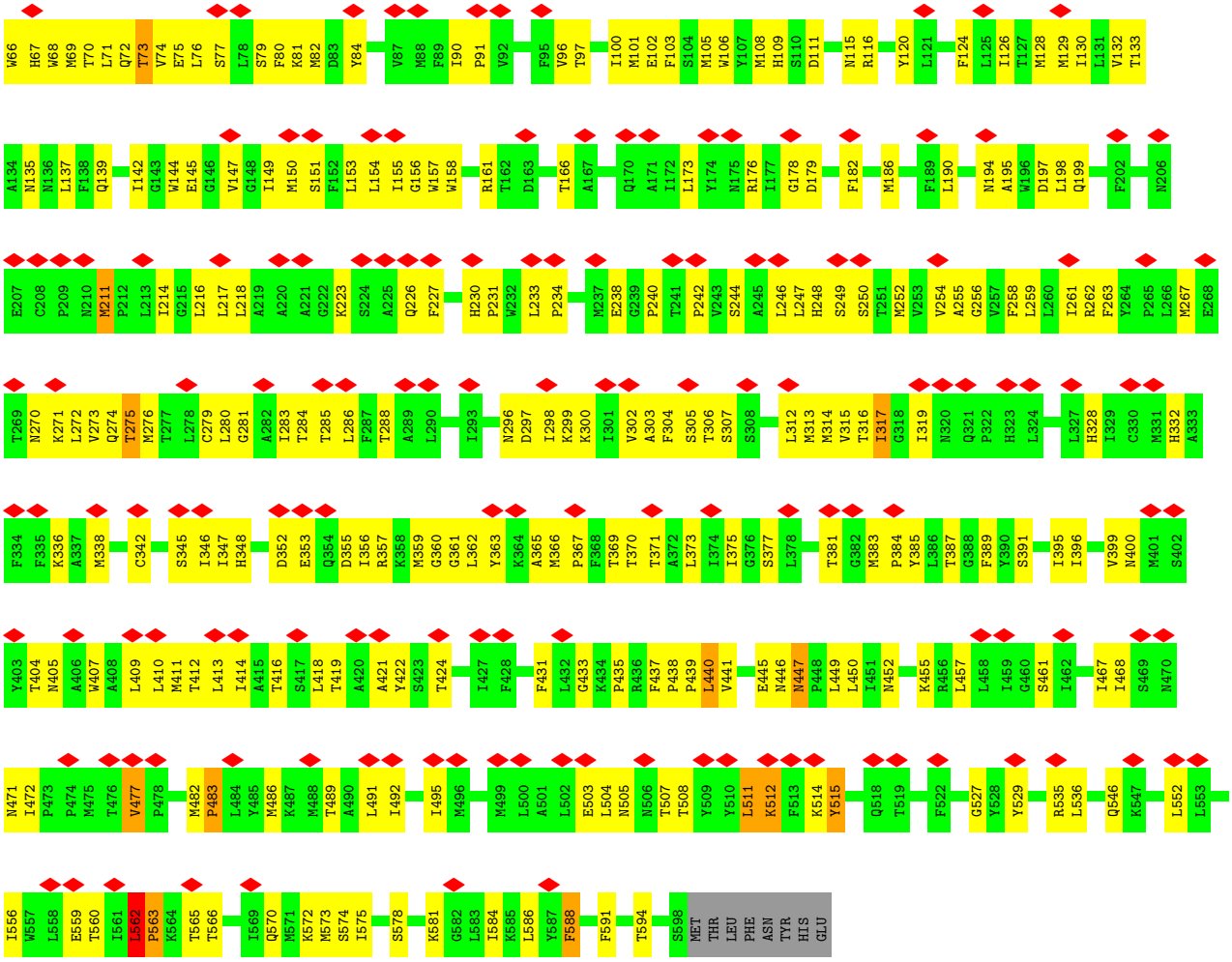
Chain i:



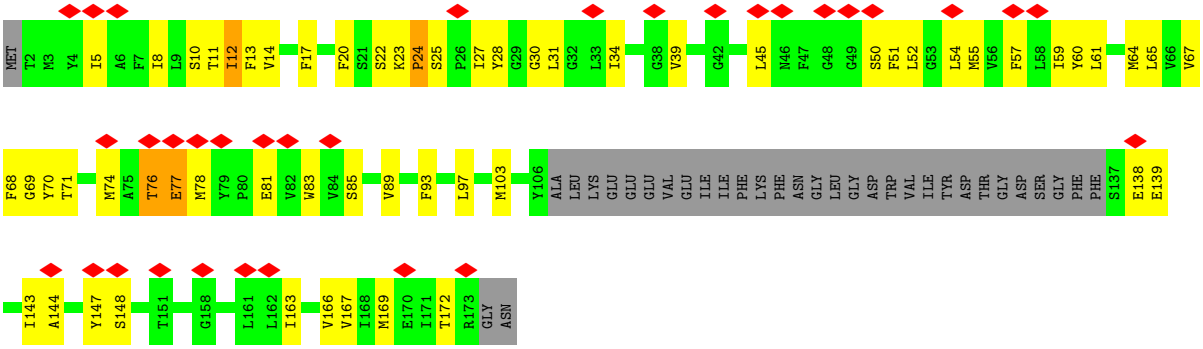
• Molecule 24: NADH-ubiquinone oxidoreductase chain 5

Chain j:

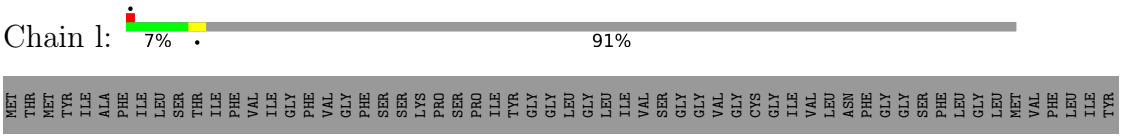


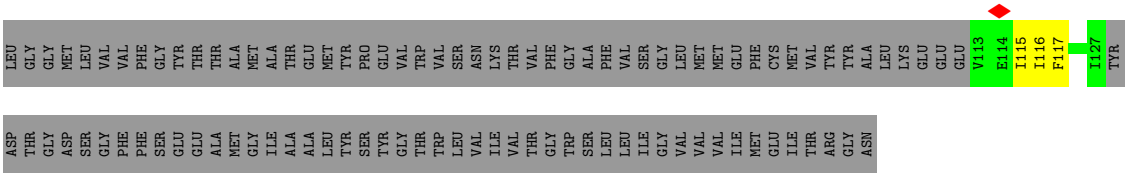


• Molecule 25: NADH-ubiquinone oxidoreductase chain 6



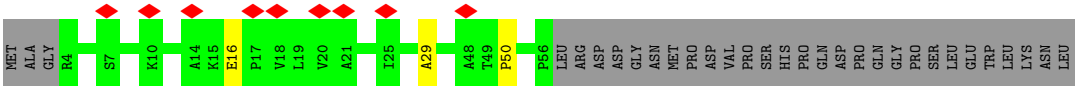
• Molecule 25: NADH-ubiquinone oxidoreductase chain 6





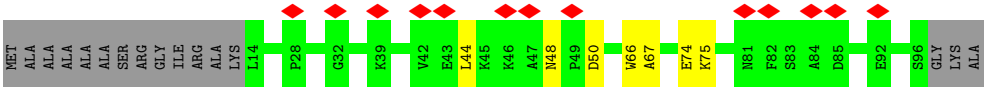
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain m:



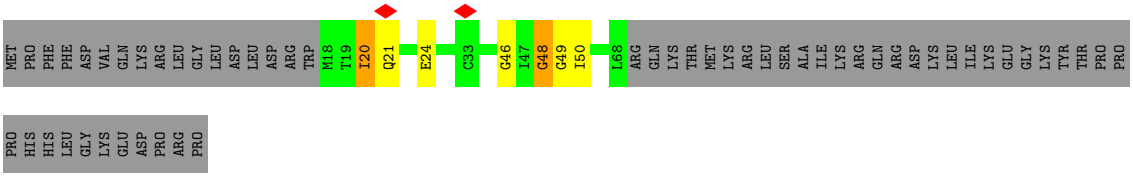
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain n:



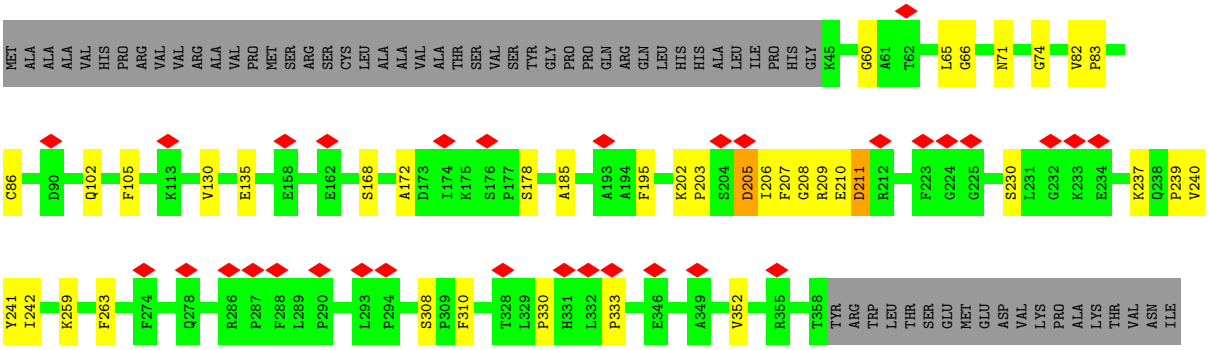
• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain o:



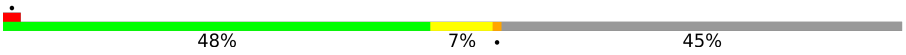
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9

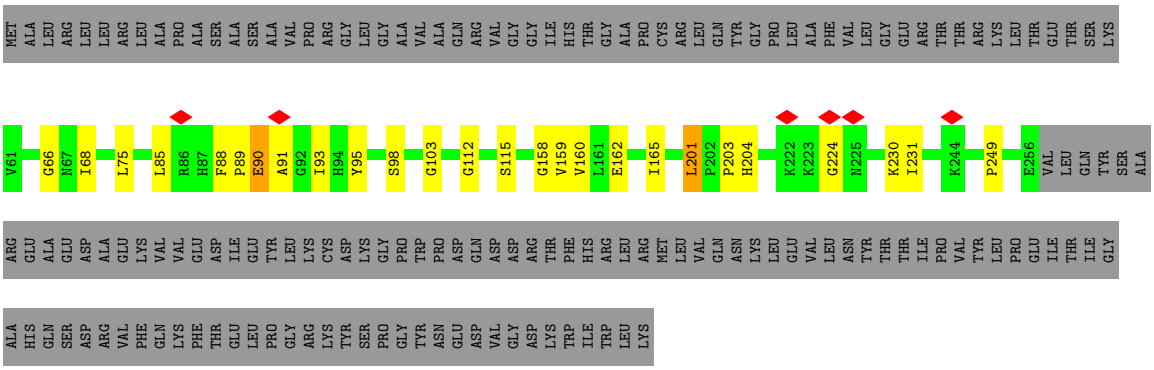
Chain p:



• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

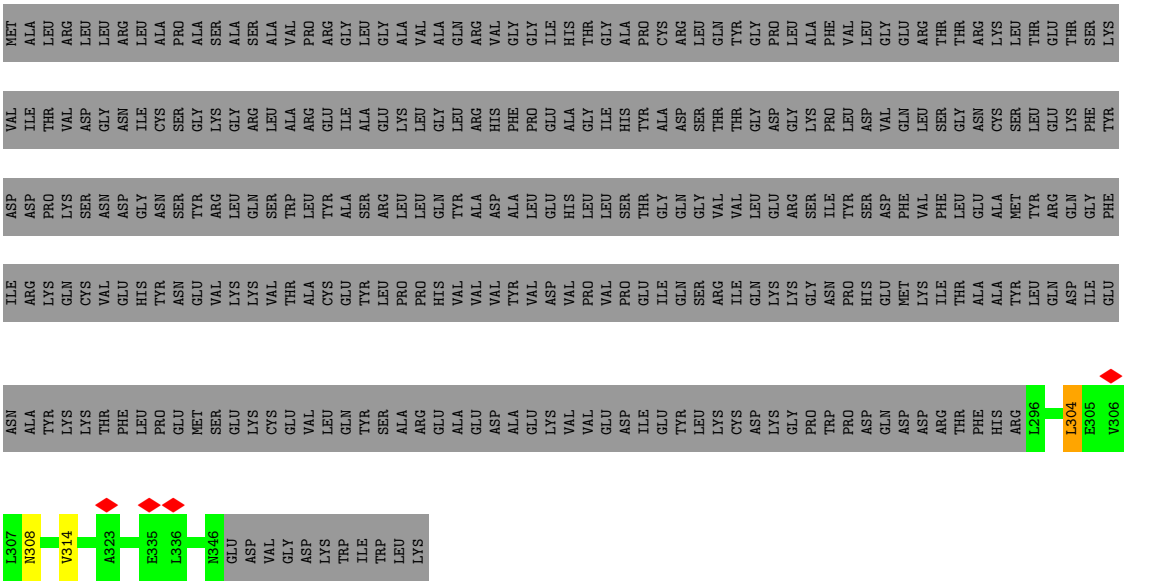
Chain q:





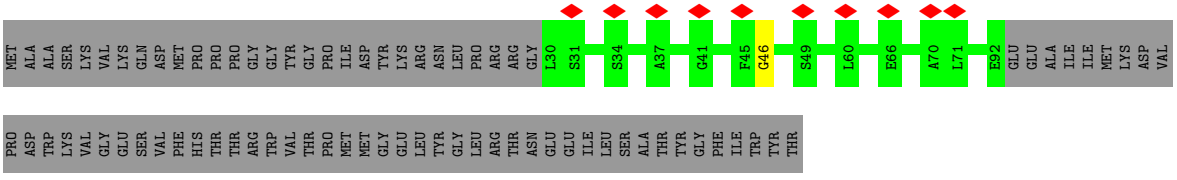
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain v:



• Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain r:

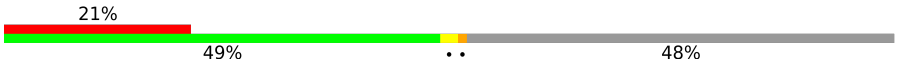


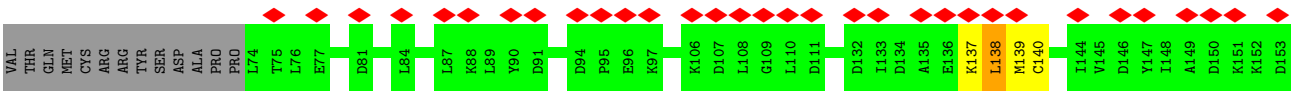
• Molecule 32: Acyl carrier protein

Chain t:

• Molecule 32: Acyl carrier protein

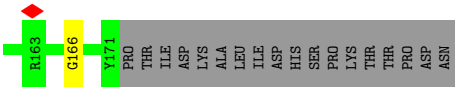
Chain Aa:





• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5

Chain u:

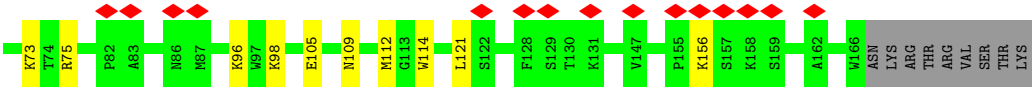


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5

Chain Ai:

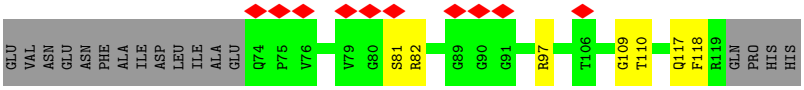
• Molecule 34: Mitochondrial NADH dehydrogenase Fe-S protein 4

Chain w:



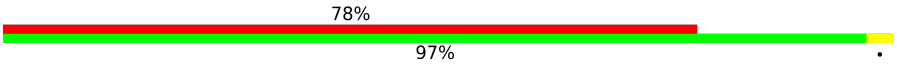
• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

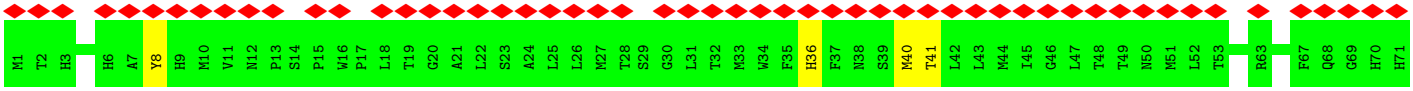
Chain x:

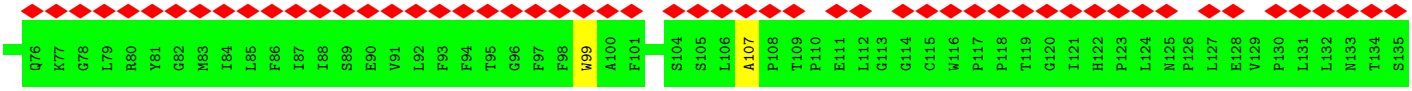


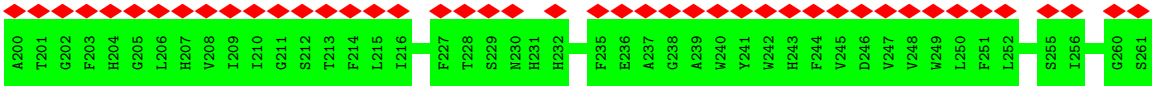
• Molecule 36: Cytochrome c oxidase subunit 3

Chain 0:



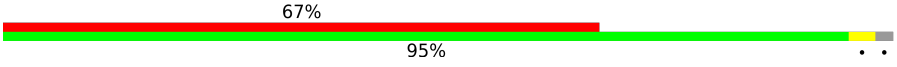


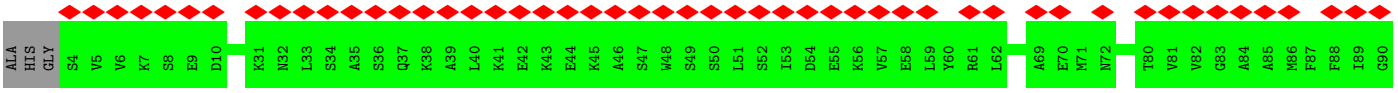


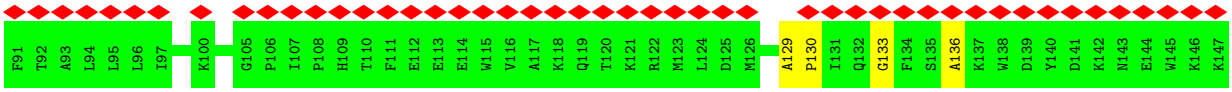


• Molecule 37: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain 1:

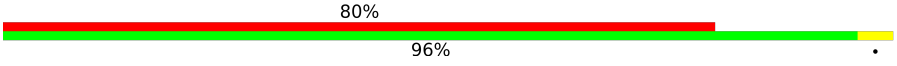


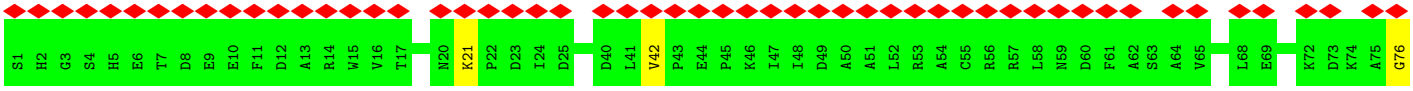


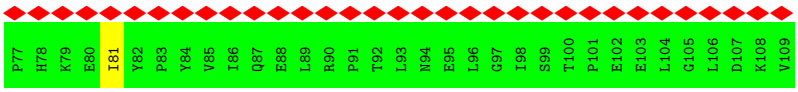


• Molecule 38: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 2:

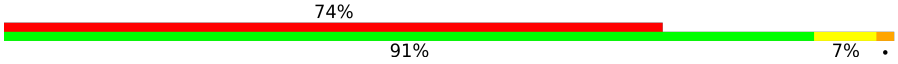


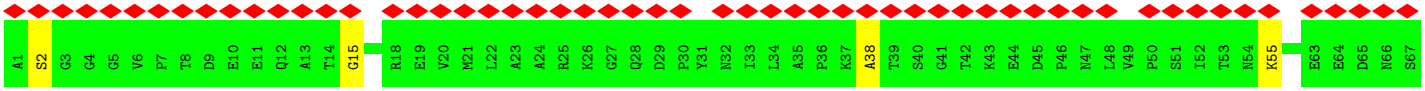


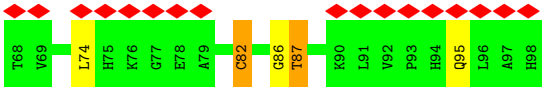


• Molecule 39: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 3:

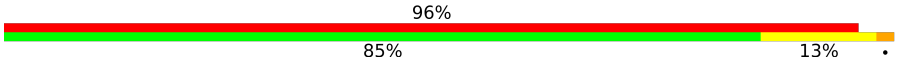


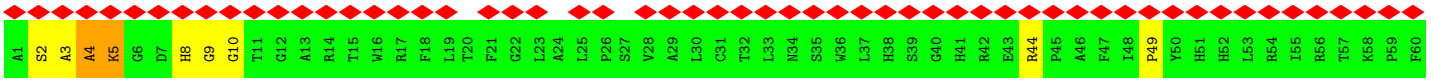


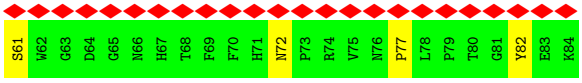


• Molecule 40: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 4:

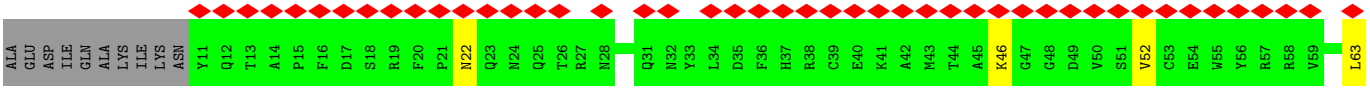


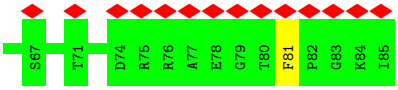




• Molecule 41: Cytochrome c oxidase subunit 6B1

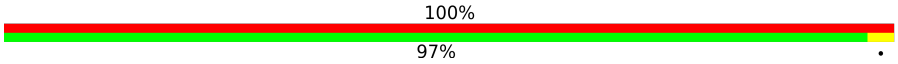
Chain 5:

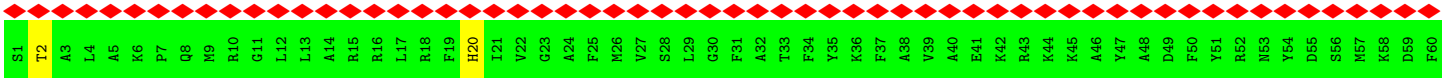


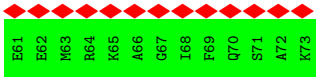


• Molecule 42: Cytochrome c oxidase subunit 6C

Chain 6:

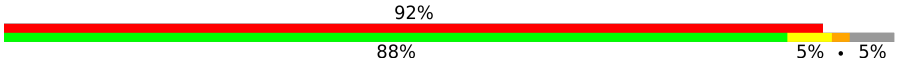


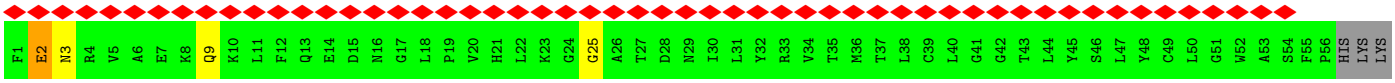




• Molecule 43: Cytochrome c oxidase subunit 7A1, mitochondrial

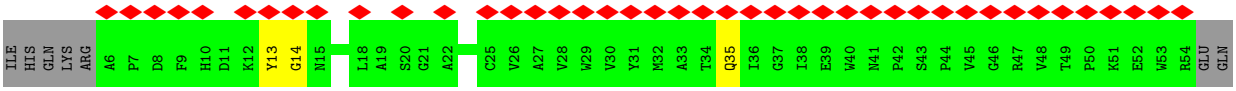
Chain 7:





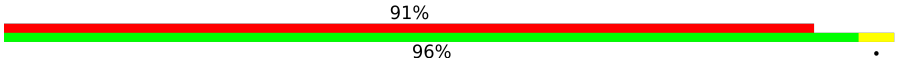
• Molecule 44: Cytochrome c oxidase subunit 7B, mitochondrial

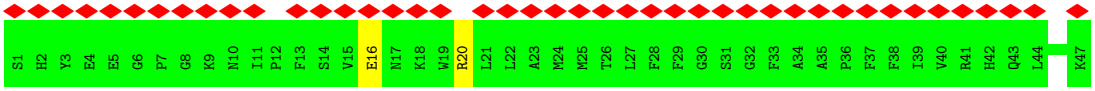
Chain 8:



• Molecule 45: Cytochrome c oxidase subunit 7C, mitochondrial

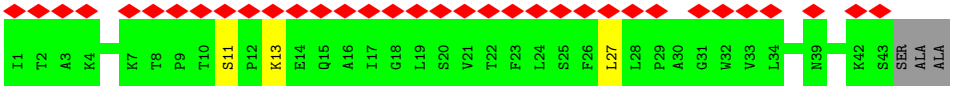
Chain 9:





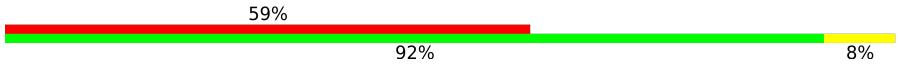
• Molecule 46: Cytochrome c oxidase subunit 8B, mitochondrial

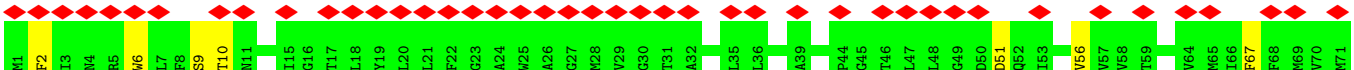
Chain s:

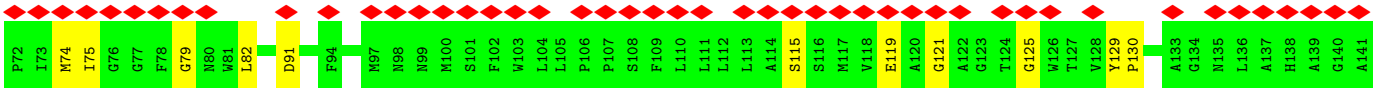


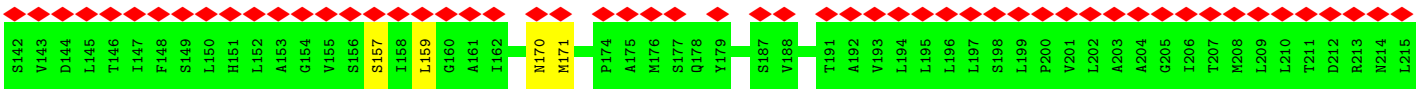
• Molecule 47: Cytochrome c oxidase subunit 1

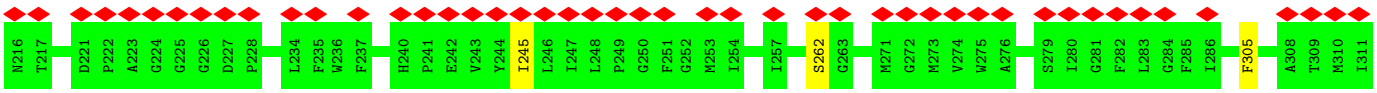
Chain y:

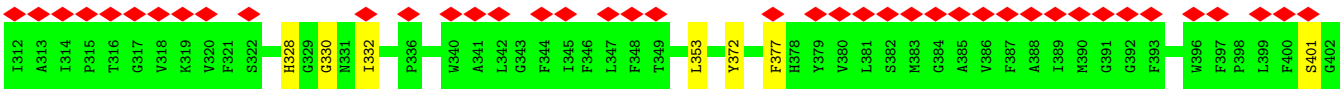


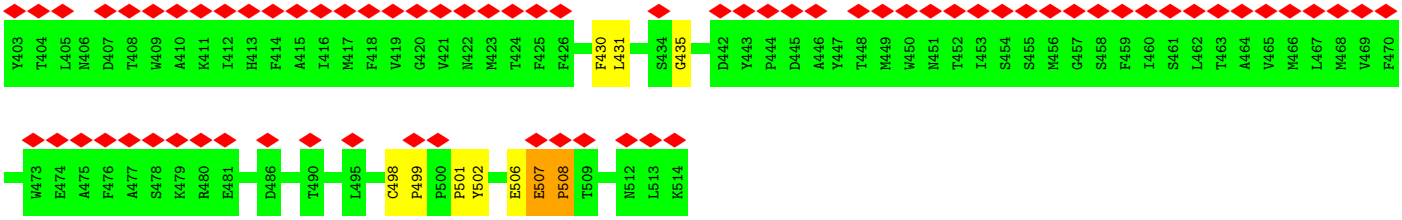




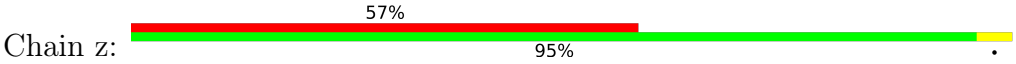


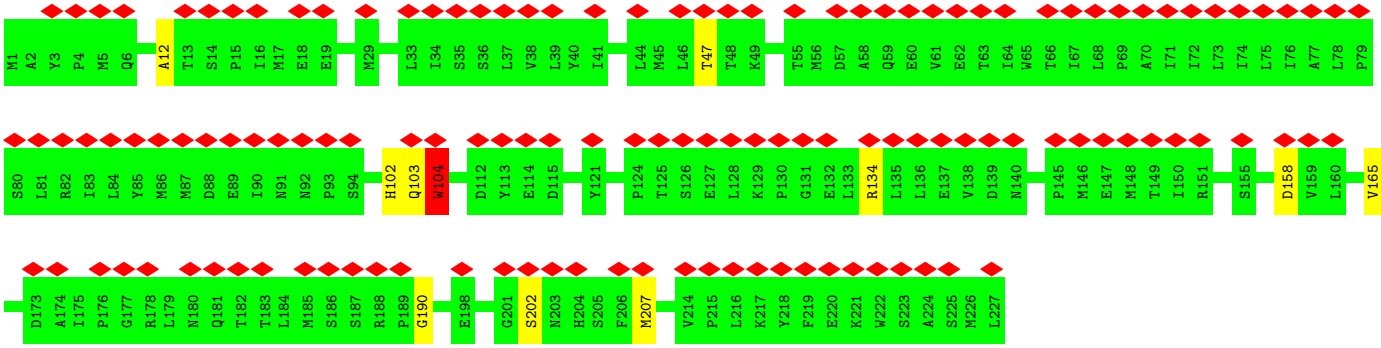




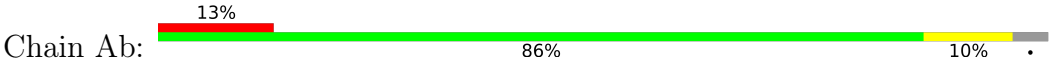


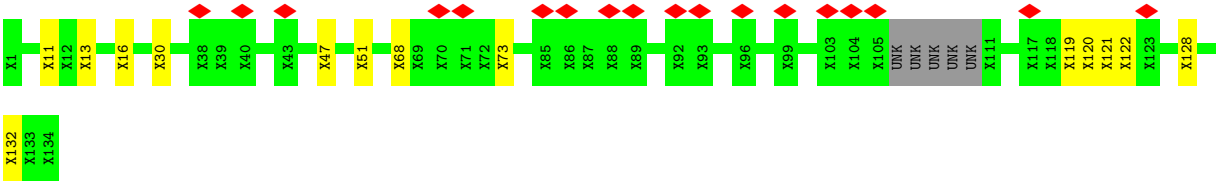
• Molecule 48: Cytochrome c oxidase subunit 2



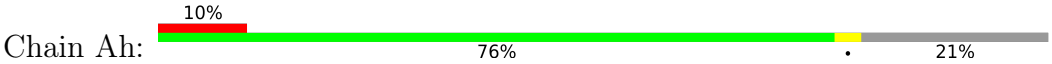


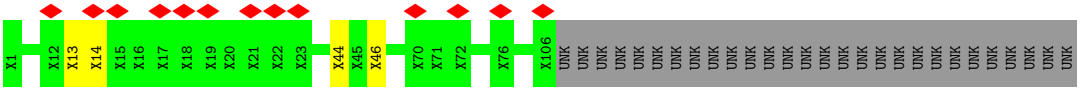
• Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



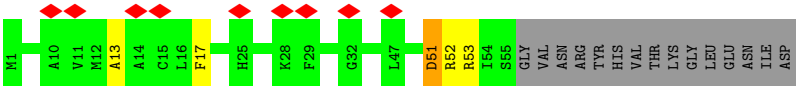


• Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



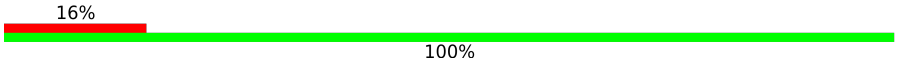


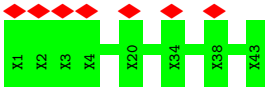
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



• Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

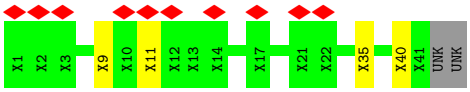
Chain Ad:





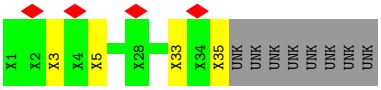
• Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ao:



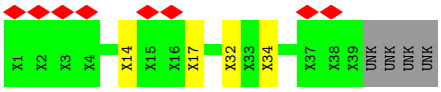
• Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ap:



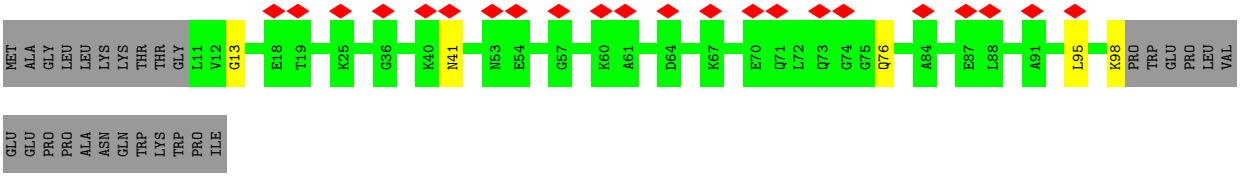
• Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Av:



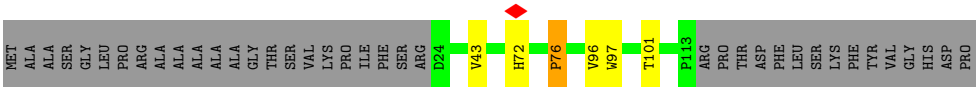
• Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain Ae:



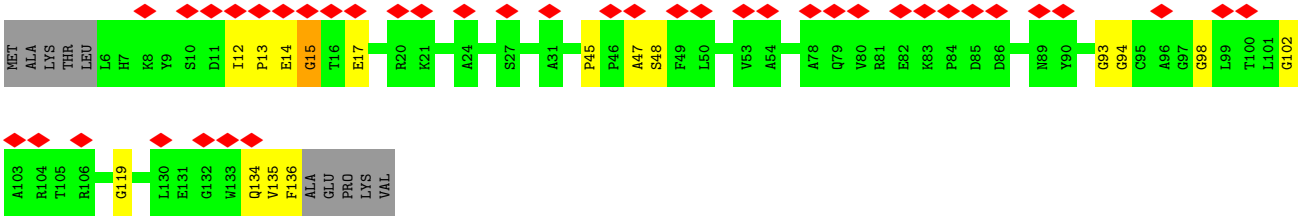
• Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Af:



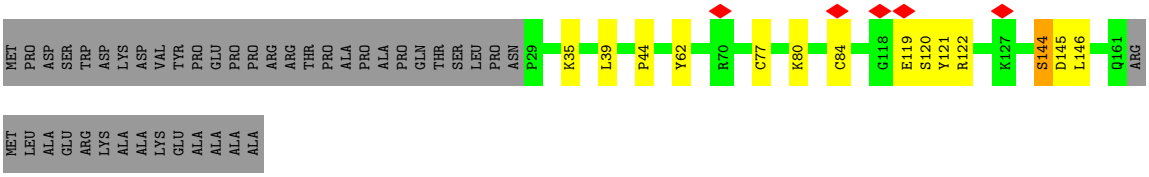
• Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Ag:



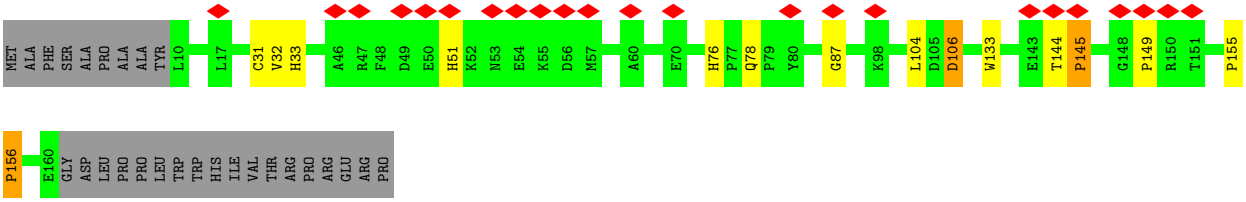
• Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain Aj:



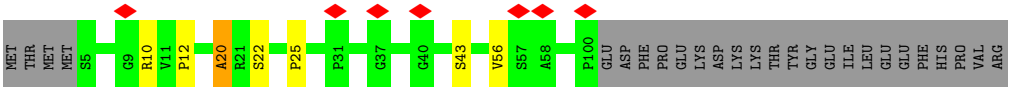
• Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain Ak:



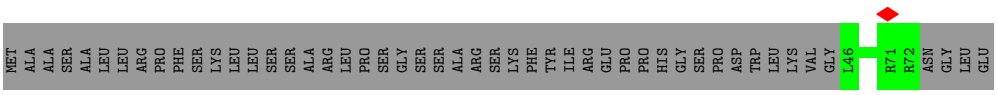
• Molecule 57: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain Al:



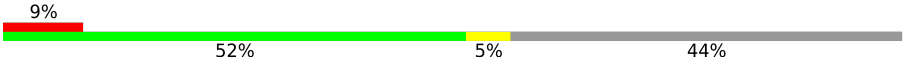
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 subunit C1

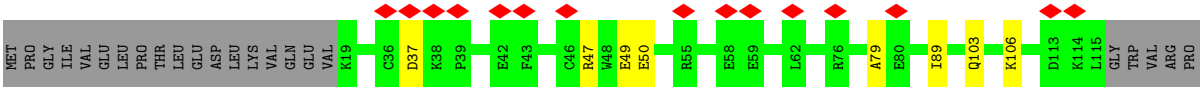
Chain Am:



• Molecule 59: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

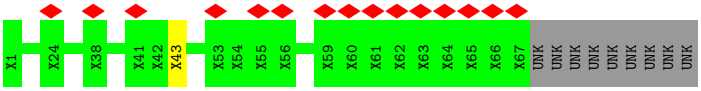
Chain An:





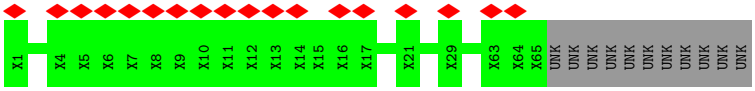
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Aq:



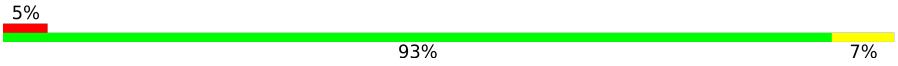
• Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

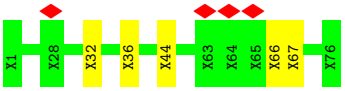
Chain As:



• Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

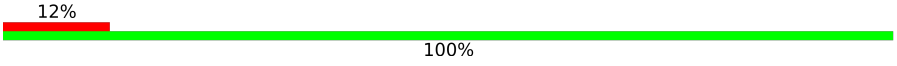
Chain Aw:

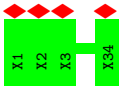




• Molecule 61: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

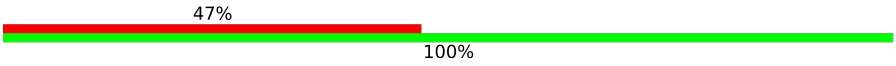
Chain Ar:

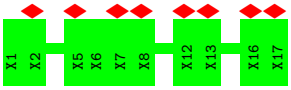




• Molecule 62: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

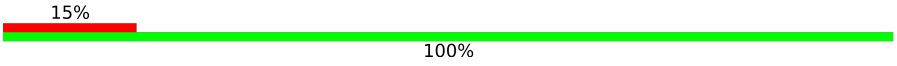
Chain At:





• Molecule 63: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Au:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	505.4208, 505.4208, 505.4208	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05296, 1.05296, 1.05296	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	2/2197 (0.1%)	2.24	107/3055 (3.5%)
1	M	0.97	4/2197 (0.2%)	2.26	91/3055 (3.0%)
2	B	0.78	2/2060 (0.1%)	2.09	66/2862 (2.3%)
2	N	0.75	0/2060	1.99	59/2862 (2.1%)
3	C	1.06	2/1869 (0.1%)	2.44	108/2600 (4.2%)
3	O	1.08	5/1869 (0.3%)	2.33	90/2600 (3.5%)
4	D	0.71	0/1187	1.84	31/1650 (1.9%)
4	P	0.70	0/1187	1.83	34/1650 (2.1%)
5	E	0.45	0/966	1.26	9/1343 (0.7%)
5	Q	0.76	0/965	2.04	32/1341 (2.4%)
6	F	0.81	1/526 (0.2%)	1.85	13/733 (1.8%)
6	R	0.85	0/526	1.98	12/733 (1.6%)
7	G	0.87	0/400	2.21	22/556 (4.0%)
7	S	0.80	0/385	1.67	11/535 (2.1%)
8	H	0.68	0/319	1.74	5/445 (1.1%)
8	T	0.60	0/319	1.62	1/445 (0.2%)
9	I	0.73	0/162	2.14	4/224 (1.8%)
9	U	0.60	0/162	1.89	5/224 (2.2%)
10	J	0.72	0/306	1.81	7/425 (1.6%)
10	L	0.75	0/306	1.85	4/425 (0.9%)
11	K	0.43	0/210	1.18	1/290 (0.3%)
11	V	0.38	0/181	1.12	1/250 (0.4%)
12	W	0.58	0/1401	1.03	4/1906 (0.2%)
13	Y	0.57	0/5077	0.98	23/6888 (0.3%)
14	Z	0.77	0/3075	0.94	8/4155 (0.2%)
15	a	0.83	0/1174	0.97	1/1591 (0.1%)
16	b	0.81	0/1215	1.05	6/1644 (0.4%)
17	c	0.49	0/3196	0.95	11/4323 (0.3%)
18	d	0.51	0/1353	0.95	4/1841 (0.2%)
19	e	0.76	0/2558	1.01	5/3497 (0.1%)
20	f	0.85	0/2761	0.99	4/3754 (0.1%)
21	g	0.71	0/850	0.87	2/1163 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
22	h	0.80	0/3700	0.98	12/5045 (0.2%)
23	i	0.87	0/687	1.06	3/931 (0.3%)
24	j	0.67	0/4831	0.95	9/6572 (0.1%)
25	k	0.72	0/1084	0.94	1/1470 (0.1%)
25	l	0.58	0/72	0.88	0/98
26	m	0.75	0/262	1.22	2/364 (0.5%)
27	n	0.51	0/410	1.13	0/570
28	o	0.81	0/250	1.14	1/346 (0.3%)
29	p	0.56	0/1545	1.05	7/2147 (0.3%)
30	q	0.61	0/966	1.24	8/1343 (0.6%)
30	v	0.74	0/251	1.20	2/348 (0.6%)
31	r	0.73	0/310	0.97	0/430
32	Aa	0.52	0/402	1.00	0/560
32	t	0.69	0/402	1.08	1/560 (0.2%)
33	Ai	0.83	0/166	1.02	0/229
33	u	0.86	0/266	1.10	2/369 (0.5%)
34	w	0.63	0/529	1.11	1/736 (0.1%)
35	x	0.63	0/220	0.85	0/301
36	0	0.88	0/1283	1.25	7/1782 (0.4%)
37	1	0.78	0/715	1.17	3/997 (0.3%)
38	2	0.75	0/538	1.22	6/748 (0.8%)
39	3	0.82	0/480	1.33	3/665 (0.5%)
40	4	0.82	0/410	1.34	6/567 (1.1%)
41	5	0.79	0/370	1.46	5/514 (1.0%)
42	6	0.81	0/360	1.12	2/500 (0.4%)
43	7	0.80	0/273	1.27	3/377 (0.8%)
44	8	0.89	0/240	1.23	1/332 (0.3%)
45	9	0.87	0/230	1.19	2/318 (0.6%)
46	s	0.81	0/212	1.15	1/294 (0.3%)
47	y	0.90	0/2522	1.34	28/3501 (0.8%)
48	z	0.88	0/1126	1.33	10/1570 (0.6%)
50	Ac	0.83	0/270	1.01	0/374
52	Ae	0.61	0/434	1.10	0/603
53	Af	0.66	0/447	1.15	3/623 (0.5%)
54	Ag	0.74	0/636	1.06	1/878 (0.1%)
55	Aj	0.78	0/662	1.06	3/924 (0.3%)
56	Ak	0.75	0/749	1.29	10/1044 (1.0%)
57	Al	0.74	0/472	1.15	1/655 (0.2%)
58	Am	0.72	0/133	0.85	0/184
59	An	0.70	0/481	1.10	1/670 (0.1%)
All	All	0.76	16/72415 (0.0%)	1.42	926/99604 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	M	0	3
2	B	0	9
2	N	0	5
3	C	0	14
3	O	0	6
4	D	0	1
4	P	0	2
5	Q	0	5
6	F	0	1
7	G	0	2
7	S	0	2
8	T	0	1
9	I	0	1
10	J	0	1
17	c	0	1
34	w	0	1
54	Ag	0	1
All	All	0	69

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	253	VAL	C-O	11.11	1.36	1.24
3	O	37	LEU	C-N	-8.12	1.24	1.33
3	O	19	ILE	CA-C	-6.33	1.44	1.52
3	O	44	GLN	C-N	-6.31	1.26	1.33
1	M	169	GLY	N-CA	-6.16	1.36	1.44
1	A	153	LEU	N-CA	-6.15	1.39	1.46
3	O	185	LEU	CA-CB	-6.08	1.45	1.53
1	M	340	GLY	C-O	-5.89	1.16	1.23
3	O	328	LEU	C-N	5.88	1.41	1.33
2	B	148	LYS	C-N	-5.76	1.26	1.33
3	C	97	HIS	C-O	-5.65	1.17	1.24
3	C	126	THR	N-CA	-5.54	1.39	1.46
1	A	373	THR	C-O	5.53	1.29	1.24
6	F	68	LEU	C-O	-5.52	1.17	1.24
1	M	333	ASP	C-O	-5.27	1.18	1.24
2	B	173	ALA	CA-CB	-5.14	1.44	1.53

All (926) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	253	VAL	O-C-N	-23.33	98.92	123.18
1	M	253	VAL	CA-C-O	16.90	137.34	120.27
3	O	44	GLN	CA-C-N	15.27	139.79	120.70
3	O	44	GLN	C-N-CA	15.27	139.79	120.70
56	Ak	155	PRO	N-CA-CB	14.56	110.79	103.22
1	M	168	GLU	CA-C-N	14.32	144.36	121.87
1	M	168	GLU	C-N-CA	14.32	144.36	121.87
3	C	204	GLY	CA-C-N	14.24	142.10	121.02
3	C	204	GLY	C-N-CA	14.24	142.10	121.02
1	A	168	GLU	CA-C-O	13.37	135.21	120.10
3	C	318	ARG	O-C-N	-13.15	109.63	121.34
6	R	65	ALA	CA-C-O	13.13	134.22	120.70
1	A	251	ALA	CA-C-O	11.33	132.60	120.36
1	M	307	PHE	CA-C-O	11.28	135.43	120.21
2	B	178	CYS	O-C-N	10.79	131.74	121.27
2	B	177	TYR	O-C-N	10.56	135.75	123.29
1	M	437	ILE	N-CA-C	-10.21	100.75	111.58
3	O	47	THR	O-C-N	-10.20	111.57	122.07
1	M	334	MET	O-C-N	-10.16	110.57	122.15
1	A	294	LEU	CA-C-N	10.13	134.67	120.29
1	A	294	LEU	C-N-CA	10.13	134.67	120.29
7	G	13	VAL	CA-C-O	9.98	130.87	120.39
13	Y	435	PRO	N-CA-CB	9.95	110.19	101.83
9	I	75	SER	N-CA-C	9.87	120.95	107.73
3	C	196	HIS	CA-C-O	-9.81	110.70	121.00
3	C	185	LEU	O-C-N	-9.66	112.75	120.38
3	O	19	ILE	O-C-N	-9.57	110.61	122.57
16	b	170	GLY	CA-C-N	9.57	129.81	119.28
16	b	170	GLY	C-N-CA	9.57	129.81	119.28
10	L	39	ALA	O-C-N	9.41	132.09	122.12
19	e	280	PHE	N-CA-C	9.37	122.69	111.82
29	p	242	ILE	N-CA-C	9.32	120.13	110.62
1	A	373	THR	CA-C-O	9.28	127.16	118.44
30	q	201	LEU	CA-C-N	-9.24	110.86	120.38
30	q	201	LEU	C-N-CA	-9.24	110.86	120.38
3	C	41	LEU	N-CA-CB	9.17	123.74	110.16
1	M	259	GLY	CA-C-N	9.12	129.68	119.92
1	M	259	GLY	C-N-CA	9.12	129.68	119.92
3	C	115	ILE	CA-C-N	-9.08	109.73	119.99
3	C	115	ILE	C-N-CA	-9.08	109.73	119.99
9	U	75	SER	N-CA-C	9.05	119.86	107.73
2	B	178	CYS	CA-C-O	-9.02	111.27	120.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	42	ALA	CA-C-N	8.97	128.61	119.82
2	B	42	ALA	C-N-CA	8.97	128.61	119.82
3	O	47	THR	CA-C-O	8.97	130.24	120.82
3	O	221	HIS	N-CA-CB	8.95	118.89	110.39
41	5	52	VAL	N-CA-C	8.90	121.16	108.17
41	5	81	PHE	CA-C-N	8.81	128.45	119.56
41	5	81	PHE	C-N-CA	8.81	128.45	119.56
17	c	120	GLY	N-CA-C	8.76	123.25	112.73
1	A	256	ALA	N-CA-C	8.65	123.17	109.50
1	A	341	GLN	O-C-N	8.63	131.41	122.09
3	C	43	LEU	O-C-N	-8.62	112.78	122.09
5	Q	192	MET	CA-C-O	8.62	129.37	120.24
1	M	320	LEU	CA-C-O	8.59	129.98	120.70
3	C	196	HIS	O-C-N	8.52	130.89	122.03
3	C	175	LEU	N-CA-CB	8.49	123.38	110.30
2	B	92	VAL	O-C-N	-8.45	114.47	122.16
1	A	434	TYR	CA-C-O	-8.44	111.52	120.63
5	Q	183	PRO	CA-C-O	-8.43	110.17	122.31
3	C	246	ALA	N-CA-CB	-8.40	101.21	110.71
2	B	85	ILE	CB-CA-C	-8.39	101.15	111.88
1	A	292	SER	CA-C-O	8.38	125.52	119.32
7	G	13	VAL	O-C-N	-8.28	114.31	123.26
24	j	562	LEU	CA-C-N	-8.28	109.50	119.84
24	j	562	LEU	C-N-CA	-8.28	109.50	119.84
2	B	369	LEU	CA-C-O	8.24	129.19	120.70
3	O	242	LEU	CB-CA-C	-8.23	98.19	110.95
6	F	43	VAL	CA-C-O	8.20	131.03	120.78
2	B	148	LYS	CA-C-N	8.18	131.08	120.44
2	B	148	LYS	C-N-CA	8.18	131.08	120.44
17	c	227	PRO	CA-C-N	-8.16	111.37	119.78
17	c	227	PRO	C-N-CA	-8.16	111.37	119.78
6	R	63	LYS	CB-CA-C	8.11	123.62	110.88
1	M	419	CYS	CA-C-N	8.11	128.16	119.89
1	M	419	CYS	C-N-CA	8.11	128.16	119.89
12	W	159	VAL	N-CA-C	8.10	118.20	110.42
20	f	255	PRO	N-CA-C	8.07	120.55	110.70
45	9	20	ARG	N-CA-C	-8.06	102.58	111.36
17	c	327	ILE	CB-CA-C	-8.03	103.48	114.00
47	y	82	LEU	N-CA-C	8.03	122.35	112.23
3	C	13	ILE	CB-CA-C	-8.00	101.34	112.14
1	A	294	LEU	O-C-N	-8.00	113.64	122.12
1	A	431	LEU	CA-C-N	7.99	129.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	LEU	C-N-CA	7.99	129.82	119.84
1	A	341	GLN	CA-C-O	-7.95	112.52	120.70
3	C	43	LEU	CA-C-O	7.92	128.86	120.70
5	Q	183	PRO	O-C-N	7.90	132.19	122.71
3	C	30	TRP	CA-C-O	7.90	129.16	120.63
3	O	257	THR	N-CA-CB	7.88	121.52	110.01
4	P	7	PRO	N-CA-C	7.87	120.30	110.70
5	Q	135	LEU	O-C-N	-7.84	113.59	123.24
3	C	321	SER	CA-C-N	7.84	131.57	120.28
3	C	321	SER	C-N-CA	7.84	131.57	120.28
4	D	97	ASN	CA-C-N	7.84	129.64	119.84
4	D	97	ASN	C-N-CA	7.84	129.64	119.84
1	M	325	VAL	O-C-N	-7.80	114.37	123.03
1	A	168	GLU	O-C-N	-7.79	113.11	122.22
2	B	320	GLY	O-C-N	-7.78	117.96	123.95
47	y	435	GLY	N-CA-C	7.71	126.15	115.27
3	O	82	MET	CA-C-O	7.71	128.59	120.42
3	C	303	LEU	N-CA-CB	7.69	121.54	110.16
3	C	195	VAL	CA-C-O	-7.68	112.97	120.95
1	M	392	LEU	N-CA-C	7.66	120.30	111.11
3	C	185	LEU	CA-C-O	7.65	126.35	119.08
10	L	39	ALA	CA-C-O	-7.64	112.45	120.55
3	C	123	VAL	CA-C-O	7.64	129.27	120.03
1	M	420	PRO	N-CA-CB	7.63	109.73	103.32
1	A	242	CYS	CA-C-O	7.63	128.75	120.43
5	Q	168	SER	N-CA-C	-7.63	103.98	113.28
19	e	200	LEU	N-CA-C	7.62	120.48	111.71
18	d	183	ALA	CA-C-N	-7.62	111.91	119.76
18	d	183	ALA	C-N-CA	-7.62	111.91	119.76
59	An	89	ILE	N-CA-C	7.61	118.41	110.72
2	B	179	PRO	N-CA-CB	7.59	110.40	103.34
6	R	65	ALA	O-C-N	-7.59	113.90	122.09
13	Y	166	GLY	CA-C-N	7.59	127.62	119.28
13	Y	166	GLY	C-N-CA	7.59	127.62	119.28
3	O	149	LEU	CA-C-O	7.58	128.91	119.05
3	C	106	SER	CA-C-O	7.52	128.67	119.79
2	N	145	ARG	O-C-N	7.52	129.81	122.07
3	O	242	LEU	N-CA-CB	7.50	120.85	109.98
7	G	26	PHE	CA-C-N	7.48	129.19	119.84
7	G	26	PHE	C-N-CA	7.48	129.19	119.84
46	s	27	LEU	N-CA-C	7.47	119.50	111.36
1	M	434	TYR	O-C-N	-7.43	114.36	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	205	SER	O-C-N	-7.43	113.13	123.01
56	Ak	145	PRO	CA-C-N	-7.43	111.11	119.28
56	Ak	145	PRO	C-N-CA	-7.43	111.11	119.28
3	C	303	LEU	N-CA-C	7.42	119.44	111.36
1	M	275	ALA	N-CA-C	-7.41	103.15	111.07
7	G	13	VAL	CA-C-N	-7.38	110.75	122.64
7	G	13	VAL	C-N-CA	-7.38	110.75	122.64
47	y	56	VAL	N-CA-C	-7.38	103.27	110.72
4	D	160	MET	N-CA-C	7.37	120.43	108.41
5	E	67	ASP	N-CA-C	7.37	119.51	108.31
1	A	364	ALA	O-C-N	7.36	129.92	122.12
3	C	195	VAL	O-C-N	7.34	128.99	121.87
3	O	222	PRO	CA-C-N	7.33	131.89	120.89
3	O	222	PRO	C-N-CA	7.33	131.89	120.89
47	y	330	GLY	N-CA-C	7.32	120.38	112.33
3	O	88	SER	N-CA-C	-7.30	103.26	111.07
2	B	92	VAL	CA-C-O	7.29	127.00	119.35
1	A	435	ASN	CA-C-O	7.28	128.34	119.97
2	N	188	PRO	O-C-N	-7.27	112.82	122.64
1	M	424	GLY	CA-C-O	-7.26	113.56	121.48
3	C	30	TRP	O-C-N	-7.26	114.43	122.12
2	N	385	GLN	CA-C-O	7.25	128.11	120.42
6	F	73	GLN	CB-CA-C	7.25	122.43	109.38
1	A	281	ASP	CA-C-N	7.24	130.29	120.38
1	A	281	ASP	C-N-CA	7.24	130.29	120.38
38	2	76	GLY	CA-C-N	7.23	128.47	120.45
38	2	76	GLY	C-N-CA	7.23	128.47	120.45
1	M	256	ALA	CB-CA-C	-7.22	93.52	109.56
3	O	37	LEU	CA-C-N	7.21	127.93	120.00
3	O	37	LEU	C-N-CA	7.21	127.93	120.00
5	Q	72	SER	CA-C-O	-7.21	113.26	121.19
47	y	332	ILE	N-CA-C	7.21	119.10	109.37
3	C	113	TRP	O-C-N	-7.20	114.60	122.09
1	A	419	CYS	N-CA-CB	7.19	119.64	110.23
5	E	143	GLY	N-CA-C	7.16	125.19	115.32
3	C	106	SER	N-CA-C	-7.14	103.23	112.23
47	y	9	SER	N-CA-C	7.13	119.77	110.43
1	M	417	ASP	CA-C-N	-7.12	109.78	122.74
1	M	417	ASP	C-N-CA	-7.12	109.78	122.74
3	O	256	TYR	N-CA-C	-7.12	104.52	112.57
1	A	242	CYS	O-C-N	-7.11	115.23	123.27
1	M	138	LEU	CA-C-O	-7.10	112.72	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	2	42	VAL	N-CA-C	-7.08	99.69	108.05
4	D	175	THR	CA-C-O	7.08	125.75	119.59
1	M	443	TRP	N-CA-C	7.08	121.70	107.41
3	C	264	THR	CB-CA-C	-7.06	100.47	109.65
6	R	50	LEU	CA-C-N	7.06	128.66	119.84
6	R	50	LEU	C-N-CA	7.06	128.66	119.84
3	O	244	LEU	O-C-N	7.05	131.55	122.10
55	Aj	44	PRO	N-CA-CB	7.05	110.77	103.23
2	B	108	THR	N-CA-C	7.04	119.92	110.35
2	N	291	ALA	N-CA-C	-7.04	104.82	113.41
5	Q	135	LEU	CA-C-N	7.02	133.64	122.33
5	Q	135	LEU	C-N-CA	7.02	133.64	122.33
3	O	231	GLY	CA-C-O	7.01	128.01	120.30
13	Y	346	VAL	CA-C-N	6.99	134.28	121.70
13	Y	346	VAL	C-N-CA	6.99	134.28	121.70
25	k	69	GLY	N-CA-C	-6.96	106.20	115.32
5	Q	182	VAL	CA-C-O	-6.96	116.15	120.88
3	O	230	LEU	CA-C-N	6.94	129.04	120.22
3	O	230	LEU	C-N-CA	6.94	129.04	120.22
1	M	414	TYR	N-CA-C	6.93	120.96	112.23
2	B	97	SER	N-CA-C	6.93	120.96	109.46
3	O	284	ILE	CA-C-O	6.92	123.69	119.19
14	Z	162	GLN	CA-C-N	6.92	124.71	119.66
14	Z	162	GLN	C-N-CA	6.92	124.71	119.66
2	N	187	THR	N-CA-C	6.91	118.77	110.07
24	j	477	VAL	CA-C-N	6.90	126.87	119.76
24	j	477	VAL	C-N-CA	6.90	126.87	119.76
3	O	241	LEU	O-C-N	6.89	130.01	122.15
36	0	36	HIS	N-CA-C	6.89	122.11	113.43
5	Q	87	MET	CA-C-O	6.89	127.83	120.46
7	G	12	HIS	CA-C-N	-6.89	114.12	123.14
7	G	12	HIS	C-N-CA	-6.89	114.12	123.14
4	P	83	ARG	CA-C-N	6.88	126.91	119.89
4	P	83	ARG	C-N-CA	6.88	126.91	119.89
5	Q	25	SER	CA-C-O	6.88	127.00	119.15
3	C	40	CYS	N-CA-C	-6.88	103.23	111.69
6	F	45	GLU	CA-C-N	-6.88	111.57	120.65
6	F	45	GLU	C-N-CA	-6.88	111.57	120.65
2	N	186	VAL	N-CA-CB	6.86	119.31	111.90
1	A	283	THR	N-CA-C	6.85	121.24	113.02
47	y	130	PRO	N-CA-C	-6.84	102.35	110.70
1	A	415	PHE	O-C-N	-6.84	111.87	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	c	318	ILE	N-CA-C	6.84	114.67	107.76
2	B	173	ALA	CA-C-O	6.80	128.03	119.12
1	M	320	LEU	O-C-N	-6.80	114.39	123.23
5	E	5	ILE	N-CA-C	6.80	118.08	108.36
2	N	258	VAL	N-CA-C	6.79	117.31	108.35
30	q	224	GLY	N-CA-C	6.79	120.87	112.73
1	M	334	MET	N-CA-CB	-6.78	100.12	110.16
4	P	97	ASN	CA-C-N	6.77	128.31	119.84
4	P	97	ASN	C-N-CA	6.77	128.31	119.84
37	1	133	GLY	N-CA-C	6.76	129.21	113.18
3	O	298	ILE	N-CA-C	6.75	116.88	110.53
1	A	436	ARG	O-C-N	6.75	129.38	122.09
53	Af	43	VAL	CB-CA-C	-6.74	107.30	113.70
47	y	507	GLU	N-CA-C	-6.72	97.93	109.15
40	4	5	LYS	N-CA-C	6.72	125.11	110.80
5	Q	194	ILE	N-CA-CB	-6.72	103.44	111.90
1	A	338	LEU	CA-C-O	6.71	128.05	121.00
3	C	218	ILE	O-C-N	6.70	128.74	121.10
3	O	328	LEU	CA-C-N	-6.70	112.12	120.56
3	O	328	LEU	C-N-CA	-6.70	112.12	120.56
1	M	268	VAL	N-CA-C	-6.69	106.27	112.96
1	A	259	GLY	CA-C-N	6.68	128.19	119.84
1	A	259	GLY	C-N-CA	6.68	128.19	119.84
3	O	13	ILE	CB-CA-C	-6.68	103.27	112.02
53	Af	76	PRO	N-CA-CB	6.67	110.25	103.25
3	C	135	TRP	CA-C-O	-6.67	113.85	121.65
4	D	7	PRO	N-CA-C	6.67	118.84	110.70
5	Q	192	MET	N-CA-C	6.65	119.25	108.34
1	A	169	GLY	CA-C-N	6.65	128.15	119.84
1	A	169	GLY	C-N-CA	6.65	128.15	119.84
3	C	143	ALA	N-CA-C	-6.65	104.12	111.36
6	R	35	ASP	CA-C-O	6.64	127.55	119.31
4	D	32	VAL	N-CA-CB	6.64	117.88	110.51
5	Q	129	LYS	CA-C-N	6.63	128.13	119.84
5	Q	129	LYS	C-N-CA	6.63	128.13	119.84
2	N	141	GLN	CA-C-N	6.63	128.13	119.84
2	N	141	GLN	C-N-CA	6.63	128.13	119.84
6	R	79	GLN	N-CA-C	6.62	120.35	112.93
3	O	222	PRO	CB-CA-C	6.62	122.49	111.56
16	b	162	CYS	CA-C-N	6.61	126.55	119.28
16	b	162	CYS	C-N-CA	6.61	126.55	119.28
47	y	74	MET	N-CA-C	6.61	118.14	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	ILE	N-CA-C	6.60	117.29	110.36
1	M	334	MET	CA-C-O	6.60	127.41	120.42
3	O	299	LEU	CA-C-O	6.59	127.47	119.49
2	N	173	ALA	CA-C-O	6.59	127.54	119.11
4	D	83	ARG	CA-C-N	6.58	126.60	119.89
4	D	83	ARG	C-N-CA	6.58	126.60	119.89
4	D	92	PRO	N-CA-CB	6.58	107.64	103.23
38	2	81	ILE	N-CA-C	6.57	116.71	110.53
13	Y	449	PRO	N-CA-CB	6.57	110.48	103.39
1	A	199	ALA	CA-C-N	-6.56	112.28	122.59
1	A	199	ALA	C-N-CA	-6.56	112.28	122.59
3	O	244	LEU	CA-C-O	-6.56	111.83	119.64
1	A	436	ARG	N-CA-CB	6.56	119.58	110.07
9	I	68	VAL	CB-CA-C	-6.55	101.74	110.98
20	f	115	VAL	CA-C-N	-6.55	112.07	119.28
20	f	115	VAL	C-N-CA	-6.55	112.07	119.28
3	O	93	CYS	N-CA-CB	6.55	119.85	110.16
1	M	229	PRO	N-CA-CB	6.54	110.53	103.33
1	M	307	PHE	O-C-N	-6.54	115.39	123.44
3	O	19	ILE	CA-C-N	6.54	134.22	122.06
3	O	19	ILE	C-N-CA	6.54	134.22	122.06
6	F	37	ILE	N-CA-C	6.53	119.03	109.63
2	B	177	TYR	CA-C-O	-6.52	113.28	120.38
3	C	293	ALA	CA-C-N	-6.52	111.03	120.29
3	C	293	ALA	C-N-CA	-6.52	111.03	120.29
3	C	186	PRO	O-C-N	-6.52	114.75	122.24
9	U	53	GLU	N-CA-C	6.51	118.38	111.28
2	B	187	THR	CA-C-N	6.51	127.98	119.84
2	B	187	THR	C-N-CA	6.51	127.98	119.84
1	A	280	TYR	O-C-N	-6.50	115.99	123.33
3	C	246	ALA	O-C-N	6.50	125.93	121.19
2	B	75	LEU	CA-C-O	-6.49	114.48	121.94
5	Q	24	SER	N-CA-C	6.49	119.63	110.23
18	d	49	PRO	N-CA-CB	6.48	110.06	103.25
47	y	506	GLU	N-CA-C	-6.47	104.22	111.28
56	Ak	156	PRO	N-CA-CB	6.47	110.05	103.25
3	C	312	GLN	O-C-N	-6.47	114.74	122.63
5	Q	66	ALA	CA-C-O	6.47	127.11	119.28
5	Q	70	ALA	CA-C-O	6.46	127.27	120.42
3	C	224	TYR	N-CA-C	6.46	120.42	112.54
3	C	230	LEU	CA-C-N	6.45	127.28	119.99
3	C	230	LEU	C-N-CA	6.45	127.28	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	29	SER	N-CA-C	6.45	118.31	111.28
1	A	420	PRO	N-CA-CB	6.43	109.44	103.39
13	Y	540	ASN	CA-C-N	6.43	127.00	120.38
13	Y	540	ASN	C-N-CA	6.43	127.00	120.38
2	B	91	ALA	CA-C-N	6.42	132.26	122.69
2	B	91	ALA	C-N-CA	6.42	132.26	122.69
2	B	29	LEU	CA-C-N	6.42	126.17	119.05
2	B	29	LEU	C-N-CA	6.42	126.17	119.05
22	h	189	SER	CB-CA-C	-6.41	109.17	116.54
1	A	11	VAL	CA-C-N	6.41	127.85	119.84
1	A	11	VAL	C-N-CA	6.41	127.85	119.84
16	b	116	CYS	N-CA-C	-6.41	105.43	113.18
3	C	107	TYR	CA-C-N	-6.40	111.61	120.38
3	C	107	TYR	C-N-CA	-6.40	111.61	120.38
1	M	100	LYS	CA-C-O	-6.40	113.45	120.43
2	N	204	MET	N-CA-C	6.38	120.44	110.17
2	B	73	SER	CA-C-O	-6.37	111.40	120.51
1	A	32	GLN	CA-C-N	6.37	127.80	119.84
1	A	32	GLN	C-N-CA	6.37	127.80	119.84
1	A	251	ALA	CA-C-N	-6.36	114.31	122.77
1	A	251	ALA	C-N-CA	-6.36	114.31	122.77
30	v	304	LEU	N-CA-C	-6.35	104.36	111.28
5	E	136	ILE	N-CA-C	-6.34	99.16	108.54
3	O	256	TYR	O-C-N	6.33	130.35	122.19
2	N	178	CYS	CA-C-N	6.33	126.09	119.76
2	N	178	CYS	C-N-CA	6.33	126.09	119.76
1	A	147	ASP	CA-C-O	6.32	127.26	120.24
1	A	436	ARG	CA-C-O	-6.30	114.21	120.70
3	C	109	PHE	O-C-N	-6.29	114.22	122.59
1	M	239	SER	CA-C-O	-6.29	114.28	121.58
2	B	291	ALA	N-CA-C	-6.28	105.74	113.41
4	D	168	VAL	CB-CA-C	-6.28	103.82	112.24
1	M	342	TRP	CA-C-N	6.28	129.01	120.54
1	M	342	TRP	C-N-CA	6.28	129.01	120.54
3	C	78	ILE	CA-C-N	-6.28	111.51	120.42
3	C	78	ILE	C-N-CA	-6.28	111.51	120.42
3	O	325	PHE	O-C-N	6.27	128.56	122.03
2	N	254	HIS	CA-C-O	-6.27	113.93	120.70
2	N	167	ALA	CA-C-O	6.27	127.18	119.97
47	y	10	THR	N-CA-C	-6.27	103.82	112.03
3	C	301	LEU	N-CA-C	6.26	118.63	111.11
1	M	161	THR	CA-C-N	6.26	126.74	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	161	THR	C-N-CA	6.26	126.74	119.47
1	A	434	TYR	O-C-N	6.26	128.76	122.12
2	B	145	ARG	CA-C-O	-6.26	114.20	120.90
1	M	319	LEU	N-CA-CB	-6.26	100.72	110.55
13	Y	179	CYS	N-CA-C	-6.26	100.39	109.59
29	p	240	VAL	N-CA-C	6.26	117.04	110.72
1	A	196	VAL	CA-C-O	-6.24	113.90	120.76
40	4	2	SER	N-CA-C	6.23	119.50	109.79
4	P	110	PRO	CA-C-N	6.20	126.15	119.76
4	P	110	PRO	C-N-CA	6.20	126.15	119.76
1	A	69	ASN	O-C-N	-6.20	115.58	122.03
1	A	392	LEU	N-CA-CB	6.19	119.16	109.94
22	h	207	MET	N-CA-C	-6.19	100.64	109.24
38	2	21	LYS	CA-C-N	6.19	126.37	119.32
38	2	21	LYS	C-N-CA	6.19	126.37	119.32
7	G	14	ILE	CA-C-N	6.18	131.90	122.93
7	G	14	ILE	C-N-CA	6.18	131.90	122.93
4	P	160	MET	N-CA-C	6.18	118.84	108.02
47	y	157	SER	N-CA-C	6.18	118.99	111.82
1	M	416	TYR	N-CA-C	6.18	118.25	108.67
6	R	98	ILE	CA-C-O	6.18	127.70	121.27
30	q	249	PRO	N-CA-CB	6.17	110.06	103.39
1	M	142	ASP	N-CA-C	-6.17	105.71	113.18
1	A	343	MET	CA-C-N	-6.17	111.93	120.38
1	A	343	MET	C-N-CA	-6.17	111.93	120.38
3	C	257	THR	CA-C-O	6.16	123.88	119.32
1	A	440	GLY	CA-C-N	-6.16	111.97	122.56
1	A	440	GLY	C-N-CA	-6.16	111.97	122.56
10	J	8	ARG	CA-C-N	6.15	128.85	120.54
10	J	8	ARG	C-N-CA	6.15	128.85	120.54
2	N	66	SER	N-CA-CB	6.14	118.91	110.01
2	B	46	ARG	N-CA-C	6.13	118.41	107.80
1	M	277	ILE	CA-C-O	-6.13	114.90	121.27
1	A	153	LEU	N-CA-CB	6.09	119.08	109.82
2	B	306	PRO	N-CA-CB	6.09	108.17	103.30
3	C	231	GLY	CA-C-O	6.09	127.33	121.05
47	y	170	ASN	N-CA-C	6.09	120.78	113.23
1	A	418	GLN	CA-C-N	-6.09	113.15	121.61
1	A	418	GLN	C-N-CA	-6.09	113.15	121.61
19	e	196	ALA	CA-C-N	-6.09	112.58	119.28
19	e	196	ALA	C-N-CA	-6.09	112.58	119.28
3	C	180	ALA	N-CA-CB	6.08	119.14	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	233	LEU	O-C-N	6.08	128.41	122.09
55	Aj	122	ARG	N-CA-C	-6.08	104.45	112.24
1	A	277	ILE	CB-CA-C	-6.07	103.95	112.14
3	O	221	HIS	CB-CA-C	-6.07	104.04	113.57
2	B	187	THR	CA-C-O	-6.06	115.15	120.60
1	M	416	TYR	CA-C-O	-6.06	113.75	120.60
1	M	292	SER	CA-C-N	6.05	127.41	119.84
1	M	292	SER	C-N-CA	6.05	127.41	119.84
5	Q	7	VAL	N-CA-C	6.04	115.61	108.96
5	Q	63	SER	N-CA-C	6.04	117.86	111.28
10	J	22	LEU	N-CA-C	-6.04	104.61	111.07
30	q	160	VAL	N-CA-C	6.03	116.30	107.37
41	5	63	LEU	N-CA-C	6.03	119.11	111.69
7	S	10	VAL	CA-C-O	-6.02	114.19	120.27
36	0	8	TYR	N-CA-C	6.02	118.29	110.53
8	H	55	THR	CA-C-O	6.01	127.13	120.82
40	4	44	ARG	CA-C-N	6.01	126.03	119.90
40	4	44	ARG	C-N-CA	6.01	126.03	119.90
3	C	186	PRO	CA-C-O	6.00	129.98	119.84
13	Y	612	PRO	CA-C-N	6.00	125.88	119.28
13	Y	612	PRO	C-N-CA	6.00	125.88	119.28
1	A	166	SER	CA-C-O	6.00	127.88	121.16
3	O	320	LEU	CA-C-N	-6.00	111.20	120.31
3	O	320	LEU	C-N-CA	-6.00	111.20	120.31
3	C	19	ILE	CA-C-O	-5.99	113.83	120.96
2	N	87	ARG	O-C-N	5.99	129.23	122.22
3	C	143	ALA	CA-C-O	5.99	126.77	120.42
2	N	85	ILE	O-C-N	5.98	130.05	122.57
2	B	409	ASP	CA-C-N	5.98	128.61	120.77
2	B	409	ASP	C-N-CA	5.98	128.61	120.77
47	y	125	GLY	N-CA-C	-5.98	104.16	112.18
1	A	338	LEU	O-C-N	-5.98	115.81	122.03
1	A	220	SER	CA-C-N	5.98	126.95	120.44
1	A	220	SER	C-N-CA	5.98	126.95	120.44
3	O	210	GLY	N-CA-C	-5.98	107.15	114.92
21	g	98	LEU	N-CA-C	-5.98	104.67	111.07
1	M	54	GLY	O-C-N	5.97	127.64	121.97
1	A	284	TYR	O-C-N	-5.96	115.60	122.93
1	A	425	PHE	N-CA-CB	5.96	121.10	110.79
2	B	145	ARG	O-C-N	5.95	128.28	122.09
22	h	278	ARG	N-CA-C	5.95	118.57	110.06
1	A	248	LEU	CA-C-N	5.94	125.82	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	LEU	C-N-CA	5.94	125.82	119.28
48	z	207	MET	CA-C-N	5.94	127.27	119.84
48	z	207	MET	C-N-CA	5.94	127.27	119.84
1	A	440	GLY	N-CA-C	-5.94	107.54	115.32
7	S	71	ARG	N-CA-C	5.93	117.75	111.28
4	D	110	PRO	CA-C-N	5.93	125.87	119.76
4	D	110	PRO	C-N-CA	5.93	125.87	119.76
48	z	47	THR	N-CA-C	5.93	119.82	112.59
2	N	75	LEU	N-CA-CB	5.92	118.91	110.44
4	D	86	LYS	N-CA-C	5.92	118.40	110.35
1	M	364	ALA	CA-C-O	5.92	126.82	120.55
24	j	588	PHE	N-CA-C	-5.92	104.75	111.14
3	C	127	ALA	CA-C-O	5.91	126.77	119.97
2	N	167	ALA	O-C-N	-5.91	115.00	122.27
2	N	285	VAL	N-CA-C	5.91	116.79	108.17
3	O	206	ASN	O-C-N	-5.90	115.72	122.68
3	C	177	ARG	CB-CA-C	-5.90	101.87	110.96
1	A	292	SER	O-C-N	-5.89	115.93	121.35
4	D	92	PRO	CB-CA-C	5.89	116.76	111.40
5	Q	132	TRP	N-CA-C	5.89	119.42	109.76
3	C	160	LEU	N-CA-C	5.89	118.46	111.33
2	N	42	ALA	CA-C-N	5.89	127.20	119.84
2	N	42	ALA	C-N-CA	5.89	127.20	119.84
3	O	126	THR	O-C-N	5.89	128.13	122.07
2	N	157	ALA	N-CA-C	5.88	117.36	111.07
14	Z	236	LEU	CA-C-N	5.88	125.84	119.78
14	Z	236	LEU	C-N-CA	5.88	125.84	119.78
48	z	134	ARG	N-CA-C	5.88	123.31	110.80
47	y	171	MET	N-CA-C	5.87	120.15	111.87
7	S	15	THR	CB-CA-C	-5.87	98.97	109.71
47	y	67	PHE	N-CA-C	5.87	119.63	112.23
3	C	22	PRO	CB-CA-C	-5.87	101.88	111.56
3	O	38	GLY	O-C-N	-5.87	116.50	122.19
3	O	54	HIS	CA-C-N	5.86	132.09	122.07
3	O	54	HIS	C-N-CA	5.86	132.09	122.07
12	W	85	GLU	N-CA-C	5.85	117.15	107.20
3	C	320	LEU	CA-C-N	-5.85	111.42	120.31
3	C	320	LEU	C-N-CA	-5.85	111.42	120.31
3	O	102	LEU	O-C-N	5.85	130.53	122.46
36	0	198	PHE	N-CA-C	5.85	117.65	111.28
4	D	182	VAL	N-CA-CB	5.83	119.33	110.58
47	y	119	GLU	CB-CA-C	-5.83	109.83	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	227	LYS	O-C-N	5.83	128.08	122.07
2	N	167	ALA	CA-C-N	-5.83	112.33	122.64
2	N	167	ALA	C-N-CA	-5.83	112.33	122.64
2	B	94	GLY	CA-C-O	-5.82	114.30	122.51
1	M	339	GLN	O-C-N	5.82	130.33	122.59
48	z	202	SER	N-CA-C	5.80	118.07	111.11
48	z	190	GLY	N-CA-C	5.79	117.79	110.38
4	D	151	PRO	N-CA-CB	5.79	108.85	103.41
3	C	205	SER	CA-C-O	5.78	127.35	120.70
2	B	139	ALA	CA-C-O	5.78	126.89	120.82
3	O	201	HIS	CA-C-O	5.78	126.06	119.18
3	C	75	TYR	N-CA-C	-5.76	106.20	113.23
2	N	157	ALA	N-CA-CB	5.76	118.36	110.01
3	C	153	ILE	CA-C-N	5.75	127.03	119.84
3	C	153	ILE	C-N-CA	5.75	127.03	119.84
1	A	23	LEU	CA-C-N	-5.75	114.79	122.72
1	A	23	LEU	C-N-CA	-5.75	114.79	122.72
4	P	50	HIS	N-CA-C	-5.75	106.10	113.23
43	7	25	GLY	N-CA-C	5.75	118.99	110.60
7	G	58	VAL	N-CA-CB	5.75	117.65	110.47
1	M	56	GLY	O-C-N	-5.74	115.23	122.70
1	M	436	ARG	CA-C-N	-5.74	112.05	121.34
1	M	436	ARG	C-N-CA	-5.74	112.05	121.34
2	B	138	ALA	CA-C-O	-5.74	114.34	120.42
3	O	185	LEU	CA-C-O	-5.73	113.29	118.79
3	C	189	ILE	CB-CA-C	-5.73	104.53	112.04
4	D	9	SER	N-CA-C	-5.73	101.03	109.62
56	Ak	149	PRO	N-CA-CB	5.73	109.59	103.52
1	M	292	SER	CA-C-O	5.72	124.17	119.36
12	W	216	VAL	N-CA-C	-5.72	107.41	112.90
22	h	112	ALA	CA-C-N	5.72	131.99	121.70
22	h	112	ALA	C-N-CA	5.72	131.99	121.70
1	M	138	LEU	O-C-N	5.71	129.11	122.20
2	N	85	ILE	CA-C-O	-5.71	113.64	120.78
3	O	63	PHE	O-C-N	5.71	129.11	122.20
1	M	428	ILE	O-C-N	-5.71	116.23	122.05
47	y	129	TYR	CB-CA-C	-5.71	100.46	109.42
24	j	438	PRO	CA-C-N	5.70	125.64	119.76
24	j	438	PRO	C-N-CA	5.70	125.64	119.76
5	Q	184	SER	CA-C-O	-5.70	114.55	121.05
3	O	22	PRO	N-CA-CB	5.69	108.23	103.17
28	o	46	GLY	N-CA-C	-5.69	108.41	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	j	111	ASP	CA-C-N	5.69	125.60	119.85
24	j	111	ASP	C-N-CA	5.69	125.60	119.85
2	B	310	SER	N-CA-C	5.68	118.72	109.06
2	B	157	ALA	N-CA-C	5.68	117.15	111.07
2	N	187	THR	CA-C-N	5.68	126.94	119.84
2	N	187	THR	C-N-CA	5.68	126.94	119.84
3	O	264	THR	CB-CA-C	-5.67	102.28	109.65
4	P	38	SER	CA-C-N	5.67	128.44	120.28
4	P	38	SER	C-N-CA	5.67	128.44	120.28
3	O	256	TYR	CA-C-O	-5.67	112.84	120.15
3	C	182	HIS	N-CA-C	-5.66	105.11	111.28
2	N	201	SER	N-CA-C	5.66	117.14	110.97
2	N	108	THR	N-CA-C	5.66	118.05	110.35
17	c	150	GLY	N-CA-C	-5.66	106.37	115.08
1	A	11	VAL	N-CA-C	5.65	114.28	109.02
37	1	129	ALA	CA-C-N	5.65	126.90	119.84
37	1	129	ALA	C-N-CA	5.65	126.90	119.84
3	O	257	THR	CB-CA-C	-5.65	103.41	109.85
34	w	121	LEU	N-CA-C	5.65	117.67	110.61
1	A	193	PRO	N-CA-CB	5.64	108.81	102.60
1	A	392	LEU	N-CA-C	5.64	117.88	111.11
3	C	96	MET	N-CA-C	-5.64	105.21	111.36
4	P	109	LEU	CA-C-N	5.64	126.19	120.38
4	P	109	LEU	C-N-CA	5.64	126.19	120.38
6	F	43	VAL	O-C-N	-5.64	115.52	122.57
3	C	191	ALA	N-CA-C	-5.64	105.03	111.07
3	O	100	ARG	N-CA-C	-5.64	105.12	112.23
3	C	22	PRO	N-CA-CB	5.64	109.17	103.25
2	N	45	SER	O-C-N	-5.64	116.60	123.19
2	N	165	ALA	CA-C-O	5.64	126.30	119.31
5	Q	76	ILE	CA-C-O	-5.64	115.39	121.19
20	f	165	GLY	N-CA-C	-5.64	107.94	115.32
3	O	196	HIS	N-CA-C	-5.63	105.04	111.07
3	O	46	LEU	N-CA-C	-5.63	105.06	111.14
9	U	56	ARG	CA-C-N	5.63	128.70	121.27
9	U	56	ARG	C-N-CA	5.63	128.70	121.27
1	A	242	CYS	N-CA-C	5.63	118.41	109.24
3	C	143	ALA	CA-C-N	-5.63	113.13	120.44
3	C	143	ALA	C-N-CA	-5.63	113.13	120.44
1	M	32	GLN	CA-C-N	5.63	126.87	119.84
1	M	32	GLN	C-N-CA	5.63	126.87	119.84
56	Ak	78	GLN	CA-C-N	5.62	125.60	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Ak	78	GLN	C-N-CA	5.62	125.60	120.03
1	A	279	HIS	O-C-N	-5.62	117.18	123.48
3	O	45	ILE	CB-CA-C	-5.62	104.78	111.81
3	C	123	VAL	CA-C-N	-5.62	111.13	120.68
3	C	123	VAL	C-N-CA	-5.62	111.13	120.68
3	O	56	THR	O-C-N	-5.61	116.34	123.24
30	q	204	HIS	N-CA-C	5.60	116.29	108.00
14	Z	365	PRO	CA-C-N	5.60	125.55	119.78
14	Z	365	PRO	C-N-CA	5.60	125.55	119.78
1	A	414	TYR	N-CA-C	5.60	120.24	112.90
4	D	31	GLN	CA-C-O	-5.60	114.91	120.90
13	Y	471	LYS	CA-C-N	5.60	125.53	119.76
13	Y	471	LYS	C-N-CA	5.60	125.53	119.76
16	b	178	GLU	N-CA-C	5.59	117.38	111.28
3	C	164	ILE	CA-C-O	-5.59	115.46	121.27
8	H	54	CYS	CA-C-N	5.59	127.70	120.44
8	H	54	CYS	C-N-CA	5.59	127.70	120.44
42	6	20	HIS	N-CA-C	5.59	118.14	111.71
48	z	104	TRP	N-CA-C	5.59	122.70	110.80
3	C	205	SER	N-CA-C	5.58	118.27	109.96
2	B	197	ASN	N-CA-C	5.57	117.43	111.36
22	h	72	LEU	N-CA-C	5.57	118.28	111.82
39	3	82	CYS	CA-C-N	5.57	125.40	119.28
39	3	82	CYS	C-N-CA	5.57	125.40	119.28
30	v	314	VAL	N-CA-C	-5.56	108.42	113.71
56	Ak	133	TRP	N-CA-C	5.56	117.34	111.28
32	t	130	ILE	N-CA-C	5.56	114.00	107.77
1	A	22	GLY	N-CA-C	-5.56	107.11	114.95
21	g	28	ASN	N-CA-C	5.56	117.77	107.99
11	V	39	ARG	N-CA-C	5.55	117.33	111.28
45	9	16	GLU	N-CA-C	5.55	117.41	111.36
3	O	35	SER	CA-C-N	5.55	127.98	120.38
3	O	35	SER	C-N-CA	5.55	127.98	120.38
23	i	87	THR	N-CA-C	5.55	117.90	110.35
3	C	282	ARG	N-CA-C	5.55	117.33	111.28
56	Ak	144	THR	CA-C-N	5.55	126.09	120.38
56	Ak	144	THR	C-N-CA	5.55	126.09	120.38
3	C	111	GLU	CA-C-O	-5.54	114.97	120.90
3	O	185	LEU	O-C-N	5.54	124.75	120.38
1	A	69	ASN	CA-C-O	5.54	126.81	121.00
2	B	85	ILE	N-CA-C	5.54	116.17	110.36
3	C	120	LEU	CA-C-O	5.53	126.82	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	102	ARG	N-CA-C	-5.53	105.63	112.38
40	4	72	ASN	CA-C-N	5.53	125.88	119.47
40	4	72	ASN	C-N-CA	5.53	125.88	119.47
10	L	8	ARG	CA-C-N	5.52	128.00	120.54
10	L	8	ARG	C-N-CA	5.52	128.00	120.54
1	M	47	TYR	N-CA-C	-5.52	106.59	113.38
1	A	360	LEU	N-CA-C	-5.52	105.34	111.36
6	R	99	ARG	CA-C-N	-5.52	112.89	120.28
6	R	99	ARG	C-N-CA	-5.52	112.89	120.28
4	P	16	GLY	N-CA-C	5.51	120.09	112.37
6	R	98	ILE	O-C-N	-5.51	116.43	121.94
3	C	26	ASN	O-C-N	-5.50	116.53	123.12
7	S	19	SER	CA-C-N	5.49	124.95	119.24
7	S	19	SER	C-N-CA	5.49	124.95	119.24
3	O	126	THR	CA-C-O	-5.49	115.06	120.82
1	A	149	VAL	N-CA-CB	5.49	116.97	110.55
2	B	190	GLU	CA-C-O	-5.49	115.03	120.90
2	B	46	ARG	CB-CA-C	-5.49	102.61	110.62
7	G	10	VAL	CA-C-O	5.49	125.68	120.25
3	C	21	LEU	N-CA-C	5.48	116.60	109.64
7	G	15	THR	N-CA-C	5.48	118.42	109.59
30	q	165	ILE	N-CA-C	5.48	116.21	110.62
1	M	341	GLN	CA-C-O	-5.48	114.62	120.42
2	N	329	GLN	CB-CA-C	5.47	119.92	110.45
4	D	109	LEU	CA-C-N	5.47	126.01	120.38
4	D	109	LEU	C-N-CA	5.47	126.01	120.38
36	0	188	ILE	CB-CA-C	-5.46	104.77	112.14
2	B	320	GLY	CA-C-O	5.46	126.43	121.47
3	C	188	ILE	N-CA-CB	5.45	117.55	110.57
4	D	40	CYS	CB-CA-C	5.45	116.19	109.16
3	C	18	PHE	CA-C-N	5.45	128.54	120.74
3	C	18	PHE	C-N-CA	5.45	128.54	120.74
1	A	208	LEU	N-CA-C	-5.45	105.03	110.97
29	p	195	PHE	CA-C-N	5.45	125.27	119.28
29	p	195	PHE	C-N-CA	5.45	125.27	119.28
9	U	58	GLN	N-CA-C	5.45	118.36	109.59
43	7	2	GLU	N-CA-C	5.45	122.40	110.80
13	Y	364	ASP	N-CA-C	5.44	117.12	108.79
13	Y	685	VAL	N-CA-C	5.44	113.93	107.73
3	C	74	ASN	N-CA-C	5.44	116.98	109.15
2	B	309	VAL	N-CA-C	5.43	115.01	108.06
5	Q	69	LEU	CA-C-N	5.43	128.00	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	69	LEU	C-N-CA	5.43	128.00	120.29
3	C	195	VAL	CA-C-N	5.43	127.81	120.65
3	C	195	VAL	C-N-CA	5.43	127.81	120.65
1	M	421	ALA	CB-CA-C	5.43	119.64	110.79
5	E	65	SER	N-CA-C	-5.42	99.25	110.80
3	O	261	PRO	N-CA-CB	5.42	108.94	103.25
2	B	44	ALA	N-CA-C	5.42	117.36	108.52
1	A	443	TRP	N-CA-C	5.42	119.19	107.49
1	M	375	VAL	O-C-N	5.42	127.20	121.89
6	F	97	VAL	N-CA-CB	-5.41	102.30	111.23
7	G	50	PRO	N-CA-CB	5.41	108.33	103.08
1	A	343	MET	O-C-N	-5.41	115.39	122.59
2	N	92	VAL	N-CA-CB	-5.41	105.28	112.26
4	P	48	TYR	CA-C-N	5.41	130.14	122.24
4	P	48	TYR	C-N-CA	5.41	130.14	122.24
12	W	104	THR	N-CA-C	-5.41	99.28	110.80
6	F	76	PRO	N-CA-CB	5.41	108.06	103.35
1	A	373	THR	O-C-N	-5.41	115.48	120.51
30	q	93	ILE	N-CA-C	5.41	116.13	110.62
7	S	12	HIS	CA-C-N	-5.40	115.91	123.10
7	S	12	HIS	C-N-CA	-5.40	115.91	123.10
1	A	94	HIS	CB-CA-C	-5.40	104.03	110.94
3	C	19	ILE	N-CA-C	5.39	116.05	110.82
22	h	168	GLN	N-CA-C	-5.39	106.66	113.18
3	O	234	LEU	N-CA-C	-5.38	105.50	111.36
2	B	89	ILE	O-C-N	-5.38	116.65	121.87
5	E	179	ASN	N-CA-C	-5.38	103.43	110.53
1	M	390	ILE	N-CA-CB	5.38	118.74	111.21
47	y	372	TYR	N-CA-C	-5.38	105.32	111.07
5	Q	172	ARG	CA-C-N	5.37	129.87	121.76
5	Q	172	ARG	C-N-CA	5.37	129.87	121.76
1	A	153	LEU	O-C-N	5.37	127.83	122.08
4	D	32	VAL	CB-CA-C	-5.37	105.01	111.88
7	G	18	LEU	O-C-N	-5.37	115.59	122.94
9	I	51	CYS	N-CA-C	5.36	118.36	109.94
10	J	55	ILE	N-CA-C	5.36	118.96	112.80
4	P	84	PRO	N-CA-CB	5.36	107.82	103.32
54	Ag	93	GLY	N-CA-C	-5.35	105.92	112.77
1	A	142	ASP	CA-C-O	5.35	125.96	119.49
47	y	159	LEU	N-CA-C	-5.34	105.53	111.36
47	y	305	PHE	N-CA-C	5.34	118.90	112.38
1	M	415	PHE	CA-C-O	5.34	126.24	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	90	LEU	O-C-N	5.34	129.49	122.33
1	A	170	PRO	N-CA-CB	5.34	108.85	103.25
6	R	36	THR	CA-C-O	5.34	126.11	119.12
3	O	259	ALA	CA-C-O	-5.33	114.67	120.81
47	y	245	ILE	N-CA-C	-5.33	104.38	111.05
3	C	356	VAL	O-C-N	-5.33	116.70	121.87
2	N	162	ASN	CB-CA-C	5.33	119.58	110.74
2	B	107	TYR	CA-C-N	5.32	128.78	120.75
2	B	107	TYR	C-N-CA	5.32	128.78	120.75
4	D	116	ILE	N-CA-C	5.32	116.04	110.62
1	M	25	VAL	CA-C-N	-5.32	114.24	122.59
1	M	25	VAL	C-N-CA	-5.32	114.24	122.59
22	h	456	GLY	CA-C-N	5.32	125.13	119.28
22	h	456	GLY	C-N-CA	5.32	125.13	119.28
3	O	141	TRP	CA-C-N	5.32	125.84	119.94
3	O	141	TRP	C-N-CA	5.32	125.84	119.94
1	M	162	PRO	CB-CA-C	-5.31	103.39	112.26
33	u	166	GLY	CA-C-N	5.31	125.12	119.28
33	u	166	GLY	C-N-CA	5.31	125.12	119.28
1	M	145	MET	CA-C-N	-5.31	113.11	120.38
1	M	145	MET	C-N-CA	-5.31	113.11	120.38
2	B	33	LEU	O-C-N	5.31	129.31	123.16
6	F	55	TYR	CA-C-O	-5.31	114.92	120.55
1	A	161	THR	CA-C-N	5.30	125.11	119.28
1	A	161	THR	C-N-CA	5.30	125.11	119.28
3	C	210	GLY	CA-C-N	5.30	132.03	122.43
3	C	210	GLY	C-N-CA	5.30	132.03	122.43
3	O	106	SER	CA-C-O	5.30	125.91	119.38
5	E	66	ALA	N-CA-C	-5.30	105.42	111.14
2	N	274	VAL	O-C-N	5.30	127.29	121.83
5	Q	136	ILE	N-CA-CB	-5.30	106.18	111.90
1	M	428	ILE	CA-C-O	5.30	125.44	120.14
3	C	233	LEU	CA-C-O	-5.29	115.23	120.90
7	G	19	SER	CA-C-N	5.29	125.35	119.32
7	G	19	SER	C-N-CA	5.29	125.35	119.32
1	A	358	LYS	CA-C-N	5.28	127.62	120.38
1	A	358	LYS	C-N-CA	5.28	127.62	120.38
2	B	94	GLY	CA-C-N	5.28	131.46	122.37
2	B	94	GLY	C-N-CA	5.28	131.46	122.37
3	O	160	LEU	N-CA-C	5.28	117.45	111.11
23	i	54	THR	N-CA-C	5.28	117.78	111.71
1	M	315	ALA	CA-C-O	5.28	126.36	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Y	184	ARG	N-CA-C	-5.28	106.10	112.54
22	h	44	GLN	CB-CA-C	-5.28	109.51	115.79
1	A	357	GLY	N-CA-C	-5.27	106.02	112.77
2	N	107	TYR	CA-C-N	5.27	128.71	120.75
2	N	107	TYR	C-N-CA	5.27	128.71	120.75
2	N	394	PRO	CA-C-N	5.27	126.42	119.84
2	N	394	PRO	C-N-CA	5.27	126.42	119.84
4	P	175	THR	CA-C-O	5.27	124.17	119.59
1	M	277	ILE	CB-CA-C	-5.26	105.14	111.88
47	y	6	TRP	N-CA-C	5.26	119.75	113.23
3	C	135	TRP	O-C-N	5.26	128.89	122.58
4	D	46	VAL	N-CA-CB	5.26	117.00	111.00
2	N	416	LYS	N-CA-C	5.26	117.76	111.71
2	B	75	LEU	O-C-N	5.25	129.11	122.65
1	M	392	LEU	N-CA-CB	5.25	117.77	109.94
3	C	361	LEU	CA-C-O	-5.25	114.96	120.63
3	O	226	ILE	CA-C-O	5.25	126.41	120.85
3	C	126	THR	N-CA-CB	5.25	118.33	109.78
1	A	425	PHE	CA-C-N	5.24	130.10	121.87
1	A	425	PHE	C-N-CA	5.24	130.10	121.87
47	y	262	SER	N-CA-C	-5.24	106.56	113.17
3	O	219	PRO	CA-C-O	5.24	126.84	121.23
1	M	440	GLY	N-CA-C	-5.24	107.82	114.16
23	i	24	SER	CB-CA-C	-5.24	109.56	115.79
18	d	91	GLY	N-CA-C	-5.24	108.02	115.30
57	Al	25	PRO	O-C-N	5.24	123.61	121.15
1	A	391	PRO	CA-C-N	5.23	127.60	120.54
1	A	391	PRO	C-N-CA	5.23	127.60	120.54
3	C	196	HIS	N-CA-CB	5.23	117.55	109.91
1	M	260	PRO	N-CA-CB	5.23	108.30	103.39
3	O	45	ILE	O-C-N	5.23	127.33	121.94
36	0	99	TRP	N-CA-C	-5.23	105.48	111.07
6	F	99	ARG	O-C-N	-5.22	116.10	122.11
1	M	416	TYR	N-CA-CB	5.22	118.30	109.94
7	S	17	SER	CA-C-O	-5.22	115.33	121.44
2	B	353	SER	CA-C-N	5.22	129.81	121.62
2	B	353	SER	C-N-CA	5.22	129.81	121.62
39	3	38	ALA	N-CA-C	5.21	117.85	110.50
1	M	350	THR	CA-C-O	-5.21	115.22	121.11
3	C	289	GLY	CA-C-O	-5.21	114.77	120.40
2	N	430	LEU	N-CA-C	5.21	119.32	111.81
8	H	60	ASP	N-CA-C	-5.21	106.61	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	138	ALA	N-CA-C	5.21	117.36	111.11
29	p	237	LYS	N-CA-C	5.21	116.90	109.14
5	Q	182	VAL	O-C-N	5.20	125.96	120.96
10	J	54	HIS	CA-C-N	5.20	129.01	121.52
10	J	54	HIS	C-N-CA	5.20	129.01	121.52
13	Y	547	LEU	N-CA-C	-5.20	106.09	112.90
47	y	353	LEU	N-CA-C	-5.20	105.69	111.36
4	P	85	GLY	CA-C-N	5.20	128.60	120.75
4	P	85	GLY	C-N-CA	5.20	128.60	120.75
2	N	57	TYR	CA-C-N	-5.20	114.08	122.81
2	N	57	TYR	C-N-CA	-5.20	114.08	122.81
13	Y	124	HIS	CA-C-N	5.19	125.13	119.78
13	Y	124	HIS	C-N-CA	5.19	125.13	119.78
4	D	46	VAL	CA-C-O	5.19	126.72	120.65
47	y	377	PHE	N-CA-C	5.19	119.46	113.18
3	C	355	SER	O-C-N	-5.19	116.62	122.12
4	D	38	SER	CA-C-N	5.18	127.75	120.28
4	D	38	SER	C-N-CA	5.18	127.75	120.28
2	N	169	ARG	N-CA-C	-5.18	106.08	112.72
3	C	175	LEU	CA-C-O	5.18	125.91	119.79
7	G	19	SER	CA-C-O	-5.18	115.94	120.60
2	B	173	ALA	O-C-N	-5.18	114.72	122.39
2	B	256	ALA	CA-C-O	-5.18	115.26	121.11
9	I	69	SER	CA-C-O	-5.18	114.74	120.33
4	P	137	PRO	CA-C-N	5.18	125.98	120.13
4	P	137	PRO	C-N-CA	5.18	125.98	120.13
47	y	401	SER	N-CA-C	5.17	119.72	113.41
1	A	311	ASN	CA-C-N	-5.17	115.91	122.37
1	A	311	ASN	C-N-CA	-5.17	115.91	122.37
1	A	390	ILE	N-CA-CB	5.17	118.44	111.21
15	a	86	THR	N-CA-C	5.17	116.83	108.26
5	E	128	LYS	N-CA-C	-5.16	106.67	113.12
29	p	308	SER	CA-C-N	5.16	124.96	119.28
29	p	308	SER	C-N-CA	5.16	124.96	119.28
1	A	188	ARG	CA-C-N	-5.16	113.65	122.11
1	A	188	ARG	C-N-CA	-5.16	113.65	122.11
8	T	55	THR	CA-C-O	5.16	126.01	120.70
2	N	165	ALA	O-C-N	-5.16	115.34	122.46
3	O	35	SER	O-C-N	-5.15	115.73	122.59
3	O	60	THR	CB-CA-C	-5.15	102.56	110.81
4	P	153	PHE	CA-C-N	5.15	126.28	119.84
4	P	153	PHE	C-N-CA	5.15	126.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	295	ALA	CA-C-O	5.15	126.01	120.70
2	B	314	ALA	CA-C-O	-5.15	115.14	120.70
22	h	346	ARG	CB-CA-C	-5.15	110.22	117.23
2	N	337	ILE	CA-C-O	-5.15	115.71	121.17
3	O	124	MET	N-CA-C	5.15	116.89	111.28
17	c	412	LEU	N-CA-C	-5.15	105.56	111.07
1	A	167	VAL	N-CA-C	-5.14	105.38	110.62
7	G	12	HIS	N-CA-C	5.14	118.48	111.39
48	z	165	VAL	CA-C-N	5.14	126.26	119.84
48	z	165	VAL	C-N-CA	5.14	126.26	119.84
3	C	230	LEU	CA-C-O	-5.13	115.43	120.82
1	A	247	GLY	O-C-N	-5.13	117.21	122.19
4	P	33	TYR	CA-C-O	-5.13	115.42	121.07
2	N	66	SER	N-CA-C	-5.13	105.58	111.07
19	e	28	LEU	N-CA-C	-5.13	106.12	112.38
2	B	394	PRO	N-CA-CB	5.13	108.06	103.08
1	M	329	MET	CA-C-N	-5.13	114.47	122.37
1	M	329	MET	C-N-CA	-5.13	114.47	122.37
4	P	150	ASN	CA-C-N	5.13	124.79	119.56
4	P	150	ASN	C-N-CA	5.13	124.79	119.56
11	K	18	VAL	CB-CA-C	-5.13	108.91	114.35
1	M	319	LEU	CA-C-O	5.13	125.96	120.32
3	O	275	LEU	CA-C-O	-5.13	115.02	121.02
1	A	403	ASP	CA-C-N	-5.13	112.52	120.31
1	A	403	ASP	C-N-CA	-5.13	112.52	120.31
2	N	354	ASN	CA-C-N	5.12	125.16	119.32
2	N	354	ASN	C-N-CA	5.12	125.16	119.32
36	0	107	ALA	CA-C-N	5.12	125.92	119.98
36	0	107	ALA	C-N-CA	5.12	125.92	119.98
3	C	119	LEU	CA-C-O	5.12	126.70	121.07
1	M	157	ALA	CA-C-O	5.12	125.27	119.18
1	M	169	GLY	CA-C-N	5.12	125.12	119.90
1	M	169	GLY	C-N-CA	5.12	125.12	119.90
3	O	221	HIS	CA-C-O	5.12	123.84	119.13
4	P	143	LEU	N-CA-C	5.12	116.51	107.61
1	M	138	LEU	CA-C-N	5.12	127.39	120.38
1	M	138	LEU	C-N-CA	5.12	127.39	120.38
2	N	246	GLU	N-CA-C	5.11	117.69	107.62
3	O	79	ILE	N-CA-CB	5.11	116.19	110.51
7	S	5	GLY	CA-C-N	5.11	130.24	122.37
7	S	5	GLY	C-N-CA	5.11	130.24	122.37
43	7	9	GLN	N-CA-C	-5.11	105.60	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	h	370	PRO	O-C-N	5.11	123.66	121.31
53	Af	97	TRP	N-CA-C	-5.11	103.79	110.53
1	A	306	SER	O-C-N	-5.10	115.80	122.59
3	C	9	PRO	N-CA-CB	5.10	107.74	103.25
1	M	100	LYS	N-CA-C	-5.10	100.92	109.24
1	M	414	TYR	CA-C-O	-5.10	113.77	119.79
2	B	21	PRO	N-CA-CB	5.10	108.61	103.00
2	B	266	SER	CA-C-O	-5.10	115.49	121.46
2	B	275	LEU	CB-CA-C	-5.10	102.85	110.90
17	c	104	LYS	CA-C-N	5.10	126.21	119.84
17	c	104	LYS	C-N-CA	5.10	126.21	119.84
4	P	143	LEU	CB-CA-C	-5.09	103.71	110.79
2	B	170	ASN	N-CA-C	5.09	119.11	112.13
2	B	282	GLY	CA-C-N	5.09	126.20	119.84
2	B	282	GLY	C-N-CA	5.09	126.20	119.84
1	A	326	CYS	N-CA-C	5.09	117.74	109.24
26	m	16	GLU	CA-C-N	5.09	124.70	119.05
26	m	16	GLU	C-N-CA	5.09	124.70	119.05
7	G	34	ILE	CA-C-N	5.08	124.69	119.05
7	G	34	ILE	C-N-CA	5.08	124.69	119.05
4	P	44	ASP	N-CA-C	5.07	116.89	111.36
2	N	172	LEU	N-CA-CB	5.07	119.26	110.39
4	D	84	PRO	N-CA-CB	5.07	107.58	103.32
1	M	101	ALA	N-CA-C	5.07	116.22	108.52
13	Y	686	PRO	CA-C-N	5.06	124.85	119.28
13	Y	686	PRO	C-N-CA	5.06	124.85	119.28
2	B	126	VAL	CB-CA-C	-5.06	104.31	112.16
41	5	22	ASN	N-CA-C	5.06	117.56	109.81
1	M	23	LEU	CA-C-N	-5.06	115.74	122.72
1	M	23	LEU	C-N-CA	-5.06	115.74	122.72
3	O	26	ASN	CA-C-O	-5.06	115.58	121.15
42	6	2	THR	N-CA-C	5.06	116.09	108.46
3	C	102	LEU	N-CA-C	5.05	117.68	111.82
4	D	110	PRO	N-CA-CB	5.05	107.98	103.08
1	M	11	VAL	CA-C-O	5.05	124.41	119.71
14	Z	175	GLY	N-CA-C	-5.05	106.67	112.73
3	O	227	LYS	CA-C-O	-5.05	115.52	120.82
13	Y	85	ALA	CA-C-N	5.05	124.65	119.05
13	Y	85	ALA	C-N-CA	5.05	124.65	119.05
3	O	197	LEU	N-CA-CB	5.05	117.54	110.12
7	S	34	ILE	CB-CA-C	-5.05	109.00	114.35
3	C	325	PHE	CB-CA-C	-5.05	102.93	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	335	LEU	CA-C-O	-5.05	115.52	120.82
4	P	15	ARG	CA-C-N	5.05	125.70	120.60
4	P	15	ARG	C-N-CA	5.05	125.70	120.60
55	Aj	62	TYR	N-CA-C	5.04	116.74	109.07
3	C	329	VAL	CA-C-O	-5.04	114.48	120.78
2	N	21	PRO	N-CA-CB	5.04	108.55	103.00
1	A	328	HIS	CA-C-O	5.04	125.58	119.38
1	M	361	LEU	O-C-N	5.04	127.33	122.09
4	P	111	PRO	N-CA-CB	5.04	107.80	103.31
3	O	256	TYR	CB-CA-C	-5.04	103.25	111.06
3	O	326	TRP	CA-C-O	-5.04	115.19	120.63
44	8	35	GLN	N-CA-C	5.04	119.19	113.19
4	P	232	SER	N-CA-C	5.04	116.77	111.28
17	c	222	LYS	CA-C-N	5.04	124.95	119.76
17	c	222	LYS	C-N-CA	5.04	124.95	119.76
1	A	356	ARG	CA-C-O	5.04	125.76	120.42
10	J	51	LEU	N-CA-C	5.04	118.02	109.76
5	E	80	ASP	N-CA-C	5.03	116.76	111.28
6	F	36	THR	N-CA-C	5.03	118.52	112.38
2	N	29	LEU	CA-C-N	5.03	125.05	119.32
2	N	29	LEU	C-N-CA	5.03	125.05	119.32
6	F	44	LYS	CA-C-O	5.03	126.28	120.90
3	O	197	LEU	N-CA-C	-5.02	105.81	111.28
3	O	373	GLU	CA-C-O	5.02	126.05	120.63
47	y	2	PHE	N-CA-C	-5.02	105.70	111.07
5	Q	89	PHE	CA-C-N	-5.02	114.32	121.50
5	Q	89	PHE	C-N-CA	-5.02	114.32	121.50
1	M	420	PRO	N-CA-C	5.02	119.09	111.11
3	O	216	ASP	CA-C-N	-5.02	115.42	122.94
3	O	216	ASP	C-N-CA	-5.02	115.42	122.94
3	C	361	LEU	O-C-N	5.01	127.44	122.12
3	O	358	TYR	N-CA-C	5.01	117.13	111.11
4	D	48	TYR	CA-C-N	5.01	129.56	122.24
4	D	48	TYR	C-N-CA	5.01	129.56	122.24
7	G	15	THR	CA-C-O	-5.01	115.40	120.71
2	B	38	LEU	CB-CA-C	-5.01	104.91	111.82
48	z	12	ALA	N-CA-C	5.01	117.43	109.96
3	C	64	SER	N-CA-C	-5.01	105.71	111.07
3	O	190	MET	N-CA-CB	5.01	117.48	110.12
3	C	269	LYS	CA-C-N	5.00	125.71	120.11
3	C	269	LYS	C-N-CA	5.00	125.71	120.11
8	H	55	THR	CB-CA-C	-5.00	103.02	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	99	ILE	CB-CA-C	-5.00	103.17	110.62
14	Z	300	TRP	N-CA-C	5.00	117.48	110.23

There are no chirality outliers.

All (69) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	122	LEU	Mainchain
1	A	196	VAL	Mainchain
1	A	210	ASP	Mainchain
1	A	239	SER	Mainchain
1	A	242	CYS	Mainchain
1	A	244	ARG	Mainchain
1	A	256	ALA	Mainchain
1	A	294	LEU	Mainchain
1	A	306	SER	Mainchain
1	A	345	LEU	Mainchain
1	A	383	LEU	Mainchain
1	A	53	ASN	Mainchain
54	Ag	12	ILE	Peptide
2	B	106	ALA	Mainchain
2	B	159	VAL	Mainchain
2	B	178	CYS	Mainchain
2	B	239	TYR	Mainchain
2	B	285	VAL	Mainchain
2	B	335	ASP	Mainchain
2	B	353	SER	Mainchain
2	B	68	LEU	Mainchain
2	B	99	THR	Mainchain
3	C	134	PRO	Mainchain
3	C	164	ILE	Mainchain
3	C	20	ASP	Mainchain
3	C	21	LEU	Mainchain
3	C	222	PRO	Mainchain
3	C	235	LEU	Mainchain
3	C	318	ARG	Mainchain
3	C	322	GLN	Mainchain
3	C	326	TRP	Mainchain
3	C	335	LEU	Mainchain
3	C	355	SER	Mainchain
3	C	362	ILE	Mainchain

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Mol	Chain	Res	Type	Group
3	C	77	TRP	Mainchain
3	C	83	HIS	Mainchain
4	D	54	VAL	Mainchain
6	F	46	ALA	Mainchain
7	G	15	THR	Mainchain
7	G	73	ASN	Mainchain
9	I	69	SER	Mainchain
10	J	43	TYR	Mainchain
1	M	100	LYS	Mainchain
1	M	141	ASN	Mainchain
1	M	290	LEU	Mainchain
2	N	137	VAL	Mainchain
2	N	144	LEU	Mainchain
2	N	200	THR	Mainchain
2	N	290	ASN	Mainchain
2	N	353	SER	Mainchain
3	O	148	ASN	Mainchain
3	O	159	ASN	Mainchain
3	O	19	ILE	Mainchain
3	O	355	SER	Mainchain
3	O	55	TYR	Mainchain
3	O	77	TRP	Mainchain
4	P	24	THR	Mainchain
4	P	46	VAL	Mainchain
5	Q	125	GLU	Mainchain
5	Q	135	LEU	Mainchain
5	Q	186	GLU	Mainchain
5	Q	195	VAL	Mainchain
5	Q	97	PHE	Mainchain
7	S	17	SER	Mainchain
7	S	18	LEU	Mainchain
8	T	40	CYS	Mainchain
17	c	327	ILE	Peptide
34	w	98	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2198	0	1040	107	0
1	M	2198	0	1040	114	0
2	B	2061	0	1028	74	0
2	N	2061	0	1028	104	0
3	C	1870	0	844	114	0
3	O	1870	0	844	72	0
4	D	1188	0	533	39	0
4	P	1188	0	533	67	0
5	E	967	0	441	35	0
5	Q	966	0	440	42	0
6	F	527	0	232	21	0
6	R	527	0	232	9	0
7	G	401	0	180	24	0
7	S	386	0	174	30	0
8	H	320	0	135	7	0
8	T	320	0	135	9	0
9	I	163	0	77	8	0
9	U	163	0	77	28	0
10	J	307	0	149	13	0
10	L	307	0	149	20	0
11	K	211	0	102	9	0
11	V	182	0	90	6	0
12	W	1366	0	1316	85	0
13	Y	4998	0	4891	359	0
14	Z	3003	0	2971	172	0
15	a	1146	0	1143	88	0
16	b	1189	0	1144	49	0
17	c	3125	0	3087	198	0
18	d	1324	0	1338	84	0
19	e	2486	0	2587	129	0
20	f	2698	0	2851	123	0
21	g	829	0	863	50	0
22	h	3610	0	3816	160	0
23	i	677	0	726	45	0
24	j	4705	0	4848	205	0
25	k	1059	0	1077	66	0
25	l	73	0	31	1	0
26	m	263	0	125	1	0
27	n	411	0	177	3	0
28	o	251	0	115	4	0
29	p	1546	0	688	41	0
30	q	967	0	431	16	0
30	v	252	0	103	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	r	311	0	140	1	0
32	Aa	403	0	172	1	0
32	t	403	0	172	0	0
33	Ai	167	0	72	0	0
33	u	267	0	123	1	0
34	w	530	0	230	5	0
35	x	221	0	101	3	0
36	0	1284	0	575	1	0
37	1	716	0	321	1	0
38	2	539	0	243	0	0
39	3	481	0	224	3	0
40	4	411	0	193	3	0
41	5	371	0	161	0	0
42	6	361	0	184	0	0
43	7	274	0	127	0	0
44	8	241	0	115	1	0
45	9	231	0	106	0	0
46	s	213	0	98	8	0
47	y	2523	0	1169	6	0
48	z	1127	0	475	1	0
49	Ab	637	0	132	11	0
49	Ah	526	0	107	5	0
50	Ac	271	0	132	2	0
51	Ad	211	0	42	0	0
51	Ao	205	0	46	4	0
51	Ap	173	0	36	3	0
51	Av	193	0	40	2	0
52	Ae	435	0	195	2	0
53	Af	448	0	190	1	0
54	Ag	637	0	331	4	0
55	Aj	663	0	292	4	0
56	Ak	750	0	321	2	0
57	Al	473	0	204	3	0
58	Am	134	0	54	0	0
59	An	482	0	214	2	0
60	Aq	335	0	69	3	0
60	As	322	0	65	0	0
60	Aw	376	0	76	3	0
61	Ar	169	0	37	0	0
62	At	84	0	18	0	0
63	Au	62	0	12	0	0
64	C	86	0	60	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	O	86	0	60	9	0
65	D	43	0	32	1	0
65	P	43	0	32	2	0
66	E	4	0	0	0	0
66	Q	4	0	0	0	0
66	Y	4	0	0	0	0
66	d	4	0	0	1	0
67	Y	16	0	0	5	0
67	a	8	0	0	0	0
67	b	16	0	0	3	0
67	c	8	0	0	4	0
68	c	31	0	19	20	0
69	p	48	0	26	26	0
70	3	1	0	0	0	0
71	y	120	0	108	2	0
72	y	1	0	0	0	0
72	z	2	0	0	0	0
73	y	1	0	0	0	0
All	All	75545	0	51782	2557	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 20.

All (2557) 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)
30:q:85:LEU:CB	30:q:159:VAL:HA	1.13	1.55
1:A:84:ALA:CB	1:A:101:ALA:HB2	1.51	1.41
24:j:507:THR:HG22	46:s:11:SER:CB	1.53	1.37
30:q:85:LEU:CB	30:q:159:VAL:CA	2.02	1.36
3:C:117:VAL:N	64:C:402:HEM:HBC2	1.43	1.34
1:M:83:GLY:CA	2:N:363:LYS:HA	1.57	1.33
3:C:116:GLY:HA3	64:C:402:HEM:C3C	1.63	1.33
29:p:203:PRO:O	69:p:401:NDP:H5N	1.23	1.28
12:W:162:ALA:HB2	14:Z:286:TYR:CA	1.61	1.28
1:A:84:ALA:HB2	1:A:101:ALA:CB	1.67	1.23
3:C:73:VAL:HA	5:E:65:SER:CA	1.67	1.22
1:A:86:LEU:O	2:B:285:VAL:HA	1.35	1.21
3:C:73:VAL:HA	5:E:65:SER:CB	1.69	1.21
18:d:63:ILE:O	18:d:67:VAL:HG23	1.40	1.19
24:j:507:THR:CG2	46:s:11:SER:CB	2.22	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:119:GLU:CB	17:c:162:PHE:HZ	1.57	1.17
5:E:160:CYS:HA	3:O:266:PRO:CA	1.76	1.16
13:Y:472:PRO:HG3	13:Y:500:ILE:HG21	1.28	1.14
4:P:234:LYS:O	7:S:15:THR:HA	1.43	1.14
29:p:207:PHE:H	29:p:241:TYR:HA	1.00	1.13
1:A:86:LEU:N	2:B:284:HIS:O	1.81	1.12
3:C:117:VAL:N	64:C:402:HEM:CBC	2.11	1.11
1:M:83:GLY:HA3	2:N:363:LYS:HA	1.28	1.11
49:Ab:121:UNK:HA	60:Aq:43:UNK:CB	1.81	1.10
12:W:162:ALA:CB	14:Z:286:TYR:HA	1.81	1.10
3:C:73:VAL:HA	5:E:65:SER:HA	1.29	1.08
24:j:503:GLU:OE1	46:s:13:LYS:HA	1.50	1.08
5:E:160:CYS:HA	3:O:266:PRO:HA	1.17	1.08
13:Y:403:VAL:HG13	13:Y:432:ILE:O	1.53	1.07
4:P:234:LYS:O	7:S:15:THR:CA	2.01	1.07
17:c:119:GLU:CB	17:c:162:PHE:CZ	2.38	1.07
3:C:116:GLY:CA	64:C:402:HEM:C3C	2.37	1.06
3:C:116:GLY:O	64:C:402:HEM:CMC	2.03	1.06
5:E:159:PRO:O	3:O:266:PRO:CB	2.04	1.05
3:C:74:ASN:CB	5:E:64:ALA:O	2.04	1.05
17:c:120:GLY:HA3	17:c:204:TYR:HD1	1.16	1.05
17:c:120:GLY:HA3	17:c:204:TYR:CD1	1.91	1.03
5:Q:75:GLU:O	5:Q:194:ILE:HA	1.57	1.03
1:M:83:GLY:HA2	2:N:363:LYS:HA	1.36	1.03
13:Y:405:THR:HA	13:Y:686:PRO:HB3	1.41	1.03
29:p:209:ARG:CB	29:p:352:VAL:HA	1.89	1.02
3:C:116:GLY:O	64:C:402:HEM:HMC2	1.57	1.02
11:K:20:THR:HA	10:L:18:SER:CB	1.89	1.02
2:B:165:ALA:HA	2:B:173:ALA:HB1	1.39	1.01
29:p:207:PHE:N	29:p:241:TYR:HA	1.75	1.01
1:A:84:ALA:HB1	1:A:100:LYS:O	1.59	1.01
13:Y:407:PRO:CG	13:Y:438:LEU:HD21	1.91	1.00
3:C:34:GLY:C	64:C:402:HEM:HMA1	1.87	0.99
1:M:225:GLU:CB	49:Ah:14:UNK:HA	1.91	0.99
13:Y:370:GLU:OE1	13:Y:482:GLN:NE2	1.96	0.99
15:a:123:MET:HB2	15:a:144:MET:HE1	1.44	0.98
17:c:118:ASP:CB	68:c:502:FMN:HM73	1.92	0.98
11:K:18:VAL:O	11:K:22:SER:N	1.95	0.98
1:A:7:ALA:HB1	2:B:41:TYR:O	1.61	0.98
1:A:157:ALA:O	1:A:236:PHE:HA	1.64	0.98
3:C:116:GLY:C	64:C:402:HEM:HBC2	1.88	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:ASN:H	5:E:65:SER:HA	1.29	0.97
4:P:139:THR:CB	8:T:41:ASP:HA	1.95	0.97
65:P:301:HEC:HHD	65:P:301:HEC:HBC2	1.45	0.96
5:Q:25:SER:O	5:Q:29:SER:CB	2.13	0.96
2:N:308:ASP:CB	9:U:54:SER:O	2.14	0.95
1:M:86:LEU:N	2:N:284:HIS:O	1.98	0.95
17:c:125:CYS:HB3	18:d:181:VAL:HG23	1.49	0.95
30:q:88:PHE:CB	30:q:162:GLU:N	2.31	0.94
13:Y:405:THR:OG1	13:Y:479:SER:HB3	1.68	0.94
3:C:73:VAL:CA	5:E:65:SER:HA	1.97	0.94
5:E:160:CYS:CA	3:O:266:PRO:HA	1.97	0.93
14:Z:182:ASN:HD22	14:Z:403:PRO:HB2	1.32	0.93
2:N:313:ASN:N	9:U:58:GLN:O	2.02	0.93
29:p:205:ASP:HA	69:p:401:NDP:H41N	1.48	0.93
3:C:34:GLY:C	64:C:402:HEM:CMA	2.42	0.93
7:S:45:ILE:O	7:S:49:ALA:HB2	1.68	0.93
3:C:74:ASN:N	5:E:65:SER:HA	1.84	0.93
2:B:308:ASP:CB	9:I:54:SER:CB	2.48	0.92
3:C:117:VAL:CA	64:C:402:HEM:HBC2	1.99	0.92
11:V:17:TRP:O	11:V:21:ALA:N	2.02	0.92
13:Y:560:LEU:HD11	13:Y:566:ILE:HD11	1.52	0.92
4:P:234:LYS:N	7:S:16:TYR:O	2.02	0.91
29:p:207:PHE:H	29:p:241:TYR:CA	1.83	0.91
3:O:74:ASN:O	5:Q:61:SER:HA	1.70	0.91
13:Y:485:ASP:O	13:Y:489:ILE:CD1	2.19	0.91
2:N:310:SER:CB	9:U:55:LEU:O	2.19	0.90
10:L:50:LYS:O	4:P:23:HIS:N	2.05	0.90
29:p:130:VAL:HA	69:p:401:NDP:H8A	1.52	0.90
13:Y:472:PRO:CG	13:Y:500:ILE:HG21	2.02	0.90
5:E:93:GLY:HA3	3:O:169:SER:CB	2.01	0.90
4:P:234:LYS:O	7:S:16:TYR:N	2.04	0.89
3:C:116:GLY:HA3	64:C:402:HEM:CAC	2.01	0.89
19:e:41:GLY:HA3	19:e:44:GLY:H	1.37	0.89
1:A:7:ALA:CB	2:B:41:TYR:O	2.21	0.89
1:M:238:GLY:O	7:S:19:SER:CB	2.21	0.89
13:Y:479:SER:OG	13:Y:687:PRO:HD3	1.72	0.88
17:c:244:ASN:N	68:c:502:FMN:O2P	2.06	0.88
29:p:203:PRO:O	69:p:401:NDP:C5N	2.17	0.87
5:E:81:ILE:CB	5:E:87:MET:CB	2.52	0.87
13:Y:652:ASN:HB2	13:Y:655:ARG:HH21	1.39	0.87
13:Y:407:PRO:HD2	13:Y:438:LEU:HD11	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:140:ARG:HH12	14:Z:399:ALA:HB3	1.38	0.86
5:E:68:VAL:O	5:E:72:SER:N	2.08	0.86
1:M:86:LEU:O	2:N:285:VAL:HA	1.76	0.86
2:B:263:ALA:O	2:B:269:ALA:HB2	1.76	0.86
13:Y:472:PRO:HG3	13:Y:500:ILE:CG2	2.06	0.86
2:N:306:PRO:CB	9:U:50:LEU:O	2.24	0.85
2:N:313:ASN:N	9:U:59:ALA:HB2	1.90	0.85
9:U:70:LEU:O	9:U:73:PRO:O	1.94	0.85
24:j:503:GLU:OE1	46:s:13:LYS:CA	2.24	0.85
10:L:50:LYS:CB	4:P:22:ASP:HA	2.07	0.85
30:q:88:PHE:CB	30:q:162:GLU:CB	2.54	0.85
2:N:263:ALA:O	2:N:269:ALA:HB2	1.77	0.85
1:A:84:ALA:HB2	1:A:101:ALA:HB2	0.86	0.85
13:Y:489:ILE:H	13:Y:489:ILE:HD12	1.42	0.84
29:p:205:ASP:HA	69:p:401:NDP:C4N	2.06	0.84
24:j:226:GLN:NE2	24:j:314:MET:SD	2.51	0.84
13:Y:400:ILE:HG22	13:Y:402:LEU:CD1	2.06	0.84
19:e:60:PRO:HD3	21:g:25:PRO:HG2	1.58	0.84
3:O:72:ASP:O	5:Q:66:ALA:N	2.09	0.84
13:Y:124:HIS:NE2	67:Y:801:SF4:S1	2.49	0.84
12:W:162:ALA:HB2	14:Z:286:TYR:HA	0.84	0.84
1:M:383:LEU:HA	1:M:387:GLY:O	1.79	0.83
17:c:297:LYS:HG2	17:c:332:CYS:HB3	1.59	0.83
24:j:27:TYR:O	24:j:115:ASN:ND2	2.11	0.83
3:C:73:VAL:CA	5:E:65:SER:CB	2.54	0.83
3:C:213:SER:O	3:C:216:ASP:N	2.10	0.83
1:M:4:TYR:HA	2:N:113:ARG:CB	2.09	0.83
4:P:236:ALA:O	7:S:14:ILE:N	2.10	0.82
22:h:418:LYS:NZ	22:h:419:TYR:O	2.12	0.82
7:G:72:LYS:CB	7:G:75:ALA:HB2	2.09	0.82
3:C:266:PRO:CB	5:Q:160:CYS:HA	2.10	0.82
4:D:115:TYR:O	4:D:119:ALA:N	2.11	0.82
13:Y:643:ARG:NH1	13:Y:656:TYR:OH	2.12	0.82
30:q:88:PHE:CB	30:q:162:GLU:H	1.92	0.82
1:A:84:ALA:HB1	1:A:101:ALA:HB2	1.61	0.82
64:O:401:HEM:HBC2	64:O:401:HEM:HMC1	1.61	0.82
24:j:305:SER:OG	24:j:336:LYS:NZ	2.13	0.81
29:p:130:VAL:CA	69:p:401:NDP:H8A	2.10	0.81
1:A:84:ALA:CB	1:A:100:LYS:O	2.29	0.81
3:C:169:SER:CB	5:Q:93:GLY:HA3	2.10	0.81
29:p:205:ASP:HA	69:p:401:NDP:H71N	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:317:PHE:HA	6:F:25:GLY:H	1.46	0.80
12:W:168:ARG:HH11	12:W:185:ARG:HG3	1.45	0.80
13:Y:403:VAL:CG1	13:Y:432:ILE:O	2.29	0.80
13:Y:408:ARG:HB3	13:Y:415:ASN:ND2	1.96	0.80
11:V:33:VAL:O	11:V:37:ASP:N	2.14	0.80
12:W:162:ALA:HB2	14:Z:286:TYR:C	2.08	0.79
24:j:145:GLU:OE2	24:j:176:ARG:NH2	2.15	0.79
5:Q:10:PHE:O	5:Q:14:ARG:N	2.15	0.79
2:B:98:VAL:N	9:I:69:SER:O	2.16	0.79
20:f:25:HIS:CD2	20:f:84:TRP:HB3	2.18	0.79
5:Q:10:PHE:O	5:Q:14:ARG:CB	2.31	0.79
29:p:206:ILE:N	69:p:401:NDP:H71N	1.80	0.79
15:a:162:TYR:HD1	16:b:153:ILE:HG21	1.47	0.79
13:Y:598:ASN:N	13:Y:602:ARG:O	2.15	0.78
4:P:233:ARG:HA	7:S:16:TYR:O	1.82	0.78
12:W:115:THR:HG22	14:Z:423:LYS:HG2	1.65	0.78
23:i:37:MET:HE3	25:k:60:TYR:HE1	1.45	0.78
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.63	0.78
4:P:236:ALA:N	7:S:14:ILE:O	2.16	0.78
2:B:97:SER:HA	9:I:70:LEU:HA	1.64	0.77
12:W:168:ARG:NH1	12:W:185:ARG:HE	1.80	0.77
1:M:83:GLY:HA3	2:N:363:LYS:CA	2.13	0.77
16:b:135:ARG:HG3	16:b:137:ASP:H	1.49	0.77
14:Z:208:GLU:OE1	15:a:103:ARG:NH2	2.17	0.77
68:c:502:FMN:O4'	68:c:502:FMN:H9	1.85	0.77
50:Ac:51:ASP:O	50:Ac:53:ARG:N	2.18	0.77
13:Y:301:ARG:HE	13:Y:613:PRO:HG3	1.48	0.77
19:e:109:SER:OG	19:e:192:GLU:OE2	2.02	0.77
13:Y:217:GLU:OE2	13:Y:412:PRO:HG3	1.84	0.77
20:f:95:MET:HE2	20:f:149:ILE:HA	1.65	0.77
14:Z:358:VAL:HG12	14:Z:360:ASP:H	1.50	0.76
17:c:378:SER:O	17:c:380:GLY:N	2.18	0.76
22:h:16:TRP:HA	22:h:93:LYS:HD3	1.67	0.76
12:W:162:ALA:CB	14:Z:286:TYR:CA	2.53	0.76
13:Y:405:THR:HG23	13:Y:686:PRO:CB	2.16	0.76
14:Z:211:PHE:CE2	15:a:98:HIS:HE1	2.03	0.76
1:A:157:ALA:O	1:A:236:PHE:CA	2.33	0.76
6:F:103:GLU:O	6:F:106:GLU:N	2.18	0.76
2:N:97:SER:CB	9:U:70:LEU:CB	2.64	0.76
13:Y:305:PRO:HG2	13:Y:319:TRP:HA	1.66	0.76
29:p:60:GLY:O	69:p:401:NDP:H4B	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:139:THR:CB	8:T:41:ASP:CA	2.64	0.76
12:W:162:ALA:CB	14:Z:286:TYR:C	2.59	0.76
13:Y:374:THR:HG21	13:Y:532:PRO:HA	1.67	0.76
1:A:27:SER:HA	1:A:199:ALA:O	1.86	0.75
14:Z:141:TYR:CG	15:a:91:CYS:HB3	2.21	0.75
13:Y:400:ILE:HG22	13:Y:402:LEU:HD12	1.67	0.75
18:d:92:TRP:NE1	18:d:124:ARG:O	2.19	0.75
13:Y:407:PRO:CD	13:Y:438:LEU:HD21	2.16	0.75
14:Z:211:PHE:HE2	15:a:98:HIS:HE1	1.33	0.75
20:f:112:HIS:HB2	20:f:184:ILE:HD11	1.67	0.75
22:h:204:MET:HG2	22:h:298:ILE:HD11	1.66	0.75
13:Y:181:ARG:HD3	13:Y:225:ILE:HG12	1.67	0.75
3:C:34:GLY:CA	64:C:402:HEM:CMA	2.65	0.75
13:Y:405:THR:HG1	13:Y:479:SER:HB3	1.49	0.75
20:f:172:GLN:HG2	20:f:177:LYS:HD2	1.67	0.75
29:p:210:GLU:O	29:p:211:ASP:O	2.05	0.75
22:h:405:LEU:HD11	24:j:173:LEU:HD13	1.69	0.74
24:j:361:GLY:H	24:j:435:PRO:HA	1.50	0.74
1:A:383:LEU:HA	1:A:387:GLY:O	1.88	0.74
13:Y:36:VAL:O	13:Y:38:GLY:N	2.21	0.74
14:Z:311:TYR:HA	14:Z:314:VAL:HG22	1.68	0.74
14:Z:136:PHE:HE2	14:Z:151:TYR:CD1	2.06	0.74
12:W:209:GLU:OE2	15:a:175:ARG:NH1	2.21	0.74
17:c:149:MET:HE3	17:c:241:THR:HG21	1.69	0.74
3:C:106:SER:CB	64:C:402:HEM:HBD2	2.17	0.74
5:Q:188:THR:N	5:Q:192:MET:O	2.21	0.74
17:c:423:THR:OG1	67:c:501:SF4:S3	2.46	0.74
13:Y:76:ARG:NE	17:c:422:HIS:O	2.20	0.73
13:Y:277:MET:HA	13:Y:284:GLU:H	1.53	0.73
13:Y:615:LEU:O	13:Y:617:ARG:NH1	2.21	0.73
17:c:296:LEU:HB3	17:c:332:CYS:HB2	1.69	0.73
22:h:59:ASP:HB3	22:h:245:ARG:HH22	1.52	0.73
19:e:149:ILE:HD11	19:e:185:TRP:HE3	1.53	0.73
1:A:292:SER:O	1:A:295:ALA:HB3	1.88	0.73
2:B:140:LEU:O	2:B:141:GLN:C	2.29	0.73
1:M:207:GLN:O	1:M:211:LEU:N	2.19	0.73
13:Y:160:VAL:H	13:Y:174:THR:HG22	1.52	0.73
18:d:63:ILE:O	18:d:67:VAL:CG2	2.29	0.73
3:C:26:ASN:CB	6:F:69:SER:CB	2.66	0.73
13:Y:140:GLN:NE2	67:Y:801:SF4:S3	2.61	0.73
11:K:18:VAL:O	11:K:22:SER:CB	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:74:ASN:O	5:Q:61:SER:CA	2.37	0.73
6:R:96:GLU:O	6:R:97:VAL:C	2.32	0.73
13:Y:611:THR:HG21	34:w:105:GLU:HA	1.70	0.73
29:p:130:VAL:CB	69:p:401:NDP:C8A	2.67	0.73
5:E:84:GLY:HA2	5:E:100:HIS:O	1.89	0.73
15:a:115:ALA:O	15:a:116:SER:OG	2.03	0.73
17:c:112:TYR:HB2	17:c:240:THR:HG22	1.71	0.73
17:c:120:GLY:CA	17:c:204:TYR:CD1	2.71	0.72
1:M:225:GLU:CB	49:Ah:13:UNK:O	2.37	0.72
20:f:12:THR:HG21	25:k:163:ILE:HD13	1.71	0.72
3:C:34:GLY:HA3	64:C:402:HEM:C3A	2.24	0.72
4:P:237:TYR:HA	7:S:12:HIS:O	1.89	0.72
2:N:313:ASN:O	9:U:59:ALA:HA	1.89	0.72
2:N:313:ASN:CB	9:U:59:ALA:HB1	2.19	0.72
3:O:61:THR:O	3:O:62:ALA:C	2.29	0.72
3:O:254:ASP:O	4:P:119:ALA:O	2.07	0.72
22:h:23:ILE:HA	22:h:26:ASN:HD22	1.55	0.72
13:Y:466:LEU:HD11	13:Y:500:ILE:HD11	1.72	0.72
4:P:234:LYS:O	7:S:15:THR:C	2.32	0.72
12:W:68:ILE:HG22	12:W:69:LEU:HG	1.72	0.72
1:M:256:ALA:HA	1:M:320:LEU:O	1.89	0.72
13:Y:407:PRO:HG2	13:Y:438:LEU:HD21	1.70	0.72
13:Y:645:ARG:NH2	13:Y:648:GLU:OE2	2.23	0.72
2:N:165:ALA:HA	2:N:173:ALA:HB1	1.72	0.71
49:Ab:47:UNK:O	49:Ab:51:UNK:N	2.23	0.71
1:A:286:GLY:O	1:A:287:GLY:C	2.33	0.71
24:j:483:PRO:HD2	24:j:486:MET:HB2	1.71	0.71
4:D:51:LEU:HA	4:D:56:TYR:O	1.91	0.71
10:J:49:GLY:HA2	10:J:54:HIS:CB	2.20	0.71
24:j:267:MET:O	24:j:274:GLN:NE2	2.23	0.71
29:p:206:ILE:H	69:p:401:NDP:H71N	1.36	0.71
1:A:245:GLU:HA	7:G:11:ARG:HA	1.72	0.71
3:C:73:VAL:C	5:E:65:SER:HA	2.16	0.71
13:Y:221:ASN:ND2	13:Y:286:ILE:O	2.21	0.71
19:e:24:GLU:HG3	19:e:271:LEU:HD22	1.71	0.71
1:A:86:LEU:O	2:B:285:VAL:CA	2.29	0.71
3:C:116:GLY:HA3	64:C:402:HEM:C4C	2.25	0.71
13:Y:259:SER:HB2	13:Y:282:ASN:HB3	1.70	0.71
17:c:378:SER:OG	67:c:501:SF4:S4	2.48	0.71
17:c:118:ASP:CB	68:c:502:FMN:C7M	2.68	0.71
24:j:302:VAL:O	24:j:305:SER:OG	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:140:ARG:HH12	14:Z:399:ALA:CB	2.03	0.71
22:h:290:SER:HA	22:h:319:HIS:HE2	1.54	0.71
18:d:153:GLN:HE21	18:d:159:LYS:HE3	1.55	0.71
57:Al:20:ALA:O	57:Al:22:SER:N	2.21	0.71
1:M:239:SER:CB	7:S:17:SER:O	2.39	0.70
4:P:240:PRO:O	4:P:241:LYS:C	2.32	0.70
13:Y:489:ILE:HD12	13:Y:489:ILE:N	2.05	0.70
13:Y:697:THR:O	13:Y:702:ARG:NH1	2.17	0.70
19:e:145:THR:HG23	19:e:297:THR:HG21	1.72	0.70
18:d:163:THR:HG22	18:d:170:THR:HG22	1.72	0.70
20:f:241:THR:OG1	20:f:300:SER:OG	2.08	0.70
3:C:117:VAL:H	64:C:402:HEM:CBC	2.04	0.70
12:W:93:VAL:HG11	12:W:153:ILE:HD11	1.74	0.70
3:C:35:SER:N	64:C:402:HEM:HMA2	2.06	0.70
17:c:214:GLU:OE2	17:c:224:ARG:NH1	2.24	0.70
13:Y:265:THR:HG22	13:Y:270:VAL:HA	1.74	0.70
23:i:23:ARG:NH2	25:k:23:LYS:O	2.25	0.70
2:N:313:ASN:CB	9:U:59:ALA:CB	2.70	0.70
7:S:45:ILE:O	7:S:49:ALA:CB	2.38	0.70
22:h:208:PRO:HD3	22:h:236:LEU:HD22	1.73	0.70
24:j:270:ASN:OD1	24:j:271:LYS:N	2.25	0.70
30:q:89:PRO:O	30:q:90:GLU:CB	2.38	0.70
12:W:111:LEU:HG	12:W:160:TYR:CB	2.21	0.69
13:Y:287:SER:HB3	13:Y:290:THR:HG22	1.73	0.69
49:Ab:119:UNK:O	60:Aq:43:UNK:O	2.09	0.69
15:a:99:MET:HG2	15:a:106:MET:HB3	1.72	0.69
54:Ag:134:GLN:O	54:Ag:136:PHE:N	2.25	0.69
13:Y:490:LEU:HD23	13:Y:490:LEU:O	1.91	0.69
10:J:36:ASP:O	10:J:37:GLN:C	2.35	0.69
18:d:133:GLN:HB2	18:d:174:VAL:HG21	1.74	0.69
4:D:102:ARG:HA	4:D:108:ALA:O	1.91	0.69
1:A:85:HIS:HA	2:B:284:HIS:CB	2.22	0.69
21:g:56:PHE:HE1	25:k:70:TYR:HB3	1.57	0.69
24:j:503:GLU:HB3	46:s:13:LYS:CB	2.22	0.69
29:p:205:ASP:CA	69:p:401:NDP:H41N	2.21	0.69
1:M:285:GLY:H	9:U:71:ASN:HA	1.56	0.69
13:Y:63:PHE:O	13:Y:181:ARG:NH2	2.26	0.69
13:Y:356:ASP:OD1	13:Y:645:ARG:NH1	2.26	0.69
1:M:4:TYR:CA	2:N:113:ARG:CB	2.71	0.69
13:Y:228:VAL:HG23	13:Y:230:ALA:H	1.57	0.69
19:e:156:MET:HE1	19:e:177:THR:HG21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:25:SER:O	5:Q:29:SER:N	2.24	0.68
4:P:102:ARG:HA	4:P:108:ALA:O	1.92	0.68
22:h:376:ILE:HD11	24:j:69:MET:HE1	1.74	0.68
1:M:157:ALA:HA	1:M:237:THR:O	1.92	0.68
3:C:72:ASP:O	5:E:65:SER:C	2.37	0.68
23:i:59:MET:HG3	23:i:60:PRO:N	2.08	0.68
2:B:348:ALA:HB1	2:B:415:LYS:HA	1.76	0.68
17:c:127:ASP:HA	17:c:130:ILE:HD12	1.76	0.68
17:c:382:CYS:SG	17:c:423:THR:OG1	2.52	0.68
24:j:26:ILE:HD11	24:j:31:LEU:HD22	1.76	0.68
24:j:355:ASP:OD2	24:j:357:ARG:NH1	2.26	0.68
55:Aj:77:CYS:CB	55:Aj:84:CYS:CB	2.70	0.68
1:A:426:GLY:HA2	1:A:428:ILE:N	2.08	0.68
1:A:426:GLY:HA2	1:A:427:PRO:C	2.19	0.68
11:V:17:TRP:O	11:V:21:ALA:CB	2.41	0.68
3:C:116:GLY:C	64:C:402:HEM:CBC	2.60	0.68
2:N:140:LEU:O	2:N:141:GLN:C	2.35	0.68
2:N:310:SER:CB	9:U:57:GLY:HA3	2.24	0.68
20:f:72:MET:HE3	20:f:76:ILE:HD11	1.76	0.68
22:h:336:ARG:NH1	22:h:433:GLU:OE1	2.27	0.68
1:A:239:SER:CB	7:G:17:SER:O	2.42	0.68
3:C:34:GLY:CA	64:C:402:HEM:C3A	2.77	0.68
10:L:35:PHE:O	10:L:36:ASP:C	2.37	0.68
13:Y:309:ASN:OD1	13:Y:313:LEU:N	2.27	0.68
13:Y:391:ILE:N	13:Y:600:GLU:OE2	2.23	0.68
19:e:298:LEU:HD21	21:g:98:LEU:HD22	1.75	0.68
25:k:76:THR:HG23	25:k:77:GLU:H	1.58	0.68
13:Y:404:GLY:O	13:Y:686:PRO:HD3	1.94	0.67
15:a:108:ARG:NH1	16:b:86:TYR:O	2.27	0.67
17:c:296:LEU:N	17:c:332:CYS:SG	2.67	0.67
14:Z:135:TYR:CZ	15:a:162:TYR:HE2	2.11	0.67
69:p:401:NDP:O2X	69:p:401:NDP:H1B	1.94	0.67
16:b:76:TYR:HD1	19:e:33:LEU:HD11	1.59	0.67
4:D:116:ILE:HA	4:D:119:ALA:HB3	1.76	0.67
13:Y:97:MET:HG3	13:Y:98:LYS:HG2	1.76	0.67
21:g:46:SER:HB3	25:k:78:MET:HE2	1.77	0.67
21:g:71:LEU:O	25:k:147:TYR:OH	2.13	0.67
1:A:342:TRP:O	1:A:343:MET:C	2.38	0.67
12:W:218:ARG:HD2	53:Af:101:THR:HA	1.75	0.67
13:Y:466:LEU:HD21	13:Y:496:ILE:CG2	2.25	0.67
10:J:34:ALA:O	10:J:35:PHE:C	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:400:ILE:CG2	13:Y:402:LEU:CD1	2.73	0.67
17:c:120:GLY:C	17:c:204:TYR:CE1	2.72	0.67
17:c:224:ARG:NH2	17:c:233:VAL:O	2.28	0.67
24:j:535:ARG:NH1	49:Ab:73:UNK:O	2.28	0.67
13:Y:173:MET:O	13:Y:175:ARG:N	2.26	0.67
20:f:5:ILE:HD11	25:k:166:VAL:HG13	1.77	0.67
3:C:109:PHE:O	3:C:110:LEU:C	2.37	0.67
2:N:101:THR:N	2:N:104:ASN:O	2.25	0.67
24:j:507:THR:HG21	46:s:11:SER:CB	2.25	0.67
49:Ab:128:UNK:O	49:Ab:132:UNK:N	2.27	0.67
13:Y:597:VAL:HA	13:Y:603:ALA:HA	1.76	0.66
14:Z:300:TRP:CH2	14:Z:305:THR:HG21	2.30	0.66
15:a:100:ALA:HB2	15:a:113:PHE:HE2	1.60	0.66
17:c:118:ASP:O	68:c:502:FMN:C7M	2.42	0.66
1:M:27:SER:HA	1:M:199:ALA:O	1.94	0.66
14:Z:266:ARG:O	14:Z:270:ASN:ND2	2.28	0.66
17:c:378:SER:OG	17:c:385:CYS:SG	2.53	0.66
3:C:74:ASN:O	5:E:61:SER:HA	1.95	0.66
14:Z:205:GLU:OE2	14:Z:209:LYS:NZ	2.28	0.66
20:f:106:LEU:HD21	20:f:139:LEU:HD21	1.77	0.66
13:Y:394:VAL:HG22	13:Y:473:MET:HE1	1.77	0.66
1:A:198:ALA:O	1:A:199:ALA:HB2	1.95	0.66
1:A:351:GLU:HA	1:A:404:ALA:HB2	1.77	0.66
3:C:116:GLY:CA	64:C:402:HEM:C2C	2.78	0.66
19:e:134:ARG:NH1	19:e:206:GLU:OE2	2.27	0.66
18:d:133:GLN:HE21	18:d:187:GLN:HE21	1.41	0.66
19:e:228:TYR:HA	19:e:231:ILE:HG22	1.77	0.66
29:p:209:ARG:HA	29:p:352:VAL:CB	2.24	0.66
13:Y:543:LYS:N	13:Y:563:ASP:OD2	2.26	0.66
13:Y:650:SER:OG	13:Y:652:ASN:OD1	2.13	0.66
17:c:418:GLN:O	17:c:422:HIS:ND1	2.29	0.66
19:e:138:GLN:NE2	19:e:194:ASN:OD1	2.27	0.66
3:C:34:GLY:C	64:C:402:HEM:HMA2	2.21	0.66
1:M:207:GLN:O	1:M:211:LEU:CB	2.43	0.66
3:O:156:ILE:O	3:O:157:GLY:C	2.39	0.66
15:a:202:ARG:O	15:a:206:ARG:NH2	2.28	0.66
22:h:6:ILE:O	22:h:9:THR:OG1	2.13	0.66
5:E:160:CYS:HA	3:O:266:PRO:CB	2.26	0.66
1:M:371:GLY:HA2	2:N:373:GLU:O	1.94	0.66
13:Y:281:ILE:O	13:Y:417:ARG:NH1	2.29	0.66
1:M:83:GLY:HA2	2:N:363:LYS:CA	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:57:PRO:HA	18:d:60:TYR:HD2	1.61	0.66
51:Ap:3:UNK:O	51:Ap:5:UNK:N	2.29	0.66
1:A:251:ALA:O	1:A:325:VAL:HA	1.95	0.65
24:j:505:ASN:O	24:j:508:THR:OG1	2.10	0.65
5:Q:117:LEU:O	5:Q:118:ARG:C	2.39	0.65
22:h:170:THR:HG23	22:h:171:THR:HG23	1.78	0.65
23:i:41:PHE:CE1	23:i:60:PRO:HB2	2.31	0.65
51:Ao:9:UNK:O	51:Ao:11:UNK:N	2.29	0.65
13:Y:365:SER:HG	13:Y:367:CYS:HG	1.40	0.65
14:Z:372:LYS:NZ	16:b:163:PRO:O	2.29	0.65
14:Z:305:THR:HG22	14:Z:306:GLN:HG3	1.76	0.65
24:j:409:LEU:O	24:j:412:THR:OG1	2.14	0.65
13:Y:36:VAL:HG11	13:Y:56:VAL:HG11	1.79	0.65
16:b:101:HIS:ND1	16:b:149:MET:HE1	2.12	0.65
16:b:116:CYS:N	67:b:301:SF4:S4	2.70	0.65
17:c:229:PHE:O	17:c:233:VAL:N	2.29	0.65
18:d:129:LYS:HB3	18:d:168:LEU:HG	1.78	0.65
24:j:70:THR:HA	24:j:75:GLU:HG3	1.79	0.65
13:Y:149:ASP:HB2	14:Z:361:ALA:HB3	1.78	0.65
13:Y:210:ILE:HG22	13:Y:212:LYS:H	1.62	0.65
21:g:68:GLU:HG2	21:g:98:LEU:HD12	1.79	0.65
22:h:112:ALA:CB	22:h:113:THR:HA	2.26	0.65
12:W:83:GLU:OE1	12:W:142:ARG:NH1	2.29	0.65
14:Z:427:PRO:O	14:Z:431:HIS:ND1	2.30	0.65
17:c:312:ASP:HA	17:c:315:LEU:HD12	1.78	0.65
18:d:131:HIS:H	18:d:189:ASN:HD21	1.44	0.65
13:Y:275:PRO:HB3	13:Y:286:ILE:HB	1.79	0.65
1:M:6:GLN:O	1:M:7:ALA:C	2.39	0.65
13:Y:472:PRO:CG	13:Y:500:ILE:HD13	2.27	0.65
3:C:156:ILE:O	3:C:157:GLY:C	2.39	0.65
4:D:138:PRO:O	4:D:139:THR:C	2.40	0.65
13:Y:63:PHE:HB2	13:Y:75:CYS:SG	2.36	0.65
13:Y:372:PHE:CD1	13:Y:481:LEU:HD13	2.32	0.65
13:Y:421:SER:O	13:Y:425:ASN:N	2.28	0.65
18:d:182:ASN:OD1	18:d:183:ALA:N	2.28	0.65
4:P:51:LEU:HA	4:P:56:TYR:O	1.97	0.64
13:Y:368:THR:N	13:Y:533:GLY:O	2.30	0.64
17:c:118:ASP:C	68:c:502:FMN:HM73	2.22	0.64
1:A:224:ASP:O	1:A:227:ALA:N	2.31	0.64
1:M:15:GLN:O	1:M:26:ALA:HA	1.98	0.64
24:j:503:GLU:CB	46:s:13:LYS:CB	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ab:120:UNK:O	49:Ab:122:UNK:N	2.31	0.64
17:c:176:ALA:HA	17:c:181:LEU:HD12	1.79	0.64
18:d:78:ALA:HB3	18:d:105:LEU:HD21	1.79	0.64
29:p:206:ILE:N	69:p:401:NDP:N7N	2.45	0.64
3:C:72:ASP:CB	5:E:66:ALA:HB2	2.27	0.64
24:j:106:TRP:HB2	24:j:449:LEU:HD11	1.79	0.64
13:Y:68:ARG:CZ	13:Y:283:GLU:HB2	2.27	0.64
15:a:155:SER:N	15:a:185:GLY:O	2.31	0.64
15:a:161:GLY:HA2	16:b:151:LYS:HA	1.79	0.64
19:e:160:TYR:OH	21:g:73:LEU:O	2.15	0.64
1:M:225:GLU:HA	49:Ah:13:UNK:O	1.98	0.64
13:Y:401:LEU:HD23	13:Y:474:VAL:HG13	1.78	0.64
4:D:27:ARG:O	4:D:28:ARG:C	2.41	0.64
2:N:312:PHE:HA	9:U:58:GLN:O	1.98	0.64
4:P:234:LYS:H	7:S:16:TYR:C	2.05	0.64
22:h:336:ARG:HH12	22:h:429:SER:HA	1.63	0.64
29:p:205:ASP:CA	69:p:401:NDP:H71N	2.11	0.64
12:W:148:ASP:HB2	12:W:151:THR:HG22	1.79	0.64
19:e:6:ILE:HG21	21:g:9:THR:HG21	1.78	0.64
1:A:338:LEU:O	1:A:339:GLN:C	2.41	0.64
1:M:426:GLY:CA	1:M:428:ILE:N	2.61	0.64
13:Y:149:ASP:HB3	14:Z:362:LYS:HE3	1.80	0.64
13:Y:262:VAL:HG23	13:Y:276:ARG:HB2	1.80	0.64
22:h:94:LEU:O	22:h:97:THR:OG1	2.16	0.64
13:Y:37:ASP:OD1	13:Y:38:GLY:N	2.30	0.63
13:Y:405:THR:CA	13:Y:686:PRO:HB3	2.25	0.63
13:Y:464:GLN:HA	13:Y:467:LYS:HD3	1.80	0.63
13:Y:595:THR:OG1	13:Y:603:ALA:O	2.15	0.63
15:a:89:LEU:HD21	15:a:133:MET:HE2	1.79	0.63
24:j:73:THR:HG21	24:j:194:ASN:HD21	1.64	0.63
5:E:159:PRO:C	3:O:266:PRO:CB	2.70	0.63
13:Y:372:PHE:CD1	13:Y:481:LEU:CD1	2.82	0.63
19:e:199:ASP:OD2	19:e:279:ARG:NH2	2.28	0.63
22:h:403:THR:HA	22:h:406:TYR:CE2	2.34	0.63
24:j:128:MET:HE1	24:j:255:ALA:HB2	1.80	0.63
1:M:279:HIS:HA	1:M:307:PHE:O	1.97	0.63
2:N:255:ALA:HB2	2:N:426:ALA:HB2	1.81	0.63
13:Y:489:ILE:CD1	13:Y:489:ILE:H	2.11	0.63
17:c:51:TRP:HB3	17:c:133:HIS:HA	1.80	0.63
1:A:6:GLN:O	1:A:7:ALA:C	2.41	0.63
12:W:162:ALA:CB	14:Z:286:TYR:O	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:106:LEU:O	20:f:135:LYS:NZ	2.30	0.63
22:h:225:ILE:HB	22:h:331:ASN:HD22	1.63	0.63
22:h:407:SER:O	22:h:410:MET:HG2	1.99	0.63
27:n:44:LEU:O	27:n:48:ASN:N	2.31	0.63
13:Y:179:CYS:SG	13:Y:227:PRO:HG3	2.39	0.63
13:Y:341:ILE:HB	13:Y:546:PHE:HD1	1.64	0.63
15:a:170:VAL:HG11	15:a:176:ILE:HD11	1.80	0.63
1:A:158:PHE:CB	1:A:164:ALA:HB2	2.28	0.62
3:O:52:ALA:HB2	64:O:401:HEM:HMD1	1.81	0.62
22:h:175:ASN:OD1	22:h:176:PHE:N	2.32	0.62
1:M:155:ALA:HA	1:M:164:ALA:HB1	1.80	0.62
3:C:34:GLY:HA3	64:C:402:HEM:CMA	2.29	0.62
12:W:140:ARG:NH1	14:Z:397:TYR:HE2	1.98	0.62
13:Y:550:ALA:HA	13:Y:575:VAL:HB	1.81	0.62
17:c:301:GLU:HA	17:c:306:GLY:HA2	1.80	0.62
24:j:332:HIS:CE1	24:j:336:LYS:HG3	2.34	0.62
14:Z:94:VAL:HG11	14:Z:116:LEU:HD12	1.81	0.62
20:f:159:MET:HB2	20:f:278:MET:HE1	1.82	0.62
20:f:190:MET:HE2	20:f:205:LEU:HA	1.79	0.62
3:C:372:ILE:O	3:C:375:LYS:N	2.32	0.62
4:D:72:ASP:O	4:D:73:GLY:O	2.18	0.62
7:S:45:ILE:O	7:S:49:ALA:N	2.32	0.62
14:Z:345:SER:O	14:Z:349:ASN:ND2	2.33	0.62
24:j:8:THR:O	24:j:11:THR:HG22	2.00	0.62
24:j:270:ASN:OD1	24:j:272:LEU:N	2.33	0.62
12:W:154:GLU:HA	12:W:179:ALA:HB3	1.81	0.62
20:f:211:MET:SD	20:f:333:SER:HB2	2.39	0.62
24:j:14:ILE:HD11	24:j:43:ALA:HB2	1.81	0.62
1:M:309:THR:HA	1:M:322:ALA:HA	1.80	0.62
4:P:50:HIS:O	4:P:51:LEU:C	2.40	0.62
19:e:148:ILE:HG13	21:g:69:ILE:HD12	1.82	0.62
20:f:42:PRO:HG3	25:k:167:VAL:HG22	1.82	0.62
29:p:168:SER:O	29:p:202:LYS:HA	1.99	0.62
29:p:203:PRO:C	69:p:401:NDP:H5N	2.17	0.62
1:M:80:GLU:O	1:M:83:GLY:N	2.28	0.62
3:O:172:LYS:O	3:O:173:ALA:C	2.41	0.62
13:Y:650:SER:OG	13:Y:652:ASN:N	2.32	0.62
59:An:47:ARG:O	59:An:50:GLU:O	2.18	0.62
3:C:116:GLY:C	64:C:402:HEM:HMC2	2.25	0.62
5:Q:15:ARG:CB	7:S:22:GLU:O	2.48	0.62
19:e:85:MET:HB3	19:e:233:MET:SD	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:34:GLU:HG2	23:i:66:PHE:HB3	1.82	0.62
20:f:210:THR:HG22	20:f:333:SER:HB3	1.80	0.62
4:P:224:ARG:CB	7:S:25:ALA:HB1	2.30	0.62
13:Y:192:VAL:HG12	13:Y:194:ASP:H	1.63	0.62
17:c:119:GLU:C	17:c:159:ARG:HH11	2.08	0.62
17:c:331:VAL:HG23	17:c:332:CYS:H	1.64	0.62
22:h:225:ILE:HD11	22:h:328:CYS:HA	1.82	0.62
65:P:301:HEC:HBC2	65:P:301:HEC:CHD	2.26	0.61
1:A:280:TYR:O	1:A:306:SER:HA	2.00	0.61
14:Z:279:THR:HG23	52:Ae:13:GLY:HA3	1.82	0.61
6:F:42:ASP:O	6:F:43:VAL:C	2.43	0.61
14:Z:161:ILE:HD11	14:Z:358:VAL:HG11	1.82	0.61
29:p:130:VAL:CB	69:p:401:NDP:N7A	2.63	0.61
2:B:90:GLU:O	2:B:91:ALA:C	2.44	0.61
12:W:196:HIS:HB2	12:W:199:ARG:HD3	1.82	0.61
13:Y:391:ILE:HA	13:Y:394:VAL:HG23	1.82	0.61
13:Y:615:LEU:HD12	13:Y:617:ARG:HH12	1.65	0.61
18:d:182:ASN:ND2	18:d:194:GLU:OE1	2.34	0.61
20:f:173:THR:O	20:f:227:THR:OG1	2.19	0.61
13:Y:64:CYS:O	13:Y:184:ARG:NH2	2.33	0.61
14:Z:171:ARG:NH1	14:Z:231:GLY:O	2.32	0.61
17:c:146:GLY:O	17:c:151:ALA:N	2.31	0.61
19:e:24:GLU:HA	19:e:271:LEU:HD13	1.83	0.61
24:j:421:ALA:O	24:j:424:THR:HG22	2.00	0.61
5:Q:15:ARG:N	7:S:22:GLU:O	2.34	0.61
13:Y:165:ILE:HD12	13:Y:171:THR:HG21	1.81	0.61
13:Y:405:THR:HG23	13:Y:686:PRO:HB2	1.81	0.61
13:Y:472:PRO:CB	13:Y:500:ILE:HD13	2.31	0.61
17:c:297:LYS:N	17:c:332:CYS:SG	2.66	0.61
24:j:132:VAL:O	24:j:262:ARG:NH1	2.34	0.61
1:A:5:ALA:O	1:A:6:GLN:C	2.43	0.61
15:a:162:TYR:CD1	16:b:153:ILE:HG21	2.33	0.61
17:c:285:PRO:HG3	18:d:143:ARG:HH22	1.66	0.61
12:W:76:VAL:HG12	12:W:86:ILE:HG22	1.83	0.61
13:Y:133:GLN:HG3	13:Y:137:CYS:HB2	1.81	0.61
13:Y:254:MET:HE3	13:Y:289:LYS:HE3	1.82	0.61
14:Z:292:MET:HG3	14:Z:431:HIS:HD2	1.64	0.61
1:M:55:ALA:O	1:M:56:GLY:C	2.43	0.61
4:D:139:THR:CB	8:H:41:ASP:HA	2.31	0.60
15:a:157:ALA:HB1	15:a:173:CYS:HB2	1.83	0.60
17:c:275:LEU:HA	17:c:289:GLU:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:O	1:A:352:SER:C	2.42	0.60
1:A:394:GLU:O	1:A:395:TRP:C	2.44	0.60
13:Y:194:ASP:OD2	13:Y:212:LYS:NZ	2.29	0.60
22:h:270:ILE:HD13	22:h:398:MET:HE3	1.82	0.60
3:C:74:ASN:H	5:E:65:SER:CA	2.11	0.60
14:Z:235:ASP:OD1	14:Z:236:LEU:N	2.35	0.60
17:c:98:LYS:NZ	68:c:502:FMN:O3P	2.34	0.60
22:h:336:ARG:NH1	22:h:429:SER:HA	2.16	0.60
24:j:72:GLN:O	24:j:74:VAL:N	2.34	0.60
1:A:395:TRP:O	1:A:396:GLU:C	2.43	0.60
2:N:313:ASN:H	9:U:59:ALA:HB2	1.66	0.60
24:j:362:LEU:HB2	24:j:365:ALA:HB3	1.83	0.60
49:Ab:11:UNK:O	49:Ab:13:UNK:N	2.34	0.60
20:f:181:TYR:HA	20:f:184:ILE:HG22	1.84	0.60
20:f:280:THR:HG22	22:h:162:VAL:HG11	1.83	0.60
7:G:68:LYS:O	7:G:72:LYS:N	2.34	0.60
11:K:17:TRP:O	11:K:21:ALA:CB	2.49	0.60
3:O:326:TRP:O	7:S:51:PRO:CB	2.49	0.60
14:Z:316:PHE:HA	14:Z:342:ARG:HH11	1.66	0.60
14:Z:330:TYR:HD2	14:Z:331:LEU:HD12	1.65	0.60
17:c:79:GLU:OE2	17:c:259:GLY:N	2.34	0.60
20:f:255:PRO:HB2	22:h:120:ILE:HG13	1.82	0.60
22:h:59:ASP:OD1	22:h:60:SER:N	2.34	0.60
24:j:244:SER:HA	24:j:248:HIS:HD2	1.67	0.60
25:k:64:MET:O	25:k:67:VAL:N	2.35	0.60
2:N:97:SER:HA	9:U:70:LEU:CB	2.31	0.60
13:Y:47:THR:OG1	13:Y:51:GLN:OE1	2.19	0.60
24:j:391:SER:O	24:j:395:ILE:HG12	2.02	0.60
29:p:205:ASP:HA	69:p:401:NDP:N7N	2.15	0.60
11:K:17:TRP:O	11:K:21:ALA:N	2.28	0.60
2:N:99:THR:O	2:N:106:ALA:N	2.35	0.60
3:O:171:ASP:O	3:O:172:LYS:C	2.44	0.60
4:P:72:ASP:O	4:P:73:GLY:O	2.20	0.60
13:Y:407:PRO:HG3	13:Y:438:LEU:HD21	1.83	0.60
17:c:179:ALA:HB3	17:c:181:LEU:HG	1.82	0.60
22:h:204:MET:HE2	22:h:209:LEU:HD22	1.82	0.60
24:j:80:PHE:HB3	24:j:82:MET:HE2	1.83	0.60
2:B:155:PRO:O	2:B:156:GLN:C	2.43	0.60
3:C:327:ALA:O	3:C:331:ASP:N	2.32	0.60
1:M:426:GLY:HA2	1:M:428:ILE:N	2.17	0.60
2:N:255:ALA:HA	2:N:425:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:474:VAL:HG11	13:Y:493:VAL:HG23	1.84	0.60
14:Z:317:ASP:H	14:Z:339:GLN:HE21	1.49	0.60
1:A:343:MET:O	1:A:344:ARG:C	2.41	0.60
1:M:221:GLY:O	1:M:225:GLU:N	2.31	0.60
29:p:130:VAL:CB	69:p:401:NDP:H8A	2.32	0.60
1:A:151:ASN:O	1:A:152:TYR:C	2.43	0.59
9:I:58:GLN:O	9:I:59:ALA:HB2	2.01	0.59
12:W:186:ARG:NE	12:W:191:TYR:O	2.35	0.59
13:Y:124:HIS:HD2	14:Z:375:MET:HE2	1.67	0.59
17:c:427:LEU:HB3	67:c:501:SF4:S4	2.41	0.59
19:e:173:TRP:NE1	19:e:244:GLY:O	2.34	0.59
22:h:205:VAL:HG22	22:h:212:LEU:HD23	1.84	0.59
23:i:75:LEU:HD22	25:k:71:THR:HG21	1.83	0.59
5:E:66:ALA:HB1	5:E:70:ALA:HB2	1.84	0.59
4:P:233:ARG:HA	7:S:17:SER:HA	1.84	0.59
17:c:244:ASN:OD1	17:c:245:VAL:N	2.35	0.59
23:i:88:ASP:HB3	23:i:90:VAL:HG12	1.82	0.59
24:j:342:CYS:O	24:j:346:ILE:HD12	2.02	0.59
2:N:154:ASN:O	2:N:155:PRO:C	2.42	0.59
2:N:269:ALA:O	2:N:272:PHE:N	2.35	0.59
12:W:101:ARG:HH12	12:W:159:VAL:HA	1.67	0.59
13:Y:371:VAL:HA	13:Y:534:VAL:HG12	1.84	0.59
17:c:392:MET:HE3	17:c:419:ILE:HD12	1.85	0.59
24:j:467:ILE:O	24:j:471:ASN:ND2	2.35	0.59
29:p:205:ASP:H	69:p:401:NDP:H41N	1.67	0.59
12:W:97:LEU:HA	12:W:100:LEU:HD12	1.83	0.59
13:Y:326:VAL:HG11	13:Y:582:VAL:HG11	1.83	0.59
17:c:104:LYS:O	17:c:106:SER:N	2.36	0.59
22:h:32:LEU:O	22:h:35:SER:OG	2.10	0.59
22:h:106:LEU:HA	22:h:109:THR:HG22	1.84	0.59
25:l:115:ILE:O	25:l:117:PHE:N	2.35	0.59
17:c:119:GLU:CB	17:c:159:ARG:HH11	2.15	0.59
15:a:200:LEU:O	15:a:204:ILE:HD12	2.02	0.59
6:F:96:GLU:O	6:F:97:VAL:C	2.45	0.59
20:f:112:HIS:CB	20:f:184:ILE:HD11	2.33	0.59
9:U:55:LEU:O	9:U:56:ARG:C	2.46	0.59
13:Y:409:PHE:HE2	13:Y:689:LEU:O	1.85	0.59
16:b:76:TYR:CD1	19:e:33:LEU:HD11	2.38	0.59
17:c:86:ARG:NE	17:c:92:GLY:O	2.29	0.59
17:c:423:THR:HG21	17:c:428:GLY:HA3	1.84	0.59
22:h:102:LEU:HD21	22:h:230:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:152:ILE:HD11	18:d:201:ILE:HG21	1.83	0.59
1:A:15:GLN:O	1:A:26:ALA:HA	2.03	0.59
12:W:118:ASP:OD1	12:W:119:VAL:N	2.36	0.59
15:a:159:GLY:O	15:a:161:GLY:N	2.32	0.59
17:c:121:GLU:N	17:c:204:TYR:CE1	2.70	0.59
20:f:254:LEU:HD11	20:f:290:LEU:HD11	1.85	0.59
22:h:373:ILE:HA	22:h:376:ILE:HG22	1.84	0.59
56:Ak:31:CYS:O	56:Ak:33:HIS:N	2.36	0.59
3:C:52:ALA:O	3:O:180:ALA:HB2	2.02	0.58
13:Y:32:ILE:HG21	13:Y:98:LYS:H	1.67	0.58
13:Y:76:ARG:HD2	17:c:424:ILE:HG23	1.83	0.58
22:h:243:MET:HE1	22:h:298:ILE:HG13	1.85	0.58
1:A:426:GLY:CA	1:A:428:ILE:N	2.66	0.58
1:M:351:GLU:HA	1:M:404:ALA:HB2	1.85	0.58
13:Y:219:SER:O	13:Y:222:ILE:HG12	2.02	0.58
13:Y:549:GLY:H	13:Y:568:TYR:HE1	1.51	0.58
17:c:89:GLY:HA3	68:c:502:FMN:H4'	1.85	0.58
25:k:22:SER:O	25:k:24:PRO:HD3	2.03	0.58
3:O:275:LEU:O	3:O:276:PHE:C	2.45	0.58
17:c:320:GLY:HA3	17:c:350:GLY:HA3	1.85	0.58
22:h:189:SER:OG	22:h:190:TRP:N	2.37	0.58
4:P:234:LYS:C	7:S:16:TYR:H	2.11	0.58
18:d:177:LEU:N	66:d:301:FES:S1	2.67	0.58
20:f:10:ILE:HD11	20:f:129:LEU:HD11	1.86	0.58
2:B:217:LYS:O	2:B:218:GLN:C	2.45	0.58
4:D:100:ALA:O	4:D:103:ALA:N	2.37	0.58
4:P:26:ILE:O	4:P:27:ARG:C	2.47	0.58
13:Y:76:ARG:NH1	17:c:424:ILE:HG22	2.18	0.58
15:a:78:ARG:HH11	19:e:57:THR:HG22	1.67	0.58
24:j:10:THR:HA	24:j:13:ILE:HG22	1.84	0.58
1:A:62:LEU:O	1:A:63:ALA:C	2.46	0.58
3:C:171:ASP:O	3:C:172:LYS:C	2.47	0.58
3:C:213:SER:O	3:C:215:VAL:N	2.36	0.58
1:M:397:SER:O	1:M:400:ALA:HB3	2.03	0.58
5:Q:76:ILE:HA	5:Q:193:VAL:O	2.03	0.58
12:W:111:LEU:CD1	12:W:163:ALA:HB2	2.34	0.58
14:Z:385:TYR:HD1	16:b:122:VAL:HG21	1.69	0.58
16:b:100:GLU:OE2	16:b:193:ASN:ND2	2.37	0.58
19:e:199:ASP:HB3	19:e:279:ARG:HE	1.69	0.58
22:h:269:MET:HE1	22:h:296:LEU:HD21	1.86	0.58
13:Y:124:HIS:CD2	14:Z:375:MET:HE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:118:ASP:C	68:c:502:FMN:C7M	2.75	0.58
20:f:78:LEU:HD21	23:i:47:ILE:HG21	1.85	0.58
3:C:372:ILE:O	3:C:373:GLU:C	2.46	0.58
15:a:99:MET:CE	15:a:113:PHE:HZ	2.16	0.58
20:f:268:GLN:HA	22:h:165:VAL:HG11	1.85	0.58
24:j:288:THR:HG21	24:j:307:SER:OG	2.04	0.58
30:q:85:LEU:CB	30:q:159:VAL:N	2.65	0.58
1:A:55:ALA:O	1:A:58:PHE:N	2.35	0.58
2:B:99:THR:O	2:B:106:ALA:N	2.37	0.58
3:C:35:SER:N	64:C:402:HEM:CMA	2.64	0.58
4:P:113:LEU:O	4:P:114:SER:C	2.46	0.58
12:W:94:ILE:HD11	12:W:154:GLU:HB2	1.86	0.58
13:Y:138:ASP:O	13:Y:142:GLN:HG2	2.04	0.58
13:Y:485:ASP:O	13:Y:489:ILE:HD13	2.03	0.58
17:c:55:GLY:O	17:c:58:SER:OG	2.16	0.58
22:h:404:ALA:O	22:h:407:SER:OG	2.19	0.58
24:j:34:ASN:HA	24:j:105:MET:HE1	1.85	0.58
49:Ab:121:UNK:CA	60:Aq:43:UNK:CB	2.71	0.58
4:D:50:HIS:O	4:D:54:VAL:N	2.28	0.58
20:f:2:ASN:O	20:f:5:ILE:HG22	2.03	0.58
20:f:288:LEU:HD11	24:j:570:GLN:NE2	2.19	0.58
22:h:14:MET:O	22:h:18:SER:OG	2.18	0.58
1:A:338:LEU:O	1:A:341:GLN:N	2.35	0.57
1:M:152:TYR:O	1:M:153:LEU:C	2.47	0.57
12:W:115:THR:OG1	12:W:129:VAL:HB	2.04	0.57
19:e:75:PRO:HA	19:e:223:PHE:CE1	2.39	0.57
19:e:134:ARG:HD3	19:e:200:LEU:HD23	1.85	0.57
21:g:56:PHE:HZ	25:k:71:THR:HA	1.69	0.57
24:j:72:GLN:OE1	24:j:72:GLN:N	2.36	0.57
12:W:153:ILE:O	12:W:178:PHE:HA	2.04	0.57
17:c:244:ASN:HB2	68:c:502:FMN:O2P	2.04	0.57
20:f:291:TYR:HE1	22:h:147:LEU:HD21	1.69	0.57
22:h:229:MET:HE2	22:h:328:CYS:HB3	1.85	0.57
1:M:270:LEU:O	1:M:273:ALA:HB3	2.04	0.57
13:Y:319:TRP:HZ3	13:Y:585:PRO:HG2	1.70	0.57
18:d:183:ALA:HB3	18:d:195:ASP:HA	1.86	0.57
3:C:116:GLY:O	64:C:402:HEM:HMC1	1.99	0.57
13:Y:299:ARG:HD2	13:Y:705:GLN:HE21	1.69	0.57
13:Y:637:ASP:N	13:Y:641:GLN:OE1	2.37	0.57
15:a:153:MET:HA	15:a:183:VAL:HG23	1.86	0.57
21:g:83:ASN:O	21:g:86:THR:OG1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:120:TYR:HB3	24:j:154:LEU:HD11	1.86	0.57
13:Y:372:PHE:HD1	13:Y:481:LEU:CD1	2.17	0.57
13:Y:466:LEU:HD21	13:Y:496:ILE:HG22	1.85	0.57
14:Z:135:TYR:CE1	15:a:162:TYR:HE2	2.22	0.57
17:c:119:GLU:H	17:c:159:ARG:HD3	1.69	0.57
24:j:342:CYS:O	24:j:345:SER:OG	2.16	0.57
3:C:115:ILE:O	3:C:116:GLY:C	2.46	0.57
7:G:33:GLY:O	7:G:37:VAL:N	2.36	0.57
6:R:98:ILE:O	6:R:99:ARG:C	2.48	0.57
12:W:212:TYR:HA	12:W:219:VAL:HA	1.86	0.57
13:Y:340:ALA:HA	13:Y:545:LEU:HB3	1.87	0.57
13:Y:405:THR:HG23	13:Y:686:PRO:HB3	1.86	0.57
14:Z:96:ARG:HB2	14:Z:115:LEU:HD11	1.86	0.57
16:b:158:CYS:N	67:b:302:SF4:S2	2.73	0.57
20:f:255:PRO:HG3	22:h:123:GLU:HB3	1.87	0.57
21:g:78:ALA:HA	25:k:144:ALA:HB1	1.87	0.57
24:j:34:ASN:HA	24:j:37:LYS:HG2	1.85	0.57
3:C:25:SER:O	3:C:26:ASN:C	2.45	0.57
1:M:394:GLU:O	1:M:395:TRP:C	2.47	0.57
4:P:236:ALA:O	7:S:13:VAL:HA	2.05	0.57
13:Y:260:ASN:HD22	13:Y:278:HIS:HB2	1.70	0.57
14:Z:333:ARG:NH2	14:Z:455:ASP:OD2	2.38	0.57
17:c:270:ASN:HD21	17:c:340:ASP:HB2	1.70	0.57
24:j:371:THR:O	24:j:375:ILE:HD12	2.05	0.57
24:j:400:ASN:HA	24:j:409:LEU:HD11	1.87	0.57
16:b:115:ALA:O	16:b:140:ARG:NH2	2.37	0.57
20:f:172:GLN:OE1	20:f:172:GLN:N	2.37	0.57
22:h:35:SER:O	22:h:38:SER:OG	2.14	0.57
22:h:46:GLY:N	60:Aw:44:UNK:O	2.36	0.57
4:D:50:HIS:O	4:D:51:LEU:C	2.48	0.57
5:Q:185:TYR:HA	5:Q:194:ILE:O	2.04	0.57
12:W:107:GLN:HE22	12:W:136:ARG:HB3	1.70	0.57
13:Y:624:ARG:NE	13:Y:636:TYR:O	2.30	0.57
18:d:179:ALA:HB3	18:d:185:MET:SD	2.44	0.57
20:f:235:ASN:OD1	20:f:236:LYS:N	2.38	0.57
22:h:305:THR:O	22:h:308:SER:OG	2.14	0.57
4:D:69:GLU:O	4:D:73:GLY:HA3	2.05	0.56
13:Y:68:ARG:NH1	13:Y:279:GLU:OE2	2.38	0.56
16:b:135:ARG:NH1	16:b:141:ARG:HG3	2.20	0.56
19:e:41:GLY:HA3	19:e:44:GLY:N	2.15	0.56
10:J:57:HIS:O	10:J:58:LYS:C	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:57:HIS:O	10:L:58:LYS:C	2.46	0.56
2:N:248:ASN:CB	2:N:428:GLY:HA2	2.35	0.56
13:Y:278:HIS:NE2	13:Y:280:ASP:HB2	2.20	0.56
13:Y:366:LEU:HD13	13:Y:530:TYR:HA	1.87	0.56
14:Z:294:ARG:HH21	14:Z:301:ASP:CG	2.13	0.56
19:e:305:ILE:HG12	21:g:75:LEU:HD21	1.87	0.56
1:A:30:SER:N	1:A:201:GLY:O	2.38	0.56
1:A:33:PRO:O	1:A:103:SER:N	2.36	0.56
1:A:309:THR:HA	1:A:322:ALA:HA	1.86	0.56
1:A:394:GLU:O	1:A:397:SER:N	2.38	0.56
1:A:425:PHE:O	1:A:426:GLY:O	2.23	0.56
9:I:53:GLU:O	9:I:54:SER:C	2.47	0.56
2:N:99:THR:N	2:N:106:ALA:O	2.19	0.56
3:O:327:ALA:O	3:O:331:ASP:N	2.35	0.56
5:Q:147:ILE:N	5:Q:157:TYR:O	2.36	0.56
13:Y:209:TYR:CD2	13:Y:210:ILE:HG13	2.41	0.56
14:Z:116:LEU:O	14:Z:116:LEU:HD23	2.05	0.56
17:c:236:PHE:CE1	18:d:74:HIS:HB2	2.40	0.56
24:j:150:MET:HE1	24:j:153:LEU:HD22	1.86	0.56
24:j:161:ARG:NH1	24:j:238:GLU:OE2	2.37	0.56
1:M:245:GLU:O	1:M:247:GLY:N	2.39	0.56
13:Y:485:ASP:O	13:Y:489:ILE:HD12	2.03	0.56
19:e:287:HIS:CE1	19:e:291:LYS:HG3	2.40	0.56
22:h:14:MET:HE1	22:h:30:HIS:NE2	2.21	0.56
6:F:103:GLU:O	6:F:104:ARG:C	2.47	0.56
19:e:294:LEU:HD22	21:g:102:LEU:HD22	1.87	0.56
12:W:168:ARG:HH11	12:W:185:ARG:CG	2.17	0.56
14:Z:117:HIS:HA	14:Z:462:ASP:HB3	1.88	0.56
14:Z:223:HIS:HD2	15:a:187:PRO:HD3	1.70	0.56
18:d:205:ILE:HA	18:d:208:LEU:HD12	1.86	0.56
20:f:25:HIS:HD2	20:f:84:TRP:HB3	1.69	0.56
24:j:155:ILE:HD11	24:j:248:HIS:NE2	2.21	0.56
1:M:435:ASN:CB	3:O:222:PRO:CB	2.83	0.56
13:Y:605:GLN:OE1	13:Y:643:ARG:NH2	2.38	0.56
14:Z:293:LEU:HB3	14:Z:298:ILE:HD11	1.88	0.56
15:a:82:LEU:HD13	15:a:122:VAL:HG11	1.88	0.56
18:d:201:ILE:O	18:d:205:ILE:HD12	2.06	0.56
18:d:207:GLU:HG2	18:d:212:LYS:O	2.06	0.56
19:e:151:LEU:HD12	21:g:73:LEU:HD23	1.87	0.56
19:e:157:ASN:OD1	19:e:158:GLY:N	2.39	0.56
1:A:55:ALA:O	1:A:56:GLY:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:240:GLN:HA	1:M:422:VAL:O	2.06	0.56
3:O:132:VAL:HA	3:O:139:SER:CB	2.36	0.56
13:Y:180:THR:O	13:Y:182:CYS:N	2.39	0.56
13:Y:180:THR:OG1	13:Y:184:ARG:NH1	2.38	0.56
17:c:184:LYS:O	17:c:186:ALA:N	2.39	0.56
18:d:140:CYS:SG	18:d:185:MET:HE3	2.46	0.56
3:C:318:ARG:O	3:C:319:PRO:C	2.48	0.56
1:M:225:GLU:CA	49:Ah:13:UNK:O	2.54	0.56
1:M:270:LEU:O	1:M:271:GLN:C	2.47	0.56
13:Y:266:ARG:H	13:Y:271:MET:HG2	1.70	0.56
14:Z:335:GLU:O	14:Z:339:GLN:HG2	2.05	0.56
15:a:100:ALA:HB2	15:a:113:PHE:CE2	2.40	0.56
15:a:150:VAL:CG2	15:a:179:VAL:HA	2.36	0.56
18:d:56:THR:OG1	18:d:59:ASN:ND2	2.39	0.56
24:j:144:TRP:NE1	24:j:179:ASP:OD1	2.34	0.56
4:D:69:GLU:HA	4:D:73:GLY:HA2	1.88	0.56
17:c:88:ARG:N	68:c:502:FMN:O1P	2.39	0.56
17:c:288:VAL:HG21	17:c:303:HIS:HB3	1.88	0.56
22:h:364:LEU:HD11	24:j:149:ILE:HG12	1.88	0.56
1:M:270:LEU:O	1:M:273:ALA:N	2.38	0.55
12:W:192:GLY:O	12:W:194:GLU:N	2.37	0.55
13:Y:48:THR:HA	13:Y:95:PRO:HA	1.88	0.55
13:Y:540:ASN:HD21	13:Y:559:ASP:HA	1.71	0.55
13:Y:652:ASN:HA	13:Y:655:ARG:HE	1.71	0.55
15:a:99:MET:HE3	15:a:113:PHE:HZ	1.71	0.55
25:k:45:LEU:HD23	25:k:50:SER:HA	1.87	0.55
10:L:34:ALA:O	10:L:35:PHE:C	2.45	0.55
5:Q:150:ALA:HB3	5:Q:157:TYR:CB	2.36	0.55
18:d:95:ILE:HG22	18:d:99:ASN:HD21	1.71	0.55
29:p:210:GLU:O	29:p:211:ASP:C	2.49	0.55
2:N:155:PRO:O	2:N:156:GLN:C	2.49	0.55
64:O:401:HEM:HBC2	64:O:401:HEM:CMC	2.35	0.55
14:Z:396:THR:O	14:Z:410:TYR:HA	2.06	0.55
17:c:118:ASP:CA	68:c:502:FMN:HM73	2.36	0.55
1:M:219:LEU:O	1:M:220:SER:O	2.25	0.55
20:f:217:MET:CB	20:f:326:LEU:HD13	2.37	0.55
20:f:318:GLU:OE1	20:f:318:GLU:N	2.37	0.55
22:h:106:LEU:HD13	22:h:234:VAL:HG11	1.88	0.55
30:q:91:ALA:HA	30:q:95:TYR:CB	2.35	0.55
1:M:81:SER:HA	2:N:359:ALA:HB1	1.87	0.55
12:W:114:LEU:HD23	12:W:166:TYR:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:287:SER:OG	13:Y:288:ASP:N	2.38	0.55
18:d:186:VAL:HG23	18:d:196:LEU:HD21	1.88	0.55
24:j:247:LEU:HB2	24:j:252:MET:HB2	1.88	0.55
24:j:303:ALA:O	24:j:306:THR:HG22	2.07	0.55
5:E:10:PHE:O	5:E:14:ARG:N	2.34	0.55
14:Z:368:ARG:HA	14:Z:371:MET:HG2	1.89	0.55
17:c:105:PRO:O	17:c:107:ASP:N	2.39	0.55
18:d:53:PHE:HE1	18:d:90:ASN:HD21	1.53	0.55
24:j:410:LEU:O	24:j:414:ILE:HD12	2.07	0.55
2:B:280:GLY:HA2	2:B:311:ALA:HB3	1.88	0.55
3:C:337:TRP:O	3:C:338:ILE:C	2.48	0.55
5:Q:89:PHE:O	5:Q:96:LEU:N	2.23	0.55
13:Y:86:PRO:O	13:Y:108:LYS:NZ	2.29	0.55
13:Y:382:ARG:HA	13:Y:385:TYR:CE2	2.42	0.55
14:Z:217:VAL:HG12	14:Z:237:PRO:HD2	1.89	0.55
14:Z:233:HIS:CD2	14:Z:234:GLN:HG3	2.42	0.55
15:a:121:ASP:OD1	15:a:121:ASP:N	2.36	0.55
17:c:116:ASN:ND2	68:c:502:FMN:C9	2.70	0.55
17:c:262:PHE:CZ	17:c:272:GLY:HA3	2.42	0.55
1:A:397:SER:O	1:A:400:ALA:HB3	2.07	0.55
3:O:371:THR:O	3:O:372:ILE:C	2.49	0.55
4:P:50:HIS:O	4:P:54:VAL:N	2.32	0.55
13:Y:217:GLU:OE2	13:Y:412:PRO:CG	2.53	0.55
2:N:88:GLY:O	2:N:91:ALA:HB3	2.07	0.55
15:a:164:HIS:CE1	15:a:171:ARG:HD2	2.42	0.55
17:c:88:ARG:C	17:c:244:ASN:HD22	2.15	0.55
19:e:32:GLN:HB2	19:e:34:ARG:HG2	1.89	0.55
19:e:60:PRO:HB3	19:e:217:ALA:HB3	1.89	0.55
20:f:167:TRP:CE3	24:j:573:MET:HB3	2.42	0.55
2:B:266:SER:O	2:B:269:ALA:HB3	2.07	0.55
1:M:445:ARG:O	1:M:446:PHE:CB	2.55	0.55
2:N:408:ALA:O	2:N:411:ILE:N	2.40	0.55
3:O:109:PHE:O	3:O:110:LEU:C	2.49	0.55
14:Z:182:ASN:ND2	14:Z:403:PRO:HB2	2.14	0.55
17:c:74:ASP:O	17:c:78:GLY:N	2.34	0.55
24:j:297:ASP:OD1	24:j:298:ILE:N	2.38	0.55
29:p:205:ASP:N	69:p:401:NDP:H41N	2.21	0.55
3:C:117:VAL:HA	64:C:402:HEM:HBC2	1.85	0.54
7:G:64:GLN:O	7:G:65:GLU:C	2.50	0.54
10:L:7:ALA:HB2	5:Q:31:ALA:HA	1.88	0.54
2:N:359:ALA:O	2:N:360:ALA:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:292:PHE:HB3	13:Y:706:THR:HG21	1.88	0.54
17:c:76:ILE:HA	17:c:79:GLU:HB3	1.89	0.54
17:c:383:THR:HG23	17:c:384:PRO:HD3	1.89	0.54
20:f:84:TRP:HE1	23:i:53:PHE:HE2	1.53	0.54
20:f:112:HIS:CE1	20:f:164:ILE:HG21	2.42	0.54
20:f:174:GLN:OE1	20:f:174:GLN:N	2.30	0.54
3:C:236:ILE:O	3:C:237:LEU:C	2.48	0.54
2:N:98:VAL:O	9:U:69:SER:O	2.25	0.54
12:W:168:ARG:NH1	12:W:185:ARG:NE	2.51	0.54
13:Y:585:PRO:HB2	13:Y:616:ALA:HB2	1.88	0.54
14:Z:324:GLY:O	14:Z:329:ARG:NH2	2.40	0.54
17:c:207:GLY:HA3	68:c:502:FMN:N5	2.23	0.54
1:A:342:TRP:O	1:A:345:LEU:N	2.40	0.54
2:B:89:ILE:O	2:B:90:GLU:C	2.47	0.54
2:B:90:GLU:O	2:B:92:VAL:N	2.41	0.54
3:C:61:THR:O	3:C:64:SER:N	2.41	0.54
3:C:85:ASN:O	3:C:86:GLY:C	2.50	0.54
13:Y:32:ILE:HG21	13:Y:98:LYS:N	2.22	0.54
13:Y:404:GLY:HA2	13:Y:684:LEU:HG	1.89	0.54
14:Z:178:THR:OG1	14:Z:214:TYR:OH	2.23	0.54
14:Z:271:ARG:NH2	19:e:281:ARG:HB2	2.22	0.54
15:a:131:ASN:ND2	15:a:168:SER:HA	2.23	0.54
22:h:82:SER:HB2	22:h:432:ARG:NH1	2.22	0.54
22:h:329:LEU:HD21	22:h:359:TRP:CD2	2.42	0.54
1:A:109:ALA:O	1:A:112:LEU:N	2.40	0.54
3:C:116:GLY:C	64:C:402:HEM:C2C	2.86	0.54
3:C:312:GLN:O	3:C:314:SER:N	2.40	0.54
1:M:106:LEU:O	1:M:107:PRO:C	2.51	0.54
8:T:68:CYS:O	8:T:69:VAL:C	2.51	0.54
13:Y:35:PHE:O	13:Y:101:ASN:HA	2.06	0.54
13:Y:124:HIS:NE2	67:Y:801:SF4:S4	2.80	0.54
14:Z:438:MET:HG2	14:Z:450:ILE:HD11	1.87	0.54
22:h:10:MET:O	22:h:13:PRO:HD2	2.06	0.54
22:h:196:TRP:HE3	22:h:197:LEU:HD23	1.72	0.54
22:h:286:ILE:O	22:h:289:SER:OG	2.14	0.54
5:E:160:CYS:HA	3:O:266:PRO:C	2.31	0.54
8:H:66:ASP:O	8:H:67:HIS:C	2.50	0.54
1:M:7:ALA:HB1	2:N:41:TYR:O	2.07	0.54
1:M:51:LYS:O	1:M:53:ASN:N	2.38	0.54
1:M:426:GLY:HA3	1:M:428:ILE:H	1.71	0.54
2:N:133:ARG:O	2:N:134:ARG:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:241:ARG:HG2	13:Y:243:TRP:CZ2	2.43	0.54
15:a:160:GLY:N	15:a:171:ARG:O	2.40	0.54
17:c:199:ARG:NH2	18:d:84:ASP:OD2	2.40	0.54
30:v:304:LEU:O	30:v:308:ASN:N	2.40	0.54
1:A:236:PHE:H	5:E:25:SER:CB	2.20	0.54
10:J:25:VAL:CB	11:V:31:GLY:HA3	2.38	0.54
3:O:106:SER:CB	64:O:402:HEM:HBD2	2.36	0.54
3:O:274:PHE:O	3:O:275:LEU:C	2.47	0.54
14:Z:100:GLU:HG2	14:Z:100:GLU:O	2.08	0.54
17:c:88:ARG:O	17:c:244:ASN:ND2	2.36	0.54
5:Q:139:CYS:O	5:Q:143:GLY:HA2	2.08	0.54
13:Y:349:GLU:HG3	13:Y:620:TRP:CG	2.42	0.54
18:d:200:ASP:O	18:d:204:ILE:HG12	2.08	0.54
19:e:20:LEU:HD23	19:e:228:TYR:HB3	1.90	0.54
22:h:360:LEU:O	22:h:364:LEU:HB2	2.08	0.54
23:i:32:CYS:HA	25:k:20:PHE:CZ	2.42	0.54
24:j:79:SER:OG	24:j:135:ASN:HB3	2.08	0.54
24:j:560:THR:O	24:j:565:THR:HG23	2.08	0.54
4:D:113:LEU:O	4:D:114:SER:C	2.48	0.54
5:Q:187:PHE:HA	5:Q:193:VAL:HA	1.89	0.54
13:Y:476:LEU:HD22	13:Y:493:VAL:HG11	1.87	0.54
22:h:138:ASN:O	22:h:139:GLN:HG2	2.08	0.54
25:k:64:MET:O	25:k:67:VAL:HG12	2.07	0.54
10:J:35:PHE:O	10:J:36:ASP:C	2.50	0.54
1:M:55:ALA:O	1:M:58:PHE:N	2.39	0.54
1:M:256:ALA:HB3	1:M:421:ALA:HB3	1.89	0.54
3:O:72:ASP:CB	5:Q:67:ASP:N	2.71	0.54
13:Y:136:GLU:N	13:Y:136:GLU:OE1	2.41	0.54
13:Y:523:VAL:HG13	13:Y:597:VAL:HB	1.89	0.54
14:Z:427:PRO:HD2	14:Z:460:GLU:OE2	2.08	0.54
17:c:273:THR:HG22	17:c:291:GLU:HA	1.90	0.54
19:e:1:MET:O	19:e:4:ILE:HG22	2.08	0.54
19:e:293:PHE:O	19:e:297:THR:HG23	2.07	0.54
21:g:52:SER:H	25:k:74:MET:HE1	1.73	0.54
29:p:172:ALA:O	29:p:185:ALA:HB2	2.08	0.54
3:C:251:GLY:O	3:C:252:ASP:C	2.50	0.54
4:P:138:PRO:O	4:P:139:THR:C	2.50	0.54
15:a:159:GLY:HA2	15:a:172:GLY:HA2	1.90	0.54
17:c:62:TRP:CE2	17:c:140:GLU:HG2	2.43	0.54
17:c:89:GLY:HA3	68:c:502:FMN:O5'	2.08	0.54
23:i:53:PHE:CD1	28:o:21:GLN:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:334:MET:O	1:M:335:MET:C	2.48	0.53
3:O:7:SER:O	3:O:8:HIS:O	2.26	0.53
16:b:196:LYS:HD2	16:b:197:TRP:NE1	2.23	0.53
17:c:229:PHE:H	17:c:232:ASP:HB3	1.73	0.53
17:c:328:PRO:HB2	17:c:330:SER:C	2.33	0.53
19:e:72:ILE:O	19:e:75:PRO:HD2	2.08	0.53
19:e:118:TRP:HH2	25:k:31:LEU:HD13	1.72	0.53
19:e:291:LYS:HA	21:g:106:TRP:CZ3	2.43	0.53
22:h:61:LEU:HD22	22:h:241:TYR:HD1	1.73	0.53
24:j:363:TYR:HB2	24:j:431:PHE:HB3	1.90	0.53
30:q:85:LEU:CB	30:q:158:GLY:O	2.56	0.53
3:C:116:GLY:O	64:C:402:HEM:C2C	2.59	0.53
10:L:49:GLY:HA2	10:L:54:HIS:CB	2.38	0.53
1:M:338:LEU:O	1:M:341:GLN:N	2.38	0.53
2:N:100:SER:O	9:U:67:SER:O	2.26	0.53
13:Y:566:ILE:O	13:Y:580:ALA:HB1	2.08	0.53
17:c:94:PRO:HB2	17:c:97:LEU:HB3	1.90	0.53
19:e:186:PHE:O	19:e:189:THR:OG1	2.20	0.53
21:g:24:LEU:HB3	21:g:25:PRO:HD3	1.89	0.53
21:g:31:SER:HA	21:g:34:THR:HG22	1.90	0.53
22:h:244:MET:HG2	22:h:301:ILE:HD12	1.89	0.53
1:A:256:ALA:HA	1:A:320:LEU:O	2.06	0.53
2:N:294:SER:O	2:N:295:LEU:C	2.51	0.53
13:Y:201:GLY:N	17:c:379:CYS:O	2.40	0.53
20:f:175:LEU:HG	20:f:296:LEU:HD11	1.91	0.53
24:j:288:THR:HG23	24:j:304:PHE:HD1	1.73	0.53
30:q:85:LEU:CB	30:q:159:VAL:C	2.79	0.53
1:M:33:PRO:O	1:M:103:SER:N	2.34	0.53
12:W:109:LYS:O	12:W:110:SER:OG	2.22	0.53
13:Y:400:ILE:CG2	13:Y:402:LEU:HD11	2.38	0.53
17:c:126:LYS:HZ1	17:c:274:LYS:HE2	1.71	0.53
22:h:337:VAL:HG13	22:h:339:SER:H	1.73	0.53
39:3:82:CYS:N	39:3:86:GLY:O	2.41	0.53
1:A:76:GLU:O	1:A:80:GLU:N	2.33	0.53
2:B:276:GLN:O	2:B:280:GLY:N	2.40	0.53
3:C:43:LEU:O	3:C:44:GLN:C	2.51	0.53
5:E:160:CYS:O	3:O:266:PRO:O	2.27	0.53
2:N:217:LYS:O	2:N:218:GLN:C	2.51	0.53
13:Y:39:GLN:HE21	13:Y:56:VAL:HG21	1.73	0.53
15:a:162:TYR:CD1	16:b:153:ILE:HD13	2.42	0.53
17:c:267:ARG:HH21	17:c:336:LEU:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:SER:O	3:C:89:MET:C	2.47	0.53
2:N:255:ALA:HB2	2:N:426:ALA:CB	2.37	0.53
17:c:119:GLU:CB	17:c:159:ARG:NH1	2.72	0.53
17:c:235:VAL:O	17:c:237:GLY:N	2.42	0.53
22:h:103:GLN:O	22:h:107:ILE:HD12	2.09	0.53
24:j:482:MET:HE3	24:j:483:PRO:HB3	1.90	0.53
4:D:178:THR:O	4:D:179:MET:C	2.50	0.53
20:f:112:HIS:O	20:f:115:VAL:HG12	2.09	0.53
20:f:231:SER:HB2	20:f:305:PHE:HB2	1.90	0.53
22:h:251:ASN:OD1	22:h:304:GLN:NE2	2.37	0.53
24:j:258:PHE:HA	24:j:261:ILE:HD12	1.90	0.53
3:C:34:GLY:O	3:C:37:LEU:CB	2.57	0.53
3:C:103:TYR:O	3:C:315:MET:CB	2.57	0.53
13:Y:337:ASP:HA	13:Y:542:PRO:HD2	1.90	0.53
13:Y:465:ILE:HA	13:Y:468:GLU:OE1	2.09	0.53
17:c:174:ARG:O	17:c:178:GLU:HG2	2.09	0.53
17:c:327:ILE:HD11	17:c:441:HIS:CD2	2.43	0.53
17:c:369:ARG:HE	18:d:136:THR:HG22	1.72	0.53
18:d:158:ILE:HD11	18:d:164:THR:HB	1.91	0.53
22:h:204:MET:HE1	22:h:261:PHE:HB3	1.90	0.53
39:3:55:LYS:HA	39:3:74:LEU:O	2.08	0.53
1:M:292:SER:O	1:M:295:ALA:HB3	2.09	0.53
4:P:69:GLU:O	4:P:73:GLY:HA3	2.09	0.53
8:T:66:ASP:O	8:T:67:HIS:C	2.49	0.53
13:Y:250:SER:HB2	13:Y:606:THR:HG23	1.91	0.53
14:Z:131:GLN:HE21	16:b:122:VAL:HA	1.74	0.53
14:Z:138:ARG:HH12	14:Z:223:HIS:HB3	1.73	0.53
14:Z:196:ALA:O	14:Z:198:THR:N	2.41	0.53
15:a:123:MET:HB3	15:a:150:VAL:HG12	1.91	0.53
22:h:252:PRO:O	22:h:255:ASN:ND2	2.41	0.53
22:h:355:MET:HA	22:h:358:TRP:HD1	1.73	0.53
22:h:451:PRO:O	22:h:454:ILE:HG22	2.09	0.53
13:Y:222:ILE:HA	13:Y:225:ILE:HG22	1.91	0.53
13:Y:258:GLY:O	13:Y:604:GLN:NE2	2.42	0.53
13:Y:472:PRO:HG3	13:Y:500:ILE:HD13	1.91	0.53
17:c:288:VAL:HG11	17:c:303:HIS:CD2	2.44	0.53
17:c:328:PRO:O	17:c:331:VAL:HG13	2.09	0.53
48:z:102:HIS:O	48:z:104:TRP:N	2.42	0.53
4:D:10:TYR:HA	8:H:70:ALA:HB1	1.91	0.52
3:O:251:GLY:O	3:O:252:ASP:C	2.51	0.52
4:P:139:THR:CB	8:T:41:ASP:CB	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:141:TYR:CD2	15:a:91:CYS:HB3	2.44	0.52
20:f:217:MET:HB2	20:f:326:LEU:HD13	1.91	0.52
21:g:87:MET:HG3	25:k:147:TYR:HB3	1.91	0.52
22:h:325:MET:HE2	22:h:362:ALA:HB2	1.91	0.52
22:h:373:ILE:HG23	22:h:448:THR:HG22	1.90	0.52
23:i:67:ALA:O	23:i:70:GLU:HG2	2.09	0.52
24:j:97:THR:O	24:j:101:MET:HG2	2.09	0.52
4:D:153:PHE:O	4:D:156:GLN:N	2.35	0.52
13:Y:525:ALA:HB1	13:Y:530:TYR:HB2	1.91	0.52
14:Z:391:VAL:O	14:Z:415:GLY:HA2	2.09	0.52
22:h:76:MET:SD	22:h:230:VAL:HG23	2.49	0.52
24:j:385:TYR:HE2	51:Ao:35:UNK:HA	1.73	0.52
2:N:164:HIS:O	2:N:173:ALA:HA	2.09	0.52
2:N:276:GLN:O	2:N:280:GLY:N	2.40	0.52
12:W:75:GLN:HB3	51:Ap:35:UNK:HA	1.92	0.52
12:W:140:ARG:NH2	14:Z:406:GLU:OE1	2.42	0.52
13:Y:264:SER:OG	13:Y:272:ARG:O	2.23	0.52
13:Y:581:ASP:OD1	13:Y:582:VAL:N	2.43	0.52
17:c:220:GLN:NE2	18:d:114:GLU:HB3	2.24	0.52
24:j:306:THR:HB	24:j:336:LYS:HE2	1.91	0.52
2:N:262:ALA:HB3	2:N:269:ALA:N	2.24	0.52
12:W:124:ASN:HB3	12:W:148:ASP:OD1	2.10	0.52
13:Y:195:LEU:HA	13:Y:208:THR:HB	1.91	0.52
13:Y:462:PHE:O	13:Y:465:ILE:HG13	2.09	0.52
19:e:120:GLY:HA3	19:e:132:ALA:HB2	1.91	0.52
24:j:67:HIS:HA	24:j:77:SER:CB	2.40	0.52
24:j:68:TRP:HE3	24:j:76:LEU:HD11	1.73	0.52
24:j:342:CYS:HB2	24:j:369:THR:HG23	1.91	0.52
3:C:116:GLY:C	64:C:402:HEM:C3C	2.88	0.52
3:C:117:VAL:CA	64:C:402:HEM:CBC	2.76	0.52
3:O:275:LEU:O	3:O:278:TYR:N	2.42	0.52
3:O:276:PHE:O	3:O:277:ALA:C	2.52	0.52
13:Y:543:LYS:HD2	13:Y:563:ASP:OD2	2.09	0.52
13:Y:569:GLN:HE21	13:Y:622:ILE:HD12	1.72	0.52
15:a:106:MET:HE3	15:a:111:VAL:HG23	1.92	0.52
18:d:131:HIS:NE2	18:d:172:ILE:HD13	2.25	0.52
20:f:248:LEU:HD21	20:f:296:LEU:HD22	1.91	0.52
13:Y:144:MET:SD	14:Z:380:HIS:ND1	2.77	0.52
13:Y:169:VAL:HG11	13:Y:222:ILE:HD11	1.91	0.52
13:Y:239:THR:O	13:Y:266:ARG:NH1	2.40	0.52
13:Y:337:ASP:O	13:Y:541:PRO:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:291:LYS:HA	21:g:106:TRP:HZ3	1.75	0.52
1:A:371:GLY:HA2	2:B:373:GLU:O	2.09	0.52
3:C:4:ILE:O	3:C:5:ARG:C	2.53	0.52
2:N:280:GLY:HA2	2:N:311:ALA:HB3	1.90	0.52
12:W:155:SER:HB3	12:W:181:HIS:HB2	1.92	0.52
17:c:120:GLY:C	17:c:204:TYR:CD1	2.88	0.52
17:c:157:TYR:HB3	17:c:212:LEU:HD11	1.90	0.52
17:c:318:ILE:HG13	17:c:357:MET:HE1	1.91	0.52
17:c:339:PHE:HB3	17:c:349:LEU:HB2	1.89	0.52
17:c:413:TRP:HB2	17:c:439:ILE:HD13	1.92	0.52
18:d:137:THR:OG1	18:d:176:CYS:N	2.39	0.52
21:g:6:THR:HA	21:g:9:THR:HG22	1.90	0.52
22:h:273:SER:O	22:h:276:CYS:HB3	2.10	0.52
24:j:559:GLU:O	24:j:563:PRO:HD2	2.10	0.52
2:B:280:GLY:HA2	2:B:311:ALA:CB	2.40	0.52
10:L:21:ALA:O	10:L:22:LEU:C	2.53	0.52
2:N:262:ALA:HB3	2:N:269:ALA:HA	1.91	0.52
2:N:313:ASN:CB	9:U:59:ALA:HB2	2.39	0.52
3:O:85:ASN:O	3:O:86:GLY:C	2.53	0.52
4:P:79:GLU:O	4:P:80:MET:C	2.52	0.52
12:W:172:ASP:O	12:W:173:MET:HE2	2.10	0.52
13:Y:387:LEU:HD23	13:Y:389:THR:O	2.09	0.52
13:Y:557:ARG:HB3	13:Y:560:LEU:HD22	1.91	0.52
15:a:203:LYS:HG3	15:a:206:ARG:NH1	2.25	0.52
3:O:52:ALA:HB2	64:O:401:HEM:CMD	2.40	0.52
13:Y:44:GLU:HG3	13:Y:45:PRO:HD2	1.91	0.52
13:Y:591:GLU:OE1	13:Y:591:GLU:N	2.43	0.52
13:Y:650:SER:HB3	13:Y:651:PRO:HA	1.92	0.52
18:d:134:VAL:O	18:d:174:VAL:N	2.42	0.52
20:f:9:LEU:O	20:f:12:THR:HG22	2.10	0.52
22:h:269:MET:HE2	22:h:399:ASN:HB2	1.92	0.52
3:C:34:GLY:HA3	64:C:402:HEM:HMA2	1.92	0.52
1:M:131:ARG:O	1:M:132:ASP:C	2.53	0.52
12:W:114:LEU:O	12:W:170:ILE:HD11	2.10	0.52
18:d:72:GLU:HA	18:d:75:LYS:HZ1	1.74	0.52
20:f:303:THR:HG21	22:h:143:LEU:HD21	1.91	0.52
21:g:71:LEU:HD11	23:i:65:VAL:HG21	1.91	0.52
27:n:66:TRP:HA	27:n:75:LYS:O	2.10	0.52
10:L:36:ASP:O	10:L:37:GLN:C	2.52	0.51
10:L:52:TRP:O	10:L:53:LYS:C	2.53	0.51
12:W:88:ILE:HB	12:W:145:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:98:LYS:NZ	13:Y:100:TRP:HE1	2.08	0.51
13:Y:648:GLU:HG3	13:Y:649:VAL:N	2.25	0.51
17:c:137:LYS:NZ	17:c:256:ARG:HH22	2.08	0.51
17:c:149:MET:HB2	17:c:151:ALA:HB2	1.92	0.51
17:c:250:VAL:O	17:c:253:THR:OG1	2.23	0.51
22:h:220:HIS:CE1	22:h:232:ALA:HB2	2.45	0.51
40:4:8:HIS:O	40:4:10:GLY:N	2.42	0.51
1:M:51:LYS:C	1:M:53:ASN:H	2.19	0.51
14:Z:271:ARG:HH22	19:e:281:ARG:HB2	1.75	0.51
19:e:287:HIS:ND1	19:e:291:LYS:HG3	2.24	0.51
20:f:331:VAL:HG13	20:f:335:LEU:HD12	1.91	0.51
22:h:447:LEU:HD21	22:h:454:ILE:HD12	1.91	0.51
24:j:14:ILE:O	24:j:17:ILE:HG22	2.10	0.51
54:Ag:94:GLY:HA3	54:Ag:119:GLY:HA2	1.92	0.51
2:B:268:GLU:O	2:B:271:ALA:HB3	2.10	0.51
2:B:383:GLY:O	2:B:386:ALA:HB3	2.10	0.51
1:M:3:THR:O	1:M:4:TYR:C	2.54	0.51
4:P:224:ARG:O	4:P:228:SER:N	2.43	0.51
13:Y:604:GLN:HA	13:Y:656:TYR:HD1	1.74	0.51
13:Y:641:GLN:O	13:Y:644:SER:HB2	2.09	0.51
22:h:127:VAL:HB	22:h:128:PRO:HD3	1.90	0.51
24:j:346:ILE:HA	24:j:366:MET:HE1	1.93	0.51
24:j:383:MET:O	24:j:389:PHE:HB2	2.10	0.51
3:C:116:GLY:C	64:C:402:HEM:CMC	2.82	0.51
3:O:117:VAL:N	64:O:402:HEM:HBC2	2.25	0.51
13:Y:544:VAL:HG23	13:Y:566:ILE:HG23	1.93	0.51
16:b:70:LEU:HG	19:e:272:TRP:CZ2	2.45	0.51
19:e:135:ALA:HB1	19:e:201:THR:HG22	1.92	0.51
22:h:152:TYR:O	22:h:205:VAL:HG11	2.11	0.51
22:h:296:LEU:HB3	22:h:381:ILE:HD11	1.91	0.51
24:j:385:TYR:CE2	51:Ao:35:UNK:HA	2.46	0.51
24:j:452:ASN:HA	24:j:455:LYS:HD3	1.93	0.51
24:j:503:GLU:HB2	46:s:13:LYS:CB	2.39	0.51
29:p:82:VAL:O	29:p:105:PHE:HA	2.10	0.51
1:M:30:SER:N	1:M:201:GLY:O	2.43	0.51
3:O:296:PHE:O	3:O:297:SER:C	2.52	0.51
12:W:56:LYS:O	12:W:59:SER:OG	2.18	0.51
13:Y:173:MET:O	13:Y:174:THR:OG1	2.28	0.51
13:Y:335:GLY:C	13:Y:363:SER:HB2	2.35	0.51
13:Y:400:ILE:HG21	13:Y:402:LEU:HD11	1.92	0.51
13:Y:655:ARG:HB3	13:Y:658:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:132:ILE:HD11	18:d:169:PHE:HD1	1.76	0.51
19:e:118:TRP:CH2	25:k:31:LEU:HD13	2.46	0.51
20:f:298:TYR:O	20:f:303:THR:OG1	2.29	0.51
22:h:112:ALA:HB3	22:h:113:THR:HA	1.92	0.51
24:j:439:PRO:O	24:j:440:LEU:HB2	2.10	0.51
47:y:75:ILE:O	47:y:79:GLY:HA3	2.11	0.51
3:C:350:ILE:O	3:C:351:GLY:C	2.53	0.51
1:M:5:ALA:O	1:M:6:GLN:C	2.53	0.51
12:W:108:PHE:HB3	12:W:132:LEU:HB3	1.93	0.51
14:Z:118:ARG:HD3	15:a:163:TYR:CZ	2.45	0.51
14:Z:181:LEU:HD21	14:Z:211:PHE:HE1	1.75	0.51
17:c:379:CYS:SG	17:c:381:GLN:HG2	2.50	0.51
20:f:40:MET:O	20:f:43:VAL:HG12	2.10	0.51
24:j:385:TYR:OH	51:Ao:40:UNK:N	2.44	0.51
3:C:327:ALA:HA	7:G:51:PRO:CB	2.40	0.51
4:D:24:THR:O	4:D:25:SER:C	2.53	0.51
12:W:85:GLU:HB2	12:W:144:LYS:NZ	2.25	0.51
13:Y:53:CYS:HA	13:Y:56:VAL:HG12	1.93	0.51
14:Z:108:LYS:HG3	14:Z:436:ASP:OD1	2.11	0.51
18:d:133:GLN:NE2	18:d:187:GLN:HE21	2.06	0.51
20:f:30:TRP:CG	20:f:71:MET:HE2	2.46	0.51
24:j:33:PRO:HB2	24:j:105:MET:HE2	1.93	0.51
24:j:297:ASP:CG	24:j:300:LYS:H	2.19	0.51
25:k:93:PHE:CE2	25:k:97:LEU:HD11	2.46	0.51
1:A:21:ASN:CB	1:A:217:SER:CB	2.89	0.51
11:K:23:LEU:CB	10:L:18:SER:O	2.59	0.51
1:M:45:SER:CB	1:M:92:ARG:HA	2.40	0.51
12:W:111:LEU:HD12	12:W:163:ALA:HB2	1.92	0.51
17:c:73:PRO:O	17:c:76:ILE:HG12	2.11	0.51
17:c:244:ASN:CB	68:c:502:FMN:O2P	2.59	0.51
4:D:30:PHE:O	4:D:31:GLN:C	2.53	0.51
2:N:112:LEU:O	2:N:113:ARG:C	2.54	0.51
9:U:58:GLN:O	9:U:59:ALA:HB2	2.11	0.51
17:c:119:GLU:CB	17:c:162:PHE:CE2	2.92	0.51
17:c:222:LYS:HB3	17:c:381:GLN:OE1	2.10	0.51
20:f:31:ILE:HG23	23:i:66:PHE:HE2	1.76	0.51
24:j:106:TRP:O	24:j:109:HIS:ND1	2.33	0.51
24:j:199:GLN:N	24:j:199:GLN:OE1	2.42	0.51
29:p:263:PHE:HA	29:p:333:PRO:O	2.09	0.51
3:C:341:GLN:O	3:C:342:PRO:C	2.52	0.51
13:Y:121:LEU:HD21	13:Y:139:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:365:SER:OG	13:Y:367:CYS:SG	2.58	0.51
13:Y:456:ALA:O	13:Y:499:ASN:ND2	2.42	0.51
14:Z:272:THR:O	14:Z:327:TYR:HB2	2.11	0.51
20:f:277:ILE:O	20:f:280:THR:OG1	2.24	0.51
22:h:319:HIS:HA	22:h:322:THR:HG22	1.92	0.51
2:B:88:GLY:O	2:B:91:ALA:HB3	2.11	0.50
4:P:146:GLY:O	4:P:148:TYR:N	2.42	0.50
13:Y:34:VAL:HG21	13:Y:96:VAL:HB	1.93	0.50
13:Y:50:LEU:O	13:Y:54:GLU:HG2	2.11	0.50
16:b:148:ASP:OD1	16:b:148:ASP:N	2.41	0.50
17:c:77:LEU:HG	17:c:81:LYS:HE3	1.93	0.50
17:c:320:GLY:HA2	17:c:353:ALA:HB3	1.92	0.50
20:f:337:LEU:C	20:f:339:MET:H	2.19	0.50
22:h:196:TRP:CD1	22:h:250:LEU:HD22	2.45	0.50
2:B:38:LEU:O	2:B:40:ASN:N	2.45	0.50
4:D:153:PHE:O	4:D:154:PRO:C	2.54	0.50
8:H:27:LEU:O	8:H:30:CYS:N	2.38	0.50
1:M:151:ASN:O	1:M:152:TYR:C	2.53	0.50
1:M:426:GLY:HA2	1:M:427:PRO:C	2.36	0.50
4:P:27:ARG:O	4:P:28:ARG:C	2.52	0.50
13:Y:372:PHE:HD1	13:Y:481:LEU:HD12	1.76	0.50
13:Y:372:PHE:CE1	13:Y:481:LEU:HD13	2.46	0.50
15:a:78:ARG:NH1	19:e:57:THR:HG22	2.26	0.50
15:a:154:GLY:O	15:a:158:ASN:ND2	2.45	0.50
18:d:213:ILE:HG22	18:d:214:PRO:O	2.12	0.50
20:f:34:GLU:OE2	23:i:70:GLU:HB3	2.12	0.50
21:g:104:TYR:HE2	25:k:169:MET:HG3	1.76	0.50
22:h:12:LEU:HB2	22:h:13:PRO:HD3	1.93	0.50
22:h:237:LYS:HZ1	22:h:319:HIS:CE1	2.28	0.50
3:C:210:GLY:HA3	3:C:314:SER:CB	2.40	0.50
5:E:145:VAL:CB	3:O:262:LEU:O	2.60	0.50
2:N:97:SER:CA	9:U:70:LEU:CB	2.89	0.50
2:N:395:PRO:O	2:N:396:SER:C	2.52	0.50
18:d:214:PRO:HG2	18:d:216:PRO:HG3	1.94	0.50
6:F:96:GLU:O	6:F:99:ARG:N	2.45	0.50
2:N:98:VAL:O	9:U:69:SER:N	2.44	0.50
2:N:100:SER:N	9:U:67:SER:O	2.44	0.50
13:Y:560:LEU:HA	13:Y:563:ASP:O	2.11	0.50
16:b:64:THR:O	16:b:67:VAL:HG12	2.11	0.50
17:c:125:CYS:HB2	18:d:180:CYS:N	2.26	0.50
17:c:446:LEU:O	17:c:450:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:24:SER:HA	20:f:86:ILE:HD11	1.93	0.50
1:A:243:HIS:HA	7:G:13:VAL:O	2.12	0.50
3:O:130:GLY:O	64:O:401:HEM:HAA1	2.11	0.50
4:P:69:GLU:HA	4:P:73:GLY:HA2	1.93	0.50
13:Y:403:VAL:HA	13:Y:432:ILE:O	2.10	0.50
15:a:84:PRO:HA	15:a:122:VAL:O	2.11	0.50
17:c:125:CYS:SG	18:d:179:ALA:HA	2.52	0.50
18:d:104:ILE:HG22	18:d:105:LEU:HD12	1.92	0.50
20:f:112:HIS:HB2	20:f:184:ILE:CD1	2.37	0.50
24:j:396:ILE:HD11	24:j:413:LEU:HD23	1.93	0.50
1:A:272:VAL:O	1:A:275:ALA:HB3	2.12	0.50
2:N:255:ALA:CB	2:N:426:ALA:HB2	2.42	0.50
13:Y:341:ILE:HB	13:Y:546:PHE:CD1	2.45	0.50
15:a:179:VAL:HG21	15:a:182:TYR:OH	2.11	0.50
19:e:70:MET:HA	19:e:73:ILE:HG22	1.94	0.50
20:f:331:VAL:HG21	57:Al:43:SER:HA	1.93	0.50
21:g:6:THR:O	21:g:10:ASN:ND2	2.34	0.50
21:g:71:LEU:O	21:g:74:PRO:HD2	2.11	0.50
1:A:296:SER:O	1:A:297:ILE:C	2.55	0.50
2:B:342:ASN:O	2:B:345:LYS:CB	2.60	0.50
7:G:52:PHE:O	7:G:53:VAL:C	2.54	0.50
5:Q:75:GLU:O	5:Q:194:ILE:CA	2.47	0.50
14:Z:292:MET:HG3	14:Z:431:HIS:CD2	2.47	0.50
22:h:207:MET:HE1	22:h:240:GLY:HA2	1.92	0.50
24:j:313:MET:HB3	24:j:328:HIS:HD2	1.76	0.50
1:A:286:GLY:O	1:A:287:GLY:O	2.30	0.50
12:W:113:ASP:CG	12:W:131:ASN:HD22	2.20	0.50
13:Y:161:GLU:OE1	13:Y:161:GLU:N	2.36	0.50
17:c:330:SER:HA	17:c:333:GLU:HB2	1.94	0.50
19:e:126:LYS:HD2	21:g:38:GLU:OE2	2.12	0.50
20:f:163:LEU:HD23	20:f:285:THR:HG21	1.93	0.50
21:g:67:LEU:HD21	23:i:68:ALA:HB3	1.94	0.50
7:G:40:ARG:O	7:G:41:THR:C	2.55	0.50
3:O:4:ILE:O	3:O:5:ARG:C	2.55	0.50
4:P:24:THR:O	4:P:25:SER:C	2.54	0.50
4:P:100:ALA:O	4:P:103:ALA:N	2.45	0.50
6:R:46:ALA:O	6:R:47:ILE:C	2.53	0.50
13:Y:299:ARG:HD2	13:Y:705:GLN:NE2	2.26	0.50
13:Y:299:ARG:HG2	13:Y:300:GLN:H	1.77	0.50
13:Y:333:PHE:HB3	13:Y:337:ASP:HB2	1.94	0.50
13:Y:358:LEU:HB3	13:Y:364:ASP:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:203:LYS:HD2	16:b:178:GLU:OE2	2.11	0.50
24:j:347:ILE:HG23	24:j:352:ASP:HA	1.93	0.50
29:p:206:ILE:HA	29:p:241:TYR:H	1.76	0.50
54:Ag:13:PRO:O	54:Ag:15:GLY:N	2.45	0.50
3:C:125:ALA:O	3:C:126:THR:C	2.53	0.49
1:M:307:PHE:HA	1:M:323:HIS:O	2.12	0.49
13:Y:158:ARG:HH22	13:Y:178:GLN:HE22	1.60	0.49
13:Y:372:PHE:CE1	13:Y:481:LEU:CD1	2.95	0.49
13:Y:645:ARG:HA	13:Y:648:GLU:HG2	1.93	0.49
17:c:183:GLY:O	17:c:192:ASP:HA	2.12	0.49
24:j:527:GLY:C	24:j:529:TYR:H	2.20	0.49
3:O:64:SER:O	3:O:65:SER:C	2.55	0.49
14:Z:230:GLY:O	14:Z:358:VAL:HG23	2.12	0.49
17:c:121:GLU:N	17:c:204:TYR:HE1	2.08	0.49
23:i:26:LEU:HD11	23:i:78:LEU:HD13	1.93	0.49
2:B:97:SER:HA	9:I:70:LEU:CA	2.39	0.49
3:C:132:VAL:HA	3:C:139:SER:CB	2.42	0.49
4:D:23:HIS:O	4:D:24:THR:C	2.55	0.49
9:I:60:ALA:HB3	9:I:63:PRO:O	2.13	0.49
13:Y:172:ILE:HG13	13:Y:175:ARG:HH22	1.76	0.49
13:Y:383:SER:HA	13:Y:386:LEU:HD12	1.93	0.49
13:Y:595:THR:HA	13:Y:605:GLN:HA	1.94	0.49
17:c:406:PRO:O	17:c:409:ILE:HG12	2.12	0.49
20:f:159:MET:HB2	20:f:278:MET:CE	2.41	0.49
22:h:208:PRO:HG3	22:h:216:LEU:HD13	1.94	0.49
1:A:395:TRP:O	1:A:398:ARG:N	2.45	0.49
4:D:161:ALA:O	4:D:163:PRO:N	2.45	0.49
5:Q:107:ASP:O	5:Q:108:GLN:C	2.55	0.49
13:Y:126:LEU:HD21	14:Z:375:MET:HA	1.95	0.49
13:Y:525:ALA:O	13:Y:529:GLY:N	2.45	0.49
15:a:150:VAL:HG23	15:a:179:VAL:HA	1.95	0.49
16:b:83:THR:OG1	19:e:35:LYS:HE2	2.11	0.49
17:c:120:GLY:HA3	17:c:204:TYR:CE1	2.46	0.49
19:e:280:PHE:O	19:e:281:ARG:HB3	2.12	0.49
20:f:7:THR:HA	20:f:10:ILE:HG22	1.93	0.49
20:f:33:PHE:HE1	20:f:137:ALA:HB1	1.75	0.49
22:h:418:LYS:HG2	22:h:419:TYR:O	2.12	0.49
24:j:74:VAL:HG21	24:j:190:LEU:HD11	1.93	0.49
24:j:139:GLN:HA	24:j:142:ILE:HG22	1.93	0.49
24:j:178:GLY:HA2	24:j:218:LEU:HD23	1.95	0.49
2:B:112:LEU:O	2:B:113:ARG:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:51:GLN:NE2	34:w:156:LYS:O	2.43	0.49
13:Y:131:CYS:SG	13:Y:229:GLY:HA3	2.52	0.49
13:Y:341:ILE:HD11	13:Y:538:ARG:HH12	1.77	0.49
14:Z:447:VAL:O	14:Z:450:ILE:HG22	2.12	0.49
17:c:132:ARG:HA	17:c:165:GLU:CD	2.37	0.49
18:d:129:LYS:H	18:d:168:LEU:HA	1.77	0.49
22:h:221:VAL:HG13	22:h:340:ARG:HH11	1.77	0.49
23:i:10:MET:HE1	25:k:103:MET:SD	2.53	0.49
23:i:53:PHE:CE1	28:o:21:GLN:HA	2.47	0.49
24:j:416:THR:O	24:j:419:THR:OG1	2.29	0.49
55:Aj:35:LYS:O	55:Aj:39:LEU:N	2.44	0.49
3:O:91:PHE:O	3:O:92:ILE:C	2.52	0.49
13:Y:136:GLU:OE1	13:Y:242:PRO:HG2	2.13	0.49
13:Y:405:THR:OG1	13:Y:479:SER:CB	2.52	0.49
17:c:371:ILE:HD12	17:c:396:MET:HG3	1.94	0.49
20:f:311:MET:HG3	20:f:315:TRP:HE1	1.78	0.49
23:i:52:HIS:ND1	25:k:138:GLU:OE1	2.45	0.49
24:j:51:LEU:O	24:j:55:MET:HG2	2.13	0.49
24:j:449:LEU:HD12	24:j:450:LEU:N	2.27	0.49
2:B:122:PHE:O	2:B:123:LEU:C	2.52	0.49
4:D:26:ILE:O	4:D:27:ARG:C	2.56	0.49
3:O:315:MET:O	3:O:318:ARG:N	2.40	0.49
6:R:95:LYS:O	6:R:96:GLU:C	2.53	0.49
14:Z:139:LEU:O	14:Z:141:TYR:N	2.46	0.49
17:c:79:GLU:HG3	17:c:254:ILE:HG22	1.93	0.49
17:c:137:LYS:HZ1	17:c:256:ARG:HH22	1.61	0.49
24:j:26:ILE:O	24:j:29:THR:OG1	2.18	0.49
25:k:34:ILE:HG12	25:k:61:LEU:CD1	2.43	0.49
32:Aa:138:LEU:O	32:Aa:140:CYS:N	2.45	0.49
2:B:255:ALA:HA	2:B:425:ALA:O	2.12	0.49
2:B:294:SER:O	2:B:295:LEU:C	2.55	0.49
4:D:180:SER:CB	8:H:17:LEU:CB	2.91	0.49
1:M:4:TYR:O	1:M:5:ALA:C	2.56	0.49
4:P:153:PHE:O	4:P:156:GLN:N	2.36	0.49
15:a:136:ALA:HB2	21:g:41:PHE:CE1	2.48	0.49
20:f:111:PHE:HA	24:j:591:PHE:CE1	2.48	0.49
22:h:18:SER:HB2	22:h:23:ILE:HG22	1.93	0.49
24:j:296:ASN:HA	24:j:356:ILE:HG12	1.94	0.49
3:O:210:GLY:HA3	3:O:314:SER:CB	2.42	0.49
4:P:31:GLN:O	4:P:32:VAL:C	2.56	0.49
13:Y:223:ILE:HD13	13:Y:233:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:234:LYS:N	13:Y:235:PRO:HD2	2.28	0.49
13:Y:308:ARG:HG2	13:Y:581:ASP:HA	1.94	0.49
15:a:102:PRO:O	16:b:83:THR:HG22	2.13	0.49
19:e:87:VAL:HG23	19:e:95:LEU:HD22	1.94	0.49
19:e:105:MET:HG3	19:e:237:PHE:CE1	2.48	0.49
22:h:25:ILE:O	22:h:29:VAL:HG12	2.13	0.49
24:j:109:HIS:HE1	24:j:348:HIS:HE1	1.60	0.49
25:k:76:THR:HG23	25:k:77:GLU:N	2.27	0.49
4:P:235:LEU:HA	7:S:14:ILE:O	2.12	0.49
13:Y:213:MET:HG2	13:Y:215:MET:HG3	1.95	0.49
13:Y:336:ASN:N	13:Y:363:SER:HB2	2.27	0.49
13:Y:574:ASP:O	13:Y:576:GLY:N	2.46	0.49
14:Z:346:GLN:O	14:Z:350:LYS:HG2	2.13	0.49
17:c:53:LEU:O	17:c:57:GLN:HG3	2.13	0.49
17:c:62:TRP:NE1	17:c:140:GLU:HG2	2.28	0.49
1:A:51:LYS:O	1:A:53:ASN:N	2.46	0.48
8:H:68:CYS:O	8:H:69:VAL:C	2.55	0.48
2:N:254:HIS:O	2:N:426:ALA:HA	2.13	0.48
15:a:79:ARG:O	15:a:201:GLN:NE2	2.46	0.48
15:a:190:ALA:O	15:a:193:LEU:HB3	2.12	0.48
19:e:290:TRP:HZ3	21:g:65:PHE:CE2	2.30	0.48
20:f:59:TYR:OH	20:f:134:GLN:NE2	2.46	0.48
20:f:125:GLN:O	20:f:128:LEU:HG	2.13	0.48
22:h:7:PRO:HA	22:h:10:MET:HB2	1.94	0.48
22:h:71:TRP:O	22:h:74:PRO:HD2	2.12	0.48
22:h:297:VAL:O	22:h:301:ILE:HG12	2.13	0.48
24:j:223:LYS:HB2	24:j:256:GLY:HA3	1.94	0.48
24:j:297:ASP:OD1	24:j:299:LYS:N	2.45	0.48
29:p:205:ASP:C	69:p:401:NDP:H71N	2.19	0.48
1:A:106:LEU:O	1:A:107:PRO:C	2.56	0.48
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.48
3:C:213:SER:O	3:C:214:ASP:C	2.56	0.48
1:M:184:GLU:O	1:M:185:TYR:C	2.56	0.48
5:Q:102:THR:O	5:Q:105:GLU:N	2.46	0.48
12:W:94:ILE:HB	12:W:95:PRO:HD3	1.94	0.48
15:a:159:GLY:C	15:a:161:GLY:H	2.19	0.48
17:c:317:VAL:HG22	17:c:356:VAL:HA	1.95	0.48
24:j:15:LEU:O	24:j:18:PRO:HD2	2.13	0.48
1:A:426:GLY:CA	1:A:427:PRO:C	2.86	0.48
3:C:73:VAL:CB	5:E:65:SER:CB	2.91	0.48
11:K:18:VAL:O	11:K:22:SER:CA	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:GLU:O	1:M:82:MET:N	2.46	0.48
4:P:178:THR:O	4:P:179:MET:C	2.55	0.48
6:R:103:GLU:O	6:R:104:ARG:C	2.55	0.48
12:W:71:LYS:HB3	12:W:72:TYR:CD2	2.48	0.48
14:Z:102:SER:OG	14:Z:103:GLY:N	2.46	0.48
14:Z:329:ARG:O	14:Z:333:ARG:HG2	2.14	0.48
15:a:102:PRO:HA	19:e:34:ARG:HB3	1.94	0.48
16:b:159:GLN:HE21	16:b:212:ARG:NH1	2.11	0.48
19:e:257:ILE:O	19:e:261:LEU:HD13	2.13	0.48
20:f:172:GLN:NE2	24:j:578:SER:OG	2.46	0.48
20:f:312:LYS:HA	20:f:315:TRP:CE2	2.48	0.48
21:g:73:LEU:O	21:g:76:PRO:HD2	2.13	0.48
1:A:289:HIS:O	1:A:290:LEU:C	2.55	0.48
10:L:4:THR:O	10:L:5:LEU:C	2.57	0.48
1:M:286:GLY:O	1:M:287:GLY:C	2.56	0.48
13:Y:454:ASP:O	13:Y:459:ASN:N	2.41	0.48
15:a:129:LEU:HD23	15:a:130:THR:N	2.29	0.48
2:B:140:LEU:O	2:B:142:PRO:N	2.47	0.48
3:C:312:GLN:O	3:C:313:ARG:C	2.53	0.48
65:D:301:HEC:HHA	65:D:301:HEC:HBD1	1.95	0.48
6:F:46:ALA:O	6:F:47:ILE:C	2.56	0.48
12:W:88:ILE:HG22	12:W:89:HIS:O	2.12	0.48
14:Z:242:ASP:OD1	14:Z:243:ASP:N	2.47	0.48
14:Z:444:LEU:O	14:Z:447:VAL:HG12	2.14	0.48
17:c:147:ARG:C	17:c:150:GLY:H	2.21	0.48
20:f:71:MET:HG3	23:i:40:LEU:HD23	1.94	0.48
20:f:175:LEU:HD21	20:f:230:LEU:HD22	1.95	0.48
30:q:85:LEU:CB	30:q:158:GLY:C	2.87	0.48
59:An:103:GLN:O	59:An:106:LYS:N	2.45	0.48
6:F:45:GLU:O	6:F:46:ALA:O	2.31	0.48
7:G:33:GLY:O	7:G:34:ILE:C	2.56	0.48
2:N:360:ALA:O	2:N:363:LYS:N	2.47	0.48
6:R:32:MET:O	6:R:33:ARG:C	2.55	0.48
13:Y:76:ARG:HH11	17:c:424:ILE:HG22	1.78	0.48
14:Z:252:SER:HA	14:Z:255:ILE:HG22	1.96	0.48
16:b:131:GLU:O	16:b:143:THR:OG1	2.19	0.48
18:d:110:MET:O	18:d:114:GLU:HG3	2.14	0.48
18:d:197:THR:O	18:d:201:ILE:HD12	2.13	0.48
20:f:174:GLN:HA	20:f:226:THR:HA	1.96	0.48
20:f:244:MET:O	20:f:248:LEU:HD13	2.12	0.48
24:j:124:PHE:HE1	24:j:147:VAL:HG13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:489:THR:HA	24:j:492:ILE:HG22	1.94	0.48
1:A:157:ALA:O	1:A:236:PHE:C	2.56	0.48
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.44	0.48
1:M:426:GLY:HA3	1:M:428:ILE:N	2.24	0.48
5:Q:163:SER:HA	5:Q:173:LYS:O	2.14	0.48
13:Y:302:LEU:HD22	13:Y:570:GLY:O	2.14	0.48
13:Y:546:PHE:CD2	13:Y:549:GLY:HA3	2.48	0.48
14:Z:156:GLU:OE2	14:Z:163:PRO:HG3	2.14	0.48
14:Z:270:ASN:C	19:e:284:GLN:HE22	2.21	0.48
14:Z:288:PHE:CE1	14:Z:431:HIS:HA	2.48	0.48
17:c:295:PRO:O	17:c:298:GLU:HB3	2.14	0.48
18:d:183:ALA:HB1	18:d:184:PRO:HD2	1.93	0.48
21:g:81:THR:HG21	25:k:148:SER:HB3	1.95	0.48
24:j:281:GLY:O	24:j:285:THR:HG23	2.14	0.48
24:j:312:LEU:O	24:j:315:VAL:HG22	2.14	0.48
24:j:504:LEU:O	24:j:507:THR:OG1	2.23	0.48
25:k:8:ILE:O	25:k:12:ILE:HD12	2.14	0.48
47:y:507:GLU:O	47:y:508:PRO:O	2.32	0.48
1:A:157:ALA:HA	1:A:237:THR:O	2.13	0.48
2:B:235:ALA:O	2:B:236:LYS:CB	2.61	0.48
12:W:55:HIS:HD2	12:W:78:VAL:HG11	1.77	0.48
12:W:187:ILE:HD12	14:Z:113:ILE:HD11	1.96	0.48
13:Y:83:GLU:HB2	13:Y:101:ASN:O	2.12	0.48
13:Y:133:GLN:HB3	67:Y:801:SF4:S2	2.54	0.48
13:Y:236:TYR:CE2	13:Y:272:ARG:HD3	2.48	0.48
13:Y:308:ARG:NE	13:Y:312:GLY:O	2.47	0.48
13:Y:543:LYS:HG3	13:Y:565:PHE:CD2	2.49	0.48
14:Z:408:GLY:O	14:Z:425:LYS:N	2.46	0.48
15:a:106:MET:HE1	15:a:113:PHE:CE1	2.48	0.48
17:c:331:VAL:O	17:c:335:VAL:HG22	2.14	0.48
19:e:28:LEU:O	19:e:32:GLN:HG2	2.13	0.48
20:f:174:GLN:HE21	20:f:177:LYS:HE2	1.79	0.48
24:j:96:VAL:O	24:j:100:ILE:HG12	2.14	0.48
47:y:115:SER:O	47:y:121:GLY:HA2	2.13	0.48
1:M:170:PRO:O	1:M:171:SER:C	2.55	0.48
2:N:194:TYR:O	2:N:195:VAL:C	2.55	0.48
13:Y:39:GLN:NE2	13:Y:56:VAL:HG21	2.29	0.48
13:Y:301:ARG:NE	13:Y:613:PRO:HG3	2.21	0.48
14:Z:426:ALA:HB1	14:Z:460:GLU:HG2	1.96	0.48
19:e:172:ILE:O	19:e:173:TRP:HB2	2.14	0.48
23:i:7:ASN:HD22	25:k:10:SER:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:227:PHE:O	24:j:230:HIS:ND1	2.46	0.48
10:J:51:LEU:O	10:J:54:HIS:N	2.46	0.48
1:M:276:ILE:O	1:M:277:ILE:C	2.57	0.48
1:M:280:TYR:O	1:M:306:SER:HA	2.14	0.48
13:Y:153:PHE:C	13:Y:154:LEU:HD12	2.39	0.48
24:j:338:MET:SD	24:j:457:LEU:HB3	2.53	0.48
29:p:208:GLY:O	29:p:211:ASP:CB	2.62	0.48
3:C:37:LEU:CB	64:C:402:HEM:HMB2	2.44	0.47
1:M:239:SER:CB	7:S:18:LEU:HA	2.44	0.47
3:O:278:TYR:O	3:O:279:ALA:C	2.55	0.47
12:W:114:LEU:HG	12:W:170:ILE:HD11	1.96	0.47
12:W:204:LEU:HD23	14:Z:126:TYR:CE1	2.49	0.47
13:Y:170:LYS:HB3	13:Y:232:THR:O	2.14	0.47
13:Y:173:MET:C	13:Y:175:ARG:N	2.72	0.47
13:Y:342:ALA:HA	13:Y:547:LEU:HB2	1.96	0.47
20:f:88:LYS:HG2	20:f:89:MET:O	2.14	0.47
1:A:77:LYS:O	1:A:81:SER:N	2.38	0.47
4:D:93:LYS:O	4:D:94:PRO:C	2.56	0.47
3:O:341:GLN:O	3:O:342:PRO:C	2.55	0.47
13:Y:540:ASN:HA	13:Y:541:PRO:HD3	1.63	0.47
13:Y:557:ARG:O	13:Y:560:LEU:HB2	2.14	0.47
15:a:131:ASN:N	15:a:168:SER:O	2.48	0.47
16:b:76:TYR:HA	16:b:79:ARG:HH21	1.79	0.47
20:f:181:TYR:O	20:f:184:ILE:HG22	2.14	0.47
22:h:282:LEU:HD11	22:h:410:MET:HE3	1.96	0.47
23:i:27:MET:HE2	25:k:71:THR:OG1	2.14	0.47
24:j:562:LEU:HG	24:j:563:PRO:HD3	1.97	0.47
55:Aj:144:SER:O	55:Aj:146:LEU:N	2.40	0.47
1:A:261:GLY:HA2	1:A:314:TYR:O	2.13	0.47
6:F:43:VAL:O	6:F:44:LYS:C	2.58	0.47
6:F:95:LYS:O	6:F:96:GLU:C	2.57	0.47
8:H:22:GLU:O	8:H:23:GLN:C	2.57	0.47
2:N:267:ALA:O	2:N:268:GLU:C	2.56	0.47
2:N:360:ALA:O	2:N:361:LYS:C	2.58	0.47
3:O:277:ALA:O	3:O:278:TYR:C	2.57	0.47
4:P:74:PRO:O	4:P:79:GLU:N	2.42	0.47
6:R:32:MET:O	6:R:35:ASP:N	2.40	0.47
13:Y:598:ASN:HB3	13:Y:602:ARG:HB3	1.96	0.47
17:c:324:THR:OG1	17:c:437:GLY:HA3	2.14	0.47
20:f:120:GLN:HE21	20:f:177:LYS:HE2	1.79	0.47
24:j:109:HIS:HE1	24:j:348:HIS:CE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:LEU:O	2:B:217:LYS:C	2.58	0.47
3:C:317:PHE:O	6:F:24:ALA:CB	2.61	0.47
6:F:45:GLU:O	6:F:46:ALA:C	2.56	0.47
1:M:251:ALA:O	1:M:325:VAL:HA	2.15	0.47
5:Q:114:VAL:O	5:Q:117:LEU:CB	2.63	0.47
17:c:119:GLU:H	17:c:159:ARG:CD	2.26	0.47
18:d:183:ALA:HB1	18:d:184:PRO:CD	2.45	0.47
20:f:124:LEU:HB2	20:f:220:ILE:HD11	1.95	0.47
20:f:228:LEU:O	20:f:231:SER:OG	2.12	0.47
22:h:355:MET:HE2	22:h:358:TRP:CD1	2.49	0.47
1:A:152:TYR:O	1:A:153:LEU:C	2.57	0.47
6:F:99:ARG:O	6:F:100:GLU:C	2.57	0.47
1:M:81:SER:CB	2:N:359:ALA:HB1	2.44	0.47
2:N:262:ALA:HB3	2:N:269:ALA:CA	2.44	0.47
14:Z:198:THR:OG1	19:e:275:ALA:O	2.26	0.47
14:Z:325:ASP:N	14:Z:325:ASP:OD1	2.46	0.47
20:f:124:LEU:HD21	20:f:176:ARG:HG2	1.96	0.47
3:C:254:ASP:O	4:D:119:ALA:HA	2.14	0.47
7:G:56:TYR:O	7:G:57:LEU:C	2.56	0.47
2:N:313:ASN:CA	9:U:59:ALA:HB2	2.44	0.47
12:W:124:ASN:ND2	12:W:146:TYR:HD2	2.12	0.47
12:W:147:THR:HG22	12:W:148:ASP:O	2.14	0.47
13:Y:421:SER:HA	13:Y:424:HIS:HB2	1.95	0.47
14:Z:135:TYR:CZ	15:a:162:TYR:CE2	2.99	0.47
19:e:126:LYS:NZ	21:g:45:GLY:O	2.43	0.47
19:e:135:ALA:CB	19:e:201:THR:HG22	2.44	0.47
20:f:106:LEU:HD12	20:f:138:PRO:HB2	1.96	0.47
24:j:233:LEU:HB3	24:j:234:PRO:HD3	1.96	0.47
29:p:209:ARG:CB	29:p:352:VAL:CA	2.78	0.47
2:B:271:ALA:O	2:B:272:PHE:C	2.58	0.47
3:C:74:ASN:N	5:E:64:ALA:O	2.46	0.47
4:D:117:VAL:O	4:D:123:GLY:HA2	2.15	0.47
1:M:134:ILE:O	1:M:137:GLU:N	2.47	0.47
2:N:84:LYS:O	2:N:85:ILE:C	2.56	0.47
3:O:61:THR:O	3:O:64:SER:N	2.48	0.47
3:O:347:TYR:O	3:O:348:ILE:C	2.58	0.47
4:P:190:LEU:O	4:P:191:ARG:C	2.55	0.47
13:Y:35:PHE:N	13:Y:100:TRP:O	2.41	0.47
13:Y:173:MET:C	13:Y:175:ARG:H	2.18	0.47
13:Y:348:ALA:HA	13:Y:351:LEU:HG	1.96	0.47
13:Y:568:TYR:CE1	13:Y:576:GLY:HA3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:266:ARG:HG2	14:Z:270:ASN:HD21	1.79	0.47
15:a:159:GLY:HA2	15:a:172:GLY:CA	2.44	0.47
17:c:320:GLY:N	17:c:353:ALA:O	2.48	0.47
17:c:357:MET:HG2	18:d:142:LEU:HD21	1.96	0.47
18:d:70:TYR:HE2	18:d:78:ALA:HA	1.79	0.47
19:e:111:LEU:HD21	25:k:61:LEU:HD21	1.96	0.47
19:e:196:ALA:O	19:e:199:ASP:HB2	2.15	0.47
20:f:279:PRO:HA	20:f:282:MET:HE2	1.97	0.47
22:h:325:MET:HA	22:h:440:HIS:ND1	2.30	0.47
22:h:339:SER:OG	22:h:344:LEU:HB2	2.15	0.47
22:h:400:MET:HG2	24:j:176:ARG:HD2	1.97	0.47
24:j:126:ILE:O	24:j:130:ILE:HG12	2.14	0.47
4:D:74:PRO:O	4:D:79:GLU:N	2.35	0.47
1:M:130:GLU:O	1:M:131:ARG:C	2.57	0.47
1:M:222:THR:O	1:M:226:ASP:N	2.33	0.47
5:Q:147:ILE:O	5:Q:148:ALA:C	2.57	0.47
13:Y:93:ALA:HB2	17:c:225:LEU:HD21	1.96	0.47
13:Y:472:PRO:HB2	13:Y:500:ILE:HD13	1.96	0.47
14:Z:211:PHE:CE2	15:a:98:HIS:CE1	2.93	0.47
17:c:220:GLN:O	17:c:222:LYS:N	2.46	0.47
17:c:398:ARG:O	17:c:402:GLY:N	2.47	0.47
23:i:10:MET:SD	25:k:103:MET:HG3	2.55	0.47
24:j:67:HIS:HA	24:j:77:SER:HB2	1.96	0.47
24:j:246:LEU:HD23	24:j:247:LEU:HD23	1.96	0.47
24:j:419:THR:HA	24:j:422:TYR:CE2	2.49	0.47
29:p:205:ASP:CA	69:p:401:NDP:C4N	2.84	0.47
60:Aw:32:UNK:O	60:Aw:36:UNK:N	2.48	0.47
1:A:246:ASP:CB	7:G:10:VAL:H	2.28	0.47
7:G:44:CYS:O	7:G:45:ILE:C	2.57	0.47
2:N:99:THR:HA	9:U:68:VAL:HA	1.96	0.47
3:O:372:ILE:O	3:O:375:LYS:N	2.45	0.47
4:P:235:LEU:HA	7:S:15:THR:HA	1.95	0.47
12:W:124:ASN:HD21	12:W:146:TYR:HD2	1.62	0.47
15:a:99:MET:HE3	15:a:113:PHE:CZ	2.50	0.47
1:M:62:LEU:O	1:M:63:ALA:C	2.57	0.47
1:M:395:TRP:O	1:M:396:GLU:C	2.57	0.47
13:Y:123:ASN:ND2	17:c:387:GLU:OE2	2.27	0.47
13:Y:226:CYS:SG	13:Y:227:PRO:HD2	2.55	0.47
13:Y:372:PHE:CD1	13:Y:481:LEU:HD12	2.50	0.47
18:d:143:ARG:HB3	18:d:184:PRO:HD3	1.96	0.47
22:h:50:LEU:HD23	22:h:51:ASN:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:21:MET:O	24:j:24:SER:OG	2.23	0.47
24:j:124:PHE:CE1	24:j:147:VAL:HG13	2.50	0.47
24:j:158:TRP:CZ2	24:j:240:PRO:HB3	2.50	0.47
24:j:511:LEU:HB3	24:j:512:LYS:H	1.48	0.47
25:k:55:MET:O	25:k:59:ILE:N	2.38	0.47
10:L:50:LYS:CB	4:P:21:LEU:O	2.63	0.46
1:M:219:LEU:O	1:M:220:SER:C	2.57	0.46
13:Y:206:VAL:HG11	67:Y:802:SF4:S2	2.56	0.46
14:Z:177:ILE:HG23	14:Z:210:MET:HE2	1.97	0.46
14:Z:395:ALA:CB	14:Z:412:VAL:HG12	2.45	0.46
15:a:117:PRO:HA	15:a:120:SER:OG	2.15	0.46
17:c:75:TRP:O	17:c:79:GLU:N	2.43	0.46
17:c:85:LEU:HD21	17:c:247:THR:HG23	1.98	0.46
17:c:278:ILE:HG13	17:c:282:VAL:HG11	1.96	0.46
17:c:297:LYS:HG2	17:c:332:CYS:CB	2.39	0.46
18:d:132:ILE:HA	18:d:188:ILE:HG12	1.97	0.46
20:f:68:MET:HB3	23:i:36:MET:SD	2.56	0.46
23:i:53:PHE:HE1	28:o:20:ILE:O	1.97	0.46
24:j:270:ASN:O	24:j:274:GLN:NE2	2.43	0.46
54:Ag:98:GLY:O	54:Ag:102:GLY:N	2.47	0.46
1:A:84:ALA:CA	1:A:100:LYS:O	2.63	0.46
3:C:8:HIS:O	3:C:9:PRO:C	2.57	0.46
7:G:36:ASN:O	7:G:37:VAL:C	2.56	0.46
1:M:255:ILE:O	1:M:321:GLY:HA3	2.14	0.46
2:N:362:ASN:O	2:N:363:LYS:C	2.57	0.46
3:O:116:GLY:HA3	64:O:402:HEM:C3C	2.51	0.46
4:P:188:THR:O	4:P:189:PHE:C	2.55	0.46
13:Y:32:ILE:HG22	13:Y:33:GLU:O	2.15	0.46
15:a:78:ARG:CZ	15:a:147:PRO:HG3	2.45	0.46
19:e:146:LEU:O	19:e:149:ILE:HG13	2.15	0.46
19:e:172:ILE:CD1	31:r:46:GLY:HA2	2.45	0.46
19:e:303:TRP:CE2	19:e:307:LEU:HD11	2.50	0.46
22:h:235:LEU:O	22:h:238:LEU:HG	2.16	0.46
24:j:124:PHE:HA	24:j:150:MET:HG3	1.97	0.46
25:k:81:GLU:HB2	25:k:85:SER:HB3	1.96	0.46
2:B:341:TYR:O	2:B:342:ASN:C	2.57	0.46
1:M:252:HIS:O	1:M:424:GLY:HA2	2.16	0.46
2:N:99:THR:CB	2:N:106:ALA:HB3	2.44	0.46
13:Y:466:LEU:CD2	13:Y:496:ILE:CG2	2.92	0.46
14:Z:95:LEU:HD22	14:Z:458:PHE:HZ	1.79	0.46
24:j:399:VAL:HG12	24:j:409:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ae:95:LEU:C	52:Ae:98:LYS:H	2.23	0.46
2:N:269:ALA:O	2:N:270:ASN:C	2.58	0.46
2:N:338:LYS:O	2:N:339:ALA:C	2.58	0.46
13:Y:624:ARG:HH21	13:Y:637:ASP:HB2	1.79	0.46
19:e:77:LEU:HD22	19:e:115:SER:HB3	1.97	0.46
24:j:446:ASN:O	24:j:447:ASN:HB2	2.14	0.46
25:k:17:PHE:HA	25:k:20:PHE:HB3	1.98	0.46
1:A:372:THR:O	1:A:373:THR:C	2.58	0.46
1:A:433:ASP:O	1:A:434:TYR:C	2.56	0.46
3:C:136:GLY:O	3:C:139:SER:N	2.48	0.46
3:C:347:TYR:O	3:C:348:ILE:C	2.59	0.46
10:L:50:LYS:CA	4:P:22:ASP:HA	2.46	0.46
1:M:287:GLY:O	1:M:289:HIS:N	2.48	0.46
3:O:236:ILE:O	3:O:237:LEU:C	2.57	0.46
12:W:181:HIS:HD2	12:W:184:LEU:N	2.12	0.46
13:Y:32:ILE:HD12	13:Y:45:PRO:HA	1.97	0.46
13:Y:335:GLY:HA2	13:Y:362:ASP:HB2	1.96	0.46
16:b:77:LEU:HD12	19:e:31:MET:HE2	1.98	0.46
17:c:70:LEU:HD12	17:c:75:TRP:CE2	2.50	0.46
22:h:148:TYR:HE2	22:h:218:LYS:NZ	2.14	0.46
22:h:346:ARG:HG3	22:h:420:THR:OG1	2.15	0.46
25:k:54:LEU:HA	25:k:54:LEU:HD23	1.67	0.46
2:B:38:LEU:O	2:B:39:GLU:C	2.56	0.46
2:B:262:ALA:HB3	2:B:269:ALA:N	2.31	0.46
11:K:27:VAL:HA	10:L:25:VAL:CB	2.45	0.46
12:W:55:HIS:CD2	12:W:78:VAL:HG11	2.49	0.46
12:W:64:TYR:O	12:W:68:ILE:HG13	2.15	0.46
13:Y:49:VAL:HG23	13:Y:94:MET:O	2.15	0.46
13:Y:639:LEU:O	13:Y:643:ARG:HG3	2.16	0.46
14:Z:447:VAL:O	14:Z:451:ILE:HG13	2.16	0.46
15:a:199:GLN:HA	15:a:202:ARG:HE	1.81	0.46
18:d:148:ILE:O	18:d:152:ILE:HD12	2.16	0.46
22:h:225:ILE:HB	22:h:331:ASN:ND2	2.28	0.46
23:i:75:LEU:HD11	25:k:68:PHE:HE1	1.80	0.46
24:j:572:LYS:O	24:j:575:ILE:HG13	2.16	0.46
24:j:584:ILE:O	24:j:588:PHE:HB2	2.15	0.46
30:q:88:PHE:CB	30:q:162:GLU:CA	2.93	0.46
1:A:192:ALA:HA	1:A:194:ARG:N	2.31	0.46
1:M:256:ALA:CA	1:M:320:LEU:O	2.59	0.46
2:N:271:ALA:O	2:N:272:PHE:C	2.57	0.46
14:Z:223:HIS:CD2	15:a:187:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:431:HIS:HB3	14:Z:454:GLN:NE2	2.31	0.46
22:h:211:GLY:C	22:h:212:LEU:HD12	2.41	0.46
25:k:34:ILE:HG12	25:k:61:LEU:HD11	1.98	0.46
29:p:65:LEU:HA	29:p:66:GLY:HA2	1.65	0.46
2:B:57:TYR:O	2:B:233:SER:CB	2.63	0.46
1:M:245:GLU:C	1:M:247:GLY:H	2.24	0.46
13:Y:49:VAL:HA	13:Y:96:VAL:HG13	1.98	0.46
13:Y:403:VAL:HB	13:Y:476:LEU:HD12	1.97	0.46
15:a:76:TRP:HA	15:a:79:ARG:HG2	1.97	0.46
20:f:189:TRP:CZ2	20:f:282:MET:HG2	2.50	0.46
22:h:42:LEU:HD21	22:h:453:MET:HB3	1.98	0.46
1:A:198:ALA:O	1:A:199:ALA:CB	2.63	0.46
2:B:267:ALA:O	2:B:268:GLU:C	2.59	0.46
5:Q:138:VAL:O	5:Q:139:CYS:C	2.59	0.46
13:Y:173:MET:C	13:Y:174:THR:HG1	2.21	0.46
13:Y:490:LEU:HD23	13:Y:490:LEU:C	2.41	0.46
17:c:118:ASP:O	68:c:502:FMN:HM72	2.15	0.46
17:c:208:GLU:HA	68:c:502:FMN:O2'	2.16	0.46
20:f:142:LEU:HA	20:f:142:LEU:HD23	1.74	0.46
21:g:52:SER:HB3	21:g:55:PHE:CD2	2.51	0.46
22:h:59:ASP:CB	22:h:245:ARG:HH22	2.26	0.46
23:i:7:ASN:HD22	25:k:10:SER:HB2	1.81	0.46
24:j:491:LEU:O	24:j:495:ILE:HG12	2.16	0.46
10:L:23:THR:O	10:L:24:ILE:C	2.58	0.46
1:M:243:HIS:O	1:M:425:PHE:HA	2.16	0.46
1:M:378:ASP:O	1:M:382:SER:CB	2.64	0.46
12:W:204:LEU:HD12	12:W:205:SER:N	2.31	0.46
14:Z:197:MET:HE3	19:e:32:GLN:NE2	2.31	0.46
15:a:108:ARG:HA	19:e:37:PRO:HA	1.98	0.46
16:b:66:LEU:O	19:e:277:TYR:OH	2.34	0.46
20:f:91:ASN:OD1	20:f:93:VAL:HG12	2.16	0.46
22:h:130:LEU:HD22	22:h:150:LEU:HD12	1.98	0.46
22:h:406:TYR:O	22:h:409:TYR:HB3	2.16	0.46
29:p:205:ASP:H	69:p:401:NDP:C4N	2.28	0.46
4:P:102:ARG:O	4:P:106:ASN:N	2.49	0.45
13:Y:65:TYR:OH	13:Y:67:GLU:HB3	2.16	0.45
13:Y:346:VAL:HA	13:Y:347:ASP:HB2	1.98	0.45
14:Z:172:VAL:O	14:Z:176:GLU:HG2	2.17	0.45
14:Z:298:ILE:HD12	14:Z:300:TRP:H	1.81	0.45
14:Z:316:PHE:HB3	14:Z:343:ILE:HD11	1.98	0.45
16:b:86:TYR:CD1	16:b:90:LYS:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:102:ALA:HB2	18:d:112:VAL:HG21	1.99	0.45
19:e:105:MET:HG3	19:e:237:PHE:HE1	1.80	0.45
20:f:337:LEU:HD21	22:h:120:ILE:HD11	1.97	0.45
24:j:132:VAL:HG23	24:j:133:THR:HG23	1.97	0.45
49:Ah:44:UNK:O	49:Ah:46:UNK:N	2.48	0.45
2:B:334:GLY:O	2:B:335:ASP:C	2.59	0.45
4:D:98:PRO:O	4:D:101:ALA:HB3	2.16	0.45
1:M:253:VAL:O	1:M:323:HIS:HA	2.16	0.45
12:W:89:HIS:CG	12:W:90:PRO:HD2	2.51	0.45
13:Y:209:TYR:H	18:d:110:MET:HE1	1.81	0.45
13:Y:566:ILE:HD12	13:Y:579:MET:O	2.16	0.45
19:e:204:GLU:O	19:e:208:VAL:N	2.49	0.45
20:f:256:PRO:HD3	22:h:124:ALA:HA	1.98	0.45
22:h:196:TRP:CE3	22:h:197:LEU:HD23	2.52	0.45
22:h:296:LEU:HB3	22:h:381:ILE:CD1	2.46	0.45
3:C:34:GLY:CA	64:C:402:HEM:HMA2	2.41	0.45
12:W:124:ASN:HB2	12:W:147:THR:C	2.42	0.45
13:Y:235:PRO:HG3	13:Y:292:PHE:CE1	2.50	0.45
23:i:4:VAL:O	23:i:8:ILE:HD12	2.16	0.45
23:i:54:THR:HA	23:i:57:ASN:ND2	2.31	0.45
24:j:35:TYR:O	24:j:39:THR:OG1	2.28	0.45
24:j:38:THR:O	24:j:41:SER:OG	2.19	0.45
27:n:67:ALA:O	27:n:74:GLU:HA	2.16	0.45
1:M:192:ALA:HA	1:M:194:ARG:N	2.31	0.45
1:M:233:PRO:CB	5:Q:24:SER:N	2.80	0.45
12:W:162:ALA:HB1	14:Z:286:TYR:O	2.17	0.45
15:a:132:LYS:O	15:a:135:PRO:HD2	2.16	0.45
17:c:114:VAL:HA	17:c:155:TYR:O	2.16	0.45
17:c:274:LYS:HD2	17:c:275:LEU:H	1.80	0.45
17:c:425:CYS:N	67:c:501:SF4:S3	2.84	0.45
21:g:74:PRO:HB2	25:k:147:TYR:HE2	1.79	0.45
22:h:318:ALA:HB2	22:h:373:ILE:HG13	1.99	0.45
24:j:49:VAL:N	24:j:50:PRO:HD2	2.32	0.45
24:j:276:MET:HA	24:j:279:CYS:SG	2.56	0.45
4:D:25:SER:O	4:D:26:ILE:C	2.58	0.45
1:M:43:ALA:CB	1:M:189:HIS:CB	2.94	0.45
1:M:394:GLU:O	1:M:397:SER:N	2.49	0.45
13:Y:355:LYS:HD2	13:Y:530:TYR:OH	2.15	0.45
13:Y:422:TRP:HE3	13:Y:423:LEU:HD12	1.81	0.45
14:Z:241:LEU:HD23	14:Z:241:LEU:HA	1.75	0.45
14:Z:300:TRP:CZ3	14:Z:305:THR:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:322:SER:OG	14:Z:323:ARG:N	2.49	0.45
15:a:163:TYR:O	15:a:169:VAL:HG21	2.16	0.45
17:c:118:ASP:CA	68:c:502:FMN:C7M	2.95	0.45
21:g:73:LEU:HD13	25:k:55:MET:HE1	1.98	0.45
22:h:201:MET:O	22:h:205:VAL:HG23	2.17	0.45
24:j:108:MET:HE1	24:j:240:PRO:HB2	1.98	0.45
24:j:316:THR:O	24:j:319:ILE:HG22	2.16	0.45
24:j:503:GLU:O	24:j:507:THR:HG23	2.16	0.45
2:B:395:PRO:O	2:B:396:SER:C	2.59	0.45
7:G:75:ALA:O	7:G:76:ALA:C	2.60	0.45
2:N:338:LYS:O	2:N:341:TYR:N	2.50	0.45
13:Y:356:ASP:HB3	13:Y:634:LEU:HD22	1.99	0.45
14:Z:393:PRO:HG3	14:Z:415:GLY:HA3	1.98	0.45
17:c:235:VAL:HG22	17:c:240:THR:HG21	1.99	0.45
17:c:299:LEU:HD21	17:c:337:MET:HG3	1.99	0.45
18:d:160:VAL:HG12	18:d:161:GLY:N	2.32	0.45
24:j:211:MET:O	24:j:214:ILE:HG13	2.16	0.45
25:k:8:ILE:O	25:k:11:THR:OG1	2.21	0.45
30:q:98:SER:O	30:q:103:GLY:HA2	2.16	0.45
7:G:60:THR:O	7:G:61:TRP:C	2.59	0.45
10:J:27:GLY:O	10:J:28:ALA:C	2.59	0.45
13:Y:252:ASP:OD2	13:Y:259:SER:OG	2.28	0.45
14:Z:232:VAL:CG1	14:Z:356:ILE:HB	2.47	0.45
18:d:92:TRP:CZ3	18:d:94:PRO:HB3	2.51	0.45
22:h:167:ILE:HA	22:h:170:THR:HG22	1.98	0.45
22:h:383:THR:HG21	24:j:190:LEU:HD23	1.98	0.45
3:C:136:GLY:O	3:C:138:MET:N	2.49	0.45
3:O:278:TYR:O	3:O:281:LEU:N	2.48	0.45
14:Z:181:LEU:HD21	14:Z:211:PHE:CE1	2.51	0.45
14:Z:194:ILE:HD11	14:Z:268:TRP:NE1	2.32	0.45
15:a:152:SER:HB3	15:a:182:TYR:CD1	2.51	0.45
17:c:135:PRO:O	17:c:139:VAL:HG23	2.17	0.45
17:c:412:LEU:HD21	17:c:435:VAL:HG11	1.98	0.45
19:e:82:ALA:HB1	19:e:229:ALA:HB3	1.99	0.45
22:h:203:PHE:HB3	22:h:243:MET:HB2	1.98	0.45
24:j:552:LEU:HA	24:j:556:ILE:HG22	1.98	0.45
40:4:3:ALA:O	40:4:4:ALA:HB2	2.17	0.45
71:y:602:HEA:HHC	71:y:602:HEA:O11	2.17	0.45
2:B:243:GLU:HA	2:B:424:MET:O	2.17	0.45
1:M:56:GLY:O	1:M:57:TYR:C	2.59	0.45
1:M:76:GLU:O	1:M:77:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:101:ASN:OD1	13:Y:102:ILE:N	2.49	0.45
13:Y:486:GLY:HA2	13:Y:489:ILE:HD13	1.97	0.45
18:d:60:TYR:O	18:d:63:ILE:HG13	2.17	0.45
19:e:74:ALA:HB3	19:e:75:PRO:HD3	1.99	0.45
19:e:186:PHE:CE1	19:e:270:PHE:HE1	2.34	0.45
19:e:230:ASN:HA	19:e:233:MET:HE2	1.99	0.45
19:e:307:LEU:HA	19:e:310:MET:HG2	1.99	0.45
21:g:92:LEU:O	21:g:96:ILE:HD12	2.17	0.45
24:j:12:LEU:HD22	24:j:129:MET:HB3	1.99	0.45
24:j:19:ILE:O	24:j:22:SER:HB3	2.17	0.45
3:C:108:THR:O	3:C:110:LEU:N	2.46	0.45
3:C:328:LEU:O	3:C:329:VAL:C	2.56	0.45
7:G:71:ARG:O	7:G:73:ASN:N	2.50	0.45
13:Y:163:LYS:HD2	13:Y:207:GLY:HA3	1.99	0.45
15:a:162:TYR:CE1	16:b:153:ILE:HD13	2.52	0.45
16:b:175:PHE:O	16:b:177:THR:HG23	2.17	0.45
18:d:95:ILE:HG22	18:d:99:ASN:ND2	2.32	0.45
19:e:73:ILE:HA	19:e:76:ILE:HD12	1.98	0.45
20:f:102:LEU:HD23	20:f:102:LEU:HA	1.75	0.45
20:f:201:THR:OG1	20:f:202:ILE:N	2.50	0.45
24:j:150:MET:HE2	24:j:150:MET:HA	1.99	0.45
56:Ak:104:LEU:O	56:Ak:106:ASP:N	2.48	0.45
1:A:51:LYS:C	1:A:53:ASN:H	2.25	0.44
3:C:131:TYR:HA	64:C:401:HEM:CAA	2.47	0.44
1:M:426:GLY:CA	1:M:427:PRO:C	2.90	0.44
2:N:332:SER:O	2:N:333:ALA:C	2.60	0.44
12:W:126:PHE:HZ	12:W:199:ARG:HE	1.64	0.44
13:Y:348:ALA:O	13:Y:351:LEU:HG	2.16	0.44
17:c:88:ARG:HD2	17:c:274:LYS:HD3	1.99	0.44
18:d:164:THR:HG22	18:d:169:PHE:H	1.82	0.44
21:g:96:ILE:O	21:g:100:ALA:N	2.45	0.44
22:h:416:ARG:HH21	24:j:156:GLY:HA3	1.82	0.44
24:j:377:SER:O	24:j:381:THR:OG1	2.30	0.44
29:p:205:ASP:HA	69:p:401:NDP:H42N	1.98	0.44
1:A:257:VAL:N	1:A:320:LEU:O	2.48	0.44
2:B:270:ASN:O	2:B:271:ALA:C	2.59	0.44
2:B:367:GLY:O	2:B:368:TYR:C	2.59	0.44
2:N:98:VAL:N	9:U:69:SER:O	2.46	0.44
11:V:17:TRP:O	11:V:21:ALA:HB3	2.15	0.44
12:W:92:GLY:O	12:W:96:VAL:HG23	2.17	0.44
13:Y:597:VAL:HG12	13:Y:598:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:115:ALA:O	15:a:116:SER:CB	2.65	0.44
15:a:179:VAL:HG21	15:a:182:TYR:CE1	2.53	0.44
17:c:75:TRP:CE2	17:c:76:ILE:HG23	2.51	0.44
17:c:316:ALA:HB1	17:c:325:PRO:HB2	1.99	0.44
18:d:153:GLN:HG3	18:d:158:ILE:O	2.17	0.44
19:e:59:GLU:HA	19:e:60:PRO:HD3	1.82	0.44
19:e:149:ILE:HD11	19:e:185:TRP:CE3	2.43	0.44
19:e:165:LEU:HD23	19:e:240:ILE:HD12	1.99	0.44
1:A:184:GLU:O	1:A:185:TYR:C	2.59	0.44
1:A:243:HIS:HA	7:G:14:ILE:HA	1.99	0.44
3:C:172:LYS:O	3:C:173:ALA:C	2.60	0.44
4:P:161:ALA:O	4:P:163:PRO:N	2.50	0.44
4:P:233:ARG:CA	7:S:16:TYR:O	2.59	0.44
14:Z:400:ILE:O	14:Z:406:GLU:HA	2.17	0.44
15:a:118:ARG:NE	19:e:214:GLU:OE1	2.51	0.44
20:f:17:THR:HG23	20:f:137:ALA:HB2	1.99	0.44
22:h:10:MET:C	22:h:13:PRO:HD2	2.43	0.44
22:h:416:ARG:NH2	24:j:156:GLY:HA3	2.33	0.44
24:j:313:MET:O	24:j:317:ILE:HD12	2.17	0.44
24:j:360:GLY:HA3	24:j:437:PHE:HD1	1.81	0.44
35:x:110:THR:HA	35:x:117:GLN:HA	1.99	0.44
2:B:360:ALA:O	2:B:361:LYS:C	2.60	0.44
12:W:74:GLN:HE22	12:W:89:HIS:HB2	1.82	0.44
13:Y:319:TRP:CZ3	13:Y:585:PRO:HG2	2.49	0.44
13:Y:397:ALA:O	13:Y:427:LEU:HD22	2.17	0.44
13:Y:691:ILE:O	13:Y:694:PHE:HB3	2.17	0.44
14:Z:133:LEU:HB3	14:Z:134:PRO:HD3	1.99	0.44
17:c:188:GLY:C	17:c:190:GLY:H	2.26	0.44
19:e:228:TYR:O	19:e:231:ILE:HG22	2.16	0.44
20:f:238:PRO:O	20:f:241:THR:HG22	2.17	0.44
22:h:112:ALA:HB1	22:h:113:THR:HA	1.98	0.44
22:h:297:VAL:HG23	22:h:315:LEU:HD22	1.99	0.44
24:j:27:TYR:OH	24:j:116:ARG:HG2	2.18	0.44
24:j:414:ILE:O	24:j:418:LEU:HG	2.18	0.44
25:k:12:ILE:HG22	25:k:39:VAL:HG21	2.00	0.44
25:k:61:LEU:HD13	25:k:65:LEU:HD12	1.98	0.44
1:M:158:PHE:O	1:M:164:ALA:HB2	2.18	0.44
2:N:334:GLY:O	2:N:335:ASP:C	2.60	0.44
2:N:367:GLY:O	2:N:368:TYR:C	2.61	0.44
3:O:282:ARG:O	3:O:283:SER:C	2.59	0.44
8:T:22:GLU:O	8:T:23:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:237:ALA:C	13:Y:239:THR:H	2.26	0.44
13:Y:339:ALA:HB3	13:Y:544:VAL:HG12	1.99	0.44
13:Y:390:THR:OG1	13:Y:393:GLY:N	2.51	0.44
14:Z:254:ARG:HD3	14:Z:254:ARG:HA	1.76	0.44
15:a:86:THR:HB	15:a:96:MET:HE1	1.99	0.44
17:c:266:GLY:HA2	17:c:293:SER:HB3	2.00	0.44
20:f:189:TRP:CZ3	20:f:282:MET:HE3	2.53	0.44
20:f:230:LEU:O	20:f:233:THR:HG22	2.18	0.44
22:h:229:MET:CE	22:h:328:CYS:HB3	2.46	0.44
22:h:295:ALA:O	22:h:298:ILE:HG22	2.17	0.44
24:j:182:PHE:HE1	24:j:259:LEU:HD11	1.82	0.44
24:j:270:ASN:ND2	24:j:273:VAL:HG23	2.32	0.44
24:j:514:LYS:O	24:j:515:TYR:HB2	2.18	0.44
29:p:207:PHE:H	29:p:241:TYR:N	2.16	0.44
49:Ab:16:UNK:O	49:Ab:30:UNK:CB	2.65	0.44
2:N:97:SER:O	2:N:108:THR:N	2.50	0.44
2:N:235:ALA:O	2:N:236:LYS:CB	2.65	0.44
13:Y:333:PHE:HE2	13:Y:543:LYS:HD3	1.82	0.44
14:Z:279:THR:HG22	14:Z:281:GLU:HG2	1.99	0.44
17:c:123:GLY:N	18:d:180:CYS:SG	2.90	0.44
17:c:276:PHE:CD1	17:c:352:ALA:HB1	2.53	0.44
20:f:261:MET:SD	20:f:340:THR:HG22	2.58	0.44
21:g:104:TYR:O	21:g:108:GLN:HG2	2.18	0.44
22:h:24:TRP:CH2	22:h:84:LEU:HD11	2.53	0.44
25:k:28:TYR:HB3	25:k:83:TRP:CH2	2.52	0.44
30:q:91:ALA:CA	30:q:95:TYR:CB	2.95	0.44
60:Aw:66:UNK:HA	60:Aw:67:UNK:HA	1.80	0.44
3:C:257:THR:O	3:C:258:PRO:C	2.61	0.44
6:F:46:ALA:O	6:F:49:ARG:N	2.30	0.44
7:G:44:CYS:O	7:G:47:ARG:N	2.47	0.44
12:W:83:GLU:HB3	12:W:142:ARG:HH12	1.82	0.44
13:Y:203:ASP:O	13:Y:205:GLN:HG3	2.18	0.44
13:Y:379:THR:HG21	13:Y:531:LYS:HD3	1.99	0.44
13:Y:532:PRO:C	13:Y:534:VAL:H	2.26	0.44
14:Z:129:TYR:CZ	14:Z:419:PRO:HB3	2.53	0.44
14:Z:320:ILE:HG22	14:Z:321:GLY:O	2.18	0.44
14:Z:399:ALA:HA	14:Z:407:PHE:O	2.17	0.44
16:b:86:TYR:CE1	16:b:90:LYS:HG2	2.53	0.44
17:c:226:LYS:HB3	17:c:227:PRO:HA	1.99	0.44
20:f:233:THR:HG23	20:f:241:THR:HB	1.99	0.44
51:Av:32:UNK:O	51:Av:34:UNK:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:357:VAL:O	2:N:360:ALA:HB3	2.18	0.44
16:b:162:CYS:SG	16:b:165:ASP:N	2.91	0.44
17:c:106:SER:C	17:c:108:GLY:H	2.25	0.44
18:d:164:THR:HG23	18:d:167:LYS:H	1.82	0.44
19:e:248:ASP:OD2	19:e:250:HIS:HB2	2.18	0.44
21:g:52:SER:HB3	21:g:55:PHE:CE2	2.53	0.44
22:h:201:MET:HA	22:h:201:MET:HE2	1.99	0.44
23:i:7:ASN:OD1	25:k:14:VAL:HG21	2.18	0.44
23:i:79:VAL:O	23:i:83:ASN:N	2.49	0.44
24:j:54:PHE:O	24:j:58:GLY:HA2	2.17	0.44
1:A:29:GLN:HA	1:A:201:GLY:O	2.18	0.44
2:B:346:THR:O	2:B:347:ILE:C	2.60	0.44
3:C:7:SER:O	3:C:8:HIS:O	2.36	0.44
1:M:191:LYS:CB	1:M:218:GLY:HA3	2.47	0.44
2:N:161:GLU:O	2:N:162:ASN:C	2.60	0.44
12:W:111:LEU:HD11	12:W:163:ALA:HB2	1.99	0.44
13:Y:379:THR:HA	13:Y:385:TYR:CE2	2.53	0.44
14:Z:154:ALA:HA	14:Z:398:THR:HG21	2.00	0.44
14:Z:412:VAL:HG23	14:Z:420:TYR:HB3	2.00	0.44
16:b:73:THR:HG23	19:e:272:TRP:HE1	1.83	0.44
17:c:159:ARG:HB3	17:c:161:GLU:OE1	2.18	0.44
17:c:236:PHE:HE1	18:d:74:HIS:HB2	1.81	0.44
19:e:22:LEU:HD12	19:e:47:GLN:HB3	1.99	0.44
19:e:107:ALA:HB1	25:k:57:PHE:HD2	1.82	0.44
20:f:241:THR:C	20:f:243:LEU:H	2.25	0.44
22:h:159:PRO:O	22:h:162:VAL:HG12	2.18	0.44
3:C:157:GLY:O	3:C:160:LEU:N	2.51	0.43
1:M:257:VAL:N	1:M:320:LEU:O	2.47	0.43
2:N:81:SER:O	2:N:84:LYS:N	2.50	0.43
13:Y:560:LEU:O	13:Y:564:CYS:N	2.51	0.43
14:Z:188:THR:HG23	14:Z:200:PHE:HA	1.99	0.43
14:Z:317:ASP:H	14:Z:339:GLN:NE2	2.13	0.43
19:e:46:LEU:O	19:e:46:LEU:HD23	2.18	0.43
20:f:298:TYR:CE1	22:h:134:THR:HG21	2.53	0.43
24:j:275:THR:HG22	24:j:279:CYS:SG	2.58	0.43
25:k:24:PRO:HB3	25:k:89:VAL:HG11	1.99	0.43
3:C:365:LEU:O	3:C:366:MET:C	2.61	0.43
3:O:136:GLY:O	3:O:137:GLN:C	2.61	0.43
12:W:100:LEU:HD11	12:W:143:VAL:HG11	1.99	0.43
13:Y:85:ALA:HA	13:Y:86:PRO:HD3	1.79	0.43
13:Y:246:ARG:HH12	13:Y:267:THR:HG22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:283:GLU:C	13:Y:285:TRP:H	2.25	0.43
14:Z:365:PRO:HA	14:Z:366:PRO:HD3	1.75	0.43
15:a:148:ARG:NH1	21:g:30:TYR:OH	2.51	0.43
17:c:62:TRP:CZ2	17:c:181:LEU:HD13	2.53	0.43
17:c:280:GLY:O	17:c:282:VAL:N	2.51	0.43
19:e:181:LEU:HG	19:e:300:LEU:HD23	1.98	0.43
19:e:243:LEU:O	19:e:262:LYS:NZ	2.35	0.43
19:e:284:GLN:HA	19:e:287:HIS:HB3	2.00	0.43
22:h:172:GLY:HA3	33:u:147:ALA:HB1	1.98	0.43
22:h:237:LYS:N	22:h:237:LYS:HD2	2.33	0.43
22:h:278:ARG:HE	24:j:546:GLN:HB2	1.83	0.43
24:j:197:ASP:OD1	24:j:198:LEU:N	2.52	0.43
1:A:224:ASP:O	1:A:225:GLU:C	2.62	0.43
1:M:333:ASP:O	1:M:334:MET:C	2.58	0.43
2:N:140:LEU:O	2:N:142:PRO:N	2.51	0.43
4:P:136:GLU:O	4:P:137:PRO:C	2.60	0.43
12:W:119:VAL:HA	12:W:120:PRO:HD3	1.84	0.43
13:Y:103:LEU:HB2	13:Y:106:SER:HB2	2.00	0.43
13:Y:301:ARG:HH22	13:Y:588:ALA:HB2	1.84	0.43
15:a:194:LEU:HD12	15:a:194:LEU:HA	1.71	0.43
17:c:412:LEU:HD22	17:c:439:ILE:HD11	1.98	0.43
22:h:310:MET:HE1	24:j:71:LEU:HG	2.00	0.43
22:h:440:HIS:O	22:h:443:PRO:HD2	2.17	0.43
23:i:11:ALA:HB1	25:k:17:PHE:HD2	1.83	0.43
1:A:88:ALA:H	2:B:286:LYS:CB	2.31	0.43
2:B:259:ALA:O	2:B:260:GLU:C	2.61	0.43
5:E:32:ARG:CB	7:G:21:PHE:O	2.66	0.43
1:M:52:ASN:CB	1:M:55:ALA:HB2	2.48	0.43
2:N:129:ALA:O	2:N:130:PRO:C	2.58	0.43
2:N:275:LEU:O	2:N:276:GLN:C	2.60	0.43
3:O:248:ASP:O	3:O:249:LEU:C	2.58	0.43
4:P:28:ARG:O	4:P:29:GLY:C	2.61	0.43
13:Y:83:GLU:HB2	13:Y:101:ASN:HB3	2.01	0.43
13:Y:381:LEU:O	13:Y:383:SER:N	2.42	0.43
17:c:76:ILE:O	17:c:80:VAL:HG23	2.18	0.43
19:e:144:VAL:HG23	19:e:145:THR:H	1.82	0.43
20:f:184:ILE:HG21	20:f:184:ILE:HD13	1.64	0.43
20:f:263:LYS:O	20:f:267:ILE:HG12	2.17	0.43
22:h:221:VAL:HA	22:h:340:ARG:NH1	2.33	0.43
24:j:37:LYS:HG3	24:j:38:THR:N	2.33	0.43
24:j:369:THR:OG1	24:j:445:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Ac:13:ALA:O	50:Ac:17:PHE:N	2.50	0.43
2:B:369:LEU:O	2:B:370:MET:C	2.61	0.43
2:B:395:PRO:O	2:B:398:VAL:CB	2.66	0.43
4:D:14:HIS:HA	4:D:19:SER:CB	2.49	0.43
1:M:292:SER:O	1:M:295:ALA:N	2.52	0.43
3:O:48:GLY:HA3	64:O:401:HEM:C3C	2.52	0.43
4:P:116:ILE:O	4:P:117:VAL:C	2.60	0.43
5:Q:182:VAL:C	5:Q:183:PRO:O	2.57	0.43
13:Y:170:LYS:HG2	13:Y:172:ILE:HD11	2.00	0.43
13:Y:697:THR:OG1	13:Y:698:ASP:N	2.50	0.43
14:Z:447:VAL:HA	14:Z:450:ILE:HG22	2.00	0.43
17:c:220:GLN:NE2	18:d:118:PHE:HB2	2.33	0.43
17:c:381:GLN:NE2	17:c:424:ILE:HD11	2.33	0.43
18:d:111:ARG:NH1	18:d:114:GLU:OE1	2.52	0.43
19:e:169:GLN:HB3	19:e:244:GLY:HA3	2.00	0.43
19:e:286:MET:HE3	19:e:286:MET:HB2	1.85	0.43
22:h:225:ILE:CD1	22:h:328:CYS:HA	2.47	0.43
24:j:151:SER:O	24:j:155:ILE:HG12	2.18	0.43
3:C:34:GLY:O	64:C:402:HEM:HMA1	2.14	0.43
10:J:24:ILE:O	10:J:25:VAL:C	2.62	0.43
3:O:88:SER:O	3:O:89:MET:C	2.61	0.43
3:O:257:THR:O	3:O:258:PRO:C	2.62	0.43
13:Y:97:MET:HE3	13:Y:100:TRP:CH2	2.54	0.43
13:Y:489:ILE:CD1	13:Y:489:ILE:N	2.75	0.43
13:Y:540:ASN:ND2	13:Y:562:LYS:HG3	2.34	0.43
14:Z:438:MET:HE1	14:Z:454:GLN:CD	2.43	0.43
16:b:117:LYS:N	67:b:301:SF4:S4	2.83	0.43
17:c:208:GLU:OE1	17:c:210:THR:N	2.52	0.43
18:d:164:THR:HG23	18:d:167:LYS:N	2.33	0.43
23:i:31:LEU:HB3	25:k:20:PHE:HE1	1.83	0.43
23:i:68:ALA:HB1	25:k:64:MET:HE2	2.01	0.43
24:j:286:LEU:HD22	24:j:411:MET:SD	2.58	0.43
35:x:109:GLY:N	35:x:118:PHE:O	2.28	0.43
2:B:78:LYS:CB	2:B:129:ALA:HB1	2.48	0.43
2:N:84:LYS:O	2:N:88:GLY:N	2.47	0.43
4:P:33:TYR:O	4:P:37:CYS:N	2.41	0.43
13:Y:64:CYS:SG	13:Y:65:TYR:N	2.92	0.43
13:Y:202:ASN:O	13:Y:203:ASP:HB2	2.17	0.43
13:Y:299:ARG:HG2	13:Y:300:GLN:N	2.34	0.43
14:Z:330:TYR:CD2	14:Z:331:LEU:HD12	2.50	0.43
15:a:118:ARG:HD2	19:e:214:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:125:VAL:HG11	15:a:173:CYS:SG	2.58	0.43
17:c:277:ASN:OD1	17:c:278:ILE:N	2.51	0.43
19:e:14:LEU:O	19:e:17:VAL:HG22	2.18	0.43
19:e:22:LEU:HB2	19:e:48:PRO:HG3	2.01	0.43
21:g:66:ASP:O	21:g:69:ILE:HG22	2.18	0.43
22:h:11:LEU:HB2	22:h:100:ILE:CD1	2.48	0.43
24:j:249:SER:O	24:j:332:HIS:HE1	2.01	0.43
24:j:281:GLY:O	24:j:284:THR:HG22	2.18	0.43
51:Ap:33:UNK:O	51:Ap:35:UNK:N	2.52	0.43
1:A:7:ALA:O	1:A:8:LEU:C	2.60	0.43
2:B:129:ALA:O	2:B:130:PRO:C	2.62	0.43
2:B:346:THR:O	2:B:349:GLN:N	2.38	0.43
64:C:401:HEM:CMB	64:C:401:HEM:HBB2	2.48	0.43
4:D:69:GLU:O	4:D:73:GLY:CA	2.67	0.43
4:D:165:TYR:O	4:D:166:ASN:C	2.61	0.43
13:Y:306:MET:HB2	13:Y:583:ILE:HD12	2.00	0.43
17:c:395:VAL:HG11	17:c:412:LEU:HD12	2.00	0.43
18:d:188:ILE:HG22	18:d:189:ASN:HD22	1.83	0.43
22:h:406:TYR:HA	22:h:409:TYR:HB3	2.00	0.43
1:A:433:ASP:O	1:A:436:ARG:N	2.52	0.43
10:L:51:LEU:O	10:L:52:TRP:C	2.61	0.43
1:M:360:LEU:HA	2:N:93:GLY:HA3	2.00	0.43
3:O:207:ASN:O	3:O:208:PRO:C	2.62	0.43
13:Y:223:ILE:HG21	13:Y:233:SER:HB3	2.01	0.43
13:Y:333:PHE:HB3	13:Y:337:ASP:CB	2.49	0.43
14:Z:123:LEU:HB3	14:Z:135:TYR:OH	2.18	0.43
17:c:285:PRO:HB3	18:d:143:ARG:HH12	1.84	0.43
19:e:303:TRP:HE3	26:m:29:ALA:HB2	1.82	0.43
21:g:73:LEU:HD23	21:g:73:LEU:HA	1.73	0.43
22:h:352:LEU:CD1	22:h:355:MET:HB2	2.49	0.43
25:k:10:SER:O	25:k:13:PHE:HB3	2.19	0.43
25:k:30:GLY:O	25:k:34:ILE:HG13	2.19	0.43
1:A:7:ALA:HB2	2:B:41:TYR:O	2.14	0.43
1:A:43:ALA:CB	1:A:189:HIS:CB	2.97	0.43
4:D:74:PRO:CB	4:D:79:GLU:CB	2.97	0.43
6:F:91:GLU:O	6:F:92:PRO:C	2.62	0.43
1:M:106:LEU:HA	1:M:109:ALA:HB3	2.01	0.43
1:M:271:GLN:O	1:M:272:VAL:C	2.59	0.43
3:O:319:PRO:O	3:O:320:LEU:C	2.61	0.43
8:T:67:HIS:O	8:T:68:CYS:C	2.62	0.43
12:W:70:PRO:HA	12:W:73:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:351:LEU:HD13	13:Y:530:TYR:CE2	2.53	0.43
14:Z:219:GLY:O	16:b:97:PHE:HA	2.19	0.43
15:a:154:GLY:HA2	15:a:188:PRO:HD3	2.01	0.43
17:c:114:VAL:O	17:c:242:VAL:HA	2.18	0.43
17:c:403:ASP:HA	17:c:453:PHE:CD2	2.54	0.43
19:e:114:TYR:HE2	19:e:118:TRP:CZ2	2.36	0.43
22:h:14:MET:HE2	22:h:26:ASN:HB3	2.01	0.43
22:h:29:VAL:HG13	22:h:30:HIS:N	2.34	0.43
24:j:81:LYS:HB3	24:j:135:ASN:HB2	2.01	0.43
24:j:216:LEU:HD11	24:j:263:PHE:CE2	2.54	0.43
3:O:7:SER:O	3:O:8:HIS:C	2.61	0.42
3:O:254:ASP:O	4:P:119:ALA:HA	2.19	0.42
13:Y:379:THR:HG22	13:Y:526:LEU:HD22	2.01	0.42
13:Y:644:SER:O	13:Y:647:GLU:HB3	2.19	0.42
17:c:207:GLY:HA3	68:c:502:FMN:C5A	2.49	0.42
18:d:132:ILE:HD11	18:d:169:PHE:CD1	2.52	0.42
19:e:28:LEU:HD12	19:e:275:ALA:HB2	2.01	0.42
20:f:113:PHE:O	20:f:116:PRO:HD2	2.19	0.42
20:f:137:ALA:HB3	20:f:138:PRO:HD3	2.01	0.42
22:h:210:TYR:CG	22:h:268:GLY:HA3	2.54	0.42
23:i:9:ILE:O	23:i:12:PHE:HB3	2.19	0.42
23:i:57:ASN:O	23:i:60:PRO:HD2	2.19	0.42
24:j:65:ASN:OD1	24:j:66:TRP:N	2.52	0.42
39:3:86:GLY:O	39:3:87:THR:O	2.37	0.42
2:B:97:SER:HA	9:I:70:LEU:CB	2.50	0.42
3:C:116:GLY:CA	64:C:402:HEM:CAC	2.82	0.42
3:C:371:THR:O	3:C:372:ILE:C	2.61	0.42
2:N:294:SER:O	2:N:297:GLN:N	2.52	0.42
4:P:12:TRP:O	4:P:13:SER:C	2.61	0.42
5:Q:107:ASP:O	5:Q:110:ALA:N	2.51	0.42
13:Y:382:ARG:HA	13:Y:385:TYR:CZ	2.54	0.42
14:Z:317:ASP:HB2	14:Z:339:GLN:NE2	2.35	0.42
17:c:338:ASP:N	17:c:338:ASP:OD1	2.52	0.42
17:c:375:LYS:HD3	17:c:393:ASN:HD22	1.83	0.42
19:e:107:ALA:HB1	25:k:57:PHE:CD2	2.54	0.42
19:e:144:VAL:HG23	19:e:145:THR:N	2.34	0.42
19:e:288:LEU:O	19:e:292:SER:HB2	2.19	0.42
20:f:28:LEU:HD23	20:f:28:LEU:HA	1.76	0.42
21:g:59:ALA:O	21:g:62:PHE:HB3	2.20	0.42
24:j:68:TRP:CE3	24:j:76:LEU:HD11	2.53	0.42
24:j:367:PRO:O	24:j:370:THR:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:387:THR:OG1	24:j:461:SER:O	2.35	0.42
36:0:40:MET:O	36:0:41:THR:C	2.62	0.42
3:C:226:ILE:O	3:C:227:LYS:C	2.61	0.42
2:N:90:GLU:O	2:N:91:ALA:C	2.62	0.42
2:N:363:LYS:O	2:N:364:LEU:C	2.61	0.42
13:Y:44:GLU:CG	13:Y:45:PRO:HD2	2.49	0.42
13:Y:382:ARG:HG2	13:Y:386:LEU:HD11	2.01	0.42
14:Z:148:GLU:HB3	14:Z:227:ILE:HB	2.01	0.42
15:a:91:CYS:O	15:a:94:VAL:HG22	2.19	0.42
17:c:370:LEU:O	17:c:373:PHE:HB3	2.19	0.42
19:e:32:GLN:O	19:e:33:LEU:HB2	2.20	0.42
24:j:226:GLN:HB3	24:j:280:LEU:CD2	2.48	0.42
24:j:409:LEU:O	24:j:413:LEU:HG	2.19	0.42
1:A:3:THR:O	1:A:4:TYR:C	2.62	0.42
2:B:177:TYR:C	2:B:178:CYS:O	2.60	0.42
3:C:34:GLY:O	3:C:37:LEU:N	2.53	0.42
3:C:307:LEU:O	3:C:308:HIS:C	2.62	0.42
1:M:245:GLU:C	1:M:247:GLY:N	2.76	0.42
4:P:25:SER:O	4:P:26:ILE:C	2.61	0.42
14:Z:412:VAL:HG23	14:Z:412:VAL:O	2.19	0.42
16:b:92:PRO:O	16:b:93:LEU:HD12	2.19	0.42
17:c:258:GLY:O	17:c:261:TRP:HB3	2.19	0.42
24:j:556:ILE:O	24:j:560:THR:OG1	2.32	0.42
1:A:54:GLY:O	1:A:55:ALA:O	2.37	0.42
2:B:406:ALA:HB3	2:B:409:ASP:CB	2.49	0.42
3:C:116:GLY:CA	64:C:402:HEM:CBC	2.97	0.42
3:O:58:ASP:O	3:O:59:THR:C	2.60	0.42
5:Q:114:VAL:O	5:Q:117:LEU:N	2.48	0.42
13:Y:422:TRP:CE2	13:Y:440:TYR:HB2	2.54	0.42
17:c:93:PHE:HD2	17:c:98:LYS:HB2	1.84	0.42
20:f:255:PRO:HA	20:f:260:PHE:CG	2.54	0.42
21:g:68:GLU:CG	21:g:98:LEU:HD12	2.49	0.42
23:i:19:LEU:N	23:i:32:CYS:SG	2.93	0.42
24:j:591:PHE:O	24:j:594:THR:HG22	2.19	0.42
40:4:77:PRO:HA	40:4:82:TYR:HA	2.02	0.42
1:A:66:GLY:O	1:A:121:SER:N	2.50	0.42
2:B:81:SER:O	2:B:82:SER:C	2.62	0.42
2:B:312:PHE:N	2:B:323:GLY:O	2.47	0.42
5:E:68:VAL:CB	5:E:72:SER:CB	2.97	0.42
11:K:17:TRP:O	11:K:21:ALA:HB3	2.19	0.42
1:M:372:THR:O	1:M:373:THR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:102:THR:H	5:Q:105:GLU:CB	2.32	0.42
12:W:114:LEU:HD13	12:W:130:TYR:CE2	2.55	0.42
13:Y:566:ILE:HB	13:Y:580:ALA:HA	2.02	0.42
14:Z:97:LEU:HD21	14:Z:109:CYS:HB2	2.02	0.42
14:Z:129:TYR:CE2	14:Z:419:PRO:HB3	2.55	0.42
15:a:95:GLU:HG3	15:a:187:PRO:HB2	2.01	0.42
17:c:316:ALA:HA	17:c:326:LEU:O	2.18	0.42
20:f:337:LEU:O	20:f:340:THR:HG23	2.19	0.42
23:i:80:MET:CE	25:k:172:THR:HA	2.50	0.42
24:j:231:PRO:C	24:j:234:PRO:HD2	2.44	0.42
24:j:407:TRP:O	24:j:411:MET:HG2	2.19	0.42
25:k:5:ILE:HA	25:k:8:ILE:HG12	2.00	0.42
3:C:319:PRO:O	3:C:322:GLN:N	2.52	0.42
13:Y:197:THR:O	18:d:114:GLU:HG2	2.20	0.42
13:Y:282:ASN:HB2	13:Y:285:TRP:O	2.20	0.42
13:Y:531:LYS:HA	13:Y:532:PRO:C	2.45	0.42
16:b:95:PRO:HA	16:b:204:ASN:OD1	2.19	0.42
16:b:129:THR:HB	16:b:146:ASP:OD1	2.19	0.42
17:c:447:GLU:O	17:c:450:MET:HB2	2.19	0.42
18:d:138:THR:HA	18:d:141:MET:HB3	2.00	0.42
19:e:84:THR:O	19:e:87:VAL:HG12	2.20	0.42
20:f:287:LEU:HD11	22:h:151:PHE:CD1	2.54	0.42
22:h:196:TRP:CH2	22:h:200:ILE:HG13	2.55	0.42
22:h:296:LEU:HA	22:h:296:LEU:HD23	1.76	0.42
22:h:450:ASN:OD1	22:h:452:LYS:HG2	2.19	0.42
24:j:566:THR:O	24:j:570:GLN:HG2	2.20	0.42
44:8:13:TYR:O	44:8:14:GLY:C	2.63	0.42
2:B:342:ASN:O	2:B:345:LYS:N	2.52	0.42
3:C:368:THR:O	3:C:369:ALA:C	2.62	0.42
4:P:115:TYR:O	4:P:119:ALA:N	2.47	0.42
4:P:139:THR:O	8:T:54:CYS:CB	2.67	0.42
4:P:234:LYS:CA	7:S:16:TYR:H	2.32	0.42
13:Y:182:CYS:O	13:Y:185:PHE:HB3	2.20	0.42
13:Y:708:ALA:HA	13:Y:711:VAL:HG12	2.02	0.42
14:Z:153:LEU:HD12	14:Z:171:ARG:HH21	1.83	0.42
14:Z:172:VAL:HG23	14:Z:311:TYR:CZ	2.54	0.42
17:c:272:GLY:O	17:c:292:MET:HG2	2.18	0.42
17:c:314:LEU:HA	17:c:329:LYS:HA	2.01	0.42
19:e:202:GLU:O	19:e:204:GLU:N	2.46	0.42
22:h:204:MET:HE3	22:h:298:ILE:HD11	2.02	0.42
24:j:313:MET:HB3	24:j:328:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:y:601:HEA:HHC	71:y:601:HEA:H122	2.02	0.42
1:A:33:PRO:O	1:A:103:SER:CB	2.67	0.42
3:C:61:THR:O	3:C:62:ALA:C	2.63	0.42
2:N:81:SER:O	2:N:82:SER:C	2.63	0.42
2:N:346:THR:O	2:N:347:ILE:C	2.62	0.42
5:Q:150:ALA:CB	5:Q:157:TYR:CB	2.98	0.42
13:Y:128:CYS:N	13:Y:129:PRO:HD2	2.35	0.42
13:Y:301:ARG:HH22	13:Y:588:ALA:N	2.18	0.42
19:e:20:LEU:HD22	19:e:232:ILE:HG23	2.01	0.42
19:e:165:LEU:HD21	19:e:241:LEU:HA	2.00	0.42
22:h:200:ILE:HG23	22:h:200:ILE:HD12	1.76	0.42
24:j:137:LEU:HD22	24:j:186:MET:HG3	2.01	0.42
24:j:313:MET:O	24:j:316:THR:HB	2.19	0.42
25:k:51:PHE:O	25:k:55:MET:HG2	2.20	0.42
1:A:5:ALA:O	1:A:6:GLN:O	2.38	0.42
1:A:252:HIS:O	1:A:424:GLY:HA2	2.20	0.42
3:C:315:MET:O	3:C:318:ARG:N	2.35	0.42
1:M:43:ALA:HB1	1:M:189:HIS:CB	2.50	0.42
3:O:254:ASP:CB	4:P:119:ALA:O	2.68	0.42
4:P:233:ARG:HA	7:S:17:SER:CA	2.48	0.42
12:W:140:ARG:NH1	14:Z:397:TYR:CE2	2.84	0.42
13:Y:236:TYR:O	13:Y:236:TYR:CG	2.73	0.42
13:Y:402:LEU:O	13:Y:432:ILE:N	2.52	0.42
16:b:148:ASP:OD2	16:b:151:LYS:HE2	2.19	0.42
21:g:83:ASN:OD1	25:k:148:SER:HB2	2.19	0.42
25:k:139:GLU:OE2	25:k:143:ILE:HD12	2.19	0.42
47:y:501:PRO:O	47:y:502:TYR:C	2.63	0.42
3:C:37:LEU:CB	64:C:402:HEM:CMB	2.98	0.41
7:G:63:THR:O	7:G:64:GLN:C	2.63	0.41
2:N:78:LYS:CB	2:N:129:ALA:HB1	2.49	0.41
9:U:55:LEU:O	9:U:56:ARG:O	2.38	0.41
13:Y:126:LEU:HD12	35:x:97:ARG:O	2.20	0.41
13:Y:171:THR:HG22	13:Y:231:LEU:CD2	2.51	0.41
13:Y:252:ASP:OD1	13:Y:259:SER:N	2.52	0.41
14:Z:429:PHE:HD1	14:Z:461:VAL:HG13	1.84	0.41
14:Z:450:ILE:O	14:Z:453:THR:HG22	2.19	0.41
19:e:260:VAL:HA	19:e:263:THR:HG22	2.02	0.41
20:f:72:MET:HE1	23:i:43:MET:SD	2.60	0.41
20:f:172:GLN:HG2	20:f:177:LYS:CD	2.44	0.41
20:f:181:TYR:HA	20:f:184:ILE:CG2	2.49	0.41
20:f:221:HIS:HD2	20:f:240:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:262:PRO:O	20:f:266:ILE:HG12	2.19	0.41
24:j:166:THR:HG22	49:Ab:68:UNK:HA	2.02	0.41
30:q:66:GLY:HA3	30:q:75:LEU:CB	2.50	0.41
1:A:185:TYR:O	1:A:186:LEU:C	2.62	0.41
2:B:248:ASN:CB	2:B:428:GLY:HA2	2.50	0.41
10:J:3:PRO:O	10:J:4:THR:C	2.63	0.41
1:M:31:SER:N	1:M:202:GLY:HA2	2.35	0.41
1:M:83:GLY:HA2	2:N:363:LYS:CB	2.51	0.41
13:Y:126:LEU:CD2	14:Z:375:MET:HA	2.49	0.41
13:Y:217:GLU:O	13:Y:288:ASP:HB2	2.20	0.41
13:Y:400:ILE:HD13	13:Y:473:MET:HB3	2.02	0.41
13:Y:462:PHE:CE1	13:Y:465:ILE:HD11	2.56	0.41
13:Y:479:SER:CB	13:Y:687:PRO:HD3	2.49	0.41
13:Y:639:LEU:O	13:Y:642:VAL:HG12	2.20	0.41
14:Z:395:ALA:HB2	14:Z:412:VAL:HG12	2.00	0.41
15:a:116:SER:HB3	19:e:208:VAL:HG22	2.02	0.41
17:c:137:LYS:HA	17:c:137:LYS:HD2	1.88	0.41
17:c:327:ILE:N	17:c:328:PRO:HD3	2.34	0.41
19:e:111:LEU:HD11	25:k:61:LEU:HG	2.01	0.41
20:f:207:ILE:O	20:f:211:MET:HG2	2.19	0.41
20:f:211:MET:HE1	20:f:250:SER:HB3	2.03	0.41
20:f:298:TYR:HE1	22:h:134:THR:HG21	1.84	0.41
22:h:378:GLU:O	22:h:381:ILE:HG12	2.20	0.41
24:j:404:THR:OG1	24:j:405:ASN:N	2.53	0.41
34:w:73:LYS:O	34:w:75:ARG:N	2.50	0.41
1:A:253:VAL:O	1:A:323:HIS:HA	2.20	0.41
1:A:381:ARG:O	1:A:382:SER:C	2.62	0.41
2:B:154:ASN:O	2:B:155:PRO:C	2.60	0.41
13:Y:149:ASP:OD1	13:Y:150:ARG:N	2.52	0.41
13:Y:198:THR:O	13:Y:204:MET:HA	2.20	0.41
13:Y:266:ARG:O	13:Y:267:THR:OG1	2.34	0.41
13:Y:345:LEU:HD11	13:Y:698:ASP:HB2	2.03	0.41
13:Y:354:LEU:O	13:Y:357:LEU:HB3	2.19	0.41
13:Y:653:LEU:C	13:Y:655:ARG:H	2.27	0.41
15:a:99:MET:CE	15:a:113:PHE:CZ	3.02	0.41
18:d:134:VAL:HG23	18:d:186:VAL:HG22	2.01	0.41
20:f:323:MET:H	20:f:323:MET:HG2	1.66	0.41
1:A:256:ALA:HB3	1:A:421:ALA:HB3	2.02	0.41
3:C:89:MET:O	3:C:90:PHE:C	2.62	0.41
10:J:25:VAL:CB	11:V:31:GLY:CA	2.98	0.41
2:N:382:VAL:O	2:N:383:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:330:ALA:CB	7:S:51:PRO:O	2.68	0.41
4:P:115:TYR:O	4:P:116:ILE:C	2.60	0.41
5:Q:184:SER:O	5:Q:195:VAL:HA	2.20	0.41
13:Y:177:ILE:O	13:Y:179:CYS:N	2.54	0.41
13:Y:236:TYR:CZ	13:Y:272:ARG:HD3	2.55	0.41
14:Z:275:ILE:HA	14:Z:276:GLY:HA2	1.67	0.41
16:b:101:HIS:NE2	16:b:169:GLU:OE2	2.53	0.41
17:c:51:TRP:HB2	17:c:135:PRO:HD3	2.02	0.41
20:f:10:ILE:HD12	20:f:10:ILE:HA	1.85	0.41
22:h:196:TRP:CZ3	22:h:200:ILE:HG13	2.56	0.41
22:h:321:LEU:HD23	22:h:321:LEU:HA	1.91	0.41
24:j:247:LEU:HB2	24:j:252:MET:CB	2.49	0.41
24:j:353:GLU:OE1	24:j:353:GLU:N	2.53	0.41
30:q:230:LYS:O	30:q:231:ILE:C	2.63	0.41
1:A:367:SER:O	1:A:368:HIS:C	2.63	0.41
4:D:187:CYS:O	4:D:188:THR:C	2.60	0.41
6:F:30:GLY:HA2	6:F:81:THR:H	1.86	0.41
9:U:60:ALA:HB3	9:U:63:PRO:O	2.21	0.41
13:Y:31:LEU:HD12	13:Y:31:LEU:O	2.20	0.41
13:Y:355:LYS:HD2	13:Y:530:TYR:CE1	2.56	0.41
13:Y:620:TRP:CG	13:Y:621:LYS:N	2.89	0.41
14:Z:169:TRP:CZ2	14:Z:350:LYS:HE2	2.55	0.41
14:Z:228:ARG:HH11	14:Z:233:HIS:CE1	2.38	0.41
14:Z:268:TRP:HZ3	14:Z:327:TYR:HD1	1.68	0.41
14:Z:279:THR:HB	14:Z:282:ASP:CB	2.50	0.41
16:b:123:CYS:HA	16:b:124:PRO:HD2	1.90	0.41
17:c:369:ARG:HH21	18:d:136:THR:HB	1.86	0.41
17:c:373:PHE:CD1	18:d:175:GLU:HB3	2.56	0.41
19:e:94:PRO:HB2	19:e:96:ILE:O	2.21	0.41
22:h:106:LEU:HA	22:h:106:LEU:HD23	1.73	0.41
24:j:157:TRP:HD1	24:j:158:TRP:CD1	2.38	0.41
24:j:250:SER:O	24:j:254:VAL:HG22	2.20	0.41
24:j:383:MET:HB3	24:j:384:PRO:HD2	2.02	0.41
37:1:130:PRO:O	37:1:136:ALA:HB2	2.20	0.41
47:y:498:CYS:HA	47:y:499:PRO:HA	1.79	0.41
49:Ab:16:UNK:O	49:Ab:30:UNK:N	2.54	0.41
57:Al:20:ALA:C	57:Al:22:SER:N	2.79	0.41
4:D:136:GLU:O	4:D:137:PRO:C	2.62	0.41
5:E:190:ASP:O	5:E:191:ASP:C	2.63	0.41
6:F:30:GLY:HA2	6:F:81:THR:CB	2.50	0.41
1:M:137:GLU:O	1:M:138:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:116:ALA:HB3	12:W:174:PHE:CE2	2.55	0.41
13:Y:351:LEU:HD13	13:Y:530:TYR:HE2	1.86	0.41
13:Y:358:LEU:HB3	13:Y:364:ASP:HB2	2.01	0.41
13:Y:403:VAL:HG22	13:Y:432:ILE:CB	2.51	0.41
13:Y:464:GLN:O	13:Y:467:LYS:HB2	2.20	0.41
14:Z:228:ARG:HH22	16:b:157:PHE:HE1	1.69	0.41
17:c:99:TRP:CD1	17:c:99:TRP:N	2.88	0.41
17:c:116:ASN:HB2	17:c:242:VAL:CG1	2.51	0.41
17:c:135:PRO:O	17:c:138:LEU:HB3	2.21	0.41
18:d:48:ASN:O	18:d:50:ASP:N	2.52	0.41
19:e:202:GLU:C	19:e:204:GLU:H	2.27	0.41
19:e:269:THR:O	19:e:273:ILE:HG12	2.20	0.41
20:f:171:ASN:HB2	24:j:574:SER:OG	2.21	0.41
20:f:199:THR:HA	20:f:202:ILE:HG22	2.02	0.41
20:f:216:PHE:O	20:f:220:ILE:HG12	2.20	0.41
20:f:288:LEU:HD11	24:j:570:GLN:HE21	1.83	0.41
22:h:373:ILE:HD13	22:h:447:LEU:HD23	2.02	0.41
24:j:52:LEU:HA	24:j:55:MET:HG2	2.03	0.41
24:j:297:ASP:OD2	24:j:300:LYS:HG2	2.21	0.41
24:j:347:ILE:HG22	24:j:352:ASP:OD1	2.21	0.41
25:k:27:ILE:HG23	25:k:28:TYR:N	2.35	0.41
34:w:109:ASN:N	34:w:114:TRP:O	2.34	0.41
3:C:192:ILE:O	3:C:193:ALA:C	2.62	0.41
4:D:90:TYR:O	4:D:91:PHE:C	2.62	0.41
5:E:160:CYS:HA	3:O:266:PRO:O	2.21	0.41
6:F:98:ILE:O	6:F:99:ARG:C	2.63	0.41
2:N:243:GLU:HA	2:N:424:MET:O	2.20	0.41
13:Y:65:TYR:CG	13:Y:66:HIS:N	2.88	0.41
13:Y:540:ASN:ND2	13:Y:559:ASP:HA	2.36	0.41
14:Z:159:LEU:HD12	14:Z:159:LEU:HA	1.93	0.41
17:c:73:PRO:HB2	17:c:74:ASP:H	1.59	0.41
17:c:319:PRO:O	17:c:350:GLY:HA3	2.20	0.41
18:d:53:PHE:CD2	18:d:97:ALA:HA	2.56	0.41
24:j:356:ILE:HA	24:j:359:MET:HB2	2.02	0.41
24:j:361:GLY:HA3	24:j:433:GLY:O	2.21	0.41
1:A:43:ALA:HB1	1:A:189:HIS:CB	2.51	0.41
1:A:134:ILE:O	1:A:137:GLU:N	2.53	0.41
2:B:397:THR:O	2:B:398:VAL:C	2.63	0.41
10:L:24:ILE:O	10:L:25:VAL:C	2.61	0.41
2:N:341:TYR:O	2:N:342:ASN:C	2.64	0.41
2:N:380:ASP:O	2:N:381:GLU:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:91:TRP:O	5:Q:92:ARG:CB	2.69	0.41
5:Q:136:ILE:O	5:Q:138:VAL:N	2.49	0.41
6:R:99:ARG:O	6:R:100:GLU:C	2.63	0.41
13:Y:68:ARG:NH2	13:Y:277:MET:HE3	2.36	0.41
13:Y:306:MET:HA	13:Y:315:THR:O	2.21	0.41
13:Y:368:THR:H	13:Y:533:GLY:HA2	1.86	0.41
14:Z:136:PHE:CE2	14:Z:151:TYR:CD1	2.98	0.41
14:Z:179:ARG:HH12	14:Z:303:ARG:CZ	2.33	0.41
14:Z:261:MET:HE2	14:Z:261:MET:HB3	1.98	0.41
19:e:307:LEU:N	19:e:308:PRO:HD2	2.35	0.41
20:f:203:LEU:HD11	20:f:261:MET:HE3	2.03	0.41
21:g:26:GLN:O	21:g:27:LEU:HD12	2.21	0.41
22:h:55:THR:HG23	22:h:56:PHE:CD2	2.56	0.41
22:h:354:LEU:HG	22:h:358:TRP:NE1	2.35	0.41
22:h:426:ILE:O	22:h:427:LYS:HD2	2.20	0.41
24:j:103:PHE:HE2	24:j:242:PRO:HG3	1.85	0.41
1:A:4:TYR:O	1:A:5:ALA:C	2.63	0.41
1:A:151:ASN:O	1:A:154:HIS:N	2.53	0.41
1:A:176:LYS:O	1:A:177:LEU:C	2.64	0.41
2:B:133:ARG:O	2:B:134:ARG:C	2.64	0.41
2:B:335:ASP:O	2:B:336:VAL:C	2.64	0.41
2:B:338:LYS:O	2:B:339:ALA:C	2.64	0.41
2:B:408:ALA:O	2:B:411:ILE:N	2.54	0.41
7:G:68:LYS:O	7:G:69:SER:C	2.64	0.41
10:J:44:GLU:O	10:J:45:HIS:C	2.62	0.41
1:M:185:TYR:O	1:M:186:LEU:C	2.64	0.41
2:N:374:SER:O	2:N:375:SER:C	2.64	0.41
3:O:146:ILE:O	3:O:147:THR:C	2.62	0.41
3:O:156:ILE:O	3:O:158:THR:N	2.53	0.41
4:P:8:PRO:CB	8:T:70:ALA:HB2	2.51	0.41
12:W:100:LEU:HD23	12:W:100:LEU:HA	1.90	0.41
13:Y:337:ASP:HB3	13:Y:542:PRO:HG2	2.03	0.41
13:Y:617:ARG:HB3	13:Y:621:LYS:HE2	2.02	0.41
14:Z:162:GLN:HA	14:Z:163:PRO:HD3	1.83	0.41
14:Z:202:TRP:CZ3	14:Z:261:MET:SD	3.14	0.41
14:Z:229:PRO:HG3	14:Z:389:TYR:OH	2.21	0.41
14:Z:323:ARG:N	14:Z:328:ASP:OD2	2.53	0.41
14:Z:383:LYS:HA	14:Z:386:THR:OG1	2.20	0.41
14:Z:386:THR:OG1	14:Z:387:GLU:N	2.49	0.41
15:a:118:ARG:NH2	21:g:35:SER:O	2.54	0.41
15:a:159:GLY:C	15:a:161:GLY:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:291:GLU:HB3	17:c:294:VAL:HG13	2.03	0.41
17:c:313:ASN:O	17:c:329:LYS:HA	2.21	0.41
17:c:363:ILE:HG21	17:c:442:PHE:HD2	1.85	0.41
17:c:380:GLY:O	17:c:386:ARG:HB2	2.20	0.41
17:c:442:PHE:HB3	17:c:445:GLU:CD	2.46	0.41
18:d:185:MET:HA	18:d:196:LEU:HD13	2.02	0.41
19:e:64:ALA:N	21:g:34:THR:OG1	2.54	0.41
19:e:152:SER:OG	19:e:301:CYS:SG	2.76	0.41
19:e:196:ALA:HB3	19:e:197:PRO:CD	2.51	0.41
20:f:298:TYR:HE2	22:h:147:LEU:HD11	1.86	0.41
22:h:34:ILE:HD12	22:h:34:ILE:HA	1.89	0.41
22:h:115:LEU:HA	22:h:118:PHE:HB3	2.02	0.41
23:i:34:GLU:HA	23:i:37:MET:HE2	2.03	0.41
24:j:102:GLU:O	24:j:449:LEU:HD13	2.20	0.41
24:j:214:ILE:O	24:j:217:LEU:HB3	2.21	0.41
28:o:48:GLY:O	28:o:50:ILE:N	2.48	0.41
3:C:122:THR:C	3:C:124:MET:N	2.79	0.41
6:F:103:GLU:O	6:F:105:GLU:N	2.54	0.41
10:L:44:GLU:O	10:L:45:HIS:C	2.62	0.41
13:Y:646:LEU:HD22	13:Y:653:LEU:HD22	2.03	0.41
14:Z:97:LEU:HD21	14:Z:109:CYS:CB	2.51	0.41
14:Z:188:THR:CG2	14:Z:200:PHE:HA	2.51	0.41
14:Z:356:ILE:HD12	14:Z:357:LYS:N	2.36	0.41
14:Z:414:ASP:OD1	14:Z:416:SER:N	2.47	0.41
19:e:210:GLY:O	19:e:213:VAL:HG23	2.21	0.41
22:h:80:SER:OG	22:h:226:ALA:HB2	2.21	0.41
22:h:182:TRP:CH2	55:Aj:80:LYS:HA	2.55	0.41
23:i:59:MET:HG3	23:i:60:PRO:CD	2.51	0.41
24:j:90:ILE:HB	24:j:91:PRO:HD3	2.03	0.41
2:B:140:LEU:O	2:B:143:GLN:N	2.40	0.40
64:C:401:HEM:CMB	64:C:401:HEM:CBB	3.00	0.40
4:D:161:ALA:O	4:D:162:PRO:C	2.63	0.40
7:G:27:PRO:O	7:G:28:HIS:C	2.62	0.40
1:M:338:LEU:O	1:M:339:GLN:C	2.65	0.40
3:O:73:VAL:HA	5:Q:65:SER:HA	2.04	0.40
3:O:350:ILE:O	3:O:351:GLY:C	2.64	0.40
5:Q:113:GLU:O	5:Q:114:VAL:C	2.63	0.40
5:Q:115:SER:C	5:Q:117:LEU:H	2.28	0.40
12:W:56:LYS:C	12:W:59:SER:HG	2.23	0.40
12:W:114:LEU:HB3	12:W:166:TYR:CD2	2.57	0.40
12:W:140:ARG:HH22	14:Z:302:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:94:VAL:HG11	14:Z:116:LEU:CD1	2.51	0.40
14:Z:224:ALA:O	14:Z:226:TYR:N	2.53	0.40
14:Z:326:CYS:SG	14:Z:453:THR:HB	2.61	0.40
15:a:76:TRP:HD1	15:a:79:ARG:NH2	2.19	0.40
16:b:85:ASN:O	16:b:89:GLU:N	2.49	0.40
18:d:84:ASP:O	18:d:88:ARG:N	2.51	0.40
18:d:140:CYS:O	18:d:145:SER:N	2.54	0.40
18:d:156:LEU:HD13	18:d:158:ILE:HD12	2.03	0.40
20:f:2:ASN:OD1	20:f:2:ASN:N	2.55	0.40
20:f:41:ILE:N	20:f:42:PRO:HD2	2.37	0.40
22:h:61:LEU:HD23	22:h:61:LEU:O	2.21	0.40
23:i:31:LEU:O	25:k:20:PHE:HZ	2.04	0.40
24:j:84:TYR:HE1	24:j:472:ILE:HD12	1.85	0.40
24:j:226:GLN:CD	24:j:280:LEU:HD22	2.45	0.40
25:k:52:LEU:HA	25:k:52:LEU:HD23	1.83	0.40
69:p:401:NDP:O3B	69:p:401:NDP:P2B	2.79	0.40
1:A:445:ARG:O	1:A:446:PHE:CB	2.68	0.40
13:Y:366:LEU:HD13	13:Y:530:TYR:HD1	1.85	0.40
13:Y:401:LEU:HB3	13:Y:474:VAL:HA	2.01	0.40
13:Y:549:GLY:N	13:Y:568:TYR:HE1	2.16	0.40
13:Y:588:ALA:O	13:Y:592:LYS:HE3	2.21	0.40
14:Z:179:ARG:CD	14:Z:183:HIS:HE1	2.35	0.40
16:b:144:ARG:NH2	34:w:112:MET:O	2.55	0.40
19:e:291:LYS:HD3	21:g:106:TRP:CZ3	2.57	0.40
22:h:148:TYR:HD1	22:h:148:TYR:HA	1.79	0.40
22:h:420:THR:HB	22:h:423:ILE:HD12	2.03	0.40
24:j:247:LEU:HD13	24:j:252:MET:SD	2.61	0.40
24:j:418:LEU:HD23	24:j:418:LEU:HA	1.84	0.40
3:C:120:LEU:H	64:C:402:HEM:HMC1	1.86	0.40
2:N:38:LEU:O	2:N:40:ASN:N	2.54	0.40
2:N:154:ASN:O	2:N:157:ALA:N	2.54	0.40
2:N:255:ALA:HA	2:N:426:ALA:HA	2.02	0.40
3:O:34:GLY:O	3:O:37:LEU:N	2.53	0.40
4:P:69:GLU:O	4:P:73:GLY:CA	2.70	0.40
4:P:153:PHE:O	4:P:154:PRO:C	2.64	0.40
12:W:114:LEU:HG	12:W:170:ILE:CD1	2.52	0.40
12:W:153:ILE:HG23	12:W:178:PHE:CD1	2.56	0.40
13:Y:369:GLU:OE2	13:Y:555:ILE:HD11	2.22	0.40
14:Z:139:LEU:HD11	14:Z:424:ILE:HD13	2.02	0.40
14:Z:438:MET:HE3	14:Z:450:ILE:HG12	2.04	0.40
15:a:119:GLN:HE22	19:e:213:VAL:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:123:CYS:SG	16:b:126:GLN:N	2.94	0.40
17:c:355:ILE:HG22	17:c:357:MET:HG3	2.04	0.40
18:d:78:ALA:O	18:d:82:VAL:HG23	2.21	0.40
19:e:180:PRO:HB2	19:e:300:LEU:HD21	2.03	0.40
23:i:25:HIS:HA	23:i:88:ASP:HA	2.03	0.40
24:j:373:LEU:HD23	24:j:431:PHE:CE2	2.56	0.40
25:k:22:SER:C	25:k:24:PRO:HD3	2.46	0.40
29:p:71:ASN:O	29:p:74:GLY:N	2.54	0.40
1:A:133:VAL:O	1:A:134:ILE:C	2.63	0.40
4:D:162:PRO:O	4:D:163:PRO:C	2.63	0.40
2:N:397:THR:O	2:N:398:VAL:C	2.65	0.40
4:P:174:GLY:O	4:P:175:THR:C	2.61	0.40
7:S:45:ILE:O	7:S:49:ALA:CA	2.69	0.40
16:b:73:THR:HG23	19:e:272:TRP:NE1	2.36	0.40
16:b:131:GLU:OE1	16:b:144:ARG:HD3	2.22	0.40
19:e:11:ILE:HB	19:e:12:PRO:HD3	2.03	0.40
19:e:135:ALA:O	19:e:139:THR:HG23	2.21	0.40
20:f:284:MET:O	20:f:287:LEU:HB3	2.21	0.40
22:h:217:PRO:O	22:h:221:VAL:HG23	2.22	0.40
24:j:247:LEU:HD12	24:j:248:HIS:N	2.37	0.40
47:y:430:PHE:O	47:y:431:LEU:C	2.64	0.40
51:Av:14:UNK:O	51:Av:17:UNK:N	2.54	0.40
2:B:156:GLN:O	2:B:157:ALA:C	2.63	0.40
6:F:51:PRO:O	6:F:52:GLU:C	2.63	0.40
10:J:40:ASP:O	10:J:41:ALA:C	2.65	0.40
6:R:104:ARG:O	6:R:105:GLU:C	2.64	0.40
12:W:66:ALA:O	12:W:70:PRO:HB3	2.21	0.40
13:Y:94:MET:HA	13:Y:95:PRO:HD2	1.91	0.40
13:Y:121:LEU:HD23	13:Y:121:LEU:HA	1.87	0.40
13:Y:278:HIS:HB3	13:Y:282:ASN:OD1	2.21	0.40
13:Y:347:ASP:HA	13:Y:596:TYR:HE1	1.87	0.40
13:Y:557:ARG:HD2	13:Y:560:LEU:HD22	2.02	0.40
14:Z:95:LEU:HD13	14:Z:458:PHE:CE2	2.55	0.40
14:Z:408:GLY:HA3	14:Z:425:LYS:HB3	2.04	0.40
15:a:152:SER:HB3	15:a:182:TYR:HD1	1.85	0.40
17:c:177:TYR:CD2	17:c:182:ILE:HD11	2.56	0.40
17:c:201:ALA:O	18:d:119:TYR:HB3	2.22	0.40
19:e:137:ALA:HB1	19:e:286:MET:HE1	2.03	0.40
20:f:211:MET:HB3	20:f:251:MET:CE	2.52	0.40
22:h:176:PHE:HA	22:h:179:ILE:HG22	2.02	0.40
23:i:75:LEU:HD11	25:k:68:PHE:CE1	2.56	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	444/446 (100%)	359 (81%)	63 (14%)	22 (5%)	1 15
1	M	444/446 (100%)	377 (85%)	47 (11%)	20 (4%)	2 16
2	B	417/439 (95%)	342 (82%)	66 (16%)	9 (2%)	5 28
2	N	417/439 (95%)	345 (83%)	60 (14%)	12 (3%)	3 23
3	C	377/379 (100%)	307 (81%)	56 (15%)	14 (4%)	2 19
3	O	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3 23
4	D	239/241 (99%)	199 (83%)	28 (12%)	12 (5%)	1 15
4	P	239/241 (99%)	201 (84%)	26 (11%)	12 (5%)	1 15
5	E	194/274 (71%)	178 (92%)	12 (6%)	4 (2%)	5 28
5	Q	194/274 (71%)	158 (81%)	28 (14%)	8 (4%)	2 17
6	F	104/110 (94%)	90 (86%)	11 (11%)	3 (3%)	3 23
6	R	104/110 (94%)	89 (86%)	12 (12%)	3 (3%)	3 23
7	G	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	2 18
7	S	76/81 (94%)	72 (95%)	2 (3%)	2 (3%)	4 24
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100 100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	7 36
9	I	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1 12
9	U	31/78 (40%)	20 (64%)	7 (23%)	4 (13%)	0 4
10	J	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0 7
10	L	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1 11
11	K	41/56 (73%)	40 (98%)	0	1 (2%)	4 26
11	V	35/56 (62%)	33 (94%)	2 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	W	167/264 (63%)	136 (81%)	23 (14%)	8 (5%)	2 15
13	Y	668/727 (92%)	575 (86%)	65 (10%)	28 (4%)	2 17
14	Z	373/463 (81%)	343 (92%)	20 (5%)	10 (3%)	4 24
15	a	145/216 (67%)	126 (87%)	11 (8%)	8 (6%)	1 14
16	b	147/212 (69%)	140 (95%)	6 (4%)	1 (1%)	18 55
17	c	408/464 (88%)	369 (90%)	27 (7%)	12 (3%)	3 23
18	d	167/249 (67%)	152 (91%)	11 (7%)	4 (2%)	4 26
19	e	313/318 (98%)	282 (90%)	27 (9%)	4 (1%)	9 40
20	f	344/347 (99%)	324 (94%)	17 (5%)	3 (1%)	14 50
21	g	104/115 (90%)	96 (92%)	7 (7%)	1 (1%)	12 47
22	h	455/459 (99%)	424 (93%)	21 (5%)	10 (2%)	5 28
23	i	88/98 (90%)	82 (93%)	4 (4%)	2 (2%)	5 27
24	j	592/606 (98%)	534 (90%)	40 (7%)	18 (3%)	3 22
25	k	138/175 (79%)	126 (91%)	8 (6%)	4 (3%)	3 23
25	l	13/175 (7%)	11 (85%)	1 (8%)	1 (8%)	1 9
26	m	51/84 (61%)	48 (94%)	2 (4%)	1 (2%)	6 30
27	n	81/99 (82%)	74 (91%)	6 (7%)	1 (1%)	10 43
28	o	49/106 (46%)	42 (86%)	3 (6%)	4 (8%)	0 9
29	p	312/377 (83%)	281 (90%)	19 (6%)	12 (4%)	2 18
30	q	194/357 (54%)	172 (89%)	16 (8%)	6 (3%)	3 21
30	v	49/357 (14%)	46 (94%)	3 (6%)	0	100 100
31	r	61/144 (42%)	60 (98%)	1 (2%)	0	100 100
32	Aa	79/156 (51%)	75 (95%)	1 (1%)	3 (4%)	2 18
32	t	79/156 (51%)	74 (94%)	3 (4%)	2 (2%)	4 25
33	Ai	32/189 (17%)	31 (97%)	1 (3%)	0	100 100
33	u	52/189 (28%)	48 (92%)	4 (8%)	0	100 100
34	w	105/175 (60%)	93 (89%)	11 (10%)	1 (1%)	12 47
35	x	44/123 (36%)	41 (93%)	1 (2%)	2 (4%)	2 16
36	0	259/261 (99%)	249 (96%)	10 (4%)	0	100 100
37	1	142/147 (97%)	135 (95%)	7 (5%)	0	100 100
38	2	107/109 (98%)	104 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2 17
40	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1 12
41	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9 38
42	6	71/73 (97%)	65 (92%)	6 (8%)	0	100 100
43	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2 19
44	8	47/56 (84%)	41 (87%)	6 (13%)	0	100 100
45	9	45/47 (96%)	42 (93%)	3 (7%)	0	100 100
46	s	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
47	y	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16 53
48	z	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9 40
50	Ac	53/70 (76%)	49 (92%)	2 (4%)	2 (4%)	2 18
52	Ae	86/116 (74%)	82 (95%)	2 (2%)	2 (2%)	5 27
53	Af	88/128 (69%)	81 (92%)	4 (4%)	3 (3%)	3 20
54	Ag	129/141 (92%)	120 (93%)	2 (2%)	7 (5%)	1 14
55	Aj	131/176 (74%)	124 (95%)	2 (2%)	5 (4%)	2 18
56	Ak	149/178 (84%)	131 (88%)	11 (7%)	7 (5%)	2 16
57	Al	94/122 (77%)	83 (88%)	7 (7%)	4 (4%)	2 16
58	Am	25/76 (33%)	23 (92%)	2 (8%)	0	100 100
59	An	95/172 (55%)	87 (92%)	5 (5%)	3 (3%)	3 20
All	All	12001/14873 (81%)	10603 (88%)	1047 (9%)	351 (3%)	5 23

All (351) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	A	426	GLY
1	A	427	PRO
2	B	141	GLN
2	B	183	ILE
2	B	305	GLN
3	C	8	HIS
3	C	27	ILE
3	C	109	PHE
3	C	319	PRO
4	D	51	LEU

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Mol	Chain	Res	Type
4	D	73	GLY
4	D	98	PRO
5	E	82	PRO
9	I	72	VAL
10	L	58	LYS
1	M	55	ALA
1	M	220	SER
1	M	427	PRO
2	N	141	GLN
2	N	183	ILE
2	N	351	ASN
3	O	8	HIS
3	O	27	ILE
3	O	157	GLY
4	P	51	LEU
4	P	73	GLY
5	Q	114	VAL
5	Q	141	HIS
9	U	73	PRO
13	Y	37	ASP
13	Y	47	THR
13	Y	181	ARG
13	Y	287	SER
13	Y	347	ASP
13	Y	448	SER
17	c	73	PRO
17	c	105	PRO
17	c	379	CYS
18	d	183	ALA
19	e	208	VAL
22	h	429	SER
24	j	562	LEU
24	j	581	LYS
25	k	76	THR
27	n	50	ASP
29	p	211	ASP
30	q	201	LEU
35	x	81	SER
39	3	2	SER
39	3	87	THR
39	3	95	GLN
40	4	4	ALA

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Mol	Chain	Res	Type
40	4	9	GLY
41	5	46	LYS
43	7	2	GLU
47	y	328	HIS
47	y	508	PRO
50	Ac	52	ARG
54	Ag	135	VAL
55	Aj	121	TYR
56	Ak	156	PRO
57	Al	10	ARG
57	Al	20	ALA
59	An	49	GLU
1	A	55	ALA
1	A	56	GLY
1	A	72	GLY
1	A	227	ALA
1	A	287	GLY
1	A	288	ALA
1	A	342	TRP
2	B	236	LYS
2	B	351	ASN
3	C	28	SER
3	C	137	GLN
3	C	157	GLY
3	C	313	ARG
4	D	154	PRO
5	E	78	LEU
5	E	191	ASP
7	G	68	LYS
9	I	59	ALA
10	J	58	LYS
10	L	23	THR
10	L	24	ILE
1	M	52	ASN
1	M	72	GLY
1	M	246	ASP
1	M	282	CYS
1	M	385	THR
2	N	236	LYS
5	Q	137	GLY
7	S	73	ASN
9	U	56	ARG

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Mol	Chain	Res	Type
9	U	59	ALA
12	W	138	ASN
12	W	192	GLY
13	Y	210	ILE
13	Y	288	ASP
13	Y	336	ASN
13	Y	368	THR
13	Y	450	LYS
13	Y	541	PRO
13	Y	555	ILE
14	Z	104	GLU
14	Z	265	ASN
14	Z	273	VAL
14	Z	386	THR
17	c	50	ASP
17	c	331	VAL
17	c	378	SER
20	f	86	ILE
22	h	22	MET
22	h	139	GLN
22	h	188	ASN
23	i	22	TYR
24	j	73	THR
24	j	440	LEU
24	j	586	LEU
25	k	24	PRO
26	m	50	PRO
28	o	20	ILE
28	o	24	GLU
28	o	48	GLY
28	o	49	GLY
29	p	86	CYS
29	p	135	GLU
29	p	230	SER
29	p	239	PRO
29	p	310	PHE
30	q	90	GLU
30	q	115	SER
30	q	203	PRO
40	4	5	LYS
32	Aa	137	LYS
32	Aa	139	MET

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Mol	Chain	Res	Type
52	Ae	41	ASN
53	Af	76	PRO
54	Ag	14	GLU
54	Ag	47	ALA
55	Aj	119	GLU
55	Aj	120	SER
56	Ak	106	ASP
57	Al	12	PRO
1	A	52	ASN
1	A	352	SER
1	A	385	THR
1	A	395	TRP
2	B	91	ALA
4	D	27	ARG
4	D	162	PRO
10	J	23	THR
10	J	35	PHE
11	K	11	ARG
10	L	57	HIS
1	M	81	SER
1	M	107	PRO
1	M	426	GLY
2	N	24	LEU
2	N	305	GLN
3	O	28	SER
3	O	62	ALA
3	O	316	MET
3	O	319	PRO
4	P	80	MET
4	P	162	PRO
5	Q	177	PRO
6	R	33	ARG
12	W	194	GLU
13	Y	174	THR
13	Y	283	GLU
13	Y	377	ALA
13	Y	663	ASN
13	Y	665	PHE
13	Y	677	GLN
13	Y	689	LEU
14	Z	102	SER
14	Z	139	LEU

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Mol	Chain	Res	Type
14	Z	197	MET
14	Z	233	HIS
15	a	105	ASP
15	a	116	SER
15	a	156	CYS
17	c	236	PHE
18	d	176	CYS
19	e	60	PRO
21	g	24	LEU
22	h	251	ASN
22	h	353	PRO
23	i	50	ASN
24	j	55	MET
24	j	447	ASN
25	k	77	GLU
25	l	116	ILE
29	p	178	SER
29	p	259	LYS
30	q	112	GLY
32	t	108	LEU
35	x	82	ARG
40	4	61	SER
48	z	104	TRP
32	Aa	138	LEU
54	Ag	48	SER
55	Aj	144	SER
55	Aj	145	ASP
56	Ak	51	HIS
1	A	107	PRO
1	A	246	ASP
1	A	391	PRO
3	C	236	ILE
3	C	365	LEU
4	D	147	LEU
6	F	95	LYS
1	M	6	GLN
1	M	109	ALA
2	N	269	ALA
2	N	409	ASP
3	O	24	PRO
3	O	109	PHE
4	P	147	LEU

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Mol	Chain	Res	Type
5	Q	130	PRO
6	R	95	LYS
7	S	27	PRO
12	W	105	ASN
12	W	121	THR
12	W	202	PHE
13	Y	69	LEU
13	Y	337	ASP
13	Y	575	VAL
13	Y	650	SER
15	a	89	LEU
16	b	175	PHE
17	c	186	ALA
17	c	237	GLY
18	d	160	VAL
19	e	196	ALA
20	f	48	PHE
20	f	81	SER
24	j	477	VAL
24	j	511	LEU
24	j	512	LYS
24	j	536	LEU
25	k	25	SER
29	p	102	GLN
29	p	205	ASP
47	y	51	ASP
50	Ac	51	ASP
52	Ae	76	GLN
53	Af	72	HIS
54	Ag	15	GLY
54	Ag	17	GLU
56	Ak	32	VAL
56	Ak	145	PRO
59	An	37	ASP
1	A	6	GLN
1	A	152	TYR
2	B	39	GLU
3	C	316	MET
6	F	104	ARG
7	G	72	LYS
10	J	4	THR
10	J	57	HIS

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Mol	Chain	Res	Type
1	M	338	LEU
1	M	391	PRO
3	O	247	PRO
3	O	255	ASN
4	P	83	ARG
4	P	98	PRO
4	P	110	PRO
4	P	154	PRO
5	Q	69	LEU
5	Q	188	THR
12	W	191	TYR
13	Y	281	ILE
13	Y	582	VAL
13	Y	654	VAL
18	d	214	PRO
19	e	281	ARG
22	h	85	SER
22	h	368	ALA
24	j	195	ALA
24	j	211	MET
24	j	441	VAL
29	p	330	PRO
30	q	68	ILE
32	t	137	LYS
34	w	96	LYS
43	7	3	ASN
48	z	103	GLN
56	Ak	76	HIS
56	Ak	87	GLY
59	An	79	ALA
1	A	33	PRO
1	A	109	ALA
2	B	52	LYS
4	D	110	PRO
4	D	163	PRO
4	D	176	PRO
7	G	45	ILE
1	M	185	TYR
2	N	52	LYS
2	N	260	GLU
4	P	176	PRO
12	W	122	ARG

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Mol	Chain	Res	Type
13	Y	267	THR
14	Z	94	VAL
15	a	159	GLY
15	a	171	ARG
17	c	74	ASP
24	j	275	THR
29	p	83	PRO
40	4	49	PRO
47	y	91	ASP
48	z	158	ASP
53	Af	96	VAL
2	B	129	ALA
6	F	51	PRO
1	M	56	GLY
1	M	293	PRO
3	C	339	GLY
4	D	83	ARG
2	N	85	ILE
2	N	109	VAL
4	P	123	GLY
5	Q	84	GLY
8	T	69	VAL
15	a	160	GLY
17	c	94	PRO
24	j	563	PRO
5	E	76	ILE
10	J	24	ILE
6	R	51	PRO
15	a	147	PRO
22	h	249	ILE
24	j	515	TYR
39	3	15	GLY
54	Ag	45	PRO
57	Al	56	VAL
1	A	260	PRO
4	P	163	PRO
9	U	65	VAL
14	Z	319	PRO
17	c	221	GLY
22	h	172	GLY
3	C	348	ILE
3	C	372	ILE

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Mol	Chain	Res	Type
4	D	26	ILE
1	M	71	PRO
1	M	193	PRO
24	j	483	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	145/228 (64%)	144 (99%)	1 (1%)	76	80
13	Y	517/610 (85%)	515 (100%)	2 (0%)	84	83
14	Z	322/393 (82%)	321 (100%)	1 (0%)	86	84
15	a	120/177 (68%)	119 (99%)	1 (1%)	73	78
16	b	126/176 (72%)	126 (100%)	0	100	100
17	c	321/368 (87%)	320 (100%)	1 (0%)	86	84
18	d	145/207 (70%)	145 (100%)	0	100	100
19	e	272/275 (99%)	270 (99%)	2 (1%)	76	80
20	f	309/311 (99%)	309 (100%)	0	100	100
21	g	91/100 (91%)	90 (99%)	1 (1%)	65	74
22	h	407/409 (100%)	404 (99%)	3 (1%)	76	80
23	i	76/85 (89%)	75 (99%)	1 (1%)	61	72
24	j	527/540 (98%)	523 (99%)	4 (1%)	73	78
25	k	112/141 (79%)	111 (99%)	1 (1%)	70	77
All	All	3490/4020 (87%)	3472 (100%)	18 (0%)	78	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	W	157	VAL
13	Y	478	SER
13	Y	489	ILE

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Mol	Chain	Res	Type
14	Z	356	ILE
15	a	91	CYS
17	c	331	VAL
19	e	187	ILE
19	e	309	ILE
21	g	96	ILE
22	h	37	ILE
22	h	96	ILE
22	h	107	ILE
23	i	8	ILE
24	j	63	ILE
24	j	283	ILE
24	j	317	ILE
24	j	468	ILE
25	k	12	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
12	W	55	HIS
12	W	107	GLN
12	W	124	ASN
12	W	181	HIS
13	Y	522	GLN
13	Y	569	GLN
13	Y	571	HIS
13	Y	705	GLN
14	Z	92	HIS
14	Z	250	ASN
14	Z	270	ASN
14	Z	299	GLN
14	Z	339	GLN
14	Z	381	HIS
14	Z	442	HIS
15	a	98	HIS
15	a	119	GLN
15	a	164	HIS
15	a	201	GLN
16	b	159	GLN
17	c	220	GLN
17	c	376	HIS
17	c	393	ASN

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Mol	Chain	Res	Type
17	c	418	GLN
17	c	441	HIS
18	d	59	ASN
18	d	69	ASN
18	d	90	ASN
18	d	99	ASN
18	d	153	GLN
18	d	187	GLN
18	d	189	ASN
18	d	191	ASN
19	e	47	GLN
19	e	230	ASN
19	e	235	ASN
19	e	247	HIS
19	e	284	GLN
19	e	304	HIS
20	f	2	ASN
20	f	47	ASN
20	f	120	GLN
20	f	134	GLN
20	f	221	HIS
20	f	319	HIS
22	h	20	HIS
22	h	26	ASN
22	h	30	HIS
22	h	83	HIS
22	h	220	HIS
22	h	251	ASN
22	h	304	GLN
22	h	331	ASN
22	h	424	ASN
22	h	434	ASN
22	h	440	HIS
24	j	165	ASN
24	j	192	HIS
24	j	194	ASN
24	j	328	HIS
24	j	332	HIS
24	j	518	GLN
24	j	546	GLN
24	j	570	GLN
24	j	580	GLN

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Mol	Chain	Res	Type
25	k	46	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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	SF4	c	501	17	0,12,12	-	-	-		
66	FES	Q	201	-	0,4,4	-	-	-		
69	NDP	p	401	-	51,52,52	1.16	6 (11%)	71,80,80	1.58	10 (14%)
67	SF4	a	301	15	0,12,12	-	-	-		
64	HEM	C	402	-	50,50,50	1.26	6 (12%)	67,82,82	1.72	17 (25%)
66	FES	Y	803	13	0,4,4	-	-	-		
67	SF4	Y	801	13	0,12,12	-	-	-		
67	SF4	b	301	16	0,12,12	-	-	-		
64	HEM	O	401	-	50,50,50	1.40	8 (16%)	67,82,82	1.87	18 (26%)
66	FES	d	301	-	0,4,4	-	-	-		
67	SF4	b	302	16	0,12,12	-	-	-		
64	HEM	C	401	-	50,50,50	1.31	7 (14%)	67,82,82	1.52	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
71	HEA	y	602	-	67,67,67	1.20	7 (10%)	81,103,103	1.35	13 (16%)
65	HEC	P	301	-	46,50,50	1.88	7 (15%)	58,82,82	1.55	4 (6%)
67	SF4	Y	802	13	0,12,12	-	-	-		
66	FES	E	201	-	0,4,4	-	-	-		
64	HEM	O	402	-	50,50,50	1.37	7 (14%)	67,82,82	1.73	14 (20%)
65	HEC	D	301	-	46,50,50	1.85	6 (13%)	58,82,82	1.53	8 (13%)
68	FMN	c	502	-	33,33,33	1.45	5 (15%)	48,50,50	1.31	8 (16%)
71	HEA	y	601	-	67,67,67	1.21	4 (5%)	81,103,103	1.33	10 (12%)

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	SF4	c	501	17	-	-	0/6/5/5
66	FES	Q	201	-	-	-	0/1/1/1
69	NDP	p	401	-	-	15/34/77/77	0/5/5/5
67	SF4	a	301	15	-	-	0/6/5/5
64	HEM	C	402	-	-	6/14/54/54	-
66	FES	Y	803	13	-	-	0/1/1/1
67	SF4	Y	801	13	-	-	0/6/5/5
67	SF4	b	301	16	-	-	0/6/5/5
64	HEM	O	401	-	-	6/14/54/54	-
66	FES	d	301	-	-	-	0/1/1/1
67	SF4	b	302	16	-	-	0/6/5/5
64	HEM	C	401	-	-	4/14/54/54	-
71	HEA	y	602	-	-	7/36/76/76	-
65	HEC	P	301	-	-	10/14/54/54	-
67	SF4	Y	802	13	-	-	0/6/5/5
66	FES	E	201	-	-	-	0/1/1/1
64	HEM	O	402	-	-	4/14/54/54	-
65	HEC	D	301	-	-	8/14/54/54	-
68	FMN	c	502	-	-	4/18/18/18	0/3/3/3
71	HEA	y	601	-	-	7/36/76/76	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	P	301	HEC	CAB-C3B	6.65	1.56	1.35
65	D	301	HEC	CAB-C3B	6.48	1.56	1.35
65	P	301	HEC	CAC-C3C	6.45	1.55	1.35
65	D	301	HEC	CAC-C3C	6.29	1.55	1.35
68	c	502	FMN	C9A-C5A	4.75	1.48	1.41
71	y	601	HEA	C11-C3B	-4.12	1.46	1.51
69	p	401	NDP	C5A-C4A	4.10	1.46	1.39
65	D	301	HEC	CBB-CAB	-3.72	1.35	1.49
71	y	602	HEA	CMA-C3A	-3.66	1.37	1.45
65	P	301	HEC	CBC-CAC	-3.64	1.36	1.49
65	D	301	HEC	CBC-CAC	-3.53	1.36	1.49
65	P	301	HEC	CBB-CAB	-3.46	1.36	1.49
64	C	401	HEM	CAB-C3B	3.39	1.56	1.47
64	O	402	HEM	FE-NA	3.39	2.06	1.95
64	O	402	HEM	FE-NC	3.39	2.06	1.95
64	O	401	HEM	CAB-C3B	3.36	1.56	1.47
68	c	502	FMN	C8-C7	3.28	1.48	1.40
64	C	401	HEM	FE-NB	3.22	2.04	1.94
64	C	402	HEM	CHB-C4A	-3.14	1.32	1.39
64	O	401	HEM	FE-NB	3.11	2.04	1.94
68	c	502	FMN	C4-N3	-2.99	1.33	1.38
71	y	602	HEA	FE-NA	2.98	2.05	1.95
64	C	401	HEM	C3B-C2B	-2.97	1.31	1.37
69	p	401	NDP	C5A-N7A	-2.93	1.33	1.39
64	O	401	HEM	C1B-C2B	2.74	1.50	1.44
64	O	402	HEM	CAC-C3C	2.70	1.54	1.47
71	y	601	HEA	C1A-C2A	-2.68	1.40	1.45
71	y	602	HEA	C1D-ND	-2.64	1.35	1.40
71	y	601	HEA	CMA-C3A	-2.64	1.39	1.45
64	O	401	HEM	CAC-C3C	2.60	1.54	1.47
71	y	602	HEA	C1D-C2D	2.56	1.49	1.44
64	C	401	HEM	FE-ND	2.48	2.02	1.94
64	O	402	HEM	C1A-NA	2.46	1.44	1.39
64	C	401	HEM	CAC-C3C	2.41	1.53	1.47
64	O	402	HEM	FE-NB	2.41	2.02	1.94
68	c	502	FMN	C5A-N5	-2.37	1.35	1.39
71	y	602	HEA	CMD-C2D	2.36	1.55	1.50
71	y	602	HEA	C3A-C2A	-2.35	1.31	1.37
65	P	301	HEC	C3C-C2C	-2.32	1.33	1.41
71	y	601	HEA	C3A-C4A	-2.31	1.42	1.46
64	C	402	HEM	FE-ND	2.31	2.02	1.94
65	D	301	HEC	C3B-C2B	-2.30	1.33	1.41
64	O	402	HEM	CAB-C3B	2.30	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	C	401	HEM	C2A-C3A	-2.30	1.32	1.38
64	O	401	HEM	C2A-C3A	-2.29	1.32	1.38
64	C	402	HEM	FE-NC	2.26	2.02	1.95
64	O	401	HEM	C3D-C2D	-2.26	1.31	1.36
65	P	301	HEC	C3B-C2B	-2.23	1.33	1.41
68	c	502	FMN	C2-N3	-2.22	1.34	1.39
69	p	401	NDP	C5A-C6A	2.17	1.47	1.41
65	D	301	HEC	C3C-C2C	-2.16	1.33	1.41
64	O	402	HEM	C2A-C3A	-2.16	1.33	1.38
64	C	402	HEM	CAB-C3B	2.15	1.53	1.47
64	O	401	HEM	FE-NA	2.14	2.02	1.95
64	C	402	HEM	FE-NB	2.14	2.01	1.94
69	p	401	NDP	C4A-N9A	-2.11	1.33	1.37
69	p	401	NDP	C8A-N9A	-2.09	1.34	1.37
65	P	301	HEC	C3D-C2D	-2.09	1.33	1.38
69	p	401	NDP	C8A-N7A	2.07	1.35	1.31
64	C	402	HEM	C1C-C2C	2.06	1.49	1.45
64	C	401	HEM	CMB-C2B	2.06	1.55	1.50
71	y	602	HEA	FE-NC	2.04	2.01	1.95
64	O	401	HEM	CMD-C2D	2.01	1.54	1.50

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	P	301	HEC	CBB-CAB-C3B	-6.71	114.02	127.43
65	D	301	HEC	CBC-CAC-C3C	-6.71	114.02	127.43
65	P	301	HEC	CBC-CAC-C3C	-6.13	115.17	127.43
69	p	401	NDP	C5A-C4A-N3A	-5.90	118.59	126.72
64	O	401	HEM	C3B-C2B-C1B	-5.33	102.41	106.41
64	O	402	HEM	C3B-C2B-C1B	5.10	110.24	106.41
65	D	301	HEC	CBB-CAB-C3B	-4.99	117.46	127.43
64	O	401	HEM	CMA-C3A-C4A	-4.96	117.87	125.42
69	p	401	NDP	N3A-C4A-N9A	4.79	135.32	127.17
64	C	401	HEM	CBD-CAD-C3D	4.78	125.76	112.53
64	O	402	HEM	CHC-C4B-NB	4.19	128.94	124.42
64	O	402	HEM	C2A-C1A-NA	-4.18	105.52	110.15
71	y	601	HEA	C17-C18-C19	-4.15	118.13	127.62
64	C	401	HEM	O1D-CGD-CBD	-4.04	110.29	123.09
69	p	401	NDP	C2A-N3A-C4A	3.88	121.32	111.83
64	O	402	HEM	CHA-C1A-C2A	3.87	133.77	125.30
64	C	401	HEM	CBB-CAB-C3B	-3.86	108.24	127.53
69	p	401	NDP	N3A-C2A-N1A	-3.82	122.79	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	C	402	HEM	CAA-CBA-CGA	3.82	123.79	113.67
64	O	402	HEM	CHB-C1B-NB	-3.77	119.71	124.37
64	O	401	HEM	C2B-C1B-NB	3.66	114.05	109.84
64	O	401	HEM	O1D-CGD-CBD	-3.62	111.60	123.09
64	O	401	HEM	C4B-C3B-C2B	3.58	110.57	107.28
64	O	401	HEM	CHB-C1B-NB	-3.47	120.08	124.37
64	C	402	HEM	C3C-C2C-C1C	-3.47	103.77	107.05
64	C	402	HEM	CMA-C3A-C4A	-3.44	120.19	125.42
64	O	401	HEM	O2D-CGD-O1D	3.43	132.16	123.33
64	O	401	HEM	CMA-C3A-C2A	3.33	132.69	125.62
69	p	401	NDP	C4A-C5A-N7A	-3.31	106.79	110.58
71	y	601	HEA	C13-C14-C15	-3.28	120.12	127.62
64	C	402	HEM	CHD-C1D-ND	3.27	127.94	124.42
71	y	602	HEA	CHA-C1A-NA	-3.16	121.01	124.45
64	C	402	HEM	C4D-ND-C1D	3.09	108.87	105.21
64	O	402	HEM	O1D-CGD-CBD	-3.08	113.32	123.09
64	C	402	HEM	O2A-CGA-CBA	3.06	123.66	114.00
64	C	402	HEM	C4A-CHB-C1B	3.00	133.30	126.25
71	y	601	HEA	C1B-C2B-C3B	2.93	110.18	106.80
64	C	402	HEM	CHB-C1B-NB	-2.87	120.82	124.37
64	C	402	HEM	CHC-C1C-NC	-2.85	121.34	124.45
69	p	401	NDP	C4A-N9A-C8A	2.83	108.71	105.74
64	C	402	HEM	CMA-C3A-C2A	2.80	131.57	125.62
64	C	402	HEM	O2A-CGA-O1A	-2.79	116.16	123.33
64	C	401	HEM	O2A-CGA-O1A	2.79	130.50	123.33
68	c	502	FMN	C4-C4A-N5	2.77	122.04	118.21
64	O	401	HEM	CMD-C2D-C1D	-2.73	120.76	125.03
65	P	301	HEC	O1D-CGD-CBD	-2.71	114.49	123.09
64	O	402	HEM	CAA-C2A-C1A	-2.71	119.65	124.94
64	C	401	HEM	CMB-C2B-C1B	-2.70	120.81	125.03
64	C	402	HEM	CAD-CBD-CGD	2.66	120.73	113.67
68	c	502	FMN	C4A-C10-N1	-2.64	118.11	124.59
64	C	402	HEM	CBD-CAD-C3D	2.62	119.78	112.53
68	c	502	FMN	C4'-C3'-C2'	-2.61	109.23	113.57
69	p	401	NDP	C5A-N7A-C8A	2.61	107.55	103.45
64	O	401	HEM	CAB-C3B-C2B	-2.60	119.98	128.43
65	D	301	HEC	O1A-CGA-CBA	-2.57	114.94	123.09
64	O	401	HEM	C1B-NB-C4B	-2.54	102.20	105.21
71	y	602	HEA	CMD-C2D-C1D	2.53	128.99	125.03
64	O	401	HEM	CBD-CAD-C3D	2.52	119.51	112.53
64	C	401	HEM	O2D-CGD-CBD	2.50	121.89	114.00
64	C	401	HEM	CMA-C3A-C4A	-2.49	121.63	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	y	601	HEA	C17-C16-C15	-2.46	105.03	113.19
64	O	401	HEM	CHA-C4D-ND	-2.45	121.33	124.37
71	y	602	HEA	C1D-C2D-C3D	-2.45	104.40	106.98
64	O	401	HEM	CMB-C2B-C3B	2.45	134.36	128.43
64	O	402	HEM	CMB-C2B-C3B	-2.44	122.53	128.43
65	D	301	HEC	O2D-CGD-O1D	2.43	129.57	123.33
64	C	402	HEM	CAA-C2A-C1A	-2.42	120.22	124.94
64	C	402	HEM	C3D-C4D-ND	-2.42	107.52	110.17
71	y	602	HEA	C12-C11-C3B	2.42	115.90	112.12
64	C	402	HEM	C4C-NC-C1C	-2.41	101.89	105.82
71	y	602	HEA	C4A-C3A-C2A	2.39	108.89	106.81
68	c	502	FMN	C4-N3-C2	-2.36	121.45	125.64
71	y	601	HEA	C3C-C4C-NC	2.33	111.76	109.80
71	y	602	HEA	C13-C14-C15	-2.33	122.30	127.62
65	D	301	HEC	O1D-CGD-CBD	-2.30	115.79	123.09
64	O	402	HEM	C4B-C3B-C2B	-2.30	105.17	107.28
68	c	502	FMN	C4A-C4-N3	2.29	119.09	113.25
71	y	602	HEA	CMB-C2B-C3B	-2.28	125.86	130.28
71	y	602	HEA	C25-C23-C24	2.27	119.82	114.59
71	y	602	HEA	CAA-C2A-C1A	2.27	129.47	124.85
64	C	401	HEM	CHC-C1C-NC	2.25	126.91	124.45
71	y	601	HEA	CAD-C3D-C4D	2.25	128.62	124.70
64	O	402	HEM	O2D-CGD-CBD	2.24	121.06	114.00
65	D	301	HEC	CAD-C3D-C2D	2.23	132.06	127.07
64	O	401	HEM	C4A-C3A-C2A	2.22	109.36	106.82
69	p	401	NDP	C3D-C2D-C1D	2.22	105.66	101.46
71	y	601	HEA	C4B-C3B-C2B	-2.22	103.71	107.44
68	c	502	FMN	O4-C4-C4A	-2.19	120.74	126.53
71	y	602	HEA	C26-C15-C16	2.19	119.03	115.23
64	O	401	HEM	C3C-C2C-C1C	2.19	109.11	107.05
69	p	401	NDP	N9A-C8A-N7A	-2.17	110.86	113.94
64	O	402	HEM	CMD-C2D-C1D	-2.17	121.64	125.03
71	y	601	HEA	C20-C19-C18	2.16	126.02	121.17
71	y	601	HEA	C12-C13-C14	-2.15	106.52	112.16
64	O	402	HEM	CHA-C1A-NA	-2.13	120.00	123.86
68	c	502	FMN	C4A-C10-N10	2.12	119.52	116.48
71	y	602	HEA	C3A-C2A-C1A	-2.10	105.05	107.05
64	O	402	HEM	CMC-C2C-C1C	-2.10	121.03	124.73
71	y	602	HEA	CBD-CAD-C3D	2.10	118.34	112.53
64	O	401	HEM	O1A-CGA-CBA	-2.09	116.48	123.09
71	y	601	HEA	C27-C19-C18	-2.08	118.29	123.63
68	c	502	FMN	C10-N1-C2	2.07	121.34	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	C	402	HEM	C2A-C1A-NA	-2.07	107.86	110.15
64	O	402	HEM	CHC-C4B-C3B	-2.07	120.95	125.07
69	p	401	NDP	C6A-C5A-N7A	2.05	136.04	132.09
64	O	401	HEM	CHA-C4D-C3D	2.04	129.00	125.23
65	P	301	HEC	O1A-CGA-CBA	-2.04	116.62	123.09
65	D	301	HEC	CAD-C3D-C4D	-2.04	120.96	124.94
65	D	301	HEC	CBD-CAD-C3D	2.03	118.14	112.53
64	C	401	HEM	CMA-C3A-C2A	2.03	129.92	125.62
71	y	602	HEA	C3C-C4C-NC	2.02	111.50	109.80

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	O	401	HEM	C2B-C3B-CAB-CBB
65	D	301	HEC	C2B-C3B-CAB-CBB
65	D	301	HEC	C4B-C3B-CAB-CBB
65	D	301	HEC	C2C-C3C-CAC-CBC
65	D	301	HEC	C4C-C3C-CAC-CBC
65	P	301	HEC	C2B-C3B-CAB-CBB
65	P	301	HEC	C2C-C3C-CAC-CBC
65	P	301	HEC	C4C-C3C-CAC-CBC
68	c	502	FMN	C1'-C2'-C3'-C4'
68	c	502	FMN	C3'-C4'-C5'-O5'
68	c	502	FMN	O4'-C4'-C5'-O5'
69	p	401	NDP	C5B-O5B-PA-O1A
69	p	401	NDP	C5B-O5B-PA-O3
69	p	401	NDP	C5D-O5D-PN-O1N
71	y	601	HEA	C2A-C3A-CMA-OMA
71	y	601	HEA	C4A-C3A-CMA-OMA
71	y	602	HEA	C2A-C3A-CMA-OMA
71	y	602	HEA	C4A-C3A-CMA-OMA
71	y	601	HEA	C15-C16-C17-C18
69	p	401	NDP	C1B-C2B-O2B-P2B
69	p	401	NDP	C3B-C2B-O2B-P2B
69	p	401	NDP	C3B-C4B-C5B-O5B
64	O	401	HEM	C4B-C3B-CAB-CBB
69	p	401	NDP	O4B-C4B-C5B-O5B
65	P	301	HEC	C1A-C2A-CAA-CBA
65	P	301	HEC	C3A-C2A-CAA-CBA
64	C	402	HEM	C2B-C3B-CAB-CBB
65	P	301	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
65	D	301	HEC	C1A-C2A-CAA-CBA
69	p	401	NDP	C5B-O5B-PA-O2A
69	p	401	NDP	C5D-O5D-PN-O3
69	p	401	NDP	C5D-O5D-PN-O2N
65	D	301	HEC	C3A-C2A-CAA-CBA
69	p	401	NDP	O4D-C1D-N1N-C6N
65	D	301	HEC	CAA-CBA-CGA-O1A
65	P	301	HEC	CAA-CBA-CGA-O1A
64	O	401	HEM	CAD-CBD-CGD-O2D
64	O	402	HEM	CAA-CBA-CGA-O1A
65	D	301	HEC	CAA-CBA-CGA-O2A
71	y	602	HEA	CAD-CBD-CGD-O1D
64	C	402	HEM	CAD-CBD-CGD-O1D
65	P	301	HEC	CAA-CBA-CGA-O2A
64	O	402	HEM	CAD-CBD-CGD-O2D
64	C	402	HEM	CAA-CBA-CGA-O2A
64	O	401	HEM	CAD-CBD-CGD-O1D
71	y	601	HEA	CAD-CBD-CGD-O1D
71	y	602	HEA	CAD-CBD-CGD-O2D
65	P	301	HEC	C2A-CAA-CBA-CGA
64	C	401	HEM	CAD-CBD-CGD-O1D
64	C	401	HEM	CAD-CBD-CGD-O2D
64	C	402	HEM	CAA-CBA-CGA-O1A
64	C	402	HEM	CAD-CBD-CGD-O2D
64	O	401	HEM	CAA-CBA-CGA-O2A
64	O	402	HEM	CAA-CBA-CGA-O2A
69	p	401	NDP	C2D-C1D-N1N-C6N
71	y	601	HEA	CAD-CBD-CGD-O2D
64	O	402	HEM	CAD-CBD-CGD-O1D
64	C	401	HEM	CAA-CBA-CGA-O2A
64	O	401	HEM	CAA-CBA-CGA-O1A
71	y	601	HEA	CAA-CBA-CGA-O1A
64	C	402	HEM	C4B-C3B-CAB-CBB
68	c	502	FMN	O2'-C2'-C3'-C4'
71	y	602	HEA	CAA-CBA-CGA-O2A
64	C	401	HEM	CAA-CBA-CGA-O1A
71	y	602	HEA	CAA-CBA-CGA-O1A
71	y	602	HEA	C26-C15-C16-C17
69	p	401	NDP	O4D-C4D-C5D-O5D
69	p	401	NDP	C3D-C4D-C5D-O5D
65	P	301	HEC	CAD-CBD-CGD-O2D
71	y	601	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
69	p	401	NDP	O4D-C1D-N1N-C2N

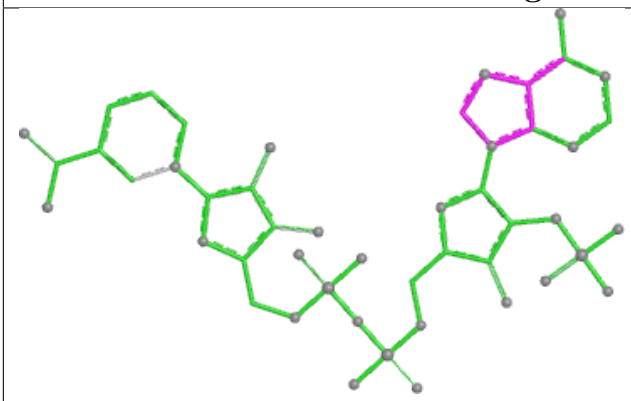
There are no ring outliers.

16 monomers are involved in 115 short contacts:

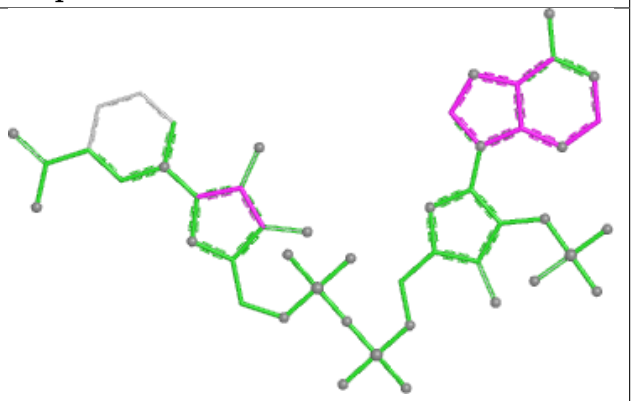
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	c	501	SF4	4	0
69	p	401	NDP	26	0
64	C	402	HEM	39	0
67	Y	801	SF4	4	0
67	b	301	SF4	2	0
64	O	401	HEM	6	0
66	d	301	FES	1	0
67	b	302	SF4	1	0
64	C	401	HEM	3	0
71	y	602	HEA	1	0
65	P	301	HEC	2	0
67	Y	802	SF4	1	0
64	O	402	HEM	3	0
65	D	301	HEC	1	0
68	c	502	FMN	20	0
71	y	601	HEA	1	0

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

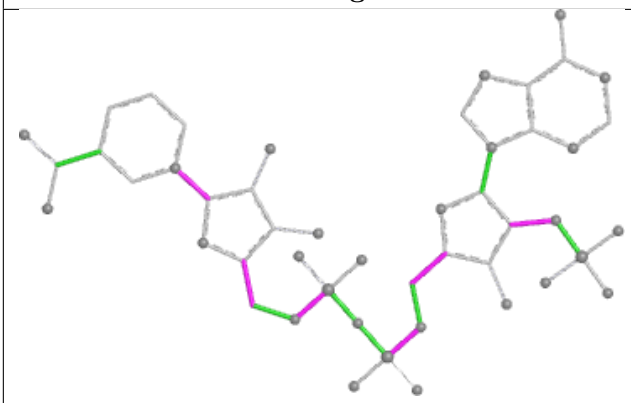
Ligand NDP p 401



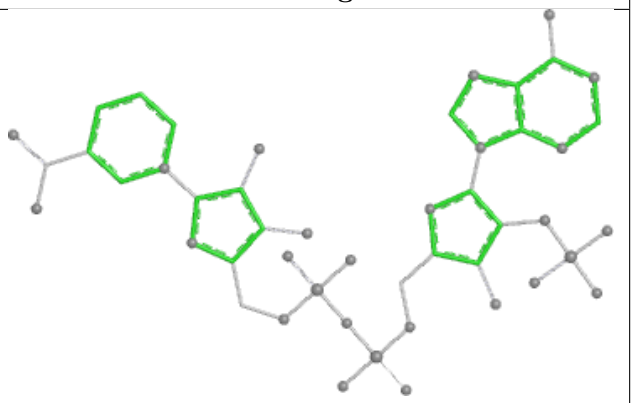
Bond lengths



Bond angles

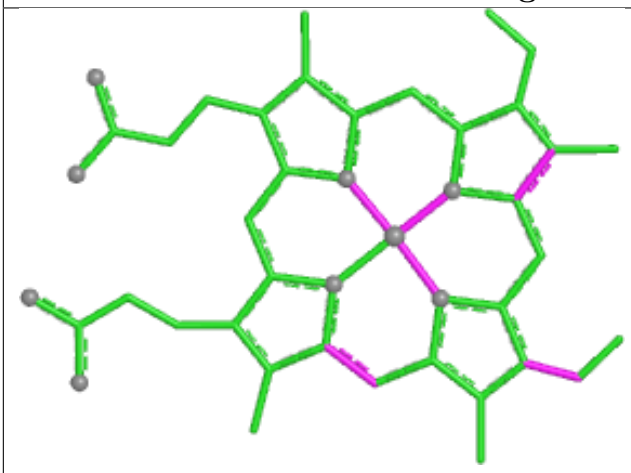


Torsions

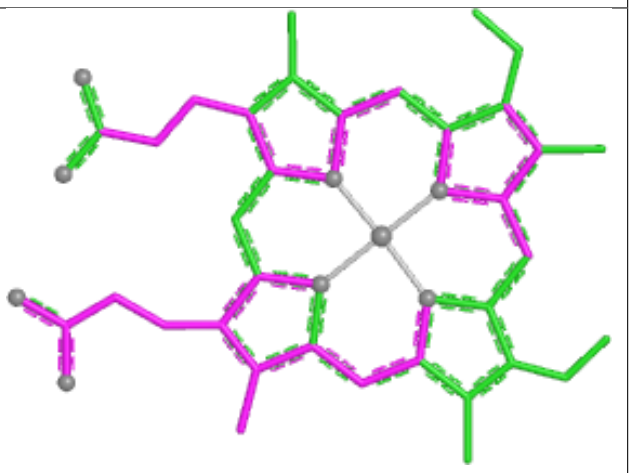


Rings

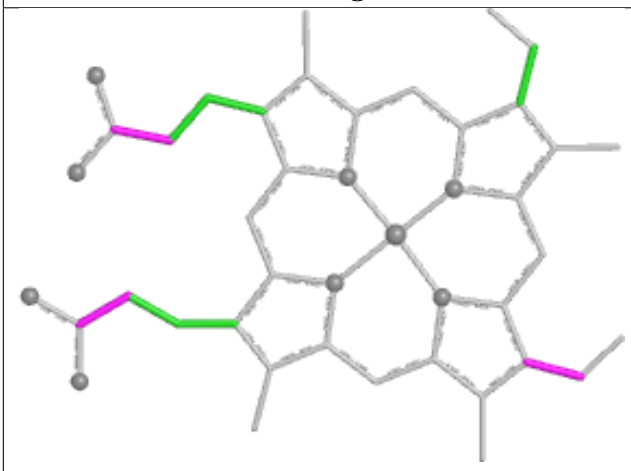
Ligand HEM C 402



Bond lengths



Bond angles



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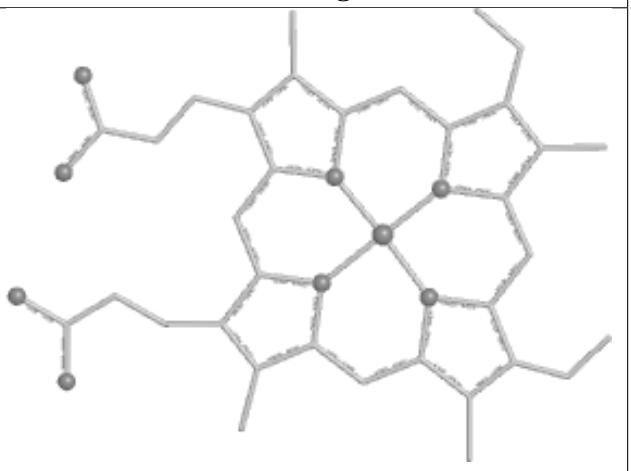
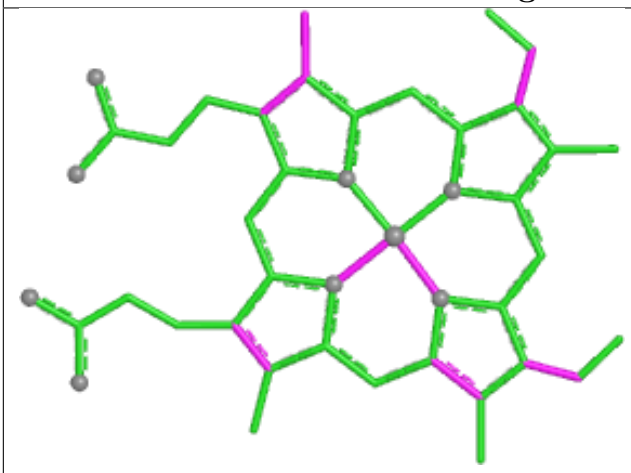
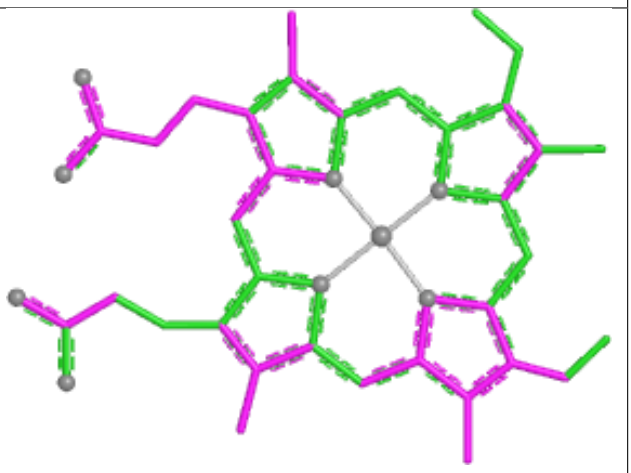


Rings

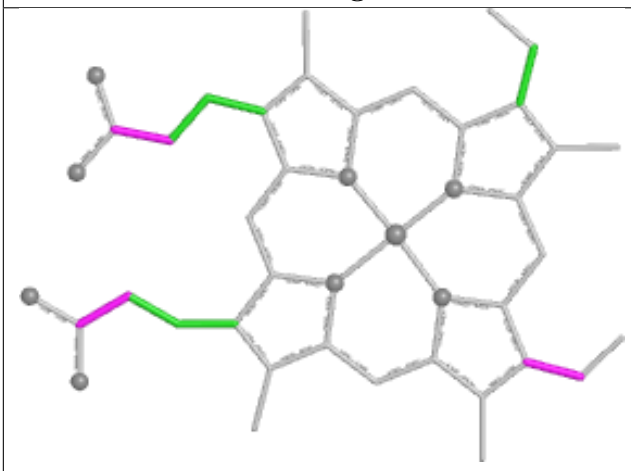
Ligand HEM O 401



Bond lengths



Bond angles



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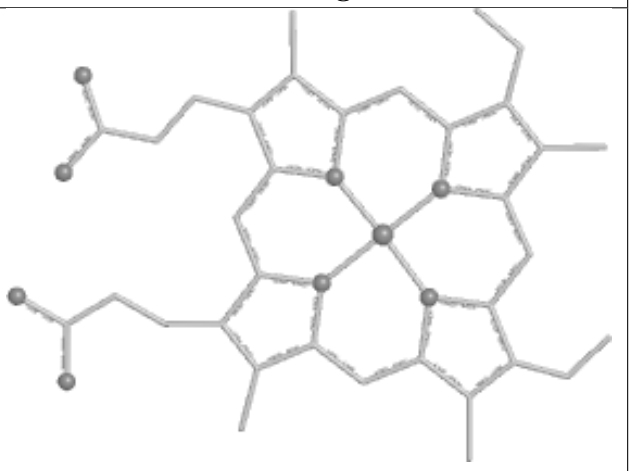
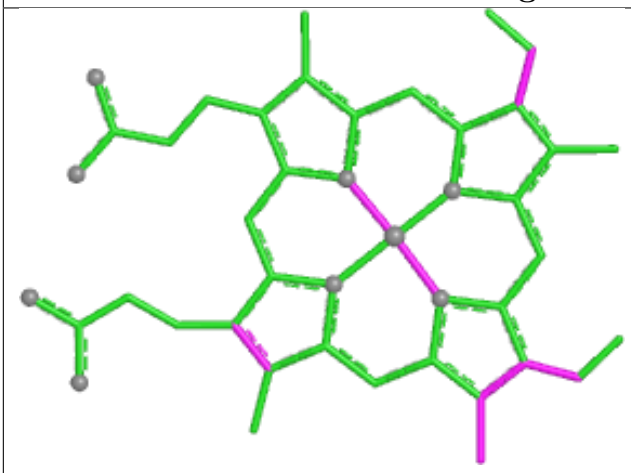
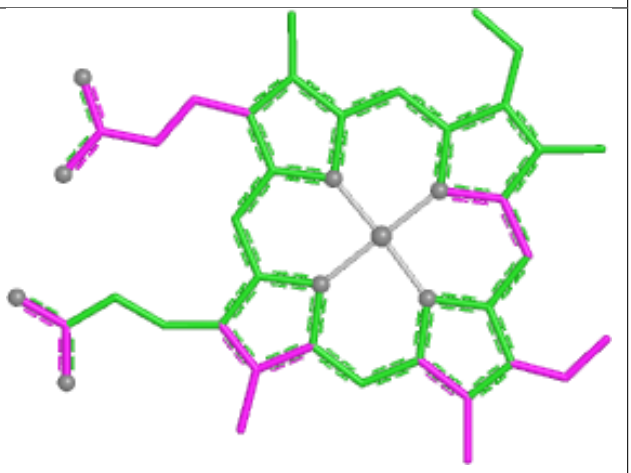


Rings

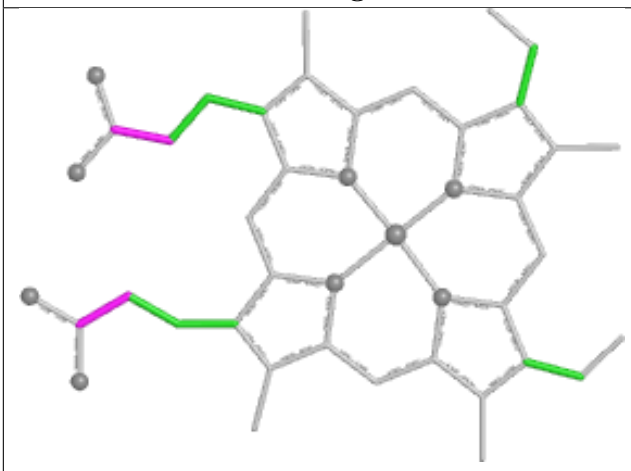
Ligand HEM C 401



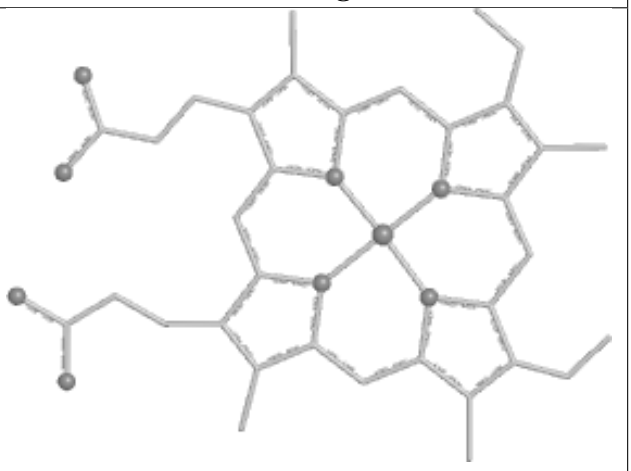
Bond lengths



Bond angles

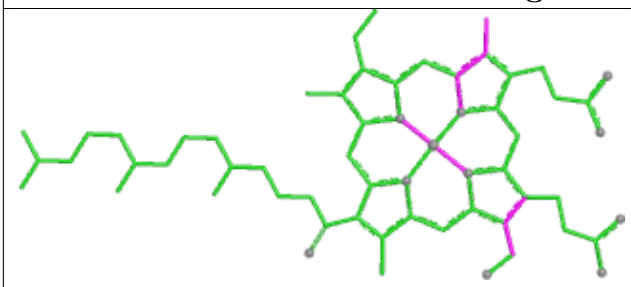


Torsions

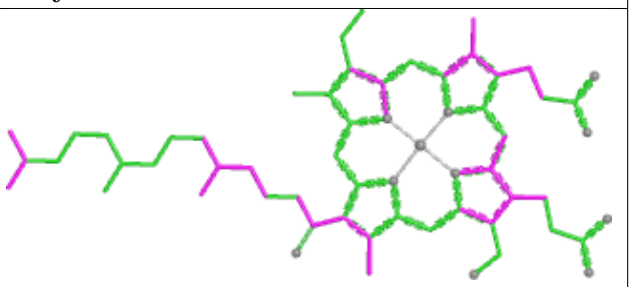


Rings

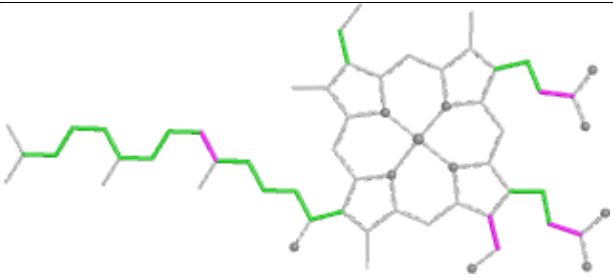
Ligand HEA y 602



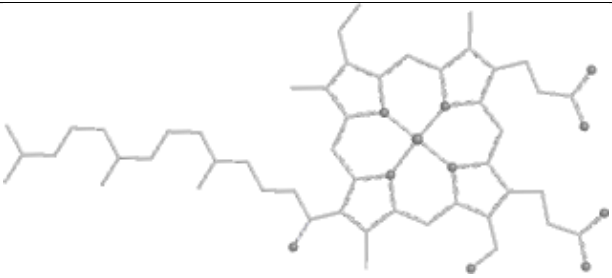
Bond lengths



Bond angles

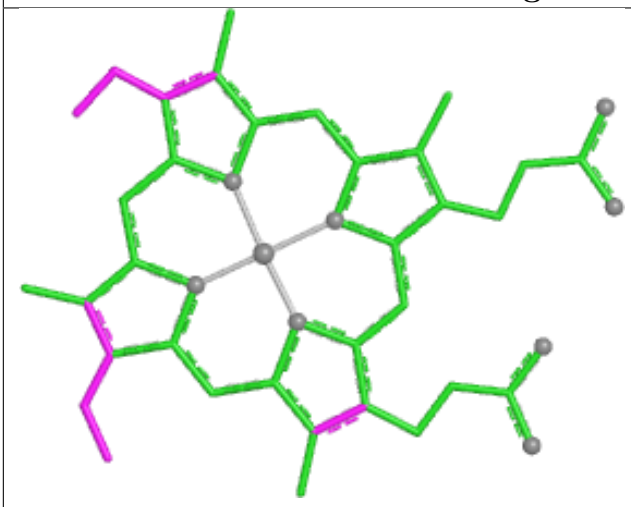


Torsions

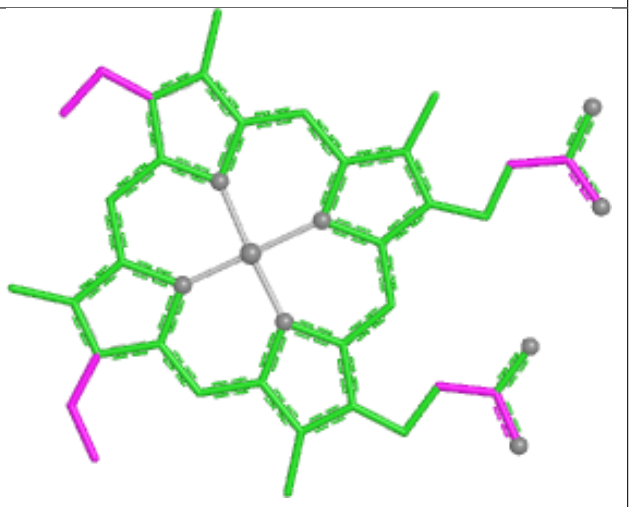


Rings

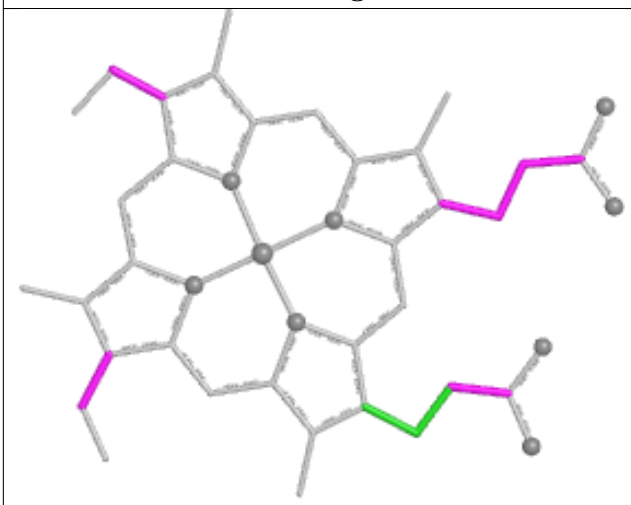
Ligand HEC P 301



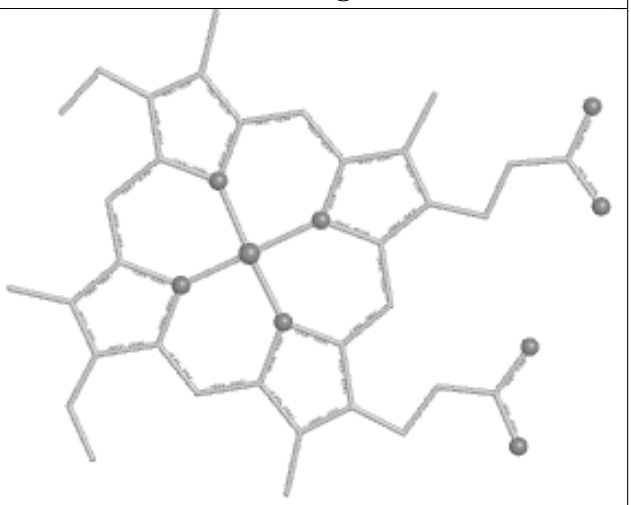
Bond lengths



Bond angles

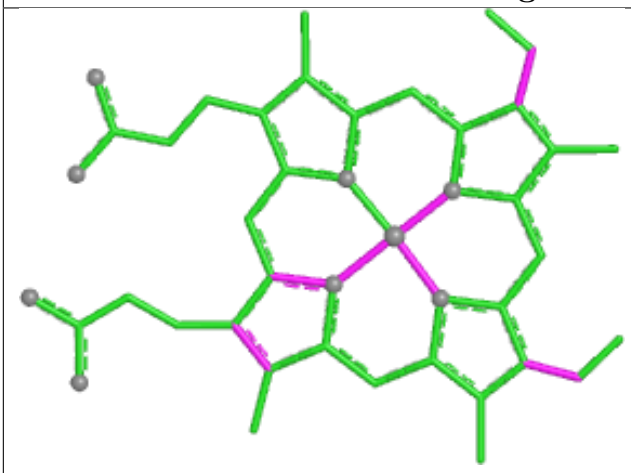


Torsions

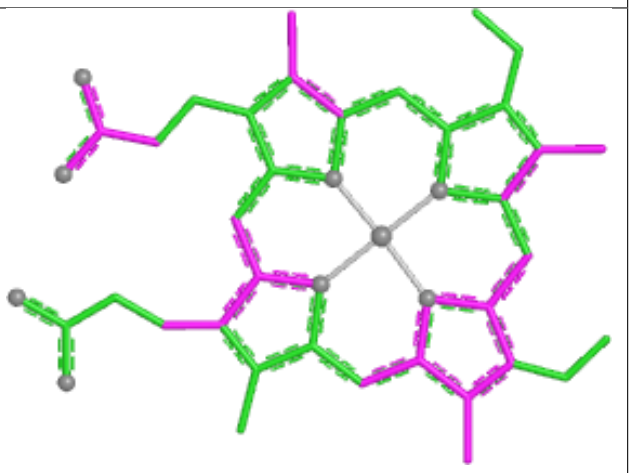


Rings

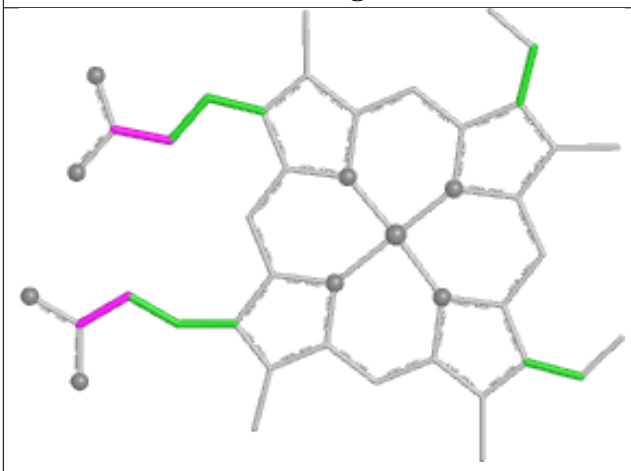
Ligand HEM O 402



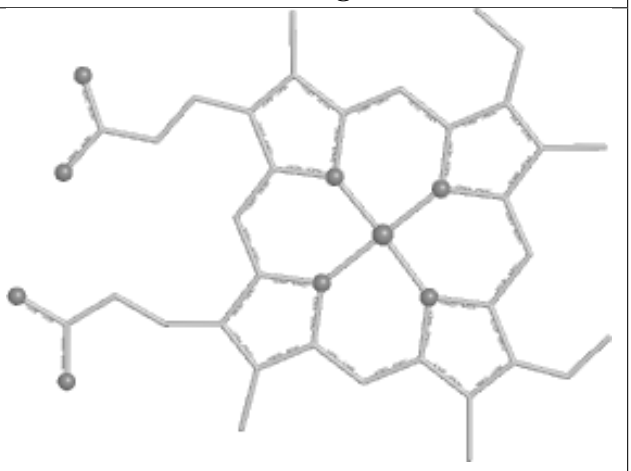
Bond lengths



Bond angles

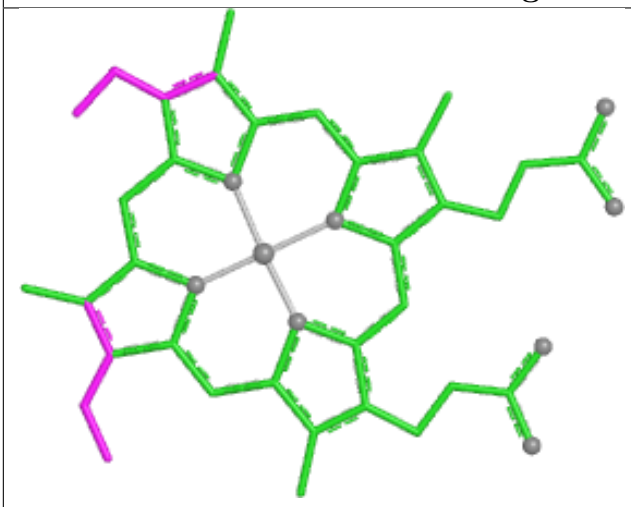


Torsions

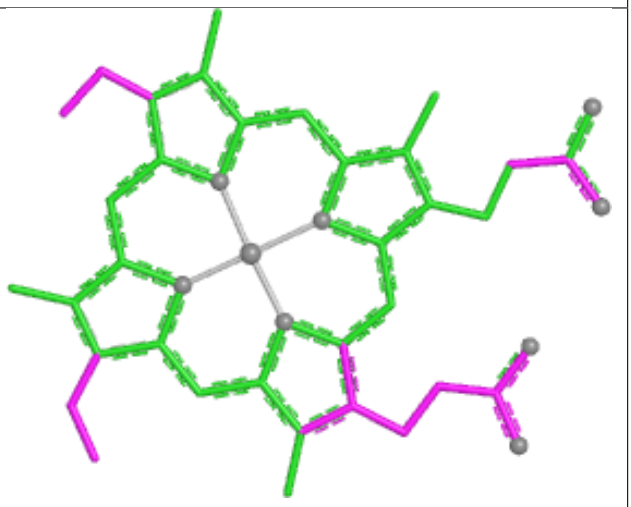


Rings

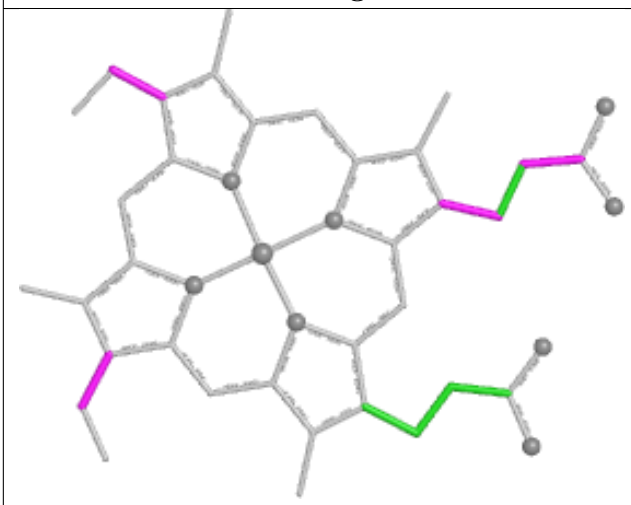
Ligand HEC D 301



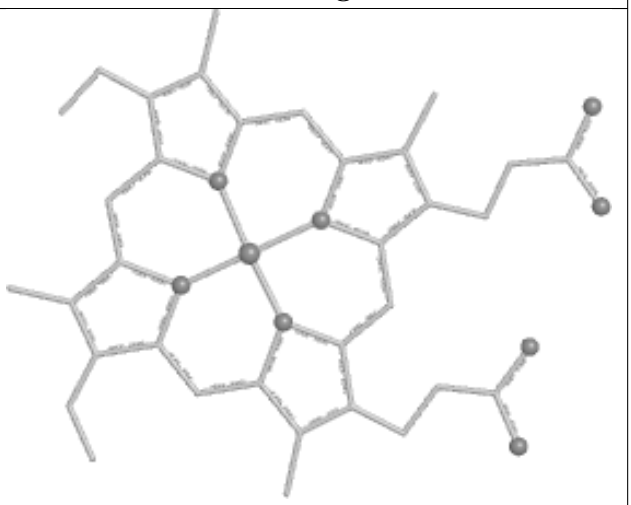
Bond lengths



Bond angles

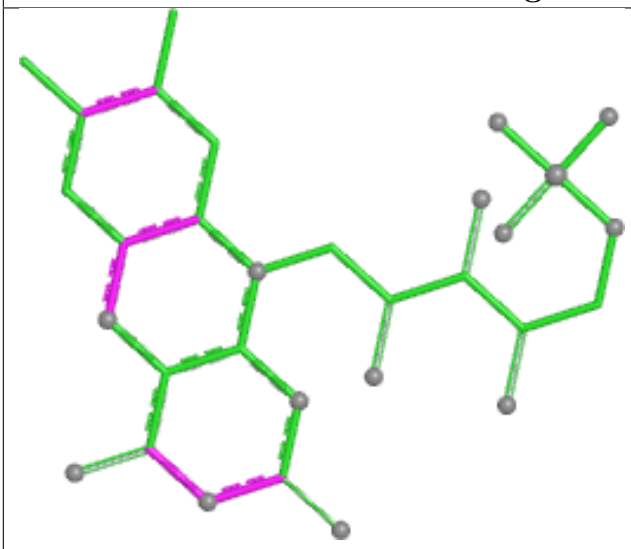


Torsions

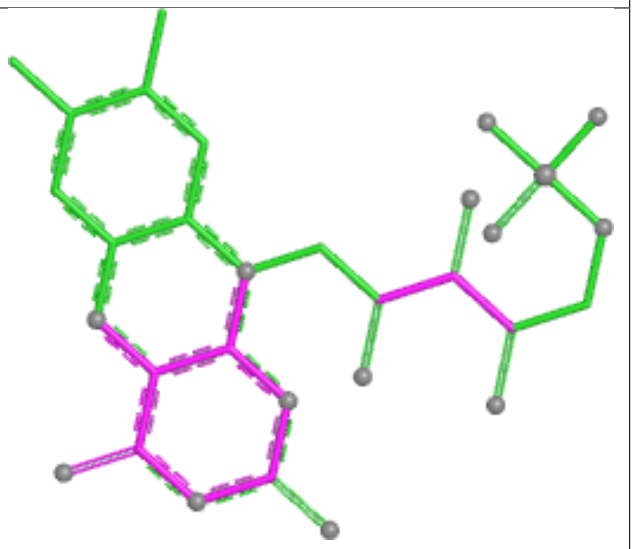


Rings

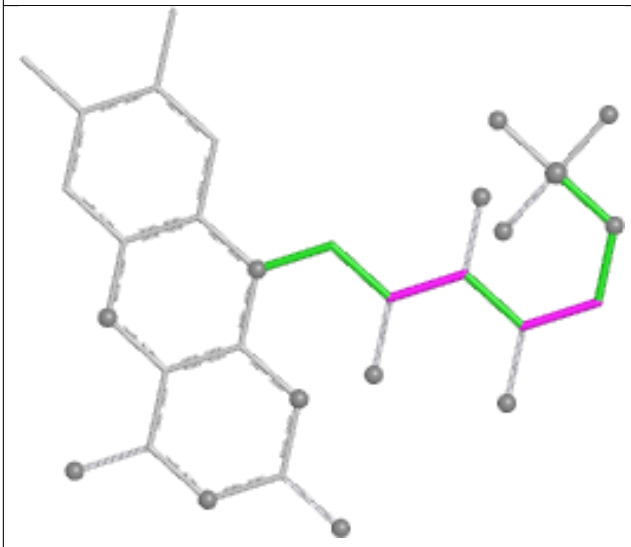
Ligand FMN c 502



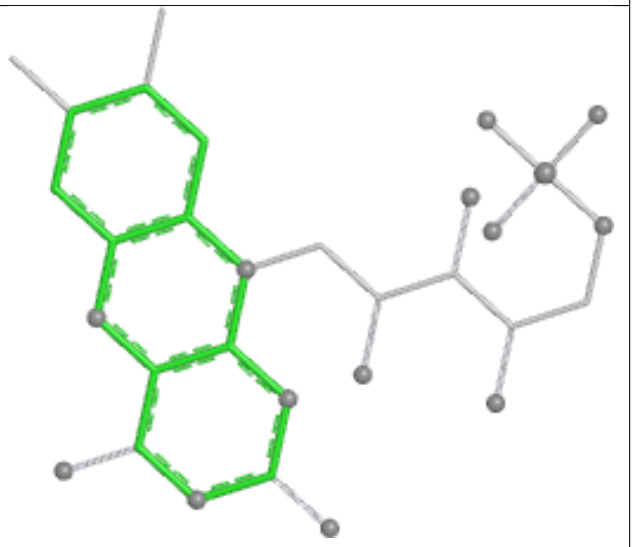
Bond lengths



Bond angles

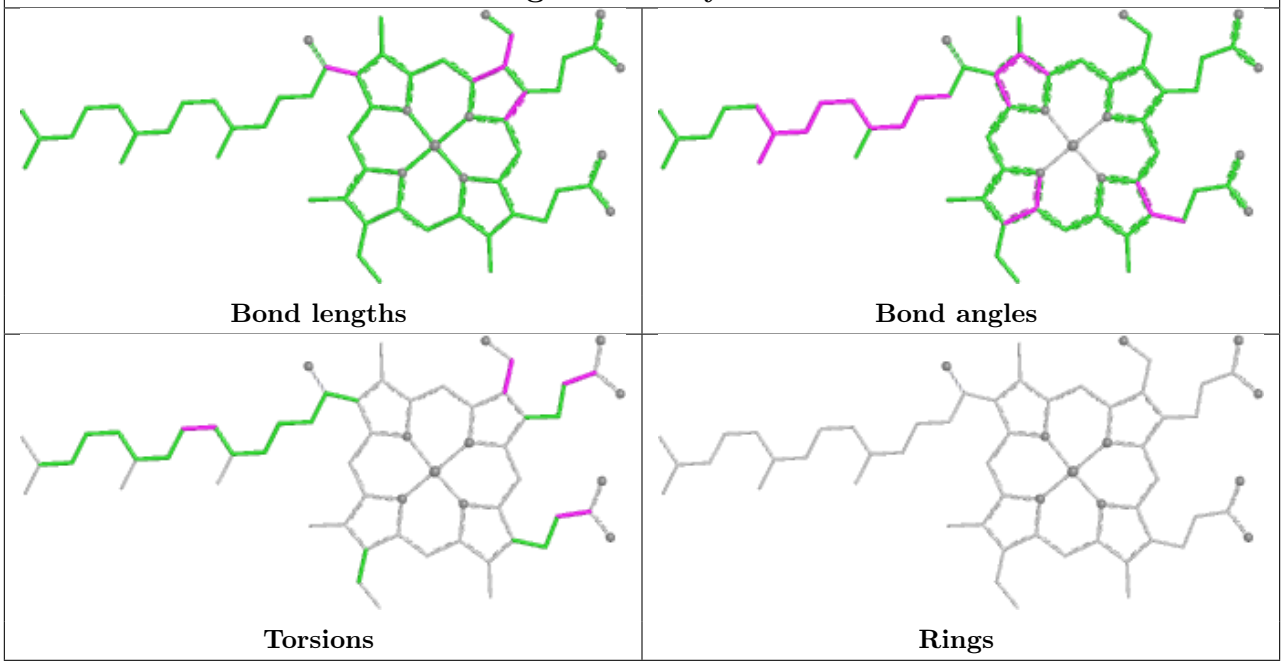


Torsions



Rings

Ligand HEA y 601



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.

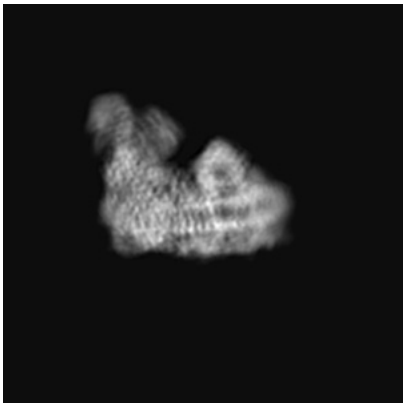
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9534. These allow visual inspection of the internal detail of the map and identification of artifacts.

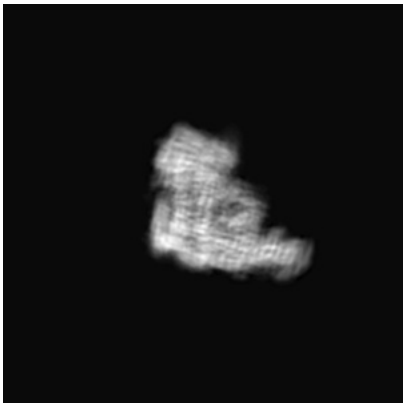
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

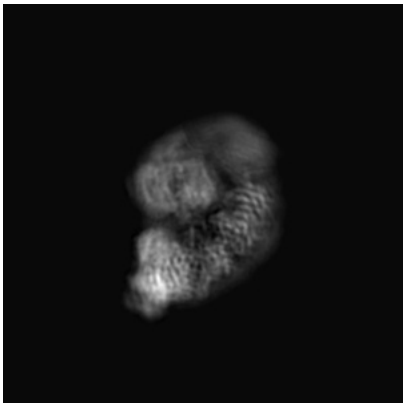
6.1.1 Primary map



X



Y



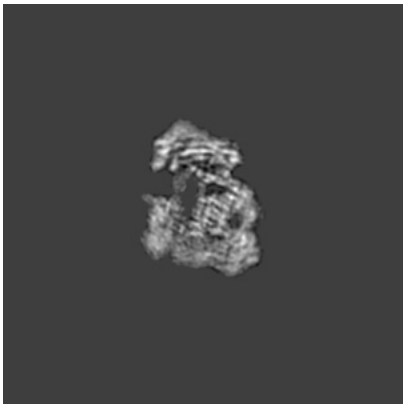
Z

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

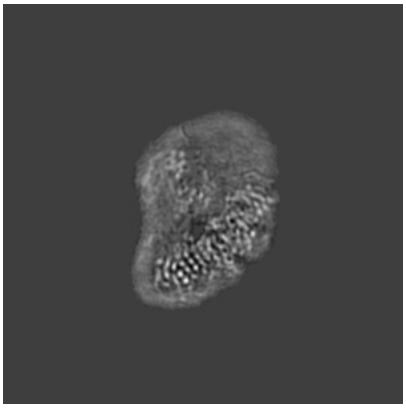
6.2 Central slices

6.2.1 Primary map

X Index: 240



Y Index: 240

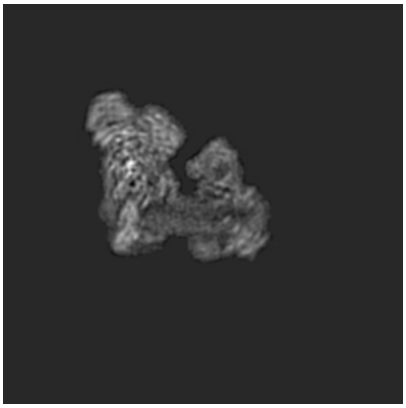


Z Index: 240

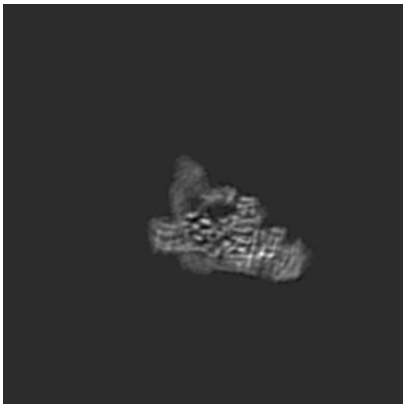
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

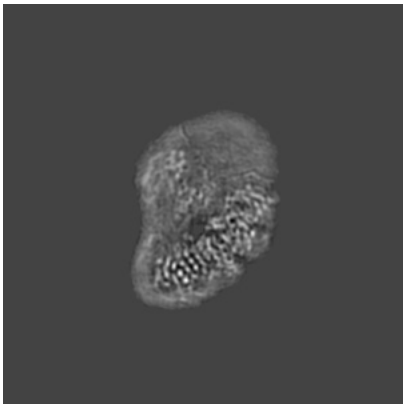
6.3.1 Primary map



X Index: 186



Y Index: 149

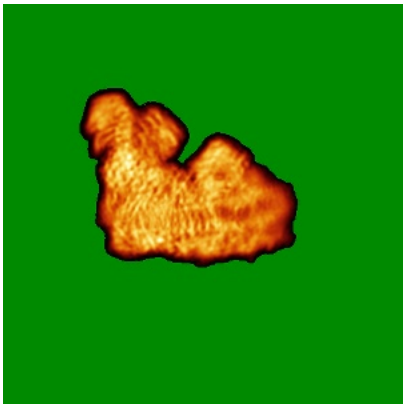


Z Index: 241

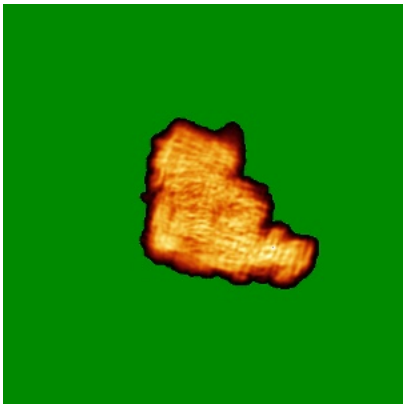
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

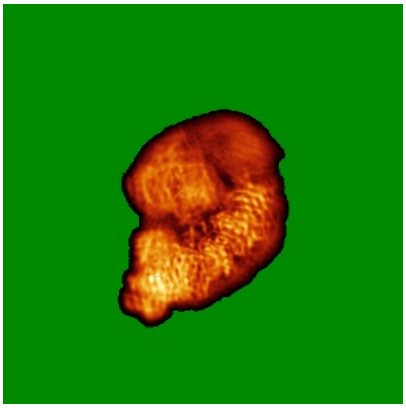
6.4.1 Primary map



X



Y

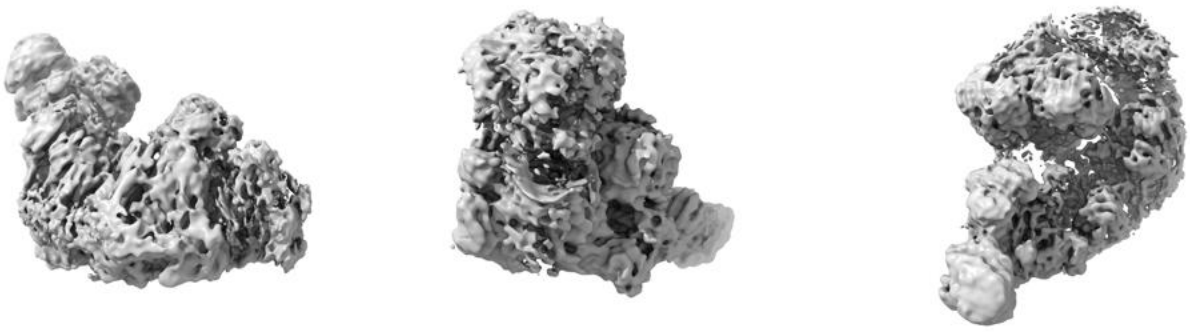


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

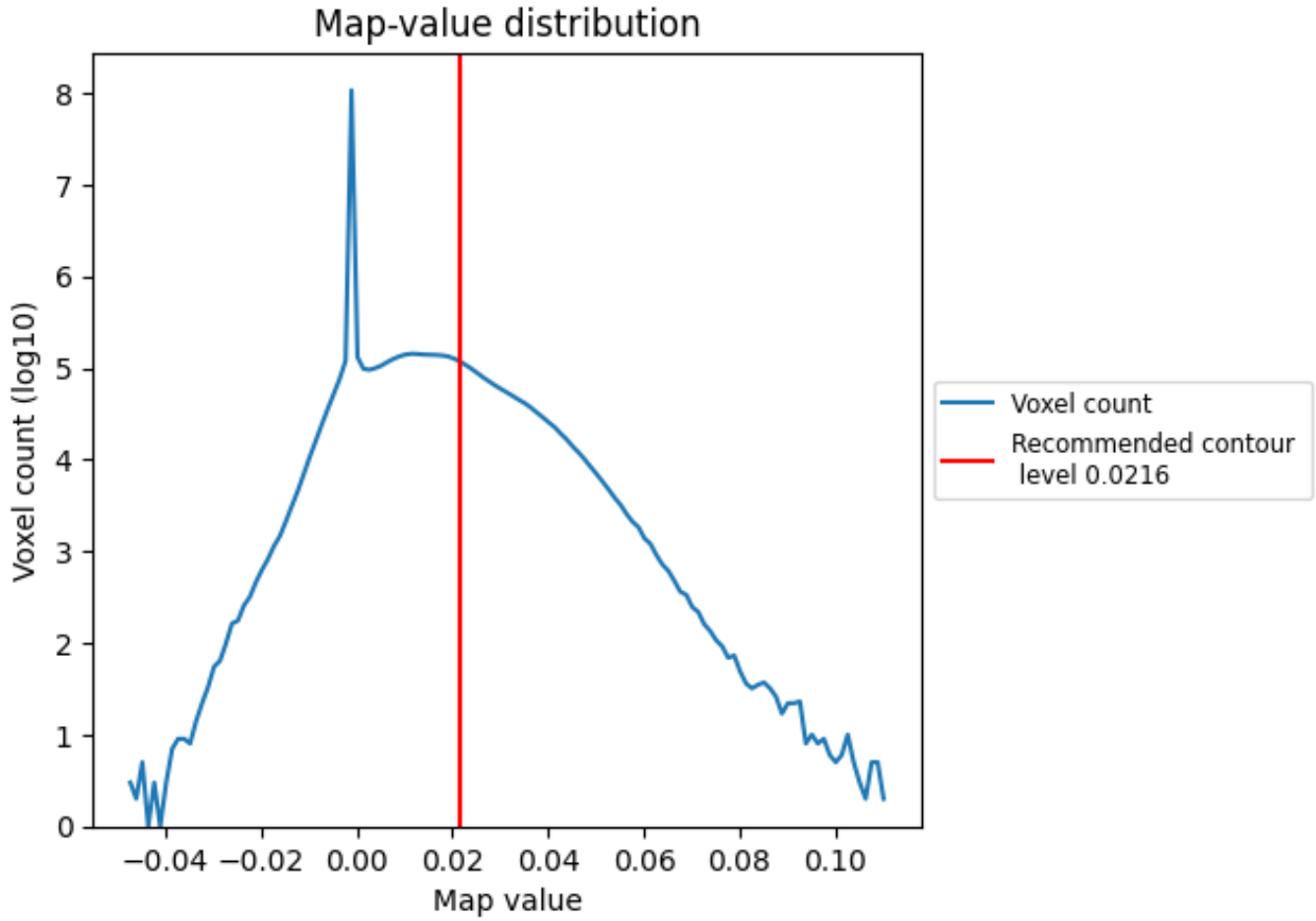
6.6 Mask visualisation (i)

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

7 Map analysis

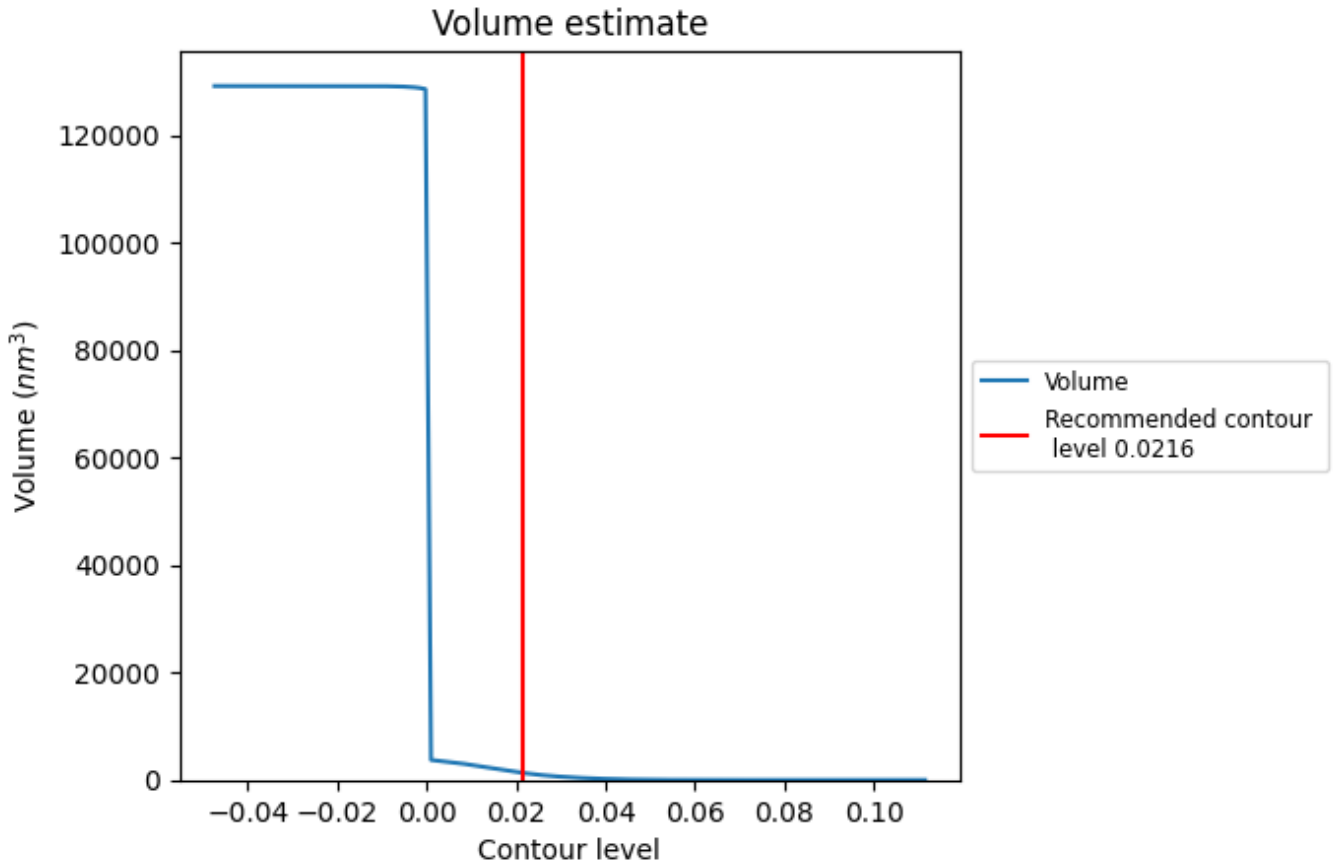
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

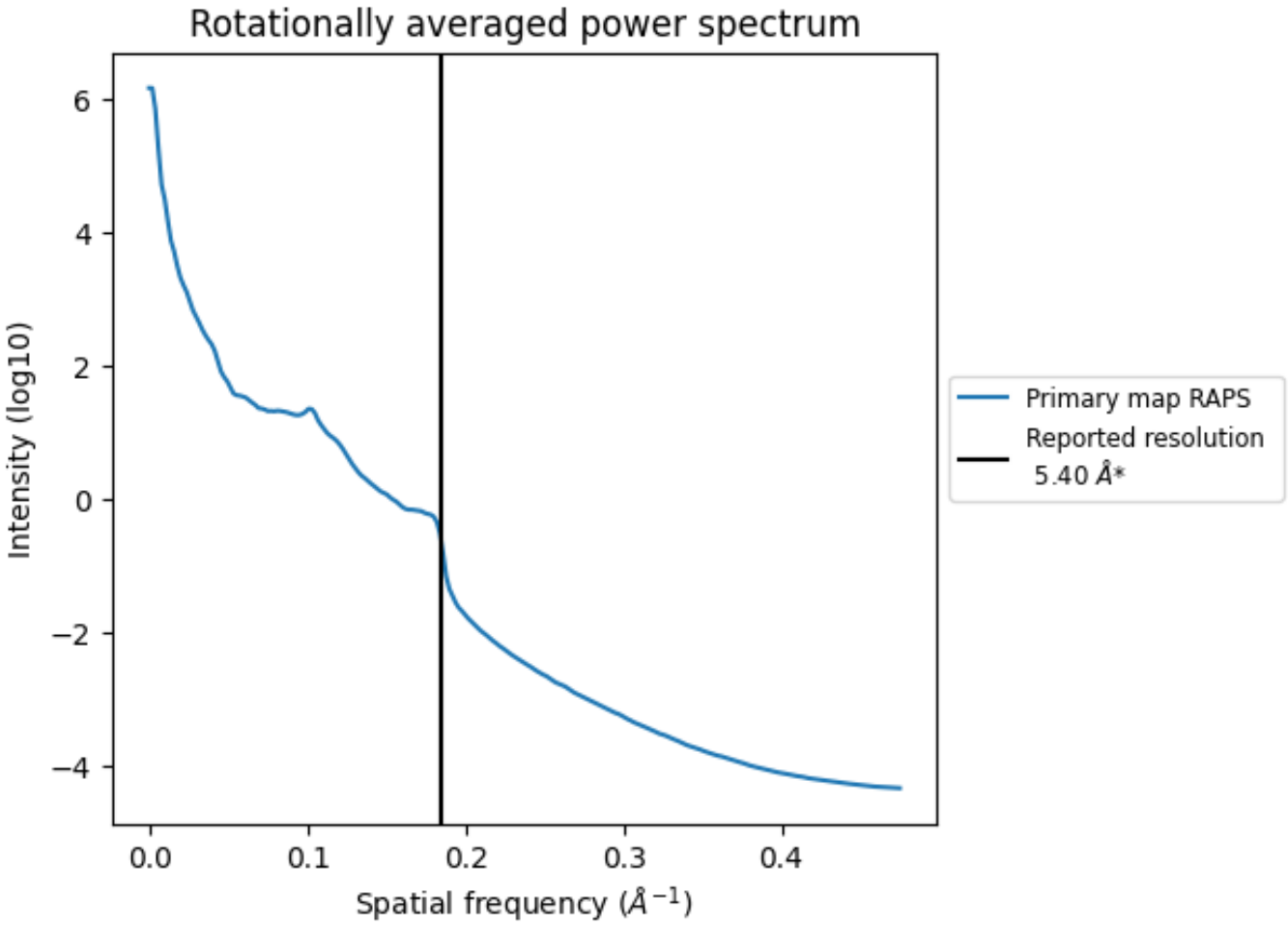
7.2 Volume estimate



The volume at the recommended contour level is 1312 nm^3; this corresponds to an approximate mass of 1185 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 0.185 $Å^{-1}$

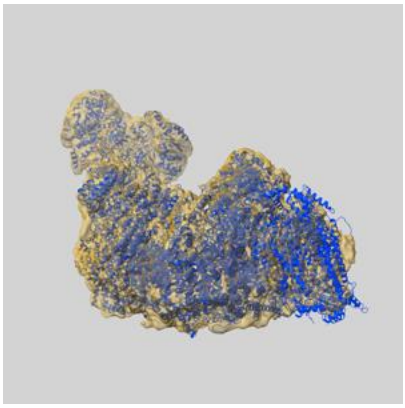
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

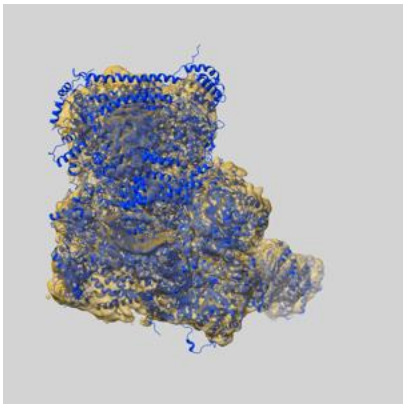
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9534 and PDB model 5GPN. Per-residue inclusion information can be found in section 3 on page 23.

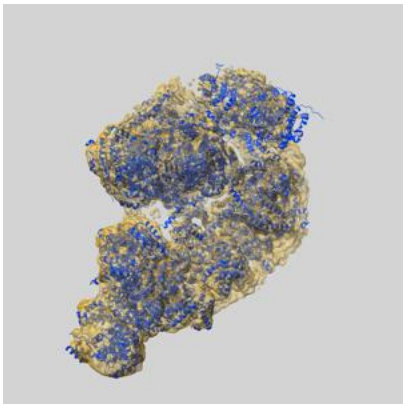
9.1 Map-model overlay



X



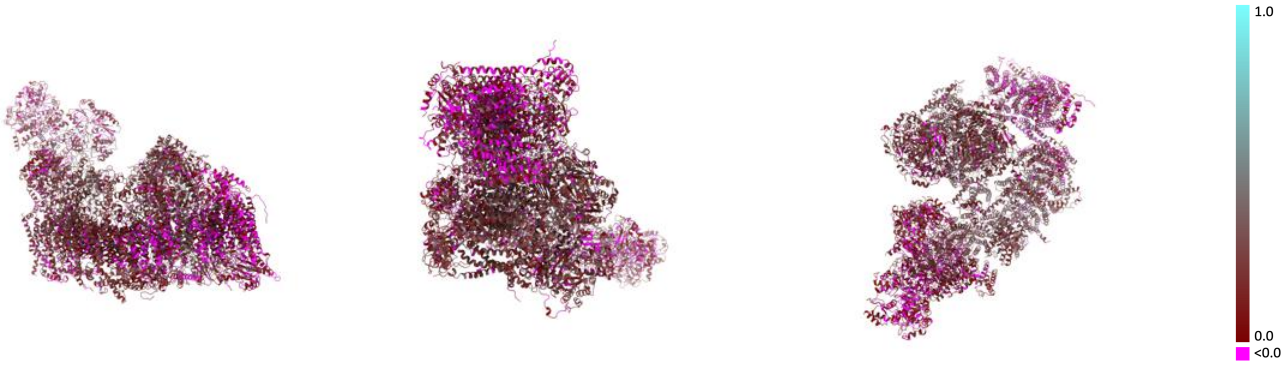
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216 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.

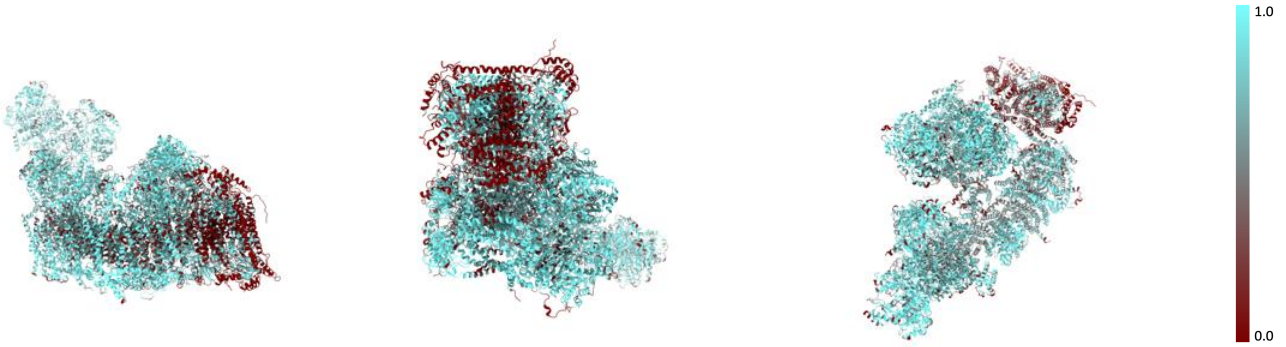
9.2 Q-score mapped to coordinate model



X Y Z

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

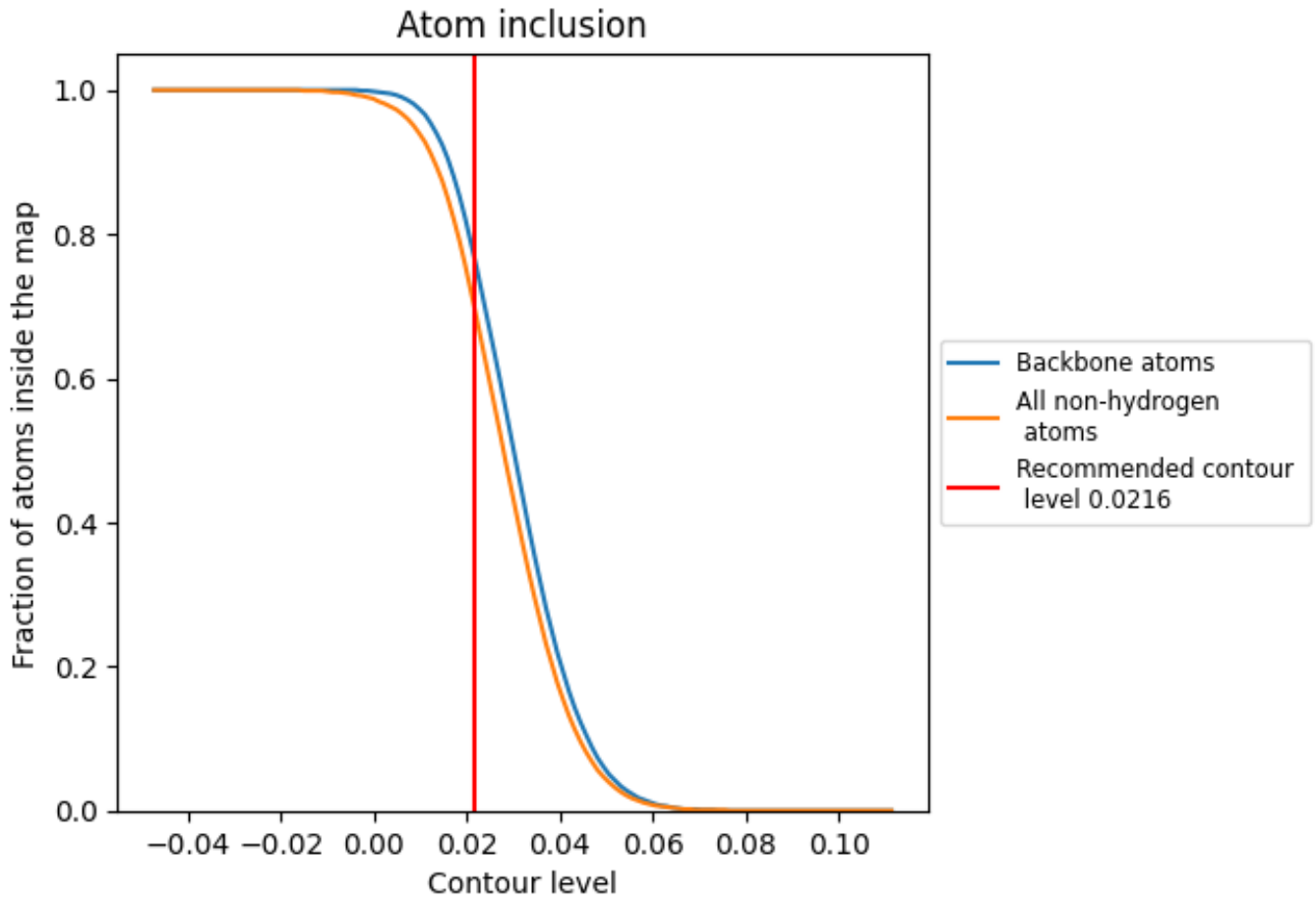
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0216).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.1430
0	0.2210	0.0520
1	0.3110	0.0940
2	0.2060	0.0300
3	0.2390	0.0480
4	0.0530	0.0860
5	0.2240	0.0490
6	0.0050	0.0050
7	0.0470	0.0620
8	0.1080	-0.0160
9	0.1260	0.0670
A	0.8130	0.1990
Aa	0.5780	0.1740
Ab	0.8100	0.1770
Ac	0.7670	0.1180
Ad	0.8100	0.0970
Ae	0.7820	0.1690
Af	0.9550	0.2780
Ag	0.6200	0.2100
Ah	0.8420	0.2330
Ai	0.9700	0.2580
Aj	0.9190	0.2090
Ak	0.8120	0.2080
Al	0.8630	0.2080
Am	0.9250	0.2200
An	0.8380	0.0810
Ao	0.7660	0.1370
Ap	0.7800	0.1640
Aq	0.7880	0.0530
Ar	0.8640	0.2430
As	0.7050	0.1470
At	0.5950	0.1800
Au	0.8060	0.0730
Av	0.7620	0.1860
Aw	0.8960	0.2190

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B	0.7550	0.1650
C	0.8050	0.2340
D	0.8380	0.1980
E	0.7900	0.1510
F	0.8480	0.2440
G	0.8160	0.2110
H	0.8380	0.2320
I	0.5710	0.0790
J	0.7560	0.2160
K	0.5690	0.2490
L	0.5900	0.2060
M	0.8030	0.2200
N	0.8930	0.2260
O	0.6290	0.2190
P	0.7830	0.1970
Q	0.6370	0.1450
R	0.6410	0.2130
S	0.6790	0.1710
T	0.7500	0.1980
U	0.4780	0.0850
V	0.7250	0.1900
W	0.7450	0.1040
Y	0.8220	0.1020
Z	0.8220	0.1240
a	0.7940	0.1260
b	0.8460	0.1190
c	0.8550	0.0580
d	0.7930	0.1080
e	0.6190	0.1080
f	0.6110	0.1430
g	0.5360	0.1410
h	0.6050	0.1370
i	0.6680	0.1390
j	0.6030	0.0970
k	0.6010	0.1320
l	0.8490	0.1710
m	0.8330	0.1610
n	0.8200	0.0880
o	0.9240	0.1520
p	0.8530	0.2180
q	0.9290	0.2520
r	0.8680	0.0510

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Chain	Atom inclusion	Q-score
s	0.2350	0.0630
t	0.7940	0.1680
u	0.9550	0.2290
v	0.9170	0.2780
w	0.8150	0.1910
x	0.7830	0.1550
y	0.4080	0.0650
z	0.4340	0.0440