



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:28 AM JST

PDB ID : 7DGS / pdb_00007dgs
EMDB ID : EMD-30675
Title : Activity optimized supercomplex state3
Authors : Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on : 2020-11-12
Resolution : 7.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

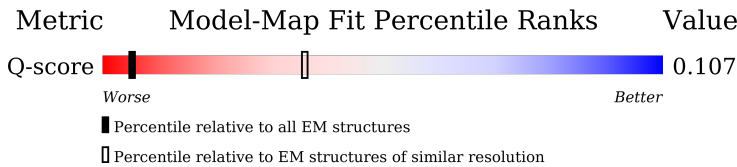
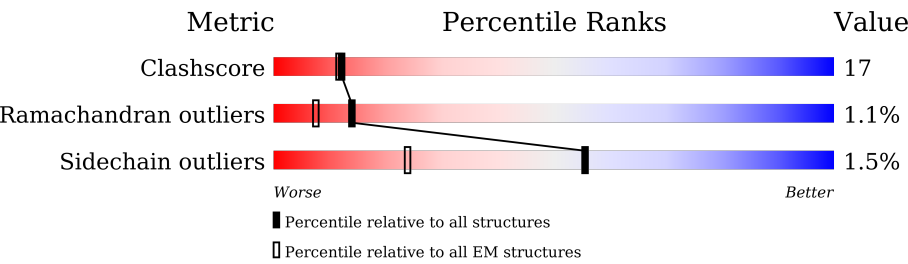
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	370 (7.30 - 8.30)

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

Mol	Chain	Length	Quality of chain
1	9	217	71%22%• 5%
2	7	175	7% 86%10%• •
3	6	606	8% 86%14%•
4	2	347	• 86%12%• •

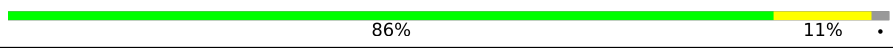
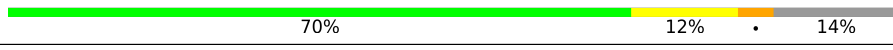
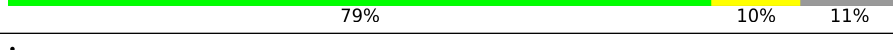
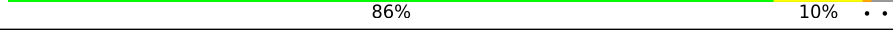
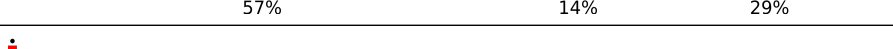
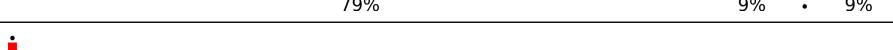
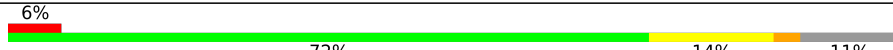
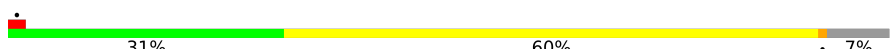
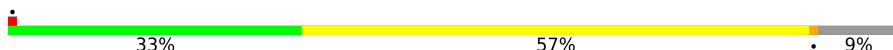
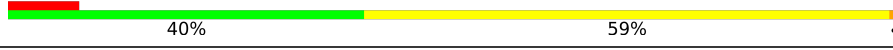
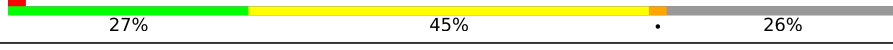
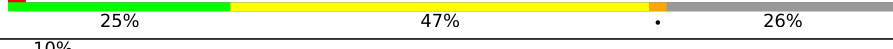
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Mol	Chain	Length	Quality of chain
5	4	459	
6	5	98	
7	8	444	
8	1	318	
9	3	115	
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	

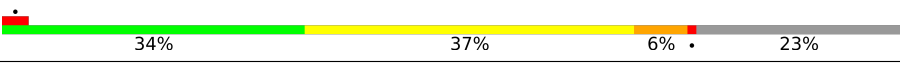
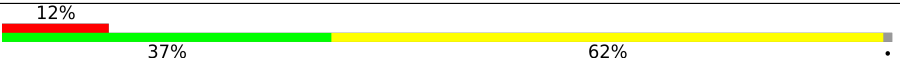
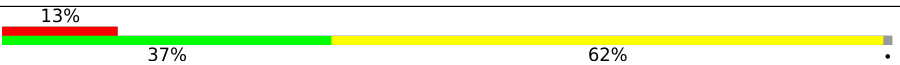
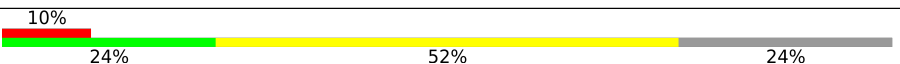
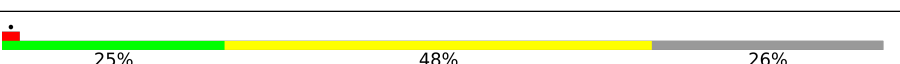
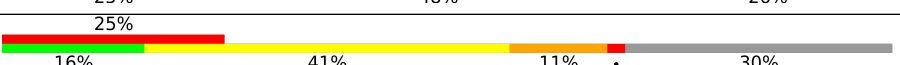
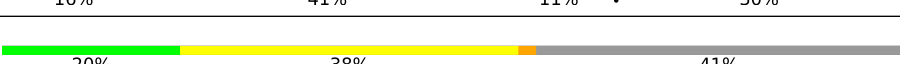
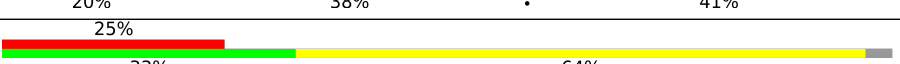
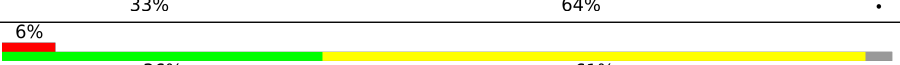
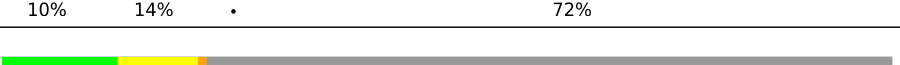
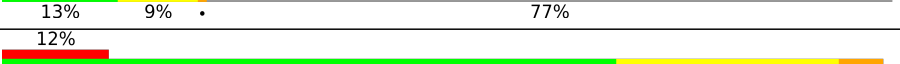
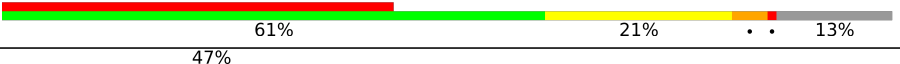
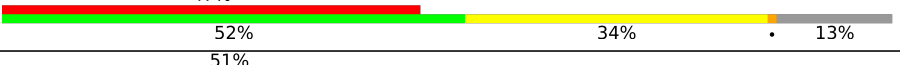
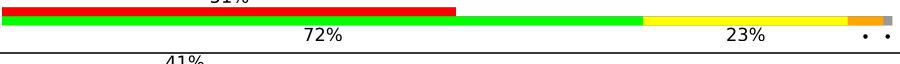
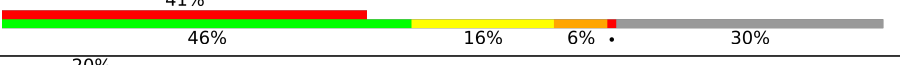
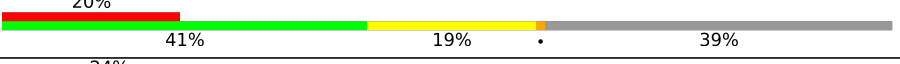
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Mol	Chain	Length	Quality of chain
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	
34	Z	97	
35	a	128	
36	b	143	
37	c	127	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	325	
48	z	325	
49	A0	196	

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Mol	Chain	Length	Quality of chain
49	p	196	
50	A1	111	
50	q	111	
51	A2	82	
51	r	82	
52	B5	91	
52	s	91	
53	A3	56	
53	t	56	
54	B4	64	
54	u	64	
55	B3	78	
55	v	78	
56	A9	514	
57	B9	227	
58	B7	261	
59	A7	169	
60	A6	152	
61	B2	129	
62	A4	97	
63	A5	86	
64	B6	74	
65	B8	80	
66	B0	80	
67	B1	63	

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Mol	Chain	Length	Quality of chain
68	A8	70	20% 43% 17% 39%

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
78	HEC	o	301	X	-	-	-
78	HEC	z	301	X	-	-	-

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 106778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	9	207	Total	C	N	O	S	0	0
			1534	978	261	285	10		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	172	Total	C	N	O	S	0	0
			1186	798	179	202	7		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	344	Total	C	N	O	S	0	0
			2582	1707	404	437	34		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	458	Total	C	N	O	S	1	0
			3447	2293	548	574	32		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	96	Total	C	N	O	S	0	0
			697	454	109	124	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	427	Total	C	N	O	S	0	0
			2965	1864	552	534	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	317	Total	C	N	O	S	0	0
			2499	1676	384	416	23		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	112	Total	C	N	O	S	0	0
			862	580	127	150	5		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	688	Total	C	N	O	S	0	0
			5179	3252	914	977	36		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	430	Total	C	N	O	S	0	0
			3416	2179	589	623	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	F	28	Total	C	N	O	0	0
			183	116	32	35		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	71	Total	C	N	O	S	0	0
			530	331	99	97	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	K	84	Total	C	N	O	0	0
			652	409	125	118		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	319	Total	C	N	O	S	0	0
			2407	1548	431	425	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	319	Total	C	N	O	S	0	0
			2297	1455	395	438	9		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	138	Total	C	N	O	S	0	0
			922	584	161	171	6		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	138	Total	C	N	O	S	0	0
			1087	699	186	193	9		

- Molecule 31 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	86	Total	C	N	O	S	0	0
			616	400	98	114	4		
31	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	a	114	Total	C	N	O	0	0
			857	550	159	148		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	c	90	Total	C	N	O	0	0
			617	391	119	107		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	84	Total	C	N	O	S	0	0
			658	423	115	118	2		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	i	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	446	Total	C	N	O	S	0	0
			3454	2159	608	667	20		
45	w	436	Total	C	N	O	S	0	0
			3385	2117	599	649	20		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	419	Total	C	N	O	S	0	0
			3135	1969	553	606	7		
46	x	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
47	y	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
48	z	241	Total	C	N	O	S	0	0
			1906	1216	329	347	14		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	151	Total	C	N	O	S	0	0
			938	572	170	194	2		
49	A0	188	Total	C	N	O	S	0	0
			1117	679	207	229	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	106	Total	C	N	O	S	0	0
			916	579	167	168	2		
50	A1	106	Total	C	N	O	S	0	0
			916	579	167	168	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
51	A2	81	Total	C	N	O	S	0	0
			676	438	125	112	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	67	Total	C	N	O	S	0	0
			548	332	99	112	5		
52	B5	69	Total	C	N	O	S	0	0
			566	342	101	118	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	33	Total	C	N	O	0	0
			262	174	46	42		
53	A3	39	Total	C	N	O	0	0
			304	202	55	47		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	u	62	Total	C	N	O	0	0
			511	335	89	87		
54	B4	62	Total	C	N	O	0	0
			511	335	89	87		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
55	v	18	Total	C	N	O	0	0
			114	70	22	22		

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Mol	Chain	Residues	Atoms				AltConf	Trace
55	B3	22	Total	C	N	O	0	0
			148	91	30	27		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A9	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B9	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	261	Total	C	N	O	S	0	0
			2125	1421	338	353	13		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	A7	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	A6	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	B2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	A4	84	Total	C	N	O	S	0	0
			671	431	129	110	1		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	A5	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	B6	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	B8	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	B0	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

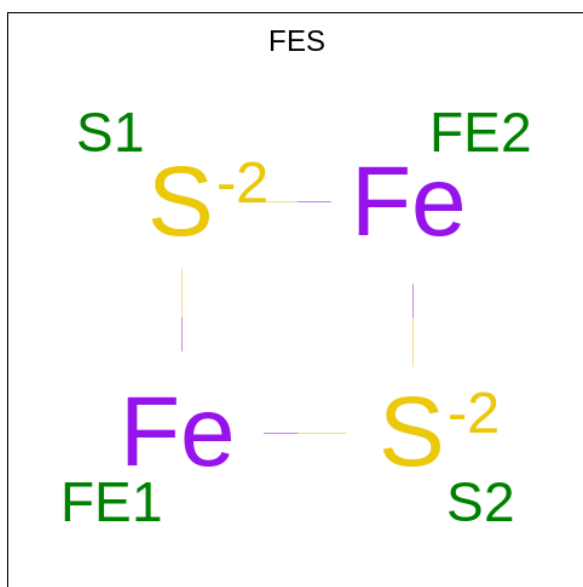
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	B1	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 68 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

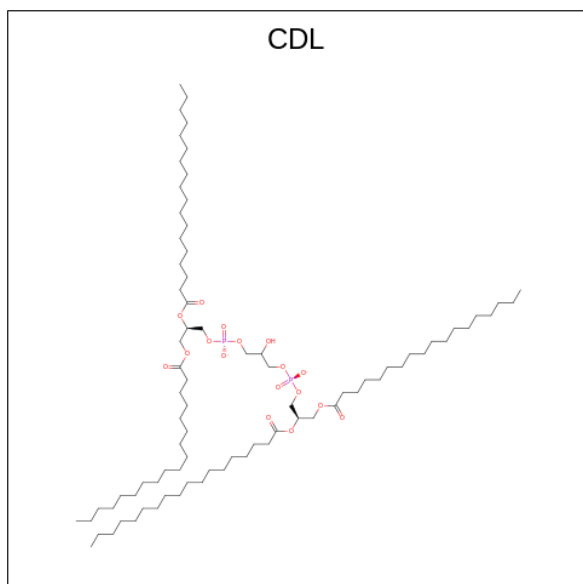
Mol	Chain	Residues	Atoms				AltConf	Trace
68	A8	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 69 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



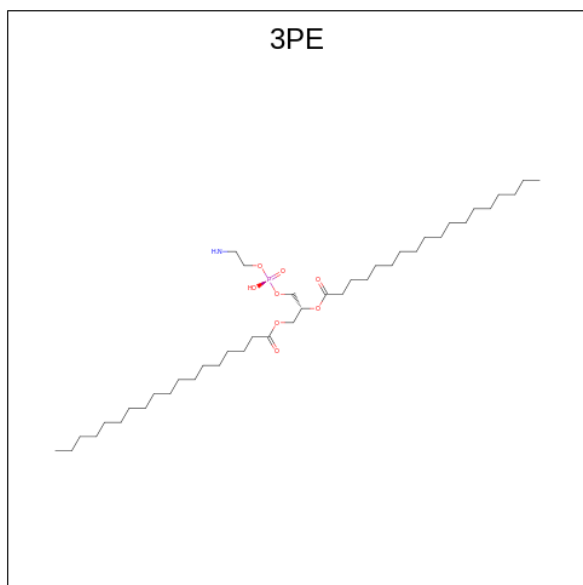
Mol	Chain	Residues	Atoms			AltConf
69	9	1	Total	Fe	S	0
			4	2	2	
69	A	1	Total	Fe	S	0
			4	2	2	
69	m	1	Total	Fe	S	0
			4	2	2	

- Molecule 70 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



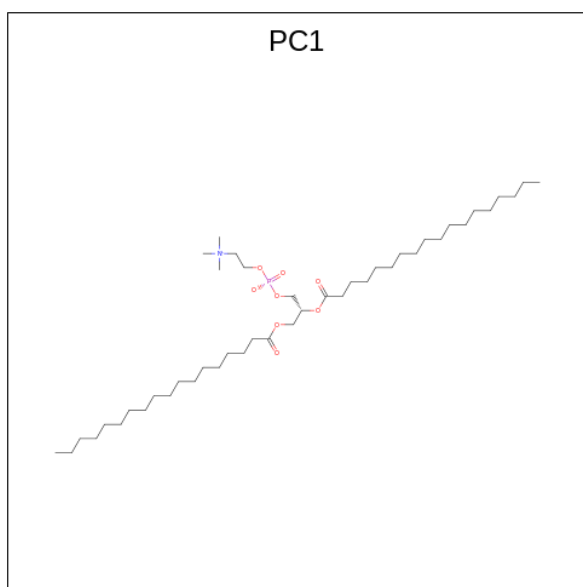
Mol	Chain	Residues	Atoms				AltConf
70	6	1	Total	C	O	P	0
			64	45	17	2	
70	4	1	Total	C	O	P	0
			82	63	17	2	
70	J	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



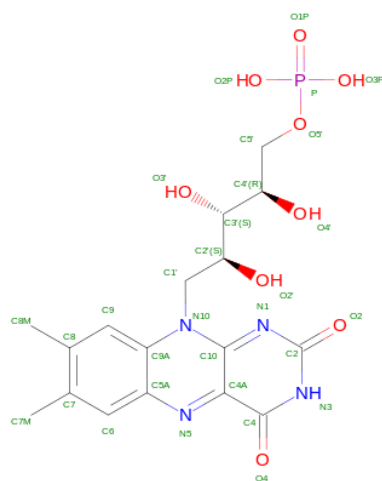
Mol	Chain	Residues	Atoms					AltConf
71	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	j	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 72 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



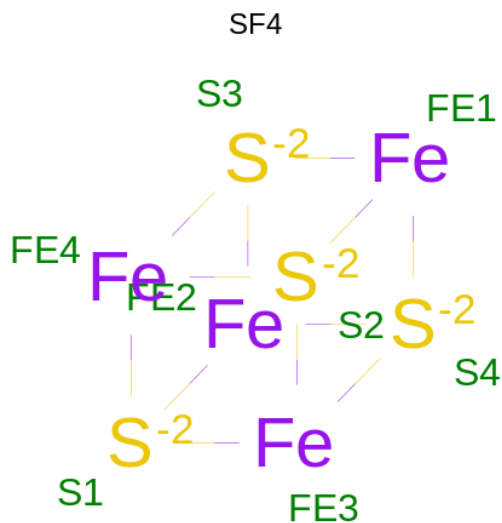
Mol	Chain	Residues	Atoms					AltConf
72	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
73	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
74	8	1	Total 8	Fe 4	S 4	0
74	A	1	Total 8	Fe 4	S 4	0
74	A	1	Total 8	Fe 4	S 4	0

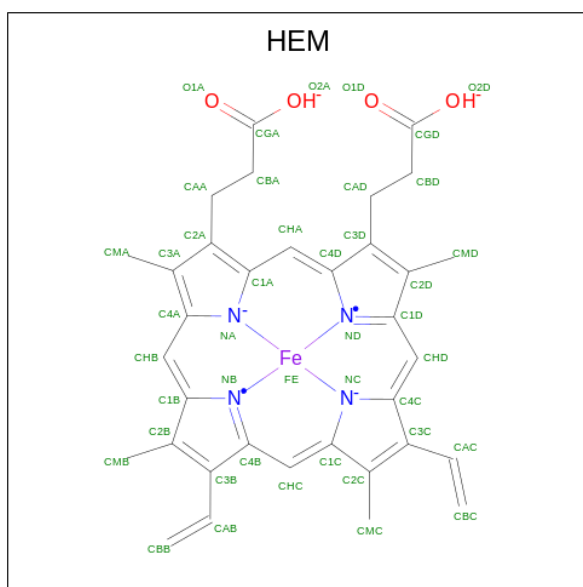
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Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total 8	Fe 4	S 4	0
74	E	1	Total 8	Fe 4	S 4	0
74	E	1	Total 8	Fe 4	S 4	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 75 | I | 1 | Total Zn
1 1 | 0 |
| 75 | B2 | 1 | Total Zn
1 1 | 0 |

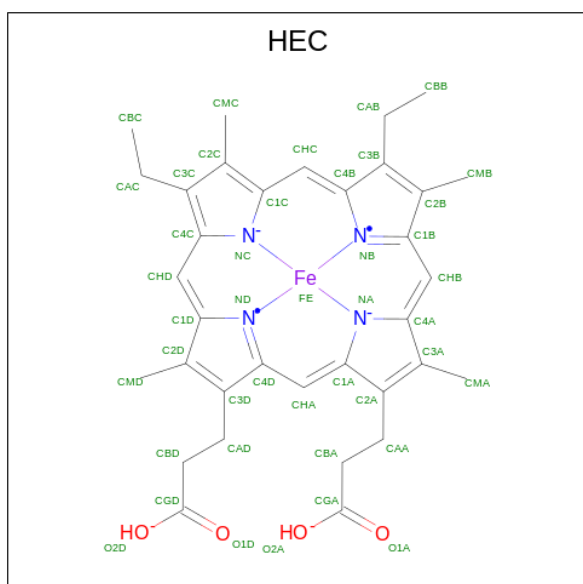
- # NAP

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



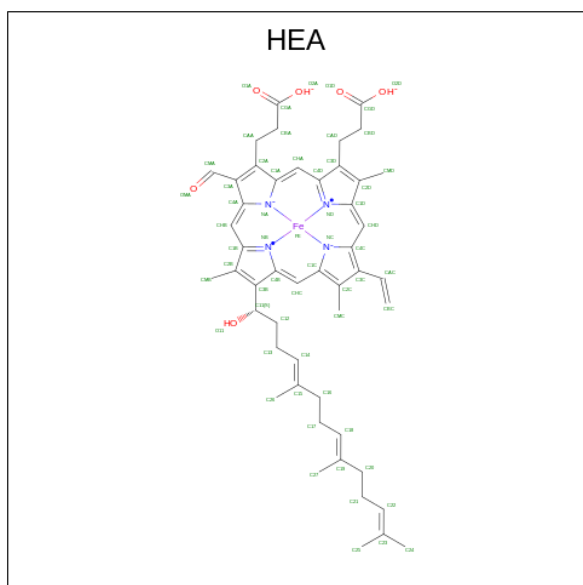
Mol	Chain	Residues	Atoms					AltConf
77	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	m	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	y	1	Total 43	C 34	Fe 1	N 4	O 4	0
77	y	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 78 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
78	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
78	z	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
79	A9	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
79	A9	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	A9	1	Total	Cu	0
			1	1	
80	B9	2	Total	Cu	0
			2	2	

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

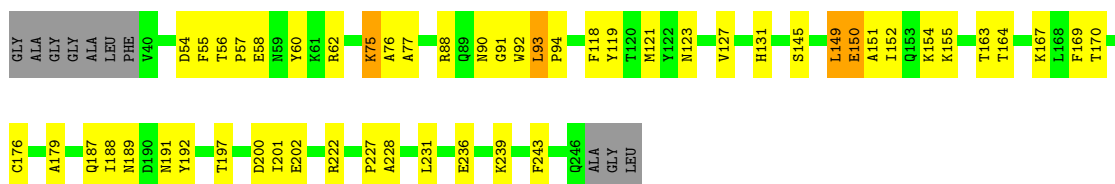
Mol	Chain	Residues	Atoms		AltConf
81	A9	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 9: 



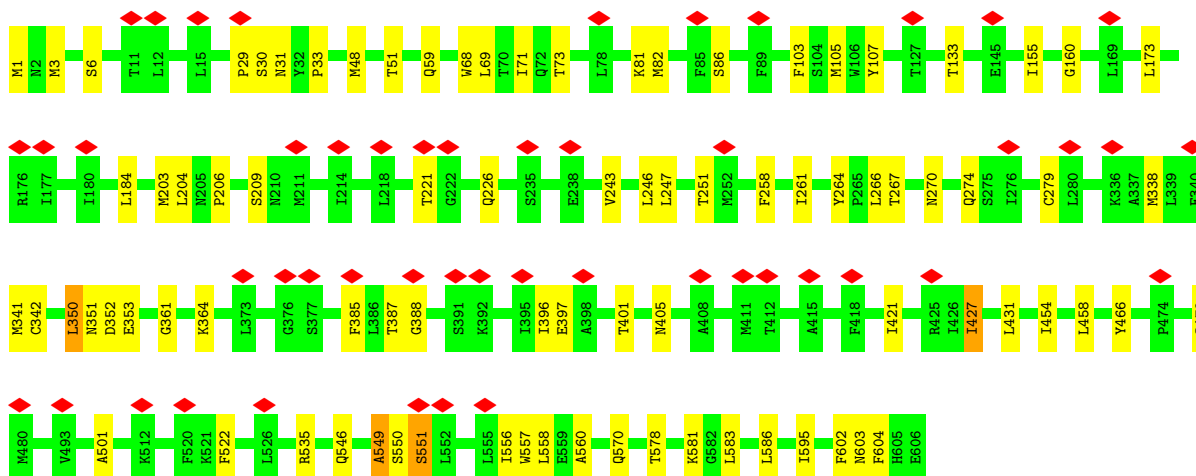
- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

Chain 7: 

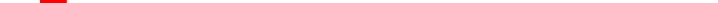


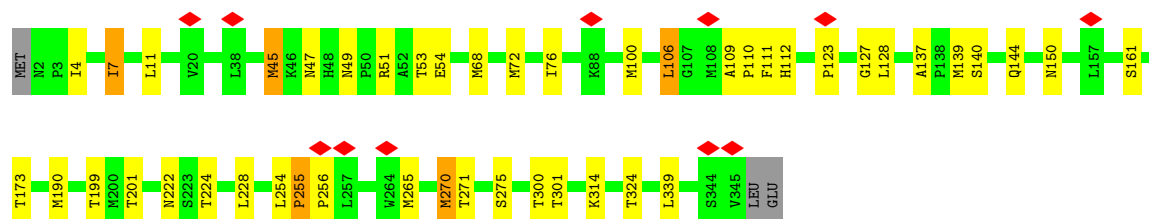
- Molecule 3: NADH-ubiquinone oxidoreductase chain 5

Chain 6: 



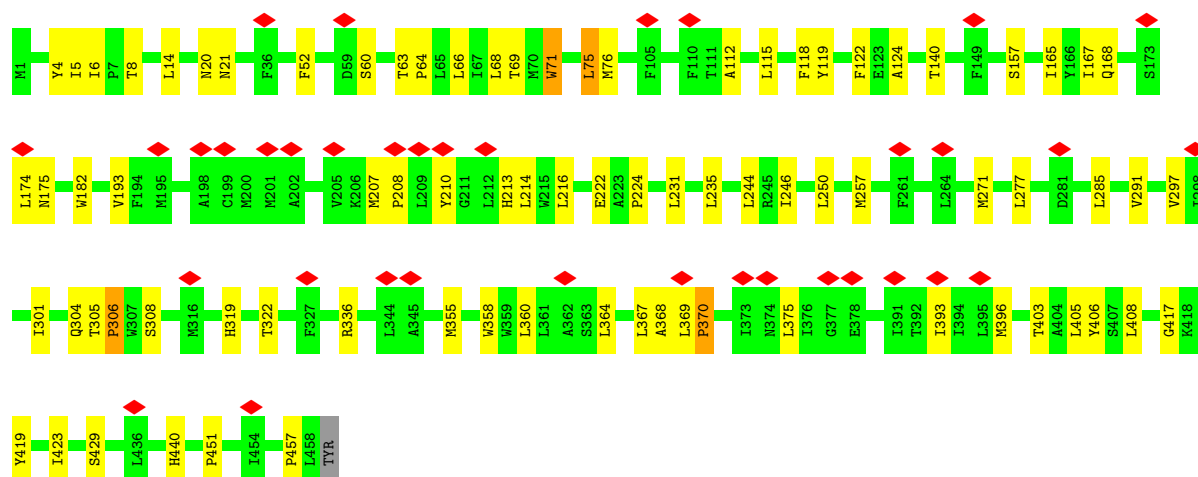
- Molecule 4: NADH-ubiquinone oxidoreductase chain 2

Chain 2:  86% 12%

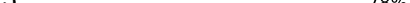


- Molecule 5: NADH-ubiquinone oxidoreductase chain 4

Chain 4: 



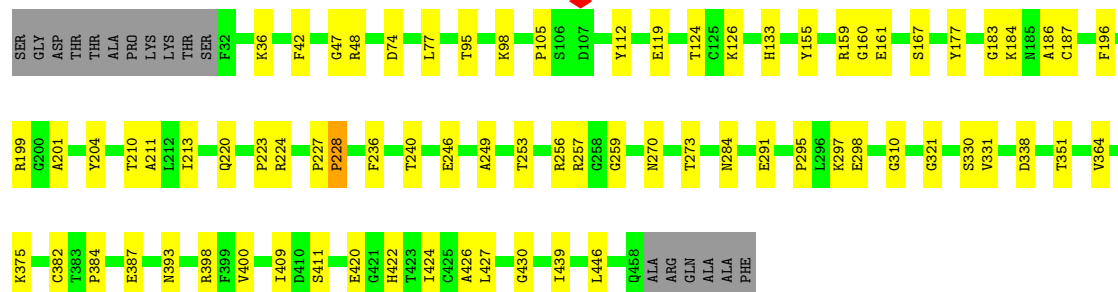
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5:  78% 19% ..



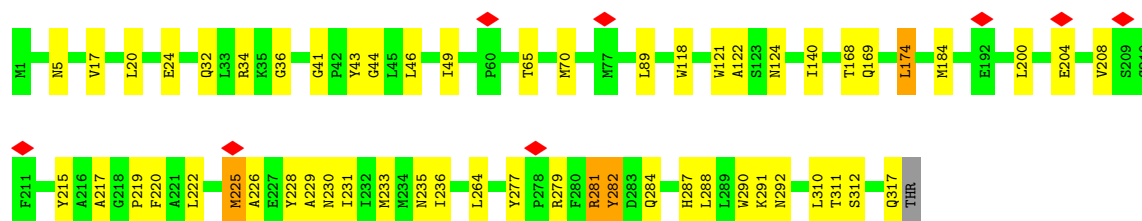
- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 8: 79% 17% .



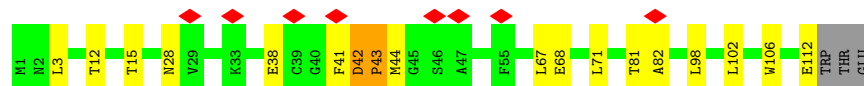
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1: 



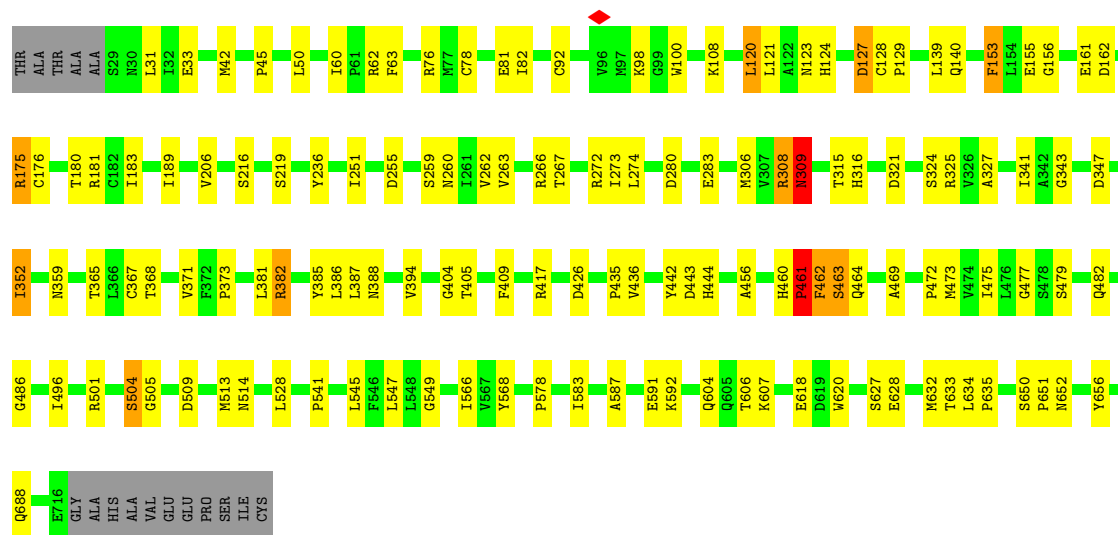
- Molecule 9: NADH-ubiquinone oxidoreductase chain 3

Chain 3: 



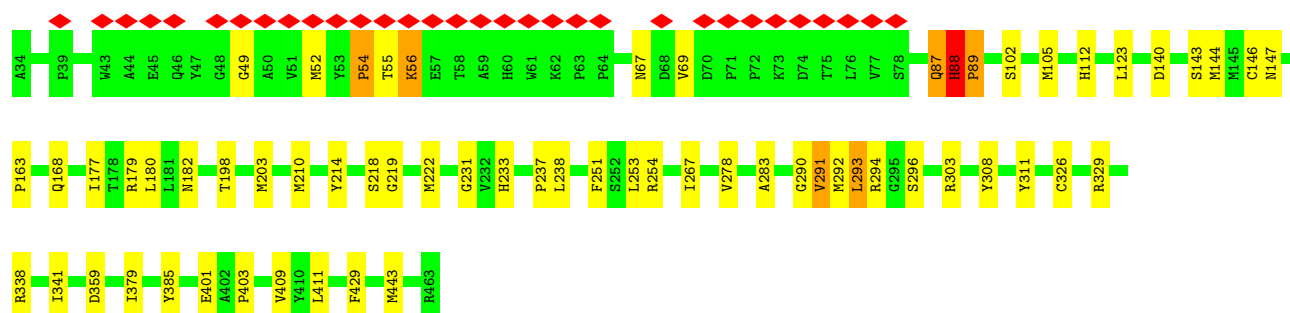
- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A: 



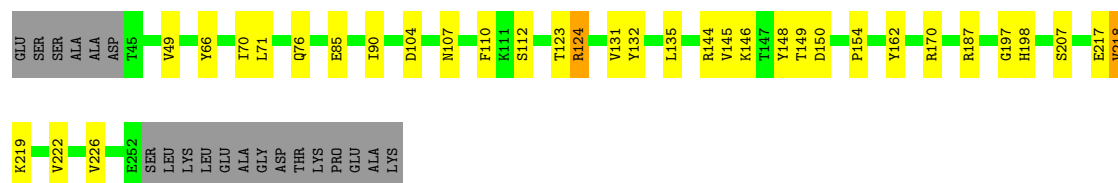
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B: 



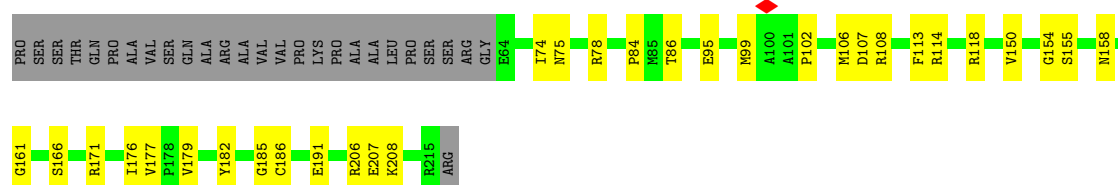
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  76% 14% 9%



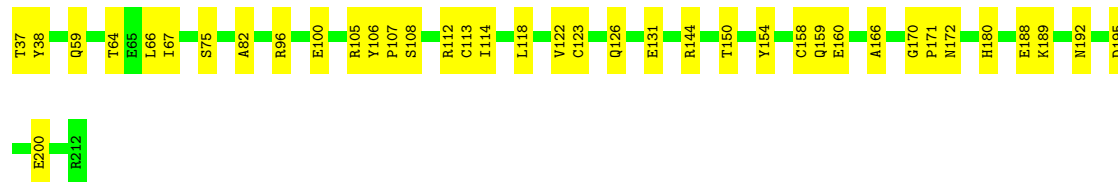
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D:  68% 17% 15%



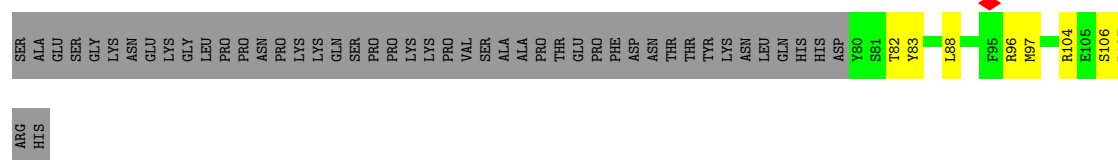
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E:  78% 22%



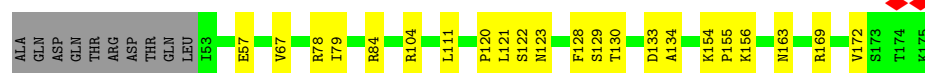
- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:  27% 11% 63%

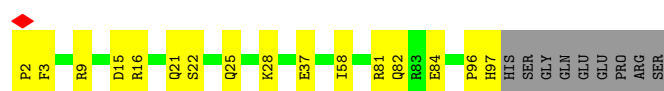
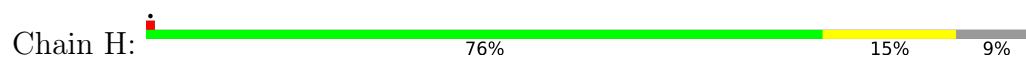


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

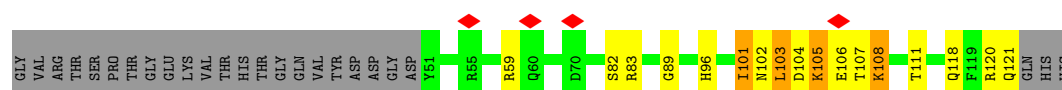
Chain G:  76% 17% 8%



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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



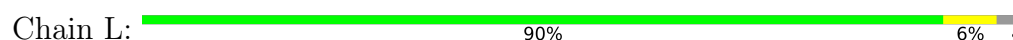
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



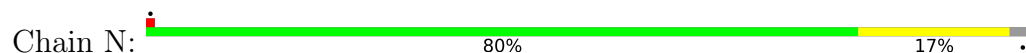
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



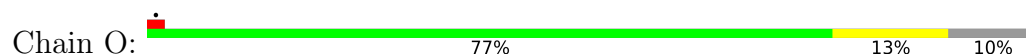
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



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



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P: 



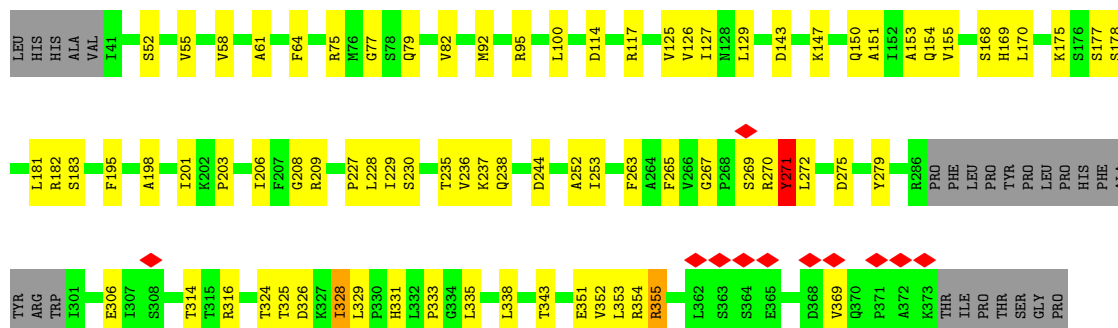
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Q: 



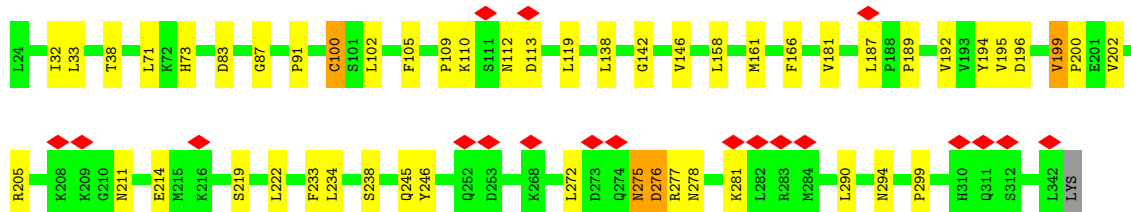
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R: 



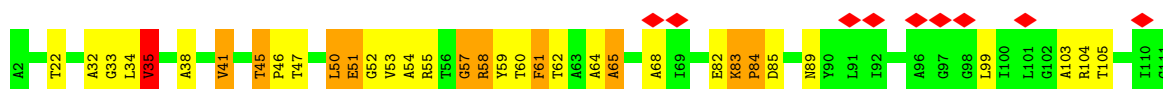
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

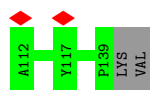
Chain S: 



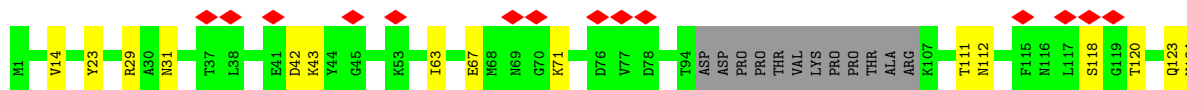
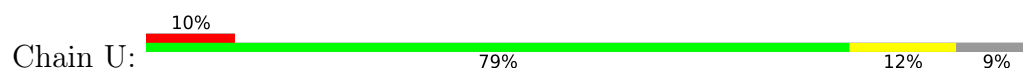
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T: 

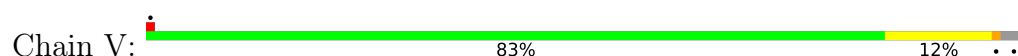




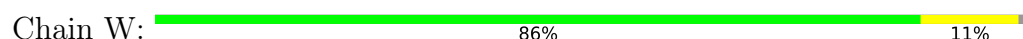
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 31: Acyl carrier protein, mitochondrial



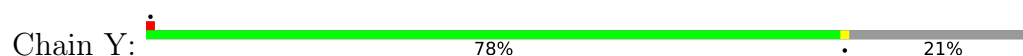
- Molecule 31: Acyl carrier protein, mitochondrial

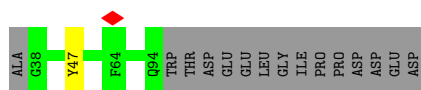


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

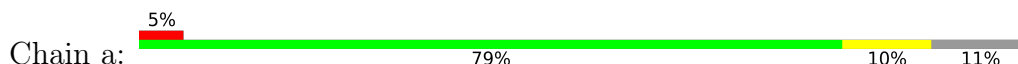




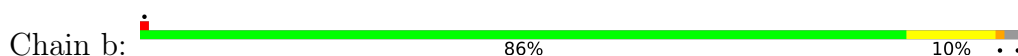
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



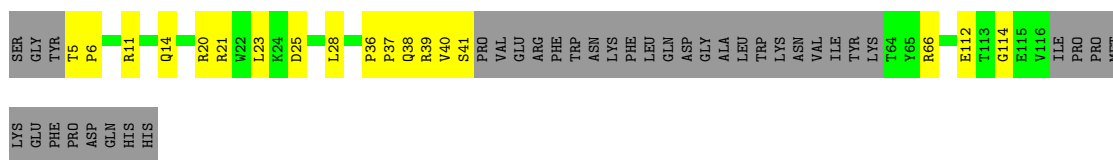
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



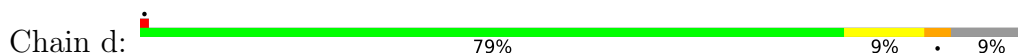
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



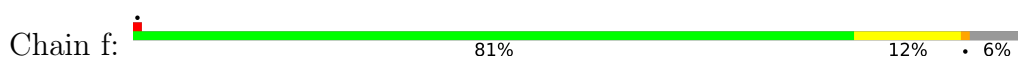
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

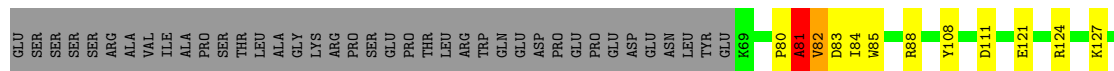


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

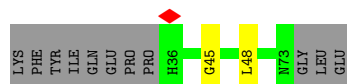




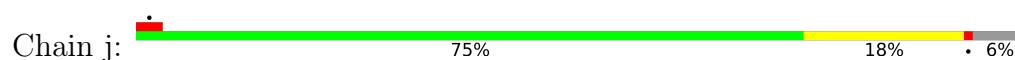
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



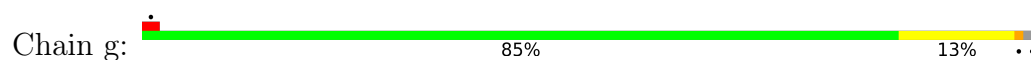
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



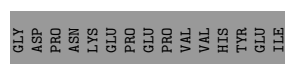
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

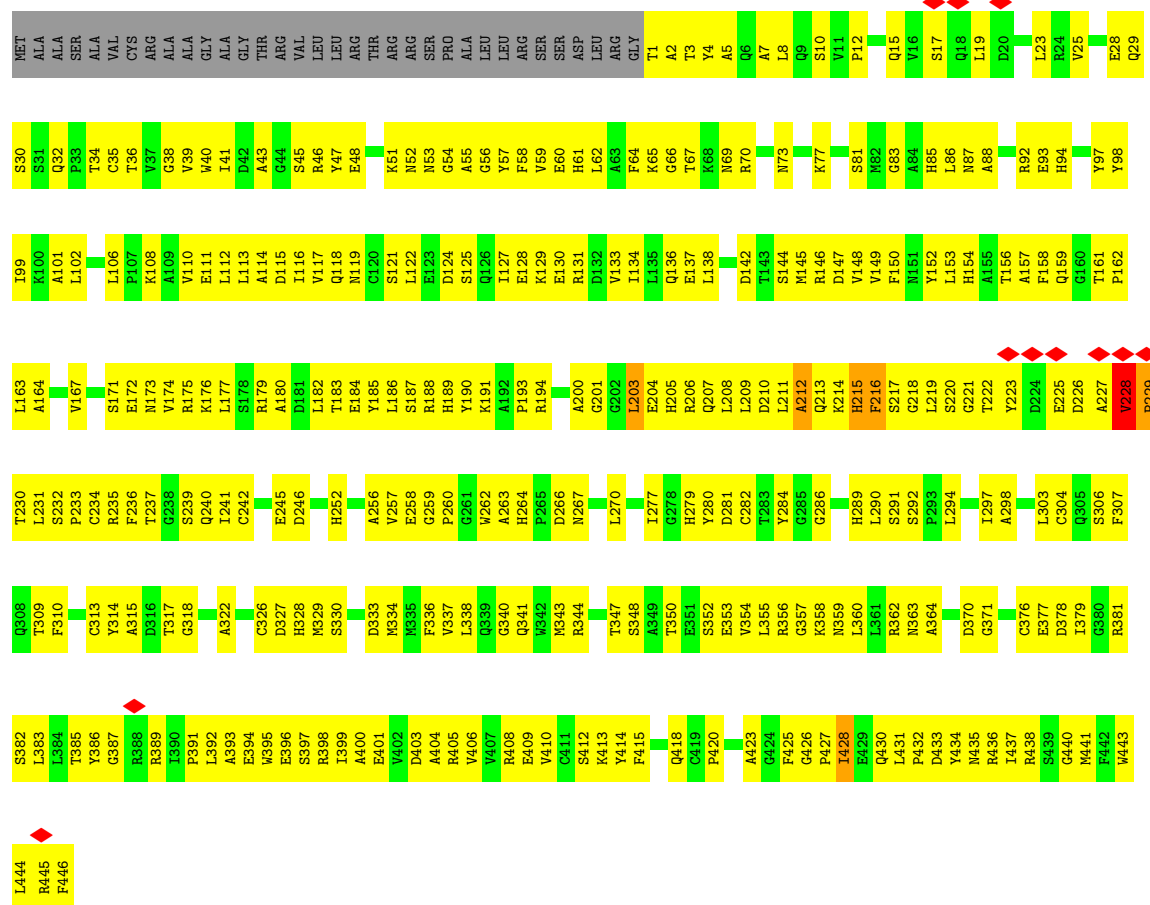


- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



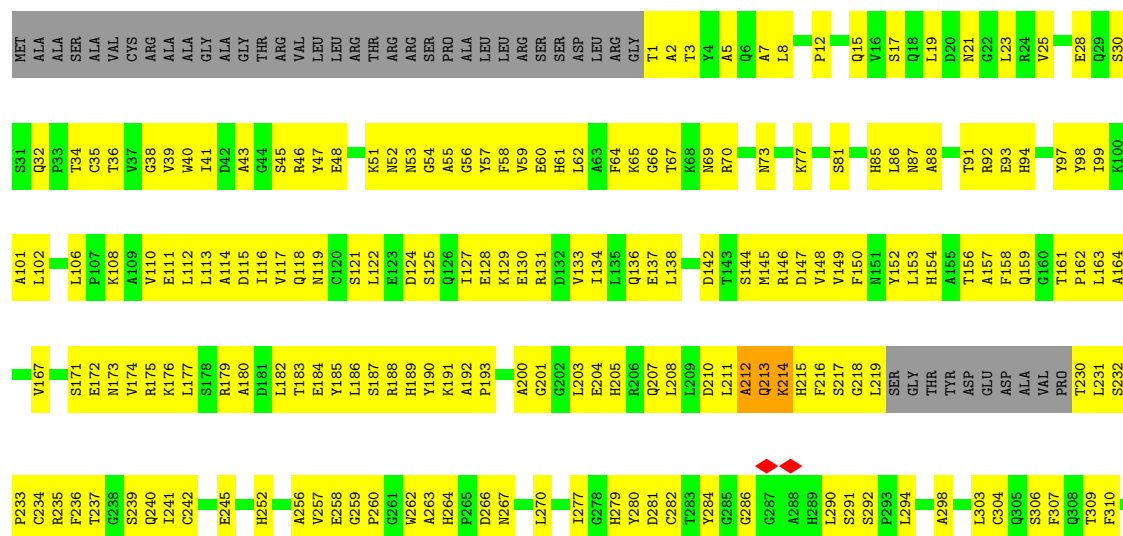
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

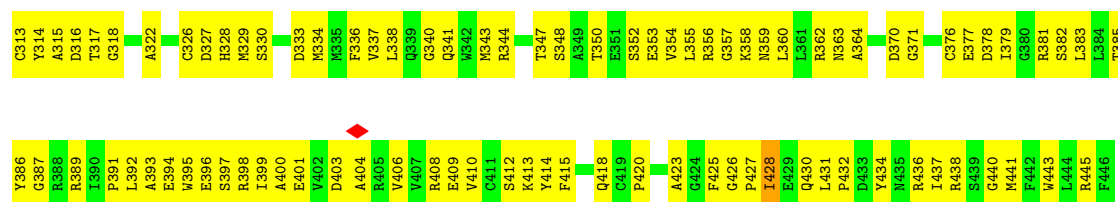
Chain k: 



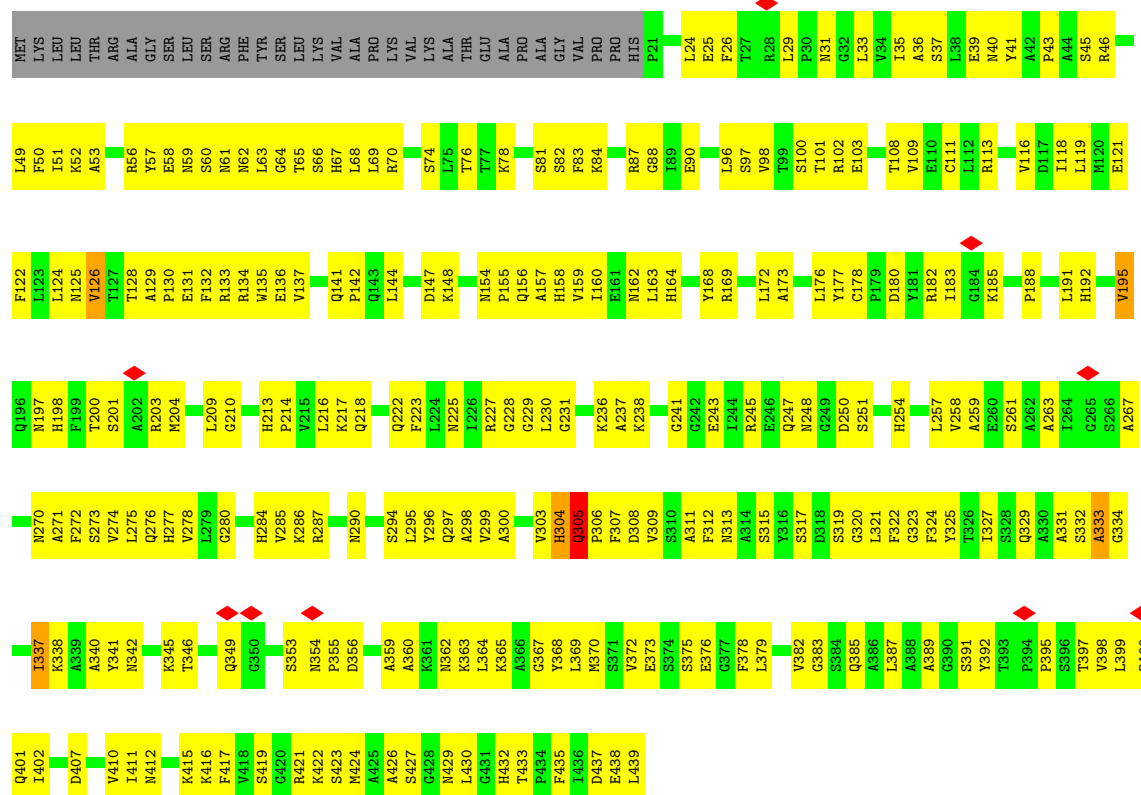
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain w: 

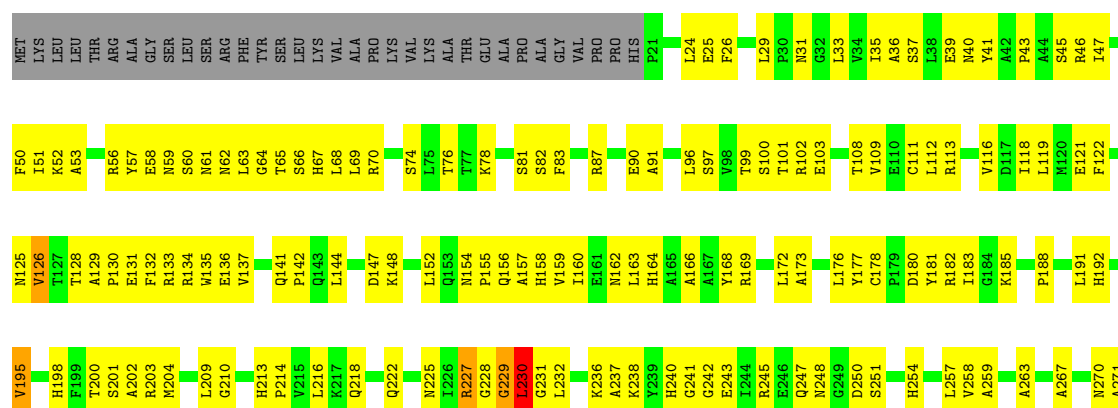


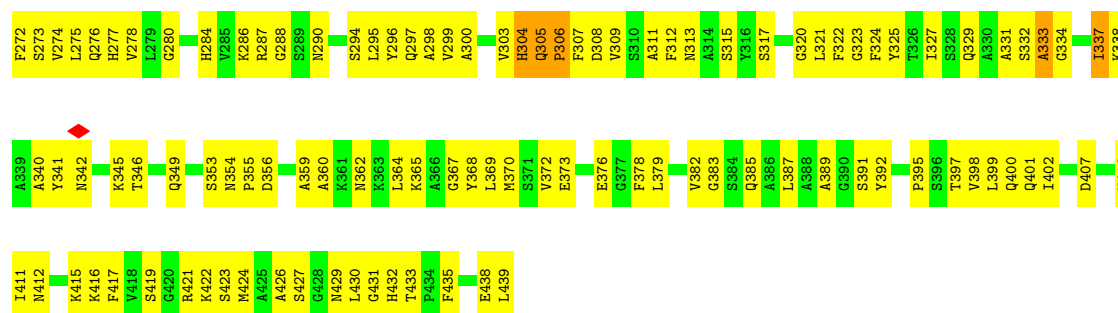


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

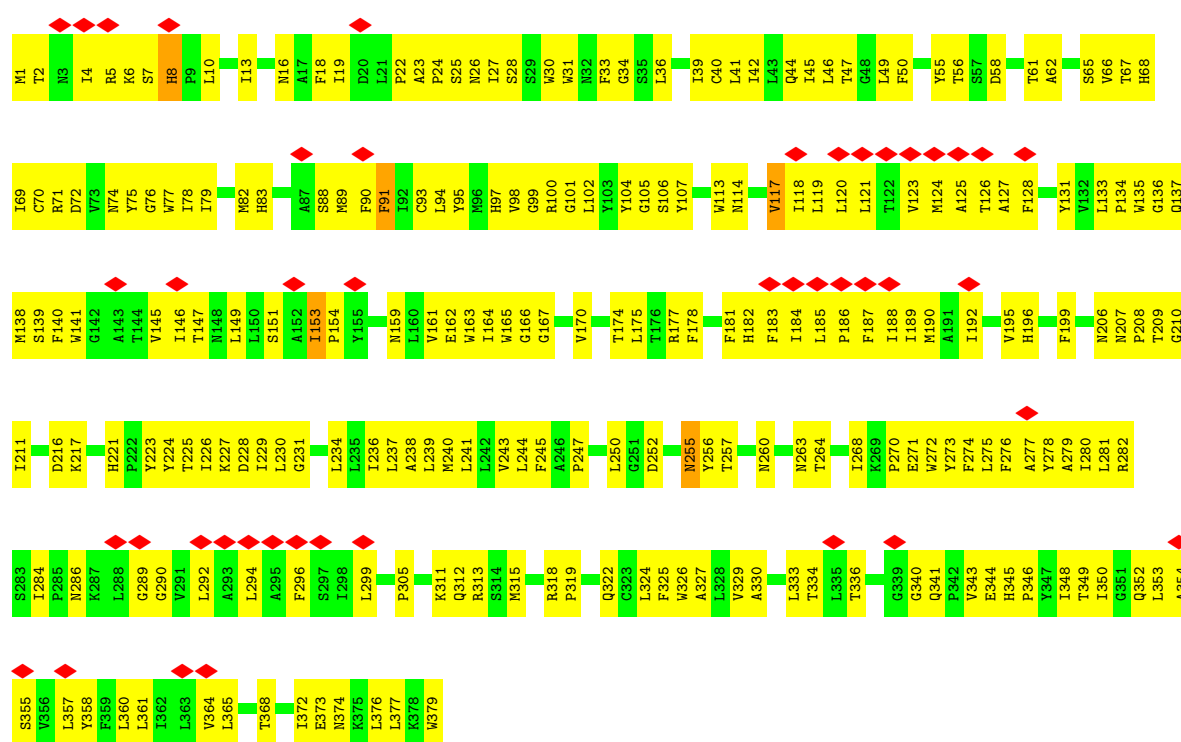
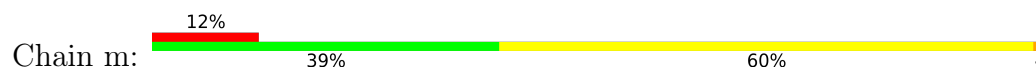


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

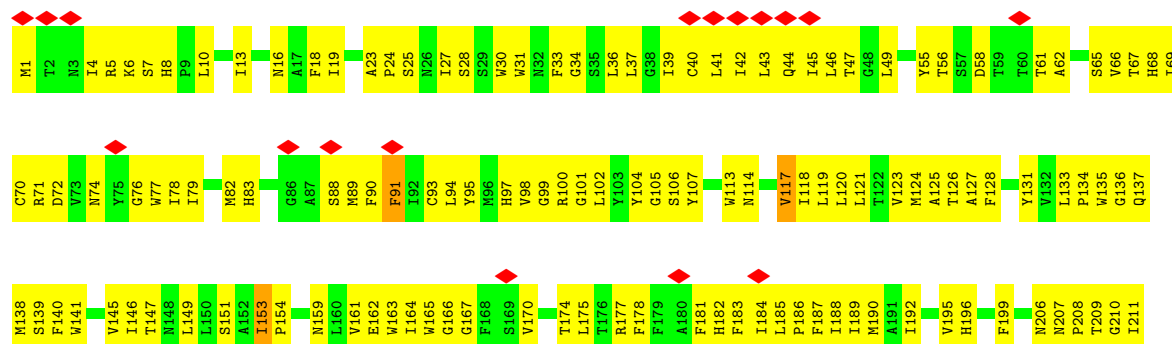
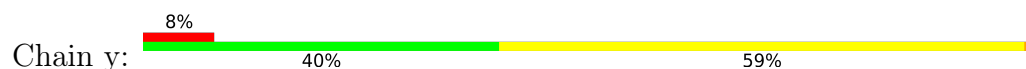


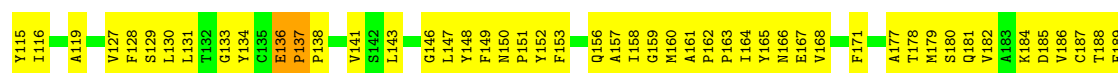


• Molecule 47: Cytochrome b



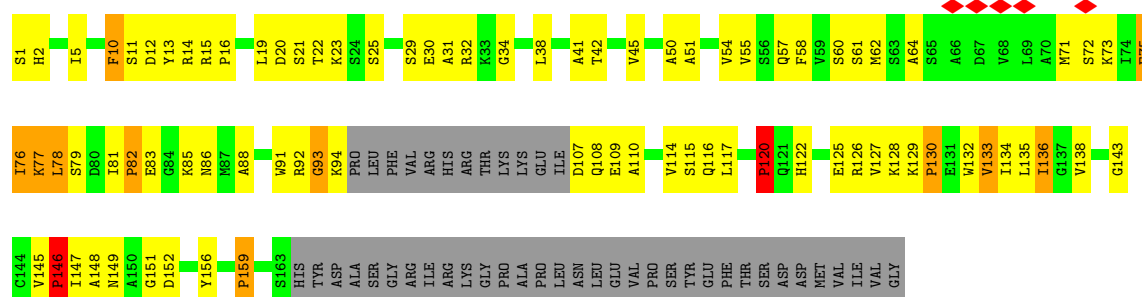
• Molecule 47: Cytochrome b



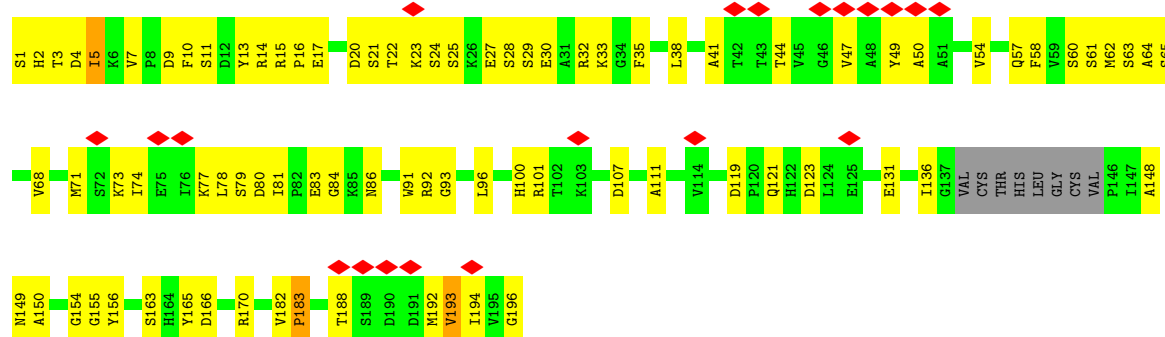




- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



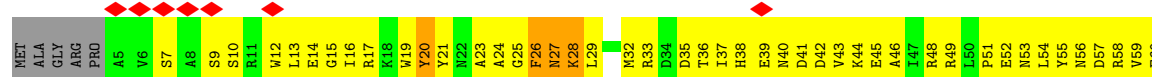
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

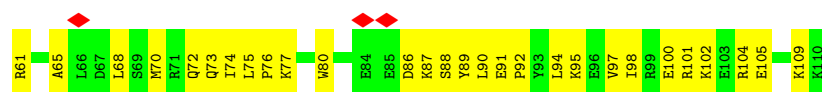


- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7

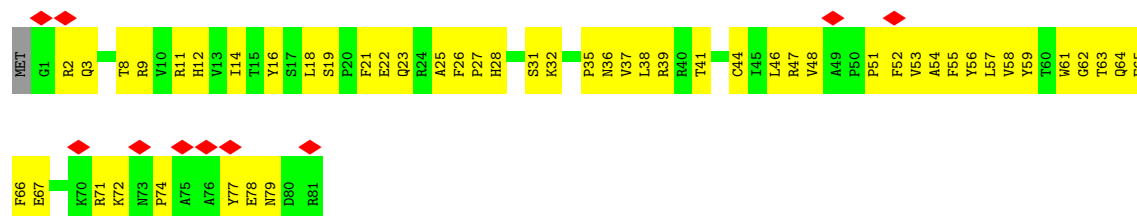




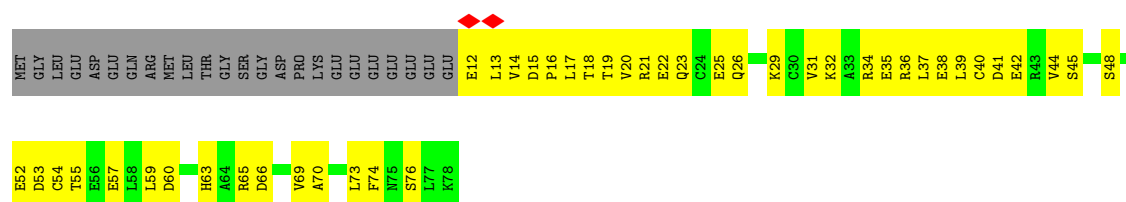
- Molecule 51: Cytochrome b-c1 complex subunit 8



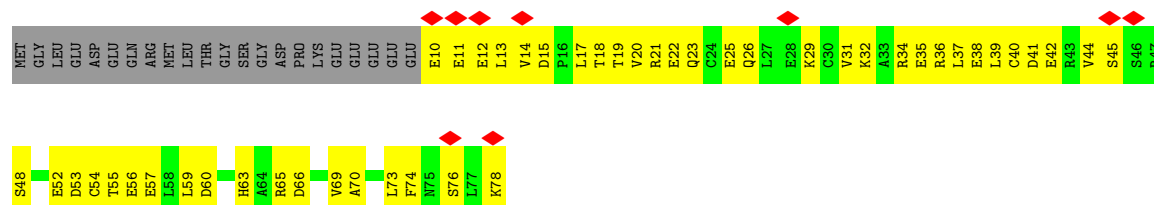
- Molecule 51: Cytochrome b-c1 complex subunit 8



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

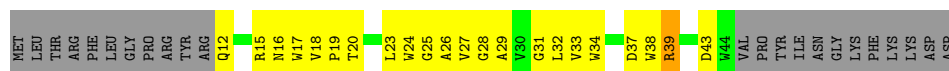


- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



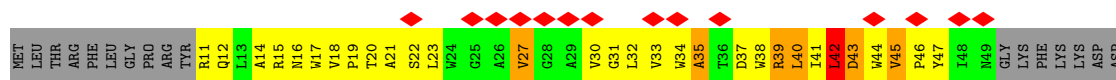
- Molecule 53: Cytochrome b-c1 complex subunit 10

Chain t: 20% 38% . 41%



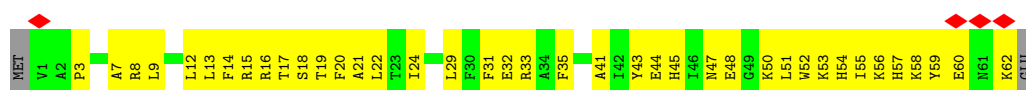
- Molecule 53: Cytochrome b-c1 complex subunit 10

Chain A3: 16% 25% 41% 11% . 30%



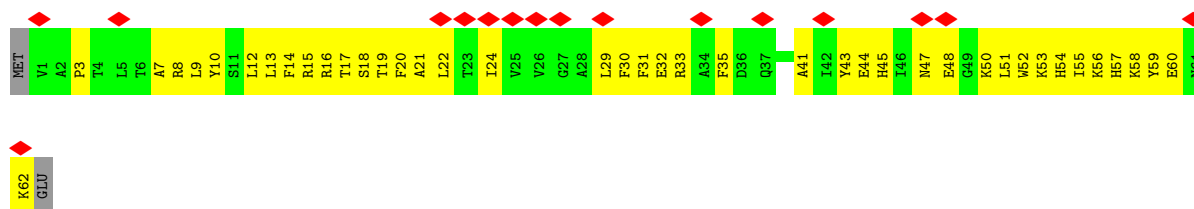
- Molecule 54: Cytochrome b-c1 complex subunit 9

Chain u: 6% 36% 61% .



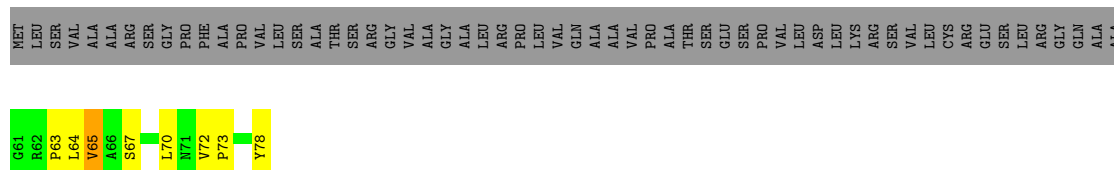
- Molecule 54: Cytochrome b-c1 complex subunit 9

Chain B4: 25% 33% 64% .



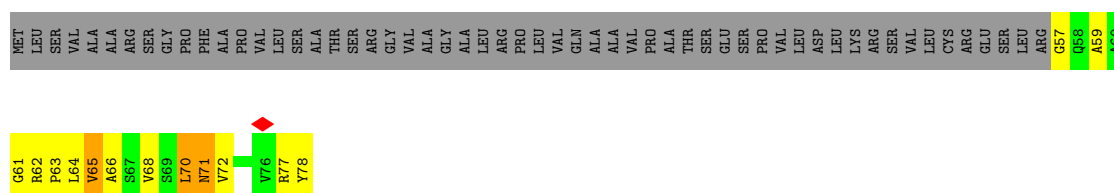
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain v: 13% 9% . 77%

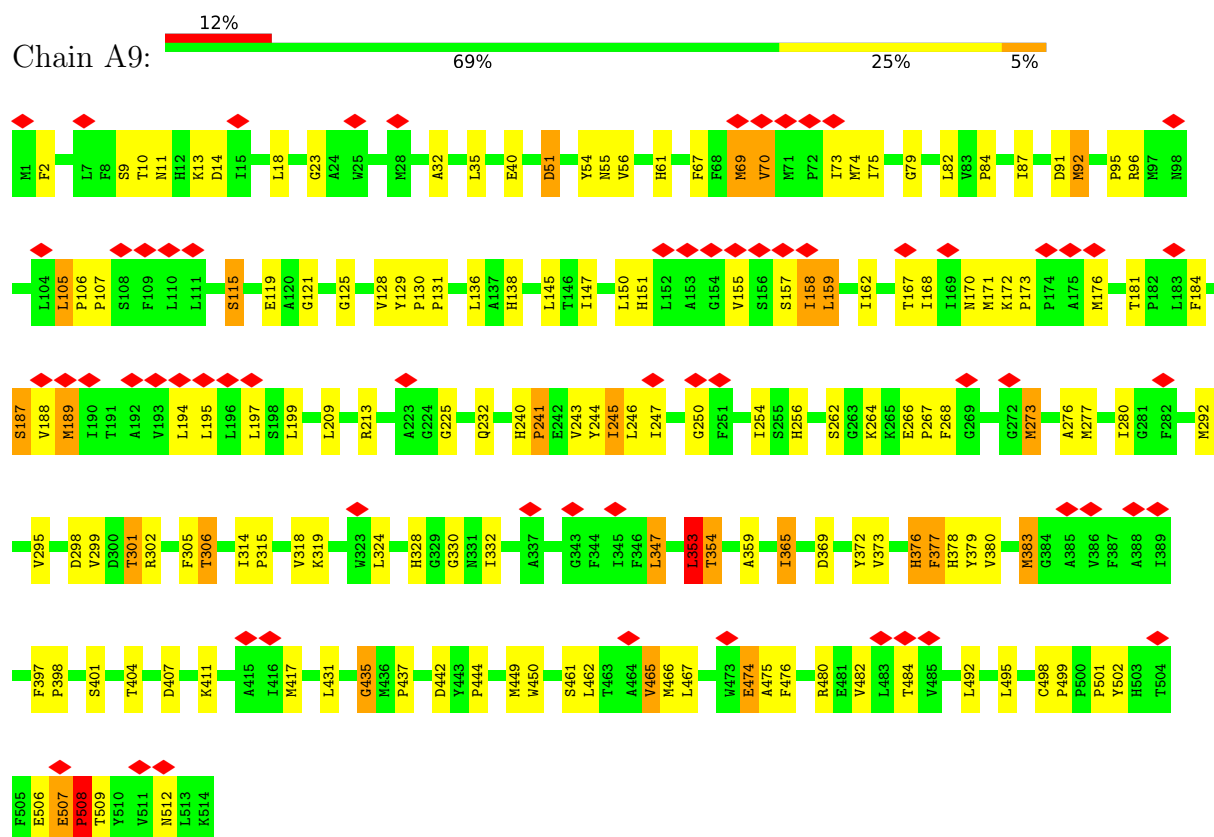


- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

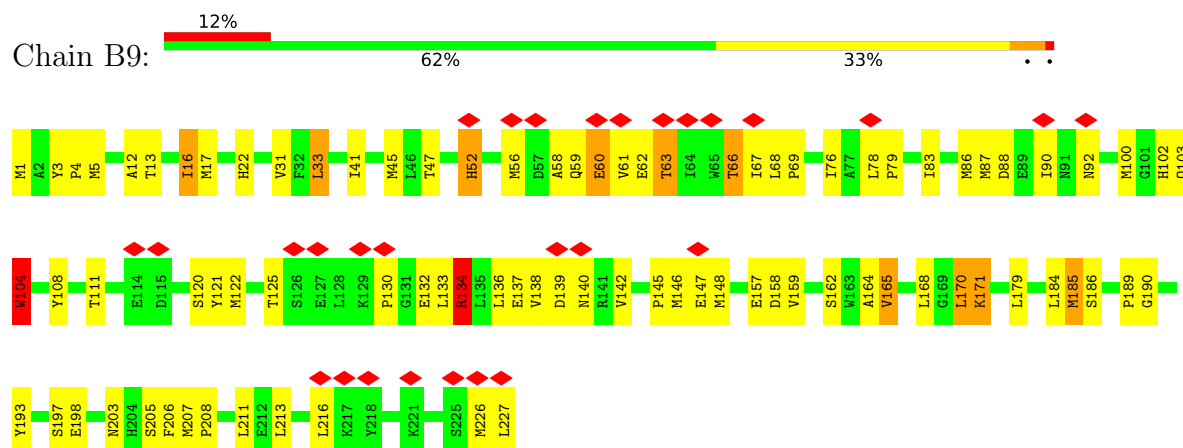
Chain B3: 10% 14% . 72%



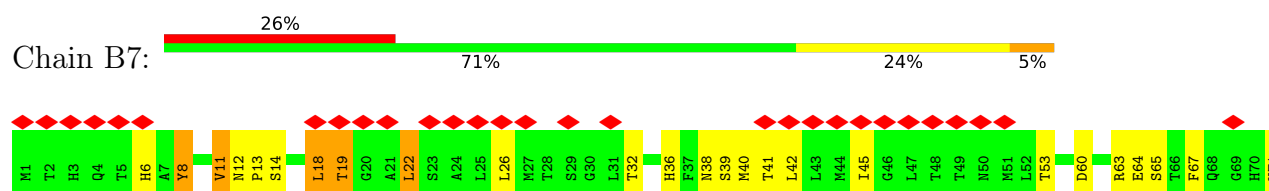
- Molecule 56: Cytochrome c oxidase subunit 1

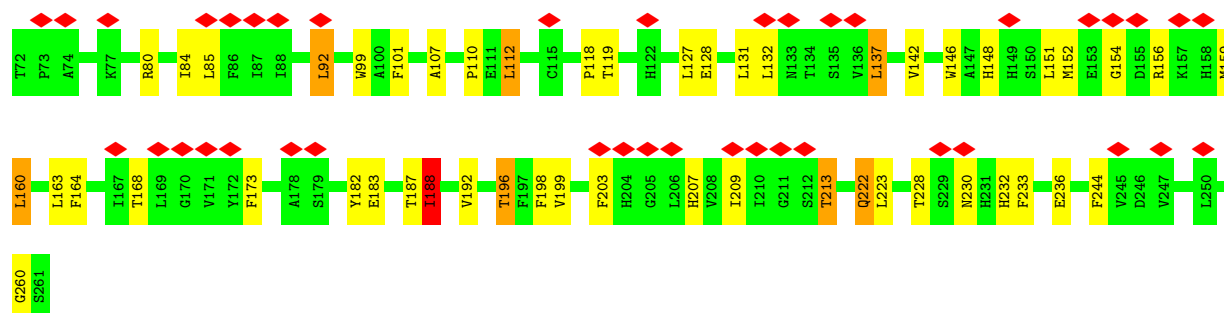


- Molecule 57: Cytochrome c oxidase subunit 2

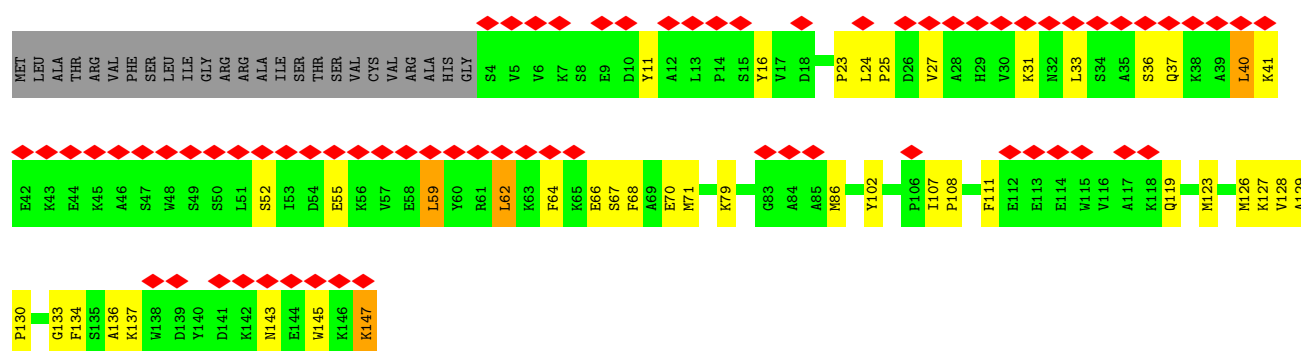
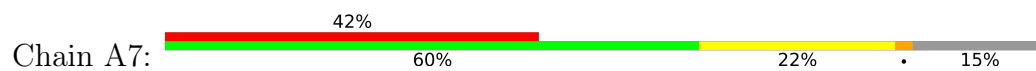


- Molecule 58: Cytochrome c oxidase subunit 3

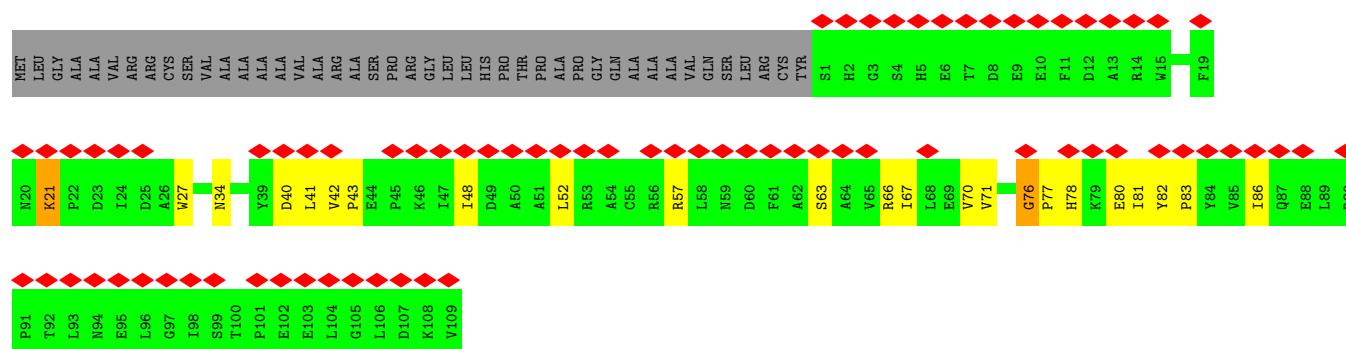




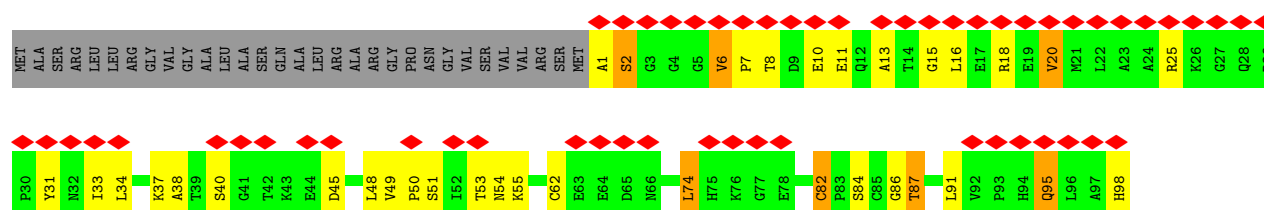
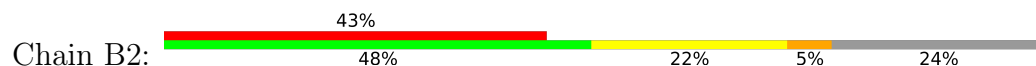
- Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



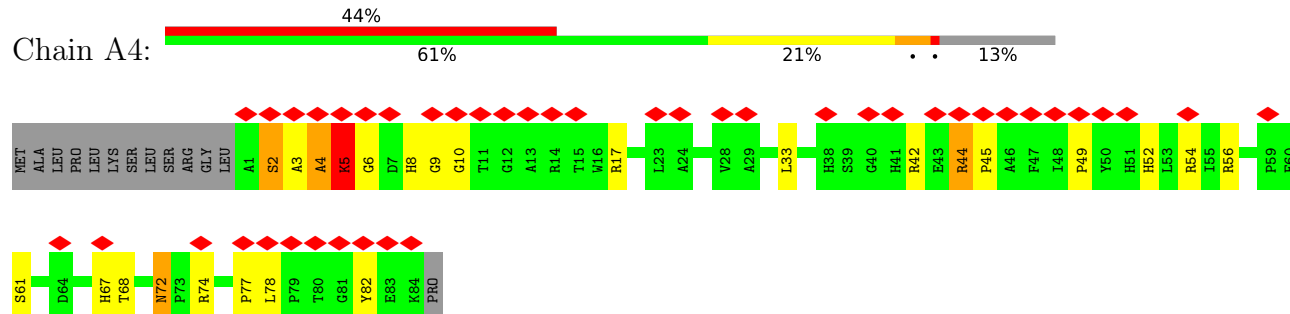
- Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial



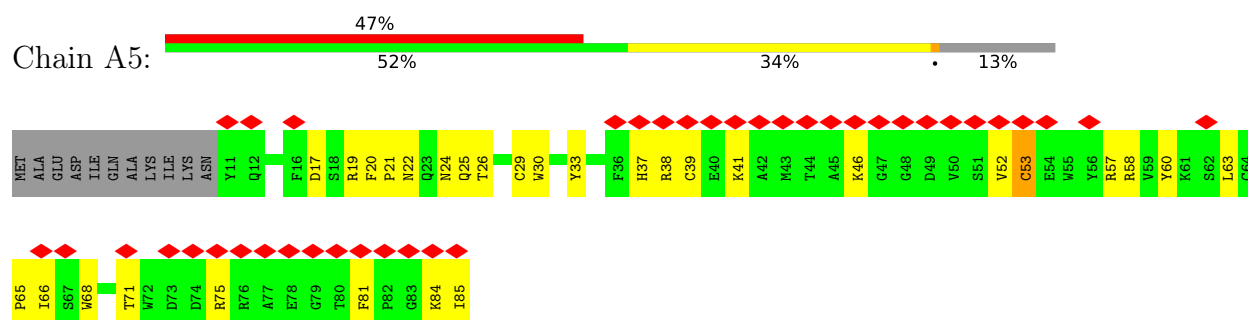
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial



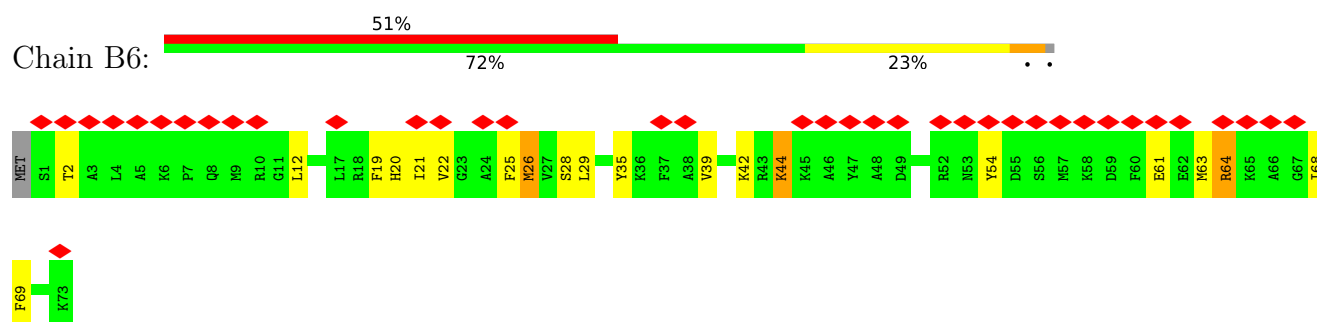
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial



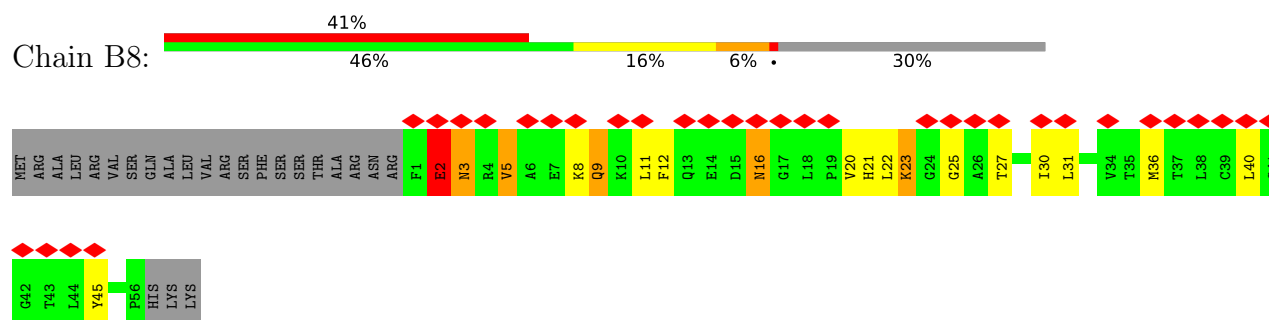
- Molecule 63: Cytochrome c oxidase subunit 6B1



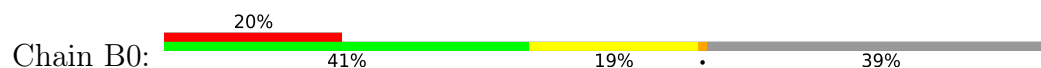
- Molecule 64: Cytochrome c oxidase subunit 6C

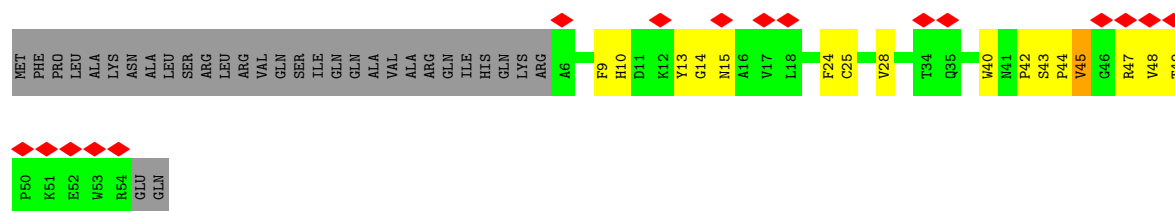


- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial

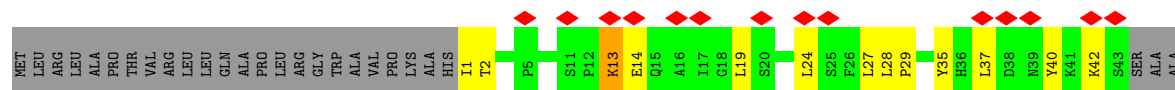
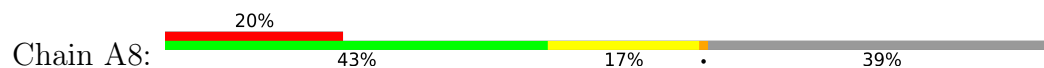




- Molecule 67: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 68: Cytochrome c oxidase subunit 8B, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	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	0.368	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PC1, CU, HEA, FES, FMN, ZN, HEM, NAP, HEC, MG, CDL, 3PE

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	9	0.29	0/1571	0.76	0/2149
2	7	0.34	0/1213	0.83	4/1659 (0.2%)
3	6	0.30	0/4892	0.73	4/6660 (0.1%)
4	2	0.41	0/2646	0.85	3/3618 (0.1%)
5	4	0.38	0/3538	0.86	10/4845 (0.2%)
6	5	0.36	0/706	0.82	0/960
7	8	0.31	0/3035	0.76	6/4130 (0.1%)
8	1	0.40	0/2571	0.83	1/3512 (0.0%)
9	3	0.34	0/885	0.89	5/1213 (0.4%)
10	A	0.36	0/5265	0.78	12/7147 (0.2%)
11	B	0.46	0/3505	0.86	5/4752 (0.1%)
12	C	0.39	0/1756	0.75	2/2394 (0.1%)
13	D	0.47	0/1231	0.85	1/1669 (0.1%)
14	E	0.45	0/1418	0.83	3/1922 (0.2%)
15	F	0.37	0/188	1.28	5/259 (1.9%)
16	G	0.41	0/1004	0.84	2/1359 (0.1%)
17	H	0.33	0/800	0.79	1/1076 (0.1%)
18	I	0.31	0/538	0.74	0/722
19	J	0.30	0/545	0.63	0/740
20	K	0.28	0/663	0.72	0/896
21	L	0.33	0/623	0.81	2/862 (0.2%)
22	N	0.27	0/882	0.72	0/1203
23	O	0.31	0/948	0.68	2/1279 (0.2%)
24	P	0.33	0/719	0.80	0/981
25	Q	0.29	0/1381	0.84	2/1869 (0.1%)
26	R	0.32	0/2465	0.85	4/3349 (0.1%)
27	S	0.31	0/2345	0.85	7/3193 (0.2%)
28	T	0.37	0/938	0.89	3/1279 (0.2%)
29	U	0.27	0/1053	0.78	3/1439 (0.2%)
30	V	0.31	0/1115	0.69	0/1508
31	M	0.27	0/651	0.77	2/876 (0.2%)
31	W	0.25	0/624	0.82	0/847

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X	0.31	0/383	0.94	4/523 (0.8%)
33	Y	0.26	0/428	0.60	0/592
34	Z	0.37	0/506	1.03	6/688 (0.9%)
35	a	0.29	0/878	0.82	5/1195 (0.4%)
36	b	0.32	0/1058	0.83	5/1434 (0.3%)
37	c	0.36	0/632	1.07	9/871 (1.0%)
38	d	0.25	0/724	0.73	2/989 (0.2%)
39	f	0.25	0/1191	0.77	2/1639 (0.1%)
40	h	0.33	0/679	0.87	0/926
41	i	0.22	0/286	0.48	0/392
42	j	0.31	0/922	0.83	5/1254 (0.4%)
43	g	0.27	0/1380	0.75	5/1872 (0.3%)
44	e	0.30	0/888	0.94	6/1234 (0.5%)
45	k	0.43	0/3527	0.69	4/4787 (0.1%)
45	w	0.42	0/3455	0.65	1/4685 (0.0%)
46	l	0.40	0/3192	0.65	3/4329 (0.1%)
46	x	0.40	0/3198	0.68	5/4336 (0.1%)
47	m	0.55	0/3108	0.68	0/4252
47	y	0.55	0/3108	0.68	0/4252
48	o	0.48	0/1978	0.71	2/2684 (0.1%)
48	z	0.48	0/1965	0.69	2/2669 (0.1%)
49	A0	0.38	0/1124	0.85	1/1538 (0.1%)
49	p	0.48	0/945	1.13	12/1288 (0.9%)
50	A1	0.52	0/935	0.70	1/1253 (0.1%)
50	q	0.52	0/935	0.64	0/1253
51	A2	0.40	0/698	0.64	0/944
51	r	0.39	0/704	0.64	0/951
52	B5	0.34	0/571	0.67	0/765
52	s	0.35	0/553	0.67	0/741
53	A3	0.44	0/314	0.74	0/434
53	t	0.28	0/272	0.54	0/377
54	B4	0.37	0/524	0.58	0/707
54	u	0.37	0/524	0.58	0/707
55	B3	0.55	0/149	1.32	1/203 (0.5%)
55	v	0.45	0/114	1.13	0/156
56	A9	0.86	7/4164 (0.2%)	1.16	35/5688 (0.6%)
57	B9	0.77	0/1868	1.12	10/2544 (0.4%)
58	B7	0.74	0/2212	1.02	8/3025 (0.3%)
59	A7	0.67	0/1229	0.96	3/1658 (0.2%)
60	A6	0.64	0/898	1.02	6/1218 (0.5%)
61	B2	0.73	0/765	1.13	3/1038 (0.3%)
62	A4	0.69	0/698	1.10	6/950 (0.6%)
63	A5	0.68	0/648	1.17	5/877 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
64	B6	0.71	0/611	0.94	2/810 (0.2%)
65	B8	0.71	0/451	1.04	3/610 (0.5%)
66	B0	0.75	0/398	1.01	0/546
67	B1	0.77	0/399	0.98	2/534 (0.4%)
68	A8	0.69	0/345	0.99	1/470 (0.2%)
All	All	0.46	7/108248 (0.0%)	0.82	254/147255 (0.2%)

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	9	0	4
2	7	0	5
3	6	0	6
4	2	0	9
5	4	0	6
6	5	0	3
7	8	0	1
8	1	0	1
10	A	0	12
11	B	0	6
12	C	0	1
13	D	0	4
14	E	0	1
17	H	0	1
22	N	0	1
24	P	0	2
25	Q	0	1
26	R	0	4
27	S	0	4
28	T	0	2
29	U	0	1
30	V	0	3
31	M	0	1
31	W	0	1
36	b	0	3
38	d	0	1
39	f	0	1
40	h	0	2
42	j	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	g	0	1
44	e	0	5
45	k	0	6
45	w	0	3
46	l	0	3
46	x	0	3
47	m	0	4
47	y	0	2
48	o	0	4
48	z	0	4
49	A0	0	6
49	p	0	6
53	A3	0	1
55	B3	0	1
All	All	0	138

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A9	61	HIS	CG-CD2	7.53	1.44	1.35
56	A9	378	HIS	ND1-CE1	7.07	1.39	1.32
56	A9	378	HIS	CE1-NE2	-6.52	1.26	1.32
56	A9	69	MET	SD-CE	-6.28	1.63	1.79
56	A9	61	HIS	ND1-CE1	5.59	1.38	1.32
56	A9	376	HIS	ND1-CE1	5.56	1.38	1.32
56	A9	378	HIS	CG-CD2	5.41	1.41	1.35

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	x	230	LEU	N-CA-C	12.17	128.14	110.24
56	A9	376	HIS	ND1-CE1-NE2	10.36	118.76	108.40
9	3	42	ASP	CA-C-N	9.84	132.14	119.84
9	3	42	ASP	C-N-CA	9.84	132.14	119.84
63	A5	52	VAL	N-CA-C	8.97	121.26	108.17
63	A5	81	PHE	CA-C-N	8.75	128.40	119.56
63	A5	81	PHE	C-N-CA	8.75	128.40	119.56
39	f	163	LEU	CA-C-N	8.71	147.91	127.00
39	f	163	LEU	C-N-CA	8.71	147.91	127.00
49	p	146	PRO	N-CA-CB	8.47	111.92	102.60
7	8	228	PRO	CA-C-N	8.18	136.43	121.70
7	8	228	PRO	C-N-CA	8.18	136.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	B1	20	ARG	N-CA-C	-8.13	102.50	111.36
56	A9	378	HIS	ND1-CE1-NE2	8.10	116.50	108.40
56	A9	82	LEU	N-CA-C	8.00	122.30	112.23
46	l	305	GLN	CA-C-N	-7.83	111.54	119.99
46	l	305	GLN	C-N-CA	-7.83	111.54	119.99
56	A9	56	VAL	N-CA-C	-7.79	103.20	110.53
9	3	3	LEU	CA-C-N	7.72	135.59	121.70
9	3	3	LEU	C-N-CA	7.72	135.59	121.70
25	Q	54	ARG	N-CA-C	-7.71	105.04	114.75
37	c	66	ARG	CA-C-N	7.67	135.50	121.70
37	c	66	ARG	C-N-CA	7.67	135.50	121.70
56	A9	435	GLY	N-CA-C	7.59	125.97	115.27
5	4	4	TYR	N-CA-C	-7.50	104.75	114.04
68	A8	27	LEU	N-CA-C	7.46	119.49	111.36
27	S	199	VAL	CA-C-N	7.45	129.16	119.84
27	S	199	VAL	C-N-CA	7.45	129.16	119.84
56	A9	330	GLY	N-CA-C	7.44	120.52	112.33
45	k	215	HIS	CA-C-N	7.39	135.00	121.70
45	k	215	HIS	C-N-CA	7.39	135.00	121.70
55	B3	71	ASN	N-CA-C	-7.34	98.20	109.14
7	8	36	LYS	CA-C-N	7.34	134.91	121.70
7	8	36	LYS	C-N-CA	7.34	134.91	121.70
37	c	36	PRO	CA-C-N	7.34	144.61	127.00
37	c	36	PRO	C-N-CA	7.34	144.61	127.00
56	A9	376	HIS	CE1-NE2-CD2	-7.25	101.75	109.00
7	8	259	GLY	CA-C-N	7.22	134.70	121.70
7	8	259	GLY	C-N-CA	7.22	134.70	121.70
34	Z	85	GLU	CA-C-N	7.22	134.69	121.70
34	Z	85	GLU	C-N-CA	7.22	134.69	121.70
46	x	229	GLY	CA-C-N	7.19	131.33	121.05
46	x	229	GLY	C-N-CA	7.19	131.33	121.05
56	A9	332	ILE	N-CA-C	7.17	119.05	109.37
37	c	114	GLY	CA-C-N	7.13	134.53	121.70
37	c	114	GLY	C-N-CA	7.13	134.53	121.70
60	A6	42	VAL	N-CA-C	-7.12	99.65	108.05
56	A9	9	SER	N-CA-C	7.12	119.75	110.43
60	A6	76	GLY	CA-C-N	7.12	128.35	120.45
60	A6	76	GLY	C-N-CA	7.12	128.35	120.45
46	l	305	GLN	N-CA-C	7.08	125.45	109.81
49	p	159	PRO	N-CA-CB	6.93	110.23	102.60
15	F	104	ARG	CA-C-N	6.93	134.18	121.70
15	F	104	ARG	C-N-CA	6.93	134.18	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A9	130	PRO	N-CA-C	-6.92	102.25	110.70
21	L	62	ASN	CA-C-N	6.89	134.11	121.70
21	L	62	ASN	C-N-CA	6.89	134.11	121.70
8	1	311	THR	N-CA-C	-6.85	104.22	114.64
10	A	461	PRO	CA-C-N	6.85	134.63	121.54
10	A	461	PRO	C-N-CA	6.85	134.63	121.54
48	o	79	GLU	N-CA-C	6.85	125.38	110.80
37	c	36	PRO	C-N-CD	-6.84	105.55	120.60
58	B7	36	HIS	N-CA-C	6.84	122.05	113.43
36	b	99	ALA	N-CA-C	6.82	119.54	111.02
59	A7	133	GLY	N-CA-C	6.75	129.18	113.18
56	A9	507	GLU	N-CA-C	-6.75	97.88	109.15
32	X	43	LEU	CA-C-N	6.74	133.84	121.70
32	X	43	LEU	C-N-CA	6.74	133.84	121.70
17	H	58	ILE	N-CA-C	-6.74	106.46	112.12
62	A4	5	LYS	N-CA-C	6.71	125.10	110.80
35	a	128	SER	CA-C-N	6.71	133.78	121.70
35	a	128	SER	C-N-CA	6.71	133.78	121.70
2	7	140	ALA	CA-C-N	6.67	133.72	121.70
2	7	140	ALA	C-N-CA	6.67	133.72	121.70
13	D	191	GLU	N-CA-C	-6.67	104.31	113.18
2	7	139	GLU	CA-C-N	6.62	133.62	121.70
2	7	139	GLU	C-N-CA	6.62	133.62	121.70
14	E	75	SER	CA-C-N	6.60	133.59	121.70
14	E	75	SER	C-N-CA	6.60	133.59	121.70
60	A6	81	ILE	N-CA-C	6.60	116.73	110.53
49	p	82	PRO	N-CA-CB	6.57	110.15	103.25
56	A9	61	HIS	CB-CG-CD2	-6.52	122.72	131.20
56	A9	61	HIS	ND1-CE1-NE2	6.50	114.90	108.40
56	A9	506	GLU	N-CA-C	-6.49	104.20	111.28
56	A9	74	MET	N-CA-C	6.48	118.00	111.07
26	R	271	TYR	CA-C-N	6.47	133.90	121.54
26	R	271	TYR	C-N-CA	6.47	133.90	121.54
16	G	155	PRO	CA-C-N	6.45	133.31	121.70
16	G	155	PRO	C-N-CA	6.45	133.31	121.70
42	j	22	PRO	CA-C-N	6.43	142.44	127.00
42	j	22	PRO	C-N-CA	6.43	142.44	127.00
27	S	87	GLY	CA-C-N	6.42	133.25	121.70
27	S	87	GLY	C-N-CA	6.42	133.25	121.70
49	p	120	PRO	N-CA-CB	6.37	109.93	103.25
38	d	31	PHE	CA-C-N	6.35	142.24	127.00
38	d	31	PHE	C-N-CA	6.35	142.24	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	292	MET	CA-C-N	6.35	133.66	121.54
11	B	292	MET	C-N-CA	6.35	133.66	121.54
49	p	130	PRO	N-CA-CB	6.34	109.91	103.25
26	R	369	VAL	CA-C-N	6.34	133.11	121.70
26	R	369	VAL	C-N-CA	6.34	133.11	121.70
11	B	293	LEU	N-CA-C	-6.33	97.31	110.80
25	Q	30	HIS	N-CA-C	-6.33	104.76	113.18
62	A4	2	SER	N-CA-C	6.29	119.60	109.79
56	A9	10	THR	N-CA-C	-6.24	103.86	112.03
50	A1	26	PHE	N-CA-C	6.24	118.67	109.69
10	A	381	LEU	CA-C-N	6.21	133.40	121.54
10	A	381	LEU	C-N-CA	6.21	133.40	121.54
4	2	127	GLY	CA-C-N	6.17	132.81	121.70
4	2	127	GLY	C-N-CA	6.17	132.81	121.70
60	A6	21	LYS	CA-C-N	6.11	126.28	119.32
60	A6	21	LYS	C-N-CA	6.11	126.28	119.32
56	A9	157	SER	N-CA-C	6.09	118.88	111.82
56	A9	170	ASN	N-CA-C	6.06	120.75	113.23
29	U	120	THR	CA-C-N	6.05	141.53	127.00
29	U	120	THR	C-N-CA	6.05	141.53	127.00
28	T	35	VAL	N-CA-C	6.03	121.89	109.34
57	B9	47	THR	N-CA-C	6.02	119.94	112.59
35	a	19	ASP	CA-C-N	6.02	141.44	127.00
35	a	19	ASP	C-N-CA	6.02	141.44	127.00
58	B7	8	TYR	N-CA-C	6.02	118.29	110.53
63	A5	63	LEU	N-CA-C	6.02	119.09	111.69
57	B9	207	MET	CA-C-N	5.99	127.32	119.84
57	B9	207	MET	C-N-CA	5.99	127.32	119.84
62	A4	44	ARG	CA-C-N	5.98	126.00	119.90
62	A4	44	ARG	C-N-CA	5.98	126.00	119.90
56	A9	67	PHE	N-CA-C	5.97	119.76	112.23
49	p	133	VAL	CA-C-N	5.97	132.44	121.70
49	p	133	VAL	C-N-CA	5.97	132.44	121.70
14	E	67	ILE	N-CA-C	-5.96	106.91	111.62
56	A9	125	GLY	N-CA-C	-5.94	104.22	112.18
56	A9	171	MET	N-CA-C	5.92	120.21	111.87
5	4	457	PRO	CA-C-N	5.91	132.33	121.70
5	4	457	PRO	C-N-CA	5.91	132.33	121.70
56	A9	119	GLU	CB-CA-C	-5.90	109.75	116.54
57	B9	134	ARG	N-CA-C	5.90	123.37	110.80
46	x	304	HIS	CA-C-N	5.89	136.18	121.80
46	x	304	HIS	C-N-CA	5.89	136.18	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B9	190	GLY	N-CA-C	5.83	117.84	110.38
42	j	22	PRO	C-N-CD	-5.81	107.81	120.60
37	c	112	GLU	CA-C-N	5.78	132.11	121.70
37	c	112	GLU	C-N-CA	5.78	132.11	121.70
3	6	350	LEU	CA-C-N	5.78	132.58	121.54
3	6	350	LEU	C-N-CA	5.78	132.58	121.54
32	X	54	VAL	CA-C-N	5.78	132.57	121.54
32	X	54	VAL	C-N-CA	5.78	132.57	121.54
65	B8	25	GLY	N-CA-C	5.75	119.00	110.60
27	S	113	ASP	CA-C-N	5.74	132.02	121.70
27	S	113	ASP	C-N-CA	5.74	132.02	121.70
59	A7	129	ALA	CA-C-N	5.73	127.00	119.84
59	A7	129	ALA	C-N-CA	5.73	127.00	119.84
58	B7	198	PHE	N-CA-C	5.72	117.52	111.28
48	z	79	GLU	CA-C-N	5.71	132.46	121.54
48	z	79	GLU	C-N-CA	5.71	132.46	121.54
49	p	75	GLU	CA-C-N	5.70	131.96	121.70
49	p	75	GLU	C-N-CA	5.70	131.96	121.70
15	F	97	MET	C-N-CD	-5.67	108.12	120.60
5	4	224	PRO	CA-C-N	5.66	128.19	120.77
5	4	224	PRO	C-N-CA	5.66	128.19	120.77
56	A9	129	TYR	CB-CA-C	-5.66	100.54	109.42
57	B9	104	TRP	N-CA-C	5.63	122.80	110.80
64	B6	20	HIS	N-CA-C	5.58	118.13	111.71
31	M	36	PHE	CA-C-N	5.57	132.18	121.54
31	M	36	PHE	C-N-CA	5.57	132.18	121.54
61	B2	82	CYS	CA-C-N	5.56	125.40	119.28
61	B2	82	CYS	C-N-CA	5.56	125.40	119.28
67	B1	16	GLU	N-CA-C	5.54	117.39	111.36
58	B7	188	ILE	CB-CA-C	-5.53	104.67	112.14
56	A9	159	LEU	N-CA-C	-5.52	105.34	111.36
29	U	120	THR	C-N-CD	-5.52	108.47	120.60
28	T	57	GLY	N-CA-C	-5.50	106.13	112.73
62	A4	72	ASN	CA-C-N	5.50	125.84	119.47
62	A4	72	ASN	C-N-CA	5.50	125.84	119.47
48	o	80	MET	CA-CB-CG	5.49	125.08	114.10
65	B8	2	GLU	N-CA-C	5.49	122.49	110.80
5	4	14	LEU	N-CA-C	-5.46	107.27	114.04
56	A9	245	ILE	N-CA-C	-5.46	104.23	111.05
35	a	76	ILE	N-CA-C	-5.45	107.54	112.12
49	A0	188	THR	CB-CA-C	-5.43	110.33	116.63
44	e	50	ALA	N-CA-C	-5.42	105.02	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	e	82	SER	N-CA-C	5.42	122.33	110.80
56	A9	305	PHE	N-CA-C	5.40	118.97	112.38
45	w	213	GLN	N-CA-C	5.38	117.74	111.02
45	k	203	LEU	CA-C-N	-5.37	111.28	121.54
45	k	203	LEU	C-N-CA	-5.37	111.28	121.54
3	6	602	PHE	CA-C-N	5.34	131.74	121.54
3	6	602	PHE	C-N-CA	5.34	131.74	121.54
11	B	231	GLY	CA-C-N	5.32	127.83	120.49
11	B	231	GLY	C-N-CA	5.32	127.83	120.49
10	A	352	ILE	N-CA-C	-5.32	107.65	112.12
44	e	98	ARG	CA-C-N	-5.31	115.21	121.90
44	e	98	ARG	C-N-CA	-5.31	115.21	121.90
42	j	115	GLU	CA-C-N	5.30	131.25	121.70
42	j	115	GLU	C-N-CA	5.30	131.25	121.70
56	A9	372	TYR	N-CA-C	-5.29	105.41	111.07
49	p	78	LEU	N-CA-C	5.28	117.01	109.14
5	4	417	GLY	CA-C-N	5.27	131.61	121.54
5	4	417	GLY	C-N-CA	5.27	131.61	121.54
27	S	276	ASP	N-CA-C	5.27	122.03	110.80
10	A	176	CYS	N-CA-C	5.26	122.00	110.80
5	4	370	PRO	N-CA-C	5.25	117.11	110.70
23	O	76	PRO	CA-C-N	5.25	131.56	121.54
23	O	76	PRO	C-N-CA	5.25	131.56	121.54
34	Z	41	LEU	CA-C-N	5.22	131.10	121.70
34	Z	41	LEU	C-N-CA	5.22	131.10	121.70
10	A	504	SER	CA-C-N	5.22	131.10	121.70
10	A	504	SER	C-N-CA	5.22	131.10	121.70
5	4	75	LEU	N-CA-C	-5.20	108.19	114.75
56	A9	262	SER	N-CA-C	-5.18	106.64	113.17
12	C	124	ARG	CA-C-N	5.18	131.43	121.54
12	C	124	ARG	C-N-CA	5.18	131.43	121.54
28	T	83	LYS	N-CA-C	5.18	121.25	109.81
58	B7	99	TRP	N-CA-C	-5.18	105.53	111.07
65	B8	9	GLN	N-CA-C	-5.17	105.54	111.07
56	A9	377	PHE	N-CA-C	5.16	119.43	113.18
61	B2	38	ALA	N-CA-C	5.16	117.78	110.50
34	Z	62	SER	CA-C-N	5.16	131.40	121.54
34	Z	62	SER	C-N-CA	5.16	131.40	121.54
43	g	124	ASN	CA-C-N	5.15	131.38	121.54
43	g	124	ASN	C-N-CA	5.15	131.38	121.54
56	A9	401	SER	N-CA-C	5.15	119.69	113.41
43	g	82	VAL	N-CA-C	-5.14	107.56	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	B7	107	ALA	CA-C-N	5.14	125.94	119.98
58	B7	107	ALA	C-N-CA	5.14	125.94	119.98
63	A5	22	ASN	N-CA-C	5.14	117.67	109.81
56	A9	353	LEU	N-CA-C	-5.13	105.77	111.36
64	B6	2	THR	N-CA-C	5.12	116.19	108.46
44	e	80	ASP	CA-C-N	5.10	131.28	121.54
44	e	80	ASP	C-N-CA	5.10	131.28	121.54
36	b	160	MET	CA-C-N	5.10	130.88	121.70
36	b	160	MET	C-N-CA	5.10	130.88	121.70
56	A9	378	HIS	CB-CG-CD2	-5.10	124.57	131.20
10	A	656	TYR	CA-C-N	5.07	131.23	121.54
10	A	656	TYR	C-N-CA	5.07	131.23	121.54
56	A9	378	HIS	N-CA-C	-5.07	106.26	112.90
4	2	255	PRO	N-CA-C	5.07	116.88	110.70
15	F	97	MET	CA-C-N	5.06	139.14	127.00
15	F	97	MET	C-N-CA	5.06	139.14	127.00
56	A9	2	PHE	N-CA-C	-5.05	105.66	111.07
36	b	100	GLU	CA-C-N	5.05	130.80	121.70
36	b	100	GLU	C-N-CA	5.05	130.80	121.70
57	B9	12	ALA	N-CA-C	5.05	117.48	109.96
57	B9	165	VAL	CA-C-N	5.05	126.15	119.84
57	B9	165	VAL	C-N-CA	5.05	126.15	119.84
57	B9	66	THR	N-CA-C	-5.05	107.78	114.04
9	3	3	LEU	N-CA-C	5.04	119.88	113.18
10	A	153	PHE	CA-C-N	5.04	130.76	121.70
10	A	153	PHE	C-N-CA	5.04	130.76	121.70
56	A9	70	VAL	N-CA-C	5.04	115.47	110.23
49	p	79	SER	CA-C-N	5.03	131.15	121.54
49	p	79	SER	C-N-CA	5.03	131.15	121.54
43	g	72	PRO	CA-C-N	-5.03	115.57	121.90
43	g	72	PRO	C-N-CA	-5.03	115.57	121.90
58	B7	244	PHE	N-CA-C	-5.02	105.26	111.33

There are no chirality outliers.

All (138) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	281	ARG	Peptide
4	2	106	LEU	Peptide
4	2	111	PHE	Peptide
4	2	128	LEU	Peptide
4	2	199	THR	Peptide

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Mol	Chain	Res	Type	Group
4	2	222	ASN	Peptide
4	2	270	MET	Peptide
4	2	271	THR	Peptide
4	2	339	LEU	Peptide
4	2	45	MET	Peptide
5	4	140	THR	Peptide
5	4	222	GLU	Peptide
5	4	306	PRO	Peptide
5	4	368	ALA	Peptide
5	4	369	LEU	Peptide
5	4	71	TRP	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
3	6	29	PRO	Peptide
3	6	351	ASN	Peptide
3	6	352	ASP	Peptide
3	6	522	PHE	Peptide
3	6	549	ALA	Peptide
3	6	71	ILE	Peptide
2	7	140	ALA	Peptide
2	7	148	SER	Peptide
2	7	170	GLU	Peptide
2	7	24	PRO	Peptide
2	7	25	SER	Peptide
7	8	228	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	179	ALA	Peptide
1	9	75	LYS	Peptide
10	A	127	ASP	Peptide
10	A	128	CYS	Peptide
10	A	175	ARG	Peptide
10	A	236	TYR	Peptide
10	A	283	GLU	Peptide
10	A	308	ARG	Peptide
10	A	309	ASN	Peptide
10	A	382	ARG	Peptide
10	A	460	HIS	Peptide
10	A	461	PRO	Peptide
10	A	462	PHE	Peptide
10	A	98	LYS	Peptide

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Mol	Chain	Res	Type	Group
49	A0	119	ASP	Peptide
49	A0	123	ASP	Peptide
49	A0	163	SER	Peptide
49	A0	165	TYR	Peptide
49	A0	183	PRO	Peptide
49	A0	193	VAL	Peptide
53	A3	45	VAL	Peptide
11	B	218	SER	Peptide
11	B	290	GLY	Peptide
11	B	291	VAL	Peptide
11	B	87	GLN	Peptide
11	B	88	HIS	Peptide
11	B	89	PRO	Peptide
55	B3	70	LEU	Peptide
12	C	198	HIS	Peptide
13	D	113	PHE	Peptide
13	D	161	GLY	Peptide
13	D	186	CYS	Peptide
13	D	84	PRO	Peptide
14	E	107	PRO	Peptide
17	H	84	GLU	Peptide
31	M	24	LYS	Peptide
22	N	40	LYS	Peptide
24	P	36	GLN	Peptide
24	P	52	ASN	Peptide
25	Q	91	TYR	Peptide
26	R	271	TYR	Peptide
26	R	324	THR	Peptide
26	R	333	PRO	Peptide
26	R	355	ARG	Peptide
27	S	100	CYS	Peptide
27	S	275	ASN	Peptide
27	S	278	ASN	Peptide
27	S	38	THR	Peptide
28	T	105	THR	Peptide
28	T	83	LYS	Peptide
29	U	118	SER	Peptide
30	V	10	MET	Peptide
30	V	142	TRP	Peptide
30	V	72	MET	Peptide
31	W	154	VAL	Peptide
36	b	110	TRP	Peptide

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Mol	Chain	Res	Type	Group
36	b	134	GLU	Peptide
36	b	96	ALA	Peptide
38	d	18	ASP	Peptide
44	e	77	LYS	Peptide
44	e	79	PRO	Peptide
44	e	81	ARG	Peptide
44	e	87	ASP	Peptide
44	e	94	HIS	Peptide
39	f	109	PRO	Peptide
43	g	160	LYS	Peptide
40	h	80	PRO	Peptide
40	h	81	ALA	Peptide
42	j	115	GLU	Peptide
42	j	21	LEU	Peptide
45	k	212	ALA	Peptide
45	k	216	PHE	Peptide
45	k	228	VAL	Peptide
45	k	229	PRO	Peptide
45	k	428	ILE	Peptide
45	k	73	ASN	Peptide
46	l	227	ARG	Peptide
46	l	229	GLY	Mainchain
46	l	304	HIS	Peptide
47	m	255	ASN	Peptide
47	m	274	PHE	Peptide
47	m	343	VAL	Mainchain
47	m	8	HIS	Peptide
48	o	50	HIS	Peptide
48	o	69	GLU	Mainchain
48	o	79	GLU	Peptide
48	o	81	PHE	Peptide
49	p	10	PHE	Peptide
49	p	133	VAL	Peptide
49	p	136	ILE	Peptide
49	p	76	ILE	Peptide
49	p	77	LYS	Peptide
49	p	78	LEU	Peptide
45	w	212	ALA	Peptide
45	w	428	ILE	Peptide
45	w	73	ASN	Peptide
46	x	227	ARG	Peptide
46	x	229	GLY	Mainchain

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Mol	Chain	Res	Type	Group
46	x	230	LEU	Peptide
47	y	255	ASN	Peptide
47	y	274	PHE	Peptide
48	z	50	HIS	Peptide
48	z	69	GLU	Peptide,Mainchain
48	z	78	GLY	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	9	1534	0	1488	33	0
2	7	1186	0	1123	11	0
3	6	4765	0	4894	51	0
4	2	2582	0	2612	28	0
5	4	3447	0	3442	46	0
6	5	697	0	708	12	0
7	8	2965	0	2596	47	0
8	1	2499	0	2612	49	0
9	3	862	0	860	14	0
10	A	5179	0	5173	76	0
11	B	3416	0	3335	52	0
12	C	1705	0	1645	24	0
13	D	1200	0	1195	22	0
14	E	1388	0	1340	24	0
15	F	183	0	132	5	0
16	G	981	0	965	14	0
17	H	780	0	753	10	0
18	I	530	0	508	22	0
19	J	530	0	503	4	0
20	K	652	0	636	7	0
21	L	602	0	592	4	0
22	N	862	0	868	11	0
23	O	925	0	907	11	0
24	P	698	0	659	11	0
25	Q	1345	0	1282	19	0
26	R	2407	0	2296	52	0
27	S	2297	0	2022	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	T	922	0	852	64	0
29	U	1019	0	900	10	0
30	V	1087	0	1037	14	0
31	M	642	0	642	11	0
31	W	616	0	579	11	0
32	X	372	0	314	4	0
33	Y	409	0	318	1	0
34	Z	493	0	395	5	0
35	a	857	0	765	9	0
36	b	1032	0	954	9	0
37	c	617	0	492	10	0
38	d	708	0	514	7	0
39	f	1156	0	892	16	0
40	h	658	0	584	10	0
41	i	277	0	240	1	0
42	j	892	0	835	13	0
43	g	1351	0	1262	16	0
44	e	864	0	567	13	0
45	k	3454	0	3350	303	0
45	w	3385	0	3293	276	0
46	l	3135	0	3112	243	0
46	x	3141	0	3123	256	0
47	m	3011	0	3077	252	0
47	y	3011	0	3077	246	0
48	o	1919	0	1870	186	0
48	z	1906	0	1841	189	0
49	A0	1117	0	808	80	0
49	p	938	0	733	72	0
50	A1	916	0	911	116	0
50	q	916	0	911	89	0
51	A2	676	0	668	74	0
51	r	682	0	679	49	0
52	B5	566	0	542	47	0
52	s	548	0	530	49	0
53	A3	304	0	299	49	0
53	t	262	0	250	25	0
54	B4	511	0	518	62	0
54	u	511	0	518	56	0
55	B3	148	0	154	18	0
55	v	114	0	107	9	0
56	A9	4025	0	4003	86	0
57	B9	1822	0	1834	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B7	2125	0	2046	52	0
59	A7	1195	0	1183	35	0
60	A6	878	0	868	21	0
61	B2	748	0	728	25	0
62	A4	671	0	645	29	0
63	A5	628	0	582	24	0
64	B6	598	0	612	16	0
65	B8	441	0	439	17	0
66	B0	384	0	366	12	0
67	B1	386	0	388	8	0
68	A8	335	0	352	12	0
69	9	4	0	0	0	0
69	A	4	0	0	0	0
69	m	4	0	0	0	0
70	4	82	0	114	1	0
70	6	64	0	72	2	0
70	J	58	0	60	1	0
71	2	41	0	59	1	0
71	4	41	0	59	1	0
71	B	51	0	82	2	0
71	V	51	0	82	0	0
71	j	46	0	69	1	0
72	2	46	0	66	2	0
72	L	47	0	71	2	0
72	Q	46	0	66	1	0
72	S	47	0	71	3	0
72	j	39	0	55	1	0
73	8	31	0	19	3	0
74	8	8	0	0	0	0
74	A	16	0	0	1	0
74	D	8	0	0	0	0
74	E	16	0	0	1	0
75	B2	1	0	0	0	0
75	I	1	0	0	0	0
76	R	48	0	23	3	0
77	m	86	0	60	28	0
77	y	86	0	60	30	0
78	o	43	0	32	10	0
78	z	43	0	32	10	0
79	A9	120	0	108	4	0
80	A9	1	0	0	0	0
80	B9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	A9	1	0	0	0	0
All	All	106778	0	102965	3613	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 17.

All (3613) 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)
8:1:17:VAL:HG21	8:1:225:MET:CE	1.21	1.57
8:1:17:VAL:CG2	8:1:225:MET:CE	1.78	1.47
50:A1:24:ALA:HB1	51:A2:47:ARG:NH2	1.33	1.43
50:A1:24:ALA:CB	51:A2:47:ARG:HH21	1.36	1.36
11:B:52:MET:O	11:B:54:PRO:HD3	1.17	1.31
28:T:41:VAL:CG1	28:T:59:TYR:OH	1.79	1.29
8:1:17:VAL:CG2	8:1:225:MET:HE1	0.81	1.27
50:A1:24:ALA:HB1	51:A2:47:ARG:CZ	1.68	1.24
18:I:104:ASP:O	18:I:105:LYS:HG3	1.35	1.23
31:W:104:PHE:O	31:W:108:LEU:HG	1.37	1.23
76:R:601:NAP:C1D	76:R:601:NAP:O4D	1.63	1.21
27:S:196:ASP:OD1	27:S:246:TYR:HB3	1.39	1.20
26:R:328:ILE:HG22	26:R:329:LEU:H	1.05	1.14
50:A1:23:ALA:HB1	51:A2:46:LEU:CD2	1.78	1.11
51:A2:37:VAL:O	51:A2:41:THR:HG23	1.50	1.11
28:T:50:LEU:O	28:T:52:GLY:N	1.86	1.08
50:q:49:ARG:O	46:x:134:ARG:NH1	1.87	1.08
53:A3:33:VAL:HA	53:A3:38:TRP:CB	1.84	1.07
28:T:41:VAL:HG11	28:T:59:TYR:OH	1.50	1.07
11:B:52:MET:O	11:B:54:PRO:CD	2.04	1.05
50:A1:23:ALA:HB1	51:A2:46:LEU:HD21	1.36	1.04
8:1:17:VAL:HG23	8:1:225:MET:HE1	1.07	1.03
27:S:196:ASP:OD1	27:S:246:TYR:CB	2.08	1.01
50:A1:24:ALA:HB1	51:A2:47:ARG:NE	1.74	1.01
28:T:32:ALA:HA	28:T:35:VAL:CG1	1.91	1.00
8:1:17:VAL:HG22	8:1:225:MET:HE1	1.43	0.98
18:I:108:LYS:HG2	18:I:118:GLN:HE21	1.24	0.98
26:R:328:ILE:CG2	26:R:329:LEU:H	1.75	0.98
28:T:32:ALA:C	28:T:35:VAL:HG13	1.89	0.97
45:k:215:HIS:HB2	45:k:216:PHE:HB2	1.45	0.97
50:A1:23:ALA:CB	51:A2:46:LEU:HD21	1.93	0.97
18:I:104:ASP:O	18:I:105:LYS:CG	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:328:ILE:HG22	26:R:329:LEU:N	1.77	0.96
48:z:158:ILE:HD11	78:z:301:HEC:HHA	1.47	0.96
48:o:158:ILE:HD11	78:o:301:HEC:HHA	1.47	0.95
56:A9:365:ILE:HD12	57:B9:87:MET:HE1	1.48	0.95
28:T:62:THR:CG2	28:T:104:ARG:HD2	1.96	0.95
47:m:344:GLU:HG2	47:m:346:PRO:HD2	1.46	0.94
46:x:247:GLN:HE22	46:x:429:ASN:HA	1.32	0.94
50:A1:24:ALA:CB	51:A2:47:ARG:HE	1.80	0.94
8:l:17:VAL:HG21	8:l:225:MET:HE3	1.50	0.94
18:I:108:LYS:HG3	18:I:120:ARG:CB	1.96	0.94
46:l:182:ARG:HD2	46:l:185:LYS:HD3	1.48	0.93
46:l:438:GLU:OE2	46:x:169:ARG:NH2	2.00	0.93
46:x:182:ARG:HD2	46:x:185:LYS:HD3	1.48	0.93
47:y:138:MET:H	47:y:255:ASN:HD22	1.16	0.93
53:A3:42:LEU:O	53:A3:44:TRP:N	2.00	0.93
28:T:62:THR:HG22	28:T:104:ARG:NH1	1.85	0.92
50:q:35:ASP:OD2	50:q:61:ARG:NH2	2.03	0.92
56:A9:449:MET:SD	57:B9:5:MET:HE2	2.09	0.92
28:T:62:THR:HG22	28:T:104:ARG:HH11	1.35	0.92
49:p:15:ARG:HH21	49:p:32:ARG:HG3	1.34	0.92
50:A1:35:ASP:OD2	50:A1:61:ARG:NH2	2.02	0.92
28:T:62:THR:CG2	28:T:104:ARG:CD	2.47	0.92
28:T:33:GLY:O	28:T:60:THR:HG23	1.70	0.91
28:T:64:ALA:O	28:T:65:ALA:CB	2.17	0.91
46:l:247:GLN:HE22	46:l:429:ASN:HA	1.32	0.91
46:l:437:ASP:OD2	46:x:240:HIS:NE2	2.02	0.91
46:l:78:LYS:HB3	46:l:129:ALA:HB1	1.52	0.91
50:A1:23:ALA:CB	51:A2:46:LEU:CD2	2.47	0.91
46:x:78:LYS:HB3	46:x:129:ALA:HB1	1.52	0.90
47:m:138:MET:H	47:m:255:ASN:HD22	1.15	0.90
50:A1:23:ALA:HB1	51:A2:46:LEU:HD22	1.54	0.90
50:A1:28:LYS:O	50:A1:29:LEU:HD23	1.72	0.90
28:T:64:ALA:O	28:T:65:ALA:HB2	1.71	0.89
49:p:14:ARG:HA	51:r:23:GLN:HA	1.54	0.89
50:A1:24:ALA:O	50:A1:26:PHE:N	2.05	0.89
54:u:52:TRP:HB2	54:u:56:LYS:HB2	1.55	0.89
48:o:99:GLU:HB3	48:z:76:GLU:HG3	1.53	0.89
45:w:329:MET:HE3	51:A2:2:ARG:HE	1.38	0.88
62:A4:5:LYS:HZ3	62:A4:6:GLY:H	0.93	0.88
11:B:55:THR:O	11:B:56:LYS:HB2	1.74	0.88
48:z:51:LEU:HD23	48:z:61:ALA:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B4:52:TRP:HB2	54:B4:56:LYS:HB2	1.55	0.87
28:T:32:ALA:HA	28:T:35:VAL:HG13	1.55	0.87
48:o:41:HIS:NE2	78:o:301:HEC:ND	2.23	0.87
48:o:51:LEU:HD23	48:o:61:ALA:HB3	1.55	0.87
28:T:41:VAL:HG11	28:T:59:TYR:CZ	2.10	0.87
28:T:32:ALA:O	28:T:35:VAL:HG13	1.75	0.87
48:z:41:HIS:NE2	78:z:301:HEC:ND	2.23	0.86
48:z:234:LYS:HB2	51:A2:16:TYR:HB2	1.57	0.86
50:A1:28:LYS:HB3	50:A1:80:TRP:CD2	2.10	0.86
28:T:41:VAL:HG13	28:T:59:TYR:OH	1.76	0.86
45:w:191:LYS:HB2	45:w:219:LEU:H	1.40	0.86
45:k:433:ASP:OD2	47:m:223:TYR:OH	1.93	0.85
46:x:247:GLN:NE2	46:x:248:ASN:O	2.09	0.85
45:k:161:THR:HG21	45:k:234:CYS:HA	1.57	0.85
50:A1:24:ALA:CB	51:A2:47:ARG:NH2	2.10	0.85
53:A3:31:GLY:O	53:A3:35:ALA:N	2.10	0.85
58:B7:112:LEU:HG	58:B7:118:PRO:HB3	1.55	0.85
28:T:32:ALA:CA	28:T:35:VAL:HG13	2.06	0.85
45:w:161:THR:HG21	45:w:234:CYS:HA	1.57	0.85
46:x:270:ASN:O	46:x:274:VAL:N	2.10	0.84
62:A4:5:LYS:HZ3	62:A4:6:GLY:N	1.75	0.84
11:B:52:MET:C	11:B:54:PRO:HD3	2.01	0.84
50:A1:24:ALA:HB3	51:A2:47:ARG:HH21	1.37	0.84
46:l:247:GLN:NE2	46:l:248:ASN:O	2.09	0.84
47:y:24:PRO:O	47:y:224:TYR:OH	1.96	0.84
28:T:32:ALA:O	28:T:35:VAL:CG1	2.26	0.83
38:d:25:PHE:CD2	38:d:40:VAL:CB	2.62	0.83
46:l:270:ASN:O	46:l:274:VAL:N	2.10	0.83
47:m:24:PRO:O	47:m:224:TYR:OH	1.96	0.83
48:z:234:LYS:HG3	49:A0:7:VAL:HG21	1.61	0.83
53:A3:19:PRO:HA	53:A3:22:SER:OG	1.76	0.83
56:A9:187:SER:HB2	56:A9:277:MET:HE1	1.60	0.83
57:B9:78:LEU:HB2	57:B9:79:PRO:HD3	1.58	0.83
54:u:56:LYS:HG2	54:u:60:GLU:HB3	1.60	0.82
45:w:21:ASN:HD21	45:w:217:SER:H	1.25	0.82
45:w:304:CYS:HA	45:w:326:CYS:HB3	1.62	0.82
48:o:197:GLU:HG2	48:o:201:ARG:HD3	1.61	0.82
47:m:244:LEU:O	48:o:201:ARG:NH1	2.12	0.82
54:B4:56:LYS:HG2	54:B4:60:GLU:HB3	1.60	0.81
54:B4:41:ALA:O	54:B4:45:HIS:N	2.13	0.81
9:3:42:ASP:N	9:3:43:PRO:CD	2.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:62:THR:HG23	28:T:104:ARG:CD	2.10	0.81
49:p:14:ARG:O	51:r:24:ARG:NH2	2.13	0.81
47:m:1:MET:SD	47:m:7:SER:OG	2.39	0.81
49:p:34:GLY:O	49:p:38:LEU:N	2.13	0.81
48:z:236:ALA:HB3	51:A2:14:ILE:HB	1.62	0.81
8:l:17:VAL:HG23	8:l:225:MET:CE	1.76	0.81
45:w:177:LEU:HD21	45:w:182:LEU:HD21	1.63	0.81
53:A3:39:ARG:HG2	53:A3:39:ARG:HH11	1.46	0.81
45:k:304:CYS:HA	45:k:326:CYS:HB3	1.61	0.81
50:q:40:ASN:HB3	50:q:43:VAL:HG23	1.60	0.81
28:T:32:ALA:CA	28:T:35:VAL:CG1	2.59	0.81
50:A1:40:ASN:HB3	50:A1:43:VAL:HG23	1.60	0.80
45:w:17:SER:OG	45:w:205:HIS:NE2	2.15	0.80
48:z:197:GLU:HG2	48:z:201:ARG:HD3	1.61	0.80
63:A5:39:CYS:SG	63:A5:53:CYS:HB3	2.22	0.80
45:k:435:ASN:OD1	48:o:226:LYS:NZ	2.12	0.80
46:l:134:ARG:NH1	50:A1:49:ARG:O	2.15	0.80
45:k:281:ASP:OD1	45:k:282:CYS:N	2.15	0.80
46:x:102:ARG:NH1	46:x:172:LEU:O	2.16	0.79
47:y:1:MET:SD	47:y:7:SER:OG	2.39	0.79
63:A5:75:ARG:HG2	63:A5:75:ARG:HH11	1.48	0.79
45:k:289:HIS:HD1	46:l:83:PHE:HD1	1.31	0.79
46:x:303:VAL:HG12	46:x:304:HIS:H	1.48	0.79
50:A1:28:LYS:HD3	50:A1:80:TRP:CZ3	2.16	0.79
54:B4:57:HIS:ND1	54:B4:60:GLU:OE2	2.16	0.79
49:p:71:MET:HG3	49:p:72:SER:H	1.46	0.79
49:p:149:ASN:N	49:p:152:ASP:O	2.10	0.79
46:l:102:ARG:NH1	46:l:172:LEU:O	2.16	0.79
50:q:77:LYS:HA	50:q:80:TRP:CE2	2.18	0.79
50:A1:77:LYS:HA	50:A1:80:TRP:CE2	2.18	0.79
47:m:74:ASN:HB2	49:p:61:SER:HA	1.64	0.79
54:B4:53:LYS:O	54:B4:57:HIS:NE2	2.15	0.79
45:k:177:LEU:HD21	45:k:182:LEU:HD21	1.63	0.78
54:u:53:LYS:O	54:u:57:HIS:NE2	2.15	0.78
62:A4:5:LYS:NZ	62:A4:6:GLY:H	1.78	0.78
18:I:108:LYS:CG	18:I:118:GLN:HE21	1.96	0.78
45:k:347:THR:O	53:t:16:ASN:ND2	2.16	0.78
46:l:303:VAL:HG12	46:l:304:HIS:H	1.48	0.78
54:u:41:ALA:O	54:u:45:HIS:N	2.14	0.78
50:A1:28:LYS:HB2	50:A1:74:ILE:HD11	1.65	0.78
47:m:361:LEU:HA	47:m:365:LEU:HD12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:57:HIS:ND1	54:u:60:GLU:OE2	2.16	0.78
47:y:207:ASN:ND2	47:y:209:THR:OG1	2.17	0.78
47:y:244:LEU:O	48:z:201:ARG:NH1	2.13	0.78
47:m:207:ASN:ND2	47:m:209:THR:OG1	2.17	0.78
63:A5:39:CYS:SG	63:A5:53:CYS:CB	2.70	0.78
45:k:17:SER:OG	45:k:205:HIS:NE2	2.15	0.78
49:A0:84:GLY:N	49:A0:100:HIS:O	2.17	0.78
50:A1:24:ALA:CB	51:A2:47:ARG:NE	2.42	0.78
28:T:33:GLY:O	28:T:60:THR:CG2	2.31	0.77
47:y:91:PHE:CZ	47:y:124:MET:HG2	2.19	0.77
28:T:54:ALA:O	28:T:58:ARG:N	2.15	0.77
46:l:83:PHE:CE2	50:A1:104:ARG:HG2	2.19	0.77
50:q:26:PHE:HB2	50:q:31:LEU:HB2	1.66	0.77
47:y:256:TYR:HB2	48:z:115:TYR:CE1	2.19	0.77
47:m:91:PHE:CZ	47:m:124:MET:HG2	2.20	0.77
45:w:281:ASP:OD1	45:w:282:CYS:N	2.15	0.77
47:y:361:LEU:HA	47:y:365:LEU:HD12	1.66	0.77
51:A2:38:LEU:HA	51:A2:41:THR:OG1	1.83	0.77
46:l:59:ASN:H	46:l:62:ASN:HB3	1.50	0.77
50:q:16:ILE:O	50:q:20:TYR:N	2.12	0.77
50:A1:28:LYS:HD2	50:A1:80:TRP:CH2	2.19	0.77
53:A3:19:PRO:O	53:A3:22:SER:OG	2.01	0.77
52:B5:44:VAL:HG22	52:B5:52:GLU:HG2	1.67	0.77
53:A3:15:ARG:HG3	53:A3:16:ASN:H	1.49	0.77
54:B4:52:TRP:HA	54:B4:55:ILE:HB	1.67	0.77
46:l:276:GLN:O	46:l:280:GLY:N	2.16	0.77
50:A1:16:ILE:O	50:A1:20:TYR:N	2.12	0.77
47:y:58:ASP:H	47:y:62:ALA:HB2	1.50	0.77
47:m:377:LEU:HD11	50:q:20:TYR:CE2	2.19	0.77
48:o:147:LEU:HB3	48:o:157:ALA:HB1	1.67	0.77
52:s:44:VAL:HG22	52:s:52:GLU:HG2	1.66	0.77
47:m:4:ILE:HG22	47:m:6:LYS:H	1.50	0.76
46:x:59:ASN:H	46:x:62:ASN:HB3	1.50	0.76
47:y:31:TRP:HA	47:y:100:ARG:HH11	1.49	0.76
57:B9:5:MET:HE3	66:B0:42:PRO:HA	1.67	0.76
28:T:32:ALA:O	28:T:35:VAL:CG2	2.34	0.76
28:T:32:ALA:O	28:T:35:VAL:HG22	1.85	0.76
47:m:31:TRP:HA	47:m:100:ARG:HH11	1.49	0.76
54:u:52:TRP:HA	54:u:55:ILE:HB	1.67	0.76
46:x:276:GLN:O	46:x:280:GLY:N	2.17	0.76
48:z:41:HIS:NE2	78:z:301:HEC:NA	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:570:GLN:O	11:B:55:THR:CB	2.34	0.76
28:T:38:ALA:HA	28:T:59:TYR:OH	1.85	0.75
38:d:31:PHE:CB	38:d:37:ARG:O	2.34	0.75
47:y:4:ILE:HG22	47:y:6:LYS:H	1.50	0.75
48:z:75:ASN:ND2	48:z:79:GLU:OE1	2.19	0.75
28:T:57:GLY:O	28:T:60:THR:N	2.19	0.75
46:l:334:GLY:HA2	46:l:337:ILE:HD12	1.69	0.75
45:w:240:GLN:NE2	45:w:242:CYS:SG	2.54	0.75
45:k:438:ARG:HH21	51:r:21:PHE:HE2	1.34	0.75
50:A1:28:LYS:CD	50:A1:80:TRP:CH2	2.69	0.75
45:k:246:ASP:OD2	51:r:10:VAL:N	2.19	0.75
48:z:224:ARG:NH2	51:A2:25:ALA:O	2.18	0.75
45:k:19:LEU:HD12	45:k:23:LEU:HB3	1.68	0.75
48:z:147:LEU:HB3	48:z:157:ALA:HB1	1.67	0.75
57:B9:59:GLN:H	57:B9:62:GLU:HG3	1.51	0.75
45:k:240:GLN:NE2	45:k:242:CYS:SG	2.54	0.75
48:o:41:HIS:NE2	78:o:301:HEC:NA	2.34	0.75
50:q:53:ASN:OD1	50:q:54:LEU:N	2.20	0.75
45:w:34:THR:HA	45:w:102:LEU:HA	1.69	0.75
48:z:129:SER:HB3	48:z:152:TYR:CZ	2.22	0.75
58:B7:187:THR:HG21	62:A4:68:THR:HG21	1.68	0.75
28:T:50:LEU:O	28:T:53:VAL:N	2.19	0.74
47:m:58:ASP:H	47:m:62:ALA:HB2	1.50	0.74
47:m:136:GLY:O	47:m:139:SER:OG	2.04	0.74
48:o:129:SER:HB3	48:o:152:TYR:CZ	2.22	0.74
45:k:348:SER:OG	53:t:17:TRP:NE1	2.20	0.74
46:l:76:THR:HG23	46:l:81:SER:HA	1.68	0.74
48:o:133:GLY:O	48:o:150:ASN:ND2	2.21	0.74
48:z:133:GLY:O	48:z:150:ASN:ND2	2.21	0.74
49:A0:79:SER:O	49:A0:81:ILE:N	2.20	0.74
11:B:55:THR:O	11:B:56:LYS:CB	2.35	0.74
47:m:162:GLU:HA	47:m:165:TRP:HB2	1.69	0.74
46:x:334:GLY:HA2	46:x:337:ILE:HD12	1.68	0.74
45:k:34:THR:HA	45:k:102:LEU:HA	1.69	0.74
47:y:136:GLY:O	47:y:139:SER:OG	2.04	0.74
45:k:142:ASP:OD1	49:p:2:HIS:ND1	2.21	0.73
45:k:216:PHE:H	45:k:219:LEU:H	1.35	0.73
57:B9:184:LEU:HD11	57:B9:211:LEU:HD21	1.69	0.73
45:w:213:GLN:OE1	45:w:214:LYS:NZ	2.17	0.73
47:y:162:GLU:HA	47:y:165:TRP:HB2	1.69	0.73
45:k:355:LEU:O	45:k:359:ASN:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:177:ARG:NH2	49:A0:62:MET:O	2.21	0.73
48:z:51:LEU:HD13	48:z:58:GLU:HA	1.70	0.73
46:l:270:ASN:HA	46:l:273:SER:HB2	1.69	0.73
53:A3:39:ARG:HG2	53:A3:39:ARG:NH1	2.01	0.73
52:s:31:VAL:HA	52:s:34:ARG:HB3	1.70	0.73
46:x:76:THR:HG23	46:x:81:SER:HA	1.68	0.73
28:T:50:LEU:O	28:T:51:GLU:C	2.31	0.73
45:w:355:LEU:O	45:w:359:ASN:N	2.19	0.73
62:A4:54:ARG:HD3	62:A4:54:ARG:N	2.04	0.73
47:m:133:LEU:HD11	47:m:182:HIS:CD2	2.24	0.73
49:A0:101:ARG:N	49:A0:131:GLU:O	2.22	0.73
47:m:208:PRO:HG2	47:m:209:THR:HG23	1.71	0.73
48:o:69:GLU:OE1	48:o:69:GLU:N	2.22	0.73
46:x:305:GLN:NE2	46:x:329:GLN:OE1	2.19	0.73
47:y:330:ALA:O	47:y:334:THR:N	2.22	0.73
45:k:57:TYR:O	45:k:61:HIS:ND1	2.22	0.73
48:o:80:MET:HG3	48:o:81:PHE:H	1.54	0.73
45:w:235:ARG:HD3	49:A0:21:SER:HA	1.71	0.73
63:A5:39:CYS:HG	63:A5:53:CYS:CB	2.01	0.73
45:k:314:TYR:N	45:k:317:THR:O	2.23	0.72
48:o:51:LEU:HD13	48:o:58:GLU:HA	1.70	0.72
50:A1:53:ASN:OD1	50:A1:54:LEU:N	2.20	0.72
44:e:68:ASP:O	44:e:75:TYR:CE2	2.42	0.72
45:w:19:LEU:HD12	45:w:23:LEU:HB3	1.69	0.72
46:x:245:ARG:HA	46:x:426:ALA:HB3	1.71	0.72
52:B5:31:VAL:HA	52:B5:34:ARG:HB3	1.70	0.72
59:A7:23:PRO:O	60:A6:66:ARG:HD3	1.89	0.72
47:m:330:ALA:O	47:m:334:THR:N	2.22	0.72
48:o:61:ALA:HA	48:o:64:LEU:HB3	1.71	0.72
45:w:158:PHE:HB2	45:w:164:ALA:HB2	1.72	0.72
46:x:270:ASN:HA	46:x:273:SER:HB2	1.69	0.72
47:y:256:TYR:HB2	48:z:115:TYR:CD1	2.24	0.72
46:l:267:ALA:O	46:l:271:ALA:N	2.23	0.72
47:y:208:PRO:HG2	47:y:209:THR:HG23	1.71	0.72
48:z:61:ALA:HA	48:z:64:LEU:HB3	1.71	0.72
47:y:133:LEU:HD11	47:y:182:HIS:CD2	2.24	0.72
46:l:245:ARG:HA	46:l:426:ALA:HB3	1.71	0.72
47:m:5:ARG:HA	47:m:8:HIS:HD2	1.53	0.72
45:w:314:TYR:N	45:w:317:THR:O	2.23	0.72
47:y:5:ARG:HA	47:y:8:HIS:HD2	1.53	0.72
48:o:53:GLY:HA2	54:u:52:TRP:CZ3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:57:TYR:O	45:w:61:HIS:ND1	2.22	0.72
31:M:35:HIS:H	31:M:39:ASP:HB3	1.53	0.71
9:3:81:THR:H	21:L:46:ASN:HD21	1.38	0.71
51:A2:37:VAL:O	51:A2:41:THR:CG2	2.35	0.71
48:z:158:ILE:HG12	48:z:160:MET:H	1.53	0.71
49:A0:71:MET:HA	49:A0:74:ILE:HD11	1.73	0.71
56:A9:176:MET:HE3	56:A9:181:THR:HG22	1.71	0.71
45:k:158:PHE:HB2	45:k:164:ALA:HB2	1.71	0.71
48:o:158:ILE:HG12	48:o:160:MET:H	1.53	0.71
46:x:97:SER:HB2	46:x:108:THR:HB	1.72	0.71
48:z:239:PRO:HB2	48:z:241:LYS:HB3	1.71	0.71
50:A1:73:GLN:HG2	51:A2:39:ARG:HH22	1.56	0.71
48:o:239:PRO:HB2	48:o:241:LYS:HB3	1.71	0.71
47:m:271:GLU:OE2	47:m:273:TYR:OH	2.08	0.71
45:w:183:THR:HA	45:w:186:LEU:HD12	1.73	0.71
46:x:267:ALA:O	46:x:271:ALA:N	2.23	0.71
50:A1:27:ASN:O	50:A1:29:LEU:N	2.24	0.71
54:u:31:PHE:O	54:u:35:PHE:N	2.20	0.71
45:k:32:GLN:NE2	45:k:34:THR:OG1	2.23	0.71
45:k:436:ARG:HH21	47:m:221:HIS:HB3	1.56	0.71
47:m:237:LEU:HD21	48:o:216:LEU:HD11	1.70	0.71
50:q:9:SER:HA	50:q:12:TRP:HB3	1.73	0.71
45:w:21:ASN:ND2	45:w:217:SER:H	1.88	0.71
46:x:148:LYS:NZ	46:x:180:ASP:OD1	2.24	0.71
47:m:45:ILE:HA	77:m:401:HEM:HMC1	1.73	0.70
50:q:52:GLU:HA	50:q:55:TYR:HB3	1.73	0.70
46:x:200:THR:HG23	46:x:203:ARG:H	1.56	0.70
47:y:244:LEU:HD12	48:z:201:ARG:HH11	1.56	0.70
1:9:131:HIS:H	1:9:189:ASN:HD21	1.38	0.70
45:w:77:LYS:O	45:w:81:SER:N	2.19	0.70
47:y:296:PHE:HA	47:y:299:LEU:HD12	1.72	0.70
50:A1:52:GLU:HA	50:A1:55:TYR:HB3	1.73	0.70
56:A9:11:ASN:HD22	56:A9:14:ASP:H	1.39	0.70
46:l:97:SER:HB2	46:l:108:THR:HB	1.73	0.70
45:w:32:GLN:NE2	45:w:34:THR:OG1	2.23	0.70
47:y:45:ILE:HA	77:y:401:HEM:HMC1	1.73	0.70
47:m:296:PHE:HA	47:m:299:LEU:HD12	1.72	0.70
48:o:127:VAL:O	48:o:131:LEU:N	2.18	0.70
52:B5:22:GLU:HA	52:B5:25:GLU:HG2	1.72	0.70
59:A7:147:LYS:HA	59:A7:147:LYS:HE3	1.72	0.70
47:y:271:GLU:OE2	47:y:273:TYR:OH	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:148:LYS:NZ	46:l:180:ASP:OD1	2.24	0.70
46:l:311:ALA:HA	46:l:324:PHE:HA	1.74	0.70
49:p:51:ALA:HA	49:p:54:VAL:HB	1.73	0.70
52:s:22:GLU:HA	52:s:25:GLU:HG2	1.73	0.70
45:w:266:ASP:OD2	45:w:413:LYS:NZ	2.25	0.70
46:x:311:ALA:HA	46:x:324:PHE:HA	1.74	0.70
45:k:17:SER:HB2	45:k:25:VAL:HB	1.73	0.70
45:k:183:THR:HA	45:k:186:LEU:HD12	1.73	0.70
45:k:309:THR:HA	45:k:322:ALA:HA	1.74	0.70
46:x:338:LYS:HA	46:x:341:TYR:HB3	1.73	0.70
49:A0:77:LYS:CB	49:A0:78:LEU:HA	2.21	0.70
45:k:15:GLN:HG3	45:k:205:HIS:HB2	1.74	0.69
46:l:59:ASN:OD1	46:l:60:SER:N	2.24	0.69
58:B7:156:ARG:HH11	58:B7:156:ARG:HG3	1.56	0.69
45:k:77:LYS:O	45:k:81:SER:N	2.19	0.69
46:l:338:LYS:HA	46:l:341:TYR:HB3	1.73	0.69
50:q:95:LYS:HA	50:q:98:ILE:HD12	1.74	0.69
45:w:15:GLN:HG3	45:w:205:HIS:HB2	1.74	0.69
54:u:48:GLU:OE1	54:u:54:HIS:NE2	2.25	0.69
45:k:431:LEU:HD12	45:k:432:PRO:HD2	1.75	0.69
50:A1:28:LYS:HB3	50:A1:80:TRP:CE2	2.27	0.69
45:k:330:SER:OG	45:k:333:ASP:OD2	2.10	0.69
46:l:40:ASN:OD1	46:l:41:TYR:N	2.25	0.69
48:z:61:ALA:O	48:z:65:ALA:N	2.20	0.69
50:A1:9:SER:HA	50:A1:12:TRP:HB3	1.73	0.69
45:k:127:ILE:HG22	45:k:131:ARG:HH12	1.57	0.69
48:o:23:HIS:CD2	54:u:51:LEU:HA	2.27	0.69
58:B7:12:ASN:HD22	65:B8:20:VAL:H	1.39	0.69
45:w:412:SER:HB3	54:B4:15:ARG:HH22	1.58	0.69
56:A9:69:MET:HE2	56:A9:70:VAL:HG23	1.74	0.69
45:k:266:ASP:OD2	45:k:413:LYS:NZ	2.25	0.69
45:k:277:ILE:O	45:k:292:SER:OG	2.10	0.69
49:p:62:MET:O	47:y:177:ARG:NH2	2.25	0.69
46:x:40:ASN:OD1	46:x:41:TYR:N	2.25	0.69
47:y:77:TRP:CD2	48:z:197:GLU:HG3	2.28	0.69
57:B9:13:THR:HB	57:B9:168:LEU:HD23	1.73	0.69
58:B7:154:GLY:HA2	61:B2:6:VAL:HG22	1.75	0.69
8:l:41:GLY:HA3	8:l:44:GLY:H	1.57	0.69
21:L:59:ASP:HB3	25:Q:130:LYS:HD2	1.75	0.69
48:o:61:ALA:O	48:o:65:ALA:N	2.20	0.69
49:p:75:GLU:HG2	49:p:76:ILE:C	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:17:SER:HB2	45:w:25:VAL:HB	1.73	0.69
54:B4:48:GLU:OE1	54:B4:54:HIS:NE2	2.25	0.69
45:k:356:ARG:O	45:k:360:LEU:N	2.23	0.69
46:l:200:THR:HG23	46:l:203:ARG:H	1.56	0.69
45:w:87:ASN:OD1	45:w:88:ALA:N	2.25	0.69
45:w:294:LEU:HD21	45:w:337:VAL:HG12	1.74	0.69
50:A1:45:GLU:OE2	50:A1:49:ARG:NH2	2.26	0.69
45:k:236:PHE:HB2	49:p:25:SER:HB2	1.74	0.68
45:k:294:LEU:HD21	45:k:337:VAL:HG12	1.74	0.68
45:w:431:LEU:HD12	45:w:432:PRO:HD2	1.75	0.68
47:y:95:TYR:O	47:y:99:GLY:N	2.25	0.68
50:q:33:ARG:NH1	50:q:91:GLU:OE2	2.21	0.68
45:w:348:SER:OG	53:A3:17:TRP:NE1	2.26	0.68
45:w:356:ARG:O	45:w:360:LEU:N	2.23	0.68
45:w:403:ASP:OD1	45:w:404:ALA:N	2.26	0.68
53:A3:45:VAL:HG11	54:B4:30:PHE:CD1	2.28	0.68
55:B3:70:LEU:HD12	55:B3:71:ASN:H	1.59	0.68
28:T:62:THR:CG2	28:T:104:ARG:NH1	2.55	0.68
52:s:17:LEU:HA	52:s:73:LEU:HD22	1.75	0.68
45:k:216:PHE:N	45:k:219:LEU:H	1.92	0.68
46:l:214:PRO:O	46:l:218:GLN:N	2.23	0.68
48:o:32:VAL:O	48:o:36:VAL:N	2.21	0.68
50:q:26:PHE:HA	50:q:29:LEU:HB2	1.75	0.68
45:w:309:THR:HA	45:w:322:ALA:HA	1.74	0.68
45:k:87:ASN:OD1	45:k:88:ALA:N	2.25	0.68
45:k:131:ARG:HE	45:k:175:ARG:HA	1.58	0.68
45:w:127:ILE:HG22	45:w:131:ARG:HH12	1.57	0.68
46:x:101:THR:HG23	46:x:103:GLU:H	1.59	0.68
51:A2:19:SER:HB3	51:A2:22:GLU:HG2	1.76	0.68
54:B4:31:PHE:O	54:B4:35:PHE:N	2.20	0.68
45:k:403:ASP:OD1	45:k:404:ALA:N	2.26	0.68
47:m:95:TYR:O	47:m:99:GLY:N	2.25	0.68
51:r:19:SER:HB3	51:r:22:GLU:HG2	1.76	0.68
46:x:214:PRO:O	46:x:218:GLN:N	2.23	0.68
50:A1:28:LYS:CD	50:A1:80:TRP:CZ3	2.77	0.68
52:B5:17:LEU:HA	52:B5:73:LEU:HD22	1.75	0.68
67:B1:19:TRP:HZ2	68:A8:14:GLU:HG2	1.59	0.68
8:l:17:VAL:HG21	8:l:225:MET:SD	2.33	0.68
46:l:101:THR:HG23	46:l:103:GLU:H	1.59	0.68
28:T:38:ALA:HA	28:T:59:TYR:HH	1.59	0.68
12:C:132:TYR:HB2	12:C:145:VAL:HB	1.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:170:LEU:O	26:R:328:ILE:HD11	1.94	0.68
46:l:155:PRO:O	46:l:159:VAL:N	2.27	0.68
46:x:155:PRO:O	46:x:159:VAL:N	2.27	0.68
49:A0:79:SER:C	49:A0:81:ILE:H	2.02	0.67
28:T:62:THR:HG21	28:T:104:ARG:HD2	1.73	0.67
46:l:247:GLN:HG3	46:x:181:TYR:OH	1.94	0.67
50:q:73:GLN:HG2	51:r:39:ARG:HH22	1.58	0.67
47:y:7:SER:HA	47:y:13:ILE:HG13	1.76	0.67
47:y:373:GLU:O	47:y:377:LEU:N	2.26	0.67
49:A0:11:SER:O	49:A0:14:ARG:N	2.27	0.67
49:A0:155:GLY:HA3	49:A0:166:ASP:C	2.18	0.67
50:A1:95:LYS:HA	50:A1:98:ILE:HD12	1.74	0.67
54:B4:21:ALA:HA	54:B4:24:ILE:HD12	1.77	0.67
45:k:327:ASP:OD1	45:k:328:HIS:N	2.27	0.67
45:w:46:ARG:NH2	45:w:232:SER:O	2.28	0.67
48:z:197:GLU:OE1	48:z:197:GLU:N	2.27	0.67
5:4:355:MET:HA	5:4:358:TRP:HD1	1.57	0.67
45:k:354:VAL:O	45:k:358:LYS:N	2.25	0.67
47:m:5:ARG:HA	47:m:8:HIS:CD2	2.29	0.67
45:w:259:GLY:N	45:w:318:GLY:O	2.28	0.67
48:o:11:PRO:HA	48:o:15:ARG:HD2	1.75	0.67
54:u:14:PHE:HA	54:u:20:PHE:HB2	1.77	0.67
54:u:21:ALA:HA	54:u:24:ILE:HD12	1.77	0.67
45:w:281:ASP:HA	45:w:306:SER:HA	1.77	0.67
47:y:5:ARG:HA	47:y:8:HIS:CD2	2.29	0.67
56:A9:273:MET:HG3	56:A9:319:LYS:HZ1	1.57	0.67
46:l:46:ARG:HH11	46:l:379:LEU:HD22	1.59	0.67
45:w:131:ARG:HE	45:w:175:ARG:HA	1.58	0.67
46:x:272:PHE:HA	46:x:275:LEU:HB3	1.77	0.67
54:B4:14:PHE:HA	54:B4:20:PHE:HB2	1.77	0.67
47:m:256:TYR:OH	48:o:118:ARG:NH2	2.27	0.67
48:o:33:TYR:CD1	48:o:37:CYS:HB2	2.30	0.67
46:x:304:HIS:CD2	46:x:305:GLN:HB3	2.30	0.67
52:B5:44:VAL:O	52:B5:48:SER:N	2.27	0.67
60:A6:43:PRO:HB2	60:A6:48:ILE:HD11	1.76	0.67
45:k:220:SER:HB2	45:k:222:THR:HG22	1.77	0.67
45:w:354:VAL:O	45:w:358:LYS:N	2.25	0.67
46:x:59:ASN:OD1	46:x:60:SER:N	2.24	0.67
56:A9:151:HIS:O	56:A9:155:VAL:HG23	1.95	0.67
45:k:46:ARG:NH2	45:k:232:SER:O	2.28	0.67
45:w:360:LEU:O	45:w:364:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:11:PRO:HA	48:z:15:ARG:HD2	1.75	0.67
48:z:127:VAL:O	48:z:131:LEU:N	2.18	0.67
63:A5:38:ARG:HG2	63:A5:85:ILE:HG23	1.77	0.67
28:T:82:GLU:HG3	28:T:84:PRO:HD2	1.76	0.66
45:k:215:HIS:CB	45:k:216:PHE:HB2	2.25	0.66
49:p:25:SER:O	49:p:29:SER:OG	2.12	0.66
45:w:329:MET:HE3	51:A2:2:ARG:NE	2.10	0.66
45:k:259:GLY:N	45:k:318:GLY:O	2.28	0.66
47:m:373:GLU:O	47:m:377:LEU:N	2.26	0.66
48:o:225:HIS:O	48:o:228:SER:OG	2.13	0.66
28:T:45:THR:C	28:T:47:THR:H	2.03	0.66
48:o:11:PRO:HB2	52:s:74:PHE:CE2	2.29	0.66
57:B9:186:SER:HB3	57:B9:213:LEU:HD22	1.76	0.66
58:B7:209:ILE:O	58:B7:213:THR:HG23	1.95	0.66
59:A7:24:LEU:H	60:A6:34:ASN:HD21	1.44	0.66
45:k:348:SER:HG	53:t:17:TRP:NE1	1.92	0.66
52:s:44:VAL:O	52:s:48:SER:N	2.27	0.66
47:m:7:SER:HA	47:m:13:ILE:HG13	1.76	0.66
46:x:74:SER:O	46:x:82:SER:OG	2.13	0.66
45:k:217:SER:N	45:k:218:GLY:HA3	2.09	0.66
46:l:272:PHE:HA	46:l:275:LEU:HB3	1.77	0.66
77:m:402:HEM:HBC2	77:m:402:HEM:HMC2	1.75	0.66
53:A3:47:TYR:HB2	54:B4:33:ARG:NH2	2.10	0.66
4:2:109:ALA:HB2	4:2:161:SER:HA	1.76	0.66
26:R:170:LEU:O	26:R:328:ILE:CD1	2.44	0.66
26:R:238:GLN:HB3	26:R:267:GLY:HA3	1.77	0.66
45:k:233:PRO:O	49:p:22:THR:HA	1.96	0.66
45:k:281:ASP:HA	45:k:306:SER:HA	1.77	0.66
46:l:74:SER:O	46:l:82:SER:OG	2.13	0.66
46:x:46:ARG:HH11	46:x:379:LEU:HD22	1.59	0.66
48:z:33:TYR:CD1	48:z:37:CYS:HB2	2.30	0.66
3:6:267:THR:O	3:6:274:GLN:NE2	2.29	0.66
47:m:100:ARG:NH2	77:m:402:HEM:HBD1	2.11	0.66
45:w:192:ALA:H	45:w:218:GLY:HA3	1.60	0.66
45:w:327:ASP:OD1	45:w:328:HIS:N	2.27	0.65
28:T:41:VAL:CG1	28:T:59:TYR:HH	2.05	0.65
44:e:68:ASP:O	44:e:75:TYR:HE2	1.80	0.65
45:w:32:GLN:HG2	45:w:34:THR:H	1.61	0.65
54:B4:9:LEU:HD11	54:B4:13:LEU:HD12	1.77	0.65
56:A9:298:ASP:HB2	56:A9:301:THR:HG23	1.77	0.65
45:k:289:HIS:ND1	46:l:83:PHE:HD1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:100:ARG:NH2	77:y:402:HEM:HBD1	2.11	0.65
52:B5:12:GLU:O	52:B5:13:LEU:HB2	1.96	0.65
18:I:108:LYS:HG2	18:I:118:GLN:NE2	2.06	0.65
46:l:338:LYS:HZ3	46:l:439:LEU:HD23	1.61	0.65
47:m:74:ASN:ND2	49:p:60:SER:O	2.27	0.65
47:m:315:MET:HG2	47:m:318:ARG:HH21	1.61	0.65
45:w:330:SER:OG	45:w:333:ASP:OD2	2.11	0.65
57:B9:120:SER:OG	57:B9:138:VAL:HG21	1.97	0.65
58:B7:101:PHE:HZ	58:B7:260:GLY:HA3	1.61	0.65
48:o:197:GLU:OE1	48:o:197:GLU:N	2.27	0.65
52:B5:21:ARG:HH11	52:B5:65:ARG:NH2	1.95	0.65
58:B7:160:LEU:HD13	58:B7:222:GLN:HG2	1.78	0.65
12:C:170:ARG:HD3	12:C:187:ARG:HB2	1.79	0.65
45:k:46:ARG:HA	45:k:162:PRO:HB2	1.78	0.65
45:k:138:LEU:HD11	45:k:174:VAL:HG21	1.79	0.65
46:l:354:ASN:ND2	46:l:407:ASP:OD2	2.30	0.65
49:p:83:GLU:HA	49:p:138:VAL:HA	1.79	0.65
50:q:45:GLU:OE2	50:q:49:ARG:NH2	2.26	0.65
52:s:12:GLU:HG2	52:s:13:LEU:H	1.62	0.65
45:w:191:LYS:HD2	45:w:219:LEU:HB3	1.77	0.65
52:B5:66:ASP:O	52:B5:70:ALA:N	2.30	0.65
63:A5:39:CYS:HG	63:A5:53:CYS:HG	0.77	0.65
46:l:83:PHE:CZ	50:A1:104:ARG:HG2	2.32	0.65
47:m:100:ARG:NH2	77:m:402:HEM:O1A	2.28	0.65
54:u:9:LEU:HD11	54:u:13:LEU:HD12	1.77	0.65
47:m:138:MET:N	47:m:255:ASN:HD22	1.92	0.65
47:m:207:ASN:HD21	47:m:211:ILE:H	1.43	0.65
45:w:277:ILE:O	45:w:292:SER:OG	2.10	0.65
49:A0:2:HIS:CG	49:A0:3:THR:H	2.15	0.65
53:A3:42:LEU:O	53:A3:43:ASP:C	2.40	0.65
45:k:360:LEU:O	45:k:364:ALA:N	2.27	0.65
46:l:305:GLN:HB3	46:l:306:PRO:HD3	1.79	0.65
47:m:66:VAL:HA	47:m:69:ILE:HD12	1.79	0.65
45:w:235:ARG:NH1	49:A0:21:SER:OG	2.30	0.65
48:z:32:VAL:O	48:z:36:VAL:N	2.21	0.65
13:D:99:MET:HG2	13:D:106:MET:HB2	1.79	0.64
46:l:182:ARG:HH11	46:l:185:LYS:HE2	1.61	0.64
50:q:21:TYR:CE2	50:q:83:TYR:HA	2.31	0.64
47:y:66:VAL:HA	47:y:69:ILE:HD12	1.79	0.64
22:N:67:LYS:HG3	22:N:71:ARG:HH11	1.61	0.64
49:p:13:TYR:HA	51:r:27:PRO:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:r:63:THR:O	51:r:67:GLU:HG3	1.97	0.64
55:v:65:VAL:HA	55:v:78:TYR:HA	1.79	0.64
47:y:164:ILE:O	47:y:177:ARG:NH1	2.31	0.64
56:A9:187:SER:CB	56:A9:277:MET:HE1	2.28	0.64
10:A:343:GLY:H	10:A:549:GLY:HA2	1.61	0.64
28:T:85:ASP:HA	28:T:89:ASN:HD22	1.63	0.64
45:k:32:GLN:HG2	45:k:34:THR:H	1.62	0.64
53:t:20:THR:HA	53:t:23:LEU:HD12	1.80	0.64
45:w:46:ARG:HA	45:w:162:PRO:HB2	1.78	0.64
46:x:182:ARG:HH11	46:x:185:LYS:HE2	1.61	0.64
46:x:354:ASN:ND2	46:x:407:ASP:OD2	2.30	0.64
51:A2:63:THR:O	51:A2:67:GLU:HG3	1.97	0.64
10:A:367:CYS:SG	10:A:368:THR:N	2.69	0.64
46:l:58:GLU:OE2	46:l:66:SER:N	2.30	0.64
46:l:286:LYS:HG2	46:l:287:ARG:HG3	1.80	0.64
47:y:315:MET:HG2	47:y:318:ARG:HH21	1.62	0.64
56:A9:84:PRO:HG3	56:A9:92:MET:HE3	1.80	0.64
56:A9:195:LEU:HD23	56:A9:245:ILE:HD13	1.79	0.64
67:B1:45:LEU:HD21	68:A8:40:TYR:HA	1.78	0.64
28:T:62:THR:HG23	28:T:104:ARG:NE	2.12	0.64
46:l:272:PHE:O	46:l:276:GLN:N	2.28	0.64
45:w:291:SER:OG	46:x:90:GLU:OE1	2.12	0.64
47:m:164:ILE:O	47:m:177:ARG:NH1	2.31	0.64
50:q:25:GLY:O	50:q:29:LEU:N	2.29	0.64
52:s:21:ARG:HH11	52:s:65:ARG:NH2	1.95	0.64
46:x:286:LYS:HG2	46:x:287:ARG:HG3	1.80	0.64
46:x:312:PHE:N	46:x:323:GLY:O	2.26	0.64
45:w:173:ASN:HA	45:w:176:LYS:HB2	1.80	0.64
46:x:325:TYR:HB3	55:B3:57:GLY:N	2.13	0.64
47:y:100:ARG:NH2	77:y:402:HEM:O1A	2.28	0.64
56:A9:172:LYS:HB2	56:A9:172:LYS:NZ	2.12	0.64
8:l:169:GLN:HE21	8:l:174:LEU:HD13	1.62	0.64
28:T:50:LEU:C	28:T:52:GLY:N	2.56	0.64
45:k:426:GLY:HA2	45:k:428:ILE:H	1.61	0.64
45:w:210:ASP:OD1	45:w:211:LEU:N	2.30	0.64
45:w:426:GLY:HA2	45:w:428:ILE:H	1.61	0.64
46:x:58:GLU:OE2	46:x:66:SER:N	2.30	0.64
47:y:33:PHE:HA	47:y:36:LEU:HB2	1.79	0.64
18:I:106:GLU:HG3	18:I:106:GLU:O	1.97	0.64
40:h:141:CYS:HA	43:g:162:ARG:HD3	1.79	0.64
48:o:69:GLU:HG2	48:o:84:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:138:LEU:HD11	45:w:174:VAL:HG21	1.79	0.64
47:y:207:ASN:HD21	47:y:211:ILE:H	1.43	0.64
50:A1:97:VAL:HA	50:A1:100:GLU:CD	2.23	0.64
45:k:210:ASP:OD1	45:k:211:LEU:N	2.30	0.63
49:p:15:ARG:NH2	49:p:32:ARG:HG3	2.12	0.63
46:x:96:LEU:O	55:B3:70:LEU:HD13	1.98	0.63
45:k:93:GLU:OE1	45:k:94:HIS:NE2	2.32	0.63
17:H:82:GLN:HE21	30:V:98:MET:HB2	1.64	0.63
52:s:66:ASP:O	52:s:70:ALA:N	2.30	0.63
48:z:31:GLN:O	48:z:35:GLN:N	2.31	0.63
26:R:92:MET:HG3	26:R:95:ARG:HH21	1.63	0.63
47:m:44:GLN:OE1	47:m:83:HIS:ND1	2.32	0.63
50:q:110:LYS:HE3	53:A3:11:ARG:HB3	1.79	0.63
47:y:138:MET:N	47:y:255:ASN:HD22	1.92	0.63
47:y:237:LEU:O	47:y:241:LEU:N	2.32	0.63
50:A1:74:ILE:HG22	51:A2:39:ARG:HH11	1.64	0.63
47:m:33:PHE:HA	47:m:36:LEU:HB2	1.80	0.63
45:w:23:LEU:HB2	45:w:217:SER:HB3	1.81	0.63
45:w:145:MET:HE3	45:w:252:HIS:HE1	1.63	0.63
45:w:213:GLN:O	45:w:215:HIS:ND1	2.23	0.63
5:4:52:PHE:O	36:b:135:ARG:NH1	2.31	0.63
7:8:211:ALA:HB2	7:8:223:PRO:HB3	1.80	0.63
27:S:71:LEU:HD23	27:S:146:VAL:HG13	1.79	0.63
49:p:71:MET:O	49:p:72:SER:OG	2.11	0.63
46:x:113:ARG:NH2	46:x:210:GLY:O	2.32	0.63
47:y:44:GLN:OE1	47:y:83:HIS:ND1	2.32	0.63
47:y:67:THR:O	47:y:71:ARG:HG2	1.99	0.63
50:A1:68:LEU:O	50:A1:72:GLN:N	2.32	0.63
11:B:182:ASN:HD22	11:B:403:PRO:HG2	1.63	0.63
46:l:67:HIS:ND1	46:l:177:TYR:HA	2.13	0.63
48:o:228:SER:HB2	51:r:23:GLN:HE21	1.62	0.63
46:x:39:GLU:HG3	46:x:210:GLY:O	1.99	0.63
50:A1:21:TYR:OH	50:A1:27:ASN:CB	2.47	0.63
50:A1:33:ARG:NH1	50:A1:91:GLU:OE2	2.21	0.63
59:A7:16:TYR:CE1	59:A7:25:PRO:HG3	2.34	0.63
45:k:348:SER:HG	53:t:17:TRP:CD1	2.17	0.63
47:m:344:GLU:OE1	51:r:66:PHE:HE1	1.82	0.63
49:p:126:ARG:HA	49:p:135:LEU:HA	1.78	0.63
45:w:436:ARG:O	45:w:440:GLY:N	2.32	0.63
49:A0:150:ALA:N	49:A0:155:GLY:O	2.32	0.63
3:6:578:THR:HA	3:6:581:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:114:GLU:HG3	42:j:115:GLU:HG2	1.81	0.62
45:k:173:ASN:HA	45:k:176:LYS:HB2	1.80	0.62
49:p:30:GLU:HG3	54:u:7:ALA:HB1	1.81	0.62
48:z:63:ALA:HA	48:z:66:GLU:CD	2.24	0.62
60:A6:82:TYR:HB3	60:A6:83:PRO:HD3	1.81	0.62
9:3:42:ASP:N	9:3:43:PRO:HD3	2.14	0.62
46:l:39:GLU:HG3	46:l:210:GLY:O	1.99	0.62
50:q:39:GLU:N	50:q:39:GLU:OE1	2.31	0.62
50:q:68:LEU:O	50:q:72:GLN:N	2.32	0.62
50:q:97:VAL:HA	50:q:100:GLU:CD	2.23	0.62
46:x:325:TYR:OH	46:x:327:ILE:HD11	1.99	0.62
47:y:72:ASP:OD1	48:z:49:ARG:NH1	2.32	0.62
47:y:74:ASN:HB2	49:A0:61:SER:HA	1.79	0.62
48:z:225:HIS:O	48:z:228:SER:OG	2.13	0.62
50:A1:39:GLU:OE1	50:A1:39:GLU:N	2.31	0.62
56:A9:128:VAL:HG22	56:A9:128:VAL:O	1.99	0.62
45:k:436:ARG:O	45:k:440:GLY:N	2.32	0.62
46:x:227:ARG:HB3	46:x:228:GLY:HA3	1.81	0.62
48:z:215:LEU:HA	48:z:218:LEU:HD12	1.81	0.62
56:A9:92:MET:HE2	56:A9:167:THR:HG21	1.82	0.62
7:8:420:GLU:H	7:8:422:HIS:HD2	1.47	0.62
38:d:25:PHE:HD2	38:d:40:VAL:CB	2.09	0.62
48:o:72:ASP:OD1	48:o:73:GLY:N	2.33	0.62
45:w:93:GLU:OE1	45:w:94:HIS:NE2	2.32	0.62
56:A9:11:ASN:HD21	56:A9:13:LYS:HB2	1.64	0.62
45:k:145:MET:HE3	45:k:252:HIS:HE1	1.63	0.62
46:l:325:TYR:OH	46:l:327:ILE:HD11	1.99	0.62
47:m:67:THR:O	47:m:71:ARG:HG2	1.99	0.62
47:m:377:LEU:HD11	50:q:20:TYR:HE2	1.64	0.62
49:p:91:TRP:C	49:p:93:GLY:H	2.08	0.62
50:q:15:GLY:O	50:q:19:TRP:N	2.22	0.62
50:A1:28:LYS:HD2	50:A1:80:TRP:CZ2	2.35	0.62
54:B4:3:PRO:HG2	54:B4:8:ARG:HE	1.64	0.62
45:k:152:TYR:O	45:k:156:THR:OG1	2.14	0.62
47:m:237:LEU:O	47:m:241:LEU:N	2.31	0.62
47:m:272:TRP:NE1	47:m:273:TYR:HD2	1.98	0.62
68:A8:13:LYS:H	68:A8:13:LYS:HD3	1.65	0.62
45:k:262:TRP:N	45:k:314:TYR:O	2.32	0.62
46:l:329:GLN:H	46:l:332:SER:HB2	1.65	0.62
45:w:262:TRP:N	45:w:314:TYR:O	2.32	0.62
45:k:403:ASP:HB3	45:k:406:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:315:SER:HA	46:l:320:GLY:HA2	1.82	0.62
45:w:131:ARG:NE	45:w:175:ARG:HA	2.15	0.62
50:A1:28:LYS:HD3	50:A1:80:TRP:CH2	2.35	0.62
4:2:68:MET:HE2	6:5:37:MET:HE2	1.80	0.62
10:A:81:GLU:HG3	10:A:108:LYS:HB3	1.81	0.62
45:k:235:ARG:NH1	49:p:21:SER:OG	2.33	0.62
48:o:31:GLN:O	48:o:35:GLN:N	2.31	0.62
45:w:353:GLU:HB2	45:w:356:ARG:HH21	1.64	0.62
46:l:113:ARG:NH2	46:l:210:GLY:O	2.32	0.62
48:o:237:TYR:HB2	50:q:60:PHE:CE1	2.34	0.62
3:6:69:LEU:HD23	5:4:451:PRO:HG2	1.82	0.61
8:1:17:VAL:HG21	8:1:225:MET:HE1	0.63	0.61
44:e:67:ASP:O	44:e:68:ASP:C	2.41	0.61
48:o:63:ALA:HA	48:o:66:GLU:CD	2.24	0.61
46:x:67:HIS:ND1	46:x:177:TYR:HA	2.13	0.61
46:x:133:ARG:O	46:x:137:VAL:N	2.28	0.61
7:8:167:SER:HA	15:F:88:LEU:HD21	1.82	0.61
36:b:160:MET:HE2	36:b:166:GLY:H	1.64	0.61
45:k:294:LEU:HD11	45:k:338:LEU:HA	1.83	0.61
46:l:59:ASN:N	46:l:62:ASN:HB3	2.15	0.61
51:r:62:GLY:O	51:r:66:PHE:N	2.25	0.61
46:x:59:ASN:N	46:x:62:ASN:HB3	2.15	0.61
47:y:100:ARG:HH21	77:y:402:HEM:HBD1	1.64	0.61
26:R:201:ILE:HG23	26:R:203:PRO:HD3	1.82	0.61
29:U:29:ARG:HH12	29:U:63:ILE:HG23	1.66	0.61
50:q:87:LYS:HG3	50:q:89:TYR:HD2	1.65	0.61
49:A0:10:PHE:CE2	51:A2:18:LEU:HD21	2.35	0.61
50:A1:24:ALA:HB2	51:A2:47:ARG:HE	1.65	0.61
8:1:222:LEU:O	8:1:226:ALA:N	2.22	0.61
45:k:131:ARG:NE	45:k:175:ARG:HA	2.15	0.61
46:l:312:PHE:N	46:l:323:GLY:O	2.27	0.61
48:o:238:ARG:CZ	49:p:5:ILE:HG22	2.31	0.61
46:x:272:PHE:O	46:x:276:GLN:N	2.28	0.61
46:x:329:GLN:H	46:x:332:SER:HB2	1.65	0.61
27:S:219:SER:HA	27:S:222:LEU:HB2	1.81	0.61
39:f:16:VAL:HG22	39:f:64:LEU:HD21	1.83	0.61
48:o:143:LEU:HD11	48:o:149:PHE:HB2	1.81	0.61
49:p:75:GLU:HG2	49:p:76:ILE:HA	1.82	0.61
45:w:403:ASP:HB3	45:w:406:VAL:HG23	1.82	0.61
46:x:250:ASP:OD1	46:x:251:SER:N	2.34	0.61
48:z:33:TYR:HD1	48:z:37:CYS:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:143:LEU:HD11	48:z:149:PHE:HB2	1.81	0.61
49:A0:20:ASP:HB3	49:A0:23:LYS:HG2	1.83	0.61
51:A2:28:HIS:HB3	51:A2:31:SER:OG	2.00	0.61
53:A3:18:VAL:HB	53:A3:19:PRO:HD3	1.82	0.61
61:B2:13:ALA:O	61:B2:18:ARG:HD2	2.00	0.61
10:A:124:HIS:NE2	74:A:801:SF4:S3	2.74	0.61
46:l:197:ASN:O	46:l:230:LEU:HB3	2.00	0.61
45:w:128:GLU:OE2	45:w:131:ARG:NH1	2.33	0.61
46:x:315:SER:HA	46:x:320:GLY:HA2	1.82	0.61
46:l:200:THR:OG1	46:l:228:GLY:N	2.29	0.61
50:q:13:LEU:O	50:q:16:ILE:HG12	2.01	0.61
47:y:127:ALA:O	47:y:131:TYR:N	2.31	0.61
57:B9:16:ILE:HD12	57:B9:17:MET:N	2.15	0.61
45:k:353:GLU:HB2	45:k:356:ARG:HH21	1.64	0.61
47:m:100:ARG:HH21	77:m:402:HEM:HBD1	1.64	0.61
48:o:81:PHE:CE1	48:o:84:PRO:HA	2.36	0.61
53:t:24:TRP:O	53:t:28:GLY:N	2.23	0.61
47:y:272:TRP:NE1	47:y:273:TYR:HD2	1.98	0.61
50:A1:61:ARG:O	50:A1:65:ALA:N	2.31	0.61
22:N:38:ILE:O	22:N:45:ARG:NH2	2.34	0.61
45:k:128:GLU:OE2	45:k:131:ARG:NH1	2.33	0.61
49:p:45:VAL:HG22	54:u:24:ILE:HG23	1.83	0.61
46:x:290:ASN:O	46:x:297:GLN:NE2	2.32	0.61
58:B7:148:HIS:O	58:B7:152:MET:HG3	2.01	0.61
28:T:41:VAL:HG12	28:T:59:TYR:OH	1.94	0.60
43:g:77:CYS:SG	43:g:78:GLN:N	2.74	0.60
77:m:401:HEM:HMC1	77:m:401:HEM:HBC2	1.83	0.60
51:r:28:HIS:HB3	51:r:31:SER:OG	2.00	0.60
54:u:3:PRO:HG2	54:u:8:ARG:HE	1.65	0.60
47:y:10:LEU:HD12	47:y:13:ILE:HD12	1.83	0.60
56:A9:92:MET:CE	56:A9:167:THR:HG21	2.31	0.60
58:B7:154:GLY:HA2	61:B2:6:VAL:CG2	2.30	0.60
65:B8:3:ASN:HD22	65:B8:3:ASN:C	2.08	0.60
7:8:98:LYS:NZ	73:8:501:FMN:O3P	2.34	0.60
10:A:501:ARG:NH2	10:A:509:ASP:OD1	2.34	0.60
12:C:112:SER:HB2	12:C:135:LEU:HB3	1.83	0.60
48:o:215:LEU:HA	48:o:218:LEU:HD12	1.82	0.60
50:A1:40:ASN:OD1	50:A1:41:ASP:N	2.34	0.60
57:B9:59:GLN:HA	57:B9:62:GLU:HB2	1.83	0.60
57:B9:226:MET:O	57:B9:227:LEU:HB2	2.01	0.60
68:A8:28:LEU:HB2	68:A8:29:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:382:CYS:HB3	7:8:384:PRO:HD2	1.83	0.60
48:o:31:GLN:O	48:o:35:GLN:HG2	2.01	0.60
49:A0:91:TRP:C	49:A0:93:GLY:H	2.09	0.60
57:B9:122:MET:HB2	57:B9:208:PRO:HD2	1.81	0.60
10:A:127:ASP:OD2	10:A:175:ARG:NH1	2.34	0.60
30:V:48:TRP:O	30:V:52:LYS:NZ	2.34	0.60
46:x:337:ILE:O	46:x:341:TYR:N	2.30	0.60
50:A1:87:LYS:HG3	50:A1:89:TYR:HD2	1.65	0.60
53:A3:32:LEU:HD11	53:A3:37:ASP:CB	2.31	0.60
54:B4:58:LYS:HG3	54:B4:59:TYR:H	1.67	0.60
12:C:90:ILE:HD12	12:C:145:VAL:HG13	1.83	0.60
48:o:33:TYR:HD1	48:o:37:CYS:HB2	1.66	0.60
49:p:16:PRO:HA	49:p:19:LEU:HB2	1.82	0.60
45:w:152:TYR:O	45:w:156:THR:OG1	2.14	0.60
48:z:138:PRO:O	48:z:141:VAL:HG12	2.01	0.60
46:l:250:ASP:OD1	46:l:251:SER:N	2.34	0.60
50:q:40:ASN:OD1	50:q:41:ASP:N	2.34	0.60
53:t:15:ARG:NH1	53:t:16:ASN:OD1	2.35	0.60
48:z:197:GLU:O	48:z:201:ARG:N	2.29	0.60
49:A0:9:ASP:OD1	49:A0:14:ARG:NH1	2.28	0.60
61:B2:62:CYS:SG	61:B2:84:SER:OG	2.60	0.60
63:A5:57:ARG:HH11	63:A5:57:ARG:HB3	1.64	0.60
7:8:297:LYS:NZ	7:8:310:GLY:O	2.34	0.60
26:R:178:SER:H	26:R:182:ARG:H	1.50	0.60
45:w:23:LEU:HB2	45:w:217:SER:CB	2.32	0.60
46:x:331:ALA:HA	46:x:432:HIS:ND1	2.17	0.60
58:B7:119:THR:O	62:A4:52:HIS:HE1	1.85	0.60
3:6:583:LEU:H	6:5:93:LEU:HD22	1.67	0.60
46:l:337:ILE:O	46:l:341:TYR:N	2.30	0.60
47:m:10:LEU:HD12	47:m:13:ILE:HD12	1.83	0.60
77:m:402:HEM:HMB1	77:m:402:HEM:HBB2	1.84	0.60
1:9:222:ARG:HD3	1:9:228:ALA:HB2	1.84	0.60
45:k:350:THR:N	45:k:353:GLU:OE2	2.34	0.60
47:m:138:MET:HE1	47:m:268:ILE:HA	1.84	0.60
48:o:138:PRO:O	48:o:141:VAL:HG12	2.01	0.60
51:r:44:CYS:O	51:r:47:ARG:N	2.31	0.60
54:u:12:LEU:HG	54:u:13:LEU:HG	1.83	0.60
45:w:294:LEU:HD11	45:w:338:LEU:HA	1.82	0.60
45:w:350:THR:N	45:w:353:GLU:OE2	2.34	0.60
48:z:167:GLU:HA	48:z:177:ALA:HB3	1.84	0.60
50:A1:13:LEU:O	50:A1:16:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:21:TYR:OH	50:A1:27:ASN:ND2	2.33	0.60
54:B4:12:LEU:HG	54:B4:13:LEU:HG	1.83	0.60
1:9:118:PHE:HB2	7:8:220:GLN:HE21	1.67	0.60
47:m:312:GLN:HE21	47:m:318:ARG:HG3	1.67	0.60
47:m:344:GLU:O	47:m:348:ILE:HG13	2.02	0.60
50:q:101:ARG:HA	50:q:104:ARG:HE	1.67	0.60
54:u:55:ILE:HG23	54:u:58:LYS:HE3	1.84	0.60
54:u:58:LYS:HG3	54:u:59:TYR:H	1.67	0.60
45:w:404:ALA:HB1	45:w:408:ARG:HH12	1.67	0.60
58:B7:6:HIS:HD2	58:B7:8:TYR:H	1.49	0.60
60:A6:80:GLU:CD	60:A6:80:GLU:H	2.10	0.60
5:4:175:ASN:ND2	25:Q:168:PHE:O	2.35	0.59
5:4:246:ILE:HG23	5:4:250:LEU:HD23	1.83	0.59
46:l:133:ARG:HD2	46:l:136:GLU:OE2	2.02	0.59
47:m:330:ALA:HB2	51:r:52:PHE:CE1	2.37	0.59
47:y:312:GLN:HE21	47:y:318:ARG:HG3	1.67	0.59
8:1:65:THR:OG1	8:1:124:ASN:ND2	2.35	0.59
46:l:154:ASN:HB3	46:l:156:GLN:HG2	1.84	0.59
48:o:197:GLU:O	48:o:201:ARG:N	2.29	0.59
46:x:154:ASN:HB3	46:x:156:GLN:HG2	1.84	0.59
47:y:138:MET:HE1	47:y:268:ILE:HA	1.84	0.59
48:z:13:SER:O	48:z:19:SER:HB3	2.02	0.59
50:A1:101:ARG:HA	50:A1:104:ARG:HE	1.67	0.59
46:l:259:ALA:HB2	46:l:422:LYS:HG2	1.85	0.59
47:m:127:ALA:O	47:m:131:TYR:N	2.31	0.59
49:p:75:GLU:OE1	49:p:75:GLU:N	2.34	0.59
5:4:60:SER:OG	5:4:63:THR:O	2.20	0.59
46:l:156:GLN:O	46:l:160:ILE:HG12	2.03	0.59
47:m:311:LYS:NZ	47:m:379:TRP:HB3	2.18	0.59
45:w:145:MET:HE3	45:w:252:HIS:CE1	2.38	0.59
47:y:317:PHE:CD1	50:A1:26:PHE:HE1	2.20	0.59
52:B5:20:VAL:HG21	52:B5:73:LEU:HB3	1.84	0.59
3:6:549:ALA:HB3	5:4:271:MET:HE2	1.85	0.59
48:o:97:ASN:O	48:o:101:ALA:N	2.32	0.59
50:q:61:ARG:O	50:q:65:ALA:N	2.31	0.59
77:y:401:HEM:HMC1	77:y:401:HEM:HBC2	1.83	0.59
45:k:41:ILE:HG22	45:k:43:ALA:H	1.68	0.59
46:l:50:PHE:CE2	46:l:383:GLY:HA3	2.38	0.59
46:l:295:LEU:O	46:l:299:VAL:N	2.34	0.59
48:o:167:GLU:HA	48:o:177:ALA:HB3	1.84	0.59
49:p:41:ALA:HB2	54:u:20:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:20:VAL:HG21	52:s:73:LEU:HB3	1.84	0.59
47:y:317:PHE:HA	50:A1:26:PHE:CE1	2.37	0.59
77:y:402:HEM:HBB2	77:y:402:HEM:HMB1	1.84	0.59
48:z:31:GLN:O	48:z:35:GLN:HG2	2.01	0.59
45:k:1:THR:OG1	46:l:39:GLU:OE2	2.13	0.59
45:k:396:GLU:O	45:k:400:ALA:N	2.27	0.59
48:o:55:CYS:SG	54:u:52:TRP:HB3	2.43	0.59
57:B9:145:PRO:CG	57:B9:148:MET:HE2	2.33	0.59
4:2:173:THR:HG21	11:B:49:GLY:HA2	1.85	0.59
7:8:411:SER:HB3	24:P:49:LEU:HD13	1.84	0.59
31:M:33:ASN:OD1	31:M:74:GLN:NE2	2.36	0.59
46:l:31:ASN:HB3	46:l:201:SER:HB3	1.85	0.59
50:q:108:ALA:O	53:A3:11:ARG:NH2	2.36	0.59
45:w:41:ILE:HG22	45:w:43:ALA:H	1.68	0.59
46:x:245:ARG:NH2	46:x:430:LEU:HB3	2.17	0.59
51:A2:48:VAL:O	51:A2:51:PRO:HD2	2.03	0.59
52:B5:11:GLU:N	52:B5:12:GLU:OE1	2.36	0.59
54:B4:55:ILE:HG23	54:B4:58:LYS:HE3	1.84	0.59
49:p:11:SER:HA	49:p:14:ARG:HG3	1.85	0.59
45:w:445:ARG:NH2	54:B4:17:THR:H	2.01	0.59
46:x:50:PHE:CE2	46:x:383:GLY:HA3	2.38	0.59
46:x:156:GLN:O	46:x:160:ILE:HG12	2.02	0.59
47:y:102:LEU:C	47:y:105:GLY:H	2.11	0.59
58:B7:192:VAL:O	58:B7:196:THR:HB	2.01	0.59
8:1:317:GLN:NE2	19:J:41:TYR:OH	2.36	0.59
45:k:404:ALA:HB1	45:k:408:ARG:HH12	1.67	0.59
46:l:331:ALA:HA	46:l:432:HIS:ND1	2.17	0.59
48:o:13:SER:O	48:o:19:SER:HB3	2.02	0.59
45:w:163:LEU:HD11	45:w:314:TYR:CE2	2.38	0.59
49:A0:5:ILE:HD13	51:A2:16:TYR:CE1	2.38	0.59
53:A3:39:ARG:HH11	53:A3:39:ARG:CG	2.16	0.59
46:l:245:ARG:NH2	46:l:430:LEU:HB3	2.17	0.58
53:t:25:GLY:O	53:t:29:ALA:N	2.35	0.58
54:u:18:SER:O	54:u:22:LEU:N	2.35	0.58
46:x:133:ARG:HD2	46:x:136:GLU:OE2	2.02	0.58
46:x:200:THR:OG1	46:x:228:GLY:N	2.29	0.58
47:y:374:ASN:HA	47:y:379:TRP:HD1	1.68	0.58
51:A2:62:GLY:O	51:A2:66:PHE:N	2.25	0.58
1:9:163:THR:HA	1:9:170:THR:HA	1.85	0.58
10:A:183:ILE:HD11	10:A:206:VAL:HG13	1.84	0.58
11:B:179:ARG:HH22	11:B:303:ARG:HD3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:403:ASP:H	45:k:406:VAL:HB	1.68	0.58
48:o:80:MET:CG	48:o:81:PHE:H	2.15	0.58
48:o:224:ARG:O	48:o:228:SER:N	2.36	0.58
46:x:200:THR:HG21	46:x:230:LEU:HB3	1.85	0.58
53:A3:42:LEU:O	53:A3:44:TRP:CB	2.51	0.58
63:A5:57:ARG:HG3	63:A5:60:TYR:CE2	2.38	0.58
66:B0:43:SER:OG	66:B0:45:VAL:HG12	2.04	0.58
4:2:144:GLN:HE21	17:H:3:PHE:HB2	1.69	0.58
45:k:56:GLY:HA2	45:k:59:VAL:HB	1.84	0.58
50:q:28:LYS:HG2	50:q:80:TRP:CE3	2.39	0.58
52:s:34:ARG:HA	52:s:37:LEU:HD12	1.85	0.58
1:9:228:ALA:HB3	7:8:284:ASN:HD22	1.68	0.58
14:E:105:ARG:NH1	14:E:195:ASP:OD2	2.36	0.58
46:l:24:LEU:HD22	46:l:392:TYR:CG	2.38	0.58
46:x:24:LEU:HD22	46:x:392:TYR:CG	2.38	0.58
46:x:338:LYS:HZ3	46:x:439:LEU:HD23	1.68	0.58
47:y:311:LYS:NZ	47:y:379:TRP:HB3	2.18	0.58
1:9:243:PHE:HB2	7:8:257:ARG:HA	1.85	0.58
45:w:8:LEU:HB3	45:w:393:ALA:HB2	1.85	0.58
45:w:56:GLY:HA2	45:w:59:VAL:HB	1.84	0.58
57:B9:193:TYR:HE1	59:A7:126:MET:HE1	1.68	0.58
7:8:424:ILE:HG12	10:A:76:ARG:HH21	1.68	0.58
27:S:211:ASN:HB3	27:S:214:GLU:HB2	1.86	0.58
45:k:45:SER:N	45:k:92:ARG:O	2.26	0.58
45:w:266:ASP:O	45:w:270:LEU:HG	2.03	0.58
45:w:403:ASP:H	45:w:406:VAL:HB	1.68	0.58
9:3:38:GLU:O	13:D:118:ARG:NH2	2.37	0.58
10:A:388:ASN:ND2	10:A:513:MET:O	2.35	0.58
25:Q:49:GLU:OE1	25:Q:135:ARG:NH2	2.36	0.58
31:W:105:MET:HB3	31:W:108:LEU:HD12	1.84	0.58
40:h:141:CYS:HB2	40:h:144:PRO:HG3	1.86	0.58
45:k:56:GLY:O	45:k:60:GLU:N	2.27	0.58
45:k:145:MET:HE3	45:k:252:HIS:CE1	2.38	0.58
49:p:107:ASP:HA	49:p:108:GLN:C	2.28	0.58
3:6:604:PHE:HA	4:2:150:ASN:HD22	1.68	0.58
5:4:115:LEU:HB2	5:4:174:LEU:HD13	1.85	0.58
10:A:50:LEU:HD21	10:A:62:ARG:HE	1.69	0.58
45:k:8:LEU:HB3	45:k:393:ALA:HB2	1.85	0.58
45:k:30:SER:N	45:k:201:GLY:O	2.29	0.58
45:k:163:LEU:HD11	45:k:314:TYR:CE2	2.38	0.58
45:w:56:GLY:O	45:w:60:GLU:N	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:45:ILE:HA	77:y:401:HEM:CMC	2.33	0.58
67:B1:46:LYS:O	67:B1:47:LYS:HB2	2.03	0.58
52:s:13:LEU:O	52:s:15:ASP:N	2.36	0.58
45:w:157:ALA:HB1	45:w:237:THR:H	1.67	0.58
45:w:438:ARG:HH21	51:A2:21:PHE:HE2	1.52	0.58
49:A0:30:GLU:HG3	54:B4:7:ALA:HA	1.86	0.58
5:4:336:ARG:HH22	5:4:429:SER:HA	1.69	0.58
17:H:9:ARG:NH2	42:j:12:GLN:OE1	2.37	0.58
50:q:44:LYS:O	50:q:48:ARG:HG2	2.04	0.58
46:x:295:LEU:O	46:x:299:VAL:N	2.34	0.58
48:z:72:ASP:OD1	48:z:73:GLY:N	2.36	0.58
50:A1:15:GLY:O	50:A1:19:TRP:N	2.22	0.58
7:8:398:ARG:NH2	10:A:155:GLU:OE2	2.37	0.57
23:O:92:GLU:HG3	23:O:97:TRP:HE3	1.67	0.57
28:T:62:THR:HG21	28:T:104:ARG:CD	2.28	0.57
31:W:105:MET:HA	31:W:108:LEU:HB2	1.85	0.57
46:l:133:ARG:O	46:l:137:VAL:N	2.29	0.57
47:m:102:LEU:C	47:m:105:GLY:H	2.11	0.57
49:p:76:ILE:N	49:p:77:LYS:HA	2.19	0.57
45:w:157:ALA:HA	45:w:237:THR:HB	1.85	0.57
45:w:262:TRP:HD1	45:w:315:ALA:HA	1.69	0.57
46:x:31:ASN:HB3	46:x:201:SER:HB3	1.85	0.57
46:x:245:ARG:HH22	46:x:430:LEU:HB3	1.69	0.57
47:y:277:ALA:HB1	47:y:294:LEU:HD11	1.86	0.57
77:y:402:HEM:HMC1	77:y:402:HEM:HBC2	1.86	0.57
51:A2:44:CYS:O	51:A2:47:ARG:N	2.31	0.57
52:B5:12:GLU:OE1	52:B5:12:GLU:N	2.36	0.57
57:B9:193:TYR:CE1	59:A7:126:MET:HE1	2.39	0.57
18:I:108:LYS:CG	18:I:118:GLN:NE2	2.65	0.57
26:R:227:PRO:HG2	26:R:230:SER:HA	1.85	0.57
45:k:157:ALA:HA	45:k:237:THR:HB	1.85	0.57
45:k:262:TRP:HD1	45:k:315:ALA:HA	1.69	0.57
46:l:67:HIS:CE1	46:l:177:TYR:HA	2.39	0.57
51:r:48:VAL:O	51:r:51:PRO:HD2	2.03	0.57
46:x:168:TYR:HE2	46:x:321:LEU:HD11	1.69	0.57
48:z:51:LEU:O	48:z:56:TYR:N	2.38	0.57
50:A1:44:LYS:O	50:A1:48:ARG:HG2	2.04	0.57
54:B4:18:SER:O	54:B4:22:LEU:N	2.35	0.57
56:A9:404:THR:O	56:A9:480:ARG:NH1	2.37	0.57
45:k:313:CYS:HA	45:k:318:GLY:HA2	1.86	0.57
46:l:63:LEU:O	46:l:182:ARG:NE	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:248:ASN:HA	46:x:181:TYR:CE2	2.40	0.57
46:l:416:LYS:HA	46:l:419:SER:HB3	1.86	0.57
47:m:374:ASN:HA	47:m:379:TRP:HD1	1.68	0.57
46:x:259:ALA:HB2	46:x:422:LYS:HG2	1.85	0.57
1:9:228:ALA:HA	1:9:231:LEU:HD23	1.86	0.57
48:o:51:LEU:O	48:o:56:TYR:N	2.38	0.57
46:x:67:HIS:CE1	46:x:177:TYR:HA	2.39	0.57
50:A1:77:LYS:HA	50:A1:80:TRP:CD2	2.39	0.57
11:B:179:ARG:NH2	11:B:401:GLU:O	2.37	0.57
46:x:296:TYR:HD2	46:x:297:GLN:NE2	2.03	0.57
46:x:416:LYS:HA	46:x:419:SER:HB3	1.86	0.57
48:z:23:HIS:HA	48:z:26:ILE:HD12	1.87	0.57
1:9:197:THR:HG23	1:9:200:ASP:H	1.68	0.57
25:Q:5:VAL:N	30:V:107:GLY:O	2.38	0.57
40:h:81:ALA:O	40:h:83:ASP:N	2.37	0.57
45:k:256:ALA:HB2	45:k:310:PHE:HZ	1.70	0.57
45:k:381:ARG:O	45:k:385:THR:N	2.38	0.57
47:m:263:ASN:OD1	47:m:264:THR:N	2.38	0.57
49:p:75:GLU:HG2	49:p:76:ILE:CA	2.34	0.57
47:y:272:TRP:CE2	47:y:273:TYR:HD2	2.23	0.57
48:z:97:ASN:O	48:z:101:ALA:N	2.32	0.57
1:9:56:THR:HG22	1:9:58:GLU:H	1.70	0.57
45:k:266:ASP:O	45:k:270:LEU:HG	2.03	0.57
47:m:277:ALA:HB1	47:m:294:LEU:HD11	1.86	0.57
47:m:344:GLU:HG2	47:m:346:PRO:CD	2.29	0.57
48:z:160:MET:HE3	78:z:301:HEC:C4B	2.35	0.57
48:z:224:ARG:HH21	51:A2:25:ALA:C	2.11	0.57
3:6:454:ILE:HG22	3:6:458:LEU:HD23	1.85	0.57
5:4:193:VAL:HG22	5:4:257:MET:HE1	1.85	0.57
26:R:328:ILE:CG2	26:R:329:LEU:N	2.46	0.57
48:o:70:VAL:HA	48:o:82:MET:HA	1.86	0.57
48:o:146:GLY:O	48:o:159:GLY:HA2	2.04	0.57
45:w:21:ASN:HD21	45:w:217:SER:N	2.01	0.57
45:w:183:THR:O	45:w:187:SER:N	2.37	0.57
45:w:313:CYS:HA	45:w:318:GLY:HA2	1.87	0.57
48:z:146:GLY:O	48:z:159:GLY:HA2	2.04	0.57
57:B9:132:GLU:HB3	57:B9:137:GLU:HG3	1.87	0.57
57:B9:179:LEU:HD21	63:A5:65:PRO:HD3	1.85	0.57
45:k:8:LEU:HD22	45:k:393:ALA:HA	1.87	0.57
45:k:183:THR:O	45:k:187:SER:N	2.37	0.57
46:l:168:TYR:HE2	46:l:321:LEU:HD11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:85:LYS:HA	49:p:86:ASN:C	2.30	0.57
45:w:348:SER:HG	53:A3:17:TRP:CD1	2.23	0.57
46:x:305:GLN:OE1	46:x:305:GLN:N	2.37	0.57
46:x:398:VAL:HA	46:x:401:GLN:OE1	2.05	0.57
47:y:236:ILE:O	47:y:240:MET:N	2.32	0.57
57:B9:189:PRO:HD2	64:B6:54:TYR:OH	2.05	0.57
3:6:558:LEU:HB3	5:4:214:LEU:HD11	1.86	0.57
31:M:70:LEU:HD13	31:M:76:ILE:HG12	1.87	0.57
45:k:46:ARG:NH2	45:k:234:CYS:SG	2.78	0.57
47:m:272:TRP:CE2	47:m:273:TYR:HD2	2.23	0.57
48:o:79:GLU:O	48:o:80:MET:HG2	2.05	0.57
52:s:38:GLU:O	52:s:42:GLU:N	2.24	0.57
45:w:130:GLU:O	45:w:134:ILE:N	2.29	0.57
45:w:348:SER:HG	53:A3:17:TRP:NE1	2.03	0.57
46:x:254:HIS:HB2	46:x:427:SER:HB2	1.87	0.57
52:B5:34:ARG:HA	52:B5:37:LEU:HD12	1.86	0.57
67:B1:41:ARG:HG3	68:A8:40:TYR:CE2	2.40	0.57
16:G:111:LEU:HD13	26:R:100:LEU:HD23	1.87	0.56
45:k:154:HIS:HB3	45:k:164:ALA:HA	1.86	0.56
45:k:204:GLU:OE1	45:k:204:GLU:N	2.38	0.56
47:m:45:ILE:HA	77:m:401:HEM:CMC	2.33	0.56
54:u:32:GLU:HA	54:u:35:PHE:HB3	1.87	0.56
45:w:8:LEU:HD22	45:w:393:ALA:HA	1.87	0.56
45:w:45:SER:N	45:w:92:ARG:O	2.26	0.56
45:w:46:ARG:NH2	45:w:234:CYS:SG	2.78	0.56
46:x:438:GLU:OE1	46:x:438:GLU:N	2.34	0.56
47:y:181:PHE:HA	47:y:184:ILE:HG22	1.87	0.56
49:A0:28:SER:HB2	49:A0:32:ARG:NH1	2.20	0.56
10:A:82:ILE:HD11	10:A:100:TRP:HB3	1.87	0.56
45:w:396:GLU:O	45:w:400:ALA:N	2.27	0.56
47:y:196:HIS:NE2	77:y:402:HEM:ND	2.53	0.56
50:A1:28:LYS:HB3	50:A1:80:TRP:CG	2.40	0.56
51:A2:72:LYS:HG2	52:B5:56:GLU:OE2	2.06	0.56
53:A3:15:ARG:CG	53:A3:16:ASN:H	2.17	0.56
57:B9:145:PRO:HG3	57:B9:148:MET:HE2	1.87	0.56
5:4:285:LEU:O	5:4:406:TYR:OH	2.23	0.56
8:1:70:MET:HG3	8:1:121:TRP:HZ3	1.70	0.56
11:B:163:PRO:HG2	11:B:168:GLN:HE21	1.70	0.56
11:B:278:VAL:HG12	11:B:283:ALA:HB2	1.87	0.56
35:a:79:ASN:ND2	44:e:73:GLY:O	2.38	0.56
45:k:130:GLU:O	45:k:134:ILE:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:239:SER:HB2	51:r:17:SER:O	2.06	0.56
45:k:395:TRP:O	45:k:399:ILE:N	2.37	0.56
46:l:398:VAL:HA	46:l:401:GLN:OE1	2.04	0.56
47:m:196:HIS:NE2	77:m:402:HEM:ND	2.53	0.56
49:p:73:LYS:HD3	49:p:94:LYS:HA	1.88	0.56
45:w:381:ARG:O	45:w:385:THR:N	2.37	0.56
47:y:91:PHE:O	47:y:94:LEU:HB3	2.06	0.56
47:y:263:ASN:OD1	47:y:264:THR:N	2.38	0.56
47:y:326:TRP:CD2	51:A:48:VAL:HG13	2.39	0.56
48:z:178:THR:O	48:z:182:VAL:N	2.35	0.56
48:z:238:ARG:NH2	49:A0:5:ILE:HG22	2.20	0.56
58:B7:203:PHE:O	58:B7:207:HIS:HD2	1.87	0.56
4:2:173:THR:HG22	11:B:52:MET:HE2	1.88	0.56
10:A:266:ARG:HG3	10:A:267:THR:HG23	1.86	0.56
12:C:197:GLY:HA2	16:G:67:VAL:HG13	1.88	0.56
45:k:53:ASN:OD1	45:k:54:GLY:N	2.39	0.56
45:k:157:ALA:HB1	45:k:237:THR:H	1.67	0.56
48:o:160:MET:HE3	78:o:301:HEC:C4B	2.35	0.56
45:w:256:ALA:HB2	45:w:310:PHE:HZ	1.69	0.56
2:7:83:TRP:HB2	2:7:89:VAL:HG11	1.86	0.56
47:m:22:PRO:HG3	51:r:4:PHE:CZ	2.41	0.56
47:m:120:LEU:O	47:m:123:VAL:N	2.37	0.56
47:m:377:LEU:HD11	50:q:20:TYR:CD2	2.40	0.56
48:o:136:GLU:O	48:o:137:PRO:C	2.49	0.56
45:w:186:LEU:HD23	45:w:190:TYR:HE2	1.70	0.56
48:z:80:MET:O	48:z:81:PHE:HB2	2.06	0.56
49:A0:96:LEU:HA	49:A0:136:ILE:HA	1.87	0.56
52:B5:20:VAL:HB	52:B5:73:LEU:HD23	1.86	0.56
56:A9:184:PHE:H	56:A9:256:HIS:HE1	1.52	0.56
12:C:66:TYR:OH	12:C:107:ASN:ND2	2.38	0.56
37:c:14:GLN:NE2	39:f:155:PRO:O	2.38	0.56
43:g:13:PRO:O	43:g:116:ARG:NH2	2.39	0.56
48:o:23:HIS:HA	48:o:26:ILE:HD12	1.86	0.56
48:o:62:LYS:O	48:o:66:GLU:HG3	2.06	0.56
52:s:20:VAL:HB	52:s:73:LEU:HD23	1.86	0.56
45:w:395:TRP:O	45:w:399:ILE:N	2.37	0.56
46:x:25:GLU:OE2	46:x:213:HIS:ND1	2.39	0.56
53:A3:42:LEU:O	53:A3:44:TRP:HB2	2.06	0.56
53:A3:45:VAL:O	54:B4:33:ARG:NH2	2.39	0.56
10:A:324:SER:HA	10:A:327:ALA:HB3	1.88	0.56
25:Q:45:LEU:O	25:Q:135:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:168:PHE:H	25:Q:170:TRP:HD1	1.53	0.56
46:l:37:SER:HB3	46:l:216:LEU:HD22	1.88	0.56
46:l:290:ASN:O	46:l:297:GLN:NE2	2.33	0.56
47:m:91:PHE:O	47:m:94:LEU:HB3	2.06	0.56
50:q:77:LYS:HA	50:q:80:TRP:CD2	2.39	0.56
47:y:120:LEU:O	47:y:123:VAL:N	2.37	0.56
48:z:57:THR:HB	48:z:60:GLU:HB2	1.88	0.56
48:z:102:ARG:CZ	48:z:109:LEU:HB2	2.36	0.56
49:A0:29:SER:HB3	49:A0:33:LYS:HE2	1.87	0.56
1:9:90:ASN:ND2	1:9:92:TRP:O	2.39	0.56
36:b:133:TYR:HE2	43:g:90:MET:HG3	1.71	0.56
45:k:186:LEU:HD23	45:k:190:TYR:HE2	1.70	0.56
45:k:191:LYS:HZ1	45:k:225:GLU:N	2.04	0.56
46:l:100:SER:OG	55:v:67:SER:OG	2.13	0.56
48:o:77:ASP:O	48:o:79:GLU:HG3	2.06	0.56
48:o:148:TYR:N	48:o:158:ILE:O	2.37	0.56
48:o:165:TYR:CZ	48:o:168:VAL:HA	2.41	0.56
50:q:58:ARG:HA	50:q:61:ARG:NH2	2.21	0.56
45:w:39:VAL:HG23	45:w:113:LEU:HD21	1.88	0.56
50:A1:28:LYS:O	50:A1:29:LEU:CD2	2.49	0.56
56:A9:95:PRO:HB2	58:B7:11:VAL:HG13	1.87	0.56
62:A4:5:LYS:HD2	62:A4:6:GLY:N	2.21	0.56
45:k:39:VAL:HG23	45:k:113:LEU:HD21	1.88	0.56
46:l:25:GLU:OE2	46:l:213:HIS:ND1	2.39	0.56
47:m:77:TRP:CH2	47:m:78:ILE:HG22	2.41	0.56
48:o:57:THR:HB	48:o:60:GLU:HB2	1.88	0.56
47:y:77:TRP:CH2	47:y:78:ILE:HG22	2.41	0.56
50:A1:75:LEU:HD12	50:A1:76:PRO:HD2	1.87	0.56
63:A5:71:THR:O	63:A5:75:ARG:HD3	2.05	0.56
26:R:147:LYS:O	26:R:151:ALA:N	2.39	0.56
46:l:296:TYR:HD2	46:l:297:GLN:NE2	2.03	0.56
45:w:204:GLU:HG2	45:w:205:HIS:N	2.21	0.56
45:w:329:MET:HG3	51:A2:2:ARG:HH21	1.70	0.56
48:z:224:ARG:O	48:z:228:SER:N	2.36	0.56
54:B4:32:GLU:HA	54:B4:35:PHE:HB3	1.87	0.56
56:A9:69:MET:HE2	56:A9:70:VAL:CG2	2.35	0.56
58:B7:42:LEU:HD13	65:B8:45:TYR:CD2	2.41	0.56
3:6:387:THR:OG1	3:6:388:GLY:N	2.38	0.55
4:2:47:ASN:HD21	4:2:123:PRO:HB2	1.69	0.55
18:I:108:LYS:CG	18:I:120:ARG:CB	2.78	0.55
28:T:62:THR:HG23	28:T:104:ARG:CZ	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:117:VAL:HG12	45:k:118:GLN:HG3	1.88	0.55
46:l:245:ARG:HH22	46:l:430:LEU:HB3	1.69	0.55
47:m:231:GLY:HA2	47:m:234:LEU:HD12	1.88	0.55
48:o:102:ARG:CZ	48:o:109:LEU:HB2	2.36	0.55
48:o:180:SER:HB3	52:s:17:LEU:HD22	1.87	0.55
47:y:74:ASN:ND2	49:A0:64:ALA:O	2.38	0.55
49:A0:10:PHE:CG	51:A2:18:LEU:HD11	2.40	0.55
55:B3:66:ALA:HB2	55:B3:77:ARG:CZ	2.37	0.55
10:A:382:ARG:HD2	10:A:386:LEU:HD23	1.88	0.55
45:k:55:ALA:O	45:k:59:VAL:N	2.31	0.55
47:m:181:PHE:HA	47:m:184:ILE:HG22	1.87	0.55
51:r:11:ARG:HB3	51:r:12:HIS:CD2	2.42	0.55
46:x:164:HIS:HB3	46:x:173:ALA:HA	1.87	0.55
48:z:71:GLN:HG3	48:z:72:ASP:CG	2.32	0.55
51:A2:11:ARG:HB3	51:A2:12:HIS:CD2	2.42	0.55
2:7:111:LYS:HA	17:H:81:ARG:HH21	1.71	0.55
3:6:361:GLY:O	3:6:364:LYS:NZ	2.39	0.55
8:1:204:GLU:HG2	8:1:279:ARG:HD3	1.88	0.55
46:l:254:HIS:HB2	46:l:427:SER:HB2	1.87	0.55
46:l:438:GLU:N	46:l:438:GLU:OE1	2.34	0.55
48:o:14:HIS:HB3	48:o:21:LEU:HD23	1.88	0.55
48:o:52:VAL:HG12	54:u:52:TRP:CD1	2.41	0.55
45:w:124:ASP:HA	45:w:127:ILE:HG12	1.88	0.55
45:w:154:HIS:HB3	45:w:164:ALA:HA	1.87	0.55
47:y:178:PHE:O	47:y:181:PHE:N	2.39	0.55
50:A1:21:TYR:OH	50:A1:27:ASN:HB2	2.06	0.55
55:B3:66:ALA:HB2	55:B3:77:ARG:NE	2.21	0.55
10:A:587:ALA:HB1	10:A:591:GLU:HB2	1.88	0.55
14:E:131:GLU:OE1	14:E:144:ARG:NH1	2.39	0.55
47:m:178:PHE:O	47:m:181:PHE:N	2.39	0.55
50:q:75:LEU:HD12	50:q:76:PRO:HD2	1.87	0.55
45:w:117:VAL:HG12	45:w:118:GLN:HG3	1.88	0.55
48:z:23:HIS:CD2	54:B4:55:ILE:HD12	2.40	0.55
38:d:18:ASP:O	38:d:20:LEU:N	2.38	0.55
45:k:34:THR:HG22	45:k:102:LEU:HD23	1.89	0.55
45:k:113:LEU:O	45:k:117:VAL:HG23	2.07	0.55
46:l:164:HIS:HB3	46:l:173:ALA:HA	1.87	0.55
47:y:354:ALA:HA	47:y:357:LEU:HB3	1.88	0.55
48:z:165:TYR:CZ	48:z:168:VAL:HA	2.41	0.55
60:A6:78:HIS:ND1	64:B6:12:LEU:HD22	2.21	0.55
8:1:208:VAL:HG11	11:B:87:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:387:LEU:HD12	10:A:514:ASN:HB2	1.88	0.55
45:k:245:GLU:H	45:k:426:GLY:HA3	1.72	0.55
45:w:30:SER:N	45:w:201:GLY:O	2.29	0.55
45:w:34:THR:HG22	45:w:102:LEU:HD23	1.89	0.55
47:y:270:PRO:O	47:y:275:LEU:HD21	2.06	0.55
47:y:346:PRO:HG3	51:A2:66:PHE:HA	1.89	0.55
48:z:53:GLY:HA2	54:B4:52:TRP:CZ3	2.40	0.55
48:z:136:GLU:O	48:z:137:PRO:C	2.49	0.55
55:B3:71:ASN:O	55:B3:72:VAL:HG22	2.06	0.55
64:B6:63:MET:HB3	64:B6:68:ILE:HD11	1.89	0.55
7:8:159:ARG:HG2	7:8:161:GLU:H	1.72	0.55
45:w:53:ASN:OD1	45:w:54:GLY:N	2.39	0.55
45:w:125:SER:O	45:w:129:LYS:NZ	2.37	0.55
47:y:102:LEU:O	47:y:105:GLY:N	2.40	0.55
48:z:97:ASN:ND2	48:z:99:GLU:HB2	2.22	0.55
48:z:228:SER:HB2	51:A2:23:GLN:HE21	1.71	0.55
48:z:234:LYS:HE3	49:A0:7:VAL:HG11	1.89	0.55
56:A9:407:ASP:O	56:A9:411:LYS:HG3	2.07	0.55
62:A4:5:LYS:HZ3	62:A4:5:LYS:HB3	1.71	0.55
2:7:49:GLY:H	6:5:49:LEU:HD21	1.72	0.55
25:Q:8:PRO:O	30:V:88:ARG:NH2	2.40	0.55
28:T:57:GLY:O	28:T:58:ARG:C	2.49	0.55
46:l:338:LYS:NZ	46:l:439:LEU:HD23	2.22	0.55
47:m:270:PRO:O	47:m:275:LEU:HD21	2.06	0.55
48:o:23:HIS:NE2	54:u:51:LEU:HA	2.22	0.55
49:p:20:ASP:HB3	49:p:23:LYS:HG2	1.88	0.55
46:x:37:SER:HB3	46:x:216:LEU:HD22	1.88	0.55
58:B7:151:LEU:HB2	58:B7:159:MET:HG3	1.89	0.55
5:4:69:THR:HG22	5:4:235:LEU:HD11	1.89	0.55
8:1:17:VAL:CG2	8:1:225:MET:SD	2.92	0.55
10:A:473:MET:HE2	10:A:475:ILE:HD11	1.89	0.55
26:R:114:ASP:HA	26:R:117:ARG:HB2	1.88	0.55
46:l:98:VAL:H	55:v:70:LEU:HB3	1.71	0.55
47:m:102:LEU:O	47:m:105:GLY:N	2.40	0.55
48:o:131:LEU:HD22	48:o:164:ILE:HD12	1.88	0.55
50:q:28:LYS:HB3	50:q:74:ILE:HD11	1.89	0.55
54:u:51:LEU:O	54:u:55:ILE:N	2.28	0.55
45:w:211:LEU:HA	45:w:213:GLN:HB2	1.89	0.55
46:x:304:HIS:CG	46:x:305:GLN:H	2.24	0.55
47:y:6:LYS:HD3	47:y:16:ASN:HD21	1.72	0.55
37:c:21:ARG:HG3	39:f:125:TRP:HH2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:t:23:LEU:O	53:t:27:VAL:N	2.23	0.55
45:w:159:GLN:O	45:w:235:ARG:NH2	2.40	0.55
46:x:275:LEU:HB2	46:x:410:VAL:HG13	1.89	0.55
47:y:231:GLY:HA2	47:y:234:LEU:HD12	1.88	0.55
48:z:14:HIS:HB3	48:z:21:LEU:HD23	1.87	0.55
50:A1:58:ARG:HA	50:A1:61:ARG:NH2	2.21	0.55
63:A5:75:ARG:HG2	63:A5:75:ARG:NH1	2.19	0.55
10:A:568:TYR:HB3	10:A:583:ILE:HG22	1.88	0.54
48:o:238:ARG:NE	49:p:5:ILE:HG22	2.22	0.54
45:w:55:ALA:O	45:w:59:VAL:N	2.31	0.54
45:w:152:TYR:HB3	45:w:241:ILE:HD13	1.89	0.54
47:y:77:TRP:CZ2	47:y:78:ILE:HG22	2.43	0.54
47:y:207:ASN:OD1	47:y:210:GLY:N	2.39	0.54
48:z:102:ARG:NH1	48:z:107:GLY:O	2.39	0.54
51:A2:37:VAL:HG12	51:A2:41:THR:HG21	1.88	0.54
53:A3:17:TRP:O	53:A3:21:ALA:N	2.24	0.54
45:k:159:GLN:O	45:k:235:ARG:NH2	2.40	0.54
47:m:78:ILE:HG12	47:m:79:ILE:HG13	1.89	0.54
52:s:18:THR:HG22	52:s:21:ARG:HE	1.73	0.54
58:B7:156:ARG:HG3	58:B7:156:ARG:NH1	2.22	0.54
61:B2:82:CYS:N	61:B2:86:GLY:O	2.41	0.54
10:A:251:ILE:HG13	10:A:604:GLN:HB3	1.89	0.54
46:l:295:LEU:HD11	46:l:340:ALA:HA	1.89	0.54
46:x:295:LEU:HD11	46:x:340:ALA:HA	1.89	0.54
48:z:231:LYS:HG2	50:A1:70:MET:HE3	1.89	0.54
53:A3:43:ASP:OD1	53:A3:47:TYR:N	2.40	0.54
46:l:132:PHE:HB3	46:l:188:PRO:HB3	1.90	0.54
47:m:354:ALA:HA	47:m:357:LEU:HB3	1.88	0.54
48:o:97:ASN:ND2	48:o:99:GLU:HB2	2.22	0.54
51:r:64:GLN:HA	51:r:67:GLU:OE1	2.07	0.54
46:x:338:LYS:NZ	46:x:439:LEU:HD23	2.22	0.54
47:y:131:TYR:O	47:y:134:PRO:HD2	2.07	0.54
48:z:215:LEU:HD23	48:z:218:LEU:HD12	1.89	0.54
62:A4:5:LYS:HD2	62:A4:5:LYS:C	2.32	0.54
8:1:230:ASN:HA	8:1:233:MET:HE2	1.89	0.54
47:m:104:TYR:CD1	47:m:208:PRO:HA	2.42	0.54
47:m:131:TYR:O	47:m:134:PRO:HD2	2.07	0.54
48:o:176:PRO:HB2	52:s:13:LEU:HD21	1.88	0.54
45:w:245:GLU:H	45:w:426:GLY:HA3	1.71	0.54
46:x:258:VAL:HG22	46:x:323:GLY:HA3	1.90	0.54
47:y:226:ILE:HG21	48:z:223:LYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:131:LEU:HD22	48:z:164:ILE:HD12	1.88	0.54
51:A2:64:GLN:HA	51:A2:67:GLU:OE1	2.08	0.54
52:B5:18:THR:HG22	52:B5:21:ARG:HE	1.73	0.54
7:8:74:ASP:HA	7:8:77:LEU:HB2	1.89	0.54
47:m:98:VAL:O	47:m:101:GLY:N	2.40	0.54
50:q:43:VAL:HA	50:q:46:ALA:HB3	1.90	0.54
50:q:109:LYS:O	53:A3:11:ARG:NE	2.41	0.54
47:y:104:TYR:CD1	47:y:208:PRO:HA	2.42	0.54
48:z:81:PHE:CG	48:z:82:MET:N	2.76	0.54
53:A3:19:PRO:C	53:A3:22:SER:HG	2.07	0.54
57:B9:111:THR:HG21	63:A5:66:ILE:HD11	1.88	0.54
9:3:28:ASN:ND2	26:R:306:GLU:O	2.40	0.54
10:A:426:ASP:HA	16:G:169:ARG:HH12	1.73	0.54
46:l:329:GLN:N	46:l:332:SER:HB2	2.22	0.54
50:q:101:ARG:N	50:q:104:ARG:HH21	2.05	0.54
45:w:113:LEU:O	45:w:117:VAL:HG23	2.07	0.54
45:w:233:PRO:O	49:A0:22:THR:HA	2.08	0.54
46:x:58:GLU:HA	46:x:62:ASN:HD22	1.73	0.54
46:x:257:LEU:HD12	46:x:423:SER:O	2.08	0.54
47:y:133:LEU:HB2	47:y:134:PRO:HD3	1.89	0.54
48:z:62:LYS:O	48:z:66:GLU:HG3	2.06	0.54
49:A0:2:HIS:CD2	49:A0:3:THR:H	2.25	0.54
57:B9:165:VAL:HB	57:B9:170:LEU:HD12	1.90	0.54
45:k:443:TRP:HB3	45:k:445:ARG:H	1.73	0.54
47:m:77:TRP:CZ2	47:m:78:ILE:HG22	2.43	0.54
48:o:57:THR:HA	54:u:56:LYS:NZ	2.23	0.54
48:z:12:TRP:HB2	48:z:15:ARG:HB2	1.89	0.54
58:B7:222:GLN:HE21	58:B7:222:GLN:HA	1.72	0.54
1:9:119:TYR:HB3	7:8:201:ALA:HB3	1.90	0.54
10:A:161:GLU:OE1	18:I:102:ASN:ND2	2.40	0.54
23:O:50:PHE:HE1	23:O:96:VAL:HG12	1.73	0.54
46:l:160:ILE:O	46:l:163:LEU:HB3	2.07	0.54
46:l:257:LEU:HD12	46:l:423:SER:O	2.08	0.54
46:l:258:VAL:HG22	46:l:323:GLY:HA3	1.90	0.54
48:o:12:TRP:HB2	48:o:15:ARG:HB2	1.89	0.54
47:y:42:ILE:O	47:y:45:ILE:N	2.41	0.54
47:y:97:HIS:CD2	77:y:402:HEM:C1C	2.96	0.54
47:y:349:THR:O	47:y:353:LEU:HG	2.08	0.54
52:B5:13:LEU:O	52:B5:15:ASP:N	2.36	0.54
59:A7:40:LEU:HD13	59:A7:59:LEU:HD13	1.90	0.54
61:B2:55:LYS:HA	61:B2:74:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:188:GLU:O	14:E:192:ASN:ND2	2.41	0.54
28:T:61:PHE:C	28:T:61:PHE:CD1	2.85	0.54
45:k:124:ASP:HA	45:k:127:ILE:HG12	1.89	0.54
45:k:188:ARG:HB2	45:k:189:HIS:ND1	2.23	0.54
45:k:356:ARG:HG3	45:k:357:GLY:H	1.73	0.54
52:s:53:ASP:OD1	52:s:54:CYS:N	2.41	0.54
46:x:329:GLN:N	46:x:332:SER:HB2	2.22	0.54
47:y:31:TRP:HA	47:y:100:ARG:NH1	2.21	0.54
10:A:263:VAL:HA	10:A:273:ILE:HG22	1.89	0.53
13:D:150:VAL:HG12	13:D:179:VAL:HG13	1.90	0.53
26:R:329:LEU:HG	26:R:331:HIS:H	1.73	0.53
27:S:100:CYS:HB3	27:S:119:LEU:HB2	1.88	0.53
47:m:349:THR:O	47:m:353:LEU:HG	2.08	0.53
46:x:61:ASN:O	46:x:182:ARG:NH2	2.39	0.53
46:x:63:LEU:O	46:x:182:ARG:NE	2.36	0.53
60:A6:41:LEU:HD12	60:A6:41:LEU:O	2.08	0.53
6:5:79:VAL:O	6:5:83:ASN:N	2.40	0.53
11:B:237:PRO:HD3	14:E:96:ARG:HH22	1.73	0.53
45:k:294:LEU:HG	45:k:341:GLN:HG3	1.91	0.53
45:k:336:PHE:HD2	45:k:337:VAL:HG22	1.73	0.53
46:l:58:GLU:HA	46:l:62:ASN:HD22	1.73	0.53
46:l:392:TYR:OH	46:l:395:PRO:HD3	2.08	0.53
47:m:97:HIS:CD2	77:m:402:HEM:C1C	2.96	0.53
50:q:87:LYS:HE3	50:q:89:TYR:HB3	1.90	0.53
50:q:91:GLU:O	50:q:95:LYS:HG3	2.08	0.53
47:y:67:THR:HG21	48:z:45:TYR:CG	2.42	0.53
50:A1:101:ARG:N	50:A1:104:ARG:HH21	2.04	0.53
59:A7:108:PRO:HG2	59:A7:111:PHE:CE2	2.42	0.53
61:B2:48:LEU:O	61:B2:50:PRO:HD3	2.08	0.53
7:8:160:GLY:HA2	7:8:199:ARG:HD2	1.89	0.53
8:1:281:ARG:NH1	11:B:443:MET:SD	2.81	0.53
26:R:154:GLN:HG3	26:R:155:VAL:HG23	1.90	0.53
45:k:114:ALA:HB1	45:k:216:PHE:CD2	2.43	0.53
45:k:370:ASP:OD1	45:k:371:GLY:N	2.41	0.53
45:w:279:HIS:HA	45:w:307:PHE:CE1	2.44	0.53
46:x:160:ILE:O	46:x:163:LEU:HB3	2.07	0.53
47:y:28:SER:HB3	47:y:30:TRP:HD1	1.74	0.53
48:z:23:HIS:CD2	54:B4:51:LEU:HA	2.44	0.53
52:B5:38:GLU:O	52:B5:42:GLU:N	2.24	0.53
59:A7:52:SER:OG	59:A7:55:GLU:HG3	2.08	0.53
45:k:279:HIS:HA	45:k:307:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:215:LEU:HD23	48:o:218:LEU:HD12	1.89	0.53
46:x:254:HIS:CD2	46:x:327:ILE:HG12	2.43	0.53
46:x:276:GLN:HG3	46:x:277:HIS:N	2.24	0.53
50:A1:43:VAL:HA	50:A1:46:ALA:HB3	1.90	0.53
5:4:216:LEU:HD23	5:4:291:VAL:HG22	1.90	0.53
37:c:28:LEU:HD13	39:f:118:TYR:HD1	1.74	0.53
42:j:35:GLY:O	42:j:39:TYR:N	2.41	0.53
44:e:39:GLY:HA3	44:e:77:LYS:HB3	1.90	0.53
45:k:152:TYR:HB3	45:k:241:ILE:HD13	1.89	0.53
47:m:28:SER:HB3	47:m:30:TRP:HD1	1.74	0.53
47:m:42:ILE:O	47:m:45:ILE:N	2.41	0.53
47:m:311:LYS:HZ2	47:m:379:TRP:HB3	1.73	0.53
48:o:178:THR:HB	48:o:181:GLN:HB2	1.91	0.53
53:t:34:TRP:HD1	54:u:29:LEU:HD13	1.74	0.53
45:w:356:ARG:HG3	45:w:357:GLY:H	1.73	0.53
50:A1:40:ASN:ND2	50:A1:42:ASP:HB2	2.23	0.53
53:A3:42:LEU:N	53:A3:42:LEU:HD23	2.22	0.53
57:B9:136:LEU:HB3	57:B9:193:TYR:HD2	1.73	0.53
57:B9:203:ASN:HD22	57:B9:206:PHE:HD2	1.55	0.53
59:A7:67:SER:OG	59:A7:70:GLU:HG3	2.08	0.53
1:9:176:CYS:O	7:8:159:ARG:NH1	2.40	0.53
2:7:66:VAL:O	2:7:70:TYR:N	2.42	0.53
47:m:100:ARG:HH22	77:m:402:HEM:CGA	2.20	0.53
47:m:133:LEU:HB2	47:m:134:PRO:HD3	1.89	0.53
47:m:325:PHE:O	47:m:329:VAL:HG23	2.09	0.53
48:o:178:THR:O	48:o:182:VAL:N	2.34	0.53
52:s:13:LEU:C	52:s:15:ASP:H	2.15	0.53
45:w:370:ASP:OD1	45:w:371:GLY:N	2.41	0.53
47:y:325:PHE:O	47:y:329:VAL:HG23	2.09	0.53
50:A1:91:GLU:O	50:A1:95:LYS:HG3	2.08	0.53
52:B5:53:ASP:OD1	52:B5:54:CYS:N	2.41	0.53
62:A4:2:SER:OG	62:A4:3:ALA:N	2.41	0.53
26:R:275:ASP:O	26:R:279:TYR:N	2.40	0.53
40:h:121:GLU:OE2	40:h:124:ARG:NH2	2.41	0.53
45:w:146:ARG:HG2	45:w:150:PHE:HE2	1.73	0.53
45:w:336:PHE:HD2	45:w:337:VAL:HG22	1.73	0.53
46:x:392:TYR:OH	46:x:395:PRO:HD3	2.08	0.53
48:z:116:ILE:HD12	48:z:119:ALA:HB3	1.91	0.53
56:A9:398:PRO:O	56:A9:498:CYS:HB3	2.09	0.53
3:6:73:THR:O	43:g:104:ASN:ND2	2.41	0.53
10:A:627:SER:OG	10:A:632:MET:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:61:ASN:O	46:l:182:ARG:NH2	2.39	0.53
47:m:26:ASN:HD22	50:q:69:SER:CB	2.21	0.53
48:o:102:ARG:NH1	48:o:107:GLY:O	2.39	0.53
49:p:88:ALA:HA	49:p:120:PRO:O	2.09	0.53
45:w:62:LEU:HA	45:w:65:LYS:HD2	1.91	0.53
61:B2:51:SER:HB2	61:B2:91:LEU:HD11	1.90	0.53
7:8:426:ALA:O	7:8:430:GLY:N	2.42	0.53
26:R:209:ARG:NH1	26:R:351:GLU:OE2	2.37	0.53
45:k:436:ARG:HH22	47:m:19:ILE:CG2	2.22	0.53
46:l:254:HIS:CD2	46:l:327:ILE:HG12	2.43	0.53
46:l:275:LEU:HB2	46:l:410:VAL:HG13	1.89	0.53
46:l:360:ALA:O	46:l:364:LEU:N	2.24	0.53
47:m:6:LYS:HD3	47:m:16:ASN:HD21	1.72	0.53
47:y:34:GLY:HA3	77:y:402:HEM:HBA2	1.91	0.53
59:A7:128:VAL:O	59:A7:134:PHE:HB3	2.09	0.53
62:A4:8:HIS:O	62:A4:10:GLY:N	2.42	0.53
3:6:427:ILE:HG13	3:6:431:LEU:HD12	1.91	0.53
3:6:583:LEU:HB3	3:6:586:LEU:HB2	1.90	0.53
5:4:301:ILE:O	5:4:304:GLN:NE2	2.41	0.53
16:G:57:GLU:OE1	23:O:15:THR:N	2.42	0.53
28:T:22:THR:OG1	28:T:68:ALA:O	2.26	0.53
31:W:105:MET:HA	31:W:108:LEU:HD12	1.91	0.53
42:j:108:THR:OG1	43:g:75:THR:O	2.27	0.53
45:k:7:ALA:HB1	46:l:43:PRO:HD3	1.91	0.53
45:k:131:ARG:NE	45:k:174:VAL:O	2.42	0.53
45:k:146:ARG:HE	45:k:150:PHE:HZ	1.57	0.53
47:m:6:LYS:HD3	47:m:16:ASN:ND2	2.24	0.53
50:q:87:LYS:HG3	50:q:89:TYR:H	1.74	0.53
45:w:188:ARG:HB2	45:w:189:HIS:ND1	2.23	0.53
46:x:227:ARG:HB3	46:x:228:GLY:CA	2.39	0.53
47:y:165:TRP:HE3	47:y:167:GLY:O	1.92	0.53
47:y:360:LEU:HD12	47:y:364:VAL:HB	1.90	0.53
48:z:31:GLN:HA	48:z:34:LYS:HB3	1.91	0.53
57:B9:104:TRP:CG	57:B9:203:ASN:HB2	2.44	0.53
7:8:119:GLU:O	7:8:159:ARG:NH2	2.42	0.52
13:D:154:GLY:O	13:D:158:ASN:ND2	2.42	0.52
45:k:125:SER:O	45:k:129:LYS:NZ	2.38	0.52
46:l:276:GLN:HG3	46:l:277:HIS:N	2.24	0.52
48:o:116:ILE:HD12	48:o:119:ALA:HB3	1.91	0.52
50:q:110:LYS:NZ	53:A3:11:ARG:O	2.34	0.52
47:y:6:LYS:HD3	47:y:16:ASN:ND2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:100:ARG:HH22	77:y:402:HEM:CGA	2.20	0.52
48:z:178:THR:HB	48:z:181:GLN:HB2	1.91	0.52
49:A0:15:ARG:NE	51:A2:21:PHE:O	2.42	0.52
53:A3:17:TRP:HA	53:A3:20:THR:HB	1.91	0.52
57:B9:102:HIS:O	57:B9:104:TRP:N	2.42	0.52
59:A7:23:PRO:HD2	60:A6:34:ASN:HD22	1.74	0.52
2:7:147:TYR:OH	9:3:71:LEU:O	2.24	0.52
28:T:33:GLY:C	28:T:60:THR:CG2	2.81	0.52
31:W:105:MET:CB	31:W:108:LEU:HD12	2.39	0.52
45:k:2:ALA:HB2	46:l:40:ASN:O	2.09	0.52
45:k:146:ARG:HG2	45:k:150:PHE:HE2	1.73	0.52
49:p:127:VAL:CB	49:p:132:TRP:H	2.22	0.52
31:M:26:ASP:HB3	31:M:40:LEU:HD21	1.89	0.52
47:m:34:GLY:HA3	77:m:402:HEM:HBA2	1.91	0.52
47:m:131:TYR:CE2	47:m:139:SER:HA	2.45	0.52
47:m:207:ASN:OD1	47:m:210:GLY:N	2.39	0.52
49:p:51:ALA:O	49:p:55:VAL:N	2.37	0.52
47:y:131:TYR:CE2	47:y:139:SER:HA	2.44	0.52
50:A1:87:LYS:HE3	50:A1:89:TYR:HB3	1.90	0.52
3:6:583:LEU:HD23	3:6:586:LEU:HD22	1.90	0.52
12:C:149:THR:OG1	12:C:150:ASP:N	2.42	0.52
12:C:207:SER:OG	13:D:171:ARG:NH2	2.42	0.52
13:D:86:THR:OG1	13:D:114:ARG:NH2	2.42	0.52
14:E:59:GLN:HA	14:E:64:THR:HG22	1.92	0.52
21:L:56:PRO:HA	25:Q:128:VAL:HG23	1.92	0.52
45:w:146:ARG:HE	45:w:150:PHE:HZ	1.57	0.52
45:w:443:TRP:HB3	45:w:445:ARG:H	1.73	0.52
46:x:132:PHE:HB3	46:x:188:PRO:HB3	1.90	0.52
47:y:83:HIS:HE1	77:y:401:HEM:C1C	2.27	0.52
48:z:138:PRO:HD2	48:z:141:VAL:HG11	1.90	0.52
57:B9:33:LEU:HD23	64:B6:28:SER:HB2	1.91	0.52
57:B9:100:MET:CE	57:B9:157:GLU:HG3	2.40	0.52
59:A7:40:LEU:HD22	59:A7:59:LEU:HD13	1.91	0.52
45:k:111:GLU:HG2	45:k:215:HIS:CE1	2.45	0.52
45:k:216:PHE:N	45:k:218:GLY:HA3	2.25	0.52
48:o:23:HIS:CD2	54:u:55:ILE:HD12	2.45	0.52
45:w:133:VAL:O	45:w:136:GLN:HB3	2.10	0.52
45:w:294:LEU:HG	45:w:341:GLN:HG3	1.91	0.52
45:w:392:LEU:HA	45:w:395:TRP:HD1	1.75	0.52
46:x:68:LEU:HD13	46:x:144:LEU:HD21	1.91	0.52
46:x:399:LEU:HD23	46:x:402:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:550:SER:OG	3:6:551:SER:N	2.39	0.52
29:U:67:GLU:HA	29:U:71:LYS:HB2	1.92	0.52
47:m:123:VAL:HG22	47:m:189:ILE:HD13	1.91	0.52
47:m:360:LEU:HD12	47:m:364:VAL:HB	1.90	0.52
48:o:12:TRP:HA	52:s:74:PHE:CZ	2.44	0.52
45:w:106:LEU:HD22	45:w:203:LEU:HD21	1.90	0.52
48:z:110:PRO:HG3	78:z:301:HEC:HMD3	1.91	0.52
9:3:68:GLU:HG3	9:3:98:LEU:HD12	1.92	0.52
26:R:252:ALA:HB2	26:R:338:LEU:HD11	1.91	0.52
28:T:45:THR:O	28:T:47:THR:N	2.43	0.52
46:l:68:LEU:HD13	46:l:144:LEU:HD21	1.91	0.52
45:w:159:GLN:HG3	45:w:235:ARG:HH21	1.75	0.52
46:x:67:HIS:HA	46:x:70:ARG:NH2	2.24	0.52
47:y:78:ILE:HG12	47:y:79:ILE:HG13	1.89	0.52
48:z:222:MET:O	48:z:225:HIS:HB3	2.10	0.52
52:B5:41:ASP:HA	52:B5:44:VAL:HB	1.91	0.52
12:C:70:ILE:HG13	12:C:71:LEU:HD12	1.91	0.52
12:C:154:PRO:HG2	23:O:18:LYS:HE2	1.92	0.52
39:f:139:GLN:HE22	39:f:157:ALA:HB1	1.74	0.52
43:g:141:ASP:N	43:g:141:ASP:OD1	2.41	0.52
45:k:62:LEU:HA	45:k:65:LYS:HD2	1.91	0.52
45:k:106:LEU:HD22	45:k:203:LEU:HD21	1.90	0.52
45:k:133:VAL:O	45:k:136:GLN:HB3	2.10	0.52
45:k:227:ALA:O	45:k:228:VAL:HG23	2.10	0.52
47:m:345:HIS:HA	47:m:348:ILE:HB	1.92	0.52
48:o:27:ARG:NH1	54:u:58:LYS:HD2	2.25	0.52
48:o:138:PRO:HD2	48:o:141:VAL:HG11	1.90	0.52
46:x:294:SER:O	46:x:298:ALA:N	2.25	0.52
47:y:58:ASP:N	47:y:62:ALA:HB2	2.23	0.52
47:y:97:HIS:HE1	77:y:402:HEM:C1A	2.28	0.52
47:y:123:VAL:HG22	47:y:189:ILE:HD13	1.91	0.52
5:4:118:PHE:O	5:4:122:PHE:N	2.40	0.52
20:K:31:GLN:HB3	20:K:34:ARG:HH21	1.74	0.52
47:m:83:HIS:HE1	77:m:401:HEM:C1C	2.27	0.52
45:w:111:GLU:HG2	45:w:215:HIS:CE1	2.45	0.52
47:y:71:ARG:HB3	48:z:49:ARG:HH22	1.74	0.52
51:A2:8:THR:HG22	51:A2:9:ARG:H	1.73	0.52
53:A3:16:ASN:O	53:A3:20:THR:N	2.19	0.52
56:A9:302:ARG:O	56:A9:306:THR:HG23	2.09	0.52
1:9:149:LEU:HD23	1:9:150:GLU:H	1.74	0.52
22:N:36:GLY:O	22:N:45:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:297:ILE:HG21	47:m:2:THR:HG21	1.91	0.52
47:m:41:LEU:O	47:m:45:ILE:HG13	2.10	0.52
52:s:41:ASP:HA	52:s:44:VAL:HB	1.91	0.52
54:u:44:GLU:O	54:u:47:ASN:N	2.43	0.52
45:w:215:HIS:O	45:w:216:PHE:HB2	2.08	0.52
45:w:391:PRO:HB3	45:w:394:GLU:OE1	2.10	0.52
46:x:148:LYS:NZ	46:x:178:CYS:O	2.41	0.52
46:x:228:GLY:C	46:x:230:LEU:H	2.17	0.52
50:A1:87:LYS:HG3	50:A1:89:TYR:H	1.74	0.52
55:B3:59:ALA:O	55:B3:61:GLY:N	2.40	0.52
56:A9:225:GLY:HA3	58:B7:112:LEU:HD13	1.92	0.52
18:I:59:ARG:NH1	29:U:123:GLN:OE1	2.43	0.51
39:f:154:LEU:HB2	39:f:157:ALA:HA	1.92	0.51
45:k:17:SER:HG	45:k:205:HIS:CE1	2.22	0.51
45:k:303:LEU:HD11	47:m:2:THR:OG1	2.10	0.51
46:l:29:LEU:HD12	46:l:33:LEU:CD1	2.41	0.51
48:z:163:PRO:HG2	78:z:301:HEC:HBB2	1.92	0.51
53:A3:19:PRO:O	53:A3:23:LEU:HG	2.09	0.51
56:A9:268:PHE:CZ	57:B9:58:ALA:HA	2.44	0.51
10:A:352:ILE:HD11	10:A:528:LEU:HD22	1.93	0.51
47:m:257:THR:HA	48:o:115:TYR:OH	2.10	0.51
50:q:21:TYR:CD2	50:q:83:TYR:HD1	2.28	0.51
50:q:40:ASN:ND2	50:q:42:ASP:HB2	2.24	0.51
48:z:148:TYR:N	48:z:158:ILE:O	2.37	0.51
51:A2:37:VAL:CG1	51:A2:41:THR:HG21	2.41	0.51
56:A9:75:ILE:O	56:A9:79:GLY:HA3	2.11	0.51
10:A:50:LEU:HG	10:A:60:ILE:HD11	1.93	0.51
45:k:2:ALA:HB3	46:l:113:ARG:CZ	2.40	0.51
46:l:245:ARG:CZ	46:l:430:LEU:HD13	2.40	0.51
45:w:334:MET:O	45:w:338:LEU:N	2.41	0.51
49:A0:148:ALA:HA	49:A0:156:TYR:HA	1.93	0.51
61:B2:8:THR:OG1	61:B2:11:GLU:HG2	2.09	0.51
11:B:326:CYS:HA	11:B:329:ARG:HG2	1.92	0.51
26:R:64:PHE:HZ	26:R:208:GLY:HA3	1.74	0.51
26:R:143:ASP:O	26:R:147:LYS:N	2.41	0.51
45:k:392:LEU:HA	45:k:395:TRP:HD1	1.75	0.51
46:l:67:HIS:CD2	46:l:178:CYS:H	2.29	0.51
46:l:271:ALA:O	46:l:275:LEU:N	2.37	0.51
47:m:36:LEU:HA	47:m:39:ILE:HD12	1.91	0.51
47:m:165:TRP:HE3	47:m:167:GLY:O	1.92	0.51
48:o:110:PRO:HG3	78:o:301:HEC:HMD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:112:ASP:OD1	48:o:113:LEU:N	2.43	0.51
50:q:104:ARG:HG2	46:x:83:PHE:CE2	2.45	0.51
54:u:16:ARG:HB2	54:u:19:THR:OG1	2.11	0.51
45:w:3:THR:HG22	45:w:5:ALA:H	1.75	0.51
47:y:223:TYR:O	47:y:226:ILE:N	2.43	0.51
48:z:102:ARG:NH2	48:z:109:LEU:HB2	2.25	0.51
48:z:184:LYS:HD2	52:B5:74:PHE:CE1	2.46	0.51
34:Z:22:TRP:NE1	34:Z:51:TRP:O	2.43	0.51
45:k:3:THR:HG22	45:k:5:ALA:H	1.75	0.51
45:k:217:SER:N	45:k:218:GLY:CA	2.74	0.51
46:l:67:HIS:HA	46:l:70:ARG:NH2	2.24	0.51
51:r:8:THR:HG22	51:r:9:ARG:H	1.73	0.51
45:w:159:GLN:NE2	45:w:237:THR:HG21	2.26	0.51
46:x:29:LEU:HD12	46:x:33:LEU:CD1	2.41	0.51
77:y:402:HEM:O2A	77:y:402:HEM:HHA	2.11	0.51
48:z:20:SER:OG	54:B4:51:LEU:HD21	2.11	0.51
7:8:204:TYR:HE1	7:8:427:LEU:HD13	1.74	0.51
45:k:66:GLY:O	45:k:121:SER:OG	2.27	0.51
77:m:402:HEM:O2A	77:m:402:HEM:HHA	2.11	0.51
48:o:164:ILE:HG22	48:o:179:MET:HG3	1.92	0.51
48:o:222:MET:O	48:o:225:HIS:HB3	2.10	0.51
48:o:237:TYR:HB2	50:q:60:PHE:CD1	2.46	0.51
52:s:57:GLU:OE1	52:s:57:GLU:N	2.29	0.51
48:z:48:TYR:HE1	48:z:91:PHE:HE1	1.58	0.51
48:z:164:ILE:HG22	48:z:179:MET:HG3	1.93	0.51
48:z:204:MET:HE3	49:A0:57:GLN:HE22	1.75	0.51
56:A9:240:HIS:HB3	56:A9:241:PRO:HD3	1.92	0.51
57:B9:136:LEU:HB3	57:B9:193:TYR:CD2	2.46	0.51
58:B7:18:LEU:HD22	58:B7:22:LEU:HD22	1.92	0.51
5:4:68:LEU:HA	5:4:71:TRP:HD1	1.75	0.51
6:5:2:SER:OG	6:5:3:MET:N	2.43	0.51
11:B:385:TYR:HD2	14:E:122:VAL:HG11	1.75	0.51
45:k:193:PRO:HD3	45:k:223:TYR:CD1	2.45	0.51
45:k:347:THR:HG1	53:t:17:TRP:HZ2	1.59	0.51
46:l:399:LEU:HD23	46:l:402:ILE:HD12	1.92	0.51
47:m:97:HIS:HE1	77:m:402:HEM:C1A	2.28	0.51
47:m:223:TYR:O	47:m:226:ILE:N	2.43	0.51
48:o:69:GLU:OE1	48:o:84:PRO:HD3	2.10	0.51
48:o:163:PRO:HG2	78:o:301:HEC:HBB2	1.92	0.51
51:r:58:VAL:HA	51:r:61:TRP:HB3	1.93	0.51
52:s:66:ASP:HA	52:s:69:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:118:GLN:NE2	45:w:217:SER:O	2.36	0.51
47:y:225:THR:O	47:y:228:ASP:HB2	2.11	0.51
52:B5:66:ASP:HA	52:B5:69:VAL:HB	1.92	0.51
54:B4:16:ARG:HB2	54:B4:19:THR:OG1	2.11	0.51
56:A9:347:LEU:HG	56:A9:383:MET:HE3	1.93	0.51
60:A6:63:SER:O	60:A6:67:ILE:HG13	2.10	0.51
3:6:204:LEU:HD12	43:g:129:LEU:HD11	1.91	0.51
7:8:409:ILE:HG23	7:8:439:ILE:HD12	1.93	0.51
8:1:290:TRP:NE1	9:3:112:GLU:OE2	2.44	0.51
48:o:11:PRO:HB2	52:s:74:PHE:CD2	2.46	0.51
48:o:208:MET:O	48:o:212:MET:N	2.44	0.51
47:y:41:LEU:O	47:y:45:ILE:HG13	2.10	0.51
48:z:112:ASP:OD1	48:z:113:LEU:N	2.43	0.51
52:B5:13:LEU:C	52:B5:15:ASP:H	2.14	0.51
52:B5:41:ASP:O	52:B5:45:SER:N	2.44	0.51
54:B4:44:GLU:O	54:B4:47:ASN:N	2.43	0.51
56:A9:250:GLY:O	56:A9:254:ILE:HG12	2.11	0.51
57:B9:1:MET:SD	57:B9:133:LEU:CD1	2.99	0.51
63:A5:60:TYR:CD1	63:A5:60:TYR:C	2.88	0.51
18:I:108:LYS:HE2	18:I:118:GLN:NE2	2.26	0.51
26:R:182:ARG:O	26:R:183:SER:OG	2.27	0.51
45:k:58:PHE:O	45:k:62:LEU:HG	2.11	0.51
45:k:172:GLU:HB2	45:k:176:LYS:NZ	2.26	0.51
45:k:191:LYS:HE2	45:k:226:ASP:HB2	1.93	0.51
45:k:263:ALA:HA	45:k:386:TYR:CE1	2.46	0.51
46:l:144:LEU:O	46:l:147:ASP:HB3	2.11	0.51
47:m:77:TRP:CE2	47:m:78:ILE:HG22	2.46	0.51
48:o:31:GLN:HA	48:o:34:LYS:HB3	1.91	0.51
48:o:102:ARG:NH2	48:o:109:LEU:HB2	2.25	0.51
50:q:22:ASN:OD1	50:q:27:ASN:ND2	2.44	0.51
52:s:40:CYS:O	52:s:44:VAL:HG23	2.11	0.51
54:u:58:LYS:HG3	54:u:59:TYR:N	2.26	0.51
45:w:153:LEU:HD13	45:w:423:ALA:HB2	1.93	0.51
52:B5:40:CYS:O	52:B5:44:VAL:HG23	2.11	0.51
1:9:54:ASP:OD1	1:9:60:TYR:OH	2.29	0.51
4:2:265:MET:HE1	25:Q:167:LEU:HD11	1.93	0.51
11:B:303:ARG:HB3	11:B:311:TYR:HE2	1.75	0.51
17:H:22:SER:HA	17:H:25:GLN:HE22	1.75	0.51
28:T:41:VAL:HG11	28:T:59:TYR:CE1	2.46	0.51
47:m:58:ASP:N	47:m:62:ALA:HB2	2.23	0.51
47:m:127:ALA:HB1	77:m:401:HEM:HMA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:225:THR:O	47:m:228:ASP:HB2	2.11	0.51
51:A2:36:ASN:CG	51:A2:39:ARG:HE	2.19	0.51
62:A4:42:ARG:HH11	62:A4:42:ARG:HG3	1.75	0.51
8:1:32:GLN:HE22	11:B:198:THR:HG22	1.75	0.50
45:k:142:ASP:OD2	49:p:1:SER:OG	2.29	0.50
49:p:151:GLY:N	49:p:152:ASP:HA	2.25	0.50
45:w:58:PHE:O	45:w:62:LEU:HG	2.11	0.50
47:y:36:LEU:HA	47:y:39:ILE:HD12	1.91	0.50
48:z:3:LEU:HD21	51:A2:71:ARG:HG3	1.93	0.50
49:A0:58:PHE:O	49:A0:61:SER:OG	2.22	0.50
56:A9:184:PHE:H	56:A9:256:HIS:CE1	2.29	0.50
57:B9:68:LEU:HB3	57:B9:69:PRO:HD3	1.91	0.50
58:B7:119:THR:O	62:A4:52:HIS:CE1	2.63	0.50
11:B:238:LEU:HD23	30:V:10:MET:HE1	1.93	0.50
19:J:3:PHE:HZ	70:J:101:CDL:HA21	1.76	0.50
28:T:32:ALA:C	28:T:35:VAL:CG1	2.68	0.50
45:k:213:GLN:O	45:k:217:SER:OG	2.28	0.50
48:o:11:PRO:HA	48:o:15:ARG:HH11	1.76	0.50
48:o:83:ARG:O	48:o:85:GLY:N	2.44	0.50
53:t:18:VAL:HB	53:t:19:PRO:HD3	1.93	0.50
45:w:263:ALA:HA	45:w:386:TYR:CE1	2.46	0.50
46:x:67:HIS:CD2	46:x:178:CYS:H	2.29	0.50
46:x:245:ARG:CZ	46:x:430:LEU:HD13	2.40	0.50
47:y:345:HIS:HA	47:y:348:ILE:HB	1.92	0.50
52:B5:55:THR:O	52:B5:59:LEU:HG	2.12	0.50
56:A9:172:LYS:HB2	56:A9:172:LYS:HZ3	1.76	0.50
57:B9:139:ASP:OD1	57:B9:140:ASN:N	2.44	0.50
16:G:128:PHE:HD2	16:G:134:ALA:HA	1.74	0.50
47:m:56:THR:HG21	47:y:58:ASP:CG	2.36	0.50
47:m:163:TRP:HE3	47:m:164:ILE:HG13	1.76	0.50
48:o:128:PHE:HD1	48:o:187:CYS:HG	1.56	0.50
50:q:25:GLY:HA2	50:q:28:LYS:NZ	2.25	0.50
52:s:41:ASP:O	52:s:45:SER:N	2.44	0.50
53:t:28:GLY:O	53:t:32:LEU:HB2	2.11	0.50
45:w:150:PHE:O	45:w:153:LEU:N	2.42	0.50
45:w:172:GLU:HB2	45:w:176:LYS:NZ	2.26	0.50
46:x:303:VAL:HG12	46:x:304:HIS:N	2.22	0.50
47:y:77:TRP:CE2	47:y:78:ILE:HG22	2.46	0.50
47:y:127:ALA:HB1	77:y:401:HEM:HMA2	1.93	0.50
47:y:330:ALA:HB2	51:A2:52:PHE:CE1	2.46	0.50
49:A0:78:LEU:H	49:A0:192:MET:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:225:MET:SD	8:1:225:MET:C	2.94	0.50
10:A:309:ASN:ND2	10:A:315:THR:OG1	2.45	0.50
11:B:203:MET:HE1	11:B:254:ARG:HB3	1.94	0.50
12:C:226:VAL:HG11	16:G:120:PRO:HB3	1.92	0.50
48:o:70:VAL:HA	48:o:83:ARG:H	1.77	0.50
52:s:55:THR:O	52:s:59:LEU:HG	2.12	0.50
52:s:73:LEU:HA	52:s:76:SER:HB2	1.94	0.50
45:w:205:HIS:O	45:w:208:LEU:HB3	2.11	0.50
46:x:313:ASN:HB2	46:x:322:PHE:HD1	1.76	0.50
47:y:163:TRP:HE3	47:y:164:ILE:HG13	1.76	0.50
48:z:52:VAL:HG13	54:B4:56:LYS:HZ3	1.76	0.50
61:B2:37:LYS:HD3	61:B2:37:LYS:N	2.27	0.50
1:9:62:ARG:NH1	15:F:83:TYR:OH	2.39	0.50
10:A:255:ASP:N	10:A:255:ASP:OD1	2.43	0.50
10:A:306:MET:HG2	10:A:316:HIS:HA	1.94	0.50
35:a:109:ARG:HH22	42:j:119:VAL:HG13	1.76	0.50
44:e:88:PRO:HD2	44:e:114:ARG:HB3	1.93	0.50
45:k:40:TRP:HH2	45:k:376:CYS:SG	2.35	0.50
45:k:150:PHE:O	45:k:153:LEU:N	2.42	0.50
45:k:159:GLN:HG3	45:k:235:ARG:HH21	1.75	0.50
45:k:391:PRO:HB3	45:k:394:GLU:OE1	2.10	0.50
46:l:50:PHE:HE2	46:l:383:GLY:HA3	1.74	0.50
46:l:313:ASN:HB2	46:l:322:PHE:HD1	1.76	0.50
47:m:31:TRP:HA	47:m:100:ARG:NH1	2.21	0.50
47:m:227:LYS:HG3	48:o:223:LYS:HE3	1.93	0.50
47:m:236:ILE:O	47:m:240:MET:N	2.32	0.50
48:o:166:ASN:HA	48:o:179:MET:N	2.27	0.50
50:q:52:GLU:O	50:q:56:ASN:N	2.24	0.50
46:x:52:LYS:HD2	46:x:203:ARG:HG2	1.93	0.50
46:x:144:LEU:O	46:x:147:ASP:HB3	2.11	0.50
46:x:243:GLU:HB2	46:x:424:MET:HB3	1.94	0.50
48:z:11:PRO:HA	48:z:15:ARG:HH11	1.76	0.50
48:z:208:MET:O	48:z:212:MET:N	2.44	0.50
3:6:350:LEU:HD22	3:6:353:GLU:HB2	1.94	0.50
11:B:338:ARG:NH1	30:V:22:LYS:O	2.44	0.50
45:k:205:HIS:O	45:k:208:LEU:HB3	2.11	0.50
47:m:83:HIS:HD2	77:m:401:HEM:CHA	2.25	0.50
48:o:210:LEU:O	48:o:214:LEU:HG	2.12	0.50
48:o:223:LYS:O	48:o:227:TRP:HD1	1.95	0.50
55:v:63:PRO:N	55:v:64:LEU:HA	2.27	0.50
45:w:340:GLY:O	45:w:343:MET:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:210:LEU:O	48:z:214:LEU:HG	2.12	0.50
51:A2:58:VAL:HA	51:A2:61:TRP:HB3	1.93	0.50
52:B5:29:LYS:HA	52:B5:32:LYS:HD3	1.94	0.50
54:B4:58:LYS:HG3	54:B4:59:TYR:N	2.26	0.50
62:A4:5:LYS:NZ	62:A4:5:LYS:HB3	2.27	0.50
12:C:85:GLU:OE1	12:C:144:ARG:NH1	2.43	0.50
25:Q:110:CYS:O	25:Q:114:LYS:N	2.41	0.50
26:R:354:ARG:O	26:R:355:ARG:NH2	2.38	0.50
27:S:32:ILE:HG13	27:S:33:LEU:HD12	1.94	0.50
27:S:83:ASP:HB3	27:S:91:PRO:HA	1.93	0.50
45:k:118:GLN:HE22	45:k:221:GLY:HA2	1.77	0.50
45:k:389:ARG:C	45:k:391:PRO:HD3	2.37	0.50
46:l:303:VAL:HG12	46:l:304:HIS:N	2.22	0.50
46:l:397:THR:HA	46:l:400:GLN:OE1	2.12	0.50
47:m:56:THR:HG21	47:y:58:ASP:OD1	2.12	0.50
51:r:74:PRO:HA	51:r:77:TYR:O	2.12	0.50
45:w:40:TRP:HH2	45:w:376:CYS:SG	2.35	0.50
46:x:50:PHE:HE2	46:x:383:GLY:HA3	1.74	0.50
46:x:70:ARG:NH1	46:x:100:SER:OG	2.33	0.50
46:x:271:ALA:O	46:x:275:LEU:N	2.37	0.50
47:y:350:ILE:HA	47:y:353:LEU:HD12	1.94	0.50
56:A9:40:GLU:HG2	56:A9:54:TYR:CD1	2.47	0.50
59:A7:64:PHE:CE1	60:A6:66:ARG:HD2	2.47	0.50
1:9:151:ALA:HA	1:9:154:LYS:HB2	1.94	0.50
10:A:251:ILE:HB	10:A:606:THR:HG22	1.94	0.50
26:R:52:SER:OG	26:R:77:GLY:O	2.27	0.50
27:S:196:ASP:OD1	27:S:246:TYR:HB2	2.06	0.50
45:k:156:THR:HG22	45:k:239:SER:OG	2.11	0.50
46:l:125:ASN:HA	46:l:128:THR:HB	1.94	0.50
46:l:213:HIS:O	46:l:216:LEU:HB3	2.12	0.50
48:o:51:LEU:CD2	48:o:61:ALA:HB3	2.36	0.50
47:y:226:ILE:O	47:y:229:ILE:N	2.45	0.50
56:A9:168:ILE:HG21	56:A9:189:MET:HG3	1.94	0.50
3:6:535:ARG:NH1	44:e:119:THR:O	2.44	0.50
4:2:45:MET:HE1	4:2:53:THR:HA	1.93	0.50
7:8:213:ILE:HD11	7:8:236:PHE:HB2	1.94	0.50
26:R:125:VAL:HG21	26:R:253:ILE:HD11	1.94	0.50
46:l:257:LEU:HD11	46:l:422:LYS:HB3	1.94	0.50
47:m:244:LEU:HD21	48:o:201:ARG:O	2.12	0.50
50:q:87:LYS:CG	50:q:89:TYR:HD2	2.25	0.50
51:r:36:ASN:CG	51:r:39:ARG:HE	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:134:ARG:HG3	46:x:135:TRP:N	2.27	0.50
47:y:98:VAL:O	47:y:101:GLY:N	2.40	0.50
57:B9:186:SER:HB3	57:B9:213:LEU:CD2	2.42	0.50
57:B9:186:SER:CB	57:B9:213:LEU:HD22	2.40	0.50
7:8:48:ARG:HA	7:8:133:HIS:CG	2.47	0.49
12:C:222:VAL:HG21	23:O:110:THR:HG21	1.94	0.49
26:R:237:LYS:HG2	26:R:325:THR:HG23	1.94	0.49
45:k:153:LEU:HD13	45:k:423:ALA:HB2	1.93	0.49
46:l:52:LYS:HB2	46:l:203:ARG:HE	1.77	0.49
46:l:52:LYS:HD2	46:l:203:ARG:HG2	1.93	0.49
46:l:354:ASN:N	46:l:355:PRO:HD2	2.27	0.49
47:m:290:GLY:O	47:m:294:LEU:N	2.35	0.49
45:w:40:TRP:HZ2	45:w:377:GLU:HA	1.77	0.49
45:w:389:ARG:C	45:w:391:PRO:HD3	2.37	0.49
46:x:338:LYS:O	46:x:342:ASN:N	2.35	0.49
52:B5:29:LYS:HA	52:B5:32:LYS:HB3	1.94	0.49
56:A9:145:LEU:HD21	58:B7:32:THR:HG21	1.93	0.49
1:9:236:GLU:OE1	1:9:239:LYS:NZ	2.45	0.49
7:8:177:TYR:O	15:F:96:ARG:NH1	2.44	0.49
10:A:461:PRO:HA	10:A:463:SER:HB3	1.94	0.49
46:l:243:GLU:HB2	46:l:424:MET:HB3	1.94	0.49
48:o:21:LEU:O	54:u:50:LYS:HB3	2.12	0.49
48:o:150:ASN:HD21	48:o:152:TYR:HD2	1.60	0.49
48:o:231:LYS:HB3	50:q:71:ARG:HD3	1.93	0.49
45:w:1:THR:OG1	45:w:2:ALA:N	2.45	0.49
46:x:29:LEU:HD12	46:x:33:LEU:HD12	1.94	0.49
46:x:109:VAL:HG22	46:x:119:LEU:HD21	1.94	0.49
47:y:125:ALA:O	47:y:128:PHE:HB3	2.12	0.49
47:y:257:THR:HA	48:z:115:TYR:OH	2.12	0.49
49:A0:41:ALA:HB1	54:B4:24:ILE:HG12	1.93	0.49
56:A9:508:PRO:HG3	58:B7:6:HIS:HB3	1.94	0.49
4:2:137:ALA:O	4:2:140:SER:OG	2.29	0.49
10:A:462:PHE:O	10:A:464:GLN:N	2.44	0.49
12:C:123:THR:HG21	16:G:129:SER:H	1.76	0.49
45:k:35:CYS:N	45:k:101:ALA:O	2.28	0.49
45:k:159:GLN:NE2	45:k:237:THR:HG21	2.26	0.49
45:k:193:PRO:HD3	45:k:223:TYR:HD1	1.78	0.49
45:k:356:ARG:O	45:k:360:LEU:HG	2.13	0.49
46:l:241:GLY:HA3	46:l:421:ARG:NE	2.27	0.49
46:l:300:ALA:HB2	46:l:307:PHE:HZ	1.77	0.49
47:m:125:ALA:O	47:m:128:PHE:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:226:ILE:O	47:m:229:ILE:N	2.45	0.49
50:q:73:GLN:HG2	51:r:39:ARG:NH2	2.27	0.49
46:x:97:SER:CB	55:B3:70:LEU:HD22	2.42	0.49
46:x:125:ASN:HA	46:x:128:THR:HB	1.93	0.49
47:y:44:GLN:O	47:y:47:THR:N	2.44	0.49
48:z:223:LYS:O	48:z:227:TRP:HD1	1.95	0.49
52:B5:73:LEU:HA	52:B5:76:SER:HB2	1.94	0.49
53:A3:46:PRO:O	54:B4:33:ARG:NH2	2.45	0.49
62:A4:42:ARG:NH1	62:A4:74:ARG:HH21	2.10	0.49
9:3:41:PHE:C	9:3:43:PRO:CD	2.84	0.49
10:A:33:GLU:HG2	10:A:42:MET:HG2	1.93	0.49
10:A:382:ARG:HB2	10:A:385:TYR:HB3	1.93	0.49
45:k:235:ARG:NH1	49:p:14:ARG:HH12	2.10	0.49
46:l:46:ARG:HD3	46:l:379:LEU:HD22	1.95	0.49
47:m:350:ILE:HA	47:m:353:LEU:HD12	1.94	0.49
48:o:48:TYR:HE1	48:o:91:PHE:HE1	1.58	0.49
48:o:68:VAL:HB	48:o:69:GLU:OE2	2.12	0.49
48:o:165:TYR:CD2	48:o:168:VAL:HG22	2.47	0.49
48:o:198:HIS:O	48:o:201:ARG:HG2	2.12	0.49
48:o:224:ARG:NH2	51:r:25:ALA:O	2.41	0.49
45:w:131:ARG:NE	45:w:174:VAL:O	2.42	0.49
45:w:156:THR:HG22	45:w:239:SER:OG	2.11	0.49
46:x:113:ARG:HH12	46:x:210:GLY:C	2.20	0.49
50:A1:26:PHE:O	50:A1:28:LYS:HG3	2.13	0.49
52:B5:10:GLU:OE1	52:B5:12:GLU:N	2.45	0.49
26:R:265:PHE:HA	26:R:335:LEU:HB2	1.94	0.49
31:W:105:MET:CA	31:W:108:LEU:HD12	2.42	0.49
45:k:444:LEU:HB3	45:k:446:PHE:HD2	1.76	0.49
46:l:169:ARG:NE	46:x:435:PHE:CE2	2.80	0.49
48:o:180:SER:HB3	52:s:17:LEU:HB2	1.93	0.49
46:x:257:LEU:HD11	46:x:422:LYS:HB3	1.94	0.49
47:y:355:SER:O	47:y:358:TYR:HB3	2.13	0.49
49:A0:30:GLU:OE2	54:B4:10:TYR:HD2	1.95	0.49
56:A9:377:PHE:HA	56:A9:380:VAL:HG22	1.93	0.49
57:B9:13:THR:HG22	57:B9:13:THR:O	2.12	0.49
5:4:208:PRO:HG2	5:4:216:LEU:HD22	1.94	0.49
5:4:370:PRO:HA	5:4:375:LEU:HB2	1.94	0.49
16:G:79:ILE:HD13	16:G:134:ALA:HB1	1.94	0.49
17:H:21:GLN:HB3	17:H:37:GLU:HG3	1.95	0.49
23:O:25:MET:SD	23:O:29:LYS:NZ	2.85	0.49
26:R:314:THR:HG22	26:R:316:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:62:THR:CG2	28:T:104:ARG:CZ	2.90	0.49
28:T:62:THR:CG2	28:T:104:ARG:HD3	2.39	0.49
31:W:104:PHE:C	31:W:108:LEU:HG	2.27	0.49
46:l:134:ARG:HG3	46:l:135:TRP:N	2.27	0.49
46:l:182:ARG:NH1	46:l:185:LYS:HE2	2.28	0.49
46:l:276:GLN:HG3	46:l:277:HIS:H	1.78	0.49
46:x:411:ILE:O	46:x:415:LYS:HG3	2.13	0.49
47:y:83:HIS:HD2	77:y:401:HEM:CHA	2.25	0.49
47:y:250:LEU:C	47:y:252:ASP:H	2.21	0.49
48:z:166:ASN:HA	48:z:179:MET:N	2.27	0.49
50:A1:57:ASP:O	50:A1:61:ARG:NH1	2.46	0.49
62:A4:44:ARG:HD2	62:A4:74:ARG:O	2.12	0.49
5:4:119:TYR:HE1	5:4:157:SER:HB2	1.78	0.49
45:k:40:TRP:HZ2	45:k:377:GLU:HA	1.77	0.49
45:k:329:MET:HB3	51:r:2:ARG:HE	1.78	0.49
45:k:340:GLY:O	45:k:343:MET:N	2.45	0.49
45:k:357:GLY:HA2	45:k:360:LEU:HD12	1.95	0.49
46:l:29:LEU:HD12	46:l:33:LEU:HD12	1.94	0.49
46:l:66:SER:HA	46:l:69:LEU:HB3	1.94	0.49
46:l:367:GLY:HA2	46:l:370:MET:HE3	1.95	0.49
47:m:74:ASN:ND2	49:p:64:ALA:O	2.46	0.49
47:m:345:HIS:HA	47:m:348:ILE:HD12	1.95	0.49
50:q:49:ARG:HD3	46:x:135:TRP:CE2	2.47	0.49
45:w:203:LEU:HA	45:w:207:GLN:HE21	1.77	0.49
45:w:260:PRO:HG3	45:w:414:TYR:OH	2.13	0.49
46:x:397:THR:HA	46:x:400:GLN:OE1	2.12	0.49
47:y:311:LYS:O	50:A1:38:HIS:N	2.34	0.49
48:z:23:HIS:HD2	54:B4:55:ILE:HD12	1.78	0.49
56:A9:232:GLN:HB2	56:A9:292:MET:HE3	1.93	0.49
62:A4:42:ARG:HD2	62:A4:42:ARG:O	2.13	0.49
3:6:258:PHE:HA	3:6:261:ILE:HD12	1.95	0.49
11:B:251:PHE:HD2	11:B:341:ILE:HD11	1.77	0.49
45:k:334:MET:O	45:k:338:LEU:N	2.41	0.49
46:l:67:HIS:HD1	46:l:70:ARG:HH22	1.61	0.49
50:q:74:ILE:HG22	51:r:39:ARG:HH11	1.78	0.49
45:w:59:VAL:O	45:w:62:LEU:N	2.44	0.49
45:w:406:VAL:O	45:w:410:VAL:HG23	2.13	0.49
46:x:66:SER:HA	46:x:69:LEU:HB3	1.94	0.49
48:z:231:LYS:HA	50:A1:70:MET:HE3	1.94	0.49
50:A1:52:GLU:O	50:A1:56:ASN:N	2.24	0.49
52:B5:57:GLU:OE1	52:B5:57:GLU:N	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:266:GLU:HB2	56:A9:267:PRO:HD2	1.95	0.49
7:8:364:VAL:HG12	7:8:400:VAL:HG22	1.94	0.49
10:A:650:SER:OG	10:A:652:ASN:OD1	2.31	0.49
37:c:25:ASP:OD2	39:f:125:TRP:NE1	2.46	0.49
45:k:406:VAL:O	45:k:410:VAL:HG23	2.13	0.49
46:l:134:ARG:NH2	50:A1:51:PRO:HB3	2.28	0.49
47:m:44:GLN:O	47:m:47:THR:N	2.44	0.49
47:m:207:ASN:HB2	47:m:208:PRO:HD2	1.95	0.49
47:m:250:LEU:C	47:m:252:ASP:H	2.21	0.49
47:m:355:SER:O	47:m:358:TYR:HB3	2.13	0.49
50:q:44:LYS:HE3	50:q:48:ARG:NH2	2.28	0.49
50:q:86:ASP:OD1	50:q:87:LYS:N	2.46	0.49
52:s:29:LYS:HA	52:s:32:LYS:HD3	1.94	0.49
46:x:354:ASN:N	46:x:355:PRO:HD2	2.28	0.49
48:z:198:HIS:O	48:z:201:ARG:HG2	2.13	0.49
50:A1:44:LYS:HE3	50:A1:48:ARG:NH2	2.28	0.49
50:A1:86:ASP:OD1	50:A1:87:LYS:N	2.46	0.49
53:A3:47:TYR:HB2	54:B4:33:ARG:HH21	1.77	0.49
63:A5:24:ASN:ND2	63:A5:26:THR:H	2.11	0.49
10:A:578:PRO:HB3	29:U:140:PRO:HG3	1.95	0.49
27:S:202:VAL:HA	27:S:205:ARG:HB2	1.95	0.49
45:k:260:PRO:HG3	45:k:414:TYR:OH	2.13	0.49
46:l:113:ARG:HH12	46:l:210:GLY:C	2.20	0.49
46:l:411:ILE:O	46:l:415:LYS:HG3	2.12	0.49
48:o:165:TYR:CE2	48:o:168:VAL:HG22	2.48	0.49
50:q:57:ASP:O	50:q:61:ARG:NH1	2.46	0.49
53:t:16:ASN:C	53:t:18:VAL:H	2.21	0.49
50:A1:51:PRO:HG2	50:A1:54:LEU:HD13	1.94	0.49
61:B2:49:VAL:HG21	61:B2:74:LEU:HD12	1.95	0.49
6:5:36:MET:O	6:5:39:SER:OG	2.25	0.48
7:8:409:ILE:HD11	7:8:446:LEU:HD11	1.95	0.48
17:H:15:ASP:OD1	17:H:15:ASP:N	2.45	0.48
45:k:1:THR:OG1	45:k:2:ALA:N	2.45	0.48
45:k:59:VAL:O	45:k:62:LEU:N	2.44	0.48
45:k:203:LEU:HA	45:k:207:GLN:HE21	1.78	0.48
47:m:114:ASN:O	47:m:117:VAL:HB	2.13	0.48
48:o:11:PRO:HA	48:o:15:ARG:CD	2.43	0.48
48:o:57:THR:HA	54:u:56:LYS:HZ1	1.76	0.48
48:o:71:GLN:OE1	48:o:71:GLN:N	2.46	0.48
48:o:166:ASN:OD1	48:o:178:THR:HG23	2.13	0.48
50:q:51:PRO:HG2	50:q:54:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:29:LYS:HA	52:s:32:LYS:HB3	1.94	0.48
45:w:356:ARG:O	45:w:360:LEU:HG	2.13	0.48
46:x:46:ARG:HD3	46:x:379:LEU:HD22	1.95	0.48
46:x:52:LYS:HB2	46:x:203:ARG:HE	1.77	0.48
46:x:203:ARG:NH1	46:x:231:GLY:HA2	2.28	0.48
46:x:241:GLY:HA3	46:x:421:ARG:NE	2.27	0.48
46:x:258:VAL:HG11	46:x:321:LEU:HB3	1.95	0.48
46:x:300:ALA:HB2	46:x:307:PHE:HZ	1.77	0.48
47:y:97:HIS:CE1	77:y:402:HEM:C1A	3.01	0.48
47:y:345:HIS:HA	47:y:348:ILE:HD12	1.95	0.48
48:z:165:TYR:CE2	48:z:168:VAL:HG22	2.48	0.48
8:1:168:THR:HG23	8:1:169:GLN:HG3	1.96	0.48
27:S:234:LEU:O	27:S:238:SER:N	2.45	0.48
28:T:62:THR:CG2	28:T:104:ARG:HH11	2.15	0.48
31:W:115:GLN:HE21	31:W:135:ALA:HB1	1.77	0.48
45:k:159:GLN:HE21	45:k:237:THR:HG21	1.77	0.48
45:k:236:PHE:HB3	45:k:258:GLU:CD	2.38	0.48
45:k:245:GLU:HG3	51:r:12:HIS:CE1	2.49	0.48
48:o:22:ASP:HA	54:u:50:LYS:O	2.14	0.48
48:o:150:ASN:O	48:o:156:GLN:HA	2.13	0.48
49:p:31:ALA:HB2	54:u:7:ALA:HB2	1.95	0.48
49:p:125:GLU:O	49:p:128:LYS:N	2.46	0.48
50:q:87:LYS:HG3	50:q:89:TYR:CD2	2.48	0.48
52:s:23:GLN:O	52:s:26:GLN:HB3	2.13	0.48
45:w:66:GLY:O	45:w:121:SER:OG	2.27	0.48
45:w:236:PHE:HB3	45:w:258:GLU:CD	2.38	0.48
46:x:133:ARG:HB2	46:x:136:GLU:CD	2.38	0.48
46:x:304:HIS:HB3	46:x:305:GLN:OE1	2.13	0.48
47:y:207:ASN:HB2	47:y:208:PRO:HD2	1.95	0.48
48:z:28:ARG:HH22	52:B5:78:LYS:HE2	1.79	0.48
48:z:52:VAL:HG12	54:B4:52:TRP:CD1	2.48	0.48
48:z:165:TYR:CD2	48:z:168:VAL:HG22	2.47	0.48
49:A0:10:PHE:O	49:A0:14:ARG:HG3	2.12	0.48
56:A9:197:LEU:O	58:B7:92:LEU:HD22	2.13	0.48
70:4:501:CDL:H171	70:4:501:CDL:H321	1.94	0.48
7:8:273:THR:HA	7:8:291:GLU:HA	1.96	0.48
13:D:155:SER:OG	14:E:150:THR:O	2.31	0.48
26:R:55:VAL:HG13	26:R:79:GLN:HB3	1.95	0.48
30:V:51:MET:HG3	30:V:55:ARG:HH21	1.77	0.48
45:k:220:SER:HA	45:k:221:GLY:C	2.38	0.48
48:o:147:LEU:HA	48:o:158:ILE:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:12:GLU:HG2	52:s:13:LEU:N	2.28	0.48
45:w:182:LEU:O	45:w:186:LEU:N	2.25	0.48
46:x:213:HIS:O	46:x:216:LEU:HB3	2.12	0.48
46:x:378:PHE:O	46:x:382:VAL:HG23	2.14	0.48
48:z:66:GLU:HA	48:z:84:PRO:HD2	1.96	0.48
48:z:147:LEU:HA	48:z:158:ILE:C	2.38	0.48
48:z:165:TYR:O	48:z:168:VAL:HG23	2.13	0.48
53:A3:15:ARG:O	53:A3:18:VAL:N	2.39	0.48
2:7:66:VAL:HG11	8:1:140:ILE:HG21	1.94	0.48
25:Q:59:GLU:HA	25:Q:62:LEU:HB2	1.95	0.48
45:k:145:MET:O	45:k:148:VAL:HB	2.13	0.48
46:l:133:ARG:HD2	46:l:136:GLU:CD	2.39	0.48
46:l:133:ARG:HB2	46:l:136:GLU:CD	2.38	0.48
47:m:230:LEU:HG	47:m:234:LEU:HD11	1.96	0.48
51:r:8:THR:HG22	51:r:9:ARG:N	2.29	0.48
52:s:35:GLU:O	52:s:39:LEU:HG	2.13	0.48
45:w:145:MET:O	45:w:148:VAL:HB	2.13	0.48
47:y:230:LEU:HG	47:y:234:LEU:HD11	1.95	0.48
51:A2:8:THR:HG22	51:A2:9:ARG:N	2.29	0.48
58:B7:65:SER:HB3	58:B7:71:HIS:CE1	2.48	0.48
59:A7:68:PHE:HA	59:A7:71:MET:HG2	1.95	0.48
20:K:82:PHE:HB3	20:K:86:GLN:HB2	1.95	0.48
45:k:206:ARG:NH1	45:k:209:LEU:HD23	2.28	0.48
45:k:214:LYS:HA	45:k:217:SER:OG	2.13	0.48
48:z:70:VAL:O	48:z:82:MET:HA	2.13	0.48
48:z:150:ASN:HD21	48:z:152:TYR:HD2	1.60	0.48
48:z:150:ASN:O	48:z:156:GLN:HA	2.13	0.48
56:A9:476:PHE:CD1	67:B1:15:VAL:HG21	2.49	0.48
57:B9:90:ILE:HD12	57:B9:90:ILE:H	1.77	0.48
4:2:224:THR:H	4:2:228:LEU:HD23	1.79	0.48
11:B:267:ILE:HD11	71:B:501:3PE:H271	1.95	0.48
14:E:38:TYR:HB2	24:P:106:LEU:HA	1.95	0.48
36:b:118:SER:OG	40:h:108:TYR:O	2.31	0.48
46:l:109:VAL:HG22	46:l:119:LEU:HD21	1.94	0.48
46:l:203:ARG:NH1	46:l:231:GLY:HA2	2.28	0.48
47:m:106:SER:OG	47:m:206:ASN:ND2	2.37	0.48
53:t:26:ALA:O	53:t:29:ALA:N	2.47	0.48
46:x:312:PHE:CZ	55:B3:64:LEU:HD13	2.48	0.48
46:x:367:GLY:HA2	46:x:370:MET:HE3	1.95	0.48
47:y:31:TRP:CE2	47:y:100:ARG:HD2	2.49	0.48
47:y:77:TRP:CE2	48:z:197:GLU:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:38:HIS:ND1	50:A1:39:GLU:O	2.47	0.48
51:A2:64:GLN:HA	51:A2:67:GLU:CD	2.39	0.48
52:B5:23:GLN:O	52:B5:26:GLN:HB3	2.13	0.48
57:B9:22:HIS:CE1	64:B6:44:LYS:HD3	2.49	0.48
58:B7:42:LEU:HD13	65:B8:45:TYR:HD2	1.77	0.48
10:A:371:VAL:HB	10:A:482:GLN:HG3	1.96	0.48
47:m:97:HIS:CE1	77:m:402:HEM:C1A	3.01	0.48
47:m:141:TRP:O	47:m:145:VAL:HG23	2.14	0.48
48:o:166:ASN:HA	48:o:179:MET:H	1.79	0.48
50:q:37:ILE:HG12	50:q:38:HIS:O	2.14	0.48
50:q:38:HIS:ND1	50:q:39:GLU:O	2.47	0.48
45:w:357:GLY:HA2	45:w:360:LEU:HD12	1.95	0.48
46:x:276:GLN:HG3	46:x:277:HIS:H	1.78	0.48
47:y:114:ASN:O	47:y:117:VAL:HB	2.13	0.48
48:z:83:ARG:O	48:z:85:GLY:N	2.47	0.48
48:z:166:ASN:HA	48:z:179:MET:H	1.79	0.48
48:z:237:TYR:HB2	50:A1:60:PHE:CE1	2.49	0.48
48:z:240:PRO:HD3	51:A2:12:HIS:ND1	2.28	0.48
51:A2:74:PRO:HA	51:A2:77:TYR:O	2.12	0.48
52:B5:35:GLU:O	52:B5:39:LEU:HG	2.13	0.48
56:A9:507:GLU:O	56:A9:508:PRO:O	2.32	0.48
64:B6:39:VAL:O	64:B6:42:LYS:HE2	2.14	0.48
8:1:46:LEU:HG	8:1:49:ILE:HD11	1.96	0.48
8:1:277:TYR:OH	14:E:66:LEU:O	2.31	0.48
22:N:31:ILE:O	22:N:35:LEU:N	2.45	0.48
26:R:203:PRO:HG2	76:R:601:NAP:H72N	1.79	0.48
26:R:269:SER:HA	26:R:270:ARG:HA	1.59	0.48
45:k:86:LEU:HD23	46:l:285:VAL:HG22	1.95	0.48
45:k:382:SER:O	45:k:387:GLY:N	2.47	0.48
46:l:45:SER:OG	46:l:116:VAL:HG21	2.13	0.48
46:l:294:SER:O	46:l:298:ALA:N	2.25	0.48
47:m:319:PRO:O	47:m:322:GLN:HB3	2.14	0.48
48:o:217:PRO:HA	48:o:220:TYR:HB3	1.96	0.48
45:w:291:SER:HA	46:x:87:ARG:NH2	2.28	0.48
45:w:412:SER:HB3	54:B4:15:ARG:NH2	2.26	0.48
48:z:166:ASN:OD1	48:z:178:THR:HG23	2.13	0.48
48:z:238:ARG:CZ	49:A0:5:ILE:HG22	2.44	0.48
51:A2:62:GLY:HA2	51:A2:65:GLU:HB3	1.96	0.48
56:A9:87:ILE:O	56:A9:173:PRO:HD3	2.13	0.48
10:A:545:LEU:H	10:A:566:ILE:HG22	1.78	0.48
11:B:293:LEU:HD23	11:B:293:LEU:HA	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:53:PRO:HD2	30:V:116:TRP:CD1	2.49	0.48
28:T:64:ALA:O	28:T:65:ALA:HB3	2.10	0.48
47:m:186:PRO:O	47:m:189:ILE:HB	2.14	0.48
48:o:3:LEU:HB2	52:s:59:LEU:HD13	1.94	0.48
49:p:41:ALA:HB2	54:u:20:PHE:HE1	1.77	0.48
45:w:347:THR:O	53:A3:15:ARG:HG2	2.14	0.48
45:w:382:SER:O	45:w:387:GLY:N	2.47	0.48
47:y:74:ASN:ND2	49:A0:60:SER:O	2.47	0.48
49:A0:10:PHE:CD2	51:A2:18:LEU:HD21	2.49	0.48
50:A1:87:LYS:HG3	50:A1:89:TYR:CD2	2.48	0.48
57:B9:4:PRO:HB2	66:B0:43:SER:HA	1.96	0.48
1:9:121:MET:HB2	7:8:201:ALA:HB1	1.95	0.48
4:2:7:ILE:O	4:2:11:LEU:N	2.41	0.48
11:B:88:HIS:CG	13:D:114:ARG:HH11	2.32	0.48
45:k:147:ASP:HA	45:k:150:PHE:HD2	1.78	0.48
46:l:51:ILE:HG12	46:l:204:MET:HG2	1.96	0.48
46:l:98:VAL:N	55:v:70:LEU:HB3	2.29	0.48
46:l:345:LYS:O	46:l:349:GLN:HG3	2.13	0.48
48:o:165:TYR:O	48:o:168:VAL:HG23	2.13	0.48
49:p:73:LYS:HG2	49:p:75:GLU:OE2	2.14	0.48
51:r:26:PHE:N	51:r:27:PRO:HD3	2.29	0.48
47:y:360:LEU:O	47:y:365:LEU:HG	2.14	0.48
48:z:217:PRO:HA	48:z:220:TYR:HB3	1.96	0.48
56:A9:115:SER:O	56:A9:121:GLY:HA2	2.14	0.48
57:B9:16:ILE:HD12	57:B9:17:MET:H	1.77	0.48
45:k:58:PHE:CE2	45:k:62:LEU:HD11	2.49	0.47
45:k:280:TYR:HB3	45:k:307:PHE:CE2	2.49	0.47
46:l:58:GLU:OE1	46:l:64:GLY:N	2.46	0.47
47:m:83:HIS:CD2	77:m:401:HEM:CHA	2.96	0.47
48:o:69:GLU:HB2	48:o:84:PRO:HD3	1.96	0.47
51:r:64:GLN:HA	51:r:67:GLU:CD	2.39	0.47
46:x:45:SER:OG	46:x:116:VAL:HG21	2.13	0.47
47:y:83:HIS:CD2	77:y:401:HEM:CHA	2.96	0.47
47:y:141:TRP:O	47:y:145:VAL:HG23	2.14	0.47
49:A0:2:HIS:CG	49:A0:3:THR:N	2.81	0.47
49:A0:10:PHE:CB	51:A2:18:LEU:HD11	2.44	0.47
50:A1:87:LYS:CG	50:A1:89:TYR:HD2	2.25	0.47
51:A2:26:PHE:N	51:A2:27:PRO:HD3	2.29	0.47
53:A3:11:ARG:N	53:A3:12:GLN:HA	2.29	0.47
56:A9:397:PHE:HB3	56:A9:398:PRO:HD3	1.95	0.47
46:l:183:ILE:C	46:l:185:LYS:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:245:ARG:HH21	46:l:433:THR:HB	1.78	0.47
46:l:258:VAL:HG11	46:l:321:LEU:HB3	1.95	0.47
52:s:12:GLU:CG	52:s:13:LEU:H	2.27	0.47
45:w:147:ASP:HA	45:w:150:PHE:HD2	1.78	0.47
47:y:311:LYS:HZ2	47:y:379:TRP:HB3	1.79	0.47
47:y:336:THR:O	47:y:340:GLY:N	2.47	0.47
4:2:324:THR:O	42:j:41:SER:OG	2.30	0.47
46:l:26:PHE:HA	46:l:36:ALA:HA	1.95	0.47
46:l:111:CYS:SG	46:l:116:VAL:HG22	2.54	0.47
46:l:338:LYS:O	46:l:342:ASN:N	2.35	0.47
46:l:378:PHE:O	46:l:382:VAL:HG23	2.14	0.47
46:x:26:PHE:HA	46:x:36:ALA:HA	1.95	0.47
46:x:118:ILE:H	46:x:118:ILE:HD12	1.79	0.47
46:x:182:ARG:NH1	46:x:185:LYS:HE2	2.27	0.47
46:x:245:ARG:HH21	46:x:433:THR:HB	1.78	0.47
47:y:159:ASN:O	47:y:163:TRP:N	2.42	0.47
47:y:312:GLN:HA	50:A1:38:HIS:N	2.29	0.47
53:A3:19:PRO:CA	53:A3:22:SER:OG	2.55	0.47
56:A9:11:ASN:ND2	56:A9:13:LYS:HB2	2.28	0.47
56:A9:11:ASN:ND2	56:A9:14:ASP:H	2.07	0.47
3:6:68:TRP:CD1	3:6:69:LEU:HG	2.49	0.47
7:8:420:GLU:H	7:8:422:HIS:CD2	2.31	0.47
8:1:284:GLN:HA	8:1:287:HIS:HB3	1.96	0.47
16:G:121:LEU:O	16:G:123:ASN:N	2.45	0.47
48:o:49:ARG:HA	48:o:87:LEU:HD23	1.96	0.47
45:w:39:VAL:N	45:w:97:TYR:O	2.41	0.47
46:x:51:ILE:HG12	46:x:204:MET:HG2	1.96	0.47
46:x:97:SER:HA	55:B3:70:LEU:HD22	1.96	0.47
46:x:111:CYS:SG	46:x:116:VAL:HG22	2.54	0.47
48:z:237:TYR:CD2	48:z:239:PRO:HD3	2.49	0.47
57:B9:59:GLN:O	57:B9:62:GLU:HB2	2.13	0.47
65:B8:8:LYS:HB3	65:B8:8:LYS:NZ	2.28	0.47
1:9:91:GLY:O	1:9:123:ASN:ND2	2.47	0.47
18:I:104:ASP:O	18:I:105:LYS:CB	2.62	0.47
45:k:10:SER:HG	46:l:41:TYR:HD1	1.61	0.47
45:k:262:TRP:HB3	45:k:385:THR:HG23	1.96	0.47
46:l:135:TRP:CE2	50:A1:49:ARG:HD3	2.50	0.47
46:l:359:ALA:HA	46:l:362:ASN:ND2	2.30	0.47
47:m:27:ILE:HD12	47:m:224:TYR:CZ	2.49	0.47
49:p:143:GLY:O	49:p:146:PRO:N	2.48	0.47
45:w:213:GLN:O	45:w:214:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:155:PRO:HB2	46:x:254:HIS:ND1	2.30	0.47
46:x:338:LYS:NZ	46:x:438:GLU:O	2.31	0.47
46:x:360:ALA:O	46:x:364:LEU:N	2.24	0.47
47:y:27:ILE:HD12	47:y:224:TYR:CZ	2.49	0.47
47:y:258:PRO:HD3	48:z:115:TYR:OH	2.14	0.47
4:2:109:ALA:O	4:2:112:HIS:ND1	2.47	0.47
7:8:270:ASN:HD21	7:8:338:ASP:HA	1.79	0.47
48:o:41:HIS:CD2	78:o:301:HEC:NB	2.83	0.47
52:s:44:VAL:HG21	52:s:54:CYS:SG	2.55	0.47
45:w:262:TRP:HB3	45:w:385:THR:HG23	1.96	0.47
46:x:58:GLU:OE1	46:x:64:GLY:N	2.46	0.47
47:y:319:PRO:O	47:y:322:GLN:HB3	2.14	0.47
48:z:41:HIS:CD2	78:z:301:HEC:NB	2.83	0.47
48:z:127:VAL:HA	48:z:130:LEU:HB3	1.96	0.47
48:z:128:PHE:HD1	48:z:187:CYS:HG	1.60	0.47
54:B4:51:LEU:O	54:B4:55:ILE:N	2.28	0.47
27:S:109:PRO:HB2	27:S:112:ASN:HB3	1.96	0.47
42:j:58:LEU:O	42:j:62:LEU:N	2.43	0.47
45:k:61:HIS:HB3	45:k:65:LYS:HZ3	1.79	0.47
45:k:215:HIS:C	45:k:219:LEU:H	2.22	0.47
46:l:128:THR:C	46:l:130:PRO:HD3	2.39	0.47
47:m:226:ILE:HD13	47:m:229:ILE:HD12	1.96	0.47
47:m:349:THR:O	47:m:353:LEU:N	2.48	0.47
47:m:360:LEU:O	47:m:365:LEU:HG	2.14	0.47
48:o:66:GLU:HA	48:o:84:PRO:HD2	1.96	0.47
45:w:7:ALA:HB1	46:x:43:PRO:HD3	1.95	0.47
45:w:280:TYR:HB3	45:w:307:PHE:CE2	2.49	0.47
46:x:67:HIS:HD1	46:x:70:ARG:HH22	1.61	0.47
46:x:133:ARG:HD2	46:x:136:GLU:CD	2.39	0.47
46:x:312:PHE:HB2	55:B3:57:GLY:HA3	1.96	0.47
46:x:345:LYS:O	46:x:349:GLN:HG3	2.13	0.47
47:y:226:ILE:HD13	47:y:229:ILE:HD12	1.95	0.47
48:z:23:HIS:NE2	54:B4:51:LEU:HA	2.30	0.47
49:A0:10:PHE:C	49:A0:14:ARG:HG3	2.40	0.47
49:A0:91:TRP:C	49:A0:93:GLY:N	2.73	0.47
49:A0:107:ASP:O	49:A0:111:ALA:N	2.48	0.47
50:A1:37:ILE:HG12	50:A1:38:HIS:O	2.14	0.47
51:A2:74:PRO:HA	51:A2:78:GLU:HA	1.96	0.47
57:B9:63:THR:O	57:B9:66:THR:HG22	2.15	0.47
57:B9:83:ILE:O	57:B9:87:MET:HG3	2.14	0.47
57:B9:108:TYR:N	57:B9:108:TYR:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B7:173:PHE:C	58:B7:173:PHE:CD1	2.92	0.47
59:A7:23:PRO:HB3	60:A6:70:VAL:CG2	2.45	0.47
59:A7:41:LYS:HD3	59:A7:62:LEU:HD23	1.97	0.47
61:B2:31:TYR:HE1	61:B2:98:HIS:HE1	1.62	0.47
62:A4:67:HIS:CD2	62:A4:78:LEU:HD11	2.50	0.47
1:9:164:THR:N	1:9:169:PHE:O	2.38	0.47
2:7:25:SER:O	2:7:27:ILE:N	2.43	0.47
10:A:443:ASP:N	10:A:443:ASP:OD1	2.48	0.47
45:k:215:HIS:O	45:k:219:LEU:N	2.47	0.47
45:k:405:ARG:HE	53:t:15:ARG:HH21	1.63	0.47
46:l:97:SER:HA	55:v:70:LEU:CB	2.45	0.47
47:m:31:TRP:CE2	47:m:100:ARG:HD2	2.49	0.47
47:m:374:ASN:HA	47:m:379:TRP:CD1	2.49	0.47
48:o:28:ARG:HB3	48:o:171:PHE:CD1	2.50	0.47
46:x:359:ALA:HA	46:x:362:ASN:ND2	2.30	0.47
46:x:370:MET:O	46:x:373:GLU:HG2	2.15	0.47
46:x:385:GLN:O	46:x:389:ALA:N	2.41	0.47
47:y:6:LYS:HB3	47:y:16:ASN:HD21	1.80	0.47
48:z:55:CYS:SG	54:B4:52:TRP:HB3	2.54	0.47
52:B5:44:VAL:HG21	52:B5:54:CYS:SG	2.55	0.47
58:B7:164:PHE:O	58:B7:168:THR:HG23	2.14	0.47
5:4:76:MET:HG2	5:4:231:LEU:HD12	1.97	0.47
10:A:31:LEU:HA	10:A:45:PRO:HD3	1.97	0.47
10:A:120:LEU:HD12	10:A:121:LEU:HG	1.97	0.47
10:A:587:ALA:O	10:A:592:LYS:NZ	2.38	0.47
11:B:123:LEU:HD22	13:D:166:SER:HB3	1.96	0.47
46:l:67:HIS:ND1	46:l:176:LEU:O	2.47	0.47
46:l:395:PRO:O	46:l:399:LEU:HG	2.14	0.47
47:m:237:LEU:HG	48:o:212:MET:HE3	1.96	0.47
47:m:344:GLU:CD	51:r:66:PHE:HE1	2.22	0.47
48:o:165:TYR:H	48:o:168:VAL:CG2	2.28	0.47
51:r:62:GLY:HA2	51:r:65:GLU:HB3	1.96	0.47
45:w:64:PHE:CD1	45:w:86:LEU:HD21	2.50	0.47
45:w:412:SER:O	54:B4:15:ARG:NH2	2.48	0.47
46:x:183:ILE:C	46:x:185:LYS:H	2.23	0.47
47:y:206:ASN:OD1	47:y:313:ARG:NH1	2.48	0.47
47:y:207:ASN:CG	47:y:209:THR:H	2.23	0.47
47:y:315:MET:HG2	47:y:318:ARG:NH2	2.30	0.47
48:z:11:PRO:HA	48:z:15:ARG:CD	2.43	0.47
48:z:165:TYR:H	48:z:168:VAL:CG2	2.28	0.47
53:A3:30:VAL:O	53:A3:34:TRP:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:306:THR:HB	56:A9:359:ALA:O	2.15	0.47
3:6:48:MET:O	3:6:51:THR:OG1	2.28	0.47
3:6:160:GLY:HA3	39:f:95:GLU:HG2	1.97	0.47
3:6:203:MET:HG2	43:g:110:LEU:HD11	1.97	0.47
3:6:546:GLN:HE22	5:4:277:LEU:HB2	1.80	0.47
5:4:306:PRO:HD3	43:g:150:TYR:HA	1.96	0.47
11:B:112:HIS:CD2	12:C:187:ARG:HH22	2.33	0.47
11:B:140:ASP:OD2	11:B:143:SER:OG	2.33	0.47
26:R:150:GLN:HA	26:R:153:ALA:HB3	1.97	0.47
76:R:601:NAP:O4D	76:R:601:NAP:C2N	2.63	0.47
45:k:182:LEU:O	45:k:186:LEU:N	2.25	0.47
45:k:220:SER:O	45:k:222:THR:HG23	2.15	0.47
45:k:340:GLY:O	45:k:344:ARG:HG2	2.15	0.47
46:l:397:THR:O	46:l:401:GLN:HG3	2.15	0.47
47:m:27:ILE:CG2	47:m:31:TRP:HB2	2.45	0.47
49:p:1:SER:OG	49:p:2:HIS:N	2.42	0.47
53:A3:19:PRO:O	53:A3:23:LEU:N	2.48	0.47
54:B4:16:ARG:O	54:B4:19:THR:OG1	2.30	0.47
3:6:421:ILE:HG22	3:6:501:ALA:HB2	1.97	0.46
5:4:403:THR:HA	5:4:406:TYR:HB3	1.97	0.46
27:S:187:LEU:HD13	27:S:277:ARG:HB2	1.97	0.46
43:g:146:LEU:HA	43:g:147:GLY:HA2	1.65	0.46
45:k:291:SER:OG	46:l:90:GLU:OE1	2.25	0.46
46:l:70:ARG:NH1	46:l:100:SER:OG	2.33	0.46
46:l:148:LYS:NZ	46:l:178:CYS:O	2.41	0.46
48:o:237:TYR:CD2	48:o:239:PRO:HD3	2.49	0.46
45:w:58:PHE:CE2	45:w:62:LEU:HD11	2.49	0.46
45:w:257:VAL:HG12	45:w:420:PRO:HA	1.97	0.46
45:w:340:GLY:O	45:w:344:ARG:HG2	2.15	0.46
46:x:128:THR:C	46:x:130:PRO:HD3	2.40	0.46
47:y:240:MET:O	47:y:243:VAL:HG12	2.15	0.46
48:z:215:LEU:O	48:z:218:LEU:HB2	2.15	0.46
58:B7:80:ARG:O	58:B7:84:ILE:HG12	2.14	0.46
59:A7:102:TYR:CD2	68:A8:35:TYR:HE1	2.33	0.46
65:B8:16:ASN:ND2	65:B8:16:ASN:H	2.12	0.46
3:6:1:MET:HG2	3:6:59:GLN:HE22	1.81	0.46
5:4:367:LEU:HD11	5:4:408:LEU:HD11	1.97	0.46
8:1:264:LEU:HD21	19:J:9:ILE:HG23	1.97	0.46
9:3:41:PHE:C	9:3:43:PRO:HD3	2.40	0.46
10:A:394:VAL:HG22	10:A:473:MET:HE1	1.96	0.46
18:I:89:GLY:H	18:I:96:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:92:GLU:HA	20:K:95:LEU:HB3	1.95	0.46
45:k:146:ARG:O	45:k:149:VAL:HG12	2.15	0.46
46:l:26:PHE:HB3	46:l:36:ALA:HB2	1.97	0.46
46:l:155:PRO:HB2	46:l:254:HIS:ND1	2.30	0.46
46:l:258:VAL:HA	46:l:323:GLY:HA3	1.96	0.46
47:m:26:ASN:HD22	50:q:69:SER:HB3	1.80	0.46
47:m:72:ASP:OD1	48:o:49:ARG:NH1	2.47	0.46
47:m:336:THR:O	47:m:340:GLY:N	2.47	0.46
49:p:109:GLU:N	49:p:110:ALA:HB3	2.30	0.46
54:u:52:TRP:HA	54:u:56:LYS:H	1.80	0.46
45:w:122:LEU:HB3	45:w:179:ARG:HD2	1.97	0.46
45:w:208:LEU:O	45:w:212:ALA:N	2.49	0.46
45:w:391:PRO:O	45:w:395:TRP:N	2.47	0.46
46:x:296:TYR:CD2	46:x:297:GLN:NE2	2.82	0.46
47:y:226:ILE:HA	47:y:229:ILE:HD12	1.97	0.46
56:A9:195:LEU:CD2	56:A9:245:ILE:HD13	2.45	0.46
66:B0:9:PHE:HD1	66:B0:10:HIS:HD2	1.63	0.46
68:A8:1:ILE:HG23	68:A8:1:ILE:O	2.15	0.46
1:9:123:ASN:HD22	1:9:127:VAL:HG11	1.79	0.46
3:6:535:ARG:HD2	35:a:16:THR:O	2.15	0.46
6:5:26:LEU:HD23	6:5:78:LEU:HD13	1.98	0.46
10:A:341:ILE:HD11	10:A:547:LEU:HG	1.97	0.46
28:T:55:ARG:HA	28:T:58:ARG:CB	2.46	0.46
34:Z:65:GLY:HA2	34:Z:68:LEU:HB2	1.97	0.46
40:h:138:GLU:OE1	40:h:140:ASN:ND2	2.48	0.46
45:k:47:TYR:HE1	45:k:231:LEU:HG	1.81	0.46
46:l:118:ILE:H	46:l:118:ILE:HD12	1.79	0.46
47:m:207:ASN:CG	47:m:209:THR:H	2.23	0.46
54:u:55:ILE:O	54:u:58:LYS:HG2	2.15	0.46
46:x:182:ARG:O	46:x:185:LYS:HB3	2.16	0.46
46:x:376:GLU:HA	46:x:379:LEU:HB3	1.97	0.46
47:y:286:ASN:CG	47:y:289:GLY:H	2.24	0.46
47:y:292:LEU:O	47:y:296:PHE:HB3	2.15	0.46
48:z:28:ARG:HB3	48:z:171:PHE:CD1	2.50	0.46
51:A2:74:PRO:HB3	51:A2:79:ASN:ND2	2.30	0.46
57:B9:148:MET:HE3	57:B9:148:MET:HB3	1.78	0.46
59:A7:108:PRO:HG2	59:A7:111:PHE:CD2	2.50	0.46
3:6:557:TRP:NE1	35:a:87:SER:O	2.40	0.46
5:4:66:LEU:O	5:4:69:THR:OG1	2.27	0.46
8:1:291:LYS:HB3	72:L:200:PC1:H141	1.97	0.46
8:1:312:SER:HG	30:V:55:ARG:HH22	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:189:LYS:HB2	29:U:124:TYR:CZ	2.51	0.46
45:k:64:PHE:CD1	45:k:86:LEU:HD21	2.50	0.46
45:k:391:PRO:O	45:k:395:TRP:N	2.47	0.46
46:l:122:PHE:O	46:l:126:VAL:HG23	2.16	0.46
47:m:315:MET:HG2	47:m:318:ARG:NH2	2.29	0.46
48:o:215:LEU:O	48:o:218:LEU:HB2	2.15	0.46
46:x:119:LEU:HA	46:x:122:PHE:CD2	2.50	0.46
46:x:258:VAL:HA	46:x:323:GLY:HA3	1.96	0.46
46:x:395:PRO:O	46:x:399:LEU:HG	2.14	0.46
47:y:55:TYR:CG	47:y:56:THR:N	2.83	0.46
49:A0:155:GLY:H	49:A0:166:ASP:HA	1.80	0.46
56:A9:172:LYS:HB3	56:A9:176:MET:HE2	1.96	0.46
56:A9:240:HIS:NE2	56:A9:244:TYR:CE2	2.81	0.46
59:A7:33:LEU:HD13	59:A7:41:LYS:HG3	1.97	0.46
16:G:154:LYS:HB2	16:G:156:LYS:HE2	1.96	0.46
23:O:83:VAL:O	23:O:87:LYS:N	2.44	0.46
34:Z:68:LEU:HD22	34:Z:71:PHE:HD1	1.79	0.46
46:l:370:MET:O	46:l:373:GLU:HG2	2.15	0.46
46:l:376:GLU:HA	46:l:379:LEU:HB3	1.97	0.46
47:m:6:LYS:HB3	47:m:16:ASN:HD21	1.80	0.46
47:m:206:ASN:OD1	47:m:313:ARG:NH1	2.48	0.46
47:m:240:MET:O	47:m:243:VAL:HG12	2.15	0.46
48:o:113:LEU:O	48:o:116:ILE:HG22	2.16	0.46
51:r:74:PRO:HA	51:r:78:GLU:HA	1.96	0.46
45:w:146:ARG:O	45:w:149:VAL:HG12	2.15	0.46
45:w:159:GLN:HE21	45:w:237:THR:HG21	1.77	0.46
45:w:412:SER:CB	54:B4:15:ARG:HH22	2.26	0.46
46:x:122:PHE:O	46:x:126:VAL:HG23	2.16	0.46
46:x:274:VAL:O	46:x:278:VAL:HG23	2.15	0.46
47:y:83:HIS:CE1	77:y:401:HEM:C1C	3.04	0.46
47:y:349:THR:O	47:y:353:LEU:N	2.48	0.46
56:A9:484:THR:HB	68:A8:2:THR:OG1	2.15	0.46
3:6:427:ILE:HA	3:6:431:LEU:HB2	1.98	0.46
11:B:67:ASN:ND2	27:S:181:VAL:O	2.49	0.46
13:D:75:ASN:OD1	13:D:78:ARG:NH2	2.49	0.46
26:R:168:SER:OG	26:R:169:HIS:N	2.47	0.46
45:k:215:HIS:H	45:k:216:PHE:C	2.23	0.46
45:k:286:GLY:HA3	45:k:290:LEU:HD11	1.97	0.46
47:m:55:TYR:CG	47:m:56:THR:N	2.83	0.46
47:m:62:ALA:O	47:m:65:SER:OG	2.26	0.46
49:p:109:GLU:HA	49:p:110:ALA:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:145:VAL:HA	49:p:156:TYR:CB	2.46	0.46
50:q:38:HIS:CE1	50:q:39:GLU:O	2.69	0.46
51:r:74:PRO:HB3	51:r:79:ASN:ND2	2.30	0.46
46:x:97:SER:HA	55:B3:70:LEU:HB3	1.98	0.46
46:x:236:LYS:NZ	46:x:238:LYS:HB2	2.30	0.46
46:x:258:VAL:HG13	46:x:322:PHE:O	2.16	0.46
47:y:27:ILE:CG2	47:y:31:TRP:HB2	2.45	0.46
47:y:88:SER:CB	47:y:250:LEU:HD21	2.46	0.46
47:y:278:TYR:O	47:y:281:LEU:HB3	2.16	0.46
47:y:322:GLN:O	47:y:325:PHE:HB3	2.16	0.46
48:z:113:LEU:O	48:z:116:ILE:HG22	2.16	0.46
57:B9:58:ALA:O	57:B9:60:GLU:HG3	2.16	0.46
1:9:75:LYS:O	1:9:77:ALA:N	2.41	0.46
3:6:385:PHE:O	3:6:466:TYR:OH	2.31	0.46
5:4:360:LEU:O	5:4:364:LEU:N	2.48	0.46
25:Q:57:LEU:O	25:Q:61:LYS:NZ	2.42	0.46
31:W:104:PHE:O	31:W:108:LEU:CG	2.32	0.46
40:h:84:ILE:HG22	40:h:88:ARG:HH12	1.80	0.46
45:k:356:ARG:HG3	45:k:357:GLY:N	2.31	0.46
46:l:46:ARG:HG2	46:l:209:LEU:HD22	1.98	0.46
48:o:134:TYR:CE1	48:o:162:PRO:HG3	2.51	0.46
47:y:106:SER:OG	47:y:206:ASN:ND2	2.37	0.46
47:y:186:PRO:O	47:y:189:ILE:HB	2.14	0.46
48:z:238:ARG:NH1	49:A0:2:HIS:HB2	2.30	0.46
50:A1:28:LYS:HG2	50:A1:80:TRP:CE3	2.51	0.46
56:A9:147:ILE:HD11	56:A9:209:LEU:HD23	1.98	0.46
56:A9:435:GLY:O	56:A9:437:PRO:HD3	2.16	0.46
57:B9:76:ILE:O	57:B9:79:PRO:HD2	2.16	0.46
61:B2:40:SER:OG	61:B2:45:ASP:HB3	2.16	0.46
3:6:33:PRO:HB2	3:6:105:MET:HE2	1.98	0.46
11:B:238:LEU:HD13	24:P:37:PRO:HD2	1.96	0.46
14:E:123:CYS:SG	14:E:126:GLN:N	2.89	0.46
71:j:202:3PE:H2B1	71:j:202:3PE:H362	1.98	0.46
46:l:118:ILE:O	46:l:121:GLU:HB3	2.16	0.46
46:l:155:PRO:HA	46:l:158:HIS:HB3	1.98	0.46
46:l:274:VAL:O	46:l:278:VAL:HG23	2.15	0.46
47:m:195:VAL:HG12	47:m:199:PHE:HE2	1.80	0.46
47:m:292:LEU:O	47:m:296:PHE:HB3	2.15	0.46
48:o:204:MET:HA	48:o:207:LYS:HB3	1.98	0.46
45:w:404:ALA:HB1	45:w:408:ARG:NH1	2.31	0.46
46:x:78:LYS:HA	46:x:131:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:151:SER:HB3	47:y:161:VAL:HG21	1.97	0.46
47:y:290:GLY:O	47:y:294:LEU:N	2.35	0.46
50:A1:73:GLN:HA	51:A2:39:ARG:NH1	2.31	0.46
3:6:3:MET:HA	3:6:6:SER:HB2	1.98	0.46
45:k:359:ASN:O	45:k:363:ASN:ND2	2.49	0.46
46:l:119:LEU:HA	46:l:122:PHE:CD2	2.51	0.46
46:l:258:VAL:HG13	46:l:322:PHE:O	2.16	0.46
46:l:296:TYR:CD2	46:l:297:GLN:NE2	2.82	0.46
47:m:88:SER:CB	47:m:250:LEU:HD21	2.46	0.46
48:o:72:ASP:OD2	48:o:80:MET:HE3	2.16	0.46
48:o:160:MET:HB2	78:o:301:HEC:C4D	2.46	0.46
45:w:61:HIS:HB3	45:w:65:LYS:HZ3	1.81	0.46
45:w:124:ASP:HA	45:w:127:ILE:CG1	2.46	0.46
45:w:230:THR:O	45:w:231:LEU:HG	2.16	0.46
45:w:303:LEU:HD22	45:w:333:ASP:OD2	2.16	0.46
46:x:200:THR:HG1	46:x:228:GLY:H	1.58	0.46
47:y:47:THR:CG2	47:y:83:HIS:HB2	2.46	0.46
48:z:41:HIS:CE1	48:z:110:PRO:HB3	2.51	0.46
48:z:240:PRO:HD3	51:A2:12:HIS:CE1	2.51	0.46
50:A1:101:ARG:HA	50:A1:104:ARG:NE	2.30	0.46
53:A3:41:ILE:H	53:A3:41:ILE:HG12	1.60	0.46
54:B4:52:TRP:HA	54:B4:56:LYS:H	1.80	0.46
55:B3:64:LEU:HG	55:B3:65:VAL:HG22	1.97	0.46
65:B8:11:LEU:O	65:B8:11:LEU:HD23	2.15	0.46
1:9:55:PHE:HB2	1:9:60:TYR:CZ	2.51	0.46
5:4:167:ILE:HD13	5:4:250:LEU:HD11	1.96	0.46
35:a:84:THR:OG1	35:a:85:LYS:N	2.49	0.46
45:k:208:LEU:O	45:k:212:ALA:N	2.49	0.46
45:k:257:VAL:HG12	45:k:420:PRO:HA	1.97	0.46
46:l:213:HIS:HD2	46:l:216:LEU:HD23	1.81	0.46
48:o:127:VAL:HA	48:o:130:LEU:HB3	1.97	0.46
49:p:91:TRP:C	49:p:93:GLY:N	2.74	0.46
45:w:147:ASP:HA	45:w:150:PHE:CD2	2.50	0.46
45:w:216:PHE:CG	45:w:217:SER:N	2.83	0.46
45:w:359:ASN:O	45:w:363:ASN:ND2	2.49	0.46
46:x:46:ARG:HG2	46:x:209:LEU:HD22	1.98	0.46
46:x:376:GLU:O	46:x:379:LEU:HB3	2.16	0.46
48:z:21:LEU:HD22	48:z:188:THR:HG23	1.97	0.46
48:z:27:ARG:NH1	54:B4:58:LYS:HD2	2.31	0.46
48:z:49:ARG:HA	48:z:87:LEU:HD23	1.97	0.46
48:z:160:MET:HB2	78:z:301:HEC:C4D	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A0:84:GLY:H	49:A0:101:ARG:HA	1.80	0.46
49:A0:136:ILE:N	49:A0:182:VAL:O	2.48	0.46
57:B9:1:MET:SD	57:B9:133:LEU:HD11	2.56	0.46
57:B9:185:MET:SD	57:B9:185:MET:C	2.99	0.46
1:9:57:PRO:HA	1:9:60:TYR:HD2	1.80	0.45
5:4:119:TYR:HA	5:4:122:PHE:HB3	1.97	0.45
30:V:28:ARG:HA	30:V:29:GLY:HA3	1.66	0.45
43:g:173:ALA:HB3	43:g:176:ALA:HB3	1.97	0.45
45:k:124:ASP:HA	45:k:127:ILE:CG1	2.46	0.45
45:k:297:ILE:CG2	47:m:2:THR:HG21	2.46	0.45
45:k:386:TYR:HB3	45:k:389:ARG:HD2	1.99	0.45
47:m:151:SER:HB3	47:m:161:VAL:HG21	1.97	0.45
45:w:329:MET:HB3	51:A2:2:ARG:HE	1.81	0.45
45:w:356:ARG:HG3	45:w:357:GLY:N	2.31	0.45
46:x:213:HIS:HD2	46:x:216:LEU:HD23	1.81	0.45
46:x:397:THR:O	46:x:401:GLN:HG3	2.15	0.45
49:A0:24:SER:HB3	49:A0:27:GLU:HG2	1.97	0.45
49:A0:30:GLU:CD	54:B4:10:TYR:HD2	2.23	0.45
54:B4:60:GLU:N	54:B4:62:LYS:O	2.49	0.45
57:B9:78:LEU:HB2	57:B9:79:PRO:CD	2.38	0.45
58:B7:223:LEU:HA	58:B7:223:LEU:HD23	1.79	0.45
10:A:140:GLN:HG3	11:B:379:ILE:HG23	1.98	0.45
11:B:102:SER:N	11:B:105:MET:O	2.50	0.45
42:j:115:GLU:HB3	42:j:117:HIS:ND1	2.31	0.45
45:k:194:ARG:HH22	45:k:229:PRO:HA	1.81	0.45
46:l:78:LYS:HA	46:l:131:GLU:OE2	2.16	0.45
46:l:236:LYS:NZ	46:l:238:LYS:HB2	2.30	0.45
48:o:151:PRO:HA	48:o:156:GLN:HG2	1.99	0.45
48:o:214:LEU:O	48:o:218:LEU:HG	2.15	0.45
46:x:26:PHE:HB3	46:x:36:ALA:HB2	1.97	0.45
48:z:204:MET:HA	48:z:207:LYS:HB3	1.98	0.45
48:z:214:LEU:O	48:z:218:LEU:HG	2.15	0.45
49:A0:10:PHE:O	49:A0:13:TYR:HB2	2.16	0.45
50:A1:38:HIS:CE1	50:A1:39:GLU:O	2.69	0.45
57:B9:41:ILE:O	57:B9:45:MET:HG2	2.16	0.45
57:B9:59:GLN:CA	57:B9:62:GLU:HB2	2.46	0.45
7:8:330:SER:OG	7:8:331:VAL:N	2.43	0.45
25:Q:9:SER:HA	30:V:88:ARG:HH12	1.81	0.45
26:R:238:GLN:HE22	26:R:271:TYR:HA	1.82	0.45
26:R:329:LEU:HD11	26:R:331:HIS:HD2	1.81	0.45
28:T:55:ARG:O	28:T:58:ARG:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:62:THR:HG22	28:T:104:ARG:HD2	1.92	0.45
30:V:91:LEU:HD11	30:V:106:VAL:HG13	1.99	0.45
45:k:4:TYR:HB2	46:l:113:ARG:HB3	1.97	0.45
45:k:69:ASN:HB2	45:k:115:ASP:OD2	2.16	0.45
47:m:90:PHE:O	47:m:93:CYS:HB2	2.16	0.45
48:o:41:HIS:CE1	48:o:110:PRO:HB3	2.51	0.45
52:s:29:LYS:O	52:s:32:LYS:HB3	2.17	0.45
53:t:24:TRP:HA	53:t:27:VAL:HB	1.98	0.45
48:z:134:TYR:CE1	48:z:162:PRO:HG3	2.51	0.45
50:A1:41:ASP:HA	50:A1:44:LYS:HG2	1.99	0.45
65:B8:2:GLU:CG	65:B8:3:ASN:H	2.30	0.45
8:1:288:LEU:HA	8:1:292:ASN:HD22	1.81	0.45
10:A:280:ASP:O	10:A:417:ARG:NH2	2.42	0.45
12:C:49:VAL:HG22	24:P:59:GLY:HA2	1.97	0.45
14:E:158:CYS:SG	14:E:159:GLN:N	2.88	0.45
45:k:404:ALA:HB1	45:k:408:ARG:NH1	2.31	0.45
46:l:267:ALA:HA	46:l:270:ASN:HB3	1.99	0.45
47:m:226:ILE:HA	47:m:229:ILE:HD12	1.97	0.45
47:m:278:TYR:O	47:m:281:LEU:HB3	2.16	0.45
47:m:324:LEU:HA	47:m:327:ALA:HB3	1.98	0.45
48:o:21:LEU:HD22	48:o:188:THR:HG23	1.97	0.45
48:o:23:HIS:HA	48:o:26:ILE:HB	1.98	0.45
50:q:101:ARG:HA	50:q:104:ARG:NE	2.30	0.45
54:u:57:HIS:HA	54:u:60:GLU:HG2	1.98	0.45
45:w:48:GLU:HB3	45:w:52:ASN:HB2	1.99	0.45
45:w:110:VAL:O	45:w:114:ALA:N	2.26	0.45
47:y:83:HIS:CD2	77:y:401:HEM:C4D	3.05	0.45
49:A0:17:GLU:HB3	49:A0:28:SER:OG	2.15	0.45
50:A1:74:ILE:H	51:A2:39:ARG:NH1	2.15	0.45
50:A1:94:LEU:HG	50:A1:98:ILE:HD11	1.98	0.45
52:B5:29:LYS:O	52:B5:32:LYS:HB3	2.17	0.45
54:B4:55:ILE:O	54:B4:58:LYS:HG2	2.15	0.45
54:B4:57:HIS:HA	54:B4:60:GLU:HG2	1.98	0.45
59:A7:33:LEU:HD22	59:A7:37:GLN:HB3	1.97	0.45
59:A7:66:GLU:O	60:A6:66:ARG:NH2	2.49	0.45
7:8:124:THR:HG22	7:8:126:LYS:H	1.81	0.45
8:1:231:ILE:O	8:1:235:ASN:ND2	2.50	0.45
9:3:12:THR:HA	9:3:15:THR:HG22	1.98	0.45
12:C:110:PHE:O	12:C:162:TYR:OH	2.34	0.45
21:L:19:LEU:HD22	72:L:200:PC1:H232	1.99	0.45
34:Z:36:LEU:O	34:Z:40:GLY:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:86:LEU:N	46:l:284:HIS:O	2.46	0.45
45:k:215:HIS:H	45:k:217:SER:N	2.13	0.45
46:l:182:ARG:O	46:l:185:LYS:HB3	2.16	0.45
47:m:47:THR:CG2	47:m:83:HIS:HB2	2.46	0.45
47:m:83:HIS:CE1	77:m:401:HEM:C1C	3.04	0.45
47:m:349:THR:HA	47:m:352:GLN:OE1	2.17	0.45
48:o:69:GLU:O	48:o:70:VAL:HG22	2.17	0.45
50:q:41:ASP:HA	50:q:44:LYS:HG2	1.99	0.45
54:u:60:GLU:N	54:u:62:LYS:O	2.49	0.45
47:y:195:VAL:HG12	47:y:199:PHE:HE2	1.80	0.45
48:z:56:TYR:HB3	48:z:61:ALA:HB2	1.99	0.45
56:A9:431:LEU:HD21	56:A9:450:TRP:HB2	1.99	0.45
57:B9:60:GLU:CD	57:B9:61:VAL:H	2.25	0.45
4:2:270:MET:O	4:2:275:SER:OG	2.34	0.45
11:B:293:LEU:O	11:B:296:SER:N	2.35	0.45
14:E:82:ALA:HB2	24:P:25:GLN:HE21	1.82	0.45
28:T:32:ALA:CA	28:T:35:VAL:HG11	2.45	0.45
31:M:20:LYS:HD3	31:M:28:GLU:H	1.80	0.45
45:k:122:LEU:HB3	45:k:179:ARG:HD2	1.97	0.45
45:k:298:ALA:O	45:k:303:LEU:N	2.50	0.45
46:l:53:ALA:HB2	46:l:198:HIS:HB3	1.98	0.45
46:l:97:SER:HA	55:v:70:LEU:HB3	1.98	0.45
48:o:68:VAL:HB	48:o:69:GLU:CD	2.40	0.45
45:w:286:GLY:HA3	45:w:290:LEU:HD11	1.97	0.45
46:x:155:PRO:HA	46:x:158:HIS:HB3	1.98	0.45
47:y:373:GLU:HA	47:y:376:LEU:HB2	1.99	0.45
47:y:374:ASN:HA	47:y:379:TRP:CD1	2.49	0.45
50:A1:32:MET:SD	50:A1:89:TYR:HE2	2.40	0.45
56:A9:240:HIS:O	56:A9:243:VAL:HG22	2.17	0.45
59:A7:79:LYS:NZ	66:B0:15:ASN:HD21	2.15	0.45
6:5:38:LEU:HA	6:5:41:PHE:HB3	1.99	0.45
9:3:102:LEU:O	9:3:106:TRP:N	2.48	0.45
10:A:153:PHE:HE2	10:A:156:GLY:HA3	1.81	0.45
10:A:504:SER:H	10:A:505:GLY:HA2	1.81	0.45
15:F:106:SER:OG	15:F:107:PRO:O	2.31	0.45
35:a:84:THR:HG23	35:a:87:SER:H	1.82	0.45
44:e:88:PRO:CD	44:e:114:ARG:HB3	2.47	0.45
45:k:378:ASP:OD1	45:k:382:SER:OG	2.35	0.45
45:k:426:GLY:HA2	45:k:428:ILE:N	2.29	0.45
47:m:312:GLN:HE21	47:m:318:ARG:CG	2.29	0.45
47:m:326:TRP:CD2	51:r:48:VAL:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:330:ALA:HB2	51:r:52:PHE:HE1	1.81	0.45
45:w:69:ASN:HB2	45:w:115:ASP:OD2	2.16	0.45
45:w:127:ILE:HG22	45:w:131:ARG:NH1	2.28	0.45
47:y:107:TYR:HB3	47:y:113:TRP:CZ3	2.52	0.45
47:y:182:HIS:NE2	77:y:401:HEM:C1D	2.79	0.45
47:y:349:THR:HA	47:y:352:GLN:OE1	2.17	0.45
56:A9:32:ALA:HB3	67:B1:36:PRO:HG2	1.98	0.45
56:A9:273:MET:HG3	56:A9:319:LYS:NZ	2.30	0.45
59:A7:40:LEU:HD22	59:A7:59:LEU:CD1	2.47	0.45
61:B2:98:HIS:ND1	61:B2:98:HIS:N	2.64	0.45
1:9:187:GLN:HA	1:9:192:TYR:HA	1.99	0.45
73:8:501:FMN:H9	73:8:501:FMN:H1'1	1.58	0.45
10:A:31:LEU:HD13	10:A:42:MET:HB3	1.99	0.45
10:A:162:ASP:O	18:I:105:LYS:NZ	2.50	0.45
10:A:259:SER:OG	10:A:260:ASN:N	2.48	0.45
11:B:143:SER:HB2	11:B:146:CYS:HB3	1.98	0.45
12:C:217:GLU:OE1	26:R:75:ARG:NH2	2.47	0.45
45:k:48:GLU:HB3	45:k:52:ASN:HB2	1.98	0.45
45:k:183:THR:HA	45:k:186:LEU:HB2	1.99	0.45
47:m:286:ASN:CG	47:m:289:GLY:H	2.24	0.45
53:t:38:TRP:CE3	53:t:39:ARG:HG2	2.52	0.45
46:x:67:HIS:ND1	46:x:176:LEU:O	2.47	0.45
47:y:77:TRP:CZ3	47:y:78:ILE:HG22	2.51	0.45
47:y:330:ALA:HB2	51:A2:52:PHE:CD1	2.52	0.45
53:A3:27:VAL:HG22	54:B4:22:LEU:HD13	1.99	0.45
57:B9:59:GLN:N	57:B9:62:GLU:HG3	2.24	0.45
4:2:110:PRO:HA	4:2:112:HIS:CE1	2.52	0.45
8:1:36:GLY:HA2	13:D:108:ARG:HD3	1.99	0.45
27:S:73:HIS:HA	27:S:146:VAL:HG23	1.99	0.45
45:k:147:ASP:HA	45:k:150:PHE:CD2	2.51	0.45
45:k:303:LEU:HD22	45:k:333:ASP:OD2	2.16	0.45
47:m:50:PHE:CE2	49:p:58:PHE:HB3	2.51	0.45
47:m:107:TYR:HB3	47:m:113:TRP:CZ3	2.52	0.45
48:o:47:ALA:HB3	48:o:49:ARG:HG2	1.99	0.45
46:x:57:TYR:HB3	46:x:198:HIS:NE2	2.32	0.45
46:x:99:THR:OG1	55:B3:68:VAL:HG22	2.16	0.45
47:y:90:PHE:O	47:y:93:CYS:HB2	2.16	0.45
47:y:221:HIS:O	47:y:225:THR:OG1	2.24	0.45
3:6:173:LEU:HG	5:4:405:LEU:HD11	1.99	0.45
10:A:373:PRO:HG3	10:A:486:GLY:HA3	1.98	0.45
25:Q:86:TRP:HA	25:Q:89:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:S:401:PC1:H292	72:S:401:PC1:H262	1.78	0.45
45:k:127:ILE:HG22	45:k:131:ARG:NH1	2.28	0.45
45:k:347:THR:OG1	45:k:348:SER:N	2.50	0.45
46:l:376:GLU:O	46:l:379:LEU:HB3	2.16	0.45
47:m:315:MET:O	47:m:318:ARG:N	2.42	0.45
47:m:322:GLN:O	47:m:325:PHE:HB3	2.16	0.45
48:o:48:TYR:HB2	48:o:87:LEU:HA	2.00	0.45
45:w:434:TYR:O	45:w:437:ILE:N	2.50	0.45
46:x:53:ALA:HB2	46:x:198:HIS:HB3	1.98	0.45
46:x:303:VAL:CG1	46:x:304:HIS:H	2.26	0.45
48:z:235:LEU:HA	51:A2:14:ILE:O	2.17	0.45
56:A9:299:VAL:HA	56:A9:302:ARG:NH1	2.31	0.45
60:A6:78:HIS:CE1	64:B6:12:LEU:HD22	2.52	0.45
61:B2:33:ILE:HG22	61:B2:34:LEU:HD12	1.98	0.45
1:9:227:PRO:HD2	1:9:231:LEU:HA	1.99	0.44
3:6:264:TYR:HA	3:6:267:THR:HG22	1.97	0.44
5:4:210:TYR:O	5:4:213:HIS:ND1	2.44	0.44
10:A:321:ASP:OD2	10:A:325:ARG:NH2	2.50	0.44
22:N:60:LYS:HA	22:N:61:ALA:HA	1.78	0.44
24:P:29:GLN:HG3	24:P:30:GLU:H	1.83	0.44
25:Q:121:ASP:OD1	25:Q:121:ASP:N	2.50	0.44
25:Q:171:THR:OG1	25:Q:172:MET:N	2.50	0.44
27:S:290:LEU:O	27:S:294:ASN:N	2.50	0.44
38:d:75:PRO:HG2	43:g:26:LEU:HB3	1.98	0.44
45:k:32:GLN:NE2	46:l:373:GLU:OE1	2.51	0.44
45:k:146:ARG:HG2	45:k:150:PHE:CE2	2.52	0.44
45:k:434:TYR:O	45:k:437:ILE:N	2.51	0.44
46:l:58:GLU:HA	46:l:62:ASN:ND2	2.32	0.44
47:m:187:PHE:O	47:m:190:MET:N	2.51	0.44
47:m:275:LEU:O	47:m:279:ALA:N	2.36	0.44
48:o:41:HIS:NE2	78:o:301:HEC:C1D	2.80	0.44
48:o:165:TYR:HA	48:o:179:MET:HE3	1.99	0.44
50:q:104:ARG:HG2	46:x:83:PHE:CD2	2.51	0.44
45:w:35:CYS:N	45:w:101:ALA:O	2.28	0.44
45:w:172:GLU:HB2	45:w:176:LYS:CE	2.47	0.44
45:w:426:GLY:HA2	45:w:428:ILE:N	2.29	0.44
46:x:305:GLN:HG2	46:x:306:PRO:HD2	1.99	0.44
49:A0:17:GLU:OE1	49:A0:32:ARG:HB2	2.17	0.44
50:A1:97:VAL:HA	50:A1:100:GLU:OE1	2.17	0.44
56:A9:379:TYR:CE2	56:A9:383:MET:HE2	2.53	0.44
62:A4:44:ARG:HA	62:A4:45:PRO:HD2	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:A5:57:ARG:HB3	63:A5:57:ARG:NH1	2.31	0.44
9:3:42:ASP:N	9:3:43:PRO:HD2	2.29	0.44
10:A:409:PHE:HB2	10:A:688:GLN:HG2	2.00	0.44
12:C:131:VAL:HG22	12:C:146:LYS:HG2	1.98	0.44
18:I:108:LYS:CB	18:I:118:GLN:NE2	2.80	0.44
44:e:128:LEU:O	44:e:132:HIS:N	2.50	0.44
46:l:353:SER:HB2	46:l:356:ASP:OD2	2.17	0.44
47:m:58:ASP:OD1	47:y:56:THR:HG21	2.18	0.44
47:m:65:SER:O	47:m:69:ILE:HG13	2.17	0.44
47:m:77:TRP:CZ3	47:m:78:ILE:HG22	2.51	0.44
47:m:373:GLU:HA	47:m:376:LEU:HB2	1.98	0.44
48:o:56:TYR:HB3	48:o:61:ALA:HB2	1.99	0.44
48:o:72:ASP:OD1	48:o:80:MET:HG2	2.17	0.44
50:q:97:VAL:HA	50:q:100:GLU:OE1	2.17	0.44
51:r:52:PHE:O	51:r:55:PHE:HB3	2.17	0.44
45:w:298:ALA:O	45:w:303:LEU:N	2.50	0.44
46:x:87:ARG:HD3	46:x:87:ARG:HA	1.75	0.44
46:x:118:ILE:O	46:x:121:GLU:HB3	2.16	0.44
47:y:97:HIS:CE1	77:y:402:HEM:NA	2.86	0.44
47:y:187:PHE:O	47:y:190:MET:N	2.50	0.44
47:y:284:ILE:HG21	47:y:289:GLY:HA3	2.00	0.44
48:z:136:GLU:O	48:z:136:GLU:HG2	2.14	0.44
48:z:190:LEU:O	48:z:193:ALA:N	2.50	0.44
50:A1:33:ARG:HH12	50:A1:91:GLU:CD	2.20	0.44
54:B4:8:ARG:O	54:B4:12:LEU:N	2.46	0.44
79:A9:602:HEA:HH1	79:A9:602:HEA:O11	2.17	0.44
58:B7:19:THR:CG2	58:B7:53:THR:OG1	2.66	0.44
60:A6:70:VAL:HG12	60:A6:71:VAL:N	2.32	0.44
64:B6:19:PHE:CD1	64:B6:19:PHE:C	2.94	0.44
67:B1:35:ALA:HB3	67:B1:36:PRO:HD3	1.99	0.44
7:8:387:GLU:HG2	10:A:123:ASN:HD22	1.82	0.44
8:1:281:ARG:HH21	8:1:284:GLN:HE21	1.65	0.44
11:B:308:TYR:OH	11:B:401:GLU:N	2.46	0.44
30:V:20:ASP:HB2	30:V:22:LYS:HG2	1.98	0.44
43:g:76:GLU:HA	43:g:77:CYS:HA	1.77	0.44
45:k:85:HIS:CE1	46:l:284:HIS:ND1	2.85	0.44
45:k:153:LEU:HD12	45:k:153:LEU:HA	1.77	0.44
45:k:328:HIS:CD2	45:k:329:MET:SD	3.10	0.44
46:l:154:ASN:O	46:l:157:ALA:HB3	2.18	0.44
47:m:75:TYR:CE2	49:p:57:GLN:HG2	2.51	0.44
47:m:83:HIS:CD2	77:m:401:HEM:C4D	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:182:HIS:O	47:m:182:HIS:CG	2.70	0.44
48:o:190:LEU:O	48:o:193:ALA:N	2.50	0.44
50:q:94:LEU:HG	50:q:98:ILE:HD11	1.98	0.44
51:r:38:LEU:HA	51:r:41:THR:OG1	2.17	0.44
45:w:328:HIS:CD2	45:w:329:MET:SD	3.10	0.44
47:y:324:LEU:HA	47:y:327:ALA:HB3	1.98	0.44
48:z:165:TYR:HA	48:z:179:MET:HE3	1.99	0.44
57:B9:162:SER:HB2	57:B9:198:GLU:HB2	1.99	0.44
59:A7:79:LYS:HZ3	66:B0:15:ASN:HD21	1.65	0.44
61:B2:31:TYR:HE1	61:B2:98:HIS:CE1	2.34	0.44
1:9:239:LYS:HG3	7:8:42:PHE:HB2	1.99	0.44
2:7:59:ILE:HD11	9:3:67:LEU:HA	1.98	0.44
10:A:121:LEU:HD21	10:A:139:LEU:HB3	1.99	0.44
10:A:404:GLY:O	10:A:479:SER:OG	2.36	0.44
11:B:67:ASN:HB2	27:S:181:VAL:HG13	1.99	0.44
16:G:104:ARG:NH1	23:O:127:ASP:O	2.51	0.44
29:U:42:ASP:HA	29:U:43:LYS:HA	1.76	0.44
46:l:57:TYR:HB3	46:l:198:HIS:NE2	2.32	0.44
47:m:1:MET:HA	47:m:4:ILE:HG13	1.99	0.44
47:m:162:GLU:O	47:m:166:GLY:N	2.45	0.44
47:m:170:VAL:O	47:m:174:THR:HB	2.18	0.44
49:p:14:ARG:O	51:r:24:ARG:CZ	2.66	0.44
45:w:183:THR:HA	45:w:186:LEU:HB2	1.99	0.44
45:w:347:THR:OG1	45:w:348:SER:N	2.50	0.44
46:x:141:GLN:HB2	46:x:142:PRO:HD3	1.99	0.44
47:y:312:GLN:HE21	47:y:318:ARG:CG	2.29	0.44
48:z:151:PRO:HA	48:z:156:GLN:HG2	1.99	0.44
56:A9:131:PRO:HB2	57:B9:159:VAL:HA	2.00	0.44
56:A9:449:MET:HE3	66:B0:40:TRP:HB3	1.98	0.44
57:B9:1:MET:SD	57:B9:133:LEU:HD13	2.58	0.44
65:B8:30:ILE:HG13	65:B8:31:LEU:N	2.32	0.44
3:6:206:PRO:HD2	3:6:266:LEU:HD13	2.00	0.44
10:A:308:ARG:HA	10:A:308:ARG:HD2	1.85	0.44
14:E:37:THR:HA	24:P:104:TRP:HB3	2.00	0.44
39:f:166:LEU:HA	39:f:167:TRP:HA	1.62	0.44
43:g:90:MET:HB3	43:g:94:ARG:HH12	1.82	0.44
45:k:110:VAL:O	45:k:114:ALA:N	2.26	0.44
46:l:141:GLN:HB2	46:l:142:PRO:HD3	1.99	0.44
47:m:137:GLN:HE21	47:m:141:TRP:NE1	2.16	0.44
47:m:182:HIS:NE2	77:m:401:HEM:C1D	2.79	0.44
47:m:225:THR:O	47:m:229:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:23:HIS:HD2	54:u:55:ILE:HD12	1.83	0.44
45:w:350:THR:HB	45:w:353:GLU:CD	2.43	0.44
46:x:154:ASN:O	46:x:157:ALA:HB3	2.18	0.44
48:z:23:HIS:HA	48:z:26:ILE:HB	1.98	0.44
48:z:98:PRO:HA	48:z:101:ALA:HB3	1.99	0.44
49:A0:149:ASN:HA	49:A0:154:GLY:O	2.18	0.44
50:A1:16:ILE:HA	50:A1:19:TRP:HB3	2.00	0.44
50:A1:55:TYR:O	50:A1:59:VAL:HG23	2.17	0.44
51:A2:56:TYR:O	51:A2:59:TYR:HB3	2.18	0.44
55:B3:59:ALA:HB1	55:B3:62:ARG:O	2.18	0.44
58:B7:183:GLU:O	62:A4:42:ARG:NH2	2.50	0.44
5:4:423:ILE:HD12	35:a:56:ARG:HB3	2.00	0.44
10:A:78:CYS:SG	10:A:92:CYS:N	2.91	0.44
12:C:104:ASP:N	12:C:104:ASP:OD1	2.50	0.44
27:S:138:LEU:O	27:S:142:GLY:N	2.51	0.44
27:S:194:TYR:HB3	27:S:245:GLN:HG3	1.99	0.44
29:U:111:THR:OG1	29:U:112:ASN:N	2.51	0.44
32:X:37:PHE:HD2	36:b:137:MET:HB3	1.83	0.44
31:M:20:LYS:HE3	31:M:28:GLU:HG2	2.00	0.44
46:l:191:LEU:O	46:l:195:VAL:N	2.39	0.44
47:m:65:SER:O	47:m:68:HIS:HB3	2.17	0.44
47:m:70:CYS:SG	47:m:77:TRP:HA	2.58	0.44
48:o:73:GLY:O	48:o:79:GLU:HG2	2.18	0.44
50:q:55:TYR:O	50:q:59:VAL:HG23	2.17	0.44
46:x:353:SER:HB2	46:x:356:ASP:OD2	2.17	0.44
48:z:226:LYS:HA	48:z:226:LYS:HD2	1.81	0.44
49:A0:10:PHE:HB2	49:A0:14:ARG:HD2	1.99	0.44
53:A3:19:PRO:C	53:A3:22:SER:OG	2.59	0.44
56:A9:158:ILE:O	56:A9:162:ILE:HG13	2.17	0.44
58:B7:63:ARG:HA	58:B7:67:PHE:CD2	2.53	0.44
64:B6:21:ILE:HD12	64:B6:21:ILE:HA	1.82	0.44
6:5:7:ASN:HA	6:5:8:ILE:HA	1.71	0.44
10:A:628:GLU:HA	10:A:633:THR:HG22	1.99	0.44
13:D:99:MET:HE2	13:D:99:MET:HB3	1.91	0.44
27:S:158:LEU:HA	27:S:161:MET:HB3	1.99	0.44
27:S:192:VAL:HG11	27:S:233:PHE:HZ	1.83	0.44
31:W:108:LEU:HD23	31:W:114:ASP:CB	2.48	0.44
45:k:131:ARG:HE	45:k:175:ARG:CA	2.30	0.44
45:k:172:GLU:HB2	45:k:176:LYS:CE	2.47	0.44
49:p:10:PHE:O	49:p:12:ASP:N	2.51	0.44
51:r:56:TYR:O	51:r:59:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:276:PHE:CG	47:y:277:ALA:N	2.85	0.44
48:z:51:LEU:CD2	48:z:61:ALA:HB3	2.36	0.44
48:z:110:PRO:HG3	78:z:301:HEC:CMD	2.48	0.44
50:A1:91:GLU:N	50:A1:92:PRO:HD2	2.33	0.44
51:A2:52:PHE:O	51:A2:55:PHE:HB3	2.17	0.44
55:B3:77:ARG:HG2	55:B3:78:TYR:H	1.82	0.44
56:A9:51:ASP:O	56:A9:55:ASN:HB2	2.17	0.44
57:B9:63:THR:HA	57:B9:66:THR:HG22	2.00	0.44
57:B9:86:MET:HE3	57:B9:86:MET:HB2	1.80	0.44
57:B9:122:MET:HB2	57:B9:208:PRO:CD	2.47	0.44
3:6:221:THR:HG22	3:6:226:GLN:HG3	2.00	0.44
18:I:111:THR:HG22	18:I:118:GLN:HA	2.00	0.44
22:N:67:LYS:HE3	22:N:71:ARG:HE	1.83	0.44
26:R:64:PHE:CZ	26:R:208:GLY:HA3	2.53	0.44
26:R:326:ASP:O	26:R:328:ILE:HG13	2.18	0.44
42:j:83:TYR:HD1	42:j:86:ARG:HE	1.64	0.44
46:l:87:ARG:HA	46:l:87:ARG:HD3	1.75	0.44
47:m:120:LEU:O	47:m:121:LEU:C	2.61	0.44
47:m:272:TRP:CZ2	47:m:273:TYR:HB3	2.53	0.44
48:o:48:TYR:CE1	48:o:91:PHE:HE1	2.35	0.44
49:p:71:MET:HG3	49:p:72:SER:N	2.23	0.44
50:q:32:MET:SD	50:q:89:TYR:HE2	2.40	0.44
45:w:21:ASN:HB2	45:w:218:GLY:O	2.18	0.44
45:w:142:ASP:OD1	49:A0:1:SER:N	2.50	0.44
45:w:214:LYS:O	45:w:215:HIS:ND1	2.51	0.44
45:w:386:TYR:HB3	45:w:389:ARG:HD2	1.98	0.44
46:x:267:ALA:HA	46:x:270:ASN:HB3	1.99	0.44
46:x:325:TYR:HD2	55:B3:57:GLY:N	2.15	0.44
47:y:137:GLN:HE21	47:y:141:TRP:NE1	2.16	0.44
57:B9:121:TYR:C	57:B9:138:VAL:HG23	2.42	0.44
5:4:207:MET:HA	5:4:208:PRO:HD3	1.86	0.44
11:B:143:SER:HB3	11:B:182:ASN:HD21	1.83	0.44
18:I:103:LEU:HD13	18:I:121:GLN:HB3	1.99	0.44
45:k:144:SER:O	45:k:148:VAL:HG23	2.18	0.44
45:k:214:LYS:O	45:k:215:HIS:ND1	2.51	0.44
47:m:97:HIS:CE1	77:m:402:HEM:NA	2.86	0.44
47:m:135:TRP:CG	47:m:135:TRP:O	2.70	0.44
47:m:276:PHE:CG	47:m:277:ALA:N	2.85	0.44
48:o:181:GLN:O	48:o:185:ASP:N	2.37	0.44
50:q:105:GLU:HB3	50:q:109:LYS:NZ	2.33	0.44
46:x:155:PRO:O	46:x:159:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:200:THR:HG1	46:x:228:GLY:N	2.15	0.44
46:x:230:LEU:HD12	46:x:230:LEU:O	2.17	0.44
46:x:304:HIS:CD2	46:x:305:GLN:H	2.36	0.44
47:y:146:ILE:O	47:y:149:LEU:HB3	2.17	0.44
47:y:170:VAL:O	47:y:174:THR:HB	2.18	0.44
48:z:22:ASP:HA	54:B4:50:LYS:O	2.18	0.44
48:z:48:TYR:HB2	48:z:87:LEU:HA	1.99	0.44
48:z:181:GLN:O	48:z:185:ASP:N	2.37	0.44
56:A9:70:VAL:HG11	56:A9:246:LEU:HD22	2.00	0.44
3:6:82:MET:HA	3:6:86:SER:HB3	2.00	0.43
3:6:209:SER:OG	3:6:270:ASN:ND2	2.51	0.43
11:B:254:ARG:HH21	24:P:24:LEU:HA	1.83	0.43
32:X:30:ASN:OD1	32:X:31:ASP:N	2.52	0.43
45:k:220:SER:C	45:k:222:THR:N	2.76	0.43
45:k:267:ASN:ND2	45:k:386:TYR:OH	2.45	0.43
45:k:438:ARG:NH2	51:r:21:PHE:HE2	2.11	0.43
50:q:91:GLU:N	50:q:92:PRO:HD2	2.33	0.43
54:u:17:THR:O	54:u:20:PHE:HB3	2.18	0.43
55:v:72:VAL:HB	55:v:73:PRO:HD3	2.00	0.43
45:w:15:GLN:HE21	45:w:205:HIS:CG	2.36	0.43
45:w:415:PHE:O	45:w:418:GLN:HG2	2.18	0.43
46:x:46:ARG:HH12	46:x:376:GLU:HB2	1.83	0.43
47:y:70:CYS:SG	47:y:77:TRP:HA	2.58	0.43
47:y:312:GLN:HA	50:A1:38:HIS:H	1.82	0.43
48:z:83:ARG:O	48:z:83:ARG:HG3	2.18	0.43
49:A0:121:GLN:CB	49:A0:170:ARG:HA	2.48	0.43
53:A3:14:ALA:HB1	53:A3:18:VAL:CG2	2.47	0.43
71:4:502:3PE:H2B1	71:4:502:3PE:H2E1	1.75	0.43
10:A:456:ALA:HA	10:A:496:ILE:HD13	2.00	0.43
10:A:607:LYS:HE2	16:G:78:ARG:HE	1.83	0.43
23:O:18:LYS:O	23:O:77:ARG:NH2	2.52	0.43
26:R:178:SER:H	26:R:181:LEU:HB3	1.82	0.43
26:R:178:SER:N	26:R:182:ARG:H	2.14	0.43
26:R:244:ASP:OD2	26:R:343:THR:OG1	2.31	0.43
46:l:155:PRO:O	46:l:159:VAL:HG23	2.18	0.43
46:l:385:GLN:O	46:l:389:ALA:N	2.41	0.43
53:t:33:VAL:HG13	53:t:38:TRP:CD1	2.54	0.43
45:w:2:ALA:HB3	46:x:113:ARG:CZ	2.47	0.43
46:x:58:GLU:HA	46:x:62:ASN:ND2	2.32	0.43
47:y:135:TRP:O	47:y:135:TRP:CG	2.71	0.43
48:z:41:HIS:NE2	78:z:301:HEC:C1D	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:48:TYR:CE1	48:z:91:PHE:HE1	2.35	0.43
50:A1:26:PHE:O	50:A1:28:LYS:N	2.49	0.43
62:A4:42:ARG:HG3	62:A4:42:ARG:NH1	2.32	0.43
64:B6:26:MET:SD	64:B6:26:MET:N	2.91	0.43
3:6:595:ILE:HD12	4:2:100:MET:HE2	2.00	0.43
7:8:246:GLU:HA	7:8:249:ALA:HB3	2.00	0.43
7:8:321:GLY:N	7:8:351:THR:OG1	2.46	0.43
16:G:130:THR:HG23	16:G:133:ASP:H	1.83	0.43
18:I:106:GLU:HA	18:I:107:THR:HA	1.64	0.43
37:c:37:PRO:HB2	37:c:38:GLN:H	1.64	0.43
45:k:3:THR:O	45:k:7:ALA:N	2.36	0.43
45:k:15:GLN:HE21	45:k:205:HIS:CG	2.36	0.43
47:m:146:ILE:O	47:m:149:LEU:HB3	2.17	0.43
47:m:230:LEU:O	47:m:234:LEU:HG	2.19	0.43
47:m:260:ASN:HB2	47:m:263:ASN:HB3	2.00	0.43
50:q:48:ARG:HA	50:q:48:ARG:HD3	1.77	0.43
45:w:86:LEU:HD13	45:w:99:ILE:HD11	2.00	0.43
45:w:133:VAL:O	45:w:137:GLU:HG3	2.19	0.43
47:y:182:HIS:O	47:y:182:HIS:CG	2.70	0.43
47:y:260:ASN:HB2	47:y:263:ASN:HB3	2.00	0.43
77:y:402:HEM:HBC2	77:y:402:HEM:CMC	2.47	0.43
48:z:238:ARG:HD3	49:A0:2:HIS:CB	2.47	0.43
49:A0:83:GLU:HA	49:A0:100:HIS:C	2.43	0.43
59:A7:37:GLN:O	59:A7:41:LYS:HG2	2.18	0.43
62:A4:3:ALA:O	62:A4:4:ALA:HB2	2.17	0.43
64:B6:68:ILE:HG13	64:B6:69:PHE:N	2.33	0.43
8:1:226:ALA:O	8:1:229:ALA:HB3	2.18	0.43
13:D:182:TYR:HE2	14:E:180:HIS:HB2	1.84	0.43
38:d:34:ARG:HA	38:d:35:LYS:HA	1.80	0.43
45:k:133:VAL:O	45:k:137:GLU:HG3	2.18	0.43
45:k:281:ASP:OD1	45:k:306:SER:HB3	2.19	0.43
48:o:83:ARG:O	48:o:83:ARG:HG3	2.18	0.43
48:o:98:PRO:HA	48:o:101:ALA:HB3	1.99	0.43
50:q:33:ARG:HH12	50:q:91:GLU:CD	2.20	0.43
53:t:31:GLY:HA2	53:t:34:TRP:HB3	2.00	0.43
54:u:9:LEU:HA	54:u:12:LEU:HB3	2.01	0.43
55:v:70:LEU:HD11	55:v:73:PRO:HG2	2.00	0.43
45:w:280:TYR:HA	45:w:284:TYR:CE2	2.53	0.43
45:w:355:LEU:O	45:w:358:LYS:HB3	2.19	0.43
45:w:437:ILE:O	45:w:441:MET:HG2	2.19	0.43
46:x:168:TYR:HD1	46:x:237:ALA:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:191:LEU:O	46:x:195:VAL:N	2.39	0.43
47:y:1:MET:HA	47:y:4:ILE:HG13	1.99	0.43
47:y:225:THR:O	47:y:229:ILE:HG13	2.18	0.43
56:A9:377:PHE:CD2	79:A9:602:HEA:HAD1	2.53	0.43
62:A4:5:LYS:CD	62:A4:6:GLY:N	2.81	0.43
66:B0:44:PRO:HA	66:B0:47:ARG:NH1	2.34	0.43
3:6:279:CYS:SG	3:6:405:ASN:ND2	2.91	0.43
71:2:401:3PE:H362	71:2:401:3PE:H331	1.81	0.43
8:1:215:TYR:HD1	8:1:219:PRO:HB2	1.83	0.43
11:B:253:LEU:HD23	11:B:254:ARG:HH12	1.83	0.43
49:p:13:TYR:CD2	49:p:13:TYR:N	2.86	0.43
49:p:38:LEU:O	49:p:42:THR:OG1	2.22	0.43
49:p:51:ALA:HB1	49:p:55:VAL:HG23	2.00	0.43
45:w:125:SER:O	45:w:129:LYS:HG3	2.19	0.43
47:y:77:TRP:CH2	48:z:201:ARG:HB2	2.54	0.43
47:y:372:ILE:HG22	47:y:376:LEU:HG	2.00	0.43
58:B7:41:THR:O	58:B7:45:ILE:HG13	2.18	0.43
58:B7:154:GLY:CA	61:B2:6:VAL:HG22	2.47	0.43
60:A6:27:TRP:CH2	61:B2:86:GLY:HA2	2.54	0.43
65:B8:11:LEU:HD23	65:B8:11:LEU:C	2.44	0.43
4:2:4:ILE:HB	72:S:401:PC1:H241	2.01	0.43
5:4:168:GLN:HE21	36:b:150:ARG:NH1	2.17	0.43
7:8:295:PRO:HG2	7:8:298:GLU:HG2	1.99	0.43
40:h:127:LYS:HA	40:h:130:GLU:HB3	2.01	0.43
45:k:86:LEU:HD13	45:k:99:ILE:HD11	2.00	0.43
45:k:262:TRP:CG	45:k:385:THR:HG23	2.54	0.43
45:k:350:THR:HB	45:k:353:GLU:CD	2.43	0.43
45:k:355:LEU:O	45:k:358:LYS:HB3	2.19	0.43
46:l:50:PHE:C	46:l:387:LEU:HD11	2.43	0.43
46:l:168:TYR:HD1	46:l:237:ALA:O	2.01	0.43
46:l:200:THR:HG1	46:l:228:GLY:H	1.59	0.43
47:m:78:ILE:O	47:m:82:MET:HG3	2.19	0.43
47:m:188:ILE:O	47:m:192:ILE:HG12	2.19	0.43
77:m:401:HEM:HBB2	77:m:401:HEM:HMB1	2.00	0.43
49:p:76:ILE:H	49:p:77:LYS:HA	1.84	0.43
50:q:91:GLU:HB3	50:q:95:LYS:HZ2	1.83	0.43
45:w:281:ASP:OD1	45:w:306:SER:HB3	2.19	0.43
46:x:97:SER:N	46:x:108:THR:O	2.52	0.43
47:y:40:CYS:HB2	47:y:90:PHE:HD1	1.84	0.43
47:y:69:ILE:O	47:y:76:GLY:HA3	2.19	0.43
47:y:107:TYR:CE1	47:y:305:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:162:GLU:O	47:y:166:GLY:N	2.45	0.43
47:y:188:ILE:O	47:y:192:ILE:HG12	2.19	0.43
47:y:230:LEU:O	47:y:234:LEU:HG	2.19	0.43
47:y:238:ALA:HA	47:y:241:LEU:HB3	2.01	0.43
47:y:272:TRP:CZ2	47:y:273:TYR:HB3	2.53	0.43
47:y:357:LEU:O	47:y:361:LEU:HG	2.18	0.43
50:A1:23:ALA:HB3	51:A2:46:LEU:HD21	1.91	0.43
54:B4:43:TYR:O	54:B4:47:ASN:ND2	2.52	0.43
56:A9:247:ILE:HB	79:A9:602:HEA:HBC1	2.01	0.43
57:B9:162:SER:HB3	57:B9:197:SER:C	2.44	0.43
58:B7:148:HIS:CE1	58:B7:152:MET:HE3	2.54	0.43
67:B1:41:ARG:HD2	68:A8:40:TYR:CZ	2.54	0.43
4:2:54:GLU:OE1	6:5:94:ASN:ND2	2.51	0.43
10:A:189:ILE:H	10:A:189:ILE:HG13	1.60	0.43
18:I:101:ILE:H	18:I:101:ILE:HG13	1.68	0.43
24:P:41:LEU:HD12	24:P:42:PRO:HD2	2.00	0.43
30:V:143:TYR:HD1	30:V:143:TYR:HA	1.78	0.43
40:h:111:ASP:OD1	40:h:111:ASP:N	2.52	0.43
46:l:56:ARG:NE	46:l:103:GLU:OE1	2.52	0.43
46:l:346:THR:O	46:l:349:GLN:HB2	2.18	0.43
46:l:368:TYR:O	46:l:372:VAL:HG23	2.19	0.43
47:m:23:ALA:N	47:m:217:LYS:HE3	2.34	0.43
47:m:166:GLY:HA2	49:A0:63:SER:O	2.19	0.43
47:m:284:ILE:HG21	47:m:289:GLY:HA3	2.00	0.43
48:o:230:LEU:O	48:o:233:ARG:HG2	2.18	0.43
49:p:50:ALA:O	49:p:54:VAL:HG23	2.19	0.43
45:w:153:LEU:HA	45:w:153:LEU:HD12	1.77	0.43
45:w:378:ASP:OD1	45:w:382:SER:OG	2.35	0.43
47:y:65:SER:O	47:y:68:HIS:HB3	2.18	0.43
47:y:65:SER:O	47:y:69:ILE:HG13	2.17	0.43
47:y:78:ILE:O	47:y:82:MET:HG3	2.19	0.43
47:y:153:ILE:HG23	47:y:154:PRO:HD2	2.00	0.43
48:z:180:SER:HB3	52:B5:17:LEU:HB2	1.99	0.43
48:z:230:LEU:O	48:z:233:ARG:HG2	2.18	0.43
58:B7:60:ASP:O	58:B7:64:GLU:HG3	2.18	0.43
7:8:47:GLY:O	7:8:133:HIS:ND1	2.52	0.43
7:8:213:ILE:HG23	7:8:224:ARG:HH12	1.83	0.43
12:C:187:ARG:HG2	23:O:88:MET:HE1	1.99	0.43
25:Q:28:ALA:O	25:Q:30:HIS:N	2.51	0.43
35:a:27:SER:HA	35:a:28:GLU:HA	1.81	0.43
36:b:161:ARG:HA	36:b:161:ARG:HD2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:82:VAL:HA	40:h:85:TRP:HD1	1.84	0.43
45:k:280:TYR:HA	45:k:284:TYR:CE2	2.53	0.43
46:l:97:SER:N	46:l:108:THR:O	2.52	0.43
47:m:91:PHE:HZ	47:m:124:MET:HG2	1.79	0.43
47:m:97:HIS:CD2	77:m:402:HEM:NC	2.87	0.43
48:o:129:SER:HB3	48:o:152:TYR:CE2	2.54	0.43
53:t:34:TRP:CD1	54:u:29:LEU:HD13	2.52	0.43
45:w:92:ARG:HG2	45:w:167:VAL:HG22	2.00	0.43
45:w:131:ARG:HE	45:w:175:ARG:CA	2.30	0.43
47:y:91:PHE:HD1	47:y:91:PHE:HA	1.73	0.43
52:B5:34:ARG:O	52:B5:37:LEU:HB2	2.19	0.43
65:B8:3:ASN:ND2	65:B8:5:VAL:HG13	2.33	0.43
1:9:152:ILE:HG12	1:9:201:ILE:HD12	2.00	0.43
7:8:155:TYR:HE1	7:8:196:PHE:HD2	1.65	0.43
8:1:20:LEU:O	8:1:24:GLU:N	2.51	0.43
26:R:58:VAL:HG13	26:R:127:ILE:HD11	2.00	0.43
31:W:109:GLY:HA2	31:W:110:LEU:HA	1.82	0.43
32:X:13:HIS:O	32:X:15:LEU:N	2.52	0.43
41:i:45:GLY:HA2	41:i:48:LEU:HB2	2.01	0.43
45:k:354:VAL:O	45:k:355:LEU:C	2.62	0.43
45:k:397:SER:O	45:k:401:GLU:HG2	2.18	0.43
47:m:238:ALA:HA	47:m:241:LEU:HB3	2.01	0.43
47:m:272:TRP:CG	47:m:273:TYR:N	2.87	0.43
48:o:65:ALA:O	48:o:69:GLU:OE1	2.36	0.43
48:o:110:PRO:HG3	78:o:301:HEC:CMD	2.48	0.43
48:o:151:PRO:HA	48:o:156:GLN:CG	2.49	0.43
49:p:58:PHE:O	49:p:61:SER:OG	2.21	0.43
45:w:85:HIS:CE1	46:x:284:HIS:ND1	2.87	0.43
45:w:138:LEU:CD1	45:w:174:VAL:HG21	2.48	0.43
45:w:144:SER:O	45:w:148:VAL:HG23	2.18	0.43
45:w:262:TRP:CG	45:w:385:THR:HG23	2.54	0.43
45:w:391:PRO:HG2	45:w:398:ARG:NH2	2.34	0.43
46:x:26:PHE:CZ	46:x:391:SER:HA	2.54	0.43
46:x:346:THR:O	46:x:349:GLN:HB2	2.18	0.43
48:z:47:ALA:HB3	48:z:49:ARG:HG2	1.99	0.43
49:A0:44:THR:O	49:A0:47:VAL:HB	2.17	0.43
50:A1:14:GLU:O	50:A1:17:ARG:HB2	2.19	0.43
50:A1:26:PHE:CG	50:A1:27:ASN:N	2.85	0.43
56:A9:353:LEU:HD12	56:A9:353:LEU:HA	1.91	0.43
57:B9:52:HIS:CD2	60:A6:40:ASP:HB2	2.54	0.43
58:B7:80:ARG:HG2	58:B7:233:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:B6:29:LEU:HD23	64:B6:29:LEU:HA	1.86	0.43
64:B6:61:GLU:OE1	64:B6:64:ARG:NH1	2.51	0.43
1:9:155:LYS:HE3	1:9:202:GLU:HA	2.00	0.43
7:8:375:LYS:HD3	7:8:393:ASN:HD22	1.84	0.43
26:R:175:LYS:O	26:R:177:SER:N	2.49	0.43
27:S:275:ASN:O	27:S:277:ARG:N	2.40	0.43
32:X:14:VAL:HA	32:X:17:PRO:HD2	2.01	0.43
45:k:92:ARG:HG2	45:k:167:VAL:HG22	2.00	0.43
45:k:235:ARG:HB2	49:p:21:SER:HA	2.01	0.43
47:m:118:ILE:O	47:m:119:LEU:C	2.62	0.43
47:m:357:LEU:O	47:m:361:LEU:HG	2.18	0.43
49:p:71:MET:CG	49:p:72:SER:H	2.24	0.43
50:q:27:ASN:O	50:q:81:THR:N	2.52	0.43
52:s:34:ARG:O	52:s:37:LEU:HB2	2.19	0.43
45:w:19:LEU:HD12	45:w:23:LEU:HD23	2.00	0.43
46:x:308:ASP:OD1	46:x:309:VAL:N	2.52	0.43
46:x:368:TYR:O	46:x:372:VAL:HG23	2.19	0.43
47:y:244:LEU:HD11	48:z:201:ARG:HG3	2.01	0.43
50:A1:105:GLU:HB3	50:A1:109:LYS:NZ	2.33	0.43
57:B9:3:TYR:CD1	57:B9:3:TYR:N	2.87	0.43
3:6:246:LEU:O	3:6:251:THR:OG1	2.27	0.42
8:1:5:ASN:HD21	19:J:23:THR:HG23	1.83	0.42
26:R:154:GLN:HG3	26:R:155:VAL:H	1.83	0.42
26:R:195:PHE:HD2	26:R:198:ALA:HB2	1.83	0.42
27:S:102:LEU:HA	27:S:105:PHE:HE1	1.84	0.42
28:T:41:VAL:CG1	28:T:59:TYR:CZ	2.81	0.42
31:M:26:ASP:OD1	31:M:26:ASP:N	2.52	0.42
45:k:415:PHE:O	45:k:418:GLN:HG2	2.18	0.42
47:m:40:CYS:HB2	47:m:90:PHE:HD1	1.84	0.42
47:m:106:SER:HG	47:m:206:ASN:HD22	1.61	0.42
50:q:7:SER:O	50:q:10:SER:HB2	2.19	0.42
50:q:16:ILE:HA	50:q:19:TRP:HB3	2.00	0.42
50:q:101:ARG:O	50:q:105:GLU:N	2.40	0.42
54:u:43:TYR:O	54:u:47:ASN:ND2	2.52	0.42
48:z:129:SER:HB3	48:z:152:TYR:CE2	2.54	0.42
48:z:151:PRO:HA	48:z:156:GLN:CG	2.49	0.42
49:A0:62:MET:HE2	49:A0:62:MET:HB3	1.91	0.42
52:B5:18:THR:HA	52:B5:21:ARG:HG3	2.00	0.42
54:B4:17:THR:O	54:B4:20:PHE:HB3	2.18	0.42
58:B7:19:THR:HG22	58:B7:53:THR:OG1	2.18	0.42
3:6:556:ILE:O	3:6:560:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:118:TRP:O	8:1:122:ALA:N	2.49	0.42
26:R:228:LEU:HA	26:R:229:ILE:HA	1.80	0.42
27:S:102:LEU:HD23	27:S:105:PHE:HE1	1.84	0.42
42:j:91:PHE:HD1	42:j:94:ILE:HD12	1.84	0.42
44:e:39:GLY:HA3	44:e:40:PRO:HA	1.75	0.42
45:k:437:ILE:O	45:k:441:MET:HG2	2.18	0.42
46:l:308:ASP:OD1	46:l:309:VAL:N	2.52	0.42
47:m:69:ILE:O	47:m:76:GLY:HA3	2.19	0.42
47:m:89:MET:HG3	47:m:239:LEU:HD13	2.01	0.42
47:m:207:ASN:ND2	47:m:211:ILE:H	2.14	0.42
47:m:244:LEU:HD11	48:o:201:ARG:HB2	2.00	0.42
50:q:18:LYS:HA	50:q:83:TYR:CD1	2.54	0.42
47:y:89:MET:HG3	47:y:239:LEU:HD13	2.01	0.42
77:y:401:HEM:HBB2	77:y:401:HEM:HMB1	2.00	0.42
48:z:29:GLY:O	48:z:32:VAL:HB	2.19	0.42
48:z:153:PHE:HD2	48:z:156:GLN:N	2.16	0.42
65:B8:36:MET:O	65:B8:40:LEU:HG	2.18	0.42
1:9:145:SER:O	1:9:149:LEU:N	2.53	0.42
3:6:81:LYS:N	3:6:133:THR:O	2.52	0.42
4:2:300:THR:HG23	4:2:301:THR:HG23	2.00	0.42
5:4:306:PRO:HA	5:4:308:SER:H	1.83	0.42
8:1:34:ARG:HD3	13:D:102:PRO:HB3	2.01	0.42
27:S:110:LYS:HA	27:S:166:PHE:HA	2.01	0.42
39:f:16:VAL:O	39:f:20:TYR:N	2.52	0.42
39:f:128:LEU:O	39:f:132:SER:OG	2.37	0.42
42:j:26:LEU:HB3	42:j:27:THR:H	1.72	0.42
45:k:171:SER:O	45:k:174:VAL:HB	2.20	0.42
48:o:11:PRO:CA	48:o:15:ARG:HH11	2.32	0.42
48:o:136:GLU:O	48:o:136:GLU:HG2	2.14	0.42
49:p:76:ILE:CB	49:p:108:GLN:HA	2.50	0.42
50:q:14:GLU:O	50:q:17:ARG:HB2	2.19	0.42
45:w:157:ALA:CB	45:w:237:THR:H	2.32	0.42
46:x:53:ALA:HA	46:x:57:TYR:CE2	2.54	0.42
46:x:228:GLY:O	46:x:230:LEU:N	2.52	0.42
46:x:365:LYS:O	46:x:369:LEU:HG	2.20	0.42
46:x:370:MET:HA	46:x:373:GLU:CD	2.44	0.42
47:y:245:PHE:O	47:y:247:PRO:HD3	2.20	0.42
48:z:28:ARG:HH12	52:B5:78:LYS:HE2	1.85	0.42
48:z:102:ARG:O	48:z:106:ASN:N	2.52	0.42
54:B4:9:LEU:HA	54:B4:12:LEU:HB3	2.01	0.42
73:8:501:FMN:O4'	73:8:501:FMN:O2'	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:76:GLN:HE22	12:C:148:TYR:HE1	1.67	0.42
39:f:58:VAL:HG11	45:w:230:THR:N	2.34	0.42
42:j:46:ASN:HA	42:j:51:ARG:HH21	1.84	0.42
45:k:106:LEU:CD2	45:k:203:LEU:HD21	2.49	0.42
46:l:46:ARG:HH12	46:l:376:GLU:HB2	1.83	0.42
47:m:107:TYR:CE1	47:m:305:PRO:HA	2.54	0.42
48:o:22:ASP:OD1	54:u:55:ILE:HD11	2.20	0.42
48:o:153:PHE:HD2	48:o:156:GLN:N	2.16	0.42
48:o:165:TYR:HA	48:o:179:MET:CE	2.49	0.42
45:w:391:PRO:HB3	45:w:394:GLU:CD	2.44	0.42
45:w:397:SER:O	45:w:401:GLU:HG2	2.18	0.42
47:y:23:ALA:N	47:y:217:LYS:HE3	2.34	0.42
47:y:97:HIS:HD2	77:y:402:HEM:C1C	2.38	0.42
47:y:102:LEU:HA	47:y:102:LEU:HD23	1.81	0.42
47:y:104:TYR:CE1	47:y:208:PRO:HA	2.54	0.42
47:y:118:ILE:O	47:y:119:LEU:C	2.62	0.42
56:A9:498:CYS:HA	56:A9:499:PRO:HA	1.78	0.42
1:9:88:ARG:NH1	15:F:82:THR:O	2.53	0.42
10:A:272:ARG:HH12	10:A:274:LEU:HD11	1.84	0.42
12:C:124:ARG:HD2	22:N:111:GLN:HG3	2.02	0.42
13:D:206:ARG:HH21	13:D:208:LYS:HE2	1.84	0.42
45:k:12:PRO:HB2	45:k:28:GLU:HG3	2.02	0.42
45:k:125:SER:O	45:k:129:LYS:HG3	2.19	0.42
45:k:185:TYR:CE1	45:k:189:HIS:CE1	3.07	0.42
45:k:395:TRP:CH2	45:k:398:ARG:NH1	2.88	0.42
45:k:412:SER:HB3	54:u:15:ARG:HH22	1.82	0.42
48:o:29:GLY:O	48:o:32:VAL:HB	2.19	0.42
52:s:18:THR:HA	52:s:21:ARG:HG3	2.00	0.42
45:w:61:HIS:HB3	45:w:65:LYS:NZ	2.34	0.42
45:w:130:GLU:OE2	45:w:134:ILE:HD11	2.20	0.42
45:w:171:SER:O	45:w:174:VAL:HB	2.20	0.42
45:w:316:ASP:OD1	45:w:316:ASP:N	2.34	0.42
46:x:46:ARG:HH12	46:x:376:GLU:CB	2.33	0.42
46:x:56:ARG:NE	46:x:103:GLU:OE1	2.51	0.42
46:x:200:THR:O	46:x:204:MET:HG3	2.19	0.42
52:B5:31:VAL:CA	52:B5:34:ARG:HB3	2.46	0.42
58:B7:137:LEU:HA	58:B7:137:LEU:HD12	1.69	0.42
62:A4:77:PRO:HA	62:A4:82:TYR:HA	2.02	0.42
1:9:188:ILE:HG13	1:9:191:ASN:H	1.84	0.42
4:2:51:ARG:HG3	11:B:69:VAL:HB	2.01	0.42
7:8:183:GLY:HA2	7:8:184:LYS:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:253:THR:HA	7:8:256:ARG:HB3	2.02	0.42
13:D:75:ASN:HD21	13:D:207:GLU:HA	1.84	0.42
17:H:28:LYS:HB3	36:b:184:LYS:HA	2.01	0.42
22:N:43:ALA:HA	22:N:46:LYS:HD3	2.00	0.42
26:R:201:ILE:HD12	26:R:263:PHE:HB2	2.01	0.42
45:k:19:LEU:HD12	45:k:23:LEU:HD23	2.00	0.42
45:k:61:HIS:HB3	45:k:65:LYS:NZ	2.34	0.42
45:k:425:PHE:C	45:k:428:ILE:HG13	2.45	0.42
46:l:200:THR:O	46:l:204:MET:HG3	2.19	0.42
51:r:32:LYS:O	51:r:35:PRO:HD2	2.20	0.42
52:s:21:ARG:HD3	52:s:65:ARG:NH2	2.35	0.42
54:u:8:ARG:O	54:u:12:LEU:N	2.46	0.42
54:u:16:ARG:O	54:u:19:THR:OG1	2.30	0.42
45:w:36:THR:N	45:w:200:ALA:O	2.47	0.42
46:x:429:ASN:OD1	46:x:431:GLY:N	2.45	0.42
47:y:120:LEU:O	47:y:121:LEU:C	2.61	0.42
47:y:227:LYS:HG3	48:z:223:LYS:HE3	2.00	0.42
47:y:272:TRP:CG	47:y:273:TYR:N	2.87	0.42
47:y:282:ARG:NH1	47:y:341:GLN:O	2.42	0.42
49:A0:91:TRP:O	49:A0:93:GLY:N	2.52	0.42
51:A2:32:LYS:O	51:A2:35:PRO:HD2	2.20	0.42
5:4:5:ILE:HA	5:4:8:THR:HG22	2.01	0.42
8:1:200:LEU:HD13	8:1:282:TYR:HB2	2.01	0.42
10:A:180:THR:HG23	10:A:183:ILE:HD12	2.02	0.42
11:B:180:LEU:HB2	11:B:210:MET:HE1	2.01	0.42
12:C:218:VAL:HG13	12:C:219:LYS:H	1.85	0.42
13:D:75:ASN:ND2	13:D:206:ARG:O	2.52	0.42
31:M:25:ILE:HD12	31:M:42:LEU:HG	2.01	0.42
45:k:350:THR:O	45:k:353:GLU:HG2	2.20	0.42
46:l:26:PHE:CZ	46:l:391:SER:HA	2.54	0.42
46:l:213:HIS:O	46:l:217:LYS:N	2.41	0.42
47:m:245:PHE:C	47:m:247:PRO:HD3	2.45	0.42
48:o:102:ARG:O	48:o:106:ASN:N	2.52	0.42
54:u:54:HIS:HA	54:u:57:HIS:CD2	2.55	0.42
46:x:50:PHE:C	46:x:387:LEU:HD11	2.44	0.42
47:y:313:ARG:HB2	50:A1:38:HIS:HD2	1.83	0.42
48:z:11:PRO:CA	48:z:15:ARG:HH11	2.32	0.42
48:z:52:VAL:HG22	54:B4:56:LYS:NZ	2.35	0.42
48:z:217:PRO:O	48:z:221:ALA:N	2.47	0.42
48:z:231:LYS:HE2	50:A1:70:MET:HG2	2.01	0.42
50:A1:7:SER:O	50:A1:10:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B7:110:PRO:HB3	63:A5:30:TRP:CD2	2.54	0.42
59:A7:126:MET:HG3	59:A7:128:VAL:HG23	2.01	0.42
64:B6:35:TYR:O	64:B6:39:VAL:HB	2.19	0.42
10:A:634:LEU:HA	10:A:635:PRO:HD3	1.83	0.42
11:B:105:MET:N	11:B:105:MET:SD	2.93	0.42
22:N:88:LEU:HD11	22:N:92:ARG:HH21	1.84	0.42
23:O:50:PHE:HE2	23:O:103:VAL:HG21	1.84	0.42
33:Y:47:TYR:HD2	34:Z:16:LEU:HD12	1.84	0.42
37:c:11:ARG:HB2	39:f:155:PRO:HB3	2.02	0.42
45:k:83:GLY:HA2	46:l:363:LYS:HG2	2.02	0.42
47:m:153:ILE:HG23	47:m:154:PRO:HD2	2.00	0.42
47:m:209:THR:O	47:m:211:ILE:HG13	2.20	0.42
47:m:330:ALA:HA	47:m:333:LEU:HB3	2.01	0.42
47:m:364:VAL:O	47:m:368:THR:OG1	2.35	0.42
47:m:372:ILE:HG22	47:m:376:LEU:HG	2.00	0.42
48:o:76:GLU:C	48:o:78:GLY:H	2.28	0.42
45:w:106:LEU:CD2	45:w:203:LEU:HD21	2.49	0.42
45:w:146:ARG:HG2	45:w:150:PHE:CE2	2.52	0.42
45:w:185:TYR:CE1	45:w:189:HIS:CE1	3.07	0.42
47:y:163:TRP:CE3	47:y:164:ILE:HG13	2.54	0.42
48:z:165:TYR:HA	48:z:179:MET:CE	2.49	0.42
49:A0:15:ARG:HB2	49:A0:16:PRO:CD	2.50	0.42
63:A5:20:PHE:N	63:A5:21:PRO:HD3	2.35	0.42
4:2:72:MET:HE3	4:2:76:ILE:HD11	2.01	0.42
72:2:402:PC1:H251	72:2:402:PC1:H222	1.94	0.42
5:4:319:HIS:HA	5:4:322:THR:HB	2.02	0.42
11:B:177:ILE:HG12	11:B:210:MET:HE3	2.02	0.42
26:R:61:ALA:H	26:R:129:LEU:HD11	1.84	0.42
28:T:34:LEU:O	28:T:35:VAL:O	2.37	0.42
44:e:49:ALA:HB2	44:e:53:LYS:HA	2.01	0.42
31:M:37:MET:HA	31:M:41:GLY:HA2	2.01	0.42
45:k:130:GLU:OE2	45:k:134:ILE:HD11	2.20	0.42
45:k:391:PRO:HG2	45:k:398:ARG:NH2	2.34	0.42
46:l:53:ALA:HA	46:l:57:TYR:CE2	2.54	0.42
46:l:200:THR:HG1	46:l:228:GLY:N	2.15	0.42
47:m:181:PHE:C	47:m:183:PHE:N	2.77	0.42
48:o:186:VAL:O	48:o:189:PHE:N	2.41	0.42
51:r:53:VAL:O	51:r:57:LEU:HG	2.20	0.42
45:w:3:THR:O	45:w:7:ALA:N	2.36	0.42
45:w:32:GLN:NE2	45:w:34:THR:HG1	2.18	0.42
45:w:57:TYR:O	45:w:61:HIS:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:267:ASN:ND2	45:w:386:TYR:OH	2.45	0.42
45:w:329:MET:CG	51:A2:2:ARG:HH21	2.32	0.42
45:w:350:THR:O	45:w:353:GLU:HG2	2.20	0.42
45:w:359:ASN:ND2	46:x:91:ALA:O	2.50	0.42
47:y:209:THR:O	47:y:211:ILE:HG13	2.20	0.42
47:y:256:TYR:N	47:y:256:TYR:CD1	2.84	0.42
49:A0:29:SER:HA	49:A0:32:ARG:NH2	2.35	0.42
50:A1:58:ARG:HA	50:A1:61:ARG:CZ	2.50	0.42
56:A9:106:PRO:HB2	56:A9:107:PRO:HD3	2.01	0.42
59:A7:127:LYS:O	59:A7:130:PRO:HD3	2.20	0.42
60:A6:86:ILE:HD13	60:A6:86:ILE:HA	1.88	0.42
61:B2:6:VAL:HA	61:B2:7:PRO:HD3	1.91	0.42
1:9:93:LEU:HA	1:9:94:PRO:HD3	1.88	0.42
3:6:338:MET:O	3:6:342:CYS:N	2.52	0.42
4:2:256:PRO:HD3	5:4:124:ALA:HA	2.01	0.42
5:4:244:LEU:HD21	5:4:301:ILE:HD12	2.02	0.42
8:1:217:ALA:HA	8:1:220:PHE:HB3	2.02	0.42
11:B:222:MET:HE2	13:D:95:GLU:HB2	2.02	0.42
14:E:106:TYR:CE1	14:E:112:ARG:HG3	2.55	0.42
37:c:5:THR:HA	37:c:6:PRO:HD3	1.91	0.42
37:c:20:ARG:HA	37:c:23:LEU:HB3	2.01	0.42
42:j:107:LYS:HD3	42:j:111:GLU:HG2	2.02	0.42
44:e:89:TRP:CD1	44:e:89:TRP:H	2.36	0.42
31:M:32:VAL:HG23	31:M:74:GLN:HE21	1.83	0.42
45:k:138:LEU:CD1	45:k:174:VAL:HG21	2.48	0.42
45:k:157:ALA:CB	45:k:237:THR:H	2.32	0.42
46:l:333:ALA:O	46:l:337:ILE:HG13	2.20	0.42
47:m:25:SER:OG	47:m:216:ASP:OD2	2.37	0.42
47:m:58:ASP:CG	47:y:56:THR:HG21	2.44	0.42
47:m:104:TYR:CE1	47:m:208:PRO:HA	2.54	0.42
47:m:326:TRP:O	47:m:329:VAL:N	2.53	0.42
48:o:164:ILE:O	48:o:179:MET:HE2	2.20	0.42
48:o:176:PRO:HB2	52:s:13:LEU:CD2	2.50	0.42
49:p:147:ILE:N	49:p:148:ALA:HB3	2.35	0.42
45:w:352:SER:HA	45:w:355:LEU:HG	2.02	0.42
46:x:128:THR:O	46:x:130:PRO:HD3	2.20	0.42
46:x:158:HIS:CE1	46:x:162:ASN:HD21	2.38	0.42
48:z:21:LEU:HD13	48:z:192:TRP:HB2	2.02	0.42
49:A0:73:LYS:HB3	49:A0:196:GLY:C	2.45	0.42
54:B4:13:LEU:O	54:B4:19:THR:OG1	2.38	0.42
56:A9:314:ILE:HB	56:A9:315:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B7:146:TRP:NE1	62:A4:17:ARG:HB2	2.35	0.42
61:B2:86:GLY:O	61:B2:87:THR:O	2.37	0.42
70:6:701:CDL:H532	70:6:701:CDL:H711	2.02	0.41
72:2:402:PC1:H143	72:2:402:PC1:H111	1.89	0.41
5:4:5:ILE:HG13	5:4:6:ILE:HG13	2.01	0.41
5:4:182:TRP:HZ3	43:g:82:VAL:HG22	1.85	0.41
8:1:233:MET:HA	8:1:236:ILE:HG22	2.01	0.41
26:R:203:PRO:HA	26:R:265:PHE:HB2	2.01	0.41
35:a:68:TRP:CH2	44:e:110:ASP:HA	2.54	0.41
37:c:40:VAL:HA	37:c:41:SER:HA	1.86	0.41
45:k:67:THR:HB	45:k:116:ILE:HG12	2.01	0.41
45:k:329:MET:SD	51:r:6:HIS:CD2	3.13	0.41
45:k:391:PRO:HB3	45:k:394:GLU:CD	2.44	0.41
45:k:430:GLN:HG2	45:k:430:GLN:O	2.20	0.41
46:l:46:ARG:HH11	46:l:379:LEU:CD2	2.30	0.41
46:l:192:HIS:O	46:l:195:VAL:HB	2.20	0.41
46:l:201:SER:OG	46:l:225:ASN:HA	2.20	0.41
47:m:175:LEU:O	47:m:178:PHE:N	2.53	0.41
47:m:245:PHE:O	47:m:247:PRO:HD3	2.19	0.41
48:o:195:GLU:HG3	48:o:198:HIS:HB2	2.02	0.41
45:w:172:GLU:H	45:w:172:GLU:HG2	1.71	0.41
46:x:192:HIS:O	46:x:195:VAL:HB	2.20	0.41
55:B3:77:ARG:HG2	55:B3:78:TYR:N	2.35	0.41
56:A9:474:GLU:HG3	56:A9:475:ALA:N	2.34	0.41
60:A6:21:LYS:O	60:A6:57:ARG:NH1	2.53	0.41
60:A6:43:PRO:HB2	60:A6:48:ILE:CD1	2.48	0.41
62:A4:5:LYS:HB3	62:A4:6:GLY:H	1.66	0.41
63:A5:24:ASN:HD22	63:A5:25:GLN:N	2.18	0.41
63:A5:84:LYS:HA	63:A5:84:LYS:HD2	1.82	0.41
66:B0:9:PHE:CD1	66:B0:9:PHE:C	2.97	0.41
8:1:222:LEU:HA	8:1:225:MET:HB3	2.02	0.41
10:A:651:PRO:HD2	20:K:56:ARG:HB3	2.02	0.41
26:R:352:VAL:HG13	26:R:353:LEU:HD12	2.02	0.41
28:T:59:TYR:CD2	28:T:59:TYR:C	2.98	0.41
45:k:352:SER:HA	45:k:355:LEU:HG	2.02	0.41
45:k:409:GLU:O	45:k:412:SER:HB2	2.20	0.41
46:l:213:HIS:N	46:l:214:PRO:HD2	2.34	0.41
46:l:365:LYS:O	46:l:369:LEU:HG	2.20	0.41
47:m:44:GLN:O	47:m:45:ILE:C	2.63	0.41
47:m:123:VAL:O	47:m:126:THR:HB	2.20	0.41
48:o:21:LEU:HD13	48:o:192:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:r:79:ASN:CG	52:s:52:GLU:HG3	2.45	0.41
52:s:36:ARG:HA	52:s:39:LEU:HD12	2.03	0.41
54:u:13:LEU:O	54:u:19:THR:OG1	2.38	0.41
45:w:314:TYR:HB2	45:w:317:THR:HB	2.02	0.41
45:w:395:TRP:CH2	45:w:398:ARG:NH1	2.88	0.41
45:w:430:GLN:O	45:w:430:GLN:HG2	2.20	0.41
46:x:201:SER:OG	46:x:225:ASN:HA	2.20	0.41
46:x:213:HIS:N	46:x:214:PRO:HD2	2.34	0.41
47:y:97:HIS:CD2	77:y:402:HEM:NC	2.87	0.41
47:y:275:LEU:O	47:y:279:ALA:N	2.36	0.41
47:y:330:ALA:HA	47:y:333:LEU:HB3	2.01	0.41
48:z:211:MET:HE2	49:A0:49:TYR:CD2	2.55	0.41
49:A0:25:SER:O	49:A0:29:SER:OG	2.27	0.41
49:A0:65:SER:HB3	49:A0:68:VAL:HG23	2.02	0.41
52:B5:21:ARG:HD3	52:B5:65:ARG:NH2	2.35	0.41
53:A3:15:ARG:C	53:A3:17:TRP:N	2.77	0.41
59:A7:130:PRO:O	59:A7:136:ALA:HB2	2.20	0.41
70:6:701:CDL:H541	70:6:701:CDL:H752	2.02	0.41
5:4:396:MET:HE2	5:4:396:MET:HB3	1.87	0.41
7:8:112:TYR:HB2	7:8:240:THR:HG22	2.01	0.41
8:1:184:MET:HE3	71:B:501:3PE:H351	2.03	0.41
10:A:436:VAL:O	10:A:442:TYR:OH	2.31	0.41
11:B:326:CYS:SG	11:B:329:ARG:NH1	2.93	0.41
13:D:107:ASP:OD1	13:D:108:ARG:N	2.52	0.41
14:E:172:ASN:ND2	14:E:200:GLU:OE1	2.54	0.41
18:I:82:SER:OG	18:I:83:ARG:N	2.53	0.41
39:f:109:PRO:HA	39:f:111:GLU:H	1.85	0.41
45:k:206:ARG:O	45:k:209:LEU:N	2.53	0.41
46:l:35:ILE:O	46:l:35:ILE:HG13	2.20	0.41
47:m:18:PHE:O	47:m:19:ILE:C	2.63	0.41
47:m:282:ARG:NH1	47:m:341:GLN:O	2.42	0.41
49:p:117:LEU:H	49:p:122:HIS:CB	2.34	0.41
52:s:36:ARG:HA	52:s:39:LEU:HB2	2.03	0.41
45:w:38:GLY:HA2	45:w:98:TYR:HA	2.01	0.41
45:w:409:GLU:O	45:w:412:SER:HB2	2.20	0.41
47:y:18:PHE:O	47:y:19:ILE:C	2.63	0.41
47:y:175:LEU:O	47:y:178:PHE:N	2.53	0.41
47:y:245:PHE:C	47:y:247:PRO:HD3	2.45	0.41
47:y:276:PHE:O	47:y:280:ILE:HG12	2.21	0.41
56:A9:264:LYS:NZ	57:B9:56:MET:HE2	2.36	0.41
57:B9:146:MET:SD	57:B9:189:PRO:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B9:193:TYR:CD1	57:B9:193:TYR:N	2.88	0.41
58:B7:146:TRP:CE2	62:A4:17:ARG:HB2	2.55	0.41
64:B6:21:ILE:O	64:B6:25:PHE:HD2	2.02	0.41
3:6:396:ILE:HD12	3:6:397:GLU:HG3	2.01	0.41
10:A:405:THR:HB	10:A:477:GLY:HA3	2.01	0.41
11:B:143:SER:OG	11:B:147:ASN:OD1	2.38	0.41
22:N:24:LEU:HB3	22:N:28:TYR:HE2	1.85	0.41
39:f:70:GLU:H	39:f:73:HIS:HB3	1.84	0.41
45:k:39:VAL:N	45:k:97:TYR:O	2.41	0.41
46:l:70:ARG:HD3	46:l:100:SER:HB3	2.01	0.41
46:l:158:HIS:CE1	46:l:162:ASN:HD21	2.37	0.41
46:l:370:MET:HA	46:l:373:GLU:CD	2.44	0.41
45:w:57:TYR:CE2	45:w:134:ILE:HD12	2.56	0.41
47:y:123:VAL:O	47:y:126:THR:HB	2.20	0.41
48:z:72:ASP:CG	48:z:73:GLY:H	2.29	0.41
48:z:195:GLU:HG3	48:z:198:HIS:HB2	2.02	0.41
50:A1:101:ARG:O	50:A1:105:GLU:N	2.40	0.41
56:A9:354:THR:HG21	56:A9:376:HIS:HA	2.03	0.41
56:A9:461:SER:O	56:A9:465:VAL:HG13	2.21	0.41
56:A9:462:LEU:O	56:A9:466:MET:HG3	2.20	0.41
58:B7:182:TYR:O	62:A4:72:ASN:HB2	2.21	0.41
59:A7:86:MET:O	66:B0:25:CYS:HB2	2.20	0.41
63:A5:65:PRO:HG2	63:A5:68:TRP:CG	2.55	0.41
68:A8:37:LEU:HA	68:A8:37:LEU:HD23	1.83	0.41
3:6:243:VAL:O	3:6:247:LEU:N	2.53	0.41
25:Q:6:GLU:O	25:Q:54:ARG:NH1	2.54	0.41
28:T:50:LEU:O	28:T:52:GLY:CA	2.66	0.41
39:f:59:LYS:HB2	45:w:193:PRO:HD2	1.54	0.41
45:k:29:GLN:CB	45:k:204:GLU:HG3	2.50	0.41
45:k:203:LEU:HA	45:k:207:GLN:NE2	2.35	0.41
46:l:96:LEU:HD23	46:l:97:SER:N	2.36	0.41
46:l:133:ARG:HB3	46:l:135:TRP:CH2	2.55	0.41
50:q:25:GLY:O	50:q:29:LEU:HG	2.20	0.41
45:w:67:THR:HB	45:w:116:ILE:HG12	2.01	0.41
45:w:145:MET:HB2	45:w:252:HIS:CE1	2.55	0.41
45:w:233:PRO:HB2	49:A0:22:THR:O	2.21	0.41
47:y:46:LEU:O	47:y:49:LEU:HB3	2.21	0.41
47:y:315:MET:O	47:y:318:ARG:N	2.42	0.41
50:A1:9:SER:O	50:A1:13:LEU:N	2.53	0.41
50:A1:28:LYS:HG3	50:A1:28:LYS:H	1.54	0.41
54:B4:54:HIS:HA	54:B4:57:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:495:LEU:HA	56:A9:495:LEU:HD23	1.68	0.41
60:A6:76:GLY:HA3	60:A6:77:PRO:HD2	1.85	0.41
61:B2:53:THR:HG22	61:B2:54:ASN:OD1	2.19	0.41
62:A4:42:ARG:NH1	62:A4:74:ARG:NH2	2.68	0.41
65:B8:5:VAL:O	65:B8:9:GLN:HG3	2.21	0.41
3:6:184:LEU:HD13	5:4:393:ILE:HG21	2.02	0.41
10:A:435:PRO:HG3	10:A:444:HIS:ND1	2.35	0.41
11:B:359:ASP:HB2	24:P:45:PRO:HG2	2.01	0.41
13:D:185:GLY:HA2	14:E:154:TYR:CE2	2.56	0.41
14:E:113:CYS:SG	14:E:114:ILE:N	2.94	0.41
28:T:33:GLY:C	28:T:60:THR:HG23	2.42	0.41
45:k:145:MET:HB2	45:k:252:HIS:CE1	2.55	0.41
46:l:323:GLY:HA2	46:l:417:PHE:CE1	2.56	0.41
77:m:402:HEM:CGA	77:m:402:HEM:HHA	2.51	0.41
48:o:81:PHE:CD1	48:o:84:PRO:HA	2.55	0.41
50:q:9:SER:O	50:q:13:LEU:N	2.53	0.41
50:q:58:ARG:HA	50:q:61:ARG:CZ	2.50	0.41
45:w:59:VAL:CG2	45:w:182:LEU:HD22	2.50	0.41
45:w:115:ASP:O	45:w:119:ASN:HB2	2.21	0.41
45:w:317:THR:HG22	45:w:318:GLY:N	2.36	0.41
45:w:354:VAL:O	45:w:355:LEU:C	2.62	0.41
46:x:96:LEU:HD23	46:x:97:SER:N	2.36	0.41
46:x:412:ASN:HA	46:x:415:LYS:HD3	2.03	0.41
47:y:25:SER:OG	47:y:216:ASP:OD2	2.37	0.41
47:y:344:GLU:C	47:y:346:PRO:HD2	2.46	0.41
48:z:76:GLU:C	48:z:78:GLY:H	2.28	0.41
50:A1:36:THR:HG22	50:A1:36:THR:O	2.21	0.41
53:A3:40:LEU:H	53:A3:40:LEU:HG	1.70	0.41
57:B9:100:MET:HE3	57:B9:100:MET:HB3	1.99	0.41
58:B7:40:MET:O	58:B7:41:THR:C	2.62	0.41
63:A5:58:ARG:HD2	63:A5:58:ARG:HA	1.74	0.41
2:7:98:LEU:O	2:7:102:PHE:N	2.48	0.41
5:4:244:LEU:HA	5:4:244:LEU:HD23	1.87	0.41
7:8:95:THR:HA	7:8:98:LYS:HG2	2.03	0.41
10:A:63:PHE:O	10:A:181:ARG:NH2	2.54	0.41
10:A:359:ASN:ND2	20:K:68:ARG:HH12	2.19	0.41
14:E:100:GLU:O	14:E:170:GLY:N	2.49	0.41
31:M:51:ILE:HD12	31:M:70:LEU:HD12	2.02	0.41
45:k:57:TYR:CE2	45:k:134:ILE:HD12	2.56	0.41
46:l:128:THR:O	46:l:130:PRO:HD3	2.20	0.41
47:m:46:LEU:O	47:m:49:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:226:ILE:HG21	48:o:223:LYS:HA	2.02	0.41
77:m:402:HEM:CGA	77:m:402:HEM:CHA	2.99	0.41
50:q:36:THR:HG22	50:q:36:THR:O	2.21	0.41
45:w:67:THR:HG22	45:w:70:ARG:HB2	2.03	0.41
45:w:379:ILE:O	45:w:383:LEU:HG	2.20	0.41
46:x:133:ARG:HB3	46:x:135:TRP:CH2	2.55	0.41
46:x:202:ALA:HB3	46:x:230:LEU:HD22	2.01	0.41
48:z:6:HIS:HA	48:z:7:PRO:HD3	1.89	0.41
48:z:164:ILE:O	48:z:179:MET:HE2	2.20	0.41
49:A0:182:VAL:HA	49:A0:183:PRO:HA	1.75	0.41
52:B5:31:VAL:O	52:B5:35:GLU:HG3	2.20	0.41
52:B5:36:ARG:HA	52:B5:39:LEU:HD12	2.03	0.41
56:A9:105:LEU:HD12	56:A9:105:LEU:HA	1.93	0.41
56:A9:240:HIS:O	56:A9:241:PRO:C	2.64	0.41
57:B9:100:MET:HE3	57:B9:157:GLU:HG3	2.01	0.41
58:B7:6:HIS:CD2	58:B7:8:TYR:HB2	2.55	0.41
58:B7:228:THR:O	58:B7:232:HIS:HD2	2.04	0.41
61:B2:16:LEU:O	61:B2:20:VAL:HG13	2.21	0.41
4:2:106:LEU:HD13	4:2:139:MET:HE2	2.02	0.41
8:1:34:ARG:CZ	13:D:108:ARG:HH12	2.34	0.41
8:1:43:TYR:HA	29:U:31:ASN:HD21	1.85	0.41
14:E:166:ALA:HB3	74:E:302:SF4:S4	2.61	0.41
36:b:58:LYS:HA	36:b:59:PRO:HD3	1.90	0.41
45:k:67:THR:HG22	45:k:70:ARG:HB2	2.03	0.41
45:k:379:ILE:O	45:k:383:LEU:HG	2.20	0.41
45:k:405:ARG:HG2	53:t:15:ARG:NH2	2.35	0.41
45:k:406:VAL:HA	45:k:409:GLU:OE1	2.21	0.41
46:l:46:ARG:HH12	46:l:376:GLU:CB	2.33	0.41
46:l:169:ARG:HD3	46:l:238:LYS:HD3	2.02	0.41
47:m:97:HIS:HD2	77:m:402:HEM:C1C	2.37	0.41
47:m:185:LEU:HB3	47:m:186:PRO:HD3	2.03	0.41
47:m:256:TYR:N	47:m:256:TYR:CD1	2.84	0.41
46:x:46:ARG:C	46:x:47:ILE:HG13	2.46	0.41
46:x:137:VAL:HG21	46:x:188:PRO:HG3	2.03	0.41
46:x:213:HIS:CD2	46:x:216:LEU:HD23	2.56	0.41
47:y:131:TYR:HE2	47:y:139:SER:HA	1.85	0.41
77:y:402:HEM:CGA	77:y:402:HEM:CHA	2.99	0.41
49:A0:50:ALA:O	49:A0:54:VAL:HG23	2.21	0.41
64:B6:42:LYS:HE2	64:B6:42:LYS:HB3	1.83	0.41
3:6:103:PHE:O	3:6:107:TYR:N	2.43	0.41
3:6:401:THR:OG1	3:6:479:GLN:NE2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:75:LEU:HD21	5:4:440:HIS:CE1	2.56	0.41
6:5:24:SER:HB3	6:5:89:TYR:HA	2.03	0.41
11:B:144:MET:HG3	11:B:214:TYR:HE2	1.86	0.41
16:G:163:ASN:HB3	16:G:172:VAL:HG22	2.01	0.41
27:S:272:LEU:HB3	27:S:275:ASN:HA	2.03	0.41
28:T:50:LEU:C	28:T:52:GLY:H	2.26	0.41
28:T:99:LEU:O	28:T:103:ALA:N	2.51	0.41
37:c:38:GLN:HA	37:c:39:ARG:HA	1.88	0.41
45:k:115:ASP:O	45:k:119:ASN:HB2	2.21	0.41
45:k:359:ASN:O	45:k:362:ARG:HB2	2.21	0.41
46:l:76:THR:O	46:l:131:GLU:HB2	2.21	0.41
46:l:137:VAL:HG21	46:l:188:PRO:HG3	2.03	0.41
46:l:258:VAL:HG13	46:l:322:PHE:C	2.45	0.41
46:l:261:SER:HB3	46:l:322:PHE:HB3	2.03	0.41
46:l:273:SER:HA	46:l:276:GLN:HG2	2.03	0.41
46:l:412:ASN:HA	46:l:415:LYS:HD3	2.03	0.41
46:l:435:PHE:CE2	46:x:169:ARG:HG2	2.55	0.41
47:m:61:THR:O	47:m:62:ALA:C	2.64	0.41
47:m:163:TRP:CE3	47:m:164:ILE:HG13	2.54	0.41
48:o:72:ASP:CG	48:o:73:GLY:H	2.29	0.41
48:o:226:LYS:HA	48:o:226:LYS:HD2	1.81	0.41
53:t:39:ARG:HG2	53:t:39:ARG:O	2.21	0.41
45:w:263:ALA:O	45:w:264:HIS:HB2	2.20	0.41
45:w:406:VAL:HA	45:w:409:GLU:OE1	2.21	0.41
45:w:425:PHE:C	45:w:428:ILE:HG13	2.45	0.41
46:x:46:ARG:HH11	46:x:379:LEU:CD2	2.30	0.41
46:x:70:ARG:HD3	46:x:100:SER:HB3	2.01	0.41
46:x:152:LEU:HD23	46:x:152:LEU:HA	1.86	0.41
46:x:169:ARG:HD3	46:x:238:LYS:HD3	2.02	0.41
46:x:305:GLN:O	46:x:306:PRO:C	2.64	0.41
46:x:372:VAL:O	46:x:378:PHE:HB2	2.20	0.41
46:x:395:PRO:O	46:x:398:VAL:HB	2.20	0.41
47:y:37:LEU:HD13	77:y:402:HEM:C3B	2.56	0.41
47:y:147:THR:HG22	47:y:161:VAL:HG13	2.03	0.41
77:y:402:HEM:CGA	77:y:402:HEM:HHA	2.51	0.41
48:z:57:THR:HA	54:B4:56:LYS:NZ	2.36	0.41
48:z:136:GLU:HA	48:z:137:PRO:HD3	1.97	0.41
49:A0:32:ARG:O	49:A0:35:PHE:HB3	2.21	0.41
51:A2:2:ARG:O	51:A2:3:GLN:C	2.63	0.41
51:A2:54:ALA:O	51:A2:58:VAL:HG23	2.21	0.41
52:B5:44:VAL:HG22	52:B5:52:GLU:CG	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A3:15:ARG:HG3	53:A3:16:ASN:N	2.25	0.41
53:A3:16:ASN:HA	53:A3:19:PRO:HD2	2.02	0.41
56:A9:442:ASP:OD2	57:B9:134:ARG:NH2	2.54	0.41
57:B9:164:ALA:HB2	57:B9:171:LYS:HD3	2.03	0.41
58:B7:22:LEU:HD12	58:B7:22:LEU:HA	1.86	0.41
59:A7:137:LYS:O	59:A7:145:TRP:HE3	2.03	0.41
61:B2:10:GLU:HG2	61:B2:25:ARG:HH22	1.86	0.41
63:A5:57:ARG:HA	63:A5:60:TYR:CD2	2.55	0.41
65:B8:3:ASN:C	65:B8:3:ASN:ND2	2.77	0.41
66:B0:13:TYR:O	66:B0:14:GLY:C	2.63	0.41
2:7:156:VAL:O	2:7:160:SER:N	2.46	0.41
4:2:190:MET:HB2	4:2:201:THR:HG23	2.03	0.41
7:8:210:THR:HA	7:8:213:ILE:HG22	2.03	0.41
10:A:618:GLU:OE2	10:A:620:TRP:NE1	2.53	0.41
11:B:233:HIS:NE2	14:E:160:GLU:OE1	2.54	0.41
18:I:108:LYS:HB3	18:I:118:GLN:NE2	2.35	0.41
38:d:88:ASP:O	38:d:92:HIS:N	2.43	0.41
45:k:38:GLY:HA2	45:k:98:TYR:HA	2.02	0.41
45:k:59:VAL:CG2	45:k:182:LEU:HD22	2.50	0.41
45:k:108:LYS:O	45:k:112:LEU:N	2.42	0.41
45:k:370:ASP:CG	46:l:375:SER:HG	2.28	0.41
45:k:436:ARG:HD3	45:k:436:ARG:HA	1.90	0.41
46:l:124:LEU:HD22	46:l:223:PHE:HB2	2.03	0.41
47:m:94:LEU:O	47:m:97:HIS:N	2.54	0.41
47:m:276:PHE:O	47:m:280:ILE:HG12	2.21	0.41
52:s:60:ASP:O	52:s:63:HIS:HB3	2.21	0.41
46:x:323:GLY:HA2	46:x:417:PHE:CE1	2.56	0.41
46:x:369:LEU:O	46:x:373:GLU:N	2.53	0.41
47:y:326:TRP:O	47:y:329:VAL:N	2.53	0.41
48:z:70:VAL:HG23	48:z:81:PHE:O	2.21	0.41
49:A0:35:PHE:O	49:A0:38:LEU:HB3	2.20	0.41
50:A1:88:SER:O	50:A1:90:LEU:N	2.54	0.41
56:A9:398:PRO:HB3	56:A9:482:VAL:HG21	2.03	0.41
79:A9:601:HEA:H122	79:A9:601:HEA:HHC	2.02	0.41
65:B8:31:LEU:HD23	65:B8:31:LEU:HA	1.82	0.41
3:6:341:MET:HE3	3:6:454:ILE:HD13	2.02	0.40
4:2:49:ASN:HD22	4:2:123:PRO:HG2	1.85	0.40
4:2:314:LYS:NZ	27:S:299:PRO:O	2.43	0.40
5:4:297:VAL:O	5:4:301:ILE:HG12	2.20	0.40
17:H:2:PRO:HB2	72:j:201:PC1:H151	2.03	0.40
26:R:235:THR:HA	26:R:236:VAL:HA	1.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:U:124:TYR:CE2	29:U:126:PRO:HG3	2.56	0.40
46:l:319:SER:OG	46:l:320:GLY:N	2.54	0.40
46:l:372:VAL:O	46:l:378:PHE:HB2	2.21	0.40
47:m:102:LEU:HD23	47:m:102:LEU:HA	1.81	0.40
50:q:105:GLU:HB3	50:q:109:LYS:HZ1	1.86	0.40
51:r:2:ARG:O	51:r:3:GLN:C	2.63	0.40
52:s:31:VAL:O	52:s:35:GLU:HG3	2.20	0.40
45:w:47:TYR:HE1	45:w:231:LEU:HG	1.86	0.40
46:x:58:GLU:OE2	46:x:65:THR:N	2.54	0.40
46:x:76:THR:O	46:x:131:GLU:HB2	2.21	0.40
46:x:258:VAL:HG13	46:x:322:PHE:C	2.45	0.40
47:y:23:ALA:HA	47:y:24:PRO:HD3	1.90	0.40
47:y:91:PHE:HZ	47:y:124:MET:HG2	1.78	0.40
52:B5:36:ARG:HA	52:B5:39:LEU:HB2	2.02	0.40
52:B5:60:ASP:O	52:B5:63:HIS:HB3	2.21	0.40
56:A9:23:GLY:HA3	56:A9:73:ILE:HG13	2.03	0.40
56:A9:365:ILE:HD12	57:B9:87:MET:CE	2.34	0.40
56:A9:501:PRO:O	56:A9:502:TYR:C	2.63	0.40
58:B7:233:PHE:HA	58:B7:236:GLU:HG3	2.03	0.40
59:A7:24:LEU:HA	59:A7:25:PRO:HD2	1.93	0.40
59:A7:102:TYR:HD2	68:A8:35:TYR:HE1	1.68	0.40
60:A6:52:LEU:HD23	60:A6:52:LEU:HA	1.93	0.40
63:A5:33:TYR:O	63:A5:37:HIS:HD2	2.05	0.40
65:B8:21:HIS:CD2	65:B8:22:LEU:HG	2.57	0.40
66:B0:24:PHE:CE1	66:B0:28:VAL:HG21	2.56	0.40
8:l:225:MET:SD	8:l:225:MET:O	2.79	0.40
11:B:409:VAL:HG12	11:B:411:LEU:HB2	2.03	0.40
13:D:176:ILE:HG22	13:D:177:VAL:HG13	2.03	0.40
24:P:53:TYR:O	24:P:56:THR:OG1	2.36	0.40
72:S:401:PC1:H12	72:S:401:PC1:H342	2.03	0.40
45:k:263:ALA:O	45:k:264:HIS:HB2	2.20	0.40
45:k:314:TYR:HB2	45:k:317:THR:HB	2.02	0.40
45:k:317:THR:HG22	45:k:318:GLY:N	2.36	0.40
46:l:58:GLU:OE2	46:l:65:THR:N	2.54	0.40
47:m:137:GLN:O	47:m:140:PHE:N	2.54	0.40
47:m:147:THR:HG22	47:m:161:VAL:HG13	2.03	0.40
47:m:284:ILE:HG22	47:m:286:ASN:N	2.37	0.40
51:r:54:ALA:O	51:r:58:VAL:HG23	2.21	0.40
53:t:12:GLN:NE2	50:A1:109:LYS:O	2.55	0.40
45:w:12:PRO:HB2	45:w:28:GLU:HG3	2.01	0.40
45:w:108:LYS:O	45:w:112:LEU:N	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:29:LEU:HD11	46:x:35:ILE:HD13	2.03	0.40
46:x:232:LEU:HD23	46:x:232:LEU:HA	1.84	0.40
46:x:286:LYS:C	46:x:288:GLY:H	2.30	0.40
47:y:44:GLN:O	47:y:45:ILE:C	2.63	0.40
47:y:61:THR:O	47:y:62:ALA:C	2.64	0.40
47:y:137:GLN:O	47:y:140:PHE:N	2.54	0.40
47:y:181:PHE:C	47:y:183:PHE:N	2.77	0.40
47:y:185:LEU:HB3	47:y:186:PRO:HD3	2.02	0.40
47:y:317:PHE:HD1	50:A1:26:PHE:HE1	1.67	0.40
48:z:167:GLU:HA	48:z:177:ALA:CB	2.49	0.40
49:A0:11:SER:HA	49:A0:14:ARG:HB2	2.03	0.40
49:A0:86:ASN:CB	49:A0:148:ALA:HB3	2.51	0.40
54:B4:53:LYS:O	54:B4:57:HIS:CD2	2.74	0.40
58:B7:188:ILE:H	58:B7:188:ILE:HG13	1.62	0.40
61:B2:49:VAL:O	61:B2:91:LEU:HD12	2.21	0.40
68:A8:19:LEU:HD23	68:A8:19:LEU:C	2.45	0.40
10:A:347:ASP:OD1	10:A:347:ASP:N	2.50	0.40
20:K:20:ARG:HG2	20:K:54:LEU:HB2	2.03	0.40
20:K:33:VAL:HA	20:K:36:PHE:HB3	2.04	0.40
22:N:107:PRO:O	22:N:109:ALA:N	2.51	0.40
28:T:54:ALA:O	28:T:58:ARG:CB	2.70	0.40
29:U:14:VAL:HG13	29:U:23:TYR:CZ	2.56	0.40
45:k:32:GLN:NE2	45:k:34:THR:HG1	2.18	0.40
45:k:36:THR:N	45:k:200:ALA:O	2.47	0.40
45:k:51:LYS:HA	45:k:173:ASN:HD21	1.87	0.40
46:l:49:LEU:HD21	46:l:51:ILE:HD11	2.03	0.40
46:l:263:ALA:HB1	46:l:317:SER:O	2.22	0.40
47:m:159:ASN:O	47:m:163:TRP:N	2.42	0.40
47:m:207:ASN:ND2	47:m:211:ILE:O	2.55	0.40
47:m:292:LEU:HD23	47:m:292:LEU:HA	1.85	0.40
48:o:20:SER:OG	54:u:51:LEU:HD21	2.21	0.40
48:o:217:PRO:O	48:o:221:ALA:N	2.47	0.40
49:p:20:ASP:OD1	49:p:22:THR:N	2.49	0.40
45:w:91:THR:N	45:w:94:HIS:O	2.55	0.40
45:w:359:ASN:O	45:w:362:ARG:HB2	2.21	0.40
45:w:362:ARG:HE	45:w:399:ILE:HG21	1.86	0.40
46:x:112:LEU:HD23	46:x:112:LEU:HA	1.86	0.40
46:x:263:ALA:HB1	46:x:317:SER:O	2.22	0.40
46:x:333:ALA:O	46:x:337:ILE:HG13	2.20	0.40
47:y:77:TRP:CD2	47:y:78:ILE:HG22	2.57	0.40
47:y:284:ILE:HG22	47:y:286:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:318:ARG:HE	47:y:318:ARG:HB2	1.60	0.40
48:z:28:ARG:HB3	48:z:171:PHE:HD1	1.86	0.40
52:B5:15:ASP:O	52:B5:19:THR:OG1	2.34	0.40
54:B4:53:LYS:HA	54:B4:53:LYS:HD2	1.92	0.40
56:A9:276:ALA:O	56:A9:280:ILE:HG13	2.21	0.40
57:B9:168:LEU:HD13	57:B9:184:LEU:HG	2.03	0.40
58:B7:42:LEU:HA	58:B7:42:LEU:HD12	1.66	0.40
63:A5:17:ASP:OD1	63:A5:19:ARG:HG2	2.22	0.40
2:7:13:PHE:HD2	6:5:8:ILE:HG21	1.87	0.40
4:2:254:LEU:HA	4:2:255:PRO:HD3	1.88	0.40
7:8:186:ALA:HA	7:8:187:CYS:HA	1.60	0.40
14:E:170:GLY:HA2	14:E:171:PRO:HD3	1.78	0.40
17:H:96:PRO:HA	17:H:97:HIS:HA	1.82	0.40
28:T:45:THR:C	28:T:47:THR:N	2.68	0.40
45:k:230:THR:O	45:k:231:LEU:HG	2.22	0.40
47:m:50:PHE:HE2	49:p:58:PHE:HB3	1.87	0.40
52:s:16:PRO:O	52:s:19:THR:HB	2.21	0.40
52:s:44:VAL:HG12	52:s:48:SER:HB2	2.03	0.40
53:t:43:ASP:HA	54:u:33:ARG:HH12	1.86	0.40
45:w:51:LYS:HA	45:w:173:ASN:HD21	1.87	0.40
45:w:64:PHE:CE1	45:w:86:LEU:HD21	2.56	0.40
45:w:235:ARG:CZ	49:A0:14:ARG:HH22	2.35	0.40
46:x:35:ILE:HG13	46:x:35:ILE:O	2.20	0.40
47:y:307:LEU:HD23	47:y:307:LEU:HA	1.86	0.40
48:z:148:TYR:CD2	48:z:161:ALA:HA	2.57	0.40
48:z:186:VAL:O	48:z:189:PHE:N	2.41	0.40
49:A0:2:HIS:C	49:A0:4:ASP:H	2.28	0.40
53:A3:11:ARG:HB2	53:A3:12:GLN:HA	2.04	0.40
56:A9:168:ILE:CG2	56:A9:189:MET:HG3	2.51	0.40
65:B8:12:PHE:O	65:B8:23:LYS:HE2	2.21	0.40
10:A:216:SER:N	10:A:219:SER:OG	2.48	0.40
10:A:469:ALA:HB3	10:A:472:PRO:HG3	2.03	0.40
14:E:118:LEU:HD23	14:E:118:LEU:HA	1.91	0.40
72:Q:201:PC1:H241	72:Q:201:PC1:H152	2.04	0.40
27:S:189:PRO:HB2	27:S:192:VAL:HG22	2.03	0.40
45:k:180:ALA:O	45:k:184:GLU:HG3	2.22	0.40
45:k:262:TRP:CD1	45:k:315:ALA:HA	2.52	0.40
45:k:396:GLU:CD	45:k:396:GLU:C	2.90	0.40
45:k:412:SER:O	54:u:15:ARG:NH2	2.54	0.40
46:l:84:LYS:O	46:l:88:GLY:N	2.51	0.40
46:l:155:PRO:HB2	46:l:254:HIS:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:131:TYR:HE2	47:m:139:SER:HA	1.86	0.40
48:o:167:GLU:HA	48:o:177:ALA:CB	2.49	0.40
51:r:73:ASN:C	51:r:75:ALA:H	2.29	0.40
45:w:180:ALA:O	45:w:184:GLU:HG3	2.22	0.40
45:w:203:LEU:HA	45:w:207:GLN:NE2	2.35	0.40
46:x:166:ALA:HB1	46:x:242:GLY:O	2.22	0.40
46:x:273:SER:HA	46:x:276:GLN:HG2	2.03	0.40
47:y:42:ILE:O	47:y:43:LEU:C	2.64	0.40
50:A1:98:ILE:O	50:A1:102:LYS:HG2	2.21	0.40
50:A1:105:GLU:HB3	50:A1:109:LYS:HZ1	1.86	0.40
51:A2:53:VAL:O	51:A2:57:LEU:HG	2.20	0.40
59:A7:11:TYR:CD1	59:A7:11:TYR:C	2.99	0.40
59:A7:119:GLN:O	59:A7:123:MET:HG3	2.22	0.40
61:B2:1:ALA:O	61:B2:2:SER:CB	2.70	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	9	205/217 (94%)	166 (81%)	38 (18%)	1 (0%)	24	63
2	7	170/175 (97%)	135 (79%)	31 (18%)	4 (2%)	4	27
3	6	604/606 (100%)	518 (86%)	82 (14%)	4 (1%)	18	56
4	2	342/347 (99%)	298 (87%)	44 (13%)	0	100	100
5	4	457/459 (100%)	374 (82%)	77 (17%)	6 (1%)	9	42
6	5	94/98 (96%)	80 (85%)	14 (15%)	0	100	100
7	8	425/444 (96%)	343 (81%)	80 (19%)	2 (0%)	24	63
8	1	315/318 (99%)	270 (86%)	43 (14%)	2 (1%)	21	59
9	3	110/115 (96%)	92 (84%)	16 (14%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	A	686/704 (97%)	563 (82%)	118 (17%)	5 (1%)	18	56
11	B	428/430 (100%)	357 (83%)	64 (15%)	7 (2%)	7	38
12	C	206/228 (90%)	175 (85%)	31 (15%)	0	100	100
13	D	150/179 (84%)	133 (89%)	17 (11%)	0	100	100
14	E	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	21	59
15	F	26/75 (35%)	17 (65%)	9 (35%)	0	100	100
16	G	121/133 (91%)	99 (82%)	20 (16%)	2 (2%)	7	36
17	H	94/105 (90%)	74 (79%)	19 (20%)	1 (1%)	11	46
18	I	69/96 (72%)	57 (83%)	11 (16%)	1 (1%)	9	40
19	J	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8	40
20	K	82/98 (84%)	62 (76%)	20 (24%)	0	100	100
21	L	78/83 (94%)	68 (87%)	10 (13%)	0	100	100
22	N	109/115 (95%)	91 (84%)	18 (16%)	0	100	100
23	O	112/127 (88%)	98 (88%)	14 (12%)	0	100	100
24	P	86/112 (77%)	66 (77%)	20 (23%)	0	100	100
25	Q	166/171 (97%)	117 (70%)	47 (28%)	2 (1%)	10	44
26	R	315/345 (91%)	249 (79%)	64 (20%)	2 (1%)	21	59
27	S	317/320 (99%)	249 (78%)	64 (20%)	4 (1%)	9	42
28	T	136/140 (97%)	112 (82%)	16 (12%)	8 (6%)	1	13
29	U	128/145 (88%)	101 (79%)	27 (21%)	0	100	100
30	V	136/143 (95%)	119 (88%)	15 (11%)	2 (2%)	8	40
31	M	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
31	W	84/88 (96%)	66 (79%)	18 (21%)	0	100	100
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
33	Y	55/72 (76%)	44 (80%)	11 (20%)	0	100	100
34	Z	72/97 (74%)	49 (68%)	23 (32%)	0	100	100
35	a	112/128 (88%)	87 (78%)	25 (22%)	0	100	100
36	b	137/143 (96%)	118 (86%)	19 (14%)	0	100	100
37	c	86/127 (68%)	67 (78%)	19 (22%)	0	100	100
38	d	105/117 (90%)	77 (73%)	24 (23%)	4 (4%)	2	19
39	f	165/178 (93%)	126 (76%)	38 (23%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	h	82/125 (66%)	57 (70%)	23 (28%)	2 (2%)	4	27
41	i	36/49 (74%)	34 (94%)	2 (6%)	0	100	100
42	j	111/120 (92%)	95 (86%)	16 (14%)	0	100	100
43	g	171/176 (97%)	143 (84%)	28 (16%)	0	100	100
44	e	139/158 (88%)	80 (58%)	52 (37%)	7 (5%)	1	16
45	k	444/480 (92%)	401 (90%)	42 (10%)	1 (0%)	43	78
45	w	432/480 (90%)	397 (92%)	33 (8%)	2 (0%)	24	63
46	l	417/453 (92%)	380 (91%)	31 (7%)	6 (1%)	9	40
46	x	417/453 (92%)	379 (91%)	31 (7%)	7 (2%)	7	36
47	m	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	36	72
47	y	377/379 (100%)	340 (90%)	36 (10%)	1 (0%)	36	72
48	o	239/325 (74%)	211 (88%)	24 (10%)	4 (2%)	7	36
48	z	239/325 (74%)	211 (88%)	23 (10%)	5 (2%)	5	30
49	A0	184/196 (94%)	135 (73%)	45 (24%)	4 (2%)	5	29
49	p	147/196 (75%)	93 (63%)	40 (27%)	14 (10%)	0	8
50	A1	104/111 (94%)	94 (90%)	7 (7%)	3 (3%)	3	23
50	q	104/111 (94%)	98 (94%)	6 (6%)	0	100	100
51	A2	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
51	r	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
52	B5	67/91 (74%)	57 (85%)	9 (13%)	1 (2%)	8	40
52	s	65/91 (71%)	55 (85%)	9 (14%)	1 (2%)	8	40
53	A3	37/56 (66%)	26 (70%)	7 (19%)	4 (11%)	0	6
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	3	21
54	B4	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
54	u	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
55	B3	20/78 (26%)	9 (45%)	9 (45%)	2 (10%)	0	7
55	v	16/78 (20%)	7 (44%)	8 (50%)	1 (6%)	1	13
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
57	B9	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
58	B7	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	A6	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	B2	96/129 (74%)	86 (90%)	6 (6%)	4 (4%)	2	17
62	A4	82/97 (84%)	67 (82%)	10 (12%)	5 (6%)	1	13
63	A5	73/86 (85%)	64 (88%)	8 (11%)	1 (1%)	9	40
64	B6	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	B8	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	20
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	B1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	13637/15129 (90%)	11563 (85%)	1924 (14%)	150 (1%)	14	46

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	7	171	ILE
9	3	43	PRO
10	A	463	SER
11	B	54	PRO
11	B	56	LYS
11	B	294	ARG
27	S	200	PRO
27	S	276	ASP
28	T	35	VAL
28	T	46	PRO
28	T	51	GLU
38	d	40	VAL
40	h	81	ALA
40	h	82	VAL
44	e	81	ARG
44	e	82	SER
49	p	82	PRO
49	p	120	PRO
49	p	129	LYS
49	p	146	PRO
49	p	159	PRO
52	s	14	VAL
48	z	80	MET
50	A1	25	GLY
50	A1	27	ASN

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Mol	Chain	Res	Type
50	A1	28	LYS
52	B5	14	VAL
53	A3	35	ALA
53	A3	43	ASP
56	A9	328	HIS
56	A9	508	PRO
61	B2	2	SER
61	B2	87	THR
61	B2	95	GLN
62	A4	4	ALA
62	A4	9	GLY
63	A5	46	LYS
65	B8	2	GLU
3	6	31	ASN
3	6	603	ASN
5	4	20	ASN
5	4	419	TYR
8	1	282	TYR
10	A	365	THR
16	G	122	SER
18	I	105	LYS
26	R	272	LEU
28	T	65	ALA
30	V	143	TYR
32	X	14	VAL
49	p	130	PRO
53	t	37	ASP
55	v	65	VAL
48	z	79	GLU
49	A0	80	ASP
49	A0	92	ARG
53	A3	42	LEU
55	B3	65	VAL
62	A4	5	LYS
1	9	76	ALA
2	7	149	TYR
5	4	21	ASN
10	A	129	PRO
10	A	309	ASN
10	A	541	PRO
17	H	16	ARG
38	d	19	PRO

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Mol	Chain	Res	Type
44	e	68	ASP
44	e	76	PRO
46	l	305	GLN
49	p	81	ILE
45	w	214	LYS
46	x	305	GLN
57	B9	104	TRP
62	A4	61	SER
2	7	170	GLU
3	6	551	SER
5	4	64	PRO
5	4	112	ALA
8	1	174	LEU
9	3	82	ALA
11	B	291	VAL
14	E	108	SER
27	S	199	VAL
28	T	50	LEU
28	T	58	ARG
38	d	38	GLU
44	e	80	ASP
44	e	83	GLN
45	k	427	PRO
49	p	115	SER
49	p	116	GLN
49	p	134	ILE
49	p	136	ILE
45	w	427	PRO
49	A0	193	VAL
56	A9	51	ASP
3	6	30	SER
11	B	89	PRO
11	B	219	GLY
25	Q	29	ALA
25	Q	166	ARG
44	e	95	PRO
48	o	51	LEU
49	p	92	ARG
48	z	51	LEU
57	B9	103	GLN
65	B8	3	ASN
7	8	227	PRO

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Mol	Chain	Res	Type
11	B	88	HIS
16	G	84	ARG
27	S	281	LYS
32	X	13	HIS
46	l	222	GLN
46	l	333	ALA
46	x	222	GLN
46	x	333	ALA
56	A9	91	ASP
57	B9	158	ASP
62	A4	49	PRO
48	o	70	VAL
48	o	74	PRO
48	z	74	PRO
39	f	145	PRO
46	l	126	VAL
46	l	195	VAL
47	m	117	VAL
49	p	93	GLY
46	x	126	VAL
46	x	195	VAL
47	y	117	VAL
49	A0	194	ILE
2	7	24	PRO
5	4	305	THR
7	8	105	PRO
46	l	337	ILE
46	x	337	ILE
53	A3	27	VAL
61	B2	15	GLY
19	J	56	GLY
28	T	84	PRO
48	o	137	PRO
49	p	114	VAL
46	x	306	PRO
48	z	137	PRO
55	B3	63	PRO
26	R	328	ILE
28	T	45	THR
30	V	73	PRO
38	d	32	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9	159/183 (87%)	157 (99%)	2 (1%)	61	74
2	7	104/142 (73%)	104 (100%)	0	100	100
3	6	523/534 (98%)	521 (100%)	2 (0%)	84	84
4	2	274/316 (87%)	273 (100%)	1 (0%)	84	84
5	4	351/413 (85%)	350 (100%)	1 (0%)	86	86
6	5	75/86 (87%)	75 (100%)	0	100	100
7	8	236/353 (67%)	236 (100%)	0	100	100
8	1	273/275 (99%)	269 (98%)	4 (2%)	57	72
9	3	89/101 (88%)	88 (99%)	1 (1%)	65	76
10	A	550/588 (94%)	548 (100%)	2 (0%)	84	84
11	B	362/371 (98%)	361 (100%)	1 (0%)	86	86
12	C	183/204 (90%)	182 (100%)	1 (0%)	81	83
13	D	126/150 (84%)	125 (99%)	1 (1%)	73	80
14	E	145/151 (96%)	145 (100%)	0	100	100
15	F	13/69 (19%)	13 (100%)	0	100	100
16	G	105/119 (88%)	105 (100%)	0	100	100
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	52/79 (66%)	49 (94%)	3 (6%)	18	40
19	J	50/59 (85%)	50 (100%)	0	100	100
20	K	66/81 (82%)	66 (100%)	0	100	100
21	L	63/71 (89%)	63 (100%)	0	100	100
22	N	88/101 (87%)	88 (100%)	0	100	100
23	O	95/113 (84%)	95 (100%)	0	100	100
24	P	72/96 (75%)	72 (100%)	0	100	100
25	Q	142/154 (92%)	139 (98%)	3 (2%)	47	65
26	R	232/298 (78%)	229 (99%)	3 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	S	204/283 (72%)	203 (100%)	1 (0%)	81	83
28	T	75/101 (74%)	73 (97%)	2 (3%)	39	61
29	U	95/131 (72%)	95 (100%)	0	100	100
30	V	106/120 (88%)	106 (100%)	0	100	100
31	M	73/81 (90%)	73 (100%)	0	100	100
31	W	57/81 (70%)	56 (98%)	1 (2%)	51	68
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/75 (37%)	28 (100%)	0	100	100
35	a	70/114 (61%)	70 (100%)	0	100	100
36	b	85/124 (68%)	85 (100%)	0	100	100
37	c	45/121 (37%)	45 (100%)	0	100	100
38	d	42/107 (39%)	42 (100%)	0	100	100
39	f	80/160 (50%)	80 (100%)	0	100	100
40	h	63/112 (56%)	63 (100%)	0	100	100
41	i	23/45 (51%)	23 (100%)	0	100	100
42	j	88/106 (83%)	88 (100%)	0	100	100
43	g	130/157 (83%)	130 (100%)	0	100	100
44	e	44/141 (31%)	44 (100%)	0	100	100
45	k	369/394 (94%)	368 (100%)	1 (0%)	86	86
45	w	362/394 (92%)	362 (100%)	0	100	100
46	l	327/355 (92%)	327 (100%)	0	100	100
46	x	328/355 (92%)	328 (100%)	0	100	100
47	m	327/327 (100%)	325 (99%)	2 (1%)	78	83
47	y	327/327 (100%)	325 (99%)	2 (1%)	78	83
48	o	206/257 (80%)	205 (100%)	1 (0%)	81	83
48	z	202/257 (79%)	201 (100%)	1 (0%)	81	83
49	A0	64/168 (38%)	63 (98%)	1 (2%)	55	70
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	95 (99%)	1 (1%)	68	78
50	q	96/99 (97%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	A2	70/72 (97%)	70 (100%)	0	100	100
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B5	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	28/46 (61%)	25 (89%)	3 (11%)	6	21
53	t	24/46 (52%)	23 (96%)	1 (4%)	26	48
54	B4	52/54 (96%)	51 (98%)	1 (2%)	50	67
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B3	15/60 (25%)	15 (100%)	0	100	100
55	v	11/60 (18%)	11 (100%)	0	100	100
56	A9	427/427 (100%)	387 (91%)	40 (9%)	8	26
57	B9	211/211 (100%)	192 (91%)	19 (9%)	9	27
58	B7	226/226 (100%)	200 (88%)	26 (12%)	5	18
59	A7	128/148 (86%)	119 (93%)	9 (7%)	14	35
60	A6	95/123 (77%)	95 (100%)	0	100	100
61	B2	81/103 (79%)	77 (95%)	4 (5%)	22	43
62	A4	68/79 (86%)	66 (97%)	2 (3%)	37	58
63	A5	67/76 (88%)	64 (96%)	3 (4%)	24	46
64	B6	58/59 (98%)	54 (93%)	4 (7%)	14	36
65	B8	47/68 (69%)	43 (92%)	4 (8%)	10	29
66	B0	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	B1	40/55 (73%)	40 (100%)	0	100	100
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10623/12909 (82%)	10463 (98%)	160 (2%)	55	72

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

Mol	Chain	Res	Type
1	9	93	LEU
1	9	149	LEU
3	6	155	ILE
3	6	427	ILE
4	2	7	ILE
5	4	165	ILE

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Mol	Chain	Res	Type
8	1	89	LEU
8	1	225	MET
8	1	228	TYR
8	1	310	LEU
9	3	44	MET
10	A	120	LEU
10	A	262	VAL
11	B	429	PHE
12	C	218	VAL
13	D	74	ILE
18	I	101	ILE
18	I	103	LEU
18	I	108	LYS
25	Q	115	LEU
25	Q	128	VAL
25	Q	154	VAL
26	R	82	VAL
26	R	126	VAL
26	R	206	ILE
27	S	195	VAL
28	T	41	VAL
28	T	61	PHE
31	W	106	LYS
45	k	228	VAL
47	m	91	PHE
47	m	153	ILE
48	o	136	GLU
53	t	39	ARG
47	y	91	PHE
47	y	153	ILE
48	z	136	GLU
49	A0	5	ILE
50	A1	20	TYR
53	A3	39	ARG
53	A3	40	LEU
53	A3	42	LEU
54	B4	29	LEU
56	A9	18	LEU
56	A9	35	LEU
56	A9	92	MET
56	A9	96	ARG
56	A9	105	LEU

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Mol	Chain	Res	Type
56	A9	115	SER
56	A9	136	LEU
56	A9	138	HIS
56	A9	150	LEU
56	A9	158	ILE
56	A9	159	LEU
56	A9	187	SER
56	A9	188	VAL
56	A9	189	MET
56	A9	194	LEU
56	A9	199	LEU
56	A9	213	ARG
56	A9	241	PRO
56	A9	273	MET
56	A9	295	VAL
56	A9	301	THR
56	A9	306	THR
56	A9	318	VAL
56	A9	324	LEU
56	A9	347	LEU
56	A9	353	LEU
56	A9	354	THR
56	A9	365	ILE
56	A9	369	ASP
56	A9	373	VAL
56	A9	383	MET
56	A9	417	MET
56	A9	444	PRO
56	A9	465	VAL
56	A9	467	LEU
56	A9	474	GLU
56	A9	492	LEU
56	A9	508	PRO
56	A9	509	THR
56	A9	512	ASN
57	B9	16	ILE
57	B9	31	VAL
57	B9	33	LEU
57	B9	52	HIS
57	B9	60	GLU
57	B9	63	THR
57	B9	67	ILE

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Mol	Chain	Res	Type
57	B9	88	ASP
57	B9	92	ASN
57	B9	125	THR
57	B9	130	PRO
57	B9	134	ARG
57	B9	142	VAL
57	B9	147	GLU
57	B9	170	LEU
57	B9	171	LYS
57	B9	185	MET
57	B9	205	SER
57	B9	216	LEU
58	B7	11	VAL
58	B7	13	PRO
58	B7	14	SER
58	B7	18	LEU
58	B7	19	THR
58	B7	22	LEU
58	B7	26	LEU
58	B7	38	ASN
58	B7	39	SER
58	B7	85	LEU
58	B7	92	LEU
58	B7	112	LEU
58	B7	127	LEU
58	B7	128	GLU
58	B7	131	LEU
58	B7	132	LEU
58	B7	137	LEU
58	B7	142	VAL
58	B7	160	LEU
58	B7	163	LEU
58	B7	188	ILE
58	B7	196	THR
58	B7	199	VAL
58	B7	213	THR
58	B7	222	GLN
58	B7	230	ASN
59	A7	27	VAL
59	A7	31	LYS
59	A7	36	SER
59	A7	40	LEU

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Mol	Chain	Res	Type
59	A7	59	LEU
59	A7	62	LEU
59	A7	107	ILE
59	A7	143	ASN
59	A7	147	LYS
61	B2	6	VAL
61	B2	20	VAL
61	B2	74	LEU
61	B2	95	GLN
62	A4	33	LEU
62	A4	56	ARG
63	A5	29	CYS
63	A5	41	LYS
63	A5	53	CYS
64	B6	22	VAL
64	B6	26	MET
64	B6	44	LYS
64	B6	64	ARG
65	B8	5	VAL
65	B8	16	ASN
65	B8	23	LYS
65	B8	27	THR
66	B0	45	VAL
66	B0	48	VAL
66	B0	49	THR
68	A8	13	LYS
68	A8	24	LEU
68	A8	42	LYS

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

Mol	Chain	Res	Type
1	9	189	ASN
2	7	46	ASN
3	6	59	GLN
3	6	113	ASN
3	6	139	GLN
3	6	192	ASN
3	6	226	GLN
3	6	270	ASN
3	6	332	HIS
3	6	405	ASN

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Mol	Chain	Res	Type
3	6	479	GLN
3	6	546	GLN
4	2	49	ASN
5	4	26	ASN
5	4	30	HIS
5	4	168	GLN
5	4	304	GLN
5	4	374	ASN
6	5	25	HIS
7	8	220	GLN
7	8	281	HIS
7	8	346	GLN
7	8	422	HIS
8	1	5	ASN
8	1	97	ASN
8	1	124	ASN
8	1	284	GLN
8	1	292	ASN
8	1	317	GLN
9	3	10	ASN
10	A	142	GLN
10	A	309	ASN
10	A	334	GLN
10	A	359	ASN
10	A	571	HIS
10	A	644	ASN
11	B	38	GLN
11	B	112	HIS
11	B	168	GLN
11	B	182	ASN
11	B	250	ASN
11	B	339	GLN
12	C	84	ASN
12	C	249	GLN
13	D	98	HIS
13	D	158	ASN
14	E	192	ASN
14	E	204	ASN
17	H	25	GLN
17	H	27	HIS
17	H	70	GLN
17	H	82	GLN

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Mol	Chain	Res	Type
18	I	118	GLN
20	K	25	GLN
21	L	46	ASN
22	N	83	GLN
22	N	111	GLN
23	O	126	HIS
26	R	43	HIS
26	R	79	GLN
26	R	323	HIS
26	R	331	HIS
28	T	89	ASN
29	U	31	ASN
30	V	112	HIS
31	W	115	GLN
32	X	13	HIS
36	b	141	GLN
36	b	170	HIS
36	b	181	HIS
37	c	14	GLN
37	c	83	HIS
39	f	139	GLN
41	i	62	HIS
42	j	88	HIS
42	j	97	HIS
43	g	55	GLN
43	g	161	GLN
31	M	74	GLN
45	k	9	GLN
45	k	15	GLN
45	k	85	HIS
45	k	118	GLN
45	k	207	GLN
45	k	243	HIS
45	k	252	HIS
45	k	267	ASN
45	k	363	ASN
46	l	162	ASN
46	l	254	HIS
46	l	277	HIS
46	l	304	HIS
46	l	354	ASN
47	m	3	ASN

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Mol	Chain	Res	Type
47	m	32	ASN
47	m	97	HIS
47	m	255	ASN
47	m	308	HIS
47	m	341	GLN
48	o	6	HIS
48	o	121	HIS
48	o	200	HIS
49	p	53	ASN
51	r	12	HIS
51	r	23	GLN
51	r	79	ASN
52	s	71	HIS
54	u	45	HIS
45	w	9	GLN
45	w	15	GLN
45	w	21	ASN
45	w	85	HIS
45	w	159	GLN
45	w	207	GLN
45	w	252	HIS
45	w	267	ASN
45	w	363	ASN
46	x	143	GLN
46	x	162	ASN
46	x	254	HIS
46	x	277	HIS
46	x	304	HIS
46	x	354	ASN
46	x	358	GLN
47	y	3	ASN
47	y	32	ASN
47	y	97	HIS
47	y	255	ASN
47	y	308	HIS
47	y	341	GLN
47	y	374	ASN
48	z	6	HIS
48	z	75	ASN
48	z	200	HIS
49	A0	57	GLN
50	A1	38	HIS

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Mol	Chain	Res	Type
50	A1	56	ASN
51	A2	12	HIS
51	A2	23	GLN
52	B5	71	HIS
53	A3	12	GLN
53	A3	16	ASN
54	B4	45	HIS
56	A9	4	ASN
56	A9	11	ASN
56	A9	12	HIS
56	A9	55	ASN
56	A9	99	ASN
56	A9	170	ASN
56	A9	178	GLN
56	A9	256	HIS
56	A9	360	ASN
56	A9	368	HIS
56	A9	413	HIS
56	A9	503	HIS
56	A9	512	ASN
57	B9	52	HIS
57	B9	102	HIS
57	B9	195	GLN
57	B9	203	ASN
58	B7	3	HIS
58	B7	6	HIS
58	B7	12	ASN
58	B7	133	ASN
58	B7	148	HIS
58	B7	149	HIS
58	B7	158	HIS
58	B7	204	HIS
58	B7	207	HIS
58	B7	222	GLN
58	B7	232	HIS
59	A7	32	ASN
59	A7	109	HIS
60	A6	34	ASN
61	B2	66	ASN
62	A4	51	HIS
62	A4	52	HIS
63	A5	23	GLN

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Mol	Chain	Res	Type
63	A5	24	ASN
63	A5	25	GLN
63	A5	28	ASN
63	A5	31	GLN
63	A5	32	ASN
63	A5	37	HIS
65	B8	3	ASN
65	B8	16	ASN
66	B0	10	HIS
66	B0	15	ASN
66	B0	35	GLN
66	B0	41	ASN
67	B1	42	HIS
68	A8	39	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 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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
77	HEM	m	402	47	50,50,50	1.90	18 (36%)	66,82,82	1.41	7 (10%)
77	HEM	y	402	47	50,50,50	1.89	17 (34%)	66,82,82	1.40	7 (10%)
71	3PE	j	202	-	45,45,50	0.91	4 (8%)	48,50,55	1.05	2 (4%)
72	PC1	Q	201	-	45,45,53	1.00	4 (8%)	51,53,61	1.07	2 (3%)
72	PC1	2	402	-	45,45,53	1.00	3 (6%)	51,53,61	1.03	2 (3%)
74	SF4	A	802	-	0,12,12	-	-	-	-	-
79	HEA	A9	602	56	66,67,67	1.22	7 (10%)	78,103,103	1.36	11 (14%)
79	HEA	A9	601	56	66,67,67	1.10	3 (4%)	78,103,103	1.38	11 (14%)
71	3PE	4	502	-	40,40,50	0.93	3 (7%)	43,45,55	1.37	3 (6%)
72	PC1	j	201	-	38,38,53	1.12	4 (10%)	44,46,61	1.10	2 (4%)
78	HEC	o	301	48	50,50,50	1.68	7 (14%)	68,82,82	1.56	11 (16%)
76	NAP	R	601	-	49,52,52	4.36	22 (44%)	69,80,80	1.86	15 (21%)
71	3PE	V	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
74	SF4	E	302	-	0,12,12	-	-	-	-	-
71	3PE	B	501	11	50,50,50	0.85	4 (8%)	53,55,55	1.12	2 (3%)
77	HEM	m	401	47	50,50,50	1.91	20 (40%)	66,82,82	1.70	12 (18%)
69	FES	9	301	-	0,4,4	-	-	-	-	-
74	SF4	8	502	-	0,12,12	-	-	-	-	-
69	FES	A	803	-	0,4,4	-	-	-	-	-
74	SF4	A	801	-	0,12,12	-	-	-	-	-
72	PC1	S	401	-	46,46,53	0.99	4 (8%)	52,54,61	0.99	2 (3%)
70	CDL	6	701	-	63,63,99	1.07	7 (11%)	69,75,111	1.28	4 (5%)
72	PC1	L	200	-	46,46,53	1.02	4 (8%)	52,54,61	1.06	2 (3%)
73	FMN	8	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.62	11 (22%)
74	SF4	E	301	-	0,12,12	-	-	-	-	-
70	CDL	J	101	-	57,57,99	1.14	7 (12%)	63,69,111	1.19	4 (6%)
77	HEM	y	401	47	50,50,50	1.90	20 (40%)	66,82,82	1.70	12 (18%)
71	3PE	2	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.18	2 (4%)
74	SF4	D	301	-	0,12,12	-	-	-	-	-
70	CDL	4	501	-	81,81,99	0.97	6 (7%)	87,93,111	1.10	5 (5%)
78	HEC	z	301	48	50,50,50	1.68	7 (14%)	68,82,82	1.56	11 (16%)
69	FES	m	403	-	0,4,4	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEM	m	402	47	-	2/14/54/54	-
77	HEM	y	402	47	-	2/14/54/54	-
71	3PE	j	202	-	-	24/49/49/54	-
72	PC1	Q	201	-	-	20/49/49/57	-
72	PC1	2	402	-	-	20/49/49/57	-
74	SF4	A	802	-	-	-	0/6/5/5
79	HEA	A9	602	56	-	7/36/76/76	-
79	HEA	A9	601	56	-	9/36/76/76	-
71	3PE	4	502	-	-	24/44/44/54	-
72	PC1	j	201	-	-	23/42/42/57	-
78	HEC	o	301	48	1/1/3/7	3/14/54/54	-
76	NAP	R	601	-	-	16/35/67/67	0/5/5/5
71	3PE	V	201	-	-	21/54/54/54	-
77	HEM	m	401	47	-	4/14/54/54	-
71	3PE	B	501	11	-	26/54/54/54	-
74	SF4	E	302	-	-	-	0/6/5/5
69	FES	9	301	-	-	-	0/1/1/1
74	SF4	8	502	-	-	-	0/6/5/5
69	FES	A	803	-	-	-	0/1/1/1
74	SF4	A	801	-	-	-	0/6/5/5
72	PC1	S	401	-	-	32/50/50/57	-
70	CDL	6	701	-	-	42/74/74/110	-
72	PC1	L	200	-	-	23/50/50/57	-
73	FMN	8	501	-	-	10/18/18/18	0/3/3/3
74	SF4	E	301	-	-	-	0/6/5/5
70	CDL	J	101	-	-	31/68/68/110	-
77	HEM	y	401	47	-	4/14/54/54	-
71	3PE	2	401	-	-	21/44/44/54	-
74	SF4	D	301	-	-	-	0/6/5/5
70	CDL	4	501	-	-	39/92/92/110	-
78	HEC	z	301	48	1/1/3/7	3/14/54/54	-
69	FES	m	403	-	-	-	0/1/1/1

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	O4D-C1D	16.09	1.63	1.41
76	R	601	NAP	C2D-C1D	-14.41	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	C2B-C1B	-9.13	1.29	1.53
76	R	601	NAP	O4B-C1B	8.26	1.61	1.42
76	R	601	NAP	C7N-N7N	6.91	1.46	1.33
78	z	301	HEC	C3D-C2D	6.89	1.51	1.36
78	o	301	HEC	C3D-C2D	6.83	1.51	1.36
76	R	601	NAP	O4D-C4D	-6.70	1.30	1.45
76	R	601	NAP	O4B-C4B	-5.84	1.31	1.45
76	R	601	NAP	C3N-C7N	5.43	1.58	1.50
77	y	402	HEM	FE-NB	-5.24	1.78	1.94
77	m	402	HEM	FE-NB	-5.22	1.78	1.94
77	m	401	HEM	FE-NC	-4.49	1.79	1.95
77	y	401	HEM	FE-NC	-4.47	1.79	1.95
76	R	601	NAP	O3D-C3D	-4.25	1.33	1.43
76	R	601	NAP	C6A-N6A	4.21	1.44	1.34
76	R	601	NAP	C5A-N7A	-4.17	1.31	1.39
76	R	601	NAP	O2D-C2D	3.80	1.51	1.43
79	A9	602	HEA	CMA-C3A	-3.68	1.37	1.45
76	R	601	NAP	O7N-C7N	-3.47	1.17	1.24
73	8	501	FMN	C4A-N5	3.40	1.37	1.30
77	y	401	HEM	CHD-C4C	-3.23	1.32	1.38
77	m	401	HEM	CHD-C4C	-3.17	1.32	1.38
77	m	402	HEM	C2A-C3A	-3.07	1.30	1.38
77	y	402	HEM	C2A-C3A	-3.05	1.30	1.38
77	m	402	HEM	CHB-C4A	-3.05	1.32	1.39
77	m	401	HEM	C2A-C3A	-3.02	1.30	1.38
77	y	401	HEM	C2A-C3A	-3.01	1.30	1.38
77	y	402	HEM	CHB-C4A	-3.00	1.32	1.39
77	m	402	HEM	C3C-C2C	-2.98	1.31	1.37
77	m	401	HEM	CHD-C1D	-2.97	1.32	1.39
77	y	401	HEM	CHD-C1D	-2.97	1.32	1.39
77	y	402	HEM	C3C-C2C	-2.94	1.31	1.37
77	m	402	HEM	C3B-C2B	-2.93	1.31	1.37
77	y	402	HEM	C3B-C2B	-2.93	1.31	1.37
79	A9	602	HEA	FE-NA	2.88	2.04	1.95
70	4	501	CDL	OB6-CB5	2.81	1.42	1.34
77	m	401	HEM	C3D-C2D	-2.79	1.30	1.36
77	m	402	HEM	C3D-C2D	-2.76	1.30	1.36
77	y	401	HEM	C3D-C2D	-2.75	1.30	1.36
77	y	402	HEM	C3D-C2D	-2.72	1.30	1.36
79	A9	601	HEA	C1A-C2A	-2.71	1.40	1.45
76	R	601	NAP	O3B-C3B	-2.70	1.36	1.43
79	A9	601	HEA	CMA-C3A	-2.66	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	A9	602	HEA	C3A-C2A	-2.65	1.31	1.36
70	6	701	CDL	OA6-CA4	-2.65	1.40	1.46
71	V	201	3PE	O21-C2	-2.63	1.40	1.46
79	A9	602	HEA	C1D-ND	-2.62	1.35	1.40
79	A9	602	HEA	C1D-C2D	2.61	1.49	1.44
77	y	401	HEM	CHA-C1A	-2.60	1.33	1.39
77	y	402	HEM	CHB-C1B	-2.59	1.33	1.38
72	Q	201	PC1	O21-C2	-2.59	1.40	1.46
77	m	401	HEM	CHA-C1A	-2.58	1.33	1.39
77	m	402	HEM	CHC-C1C	-2.58	1.33	1.38
72	S	401	PC1	O21-C2	-2.57	1.40	1.46
70	4	501	CDL	OB8-CB7	2.57	1.40	1.33
77	y	402	HEM	CHC-C1C	-2.56	1.33	1.38
71	j	202	3PE	O21-C2	-2.56	1.40	1.46
70	6	701	CDL	OB6-CB5	2.54	1.41	1.34
77	y	401	HEM	CHC-C4B	-2.52	1.33	1.39
77	m	402	HEM	CHB-C1B	-2.52	1.33	1.38
77	y	402	HEM	CHC-C4B	-2.52	1.33	1.39
77	m	401	HEM	CHC-C4B	-2.51	1.33	1.39
77	m	402	HEM	CHC-C4B	-2.51	1.33	1.39
77	m	401	HEM	C1B-NB	-2.51	1.36	1.40
70	J	101	CDL	OB8-CB7	2.51	1.40	1.33
70	4	501	CDL	OA6-CA4	-2.50	1.40	1.46
70	4	501	CDL	OA8-CA7	2.49	1.40	1.33
77	y	402	HEM	CHD-C4C	-2.49	1.33	1.38
77	m	401	HEM	C3C-C2C	-2.48	1.32	1.37
77	y	401	HEM	C3C-C2C	-2.48	1.32	1.37
77	y	401	HEM	C1B-NB	-2.47	1.36	1.40
70	J	101	CDL	OB6-CB4	-2.47	1.40	1.46
72	j	201	PC1	O21-C2	-2.47	1.40	1.46
77	m	401	HEM	C4C-NC	-2.46	1.35	1.39
77	m	402	HEM	CHD-C4C	-2.45	1.33	1.38
70	J	101	CDL	OA6-CA4	-2.45	1.40	1.46
76	R	601	NAP	C4A-N9A	-2.44	1.32	1.37
71	4	502	3PE	O21-C21	2.44	1.41	1.34
77	y	401	HEM	C4C-NC	-2.43	1.35	1.39
72	2	402	PC1	O21-C21	2.43	1.41	1.34
76	R	601	NAP	PA-O5B	2.43	1.69	1.59
77	y	402	HEM	CHD-C1D	-2.42	1.33	1.39
77	m	401	HEM	CHC-C1C	-2.41	1.33	1.38
78	o	301	HEC	C3C-C2C	-2.41	1.32	1.38
71	j	202	3PE	O31-C31	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	V	201	3PE	O31-C31	2.40	1.40	1.33
77	m	402	HEM	CHD-C1D	-2.40	1.33	1.39
70	J	101	CDL	OA8-CA7	2.40	1.40	1.33
76	R	601	NAP	C8A-N9A	-2.39	1.33	1.37
71	4	502	3PE	O31-C3	-2.39	1.39	1.45
71	B	501	3PE	O21-C2	-2.39	1.40	1.46
77	m	402	HEM	C1B-NB	-2.38	1.36	1.40
72	L	200	PC1	O31-C31	2.38	1.40	1.33
78	z	301	HEC	C3C-C2C	-2.38	1.32	1.38
77	y	401	HEM	CHC-C1C	-2.37	1.33	1.38
78	z	301	HEC	CHA-C4D	-2.37	1.33	1.39
77	y	402	HEM	C1B-NB	-2.36	1.36	1.40
79	A9	601	HEA	C3A-C4A	-2.36	1.41	1.46
73	8	501	FMN	C10-N1	2.36	1.38	1.33
78	o	301	HEC	CHA-C4D	-2.35	1.33	1.39
79	A9	602	HEA	CMD-C2D	2.34	1.55	1.50
71	2	401	3PE	O21-C21	2.34	1.40	1.34
72	j	201	PC1	O31-C31	2.34	1.40	1.33
70	6	701	CDL	OA8-CA6	-2.33	1.39	1.45
78	o	301	HEC	C4B-NB	-2.33	1.36	1.40
72	L	200	PC1	O21-C2	-2.32	1.40	1.46
77	m	401	HEM	C3C-C4C	-2.32	1.42	1.46
72	2	402	PC1	O31-C31	2.32	1.40	1.33
72	L	200	PC1	O31-C3	-2.32	1.39	1.45
72	S	401	PC1	O31-C31	2.32	1.40	1.33
71	2	401	3PE	O31-C3	-2.32	1.39	1.45
77	m	401	HEM	CAB-C3B	2.31	1.53	1.47
71	B	501	3PE	O31-C3	-2.30	1.39	1.45
77	y	401	HEM	CAB-C3B	2.30	1.53	1.47
78	z	301	HEC	C2A-C3A	-2.30	1.31	1.36
78	o	301	HEC	C2A-C3A	-2.29	1.31	1.36
77	y	401	HEM	C3C-C4C	-2.28	1.42	1.46
70	6	701	CDL	OB8-CB7	2.28	1.40	1.33
72	Q	201	PC1	O31-C3	-2.28	1.40	1.45
77	m	401	HEM	CAC-C3C	2.27	1.53	1.47
71	V	201	3PE	O31-C3	-2.27	1.40	1.45
78	z	301	HEC	C4B-NB	-2.27	1.36	1.40
76	R	601	NAP	C5A-C4A	-2.27	1.34	1.39
72	j	201	PC1	O21-C21	2.26	1.40	1.34
70	6	701	CDL	OA8-CA7	2.26	1.39	1.33
72	j	201	PC1	O31-C3	-2.26	1.40	1.45
76	R	601	NAP	P2B-O2B	2.26	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	401	HEM	FE-NB	-2.25	1.87	1.94
77	y	401	HEM	CAC-C3C	2.25	1.53	1.47
77	m	401	HEM	FE-NB	-2.25	1.87	1.94
71	2	401	3PE	O31-C31	2.23	1.39	1.33
72	S	401	PC1	O21-C21	2.22	1.40	1.34
76	R	601	NAP	C4N-C3N	-2.21	1.35	1.39
71	B	501	3PE	O21-C21	2.19	1.40	1.34
70	J	101	CDL	OB6-CB5	2.19	1.40	1.34
77	m	402	HEM	CAC-C3C	2.17	1.53	1.47
77	m	401	HEM	CHB-C4A	-2.17	1.34	1.39
72	L	200	PC1	O21-C21	2.17	1.40	1.34
77	y	402	HEM	CAB-C3B	2.17	1.53	1.47
78	z	301	HEC	FE-NC	-2.17	1.87	1.95
71	j	202	3PE	O31-C3	-2.16	1.40	1.45
78	o	301	HEC	C3B-C2B	-2.16	1.32	1.36
77	y	401	HEM	CHA-C4D	-2.16	1.34	1.38
78	o	301	HEC	FE-NC	-2.16	1.87	1.95
70	6	701	CDL	OA6-CA5	2.15	1.40	1.34
77	m	402	HEM	CAB-C3B	2.14	1.53	1.47
71	4	502	3PE	O31-C31	2.14	1.39	1.33
71	B	501	3PE	O31-C31	2.13	1.39	1.33
77	y	402	HEM	CAC-C3C	2.13	1.53	1.47
77	y	401	HEM	CHB-C4A	-2.13	1.34	1.39
70	J	101	CDL	OB8-CB6	-2.13	1.40	1.45
77	y	401	HEM	C3B-C2B	-2.13	1.33	1.37
77	y	402	HEM	C4A-NA	-2.13	1.35	1.39
77	m	401	HEM	C3B-C2B	-2.13	1.33	1.37
70	6	701	CDL	OB8-CB6	-2.12	1.40	1.45
78	z	301	HEC	C3B-C2B	-2.12	1.32	1.36
77	m	401	HEM	CHA-C4D	-2.10	1.34	1.38
71	2	401	3PE	O21-C2	-2.09	1.41	1.46
70	J	101	CDL	OA6-CA5	2.08	1.40	1.34
70	4	501	CDL	OA6-CA5	2.08	1.40	1.34
77	m	402	HEM	C3C-C4C	-2.08	1.42	1.46
77	m	402	HEM	C4A-NA	-2.08	1.35	1.39
77	y	402	HEM	C3C-C4C	-2.08	1.42	1.46
72	2	402	PC1	O31-C3	-2.07	1.40	1.45
77	m	401	HEM	FE-ND	-2.07	1.88	1.94
70	4	501	CDL	OA8-CA6	-2.07	1.40	1.45
76	R	601	NAP	PN-O5D	2.07	1.67	1.59
77	m	402	HEM	C4D-ND	-2.06	1.36	1.40
77	y	401	HEM	FE-ND	-2.06	1.88	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	401	HEM	FE-NA	-2.06	1.88	1.95
77	m	401	HEM	FE-NA	-2.05	1.88	1.95
72	S	401	PC1	O31-C3	-2.05	1.40	1.45
77	y	402	HEM	C4D-ND	-2.05	1.36	1.40
71	V	201	3PE	O21-C21	2.04	1.40	1.34
72	Q	201	PC1	O31-C31	2.04	1.39	1.33
79	A9	602	HEA	FE-NC	2.03	2.02	1.95
72	Q	201	PC1	O21-C21	2.02	1.40	1.34
71	j	202	3PE	O21-C21	2.02	1.40	1.34
76	R	601	NAP	O2B-C2B	2.01	1.51	1.44
77	m	402	HEM	C1C-NC	-2.01	1.35	1.39

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	R	601	NAP	N3A-C2A-N1A	-6.02	119.19	128.60
77	y	401	HEM	C1C-CHC-C4B	-5.74	113.67	126.06
77	m	401	HEM	C1C-CHC-C4B	-5.72	113.72	126.06
77	m	401	HEM	C1A-CHA-C4D	-5.57	113.13	126.34
77	y	401	HEM	C1A-CHA-C4D	-5.53	113.22	126.34
76	R	601	NAP	C5A-C4A-N3A	-5.14	120.05	126.75
71	4	502	3PE	O21-C21-C22	4.88	122.03	111.50
76	R	601	NAP	N6A-C6A-N1A	-4.81	107.81	118.35
72	L	200	PC1	O21-C21-C22	4.60	121.42	111.50
71	B	501	3PE	O21-C21-C22	4.52	121.24	111.50
78	o	301	HEC	C1A-CHA-C4D	-4.52	116.31	126.06
78	z	301	HEC	C1A-CHA-C4D	-4.49	116.38	126.06
76	R	601	NAP	N9A-C8A-N7A	-4.48	107.79	113.91
77	m	402	HEM	C4C-CHD-C1D	-4.46	116.44	126.06
77	y	402	HEM	C4C-CHD-C1D	-4.41	116.54	126.06
71	2	401	3PE	O21-C21-C22	4.38	120.94	111.50
70	4	501	CDL	OA6-CA5-C11	4.31	120.79	111.50
70	6	701	CDL	OB6-CB5-C51	4.26	120.67	111.50
70	J	101	CDL	OA6-CA5-C11	4.20	120.56	111.50
71	V	201	3PE	O21-C21-C22	4.17	120.48	111.50
70	J	101	CDL	OB6-CB5-C51	4.09	120.31	111.50
70	6	701	CDL	OA6-CA5-C11	3.97	120.06	111.50
79	A9	601	HEA	C17-C18-C19	-3.97	118.11	127.66
72	2	402	PC1	O21-C21-C22	3.93	119.97	111.50
77	y	401	HEM	CAD-CBD-CGD	-3.92	105.17	113.60
77	m	401	HEM	CAD-CBD-CGD	-3.91	105.18	113.60
73	8	501	FMN	C4-N3-C2	-3.86	118.52	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	8	501	FMN	C4A-C10-N1	-3.84	115.82	124.73
78	o	301	HEC	C4A-CHB-C1B	-3.83	117.80	126.06
72	S	401	PC1	O21-C21-C22	3.83	119.75	111.50
78	z	301	HEC	C4A-CHB-C1B	-3.82	117.81	126.06
71	j	202	3PE	O21-C21-C22	3.82	119.74	111.50
72	Q	201	PC1	O21-C21-C22	3.82	119.74	111.50
78	z	301	HEC	C1D-ND-C4D	3.81	109.01	105.07
77	m	402	HEM	C4A-CHB-C1B	-3.78	117.37	126.34
76	R	601	NAP	C2A-N3A-C4A	3.78	120.68	111.75
77	y	402	HEM	C4A-CHB-C1B	-3.77	117.39	126.34
78	o	301	HEC	C1C-CHC-C4B	-3.74	117.46	126.34
78	o	301	HEC	C1D-ND-C4D	3.72	108.92	105.07
78	z	301	HEC	C1C-CHC-C4B	-3.72	117.52	126.34
77	m	402	HEM	CAA-CBA-CGA	-3.69	105.66	113.60
77	y	402	HEM	CAA-CBA-CGA	-3.68	105.68	113.60
76	R	601	NAP	C5A-C6A-N6A	3.66	131.40	123.43
78	o	301	HEC	CAA-CBA-CGA	-3.56	105.94	113.60
72	j	201	PC1	O21-C21-C22	3.56	120.72	110.80
78	z	301	HEC	CAA-CBA-CGA	-3.54	105.97	113.60
77	m	402	HEM	CHC-C4B-NB	3.30	128.01	124.42
77	y	401	HEM	CAA-CBA-CGA	-3.29	106.52	113.60
77	m	401	HEM	CAA-CBA-CGA	-3.28	106.55	113.60
70	6	701	CDL	OA8-CA7-C31	3.27	122.16	111.91
78	o	301	HEC	CAD-CBD-CGD	-3.24	106.62	113.60
73	8	501	FMN	C10-N1-C2	3.23	123.37	116.90
77	y	401	HEM	C4C-CHD-C1D	-3.23	119.09	126.06
77	m	401	HEM	C4C-CHD-C1D	-3.23	119.10	126.06
77	y	402	HEM	CHC-C4B-NB	3.22	127.92	124.42
78	z	301	HEC	CAD-CBD-CGD	-3.21	106.70	113.60
70	4	501	CDL	CB4-OB6-CB5	3.21	125.69	117.79
79	A9	601	HEA	C13-C14-C15	-3.18	120.01	127.66
77	m	401	HEM	CAD-C3D-C4D	3.16	130.18	124.66
76	R	601	NAP	C5A-N7A-C8A	3.15	107.99	103.51
77	y	401	HEM	CAD-C3D-C4D	3.15	130.17	124.66
79	A9	602	HEA	CHA-C1A-NA	-3.15	121.03	124.44
78	z	301	HEC	CMD-C2D-C1D	3.06	129.70	125.04
70	4	501	CDL	OB6-CB5-C51	3.04	118.06	111.50
78	o	301	HEC	C4C-CHD-C1D	-3.03	119.16	126.34
73	8	501	FMN	C1'-N10-C9A	-3.03	115.47	120.51
78	z	301	HEC	C4C-CHD-C1D	-3.01	119.19	126.34
78	o	301	HEC	CMD-C2D-C1D	2.99	129.60	125.04
73	8	501	FMN	C4A-C4-N3	2.98	120.75	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	R	601	NAP	N3A-C4A-N9A	2.95	131.94	127.08
76	R	601	NAP	PN-O3-PA	-2.87	122.97	132.83
72	j	201	PC1	O31-C31-C32	2.87	120.90	111.91
70	4	501	CDL	OA8-CA7-C31	2.85	120.85	111.91
73	8	501	FMN	C4-C4A-C10	2.80	121.50	116.79
73	8	501	FMN	C5A-C9A-N10	2.80	120.85	117.95
70	J	101	CDL	OA8-CA7-C31	2.79	120.67	111.91
79	A9	601	HEA	C1B-C2B-C3B	2.78	110.12	106.80
71	2	401	3PE	O31-C31-C32	2.76	120.58	111.91
79	A9	602	HEA	C4A-C3A-C2A	2.76	109.02	106.75
70	6	701	CDL	OB8-CB7-C71	2.75	120.55	111.91
73	8	501	FMN	O4-C4-C4A	-2.71	119.41	126.60
77	m	402	HEM	CBD-CAD-C3D	-2.70	105.13	112.63
77	y	402	HEM	CBD-CAD-C3D	-2.68	105.19	112.63
77	y	401	HEM	CAD-C3D-C2D	-2.66	122.92	127.88
70	J	101	CDL	OB8-CB7-C71	2.66	120.26	111.91
79	A9	601	HEA	C3C-C4C-NC	2.64	111.87	110.25
72	S	401	PC1	O31-C31-C32	2.63	120.16	111.91
71	4	502	3PE	O31-C31-C32	2.63	120.15	111.91
73	8	501	FMN	C4A-C10-N10	2.62	120.31	116.48
72	L	200	PC1	O31-C31-C32	2.61	120.08	111.91
77	m	401	HEM	CAD-C3D-C2D	-2.61	123.03	127.88
79	A9	602	HEA	CMD-C2D-C1D	2.58	128.97	125.04
76	R	601	NAP	C4A-N9A-C1B	-2.56	120.49	126.59
72	2	402	PC1	O31-C31-C32	2.55	119.91	111.91
71	B	501	3PE	O31-C31-C32	2.54	119.89	111.91
71	V	201	3PE	O31-C31-C32	2.48	119.68	111.91
79	A9	602	HEA	C1D-C2D-C3D	-2.44	104.39	106.96
76	R	601	NAP	C3D-C2D-C1D	2.43	104.64	100.98
79	A9	602	HEA	CAA-C2A-C1A	2.42	129.46	124.89
79	A9	601	HEA	C17-C16-C15	-2.40	105.08	112.98
71	j	202	3PE	O31-C31-C32	2.40	119.43	111.91
70	4	501	CDL	OB8-CB7-C71	2.39	119.41	111.91
77	y	401	HEM	C4A-CHB-C1B	-2.38	120.69	126.34
79	A9	601	HEA	C20-C19-C18	2.38	125.93	121.12
78	z	301	HEC	CHC-C4B-NB	-2.36	121.46	124.37
77	m	401	HEM	CBA-CAA-C2A	-2.36	106.07	112.63
77	m	401	HEM	C4A-CHB-C1B	-2.36	120.75	126.34
77	y	401	HEM	CBA-CAA-C2A	-2.35	106.11	112.63
79	A9	602	HEA	CMB-C2B-C3B	-2.35	125.87	130.34
79	A9	601	HEA	C16-C17-C18	-2.34	104.18	111.88
78	o	301	HEC	CHC-C4B-NB	-2.33	121.50	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	y	402	HEM	C4C-NC-C1C	-2.33	103.07	105.35
79	A9	602	HEA	C13-C14-C15	-2.32	122.07	127.66
79	A9	601	HEA	CAD-C3D-C4D	2.30	128.68	124.66
77	m	402	HEM	C4C-NC-C1C	-2.30	103.10	105.35
73	8	501	FMN	C5'-C4'-C3'	-2.30	107.77	112.20
79	A9	602	HEA	C25-C23-C24	2.28	119.65	114.60
72	Q	201	PC1	O31-C31-C32	2.25	118.97	111.91
78	z	301	HEC	C1D-C2D-C3D	-2.22	104.63	106.96
79	A9	602	HEA	C26-C15-C16	2.22	119.00	115.27
79	A9	601	HEA	C12-C13-C14	-2.18	106.48	112.23
78	o	301	HEC	C1D-C2D-C3D	-2.16	104.68	106.96
79	A9	601	HEA	C4B-C3B-C2B	-2.15	103.74	107.41
71	4	502	3PE	C2-O21-C21	2.14	123.06	117.79
77	m	401	HEM	CHA-C4D-ND	-2.14	121.73	124.37
76	R	601	NAP	C4A-N9A-C8A	2.13	108.04	105.73
77	y	401	HEM	CHA-C4D-ND	-2.12	121.76	124.37
76	R	601	NAP	C4B-O4B-C1B	-2.11	104.81	109.47
79	A9	601	HEA	C27-C19-C18	-2.10	118.28	123.68
79	A9	602	HEA	C3A-C2A-C1A	-2.09	105.08	107.08
77	m	401	HEM	CHD-C4C-C3C	-2.07	121.71	125.26
77	y	401	HEM	CHD-C4C-C3C	-2.07	121.72	125.26
78	z	301	HEC	CAB-C3B-C4B	2.07	127.49	124.81
73	8	501	FMN	C9A-C5A-N5	-2.06	120.19	122.43
78	o	301	HEC	CAB-C3B-C4B	2.05	127.47	124.81
76	R	601	NAP	C6N-N1N-C2N	-2.04	120.11	121.97
79	A9	602	HEA	CBD-CAD-C3D	2.04	118.29	112.63
77	m	402	HEM	CHC-C4B-C3B	-2.04	120.75	125.13
77	y	401	HEM	C4C-NC-C1C	-2.02	103.37	105.35
77	m	401	HEM	C4C-NC-C1C	-2.02	103.37	105.35
77	y	402	HEM	CHC-C4B-C3B	-2.01	120.81	125.13
76	R	601	NAP	C4A-C5A-N7A	-2.01	108.18	110.62

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
78	o	301	HEC	NA
78	z	301	HEC	NA

All (406) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	6	701	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
70	6	701	CDL	CA3-OA5-PA1-OA2
70	6	701	CDL	CA3-OA5-PA1-OA3
70	6	701	CDL	CA3-OA5-PA1-OA4
70	6	701	CDL	CB2-OB2-PB2-OB3
70	6	701	CDL	CB2-OB2-PB2-OB4
70	6	701	CDL	CB2-OB2-PB2-OB5
70	6	701	CDL	C51-CB5-OB6-CB4
70	4	501	CDL	C1-CA2-OA2-PA1
70	4	501	CDL	CA2-OA2-PA1-OA4
70	J	101	CDL	CB2-C1-CA2-OA2
70	J	101	CDL	CA2-OA2-PA1-OA3
70	J	101	CDL	CA2-OA2-PA1-OA5
70	J	101	CDL	OA7-CA5-OA6-CA4
71	2	401	3PE	C11-O13-P-O12
71	2	401	3PE	C11-O13-P-O14
71	2	401	3PE	C22-C21-O21-C2
71	4	502	3PE	C1-O11-P-O12
71	4	502	3PE	C1-O11-P-O13
71	4	502	3PE	C1-O11-P-O14
71	4	502	3PE	C22-C21-O21-C2
71	B	501	3PE	C1-O11-P-O12
71	B	501	3PE	C1-O11-P-O13
71	B	501	3PE	C1-O11-P-O14
71	B	501	3PE	O13-C11-C12-N
71	B	501	3PE	O22-C21-O21-C2
71	B	501	3PE	C22-C21-O21-C2
71	V	201	3PE	C1-O11-P-O12
71	V	201	3PE	C1-O11-P-O14
71	V	201	3PE	O21-C2-C3-O31
71	j	202	3PE	C1-O11-P-O12
71	j	202	3PE	C1-O11-P-O14
71	j	202	3PE	C11-O13-P-O12
72	2	402	PC1	O13-C11-C12-N
72	L	200	PC1	C11-O13-P-O14
72	L	200	PC1	C1-O11-P-O12
72	L	200	PC1	C1-O11-P-O14
72	L	200	PC1	O13-C11-C12-N
72	Q	201	PC1	C1-O11-P-O12
72	Q	201	PC1	C1-O11-P-O14
72	Q	201	PC1	C1-O11-P-O13
72	Q	201	PC1	O22-C21-O21-C2
72	S	401	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
72	S	401	PC1	C1-O11-P-O14
72	S	401	PC1	O13-C11-C12-N
72	j	201	PC1	C11-O13-P-O12
72	j	201	PC1	C11-O13-P-O14
72	j	201	PC1	C1-O11-P-O14
72	j	201	PC1	C22-C21-O21-C2
73	8	501	FMN	C2'-C1'-N10-C10
73	8	501	FMN	N10-C1'-C2'-O2'
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	C1'-C2'-C3'-O3'
73	8	501	FMN	C1'-C2'-C3'-C4'
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P
76	R	601	NAP	C5B-O5B-PA-O1A
76	R	601	NAP	C5B-O5B-PA-O2A
76	R	601	NAP	C1B-C2B-O2B-P2B
76	R	601	NAP	C5D-O5D-PN-O1N
76	R	601	NAP	C5D-O5D-PN-O2N
76	R	601	NAP	C2D-C1D-N1N-C2N
76	R	601	NAP	C2D-C1D-N1N-C6N
79	A9	601	HEA	C2A-C3A-CMA-OMA
79	A9	601	HEA	C4A-C3A-CMA-OMA
79	A9	601	HEA	C12-C11-C3B-C2B
79	A9	602	HEA	C2A-C3A-CMA-OMA
79	A9	602	HEA	C4A-C3A-CMA-OMA
70	6	701	CDL	OA9-CA7-OA8-CA6
70	4	501	CDL	OB9-CB7-OB8-CB6
71	j	202	3PE	O32-C31-O31-C3
70	6	701	CDL	OB7-CB5-OB6-CB4
71	2	401	3PE	O22-C21-O21-C2
72	j	201	PC1	O22-C21-O21-C2
70	6	701	CDL	C31-CA7-OA8-CA6
70	4	501	CDL	C71-CB7-OB8-CB6
71	j	202	3PE	C32-C31-O31-C3
70	J	101	CDL	C11-CA5-OA6-CA4
72	Q	201	PC1	C22-C21-O21-C2
70	J	101	CDL	C31-CA7-OA8-CA6
70	J	101	CDL	C71-CB7-OB8-CB6
71	4	502	3PE	C32-C31-O31-C3
72	S	401	PC1	C32-C31-O31-C3
71	4	502	3PE	O22-C21-O21-C2
72	2	402	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
70	J	101	CDL	OB9-CB7-OB8-CB6
72	S	401	PC1	O32-C31-O31-C3
72	j	201	PC1	O32-C31-O31-C3
70	6	701	CDL	O1-C1-CA2-OA2
70	J	101	CDL	O1-C1-CA2-OA2
72	2	402	PC1	C22-C21-O21-C2
73	8	501	FMN	O2'-C2'-C3'-O3'
76	R	601	NAP	O4B-C4B-C5B-O5B
76	R	601	NAP	O4D-C4D-C5D-O5D
72	j	201	PC1	C32-C31-O31-C3
70	J	101	CDL	OA9-CA7-OA8-CA6
77	m	401	HEM	C2A-CAA-CBA-CGA
77	y	401	HEM	C2A-CAA-CBA-CGA
71	4	502	3PE	O32-C31-O31-C3
79	A9	601	HEA	C15-C16-C17-C18
71	2	401	3PE	C32-C31-O31-C3
70	J	101	CDL	CA2-C1-CB2-OB2
72	L	200	PC1	C32-C31-O31-C3
72	2	402	PC1	C22-C23-C24-C25
72	L	200	PC1	C31-C32-C33-C34
71	B	501	3PE	O11-C1-C2-O21
72	2	402	PC1	C21-C22-C23-C24
71	2	401	3PE	O32-C31-O31-C3
70	4	501	CDL	C11-CA5-OA6-CA4
70	6	701	CDL	CA7-C31-C32-C33
72	2	402	PC1	C31-C32-C33-C34
70	6	701	CDL	CB5-C51-C52-C53
72	L	200	PC1	O32-C31-O31-C3
70	6	701	CDL	CA5-C11-C12-C13
70	4	501	CDL	CA5-C11-C12-C13
73	8	501	FMN	O2'-C2'-C3'-C4'
72	Q	201	PC1	C31-C32-C33-C34
72	j	201	PC1	C31-C32-C33-C34
70	J	101	CDL	O1-C1-CB2-OB2
70	4	501	CDL	OA7-CA5-OA6-CA4
70	6	701	CDL	CA4-CA6-OA8-CA7
70	6	701	CDL	CB3-OB5-PB2-OB2
70	4	501	CDL	CA2-OA2-PA1-OA5
71	2	401	3PE	C11-O13-P-O11
71	V	201	3PE	C1-O11-P-O13
71	j	202	3PE	C1-O11-P-O13
72	L	200	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
72	L	200	PC1	C1-O11-P-O13
72	S	401	PC1	C11-O13-P-O11
72	S	401	PC1	C1-O11-P-O13
72	j	201	PC1	C11-O13-P-O11
72	S	401	PC1	C23-C24-C25-C26
71	2	401	3PE	C27-C28-C29-C2A
71	B	501	3PE	C32-C33-C34-C35
72	S	401	PC1	C3E-C3F-C3G-C3H
71	2	401	3PE	C3-C2-O21-C21
70	6	701	CDL	C52-C53-C54-C55
70	J	101	CDL	C54-C55-C56-C57
71	j	202	3PE	C38-C39-C3A-C3B
77	m	401	HEM	C3D-CAD-CBD-CGD
77	y	401	HEM	C3D-CAD-CBD-CGD
78	o	301	HEC	C2A-CAA-CBA-CGA
78	z	301	HEC	C2A-CAA-CBA-CGA
72	S	401	PC1	C31-C32-C33-C34
72	j	201	PC1	C36-C37-C38-C39
70	6	701	CDL	C14-C15-C16-C17
71	B	501	3PE	C2D-C2E-C2F-C2G
70	4	501	CDL	CA7-C31-C32-C33
70	4	501	CDL	C62-C63-C64-C65
72	L	200	PC1	C34-C35-C36-C37
72	L	200	PC1	C39-C3A-C3B-C3C
72	j	201	PC1	C3B-C3C-C3D-C3E
70	4	501	CDL	C77-C78-C79-C80
70	J	101	CDL	C15-C16-C17-C18
71	4	502	3PE	C28-C29-C2A-C2B
70	4	501	CDL	C78-C79-C80-C81
71	4	502	3PE	C32-C33-C34-C35
71	j	202	3PE	C22-C23-C24-C25
72	2	402	PC1	C27-C28-C29-C2A
70	6	701	CDL	C51-C52-C53-C54
70	6	701	CDL	C72-C73-C74-C75
71	B	501	3PE	C2C-C2D-C2E-C2F
71	j	202	3PE	O13-C11-C12-N
71	2	401	3PE	C26-C27-C28-C29
71	B	501	3PE	C31-C32-C33-C34
72	Q	201	PC1	C2B-C2C-C2D-C2E
70	J	101	CDL	C53-C54-C55-C56
71	B	501	3PE	C33-C34-C35-C36
72	S	401	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
72	S	401	PC1	C32-C33-C34-C35
70	4	501	CDL	C54-C55-C56-C57
77	m	401	HEM	C4D-C3D-CAD-CBD
77	y	401	HEM	C4D-C3D-CAD-CBD
71	4	502	3PE	C31-C32-C33-C34
71	V	201	3PE	C32-C33-C34-C35
71	j	202	3PE	C22-C21-O21-C2
70	4	501	CDL	C75-C76-C77-C78
71	B	501	3PE	C26-C27-C28-C29
71	j	202	3PE	C33-C34-C35-C36
71	4	502	3PE	C24-C25-C26-C27
72	j	201	PC1	C32-C33-C34-C35
70	4	501	CDL	CA2-C1-CB2-OB2
71	j	202	3PE	C24-C25-C26-C27
71	j	202	3PE	C36-C37-C38-C39
70	4	501	CDL	C13-C14-C15-C16
71	2	401	3PE	C25-C26-C27-C28
71	V	201	3PE	C26-C27-C28-C29
72	2	402	PC1	C37-C38-C39-C3A
71	V	201	3PE	C2A-C2B-C2C-C2D
71	j	202	3PE	O22-C21-O21-C2
71	B	501	3PE	C21-C22-C23-C24
70	6	701	CDL	C74-C75-C76-C77
71	V	201	3PE	C36-C37-C38-C39
72	2	402	PC1	C34-C35-C36-C37
71	j	202	3PE	C21-C22-C23-C24
72	L	200	PC1	C27-C28-C29-C2A
72	S	401	PC1	C39-C3A-C3B-C3C
71	V	201	3PE	C2E-C2F-C2G-C2H
72	L	200	PC1	C25-C26-C27-C28
70	J	101	CDL	CA7-C31-C32-C33
71	B	501	3PE	C35-C36-C37-C38
72	L	200	PC1	C3C-C3D-C3E-C3F
72	S	401	PC1	C24-C25-C26-C27
71	4	502	3PE	C2E-C2F-C2G-C2H
71	B	501	3PE	C23-C24-C25-C26
70	4	501	CDL	C80-C81-C82-C83
71	B	501	3PE	C34-C35-C36-C37
70	4	501	CDL	OA6-CA4-CA6-OA8
71	V	201	3PE	C2B-C2C-C2D-C2E
72	S	401	PC1	C22-C23-C24-C25
70	4	501	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
77	m	401	HEM	C2D-C3D-CAD-CBD
77	y	401	HEM	C2D-C3D-CAD-CBD
70	6	701	CDL	C33-C34-C35-C36
70	6	701	CDL	C53-C54-C55-C56
70	4	501	CDL	C74-C75-C76-C77
71	j	202	3PE	C11-O13-P-O11
70	6	701	CDL	OB5-CB3-CB4-CB6
71	B	501	3PE	O11-C1-C2-C3
70	4	501	CDL	C34-C35-C36-C37
71	j	202	3PE	C26-C27-C28-C29
71	j	202	3PE	C27-C28-C29-C2A
72	S	401	PC1	C21-C22-C23-C24
71	4	502	3PE	C21-C22-C23-C24
72	L	200	PC1	C26-C27-C28-C29
71	j	202	3PE	C23-C24-C25-C26
76	R	601	NAP	C3B-C4B-C5B-O5B
70	6	701	CDL	C13-C14-C15-C16
70	4	501	CDL	C52-C53-C54-C55
70	4	501	CDL	C84-C85-C86-C87
73	8	501	FMN	C5'-O5'-P-O1P
70	4	501	CDL	O1-C1-CB2-OB2
72	L	200	PC1	O21-C2-C3-O31
72	S	401	PC1	O21-C2-C3-O31
71	4	502	3PE	C35-C36-C37-C38
71	B	501	3PE	C3E-C3F-C3G-C3H
72	2	402	PC1	C35-C36-C37-C38
71	j	202	3PE	C2C-C2D-C2E-C2F
71	2	401	3PE	C28-C29-C2A-C2B
70	4	501	CDL	C15-C16-C17-C18
72	S	401	PC1	C3F-C3G-C3H-C3I
72	2	402	PC1	O11-C1-C2-C3
72	L	200	PC1	O11-C1-C2-C3
71	j	202	3PE	C2A-C2B-C2C-C2D
71	V	201	3PE	C38-C39-C3A-C3B
70	6	701	CDL	C31-C32-C33-C34
72	Q	201	PC1	C21-C22-C23-C24
72	Q	201	PC1	C2A-C2B-C2C-C2D
70	4	501	CDL	CA3-CA4-CA6-OA8
70	J	101	CDL	CA3-CA4-CA6-OA8
71	2	401	3PE	C1-C2-C3-O31
71	V	201	3PE	C1-C2-C3-O31
72	j	201	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
72	S	401	PC1	C3D-C3E-C3F-C3G
71	4	502	3PE	C23-C24-C25-C26
71	4	502	3PE	C2C-C2D-C2E-C2F
70	6	701	CDL	OB5-CB3-CB4-OB6
71	2	401	3PE	O11-C1-C2-O21
72	L	200	PC1	O11-C1-C2-O21
72	L	200	PC1	C35-C36-C37-C38
70	4	501	CDL	C81-C82-C83-C84
70	J	101	CDL	OA6-CA4-CA6-OA8
70	J	101	CDL	C12-C13-C14-C15
71	4	502	3PE	C2-C1-O11-P
71	V	201	3PE	O21-C21-C22-C23
76	R	601	NAP	PN-O3-PA-O5B
76	R	601	NAP	PA-O3-PN-O5D
70	J	101	CDL	C16-C17-C18-C19
70	4	501	CDL	OA5-CA3-CA4-CA6
70	4	501	CDL	OB5-CB3-CB4-CB6
72	S	401	PC1	O11-C1-C2-C3
71	V	201	3PE	C3F-C3G-C3H-C3I
72	2	402	PC1	C32-C31-O31-C3
72	j	201	PC1	C35-C36-C37-C38
72	2	402	PC1	C3-C2-O21-C21
70	J	101	CDL	C11-C12-C13-C14
70	6	701	CDL	C1-CA2-OA2-PA1
71	B	501	3PE	C2-C1-O11-P
72	Q	201	PC1	C1-C2-C3-O31
72	2	402	PC1	O11-C1-C2-O21
72	S	401	PC1	O11-C1-C2-O21
70	4	501	CDL	OB6-CB4-CB6-OB8
72	Q	201	PC1	O21-C2-C3-O31
72	j	201	PC1	O21-C2-C3-O31
76	R	601	NAP	C5B-O5B-PA-O3
76	R	601	NAP	C2B-O2B-P2B-O3X
70	J	101	CDL	CB7-C71-C72-C73
78	o	301	HEC	C1A-C2A-CAA-CBA
72	Q	201	PC1	C32-C33-C34-C35
72	j	201	PC1	C1-O11-P-O13
70	J	101	CDL	C31-C32-C33-C34
72	2	402	PC1	O32-C31-O31-C3
70	6	701	CDL	CB3-OB5-PB2-OB3
70	6	701	CDL	CB3-OB5-PB2-OB4
71	j	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
72	L	200	PC1	C11-O13-P-O12
72	S	401	PC1	C11-O13-P-O14
72	S	401	PC1	C1-O11-P-O12
70	J	101	CDL	OB5-CB3-CB4-CB6
71	2	401	3PE	O11-C1-C2-C3
71	4	502	3PE	O11-C1-C2-C3
72	2	402	PC1	C33-C34-C35-C36
78	z	301	HEC	C1A-C2A-CAA-CBA
70	4	501	CDL	OA5-CA3-CA4-OA6
71	B	501	3PE	C3B-C3C-C3D-C3E
72	Q	201	PC1	C35-C36-C37-C38
71	V	201	3PE	C23-C24-C25-C26
71	V	201	3PE	C2C-C2D-C2E-C2F
70	4	501	CDL	CB3-CB4-CB6-OB8
72	Q	201	PC1	O13-C11-C12-N
72	j	201	PC1	O13-C11-C12-N
71	2	401	3PE	O21-C2-C3-O31
70	4	501	CDL	C14-C15-C16-C17
71	V	201	3PE	C2-C1-O11-P
70	6	701	CDL	CB3-CB4-OB6-CB5
70	6	701	CDL	CA4-CA3-OA5-PA1
72	Q	201	PC1	C2-C1-O11-P
72	S	401	PC1	C2-C1-O11-P
70	4	501	CDL	C35-C36-C37-C38
71	4	502	3PE	C34-C35-C36-C37
70	J	101	CDL	CB2-OB2-PB2-OB5
71	4	502	3PE	C11-O13-P-O11
71	V	201	3PE	C11-O13-P-O11
72	2	402	PC1	C1-O11-P-O13
72	L	200	PC1	C1-C2-C3-O31
72	S	401	PC1	C1-C2-C3-O31
71	2	401	3PE	C33-C34-C35-C36
70	4	501	CDL	CA4-CA3-OA5-PA1
70	6	701	CDL	OA7-CA5-OA6-CA4
70	6	701	CDL	C71-CB7-OB8-CB6
71	B	501	3PE	C38-C39-C3A-C3B
76	R	601	NAP	C2B-C1B-N9A-C8A
71	B	501	3PE	C37-C38-C39-C3A
71	4	502	3PE	O13-C11-C12-N
71	B	501	3PE	C36-C37-C38-C39
70	6	701	CDL	OB9-CB7-OB8-CB6
71	V	201	3PE	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
72	j	201	PC1	C3A-C3B-C3C-C3D
72	2	402	PC1	O21-C21-C22-C23
72	2	402	PC1	C28-C29-C2A-C2B
77	m	402	HEM	CAA-CBA-CGA-O1A
77	y	402	HEM	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O1D
72	j	201	PC1	C37-C38-C39-C3A
70	4	501	CDL	CB3-CB4-OB6-CB5
71	4	502	3PE	C1-C2-O21-C21
77	m	402	HEM	CAA-CBA-CGA-O2A
77	y	402	HEM	CAA-CBA-CGA-O2A
70	6	701	CDL	CB4-CB3-OB5-PB2
71	j	202	3PE	C39-C3A-C3B-C3C
70	6	701	CDL	C11-CA5-OA6-CA4
79	A9	602	HEA	CAD-CBD-CGD-O1D
72	L	200	PC1	C32-C33-C34-C35
72	2	402	PC1	C38-C39-C3A-C3B
70	J	101	CDL	OB7-CB5-OB6-CB4
79	A9	602	HEA	CAD-CBD-CGD-O2D
78	o	301	HEC	C3A-C2A-CAA-CBA
72	L	200	PC1	C22-C23-C24-C25
79	A9	601	HEA	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O2D
70	4	501	CDL	C71-C72-C73-C74
78	z	301	HEC	C3A-C2A-CAA-CBA
72	S	401	PC1	C34-C35-C36-C37
70	J	101	CDL	C14-C15-C16-C17
71	2	401	3PE	C29-C2A-C2B-C2C
71	2	401	3PE	C21-C22-C23-C24
70	4	501	CDL	C52-C51-CB5-OB6
72	Q	201	PC1	O21-C21-C22-C23
72	Q	201	PC1	C26-C27-C28-C29
79	A9	602	HEA	CAA-CBA-CGA-O2A
72	S	401	PC1	C38-C39-C3A-C3B
70	6	701	CDL	C12-C11-CA5-OA6
70	6	701	CDL	OB6-CB4-CB6-OB8
79	A9	602	HEA	CAA-CBA-CGA-O1A
72	S	401	PC1	O31-C31-C32-C33
72	j	201	PC1	O31-C31-C32-C33
76	R	601	NAP	C5D-O5D-PN-O3
70	J	101	CDL	C51-CB5-OB6-CB4
72	S	401	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
71	4	502	3PE	C2D-C2E-C2F-C2G
70	4	501	CDL	C52-C51-CB5-OB7
72	Q	201	PC1	O22-C21-C22-C23
70	J	101	CDL	CB3-CB4-CB6-OB8
72	S	401	PC1	O32-C31-C32-C33
79	A9	601	HEA	CAA-CBA-CGA-O2A
71	4	502	3PE	C11-O13-P-O14
71	V	201	3PE	C11-O13-P-O14
72	Q	201	PC1	C11-O13-P-O14
70	6	701	CDL	C12-C11-CA5-OA7
72	j	201	PC1	O32-C31-C32-C33
72	S	401	PC1	C27-C28-C29-C2A
70	6	701	CDL	C52-C51-CB5-OB6
70	J	101	CDL	C13-C14-C15-C16
71	V	201	3PE	O22-C21-C22-C23
72	j	201	PC1	C12-C11-O13-P
70	J	101	CDL	C12-C11-CA5-OA6
71	B	501	3PE	O31-C31-C32-C33
72	Q	201	PC1	C22-C23-C24-C25
79	A9	602	HEA	C26-C15-C16-C17
72	j	201	PC1	O11-C1-C2-O21
79	A9	601	HEA	O11-C11-C3B-C2B
71	2	401	3PE	O31-C31-C32-C33
71	j	202	3PE	O21-C21-C22-C23
72	S	401	PC1	O22-C21-C22-C23
71	B	501	3PE	O32-C31-C32-C33
71	2	401	3PE	O32-C31-C32-C33

There are no ring outliers.

24 monomers are involved in 108 short contacts:

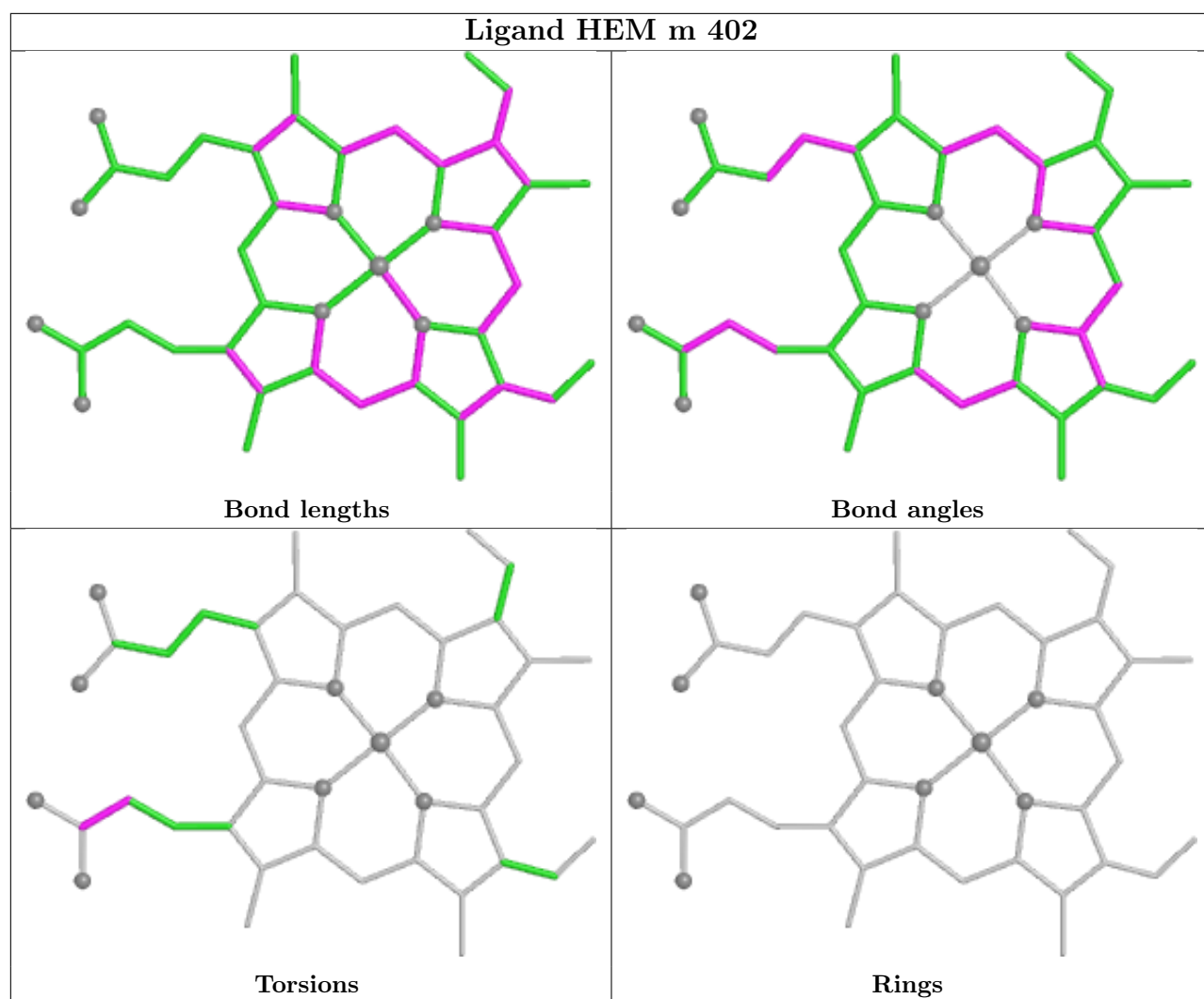
Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	m	402	HEM	17	0
77	y	402	HEM	19	0
71	j	202	3PE	1	0
72	Q	201	PC1	1	0
72	2	402	PC1	2	0
79	A9	602	HEA	3	0
79	A9	601	HEA	1	0
71	4	502	3PE	1	0
72	j	201	PC1	1	0
78	o	301	HEC	10	0

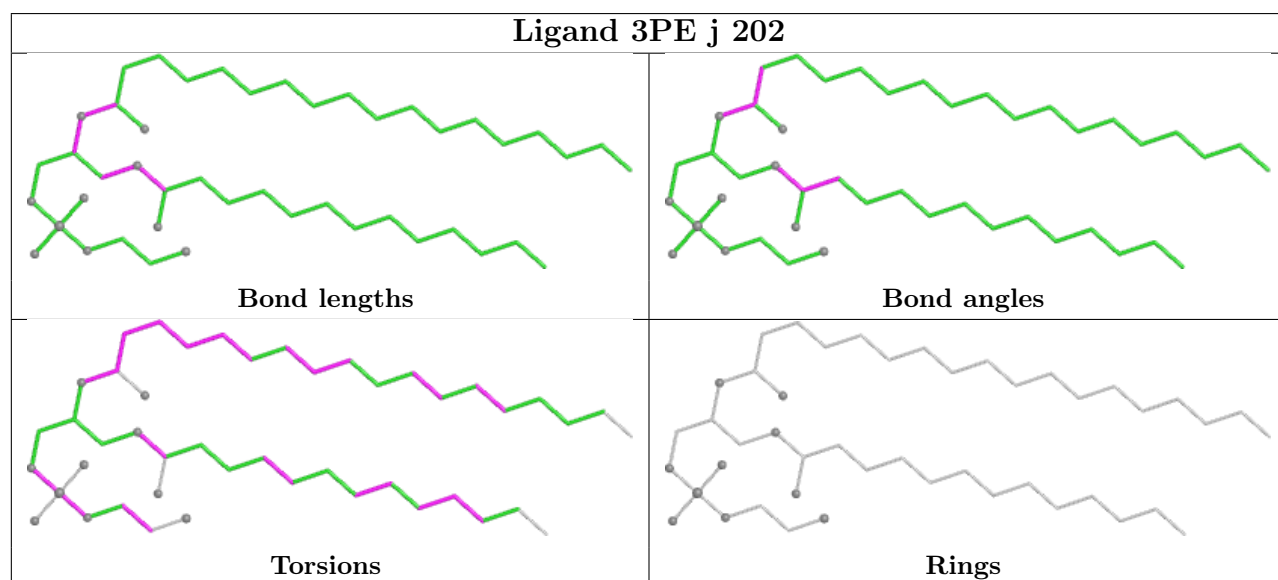
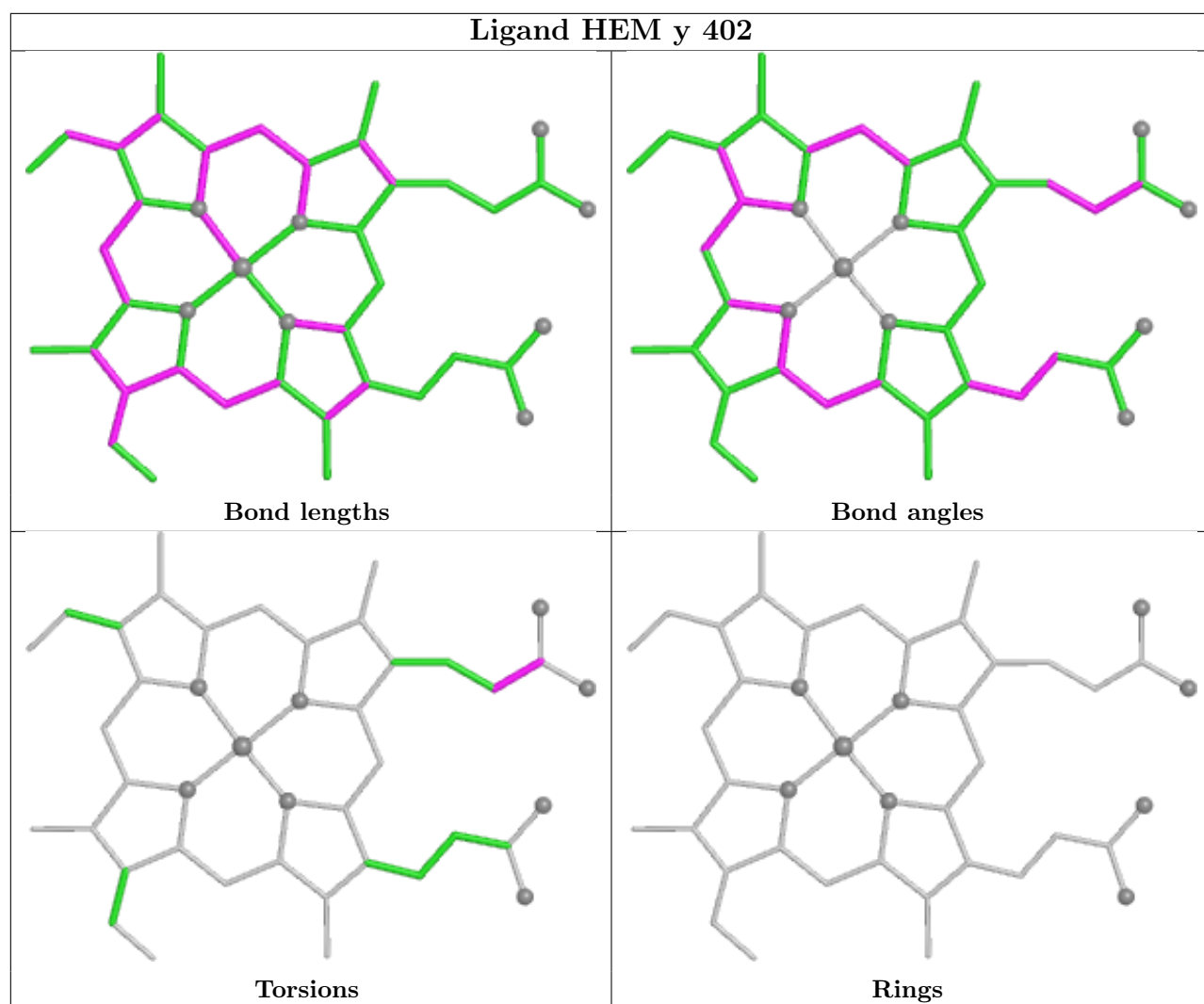
Continued on next page...

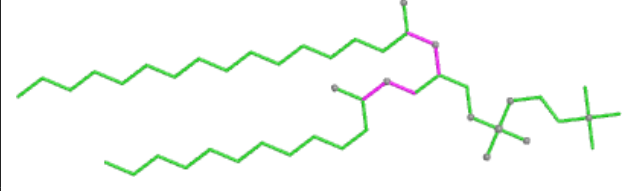
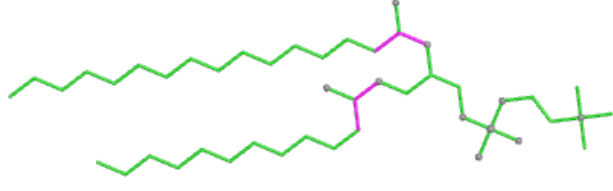
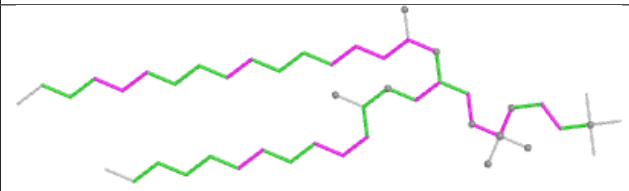
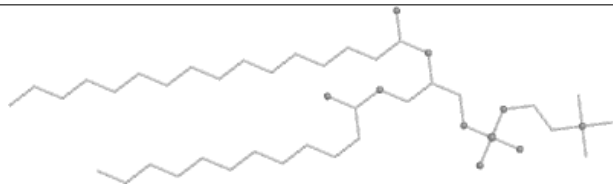
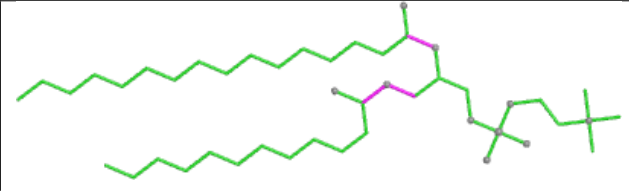
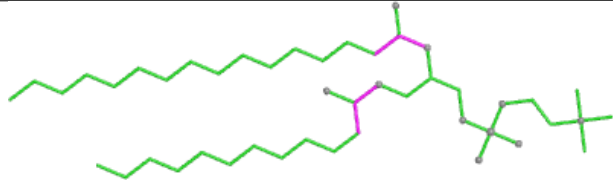
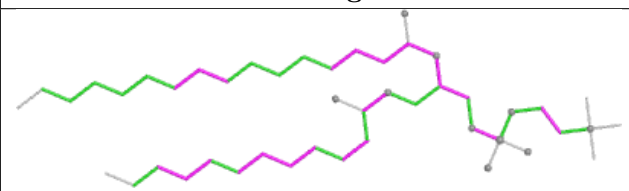
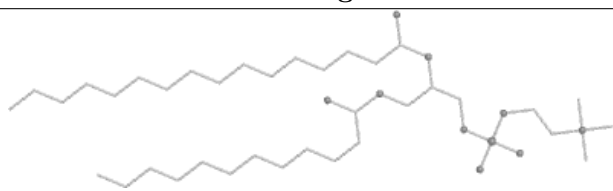
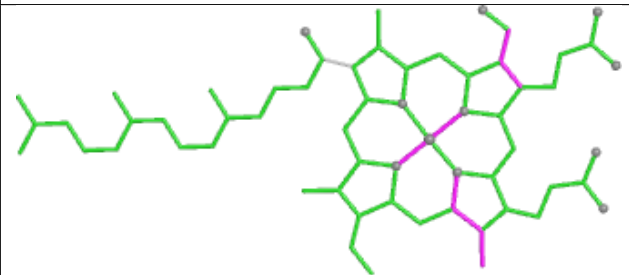
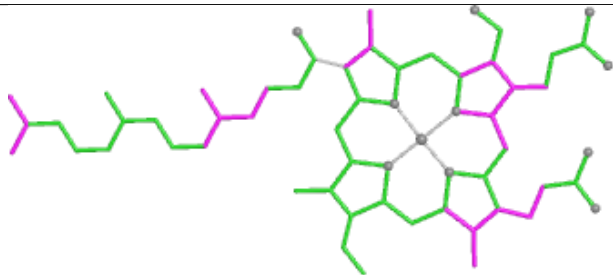
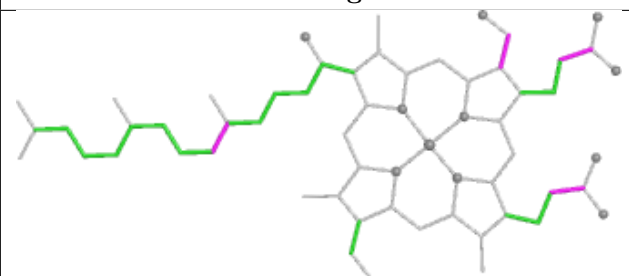
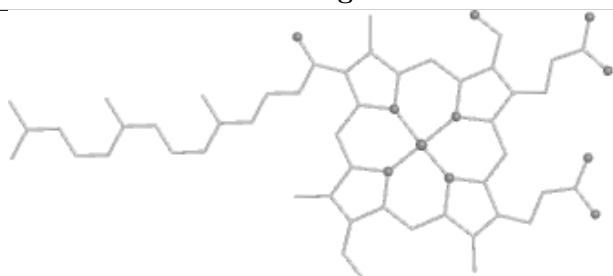
Continued from previous page...

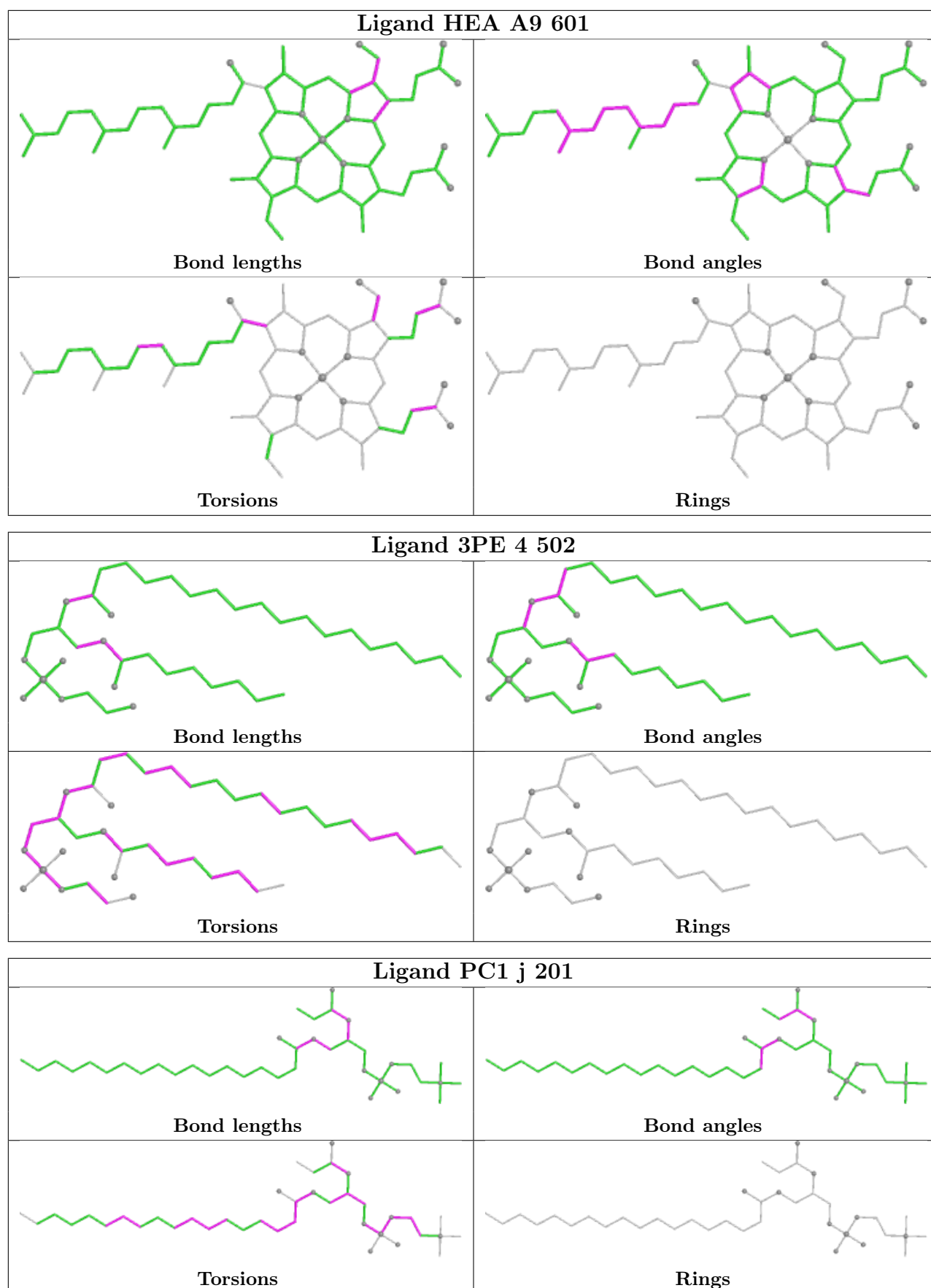
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	R	601	NAP	3	0
74	E	302	SF4	1	0
71	B	501	3PE	2	0
77	m	401	HEM	11	0
74	A	801	SF4	1	0
72	S	401	PC1	3	0
70	6	701	CDL	2	0
72	L	200	PC1	2	0
73	8	501	FMN	3	0
70	J	101	CDL	1	0
77	y	401	HEM	11	0
71	2	401	3PE	1	0
70	4	501	CDL	1	0
78	z	301	HEC	10	0

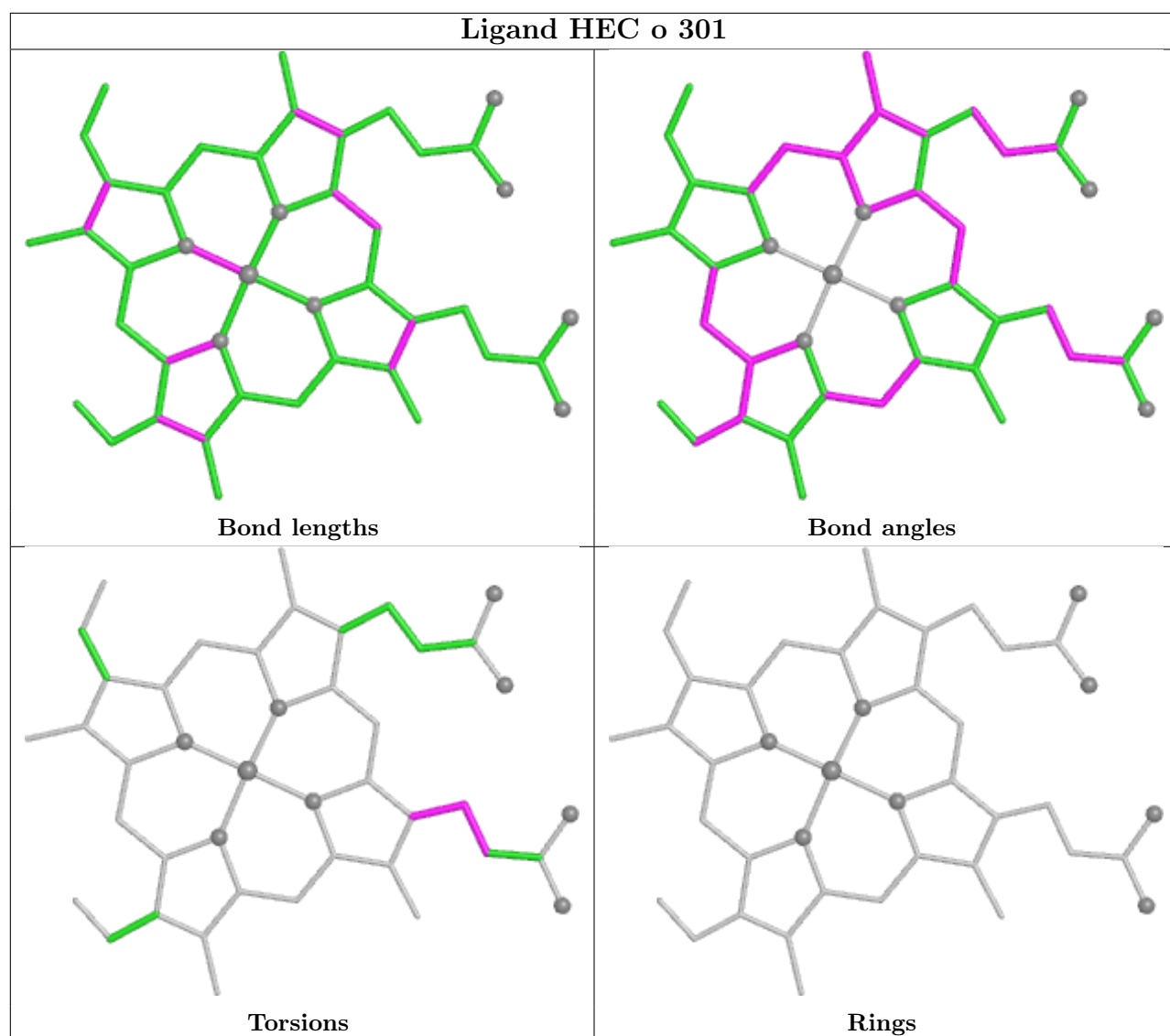
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

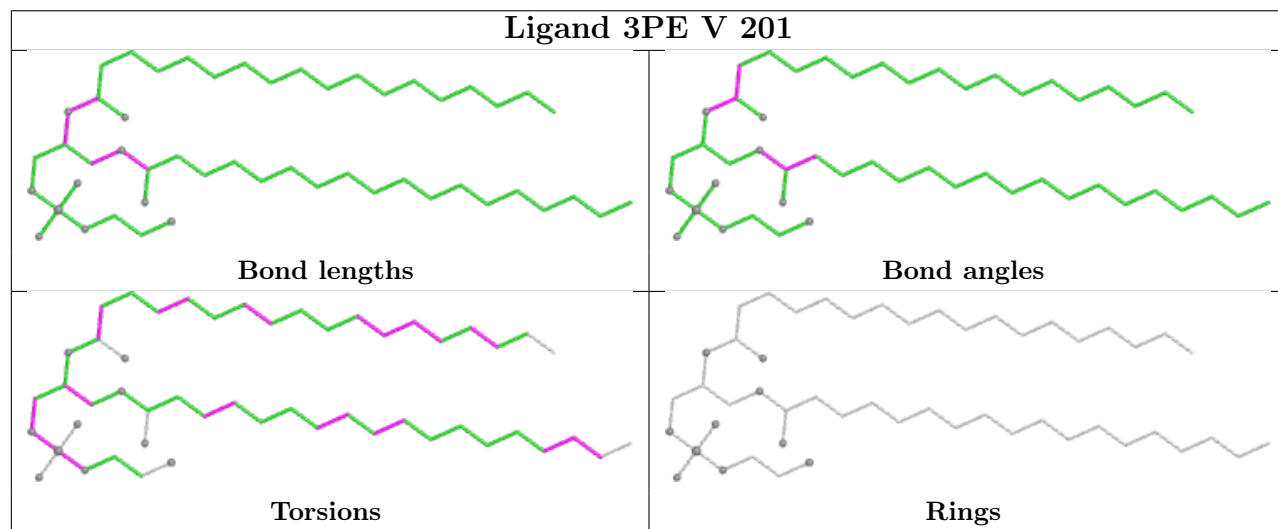
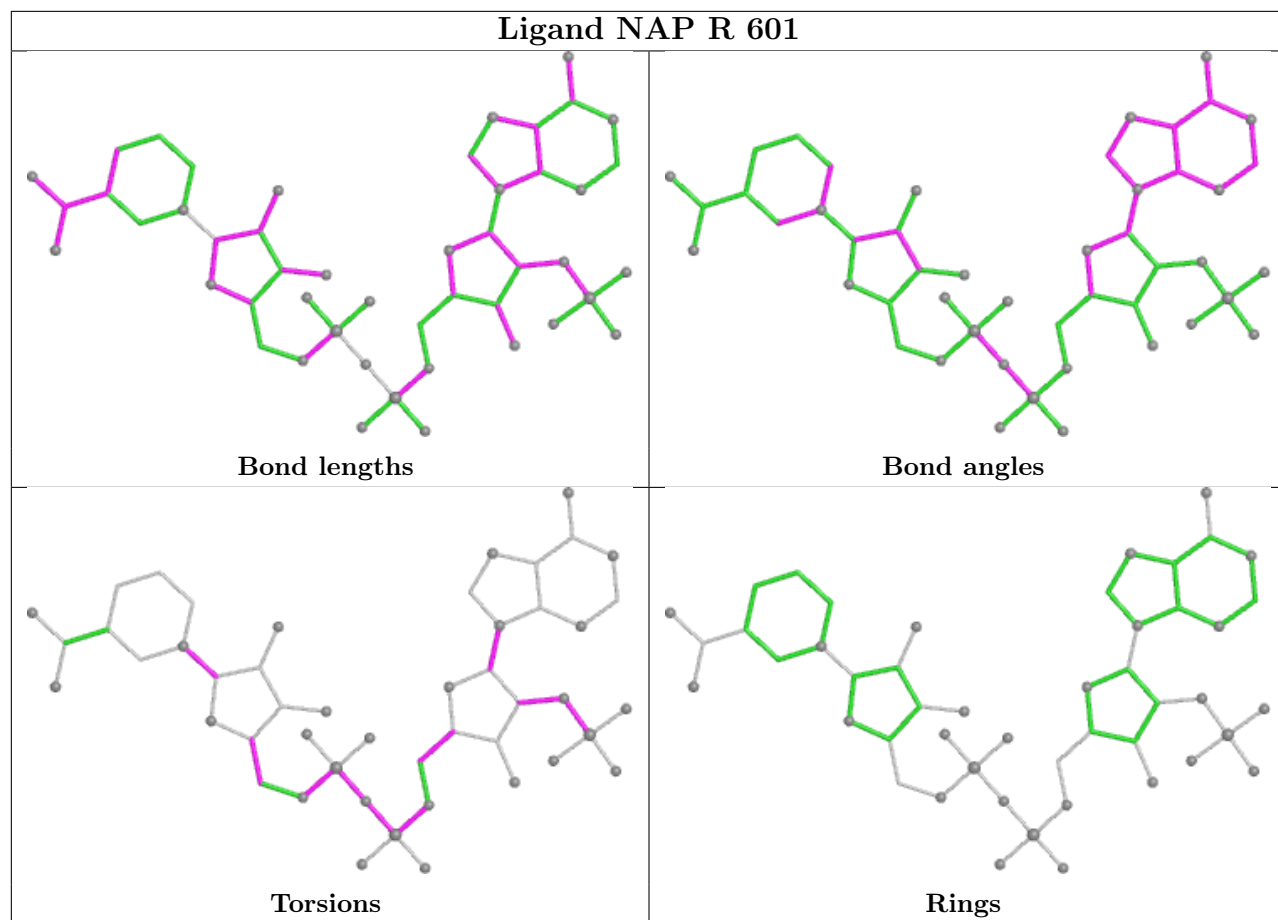


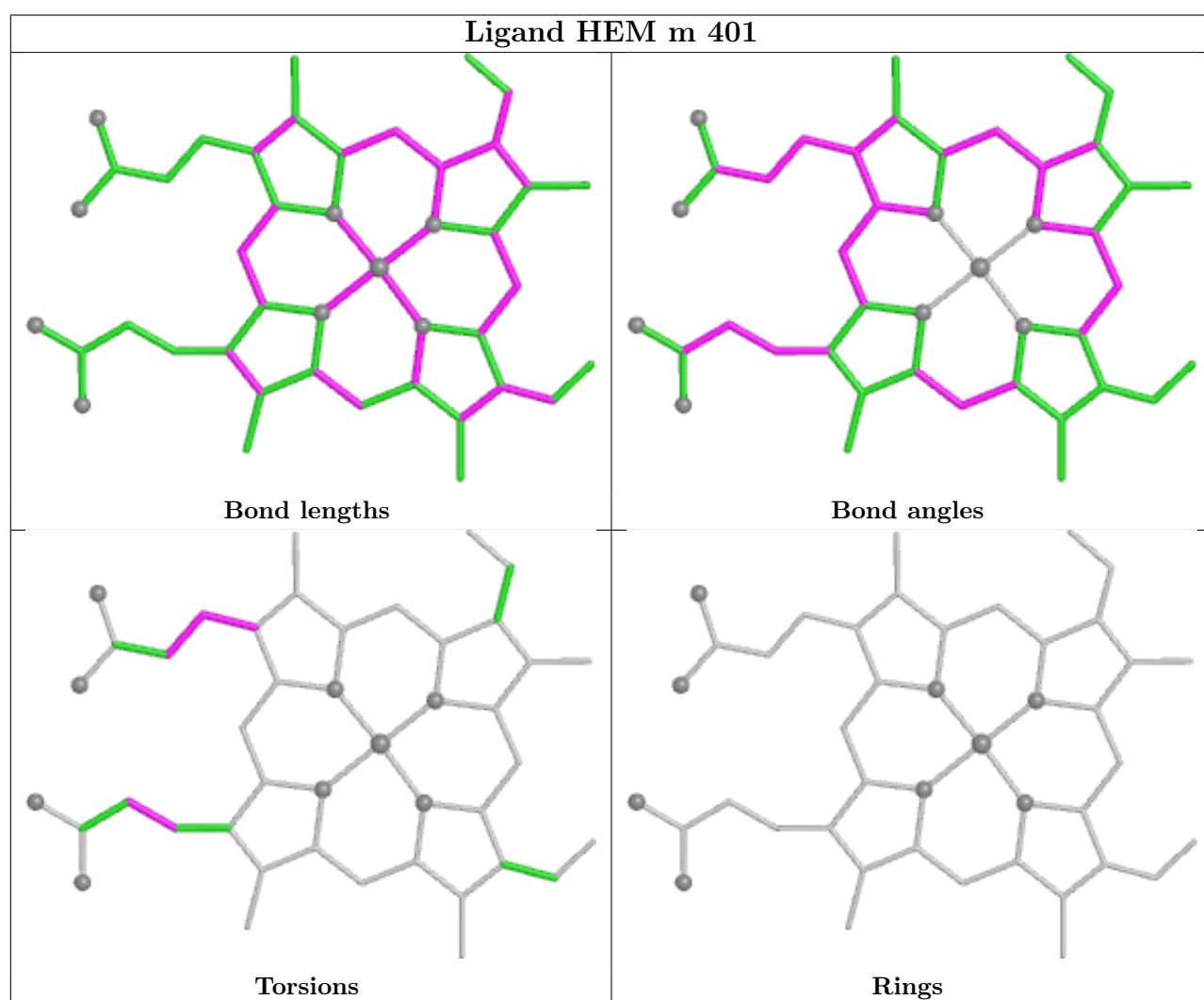
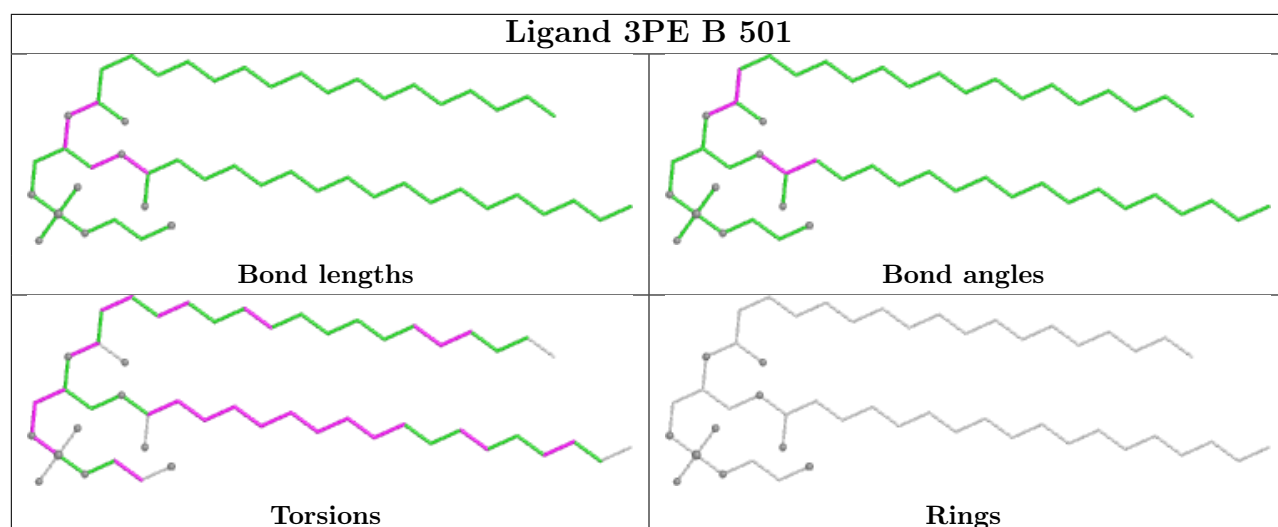


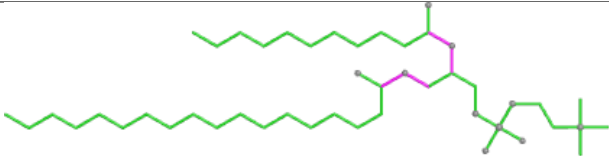
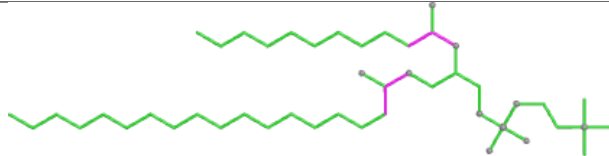
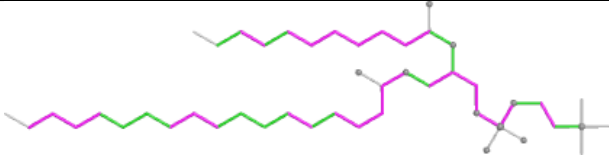
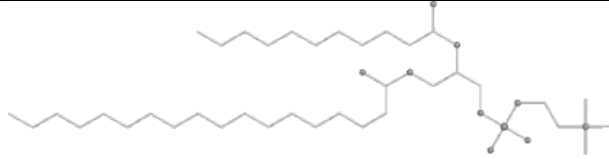
Ligand PC1 Q 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 2 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand HEA A9 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

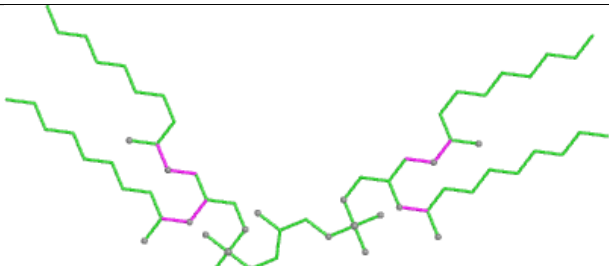
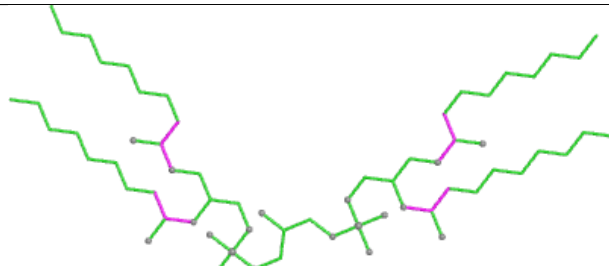
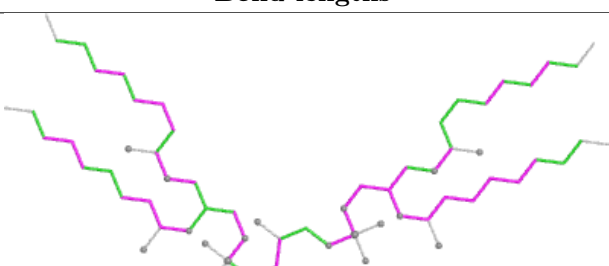
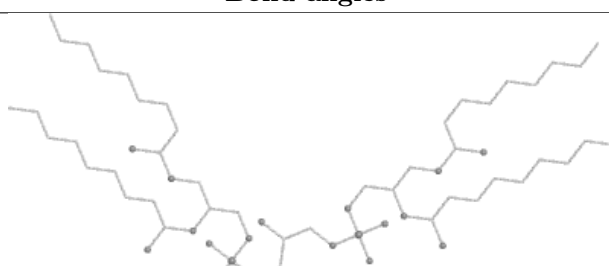


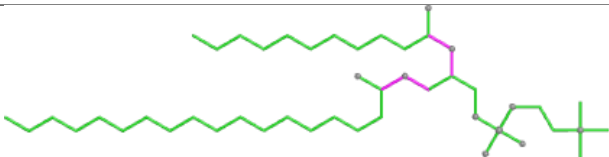
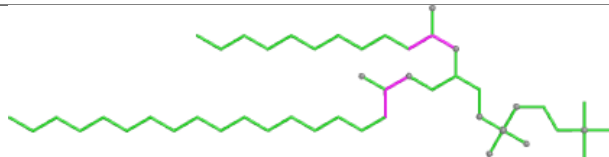
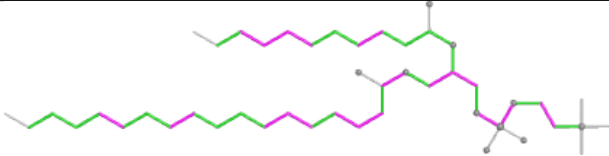
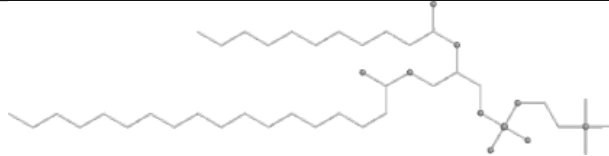


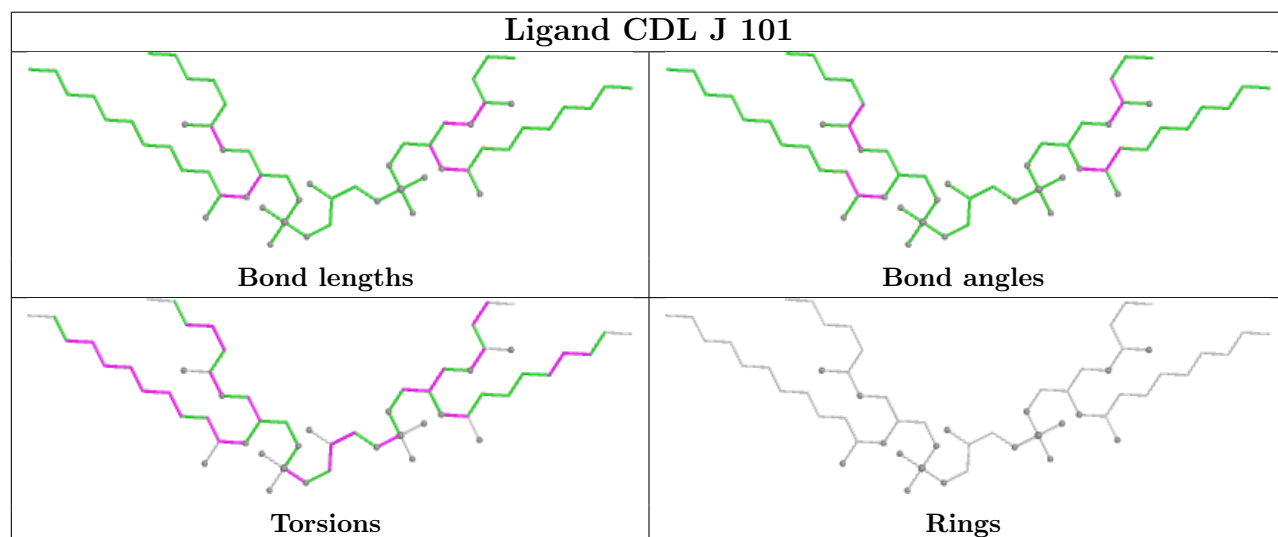
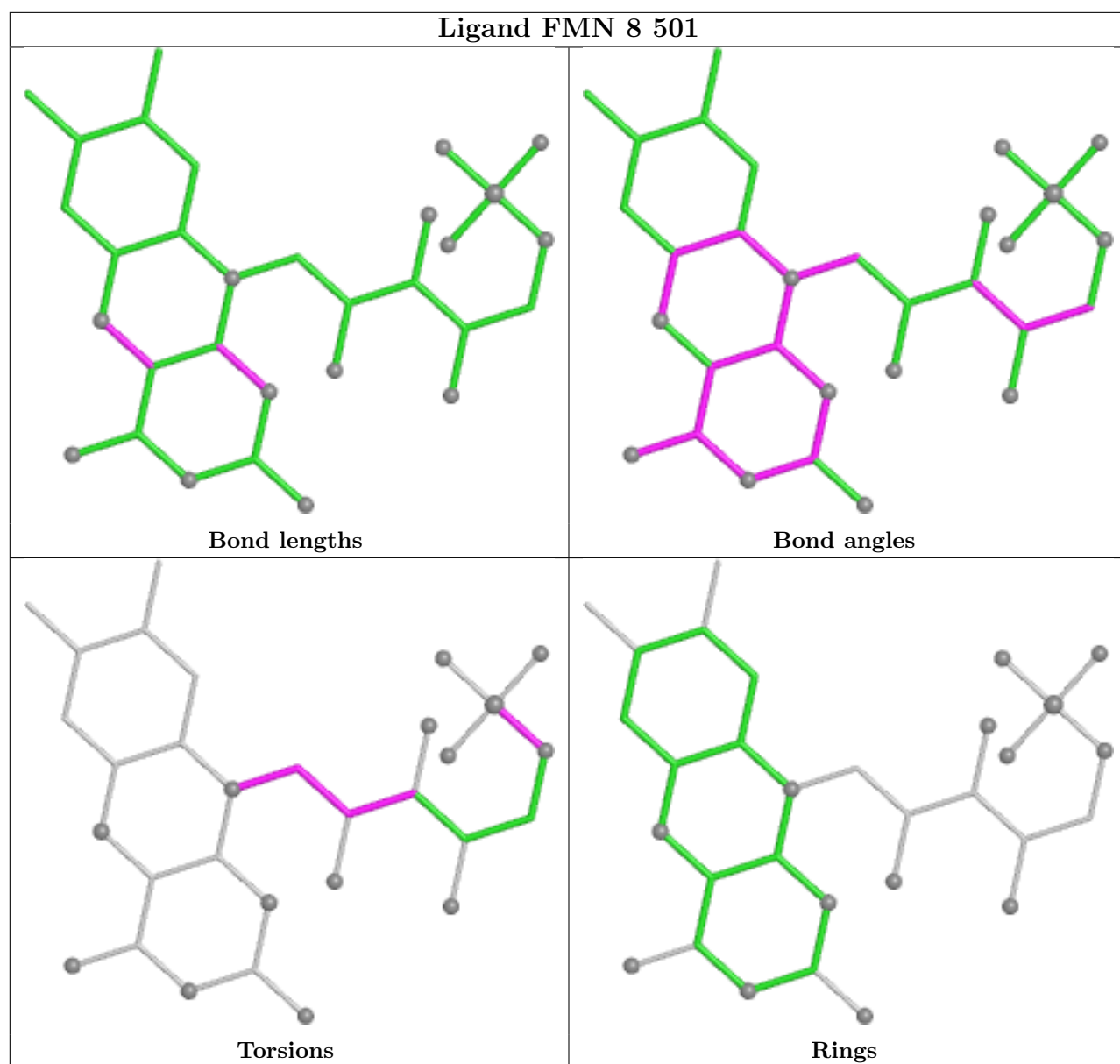


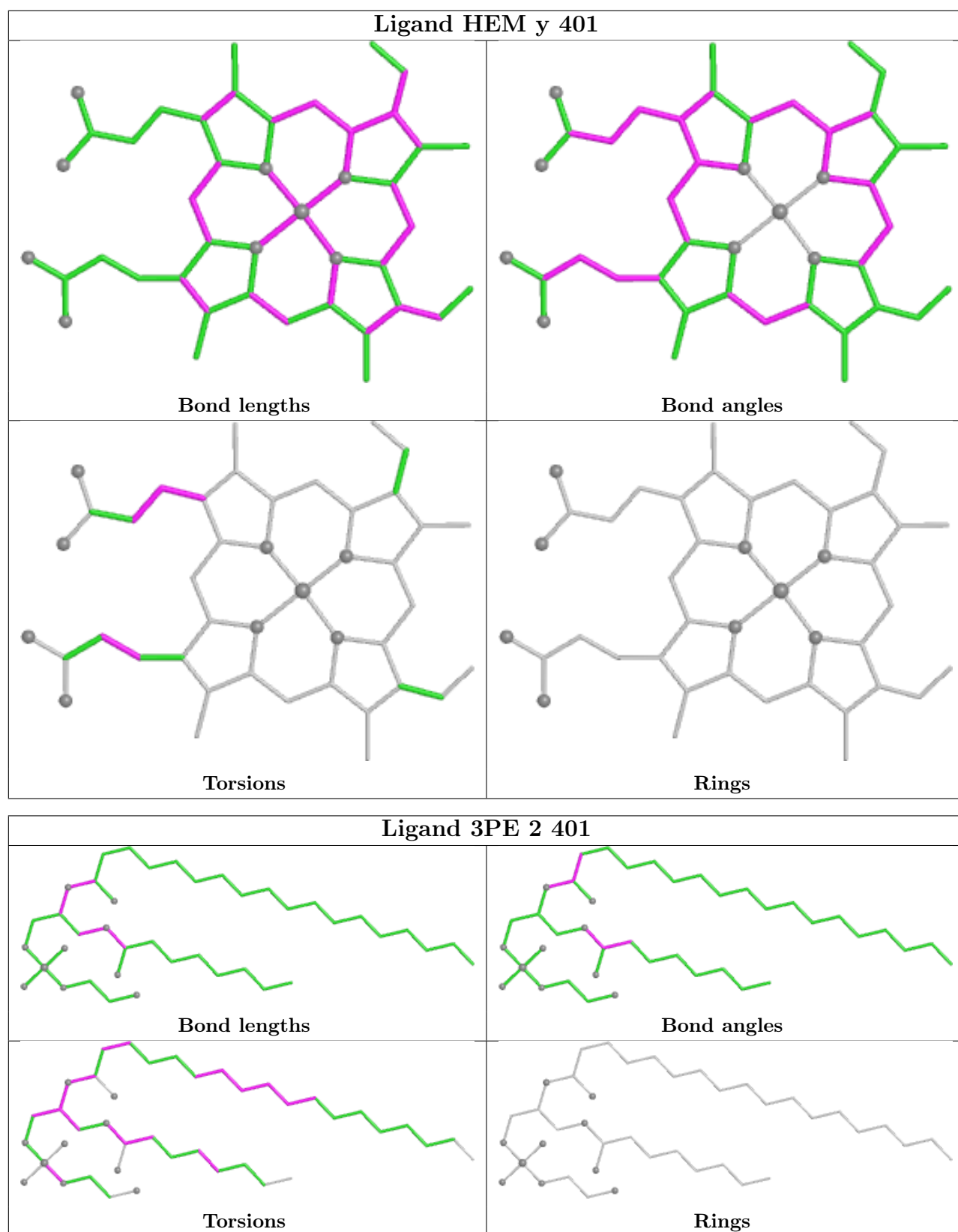


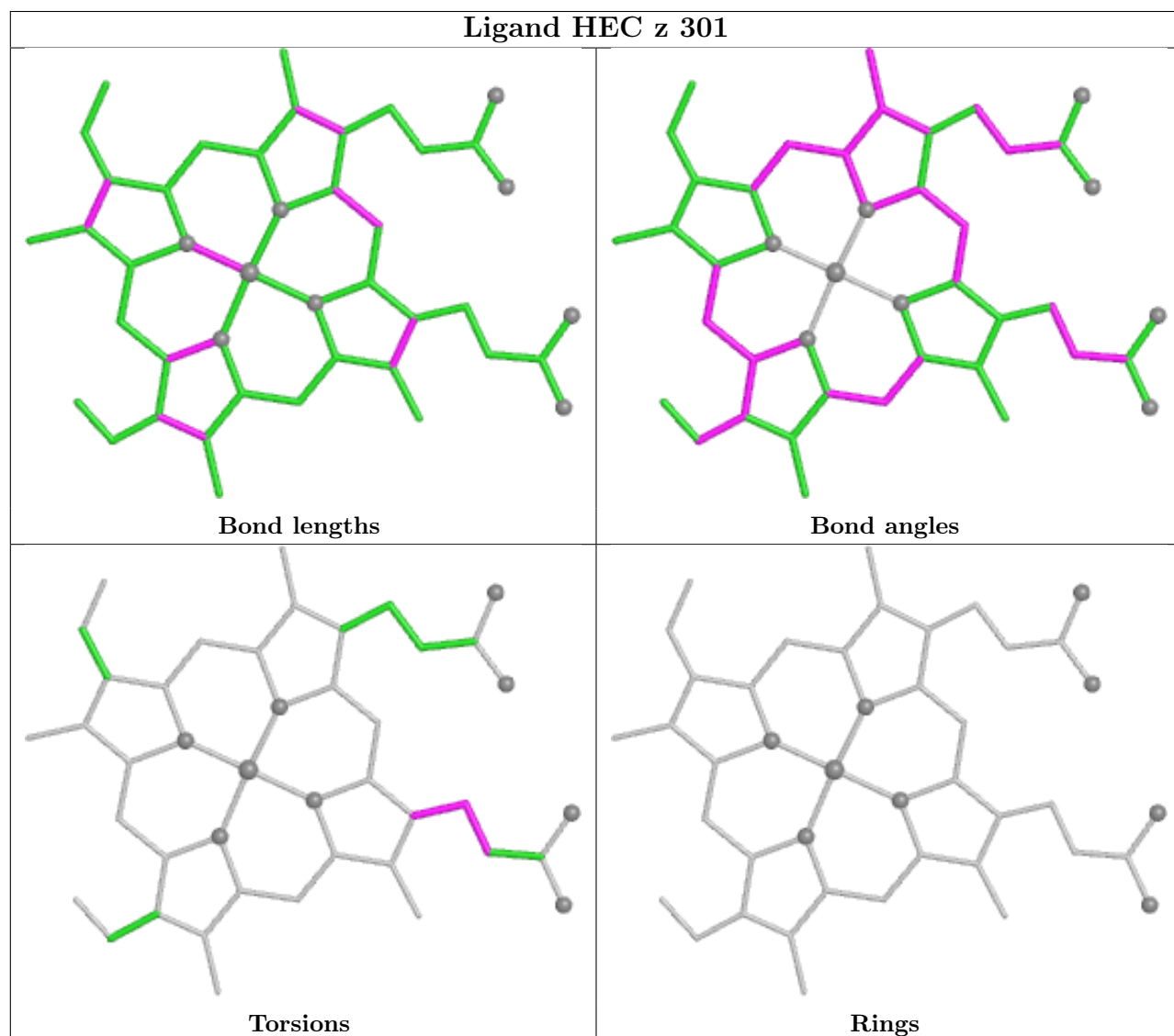
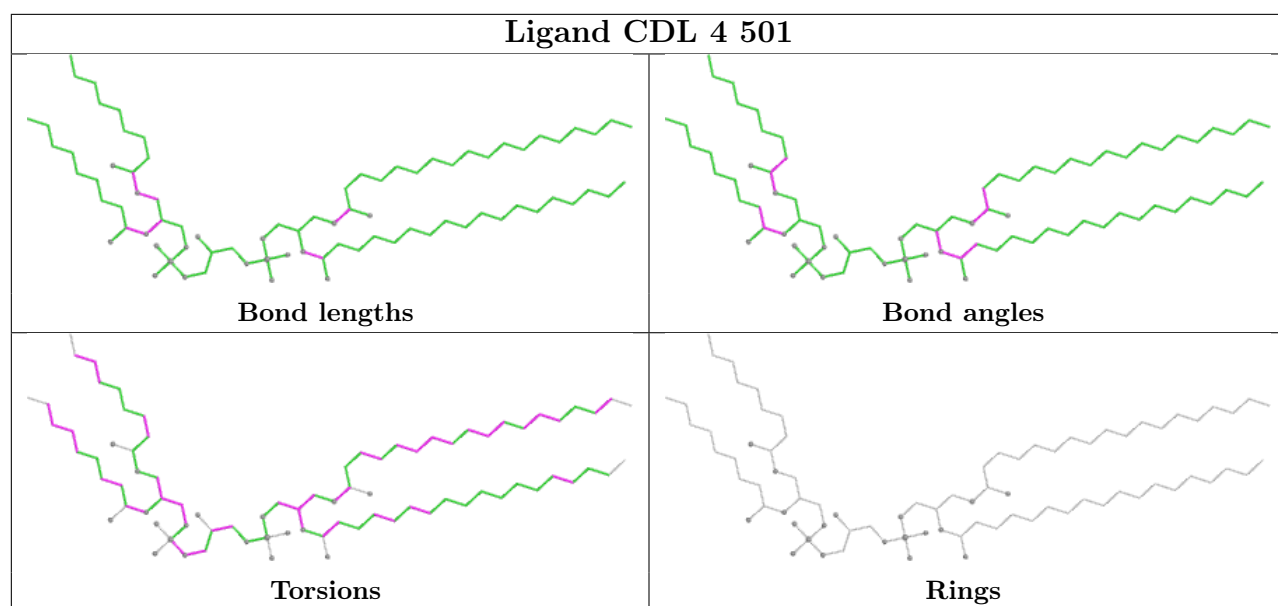
Ligand PC1 S 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL 6 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 L 200	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

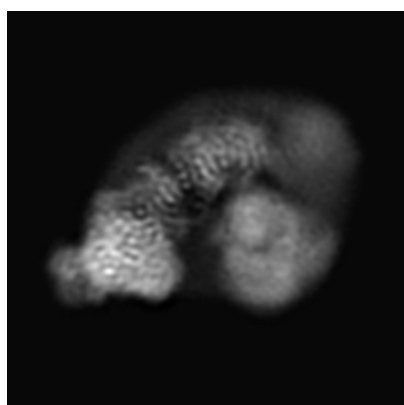
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30675. These allow visual inspection of the internal detail of the map and identification of artifacts.

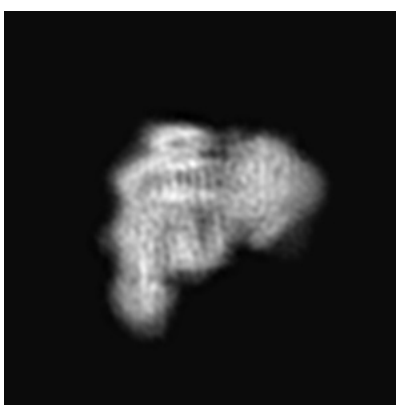
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

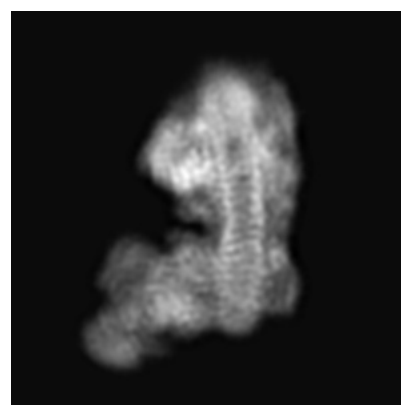
6.1.1 Primary map



X



Y

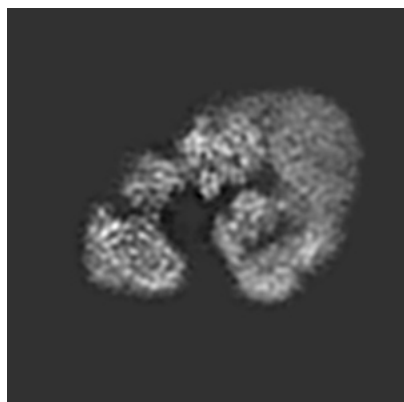


Z

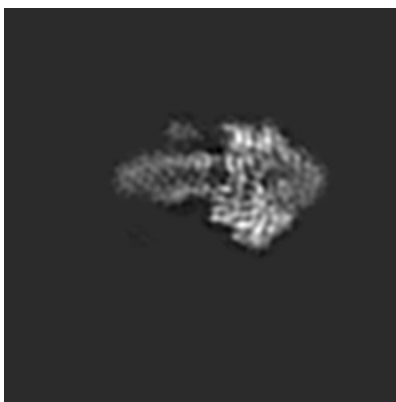
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

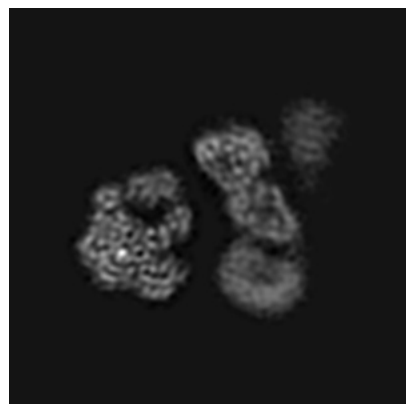


Z Index: 140

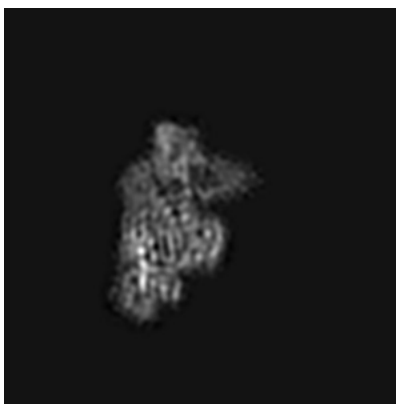
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 123



Y Index: 71

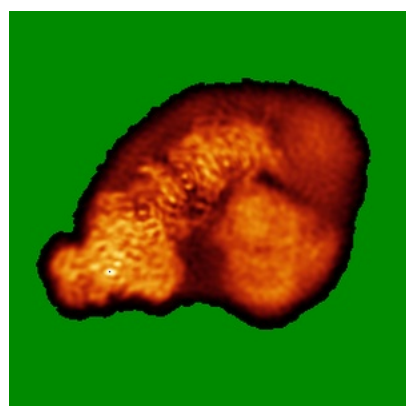


Z Index: 97

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

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

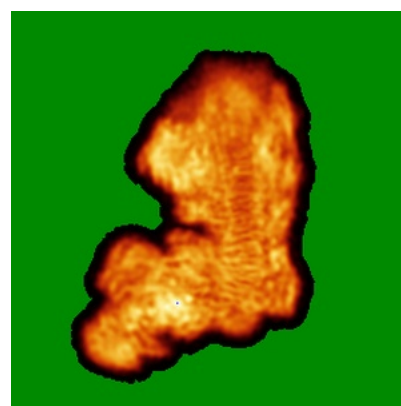
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

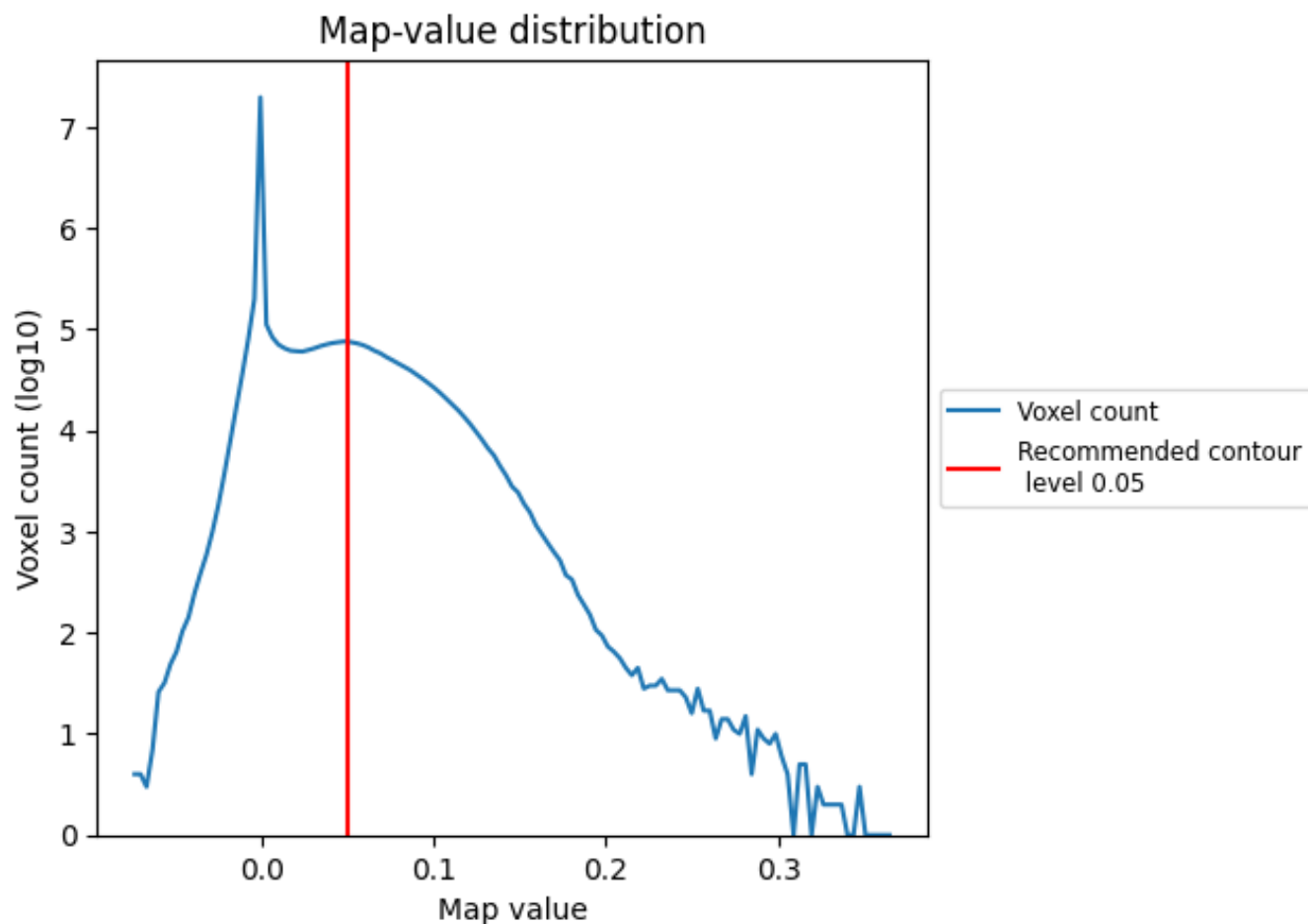
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

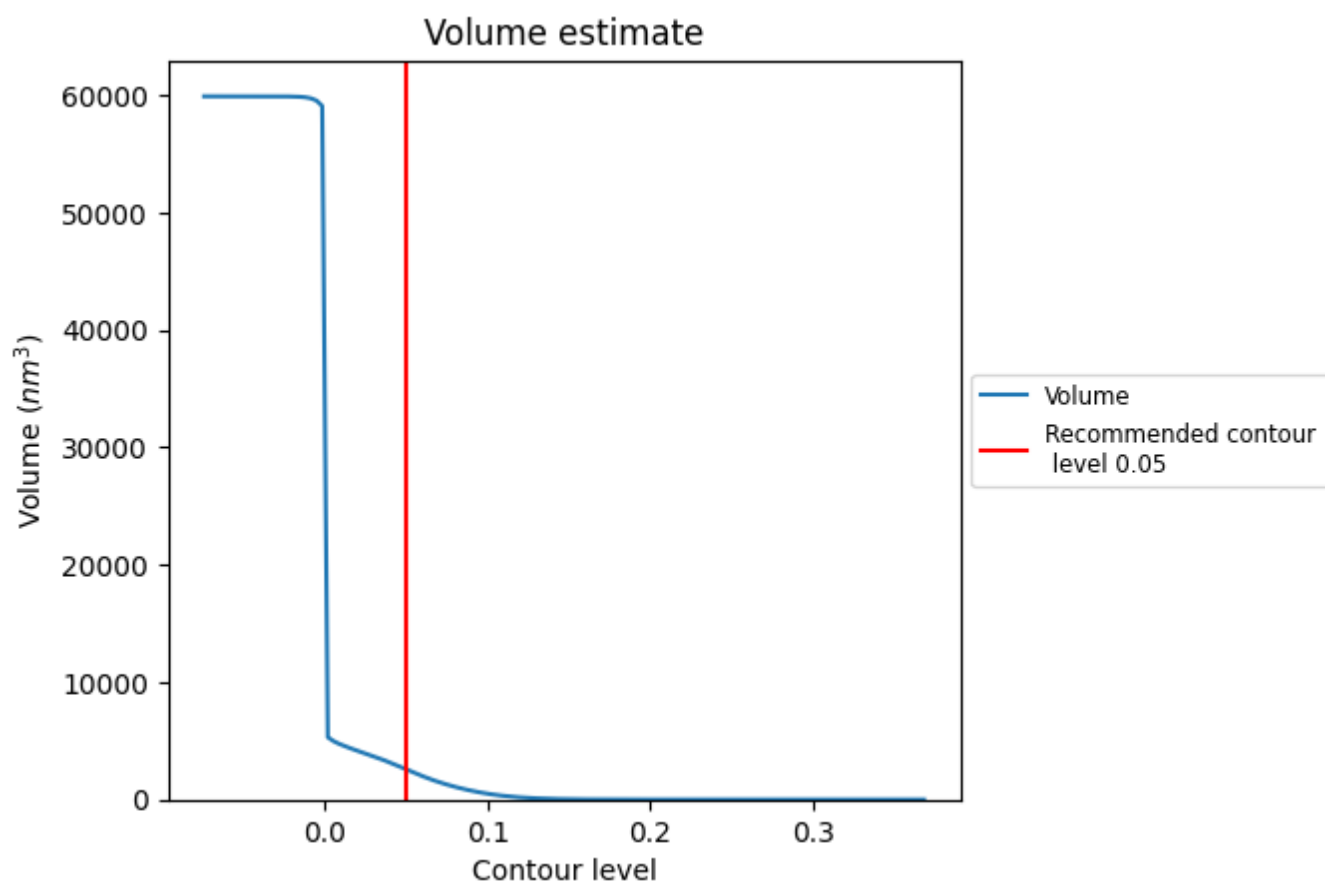
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

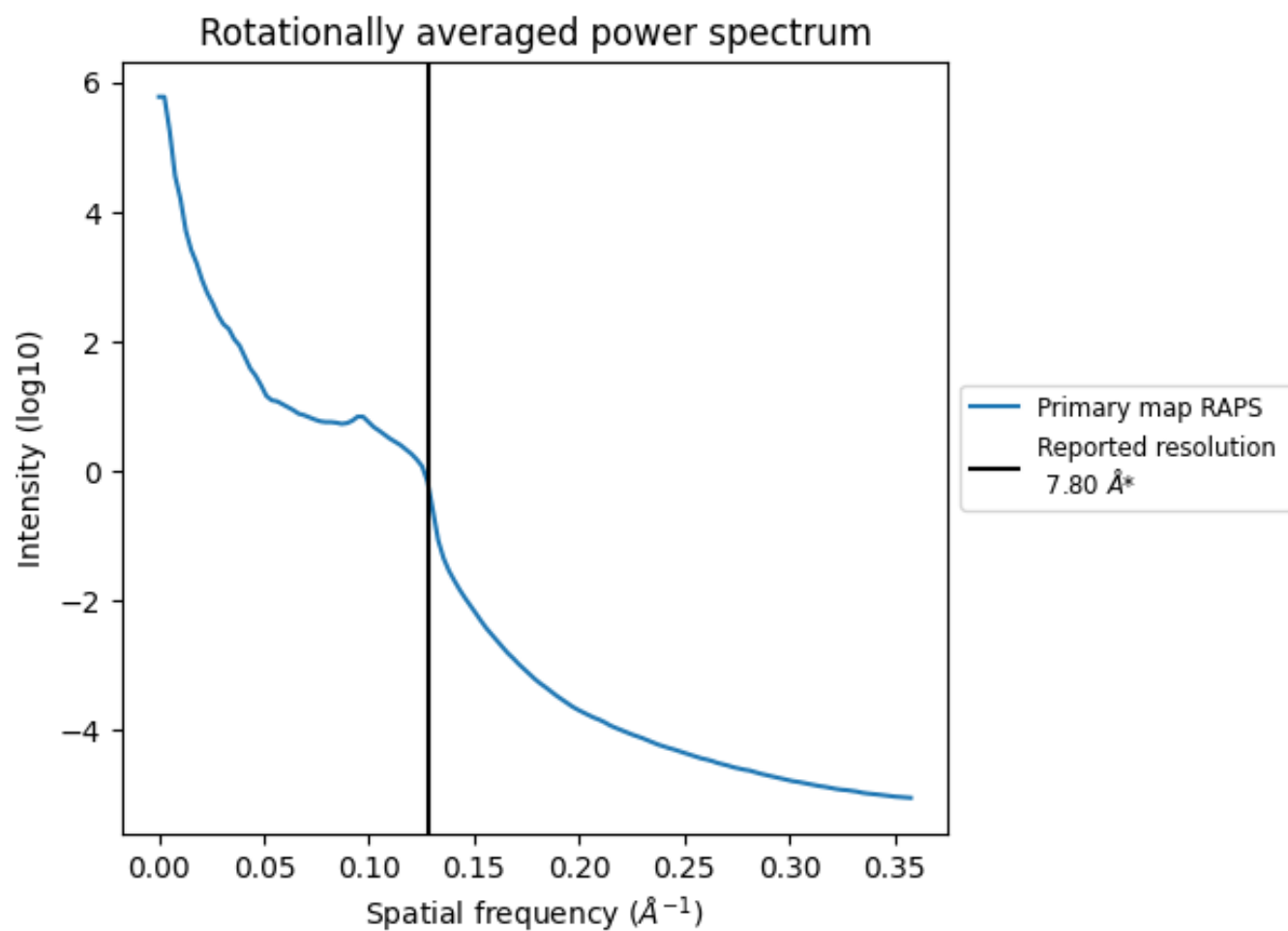
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2566 nm³; this corresponds to an approximate mass of 2318 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

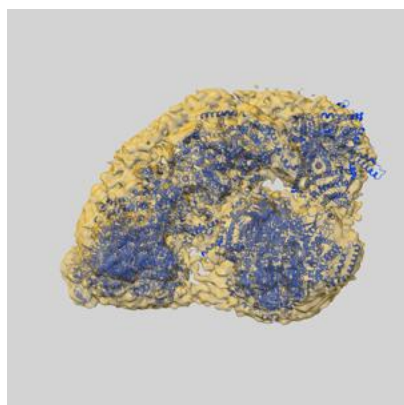
8 Fourier-Shell correlation

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

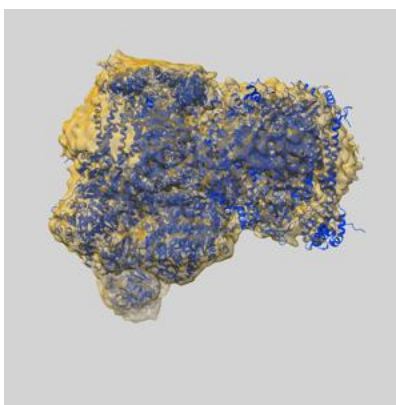
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30675 and PDB model 7DGS. Per-residue inclusion information can be found in section 3 on page 25.

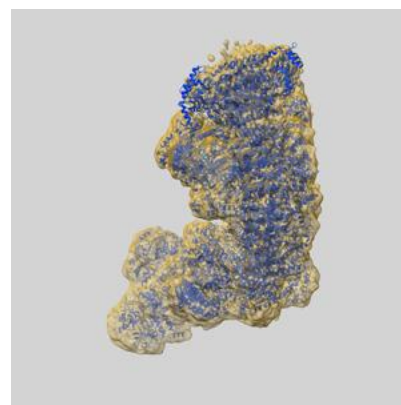
9.1 Map-model overlay [i](#)



X



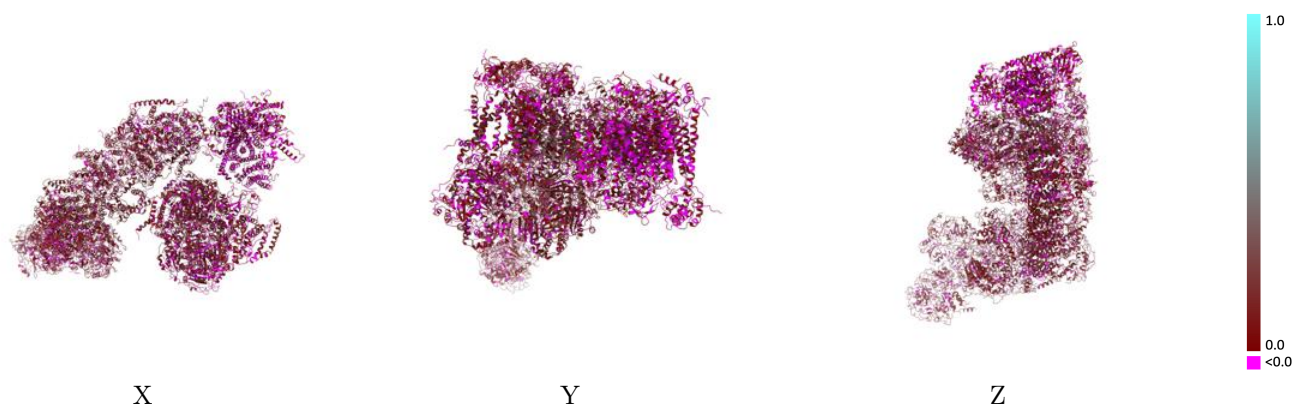
Y



Z

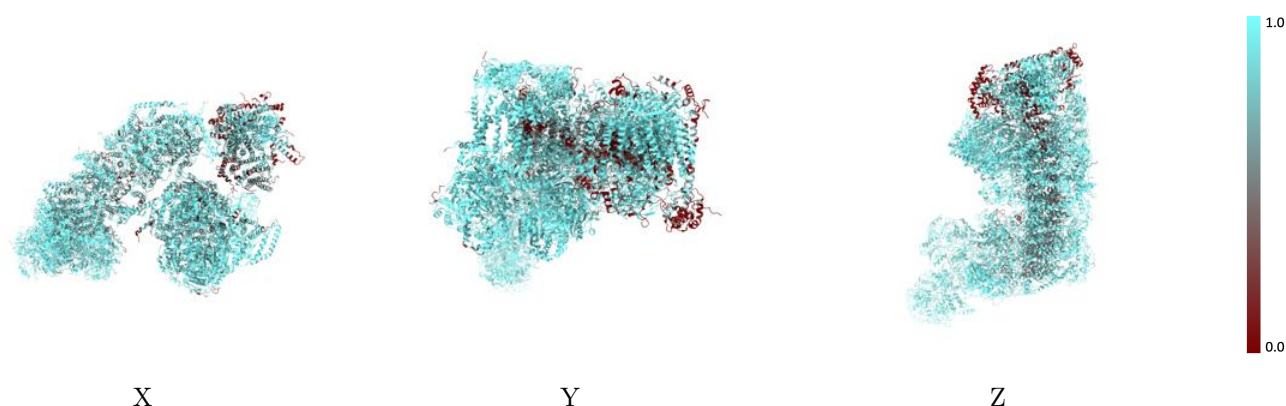
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



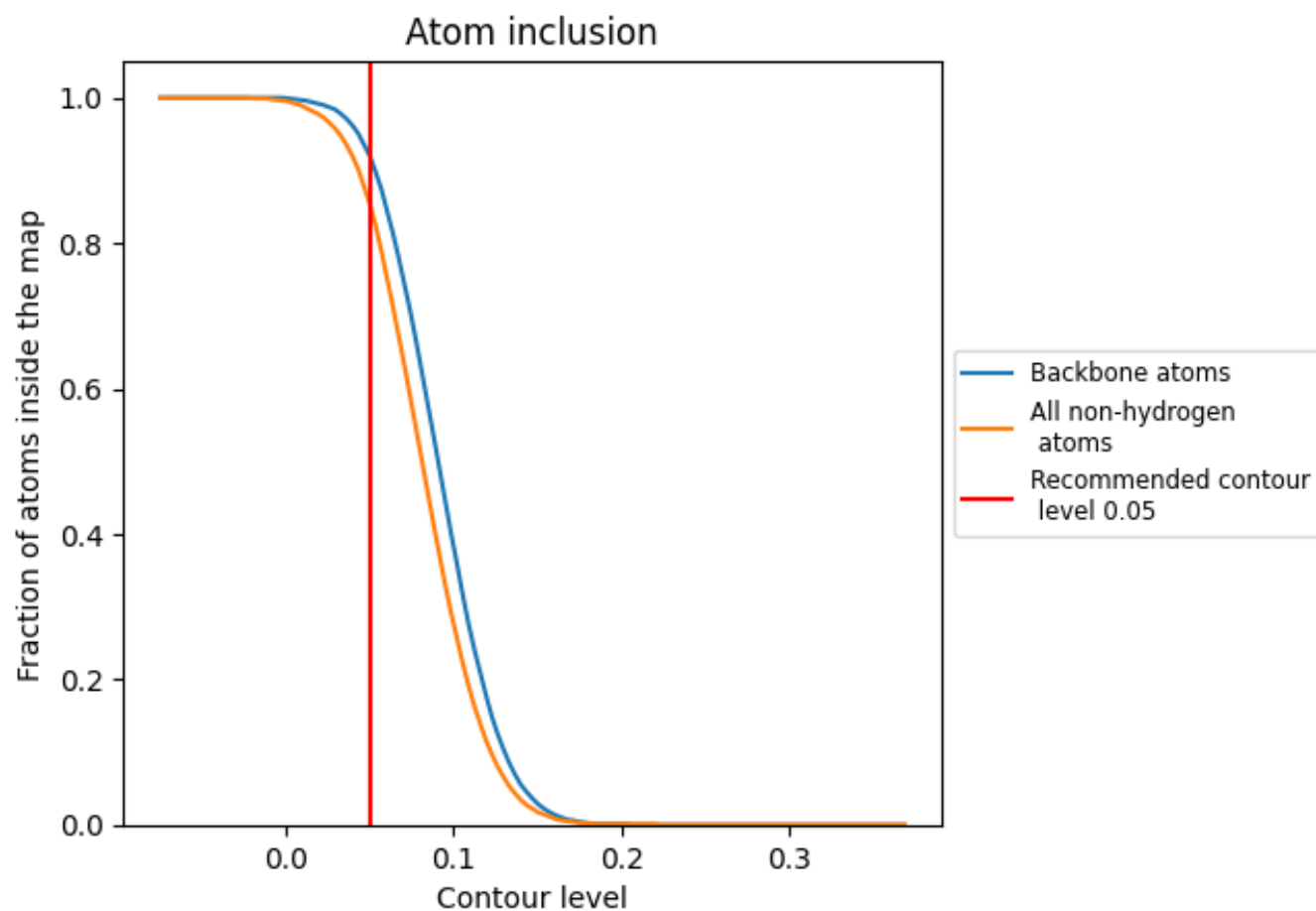
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.1070
1	 0.8100	 0.1090
2	 0.7720	 0.1360
3	 0.7320	 0.1250
4	 0.7440	 0.1310
5	 0.7720	 0.1370
6	 0.7790	 0.1090
7	 0.7820	 0.1390
8	 0.9880	 0.1220
9	 0.9760	 0.1210
A	 0.9760	 0.1180
A0	 0.8540	 0.1070
A1	 0.8090	 0.1020
A2	 0.8050	 0.1220
A3	 0.6250	 0.1390
A4	 0.4460	 0.0290
A5	 0.4850	 0.0270
A6	 0.2510	 0.0430
A7	 0.4570	 0.0200
A8	 0.5750	 0.0720
A9	 0.8320	 0.0150
B	 0.8540	 0.1110
B0	 0.6290	 0.0590
B1	 0.6550	 0.0110
B2	 0.3770	 0.0100
B3	 0.8960	 -0.0200
B4	 0.6470	 0.1520
B5	 0.7730	 0.0990
B6	 0.4400	 0.0530
B7	 0.7020	 0.0260
B8	 0.3880	 0.0110
B9	 0.8100	 0.0390
C	 0.9520	 0.1320
D	 0.9060	 0.1050
E	 0.9600	 0.1020



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Chain	Atom inclusion	Q-score
F	 0.9440	 0.0600
G	 0.9300	 0.1290
H	 0.9120	 0.1270
I	 0.8940	 0.0830
J	 0.9700	 0.1380
K	 0.9530	 0.1230
L	 0.8870	 0.1490
M	 0.8880	 0.1500
N	 0.9820	 0.1550
O	 0.9180	 0.1580
P	 0.9360	 0.1390
Q	 0.9260	 0.1460
R	 0.9260	 0.1230
S	 0.8460	 0.1300
T	 0.7900	 0.1700
U	 0.8580	 0.0850
V	 0.9380	 0.1590
W	 0.9540	 0.1440
X	 0.9100	 0.1290
Y	 0.9480	 0.1790
Z	 0.9090	 0.1270
a	 0.8210	 0.1530
b	 0.9360	 0.1410
c	 0.9470	 0.1590
d	 0.9800	 0.1240
e	 0.8620	 0.1390
f	 0.9380	 0.1520
g	 0.9550	 0.1270
h	 0.8890	 0.1200
i	 0.9190	 0.1820
j	 0.8490	 0.1320
k	 0.9560	 0.0600
l	 0.9550	 0.0930
m	 0.8260	 0.1030
o	 0.9470	 0.0840
p	 0.9450	 0.0970
q	 0.9290	 0.1420
r	 0.8370	 0.0960
s	 0.9120	 0.0940
t	 0.9090	 0.1090
u	 0.9020	 0.0550
v	 0.9460	 -0.0380

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Chain	Atom inclusion	Q-score
w	 0.9540	 0.1330
x	 0.9820	 0.1330
y	 0.8200	 0.1220
z	 0.9160	 0.1010