



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:07 AM JST

PDB ID : 7DGR / pdb_00007dgr
EMDB ID : EMD-30674
Title : Activity optimized supercomplex state2
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 : 4.60 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:

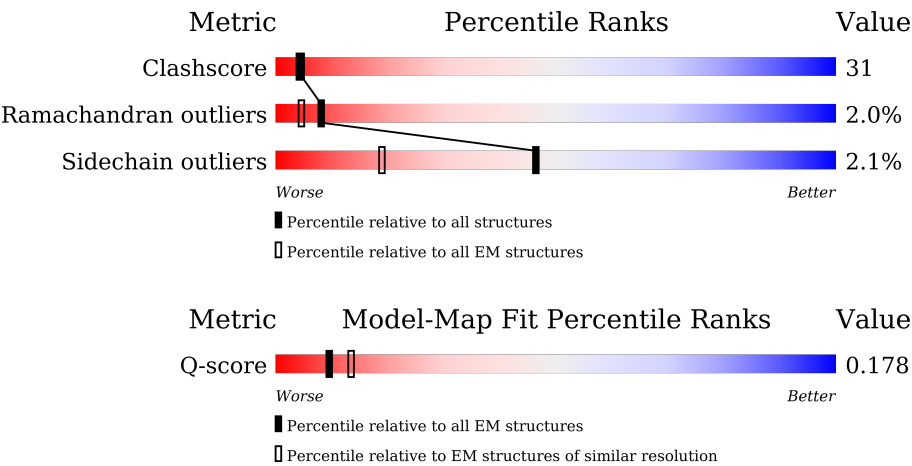
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 4.60 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.



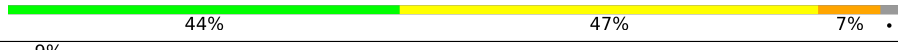
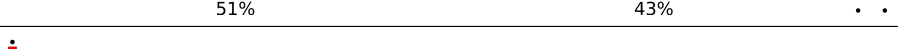
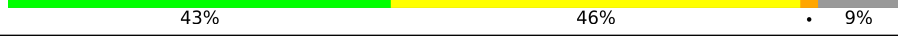
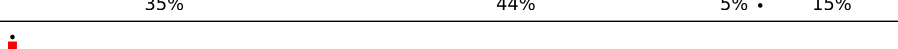
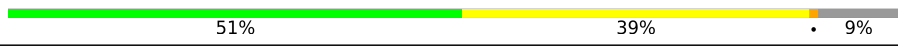
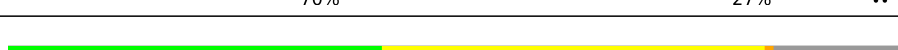
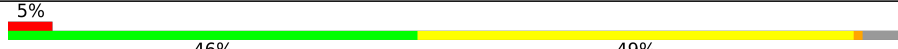
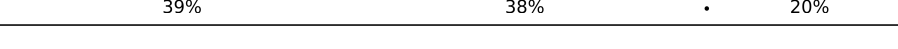
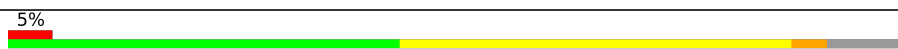
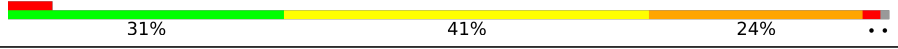
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	46% 46% 5%
2	4	459	46% 50%
3	2	347	42% 54%
4	7	175	5% 49% 43% 5%

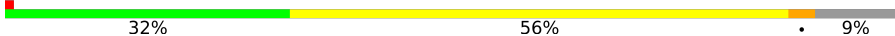
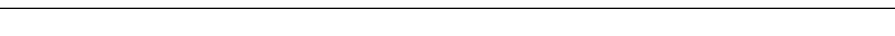
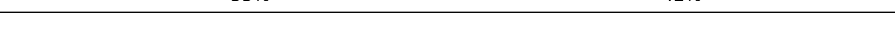
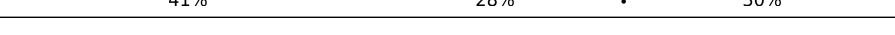
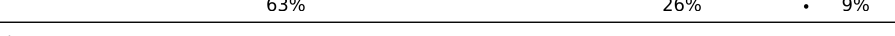
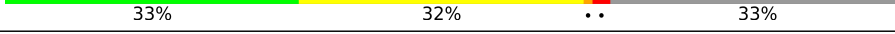
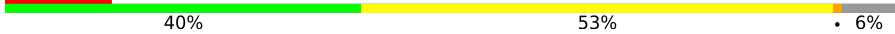
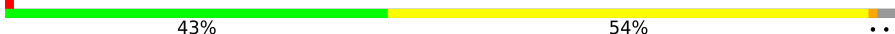
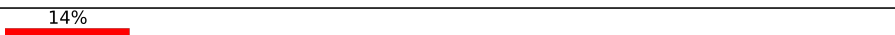
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Mol	Chain	Length	Quality of chain
5	6	606	
6	5	98	
7	3	115	
8	1	318	
9	8	444	
10	A	704	
11	B	430	
12	C	228	
13	D	179	
14	E	176	
15	F	75	
16	G	133	
17	H	105	
18	I	96	
19	J	70	
20	K	98	
21	L	83	
22	N	115	
23	O	127	
24	P	112	
25	Q	171	
26	R	345	
27	S	320	
28	T	140	
29	U	145	

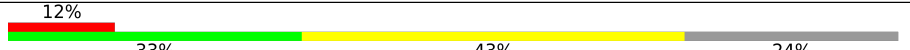
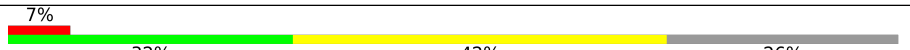
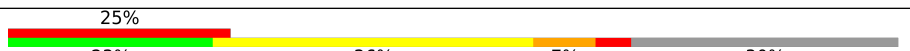
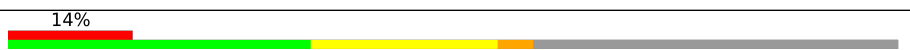
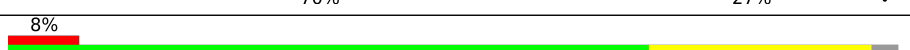
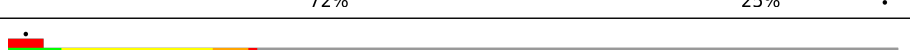
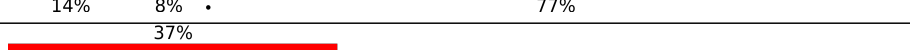
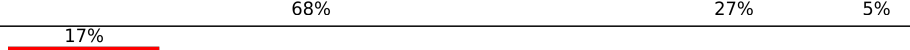
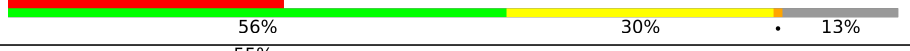
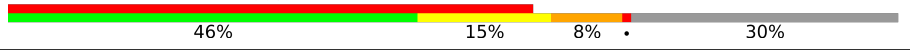
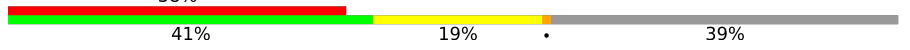
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Mol	Chain	Length	Quality of chain
30	V	143	
31	M	88	
31	W	88	
32	X	57	
33	Y	72	
34	Z	98	
35	a	128	
36	b	143	
37	c	128	
38	d	117	
39	f	178	
40	h	125	
41	i	49	
42	j	120	
43	g	176	
44	e	158	
45	k	480	
45	w	480	
46	l	453	
46	x	453	
47	m	379	
47	y	379	
48	o	241	
48	z	241	
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	B3	91	
52	s	91	
53	A3	56	
53	t	56	
54	B2	64	
54	u	64	
55	B1	78	
55	v	78	
56	A9	514	
57	C4	227	
58	C2	261	
59	A7	169	
60	C0	152	
61	A6	129	
62	A4	97	
63	A5	86	
64	B4	74	
65	C3	80	
66	B0	80	
67	C1	63	

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Mol	Chain	Length	Quality of chain
68	A8	70	

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
69	FES	A	803	-	-	X	-
70	3PE	4	501	-	-	X	-
70	3PE	4	503	-	-	X	-
70	3PE	B	501	-	-	X	-
71	CDL	4	502	-	-	X	-
71	CDL	6	701	-	-	X	-
72	PC1	2	402	-	-	X	-
72	PC1	L	200	-	-	X	-
73	FMN	8	501	-	-	X	-
74	SF4	8	502	-	-	X	-
74	SF4	A	801	-	-	X	-
74	SF4	A	802	-	-	X	-
74	SF4	D	301	-	-	X	-
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 107305 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
			1578	1006	269	293	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	458	Total	C	N	O	S	1	0
			3577	2382	561	599	35		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	344	Total	C	N	O	S	0	0
			2681	1779	413	449	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	172	Total	C	N	O	S	0	0
			1239	838	182	211	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	606	Total	C	N	O	S	0	0
			4766	3172	732	820	42		

- 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
			712	464	110	125	13		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3	112	Total	C	N	O	S	0	0
			879	593	128	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	318	Total	C	N	O	S	0	0
			2503	1678	385	417	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	427	Total	C	N	O	S	0	0
			3065	1927	563	559	16		

- 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
			5218	3273	920	988	37		

- 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
			3422	2185	588	624	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
			1726	1114	297	312	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
			1206	772	212	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
			1401	880	243	267	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	S	0	0
			186	118	32	35	1		

- 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
			985	622	178	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
			533	332	99	99	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 subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	K	84	Total	C	N	O	0	0
			656	412	126	118		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 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 subunit 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 subunit 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 subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	90	Total	C	N	O	S	0	0
			702	445	129	126	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 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 subunit 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
			2299	1457	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
			923	586	163	168	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
			713	448	134	127	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
			883	580	149	151	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	B3	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
			318	212	56	50		

- 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	B2	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	B1	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	C4	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	C2	261	Total	C	N	O	S	0	0
			2124	1420	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	C0	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	A6	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	B4	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	C3	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		

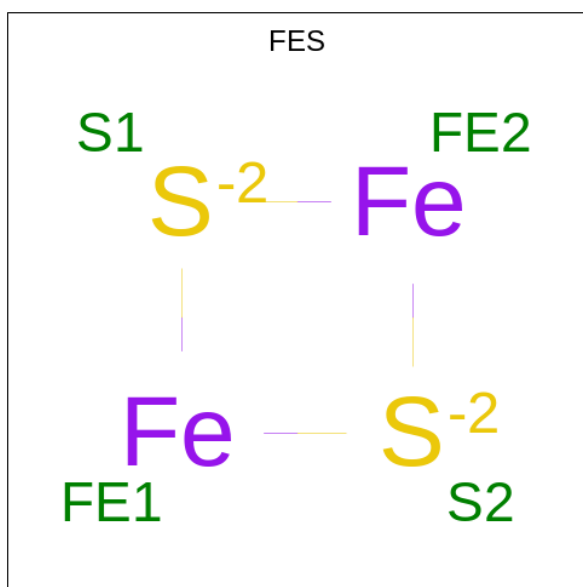
- Molecule 67 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	C1	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.

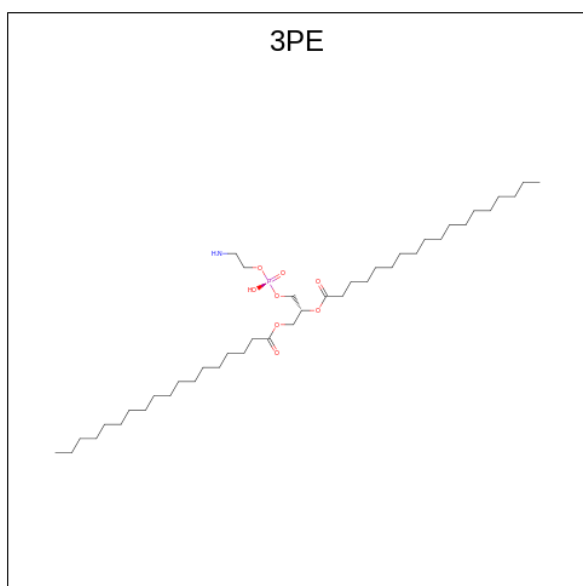
Mol	Chain	Residues	Atoms				AltConf	Trace
68	A8	43	Total	C	N	O	0	0
			335	223	53	59		

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



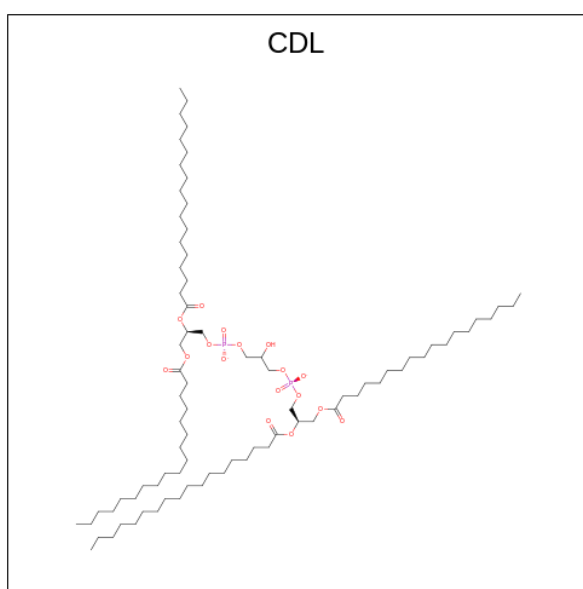
Mol	Chain	Residues	Atoms			AltConf
69	9	1	Total	Fe	S	0
			4	2	2	
69	A	1	Total	Fe	S	0
			4	2	2	
69	m	1	Total	Fe	S	0
			4	2	2	

- Molecule 70 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



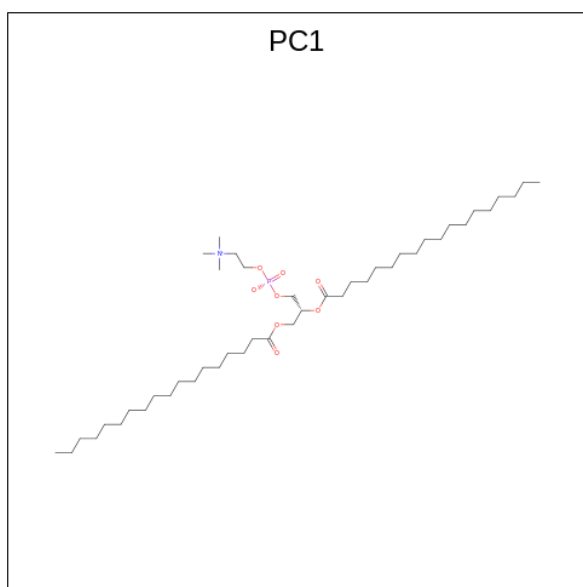
Mol	Chain	Residues	Atoms					AltConf
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 71 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



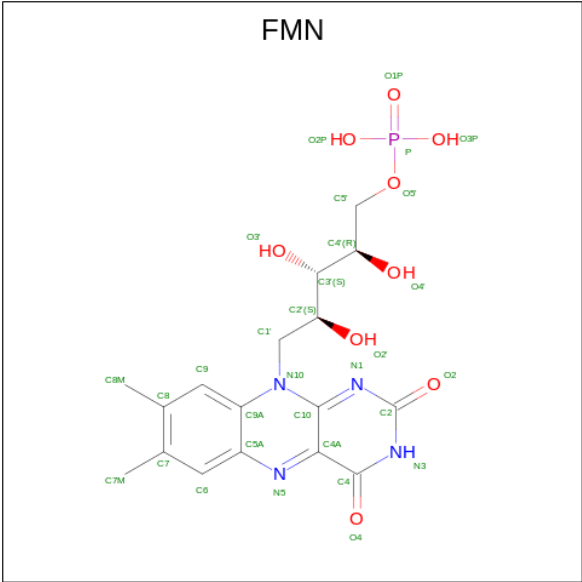
Mol	Chain	Residues	Atoms				AltConf
71	4	1	Total	C	O	P	0
			82	63	17	2	
71	6	1	Total	C	O	P	0
			64	45	17	2	
71	J	1	Total	C	O	P	0
			58	39	17	2	

- 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).



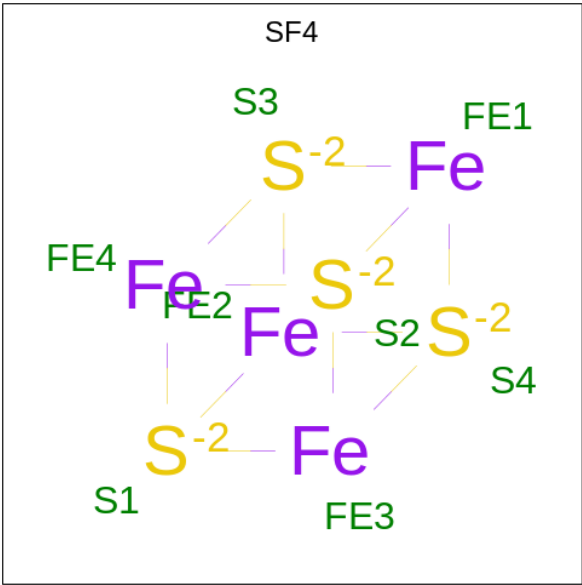
Mol	Chain	Residues	Atoms					AltConf
72	4	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	2	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
72	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- 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: Fe₄S₄).



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

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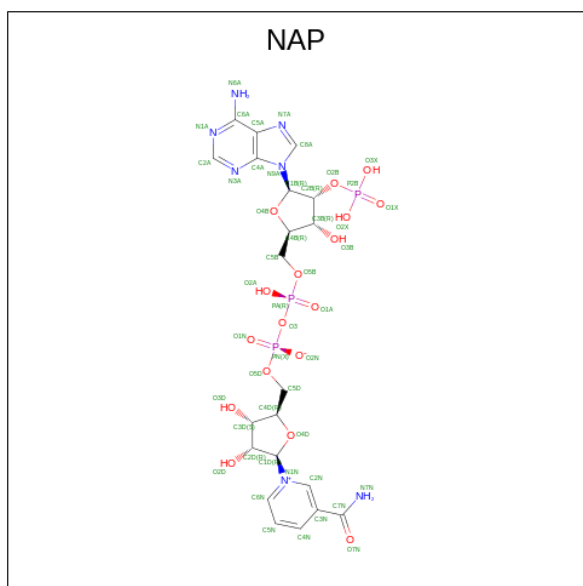
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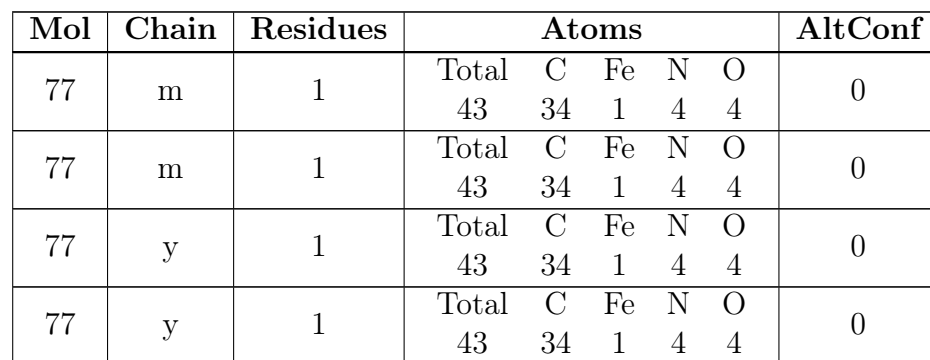
Mol	Chain	Residues	Atoms			AltConf
74	D	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	
74	E	1	Total	Fe	S	0
			8	4	4	

- Molecule 75 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
75	I	1	Total	Zn	0
			1	1	
75	A6	1	Total	Zn	0
			1	1	

- Molecule 76 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

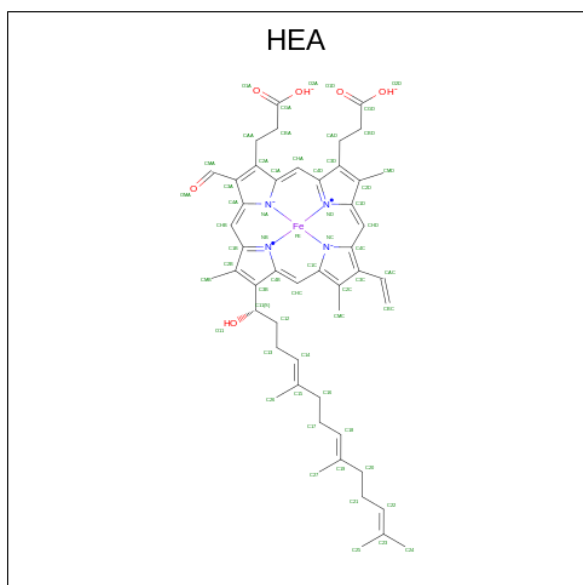




- # HEC
-
- The diagram illustrates the chemical structure of HEC (Hexaethylcobalamin). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is highly symmetrical, with various side chains (C1A through C1D, C2A through C2D, C3A through C3D, C4A through C4D, C5A through C5D, C6A through C6D) and a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is highly symmetrical, with various side chains (C1A through C1D, C2A through C2D, C3A through C3D, C4A through C4D, C5A through C5D, C6A through C6D) and a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring.

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	C4	2	Total	Cu	0
			2	2	

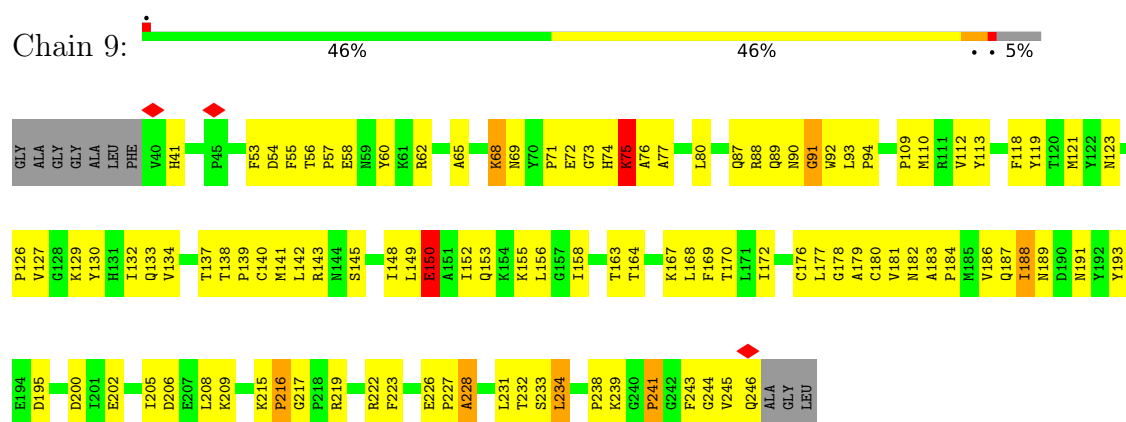
- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

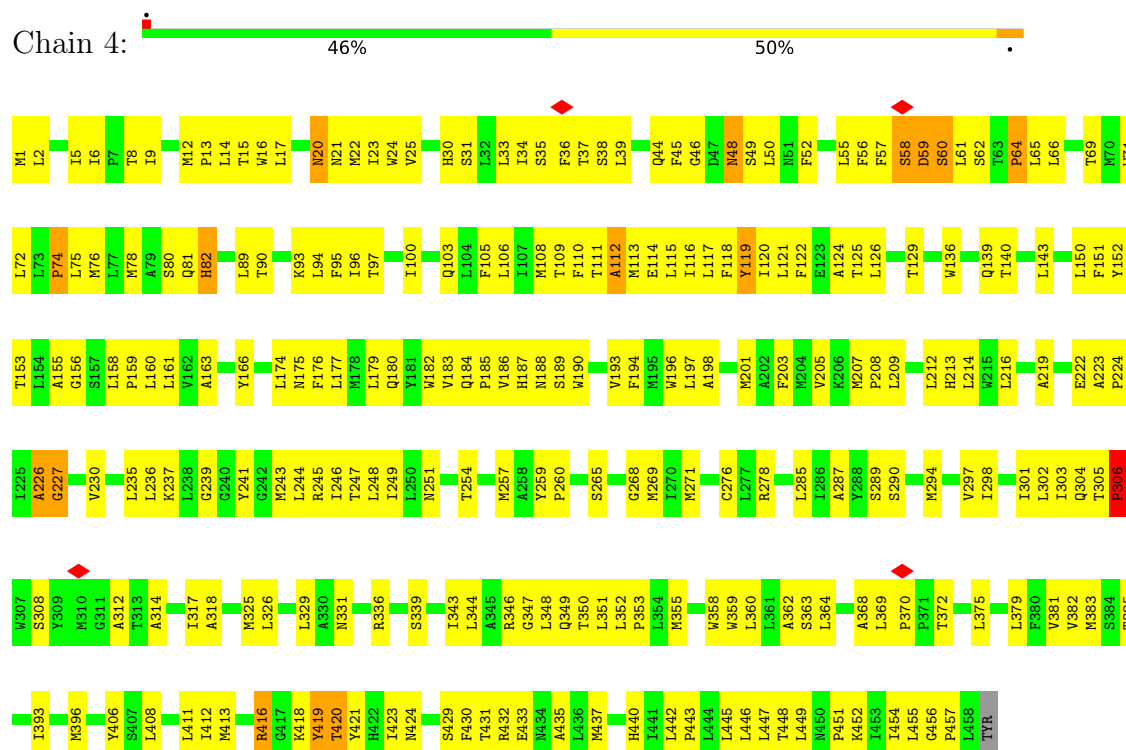
3 Residue-property plots

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.

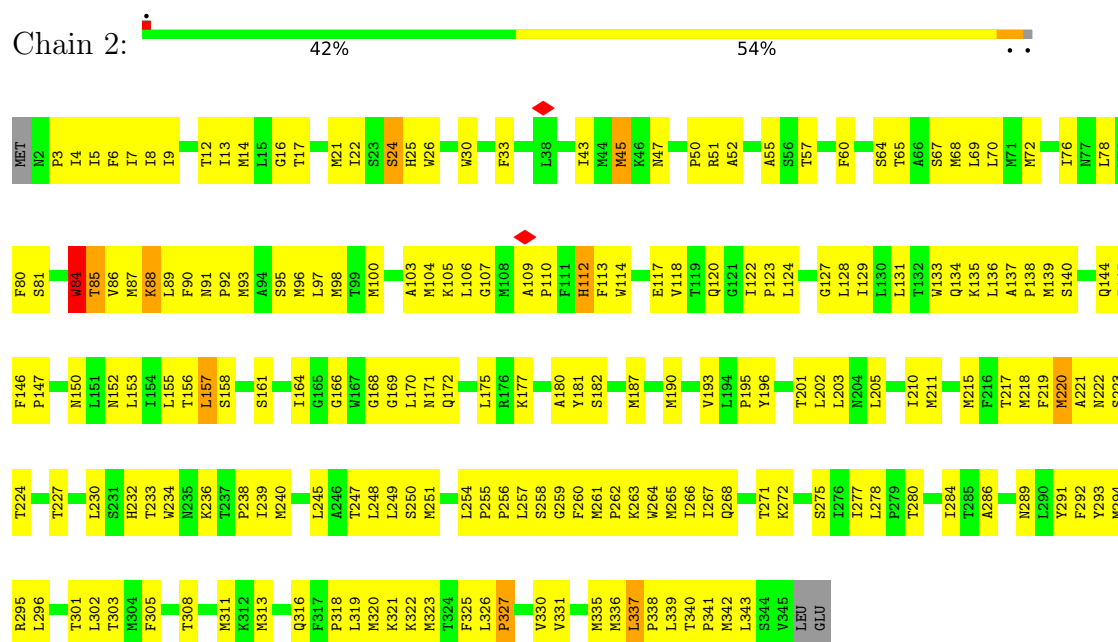
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



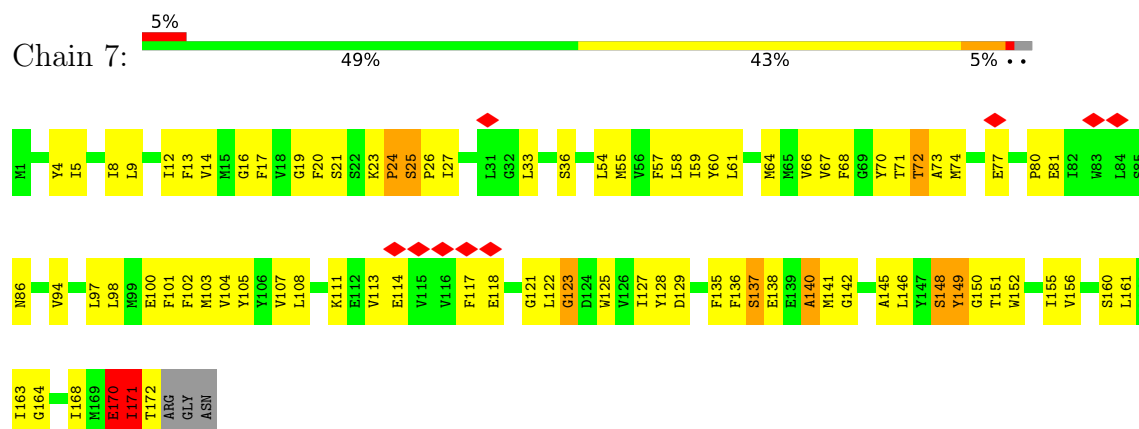
- Molecule 2: NADH-ubiquinone oxidoreductase chain 4



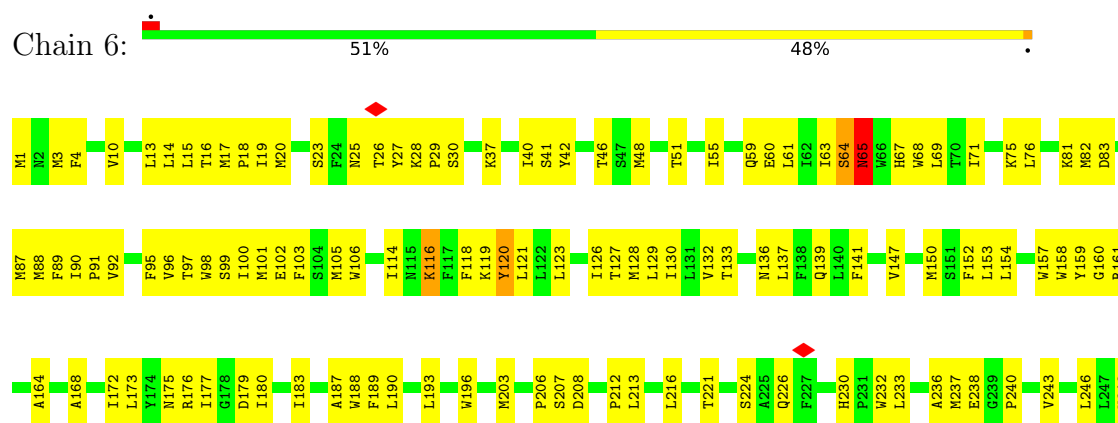
• Molecule 3: NADH-ubiquinone oxidoreductase chain 2

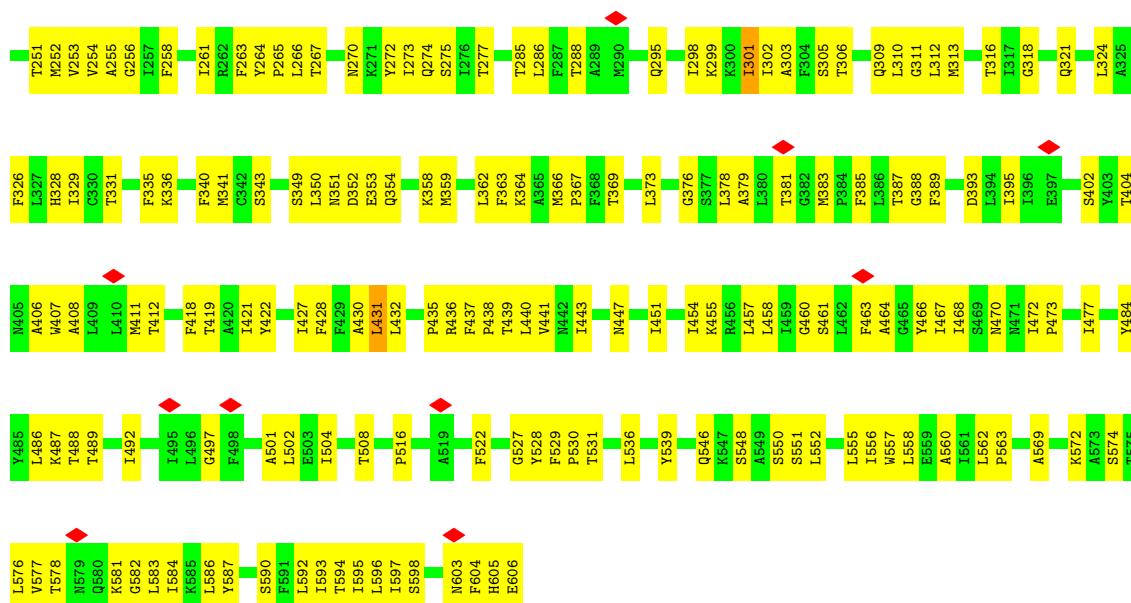


• Molecule 4: NADH-ubiquinone oxidoreductase chain 6



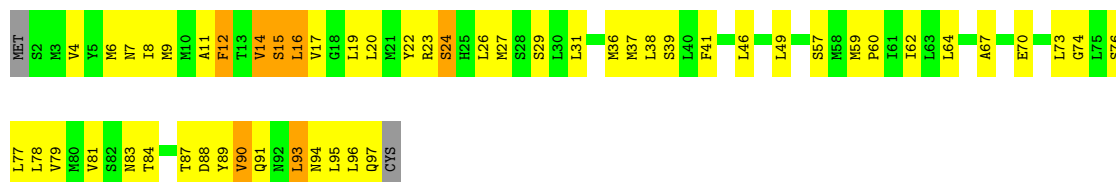
• Molecule 5: NADH-ubiquinone oxidoreductase chain 5





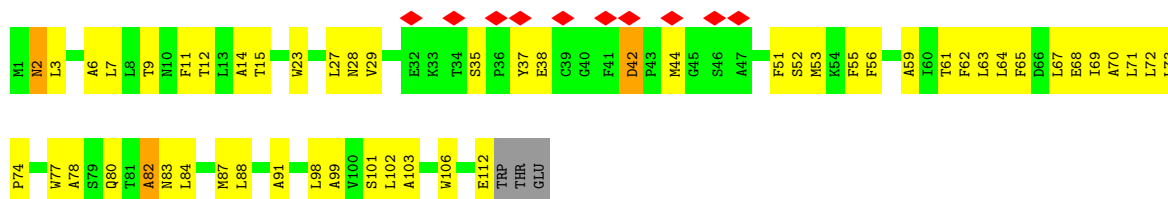
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 5: 44% 47% 7% .



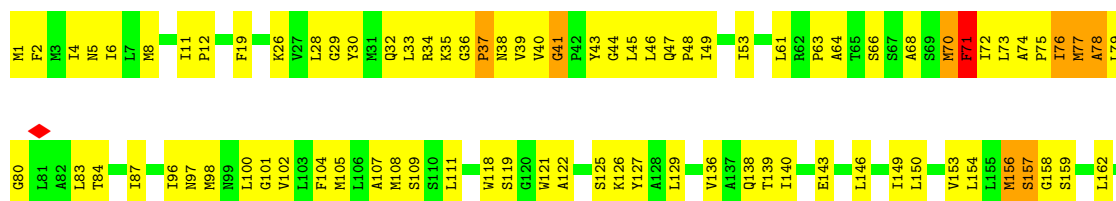
• Molecule 7: NADH-ubiquinone oxidoreductase chain 3

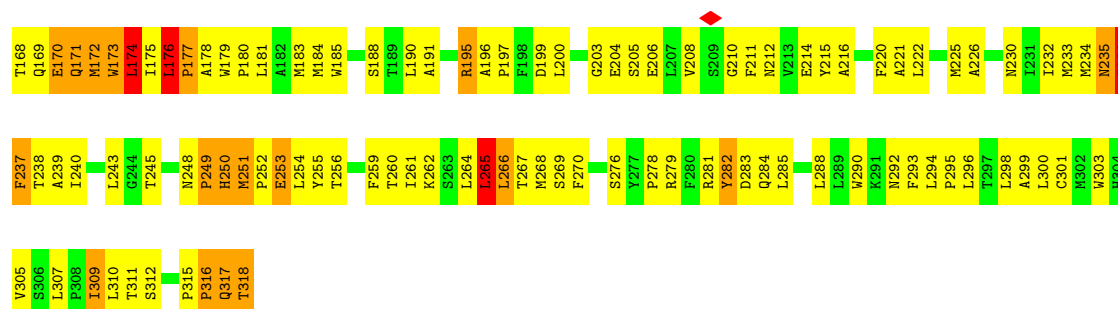
Chain 3: 9% 51% 43% . .



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

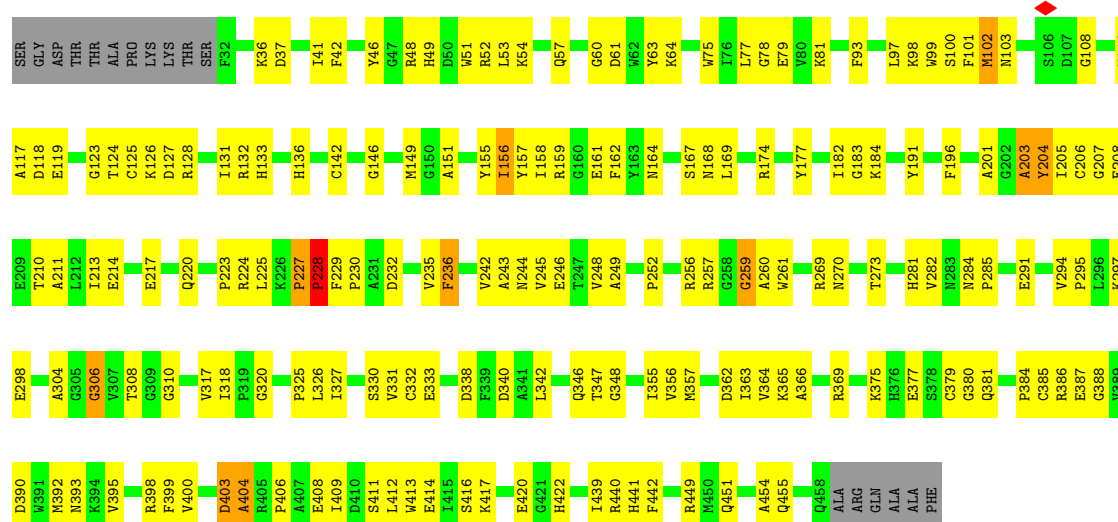
Chain 1: 41% 49% 8% .





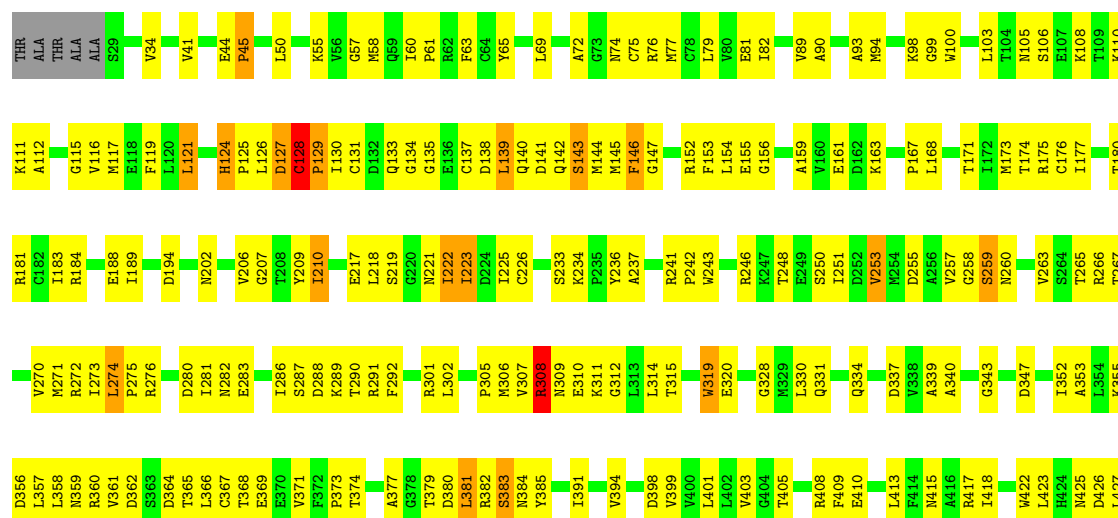
- Molecule 9: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

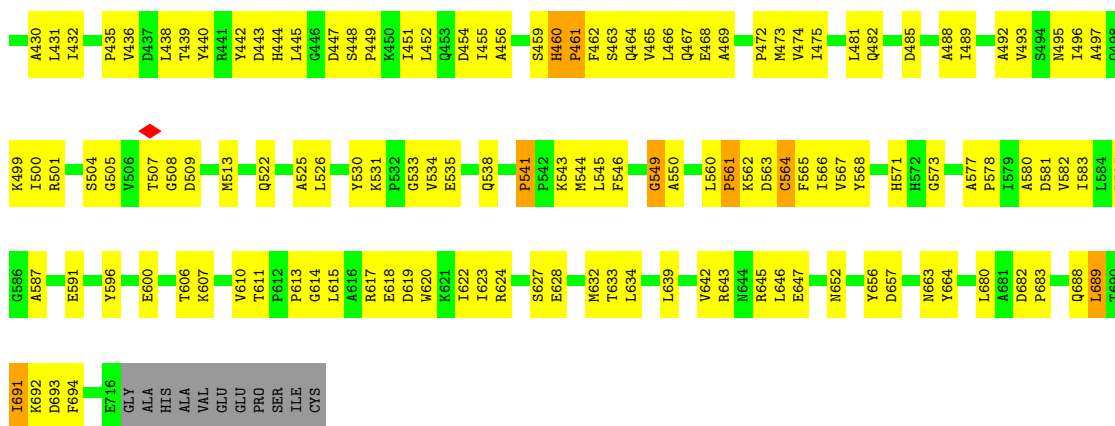
Chain 8: 55% 38%



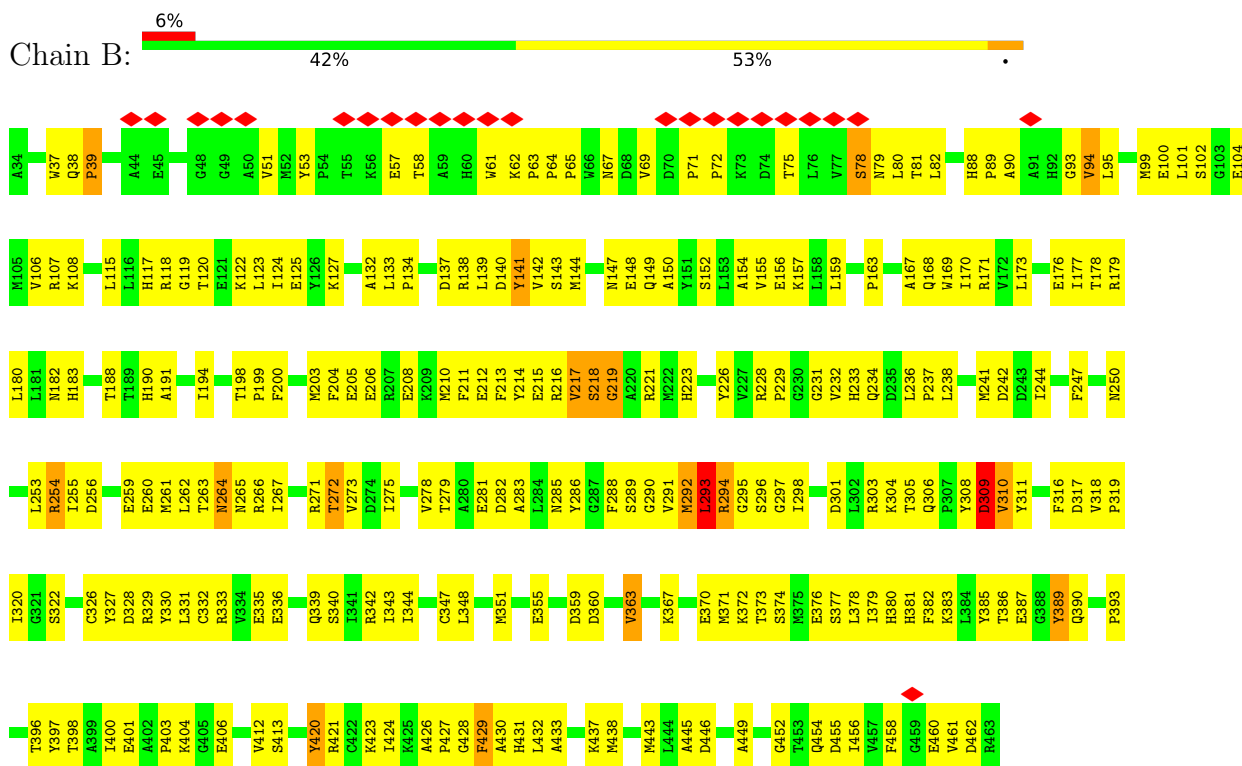
- Molecule 10: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A: 50% 44%





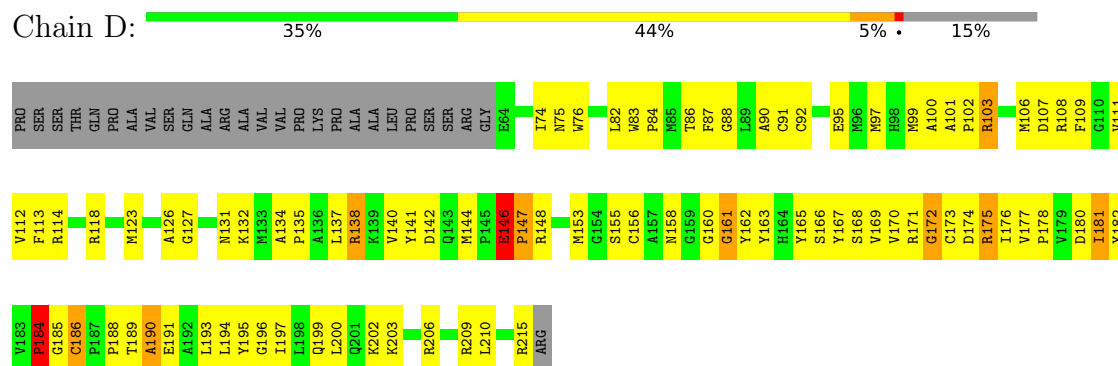
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



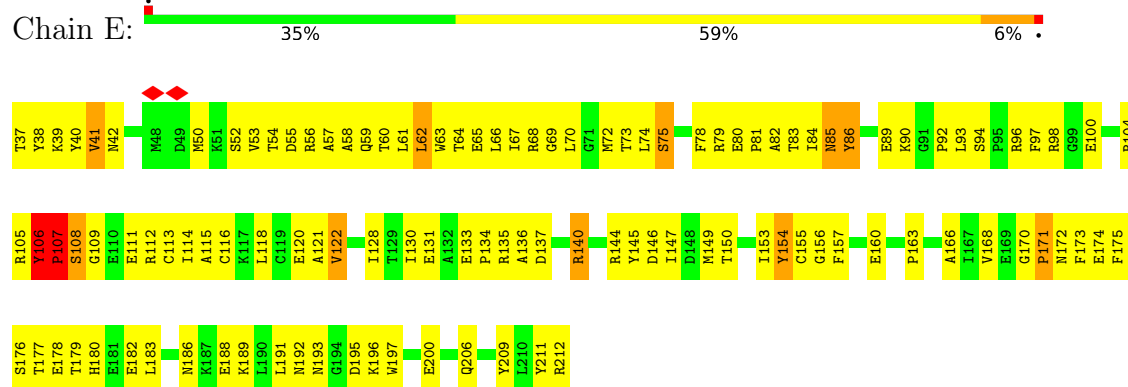
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



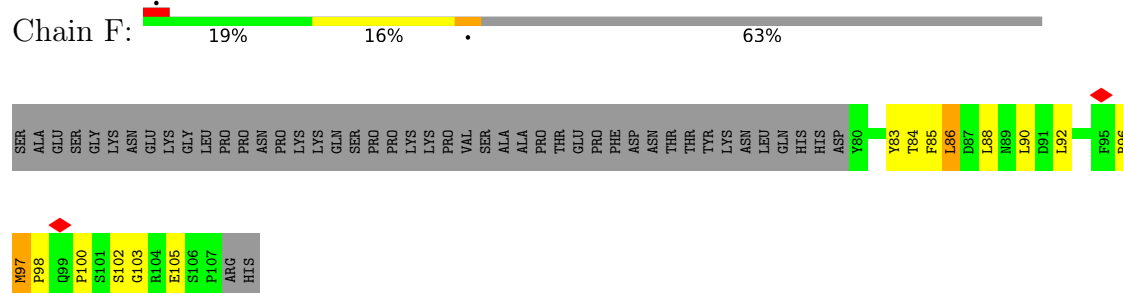
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



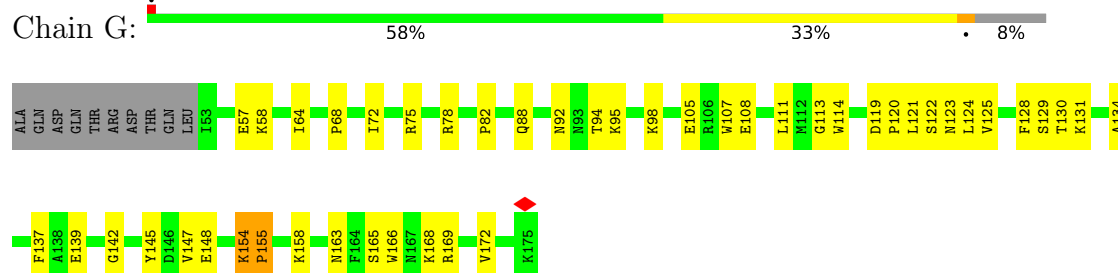
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

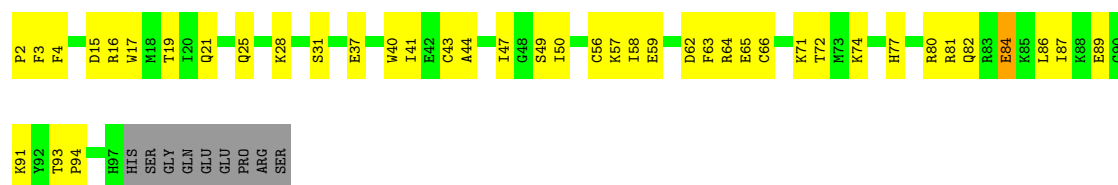


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



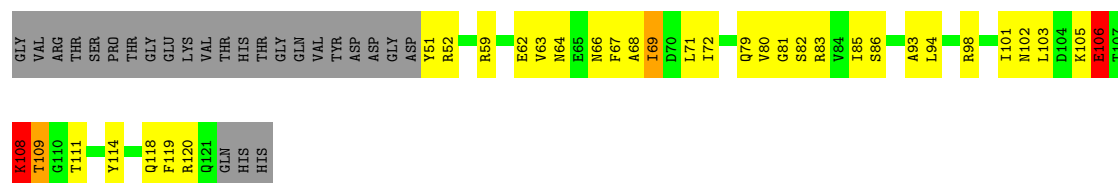
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain H: 



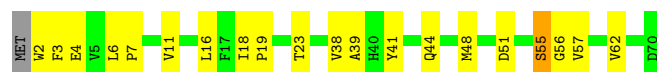
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain I: 



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

Chain J: 



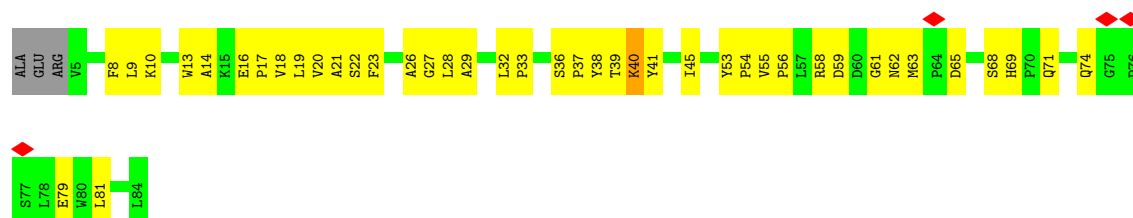
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain K: 



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

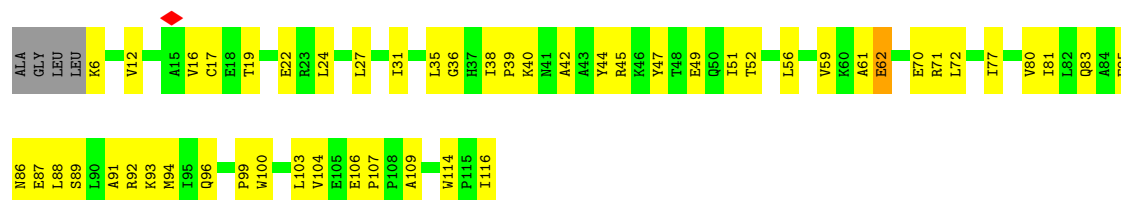
Chain L: 



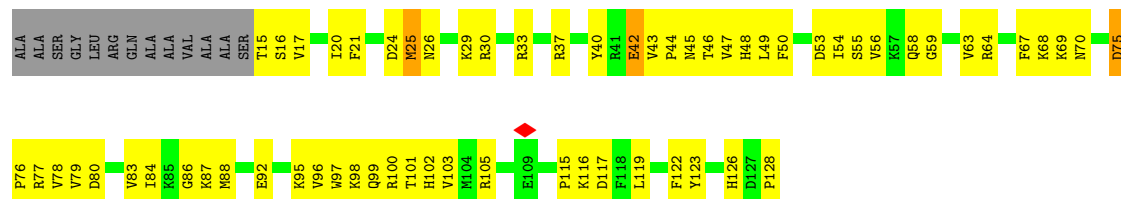
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N: 

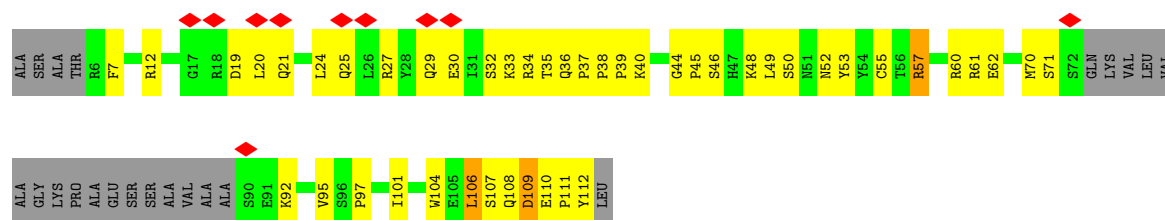
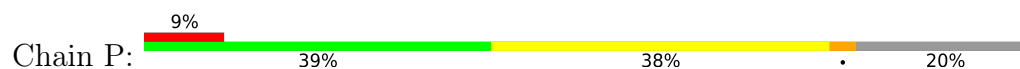




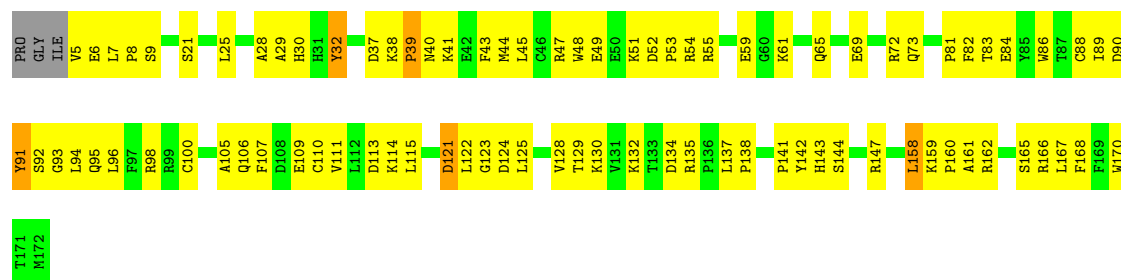
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



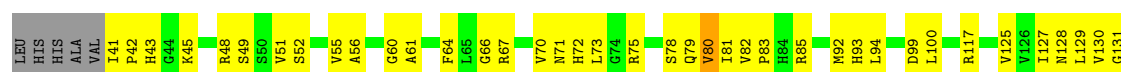
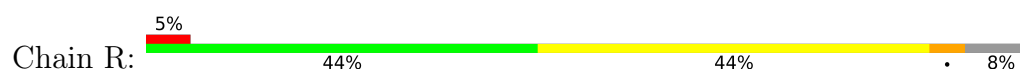
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

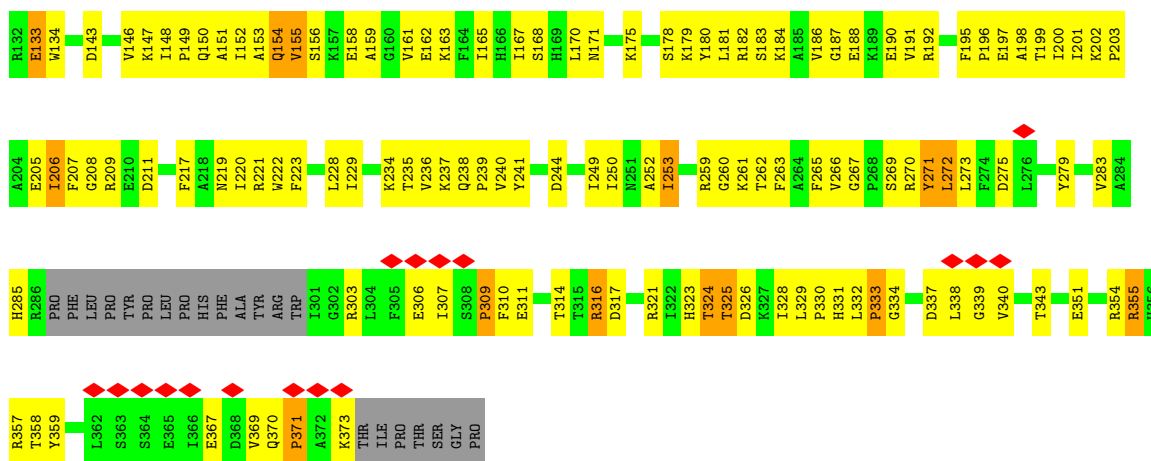


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

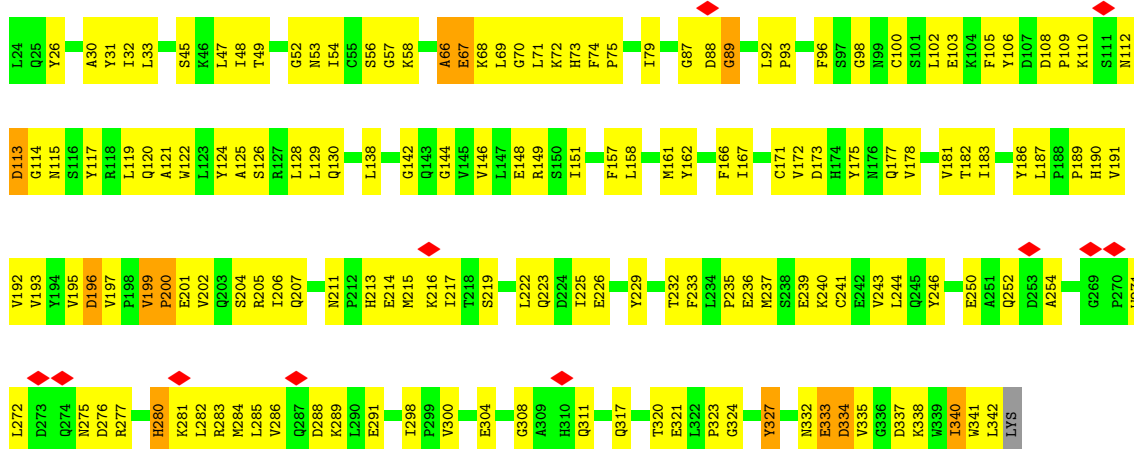


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

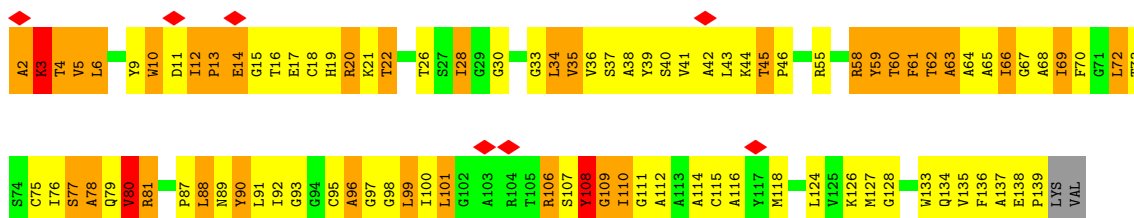




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

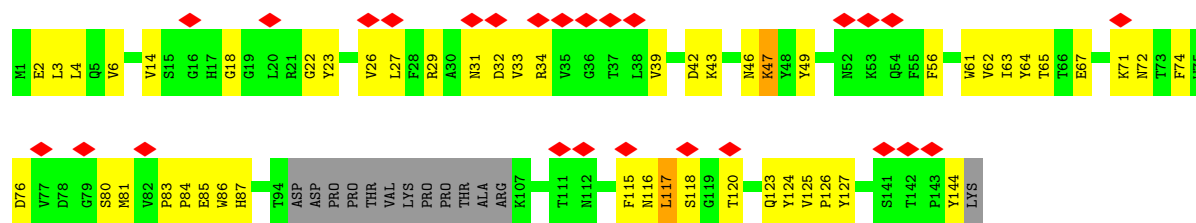


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



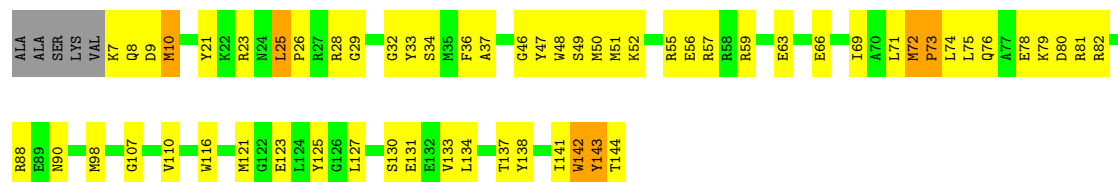
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





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

Chain V: 55% 38%



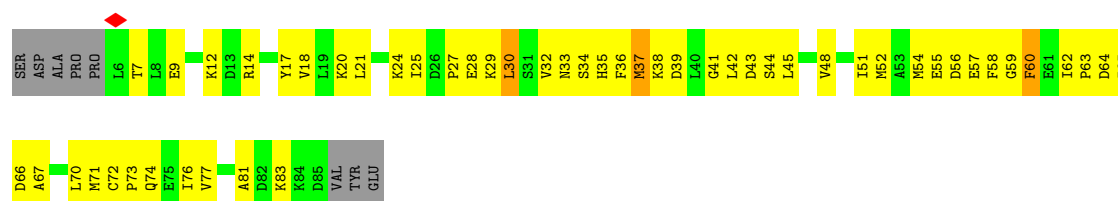
- Molecule 31: Acyl carrier protein, mitochondrial

Chain W: 53% 41%



- Molecule 31: Acyl carrier protein, mitochondrial

Chain M: 32% 56% 9%



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

Chain X: 51% 32% 14%

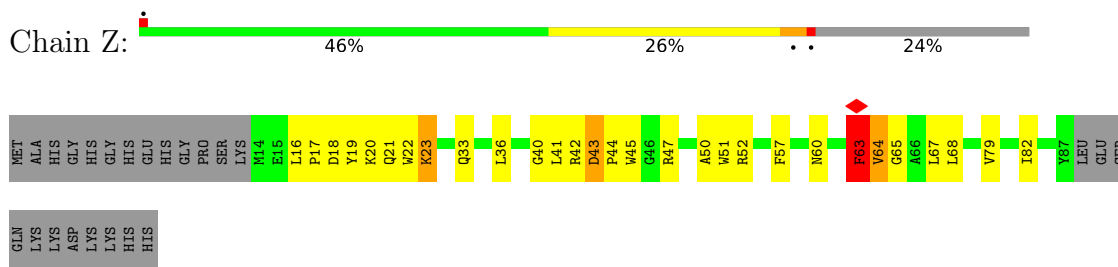


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

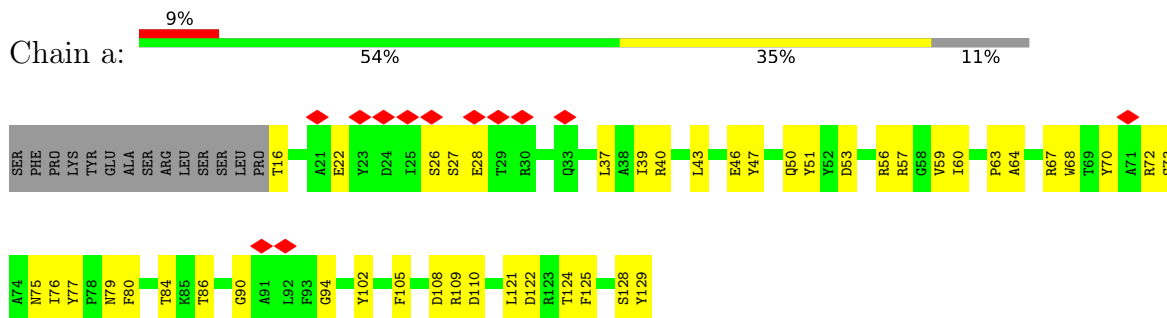
Chain Y: 54% 25% 21%



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



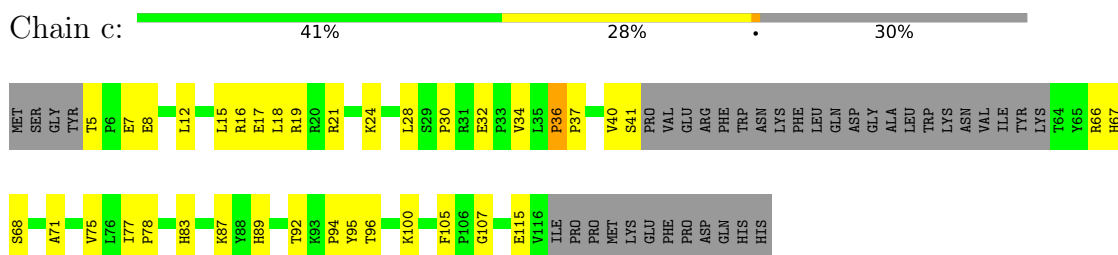
● Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



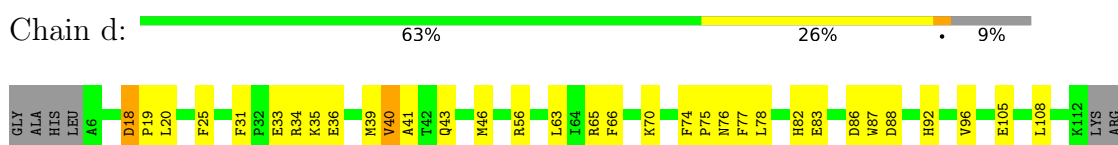
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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



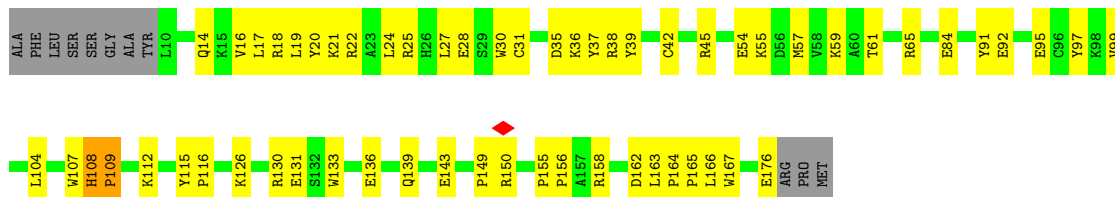
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



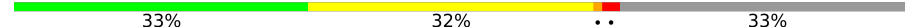
ARG
GLU
GLN
ARG

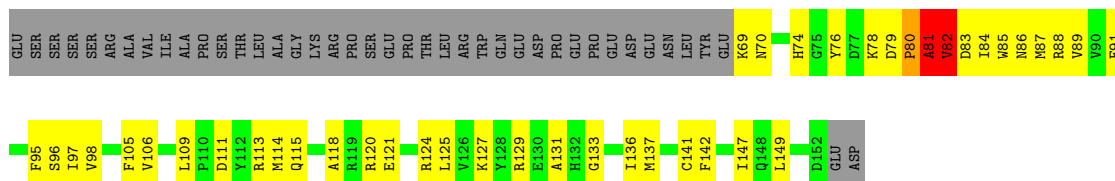
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain f:  61% 32% 6%



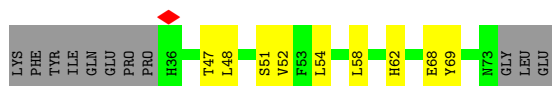
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain h:  33% 32% 33%



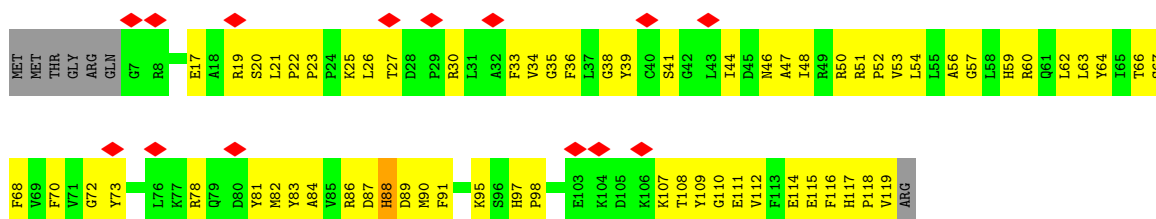
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain i:  59% 18% 22%



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

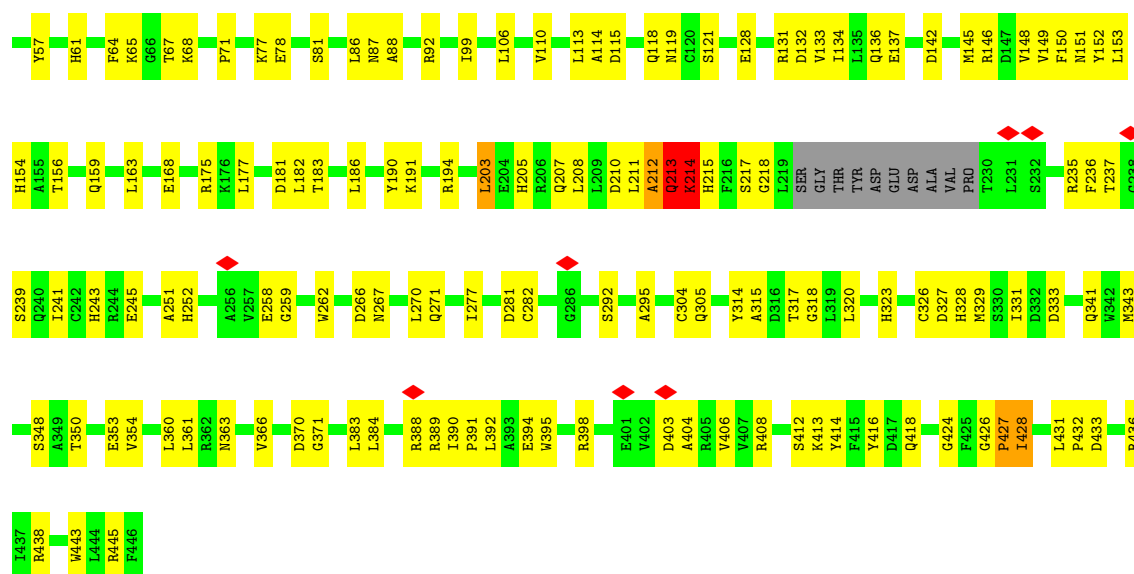
Chain j:  12% 40% 53% 6%



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

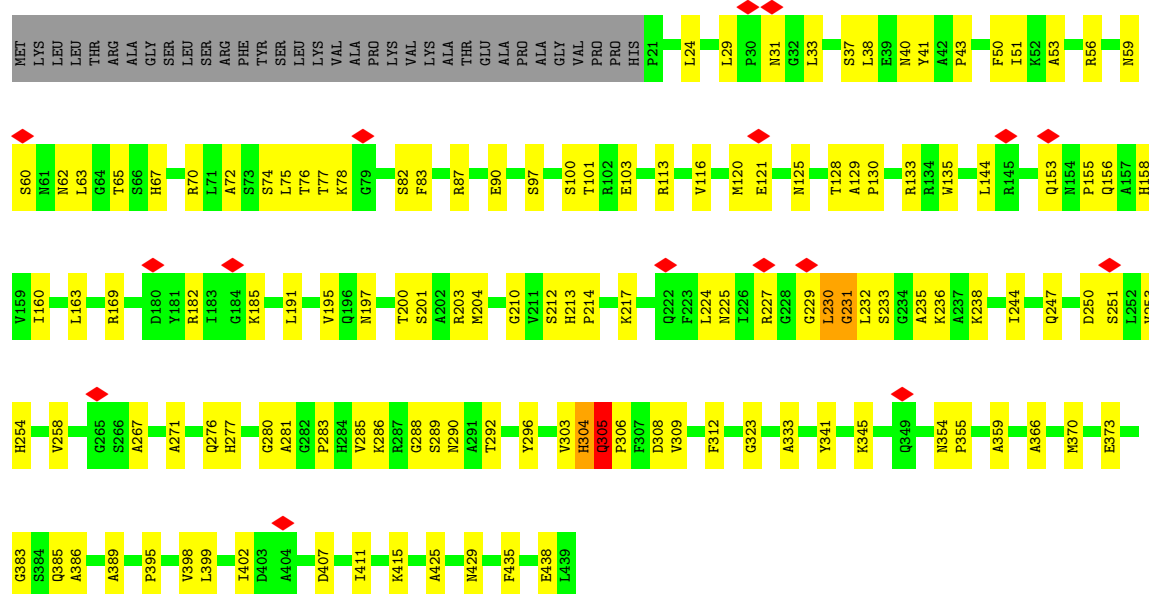
Chain g:  43% 54%





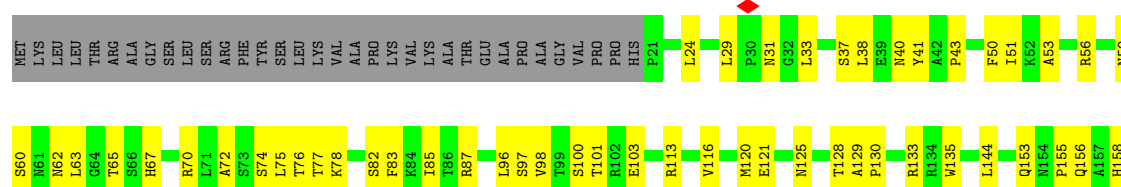
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

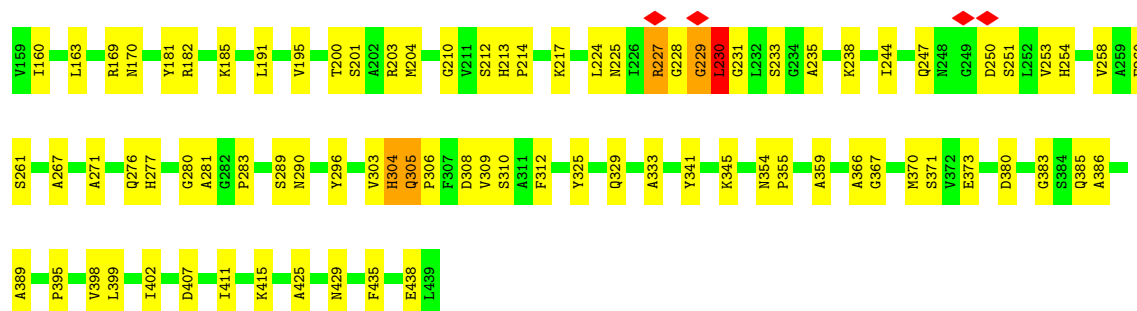
Chain 1: 64% 28% 8%



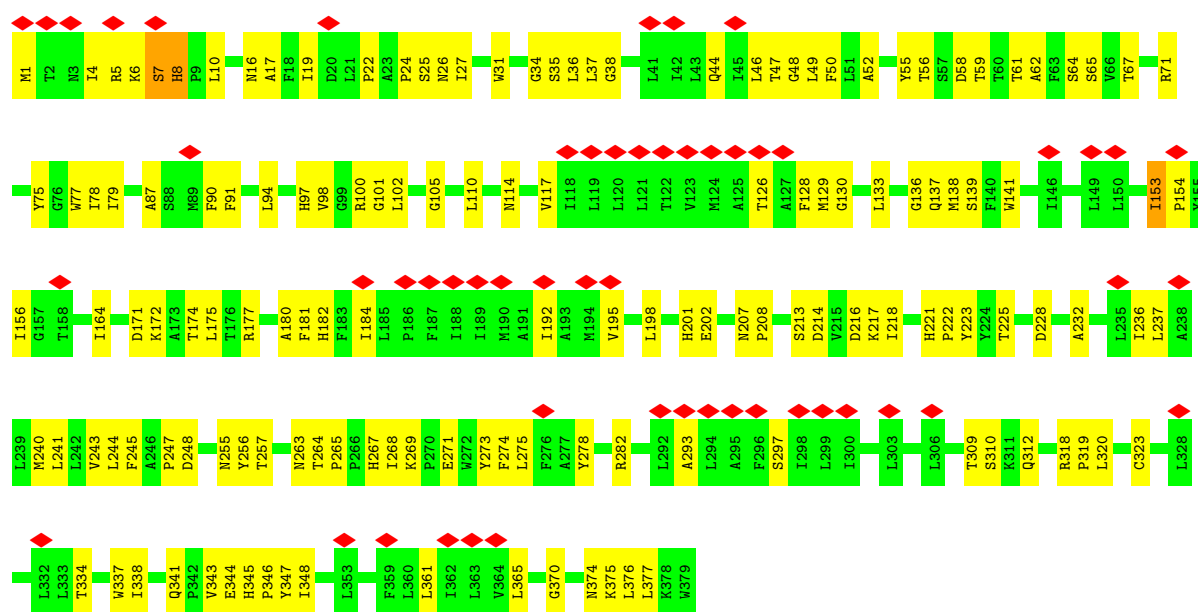
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain x: 63% 29% 8%

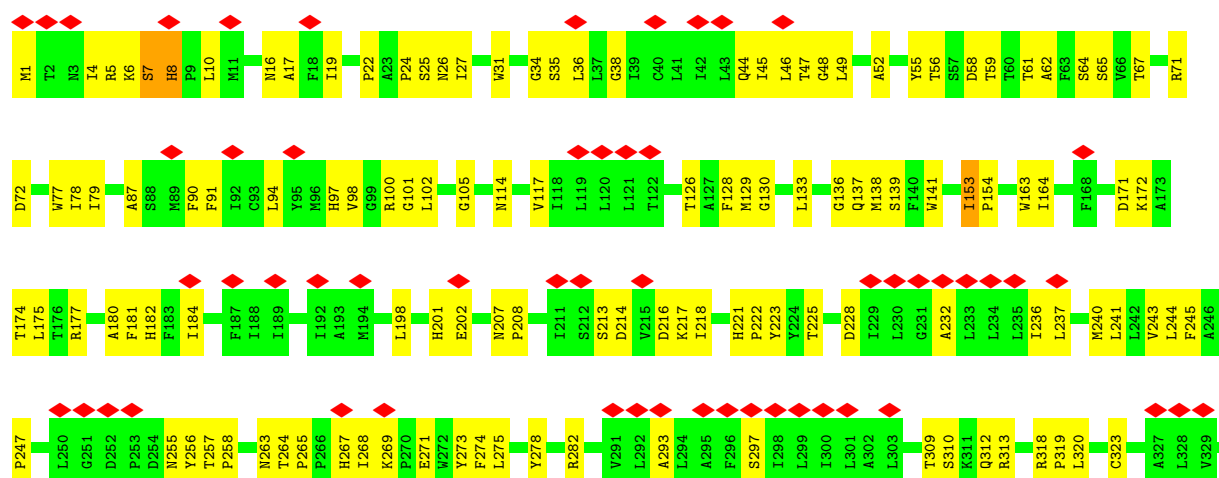


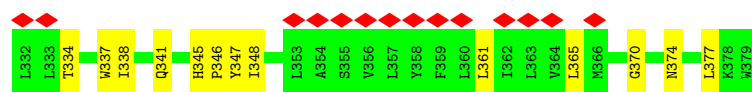


• Molecule 47: Cytochrome b

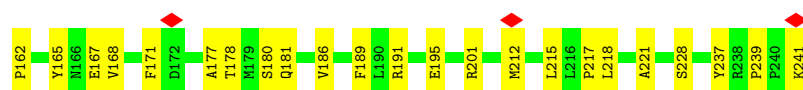


• Molecule 47: Cytochrome b

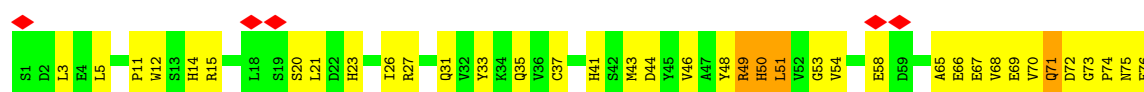




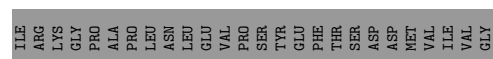
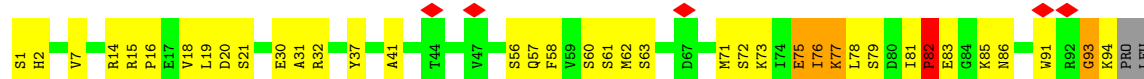
- Molecule 48: Cytochrome c1, heme protein, mitochondrial



- Molecule 48: Cytochrome c1, heme protein, mitochondrial

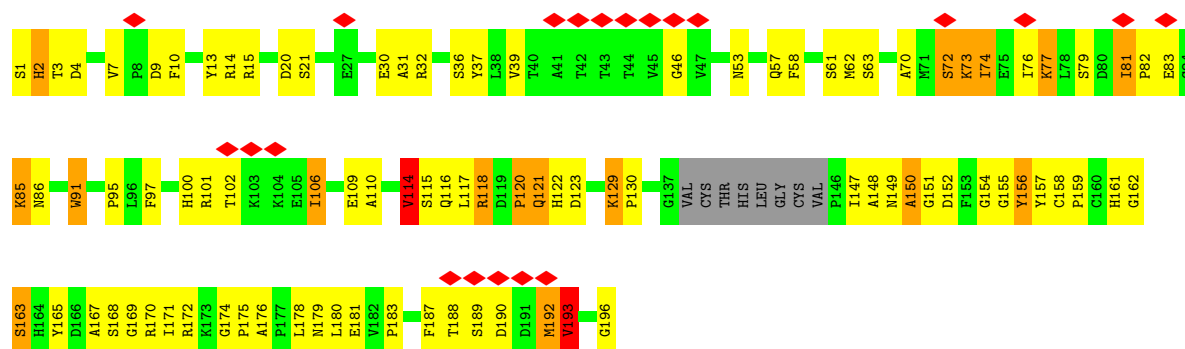


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



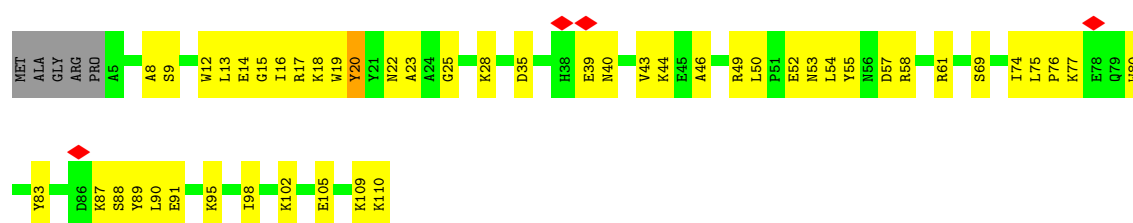
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial





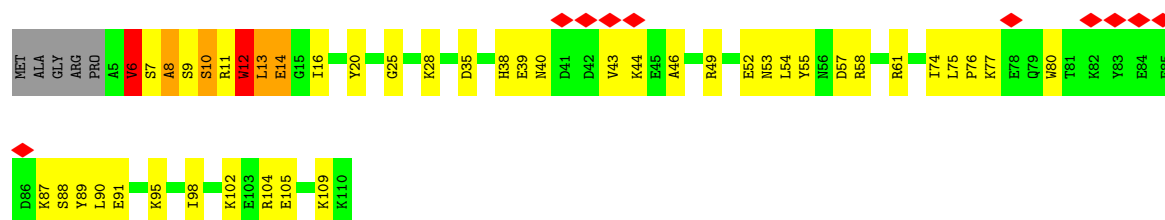
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain q: 52% 42% 5%



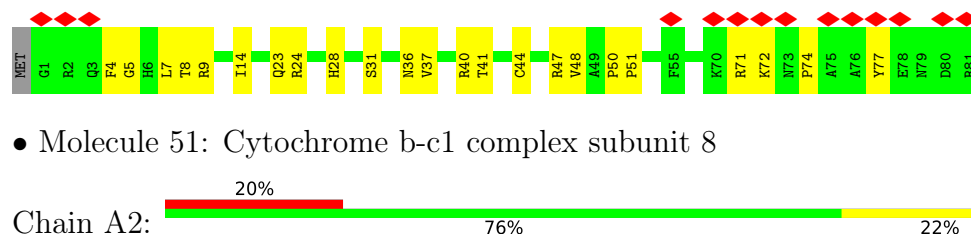
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain A1: 9% 56% 34% 5%



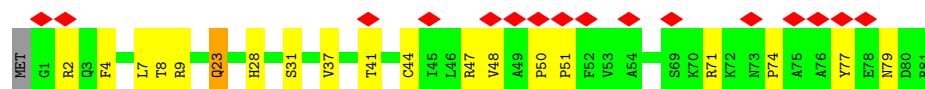
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain r: 17% 71% 28%

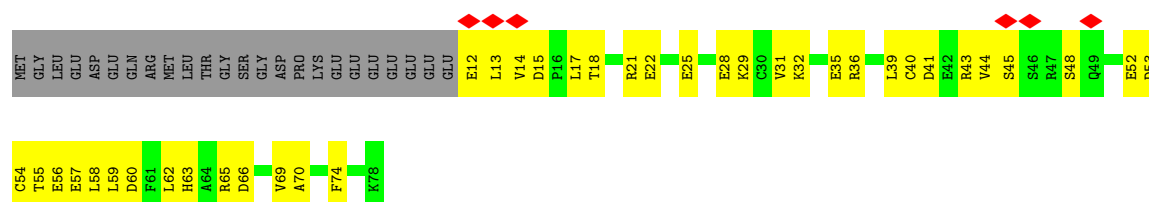


- Molecule 51: Cytochrome b-c1 complex subunit 8

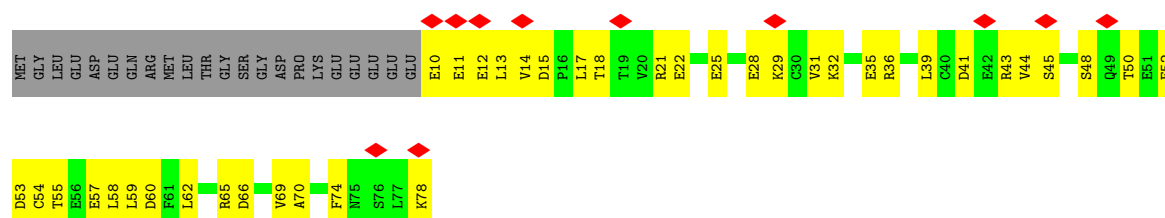
Chain A2: 20% 76% 22%



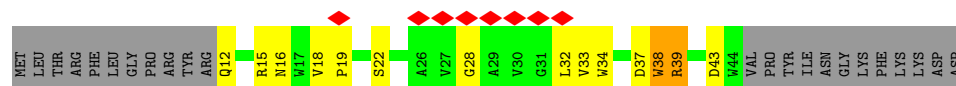
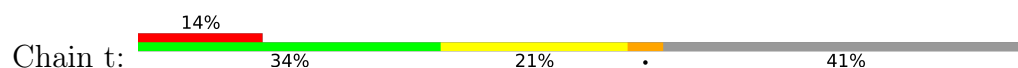
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



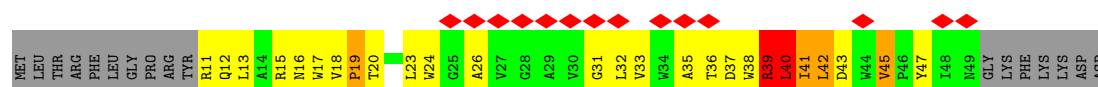
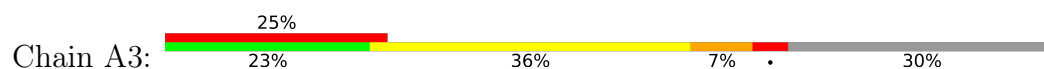
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



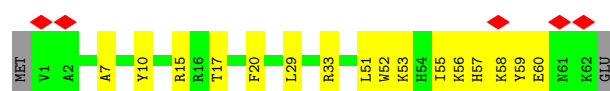
- Molecule 53: Cytochrome b-c1 complex subunit 10



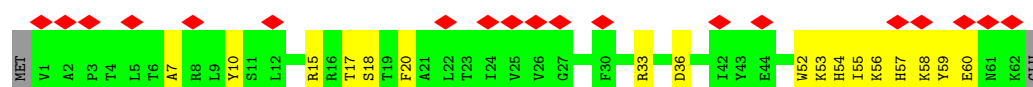
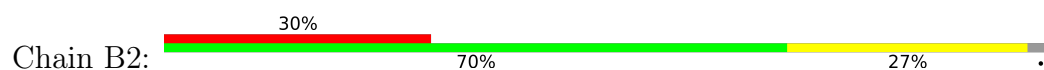
- Molecule 53: Cytochrome b-c1 complex subunit 10



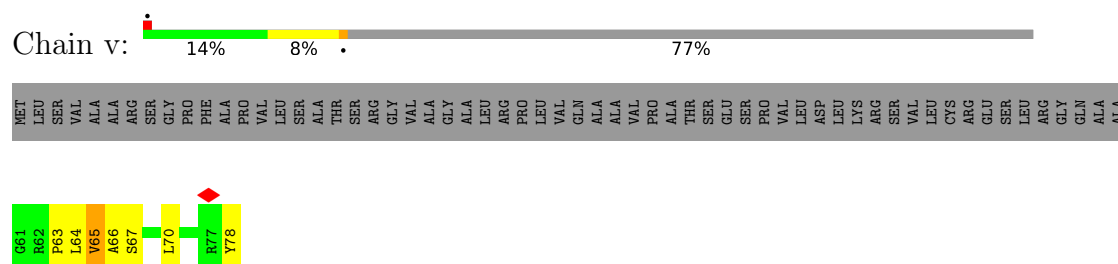
- Molecule 54: Cytochrome b-c1 complex subunit 9



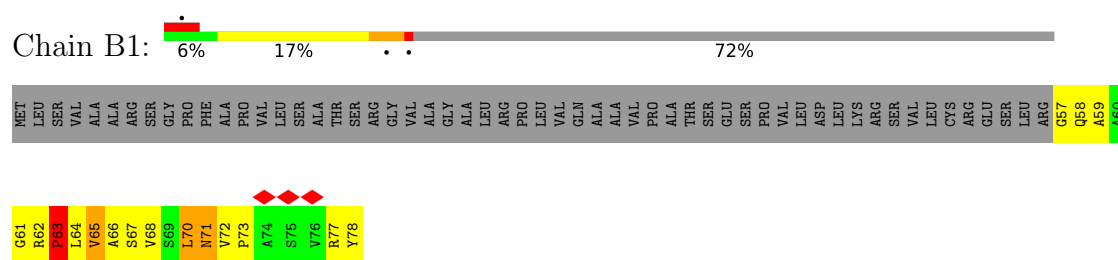
- Molecule 54: Cytochrome b-c1 complex subunit 9



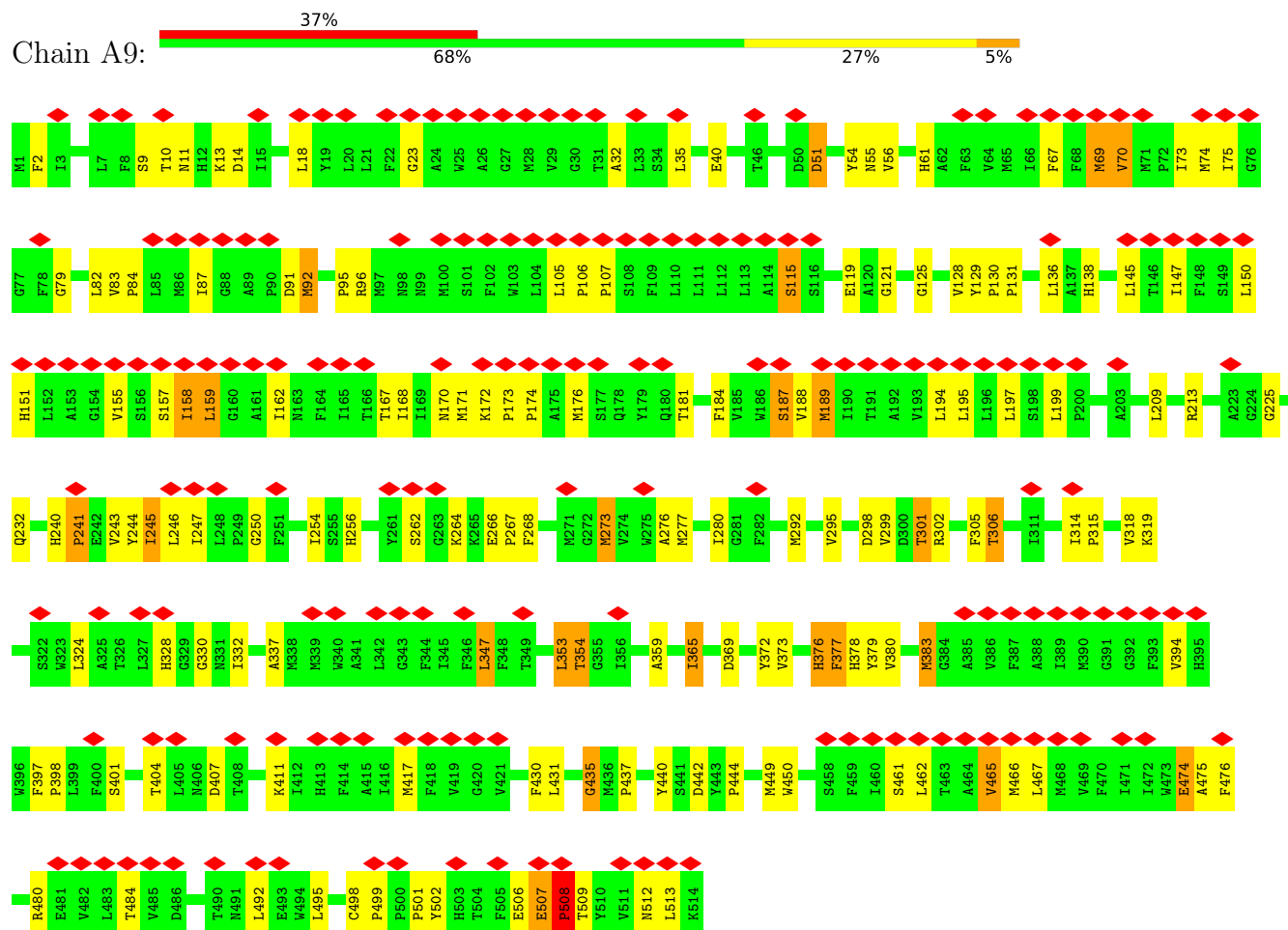
- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

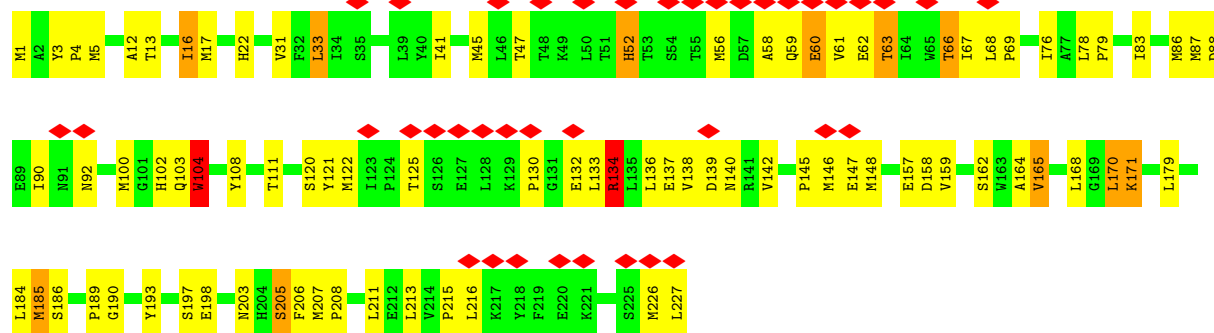


- Molecule 56: Cytochrome c oxidase subunit 1



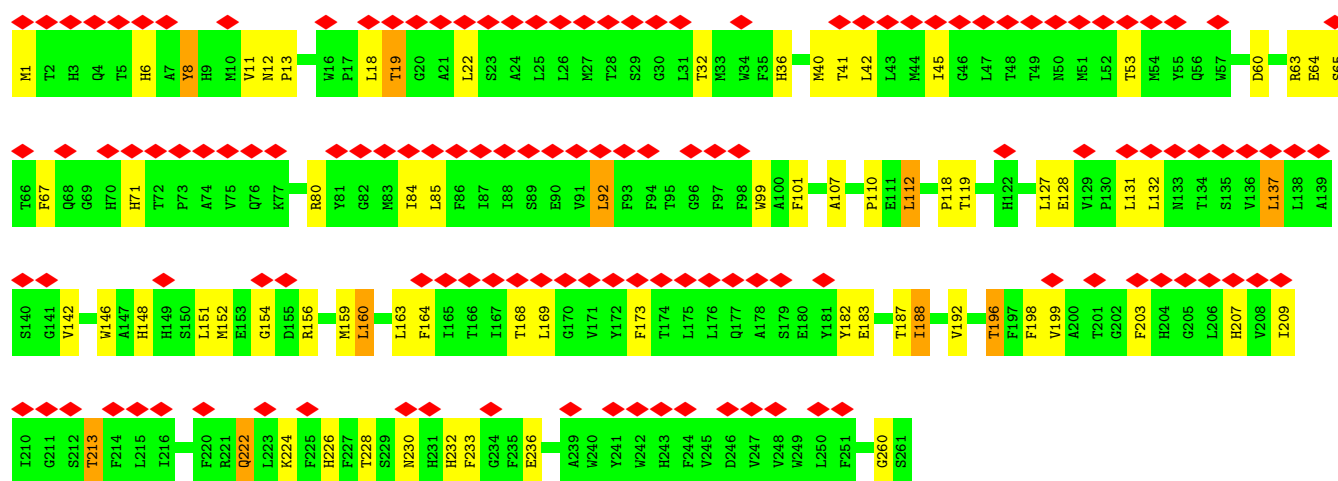
- Molecule 57: Cytochrome c oxidase subunit 2

Chain C4: 17% 61% 33% 5%



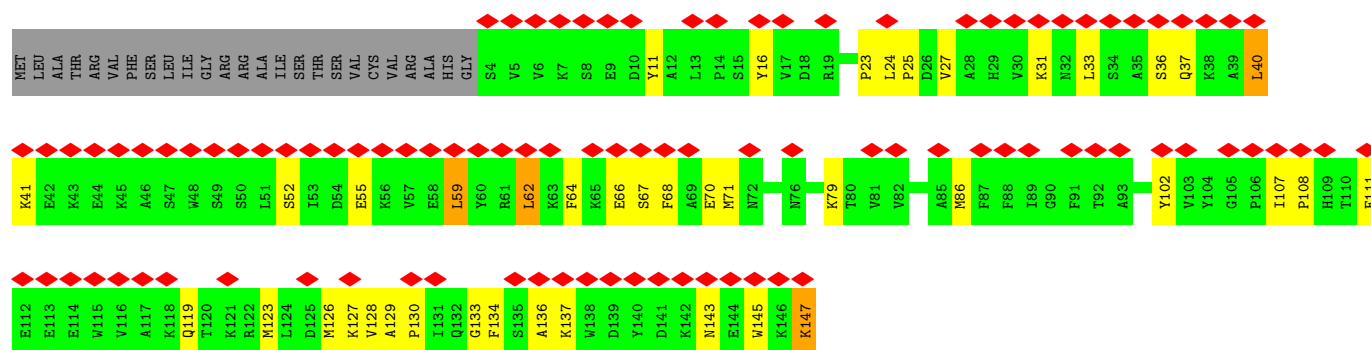
• Molecule 58: Cytochrome c oxidase subunit 3

Chain C2: 51% 72% 24%



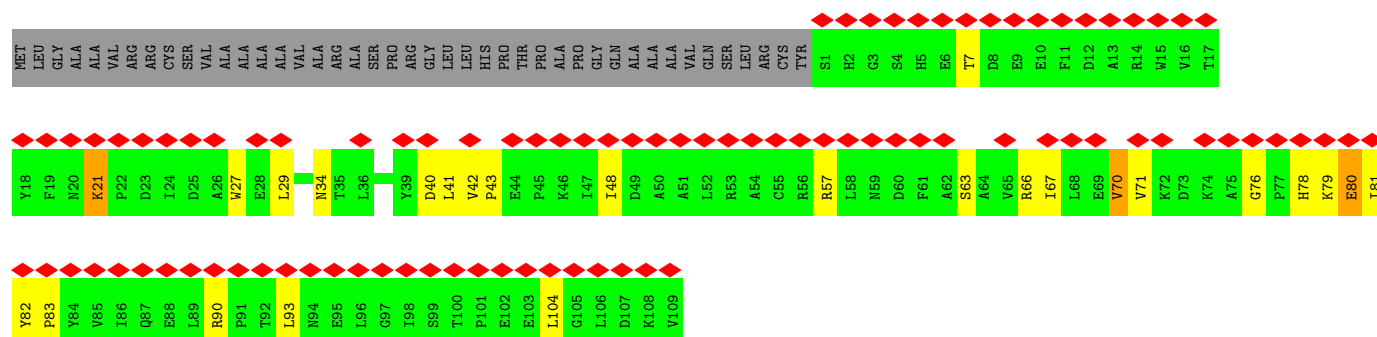
• Molecule 59: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain A7: 58% 60% 22% 15%

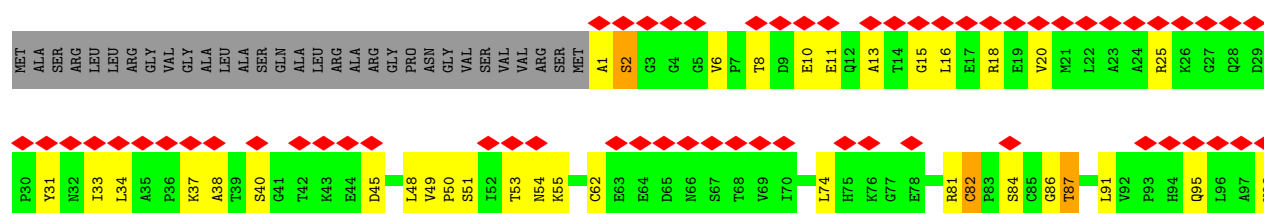


• Molecule 60: Cytochrome c oxidase subunit 5A, mitochondrial

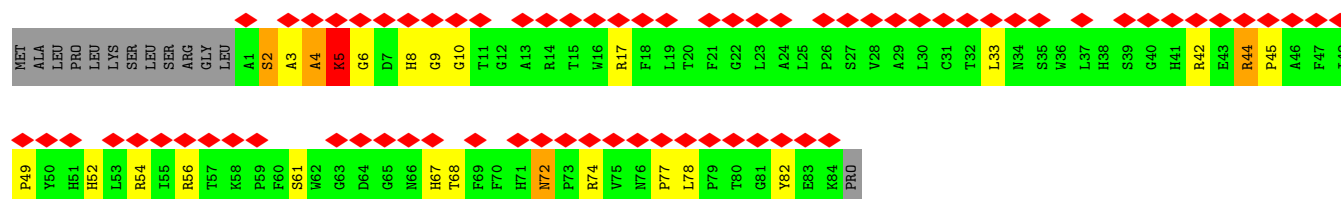
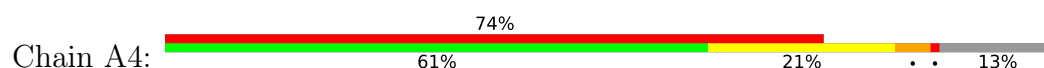
Chain C0: 61% 55% 15% 28%



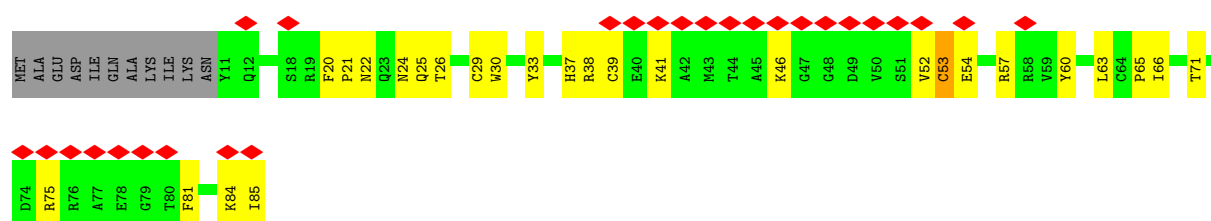
- Molecule 61: Cytochrome c oxidase subunit 5B, mitochondrial



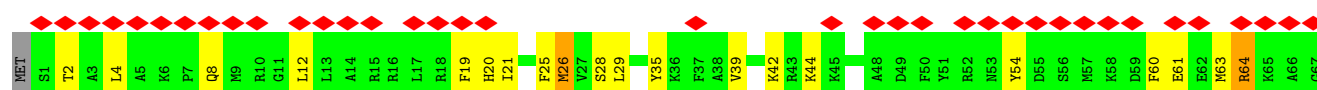
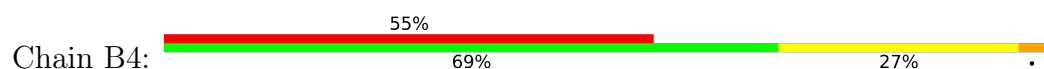
- Molecule 62: Cytochrome c oxidase subunit 6A2, mitochondrial

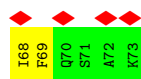


- Molecule 63: Cytochrome c oxidase subunit 6B1

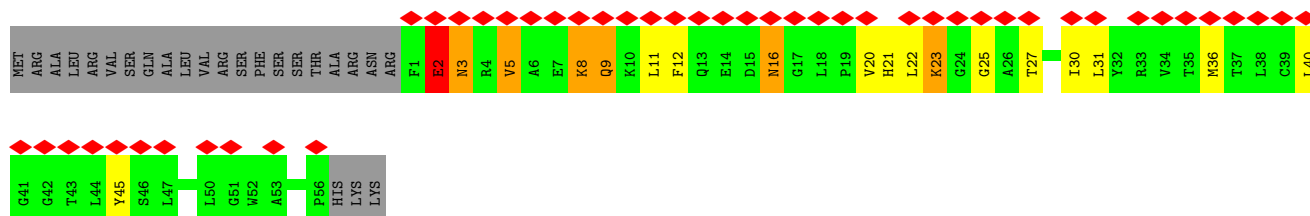


- Molecule 64: Cytochrome c oxidase subunit 6C

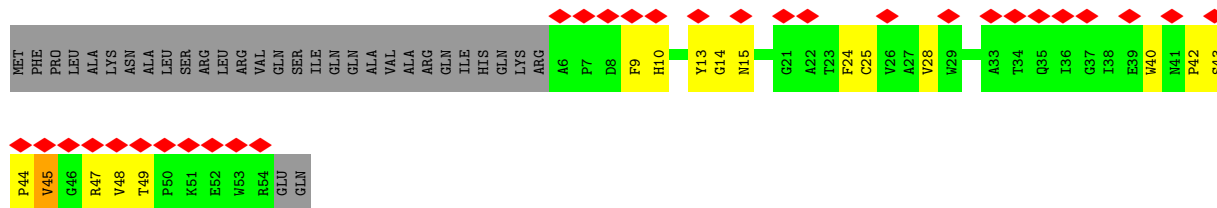
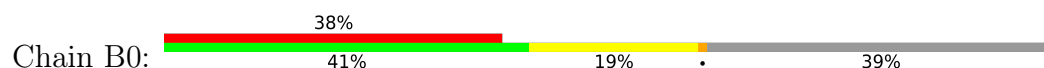




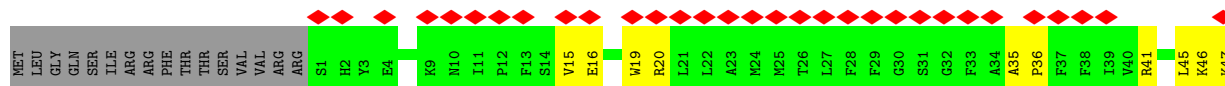
- Molecule 65: Cytochrome c oxidase subunit 7A1, mitochondrial



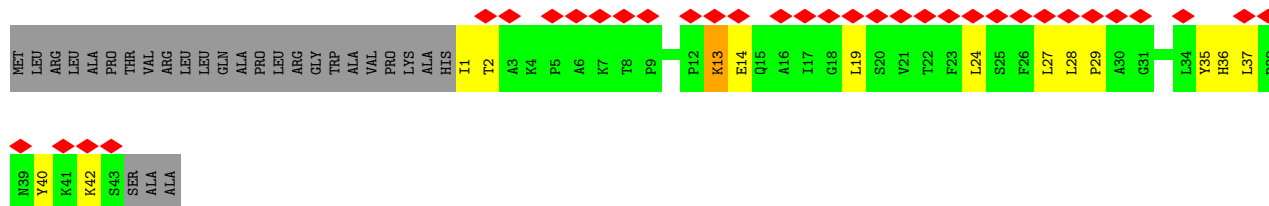
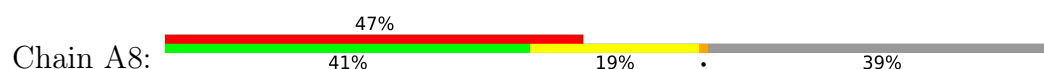
- Molecule 66: Cytochrome c oxidase subunit 7B, mitochondrial



- 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	57806	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	0.509	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	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: PC1, SF4, 3PE, CDL, CU, FES, ZN, HEA, MG, HEC, HEM, FMN, NAP

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	0.43	0/1617	0.69	0/2206
2	4	0.65	1/3674 (0.0%)	0.88	6/5020 (0.1%)
3	2	0.75	1/2749 (0.0%)	0.97	5/3744 (0.1%)
4	7	0.55	0/1271	0.85	1/1735 (0.1%)
5	6	0.44	0/4893	0.74	2/6661 (0.0%)
6	5	0.68	0/721	1.04	5/977 (0.5%)
7	3	0.54	0/902	0.82	2/1233 (0.2%)
8	1	0.70	1/2575 (0.0%)	1.05	15/3518 (0.4%)
9	8	0.46	0/3136	0.80	12/4258 (0.3%)
10	A	0.68	1/5304 (0.0%)	0.95	9/7193 (0.1%)
11	B	0.85	0/3512	1.06	13/4763 (0.3%)
12	C	0.74	0/1777	0.94	3/2420 (0.1%)
13	D	0.91	2/1237 (0.2%)	1.05	1/1676 (0.1%)
14	E	0.88	0/1431	1.11	7/1938 (0.4%)
15	F	0.40	0/191	1.08	2/262 (0.8%)
16	G	0.72	0/1008	0.97	3/1363 (0.2%)
17	H	0.54	0/800	0.80	0/1076
18	I	0.53	0/541	0.99	3/726 (0.4%)
19	J	0.56	0/545	0.68	0/740
20	K	0.42	0/667	0.68	0/900
21	L	0.44	0/623	0.75	0/862
22	N	0.48	0/882	0.88	2/1203 (0.2%)
23	O	0.50	0/948	0.83	3/1279 (0.2%)
24	P	0.49	0/723	0.81	1/985 (0.1%)
25	Q	0.45	0/1381	0.82	2/1869 (0.1%)
26	R	0.49	0/2465	0.86	8/3349 (0.2%)
27	S	0.35	0/2348	0.82	6/3198 (0.2%)
28	T	0.48	0/938	0.99	3/1278 (0.2%)
29	U	0.40	0/1053	0.85	3/1439 (0.2%)
30	V	0.50	0/1115	0.79	1/1508 (0.1%)
31	M	0.43	0/651	0.77	0/876
31	W	0.32	0/624	0.73	1/847 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X	0.36	0/383	0.71	0/523
33	Y	0.35	0/428	0.72	0/592
34	Z	0.35	0/506	0.85	2/688 (0.3%)
35	a	0.43	0/878	0.71	0/1195
36	b	0.51	0/1058	0.78	0/1434
37	c	0.39	0/632	1.01	3/871 (0.3%)
38	d	0.31	0/729	0.70	2/996 (0.2%)
39	f	0.32	0/1191	0.74	2/1639 (0.1%)
40	h	0.44	0/679	0.82	1/926 (0.1%)
41	i	0.34	0/286	0.56	0/392
42	j	0.50	0/912	0.84	4/1240 (0.3%)
43	g	0.43	1/1380 (0.1%)	0.74	2/1872 (0.1%)
44	e	0.47	0/888	1.08	9/1234 (0.7%)
45	k	0.46	0/3527	0.66	3/4787 (0.1%)
45	w	0.46	1/3455 (0.0%)	0.64	2/4685 (0.0%)
46	l	0.41	0/3192	0.58	3/4329 (0.1%)
46	x	0.41	0/3198	0.61	5/4336 (0.1%)
47	m	0.55	0/3108	0.62	0/4252
47	y	0.55	0/3108	0.62	0/4252
48	o	0.46	0/1978	0.65	1/2684 (0.0%)
48	z	0.47	0/1965	0.66	0/2669
49	A0	0.46	0/1124	0.95	5/1538 (0.3%)
49	p	0.47	0/945	1.15	10/1288 (0.8%)
50	A1	0.46	0/935	0.61	0/1253
50	q	0.45	0/935	0.65	1/1253 (0.1%)
51	A2	0.41	0/698	0.62	0/944
51	r	0.41	0/704	0.63	0/951
52	B3	0.31	0/571	0.60	0/765
52	s	0.32	0/553	0.57	0/741
53	A3	0.44	0/330	0.73	0/457
53	t	0.33	0/272	0.52	0/377
54	B2	0.34	0/524	0.50	0/707
54	u	0.34	0/524	0.50	0/707
55	B1	0.57	0/149	1.24	0/203
55	v	0.52	0/114	1.13	0/156
56	A9	0.86	7/4164 (0.2%)	1.16	35/5688 (0.6%)
57	C4	0.77	0/1868	1.12	10/2544 (0.4%)
58	C2	0.74	0/2211	1.02	7/3023 (0.2%)
59	A7	0.67	0/1229	0.96	3/1658 (0.2%)
60	C0	0.64	0/898	1.02	6/1218 (0.5%)
61	A6	0.72	0/765	1.13	4/1038 (0.4%)
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	B4	0.71	0/611	0.94	2/810 (0.2%)
65	C3	0.70	0/451	1.04	3/610 (0.5%)
66	B0	0.74	0/398	1.01	0/546
67	C1	0.77	0/399	0.97	2/534 (0.4%)
68	A8	0.68	0/345	0.99	1/470 (0.2%)
All	All	0.58	15/108846 (0.0%)	0.86	258/148004 (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	6
2	4	0	9
3	2	0	10
4	7	0	6
5	6	0	5
6	5	0	4
7	3	0	2
8	1	0	3
9	8	0	8
10	A	0	16
11	B	0	4
13	D	0	6
14	E	0	5
17	H	0	2
18	I	0	1
20	K	0	1
21	L	0	1
22	N	0	1
23	O	0	1
24	P	0	3
25	Q	0	2
26	R	0	9
27	S	0	4
29	U	0	3
30	V	0	2
31	M	0	3
31	W	0	2
34	Z	0	2
35	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	b	0	4
38	d	0	1
39	f	0	3
40	h	0	3
42	j	0	2
43	g	0	1
44	e	0	7
45	k	0	3
45	w	0	4
46	l	0	5
46	x	0	3
47	m	0	4
47	y	0	3
48	o	0	7
48	z	0	7
49	A0	0	3
49	p	0	6
53	A3	0	1
55	B1	0	5
All	All	0	194

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	161	LEU	CA-C	-9.68	1.38	1.52
56	A9	61	HIS	CG-CD2	7.59	1.44	1.35
56	A9	378	HIS	ND1-CE1	7.10	1.39	1.32
56	A9	378	HIS	CE1-NE2	-6.54	1.26	1.32
56	A9	69	MET	SD-CE	-6.26	1.64	1.79
45	w	213	GLN	CA-C	-6.12	1.44	1.52
13	D	88	GLY	C-N	-5.87	1.25	1.33
8	1	37	PRO	C-N	-5.59	1.25	1.33
56	A9	61	HIS	ND1-CE1	5.58	1.38	1.32
56	A9	376	HIS	ND1-CE1	5.58	1.38	1.32
13	D	190	ALA	C-N	-5.57	1.25	1.33
56	A9	378	HIS	CG-CD2	5.46	1.41	1.35
3	2	157	LEU	C-N	-5.39	1.26	1.33
10	A	93	ALA	CA-CB	-5.30	1.45	1.53
43	g	27	PRO	C-N	5.25	1.43	1.33

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	128	CYS	CA-C-N	-13.67	102.76	119.84
10	A	128	CYS	C-N-CA	-13.67	102.76	119.84
46	x	230	LEU	N-CA-C	11.27	126.80	110.24
9	8	227	PRO	CA-C-N	-10.59	107.96	118.97
9	8	227	PRO	C-N-CA	-10.59	107.96	118.97
56	A9	376	HIS	ND1-CE1-NE2	10.35	118.75	108.40
11	B	420	TYR	N-CA-C	-9.94	94.36	108.07
8	1	176	LEU	CA-C-N	9.78	132.06	119.84
8	1	176	LEU	C-N-CA	9.78	132.06	119.84
27	S	199	VAL	C-N-CD	-9.52	85.97	125.00
13	D	172	GLY	N-CA-C	9.47	126.31	114.37
45	k	213	GLN	N-CA-C	9.23	121.28	111.03
8	1	315	PRO	CA-C-N	8.97	131.05	119.84
8	1	315	PRO	C-N-CA	8.97	131.05	119.84
63	A5	52	VAL	N-CA-C	8.96	121.25	108.17
6	5	12	PHE	CA-C-N	-8.83	108.91	122.16
6	5	12	PHE	C-N-CA	-8.83	108.91	122.16
63	A5	81	PHE	CA-C-N	8.71	128.35	119.56
63	A5	81	PHE	C-N-CA	8.71	128.35	119.56
22	N	62	GLU	CA-C-N	8.62	128.76	120.31
22	N	62	GLU	C-N-CA	8.62	128.76	120.31
49	p	146	PRO	N-CA-CB	8.52	111.97	102.60
11	B	309	ASP	N-CA-C	-8.37	94.44	108.75
6	5	14	VAL	N-CA-C	-8.18	104.52	113.43
8	1	158	GLY	N-CA-C	8.12	126.11	114.67
67	C1	20	ARG	N-CA-C	-8.11	102.52	111.36
56	A9	378	HIS	ND1-CE1-NE2	8.06	116.46	108.40
56	A9	82	LEU	N-CA-C	8.01	122.33	112.23
14	E	140	ARG	CG-CD-NE	7.98	129.55	112.00
37	c	36	PRO	CA-C-N	7.90	145.97	127.00
37	c	36	PRO	C-N-CA	7.90	145.97	127.00
11	B	292	MET	CA-C-N	7.79	136.42	121.54
11	B	292	MET	C-N-CA	7.79	136.42	121.54
56	A9	56	VAL	N-CA-C	-7.78	103.21	110.53
37	c	36	PRO	C-N-CD	-7.73	103.60	120.60
56	A9	435	GLY	N-CA-C	7.59	125.97	115.27
11	B	293	LEU	N-CA-C	-7.56	94.70	110.80
34	Z	43	ASP	CA-C-N	7.55	128.01	119.93
34	Z	43	ASP	C-N-CA	7.55	128.01	119.93
4	7	123	GLY	N-CA-C	7.43	122.49	113.79
68	A8	27	LEU	N-CA-C	7.42	119.45	111.36
56	A9	330	GLY	N-CA-C	7.39	120.46	112.33
48	o	79	GLU	N-CA-C	7.29	126.32	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A9	376	HIS	CE1-NE2-CD2	-7.27	101.73	109.00
56	A9	9	SER	N-CA-C	7.19	119.85	110.43
60	C0	76	GLY	CA-C-N	7.14	128.38	120.45
60	C0	76	GLY	C-N-CA	7.14	128.38	120.45
56	A9	332	ILE	N-CA-C	7.12	118.98	109.37
49	p	82	PRO	N-CA-CB	7.10	110.71	103.25
14	E	156	GLY	N-CA-C	-7.10	105.00	115.72
60	C0	42	VAL	N-CA-C	-7.09	99.68	108.05
56	A9	130	PRO	N-CA-C	-6.90	102.28	110.70
44	e	119	THR	N-CA-C	6.86	125.41	110.80
58	C2	36	HIS	N-CA-C	6.84	122.05	113.43
49	p	130	PRO	N-CA-CB	6.83	110.42	103.25
8	1	265	LEU	N-CA-C	-6.80	101.16	111.56
42	j	22	PRO	N-CA-C	6.78	118.98	110.70
39	f	108	HIS	CA-C-N	6.78	128.32	119.84
39	f	108	HIS	C-N-CA	6.78	128.32	119.84
59	A7	133	GLY	N-CA-C	6.75	129.19	113.18
56	A9	507	GLU	N-CA-C	-6.75	97.89	109.15
23	O	17	VAL	CA-C-N	-6.74	111.64	120.67
23	O	17	VAL	C-N-CA	-6.74	111.64	120.67
62	A4	5	LYS	N-CA-C	6.71	125.09	110.80
8	1	237	PHE	N-CA-C	-6.66	103.00	112.13
2	4	416	ARG	CA-C-N	-6.65	115.00	120.98
2	4	416	ARG	C-N-CA	-6.65	115.00	120.98
60	C0	81	ILE	N-CA-C	6.62	116.76	110.53
27	S	308	GLY	N-CA-C	6.60	121.10	112.25
49	p	159	PRO	N-CA-CB	6.58	109.83	102.60
49	p	120	PRO	N-CA-CB	6.57	110.15	103.25
9	8	404	ALA	CA-C-N	6.54	131.33	120.86
9	8	404	ALA	C-N-CA	6.54	131.33	120.86
44	e	85	GLU	CA-C-N	6.53	134.01	121.54
44	e	85	GLU	C-N-CA	6.53	134.01	121.54
56	A9	61	HIS	CB-CG-CD2	-6.53	122.71	131.20
14	E	140	ARG	CB-CG-CD	-6.53	96.29	111.30
56	A9	506	GLU	N-CA-C	-6.52	104.18	111.28
56	A9	74	MET	N-CA-C	6.49	118.02	111.07
56	A9	61	HIS	ND1-CE1-NE2	6.45	114.84	108.40
8	1	41	GLY	N-CA-C	6.43	125.46	112.34
49	p	133	VAL	CA-C-N	6.39	133.20	121.70
49	p	133	VAL	C-N-CA	6.39	133.20	121.70
18	I	108	LYS	CA-C-N	6.31	133.60	121.54
18	I	108	LYS	C-N-CA	6.31	133.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	94	VAL	N-CA-C	6.29	115.93	106.42
14	E	122	VAL	CB-CA-C	-6.29	100.80	111.37
46	x	229	GLY	CA-C-N	6.24	129.97	121.05
46	x	229	GLY	C-N-CA	6.24	129.97	121.05
62	A4	2	SER	N-CA-C	6.24	119.52	109.79
56	A9	10	THR	N-CA-C	-6.23	103.87	112.03
14	E	140	ARG	CA-CB-CG	6.22	126.54	114.10
3	2	308	THR	CA-C-N	-6.21	111.97	121.66
3	2	308	THR	C-N-CA	-6.21	111.97	121.66
11	B	217	VAL	CA-C-N	-6.20	113.43	121.79
11	B	217	VAL	C-N-CA	-6.20	113.43	121.79
46	l	305	GLN	N-CA-C	6.17	123.45	109.81
8	1	253	GLU	CA-C-N	-6.16	108.97	121.18
8	1	253	GLU	C-N-CA	-6.16	108.97	121.18
60	C0	21	LYS	CA-C-N	6.13	126.31	119.32
60	C0	21	LYS	C-N-CA	6.13	126.31	119.32
28	T	2	ALA	CA-C-N	-6.12	109.86	121.54
28	T	2	ALA	C-N-CA	-6.12	109.86	121.54
56	A9	157	SER	N-CA-C	6.07	118.86	111.82
56	A9	170	ASN	N-CA-C	6.07	120.75	113.23
63	A5	63	LEU	N-CA-C	6.06	119.15	111.69
11	B	218	SER	CA-C-N	-6.03	109.59	121.41
11	B	218	SER	C-N-CA	-6.03	109.59	121.41
57	C4	47	THR	N-CA-C	6.02	119.94	112.59
45	w	203	LEU	CA-C-N	6.00	131.36	121.39
45	w	203	LEU	C-N-CA	6.00	131.36	121.39
57	C4	207	MET	CA-C-N	6.00	127.34	119.84
57	C4	207	MET	C-N-CA	6.00	127.34	119.84
11	B	363	VAL	CA-C-N	-5.99	105.00	122.38
11	B	363	VAL	C-N-CA	-5.99	105.00	122.38
56	A9	125	GLY	N-CA-C	-5.99	104.15	112.18
58	C2	8	TYR	N-CA-C	5.99	118.26	110.53
45	k	203	LEU	CA-C-N	-5.98	110.11	121.54
45	k	203	LEU	C-N-CA	-5.98	110.11	121.54
27	S	89	GLY	CA-C-N	-5.98	109.58	120.94
27	S	89	GLY	C-N-CA	-5.98	109.58	120.94
10	A	309	ASN	N-CA-C	5.97	118.71	110.35
62	A4	44	ARG	CA-C-N	5.97	125.99	119.90
62	A4	44	ARG	C-N-CA	5.97	125.99	119.90
18	I	106	GLU	N-CA-C	-5.96	98.10	110.80
12	C	93	ASP	CA-C-N	-5.95	115.62	120.98
12	C	93	ASP	C-N-CA	-5.95	115.62	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	p	75	GLU	CA-C-N	5.95	132.41	121.70
49	p	75	GLU	C-N-CA	5.95	132.41	121.70
56	A9	67	PHE	N-CA-C	5.93	119.71	112.23
56	A9	171	MET	N-CA-C	5.93	120.23	111.87
5	6	431	LEU	CA-C-N	-5.92	113.05	122.17
5	6	431	LEU	C-N-CA	-5.92	113.05	122.17
57	C4	134	ARG	N-CA-C	5.90	123.37	110.80
56	A9	119	GLU	CB-CA-C	-5.88	109.78	116.54
10	A	461	PRO	CA-C-N	5.86	132.74	121.54
10	A	461	PRO	C-N-CA	5.86	132.74	121.54
29	U	120	THR	C-N-CD	-5.85	107.72	120.60
26	R	80	VAL	CA-C-N	-5.83	115.08	122.43
26	R	80	VAL	C-N-CA	-5.83	115.08	122.43
57	C4	190	GLY	N-CA-C	5.82	117.83	110.38
29	U	120	THR	CA-C-N	5.80	140.93	127.00
29	U	120	THR	C-N-CA	5.80	140.93	127.00
49	A0	174	GLY	CA-C-N	5.80	127.09	119.84
49	A0	174	GLY	C-N-CA	5.80	127.09	119.84
49	A0	190	ASP	CB-CA-C	-5.73	109.44	117.23
58	C2	198	PHE	N-CA-C	5.73	117.52	111.28
42	j	22	PRO	CA-C-N	5.72	140.73	127.00
42	j	22	PRO	C-N-CA	5.72	140.73	127.00
65	C3	25	GLY	N-CA-C	5.72	118.95	110.60
59	A7	129	ALA	CA-C-N	5.70	126.96	119.84
59	A7	129	ALA	C-N-CA	5.70	126.96	119.84
56	A9	129	TYR	CB-CA-C	-5.68	100.50	109.42
43	g	27	PRO	CA-C-N	-5.67	109.04	122.31
43	g	27	PRO	C-N-CA	-5.67	109.04	122.31
9	8	228	PRO	CA-C-O	-5.67	111.81	120.03
27	S	113	ASP	N-CA-C	5.66	117.25	111.14
27	S	196	ASP	N-CA-C	-5.64	101.94	110.28
26	R	175	LYS	CA-C-N	-5.63	113.06	122.17
26	R	175	LYS	C-N-CA	-5.63	113.06	122.17
57	C4	104	TRP	N-CA-C	5.61	122.74	110.80
64	B4	20	HIS	N-CA-C	5.60	118.14	111.71
44	e	80	ASP	CA-C-N	5.59	132.22	121.54
44	e	80	ASP	C-N-CA	5.59	132.22	121.54
14	E	86	TYR	CA-CB-CG	-5.57	103.88	113.90
2	4	59	ASP	CA-C-N	-5.56	110.92	121.54
2	4	59	ASP	C-N-CA	-5.56	110.92	121.54
10	A	139	LEU	CA-CB-CG	-5.56	96.85	116.30
44	e	82	SER	N-CA-C	5.56	122.64	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	A0	114	VAL	CA-C-N	-5.56	110.92	121.54
49	A0	114	VAL	C-N-CA	-5.56	110.92	121.54
62	A4	72	ASN	CA-C-N	5.55	125.91	119.47
62	A4	72	ASN	C-N-CA	5.55	125.91	119.47
14	E	154	TYR	CA-CB-CG	-5.54	103.93	113.90
58	C2	188	ILE	CB-CA-C	-5.53	104.68	112.14
61	A6	82	CYS	CA-C-N	5.52	125.35	119.28
61	A6	82	CYS	C-N-CA	5.52	125.35	119.28
3	2	85	THR	CB-CA-C	-5.50	108.63	115.89
26	R	133	GLU	CA-C-N	5.50	129.50	121.31
26	R	133	GLU	C-N-CA	5.50	129.50	121.31
67	C1	16	GLU	N-CA-C	5.50	117.35	111.36
65	C3	2	GLU	N-CA-C	5.49	122.49	110.80
28	T	19	HIS	N-CA-C	5.47	118.30	111.24
56	A9	159	LEU	N-CA-C	-5.47	105.40	111.36
56	A9	245	ILE	N-CA-C	-5.45	104.24	111.05
8	1	252	PRO	N-CA-C	-5.41	105.73	113.47
7	3	2	ASN	CA-C-N	-5.39	113.30	120.63
7	3	2	ASN	C-N-CA	-5.39	113.30	120.63
49	p	75	GLU	CA-C-O	-5.39	115.14	120.80
56	A9	305	PHE	N-CA-C	5.37	118.93	112.38
9	8	36	LYS	CA-C-N	5.36	131.35	121.70
9	8	36	LYS	C-N-CA	5.36	131.35	121.70
3	2	157	LEU	CA-C-N	-5.35	113.35	120.63
3	2	157	LEU	C-N-CA	-5.35	113.35	120.63
10	A	121	LEU	CA-CB-CG	-5.33	97.66	116.30
44	e	87	ASP	CA-C-N	-5.30	114.33	119.90
44	e	87	ASP	C-N-CA	-5.30	114.33	119.90
56	A9	372	TYR	N-CA-C	-5.29	105.41	111.07
9	8	259	GLY	N-CA-C	-5.28	104.50	112.84
9	8	108	GLY	CA-C-N	-5.27	111.13	122.67
9	8	108	GLY	C-N-CA	-5.27	111.13	122.67
24	P	57	ARG	N-CA-C	-5.26	102.12	109.96
8	1	68	ALA	N-CA-C	5.25	117.75	111.71
2	4	227	GLY	N-CA-C	-5.25	106.82	114.90
9	8	259	GLY	CA-C-N	5.24	131.14	121.70
9	8	259	GLY	C-N-CA	5.24	131.14	121.70
2	4	119	TYR	CA-CB-CG	-5.23	104.48	113.90
12	C	159	VAL	CB-CA-C	-5.23	108.80	114.35
8	1	236	ILE	N-CA-C	-5.22	107.38	112.29
56	A9	262	SER	N-CA-C	-5.22	106.59	113.17
65	C3	9	GLN	N-CA-C	-5.22	105.49	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	428	GLY	N-CA-C	-5.21	107.80	114.37
58	C2	99	TRP	N-CA-C	-5.21	105.50	111.07
42	j	22	PRO	C-N-CD	-5.20	109.15	120.60
16	G	154	LYS	CA-C-N	-5.19	113.57	118.97
16	G	154	LYS	C-N-CA	-5.19	113.57	118.97
30	V	10	MET	N-CA-C	5.18	119.21	112.17
16	G	155	PRO	CA-C-O	-5.17	112.53	120.03
61	A6	38	ALA	N-CA-C	5.17	117.79	110.50
56	A9	377	PHE	N-CA-C	5.17	119.44	113.18
63	A5	22	ASN	N-CA-C	5.15	117.69	109.81
56	A9	401	SER	N-CA-C	5.14	119.69	113.41
25	Q	147	ARG	CA-C-N	5.14	139.33	127.00
25	Q	147	ARG	C-N-CA	5.14	139.33	127.00
10	A	308	ARG	N-CA-C	5.13	119.54	113.28
56	A9	353	LEU	N-CA-C	-5.13	105.76	111.36
64	B4	2	THR	N-CA-C	5.13	116.21	108.46
46	x	304	HIS	CA-C-N	5.11	134.26	121.80
46	x	304	HIS	C-N-CA	5.11	134.26	121.80
58	C2	107	ALA	CA-C-N	5.11	125.90	119.98
58	C2	107	ALA	C-N-CA	5.11	125.90	119.98
38	d	31	PHE	CA-C-N	5.10	139.25	127.00
38	d	31	PHE	C-N-CA	5.10	139.25	127.00
44	e	113	ILE	N-CA-C	-5.10	107.78	112.83
8	1	204	GLU	CA-C-N	5.08	129.11	120.88
8	1	204	GLU	C-N-CA	5.08	129.11	120.88
15	F	97	MET	CA-C-N	5.08	125.52	120.14
15	F	97	MET	C-N-CA	5.08	125.52	120.14
6	5	90	VAL	CA-C-N	5.07	131.22	121.54
6	5	90	VAL	C-N-CA	5.07	131.22	121.54
57	C4	66	THR	N-CA-C	-5.07	107.75	114.04
31	W	106	LYS	N-CA-C	-5.06	105.85	112.23
56	A9	2	PHE	N-CA-C	-5.06	105.65	111.07
56	A9	378	HIS	CB-CG-CD2	-5.06	124.62	131.20
57	C4	165	VAL	CA-C-N	5.05	126.16	119.84
57	C4	165	VAL	C-N-CA	5.05	126.16	119.84
23	O	75	ASP	N-CA-C	5.04	116.39	108.23
46	l	230	LEU	CA-C-N	5.03	129.94	122.30
46	l	230	LEU	C-N-CA	5.03	129.94	122.30
56	A9	378	HIS	N-CA-C	-5.03	106.31	112.90
50	q	20	TYR	N-CA-C	-5.03	105.69	111.07
57	C4	12	ALA	N-CA-C	5.03	117.45	109.96
61	A6	81	ARG	N-CA-C	5.02	117.62	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A9	70	VAL	N-CA-C	5.02	115.45	110.23
10	A	222	ILE	CB-CA-C	-5.01	105.37	112.14
40	h	82	VAL	N-CA-C	5.01	119.77	109.34
26	R	332	LEU	CA-C-N	5.01	125.28	119.47
26	R	332	LEU	C-N-CA	5.01	125.28	119.47

There are no chirality outliers.

All (194) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	125	SER	Peptide
8	1	195	ARG	Peptide
8	1	66	SER	Mainchain
3	2	106	LEU	Peptide
3	2	112	HIS	Peptide
3	2	147	PRO	Peptide
3	2	193	VAL	Peptide
3	2	220	MET	Peptide
3	2	24	SER	Peptide
3	2	327	PRO	Peptide
3	2	336	MET	Peptide
3	2	337	LEU	Peptide
3	2	45	MET	Peptide
7	3	42	ASP	Peptide
7	3	69	ILE	Peptide
2	4	20	ASN	Peptide
2	4	226	ALA	Peptide
2	4	306	PRO	Peptide
2	4	419	TYR	Peptide
2	4	48	ASN	Peptide
2	4	56	PHE	Peptide
2	4	60	SER	Peptide
2	4	64	PRO	Peptide
2	4	74	PRO	Peptide
6	5	15	SER	Peptide
6	5	16	LEU	Peptide
6	5	24	SER	Peptide
6	5	93	LEU	Peptide
5	6	30	SER	Peptide
5	6	351	ASN	Peptide
5	6	522	PHE	Peptide
5	6	64	SER	Peptide

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Mol	Chain	Res	Type	Group
5	6	65	ASN	Peptide
4	7	137	SER	Peptide
4	7	170	GLU	Peptide
4	7	24	PRO	Peptide
4	7	25	SER	Peptide
4	7	26	PRO	Peptide
4	7	72	THR	Peptide
9	8	102	MET	Peptide
9	8	203	ALA	Peptide
9	8	204	TYR	Peptide
9	8	208	GLU	Peptide
9	8	228	PRO	Peptide
9	8	260	ALA	Peptide
9	8	306	GLY	Peptide
9	8	404	ALA	Peptide
1	9	109	PRO	Peptide
1	9	150	GLU	Peptide
1	9	167	LYS	Peptide
1	9	228	ALA	Peptide
1	9	75	LYS	Peptide
1	9	91	GLY	Peptide
10	A	124	HIS	Peptide
10	A	127	ASP	Peptide
10	A	128	CYS	Peptide
10	A	143	SER	Peptide
10	A	147	GLY	Peptide
10	A	236	TYR	Peptide
10	A	253	VAL	Peptide
10	A	259	SER	Peptide
10	A	274	LEU	Peptide
10	A	308	ARG	Peptide
10	A	460	HIS	Peptide
10	A	549	GLY	Peptide
10	A	564	CYS	Peptide
10	A	689	LEU	Peptide
10	A	691	ILE	Peptide
10	A	98	LYS	Peptide
49	A0	161	HIS	Peptide
49	A0	192	MET	Peptide
49	A0	193	VAL	Peptide
53	A3	45	VAL	Peptide
11	B	219	GLY	Peptide

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Mol	Chain	Res	Type	Group
11	B	272	THR	Peptide
11	B	290	GLY	Peptide
11	B	309	ASP	Peptide
55	B1	58	GLN	Peptide
55	B1	61	GLY	Peptide
55	B1	63	PRO	Peptide
55	B1	70	LEU	Peptide
55	B1	71	ASN	Peptide
13	D	113	PHE	Peptide
13	D	126	ALA	Peptide
13	D	161	GLY	Peptide
13	D	184	PRO	Peptide
13	D	186	CYS	Peptide
13	D	188	PRO	Peptide
14	E	106	TYR	Peptide
14	E	107	PRO	Peptide
14	E	108	SER	Peptide
14	E	75	SER	Peptide
14	E	85	ASN	Peptide
17	H	84	GLU	Peptide
17	H	94	PRO	Peptide
18	I	69	ILE	Peptide
20	K	40	ARG	Peptide
21	L	40	LYS	Peptide
31	M	24	LYS	Peptide
31	M	37	MET	Peptide
31	M	63	PRO	Peptide
22	N	17	CYS	Peptide
23	O	42	GLU	Peptide
24	P	109	ASP	Peptide
24	P	44	GLY	Peptide
24	P	62	GLU	Peptide
25	Q	39	PRO	Peptide
25	Q	91	TYR	Peptide
26	R	154	GLN	Peptide
26	R	221	ARG	Peptide
26	R	253	ILE	Peptide
26	R	271	TYR	Peptide
26	R	324	THR	Peptide
26	R	333	PRO	Peptide
26	R	355	ARG	Peptide
26	R	371	PRO	Peptide

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Mol	Chain	Res	Type	Group
26	R	78	SER	Peptide
27	S	311	GLN	Peptide
27	S	337	ASP	Peptide
27	S	66	ALA	Peptide
27	S	67	GLU	Peptide
29	U	117	LEU	Peptide
29	U	118	SER	Peptide
29	U	47	LYS	Peptide
30	V	142	TRP	Peptide
30	V	72	MET	Peptide
31	W	128	PHE	Peptide
31	W	154	VAL	Peptide
34	Z	23	LYS	Peptide
34	Z	63	PHE	Peptide
35	a	26	SER	Peptide
36	b	110	TRP	Peptide
36	b	129	PRO	Peptide
36	b	132	ASN	Peptide
36	b	134	GLU	Peptide
38	d	18	ASP	Peptide
44	e	107	TRP	Peptide
44	e	60	GLU	Peptide
44	e	65	TYR	Peptide
44	e	79	PRO	Peptide
44	e	80	ASP	Peptide
44	e	81	ARG	Peptide
44	e	87	ASP	Peptide
39	f	109	PRO	Peptide
39	f	131	GLU	Peptide
39	f	150	ARG	Peptide
43	g	160	LYS	Peptide
40	h	133	GLY	Peptide
40	h	80	PRO	Peptide
40	h	81	ALA	Peptide
42	j	21	LEU	Peptide
42	j	54	LEU	Peptide
45	k	212	ALA	Peptide
45	k	228	VAL	Peptide
45	k	428	ILE	Peptide
46	l	227	ARG	Peptide
46	l	229	GLY	Mainchain,Peptide
46	l	231	GLY	Peptide

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Mol	Chain	Res	Type	Group
46	l	304	HIS	Peptide
47	m	171	ASP	Peptide
47	m	343	VAL	Mainchain
47	m	7	SER	Peptide
47	m	8	HIS	Peptide
48	o	50	HIS	Peptide
48	o	68	VAL	Peptide
48	o	69	GLU	Mainchain
48	o	78	GLY	Peptide
48	o	79	GLU	Peptide
48	o	81	PHE	Peptide
48	o	83	ARG	Peptide
49	p	116	GLN	Peptide
49	p	133	VAL	Peptide
49	p	135	LEU	Peptide
49	p	143	GLY	Peptide
49	p	76	ILE	Peptide
49	p	77	LYS	Peptide
45	w	212	ALA	Peptide
45	w	213	GLN	Peptide
45	w	214	LYS	Mainchain
45	w	428	ILE	Peptide
46	x	227	ARG	Peptide
46	x	229	GLY	Mainchain
46	x	230	LEU	Peptide
47	y	171	ASP	Peptide
47	y	7	SER	Peptide
47	y	8	HIS	Peptide
48	z	50	HIS	Peptide
48	z	68	VAL	Peptide
48	z	69	GLU	Mainchain,Peptide
48	z	71	GLN	Peptide
48	z	78	GLY	Peptide
48	z	83	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	1578	0	1553	167	0
2	4	3577	0	3674	398	0
3	2	2681	0	2823	257	0
4	7	1239	0	1193	83	0
5	6	4766	0	4897	363	0
6	5	712	0	742	82	0
7	3	879	0	906	60	0
8	1	2503	0	2617	293	0
9	8	3065	0	2801	239	0
10	A	5218	0	5232	376	0
11	B	3422	0	3345	397	0
12	C	1726	0	1676	219	0
13	D	1206	0	1203	204	0
14	E	1401	0	1353	281	0
15	F	186	0	139	29	0
16	G	985	0	976	78	0
17	H	780	0	753	45	0
18	I	533	0	511	63	0
19	J	530	0	503	30	0
20	K	656	0	647	37	0
21	L	602	0	591	102	0
22	N	862	0	868	40	0
23	O	925	0	907	122	0
24	P	702	0	670	90	0
25	Q	1345	0	1281	161	0
26	R	2407	0	2296	182	0
27	S	2299	0	2028	201	0
28	T	923	0	851	286	0
29	U	1019	0	900	72	0
30	V	1087	0	1037	110	0
31	M	642	0	642	79	0
31	W	616	0	579	44	0
32	X	372	0	314	19	0
33	Y	409	0	318	16	0
34	Z	493	0	395	58	0
35	a	857	0	765	155	0
36	b	1032	0	954	82	0
37	c	617	0	492	36	0
38	d	713	0	522	62	0
39	f	1156	0	892	56	0
40	h	658	0	584	71	0
41	i	277	0	240	54	0
42	j	883	0	823	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	1351	0	1262	190	0
44	e	864	0	567	122	0
45	k	3454	0	3350	137	0
45	w	3385	0	3296	134	0
46	l	3135	0	3112	101	0
46	x	3141	0	3123	114	0
47	m	3011	0	3077	132	0
47	y	3011	0	3077	110	0
48	o	1919	0	1870	90	0
48	z	1906	0	1841	76	0
49	A0	1117	0	807	123	0
49	p	938	0	733	52	0
50	A1	916	0	911	42	0
50	q	916	0	911	78	0
51	A2	676	0	668	20	0
51	r	682	0	679	19	0
52	B3	566	0	542	35	0
52	s	548	0	530	35	0
53	A3	318	0	314	66	0
53	t	262	0	250	13	0
54	B2	511	0	518	23	0
54	u	511	0	518	23	0
55	B1	148	0	154	23	0
55	v	114	0	107	4	0
56	A9	4025	0	4003	88	0
57	C4	1822	0	1834	73	0
58	C2	2124	0	2042	52	0
59	A7	1195	0	1183	34	0
60	C0	878	0	868	20	0
61	A6	748	0	728	25	0
62	A4	671	0	645	30	0
63	A5	628	0	582	21	0
64	B4	598	0	612	14	0
65	C3	441	0	439	17	0
66	B0	384	0	366	12	0
67	C1	386	0	388	8	0
68	A8	335	0	352	13	0
69	9	4	0	0	0	0
69	A	4	0	0	2	0
69	m	4	0	0	0	0
70	2	46	0	69	18	0
70	4	82	0	118	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	B	51	0	82	27	0
71	4	82	0	114	44	0
71	6	64	0	72	66	0
71	J	58	0	60	14	0
72	2	46	0	66	32	0
72	4	46	0	66	13	0
72	L	47	0	71	34	0
72	S	47	0	69	15	0
72	j	39	0	55	1	0
73	8	31	0	19	39	0
74	8	8	0	0	3	0
74	A	16	0	0	11	0
74	D	8	0	0	7	0
74	E	16	0	0	1	0
75	A6	1	0	0	0	0
75	I	1	0	0	0	0
76	R	48	0	23	10	0
77	m	86	0	60	10	0
77	y	86	0	60	10	0
78	o	43	0	32	1	0
78	z	43	0	32	1	0
79	A9	120	0	108	3	0
80	A9	1	0	0	0	0
80	C4	2	0	0	0	0
81	A9	1	0	0	0	0
All	All	107305	0	103928	6529	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 31.

All (6529) 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)
2:4:449:LEU:CB	71:4:502:CDL:H311	1.22	1.66
5:6:55:ILE:HD11	38:d:74:PHE:CZ	1.31	1.66
14:E:62:LEU:HD13	30:V:36:PHE:CZ	1.22	1.66
27:S:284:MET:CB	72:S:401:PC1:C12	1.76	1.61
49:A0:106:ILE:C	49:A0:167:ALA:HB1	1.27	1.60
41:i:62:HIS:HE1	42:j:23:PRO:CG	1.10	1.60
28:T:69:ILE:HD12	28:T:100:ILE:CD1	1.32	1.58
5:6:119:LYS:CD	71:6:701:CDL:H332	1.18	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:23:PHE:CE1	72:L:200:PC1:C28	1.79	1.58
27:S:342:LEU:HA	42:j:59:HIS:CD2	1.32	1.57
35:a:60:ILE:CG2	44:e:105:MET:HE1	1.29	1.57
35:a:47:TYR:CD1	44:e:105:MET:HB2	1.04	1.56
2:4:446:LEU:CD2	71:4:502:CDL:H371	1.36	1.56
49:A0:106:ILE:HA	49:A0:167:ALA:CB	1.33	1.56
23:O:33:ARG:HH22	31:M:44:SER:CB	1.19	1.54
49:A0:106:ILE:CA	49:A0:167:ALA:HB1	1.31	1.54
25:Q:158:LEU:HD12	42:j:88:HIS:CB	1.37	1.54
41:i:62:HIS:CE1	42:j:23:PRO:CG	1.88	1.53
35:a:47:TYR:CD1	44:e:105:MET:CB	1.85	1.52
21:L:23:PHE:CE1	72:L:200:PC1:H282	1.30	1.51
2:4:166:TYR:CE1	70:4:503:3PE:H11	1.46	1.51
49:A0:117:LEU:HA	49:A0:121:GLN:CB	1.33	1.50
49:A0:106:ILE:HA	49:A0:167:ALA:CA	1.38	1.49
5:6:119:LYS:HD2	71:6:701:CDL:C33	1.40	1.49
14:E:188:GLU:CD	18:I:64:ASN:HB2	1.11	1.48
8:1:172:MET:HE1	8:1:176:LEU:CD1	0.98	1.46
2:4:421:TYR:CE1	35:a:59:VAL:HA	1.47	1.45
7:3:84:LEU:HD21	8:1:309:ILE:CD1	1.47	1.44
5:6:556:ILE:CD1	35:a:76:ILE:HD12	1.43	1.44
13:D:103:ARG:NH1	14:E:84:ILE:HD11	1.24	1.44
28:T:34:LEU:HD13	28:T:35:VAL:N	1.32	1.42
21:L:23:PHE:HE1	72:L:200:PC1:C28	1.20	1.41
21:L:8:PHE:CZ	72:L:200:PC1:H322	1.53	1.41
49:A0:117:LEU:CA	49:A0:121:GLN:CB	1.97	1.41
35:a:16:THR:N	44:e:125:ASN:HB3	1.33	1.40
43:g:78:GLN:CB	43:g:81:ASP:OD2	1.66	1.40
27:S:284:MET:CB	72:S:401:PC1:C11	1.97	1.40
27:S:333:GLU:CG	42:j:52:PRO:HG2	0.92	1.39
5:6:556:ILE:HD11	35:a:76:ILE:CD1	1.53	1.39
11:B:242:ASP:CB	24:P:32:SER:OG	1.69	1.39
35:a:79:ASN:ND2	44:e:73:GLY:HA2	1.34	1.39
5:6:55:ILE:HD12	38:d:74:PHE:CE1	1.54	1.39
13:D:103:ARG:NH1	14:E:84:ILE:CD1	1.86	1.38
27:S:333:GLU:HG2	42:j:52:PRO:CG	0.92	1.38
27:S:199:VAL:CB	27:S:200:PRO:HD3	1.41	1.38
41:i:69:TYR:CD1	42:j:20:SER:O	1.77	1.38
41:i:58:LEU:HD11	42:j:73:TYR:CE2	1.56	1.38
41:i:62:HIS:CE1	42:j:23:PRO:HG2	1.47	1.38
14:E:62:LEU:CD1	30:V:36:PHE:CZ	2.06	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A0:155:GLY:O	49:A0:165:TYR:CB	1.71	1.37
24:P:40:LYS:HB3	30:V:7:LYS:N	1.34	1.37
8:1:172:MET:CE	8:1:176:LEU:HD12	0.89	1.36
10:A:355:LYS:HD2	10:A:530:TYR:CE1	1.60	1.36
23:O:33:ARG:NH2	31:M:44:SER:HB2	1.37	1.35
5:6:55:ILE:CD1	38:d:74:PHE:CZ	2.08	1.35
8:1:79:LEU:CD1	8:1:222:LEU:HD22	1.55	1.35
5:6:55:ILE:CD1	38:d:74:PHE:CE1	2.10	1.35
5:6:153:LEU:CD1	71:6:701:CDL:C55	2.05	1.34
14:E:188:GLU:CD	18:I:64:ASN:CB	1.99	1.34
27:S:284:MET:CB	72:S:401:PC1:H112	1.56	1.34
5:6:470:ASN:HD21	38:d:77:PHE:CA	1.39	1.34
14:E:50:MET:HE1	21:L:10:LYS:CB	1.58	1.34
35:a:47:TYR:CG	44:e:105:MET:HB2	1.61	1.33
18:I:109:THR:CB	18:I:119:PHE:O	1.77	1.33
3:2:326:LEU:HD11	72:2:402:PC1:C2A	1.56	1.32
53:A3:47:TYR:CD2	54:B2:33:ARG:NH2	1.96	1.32
41:i:47:THR:HB	42:j:63:LEU:CD1	1.59	1.31
27:S:342:LEU:CA	42:j:59:HIS:CD2	2.10	1.31
41:i:69:TYR:HD1	42:j:20:SER:C	1.36	1.31
11:B:261:MET:SD	14:E:70:LEU:HD21	1.70	1.30
28:T:13:PRO:HG3	28:T:20:ARG:NH2	1.45	1.30
34:Z:43:ASP:O	39:f:38:ARG:NH2	1.63	1.30
50:A1:13:LEU:O	50:A1:14:GLU:HG3	1.14	1.30
49:A0:151:GLY:H	49:A0:157:TYR:CB	1.43	1.30
21:L:23:PHE:CZ	72:L:200:PC1:H282	1.66	1.30
35:a:39:ILE:CB	44:e:56:ASN:CB	2.08	1.30
23:O:33:ARG:NH2	31:M:44:SER:CB	1.90	1.29
23:O:33:ARG:HH11	31:M:48:VAL:CG2	1.43	1.29
23:O:33:ARG:CD	31:M:48:VAL:HG21	1.61	1.29
41:i:47:THR:CB	42:j:63:LEU:HD12	1.63	1.29
2:4:185:PRO:HG3	42:j:115:GLU:OE2	1.33	1.29
5:6:470:ASN:ND2	38:d:77:PHE:CD1	1.97	1.29
12:C:227:GLU:CG	26:R:49:SER:HB3	1.60	1.29
28:T:69:ILE:CD1	28:T:100:ILE:HD11	1.61	1.29
49:A0:106:ILE:O	49:A0:167:ALA:CB	1.78	1.29
49:A0:122:HIS:CB	49:A0:168:SER:CB	2.11	1.29
10:A:111:LYS:HA	24:P:53:TYR:OH	1.15	1.28
8:1:176:LEU:HB2	8:1:177:PRO:CD	1.61	1.28
41:i:68:GLU:CG	42:j:19:ARG:HD2	1.62	1.28
35:a:60:ILE:CG2	44:e:105:MET:CE	2.10	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:68:GLU:CB	42:j:19:ARG:HD2	1.61	1.28
2:4:166:TYR:CG	70:4:503:3PE:O22	1.86	1.28
50:q:15:GLY:O	50:q:19:TRP:HB3	1.34	1.28
28:T:26:THR:CG2	28:T:68:ALA:HA	1.65	1.27
3:2:325:PHE:CD2	70:2:401:3PE:H2G1	1.69	1.27
10:A:320:GLU:HB2	23:O:123:TYR:OH	1.10	1.27
28:T:5:VAL:CG1	28:T:28:ILE:HD11	1.65	1.27
2:4:423:ILE:HB	35:a:57:ARG:CG	1.65	1.27
28:T:109:GLY:O	28:T:110:ILE:CG1	1.83	1.27
14:E:61:LEU:HD13	21:L:17:PRO:O	1.35	1.26
11:B:237:PRO:HD3	14:E:96:ARG:NH2	1.48	1.26
27:S:199:VAL:CB	27:S:200:PRO:CD	2.14	1.26
49:A0:110:ALA:HB2	49:A0:122:HIS:O	1.19	1.26
9:8:98:LYS:NZ	73:8:501:FMN:O2P	1.67	1.25
1:9:72:GLU:HB3	15:F:103:GLY:O	1.32	1.25
2:4:424:ASN:HA	35:a:57:ARG:NH2	1.49	1.25
5:6:119:LYS:CD	71:6:701:CDL:C33	2.06	1.25
31:W:156:GLU:OE2	37:c:24:LYS:HA	1.36	1.25
23:O:33:ARG:HH12	31:M:44:SER:C	1.44	1.25
34:Z:44:PRO:C	39:f:38:ARG:HH22	1.45	1.25
23:O:33:ARG:NH1	31:M:44:SER:O	1.69	1.24
8:1:233:MET:HA	8:1:236:ILE:CG2	1.67	1.24
12:C:240:PRO:HG3	16:G:88:GLN:NE2	1.52	1.24
1:9:69:ASN:OD1	15:F:97:MET:HE1	1.10	1.24
16:G:58:LYS:O	23:O:15:THR:N	1.69	1.24
41:i:62:HIS:CE1	42:j:23:PRO:HG3	1.59	1.23
2:4:446:LEU:HD23	71:4:502:CDL:C37	1.66	1.23
18:I:109:THR:CB	18:I:120:ARG:HA	1.67	1.23
23:O:33:ARG:HD3	31:M:48:VAL:CG2	1.66	1.23
27:S:196:ASP:OD1	27:S:246:TYR:CB	1.85	1.23
9:8:207:GLY:HA2	73:8:501:FMN:C9A	1.69	1.23
2:4:449:LEU:CB	71:4:502:CDL:C31	2.15	1.22
11:B:320:ILE:HD12	14:E:39:LYS:O	1.39	1.22
14:E:188:GLU:OE1	18:I:64:ASN:HB2	1.36	1.22
19:J:3:PHE:CE2	71:J:101:CDL:HB62	1.72	1.22
10:A:320:GLU:HB2	23:O:123:TYR:CZ	1.75	1.22
49:A0:110:ALA:CB	49:A0:122:HIS:O	1.88	1.22
2:4:423:ILE:CB	35:a:57:ARG:HG3	1.69	1.21
14:E:57:ALA:HB3	21:L:13:TRP:CZ3	1.75	1.21
3:2:325:PHE:CE2	70:2:401:3PE:H2I2	1.73	1.21
53:A3:47:TYR:CE2	54:B2:33:ARG:NH2	2.09	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:33:ARG:NH1	31:M:48:VAL:HG23	1.54	1.21
49:A0:117:LEU:CB	49:A0:121:GLN:CB	2.17	1.21
49:A0:156:TYR:CB	49:A0:165:TYR:CB	2.18	1.21
9:8:207:GLY:HA2	73:8:501:FMN:C9	1.72	1.20
11:B:61:TRP:CH2	11:B:64:PRO:CG	2.24	1.20
2:4:449:LEU:HB2	71:4:502:CDL:C31	1.72	1.20
14:E:188:GLU:OE2	18:I:64:ASN:CB	1.89	1.20
28:T:22:THR:O	28:T:26:THR:HG23	1.37	1.20
2:4:360:LEU:HD13	71:6:701:CDL:H511	1.24	1.19
41:i:69:TYR:CE1	42:j:20:SER:O	1.94	1.19
3:2:326:LEU:CD1	72:2:402:PC1:H2A2	1.70	1.19
49:A0:85:LYS:HA	49:A0:149:ASN:CB	1.71	1.19
35:a:60:ILE:HG21	44:e:105:MET:SD	1.82	1.19
50:q:18:LYS:HG3	50:q:83:TYR:CE2	1.76	1.19
5:6:470:ASN:ND2	38:d:77:PHE:HA	1.56	1.19
12:C:229:ALA:O	16:G:114:TRP:CE3	1.96	1.19
42:j:114:GLU:HB2	43:g:160:LYS:CE	1.70	1.19
49:A0:151:GLY:N	49:A0:157:TYR:CB	2.02	1.19
13:D:195:TYR:CE2	29:U:116:ASN:ND2	2.11	1.19
2:4:166:TYR:CZ	70:4:503:3PE:H11	1.77	1.18
41:i:69:TYR:CD1	42:j:20:SER:C	2.19	1.18
51:A2:37:VAL:O	51:A2:41:THR:HG23	1.38	1.18
21:L:8:PHE:CE2	72:L:200:PC1:H322	1.77	1.18
35:a:16:THR:N	44:e:125:ASN:CB	2.05	1.18
42:j:119:VAL:N	43:g:147:GLY:H	1.40	1.18
8:1:71:PHE:CZ	8:1:215:TYR:CE1	1.93	1.18
11:B:61:TRP:CH2	11:B:64:PRO:HG3	1.78	1.18
25:Q:158:LEU:CG	25:Q:159:LYS:H	1.55	1.18
50:q:16:ILE:O	50:q:20:TYR:N	1.76	1.18
2:4:166:TYR:CD2	70:4:503:3PE:O22	1.97	1.18
14:E:135:ARG:NH2	18:I:72:ILE:HD11	1.57	1.18
5:6:119:LYS:HE3	71:6:701:CDL:H331	1.21	1.17
11:B:61:TRP:CZ2	11:B:64:PRO:CG	2.27	1.17
23:O:48:HIS:ND1	26:R:359:TYR:OH	1.71	1.17
28:T:13:PRO:CG	28:T:20:ARG:HH22	1.56	1.17
28:T:101:LEU:CD1	28:T:110:ILE:HG22	1.74	1.17
2:4:166:TYR:OH	70:4:503:3PE:O13	1.58	1.17
10:A:176:CYS:SG	74:A:802:SF4:S4	2.41	1.17
11:B:90:ALA:HB1	11:B:93:GLY:O	1.43	1.17
11:B:242:ASP:HB2	24:P:32:SER:OG	0.99	1.17
11:B:320:ILE:O	14:E:41:VAL:CG2	1.92	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:13:LEU:O	50:A1:14:GLU:CG	1.93	1.17
3:2:319:LEU:O	72:2:402:PC1:H222	1.39	1.17
21:L:23:PHE:CE1	72:L:200:PC1:H281	1.60	1.17
50:A1:12:TRP:HZ3	50:A1:13:LEU:HD22	1.02	1.17
27:S:342:LEU:HA	42:j:59:HIS:NE2	1.57	1.16
11:B:62:LYS:CG	11:B:63:PRO:HD2	1.74	1.16
35:a:60:ILE:HG23	44:e:105:MET:HE1	1.23	1.16
42:j:114:GLU:CB	43:g:160:LYS:CD	2.21	1.16
49:A0:150:ALA:H	49:A0:155:GLY:CA	1.59	1.16
14:E:62:LEU:HD22	30:V:36:PHE:CE2	1.79	1.16
41:i:68:GLU:HG3	42:j:19:ARG:HD2	1.21	1.16
49:A0:91:TRP:CB	49:A0:196:GLY:HA3	1.73	1.16
7:3:84:LEU:CD2	8:1:309:ILE:HD11	1.76	1.16
13:D:103:ARG:CZ	14:E:84:ILE:HD13	1.74	1.16
25:Q:162:ARG:HD2	42:j:91:PHE:CZ	1.79	1.16
35:a:79:ASN:HD22	44:e:73:GLY:CA	1.57	1.16
2:4:421:TYR:CE1	35:a:59:VAL:CA	2.28	1.15
12:C:232:PHE:HB2	13:D:165:TYR:CE1	1.78	1.15
28:T:18:CYS:O	28:T:22:THR:HG22	1.45	1.15
1:9:71:PRO:HA	15:F:102:SER:CB	1.75	1.15
5:6:153:LEU:HD13	71:6:701:CDL:C54	1.76	1.15
49:A0:83:GLU:O	49:A0:100:HIS:O	1.61	1.15
49:A0:121:GLN:O	49:A0:170:ARG:CB	1.94	1.15
25:Q:9:SER:HA	30:V:88:ARG:HH12	1.12	1.15
13:D:91:CYS:HB2	74:D:301:SF4:S2	1.88	1.14
28:T:12:ILE:CB	28:T:13:PRO:CD	2.25	1.14
49:A0:121:GLN:C	49:A0:170:ARG:CB	2.20	1.14
7:3:88:LEU:HD11	8:1:309:ILE:HG21	1.29	1.14
11:B:320:ILE:O	14:E:41:VAL:HG23	1.44	1.14
11:B:322:SER:CB	14:E:42:ASN:HB3	1.76	1.14
5:6:556:ILE:CD1	35:a:76:ILE:CD1	2.15	1.14
12:C:213:ARG:HB3	13:D:175:ARG:HG2	1.23	1.14
28:T:101:LEU:HD11	28:T:110:ILE:HG22	1.19	1.14
21:L:8:PHE:CZ	72:L:200:PC1:C32	2.30	1.14
49:A0:106:ILE:O	49:A0:167:ALA:HB1	1.36	1.14
10:A:320:GLU:CB	23:O:123:TYR:OH	1.95	1.13
8:1:72:ILE:HG22	8:1:76:ILE:HD11	1.24	1.13
25:Q:162:ARG:HD2	42:j:91:PHE:HZ	0.99	1.13
27:S:335:VAL:HB	42:j:52:PRO:HD3	1.20	1.13
27:S:335:VAL:O	42:j:52:PRO:CD	1.94	1.13
10:A:110:LYS:HD3	24:P:55:CYS:SG	1.89	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:129:SER:OG	22:N:116:ILE:O	1.64	1.13
21:L:16:GLU:HG2	72:L:200:PC1:C15	1.78	1.13
8:1:79:LEU:HD12	8:1:222:LEU:HD22	1.27	1.13
8:1:172:MET:HE2	8:1:176:LEU:HD12	1.25	1.12
9:8:414:GLU:OE2	24:P:50:SER:O	1.66	1.12
2:4:446:LEU:CD2	71:4:502:CDL:C37	2.22	1.12
11:B:322:SER:HB3	14:E:42:ASN:HB3	1.25	1.12
13:D:195:TYR:OH	29:U:80:SER:CB	1.97	1.12
7:3:84:LEU:CD2	8:1:309:ILE:CD1	2.27	1.12
11:B:61:TRP:CD1	11:B:62:LYS:H	1.67	1.12
41:i:69:TYR:HD1	42:j:20:SER:CA	1.61	1.12
49:A0:150:ALA:H	49:A0:155:GLY:HA2	1.07	1.12
2:4:360:LEU:CD1	71:6:701:CDL:H511	1.78	1.12
27:S:196:ASP:OD1	27:S:246:TYR:HB3	1.40	1.12
50:A1:12:TRP:CZ3	50:A1:13:LEU:HD22	1.83	1.12
18:I:109:THR:CB	18:I:120:ARG:CA	2.28	1.12
2:4:105:PHE:HE1	72:4:504:PC1:C3C	1.63	1.11
19:J:3:PHE:HB3	71:J:101:CDL:H721	1.24	1.11
27:S:335:VAL:CB	42:j:52:PRO:HD3	1.80	1.11
42:j:116:PHE:HE1	43:g:157:ALA:HB1	1.12	1.11
42:j:114:GLU:HB2	43:g:160:LYS:HE2	1.28	1.11
1:9:191:ASN:OD1	9:8:164:ASN:ND2	1.82	1.11
8:1:38:ASN:OD1	29:U:31:ASN:OD1	1.67	1.11
25:Q:158:LEU:CD1	42:j:88:HIS:HB2	1.81	1.11
1:9:69:ASN:OD1	15:F:97:MET:CE	1.97	1.11
11:B:237:PRO:CD	14:E:96:ARG:HH22	1.64	1.11
13:D:195:TYR:OH	29:U:80:SER:HB2	1.47	1.11
11:B:242:ASP:CB	24:P:32:SER:HG	1.50	1.10
28:T:13:PRO:CG	28:T:20:ARG:NH2	2.14	1.10
8:1:176:LEU:CB	8:1:177:PRO:CD	2.25	1.10
10:A:355:LYS:CD	10:A:530:TYR:HE1	1.63	1.10
12:C:213:ARG:CB	13:D:175:ARG:HG2	1.80	1.10
14:E:62:LEU:CD1	30:V:36:PHE:CE1	2.34	1.10
28:T:26:THR:CB	28:T:68:ALA:HA	1.80	1.10
5:6:153:LEU:HD11	71:6:701:CDL:C55	1.77	1.10
21:L:56:PRO:CB	25:Q:129:THR:O	2.00	1.10
23:O:33:ARG:HB3	31:M:48:VAL:HG11	1.24	1.10
23:O:48:HIS:CE1	26:R:359:TYR:HH	1.69	1.10
42:j:119:VAL:CB	43:g:147:GLY:HA3	1.80	1.10
49:A0:106:ILE:CA	49:A0:167:ALA:CB	2.03	1.10
41:i:51:SER:OG	42:j:66:THR:HG21	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:90:THR:HG21	70:4:501:3PE:H322	1.21	1.09
5:6:153:LEU:HD11	71:6:701:CDL:H551	1.11	1.09
26:R:328:ILE:HG22	26:R:329:LEU:H	1.03	1.09
28:T:2:ALA:O	28:T:3:LYS:C	1.89	1.09
49:A0:150:ALA:N	49:A0:155:GLY:HA2	1.68	1.09
3:2:322:LYS:CD	70:2:401:3PE:H2D1	1.83	1.09
11:B:372:LYS:NZ	14:E:163:PRO:O	1.84	1.09
42:j:114:GLU:HB3	43:g:160:LYS:CD	1.79	1.09
42:j:116:PHE:CE1	43:g:157:ALA:HB1	1.87	1.09
8:1:176:LEU:HB2	8:1:177:PRO:HD2	1.26	1.09
21:L:8:PHE:HZ	72:L:200:PC1:C32	1.65	1.09
28:T:26:THR:HG22	28:T:68:ALA:HA	1.24	1.09
5:6:153:LEU:CD1	71:6:701:CDL:C54	2.30	1.08
2:4:421:TYR:CE1	35:a:59:VAL:HG12	1.87	1.08
10:A:310:GLU:OE2	10:A:311:LYS:NZ	1.85	1.08
11:B:61:TRP:CD1	11:B:62:LYS:N	2.21	1.08
28:T:12:ILE:CB	28:T:13:PRO:HD3	1.83	1.08
10:A:127:ASP:OD2	10:A:175:ARG:NH1	1.86	1.08
12:C:207:SER:OG	13:D:171:ARG:NH2	1.86	1.08
28:T:17:GLU:O	28:T:20:ARG:NH2	1.85	1.08
35:a:60:ILE:HG22	44:e:105:MET:HE1	1.31	1.08
5:6:556:ILE:CG1	35:a:76:ILE:CD1	2.30	1.08
8:1:245:THR:OG1	8:1:255:TYR:CE1	2.05	1.08
13:D:155:SER:OG	14:E:150:THR:O	1.68	1.08
31:W:85:TYR:HE1	34:Z:18:ASP:C	1.60	1.08
35:a:70:TYR:HD2	44:e:35:ASP:CB	1.66	1.08
25:Q:158:LEU:CD1	42:j:88:HIS:CB	2.32	1.08
5:6:470:ASN:ND2	38:d:77:PHE:HD1	1.42	1.07
71:4:502:CDL:C67	5:6:20:MET:O	2.02	1.07
5:6:153:LEU:CD1	71:6:701:CDL:H541	1.83	1.07
24:P:40:LYS:CB	30:V:7:LYS:N	2.16	1.07
49:A0:110:ALA:HB1	49:A0:123:ASP:CB	1.84	1.07
71:4:502:CDL:H672	5:6:20:MET:O	1.54	1.07
9:8:116:ASN:ND2	73:8:501:FMN:O3'	1.87	1.07
10:A:110:LYS:CD	24:P:55:CYS:SG	2.42	1.07
11:B:254:ARG:HD2	24:P:24:LEU:HG	1.35	1.07
5:6:119:LYS:CE	71:6:701:CDL:C33	2.32	1.06
27:S:342:LEU:CA	42:j:59:HIS:NE2	2.16	1.06
28:T:13:PRO:HB2	28:T:16:THR:O	1.55	1.06
28:T:69:ILE:CD1	28:T:100:ILE:CD1	2.26	1.06
5:6:557:TRP:CZ2	35:a:80:PHE:HZ	1.72	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:61:TRP:CH2	11:B:64:PRO:HG2	1.91	1.06
11:B:61:TRP:CG	11:B:62:LYS:H	1.67	1.06
31:W:85:TYR:OH	34:Z:22:TRP:HZ3	1.34	1.06
41:i:68:GLU:HG3	42:j:19:ARG:CD	1.83	1.06
5:6:153:LEU:HD12	71:6:701:CDL:H552	1.37	1.06
5:6:593:ILE:HD12	28:T:42:ALA:HB2	1.37	1.06
11:B:267:ILE:HD11	70:B:501:3PE:H282	1.38	1.06
25:Q:158:LEU:HD12	42:j:88:HIS:CG	1.90	1.06
12:C:227:GLU:HG3	26:R:49:SER:HB3	1.32	1.06
35:a:68:TRP:HH2	44:e:110:ASP:OD1	1.38	1.06
41:i:47:THR:CB	42:j:63:LEU:CD1	2.26	1.06
42:j:116:PHE:HE1	43:g:157:ALA:CB	1.67	1.06
3:2:326:LEU:HD11	72:2:402:PC1:H2A2	1.12	1.06
25:Q:158:LEU:HG	25:Q:159:LYS:N	1.39	1.06
27:S:338:LYS:HE2	42:j:60:ARG:NH1	1.70	1.06
21:L:55:VAL:O	25:Q:128:VAL:CG2	2.04	1.05
2:4:446:LEU:HD23	71:4:502:CDL:H371	1.09	1.05
2:4:166:TYR:CE1	70:4:503:3PE:C1	2.38	1.05
49:A0:106:ILE:HA	49:A0:167:ALA:HA	1.37	1.05
28:T:62:THR:HG22	28:T:63:ALA:H	0.89	1.05
1:9:71:PRO:HA	15:F:102:SER:HB3	1.07	1.04
1:9:71:PRO:CA	15:F:102:SER:HB3	1.85	1.04
9:8:207:GLY:HA2	73:8:501:FMN:C5A	1.86	1.04
28:T:5:VAL:HG11	28:T:28:ILE:HD11	1.08	1.04
43:g:91:GLN:NE2	43:g:95:ASP:OD2	1.90	1.04
14:E:62:LEU:HD13	30:V:36:PHE:CE1	1.92	1.04
23:O:33:ARG:HH11	31:M:48:VAL:HG23	1.07	1.04
24:P:39:PRO:CA	30:V:8:GLN:HB2	1.87	1.04
53:A3:43:ASP:HA	53:A3:47:TYR:CD2	1.93	1.04
8:1:172:MET:HE1	8:1:176:LEU:HD11	1.35	1.04
8:1:176:LEU:HB2	8:1:177:PRO:HD3	1.38	1.04
11:B:62:LYS:HG2	11:B:63:PRO:CD	1.86	1.04
11:B:237:PRO:HD3	14:E:96:ARG:HH22	0.88	1.04
27:S:333:GLU:CB	42:j:52:PRO:HG2	1.88	1.04
53:A3:43:ASP:O	53:A3:47:TYR:CD2	2.11	1.04
2:4:449:LEU:HB2	71:4:502:CDL:H311	1.07	1.04
2:4:449:LEU:HB3	71:4:502:CDL:C31	1.85	1.04
41:i:47:THR:CG2	42:j:63:LEU:CD1	2.35	1.04
14:E:50:MET:CE	21:L:10:LYS:CB	2.36	1.03
28:T:109:GLY:O	28:T:110:ILE:HG13	0.87	1.03
2:4:353:PRO:HB2	71:6:701:CDL:H1	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:312:GLY:N	29:U:144:TYR:CD1	2.26	1.03
12:C:227:GLU:HG2	26:R:49:SER:HB3	1.32	1.03
24:P:39:PRO:HA	30:V:8:GLN:HB2	1.35	1.03
42:j:119:VAL:H	43:g:147:GLY:N	1.56	1.03
5:6:593:ILE:CD1	28:T:42:ALA:HB2	1.88	1.03
14:E:54:THR:HA	21:L:13:TRP:HZ3	1.17	1.03
28:T:13:PRO:CB	28:T:20:ARG:HH22	1.71	1.03
11:B:265:ASN:ND2	14:E:70:LEU:HD12	1.74	1.03
27:S:342:LEU:C	42:j:59:HIS:NE2	2.16	1.02
28:T:62:THR:HG22	28:T:63:ALA:N	1.46	1.02
28:T:62:THR:O	28:T:64:ALA:N	1.91	1.02
8:1:79:LEU:HD11	8:1:222:LEU:HD22	1.37	1.02
8:1:176:LEU:CB	8:1:177:PRO:HD3	1.88	1.02
28:T:13:PRO:HB3	28:T:17:GLU:HB2	1.42	1.02
8:1:232:ILE:O	8:1:236:ILE:HG22	1.56	1.02
43:g:78:GLN:CB	43:g:81:ASP:CG	2.31	1.02
49:A0:106:ILE:CA	49:A0:167:ALA:CA	2.32	1.02
49:A0:151:GLY:CA	49:A0:157:TYR:CB	2.38	1.02
2:4:449:LEU:HB3	71:4:502:CDL:H311	1.07	1.02
3:2:325:PHE:CZ	70:2:401:3PE:H2I2	1.94	1.02
7:3:106:TRP:CZ2	72:L:200:PC1:H143	1.95	1.02
21:L:16:GLU:CG	72:L:200:PC1:H152	1.90	1.02
34:Z:45:TRP:N	39:f:38:ARG:HH22	1.56	1.02
47:m:376:LEU:HD23	50:q:17:ARG:HE	0.93	1.02
12:C:232:PHE:HB2	13:D:165:TYR:CD1	1.95	1.02
31:W:117:GLU:OE2	34:Z:45:TRP:HZ3	1.43	1.02
35:a:47:TYR:CE1	44:e:105:MET:HA	1.93	1.01
35:a:47:TYR:HD1	44:e:105:MET:CG	1.74	1.01
3:2:277:ILE:CG2	28:T:135:VAL:HG22	1.90	1.01
50:q:16:ILE:O	50:q:20:TYR:CB	2.07	1.01
7:3:106:TRP:HZ2	72:L:200:PC1:H143	1.23	1.01
10:A:312:GLY:N	29:U:144:TYR:HD1	1.55	1.01
12:C:212:LEU:CD2	13:D:176:ILE:HD11	1.91	1.01
16:G:57:GLU:OE2	23:O:16:SER:OG	1.77	1.01
35:a:60:ILE:HG21	44:e:105:MET:CE	1.86	1.01
38:d:105:GLU:OE2	44:e:165:ASN:N	1.93	1.01
9:8:207:GLY:HA2	73:8:501:FMN:C8	1.89	1.01
10:A:355:LYS:HB2	10:A:530:TYR:OH	1.58	1.01
35:a:68:TRP:CZ3	44:e:110:ASP:HA	1.96	1.01
2:4:446:LEU:HD21	71:4:502:CDL:H371	1.41	1.01
26:R:328:ILE:CG2	26:R:329:LEU:H	1.72	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:260:GLU:OE1	14:E:73:THR:OG1	1.77	1.00
23:O:48:HIS:HB2	26:R:359:TYR:CE1	1.96	1.00
24:P:39:PRO:HA	30:V:8:GLN:CB	1.91	1.00
3:2:338:PRO:O	42:j:83:TYR:OH	1.77	1.00
28:T:34:LEU:CD1	28:T:35:VAL:N	2.23	1.00
8:1:316:PRO:HG2	30:V:57:ARG:HE	1.21	1.00
10:A:614:GLY:O	23:O:126:HIS:NE2	1.93	1.00
25:Q:165:SER:OG	42:j:83:TYR:CD1	2.13	1.00
31:W:85:TYR:OH	34:Z:22:TRP:CZ3	2.13	1.00
14:E:135:ARG:HH21	18:I:72:ILE:HD11	1.23	1.00
8:1:157:SER:OG	8:1:168:THR:HG21	1.61	1.00
21:L:23:PHE:CZ	72:L:200:PC1:C28	2.34	1.00
27:S:335:VAL:O	42:j:52:PRO:HD2	1.57	1.00
10:A:111:LYS:HD3	24:P:53:TYR:CE2	1.97	0.99
14:E:171:PRO:HB2	14:E:200:GLU:OE2	1.61	0.99
47:m:376:LEU:HD23	50:q:17:ARG:NE	1.77	0.99
5:6:153:LEU:CD1	71:6:701:CDL:H551	1.80	0.99
49:A0:156:TYR:C	49:A0:165:TYR:CB	2.35	0.99
5:6:557:TRP:CZ2	35:a:80:PHE:CZ	2.50	0.99
26:R:170:LEU:O	26:R:328:ILE:HD12	1.62	0.99
27:S:333:GLU:HG2	42:j:52:PRO:CB	1.92	0.99
28:T:109:GLY:C	28:T:110:ILE:HG13	1.87	0.99
2:4:185:PRO:CG	42:j:115:GLU:OE2	2.09	0.99
13:D:138:ARG:NH1	13:D:141:TYR:HD2	1.61	0.99
27:S:196:ASP:OD1	27:S:246:TYR:HB2	1.58	0.99
27:S:338:LYS:CE	42:j:60:ARG:HH12	1.75	0.99
28:T:77:SER:HA	28:T:80:VAL:CG1	1.92	0.99
28:T:62:THR:CG2	28:T:63:ALA:H	1.68	0.99
1:9:143:ARG:NH1	9:8:285:PRO:HG2	1.77	0.99
27:S:335:VAL:CA	42:j:52:PRO:HD3	1.92	0.99
40:h:147:ILE:CD1	42:j:110:GLY:HA2	1.93	0.99
50:q:15:GLY:O	50:q:19:TRP:CB	2.09	0.99
27:S:338:LYS:HE2	42:j:60:ARG:HH12	0.85	0.99
14:E:62:LEU:HD11	30:V:36:PHE:CE1	1.98	0.99
23:O:33:ARG:NH1	31:M:48:VAL:CG2	2.14	0.99
25:Q:162:ARG:NH1	42:j:91:PHE:CZ	2.30	0.99
28:T:106:ARG:HA	28:T:106:ARG:NH1	1.77	0.98
53:A3:43:ASP:CG	53:A3:47:TYR:HB2	1.88	0.98
10:A:58:MET:CG	12:C:248:ARG:NH1	2.26	0.98
5:6:119:LYS:CE	71:6:701:CDL:H331	1.93	0.98
5:6:593:ILE:HD12	28:T:42:ALA:CB	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:57:ALA:HB3	21:L:13:TRP:CE3	1.97	0.98
10:A:75:CYS:SG	10:A:76:ARG:N	2.37	0.98
23:O:48:HIS:CG	26:R:359:TYR:OH	2.16	0.98
26:R:328:ILE:HG22	26:R:329:LEU:N	1.76	0.98
28:T:22:THR:HG21	28:T:75:CYS:SG	2.01	0.98
38:d:105:GLU:OE2	44:e:165:ASN:CA	2.10	0.98
1:9:233:SER:HB3	9:8:41:ILE:HD13	1.43	0.98
35:a:68:TRP:CH2	44:e:110:ASP:HA	1.98	0.98
21:L:55:VAL:O	25:Q:128:VAL:HG21	1.63	0.98
21:L:56:PRO:CA	25:Q:129:THR:O	2.11	0.98
25:Q:166:ARG:NH2	42:j:86:ARG:HH12	1.62	0.98
1:9:73:GLY:HA3	15:F:105:GLU:O	1.64	0.98
5:6:153:LEU:HD13	71:6:701:CDL:H541	0.99	0.98
49:A0:85:LYS:CA	49:A0:149:ASN:CB	2.40	0.98
1:9:176:CYS:O	9:8:159:ARG:NH1	1.95	0.97
40:h:149:LEU:HD11	43:g:167:ARG:CA	1.93	0.97
19:J:3:PHE:HB3	71:J:101:CDL:C72	1.93	0.97
2:4:90:THR:CG2	70:4:501:3PE:H322	1.94	0.97
13:D:99:MET:HG2	13:D:106:MET:HB2	1.46	0.97
3:2:239:ILE:HG21	42:j:47:ALA:O	1.65	0.97
3:2:325:PHE:CD2	70:2:401:3PE:C2G	2.47	0.97
23:O:128:PRO:HG2	26:R:45:LYS:CE	1.95	0.97
42:j:119:VAL:HB	43:g:147:GLY:HA3	1.00	0.97
27:S:335:VAL:HB	42:j:52:PRO:CD	1.93	0.97
28:T:101:LEU:HD11	28:T:110:ILE:CG2	1.94	0.97
10:A:58:MET:HG2	12:C:248:ARG:CZ	1.93	0.97
40:h:147:ILE:HD12	42:j:110:GLY:HA2	1.46	0.97
19:J:3:PHE:CG	71:J:101:CDL:H722	1.98	0.97
3:2:322:LYS:HD2	70:2:401:3PE:H2D1	1.47	0.96
25:Q:160:PRO:HA	42:j:84:ALA:HB1	1.45	0.96
38:d:105:GLU:OE2	44:e:165:ASN:CB	2.13	0.96
62:A4:5:LYS:HZ3	62:A4:6:GLY:H	0.98	0.96
10:A:111:LYS:CA	24:P:53:TYR:OH	2.12	0.96
13:D:186:CYS:SG	74:D:301:SF4:S4	2.62	0.96
27:S:333:GLU:HG2	42:j:52:PRO:CD	1.95	0.96
10:A:355:LYS:HD2	10:A:530:TYR:HE1	0.81	0.96
2:4:90:THR:HG21	70:4:501:3PE:C32	1.95	0.96
2:4:166:TYR:HH	70:4:503:3PE:C11	1.77	0.96
13:D:103:ARG:CZ	14:E:84:ILE:CD1	2.34	0.96
28:T:99:LEU:H	28:T:99:LEU:HD12	1.27	0.96
18:I:108:LYS:HZ2	18:I:108:LYS:HA	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:f:136:GLU:OE2	39:f:164:PRO:CB	2.14	0.96
21:L:16:GLU:HG2	72:L:200:PC1:H152	0.97	0.96
8:1:71:PHE:HZ	8:1:215:TYR:CE1	1.81	0.95
8:1:79:LEU:CD1	8:1:222:LEU:CD2	2.44	0.95
28:T:62:THR:CG2	28:T:63:ALA:N	2.23	0.95
12:C:229:ALA:O	16:G:114:TRP:HE3	1.39	0.95
25:Q:161:ALA:HB2	42:j:83:TYR:O	1.64	0.95
9:8:207:GLY:CA	73:8:501:FMN:C9	2.44	0.95
42:j:114:GLU:HB3	43:g:160:LYS:HD3	1.45	0.95
47:y:244:LEU:O	48:z:201:ARG:NH1	1.99	0.95
5:6:556:ILE:HG12	35:a:76:ILE:CD1	1.96	0.95
11:B:265:ASN:HD22	14:E:70:LEU:HD12	1.32	0.95
23:O:33:ARG:NH2	31:M:44:SER:OG	1.99	0.95
43:g:159:GLN:O	43:g:163:MET:HG2	1.66	0.95
8:1:203:GLY:H	8:1:210:GLY:H	1.12	0.95
41:i:69:TYR:CD1	42:j:20:SER:CA	2.49	0.95
11:B:266:ARG:HH11	70:B:501:3PE:C23	1.78	0.95
41:i:62:HIS:ND1	42:j:23:PRO:HG3	1.81	0.95
8:1:79:LEU:HD11	8:1:222:LEU:CD2	1.97	0.95
8:1:233:MET:HA	8:1:236:ILE:HG23	1.48	0.95
11:B:61:TRP:CZ2	11:B:64:PRO:HG3	1.94	0.94
27:S:333:GLU:HG3	42:j:52:PRO:O	1.66	0.94
28:T:13:PRO:HG3	28:T:20:ARG:HH22	1.09	0.94
28:T:34:LEU:HD13	28:T:35:VAL:H	1.20	0.94
42:j:118:PRO:HB2	43:g:146:LEU:O	1.67	0.94
49:A0:110:ALA:HB1	49:A0:123:ASP:CA	1.97	0.94
49:A0:156:TYR:CA	49:A0:165:TYR:CB	2.44	0.94
3:2:322:LYS:HD3	70:2:401:3PE:H2D1	1.47	0.94
11:B:215:GLU:OE2	14:E:93:LEU:HD22	1.67	0.94
5:6:119:LYS:HD3	71:6:701:CDL:H332	1.49	0.94
8:1:232:ILE:O	8:1:236:ILE:CG2	2.15	0.94
35:a:47:TYR:CE1	44:e:105:MET:CA	2.48	0.94
35:a:70:TYR:CD2	44:e:35:ASP:CB	2.50	0.94
53:A3:43:ASP:OD1	53:A3:47:TYR:HB2	1.68	0.94
25:Q:165:SER:HA	42:j:86:ARG:NH2	1.83	0.94
25:Q:166:ARG:NH2	42:j:86:ARG:NH1	2.15	0.94
41:i:58:LEU:CD1	42:j:73:TYR:HE2	1.81	0.94
1:9:233:SER:O	9:8:41:ILE:HB	1.66	0.94
14:E:188:GLU:OE2	18:I:64:ASN:HB2	1.54	0.94
27:S:333:GLU:CG	42:j:52:PRO:CB	2.46	0.94
14:E:57:ALA:CB	21:L:13:TRP:CE3	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:105:LYS:C	18:I:106:GLU:HG3	1.91	0.94
18:I:108:LYS:HA	18:I:108:LYS:NZ	1.83	0.94
2:4:421:TYR:HE1	35:a:59:VAL:CA	1.72	0.94
24:P:39:PRO:HA	30:V:8:GLN:CG	1.98	0.94
27:S:342:LEU:N	42:j:59:HIS:HD2	1.66	0.94
28:T:5:VAL:HG11	28:T:28:ILE:CD1	1.98	0.94
35:a:67:ARG:NH1	44:e:79:PRO:HB2	1.83	0.94
1:9:226:GLU:OE1	9:8:48:ARG:CZ	2.16	0.93
8:1:72:ILE:HG22	8:1:76:ILE:CD1	1.98	0.93
45:k:433:ASP:OD2	47:m:223:TYR:OH	1.85	0.93
47:m:376:LEU:HA	50:q:17:ARG:NE	1.81	0.93
41:i:58:LEU:HD11	42:j:73:TYR:HE2	0.91	0.93
10:A:127:ASP:C	74:A:801:SF4:S1	2.51	0.93
34:Z:44:PRO:C	39:f:38:ARG:NH2	2.24	0.93
42:j:114:GLU:CB	43:g:160:LYS:HE2	1.99	0.93
47:y:71:ARG:HH22	48:z:46:VAL:HG22	1.32	0.93
56:A9:365:ILE:HD12	57:C4:87:MET:HE1	1.48	0.93
28:T:95:CYS:O	28:T:97:GLY:N	2.01	0.93
50:q:110:LYS:NZ	53:A3:11:ARG:O	2.01	0.93
2:4:446:LEU:CG	71:4:502:CDL:H371	1.99	0.93
21:L:56:PRO:HB3	25:Q:129:THR:C	1.93	0.93
2:4:185:PRO:HG3	42:j:115:GLU:CD	1.94	0.93
8:1:72:ILE:CG2	8:1:76:ILE:HD11	1.92	0.93
24:P:39:PRO:CB	30:V:8:GLN:HB2	1.97	0.93
28:T:69:ILE:HG21	28:T:100:ILE:CD1	1.97	0.93
49:A0:109:GLU:CB	49:A0:167:ALA:HB2	1.98	0.93
27:S:335:VAL:H	42:j:52:PRO:HG3	1.31	0.93
53:A3:39:ARG:C	53:A3:41:ILE:H	1.71	0.93
12:C:212:LEU:HD23	13:D:176:ILE:HD11	1.51	0.93
13:D:103:ARG:HH11	14:E:84:ILE:HD11	1.24	0.93
14:E:53:VAL:CG1	21:L:14:ALA:HB2	1.98	0.93
35:a:47:TYR:CD1	44:e:105:MET:CA	2.52	0.93
11:B:233:HIS:NE2	14:E:160:GLU:OE1	2.00	0.93
25:Q:162:ARG:CD	42:j:91:PHE:HZ	1.82	0.93
27:S:48:ILE:HD13	27:S:191:VAL:HB	1.50	0.93
28:T:69:ILE:HD12	28:T:100:ILE:HD11	0.93	0.93
40:h:120:ARG:HH22	43:g:66:ARG:H	1.14	0.93
45:k:252:HIS:HD2	45:k:323:HIS:HE1	1.17	0.93
14:E:57:ALA:HB2	21:L:13:TRP:O	1.69	0.92
28:T:66:ILE:O	28:T:69:ILE:HG23	1.69	0.92
38:d:105:GLU:OE2	44:e:166:LEU:N	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:421:TYR:HE1	35:a:59:VAL:CG1	1.82	0.92
8:1:183:MET:HG2	70:B:501:3PE:H2H2	1.48	0.92
8:1:316:PRO:CG	30:V:57:ARG:HE	1.81	0.92
42:j:119:VAL:H	43:g:147:GLY:H	0.99	0.92
5:6:119:LYS:HE3	71:6:701:CDL:C33	1.93	0.92
5:6:119:LYS:CE	71:6:701:CDL:H332	1.94	0.92
13:D:138:ARG:NH1	13:D:141:TYR:CD2	2.36	0.92
47:m:376:LEU:HD22	50:q:17:ARG:CG	2.00	0.92
5:6:116:LYS:HG3	5:6:119:LYS:NZ	1.85	0.92
32:X:37:PHE:HD2	36:b:137:MET:HB3	1.32	0.92
42:j:114:GLU:CB	43:g:160:LYS:HD3	1.97	0.92
28:T:69:ILE:CG1	28:T:100:ILE:HD11	2.00	0.92
3:2:325:PHE:CE2	70:2:401:3PE:C2I	2.52	0.92
11:B:216:ARG:HG3	14:E:94:SER:OG	1.70	0.92
53:A3:39:ARG:O	53:A3:41:ILE:N	2.01	0.92
56:A9:449:MET:SD	57:C4:5:MET:HE2	2.09	0.92
5:6:470:ASN:ND2	38:d:77:PHE:CG	2.37	0.92
5:6:470:ASN:ND2	38:d:77:PHE:CB	2.33	0.92
28:T:13:PRO:CB	28:T:20:ARG:NH2	2.33	0.92
8:1:172:MET:CE	8:1:176:LEU:CD1	1.81	0.92
42:j:114:GLU:HB3	43:g:160:LYS:HD2	1.50	0.92
49:A0:85:LYS:CB	49:A0:149:ASN:CB	2.48	0.92
53:A3:43:ASP:O	53:A3:47:TYR:CE2	2.23	0.92
23:O:53:ASP:OD2	26:R:351:GLU:HA	1.69	0.91
40:h:84:ILE:HG22	40:h:88:ARG:HH12	1.33	0.91
41:i:68:GLU:HB3	42:j:19:ARG:HD2	1.51	0.91
11:B:254:ARG:CD	24:P:24:LEU:HG	1.98	0.91
5:6:120:TYR:OH	71:6:701:CDL:H512	1.68	0.91
10:A:367:CYS:SG	10:A:368:THR:N	2.39	0.91
25:Q:9:SER:HA	30:V:88:ARG:NH1	1.85	0.91
40:h:149:LEU:HD11	43:g:167:ARG:N	1.84	0.91
7:3:106:TRP:HZ2	72:L:200:PC1:C14	1.83	0.91
13:D:195:TYR:HE2	29:U:116:ASN:ND2	1.68	0.91
14:E:61:LEU:HB2	21:L:17:PRO:HB2	1.50	0.91
11:B:216:ARG:HA	14:E:94:SER:CB	2.01	0.91
53:A3:40:LEU:C	53:A3:41:ILE:HG12	1.95	0.91
2:4:278:ARG:H	5:6:546:GLN:HE22	1.06	0.91
47:m:344:GLU:HG2	47:m:346:PRO:HD2	1.52	0.91
8:1:38:ASN:CG	29:U:31:ASN:OD1	2.13	0.91
42:j:116:PHE:CD1	43:g:160:LYS:HB2	2.06	0.91
5:6:366:MET:HE3	5:6:369:THR:HG21	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:267:THR:O	8:1:269:SER:N	2.04	0.91
42:j:119:VAL:HB	43:g:147:GLY:CA	1.96	0.91
3:2:68:MET:HE2	6:5:37:MET:HE2	1.50	0.90
28:T:2:ALA:O	28:T:4:THR:N	2.05	0.90
2:4:424:ASN:CA	35:a:57:ARG:NH2	2.34	0.90
11:B:238:LEU:HD13	24:P:37:PRO:HD2	1.50	0.90
28:T:106:ARG:HA	28:T:106:ARG:HH11	1.27	0.90
44:e:114:ARG:N	44:e:114:ARG:HD3	1.85	0.90
11:B:62:LYS:HG2	11:B:63:PRO:HD2	0.94	0.90
23:O:33:ARG:HH11	31:M:48:VAL:HG21	1.33	0.90
44:e:70:THR:O	44:e:72:TYR:N	2.03	0.90
10:A:422:TRP:CZ2	16:G:169:ARG:HD3	2.07	0.90
27:S:334:ASP:CB	42:j:50:ARG:HD3	2.01	0.90
12:C:242:GLU:HB2	16:G:92:ASN:CG	1.96	0.90
41:i:58:LEU:CD1	42:j:73:TYR:CE2	2.52	0.90
45:w:252:HIS:HD2	45:w:323:HIS:HE1	1.17	0.90
21:L:56:PRO:CB	25:Q:129:THR:C	2.45	0.90
8:1:172:MET:HE1	8:1:176:LEU:CG	2.02	0.90
21:L:8:PHE:HZ	72:L:200:PC1:H322	1.09	0.90
2:4:421:TYR:CE1	35:a:59:VAL:CG1	2.54	0.90
2:4:449:LEU:HD12	71:4:502:CDL:H322	1.54	0.90
10:A:319:TRP:HH2	10:A:585:PRO:HD2	1.35	0.90
11:B:264:ASN:O	14:E:65:GLU:OE2	1.90	0.90
25:Q:158:LEU:O	25:Q:159:LYS:CD	2.19	0.90
28:T:88:LEU:O	28:T:91:LEU:HB3	1.71	0.90
48:z:239:PRO:HB2	48:z:241:LYS:HB3	1.53	0.90
14:E:54:THR:HA	21:L:13:TRP:CZ3	2.07	0.90
2:4:424:ASN:HA	35:a:57:ARG:HH21	1.19	0.90
8:1:245:THR:OG1	8:1:255:TYR:HE1	1.52	0.90
35:a:47:TYR:CD1	44:e:105:MET:SD	2.65	0.90
53:t:33:VAL:O	53:t:37:ASP:HB3	1.72	0.90
18:I:109:THR:CB	18:I:120:ARG:CB	2.50	0.89
31:W:89:LEU:HD21	34:Z:47:ARG:CB	2.01	0.89
7:3:84:LEU:CD2	8:1:309:ILE:HD13	2.01	0.89
23:O:48:HIS:CG	26:R:359:TYR:HH	1.87	0.89
28:T:139:PRO:HB3	36:b:158:ARG:HA	1.54	0.89
48:o:239:PRO:HB2	48:o:241:LYS:HB3	1.53	0.89
5:6:470:ASN:HD21	38:d:77:PHE:HA	0.73	0.89
31:W:85:TYR:CE1	34:Z:18:ASP:C	2.50	0.89
10:A:305:PRO:HB3	10:A:319:TRP:CZ3	2.07	0.89
25:Q:158:LEU:HD12	42:j:88:HIS:HB2	0.92	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:117:GLU:OE2	34:Z:45:TRP:CZ3	2.26	0.89
3:2:326:LEU:HD11	72:2:402:PC1:H2A1	1.50	0.89
5:6:153:LEU:HD12	71:6:701:CDL:C55	1.91	0.89
12:C:240:PRO:HG3	16:G:88:GLN:HE22	1.33	0.89
26:R:314:THR:HG22	26:R:316:ARG:HB2	1.55	0.89
27:S:286:VAL:CB	72:S:401:PC1:C15	2.50	0.89
27:S:335:VAL:HG23	42:j:50:ARG:O	1.73	0.89
42:j:118:PRO:HB2	43:g:146:LEU:C	1.98	0.89
10:A:110:LYS:HD2	24:P:55:CYS:SG	2.13	0.89
9:8:116:ASN:ND2	73:8:501:FMN:O2	2.06	0.89
9:8:116:ASN:HD22	73:8:501:FMN:C2	1.84	0.89
27:S:73:HIS:NE2	27:S:148:GLU:OE2	2.05	0.89
8:1:172:MET:CE	8:1:176:LEU:CG	2.51	0.88
23:O:33:ARG:NH1	31:M:44:SER:C	2.20	0.88
50:A1:13:LEU:C	50:A1:14:GLU:HG3	1.97	0.88
5:6:470:ASN:ND2	38:d:77:PHE:CA	2.21	0.88
24:P:38:PRO:O	30:V:8:GLN:HG3	1.73	0.88
3:2:319:LEU:O	72:2:402:PC1:C22	2.21	0.88
5:6:594:THR:OG1	28:T:39:TYR:OH	1.86	0.88
11:B:120:THR:OG1	11:B:462:ASP:OD2	1.90	0.88
36:b:149:LEU:HD23	42:j:90:MET:HE1	1.56	0.88
10:A:362:ASP:HB2	20:K:71:PHE:HD1	1.38	0.88
35:a:60:ILE:HG21	44:e:105:MET:HE1	1.44	0.88
34:Z:45:TRP:O	39:f:38:ARG:CZ	2.21	0.88
10:A:111:LYS:HD3	24:P:53:TYR:CZ	2.08	0.88
11:B:265:ASN:HD22	14:E:70:LEU:CD1	1.86	0.88
11:B:266:ARG:CZ	14:E:66:LEU:CD2	2.52	0.88
2:4:16:TRP:HH2	70:4:501:3PE:H2I3	1.38	0.88
25:Q:158:LEU:O	25:Q:159:LYS:HG2	1.74	0.88
28:T:80:VAL:HB	28:T:81:ARG:HD3	1.54	0.88
44:e:70:THR:C	44:e:72:TYR:H	1.82	0.88
1:9:180:CYS:HB2	9:8:123:GLY:HA2	1.54	0.88
47:m:376:LEU:HD22	50:q:17:ARG:HG2	1.55	0.88
40:h:149:LEU:HD23	43:g:171:LYS:HE2	1.54	0.87
1:9:226:GLU:OE1	9:8:48:ARG:NH1	2.07	0.87
3:2:104:MET:O	3:2:114:TRP:HZ3	1.57	0.87
9:8:206:CYS:O	73:8:501:FMN:N10	2.07	0.87
11:B:322:SER:HB3	14:E:42:ASN:CB	2.04	0.87
25:Q:8:PRO:O	30:V:88:ARG:NH2	2.08	0.87
25:Q:158:LEU:HG	25:Q:159:LYS:H	0.72	0.87
27:S:237:MET:HA	27:S:243:VAL:HG11	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:58:LEU:HD11	42:j:73:TYR:CD2	2.09	0.87
46:l:247:GLN:HE22	46:l:429:ASN:HA	1.39	0.87
8:1:71:PHE:CZ	8:1:215:TYR:CD1	2.62	0.87
11:B:266:ARG:H	14:E:66:LEU:HD13	1.40	0.87
50:q:16:ILE:O	50:q:20:TYR:CA	2.22	0.87
10:A:312:GLY:CA	29:U:144:TYR:CD1	2.56	0.87
23:O:128:PRO:CG	26:R:45:LYS:CE	2.53	0.87
46:x:247:GLN:HE22	46:x:429:ASN:HA	1.39	0.87
25:Q:53:PRO:HD2	30:V:116:TRP:HD1	1.35	0.87
36:b:140:LEU:HD23	43:g:82:VAL:CG1	2.03	0.87
38:d:74:PHE:HB3	38:d:75:PRO:HD3	1.57	0.87
58:C2:112:LEU:HG	58:C2:118:PRO:HB3	1.55	0.87
1:9:88:ARG:HG3	15:F:83:TYR:HD1	1.40	0.87
26:R:85:ARG:HH21	76:R:601:NAP:C6A	1.88	0.87
27:S:275:ASN:O	27:S:277:ARG:N	2.07	0.87
35:a:67:ARG:CZ	44:e:52:ALA:HB1	2.03	0.87
1:9:239:LYS:HE2	9:8:42:PHE:CD1	2.09	0.87
9:8:243:ALA:C	73:8:501:FMN:O3P	2.18	0.87
14:E:61:LEU:CD1	21:L:17:PRO:O	2.20	0.87
21:L:55:VAL:C	25:Q:128:VAL:HG23	2.00	0.87
2:4:105:PHE:CE1	72:4:504:PC1:C3C	2.56	0.87
9:8:207:GLY:CA	73:8:501:FMN:C9A	2.52	0.87
28:T:81:ARG:HD3	28:T:81:ARG:H	1.40	0.87
41:i:68:GLU:CB	42:j:19:ARG:CD	2.52	0.87
10:A:144:MET:HG2	11:B:380:HIS:HD2	1.37	0.86
40:h:79:ASP:N	40:h:83:ASP:OD2	2.09	0.86
2:4:139:GLN:N	2:4:222:GLU:OE2	2.08	0.86
12:C:214:TYR:CD2	13:D:176:ILE:O	2.29	0.86
12:C:218:VAL:C	12:C:219:LYS:HG3	1.98	0.86
35:a:68:TRP:CH2	44:e:110:ASP:OD1	2.26	0.86
19:J:3:PHE:HE2	71:J:101:CDL:HB62	1.37	0.86
28:T:89:ASN:O	28:T:91:LEU:N	2.07	0.86
4:7:118:GLU:O	17:H:74:LYS:NZ	2.08	0.86
28:T:34:LEU:HD13	28:T:35:VAL:CA	2.05	0.86
9:8:327:ILE:HG21	9:8:332:CYS:HB2	1.57	0.86
10:A:58:MET:HG2	12:C:248:ARG:NH1	1.89	0.86
25:Q:53:PRO:HD2	30:V:116:TRP:CD1	2.10	0.86
1:9:233:SER:O	9:8:41:ILE:CG1	2.24	0.86
10:A:124:HIS:NE2	74:A:801:SF4:S3	2.48	0.86
10:A:343:GLY:H	10:A:549:GLY:HA2	1.41	0.86
42:j:114:GLU:CB	43:g:160:LYS:HD2	2.02	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:166:TYR:CZ	70:4:503:3PE:C1	2.58	0.86
18:I:108:LYS:HA	18:I:108:LYS:CE	2.04	0.86
22:N:106:GLU:OE2	24:P:71:SER:OG	1.92	0.86
42:j:114:GLU:HB2	43:g:160:LYS:CD	1.92	0.86
2:4:360:LEU:HD13	71:6:701:CDL:C51	2.04	0.86
23:O:33:ARG:HH22	31:M:44:SER:CA	1.89	0.86
35:a:47:TYR:HD1	44:e:105:MET:HB2	1.04	0.86
47:m:376:LEU:CD2	50:q:17:ARG:HE	1.86	0.86
49:A0:122:HIS:CB	49:A0:168:SER:CA	2.53	0.86
49:A0:150:ALA:C	49:A0:155:GLY:HA2	2.00	0.86
11:B:254:ARG:HD2	24:P:24:LEU:CG	2.06	0.86
28:T:69:ILE:HD12	28:T:100:ILE:HD12	1.58	0.86
9:8:207:GLY:CA	73:8:501:FMN:C8	2.54	0.85
13:D:195:TYR:OH	29:U:80:SER:HB3	1.73	0.85
25:Q:158:LEU:O	25:Q:159:LYS:CG	2.24	0.85
31:M:7:THR:HG22	31:M:9:GLU:H	1.42	0.85
8:1:41:GLY:HA3	8:1:44:GLY:H	1.40	0.85
12:C:192:ASP:HA	13:D:132:LYS:HD2	1.56	0.85
16:G:57:GLU:CD	23:O:16:SER:OG	2.18	0.85
28:T:26:THR:HB	28:T:68:ALA:HA	1.54	0.85
3:2:217:THR:HG21	72:2:402:PC1:H261	1.56	0.85
5:6:470:ASN:HD22	38:d:77:PHE:HD1	0.92	0.85
10:A:618:GLU:OE2	10:A:620:TRP:NE1	2.09	0.85
11:B:219:GLY:HA3	14:E:98:ARG:NE	1.92	0.85
14:E:53:VAL:HG13	21:L:14:ALA:HB2	1.58	0.85
26:R:61:ALA:HA	26:R:66:GLY:HA3	1.58	0.85
27:S:333:GLU:CD	42:j:52:PRO:HG2	2.01	0.85
28:T:2:ALA:C	28:T:4:THR:N	2.34	0.85
28:T:77:SER:HA	28:T:80:VAL:HG13	1.58	0.85
49:A0:121:GLN:CA	49:A0:170:ARG:CB	2.53	0.85
25:Q:162:ARG:HH11	42:j:91:PHE:HZ	1.22	0.85
53:A3:43:ASP:HA	53:A3:47:TYR:HD2	1.41	0.85
11:B:179:ARG:NH2	11:B:401:GLU:O	2.10	0.85
70:B:501:3PE:O32	21:L:18:VAL:HG22	1.77	0.85
14:E:137:ASP:OD2	18:I:72:ILE:HD12	1.76	0.85
28:T:26:THR:HB	28:T:68:ALA:CA	2.07	0.85
2:4:190:TRP:CZ2	28:T:87:PRO:CB	2.59	0.85
7:3:44:MET:HE3	23:O:49:LEU:O	1.77	0.85
17:H:82:GLN:HE21	30:V:98:MET:HB2	1.41	0.85
21:L:68:SER:N	25:Q:130:LYS:HE3	1.92	0.85
36:b:160:MET:HB3	36:b:161:ARG:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:47:THR:HG21	42:j:63:LEU:HD13	1.58	0.85
49:A0:106:ILE:CB	49:A0:167:ALA:C	2.48	0.85
1:9:62:ARG:NE	15:F:86:LEU:HA	1.92	0.85
8:1:233:MET:CA	8:1:236:ILE:CG2	2.53	0.85
35:a:47:TYR:CD1	44:e:105:MET:CG	2.55	0.85
49:A0:155:GLY:C	49:A0:165:TYR:CB	2.49	0.85
2:4:1:MET:HG2	2:4:2:LEU:H	1.41	0.85
2:4:198:ALA:HB2	70:4:503:3PE:H271	1.58	0.85
2:4:446:LEU:CG	71:4:502:CDL:C37	2.54	0.85
3:2:326:LEU:CD1	72:2:402:PC1:C2A	2.41	0.85
9:8:207:GLY:HA2	73:8:501:FMN:C7	2.07	0.85
9:8:207:GLY:HA2	73:8:501:FMN:C6	2.07	0.85
12:C:123:THR:HG21	16:G:128:PHE:HA	1.57	0.84
28:T:26:THR:HG22	28:T:68:ALA:CA	2.05	0.84
50:q:28:LYS:HB3	50:q:74:ILE:HD11	1.59	0.84
5:6:435:PRO:HG3	34:Z:57:PHE:CD2	2.12	0.84
9:8:206:CYS:O	73:8:501:FMN:C10	2.24	0.84
47:m:375:LYS:HG2	50:q:17:ARG:NH2	1.91	0.84
3:2:87:MET:HE2	3:2:90:PHE:HZ	1.43	0.84
3:2:277:ILE:HG21	28:T:135:VAL:HG22	1.57	0.84
11:B:293:LEU:O	11:B:295:GLY:N	2.10	0.84
11:B:367:LYS:NZ	14:E:212:ARG:C	2.35	0.84
14:E:62:LEU:HD22	30:V:36:PHE:CD2	2.12	0.84
53:t:34:TRP:HD1	54:u:29:LEU:HD13	1.41	0.84
57:C4:78:LEU:HB2	57:C4:79:PRO:HD3	1.58	0.84
41:i:69:TYR:CD1	42:j:20:SER:HA	2.13	0.84
1:9:75:LYS:O	1:9:77:ALA:N	2.11	0.84
10:A:391:ILE:HG12	10:A:600:GLU:OE2	1.78	0.84
28:T:101:LEU:HD21	28:T:110:ILE:HG21	1.57	0.84
46:l:59:ASN:H	46:l:62:ASN:HB3	1.43	0.84
53:A3:43:ASP:O	53:A3:47:TYR:HD2	1.60	0.84
56:A9:187:SER:HB2	56:A9:277:MET:HE1	1.60	0.84
1:9:233:SER:HB3	9:8:41:ILE:CD1	2.08	0.84
10:A:462:PHE:O	10:A:464:GLN:N	2.11	0.83
11:B:322:SER:OG	14:E:42:ASN:HB3	1.78	0.83
23:O:128:PRO:HG3	26:R:45:LYS:HE3	1.58	0.83
47:m:244:LEU:O	48:o:201:ARG:NH1	2.11	0.83
11:B:266:ARG:NE	14:E:66:LEU:HD22	1.92	0.83
49:A0:156:TYR:CB	49:A0:165:TYR:CA	2.56	0.83
31:W:85:TYR:HH	34:Z:22:TRP:HZ3	1.13	0.83
43:g:11:PRO:HD2	43:g:109:ARG:HH12	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:28:LYS:HB3	50:A1:74:ILE:HD11	1.59	0.83
12:C:66:TYR:OH	12:C:107:ASN:ND2	2.11	0.83
12:C:123:THR:HG21	16:G:128:PHE:CA	2.08	0.83
13:D:103:ARG:HH12	14:E:84:ILE:HD11	1.38	0.83
46:l:276:GLN:O	46:l:280:GLY:N	2.11	0.83
5:6:55:ILE:HD12	38:d:74:PHE:HE1	0.97	0.83
16:G:57:GLU:CD	23:O:16:SER:HG	1.87	0.83
27:S:335:VAL:CG2	42:j:50:ARG:O	2.25	0.83
50:q:13:LEU:O	50:q:16:ILE:CG2	2.26	0.83
12:C:232:PHE:CB	13:D:165:TYR:CE1	2.61	0.83
2:4:190:TRP:CE3	28:T:127:MET:HE2	2.14	0.83
5:6:556:ILE:HG12	35:a:76:ILE:HD11	1.59	0.83
27:S:109:PRO:HB2	27:S:112:ASN:HB3	1.61	0.83
40:h:149:LEU:HD11	43:g:167:ARG:CB	2.08	0.83
46:x:59:ASN:H	46:x:62:ASN:HB3	1.43	0.83
2:4:349:GLN:NE2	71:6:701:CDL:OB3	2.11	0.83
23:O:33:ARG:HH22	31:M:44:SER:HB2	0.93	0.83
49:A0:151:GLY:HA2	49:A0:157:TYR:CB	2.09	0.83
4:7:4:TYR:HE1	4:7:123:GLY:HA2	1.44	0.83
11:B:215:GLU:OE2	14:E:97:PHE:CD1	2.32	0.83
11:B:253:LEU:HB3	11:B:254:ARG:NH1	1.94	0.83
23:O:128:PRO:CG	26:R:45:LYS:HE3	2.08	0.83
24:P:39:PRO:HB3	30:V:8:GLN:HB2	1.58	0.83
25:Q:165:SER:HB3	42:j:83:TYR:CE1	2.13	0.83
44:e:119:THR:OG1	44:e:120:SER:N	2.10	0.83
28:T:13:PRO:HB3	28:T:20:ARG:HH22	1.44	0.82
38:d:105:GLU:CD	44:e:165:ASN:H	1.86	0.82
46:x:276:GLN:O	46:x:280:GLY:N	2.11	0.82
1:9:188:ILE:HD12	1:9:189:ASN:H	1.42	0.82
2:4:16:TRP:HZ2	70:4:501:3PE:H2G2	1.43	0.82
11:B:265:ASN:ND2	14:E:70:LEU:CD1	2.42	0.82
12:C:127:ARG:HE	12:C:128:PHE:HE1	1.28	0.82
12:C:214:TYR:HB3	13:D:176:ILE:HA	1.61	0.82
50:q:13:LEU:O	50:q:16:ILE:HG22	1.77	0.82
5:6:557:TRP:CH2	35:a:80:PHE:CZ	2.67	0.82
25:Q:158:LEU:HD12	42:j:88:HIS:HB3	1.61	0.82
2:4:2:LEU:HG	72:4:504:PC1:C14	2.09	0.82
3:2:85:THR:HG22	17:H:19:THR:CG2	2.09	0.82
25:Q:165:SER:HA	42:j:86:ARG:HH21	1.45	0.82
10:A:462:PHE:O	10:A:465:VAL:N	2.11	0.82
21:L:56:PRO:HA	25:Q:129:THR:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:233:SER:O	9:8:41:ILE:CB	2.27	0.82
10:A:128:CYS:N	74:A:801:SF4:S1	2.53	0.82
12:C:192:ASP:OD1	13:D:132:LYS:HG2	1.80	0.82
25:Q:158:LEU:CD1	42:j:88:HIS:CG	2.59	0.82
2:4:64:PRO:O	2:4:66:LEU:N	2.13	0.82
8:1:311:THR:O	30:V:55:ARG:NH2	2.11	0.82
14:E:105:ARG:NH1	14:E:195:ASP:OD2	2.12	0.82
2:4:190:TRP:CE2	28:T:87:PRO:CB	2.62	0.82
12:C:221:VAL:HG22	13:D:138:ARG:HG2	1.60	0.82
28:T:10:TRP:HA	28:T:10:TRP:CE3	2.14	0.82
28:T:30:GLY:HA3	28:T:64:ALA:HB2	1.61	0.82
28:T:65:ALA:O	28:T:69:ILE:HG22	1.79	0.82
38:d:76:ASN:ND2	38:d:78:LEU:O	2.12	0.82
53:A3:38:TRP:O	53:A3:40:LEU:N	2.13	0.82
2:4:5:ILE:HD11	72:4:504:PC1:H141	1.62	0.82
14:E:135:ARG:NH1	18:I:68:ALA:O	2.13	0.82
28:T:60:THR:O	28:T:62:THR:N	2.13	0.82
38:d:108:LEU:CB	44:e:166:LEU:CD2	2.57	0.82
47:m:5:ARG:HA	47:m:8:HIS:HD2	1.45	0.82
11:B:123:LEU:CD1	12:C:206:LEU:HD21	2.10	0.81
11:B:426:ALA:HB3	11:B:460:GLU:OE2	1.80	0.81
53:A3:43:ASP:CA	53:A3:47:TYR:HD2	1.92	0.81
25:Q:165:SER:CB	42:j:83:TYR:CE1	2.63	0.81
35:a:47:TYR:CE1	44:e:105:MET:CB	2.63	0.81
35:a:47:TYR:HD1	44:e:105:MET:CB	1.54	0.81
2:4:25:VAL:HG23	40:h:89:VAL:HG11	1.60	0.81
2:4:166:TYR:CD2	70:4:503:3PE:C21	2.62	0.81
5:6:557:TRP:CH2	35:a:80:PHE:HZ	1.98	0.81
10:A:501:ARG:HA	10:A:505:GLY:HA3	1.61	0.81
14:E:197:TRP:HB3	29:U:84:PRO:HB3	1.60	0.81
47:m:164:ILE:O	47:m:177:ARG:NH1	2.14	0.81
12:C:150:ASP:OD1	12:C:151:GLU:N	2.12	0.81
13:D:138:ARG:CZ	13:D:141:TYR:HD2	1.92	0.81
16:G:111:LEU:HD13	26:R:100:LEU:HD23	1.60	0.81
28:T:70:PHE:CD1	28:T:93:GLY:HA3	2.14	0.81
39:f:163:LEU:N	39:f:164:PRO:HA	1.94	0.81
40:h:81:ALA:O	40:h:83:ASP:N	2.14	0.81
44:e:43:LYS:O	44:e:46:GLU:N	2.12	0.81
46:l:303:VAL:HG12	46:l:304:HIS:H	1.43	0.81
53:A3:38:TRP:C	53:A3:40:LEU:H	1.89	0.81
55:B1:64:LEU:HG	55:B1:65:VAL:HG22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:179:ALA:HB2	9:8:128:ARG:HH21	1.46	0.81
1:9:223:PHE:HZ	9:8:49:HIS:CD2	1.98	0.81
2:4:421:TYR:CZ	35:a:59:VAL:HG12	2.14	0.81
11:B:266:ARG:CZ	14:E:66:LEU:HD22	2.10	0.81
28:T:14:GLU:OE1	28:T:126:LYS:HE2	1.81	0.81
2:4:198:ALA:CB	70:4:503:3PE:H271	2.10	0.81
2:4:421:TYR:CZ	35:a:59:VAL:HA	2.15	0.81
5:6:116:LYS:HG3	5:6:119:LYS:HZ2	1.43	0.81
5:6:119:LYS:HD2	71:6:701:CDL:C34	2.10	0.81
40:h:121:GLU:OE2	40:h:124:ARG:NH2	2.13	0.81
41:i:54:LEU:HD22	42:j:70:PHE:CZ	2.15	0.81
41:i:68:GLU:HB3	42:j:19:ARG:HB3	1.61	0.81
49:A0:106:ILE:HA	49:A0:167:ALA:C	2.05	0.81
5:6:432:LEU:O	34:Z:60:ASN:ND2	2.13	0.81
27:S:158:LEU:HA	27:S:161:MET:HB3	1.63	0.81
31:W:113:LEU:CB	39:f:45:ARG:HH21	1.94	0.81
46:l:101:THR:HG23	46:l:103:GLU:H	1.44	0.81
2:4:16:TRP:CH2	70:4:501:3PE:H2I3	2.15	0.81
54:B2:52:TRP:HA	54:B2:55:ILE:HB	1.63	0.81
1:9:188:ILE:HD11	1:9:191:ASN:HB2	1.63	0.81
73:8:501:FMN:O3'	73:8:501:FMN:N1	2.13	0.81
12:C:214:TYR:HD2	13:D:176:ILE:O	1.63	0.81
12:C:227:GLU:HG3	26:R:49:SER:CB	2.10	0.81
28:T:72:LEU:HD12	28:T:72:LEU:O	1.81	0.81
47:y:164:ILE:O	47:y:177:ARG:NH1	2.14	0.81
46:x:101:THR:HG23	46:x:103:GLU:H	1.45	0.81
46:x:303:VAL:HG12	46:x:304:HIS:H	1.43	0.81
2:4:143:LEU:HD21	3:2:302:LEU:HD21	1.60	0.80
10:A:320:GLU:HB2	23:O:123:TYR:CE1	2.16	0.80
28:T:17:GLU:CB	28:T:20:ARG:NH2	2.44	0.80
10:A:141:ASP:HB3	12:C:241:TRP:CD1	2.17	0.80
19:J:3:PHE:CG	71:J:101:CDL:C72	2.64	0.80
25:Q:90:ASP:O	25:Q:92:SER:OG	2.00	0.80
28:T:38:ALA:O	28:T:41:VAL:HG12	1.80	0.80
50:q:16:ILE:O	50:q:20:TYR:HB2	1.80	0.80
2:4:449:LEU:HD12	71:4:502:CDL:C32	2.10	0.80
3:2:135:LYS:HD2	3:2:187:MET:HE3	1.60	0.80
11:B:61:TRP:CZ2	11:B:64:PRO:CD	2.64	0.80
11:B:234:GLN:NE2	14:E:96:ARG:HD2	1.96	0.80
11:B:266:ARG:HH12	14:E:63:TRP:CD1	2.00	0.80
28:T:20:ARG:H	28:T:20:ARG:NE	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:266:ARG:HH11	70:B:501:3PE:H232	1.43	0.80
34:Z:45:TRP:N	39:f:38:ARG:NH2	2.29	0.80
49:A0:156:TYR:CB	49:A0:165:TYR:HA	2.11	0.80
18:I:109:THR:CB	18:I:119:PHE:C	2.53	0.80
42:j:109:TYR:CB	43:g:75:THR:HA	2.11	0.80
63:A5:39:CYS:SG	63:A5:53:CYS:HB3	2.22	0.80
5:6:119:LYS:NZ	71:6:701:CDL:H311	1.97	0.80
8:1:8:MET:O	8:1:12:PRO:HG2	1.82	0.80
8:1:233:MET:HA	8:1:236:ILE:HG22	1.64	0.80
9:8:207:GLY:C	73:8:501:FMN:C9	2.54	0.80
9:8:398:ARG:HG3	9:8:403:ASP:HB3	1.63	0.80
26:R:171:ASN:HD21	26:R:324:THR:HB	1.45	0.80
27:S:92:LEU:HD13	27:S:96:PHE:HB2	1.64	0.80
13:D:138:ARG:NE	13:D:138:ARG:O	2.15	0.80
16:G:111:LEU:HD13	26:R:100:LEU:CD2	2.12	0.80
21:L:23:PHE:HE1	72:L:200:PC1:C29	1.93	0.80
45:w:118:GLN:NE2	45:w:217:SER:O	2.14	0.80
3:2:239:ILE:CG2	42:j:48:ILE:HA	2.12	0.80
4:7:100:GLU:O	4:7:104:VAL:N	2.14	0.79
5:6:3:MET:HB3	43:g:37:PHE:CE2	2.17	0.79
14:E:135:ARG:HH21	18:I:72:ILE:CD1	1.96	0.79
26:R:209:ARG:NH1	26:R:351:GLU:OE2	2.15	0.79
28:T:18:CYS:O	28:T:22:THR:CG2	2.29	0.79
36:b:137:MET:HE3	43:g:87:GLU:OE2	1.81	0.79
28:T:69:ILE:HD12	28:T:100:ILE:HD13	1.56	0.79
53:A3:43:ASP:C	53:A3:47:TYR:HD2	1.89	0.79
2:4:16:TRP:NE1	70:4:501:3PE:H2C1	1.98	0.79
9:8:116:ASN:ND2	73:8:501:FMN:C2	2.46	0.79
10:A:362:ASP:HB2	20:K:71:PHE:CD1	2.17	0.79
21:L:8:PHE:CE2	72:L:200:PC1:C32	2.59	0.79
10:A:469:ALA:HB3	10:A:472:PRO:HG3	1.63	0.79
26:R:270:ARG:NH1	26:R:373:LYS:O	2.14	0.79
49:A0:106:ILE:O	49:A0:167:ALA:HB2	1.81	0.79
47:y:5:ARG:HA	47:y:8:HIS:HD2	1.45	0.79
7:3:84:LEU:HD21	8:1:309:ILE:HD11	0.80	0.79
10:A:382:ARG:O	10:A:384:ASN:N	2.14	0.79
14:E:52:SER:O	14:E:55:ASP:N	2.16	0.79
27:S:333:GLU:CG	42:j:52:PRO:CG	1.82	0.79
28:T:77:SER:HA	28:T:80:VAL:HG11	1.63	0.79
1:9:234:LEU:O	9:8:41:ILE:HG12	1.81	0.79
10:A:545:LEU:HB2	10:A:566:ILE:HG22	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:B:501:3PE:O32	21:L:18:VAL:CG2	2.30	0.79
13:D:107:ASP:OD1	13:D:108:ARG:N	2.15	0.79
13:D:186:CYS:SG	14:E:153:ILE:HG13	2.23	0.79
19:J:3:PHE:CB	71:J:101:CDL:H721	2.11	0.79
23:O:42:GLU:OE2	23:O:45:ASN:HB3	1.83	0.79
25:Q:160:PRO:HA	42:j:84:ALA:CB	2.11	0.79
28:T:5:VAL:HG12	28:T:28:ILE:HD11	1.63	0.79
34:Z:45:TRP:O	39:f:38:ARG:NH2	2.16	0.79
35:a:47:TYR:CE1	44:e:105:MET:SD	2.76	0.79
42:j:116:PHE:HB2	43:g:160:LYS:HB3	1.65	0.79
10:A:144:MET:HG2	11:B:380:HIS:CD2	2.17	0.79
25:Q:38:LYS:HG3	25:Q:39:PRO:HD3	1.64	0.79
38:d:74:PHE:HB3	38:d:75:PRO:CD	2.13	0.79
63:A5:75:ARG:HG2	63:A5:75:ARG:HH11	1.48	0.79
71:4:502:CDL:H673	5:6:20:MET:O	1.83	0.79
5:6:120:TYR:OH	71:6:701:CDL:C51	2.31	0.79
9:8:243:ALA:HA	73:8:501:FMN:O3P	1.83	0.79
11:B:266:ARG:CZ	14:E:66:LEU:HD23	2.13	0.79
11:B:322:SER:CB	14:E:42:ASN:CB	2.60	0.79
14:E:135:ARG:NH2	18:I:72:ILE:CD1	2.41	0.79
1:9:149:LEU:HD23	1:9:150:GLU:H	1.46	0.78
2:4:60:SER:O	2:4:62:SER:N	2.16	0.78
8:1:261:ILE:O	8:1:261:ILE:HG22	1.83	0.78
9:8:243:ALA:CA	73:8:501:FMN:O3P	2.31	0.78
25:Q:110:CYS:O	25:Q:114:LYS:N	2.15	0.78
50:q:13:LEU:HA	50:q:16:ILE:HG22	1.65	0.78
1:9:72:GLU:CB	15:F:103:GLY:O	2.25	0.78
12:C:214:TYR:CZ	13:D:138:ARG:HD3	2.17	0.78
13:D:138:ARG:NH2	13:D:142:ASP:OD1	2.15	0.78
25:Q:161:ALA:N	42:j:84:ALA:HA	1.98	0.78
31:W:85:TYR:HE1	34:Z:19:TYR:N	1.81	0.78
63:A5:39:CYS:SG	63:A5:53:CYS:CB	2.70	0.78
2:4:449:LEU:CG	71:4:502:CDL:H311	2.12	0.78
25:Q:6:GLU:OE2	25:Q:55:ARG:NH2	2.16	0.78
62:A4:5:LYS:NZ	62:A4:6:GLY:H	1.78	0.78
39:f:104:LEU:HA	39:f:107:TRP:HE1	1.48	0.78
10:A:308:ARG:NH1	10:A:308:ARG:O	2.15	0.78
11:B:143:SER:HB3	11:B:182:ASN:HD21	1.48	0.78
12:C:99:LEU:O	12:C:103:ARG:N	2.16	0.78
25:Q:166:ARG:CZ	42:j:86:ARG:HH12	1.96	0.78
28:T:20:ARG:CZ	28:T:20:ARG:HB2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:u:52:TRP:HA	54:u:55:ILE:HB	1.63	0.78
47:y:237:LEU:HD11	48:z:212:MET:HG2	1.65	0.78
11:B:266:ARG:NH1	70:B:501:3PE:O22	2.17	0.78
14:E:59:GLN:HA	14:E:64:THR:HG22	1.66	0.78
27:S:335:VAL:O	42:j:52:PRO:HD3	1.82	0.78
28:T:13:PRO:CB	28:T:16:THR:O	2.32	0.78
42:j:114:GLU:H	43:g:160:LYS:HD3	1.49	0.78
3:2:321:LYS:HG3	72:2:402:PC1:H272	1.63	0.78
5:6:119:LYS:HE3	71:6:701:CDL:C71	2.13	0.78
28:T:101:LEU:CD2	28:T:110:ILE:HG21	2.14	0.78
10:A:241:ARG:HD3	10:A:243:TRP:CH2	2.18	0.78
49:p:75:GLU:HG2	49:p:76:ILE:C	2.08	0.78
49:A0:110:ALA:CB	49:A0:123:ASP:HA	2.13	0.78
11:B:233:HIS:CE1	14:E:160:GLU:OE2	2.37	0.78
27:S:239:GLU:HG2	27:S:240:LYS:H	1.48	0.78
46:x:113:ARG:NH1	46:x:210:GLY:O	2.16	0.78
41:i:47:THR:HG21	42:j:63:LEU:CD1	2.12	0.77
2:4:166:TYR:OH	70:4:503:3PE:C11	2.28	0.77
2:4:446:LEU:HG	71:4:502:CDL:C37	2.14	0.77
11:B:241:MET:HG3	30:V:10:MET:HB3	1.66	0.77
13:D:182:TYR:CD2	14:E:180:HIS:N	2.42	0.77
23:O:128:PRO:HG2	26:R:45:LYS:HE2	1.67	0.77
25:Q:124:ASP:C	30:V:66:GLU:OE2	2.28	0.77
11:B:393:PRO:HG2	12:C:247:TYR:CE1	2.19	0.77
39:f:162:ASP:C	39:f:164:PRO:HA	2.09	0.77
50:q:14:GLU:O	50:q:18:LYS:HB3	1.83	0.77
55:B1:70:LEU:HD12	55:B1:71:ASN:H	1.49	0.77
12:C:208:GLY:H	13:D:167:TYR:HA	1.47	0.77
12:C:242:GLU:HB2	16:G:92:ASN:ND2	2.00	0.77
14:E:79:ARG:NH2	24:P:19:ASP:OD2	2.16	0.77
5:6:556:ILE:CG1	35:a:76:ILE:HD13	2.13	0.77
9:8:259:GLY:HA3	9:8:261:TRP:H	1.49	0.77
11:B:215:GLU:OE2	14:E:93:LEU:CD2	2.32	0.77
28:T:26:THR:HB	28:T:68:ALA:CB	2.14	0.77
37:c:15:LEU:HA	37:c:18:LEU:HB2	1.67	0.77
41:i:47:THR:CG2	42:j:63:LEU:HD11	2.15	0.77
49:A0:122:HIS:CB	49:A0:168:SER:C	2.58	0.77
4:7:111:LYS:HA	17:H:81:ARG:HH21	1.50	0.77
10:A:355:LYS:CB	10:A:530:TYR:OH	2.30	0.77
14:E:98:ARG:NH1	14:E:155:CYS:O	2.17	0.77
22:N:19:THR:HB	22:N:22:GLU:OE2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:177:ARG:NH2	49:A0:62:MET:O	2.17	0.77
1:9:233:SER:CB	9:8:41:ILE:HD13	2.14	0.77
9:8:119:GLU:O	9:8:159:ARG:NH2	2.18	0.77
14:E:188:GLU:OE2	18:I:64:ASN:HB3	1.85	0.77
28:T:77:SER:C	28:T:80:VAL:HG22	2.10	0.77
49:p:71:MET:HG3	49:p:72:SER:H	1.48	0.77
2:4:190:TRP:CB	28:T:127:MET:HG3	2.14	0.77
2:4:370:PRO:HA	2:4:375:LEU:HD12	1.64	0.77
14:E:188:GLU:OE2	18:I:64:ASN:CG	2.27	0.77
3:2:239:ILE:HG21	42:j:48:ILE:HA	1.67	0.77
3:2:339:LEU:HD13	3:2:343:LEU:HD13	1.66	0.77
6:5:36:MET:O	6:5:39:SER:OG	2.02	0.77
10:A:501:ARG:NH2	10:A:509:ASP:OD1	2.17	0.77
11:B:216:ARG:HG3	14:E:94:SER:CB	2.14	0.77
14:E:62:LEU:CD2	30:V:36:PHE:CE2	2.65	0.77
26:R:237:LYS:O	26:R:239:PRO:HD3	1.85	0.77
35:a:47:TYR:HD1	44:e:105:MET:SD	2.03	0.77
38:d:88:ASP:O	38:d:92:HIS:N	2.18	0.77
47:m:71:ARG:HH22	48:o:46:VAL:HG22	1.49	0.77
1:9:191:ASN:CG	9:8:164:ASN:HD21	1.91	0.76
3:2:326:LEU:HD21	72:2:402:PC1:H2C2	1.65	0.76
21:L:55:VAL:C	25:Q:128:VAL:CG2	2.57	0.76
26:R:133:GLU:HG3	26:R:134:TRP:H	1.49	0.76
28:T:10:TRP:HA	28:T:10:TRP:HE3	1.47	0.76
35:a:60:ILE:CG2	44:e:105:MET:SD	2.64	0.76
42:j:119:VAL:N	43:g:147:GLY:N	2.20	0.76
49:A0:106:ILE:CB	49:A0:167:ALA:O	2.33	0.76
49:A0:147:ILE:CB	49:A0:157:TYR:O	2.33	0.76
1:9:118:PHE:HB2	9:8:220:GLN:HE21	1.51	0.76
2:4:44:GLN:HG2	2:4:45:PHE:H	1.49	0.76
5:6:116:LYS:CG	5:6:119:LYS:NZ	2.49	0.76
36:b:140:LEU:HD23	43:g:82:VAL:HG11	1.66	0.76
46:l:305:GLN:HB3	46:l:306:PRO:HD3	1.66	0.76
11:B:322:SER:OG	14:E:42:ASN:ND2	2.18	0.76
28:T:17:GLU:HB3	28:T:20:ARG:NH2	1.99	0.76
43:g:52:ILE:HA	43:g:55:GLN:HB3	1.67	0.76
1:9:178:GLY:N	9:8:119:GLU:OE2	2.19	0.76
3:2:196:TYR:HE1	28:T:137:ALA:O	1.69	0.76
6:5:26:LEU:HD23	6:5:78:LEU:HD13	1.67	0.76
10:A:334:GLN:NE2	10:A:361:VAL:O	2.19	0.76
11:B:90:ALA:CB	11:B:93:GLY:O	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:213:ARG:CB	13:D:175:ARG:CG	2.62	0.76
23:O:50:PHE:HE1	23:O:96:VAL:HG12	1.51	0.76
28:T:95:CYS:O	28:T:96:ALA:C	2.24	0.76
14:E:61:LEU:HD22	21:L:17:PRO:O	1.86	0.76
23:O:99:GLN:O	23:O:101:THR:N	2.15	0.76
35:a:60:ILE:HG22	44:e:105:MET:CE	1.97	0.76
53:A3:31:GLY:O	53:A3:35:ALA:N	2.14	0.76
2:4:355:MET:HA	2:4:358:TRP:HD1	1.49	0.76
3:2:338:PRO:HB3	25:Q:167:LEU:HD22	1.66	0.76
9:8:207:GLY:O	73:8:501:FMN:C9	2.33	0.76
14:E:188:GLU:OE2	18:I:64:ASN:ND2	2.18	0.76
28:T:17:GLU:C	28:T:20:ARG:HH21	1.92	0.76
35:a:79:ASN:HD22	44:e:73:GLY:C	1.93	0.76
3:2:57:THR:HB	6:5:77:LEU:HD23	1.68	0.76
8:1:172:MET:O	8:1:173:TRP:C	2.29	0.76
8:1:199:ASP:OD2	8:1:279:ARG:NH2	2.19	0.76
16:G:58:LYS:C	23:O:15:THR:N	2.44	0.76
27:S:226:GLU:HA	27:S:229:TYR:HD2	1.51	0.76
28:T:101:LEU:CD1	28:T:110:ILE:CG2	2.59	0.76
42:j:35:GLY:O	42:j:39:TYR:N	2.18	0.76
47:m:375:LYS:HG2	50:q:17:ARG:HH22	1.51	0.76
49:A0:15:ARG:HH21	49:A0:32:ARG:HG2	1.51	0.76
2:4:75:LEU:HD21	2:4:440:HIS:CE1	2.21	0.76
8:1:171:GLN:HE21	8:1:171:GLN:N	1.83	0.76
8:1:301:CYS:O	8:1:305:VAL:HG23	1.85	0.76
10:A:382:ARG:O	10:A:385:TYR:N	2.17	0.76
11:B:216:ARG:HA	14:E:94:SER:HB3	1.65	0.76
40:h:142:PHE:CD2	43:g:162:ARG:NH1	2.54	0.76
2:4:16:TRP:HZ2	70:4:501:3PE:C2G	1.98	0.76
13:D:103:ARG:NE	14:E:84:ILE:HD13	2.00	0.76
19:J:3:PHE:CB	71:J:101:CDL:C72	2.64	0.76
25:Q:32:TYR:OH	30:V:74:LEU:HD22	1.85	0.76
28:T:99:LEU:H	28:T:99:LEU:CD1	1.99	0.76
28:T:101:LEU:CG	28:T:110:ILE:HG22	2.16	0.76
49:A0:150:ALA:O	49:A0:155:GLY:HA2	1.86	0.76
8:1:173:TRP:O	8:1:175:ILE:N	2.19	0.75
10:A:141:ASP:HB3	12:C:241:TRP:HD1	1.48	0.75
10:A:176:CYS:CB	74:A:802:SF4:S4	2.74	0.75
26:R:55:VAL:HG12	26:R:56:ALA:H	1.51	0.75
5:6:88:MET:HE2	5:6:468:ILE:HG12	1.68	0.75
11:B:367:LYS:HZ2	14:E:212:ARG:C	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:213:ARG:NH1	12:C:224:GLU:OE2	2.18	0.75
12:C:214:TYR:CE1	13:D:138:ARG:HD3	2.22	0.75
19:J:55:SER:HB2	19:J:62:VAL:HG23	1.69	0.75
45:k:32:GLN:NE2	46:l:373:GLU:OE1	2.20	0.75
53:A3:39:ARG:HH11	53:A3:39:ARG:HG3	1.50	0.75
57:C4:5:MET:HE3	66:B0:42:PRO:HA	1.67	0.75
57:C4:59:GLN:H	57:C4:62:GLU:HG3	1.51	0.75
2:4:449:LEU:CD1	71:4:502:CDL:H322	2.16	0.75
8:1:146:LEU:HD11	8:1:185:TRP:CZ3	2.21	0.75
12:C:227:GLU:CG	26:R:49:SER:CB	2.55	0.75
25:Q:51:LYS:NZ	36:b:189:ASN:HD21	1.83	0.75
27:S:335:VAL:C	42:j:52:PRO:HD3	2.11	0.75
48:z:101:ALA:O	48:z:105:ASN:ND2	2.20	0.75
8:1:307:LEU:HD23	30:V:47:TYR:CE1	2.21	0.75
19:J:38:VAL:O	19:J:44:GLN:NE2	2.19	0.75
45:k:142:ASP:OD1	49:p:2:HIS:ND1	2.19	0.75
47:m:1:MET:SD	47:m:7:SER:OG	2.45	0.75
2:4:16:TRP:CZ2	70:4:501:3PE:H2E1	2.21	0.75
14:E:57:ALA:CB	21:L:13:TRP:CZ3	2.61	0.75
1:9:148:ILE:HD12	1:9:184:PRO:HB2	1.69	0.75
5:6:581:LYS:HB3	6:5:96:LEU:HD11	1.68	0.75
17:H:15:ASP:O	17:H:17:TRP:N	2.20	0.75
27:S:335:VAL:H	42:j:52:PRO:CG	1.99	0.75
28:T:66:ILE:HA	28:T:69:ILE:CG2	2.17	0.75
45:k:80:GLU:OE1	46:l:292:THR:OG1	2.04	0.75
48:o:158:ILE:HG12	48:o:160:MET:H	1.52	0.75
11:B:242:ASP:HB3	24:P:32:SER:OG	1.82	0.75
38:d:40:VAL:HG12	38:d:41:ALA:N	2.00	0.75
45:k:131:ARG:NH2	45:k:177:LEU:O	2.19	0.75
53:A3:33:VAL:HG13	53:A3:41:ILE:HD11	1.69	0.75
1:9:233:SER:C	9:8:41:ILE:HD13	2.11	0.75
26:R:168:SER:HB2	26:R:188:GLU:OE2	1.86	0.75
36:b:93:ILE:HG23	43:g:61:TYR:CE2	2.22	0.75
38:d:108:LEU:CB	44:e:166:LEU:HD21	2.16	0.75
41:i:51:SER:OG	42:j:66:THR:CG2	2.32	0.75
47:m:271:GLU:OE2	47:m:273:TYR:OH	2.05	0.75
55:v:65:VAL:HA	55:v:78:TYR:HA	1.69	0.75
8:1:34:ARG:HA	14:E:83:THR:HG21	1.67	0.74
8:1:38:ASN:ND2	29:U:31:ASN:OD1	2.19	0.74
10:A:111:LYS:HA	24:P:53:TYR:HH	1.51	0.74
11:B:234:GLN:HE22	14:E:96:ARG:HD2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:120:ASP:OD2	12:C:201:ARG:HA	1.87	0.74
14:E:37:THR:HB	24:P:107:SER:HB2	1.69	0.74
18:I:62:GLU:O	29:U:127:TYR:CE2	2.40	0.74
27:S:342:LEU:N	42:j:59:HIS:CD2	2.44	0.74
40:h:120:ARG:NH2	43:g:66:ARG:H	1.85	0.74
31:M:17:TYR:OH	31:M:57:GLU:OE2	2.04	0.74
42:j:115:GLU:HB3	42:j:117:HIS:ND1	2.02	0.74
45:w:131:ARG:NH2	45:w:177:LEU:O	2.19	0.74
57:C4:184:LEU:HD11	57:C4:211:LEU:HD21	1.69	0.74
3:2:316:GLN:HB3	3:2:318:PRO:HD3	1.67	0.74
3:2:325:PHE:CE2	70:2:401:3PE:H2G1	2.19	0.74
9:8:142:CYS:O	9:8:146:GLY:N	2.15	0.74
9:8:295:PRO:HG2	9:8:298:GLU:HG2	1.69	0.74
14:E:69:GLY:O	14:E:73:THR:N	2.19	0.74
1:9:200:ASP:OD2	1:9:219:ARG:HD3	1.87	0.74
3:2:30:TRP:CZ3	3:2:67:SER:HB3	2.22	0.74
10:A:259:SER:O	10:A:260:ASN:ND2	2.20	0.74
14:E:135:ARG:HD2	18:I:69:ILE:HA	1.70	0.74
21:L:8:PHE:HZ	72:L:200:PC1:C31	1.99	0.74
25:Q:110:CYS:HA	25:Q:113:ASP:HB3	1.69	0.74
26:R:154:GLN:O	26:R:156:SER:N	2.20	0.74
26:R:203:PRO:HA	26:R:265:PHE:HB2	1.70	0.74
41:i:69:TYR:HA	42:j:20:SER:HA	1.69	0.74
44:e:113:ILE:C	44:e:114:ARG:HD3	2.13	0.74
2:4:360:LEU:CD1	71:6:701:CDL:H532	2.17	0.74
3:2:109:ALA:O	3:2:112:HIS:NE2	2.20	0.74
10:A:307:VAL:HG22	10:A:308:ARG:H	1.52	0.74
71:J:101:CDL:H122	29:U:2:GLU:HB2	1.70	0.74
25:Q:52:ASP:HA	30:V:116:TRP:HB3	1.68	0.74
27:S:341:TRP:C	42:j:59:HIS:HD2	1.95	0.74
28:T:2:ALA:HB3	28:T:4:THR:OG1	1.88	0.74
35:a:124:THR:CB	43:g:137:LYS:HB2	2.17	0.74
1:9:90:ASN:ND2	1:9:92:TRP:O	2.20	0.74
1:9:227:PRO:HD2	9:8:48:ARG:HH12	1.51	0.74
10:A:241:ARG:HD3	10:A:243:TRP:CZ3	2.22	0.74
11:B:458:PHE:C	11:B:460:GLU:H	1.95	0.74
13:D:184:PRO:HG3	14:E:183:LEU:HD22	1.68	0.74
13:D:196:GLY:HA2	14:E:176:SER:HB3	1.69	0.74
26:R:275:ASP:O	26:R:279:TYR:N	2.19	0.74
28:T:101:LEU:CG	28:T:110:ILE:CG2	2.66	0.74
34:Z:41:LEU:CB	39:f:42:CYS:CB	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:133:TYR:OH	43:g:87:GLU:HG2	1.88	0.74
2:4:244:LEU:HD21	2:4:301:ILE:HD12	1.69	0.74
11:B:95:LEU:HD23	11:B:458:PHE:CZ	2.23	0.74
22:N:36:GLY:O	22:N:45:ARG:NH2	2.20	0.74
42:j:30:ARG:O	42:j:34:VAL:N	2.14	0.74
53:t:43:ASP:HA	54:u:33:ARG:HH22	1.52	0.74
2:4:2:LEU:CG	72:4:504:PC1:H142	2.18	0.74
12:C:213:ARG:HB3	13:D:175:ARG:CG	2.10	0.74
13:D:138:ARG:HH21	13:D:142:ASP:CG	1.95	0.74
47:y:1:MET:SD	47:y:7:SER:OG	2.45	0.74
1:9:183:ALA:HB3	1:9:195:ASP:HA	1.68	0.74
25:Q:7:LEU:O	30:V:88:ARG:NH2	2.19	0.74
28:T:34:LEU:CD1	28:T:35:VAL:H	1.94	0.74
33:Y:46:ARG:HA	33:Y:49:GLN:HE22	1.52	0.74
48:z:175:THR:OG1	52:B3:78:LYS:NZ	2.21	0.74
2:4:248:LEU:HD11	43:g:151:SER:HA	1.71	0.73
13:D:146:GLU:O	13:D:148:ARG:N	2.21	0.73
8:1:222:LEU:O	8:1:226:ALA:N	2.21	0.73
11:B:134:PRO:O	11:B:137:ASP:N	2.19	0.73
24:P:109:ASP:H	24:P:111:PRO:HD3	1.53	0.73
35:a:79:ASN:ND2	44:e:73:GLY:CA	2.25	0.73
40:h:149:LEU:HD21	43:g:167:ARG:HA	1.70	0.73
46:l:40:ASN:OD1	46:l:41:TYR:N	2.21	0.73
46:l:113:ARG:NH1	46:l:210:GLY:O	2.16	0.73
47:m:156:ILE:HG22	53:A3:38:TRP:CH2	2.23	0.73
47:m:237:LEU:HD11	48:o:212:MET:HG2	1.70	0.73
45:w:412:SER:O	54:B2:15:ARG:NH2	2.21	0.73
12:C:123:THR:HG21	16:G:129:SER:H	1.50	0.73
14:E:62:LEU:HD13	30:V:36:PHE:HZ	0.94	0.73
39:f:126:LYS:O	39:f:130:ARG:N	2.20	0.73
46:x:40:ASN:OD1	46:x:41:TYR:N	2.21	0.73
49:A0:83:GLU:HA	49:A0:102:THR:CB	2.18	0.73
58:C2:187:THR:HG21	62:A4:68:THR:HG21	1.68	0.73
3:2:153:LEU:O	3:2:156:THR:N	2.21	0.73
10:A:124:HIS:CD2	74:A:801:SF4:S3	2.82	0.73
14:E:60:THR:HG21	21:L:17:PRO:HD2	1.70	0.73
27:S:219:SER:O	27:S:223:GLN:N	2.19	0.73
41:i:68:GLU:HG3	42:j:19:ARG:NE	2.03	0.73
62:A4:5:LYS:HZ3	62:A4:6:GLY:N	1.81	0.73
3:2:234:TRP:CZ3	27:S:327:TYR:CE2	2.77	0.73
9:8:364:VAL:HG12	9:8:400:VAL:HG22	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:59:ASP:OD2	25:Q:130:LYS:HD2	1.87	0.73
27:S:335:VAL:HB	42:j:51:ARG:C	2.14	0.73
45:k:436:ARG:HH21	47:m:221:HIS:HB3	1.54	0.73
47:m:156:ILE:HG22	53:A3:38:TRP:HH2	1.54	0.73
3:2:196:TYR:CE1	28:T:137:ALA:O	2.41	0.73
8:1:169:GLN:O	8:1:170:GLU:O	2.07	0.73
12:C:205:PRO:HB3	16:G:120:PRO:O	1.89	0.73
12:C:240:PRO:CG	16:G:88:GLN:HE22	2.02	0.73
35:a:43:LEU:O	35:a:47:TYR:N	2.17	0.73
41:i:62:HIS:HE1	42:j:23:PRO:HG2	0.57	0.73
48:o:101:ALA:O	48:o:105:ASN:ND2	2.20	0.73
47:y:271:GLU:OE2	47:y:273:TYR:OH	2.05	0.73
8:1:317:GLN:NE2	8:1:317:GLN:HA	2.03	0.73
10:A:312:GLY:HA3	29:U:144:TYR:HA	1.71	0.73
11:B:266:ARG:NH1	70:B:501:3PE:H232	2.04	0.73
42:j:116:PHE:CE1	43:g:157:ALA:CB	2.58	0.73
50:A1:13:LEU:O	50:A1:14:GLU:CB	2.36	0.73
2:4:208:PRO:HB3	2:4:213:HIS:HB3	1.71	0.73
10:A:217:GLU:OE2	10:A:408:ARG:NE	2.21	0.73
25:Q:161:ALA:HB2	42:j:83:TYR:C	2.14	0.73
49:A0:117:LEU:O	49:A0:118:ARG:O	2.06	0.73
10:A:319:TRP:CH2	10:A:585:PRO:HD2	2.22	0.73
19:J:4:GLU:OE2	29:U:31:ASN:HB3	1.89	0.73
2:4:248:LEU:HD11	43:g:151:SER:CA	2.19	0.73
8:1:172:MET:SD	8:1:176:LEU:HD12	2.25	0.73
27:S:335:VAL:HB	42:j:51:ARG:O	1.89	0.73
42:j:114:GLU:CB	43:g:160:LYS:CE	2.46	0.73
2:4:446:LEU:HD23	71:4:502:CDL:C38	2.19	0.72
10:A:34:VAL:HG22	10:A:99:GLY:HA2	1.70	0.72
10:A:627:SER:OG	10:A:632:MET:O	2.06	0.72
28:T:20:ARG:HB2	28:T:20:ARG:NH1	2.04	0.72
28:T:30:GLY:CA	28:T:64:ALA:HB2	2.19	0.72
4:7:23:LYS:HZ2	6:5:23:ARG:HH11	1.35	0.72
11:B:266:ARG:HH11	70:B:501:3PE:H231	1.53	0.72
12:C:232:PHE:HD1	13:D:165:TYR:CE2	2.07	0.72
62:A4:54:ARG:HD3	62:A4:54:ARG:N	2.04	0.72
11:B:61:TRP:CZ2	11:B:64:PRO:HG2	2.12	0.72
11:B:238:LEU:CD1	24:P:37:PRO:O	2.36	0.72
18:I:66:ASN:OD1	18:I:67:PHE:N	2.22	0.72
40:h:142:PHE:CE2	43:g:162:ARG:NH1	2.58	0.72
12:C:240:PRO:CG	16:G:88:GLN:NE2	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:138:ARG:NH2	13:D:142:ASP:CG	2.47	0.72
28:T:22:THR:CG2	28:T:75:CYS:HG	2.03	0.72
32:X:55:THR:HG21	36:b:131:LYS:HD2	1.69	0.72
34:Z:64:VAL:HG12	34:Z:68:LEU:HG	1.69	0.72
45:w:32:GLN:NE2	46:x:373:GLU:OE1	2.22	0.72
48:z:158:ILE:HG12	48:z:160:MET:H	1.52	0.72
8:1:316:PRO:CG	30:V:57:ARG:NE	2.51	0.72
12:C:157:SER:HB2	12:C:159:VAL:HG23	1.72	0.72
28:T:99:LEU:HD12	28:T:99:LEU:N	2.03	0.72
28:T:101:LEU:HD22	28:T:101:LEU:C	2.14	0.72
3:2:93:MET:SD	5:6:605:HIS:HE1	2.11	0.72
3:2:325:PHE:CE2	70:2:401:3PE:C2G	2.72	0.72
5:6:55:ILE:HD11	38:d:74:PHE:HZ	0.91	0.72
10:A:422:TRP:CH2	16:G:169:ARG:HD3	2.25	0.72
11:B:123:LEU:HD11	12:C:206:LEU:HD21	1.71	0.72
44:e:70:THR:C	44:e:72:TYR:N	2.43	0.72
28:T:12:ILE:CB	28:T:13:PRO:HD2	2.17	0.72
28:T:88:LEU:C	28:T:88:LEU:HD23	2.14	0.72
49:A0:101:ARG:H	49:A0:129:LYS:C	1.97	0.72
1:9:41:HIS:CE1	18:I:83:ARG:HH22	2.08	0.72
1:9:181:VAL:HG22	9:8:125:CYS:SG	2.29	0.72
1:9:227:PRO:HD3	9:8:48:ARG:NH2	2.05	0.72
1:9:238:PRO:HD3	9:8:60:GLY:HA2	1.72	0.72
2:4:69:THR:HG22	2:4:235:LEU:HD11	1.72	0.72
5:6:157:TRP:HD1	5:6:158:TRP:CD1	2.08	0.72
5:6:470:ASN:CG	38:d:77:PHE:HD1	1.98	0.72
49:p:73:LYS:HD3	49:p:94:LYS:HA	1.72	0.72
45:w:408:ARG:HE	53:A3:15:ARG:NH2	1.88	0.72
28:T:22:THR:CG2	28:T:75:CYS:SG	2.77	0.72
31:W:105:MET:HA	31:W:108:LEU:HB2	1.70	0.72
35:a:63:PRO:HD2	44:e:106:HIS:CB	2.20	0.72
48:o:79:GLU:O	48:o:80:MET:HG2	1.90	0.72
53:A3:43:ASP:O	54:B2:33:ARG:NH2	2.14	0.72
13:D:184:PRO:HG3	14:E:183:LEU:CD2	2.20	0.72
26:R:182:ARG:O	26:R:183:SER:OG	2.07	0.72
28:T:18:CYS:O	28:T:75:CYS:SG	2.46	0.72
30:V:48:TRP:O	30:V:52:LYS:NZ	2.22	0.72
50:q:13:LEU:HA	50:q:16:ILE:CG2	2.20	0.72
49:A0:110:ALA:HB1	49:A0:123:ASP:HA	1.67	0.72
59:A7:23:PRO:O	60:C0:66:ARG:HD3	1.89	0.72
7:3:106:TRP:CZ2	72:L:200:PC1:C14	2.67	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:237:PHE:CD1	8:1:240:ILE:HD11	2.24	0.71
11:B:238:LEU:HD12	24:P:37:PRO:O	1.89	0.71
12:C:232:PHE:HA	13:D:165:TYR:CZ	2.25	0.71
21:L:23:PHE:HE1	72:L:200:PC1:C2A	2.03	0.71
23:O:33:ARG:HD3	31:M:48:VAL:HG21	0.79	0.71
23:O:46:THR:O	23:O:49:LEU:N	2.22	0.71
53:A3:39:ARG:C	53:A3:41:ILE:N	2.43	0.71
14:E:105:ARG:HD3	14:E:109:GLY:HA3	1.70	0.71
21:L:56:PRO:HB2	25:Q:129:THR:O	1.90	0.71
27:S:67:GLU:HA	27:S:70:GLY:H	1.55	0.71
53:A3:15:ARG:HG3	53:A3:16:ASN:H	1.54	0.71
7:3:53:MET:O	7:3:56:PHE:N	2.22	0.71
8:1:5:ASN:HD21	19:J:23:THR:HG23	1.54	0.71
10:A:217:GLU:OE1	10:A:217:GLU:N	2.20	0.71
28:T:81:ARG:H	28:T:81:ARG:CD	2.01	0.71
45:k:426:GLY:HA2	45:k:428:ILE:HG13	1.72	0.71
45:k:438:ARG:NH2	49:p:37:TYR:OH	2.24	0.71
2:4:2:LEU:HD21	72:4:504:PC1:H142	1.70	0.71
2:4:118:PHE:O	2:4:122:PHE:N	2.24	0.71
2:4:166:TYR:CE2	70:4:503:3PE:O21	2.43	0.71
9:8:317:VAL:HG23	9:8:356:VAL:HG12	1.70	0.71
11:B:94:VAL:HG12	11:B:115:LEU:HD23	1.73	0.71
14:E:53:VAL:HG11	21:L:14:ALA:HB2	1.70	0.71
28:T:90:TYR:CB	28:T:126:LYS:HD2	2.20	0.71
45:k:215:HIS:ND1	45:k:215:HIS:O	2.23	0.71
45:w:41:ILE:HG22	45:w:43:ALA:H	1.55	0.71
2:4:190:TRP:HB3	28:T:127:MET:CG	2.20	0.71
24:P:27:ARG:HA	29:U:56:PHE:HB3	1.73	0.71
24:P:40:LYS:CA	30:V:7:LYS:N	2.53	0.71
27:S:31:TYR:OH	27:S:285:LEU:O	2.06	0.71
37:c:95:TYR:HE2	43:g:10:TYR:HD1	1.36	0.71
42:j:114:GLU:N	43:g:160:LYS:CE	2.53	0.71
46:l:70:ARG:NH1	55:v:67:SER:OG	2.24	0.71
45:w:426:GLY:HA2	45:w:428:ILE:HG13	1.72	0.71
46:x:70:ARG:NH1	46:x:100:SER:OG	2.24	0.71
1:9:130:TYR:HA	1:9:189:ASN:HD21	1.53	0.71
1:9:241:PRO:HB2	9:8:63:TYR:CE2	2.25	0.71
11:B:322:SER:OG	14:E:42:ASN:CG	2.34	0.71
25:Q:158:LEU:HA	42:j:88:HIS:ND1	2.06	0.71
28:T:69:ILE:HD11	28:T:96:ALA:HB3	1.70	0.71
47:m:44:GLN:O	47:m:48:GLY:N	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:139:PRO:HB3	36:b:158:ARG:CA	2.21	0.71
35:a:79:ASN:CG	44:e:73:GLY:HA2	2.15	0.71
50:q:18:LYS:HG3	50:q:83:TYR:CD2	2.26	0.71
45:w:67:THR:HA	45:w:121:SER:H	1.56	0.71
45:w:281:ASP:OD1	45:w:282:CYS:N	2.24	0.71
49:A0:120:PRO:O	49:A0:122:HIS:N	2.19	0.71
40:h:141:CYS:HA	43:g:162:ARG:HD3	1.72	0.71
43:g:50:GLU:OE2	43:g:54:ARG:NE	2.21	0.71
44:e:65:TYR:O	44:e:67:ASP:N	2.24	0.71
45:k:41:ILE:HG22	45:k:43:ALA:H	1.55	0.71
53:A3:41:ILE:O	53:A3:42:LEU:C	2.33	0.71
58:C2:156:ARG:HH11	58:C2:156:ARG:HG3	1.56	0.71
5:6:470:ASN:HD21	38:d:77:PHE:CB	1.95	0.71
8:1:77:MET:O	8:1:80:GLY:N	2.21	0.71
11:B:139:LEU:HD21	11:B:424:ILE:HD12	1.73	0.71
11:B:264:ASN:HB2	14:E:65:GLU:OE2	1.91	0.71
28:T:17:GLU:HB3	28:T:20:ARG:CZ	2.21	0.71
46:x:304:HIS:CD2	46:x:305:GLN:HB3	2.26	0.71
8:1:171:GLN:HE21	8:1:171:GLN:H	1.36	0.71
34:Z:63:PHE:O	34:Z:65:GLY:N	2.24	0.71
44:e:111:MET:HG2	44:e:112:TYR:H	1.56	0.71
49:p:126:ARG:HA	49:p:135:LEU:HA	1.73	0.71
59:A7:147:LYS:HA	59:A7:147:LYS:HE3	1.72	0.71
1:9:72:GLU:N	15:F:102:SER:HB3	2.06	0.70
3:2:14:MET:HA	3:2:17:THR:HG22	1.73	0.70
5:6:467:ILE:HD12	38:d:77:PHE:HZ	1.56	0.70
11:B:61:TRP:CZ2	11:B:64:PRO:HD3	2.25	0.70
11:B:322:SER:OG	14:E:42:ASN:CB	2.38	0.70
26:R:168:SER:OG	26:R:202:LYS:NZ	2.20	0.70
76:R:601:NAP:O2X	76:R:601:NAP:H1B	1.87	0.70
27:S:338:LYS:NZ	42:j:57:GLY:H	1.88	0.70
28:T:98:GLY:HA2	28:T:114:ALA:HB3	1.71	0.70
58:C2:12:ASN:HD22	65:C3:20:VAL:H	1.39	0.70
11:B:378:LEU:O	11:B:381:HIS:N	2.24	0.70
13:D:180:ASP:O	14:E:178:GLU:O	2.09	0.70
53:A3:45:VAL:O	54:B2:33:ARG:NH2	2.24	0.70
2:4:20:ASN:O	2:4:22:MET:N	2.25	0.70
11:B:61:TRP:CG	11:B:62:LYS:N	2.38	0.70
23:O:48:HIS:ND1	26:R:359:TYR:CZ	2.59	0.70
28:T:5:VAL:CG1	28:T:28:ILE:CD1	2.58	0.70
28:T:13:PRO:CB	28:T:17:GLU:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:106:ARG:HD2	28:T:106:ARG:N	2.06	0.70
2:4:166:TYR:CD1	70:4:503:3PE:O22	2.44	0.70
5:6:406:ALA:HB2	44:e:147:GLY:HA2	1.74	0.70
11:B:61:TRP:HH2	11:B:64:PRO:HG2	1.57	0.70
12:C:149:THR:HB	12:C:155:ILE:HD11	1.72	0.70
18:I:108:LYS:HZ2	18:I:108:LYS:CA	2.04	0.70
28:T:20:ARG:H	28:T:20:ARG:CD	2.03	0.70
28:T:79:GLN:O	28:T:80:VAL:O	2.10	0.70
28:T:98:GLY:HA3	28:T:111:GLY:O	1.91	0.70
31:W:85:TYR:CE1	34:Z:19:TYR:N	2.57	0.70
33:Y:47:TYR:CE1	34:Z:17:PRO:HD3	2.26	0.70
45:k:347:THR:O	53:t:16:ASN:ND2	2.24	0.70
4:7:107:VAL:HG13	4:7:108:LEU:H	1.56	0.70
12:C:192:ASP:HA	13:D:132:LYS:CD	2.21	0.70
1:9:228:ALA:HA	1:9:231:LEU:HD23	1.72	0.70
34:Z:45:TRP:C	39:f:38:ARG:NH2	2.50	0.70
1:9:239:LYS:HE2	9:8:42:PHE:HD1	1.53	0.70
2:4:278:ARG:HB2	5:6:546:GLN:NE2	2.07	0.70
11:B:301:ASP:OD2	11:B:318:VAL:HG21	1.92	0.70
12:C:217:GLU:OE1	26:R:71:ASN:ND2	2.25	0.70
14:E:188:GLU:CD	18:I:64:ASN:CG	2.60	0.70
25:Q:165:SER:OG	42:j:83:TYR:CE1	2.41	0.70
35:a:67:ARG:HD2	44:e:79:PRO:HD2	1.73	0.70
3:2:261:MET:HE2	3:2:337:LEU:HD12	1.72	0.70
9:8:93:PHE:CE2	9:8:98:LYS:HB3	2.27	0.70
9:8:98:LYS:HG3	9:8:99:TRP:CD1	2.26	0.70
14:E:135:ARG:HH22	18:I:72:ILE:HD11	1.50	0.70
25:Q:109:GLU:HG3	25:Q:110:CYS:H	1.56	0.70
41:i:47:THR:HB	42:j:63:LEU:HD12	0.77	0.70
42:j:116:PHE:HE1	43:g:157:ALA:CA	2.05	0.70
56:A9:11:ASN:HD22	56:A9:14:ASP:H	1.39	0.70
10:A:312:GLY:HA2	29:U:144:TYR:CD1	2.27	0.70
11:B:278:VAL:HG23	11:B:438:MET:HG3	1.73	0.70
40:h:82:VAL:O	40:h:86:ASN:N	2.24	0.70
45:k:252:HIS:HD2	45:k:323:HIS:CE1	2.06	0.70
52:s:44:VAL:O	52:s:48:SER:N	2.25	0.70
49:A0:91:TRP:CB	49:A0:196:GLY:CA	2.64	0.70
53:A3:47:TYR:CE2	54:B2:33:ARG:CZ	2.74	0.70
56:A9:176:MET:HE3	56:A9:181:THR:HG22	1.71	0.70
4:7:170:GLU:O	4:7:172:THR:N	2.24	0.70
5:6:19:ILE:CG2	71:6:701:CDL:H372	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:312:SER:OG	30:V:55:ARG:NH1	2.25	0.70
12:C:204:PHE:HE2	13:D:167:TYR:CB	2.04	0.70
24:P:38:PRO:O	30:V:8:GLN:CG	2.40	0.70
28:T:90:TYR:CG	28:T:126:LYS:HD2	2.27	0.70
1:9:143:ARG:NH1	9:8:285:PRO:CG	2.54	0.69
2:4:2:LEU:HG	72:4:504:PC1:H141	1.74	0.69
2:4:2:LEU:CG	72:4:504:PC1:C14	2.69	0.69
6:5:24:SER:HB3	6:5:89:TYR:HA	1.72	0.69
16:G:75:ARG:NH2	16:G:119:ASP:OD1	2.24	0.69
23:O:20:ILE:HB	23:O:80:ASP:OD2	1.91	0.69
24:P:29:GLN:HG3	24:P:30:GLU:H	1.56	0.69
26:R:207:PHE:HA	26:R:211:ASP:OD2	1.92	0.69
52:B3:44:VAL:O	52:B3:48:SER:N	2.25	0.69
1:9:56:THR:HG22	1:9:58:GLU:H	1.57	0.69
4:7:17:PHE:CE2	6:5:11:ALA:HB1	2.27	0.69
5:6:237:MET:HB3	5:6:299:LYS:HD3	1.73	0.69
11:B:212:GLU:OE2	14:E:92:PRO:HG3	1.92	0.69
45:k:281:ASP:OD1	45:k:282:CYS:N	2.24	0.69
4:7:140:ALA:O	4:7:142:GLY:N	2.25	0.69
5:6:467:ILE:CD1	38:d:77:PHE:CZ	2.74	0.69
5:6:577:VAL:HG13	6:5:97:GLN:HE22	1.56	0.69
8:1:232:ILE:C	8:1:236:ILE:HG22	2.16	0.69
10:A:355:LYS:HB2	10:A:530:TYR:CZ	2.27	0.69
11:B:261:MET:SD	14:E:70:LEU:CD2	2.65	0.69
12:C:62:ALA:O	12:C:65:GLU:N	2.26	0.69
13:D:184:PRO:HG3	14:E:183:LEU:HD13	1.73	0.69
21:L:9:LEU:HD21	72:L:200:PC1:H382	1.74	0.69
25:Q:165:SER:CB	42:j:83:TYR:CD1	2.75	0.69
28:T:69:ILE:HG21	28:T:100:ILE:HD11	1.72	0.69
29:U:124:TYR:CE2	29:U:126:PRO:HG3	2.27	0.69
45:k:87:ASN:OD1	45:k:88:ALA:N	2.25	0.69
11:B:188:THR:O	11:B:191:ALA:N	2.26	0.69
11:B:289:SER:OG	11:B:406:GLU:N	2.24	0.69
12:C:175:MET:O	12:C:198:HIS:HB3	1.92	0.69
12:C:221:VAL:CG2	13:D:138:ARG:HG2	2.22	0.69
14:E:135:ARG:HH12	18:I:68:ALA:HB1	1.57	0.69
16:G:111:LEU:CD1	26:R:100:LEU:HD23	2.20	0.69
28:T:22:THR:O	28:T:26:THR:CG2	2.29	0.69
34:Z:43:ASP:C	39:f:38:ARG:HH21	1.92	0.69
31:M:70:LEU:HD13	31:M:76:ILE:HG12	1.75	0.69
47:m:376:LEU:HD22	50:q:17:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:87:ASN:OD1	45:w:88:ALA:N	2.25	0.69
45:w:252:HIS:HD2	45:w:323:HIS:CE1	2.06	0.69
7:3:112:GLU:OE2	8:1:290:TRP:NE1	2.26	0.69
10:A:226:CYS:SG	74:A:802:SF4:S1	2.91	0.69
12:C:205:PRO:CB	16:G:120:PRO:O	2.40	0.69
27:S:193:VAL:HG22	27:S:244:LEU:HB3	1.75	0.69
42:j:108:THR:CB	43:g:79:GLU:HA	2.22	0.69
47:m:5:ARG:HA	47:m:8:HIS:CD2	2.28	0.69
11:B:260:GLU:HB2	14:E:73:THR:HG21	1.72	0.69
12:C:218:VAL:HG13	12:C:219:LYS:H	1.58	0.69
31:M:60:PHE:HE1	31:M:83:LYS:HG2	1.56	0.69
46:l:70:ARG:NH1	46:l:100:SER:OG	2.24	0.69
3:2:325:PHE:CG	70:2:401:3PE:H2G1	2.25	0.69
8:1:35:LYS:O	13:D:108:ARG:HD3	1.92	0.69
17:H:84:GLU:OE2	30:V:127:LEU:HD11	1.93	0.69
28:T:34:LEU:C	28:T:34:LEU:HD22	2.17	0.69
28:T:55:ARG:O	28:T:58:ARG:HB3	1.92	0.69
45:w:203:LEU:HA	45:w:207:GLN:HE21	1.57	0.69
57:C4:13:THR:HB	57:C4:168:LEU:HD23	1.73	0.69
2:4:188:ASN:OD1	2:4:189:SER:N	2.26	0.69
2:4:278:ARG:H	5:6:546:GLN:NE2	1.86	0.69
4:7:13:PHE:O	4:7:16:GLY:N	2.26	0.69
8:1:172:MET:O	8:1:172:MET:HE3	1.93	0.69
10:A:112:ALA:O	10:A:115:GLY:N	2.23	0.69
10:A:311:LYS:O	29:U:144:TYR:HE1	1.75	0.69
11:B:253:LEU:HD23	11:B:254:ARG:NH1	2.08	0.69
11:B:355:GLU:OE1	11:B:355:GLU:N	2.21	0.69
12:C:123:THR:HG21	16:G:129:SER:N	2.08	0.69
12:C:217:GLU:HB2	26:R:71:ASN:ND2	2.08	0.69
26:R:208:GLY:N	26:R:211:ASP:OD2	2.25	0.69
27:S:162:TYR:HD1	27:S:172:VAL:HG21	1.58	0.69
27:S:333:GLU:CG	42:j:52:PRO:O	2.41	0.69
28:T:72:LEU:HD12	28:T:72:LEU:C	2.17	0.69
41:i:68:GLU:CB	42:j:19:ARG:HB3	2.22	0.69
42:j:114:GLU:N	43:g:160:LYS:HD3	2.07	0.69
45:k:67:THR:HA	45:k:121:SER:H	1.56	0.69
45:k:203:LEU:HA	45:k:207:GLN:HE21	1.58	0.69
48:o:80:MET:HG3	48:o:81:PHE:H	1.57	0.69
49:A0:122:HIS:CB	49:A0:168:SER:O	2.41	0.69
50:A1:12:TRP:CE3	50:A1:13:LEU:N	2.61	0.69
2:4:344:LEU:HD21	35:a:59:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:346:ARG:HD3	2:4:413:MET:HE3	1.75	0.69
3:2:335:MET:O	25:Q:170:TRP:CH2	2.46	0.69
8:1:176:LEU:HB3	8:1:177:PRO:HD3	1.70	0.69
31:W:79:ILE:HG12	31:W:145:VAL:HG13	1.74	0.69
58:C2:154:GLY:HA2	61:A6:6:VAL:HG22	1.75	0.69
1:9:227:PRO:HD3	9:8:48:ARG:HH22	1.57	0.69
3:2:104:MET:O	3:2:114:TRP:CZ3	2.44	0.69
9:8:242:VAL:HG12	73:8:501:FMN:H5'2	1.74	0.69
19:J:3:PHE:CD1	71:J:101:CDL:H722	2.27	0.69
30:V:121:MET:HE3	30:V:137:THR:HG22	1.75	0.69
70:4:501:3PE:H371	70:4:501:3PE:H2A1	1.75	0.68
3:2:210:ILE:HG12	72:2:402:PC1:H2F1	1.73	0.68
5:6:578:THR:HB	11:B:58:THR:OG1	1.92	0.68
5:6:593:ILE:HD11	28:T:42:ALA:HB2	1.74	0.68
10:A:168:LEU:O	10:A:234:LYS:HB2	1.93	0.68
10:A:504:SER:H	10:A:505:GLY:HA2	1.59	0.68
11:B:264:ASN:OD1	11:B:264:ASN:N	2.26	0.68
11:B:272:THR:HA	11:B:275:ILE:HD12	1.74	0.68
13:D:195:TYR:CZ	29:U:80:SER:HB2	2.27	0.68
29:U:115:PHE:HB2	29:U:117:LEU:HG	1.75	0.68
35:a:79:ASN:HD22	44:e:73:GLY:HA2	0.90	0.68
31:M:25:ILE:HD12	31:M:42:LEU:HG	1.73	0.68
3:2:227:THR:HA	3:2:230:LEU:HD13	1.76	0.68
8:1:237:PHE:O	8:1:238:THR:C	2.33	0.68
11:B:141:TYR:OH	11:B:458:PHE:O	2.08	0.68
12:C:232:PHE:HD1	13:D:165:TYR:CD2	2.11	0.68
21:L:53:TYR:HD1	30:V:69:ILE:HG23	1.58	0.68
42:j:114:GLU:N	43:g:160:LYS:HE2	2.08	0.68
47:y:5:ARG:HA	47:y:8:HIS:CD2	2.28	0.68
49:A0:150:ALA:CA	49:A0:155:GLY:HA2	2.22	0.68
49:A0:187:PHE:O	49:A0:193:VAL:CB	2.41	0.68
4:7:67:VAL:HG22	7:3:59:ALA:HB1	1.75	0.68
8:1:8:MET:O	8:1:8:MET:HG3	1.92	0.68
8:1:77:MET:C	8:1:79:LEU:H	2.01	0.68
49:p:83:GLU:HA	49:p:138:VAL:HA	1.75	0.68
8:1:183:MET:HG2	70:B:501:3PE:C2H	2.21	0.68
11:B:95:LEU:HD23	11:B:458:PHE:HZ	1.57	0.68
21:L:71:GLN:NE2	25:Q:123:GLY:HA3	2.08	0.68
42:j:119:VAL:HG23	43:g:147:GLY:C	2.18	0.68
56:A9:69:MET:HE2	56:A9:70:VAL:HG23	1.74	0.68
2:4:64:PRO:C	2:4:66:LEU:H	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:12:PHE:HB2	6:5:39:SER:HB2	1.76	0.68
7:3:88:LEU:HD21	8:1:309:ILE:HD12	1.73	0.68
11:B:125:GLU:OE1	12:C:202:LYS:HE2	1.93	0.68
13:D:184:PRO:HG3	14:E:183:LEU:CD1	2.24	0.68
25:Q:124:ASP:OD1	25:Q:125:LEU:N	2.25	0.68
28:T:26:THR:CG2	28:T:68:ALA:CA	2.59	0.68
28:T:101:LEU:HD21	28:T:110:ILE:CG2	2.23	0.68
32:X:13:HIS:O	32:X:15:LEU:N	2.26	0.68
39:f:42:CYS:HA	39:f:45:ARG:HB3	1.75	0.68
1:9:223:PHE:CZ	9:8:49:HIS:CD2	2.82	0.68
4:7:145:ALA:HB1	7:3:78:ALA:HB2	1.74	0.68
10:A:61:PRO:HG3	10:A:146:PHE:CE2	2.29	0.68
10:A:181:ARG:HA	10:A:184:ARG:HH21	1.58	0.68
11:B:150:ALA:HB2	11:B:400:ILE:HD13	1.75	0.68
21:L:68:SER:CA	25:Q:130:LYS:HE3	2.24	0.68
25:Q:38:LYS:CG	25:Q:39:PRO:HD3	2.23	0.68
28:T:70:PHE:HD1	28:T:93:GLY:HA3	1.57	0.68
35:a:67:ARG:NH1	44:e:79:PRO:CB	2.57	0.68
47:m:228:ASP:O	47:m:232:ALA:N	2.26	0.68
47:m:376:LEU:CD2	50:q:17:ARG:CG	2.72	0.68
2:4:16:TRP:CZ2	70:4:501:3PE:H2G2	2.28	0.68
25:Q:158:LEU:O	25:Q:159:LYS:HD2	1.93	0.68
26:R:150:GLN:HA	26:R:153:ALA:HB3	1.75	0.68
28:T:69:ILE:HG21	28:T:100:ILE:HD13	1.76	0.68
35:a:68:TRP:CE3	44:e:109:LEU:O	2.47	0.68
40:h:149:LEU:CD1	43:g:167:ARG:N	2.57	0.68
45:k:128:GLU:OE2	45:k:131:ARG:NH1	2.27	0.68
53:t:19:PRO:O	53:t:22:SER:OG	2.12	0.68
13:D:199:GLN:HG3	14:E:178:GLU:CG	2.24	0.68
14:E:135:ARG:NH1	18:I:68:ALA:HB1	2.09	0.68
27:S:286:VAL:CB	72:S:401:PC1:H151	2.23	0.68
35:a:108:ASP:C	35:a:110:ASP:H	2.01	0.68
1:9:73:GLY:CA	15:F:105:GLU:O	2.41	0.68
2:4:207:MET:HG3	2:4:298:ILE:HD11	1.74	0.68
3:2:84:TRP:CD1	3:2:84:TRP:H	2.11	0.68
12:C:88:ILE:HD11	12:C:143:ILE:HD11	1.76	0.68
1:9:180:CYS:CB	9:8:123:GLY:HA2	2.25	0.67
4:7:136:PHE:N	4:7:138:GLU:O	2.27	0.67
10:A:535:GLU:O	10:A:538:GLN:N	2.27	0.67
12:C:187:ARG:HG2	23:O:88:MET:HE1	1.76	0.67
28:T:13:PRO:HB3	28:T:20:ARG:NH2	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:114:GLU:CA	43:g:160:LYS:HE2	2.23	0.67
48:z:148:TYR:HE2	48:z:161:ALA:HA	1.58	0.67
53:A3:43:ASP:CA	53:A3:47:TYR:CD2	2.67	0.67
62:A4:5:LYS:HZ3	62:A4:5:LYS:HB3	1.60	0.67
67:C1:19:TRP:HZ2	68:A8:14:GLU:HG2	1.59	0.67
3:2:87:MET:O	3:2:88:LYS:C	2.37	0.67
5:6:119:LYS:HD2	71:6:701:CDL:H332	0.68	0.67
23:O:48:HIS:CE1	26:R:359:TYR:OH	2.32	0.67
45:w:128:GLU:OE2	45:w:131:ARG:NH1	2.27	0.67
2:4:16:TRP:CE2	70:4:501:3PE:H2C1	2.29	0.67
3:2:277:ILE:HG23	28:T:135:VAL:HG22	1.76	0.67
11:B:219:GLY:HA3	14:E:98:ARG:HE	1.57	0.67
12:C:192:ASP:OD1	12:C:193:TYR:N	2.26	0.67
14:E:135:ARG:CZ	18:I:68:ALA:O	2.42	0.67
28:T:26:THR:CB	28:T:68:ALA:CA	2.62	0.67
38:d:83:GLU:O	38:d:87:TRP:N	2.26	0.67
2:4:360:LEU:CD1	71:6:701:CDL:C51	2.64	0.67
5:6:119:LYS:HE3	71:6:701:CDL:H711	1.76	0.67
26:R:197:GLU:HB3	26:R:259:ARG:HB2	1.75	0.67
30:V:76:GLN:HE22	36:b:187:PRO:HG2	1.59	0.67
45:k:327:ASP:OD1	45:k:328:HIS:N	2.28	0.67
49:p:16:PRO:HA	49:p:19:LEU:HB2	1.75	0.67
54:u:52:TRP:O	54:u:56:LYS:N	2.23	0.67
1:9:179:ALA:HB1	1:9:181:VAL:HG22	1.75	0.67
11:B:234:GLN:NE2	14:E:96:ARG:CD	2.57	0.67
28:T:89:ASN:C	28:T:91:LEU:N	2.52	0.67
39:f:163:LEU:N	39:f:164:PRO:CA	2.58	0.67
43:g:43:ARG:HB2	43:g:44:PRO:HD3	1.75	0.67
57:C4:186:SER:HB3	57:C4:213:LEU:HD22	1.76	0.67
10:A:382:ARG:HG3	10:A:383:SER:H	1.59	0.67
49:A0:187:PHE:O	49:A0:192:MET:O	2.12	0.67
50:A1:16:ILE:O	50:A1:20:TYR:N	2.24	0.67
4:7:21:SER:OG	6:5:14:VAL:HG23	1.94	0.67
9:8:131:ILE:HG23	9:8:169:LEU:HD21	1.75	0.67
10:A:643:ARG:NH1	10:A:656:TYR:OH	2.27	0.67
17:H:65:GLU:OE2	17:H:71:LYS:HB2	1.94	0.67
18:I:62:GLU:O	29:U:127:TYR:CZ	2.46	0.67
42:j:116:PHE:CD2	43:g:160:LYS:O	2.47	0.67
47:m:263:ASN:OD1	47:m:264:THR:N	2.28	0.67
48:o:143:LEU:HD11	48:o:149:PHE:HB2	1.77	0.67
45:w:314:TYR:N	45:w:317:THR:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:305:GLN:NE2	46:x:329:GLN:OE1	2.24	0.67
47:y:263:ASN:OD1	47:y:264:THR:N	2.28	0.67
58:C2:209:ILE:O	58:C2:213:THR:HG23	1.95	0.67
2:4:190:TRP:HB3	28:T:127:MET:HG3	1.74	0.67
5:6:516:PRO:HB3	39:f:30:TRP:CD1	2.29	0.67
10:A:319:TRP:HA	10:A:319:TRP:CE3	2.30	0.67
11:B:308:TYR:OH	11:B:401:GLU:N	2.23	0.67
11:B:320:ILE:O	14:E:41:VAL:CB	2.43	0.67
12:C:221:VAL:HG21	13:D:138:ARG:HB2	1.77	0.67
13:D:155:SER:CB	14:E:150:THR:O	2.42	0.67
31:W:81:ASP:OD2	34:Z:17:PRO:HG2	1.94	0.67
35:a:67:ARG:NE	44:e:52:ALA:HB1	2.09	0.67
48:o:148:TYR:HE2	48:o:161:ALA:HA	1.58	0.67
16:G:107:TRP:HD1	16:G:108:GLU:O	1.78	0.67
25:Q:52:ASP:OD1	30:V:116:TRP:HB2	1.95	0.67
27:S:182:THR:HG23	27:S:183:ILE:HG13	1.77	0.67
27:S:190:HIS:HA	27:S:241:CYS:HB3	1.77	0.67
28:T:89:ASN:O	28:T:90:TYR:C	2.35	0.67
28:T:96:ALA:HA	28:T:99:LEU:HD13	1.76	0.67
45:w:329:MET:HE3	51:A2:2:ARG:HE	1.58	0.67
49:A0:31:ALA:HB2	54:B2:7:ALA:HB2	1.76	0.67
3:2:250:SER:HB2	3:2:257:LEU:HD13	1.76	0.67
5:6:68:TRP:CD1	5:6:69:LEU:HG	2.30	0.67
8:1:26:LYS:HD3	8:1:36:GLY:HA3	1.76	0.67
10:A:624:ARG:NH2	10:A:628:GLU:OE2	2.28	0.67
11:B:386:THR:OG1	11:B:387:GLU:N	2.27	0.67
27:S:199:VAL:CB	27:S:200:PRO:HD2	2.20	0.67
27:S:333:GLU:HG3	42:j:52:PRO:CB	2.25	0.67
45:w:245:GLU:H	45:w:426:GLY:HA3	1.60	0.67
48:z:51:LEU:HD22	48:z:58:GLU:HA	1.77	0.67
60:C0:43:PRO:HB2	60:C0:48:ILE:HD11	1.76	0.67
1:9:88:ARG:HG3	15:F:83:TYR:CD1	2.26	0.66
5:6:406:ALA:HB2	44:e:147:GLY:CA	2.25	0.66
8:1:190:LEU:HD11	8:1:197:PRO:HD2	1.77	0.66
8:1:312:SER:OG	30:V:55:ARG:NH2	2.28	0.66
11:B:254:ARG:HD2	24:P:24:LEU:CD2	2.25	0.66
11:B:293:LEU:O	11:B:296:SER:N	2.24	0.66
27:S:237:MET:HG3	27:S:243:VAL:HG21	1.77	0.66
9:8:207:GLY:CA	73:8:501:FMN:C7	2.73	0.66
12:C:206:LEU:HG	13:D:165:TYR:O	1.95	0.66
20:K:32:GLY:O	20:K:36:PHE:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:226:GLU:HA	27:S:229:TYR:CD2	2.30	0.66
36:b:94:GLY:O	43:g:61:TYR:HD2	1.78	0.66
31:M:60:PHE:CE1	31:M:83:LYS:HG2	2.30	0.66
45:k:314:TYR:N	45:k:317:THR:O	2.27	0.66
47:m:198:LEU:HD21	47:y:10:LEU:HD23	1.76	0.66
11:B:106:VAL:HG23	11:B:107:ARG:H	1.60	0.66
24:P:40:LYS:O	30:V:7:LYS:N	2.28	0.66
25:Q:158:LEU:C	25:Q:159:LYS:HG2	2.20	0.66
28:T:66:ILE:O	28:T:69:ILE:CG2	2.42	0.66
35:a:67:ARG:HH11	44:e:79:PRO:HD2	1.60	0.66
39:f:156:PRO:HG2	39:f:158:ARG:H	1.60	0.66
40:h:84:ILE:HG22	40:h:88:ARG:NH1	2.09	0.66
50:q:13:LEU:CA	50:q:16:ILE:HG22	2.25	0.66
49:A0:106:ILE:CA	49:A0:167:ALA:C	2.63	0.66
53:A3:40:LEU:HD11	53:A3:47:TYR:HB3	1.78	0.66
10:A:155:GLU:OE1	10:A:155:GLU:N	2.28	0.66
11:B:322:SER:OG	11:B:328:ASP:OD2	2.13	0.66
12:C:110:PHE:CD1	12:C:136:SER:HB3	2.30	0.66
13:D:203:LYS:HB2	14:E:178:GLU:OE2	1.96	0.66
22:N:38:ILE:O	22:N:45:ARG:NH2	2.29	0.66
26:R:51:VAL:HG23	26:R:52:SER:H	1.59	0.66
28:T:26:THR:HB	28:T:68:ALA:HB2	1.77	0.66
3:2:80:PHE:HB3	17:H:64:ARG:HH12	1.60	0.66
4:7:33:LEU:HD11	6:5:31:LEU:HD11	1.76	0.66
8:1:75:PRO:C	8:1:77:MET:H	2.03	0.66
10:A:58:MET:CG	12:C:248:ARG:HH12	2.09	0.66
26:R:208:GLY:H	26:R:211:ASP:CG	2.04	0.66
28:T:95:CYS:C	28:T:97:GLY:N	2.51	0.66
31:M:62:ILE:HG23	31:M:66:ASP:HB2	1.77	0.66
45:k:245:GLU:H	45:k:426:GLY:HA3	1.60	0.66
1:9:222:ARG:HD2	1:9:226:GLU:HB2	1.77	0.66
3:2:137:ALA:O	3:2:140:SER:OG	2.13	0.66
8:1:74:ALA:O	8:1:77:MET:HB2	1.95	0.66
8:1:169:GLN:HG2	8:1:174:LEU:HB2	1.77	0.66
10:A:255:ASP:N	10:A:255:ASP:OD1	2.28	0.66
22:N:88:LEU:HD11	22:N:92:ARG:HH21	1.59	0.66
53:t:34:TRP:CD1	54:u:29:LEU:HD13	2.28	0.66
45:w:327:ASP:OD1	45:w:328:HIS:N	2.28	0.66
45:w:438:ARG:NH2	49:A0:37:TYR:OH	2.27	0.66
48:z:143:LEU:HD11	48:z:149:PHE:HB2	1.77	0.66
56:A9:151:HIS:O	56:A9:155:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:128:ILE:HD13	14:E:147:ILE:HG12	1.77	0.66
46:l:97:SER:HA	55:v:70:LEU:HB3	1.77	0.66
52:s:12:GLU:HG2	52:s:13:LEU:HD12	1.77	0.66
46:x:155:PRO:HB2	46:x:254:HIS:CE1	2.31	0.66
59:A7:24:LEU:H	60:C0:34:ASN:HD21	1.44	0.66
2:4:1:MET:HB2	2:4:52:PHE:CZ	2.31	0.66
3:2:155:LEU:HD13	28:T:136:PHE:CE1	2.31	0.66
5:6:119:LYS:CE	71:6:701:CDL:H711	2.25	0.66
12:C:227:GLU:HG2	26:R:49:SER:CB	2.19	0.66
12:C:229:ALA:O	16:G:114:TRP:CZ3	2.49	0.66
2:4:16:TRP:HZ2	70:4:501:3PE:C2F	2.09	0.66
8:1:237:PHE:O	8:1:240:ILE:HG13	1.96	0.66
13:D:199:GLN:HG3	14:E:178:GLU:OE2	1.95	0.66
5:6:116:LYS:CG	5:6:119:LYS:HZ3	2.07	0.66
5:6:224:SER:HB3	5:6:256:GLY:HA3	1.76	0.66
9:8:177:TYR:HD1	9:8:182:ILE:HB	1.60	0.66
9:8:269:ARG:HG2	9:8:340:ASP:OD2	1.96	0.66
12:C:70:ILE:HD11	12:C:101:PHE:CZ	2.31	0.66
26:R:143:ASP:O	26:R:147:LYS:N	2.27	0.66
34:Z:36:LEU:O	34:Z:40:GLY:N	2.29	0.66
48:o:69:GLU:HG2	48:o:84:PRO:HB3	1.78	0.66
63:A5:38:ARG:HG2	63:A5:85:ILE:HG23	1.76	0.66
2:4:421:TYR:CE1	35:a:59:VAL:CB	2.78	0.65
5:6:1:MET:HG2	5:6:59:GLN:HE22	1.61	0.65
10:A:382:ARG:HH22	10:A:652:ASN:HD21	1.43	0.65
44:e:47:GLU:O	44:e:50:ALA:N	2.25	0.65
48:o:69:GLU:OE1	48:o:69:GLU:N	2.28	0.65
49:A0:110:ALA:CB	49:A0:123:ASP:CA	2.72	0.65
53:A3:43:ASP:C	53:A3:47:TYR:CD2	2.70	0.65
3:2:335:MET:C	25:Q:170:TRP:HH2	2.05	0.65
8:1:43:TYR:CE1	29:U:27:LEU:HD21	2.31	0.65
16:G:108:GLU:OE2	16:G:113:GLY:HA2	1.95	0.65
10:A:628:GLU:HA	10:A:633:THR:HG22	1.78	0.65
11:B:67:ASN:HB2	27:S:181:VAL:HG13	1.78	0.65
11:B:241:MET:HE3	11:B:351:MET:HE1	1.78	0.65
12:C:221:VAL:CG2	13:D:138:ARG:CB	2.74	0.65
13:D:215:ARG:CD	76:R:601:NAP:O1X	2.43	0.65
45:k:408:ARG:HH21	53:t:15:ARG:CZ	2.10	0.65
48:o:51:LEU:HD22	48:o:58:GLU:HA	1.77	0.65
58:C2:101:PHE:HZ	58:C2:260:GLY:HA3	1.61	0.65
7:3:77:TRP:CD1	8:1:318:THR:O	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:33:ARG:CB	31:M:48:VAL:HG11	2.15	0.65
23:O:48:HIS:CB	26:R:359:TYR:CE1	2.76	0.65
25:Q:45:LEU:O	25:Q:135:ARG:NH2	2.29	0.65
26:R:131:GLY:O	76:R:601:NAP:H3D	1.96	0.65
28:T:34:LEU:HD13	28:T:34:LEU:C	2.18	0.65
44:e:63:GLU:O	44:e:65:TYR:N	2.27	0.65
47:y:228:ASP:O	47:y:232:ALA:N	2.26	0.65
1:9:143:ARG:HH11	9:8:285:PRO:HG2	1.60	0.65
1:9:200:ASP:OD2	1:9:219:ARG:NH1	2.30	0.65
1:9:227:PRO:HD2	9:8:48:ARG:NH1	2.10	0.65
8:1:266:LEU:O	8:1:269:SER:HB2	1.95	0.65
14:E:106:TYR:CE1	14:E:112:ARG:HG3	2.32	0.65
25:Q:161:ALA:CB	42:j:83:TYR:O	2.42	0.65
27:S:120:GLN:O	27:S:124:TYR:N	2.29	0.65
48:o:81:PHE:CE1	48:o:84:PRO:HA	2.32	0.65
57:C4:120:SER:OG	57:C4:138:VAL:HG21	1.97	0.65
3:2:234:TRP:CZ3	27:S:327:TYR:HE2	2.15	0.65
8:1:74:ALA:HB3	8:1:75:PRO:HD3	1.79	0.65
9:8:420:GLU:H	9:8:422:HIS:HD2	1.44	0.65
10:A:311:LYS:C	29:U:144:TYR:CE1	2.75	0.65
25:Q:48:TRP:HH2	36:b:186:THR:N	1.94	0.65
35:a:16:THR:N	44:e:125:ASN:CA	2.59	0.65
54:B2:52:TRP:HB2	54:B2:56:LYS:HB2	1.78	0.65
2:4:140:THR:HB	11:B:38:GLN:HB3	1.78	0.65
9:8:207:GLY:CA	73:8:501:FMN:C5A	2.70	0.65
9:8:325:PRO:HD2	9:8:347:THR:HG21	1.78	0.65
25:Q:45:LEU:HB3	25:Q:135:ARG:HH22	1.60	0.65
39:f:133:TRP:O	39:f:136:GLU:N	2.30	0.65
40:h:149:LEU:HD23	43:g:171:LYS:CE	2.27	0.65
43:g:11:PRO:HD2	43:g:109:ARG:NH1	2.11	0.65
47:m:10:LEU:HD23	47:y:198:LEU:HD21	1.78	0.65
1:9:233:SER:O	9:8:41:ILE:HD13	1.97	0.65
5:6:577:VAL:HG13	6:5:97:GLN:NE2	2.11	0.65
9:8:380:GLY:N	74:8:502:SF4:S4	2.61	0.65
27:S:162:TYR:CD1	27:S:172:VAL:HG21	2.30	0.65
46:l:155:PRO:HB2	46:l:254:HIS:CE1	2.31	0.65
77:m:401:HEM:O2D	77:m:401:HEM:HHA	1.97	0.65
54:u:52:TRP:HB2	54:u:56:LYS:HB2	1.78	0.65
48:z:228:SER:O	51:A2:23:GLN:NE2	2.29	0.65
10:A:127:ASP:O	74:A:801:SF4:S1	2.55	0.65
10:A:464:GLN:O	10:A:468:GLU:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:385:TYR:CD1	14:E:122:VAL:HG11	2.32	0.65
12:C:192:ASP:HA	13:D:132:LYS:CG	2.27	0.65
49:A0:150:ALA:N	49:A0:155:GLY:CA	2.38	0.65
1:9:41:HIS:CE1	18:I:83:ARG:NH2	2.65	0.65
2:4:62:SER:OG	2:4:455:LEU:O	2.15	0.65
3:2:325:PHE:HE2	70:2:401:3PE:H2I2	1.54	0.65
3:2:335:MET:O	25:Q:170:TRP:HH2	1.78	0.65
8:1:311:THR:O	8:1:312:SER:OG	2.15	0.65
13:D:193:LEU:O	13:D:196:GLY:N	2.28	0.65
42:j:119:VAL:H	43:g:147:GLY:CA	2.10	0.65
46:x:247:GLN:NE2	46:x:429:ASN:HA	2.12	0.65
1:9:71:PRO:C	15:F:102:SER:HB3	2.22	0.64
1:9:73:GLY:HA3	15:F:105:GLU:CB	2.27	0.64
3:2:168:GLY:HA2	5:6:576:LEU:HD22	1.79	0.64
11:B:278:VAL:HG12	11:B:283:ALA:HB2	1.78	0.64
20:K:55:ILE:O	20:K:56:ARG:NH1	2.29	0.64
23:O:33:ARG:HH22	31:M:44:SER:C	2.05	0.64
39:f:35:ASP:OD1	39:f:36:LYS:N	2.29	0.64
51:r:36:ASN:O	51:r:40:ARG:HG2	1.96	0.64
54:B2:52:TRP:O	54:B2:56:LYS:N	2.24	0.64
58:C2:160:LEU:HD13	58:C2:222:GLN:HG2	1.78	0.64
2:4:76:MET:O	2:4:80:SER:N	2.27	0.64
3:2:13:ILE:O	3:2:16:GLY:N	2.30	0.64
4:7:66:VAL:O	4:7:70:TYR:N	2.29	0.64
8:1:77:MET:C	8:1:79:LEU:N	2.53	0.64
10:A:76:ARG:NH1	10:A:90:ALA:HB2	2.12	0.64
10:A:624:ARG:NH1	10:A:634:LEU:O	2.30	0.64
27:S:286:VAL:O	27:S:289:LYS:N	2.29	0.64
41:i:68:GLU:HB2	42:j:19:ARG:HD2	1.73	0.64
44:e:70:THR:HG22	44:e:71:GLY:H	1.61	0.64
46:x:59:ASN:OD1	46:x:60:SER:N	2.27	0.64
46:x:355:PRO:O	46:x:359:ALA:N	2.29	0.64
56:A9:298:ASP:HB2	56:A9:301:THR:HG23	1.77	0.64
67:C1:45:LEU:HD21	68:A8:40:TYR:HA	1.78	0.64
3:2:321:LYS:CG	72:2:402:PC1:H251	2.26	0.64
13:D:191:GLU:HG2	14:E:173:PHE:CD1	2.32	0.64
24:P:39:PRO:HA	30:V:8:GLN:HG2	1.78	0.64
28:T:101:LEU:HD22	28:T:101:LEU:O	1.96	0.64
45:k:235:ARG:NH1	49:p:14:ARG:HH12	1.96	0.64
47:m:375:LYS:NZ	50:q:17:ARG:NH2	2.45	0.64
5:6:440:LEU:HB2	31:W:82:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:106:SER:HB2	22:N:51:ILE:HD12	1.79	0.64
48:o:77:ASP:O	48:o:79:GLU:HG3	1.97	0.64
50:A1:35:ASP:OD1	50:A1:89:TYR:OH	2.15	0.64
2:4:71:TRP:O	2:4:74:PRO:HD2	1.97	0.64
11:B:266:ARG:NH1	70:B:501:3PE:C23	2.56	0.64
20:K:16:LEU:HD23	20:K:94:VAL:HG12	1.78	0.64
26:R:203:PRO:HB3	26:R:265:PHE:HD2	1.60	0.64
27:S:333:GLU:HG3	42:j:52:PRO:HB2	1.78	0.64
33:Y:89:TYR:O	33:Y:91:ASP:N	2.30	0.64
50:q:13:LEU:O	50:q:16:ILE:N	2.30	0.64
2:4:35:SER:O	2:4:38:SER:OG	2.12	0.64
10:A:320:GLU:HB2	23:O:123:TYR:HH	1.56	0.64
11:B:254:ARG:NE	24:P:24:LEU:HG	2.12	0.64
13:D:146:GLU:CB	13:D:147:PRO:CD	2.76	0.64
46:l:267:ALA:O	46:l:271:ALA:N	2.30	0.64
48:z:3:LEU:HB2	52:B3:59:LEU:HD13	1.78	0.64
3:2:80:PHE:O	3:2:81:SER:OG	2.12	0.64
3:2:217:THR:CG2	72:2:402:PC1:H261	2.26	0.64
3:2:321:LYS:HG3	72:2:402:PC1:H251	1.79	0.64
5:6:310:LEU:HA	5:6:313:MET:HE3	1.78	0.64
14:E:104:ARG:HH12	14:E:112:ARG:NH2	1.95	0.64
23:O:48:HIS:O	26:R:359:TYR:HE1	1.80	0.64
40:h:142:PHE:CE2	43:g:162:ARG:CZ	2.81	0.64
56:A9:84:PRO:HG3	56:A9:92:MET:HE3	1.80	0.64
2:4:2:LEU:CD2	72:4:504:PC1:H142	2.27	0.64
4:7:23:LYS:NZ	6:5:23:ARG:HH11	1.95	0.64
5:6:120:TYR:HH	71:6:701:CDL:CB5	2.10	0.64
5:6:529:PHE:HB3	5:6:530:PRO:HD3	1.80	0.64
9:8:414:GLU:CD	24:P:50:SER:O	2.41	0.64
11:B:94:VAL:HG12	11:B:115:LEU:CD2	2.28	0.64
19:J:4:GLU:OE2	29:U:31:ASN:CB	2.45	0.64
23:O:48:HIS:HB2	26:R:359:TYR:CZ	2.32	0.64
25:Q:51:LYS:NZ	36:b:189:ASN:ND2	2.46	0.64
48:o:147:LEU:HB3	48:o:157:ALA:HB1	1.80	0.64
50:q:13:LEU:C	50:q:16:ILE:HG22	2.23	0.64
6:5:9:MET:O	6:5:12:PHE:N	2.30	0.64
9:8:342:LEU:HB3	9:8:348:GLY:HA2	1.79	0.64
11:B:238:LEU:HD23	30:V:10:MET:HE1	1.80	0.64
12:C:171:GLU:OE1	12:C:172:ILE:N	2.31	0.64
21:L:71:GLN:HE22	25:Q:123:GLY:HA3	1.63	0.64
46:l:43:PRO:HA	46:l:113:ARG:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:187:SER:CB	56:A9:277:MET:HE1	2.28	0.64
2:4:276:CYS:SG	2:4:285:LEU:HD12	2.38	0.64
2:4:421:TYR:HE1	35:a:59:VAL:CB	2.09	0.64
11:B:206:GLU:OE2	11:B:247:PHE:HZ	1.81	0.64
43:g:52:ILE:O	43:g:56:HIS:N	2.28	0.64
49:A0:121:GLN:CB	49:A0:170:ARG:CB	2.76	0.64
4:7:136:PHE:O	4:7:138:GLU:N	2.31	0.63
5:6:81:LYS:N	5:6:133:THR:O	2.30	0.63
5:6:335:PHE:CE2	5:6:383:MET:HE1	2.33	0.63
10:A:126:LEU:HD13	18:I:98:ARG:O	1.98	0.63
10:A:340:ALA:HB2	10:A:546:PHE:HD2	1.63	0.63
10:A:568:TYR:HB3	10:A:583:ILE:HG22	1.80	0.63
27:S:206:ILE:HD11	27:S:214:GLU:HB3	1.80	0.63
28:T:89:ASN:OD1	28:T:92:ILE:HD12	1.98	0.63
35:a:39:ILE:CA	44:e:56:ASN:CB	2.76	0.63
1:9:179:ALA:HB2	9:8:128:ARG:NH2	2.12	0.63
9:8:78:GLY:HA2	9:8:81:LYS:HG2	1.80	0.63
11:B:264:ASN:HD21	14:E:68:ARG:NH2	1.96	0.63
17:H:28:LYS:HB3	36:b:184:LYS:HA	1.80	0.63
20:K:62:GLN:O	20:K:64:LYS:N	2.30	0.63
27:S:213:HIS:HA	27:S:215:MET:HE2	1.80	0.63
36:b:93:ILE:HG23	43:g:61:TYR:HE2	1.63	0.63
45:w:110:VAL:O	45:w:114:ALA:N	2.25	0.63
46:x:325:TYR:HB3	55:B1:57:GLY:HA2	1.81	0.63
2:4:278:ARG:HH21	35:a:72:ARG:HH22	1.44	0.63
7:3:12:THR:HA	7:3:15:THR:HG22	1.80	0.63
9:8:98:LYS:HE3	9:8:99:TRP:HE1	1.63	0.63
45:k:227:ALA:O	45:k:228:VAL:HG23	1.99	0.63
1:9:68:LYS:O	15:F:100:PRO:HG3	1.99	0.63
5:6:150:MET:HE3	71:6:701:CDL:C58	2.28	0.63
9:8:395:VAL:HG23	9:8:398:ARG:NH1	2.13	0.63
14:E:115:ALA:O	14:E:140:ARG:NH1	2.32	0.63
23:O:42:GLU:CD	23:O:45:ASN:HB3	2.23	0.63
30:V:72:MET:HE2	30:V:75:LEU:HD23	1.79	0.63
77:y:401:HEM:O2D	77:y:401:HEM:HHA	1.97	0.63
5:6:435:PRO:HB2	34:Z:52:ARG:HD3	1.81	0.63
8:1:233:MET:CA	8:1:236:ILE:HG22	2.23	0.63
13:D:169:VAL:HG12	13:D:170:VAL:O	1.98	0.63
13:D:176:ILE:HG22	13:D:177:VAL:HG13	1.80	0.63
17:H:41:ILE:HG12	36:b:174:ILE:HG21	1.81	0.63
26:R:178:SER:H	26:R:181:LEU:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:139:PRO:HA	36:b:158:ARG:HG3	1.81	0.63
41:i:47:THR:HG22	42:j:63:LEU:HD11	1.80	0.63
45:w:150:PHE:O	45:w:153:LEU:N	2.31	0.63
48:z:148:TYR:CE2	48:z:161:ALA:HA	2.33	0.63
56:A9:172:LYS:HB2	56:A9:172:LYS:NZ	2.12	0.63
2:4:2:LEU:HD11	72:4:504:PC1:H142	1.79	0.63
2:4:166:TYR:CZ	70:4:503:3PE:O13	2.49	0.63
2:4:243:MET:O	2:4:247:THR:HG22	1.98	0.63
2:4:278:ARG:N	5:6:546:GLN:HE22	1.88	0.63
71:4:502:CDL:C67	5:6:23:SER:O	2.47	0.63
8:1:153:VAL:HA	8:1:156:MET:HE2	1.80	0.63
9:8:246:GLU:HA	9:8:249:ALA:HB3	1.81	0.63
9:8:346:GLN:OE1	9:8:441:HIS:NE2	2.32	0.63
12:C:221:VAL:HG21	13:D:138:ARG:CB	2.28	0.63
13:D:195:TYR:CD2	29:U:116:ASN:ND2	2.65	0.63
27:S:275:ASN:C	27:S:277:ARG:H	2.04	0.63
28:T:9:TYR:O	28:T:12:ILE:CB	2.46	0.63
47:y:72:ASP:OD1	48:z:49:ARG:NH1	2.30	0.63
56:A9:128:VAL:HG22	56:A9:128:VAL:O	1.99	0.63
56:A9:195:LEU:HD23	56:A9:245:ILE:HD13	1.79	0.63
2:4:304:GLN:O	2:4:305:THR:OG1	2.15	0.63
5:6:137:LEU:HB3	5:6:196:TRP:HB2	1.81	0.63
9:8:116:ASN:CB	73:8:501:FMN:O2	2.47	0.63
10:A:163:LYS:HE3	10:A:207:GLY:HA3	1.79	0.63
12:C:232:PHE:CD1	13:D:165:TYR:CD2	2.86	0.63
18:I:63:VAL:HG22	18:I:64:ASN:H	1.64	0.63
28:T:10:TRP:C	28:T:12:ILE:H	2.05	0.63
34:Z:41:LEU:H	34:Z:42:ARG:HA	1.64	0.63
35:a:67:ARG:NE	44:e:52:ALA:CB	2.62	0.63
46:l:59:ASN:OD1	46:l:60:SER:N	2.27	0.63
47:m:6:LYS:HD3	47:m:16:ASN:HD21	1.64	0.63
47:m:375:LYS:HZ2	50:q:17:ARG:NH2	1.97	0.63
46:x:43:PRO:HA	46:x:113:ARG:HB2	1.80	0.63
46:x:78:LYS:HB3	46:x:129:ALA:HB1	1.80	0.63
47:y:221:HIS:O	47:y:225:THR:OG1	2.14	0.63
49:A0:2:HIS:CG	49:A0:3:THR:H	2.17	0.63
59:A7:16:TYR:CE1	59:A7:25:PRO:HG3	2.34	0.63
3:2:87:MET:HE2	3:2:90:PHE:CZ	2.29	0.63
8:1:101:GLY:O	8:1:104:PHE:N	2.28	0.63
10:A:137:CYS:SG	10:A:138:ASP:N	2.70	0.63
28:T:37:SER:HB3	28:T:60:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:68:GLU:HB3	42:j:19:ARG:CD	2.24	0.63
47:m:361:LEU:HD23	47:m:365:LEU:HD12	1.81	0.63
47:y:44:GLN:O	47:y:48:GLY:N	2.20	0.63
1:9:121:MET:HB2	9:8:201:ALA:HB1	1.78	0.63
1:9:233:SER:O	9:8:41:ILE:HG12	1.99	0.63
8:1:237:PHE:CE1	8:1:240:ILE:HD11	2.33	0.63
10:A:639:LEU:O	10:A:642:VAL:N	2.28	0.63
17:H:62:ASP:OD1	17:H:63:PHE:N	2.32	0.63
40:h:136:ILE:HD11	43:g:106:ILE:HD11	1.80	0.63
46:l:78:LYS:HB3	46:l:129:ALA:HB1	1.80	0.63
50:q:35:ASP:OD1	50:q:89:TYR:OH	2.15	0.63
2:4:372:THR:HA	2:4:448:THR:HG21	1.79	0.62
3:2:3:PRO:HG3	27:S:31:TYR:CE2	2.34	0.62
11:B:322:SER:CB	14:E:42:ASN:O	2.47	0.62
14:E:82:ALA:HB2	24:P:25:GLN:HE21	1.64	0.62
16:G:68:PRO:HG2	16:G:72:ILE:HD11	1.80	0.62
26:R:61:ALA:H	26:R:129:LEU:HD11	1.63	0.62
49:A0:72:SER:HB3	49:A0:73:LYS:HE3	1.80	0.62
2:4:308:SER:O	2:4:312:ALA:N	2.30	0.62
6:5:94:ASN:OD1	6:5:95:LEU:N	2.32	0.62
17:H:84:GLU:HG3	17:H:87:ILE:HD11	1.81	0.62
22:N:81:ILE:O	22:N:85:GLU:N	2.32	0.62
27:S:47:LEU:HD12	27:S:48:ILE:H	1.64	0.62
28:T:101:LEU:CD1	28:T:111:GLY:HA2	2.29	0.62
28:T:101:LEU:HG	28:T:110:ILE:CG2	2.28	0.62
42:j:44:ILE:O	42:j:47:ALA:N	2.32	0.62
43:g:128:GLU:O	43:g:132:PHE:N	2.28	0.62
45:k:150:PHE:O	45:k:153:LEU:N	2.31	0.62
46:x:267:ALA:O	46:x:271:ALA:N	2.30	0.62
47:y:6:LYS:HD3	47:y:16:ASN:HD21	1.64	0.62
49:A0:100:HIS:HA	49:A0:130:PRO:HA	1.81	0.62
5:6:4:PHE:HD2	5:6:61:LEU:HD12	1.64	0.62
13:D:186:CYS:CB	74:D:301:SF4:S4	2.87	0.62
25:Q:47:ARG:CZ	25:Q:53:PRO:HB3	2.30	0.62
35:a:64:ALA:HB1	44:e:108:ASP:O	1.99	0.62
38:d:105:GLU:OE2	44:e:165:ASN:C	2.41	0.62
48:o:148:TYR:CE2	48:o:161:ALA:HA	2.33	0.62
47:y:47:THR:HG23	47:y:79:ILE:HG23	1.81	0.62
48:z:147:LEU:HB3	48:z:157:ALA:HB1	1.80	0.62
8:1:33:LEU:HG	14:E:81:PRO:HA	1.82	0.62
10:A:347:ASP:OD1	10:A:347:ASP:N	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:94:VAL:HG12	11:B:94:VAL:O	1.99	0.62
11:B:253:LEU:HD23	11:B:254:ARG:HH12	1.64	0.62
12:C:174:ASP:OD2	12:C:189:ILE:N	2.30	0.62
14:E:131:GLU:OE1	14:E:144:ARG:NH1	2.31	0.62
18:I:105:LYS:C	18:I:106:GLU:CG	2.68	0.62
25:Q:165:SER:CA	42:j:86:ARG:NH2	2.61	0.62
56:A9:92:MET:HE2	56:A9:167:THR:HG21	1.82	0.62
1:9:152:ILE:O	1:9:156:LEU:N	2.30	0.62
2:4:287:ALA:O	2:4:290:SER:OG	2.16	0.62
2:4:382:VAL:HG22	2:4:396:MET:HE3	1.79	0.62
3:2:50:PRO:HB2	11:B:72:PRO:HG2	1.81	0.62
10:A:163:LYS:CE	10:A:207:GLY:HA3	2.29	0.62
23:O:50:PHE:HE2	23:O:103:VAL:HG21	1.65	0.62
3:2:217:THR:HG22	72:2:402:PC1:H252	1.82	0.62
8:1:235:ASN:N	8:1:235:ASN:OD1	2.32	0.62
10:A:259:SER:OG	10:A:260:ASN:N	2.30	0.62
28:T:17:GLU:HB2	28:T:20:ARG:NH2	2.15	0.62
45:k:208:LEU:O	45:k:212:ALA:N	2.33	0.62
46:x:227:ARG:HB3	46:x:228:GLY:HA3	1.81	0.62
49:A0:97:PHE:CB	49:A0:148:ALA:HB2	2.29	0.62
8:1:261:ILE:O	8:1:261:ILE:CG2	2.47	0.62
8:1:283:ASP:OD2	11:B:443:MET:SD	2.57	0.62
10:A:63:PHE:O	10:A:181:ARG:NH2	2.22	0.62
11:B:396:THR:OG1	11:B:397:TYR:N	2.29	0.62
39:f:133:TRP:HA	39:f:136:GLU:HB3	1.81	0.62
45:w:92:ARG:HH12	45:w:154:HIS:CG	2.18	0.62
45:w:235:ARG:NH1	49:A0:14:ARG:HH12	1.98	0.62
49:A0:2:HIS:CD2	49:A0:3:THR:H	2.18	0.62
49:A0:9:ASP:OD1	49:A0:10:PHE:N	2.32	0.62
50:A1:6:VAL:O	50:A1:6:VAL:HG12	2.00	0.62
57:C4:122:MET:HB2	57:C4:208:PRO:HD2	1.81	0.62
2:4:219:ALA:O	2:4:223:ALA:HB2	1.99	0.62
7:3:77:TRP:CD1	8:1:318:THR:C	2.77	0.62
8:1:71:PHE:HZ	8:1:215:TYR:CD1	2.12	0.62
14:E:118:LEU:O	14:E:121:ALA:N	2.30	0.62
37:c:83:HIS:CE1	37:c:87:LYS:HB2	2.35	0.62
40:h:147:ILE:HD13	42:j:110:GLY:HA2	1.79	0.62
5:6:55:ILE:CD1	38:d:74:PHE:HZ	1.76	0.62
5:6:119:LYS:HZ1	71:6:701:CDL:H311	1.63	0.62
5:6:593:ILE:HD12	28:T:42:ALA:HB3	1.81	0.62
8:1:260:THR:O	8:1:264:LEU:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:45:LYS:NZ	20:K:51:LEU:O	2.32	0.62
44:e:89:TRP:CD1	44:e:89:TRP:H	2.15	0.62
47:m:4:ILE:HG22	47:m:6:LYS:H	1.65	0.62
2:4:446:LEU:CG	71:4:502:CDL:H372	2.29	0.62
3:2:52:ALA:HB2	3:2:123:PRO:HD2	1.81	0.62
5:6:457:LEU:O	5:6:461:SER:N	2.32	0.62
10:A:305:PRO:HG3	10:A:319:TRP:CE3	2.34	0.62
12:C:214:TYR:N	13:D:176:ILE:HD13	2.15	0.62
13:D:199:GLN:CG	14:E:178:GLU:HG3	2.29	0.62
17:H:56:CYS:O	17:H:58:ILE:N	2.31	0.62
23:O:98:LYS:HB3	23:O:102:HIS:HB2	1.81	0.62
50:q:49:ARG:HD3	46:x:135:TRP:CE2	2.34	0.62
56:A9:11:ASN:HD21	56:A9:13:LYS:HB2	1.64	0.62
60:C0:82:TYR:HB3	60:C0:83:PRO:HD3	1.81	0.62
2:4:423:ILE:HB	35:a:57:ARG:HG3	0.77	0.61
2:4:449:LEU:CD1	71:4:502:CDL:C32	2.75	0.61
5:6:341:MET:HE3	5:6:454:ILE:HD13	1.80	0.61
10:A:320:GLU:N	23:O:123:TYR:HE1	1.97	0.61
11:B:259:GLU:OE2	30:V:23:ARG:NH2	2.30	0.61
14:E:57:ALA:CB	21:L:13:TRP:O	2.46	0.61
42:j:116:PHE:CG	43:g:160:LYS:O	2.52	0.61
43:g:151:SER:C	43:g:153:ARG:H	2.08	0.61
43:g:163:MET:O	43:g:167:ARG:N	2.32	0.61
68:A8:13:LYS:H	68:A8:13:LYS:HD3	1.65	0.61
7:3:29:VAL:HB	26:R:303:ARG:CB	2.30	0.61
11:B:80:LEU:HD22	11:B:82:LEU:HG	1.83	0.61
43:g:89:GLU:O	43:g:93:ARG:N	2.25	0.61
45:k:92:ARG:HH12	45:k:154:HIS:CG	2.18	0.61
1:9:54:ASP:OD1	1:9:55:PHE:N	2.33	0.61
1:9:92:TRP:CD1	1:9:126:PRO:HA	2.36	0.61
2:4:446:LEU:HG	71:4:502:CDL:C34	2.30	0.61
3:2:109:ALA:O	3:2:112:HIS:CD2	2.53	0.61
5:6:418:PHE:HA	5:6:421:ILE:HG12	1.81	0.61
10:A:111:LYS:CD	24:P:53:TYR:CE2	2.78	0.61
10:A:382:ARG:HG3	10:A:383:SER:N	2.14	0.61
17:H:84:GLU:HA	17:H:87:ILE:HG13	1.81	0.61
27:S:280:HIS:O	27:S:282:LEU:N	2.34	0.61
42:j:116:PHE:CD1	43:g:160:LYS:CB	2.82	0.61
43:g:89:GLU:O	43:g:92:TRP:N	2.33	0.61
47:m:172:LYS:O	47:m:175:LEU:N	2.30	0.61
48:o:83:ARG:O	48:o:85:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:A6:13:ALA:O	61:A6:18:ARG:HD2	2.00	0.61
1:9:223:PHE:HZ	9:8:49:HIS:HD2	1.44	0.61
9:8:60:GLY:O	9:8:256:ARG:NH1	2.33	0.61
10:A:617:ARG:HG3	23:O:122:PHE:CE1	2.35	0.61
14:E:72:MET:O	14:E:75:SER:N	2.32	0.61
28:T:37:SER:CB	28:T:60:THR:HG21	2.31	0.61
37:c:89:HIS:O	37:c:92:THR:N	2.30	0.61
42:j:119:VAL:CB	43:g:147:GLY:CA	2.69	0.61
46:l:133:ARG:HD3	46:l:135:TRP:CZ2	2.36	0.61
47:m:47:THR:HG23	47:m:79:ILE:HG23	1.81	0.61
45:w:19:LEU:HD12	45:w:23:LEU:HD23	1.81	0.61
57:C4:16:ILE:HD12	57:C4:17:MET:N	2.15	0.61
8:1:172:MET:HE2	8:1:176:LEU:HB2	1.82	0.61
9:8:395:VAL:HG23	9:8:398:ARG:HH11	1.66	0.61
11:B:303:ARG:HD2	11:B:311:TYR:OH	2.00	0.61
12:C:167:TRP:O	12:C:170:ARG:N	2.34	0.61
13:D:199:GLN:CG	14:E:178:GLU:CG	2.79	0.61
28:T:112:ALA:O	28:T:116:ALA:N	2.32	0.61
36:b:137:MET:CE	43:g:87:GLU:OE2	2.48	0.61
38:d:105:GLU:CD	44:e:166:LEU:HG	2.26	0.61
47:m:376:LEU:CD2	50:q:17:ARG:HG2	2.27	0.61
49:A0:117:LEU:CB	49:A0:121:GLN:CA	2.79	0.61
65:C3:3:ASN:C	65:C3:3:ASN:HD22	2.08	0.61
2:4:16:TRP:CD1	70:4:501:3PE:H2C1	2.34	0.61
2:4:190:TRP:HB3	28:T:127:MET:SD	2.41	0.61
2:4:446:LEU:HG	71:4:502:CDL:C35	2.31	0.61
11:B:216:ARG:HG3	14:E:94:SER:HB2	1.82	0.61
18:I:111:THR:HG21	18:I:118:GLN:HA	1.82	0.61
21:L:53:TYR:CD1	30:V:69:ILE:HG23	2.35	0.61
36:b:166:GLY:O	36:b:168:TRP:N	2.32	0.61
46:l:247:GLN:NE2	46:l:429:ASN:HA	2.12	0.61
45:w:208:LEU:O	45:w:212:ALA:N	2.33	0.61
46:x:133:ARG:HD3	46:x:135:TRP:CZ2	2.36	0.61
46:x:304:HIS:CG	46:x:305:GLN:H	2.17	0.61
49:A0:117:LEU:CB	49:A0:121:GLN:N	2.64	0.61
63:A5:39:CYS:HG	63:A5:53:CYS:HG	0.70	0.61
2:4:190:TRP:CD2	28:T:127:MET:HE2	2.35	0.61
5:6:581:LYS:HD2	6:5:96:LEU:HG	1.83	0.61
10:A:615:LEU:O	10:A:617:ARG:NH1	2.33	0.61
12:C:213:ARG:HB2	13:D:175:ARG:HG2	1.77	0.61
27:S:236:GLU:HA	27:S:239:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:19:LEU:HD12	45:k:23:LEU:HD23	1.82	0.61
56:A9:273:MET:HG3	56:A9:319:LYS:HZ1	1.64	0.61
5:6:152:PHE:HD1	5:6:168:ALA:HB1	1.64	0.61
9:8:384:PRO:HG2	9:8:422:HIS:O	2.01	0.61
10:A:614:GLY:HA2	26:R:41:ILE:HD12	1.83	0.61
11:B:170:ILE:O	11:B:173:LEU:N	2.34	0.61
13:D:155:SER:OG	13:D:155:SER:O	2.15	0.61
27:S:335:VAL:N	42:j:52:PRO:HD3	2.16	0.61
53:A3:11:ARG:N	53:A3:12:GLN:HA	2.15	0.61
56:A9:92:MET:CE	56:A9:167:THR:HG21	2.31	0.61
57:C4:59:GLN:HA	57:C4:62:GLU:HB2	1.83	0.61
2:4:48:ASN:CG	43:g:90:MET:SD	2.83	0.61
10:A:312:GLY:HA2	29:U:144:TYR:CE1	2.36	0.61
12:C:204:PHE:HE2	13:D:167:TYR:HB3	1.65	0.61
16:G:75:ARG:HH22	16:G:119:ASP:CG	2.08	0.61
37:c:15:LEU:O	37:c:19:ARG:N	2.33	0.61
2:4:57:PHE:O	2:4:111:THR:HG23	2.01	0.61
2:4:166:TYR:CE2	70:4:503:3PE:C21	2.84	0.61
3:2:109:ALA:HB3	3:2:110:PRO:HD3	1.82	0.61
3:2:129:ILE:CG2	72:2:402:PC1:H372	2.30	0.61
7:3:88:LEU:HD11	8:1:309:ILE:HD13	1.83	0.61
8:1:233:MET:HA	8:1:236:ILE:HG21	1.77	0.61
10:A:153:PHE:HE2	10:A:156:GLY:HA3	1.64	0.61
11:B:212:GLU:O	11:B:215:GLU:N	2.34	0.61
12:C:213:ARG:HB2	13:D:175:ARG:CG	2.30	0.61
13:D:95:GLU:OE1	13:D:190:ALA:HB2	2.01	0.61
27:S:173:ASP:O	27:S:177:GLN:N	2.32	0.61
28:T:13:PRO:HG2	28:T:21:LYS:CB	2.31	0.61
39:f:164:PRO:O	39:f:166:LEU:N	2.34	0.61
42:j:46:ASN:HA	42:j:51:ARG:HE	1.66	0.61
45:k:372:THR:OG1	46:l:373:GLU:OE1	2.15	0.61
52:s:53:ASP:OD1	52:s:54:CYS:N	2.34	0.61
53:A3:43:ASP:OD1	53:A3:47:TYR:CB	2.48	0.61
58:C2:154:GLY:HA2	61:A6:6:VAL:CG2	2.30	0.61
7:3:68:GLU:O	7:3:72:LEU:N	2.31	0.60
8:1:176:LEU:CB	8:1:177:PRO:HD2	2.08	0.60
24:P:40:LYS:H	30:V:8:GLN:H	1.49	0.60
29:U:29:ARG:HH12	29:U:63:ILE:HG12	1.66	0.60
46:x:308:ASP:OD1	46:x:309:VAL:N	2.35	0.60
49:A0:106:ILE:CA	49:A0:167:ALA:HA	2.17	0.60
58:C2:148:HIS:O	58:C2:152:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:163:ALA:HB2	70:4:503:3PE:H241	1.81	0.60
4:7:68:PHE:CZ	6:5:31:LEU:HD13	2.36	0.60
6:5:8:ILE:HG13	6:5:8:ILE:O	2.01	0.60
27:S:121:ALA:O	27:S:125:ALA:N	2.29	0.60
35:a:129:TYR:CE2	43:g:144:HIS:HE1	2.18	0.60
1:9:222:ARG:HH12	9:8:284:ASN:HB2	1.67	0.60
2:4:196:TRP:CD1	2:4:251:ASN:HD22	2.19	0.60
3:2:340:THR:OG1	3:2:341:PRO:HD3	2.01	0.60
5:6:82:MET:HB3	5:6:87:MET:HE2	1.81	0.60
5:6:123:LEU:HA	5:6:126:ILE:HD12	1.82	0.60
8:1:63:PRO:HG3	8:1:214:GLU:OE2	2.01	0.60
8:1:203:GLY:N	8:1:210:GLY:H	1.93	0.60
10:A:423:LEU:C	10:A:425:ASN:H	2.09	0.60
11:B:233:HIS:NE2	14:E:160:GLU:CD	2.59	0.60
12:C:90:ILE:HG22	12:C:91:HIS:O	2.01	0.60
33:Y:47:TYR:CE2	34:Z:16:LEU:HD12	2.36	0.60
48:o:23:HIS:HD2	54:u:51:LEU:HA	1.65	0.60
47:y:361:LEU:HD23	47:y:365:LEU:HD12	1.81	0.60
7:3:73:LEU:HB3	7:3:74:PRO:HD3	1.83	0.60
10:A:312:GLY:H	29:U:144:TYR:HD1	1.47	0.60
11:B:328:ASP:OD2	14:E:42:ASN:ND2	2.24	0.60
26:R:155:VAL:O	26:R:159:ALA:N	2.24	0.60
26:R:200:ILE:O	26:R:262:THR:OG1	2.16	0.60
44:e:78:LEU:O	44:e:80:ASP:N	2.34	0.60
63:A5:57:ARG:HH11	63:A5:57:ARG:HB3	1.64	0.60
3:2:150:ASN:N	3:2:150:ASN:OD1	2.31	0.60
5:6:581:LYS:CA	6:5:96:LEU:HD11	2.31	0.60
8:1:266:LEU:O	8:1:266:LEU:HD12	2.01	0.60
9:8:411:SER:HB3	24:P:49:LEU:HD13	1.84	0.60
10:A:320:GLU:CG	23:O:123:TYR:OH	2.50	0.60
10:A:691:ILE:O	10:A:693:ASP:N	2.35	0.60
11:B:322:SER:HB3	14:E:42:ASN:O	2.02	0.60
23:O:33:ARG:NH1	31:M:45:LEU:HA	2.16	0.60
2:4:347:GLY:HA2	2:4:416:ARG:O	2.01	0.60
8:1:174:LEU:O	8:1:174:LEU:HD22	2.02	0.60
8:1:311:THR:O	8:1:311:THR:HG22	2.01	0.60
10:A:251:ILE:HB	10:A:606:THR:HG22	1.82	0.60
11:B:266:ARG:HD3	70:B:501:3PE:O22	2.01	0.60
23:O:53:ASP:HB3	26:R:354:ARG:NH2	2.16	0.60
68:A8:28:LEU:HB2	68:A8:29:PRO:HD3	1.84	0.60
6:5:87:THR:HB	6:5:89:TYR:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:196:GLY:CA	14:E:176:SER:HB3	2.30	0.60
16:G:121:LEU:O	16:G:123:ASN:N	2.28	0.60
28:T:20:ARG:HG2	28:T:20:ARG:HH11	1.67	0.60
36:b:119:ARG:NH1	43:g:62:TYR:O	2.35	0.60
43:g:125:CYS:O	43:g:127:LYS:N	2.34	0.60
45:k:145:MET:HE3	45:k:252:HIS:HE1	1.67	0.60
45:w:266:ASP:OD2	45:w:413:LYS:NZ	2.35	0.60
47:y:71:ARG:NH2	48:z:46:VAL:HG22	2.11	0.60
3:2:22:ILE:HD11	17:H:4:PHE:HB2	1.83	0.60
3:2:260:PHE:CE2	3:2:264:TRP:HB2	2.37	0.60
10:A:311:LYS:O	29:U:144:TYR:CE1	2.54	0.60
12:C:233:ARG:NH2	14:E:120:GLU:OE2	2.33	0.60
14:E:100:GLU:OE2	14:E:193:ASN:ND2	2.34	0.60
16:G:139:GLU:OE2	16:G:145:TYR:HE2	1.84	0.60
28:T:3:LYS:N	28:T:3:LYS:HD2	2.17	0.60
28:T:139:PRO:CA	36:b:158:ARG:HG3	2.32	0.60
46:x:163:LEU:HD21	46:x:258:VAL:HG21	1.84	0.60
3:2:69:LEU:HD23	3:2:97:LEU:HD11	1.81	0.60
4:7:125:TRP:CD1	30:V:138:TYR:HH	2.20	0.60
7:3:88:LEU:CD1	8:1:309:ILE:HG21	2.20	0.60
10:A:418:ILE:O	10:A:422:TRP:N	2.30	0.60
12:C:207:SER:HA	13:D:166:SER:O	2.02	0.60
42:j:51:ARG:HB3	42:j:53:VAL:H	1.66	0.60
46:l:308:ASP:OD1	46:l:309:VAL:N	2.35	0.60
48:z:133:GLY:O	48:z:150:ASN:ND2	2.35	0.60
57:C4:226:MET:O	57:C4:227:LEU:HB2	2.01	0.60
61:A6:62:CYS:SG	61:A6:84:SER:OG	2.60	0.60
2:4:166:TYR:CZ	70:4:503:3PE:C2	2.84	0.60
70:4:501:3PE:O14	3:2:238:PRO:HB2	2.01	0.60
3:2:267:ILE:O	3:2:271:THR:HG22	2.02	0.60
3:2:305:PHE:HZ	27:S:317:GLN:HG2	1.67	0.60
5:6:119:LYS:HZ2	71:6:701:CDL:H311	1.66	0.60
8:1:233:MET:O	8:1:236:ILE:HG23	2.01	0.60
9:8:211:ALA:HB2	9:8:223:PRO:HB3	1.83	0.60
10:A:565:PHE:HB2	10:A:581:ASP:CB	2.31	0.60
26:R:234:LYS:HB3	26:R:323:HIS:CE1	2.37	0.60
28:T:30:GLY:N	28:T:64:ALA:HA	2.17	0.60
28:T:69:ILE:CG2	28:T:100:ILE:HD11	2.31	0.60
38:d:33:GLU:O	38:d:36:GLU:N	2.35	0.60
41:i:68:GLU:HB3	42:j:19:ARG:CB	2.32	0.60
46:l:24:LEU:HG	46:l:38:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B3:53:ASP:OD1	52:B3:54:CYS:N	2.34	0.60
53:A3:40:LEU:C	53:A3:41:ILE:CG1	2.71	0.60
3:2:249:LEU:HD21	3:2:254:LEU:HD12	1.82	0.59
8:1:267:THR:C	8:1:269:SER:N	2.59	0.59
9:8:318:ILE:HB	9:8:355:ILE:HG13	1.81	0.59
10:A:250:SER:OG	10:A:251:ILE:N	2.34	0.59
11:B:234:GLN:HE22	14:E:96:ARG:CD	2.13	0.59
11:B:326:CYS:O	11:B:329:ARG:N	2.33	0.59
23:O:48:HIS:O	26:R:359:TYR:CE1	2.55	0.59
23:O:76:PRO:O	23:O:77:ARG:HG2	2.01	0.59
27:S:286:VAL:CB	72:S:401:PC1:H152	2.30	0.59
36:b:143:GLU:O	36:b:146:LYS:N	2.28	0.59
3:2:26:TRP:CD1	3:2:85:THR:O	2.55	0.59
71:6:701:CDL:HB31	71:6:701:CDL:OA3	2.01	0.59
8:1:35:LYS:NZ	14:E:85:ASN:HD21	2.00	0.59
9:8:204:TYR:HB3	9:8:377:GLU:HG2	1.84	0.59
9:8:411:SER:O	9:8:414:GLU:N	2.35	0.59
10:A:57:GLY:O	12:C:248:ARG:HD3	2.01	0.59
12:C:71:LEU:N	12:C:72:PRO:HD3	2.17	0.59
23:O:99:GLN:C	23:O:101:THR:H	2.07	0.59
26:R:238:GLN:HE22	26:R:271:TYR:HA	1.66	0.59
28:T:97:GLY:HA2	28:T:100:ILE:HD12	1.84	0.59
40:h:78:LYS:H	40:h:83:ASP:CG	2.10	0.59
31:M:12:LYS:HD3	31:M:77:VAL:HG11	1.83	0.59
45:k:203:LEU:HA	45:k:207:GLN:NE2	2.17	0.59
45:w:203:LEU:HA	45:w:207:GLN:NE2	2.17	0.59
57:C4:145:PRO:CG	57:C4:148:MET:HE2	2.32	0.59
4:7:101:PHE:O	4:7:105:TYR:N	2.32	0.59
8:1:169:GLN:NE2	8:1:174:LEU:HB2	2.16	0.59
9:8:164:ASN:O	9:8:167:SER:OG	2.18	0.59
40:h:137:MET:O	43:g:138:ALA:HB1	2.02	0.59
53:A3:16:ASN:HA	53:A3:19:PRO:HD2	1.84	0.59
2:4:442:LEU:HB2	2:4:443:PRO:HD3	1.83	0.59
4:7:72:THR:HG23	6:5:27:MET:HE2	1.84	0.59
8:1:119:SER:HB2	8:1:211:PHE:HE1	1.66	0.59
10:A:58:MET:HG3	12:C:248:ARG:NH1	2.13	0.59
14:E:40:TYR:HE2	24:P:106:LEU:HD11	1.67	0.59
22:N:107:PRO:O	22:N:109:ALA:N	2.34	0.59
28:T:30:GLY:HA3	28:T:64:ALA:CB	2.30	0.59
30:V:78:GLU:O	30:V:82:ARG:HG2	2.02	0.59
45:w:145:MET:HE3	45:w:252:HIS:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:304:HIS:CD2	46:x:305:GLN:H	2.20	0.59
48:z:83:ARG:O	48:z:85:GLY:N	2.34	0.59
58:C2:119:THR:O	62:A4:52:HIS:HE1	1.84	0.59
1:9:227:PRO:CD	9:8:48:ARG:HH22	2.15	0.59
2:4:325:MET:HE3	2:4:362:ALA:HB2	1.84	0.59
3:2:84:TRP:HH2	6:5:59:MET:SD	2.26	0.59
4:7:71:THR:O	4:7:72:THR:OG1	2.19	0.59
9:8:49:HIS:ND1	9:8:49:HIS:O	2.36	0.59
9:8:284:ASN:OD1	9:8:304:ALA:N	2.33	0.59
9:8:362:ASP:HB3	9:8:365:LYS:HB3	1.83	0.59
10:A:371:VAL:HB	10:A:482:GLN:HG3	1.84	0.59
10:A:618:GLU:OE2	10:A:620:TRP:CD1	2.54	0.59
11:B:141:TYR:CD1	11:B:141:TYR:N	2.67	0.59
11:B:320:ILE:O	14:E:41:VAL:HG21	1.96	0.59
12:C:123:THR:CG2	16:G:128:PHE:HA	2.29	0.59
16:G:128:PHE:HD2	16:G:134:ALA:HA	1.68	0.59
27:S:161:MET:HG3	27:S:166:PHE:CE1	2.38	0.59
32:X:41:SER:OG	43:g:71:VAL:CB	2.51	0.59
47:m:377:LEU:HD11	50:q:20:TYR:HE2	1.68	0.59
58:C2:192:VAL:O	58:C2:196:THR:HB	2.01	0.59
1:9:177:LEU:HA	9:8:159:ARG:NH1	2.17	0.59
5:6:305:SER:OG	5:6:336:LYS:NZ	2.22	0.59
14:E:53:VAL:HG13	21:L:14:ALA:CB	2.32	0.59
26:R:117:ARG:NE	26:R:155:VAL:HG21	2.17	0.59
26:R:234:LYS:O	26:R:271:TYR:OH	2.17	0.59
28:T:13:PRO:HG3	28:T:20:ARG:CZ	2.25	0.59
28:T:20:ARG:HH11	28:T:20:ARG:CG	2.14	0.59
29:U:14:VAL:HG22	29:U:23:TYR:CE1	2.38	0.59
30:V:46:GLY:O	30:V:49:SER:OG	2.17	0.59
35:a:47:TYR:OH	44:e:103:GLU:O	2.14	0.59
42:j:112:VAL:HG21	43:g:79:GLU:CD	2.28	0.59
52:B3:10:GLU:OE1	52:B3:12:GLU:N	2.35	0.59
2:4:254:THR:HG21	2:4:257:MET:HE3	1.83	0.59
10:A:577:ALA:HB3	10:A:578:PRO:HD3	1.84	0.59
11:B:370:GLU:OE2	11:B:374:SER:OG	2.16	0.59
12:C:128:PHE:HD2	12:C:178:VAL:HG23	1.66	0.59
13:D:75:ASN:ND2	13:D:206:ARG:O	2.35	0.59
40:h:149:LEU:HD22	43:g:166:GLU:HB3	1.84	0.59
1:9:123:ASN:HD22	1:9:127:VAL:HG11	1.65	0.59
2:4:34:ILE:O	2:4:37:THR:OG1	2.15	0.59
5:6:67:HIS:ND1	5:6:67:HIS:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:298:ILE:HD13	5:6:354:GLN:HA	1.83	0.59
5:6:402:SER:OG	5:6:404:THR:HG23	2.02	0.59
10:A:105:ASN:OD1	10:A:110:LYS:HE2	2.02	0.59
25:Q:93:GLY:O	25:Q:95:GLN:N	2.35	0.59
26:R:250:ILE:HA	26:R:253:ILE:HB	1.85	0.59
28:T:101:LEU:CG	28:T:110:ILE:HG21	2.32	0.59
30:V:50:MET:C	30:V:52:LYS:H	2.09	0.59
34:Z:63:PHE:CE2	34:Z:64:VAL:HG23	2.38	0.59
35:a:68:TRP:CZ3	44:e:109:LEU:O	2.55	0.59
47:m:24:PRO:HD2	47:m:27:ILE:HD11	1.85	0.59
47:m:376:LEU:HA	50:q:17:ARG:HE	1.66	0.59
63:A5:57:ARG:HG3	63:A5:60:TYR:CE2	2.38	0.59
2:4:447:LEU:HD13	2:4:454:ILE:HD11	1.83	0.59
5:6:562:LEU:HB3	5:6:563:PRO:HD3	1.84	0.59
11:B:263:THR:OG1	11:B:264:ASN:OD1	2.20	0.59
12:C:151:GLU:OE1	16:G:64:ILE:HD13	2.03	0.59
12:C:183:HIS:ND1	12:C:185:ASP:O	2.36	0.59
16:G:94:THR:HG22	16:G:95:LYS:H	1.68	0.59
43:g:33:LEU:O	43:g:37:PHE:N	2.35	0.59
49:A0:20:ASP:OD1	49:A0:21:SER:N	2.36	0.59
71:6:701:CDL:H111	36:b:68:LEU:HD21	1.85	0.59
10:A:161:GLU:OE1	18:I:102:ASN:ND2	2.36	0.59
12:C:213:ARG:NE	26:R:48:ARG:NH1	2.51	0.59
13:D:99:MET:SD	13:D:193:LEU:HD22	2.43	0.59
21:L:56:PRO:HA	25:Q:128:VAL:HG22	1.84	0.59
21:L:69:HIS:NE2	21:L:71:GLN:HB2	2.18	0.59
45:k:17:SER:HB2	45:k:25:VAL:HB	1.85	0.59
46:l:355:PRO:O	46:l:359:ALA:N	2.29	0.59
48:o:133:GLY:O	48:o:150:ASN:ND2	2.35	0.59
50:q:39:GLU:N	50:q:39:GLU:OE1	2.35	0.59
45:w:156:THR:HG22	45:w:239:SER:OG	2.03	0.59
46:x:24:LEU:HG	46:x:38:LEU:HD11	1.84	0.59
1:9:233:SER:O	9:8:41:ILE:CD1	2.49	0.58
2:4:360:LEU:HD11	71:6:701:CDL:H532	1.84	0.58
3:2:169:GLY:O	3:2:172:GLN:N	2.35	0.58
12:C:221:VAL:CG2	13:D:138:ARG:CG	2.81	0.58
17:H:15:ASP:C	17:H:17:TRP:H	2.09	0.58
21:L:8:PHE:HE2	72:L:200:PC1:H322	1.59	0.58
23:O:88:MET:HE3	23:O:92:GLU:OE2	2.03	0.58
42:j:68:PHE:O	42:j:72:GLY:N	2.30	0.58
31:M:34:SER:O	31:M:72:CYS:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:M:41:GLY:O	31:M:42:LEU:HD12	2.03	0.58
47:m:77:TRP:CZ3	47:m:78:ILE:HG22	2.38	0.58
47:m:114:ASN:O	47:m:117:VAL:N	2.36	0.58
77:y:402:HEM:HMC1	77:y:402:HEM:HBC2	1.85	0.58
49:A0:114:VAL:O	49:A0:116:GLN:N	2.36	0.58
55:B1:59:ALA:HB1	55:B1:62:ARG:O	2.03	0.58
2:4:423:ILE:HD12	35:a:57:ARG:HB2	1.85	0.58
3:2:337:LEU:HB2	3:2:339:LEU:HG	1.84	0.58
7:3:88:LEU:HD11	8:1:309:ILE:CD1	2.33	0.58
8:1:76:ILE:O	8:1:76:ILE:HG22	2.03	0.58
8:1:153:VAL:O	8:1:156:MET:N	2.32	0.58
9:8:116:ASN:HB2	73:8:501:FMN:O2	2.03	0.58
13:D:197:ILE:O	13:D:200:LEU:N	2.35	0.58
14:E:188:GLU:OE1	18:I:64:ASN:CB	2.25	0.58
26:R:133:GLU:HG3	26:R:134:TRP:N	2.17	0.58
34:Z:47:ARG:HA	34:Z:50:ALA:HB3	1.84	0.58
41:i:69:TYR:CB	42:j:20:SER:HA	2.33	0.58
49:A0:106:ILE:C	49:A0:167:ALA:CB	2.16	0.58
49:A0:116:GLN:CB	49:A0:172:ARG:HA	2.33	0.58
2:4:58:SER:O	2:4:111:THR:OG1	2.16	0.58
2:4:186:VAL:HB	2:4:251:ASN:OD1	2.03	0.58
8:1:70:MET:HE1	8:1:118:TRP:CD1	2.38	0.58
12:C:77:GLN:HB3	12:C:89:CYS:HB2	1.84	0.58
12:C:95:VAL:H	12:C:97:PRO:HD2	1.67	0.58
12:C:128:PHE:CE2	12:C:176:PHE:HB3	2.38	0.58
17:H:15:ASP:OD1	17:H:15:ASP:N	2.26	0.58
23:O:53:ASP:OD2	26:R:351:GLU:CA	2.49	0.58
25:Q:47:ARG:NH2	36:b:187:PRO:HB2	2.18	0.58
31:W:85:TYR:CD1	34:Z:17:PRO:O	2.56	0.58
35:a:47:TYR:CB	44:e:105:MET:HB2	2.28	0.58
38:d:25:PHE:CE1	38:d:43:GLN:HB3	2.38	0.58
42:j:108:THR:CB	43:g:78:GLN:C	2.76	0.58
50:q:9:SER:O	50:q:13:LEU:N	2.36	0.58
47:y:4:ILE:HG22	47:y:6:LYS:H	1.65	0.58
1:9:223:PHE:CZ	9:8:49:HIS:HD2	2.20	0.58
2:4:62:SER:HB2	40:h:113:ARG:HH22	1.68	0.58
2:4:449:LEU:CD1	71:4:502:CDL:H311	2.32	0.58
10:A:260:ASN:H	10:A:282:ASN:ND2	2.00	0.58
11:B:308:TYR:HH	11:B:401:GLU:H	1.51	0.58
20:K:25:GLN:NE2	20:K:57:GLU:OE2	2.36	0.58
22:N:42:ALA:HB2	22:N:100:TRP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:92:GLU:HG3	23:O:97:TRP:HE3	1.68	0.58
25:Q:43:PHE:HD1	25:Q:59:GLU:HB2	1.69	0.58
28:T:139:PRO:CB	36:b:158:ARG:HA	2.31	0.58
43:g:70:ARG:HH22	43:g:94:ARG:HD2	1.67	0.58
43:g:114:GLN:O	43:g:117:GLU:N	2.32	0.58
50:q:17:ARG:HA	50:q:20:TYR:HB3	1.84	0.58
45:w:412:SER:C	54:B2:15:ARG:HH22	2.11	0.58
49:A0:150:ALA:O	49:A0:155:GLY:CA	2.52	0.58
52:B3:13:LEU:C	52:B3:15:ASP:H	2.12	0.58
58:C2:6:HIS:HD2	58:C2:8:TYR:H	1.49	0.58
2:4:2:LEU:HD21	72:4:504:PC1:C14	2.33	0.58
8:1:77:MET:O	8:1:79:LEU:N	2.36	0.58
52:B3:10:GLU:N	52:B3:11:GLU:HA	2.17	0.58
60:C0:80:GLU:CD	60:C0:80:GLU:H	2.10	0.58
5:6:89:PHE:HB2	5:6:326:PHE:HZ	1.68	0.58
10:A:153:PHE:HB3	10:A:154:LEU:HA	1.84	0.58
10:A:380:ASP:OD2	20:K:41:TYR:OH	2.20	0.58
35:a:64:ALA:CB	44:e:108:ASP:N	2.67	0.58
43:g:140:GLN:O	43:g:144:HIS:HB3	2.04	0.58
45:k:156:THR:HG22	45:k:239:SER:OG	2.03	0.58
46:l:163:LEU:HD21	46:l:258:VAL:HG21	1.84	0.58
47:y:24:PRO:HD2	47:y:27:ILE:HD11	1.84	0.58
47:y:77:TRP:CZ3	47:y:78:ILE:HG22	2.38	0.58
2:4:193:VAL:HG22	2:4:257:MET:HE1	1.83	0.58
3:2:264:TRP:NE1	25:Q:168:PHE:CE2	2.72	0.58
8:1:8:MET:O	8:1:12:PRO:CG	2.50	0.58
10:A:146:PHE:N	10:A:146:PHE:CD1	2.70	0.58
10:A:656:TYR:O	10:A:657:ASP:OD1	2.21	0.58
23:O:128:PRO:CG	26:R:45:LYS:NZ	2.66	0.58
27:S:120:GLN:NE2	27:S:161:MET:SD	2.77	0.58
43:g:9:VAL:O	43:g:109:ARG:NH2	2.37	0.58
47:y:114:ASN:O	47:y:117:VAL:N	2.36	0.58
52:B3:41:ASP:O	52:B3:45:SER:N	2.31	0.58
66:B0:43:SER:OG	66:B0:45:VAL:HG12	2.04	0.58
2:4:36:PHE:HZ	40:h:97:ILE:HG13	1.69	0.58
11:B:320:ILE:HD12	14:E:39:LYS:H	1.68	0.58
11:B:389:TYR:N	11:B:389:TYR:CD1	2.69	0.58
14:E:37:THR:CB	24:P:107:SER:HB2	2.34	0.58
31:W:85:TYR:HE1	34:Z:18:ASP:O	1.86	0.58
77:m:402:HEM:HBC2	77:m:402:HEM:HMC1	1.85	0.58
45:w:183:THR:HA	45:w:186:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:39:GLU:OE1	50:A1:39:GLU:N	2.35	0.58
67:C1:46:LYS:O	67:C1:47:LYS:HB2	2.02	0.58
3:2:338:PRO:C	42:j:83:TYR:OH	2.47	0.58
4:7:25:SER:O	4:7:27:ILE:N	2.37	0.58
5:6:556:ILE:CD1	35:a:76:ILE:HD11	2.30	0.58
9:8:207:GLY:O	73:8:501:FMN:H9	2.04	0.58
11:B:154:ALA:HB2	11:B:398:THR:HG21	1.86	0.58
11:B:282:ASP:HA	11:B:285:ASN:HB3	1.85	0.58
19:J:3:PHE:CB	71:J:101:CDL:H722	2.34	0.58
26:R:154:GLN:HG3	26:R:155:VAL:H	1.68	0.58
27:S:320:THR:O	27:S:324:GLY:HA3	2.03	0.58
30:V:72:MET:HG3	30:V:72:MET:O	2.03	0.58
33:Y:46:ARG:HA	33:Y:49:GLN:NE2	2.18	0.58
44:e:70:THR:HG22	44:e:71:GLY:N	2.19	0.58
50:q:20:TYR:O	50:q:23:ALA:N	2.28	0.58
45:w:277:ILE:HD12	45:w:341:GLN:HB3	1.86	0.58
2:4:2:LEU:CD1	72:4:504:PC1:H142	2.34	0.58
70:4:501:3PE:H371	70:4:501:3PE:C2A	2.34	0.58
3:2:91:ASN:OD1	3:2:92:PRO:HD2	2.04	0.58
5:6:578:THR:O	5:6:581:LYS:HG2	2.03	0.58
5:6:581:LYS:CB	6:5:96:LEU:HD11	2.33	0.58
6:5:17:VAL:HA	6:5:20:LEU:HB3	1.86	0.58
8:1:310:LEU:HD23	8:1:310:LEU:O	2.02	0.58
16:G:165:SER:HB3	16:G:168:LYS:HB2	1.86	0.58
23:O:53:ASP:HB3	26:R:354:ARG:HH22	1.69	0.58
25:Q:5:VAL:HG22	30:V:107:GLY:O	2.04	0.58
37:c:95:TYR:CE2	43:g:10:TYR:HD1	2.20	0.58
45:w:408:ARG:HE	53:A3:15:ARG:HH21	1.51	0.58
49:A0:187:PHE:O	49:A0:189:SER:N	2.35	0.58
1:9:138:THR:HB	1:9:139:PRO:HD3	1.86	0.57
3:2:112:HIS:O	3:2:112:HIS:CG	2.57	0.57
5:6:40:ILE:HG22	5:6:98:TRP:HD1	1.69	0.57
8:1:73:LEU:C	8:1:76:ILE:HD12	2.20	0.57
11:B:233:HIS:HE2	14:E:160:GLU:CD	2.10	0.57
27:S:48:ILE:HD12	27:S:49:THR:H	1.68	0.57
27:S:157:PHE:O	27:S:161:MET:N	2.34	0.57
28:T:95:CYS:C	28:T:97:GLY:H	2.12	0.57
39:f:35:ASP:O	39:f:39:TYR:N	2.31	0.57
45:k:214:LYS:O	45:k:215:HIS:CG	2.57	0.57
5:6:470:ASN:CB	38:d:77:PHE:HD1	2.16	0.57
10:A:311:LYS:C	29:U:144:TYR:CD1	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:355:LYS:CD	10:A:530:TYR:CE1	2.52	0.57
11:B:94:VAL:CG1	11:B:115:LEU:HD23	2.34	0.57
13:D:137:LEU:O	13:D:140:VAL:N	2.37	0.57
14:E:179:THR:OG1	29:U:123:GLN:NE2	2.37	0.57
42:j:114:GLU:CA	43:g:160:LYS:HD3	2.34	0.57
42:j:119:VAL:CG2	43:g:147:GLY:HA3	2.34	0.57
45:k:186:LEU:HD23	45:k:190:TYR:HE2	1.70	0.57
45:k:266:ASP:OD2	45:k:413:LYS:NZ	2.35	0.57
46:x:325:TYR:HB3	55:B1:57:GLY:CA	2.35	0.57
47:y:49:LEU:O	47:y:52:ALA:N	2.37	0.57
57:C4:193:TYR:HE1	59:A7:126:MET:HE1	1.68	0.57
5:6:203:MET:HB2	43:g:114:GLN:OE1	2.04	0.57
6:5:73:LEU:O	6:5:76:SER:N	2.29	0.57
8:1:233:MET:CA	8:1:236:ILE:HG23	2.25	0.57
10:A:44:GLU:HG2	10:A:45:PRO:HD2	1.87	0.57
10:A:452:LEU:O	10:A:455:ILE:HG22	2.04	0.57
14:E:171:PRO:CB	14:E:200:GLU:OE2	2.44	0.57
23:O:21:PHE:N	23:O:80:ASP:OD2	2.34	0.57
25:Q:83:THR:HA	25:Q:86:TRP:NE1	2.18	0.57
27:S:100:CYS:HB3	27:S:119:LEU:HB2	1.86	0.57
27:S:321:GLU:C	27:S:324:GLY:H	2.13	0.57
44:e:43:LYS:O	44:e:44:THR:C	2.47	0.57
31:M:28:GLU:HA	31:M:30:LEU:HD13	1.85	0.57
31:M:37:MET:HG2	31:M:41:GLY:HA2	1.86	0.57
48:o:12:TRP:HB2	48:o:15:ARG:HB2	1.87	0.57
45:w:17:SER:HB2	45:w:25:VAL:HB	1.85	0.57
45:w:213:GLN:O	45:w:214:LYS:C	2.47	0.57
2:4:190:TRP:CE3	28:T:127:MET:CE	2.86	0.57
3:2:275:SER:HA	28:T:134:GLN:O	2.05	0.57
5:6:497:GLY:O	5:6:501:ALA:N	2.37	0.57
8:1:43:TYR:CZ	29:U:27:LEU:HD21	2.40	0.57
45:k:277:ILE:HD12	45:k:341:GLN:HB3	1.86	0.57
45:k:343:MET:HE1	45:k:416:TYR:HD2	1.69	0.57
48:z:75:ASN:ND2	48:z:79:GLU:OE1	2.37	0.57
49:A0:117:LEU:CB	49:A0:121:GLN:H	2.15	0.57
57:C4:193:TYR:CE1	59:A7:126:MET:HE1	2.39	0.57
70:4:501:3PE:C22	70:4:501:3PE:H11	2.33	0.57
4:7:17:PHE:CD2	6:5:11:ALA:HB1	2.40	0.57
5:6:64:SER:OG	37:c:96:THR:HA	2.04	0.57
8:1:53:ILE:O	8:1:53:ILE:HG22	2.03	0.57
9:8:385:CYS:SG	74:8:502:SF4:S3	3.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:58:MET:HG2	12:C:248:ARG:NH2	2.20	0.57
12:C:227:GLU:HG2	26:R:48:ARG:O	2.04	0.57
21:L:62:ASN:HA	21:L:63:MET:HB3	1.86	0.57
27:S:71:LEU:HG	27:S:144:GLY:HA3	1.87	0.57
35:a:79:ASN:HB3	44:e:73:GLY:HA3	1.87	0.57
41:i:68:GLU:CG	42:j:19:ARG:CD	2.51	0.57
47:m:49:LEU:O	47:m:52:ALA:N	2.37	0.57
45:w:426:GLY:HA2	45:w:428:ILE:H	1.70	0.57
67:C1:41:ARG:HG3	68:A8:40:TYR:CE2	2.40	0.57
5:6:583:LEU:HB3	5:6:586:LEU:HD13	1.86	0.57
8:1:61:LEU:HD11	13:D:118:ARG:HD2	1.86	0.57
26:R:171:ASN:ND2	26:R:324:THR:HB	2.19	0.57
26:R:238:GLN:NE2	26:R:270:ARG:O	2.36	0.57
30:V:51:MET:HG3	30:V:55:ARG:HH21	1.70	0.57
35:a:47:TYR:HE1	44:e:105:MET:SD	2.27	0.57
36:b:92:PHE:HB2	36:b:93:ILE:HD12	1.87	0.57
41:i:69:TYR:CA	42:j:20:SER:HA	2.34	0.57
50:q:13:LEU:O	50:q:16:ILE:HG23	2.04	0.57
49:A0:121:GLN:HA	49:A0:170:ARG:CB	2.35	0.57
57:C4:145:PRO:HG3	57:C4:148:MET:HE2	1.87	0.57
57:C4:179:LEU:HD21	63:A5:65:PRO:HD3	1.85	0.57
2:4:160:LEU:O	2:4:163:ALA:N	2.37	0.57
2:4:306:PRO:HD3	43:g:149:HIS:C	2.29	0.57
10:A:466:LEU:HB3	10:A:500:ILE:HD11	1.86	0.57
11:B:273:VAL:O	11:B:275:ILE:HG13	2.05	0.57
13:D:172:GLY:O	13:D:174:ASP:N	2.38	0.57
30:V:90:ASN:ND2	30:V:123:GLU:O	2.37	0.57
52:s:53:ASP:OD2	52:s:55:THR:OG1	2.22	0.57
51:A2:37:VAL:C	51:A2:41:THR:HG23	2.23	0.57
56:A9:404:THR:O	56:A9:480:ARG:NH1	2.37	0.57
1:9:191:ASN:HB3	1:9:216:PRO:HB3	1.86	0.57
3:2:239:ILE:HG23	42:j:48:ILE:HA	1.84	0.57
8:1:316:PRO:HG3	30:V:57:ARG:NE	2.19	0.57
9:8:54:LYS:HA	9:8:136:HIS:CE1	2.38	0.57
12:C:128:PHE:CD2	12:C:178:VAL:HG23	2.40	0.57
26:R:329:LEU:HD12	26:R:330:PRO:HD2	1.86	0.57
31:W:80:LYS:HE2	31:W:142:GLN:HE22	1.68	0.57
37:c:115:GLU:HA	38:d:65:ARG:NH1	2.18	0.57
40:h:149:LEU:HD21	43:g:166:GLU:C	2.30	0.57
47:m:221:HIS:HB3	47:m:222:PRO:HD3	1.87	0.57
52:s:13:LEU:C	52:s:15:ASP:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:163:THR:HG22	1:9:170:THR:HB	1.86	0.57
2:4:16:TRP:CZ2	70:4:501:3PE:C2F	2.87	0.57
5:6:438:PRO:HB3	31:W:124:ASP:O	2.05	0.57
7:3:98:LEU:O	7:3:101:SER:OG	2.20	0.57
8:1:153:VAL:HA	8:1:156:MET:CE	2.35	0.57
10:A:320:GLU:CB	23:O:123:TYR:CE1	2.87	0.57
21:L:79:GLU:OE1	21:L:79:GLU:N	2.37	0.57
25:Q:49:GLU:OE2	25:Q:138:PRO:HD2	2.05	0.57
27:S:88:ASP:N	27:S:89:GLY:HA3	2.19	0.57
42:j:108:THR:O	42:j:111:GLU:HB3	2.04	0.57
45:k:426:GLY:HA2	45:k:428:ILE:H	1.70	0.57
47:m:221:HIS:O	47:m:225:THR:OG1	2.14	0.57
47:m:310:SER:OG	47:m:318:ARG:NH1	2.38	0.57
49:p:75:GLU:HG2	49:p:76:ILE:CA	2.35	0.57
45:w:366:VAL:HG11	46:x:43:PRO:HG2	1.87	0.57
49:A0:117:LEU:O	49:A0:118:ARG:C	2.47	0.57
2:4:111:THR:O	2:4:113:MET:N	2.35	0.57
3:2:84:TRP:CH2	6:5:59:MET:SD	2.98	0.57
5:6:312:LEU:HD11	5:6:395:ILE:HG21	1.87	0.57
71:6:701:CDL:H721	71:6:701:CDL:H542	1.87	0.57
10:A:218:LEU:HD21	10:A:413:LEU:HD21	1.87	0.57
24:P:108:GLN:OE1	24:P:108:GLN:N	2.35	0.57
28:T:62:THR:C	28:T:64:ALA:N	2.63	0.57
35:a:76:ILE:O	35:a:80:PHE:N	2.38	0.57
44:e:43:LYS:O	44:e:45:PRO:N	2.38	0.57
47:m:10:LEU:HB2	47:y:202:GLU:OE2	2.05	0.57
2:4:421:TYR:OH	35:a:59:VAL:HB	2.05	0.56
3:2:129:ILE:HG22	72:2:402:PC1:H372	1.87	0.56
4:7:117:PHE:CE1	6:5:6:MET:HE1	2.41	0.56
5:6:407:TRP:O	5:6:411:MET:N	2.31	0.56
71:6:701:CDL:H331	71:6:701:CDL:H712	1.85	0.56
8:1:70:MET:HE1	8:1:118:TRP:CG	2.40	0.56
9:8:116:ASN:ND2	73:8:501:FMN:HO3'	1.99	0.56
9:8:441:HIS:O	9:8:442:PHE:HD1	1.87	0.56
10:A:339:ALA:HB2	10:A:365:THR:HG23	1.87	0.56
11:B:458:PHE:C	11:B:460:GLU:N	2.63	0.56
13:D:86:THR:O	13:D:87:PHE:HD1	1.88	0.56
13:D:103:ARG:HH11	14:E:84:ILE:CD1	1.88	0.56
14:E:62:LEU:CG	30:V:36:PHE:CZ	2.86	0.56
23:O:33:ARG:CZ	31:M:44:SER:C	2.78	0.56
2:4:424:ASN:CB	35:a:57:ARG:NH2	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:455:LEU:HD23	2:4:456:GLY:O	2.05	0.56
3:2:210:ILE:HG12	72:2:402:PC1:C2F	2.35	0.56
5:6:97:THR:HA	5:6:100:ILE:HG22	1.87	0.56
5:6:285:THR:O	5:6:288:THR:OG1	2.22	0.56
6:5:37:MET:O	6:5:38:LEU:HB2	2.05	0.56
11:B:342:ARG:NH2	30:V:21:TYR:OH	2.38	0.56
14:E:80:GLU:O	24:P:25:GLN:NE2	2.38	0.56
23:O:26:ASN:O	23:O:30:ARG:N	2.36	0.56
26:R:155:VAL:HG12	26:R:159:ALA:HB2	1.86	0.56
26:R:266:VAL:HG12	26:R:267:GLY:O	2.05	0.56
27:S:280:HIS:O	27:S:283:ARG:N	2.39	0.56
28:T:139:PRO:HB2	36:b:158:ARG:O	2.05	0.56
63:A5:71:THR:O	63:A5:75:ARG:HD3	2.05	0.56
2:4:336:ARG:HH22	2:4:429:SER:HA	1.68	0.56
2:4:449:LEU:HB2	71:4:502:CDL:C33	2.35	0.56
5:6:313:MET:O	5:6:316:THR:OG1	2.21	0.56
5:6:359:MET:HB3	5:6:430:ALA:HA	1.87	0.56
9:8:281:HIS:HD2	9:8:357:MET:HA	1.69	0.56
10:A:301:ARG:HE	10:A:613:PRO:HG3	1.70	0.56
10:A:431:LEU:HD23	10:A:432:ILE:N	2.21	0.56
11:B:134:PRO:HB3	11:B:138:ARG:NH1	2.20	0.56
11:B:272:THR:O	11:B:273:VAL:HG13	2.06	0.56
23:O:44:PRO:O	23:O:47:VAL:HG12	2.05	0.56
25:Q:109:GLU:HG3	25:Q:110:CYS:N	2.19	0.56
27:S:219:SER:HA	27:S:222:LEU:HB2	1.88	0.56
42:j:116:PHE:CE1	43:g:157:ALA:CA	2.87	0.56
43:g:142:ARG:O	43:g:162:ARG:NH2	2.38	0.56
31:M:35:HIS:HA	31:M:71:MET:O	2.05	0.56
31:M:37:MET:HA	31:M:41:GLY:HA2	1.85	0.56
47:m:236:ILE:O	47:m:240:MET:N	2.25	0.56
47:m:240:MET:HA	47:m:243:VAL:HG12	1.87	0.56
48:o:73:GLY:O	48:o:79:GLU:HG2	2.06	0.56
49:p:126:ARG:O	49:p:130:PRO:N	2.38	0.56
50:q:105:GLU:O	50:q:109:LYS:NZ	2.35	0.56
47:y:221:HIS:HB3	47:y:222:PRO:HD3	1.87	0.56
52:B3:12:GLU:O	52:B3:13:LEU:HB2	2.05	0.56
53:A3:18:VAL:HB	53:A3:19:PRO:HD3	1.86	0.56
57:C4:189:PRO:HD2	64:B4:54:TYR:OH	2.05	0.56
62:A4:5:LYS:HD2	62:A4:6:GLY:N	2.21	0.56
3:2:51:ARG:O	3:2:55:ALA:N	2.38	0.56
5:6:274:GLN:O	5:6:277:THR:OG1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:64:LEU:O	6:5:67:ALA:N	2.39	0.56
27:S:197:VAL:HG11	27:S:226:GLU:OE2	2.06	0.56
28:T:33:GLY:HA3	28:T:63:ALA:HB3	1.88	0.56
28:T:101:LEU:CD2	28:T:110:ILE:CG2	2.83	0.56
47:m:1:MET:HG3	47:m:4:ILE:HB	1.88	0.56
47:m:214:ASP:HB3	51:r:8:THR:OG1	2.05	0.56
50:q:52:GLU:O	50:q:55:TYR:N	2.39	0.56
47:y:240:MET:HA	47:y:243:VAL:HG12	1.87	0.56
58:C2:203:PHE:O	58:C2:207:HIS:HD2	1.88	0.56
2:4:48:ASN:ND2	43:g:90:MET:SD	2.78	0.56
2:4:119:TYR:HA	2:4:122:PHE:HB3	1.86	0.56
5:6:42:TYR:O	5:6:46:THR:OG1	2.18	0.56
5:6:435:PRO:HG3	34:Z:57:PHE:CG	2.39	0.56
11:B:147:ASN:O	11:B:148:GLU:HB2	2.06	0.56
11:B:367:LYS:HZ1	14:E:212:ARG:C	2.11	0.56
11:B:378:LEU:O	11:B:382:PHE:N	2.33	0.56
12:C:149:THR:OG1	12:C:150:ASP:N	2.38	0.56
24:P:36:GLN:HB2	24:P:37:PRO:HD3	1.87	0.56
26:R:186:VAL:O	26:R:190:GLU:N	2.31	0.56
45:k:183:THR:HA	45:k:186:LEU:HD12	1.86	0.56
47:m:375:LYS:NZ	50:q:17:ARG:HH21	2.02	0.56
52:s:41:ASP:O	52:s:45:SER:N	2.31	0.56
47:y:257:THR:HA	48:z:115:TYR:OH	2.06	0.56
1:9:226:GLU:OE1	9:8:48:ARG:NE	2.38	0.56
5:6:119:LYS:NZ	71:6:701:CDL:C31	2.68	0.56
10:A:131:CYS:SG	74:A:801:SF4:S2	3.04	0.56
11:B:182:ASN:HD22	11:B:403:PRO:HB2	1.71	0.56
11:B:226:TYR:CE2	11:B:232:VAL:HG13	2.40	0.56
13:D:155:SER:O	13:D:161:GLY:N	2.36	0.56
25:Q:37:ASP:HA	25:Q:40:ASN:OD1	2.05	0.56
35:a:67:ARG:NH2	44:e:52:ALA:HB1	2.19	0.56
39:f:84:GLU:HA	39:f:91:TYR:HA	1.88	0.56
41:i:69:TYR:HE1	42:j:20:SER:O	1.75	0.56
43:g:13:PRO:O	43:g:116:ARG:NH2	2.37	0.56
48:o:5:LEU:HD11	52:s:63:HIS:HB2	1.87	0.56
46:x:310:SER:HB3	55:B1:57:GLY:N	2.19	0.56
47:y:310:SER:OG	47:y:318:ARG:NH1	2.38	0.56
48:z:178:THR:HG22	48:z:180:SER:H	1.71	0.56
1:9:55:PHE:HB2	1:9:60:TYR:CZ	2.41	0.56
4:7:54:LEU:HD12	8:1:100:LEU:HD11	1.88	0.56
8:1:236:ILE:O	8:1:236:ILE:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:8:501:FMN:O4'	73:8:501:FMN:O2'	2.22	0.56
10:A:61:PRO:HG3	10:A:146:PHE:CD2	2.40	0.56
10:A:359:ASN:ND2	20:K:68:ARG:NH1	2.54	0.56
10:A:362:ASP:CB	20:K:71:PHE:CD1	2.89	0.56
18:I:108:LYS:HA	18:I:108:LYS:HE3	1.85	0.56
20:K:40:ARG:HB3	20:K:44:LEU:HB2	1.87	0.56
26:R:180:TYR:N	26:R:317:ASP:OD2	2.38	0.56
27:S:202:VAL:HA	27:S:205:ARG:HB2	1.87	0.56
28:T:70:PHE:HZ	28:T:90:TYR:CZ	2.23	0.56
30:V:131:GLU:O	30:V:134:LEU:N	2.39	0.56
36:b:96:ALA:O	43:g:61:TYR:C	2.48	0.56
41:i:58:LEU:CD1	42:j:73:TYR:CD2	2.84	0.56
42:j:26:LEU:O	42:j:27:THR:HG22	2.05	0.56
45:k:110:VAL:O	45:k:114:ALA:N	2.25	0.56
47:m:309:THR:HG23	47:m:370:GLY:HA3	1.86	0.56
46:x:96:LEU:O	55:B1:70:LEU:HB2	2.06	0.56
77:y:401:HEM:HBB2	77:y:401:HEM:HMB1	1.88	0.56
57:C4:132:GLU:HB3	57:C4:137:GLU:HG3	1.87	0.56
2:4:385:THR:HG21	2:4:396:MET:HE1	1.88	0.56
3:2:233:THR:HG23	3:2:234:TRP:CD1	2.41	0.56
5:6:114:ILE:HD11	5:6:118:PHE:HE2	1.71	0.56
8:1:39:VAL:HG13	8:1:40:VAL:HG13	1.88	0.56
11:B:238:LEU:HD13	24:P:37:PRO:CD	2.31	0.56
11:B:264:ASN:ND2	14:E:68:ARG:NH2	2.53	0.56
21:L:22:SER:O	21:L:26:ALA:N	2.39	0.56
26:R:244:ASP:OD2	26:R:343:THR:HG23	2.05	0.56
29:U:71:LYS:NZ	29:U:76:ASP:OD2	2.36	0.56
35:a:79:ASN:HB3	44:e:73:GLY:CA	2.35	0.56
38:d:108:LEU:CB	44:e:166:LEU:HD22	2.26	0.56
31:M:37:MET:HG2	31:M:42:LEU:H	1.69	0.56
45:w:77:LYS:O	45:w:81:SER:OG	2.16	0.56
45:w:281:ASP:OD2	55:B1:73:PRO:HB3	2.05	0.56
48:z:80:MET:O	48:z:81:PHE:HB2	2.06	0.56
48:z:138:PRO:HG3	52:B3:58:LEU:HD22	1.88	0.56
52:B3:57:GLU:OE1	52:B3:57:GLU:N	2.37	0.56
53:A3:40:LEU:O	53:A3:41:ILE:CG1	2.54	0.56
56:A9:184:PHE:H	56:A9:256:HIS:HE1	1.52	0.56
2:4:150:LEU:C	2:4:152:TYR:H	2.14	0.56
3:2:87:MET:O	3:2:88:LYS:O	2.24	0.56
8:1:138:GLN:OE1	8:1:285:LEU:HD21	2.06	0.56
9:8:409:ILE:HG23	9:8:439:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:250:SER:O	10:A:251:ILE:HD13	2.06	0.56
10:A:355:LYS:CG	10:A:530:TYR:HE1	2.18	0.56
32:X:41:SER:OG	43:g:72:PRO:HD3	2.06	0.56
45:w:343:MET:HE1	45:w:416:TYR:HD2	1.69	0.56
48:z:12:TRP:HB2	48:z:15:ARG:HB2	1.87	0.56
48:z:241:LYS:NZ	50:A1:57:ASP:OD2	2.39	0.56
53:A3:15:ARG:CG	53:A3:16:ASN:H	2.17	0.56
60:C0:78:HIS:ND1	64:B4:12:LEU:HD22	2.21	0.56
3:2:338:PRO:HG2	42:j:83:TYR:OH	2.06	0.56
5:6:101:MET:HB3	5:6:118:PHE:HE1	1.71	0.56
5:6:603:ASN:O	5:6:606:GLU:N	2.27	0.56
19:J:39:ALA:H	30:V:144:THR:HG22	1.71	0.56
21:L:23:PHE:CE1	72:L:200:PC1:C2A	2.84	0.56
26:R:81:ILE:O	26:R:83:PRO:HD3	2.06	0.56
38:d:105:GLU:OE1	44:e:166:LEU:HG	2.05	0.56
45:k:77:LYS:O	45:k:81:SER:OG	2.16	0.56
47:m:91:PHE:O	47:m:94:LEU:N	2.39	0.56
45:w:211:LEU:C	45:w:213:GLN:HB2	2.31	0.56
46:x:74:SER:O	46:x:82:SER:OG	2.23	0.56
50:A1:52:GLU:O	50:A1:55:TYR:N	2.39	0.56
2:4:449:LEU:HB2	71:4:502:CDL:H332	1.88	0.55
11:B:124:ILE:HG22	11:B:124:ILE:O	2.06	0.55
11:B:301:ASP:O	11:B:301:ASP:OD1	2.23	0.55
11:B:430:ALA:O	11:B:433:ALA:N	2.39	0.55
21:L:23:PHE:CE1	72:L:200:PC1:C2B	2.89	0.55
28:T:69:ILE:CG2	28:T:100:ILE:CD1	2.78	0.55
43:g:162:ARG:HA	43:g:165:ALA:HB3	1.88	0.55
47:m:46:LEU:O	47:m:49:LEU:N	2.35	0.55
2:4:16:TRP:CZ2	70:4:501:3PE:C2E	2.89	0.55
8:1:311:THR:HG22	30:V:51:MET:HG3	1.88	0.55
13:D:191:GLU:HG2	14:E:173:PHE:CE1	2.41	0.55
28:T:90:TYR:CD2	28:T:126:LYS:HD2	2.40	0.55
45:k:131:ARG:HD3	45:k:175:ARG:HA	1.88	0.55
46:l:59:ASN:N	46:l:62:ASN:HB3	2.18	0.55
46:l:63:LEU:O	46:l:182:ARG:NE	2.36	0.55
48:o:3:LEU:HB2	52:s:59:LEU:HD13	1.88	0.55
47:y:172:LYS:O	47:y:175:LEU:N	2.30	0.55
47:y:309:THR:HG23	47:y:370:GLY:HA3	1.87	0.55
1:9:239:LYS:CE	9:8:42:PHE:HD1	2.18	0.55
2:4:364:LEU:HD21	2:4:369:LEU:HD12	1.88	0.55
5:6:428:PHE:O	5:6:432:LEU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:180:THR:HG23	10:A:183:ILE:HD12	1.87	0.55
11:B:254:ARG:CZ	24:P:24:LEU:HA	2.36	0.55
12:C:88:ILE:HG22	12:C:90:ILE:HG13	1.88	0.55
27:S:138:LEU:O	27:S:142:GLY:N	2.39	0.55
27:S:332:ASN:C	27:S:334:ASP:H	2.14	0.55
30:V:79:LYS:O	30:V:82:ARG:N	2.39	0.55
31:W:94:ASP:OD1	31:W:97:LYS:HB2	2.05	0.55
32:X:34:LEU:HD22	36:b:139:ILE:HG22	1.88	0.55
45:k:403:ASP:H	45:k:406:VAL:HB	1.72	0.55
48:o:178:THR:HG22	48:o:180:SER:H	1.71	0.55
49:p:73:LYS:HE2	49:p:108:GLN:H	1.71	0.55
1:9:176:CYS:C	9:8:159:ARG:HH12	2.14	0.55
3:2:127:GLY:HA3	3:2:129:ILE:H	1.71	0.55
3:2:247:THR:O	3:2:250:SER:N	2.40	0.55
5:6:25:ASN:O	5:6:26:THR:OG1	2.20	0.55
5:6:376:GLY:O	5:6:379:ALA:N	2.39	0.55
10:A:127:ASP:O	10:A:128:CYS:HB2	2.07	0.55
12:C:227:GLU:HG2	26:R:48:ARG:C	2.31	0.55
22:N:114:TRP:O	22:N:116:ILE:N	2.35	0.55
28:T:60:THR:C	28:T:62:THR:N	2.64	0.55
45:k:412:SER:O	54:u:15:ARG:NH2	2.40	0.55
53:A3:32:LEU:HA	53:A3:35:ALA:HB3	1.89	0.55
56:A9:95:PRO:HB2	58:C2:11:VAL:HG13	1.87	0.55
57:C4:111:THR:HG21	63:A5:66:ILE:HD11	1.88	0.55
3:2:4:ILE:HG13	72:S:401:PC1:H281	1.89	0.55
3:2:326:LEU:CD2	72:2:402:PC1:H2C2	2.36	0.55
5:6:502:LEU:HD22	34:Z:63:PHE:CD1	2.42	0.55
6:5:84:THR:O	11:B:75:THR:OG1	2.22	0.55
8:1:169:GLN:HE21	8:1:174:LEU:CB	2.19	0.55
10:A:367:CYS:SG	10:A:533:GLY:N	2.80	0.55
11:B:204:PHE:HE2	13:D:97:MET:HE2	1.71	0.55
13:D:162:TYR:CG	13:D:163:TYR:N	2.75	0.55
22:N:51:ILE:HD11	22:N:87:GLU:OE2	2.05	0.55
25:Q:124:ASP:CB	30:V:66:GLU:OE2	2.55	0.55
27:S:282:LEU:CB	27:S:288:ASP:H	2.19	0.55
37:c:95:TYR:HE2	43:g:10:TYR:CD1	2.20	0.55
38:d:105:GLU:CD	44:e:166:LEU:H	2.11	0.55
45:w:186:LEU:HD23	45:w:190:TYR:HE2	1.70	0.55
2:4:1:MET:HG2	2:4:2:LEU:N	2.17	0.55
2:4:115:LEU:HB2	2:4:174:LEU:HD13	1.87	0.55
2:4:348:LEU:O	2:4:349:GLN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:28:ASN:OD1	7:3:29:VAL:N	2.34	0.55
11:B:215:GLU:OE2	14:E:97:PHE:HD1	1.89	0.55
14:E:57:ALA:HB1	21:L:13:TRP:CD2	2.41	0.55
14:E:62:LEU:CD2	30:V:36:PHE:CZ	2.90	0.55
25:Q:124:ASP:HB3	30:V:66:GLU:OE2	2.07	0.55
26:R:55:VAL:HG12	26:R:56:ALA:N	2.21	0.55
26:R:72:HIS:CD2	26:R:75:ARG:HH12	2.25	0.55
28:T:40:SER:O	28:T:44:LYS:HB3	2.07	0.55
46:l:169:ARG:HG2	46:x:435:PHE:HE2	1.72	0.55
45:w:304:CYS:HA	45:w:326:CYS:HB3	1.88	0.55
45:w:433:ASP:OD2	47:y:223:TYR:OH	2.16	0.55
1:9:153:GLN:OE1	1:9:153:GLN:N	2.37	0.55
3:2:134:GLN:N	3:2:134:GLN:OE1	2.35	0.55
8:1:196:ALA:O	8:1:199:ASP:HB2	2.07	0.55
11:B:81:THR:HA	11:B:100:GLU:OE2	2.07	0.55
11:B:212:GLU:OE2	14:E:92:PRO:CG	2.54	0.55
14:E:52:SER:OG	14:E:56:ARG:NH1	2.39	0.55
25:Q:48:TRP:CH2	36:b:186:THR:N	2.73	0.55
32:X:37:PHE:CD2	36:b:137:MET:HB3	2.25	0.55
36:b:66:ARG:HG2	40:h:74:HIS:CE1	2.42	0.55
42:j:64:TYR:O	42:j:67:SER:N	2.39	0.55
53:t:12:GLN:NE2	50:A1:109:LYS:O	2.38	0.55
45:w:350:THR:HG23	53:A3:13:LEU:HD12	1.87	0.55
45:w:403:ASP:H	45:w:406:VAL:HB	1.72	0.55
46:x:325:TYR:HB3	55:B1:57:GLY:N	2.21	0.55
51:A2:28:HIS:HB3	51:A2:31:SER:OG	2.07	0.55
58:C2:42:LEU:HD13	65:C3:45:TYR:CD2	2.41	0.55
62:A4:5:LYS:HD2	62:A4:5:LYS:C	2.32	0.55
2:4:306:PRO:HD3	43:g:150:TYR:N	2.22	0.55
7:3:84:LEU:HD22	8:1:309:ILE:HD13	1.83	0.55
8:1:232:ILE:O	8:1:236:ILE:HG21	2.04	0.55
10:A:280:ASP:O	10:A:417:ARG:NH2	2.40	0.55
11:B:264:ASN:ND2	14:E:68:ARG:HH21	2.05	0.55
12:C:232:PHE:CA	13:D:165:TYR:CE1	2.90	0.55
22:N:86:ASN:O	22:N:89:SER:N	2.39	0.55
22:N:88:LEU:O	22:N:91:ALA:N	2.40	0.55
25:Q:47:ARG:NE	25:Q:53:PRO:HB3	2.22	0.55
35:a:67:ARG:HG2	44:e:35:ASP:HA	1.89	0.55
44:e:46:GLU:O	44:e:50:ALA:HB2	2.07	0.55
45:k:304:CYS:HA	45:k:326:CYS:HB3	1.88	0.55
50:q:9:SER:HA	50:q:12:TRP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:102:LEU:O	47:y:105:GLY:N	2.30	0.55
49:A0:100:HIS:CA	49:A0:130:PRO:HA	2.36	0.55
56:A9:69:MET:HE2	56:A9:70:VAL:CG2	2.36	0.55
1:9:222:ARG:NE	1:9:226:GLU:O	2.40	0.55
2:4:421:TYR:OH	35:a:59:VAL:HG12	2.06	0.55
3:2:24:SER:O	3:2:85:THR:HA	2.07	0.55
5:6:373:LEU:HD12	5:6:431:LEU:HD11	1.88	0.55
8:1:105:MET:O	8:1:109:SER:N	2.33	0.55
10:A:146:PHE:N	10:A:146:PHE:HD1	2.04	0.55
10:A:266:ARG:HG3	10:A:267:THR:HG23	1.88	0.55
23:O:33:ARG:NH1	31:M:48:VAL:HG21	1.99	0.55
23:O:43:VAL:HG11	23:O:59:GLY:HA3	1.89	0.55
25:Q:141:PRO:HG2	25:Q:144:SER:HB3	1.88	0.55
31:W:81:ASP:O	31:W:85:TYR:N	2.40	0.55
42:j:114:GLU:N	43:g:160:LYS:CD	2.69	0.55
48:o:217:PRO:O	48:o:221:ALA:N	2.40	0.55
45:w:277:ILE:O	45:w:292:SER:OG	2.25	0.55
56:A9:407:ASP:O	56:A9:411:LYS:HG3	2.07	0.55
2:4:2:LEU:CD2	72:4:504:PC1:C14	2.84	0.55
3:2:84:TRP:H	3:2:84:TRP:HD1	1.55	0.55
3:2:234:TRP:NE1	3:2:303:THR:OG1	2.40	0.55
5:6:467:ILE:HD12	38:d:77:PHE:CZ	2.37	0.55
8:1:159:SER:HB3	8:1:317:GLN:CG	2.37	0.55
8:1:264:LEU:HG	8:1:264:LEU:O	2.07	0.55
10:A:221:ASN:OD1	10:A:291:ARG:NH2	2.40	0.55
10:A:260:ASN:H	10:A:282:ASN:HD22	1.54	0.55
11:B:203:MET:O	11:B:206:GLU:N	2.35	0.55
28:T:33:GLY:HA3	28:T:63:ALA:CB	2.37	0.55
37:c:28:LEU:HG	37:c:30:PRO:HD2	1.88	0.55
42:j:62:LEU:HG	42:j:63:LEU:H	1.72	0.55
45:k:277:ILE:O	45:k:292:SER:OG	2.24	0.55
46:l:201:SER:OG	46:l:224:LEU:O	2.16	0.55
54:u:56:LYS:HG2	54:u:60:GLU:HB3	1.88	0.55
46:x:201:SER:OG	46:x:224:LEU:O	2.16	0.55
47:y:17:ALA:HB1	47:y:201:HIS:CE1	2.42	0.55
5:6:152:PHE:CD1	5:6:168:ALA:HB1	2.41	0.54
5:6:408:ALA:HA	5:6:411:MET:HB3	1.87	0.54
5:6:581:LYS:HB3	6:5:96:LEU:HD21	1.88	0.54
10:A:355:LYS:CA	10:A:530:TYR:OH	2.55	0.54
11:B:61:TRP:CE2	11:B:62:LYS:O	2.60	0.54
70:B:501:3PE:H232	14:E:63:TRP:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:335:VAL:O	42:j:52:PRO:CG	2.54	0.54
28:T:9:TYR:CD1	28:T:9:TYR:C	2.85	0.54
28:T:89:ASN:O	28:T:92:ILE:N	2.35	0.54
40:h:149:LEU:CD2	43:g:166:GLU:C	2.80	0.54
77:m:401:HEM:HBB2	77:m:401:HEM:HMB1	1.88	0.54
45:w:39:VAL:HG23	45:w:113:LEU:HD21	1.89	0.54
45:w:131:ARG:HD3	45:w:175:ARG:HA	1.88	0.54
50:A1:35:ASP:OD2	50:A1:61:ARG:NH2	2.35	0.54
2:4:227:GLY:HA2	2:4:230:VAL:HB	1.89	0.54
71:4:502:CDL:H671	5:6:23:SER:O	2.06	0.54
3:2:5:ILE:O	3:2:8:ILE:N	2.40	0.54
5:6:37:LYS:HD2	5:6:102:GLU:HG3	1.88	0.54
10:A:69:LEU:O	16:G:158:LYS:NZ	2.23	0.54
11:B:385:TYR:HD1	14:E:122:VAL:HG11	1.71	0.54
11:B:460:GLU:CD	11:B:460:GLU:C	2.75	0.54
12:C:171:GLU:OE1	12:C:172:ILE:HG13	2.07	0.54
31:W:115:GLN:HE21	31:W:135:ALA:C	2.15	0.54
40:h:149:LEU:HD21	43:g:166:GLU:O	2.07	0.54
31:M:14:ARG:HA	31:M:17:TYR:CE2	2.43	0.54
47:m:17:ALA:HB1	47:m:201:HIS:CE1	2.42	0.54
49:p:82:PRO:O	49:p:134:ILE:HA	2.07	0.54
49:p:107:ASP:HA	49:p:108:GLN:C	2.33	0.54
45:w:159:GLN:NE2	45:w:237:THR:HG21	2.23	0.54
47:y:237:LEU:O	47:y:241:LEU:N	2.38	0.54
48:z:71:GLN:HG3	48:z:72:ASP:CG	2.33	0.54
49:A0:150:ALA:H	49:A0:155:GLY:HA3	1.62	0.54
53:A3:37:ASP:OD2	53:A3:40:LEU:HA	2.06	0.54
54:B2:56:LYS:HG2	54:B2:60:GLU:HB3	1.88	0.54
1:9:228:ALA:HB3	9:8:284:ASN:HD22	1.71	0.54
2:4:248:LEU:HD11	43:g:151:SER:N	2.21	0.54
3:2:9:ILE:O	3:2:12:THR:HG22	2.07	0.54
3:2:118:VAL:O	3:2:122:ILE:HG13	2.08	0.54
9:8:398:ARG:HG3	9:8:403:ASP:OD2	2.08	0.54
10:A:176:CYS:HA	74:A:802:SF4:S4	2.48	0.54
11:B:152:SER:OG	11:B:228:ARG:O	2.22	0.54
11:B:163:PRO:HB2	11:B:167:ALA:HB3	1.90	0.54
11:B:205:GLU:OE2	14:E:82:ALA:HB1	2.07	0.54
13:D:146:GLU:HB3	13:D:147:PRO:CD	2.38	0.54
24:P:45:PRO:O	24:P:46:SER:OG	2.23	0.54
36:b:67:PHE:O	36:b:68:LEU:HB2	2.06	0.54
37:c:5:THR:HG22	37:c:7:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:138:MET:HE2	47:m:255:ASN:HD22	1.72	0.54
77:m:401:HEM:HBC2	77:m:401:HEM:HMC1	1.89	0.54
50:q:16:ILE:O	50:q:20:TYR:HB3	2.02	0.54
58:C2:151:LEU:HB2	58:C2:159:MET:HG3	1.89	0.54
1:9:123:ASN:HD22	1:9:127:VAL:CG1	2.20	0.54
5:6:48:MET:O	5:6:51:THR:OG1	2.23	0.54
7:3:106:TRP:CH2	72:L:200:PC1:H143	2.42	0.54
10:A:456:ALA:O	10:A:499:LYS:NZ	2.40	0.54
11:B:266:ARG:NH2	14:E:66:LEU:HB3	2.23	0.54
11:B:322:SER:HB3	14:E:42:ASN:C	2.33	0.54
25:Q:28:ALA:O	25:Q:30:HIS:N	2.41	0.54
27:S:333:GLU:C	27:S:335:VAL:H	2.15	0.54
28:T:2:ALA:C	28:T:4:THR:H	2.14	0.54
28:T:59:TYR:C	28:T:59:TYR:CD1	2.84	0.54
46:x:304:HIS:HB3	46:x:305:GLN:OE1	2.07	0.54
64:B4:63:MET:HB3	64:B4:68:ILE:HD11	1.89	0.54
2:4:446:LEU:HG	71:4:502:CDL:H342	1.89	0.54
2:4:449:LEU:CD1	71:4:502:CDL:C31	2.86	0.54
3:2:175:LEU:HG	3:2:224:THR:O	2.08	0.54
8:1:146:LEU:HD11	8:1:185:TRP:HZ3	1.72	0.54
8:1:253:GLU:CG	8:1:254:LEU:N	2.71	0.54
9:8:151:ALA:O	9:8:191:TYR:OH	2.21	0.54
11:B:190:HIS:ND1	11:B:452:GLY:HA3	2.23	0.54
35:a:51:TYR:HD1	35:a:56:ARG:HH12	1.55	0.54
39:f:104:LEU:CA	39:f:107:TRP:HE1	2.18	0.54
45:k:57:TYR:CD2	45:k:168:GLU:HG2	2.43	0.54
46:l:160:ILE:O	46:l:163:LEU:N	2.40	0.54
46:l:182:ARG:HD2	46:l:185:LYS:HD3	1.90	0.54
49:p:91:TRP:C	49:p:93:GLY:H	2.14	0.54
46:x:305:GLN:OE1	46:x:305:GLN:N	2.40	0.54
47:y:1:MET:HG3	47:y:4:ILE:HB	1.88	0.54
2:4:209:LEU:HD22	2:4:265:SER:HB3	1.90	0.54
2:4:359:TRP:HB3	2:4:411:LEU:HD22	1.89	0.54
3:2:278:LEU:HD12	28:T:136:PHE:CE1	2.42	0.54
4:7:170:GLU:O	4:7:172:THR:OG1	2.26	0.54
5:6:587:TYR:O	5:6:590:SER:N	2.37	0.54
6:5:20:LEU:O	6:5:29:SER:HB2	2.07	0.54
8:1:143:GLU:OE1	8:1:143:GLU:N	2.41	0.54
9:8:159:ARG:HG2	9:8:161:GLU:H	1.71	0.54
11:B:168:GLN:O	11:B:171:ARG:N	2.40	0.54
25:Q:105:ALA:O	25:Q:109:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:190:HIS:HB2	27:S:277:ARG:NE	2.23	0.54
28:T:66:ILE:HA	28:T:69:ILE:HG21	1.90	0.54
28:T:124:LEU:O	28:T:128:GLY:N	2.38	0.54
31:W:89:LEU:HD21	34:Z:47:ARG:CA	2.37	0.54
49:p:71:MET:O	49:p:72:SER:OG	2.15	0.54
51:r:48:VAL:O	51:r:51:PRO:HD2	2.08	0.54
47:y:91:PHE:O	47:y:94:LEU:N	2.39	0.54
47:y:138:MET:HE2	47:y:255:ASN:HD22	1.72	0.54
1:9:62:ARG:HG2	15:F:90:LEU:CB	2.38	0.54
1:9:130:TYR:CZ	1:9:208:LEU:HD11	2.43	0.54
3:2:311:MET:HB3	3:2:313:MET:HE3	1.89	0.54
5:6:582:GLY:N	6:5:96:LEU:CD1	2.71	0.54
9:8:103:ASN:HD22	9:8:149:MET:HE1	1.72	0.54
10:A:374:THR:OG1	10:A:377:ALA:O	2.23	0.54
11:B:215:GLU:CD	14:E:97:PHE:CD1	2.85	0.54
23:O:126:HIS:CE1	26:R:43:HIS:ND1	2.75	0.54
25:Q:158:LEU:C	25:Q:159:LYS:CG	2.79	0.54
27:S:291:GLU:OE1	27:S:291:GLU:N	2.40	0.54
28:T:22:THR:HG22	28:T:75:CYS:HG	1.71	0.54
31:W:123:GLU:HB2	31:W:130:ILE:HD12	1.90	0.54
46:x:182:ARG:HD2	46:x:185:LYS:HD3	1.90	0.54
49:A0:155:GLY:C	49:A0:157:TYR:H	2.15	0.54
57:C4:165:VAL:HB	57:C4:170:LEU:HD12	1.90	0.54
59:A7:108:PRO:HG2	59:A7:111:PHE:CE2	2.42	0.54
61:A6:55:LYS:HA	61:A6:74:LEU:O	2.08	0.54
3:2:322:LYS:HD2	70:2:401:3PE:C2D	2.29	0.54
4:7:33:LEU:O	4:7:36:SER:N	2.40	0.54
5:6:555:LEU:HD22	35:a:73:SER:O	2.08	0.54
5:6:598:SER:O	5:6:604:PHE:HD2	1.91	0.54
10:A:143:SER:O	10:A:143:SER:OG	2.19	0.54
10:A:320:GLU:OE1	23:O:123:TYR:OH	2.26	0.54
10:A:560:LEU:HD12	10:A:561:PRO:HD2	1.90	0.54
11:B:198:THR:OG1	11:B:199:PRO:HD3	2.08	0.54
14:E:57:ALA:CB	21:L:13:TRP:CD2	2.90	0.54
49:p:109:GLU:HA	49:p:110:ALA:C	2.32	0.54
50:q:87:LYS:HG3	50:q:89:TYR:HD2	1.73	0.54
45:w:57:TYR:CD2	45:w:168:GLU:HG2	2.43	0.54
50:A1:12:TRP:C	50:A1:12:TRP:CD2	2.85	0.54
59:A7:52:SER:OG	59:A7:55:GLU:HG3	2.08	0.54
61:A6:48:LEU:O	61:A6:50:PRO:HD3	2.08	0.54
3:2:112:HIS:O	3:2:112:HIS:ND1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:560:ALA:HA	35:a:77:TYR:HE1	1.73	0.54
14:E:61:LEU:CD2	21:L:17:PRO:O	2.55	0.54
22:N:93:LYS:O	22:N:96:GLN:N	2.33	0.54
45:k:159:GLN:NE2	45:k:237:THR:HG21	2.23	0.54
46:l:65:THR:HG23	46:l:191:LEU:HD23	1.90	0.54
47:m:375:LYS:HZ1	50:q:17:ARG:HH21	1.53	0.54
48:o:27:ARG:O	48:o:31:GLN:HG2	2.08	0.54
49:p:143:GLY:O	49:p:146:PRO:N	2.41	0.54
50:q:110:LYS:HE3	53:A3:11:ARG:HB3	1.89	0.54
49:A0:70:ALA:O	49:A0:74:ILE:CD1	2.55	0.54
60:C0:41:LEU:O	60:C0:41:LEU:HD12	2.08	0.54
61:A6:82:CYS:N	61:A6:86:GLY:O	2.41	0.54
2:4:423:ILE:HB	35:a:57:ARG:CB	2.33	0.54
3:2:280:THR:O	3:2:284:ILE:N	2.33	0.54
4:7:81:GLU:OE2	4:7:86:ASN:ND2	2.40	0.54
5:6:132:VAL:HG23	5:6:133:THR:HG23	1.89	0.54
8:1:190:LEU:HD12	8:1:195:ARG:HB2	1.90	0.54
8:1:266:LEU:HD12	8:1:266:LEU:C	2.33	0.54
9:8:210:THR:HG22	9:8:224:ARG:HB2	1.89	0.54
10:A:183:ILE:HD11	10:A:206:VAL:HG13	1.90	0.54
10:A:394:VAL:HG11	10:A:418:ILE:HD13	1.89	0.54
11:B:250:ASN:HB3	11:B:254:ARG:NH2	2.23	0.54
12:C:212:LEU:HD21	13:D:176:ILE:HD11	1.82	0.54
12:C:213:ARG:HH11	12:C:224:GLU:CD	2.15	0.54
13:D:99:MET:HE3	13:D:106:MET:HG2	1.89	0.54
14:E:118:LEU:C	14:E:120:GLU:N	2.62	0.54
14:E:128:ILE:CD1	14:E:147:ILE:HG12	2.38	0.54
20:K:23:LEU:HA	20:K:63:PRO:HB3	1.89	0.54
24:P:19:ASP:C	24:P:21:GLN:H	2.16	0.54
27:S:124:TYR:OH	27:S:182:THR:HG21	2.08	0.54
32:X:30:ASN:OD1	32:X:31:ASP:N	2.41	0.54
31:M:29:LYS:HE2	31:M:39:ASP:OD1	2.07	0.54
45:k:42:ASP:HB3	45:k:384:LEU:HD23	1.89	0.54
46:x:160:ILE:O	46:x:163:LEU:N	2.41	0.54
49:A0:30:GLU:OE2	54:B2:10:TYR:HD2	1.91	0.54
57:C4:136:LEU:HB3	57:C4:193:TYR:HD2	1.73	0.54
1:9:238:PRO:HG2	1:9:241:PRO:HG3	1.89	0.53
2:4:359:TRP:HB3	2:4:411:LEU:CD2	2.38	0.53
2:4:360:LEU:HD13	71:6:701:CDL:H532	1.89	0.53
3:2:217:THR:CG2	72:2:402:PC1:H252	2.38	0.53
5:6:467:ILE:CD1	38:d:77:PHE:HZ	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:355:LYS:HD2	10:A:530:TYR:CD1	2.36	0.53
11:B:215:GLU:HG3	14:E:97:PHE:HD1	1.73	0.53
28:T:70:PHE:CD1	28:T:70:PHE:C	2.85	0.53
42:j:78:ARG:O	42:j:81:TYR:HB3	2.08	0.53
44:e:37:LEU:H	44:e:77:LYS:HD3	1.72	0.53
31:M:51:ILE:HD12	31:M:70:LEU:HD12	1.91	0.53
46:l:153:GLN:O	46:l:155:PRO:HD3	2.09	0.53
48:o:55:CYS:SG	54:u:52:TRP:HB3	2.47	0.53
45:w:42:ASP:HB3	45:w:384:LEU:HD23	1.89	0.53
47:y:256:TYR:HB2	48:z:115:TYR:CE1	2.43	0.53
48:z:217:PRO:O	48:z:221:ALA:N	2.40	0.53
62:A4:2:SER:OG	62:A4:3:ALA:N	2.41	0.53
1:9:155:LYS:HE2	1:9:205:ILE:HD13	1.89	0.53
2:4:198:ALA:HB1	70:4:503:3PE:H271	1.88	0.53
2:4:449:LEU:HD12	71:4:502:CDL:C33	2.39	0.53
3:2:294:MET:O	3:2:295:ARG:HB3	2.08	0.53
5:6:232:TRP:CE3	5:6:233:LEU:HD12	2.44	0.53
5:6:546:GLN:O	5:6:550:SER:N	2.40	0.53
5:6:592:LEU:HA	5:6:595:ILE:HG22	1.89	0.53
8:1:172:MET:HE2	8:1:176:LEU:CD1	2.01	0.53
10:A:138:ASP:O	10:A:139:LEU:HD23	2.07	0.53
11:B:266:ARG:HH12	14:E:63:TRP:HD1	1.52	0.53
14:E:155:CYS:HB2	14:E:157:PHE:H	1.73	0.53
25:Q:8:PRO:O	30:V:88:ARG:CZ	2.56	0.53
28:T:95:CYS:HA	28:T:115:CYS:HA	1.89	0.53
35:a:67:ARG:HD2	44:e:79:PRO:CD	2.38	0.53
36:b:76:LEU:O	36:b:79:GLY:N	2.41	0.53
36:b:163:ARG:HB3	36:b:165:ASP:HB2	1.90	0.53
40:h:85:TRP:HA	40:h:88:ARG:HH11	1.72	0.53
45:k:39:VAL:HG23	45:k:113:LEU:HD21	1.89	0.53
45:k:159:GLN:OE1	49:p:7:VAL:HG11	2.08	0.53
51:r:28:HIS:HB3	51:r:31:SER:OG	2.07	0.53
46:x:65:THR:HG23	46:x:191:LEU:HD23	1.90	0.53
77:y:401:HEM:HBC2	77:y:401:HEM:HMC1	1.90	0.53
2:4:179:LEU:O	2:4:180:GLN:NE2	2.41	0.53
5:6:120:TYR:HE1	71:6:701:CDL:H541	1.73	0.53
6:5:79:VAL:O	6:5:83:ASN:N	2.36	0.53
7:3:88:LEU:CD2	8:1:309:ILE:HD12	2.38	0.53
8:1:84:THR:O	8:1:87:ILE:HG13	2.08	0.53
9:8:98:LYS:HG3	9:8:99:TRP:HD1	1.72	0.53
11:B:217:VAL:HG13	11:B:218:SER:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:390:GLN:O	24:P:60:ARG:HD2	2.08	0.53
12:C:129:GLU:O	12:C:130:ILE:HD13	2.09	0.53
13:D:90:ALA:HB3	13:D:127:GLY:HA2	1.91	0.53
38:d:108:LEU:CB	44:e:166:LEU:CD1	2.86	0.53
47:m:36:LEU:HD21	47:m:232:ALA:HA	1.91	0.53
50:q:53:ASN:OD1	50:q:54:LEU:N	2.41	0.53
52:s:13:LEU:O	52:s:15:ASP:N	2.41	0.53
45:w:213:GLN:OE1	45:w:214:LYS:HE2	2.07	0.53
47:y:62:ALA:O	47:y:65:SER:OG	2.25	0.53
48:z:27:ARG:O	48:z:31:GLN:HG2	2.08	0.53
49:A0:187:PHE:C	49:A0:193:VAL:CB	2.81	0.53
58:C2:156:ARG:HG3	58:C2:156:ARG:NH1	2.23	0.53
1:9:71:PRO:HA	15:F:102:SER:OG	2.06	0.53
3:2:84:TRP:CD1	3:2:84:TRP:N	2.77	0.53
3:2:190:MET:HB2	3:2:201:THR:HG23	1.90	0.53
3:2:217:THR:CG2	72:2:402:PC1:C26	2.86	0.53
3:2:239:ILE:HG21	42:j:47:ALA:C	2.31	0.53
5:6:176:ARG:O	5:6:179:ASP:HB3	2.08	0.53
5:6:305:SER:O	5:6:309:GLN:HG2	2.09	0.53
7:3:87:MET:O	7:3:91:ALA:N	2.25	0.53
8:1:284:GLN:O	8:1:288:LEU:HD23	2.08	0.53
10:A:587:ALA:HB1	10:A:591:GLU:HB2	1.89	0.53
11:B:305:THR:HG23	11:B:306:GLN:HG2	1.90	0.53
12:C:208:GLY:N	13:D:167:TYR:HA	2.22	0.53
14:E:114:ILE:O	14:E:114:ILE:HG13	2.08	0.53
28:T:69:ILE:HD11	28:T:96:ALA:CB	2.37	0.53
45:w:412:SER:HB3	54:B2:15:ARG:NH2	2.23	0.53
49:A0:81:ILE:CB	49:A0:86:ASN:HA	2.38	0.53
63:A5:75:ARG:HG2	63:A5:75:ARG:NH1	2.19	0.53
1:9:55:PHE:HA	1:9:89:GLN:HE22	1.73	0.53
3:2:80:PHE:HB3	17:H:64:ARG:NH1	2.23	0.53
5:6:504:ILE:O	5:6:508:THR:N	2.41	0.53
5:6:577:VAL:CG1	6:5:97:GLN:HE22	2.19	0.53
9:8:206:CYS:O	73:8:501:FMN:C9A	2.57	0.53
10:A:152:ARG:HG3	10:A:152:ARG:O	2.07	0.53
10:A:611:THR:HG21	16:G:105:GLU:HA	1.90	0.53
11:B:421:ARG:HG3	12:C:119:VAL:HG22	1.89	0.53
14:E:86:TYR:OH	14:E:90:LYS:NZ	2.42	0.53
25:Q:51:LYS:HZ1	36:b:189:ASN:HD21	1.57	0.53
37:c:77:ILE:HB	37:c:78:PRO:HD3	1.91	0.53
39:f:163:LEU:CB	39:f:166:LEU:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:114:GLU:H	43:g:160:LYS:CD	2.18	0.53
51:r:71:ARG:HH21	52:s:60:ASP:CG	2.15	0.53
46:x:63:LEU:O	46:x:182:ARG:NE	2.36	0.53
46:x:385:GLN:O	46:x:389:ALA:N	2.38	0.53
58:C2:222:GLN:HA	58:C2:222:GLN:HE21	1.72	0.53
1:9:72:GLU:H	15:F:102:SER:HB3	1.74	0.53
3:2:21:MET:HG2	3:2:140:SER:HB2	1.90	0.53
3:2:100:MET:HE1	5:6:598:SER:HB2	1.91	0.53
3:2:127:GLY:CA	3:2:129:ILE:H	2.22	0.53
7:3:68:GLU:HA	7:3:71:LEU:HB2	1.90	0.53
11:B:294:ARG:HH21	11:B:301:ASP:HB3	1.73	0.53
12:C:179:PHE:CE1	23:O:84:ILE:HG21	2.43	0.53
13:D:106:MET:HE3	13:D:111:VAL:HB	1.91	0.53
13:D:184:PRO:HB3	14:E:183:LEU:HD13	1.90	0.53
21:L:56:PRO:HB2	25:Q:129:THR:C	2.29	0.53
39:f:16:VAL:O	39:f:20:TYR:N	2.33	0.53
39:f:61:THR:O	39:f:65:ARG:N	2.36	0.53
42:j:119:VAL:HG23	43:g:147:GLY:O	2.08	0.53
45:k:229:PRO:HG2	45:k:231:LEU:HB2	1.91	0.53
50:A1:53:ASN:OD1	50:A1:54:LEU:N	2.41	0.53
52:B3:31:VAL:O	52:B3:35:GLU:HG3	2.09	0.53
57:C4:203:ASN:HD22	57:C4:206:PHE:HD2	1.55	0.53
1:9:113:TYR:CE2	10:A:210:ILE:HG23	2.44	0.53
2:4:93:LYS:O	2:4:97:THR:HG23	2.09	0.53
2:4:226:ALA:HA	2:4:331:ASN:ND2	2.24	0.53
8:1:46:LEU:HG	8:1:49:ILE:HD11	1.91	0.53
8:1:283:ASP:O	8:1:285:LEU:N	2.42	0.53
10:A:464:GLN:HA	10:A:467:GLN:HB3	1.90	0.53
25:Q:39:PRO:O	25:Q:43:PHE:N	2.41	0.53
27:S:333:GLU:CB	42:j:52:PRO:CG	2.52	0.53
28:T:30:GLY:CA	28:T:64:ALA:CA	2.87	0.53
43:g:14:PRO:O	43:g:116:ARG:NH2	2.41	0.53
47:m:34:GLY:HA3	77:m:402:HEM:HBA2	1.90	0.53
46:x:153:GLN:O	46:x:155:PRO:HD3	2.08	0.53
47:y:34:GLY:HA3	77:y:402:HEM:HBA2	1.90	0.53
47:y:236:ILE:O	47:y:240:MET:N	2.25	0.53
47:y:377:LEU:HD11	50:A1:20:TYR:HE2	1.73	0.53
51:A2:48:VAL:O	51:A2:51:PRO:HD2	2.08	0.53
51:A2:79:ASN:HB3	52:B3:52:GLU:HB2	1.89	0.53
59:A7:67:SER:OG	59:A7:70:GLU:HG3	2.08	0.53
4:7:80:PRO:HG2	8:1:121:TRP:HZ2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:560:ALA:HA	35:a:77:TYR:CE1	2.44	0.53
8:1:153:VAL:HG23	8:1:154:LEU:HD12	1.90	0.53
8:1:296:LEU:HD11	70:B:501:3PE:H351	1.91	0.53
10:A:72:ALA:O	69:A:803:FES:S1	2.66	0.53
11:B:234:GLN:OE1	14:E:212:ARG:HD3	2.09	0.53
11:B:286:TYR:OH	11:B:437:LYS:HD2	2.08	0.53
12:C:123:THR:CG2	16:G:129:SER:H	2.18	0.53
17:H:72:THR:OG1	30:V:110:VAL:HG11	2.09	0.53
24:P:40:LYS:N	30:V:7:LYS:N	2.56	0.53
26:R:354:ARG:O	26:R:355:ARG:NH2	2.37	0.53
28:T:34:LEU:O	28:T:35:VAL:C	2.52	0.53
30:V:32:GLY:O	30:V:33:TYR:HB3	2.09	0.53
37:c:7:GLU:OE2	39:f:155:PRO:HG3	2.09	0.53
47:m:237:LEU:O	47:m:241:LEU:N	2.38	0.53
45:w:142:ASP:OD1	49:A0:1:SER:N	2.41	0.53
46:x:59:ASN:N	46:x:62:ASN:HB3	2.18	0.53
52:B3:13:LEU:O	52:B3:15:ASP:N	2.41	0.53
52:B3:53:ASP:OD2	52:B3:55:THR:OG1	2.22	0.53
59:A7:40:LEU:HD13	59:A7:59:LEU:HD13	1.90	0.53
3:2:265:MET:HE2	3:2:341:PRO:HG2	1.90	0.53
5:6:255:ALA:HA	5:6:258:PHE:HB3	1.90	0.53
11:B:62:LYS:O	11:B:64:PRO:HD3	2.09	0.53
11:B:171:ARG:HH21	11:B:231:GLY:HA2	1.74	0.53
25:Q:110:CYS:HB2	25:Q:114:LYS:HB2	1.91	0.53
26:R:148:ILE:HB	26:R:149:PRO:HD3	1.91	0.53
45:k:327:ASP:OD1	45:k:328:HIS:ND1	2.41	0.53
47:y:36:LEU:HD21	47:y:232:ALA:HA	1.91	0.53
50:A1:87:LYS:HG3	50:A1:89:TYR:HD2	1.73	0.53
5:6:335:PHE:HE2	5:6:383:MET:HE1	1.74	0.53
5:6:358:LYS:HA	5:6:436:ARG:HG3	1.91	0.53
9:8:297:LYS:NZ	9:8:310:GLY:O	2.41	0.53
9:8:375:LYS:HD3	9:8:393:ASN:HD22	1.74	0.53
10:A:566:ILE:HD11	10:A:580:ALA:HA	1.90	0.53
11:B:294:ARG:HH21	11:B:301:ASP:CB	2.21	0.53
12:C:90:ILE:HD12	12:C:145:VAL:HG13	1.91	0.53
12:C:127:ARG:NH1	16:G:137:PHE:CZ	2.77	0.53
12:C:213:ARG:HD3	12:C:224:GLU:OE1	2.09	0.53
17:H:82:GLN:NE2	30:V:98:MET:HB2	2.19	0.53
21:L:65:ASP:HB3	21:L:74:GLN:O	2.09	0.53
23:O:33:ARG:NH2	31:M:44:SER:C	2.64	0.53
25:Q:52:ASP:CG	30:V:116:TRP:HB2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:92:LEU:HB2	27:S:93:PRO:HD2	1.90	0.53
31:M:12:LYS:HZ2	31:M:77:VAL:HG21	1.73	0.53
45:w:327:ASP:OD1	45:w:328:HIS:ND1	2.41	0.53
2:4:451:PRO:HG2	5:6:69:LEU:HD23	1.90	0.52
3:2:85:THR:HG22	17:H:19:THR:HG23	1.90	0.52
4:7:17:PHE:HE2	6:5:11:ALA:HB1	1.74	0.52
4:7:94:VAL:O	4:7:97:LEU:N	2.42	0.52
8:1:8:MET:O	8:1:12:PRO:CD	2.57	0.52
8:1:35:LYS:HZ3	14:E:85:ASN:HD21	1.56	0.52
8:1:126:LYS:HD3	8:1:129:LEU:HD23	1.90	0.52
9:8:207:GLY:CA	73:8:501:FMN:C6	2.82	0.52
11:B:256:ASP:O	11:B:256:ASP:OD1	2.27	0.52
11:B:404:LYS:HE2	11:B:455:ASP:OD2	2.09	0.52
17:H:56:CYS:C	17:H:58:ILE:H	2.17	0.52
25:Q:132:LYS:HE3	25:Q:134:ASP:OD1	2.08	0.52
40:h:79:ASP:H	40:h:83:ASP:CG	2.17	0.52
46:l:244:ILE:O	46:l:425:ALA:HA	2.09	0.52
46:l:385:GLN:O	46:l:389:ALA:N	2.38	0.52
47:m:137:GLN:HE21	47:m:141:TRP:CD1	2.27	0.52
49:p:1:SER:OG	49:p:2:HIS:N	2.41	0.52
46:x:244:ILE:O	46:x:425:ALA:HA	2.09	0.52
47:y:267:HIS:NE2	47:y:269:LYS:HD3	2.25	0.52
49:A0:36:SER:O	49:A0:39:VAL:N	2.38	0.52
49:A0:110:ALA:HB3	49:A0:123:ASP:HA	1.90	0.52
59:A7:128:VAL:O	59:A7:134:PHE:HB3	2.09	0.52
62:A4:8:HIS:O	62:A4:10:GLY:N	2.42	0.52
71:4:502:CDL:H673	5:6:23:SER:OG	2.09	0.52
5:6:437:PHE:O	34:Z:52:ARG:NH2	2.42	0.52
9:8:93:PHE:HE2	9:8:98:LYS:HB3	1.73	0.52
11:B:127:LYS:HB2	11:B:132:ALA:HB2	1.91	0.52
12:C:63:PHE:CD2	24:P:97:PRO:HG3	2.44	0.52
34:Z:63:PHE:CG	34:Z:64:VAL:N	2.78	0.52
35:a:125:PHE:HB3	43:g:133:THR:HG22	1.91	0.52
38:d:40:VAL:HG12	38:d:41:ALA:H	1.73	0.52
39:f:14:GLN:HB2	39:f:17:LEU:HD12	1.90	0.52
45:k:366:VAL:HG11	46:l:43:PRO:HG2	1.90	0.52
48:o:31:GLN:O	48:o:35:GLN:HG2	2.10	0.52
49:p:14:ARG:HA	51:r:23:GLN:HA	1.90	0.52
45:w:146:ARG:O	45:w:149:VAL:HG12	2.10	0.52
61:A6:51:SER:HB2	61:A6:91:LEU:HD11	1.90	0.52
1:9:62:ARG:O	1:9:65:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:126:LEU:HD21	2:4:153:THR:HG21	1.91	0.52
3:2:95:SER:O	3:2:98:MET:N	2.40	0.52
3:2:103:ALA:O	3:2:107:GLY:HA2	2.10	0.52
3:2:218:MET:SD	3:2:323:MET:HE2	2.49	0.52
4:7:117:PHE:CD1	6:5:6:MET:HE1	2.43	0.52
5:6:157:TRP:CD1	5:6:158:TRP:CD1	2.94	0.52
5:6:206:PRO:HD2	5:6:266:LEU:HD13	1.89	0.52
10:A:319:TRP:HA	10:A:319:TRP:HE3	1.73	0.52
11:B:385:TYR:HD1	14:E:122:VAL:CG1	2.23	0.52
23:O:48:HIS:CG	26:R:359:TYR:CZ	2.95	0.52
23:O:64:ARG:O	23:O:68:LYS:HE2	2.09	0.52
25:Q:161:ALA:HA	42:j:87:ASP:CB	2.39	0.52
27:S:52:GLY:H	27:S:195:VAL:HB	1.73	0.52
32:X:19:GLY:O	32:X:22:PHE:HB3	2.08	0.52
36:b:66:ARG:CZ	40:h:76:TYR:OH	2.58	0.52
37:c:71:ALA:O	37:c:75:VAL:HG12	2.08	0.52
43:g:76:GLU:O	43:g:85:MET:SD	2.67	0.52
43:g:120:SER:C	43:g:122:ARG:H	2.17	0.52
47:m:62:ALA:O	47:m:65:SER:OG	2.25	0.52
47:m:257:THR:HA	48:o:115:TYR:OH	2.09	0.52
46:x:227:ARG:HB3	46:x:228:GLY:CA	2.39	0.52
53:A3:40:LEU:O	53:A3:41:ILE:HG12	2.09	0.52
56:A9:302:ARG:O	56:A9:306:THR:HG23	2.09	0.52
56:A9:398:PRO:O	56:A9:498:CYS:HB3	2.09	0.52
59:A7:40:LEU:HD22	59:A7:59:LEU:HD13	1.92	0.52
1:9:129:LYS:H	1:9:168:LEU:HA	1.73	0.52
2:4:24:TRP:CG	2:4:81:GLN:HE22	2.28	0.52
2:4:166:TYR:HH	70:4:503:3PE:P	2.18	0.52
2:4:257:MET:O	2:4:260:PRO:HD2	2.09	0.52
5:6:60:GLU:CD	5:6:83:ASP:HA	2.34	0.52
8:1:78:ALA:O	8:1:226:ALA:HB1	2.08	0.52
12:C:70:ILE:HG13	12:C:71:LEU:HD12	1.91	0.52
14:E:135:ARG:HG2	14:E:136:ALA:H	1.74	0.52
28:T:30:GLY:CA	28:T:64:ALA:CB	2.86	0.52
35:a:47:TYR:O	35:a:51:TYR:N	2.38	0.52
42:j:116:PHE:CZ	43:g:157:ALA:HB1	2.41	0.52
31:M:59:GLY:O	31:M:60:PHE:HB2	2.09	0.52
47:y:46:LEU:O	47:y:49:LEU:N	2.35	0.52
51:A2:8:THR:HG22	51:A2:9:ARG:H	1.74	0.52
52:B3:10:GLU:OE1	52:B3:13:LEU:N	2.42	0.52
1:9:87:GLN:O	1:9:91:GLY:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:181:TYR:O	3:2:182:SER:OG	2.21	0.52
3:2:271:THR:O	3:2:272:LYS:HB3	2.09	0.52
5:6:487:LYS:HG3	5:6:488:THR:H	1.73	0.52
7:3:98:LEU:HD22	8:1:298:LEU:HD21	1.90	0.52
9:8:97:LEU:HD23	9:8:101:PHE:HB2	1.91	0.52
10:A:435:PRO:HG3	10:A:444:HIS:CG	2.45	0.52
12:C:123:THR:HG22	12:C:123:THR:O	2.10	0.52
20:K:23:LEU:O	20:K:58:CYS:HA	2.10	0.52
26:R:155:VAL:HA	26:R:158:GLU:HB3	1.90	0.52
26:R:270:ARG:HD2	26:R:373:LYS:CB	2.38	0.52
32:X:37:PHE:HE2	43:g:83:LEU:CD2	2.22	0.52
36:b:112:TYR:O	43:g:63:TYR:HB2	2.09	0.52
39:f:31:CYS:SG	39:f:37:TYR:HB2	2.50	0.52
40:h:147:ILE:CD1	42:j:110:GLY:CA	2.80	0.52
50:q:110:LYS:HZ1	53:A3:11:ARG:C	2.06	0.52
52:s:31:VAL:O	52:s:35:GLU:HG3	2.09	0.52
56:A9:225:GLY:HA3	58:C2:112:LEU:HD13	1.92	0.52
56:A9:268:PHE:CZ	57:C4:58:ALA:HA	2.44	0.52
57:C4:59:GLN:N	57:C4:62:GLU:HG3	2.24	0.52
1:9:118:PHE:HB2	9:8:220:GLN:NE2	2.20	0.52
2:4:57:PHE:C	2:4:111:THR:HG23	2.34	0.52
2:4:421:TYR:OH	35:a:59:VAL:CB	2.58	0.52
5:6:581:LYS:C	6:5:96:LEU:HD11	2.35	0.52
8:1:78:ALA:O	8:1:226:ALA:CB	2.58	0.52
12:C:199:PRO:O	12:C:201:ARG:N	2.43	0.52
17:H:62:ASP:O	17:H:66:CYS:N	2.41	0.52
17:H:72:THR:HG23	30:V:110:VAL:HG21	1.91	0.52
21:L:36:SER:O	21:L:39:THR:HG22	2.08	0.52
28:T:9:TYR:CE1	28:T:21:LYS:CB	2.92	0.52
42:j:115:GLU:HB2	42:j:116:PHE:HA	1.92	0.52
52:s:57:GLU:OE1	52:s:57:GLU:N	2.37	0.52
57:C4:102:HIS:O	57:C4:104:TRP:N	2.42	0.52
57:C4:104:TRP:CG	57:C4:203:ASN:HB2	2.44	0.52
59:A7:23:PRO:HD2	60:C0:34:ASN:HD22	1.74	0.52
1:9:118:PHE:CB	9:8:220:GLN:HE21	2.22	0.52
2:4:95[B]:PHE:CZ	2:4:136:TRP:CD1	2.97	0.52
8:1:1:MET:O	8:1:4:ILE:HG22	2.09	0.52
8:1:283:ASP:C	8:1:285:LEU:H	2.18	0.52
9:8:48:ARG:HG3	9:8:133:HIS:CD2	2.44	0.52
9:8:93:PHE:CZ	9:8:98:LYS:HB3	2.43	0.52
9:8:392:MET:O	9:8:395:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:307:VAL:N	10:A:315:THR:O	2.42	0.52
10:A:398:ASP:O	10:A:427:LEU:HD12	2.10	0.52
11:B:149:GLN:O	11:B:149:GLN:NE2	2.43	0.52
11:B:266:ARG:HD3	70:B:501:3PE:C21	2.40	0.52
11:B:272:THR:HG22	11:B:327:TYR:HB2	1.91	0.52
26:R:67:ARG:HH11	26:R:93:HIS:CD2	2.27	0.52
28:T:70:PHE:CE1	28:T:93:GLY:HA3	2.44	0.52
30:V:56:GLU:HA	30:V:59:ARG:NH1	2.25	0.52
38:d:46:MET:HE2	38:d:56:ARG:HA	1.91	0.52
44:e:136:PHE:O	44:e:139:PHE:N	2.41	0.52
31:M:33:ASN:OD1	31:M:74:GLN:NE2	2.42	0.52
2:4:106:LEU:HD13	2:4:235:LEU:HD22	1.91	0.52
70:4:501:3PE:O14	3:2:238:PRO:CG	2.58	0.52
8:1:143:GLU:O	8:1:146:LEU:N	2.37	0.52
10:A:473:MET:HE2	10:A:475:ILE:HD11	1.89	0.52
12:C:133:ASN:C	12:C:134:LEU:HD12	2.35	0.52
27:S:66:ALA:O	27:S:71:LEU:N	2.27	0.52
28:T:66:ILE:CA	28:T:69:ILE:CG2	2.88	0.52
43:g:5:TRP:HD1	43:g:6:ASP:O	1.93	0.52
45:k:146:ARG:O	45:k:149:VAL:HG12	2.10	0.52
46:l:74:SER:O	46:l:82:SER:OG	2.22	0.52
48:o:138:PRO:O	48:o:141:VAL:HG12	2.10	0.52
57:C4:68:LEU:HB3	57:C4:69:PRO:HD3	1.91	0.52
57:C4:100:MET:CE	57:C4:157:GLU:HG3	2.40	0.52
1:9:181:VAL:CG2	9:8:125:CYS:SG	2.96	0.52
2:4:143:LEU:CD2	3:2:302:LEU:HD21	2.34	0.52
3:2:127:GLY:HA2	3:2:128:LEU:HB2	1.91	0.52
3:2:166:GLY:O	3:2:292:PHE:HZ	1.93	0.52
5:6:484:TYR:HA	5:6:487:LYS:HD3	1.91	0.52
8:1:296:LEU:HD11	70:B:501:3PE:C35	2.40	0.52
9:8:386:ARG:C	9:8:388:GLY:H	2.18	0.52
10:A:310:GLU:HG2	10:A:311:LYS:HG3	1.91	0.52
11:B:320:ILE:O	14:E:41:VAL:HB	2.09	0.52
11:B:421:ARG:HH21	11:B:423:LYS:HB2	1.73	0.52
20:K:59:SER:C	20:K:61:VAL:H	2.18	0.52
28:T:30:GLY:CA	28:T:64:ALA:HA	2.40	0.52
39:f:17:LEU:O	39:f:21:LYS:N	2.35	0.52
41:i:69:TYR:HB2	42:j:19:ARG:O	2.09	0.52
42:j:119:VAL:CG2	43:g:147:GLY:O	2.57	0.52
48:o:11:PRO:HB2	52:s:74:PHE:CE2	2.44	0.52
48:o:99:GLU:HB3	48:z:76:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:138:PRO:O	48:z:141:VAL:HG12	2.10	0.52
49:A0:120:PRO:C	49:A0:122:HIS:H	2.12	0.52
1:9:243:PHE:CD2	9:8:257:ARG:HB2	2.44	0.52
7:3:80:GLN:HG3	8:1:317:GLN:O	2.09	0.52
10:A:167:PRO:O	10:A:168:LEU:HD23	2.10	0.52
10:A:426:ASP:OD1	16:G:169:ARG:NH1	2.36	0.52
10:A:507:THR:CB	10:A:508:GLY:HA3	2.40	0.52
70:B:501:3PE:H392	14:E:61:LEU:HD11	1.91	0.52
12:C:169:GLU:OE1	12:C:183:HIS:CD2	2.63	0.52
14:E:100:GLU:O	14:E:170:GLY:N	2.42	0.52
14:E:135:ARG:NH1	18:I:68:ALA:CB	2.73	0.52
25:Q:124:ASP:O	30:V:66:GLU:OE2	2.27	0.52
26:R:125:VAL:HG21	26:R:253:ILE:HD11	1.91	0.52
26:R:328:ILE:CG2	26:R:329:LEU:N	2.44	0.52
28:T:20:ARG:NH1	28:T:20:ARG:CB	2.73	0.52
35:a:67:ARG:CZ	44:e:79:PRO:HB2	2.37	0.52
47:y:137:GLN:HE21	47:y:141:TRP:CD1	2.27	0.52
47:y:310:SER:HA	47:y:374:ASN:HD21	1.75	0.52
1:9:74:HIS:NE2	16:G:166:TRP:O	2.39	0.51
2:4:446:LEU:HG	71:4:502:CDL:H372	1.89	0.51
11:B:260:GLU:OE2	30:V:25:LEU:CB	2.57	0.51
25:Q:51:LYS:HZ3	36:b:189:ASN:CG	2.18	0.51
26:R:128:ASN:HD21	26:R:130:VAL:HG12	1.75	0.51
27:S:32:ILE:HG13	27:S:33:LEU:HD12	1.91	0.51
35:a:67:ARG:HH12	44:e:79:PRO:HB2	1.70	0.51
42:j:33:PHE:O	42:j:36:PHE:HB3	2.10	0.51
45:k:213:GLN:O	45:k:217:SER:OG	2.23	0.51
56:A9:75:ILE:O	56:A9:79:GLY:HA3	2.11	0.51
56:A9:240:HIS:HB3	56:A9:241:PRO:HD3	1.92	0.51
58:C2:18:LEU:HD22	58:C2:22:LEU:HD22	1.92	0.51
62:A4:42:ARG:HH11	62:A4:42:ARG:HG3	1.75	0.51
2:4:1:MET:HB2	2:4:52:PHE:CE1	2.45	0.51
2:4:297:VAL:O	2:4:301:ILE:HG12	2.10	0.51
2:4:381:VAL:O	2:4:385:THR:HG22	2.10	0.51
5:6:61:LEU:H	5:6:82:MET:HB2	1.74	0.51
5:6:119:LYS:HE3	71:6:701:CDL:H712	1.90	0.51
5:6:435:PRO:O	34:Z:52:ARG:HD2	2.10	0.51
8:1:162:LEU:HD23	8:1:240:ILE:HD13	1.91	0.51
9:8:413:TRP:O	9:8:416:SER:OG	2.23	0.51
10:A:129:PRO:HD2	18:I:114:TYR:OH	2.09	0.51
10:A:307:VAL:O	10:A:314:LEU:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:443:ASP:N	10:A:443:ASP:OD1	2.42	0.51
18:I:85:ILE:HG21	18:I:119:PHE:HZ	1.76	0.51
24:P:38:PRO:C	30:V:8:GLN:HG3	2.34	0.51
37:c:66:ARG:HA	37:c:67:HIS:C	2.35	0.51
40:h:113:ARG:O	40:h:115:GLN:N	2.43	0.51
42:j:91:PHE:O	42:j:95:LYS:N	2.38	0.51
45:k:2:ALA:HB3	46:l:113:ARG:CZ	2.40	0.51
45:k:360:LEU:HA	45:k:363:ASN:HD22	1.75	0.51
47:m:267:HIS:NE2	47:m:269:LYS:HD3	2.25	0.51
47:y:25:SER:HA	47:y:218:ILE:HD12	1.93	0.51
48:z:73:GLY:HA2	48:z:79:GLU:HG3	1.92	0.51
2:4:446:LEU:O	71:4:502:CDL:H331	2.10	0.51
4:7:14:VAL:HG21	6:5:7:ASN:ND2	2.26	0.51
5:6:161:ARG:HD3	5:6:164:ALA:HB2	1.92	0.51
5:6:328:HIS:O	5:6:331:THR:OG1	2.28	0.51
9:8:37:ASP:CB	9:8:294:VAL:HB	2.40	0.51
11:B:316:PHE:HA	11:B:342:ARG:HH11	1.76	0.51
12:C:195:PHE:HE2	13:D:131:ASN:HD22	1.56	0.51
13:D:184:PRO:CG	14:E:183:LEU:HD22	2.38	0.51
18:I:79:GLN:HA	18:I:120:ARG:O	2.10	0.51
42:j:112:VAL:HG21	43:g:79:GLU:OE2	2.10	0.51
45:k:220:SER:O	45:k:222:THR:HG23	2.11	0.51
47:m:25:SER:HA	47:m:218:ILE:HD12	1.93	0.51
47:m:100:ARG:NH1	77:m:402:HEM:O1A	2.42	0.51
55:v:63:PRO:N	55:v:64:LEU:HA	2.26	0.51
47:y:341:GLN:HB3	47:y:347:TYR:CE2	2.46	0.51
48:z:31:GLN:O	48:z:35:GLN:HG2	2.10	0.51
2:4:2:LEU:HB3	2:4:6:ILE:HD12	1.92	0.51
2:4:336:ARG:NH2	2:4:433:GLU:HG3	2.25	0.51
2:4:349:GLN:NE2	2:4:349:GLN:O	2.44	0.51
3:2:133:TRP:O	3:2:136:LEU:N	2.34	0.51
5:6:264:TYR:CE1	5:6:265:PRO:HG3	2.45	0.51
8:1:169:GLN:HE21	8:1:174:LEU:HB2	1.74	0.51
8:1:203:GLY:H	8:1:210:GLY:N	1.94	0.51
11:B:266:ARG:HD2	70:B:501:3PE:H231	1.93	0.51
12:C:214:TYR:CD1	13:D:138:ARG:HG2	2.45	0.51
12:C:243:ALA:HB1	24:P:61:ARG:HH21	1.76	0.51
26:R:154:GLN:HG3	26:R:155:VAL:HG23	1.93	0.51
27:S:335:VAL:CB	42:j:51:ARG:O	2.58	0.51
27:S:338:LYS:HZ3	42:j:57:GLY:H	1.55	0.51
28:T:101:LEU:HD11	28:T:110:ILE:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:138:MET:HE2	47:m:255:ASN:ND2	2.26	0.51
45:w:360:LEU:HA	45:w:363:ASN:HD22	1.75	0.51
57:C4:33:LEU:HD23	64:B4:28:SER:HB2	1.91	0.51
2:4:423:ILE:HD12	35:a:57:ARG:CA	2.41	0.51
2:4:431:THR:O	2:4:435:ALA:N	2.41	0.51
4:7:4:TYR:CE1	4:7:123:GLY:HA2	2.35	0.51
4:7:17:PHE:O	4:7:19:GLY:N	2.43	0.51
5:6:472:ILE:HG12	5:6:473:PRO:O	2.10	0.51
7:3:88:LEU:CG	8:1:309:ILE:HD12	2.40	0.51
8:1:230:ASN:HA	8:1:233:MET:HE2	1.92	0.51
9:8:75:TRP:O	9:8:79:GLU:HB2	2.10	0.51
9:8:330:SER:OG	9:8:331:VAL:N	2.43	0.51
11:B:80:LEU:HD23	11:B:81:THR:N	2.25	0.51
11:B:102:SER:HB3	11:B:107:ARG:HH11	1.76	0.51
15:F:83:TYR:O	15:F:84:THR:OG1	2.27	0.51
31:M:35:HIS:HB3	31:M:38:LYS:HZ3	1.76	0.51
45:k:259:GLY:O	45:k:318:GLY:N	2.44	0.51
47:m:237:LEU:HD11	48:o:212:MET:CG	2.39	0.51
61:A6:8:THR:OG1	61:A6:11:GLU:HG2	2.09	0.51
2:4:49:SER:HB2	2:4:60:SER:CB	2.40	0.51
2:4:190:TRP:HB2	28:T:127:MET:HG3	1.92	0.51
3:2:64:SER:OG	3:2:65:THR:N	2.42	0.51
3:2:155:LEU:HD13	28:T:136:PHE:CD1	2.45	0.51
3:2:250:SER:O	3:2:259:GLY:HA3	2.09	0.51
3:2:325:PHE:HE2	70:2:401:3PE:C2I	2.18	0.51
5:6:1:MET:HG2	5:6:59:GLN:NE2	2.25	0.51
5:6:221:THR:HG22	5:6:226:GLN:HG3	1.91	0.51
5:6:569:ALA:O	5:6:572:LYS:N	2.43	0.51
6:5:46:LEU:O	6:5:49:LEU:N	2.43	0.51
9:8:53:LEU:C	9:8:136:HIS:HE2	2.19	0.51
10:A:306:MET:HB2	10:A:583:ILE:HD11	1.91	0.51
10:A:356:ASP:OD2	10:A:645:ARG:NE	2.44	0.51
12:C:214:TYR:HB3	13:D:176:ILE:O	2.11	0.51
13:D:184:PRO:HB2	14:E:149:MET:O	2.10	0.51
25:Q:44:MET:HE3	30:V:73:PRO:HA	1.92	0.51
25:Q:142:TYR:HD1	25:Q:143:HIS:CD2	2.28	0.51
26:R:238:GLN:HB3	26:R:267:GLY:HA3	1.92	0.51
32:X:10:HIS:HB3	32:X:13:HIS:HD2	1.74	0.51
32:X:37:PHE:HE2	43:g:83:LEU:HD22	1.76	0.51
35:a:129:TYR:CE2	43:g:144:HIS:CE1	2.99	0.51
47:m:91:PHE:HE2	47:m:273:TYR:CE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A1:105:GLU:O	50:A1:109:LYS:NZ	2.35	0.51
57:C4:1:MET:SD	57:C4:133:LEU:CD1	2.98	0.51
63:A5:60:TYR:CD1	63:A5:60:TYR:C	2.88	0.51
2:4:223:ALA:HB1	2:4:224:PRO:HD2	1.92	0.51
5:6:590:SER:HA	28:T:42:ALA:HB1	1.92	0.51
7:3:2:ASN:HB2	8:1:2:PHE:CE2	2.45	0.51
10:A:176:CYS:CA	74:A:802:SF4:S4	2.98	0.51
22:N:49:GLU:O	22:N:52:THR:OG1	2.22	0.51
23:O:101:THR:O	23:O:105:ARG:HG3	2.10	0.51
25:Q:161:ALA:HA	42:j:87:ASP:HB2	1.92	0.51
26:R:85:ARG:NH2	76:R:601:NAP:C6A	2.69	0.51
27:S:79:ILE:O	27:S:122:TRP:NE1	2.36	0.51
27:S:117:TYR:HE1	27:S:175:TYR:HD2	1.57	0.51
31:W:78:GLY:O	31:W:82:ARG:N	2.36	0.51
33:Y:73:LEU:HD22	33:Y:74:TRP:CD1	2.45	0.51
39:f:97:TYR:C	39:f:99:VAL:H	2.17	0.51
40:h:149:LEU:HD13	43:g:166:GLU:CB	2.40	0.51
43:g:22:PRO:O	43:g:24:THR:N	2.44	0.51
43:g:141:ASP:OD1	43:g:141:ASP:N	2.40	0.51
45:k:86:LEU:HD23	46:l:285:VAL:HG22	1.93	0.51
46:l:83:PHE:CZ	50:A1:104:ARG:HG2	2.46	0.51
48:o:80:MET:CG	48:o:81:PHE:H	2.23	0.51
47:y:91:PHE:HE2	47:y:273:TYR:CE1	2.29	0.51
47:y:100:ARG:NH1	77:y:402:HEM:O1A	2.42	0.51
47:y:138:MET:HE2	47:y:255:ASN:ND2	2.26	0.51
56:A9:347:LEU:HG	56:A9:383:MET:HE3	1.93	0.51
1:9:137:THR:HG22	1:9:138:THR:H	1.75	0.51
3:2:217:THR:HG21	72:2:402:PC1:C26	2.34	0.51
10:A:65:TYR:N	69:A:803:FES:S2	2.81	0.51
10:A:121:LEU:HD13	11:B:376:GLU:OE2	2.10	0.51
10:A:481:LEU:HA	10:A:489:ILE:HD11	1.93	0.51
10:A:495:ASN:O	10:A:499:LYS:N	2.33	0.51
17:H:15:ASP:O	17:H:17:TRP:CD1	2.63	0.51
20:K:35:ASP:OD1	20:K:39:LYS:NZ	2.34	0.51
26:R:252:ALA:HB2	26:R:338:LEU:HD11	1.93	0.51
26:R:369:VAL:H	26:R:370:GLN:HA	1.75	0.51
39:f:54:GLU:OE1	39:f:59:LYS:NZ	2.43	0.51
47:m:341:GLN:HB3	47:m:347:TYR:CE2	2.46	0.51
46:x:97:SER:CB	55:B1:70:LEU:HD22	2.41	0.51
49:A0:58:PHE:O	49:A0:61:SER:OG	2.23	0.51
55:B1:70:LEU:HD12	55:B1:71:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:184:PHE:H	56:A9:256:HIS:CE1	2.29	0.51
56:A9:250:GLY:O	56:A9:254:ILE:HG12	2.11	0.51
2:4:94:LEU:O	2:4:97:THR:N	2.43	0.51
2:4:194:PHE:O	2:4:198:ALA:N	2.40	0.51
2:4:196:TRP:HD1	2:4:251:ASN:HD22	1.59	0.51
3:2:93:MET:SD	5:6:605:HIS:CE1	3.00	0.51
4:7:168:ILE:O	4:7:172:THR:OG1	2.28	0.51
5:6:270:ASN:HB2	5:6:273:ILE:HD12	1.92	0.51
10:A:58:MET:HE3	12:C:248:ARG:HH22	1.76	0.51
11:B:176:GLU:HG3	11:B:176:GLU:O	2.11	0.51
13:D:146:GLU:HB3	13:D:147:PRO:HD3	1.92	0.51
22:N:44:TYR:CE1	22:N:94:MET:HE3	2.45	0.51
27:S:189:PRO:HB2	27:S:192:VAL:HG22	1.93	0.51
28:T:90:TYR:HB3	28:T:126:LYS:HD2	1.93	0.51
35:a:108:ASP:C	35:a:110:ASP:N	2.69	0.51
39:f:176:GLU:OE1	39:f:176:GLU:N	2.44	0.51
49:p:58:PHE:O	49:p:61:SER:OG	2.21	0.51
49:p:151:GLY:N	49:p:152:ASP:HA	2.25	0.51
49:A0:157:TYR:N	49:A0:165:TYR:CB	2.73	0.51
2:4:89:LEU:HD12	2:4:90:THR:N	2.26	0.51
2:4:278:ARG:HD3	5:6:546:GLN:CD	2.36	0.51
2:4:385:THR:CG2	2:4:396:MET:HE1	2.41	0.51
5:6:137:LEU:CB	5:6:196:TRP:HB2	2.41	0.51
8:1:178:ALA:O	8:1:179:TRP:C	2.52	0.51
10:A:111:LYS:HD3	24:P:53:TYR:OH	2.10	0.51
10:A:139:LEU:HD11	10:A:177:ILE:HG21	1.91	0.51
11:B:233:HIS:CE1	14:E:160:GLU:CD	2.89	0.51
11:B:242:ASP:CA	24:P:32:SER:OG	2.53	0.51
12:C:242:GLU:CB	16:G:92:ASN:ND2	2.72	0.51
71:J:101:CDL:H512	29:U:6:VAL:HG13	1.92	0.51
26:R:55:VAL:HG13	26:R:79:GLN:HB3	1.92	0.51
36:b:121:ILE:HD11	40:h:105:PHE:CE1	2.46	0.51
40:h:97:ILE:HG23	40:h:98:VAL:HG23	1.92	0.51
45:k:408:ARG:O	45:k:412:SER:OG	2.26	0.51
46:l:213:HIS:CD2	46:l:217:LYS:HB2	2.46	0.51
47:m:310:SER:HA	47:m:374:ASN:HD21	1.75	0.51
3:2:215:MET:HE2	3:2:215:MET:HA	1.92	0.50
4:7:107:VAL:HG23	4:7:117:PHE:HB3	1.92	0.50
5:6:177:ILE:O	5:6:180:ILE:N	2.37	0.50
5:6:233:LEU:HG	5:6:248:HIS:HE1	1.75	0.50
6:5:89:TYR:HB3	6:5:91:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:243:TRP:O	12:C:236:ASP:HB3	2.11	0.50
12:C:77:GLN:HG3	24:P:70:MET:CB	2.40	0.50
12:C:209:TYR:HE1	16:G:120:PRO:CG	2.24	0.50
16:G:131:LYS:NZ	16:G:147:VAL:HG11	2.26	0.50
27:S:338:LYS:HZ1	42:j:57:GLY:H	1.58	0.50
34:Z:21:GLN:HB3	34:Z:22:TRP:CE3	2.46	0.50
41:i:48:LEU:O	41:i:52:VAL:HG23	2.11	0.50
42:j:107:LYS:O	43:g:79:GLU:HB2	2.11	0.50
42:j:118:PRO:HB2	43:g:147:GLY:N	2.26	0.50
45:k:132:ASP:O	45:k:136:GLN:N	2.44	0.50
52:s:21:ARG:HB3	52:s:65:ARG:HH21	1.76	0.50
77:y:402:HEM:HBB2	77:y:402:HEM:HMB2	1.93	0.50
2:4:112:ALA:O	2:4:114:GLU:HG2	2.11	0.50
5:6:378:LEU:O	5:6:381:THR:OG1	2.15	0.50
9:8:363:ILE:H	9:8:363:ILE:HD12	1.76	0.50
10:A:320:GLU:OE1	23:O:119:LEU:HD21	2.11	0.50
12:C:169:GLU:HB3	12:C:180:PHE:HD2	1.75	0.50
13:D:215:ARG:HD2	26:R:85:ARG:HD2	1.92	0.50
23:O:75:ASP:O	23:O:79:VAL:HG23	2.11	0.50
27:S:340:ILE:HA	42:j:57:GLY:HA2	1.94	0.50
37:c:83:HIS:HE1	37:c:87:LYS:HE2	1.75	0.50
31:M:20:LYS:HB2	31:M:30:LEU:HD11	1.92	0.50
48:z:178:THR:HB	48:z:181:GLN:HB2	1.94	0.50
49:A0:106:ILE:O	49:A0:167:ALA:HB3	2.00	0.50
57:C4:139:ASP:OD1	57:C4:140:ASN:N	2.44	0.50
1:9:143:ARG:HH12	9:8:285:PRO:HG2	1.71	0.50
3:2:339:LEU:O	3:2:343:LEU:N	2.44	0.50
5:6:119:LYS:HE2	71:6:701:CDL:H711	1.93	0.50
8:1:237:PHE:O	8:1:239:ALA:N	2.43	0.50
9:8:42:PHE:HE2	9:8:261:TRP:CE2	2.30	0.50
10:A:173:MET:SD	10:A:176:CYS:SG	3.09	0.50
23:O:48:HIS:ND1	26:R:359:TYR:CE1	2.78	0.50
23:O:83:VAL:O	23:O:86:GLY:N	2.44	0.50
27:S:333:GLU:CG	42:j:52:PRO:HB2	2.28	0.50
28:T:20:ARG:NH1	28:T:20:ARG:CG	2.73	0.50
34:Z:20:LYS:HA	34:Z:23:LYS:HE2	1.92	0.50
43:g:77:CYS:HB2	43:g:84:CYS:SG	2.52	0.50
44:e:131:LYS:O	44:e:135:GLY:N	2.45	0.50
50:q:109:LYS:O	53:A3:11:ARG:HG2	2.12	0.50
45:w:259:GLY:O	45:w:318:GLY:N	2.44	0.50
56:A9:40:GLU:HG2	56:A9:54:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:C4:136:LEU:HB3	57:C4:193:TYR:CD2	2.46	0.50
59:A7:64:PHE:CE1	60:C0:66:ARG:HD2	2.47	0.50
60:C0:63:SER:O	60:C0:67:ILE:HG13	2.10	0.50
61:A6:37:LYS:HD3	61:A6:37:LYS:N	2.27	0.50
2:4:179:LEU:HD11	43:g:82:VAL:HG21	1.94	0.50
3:2:161:SER:HA	3:2:164:ILE:HG22	1.94	0.50
3:2:164:ILE:HG13	5:6:576:LEU:HD11	1.92	0.50
3:2:278:LEU:HD12	28:T:136:PHE:CD1	2.47	0.50
5:6:120:TYR:OH	71:6:701:CDL:CB5	2.57	0.50
8:1:19:PHE:CG	19:J:11:VAL:HG11	2.46	0.50
9:8:117:ALA:HB3	9:8:158:ILE:HG12	1.93	0.50
10:A:328:GLY:O	10:A:331:GLN:N	2.43	0.50
11:B:279:THR:OG1	22:N:12:VAL:HG12	2.11	0.50
11:B:371:MET:HA	11:B:377:SER:OG	2.10	0.50
12:C:232:PHE:CA	13:D:165:TYR:CZ	2.93	0.50
14:E:62:LEU:CD2	30:V:36:PHE:CD2	2.91	0.50
17:H:47:ILE:HG22	17:H:49:SER:H	1.76	0.50
17:H:71:LYS:O	17:H:74:LYS:N	2.39	0.50
40:h:141:CYS:HA	43:g:162:ARG:HH11	1.76	0.50
31:M:35:HIS:HB2	31:M:39:ASP:HB2	1.93	0.50
48:o:11:PRO:HB2	52:s:74:PHE:CD2	2.45	0.50
45:w:431:LEU:HD12	45:w:432:PRO:HD2	1.93	0.50
46:x:213:HIS:CD2	46:x:217:LYS:HB2	2.46	0.50
46:x:367:GLY:O	46:x:371:SER:OG	2.23	0.50
51:A2:74:PRO:HA	51:A2:77:TYR:O	2.11	0.50
2:4:196:TRP:CD1	2:4:251:ASN:ND2	2.78	0.50
3:2:86:VAL:O	3:2:86:VAL:HG12	2.11	0.50
5:6:147:VAL:HB	5:6:252:MET:SD	2.52	0.50
5:6:419:THR:HA	5:6:422:TYR:CD2	2.47	0.50
5:6:528:TYR:O	5:6:531:THR:OG1	2.29	0.50
6:5:19:LEU:HA	6:5:22:TYR:O	2.11	0.50
11:B:267:ILE:CD1	70:B:501:3PE:H282	2.26	0.50
11:B:309:ASP:O	11:B:310:VAL:C	2.54	0.50
12:C:221:VAL:CG2	13:D:138:ARG:HB2	2.38	0.50
13:D:103:ARG:CD	14:E:84:ILE:HD13	2.42	0.50
17:H:2:PRO:HG2	17:H:4:PHE:CE1	2.46	0.50
26:R:329:LEU:HD11	26:R:331:HIS:CD2	2.47	0.50
31:W:104:PHE:HB2	31:W:139:MET:O	2.11	0.50
36:b:87:THR:O	36:b:91:VAL:HG23	2.11	0.50
31:M:32:VAL:O	31:M:74:GLN:N	2.44	0.50
45:k:426:GLY:HA2	45:k:428:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:78:ILE:HG13	47:m:79:ILE:N	2.27	0.50
47:y:258:PRO:HD3	48:z:115:TYR:OH	2.11	0.50
1:9:132:ILE:HG22	1:9:170:THR:O	2.12	0.50
1:9:245:VAL:HG22	9:8:64:LYS:NZ	2.27	0.50
2:4:55:LEU:HA	2:4:113:MET:HG2	1.92	0.50
2:4:180:GLN:HG3	2:4:249:ILE:HD12	1.92	0.50
2:4:203:PHE:HE2	2:4:246:ILE:HD12	1.76	0.50
5:6:590:SER:CA	28:T:42:ALA:HB1	2.41	0.50
8:1:311:THR:CG2	30:V:51:MET:SD	3.00	0.50
9:8:213:ILE:HD11	9:8:236:PHE:HB2	1.93	0.50
9:8:318:ILE:HG13	9:8:326:LEU:HD23	1.93	0.50
9:8:386:ARG:O	9:8:388:GLY:N	2.45	0.50
11:B:281:GLU:OE2	22:N:12:VAL:O	2.30	0.50
12:C:123:THR:HG21	16:G:128:PHE:CB	2.42	0.50
13:D:137:LEU:O	13:D:138:ARG:C	2.55	0.50
26:R:179:LYS:HB3	26:R:317:ASP:OD1	2.12	0.50
33:Y:47:TYR:N	33:Y:49:GLN:OE1	2.42	0.50
37:c:66:ARG:HA	37:c:68:SER:N	2.26	0.50
45:k:389:ARG:HB3	45:k:391:PRO:HG3	1.94	0.50
46:l:305:GLN:HB3	46:l:306:PRO:CD	2.41	0.50
48:o:69:GLU:HB2	48:o:84:PRO:HD3	1.94	0.50
45:w:426:GLY:HA2	45:w:428:ILE:N	2.26	0.50
52:B3:21:ARG:HB3	52:B3:65:ARG:HH21	1.76	0.50
53:A3:39:ARG:HH11	53:A3:39:ARG:CG	2.20	0.50
56:A9:168:ILE:HG21	56:A9:189:MET:HG3	1.94	0.50
2:4:205:VAL:HA	2:4:212:LEU:HD13	1.92	0.50
3:2:117:GLU:OE2	6:5:97:GLN:N	2.44	0.50
5:6:451:ILE:HG22	5:6:455:LYS:HD2	1.94	0.50
10:A:276:ARG:HG2	10:A:276:ARG:O	2.11	0.50
10:A:422:TRP:CZ2	16:G:169:ARG:CD	2.88	0.50
10:A:423:LEU:O	10:A:425:ASN:N	2.44	0.50
11:B:344:ILE:O	11:B:348:LEU:HG	2.12	0.50
21:L:32:LEU:N	21:L:33:PRO:HD2	2.27	0.50
21:L:39:THR:O	21:L:40:LYS:HB3	2.11	0.50
43:g:71:VAL:N	43:g:72:PRO:HD2	2.27	0.50
45:k:431:LEU:HD12	45:k:432:PRO:HD2	1.93	0.50
45:w:115:ASP:OD1	45:w:119:ASN:HB2	2.12	0.50
45:w:292:SER:O	45:w:295:ALA:N	2.41	0.50
45:w:403:ASP:OD1	45:w:404:ALA:N	2.44	0.50
56:A9:508:PRO:HG3	58:C2:6:HIS:HB3	1.94	0.50
2:4:90:THR:CG2	70:4:501:3PE:C32	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:90:THR:HG22	70:4:501:3PE:H352	1.93	0.50
2:4:336:ARG:NH1	2:4:352:LEU:HD21	2.26	0.50
3:2:113:PHE:CE2	28:T:43:LEU:CD2	2.95	0.50
3:2:169:GLY:O	3:2:171:ASN:N	2.45	0.50
3:2:239:ILE:HG21	42:j:48:ILE:CA	2.41	0.50
10:A:76:ARG:O	10:A:116:VAL:HG21	2.12	0.50
11:B:244:ILE:HG22	11:B:348:LEU:HD11	1.93	0.50
70:B:501:3PE:C3B	21:L:21:ALA:HB1	2.41	0.50
12:C:209:TYR:CE1	16:G:120:PRO:CG	2.95	0.50
14:E:118:LEU:O	14:E:120:GLU:N	2.45	0.50
14:E:191:LEU:O	14:E:195:ASP:N	2.45	0.50
27:S:102:LEU:HD23	27:S:105:PHE:HE2	1.76	0.50
27:S:190:HIS:HE1	27:S:271:TRP:O	1.94	0.50
35:a:22:GLU:OE1	35:a:22:GLU:N	2.41	0.50
43:g:145:ASP:O	43:g:149:HIS:N	2.45	0.50
45:k:115:ASP:OD1	45:k:119:ASN:HB2	2.12	0.50
46:l:155:PRO:HB2	46:l:254:HIS:HE1	1.73	0.50
45:w:389:ARG:HB3	45:w:391:PRO:HG3	1.94	0.50
56:A9:232:GLN:HB2	56:A9:292:MET:HE3	1.93	0.50
2:4:329:LEU:HD23	2:4:437:MET:HE3	1.93	0.50
2:4:423:ILE:CG2	35:a:57:ARG:HD2	2.42	0.50
3:2:263:LYS:O	3:2:266:ILE:HG22	2.10	0.50
5:6:10:VAL:O	5:6:14:LEU:HD13	2.12	0.50
10:A:573:GLY:HA2	10:A:577:ALA:HB2	1.94	0.50
10:A:607:LYS:HE2	16:G:78:ARG:CZ	2.41	0.50
13:D:178:PRO:HB2	26:R:92:MET:HG2	1.94	0.50
13:D:203:LYS:HG3	14:E:178:GLU:OE1	2.12	0.50
31:W:85:TYR:CE1	34:Z:19:TYR:CA	2.95	0.50
36:b:167:PRO:O	36:b:168:TRP:HD1	1.95	0.50
37:c:105:PHE:O	37:c:107:GLY:N	2.40	0.50
47:m:102:LEU:O	47:m:105:GLY:N	2.30	0.50
57:C4:186:SER:HB3	57:C4:213:LEU:CD2	2.42	0.50
2:4:50:LEU:HD21	2:4:52:PHE:HD2	1.77	0.49
3:2:22:ILE:CD1	17:H:4:PHE:HB2	2.41	0.49
5:6:548:SER:HA	5:6:552:LEU:HD13	1.94	0.49
8:1:296:LEU:O	8:1:299:ALA:N	2.45	0.49
9:8:51:TRP:CH2	9:8:57:GLN:HA	2.47	0.49
27:S:113:ASP:N	27:S:114:GLY:HA2	2.27	0.49
29:U:85:GLU:OE1	29:U:86:TRP:HD1	1.94	0.49
30:V:125:TYR:CD2	30:V:133:VAL:HG22	2.47	0.49
35:a:37:LEU:HA	35:a:40:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:e:70:THR:CG2	44:e:71:GLY:H	2.22	0.49
47:m:75:TYR:CD2	49:p:57:GLN:HA	2.47	0.49
49:p:41:ALA:HB2	54:u:20:PHE:CE1	2.47	0.49
51:r:37:VAL:O	51:r:41:THR:HG23	2.12	0.49
53:t:16:ASN:C	53:t:18:VAL:H	2.20	0.49
2:4:66:LEU:O	2:4:69:THR:OG1	2.28	0.49
5:6:387:THR:OG1	5:6:388:GLY:N	2.44	0.49
5:6:582:GLY:N	6:5:96:LEU:HD11	2.27	0.49
8:1:34:ARG:HA	14:E:83:THR:CG2	2.38	0.49
8:1:53:ILE:O	8:1:53:ILE:CG2	2.60	0.49
8:1:188:SER:O	8:1:191:ALA:N	2.45	0.49
8:1:248:ASN:C	8:1:250:HIS:H	2.20	0.49
10:A:289:LYS:HB2	10:A:694:PHE:CZ	2.47	0.49
28:T:20:ARG:CD	28:T:20:ARG:N	2.73	0.49
28:T:44:LYS:HD2	28:T:45:THR:H	1.77	0.49
28:T:89:ASN:C	28:T:91:LEU:H	2.20	0.49
35:a:64:ALA:HB3	44:e:108:ASP:H	1.77	0.49
43:g:90:MET:HB3	43:g:94:ARG:HH12	1.77	0.49
77:m:402:HEM:HMB2	77:m:402:HEM:HBB2	1.93	0.49
48:o:41:HIS:HB3	48:o:113:LEU:HG	1.94	0.49
51:r:8:THR:HG22	51:r:9:ARG:H	1.75	0.49
45:w:292:SER:HB3	45:w:295:ALA:HB3	1.94	0.49
56:A9:172:LYS:HB2	56:A9:172:LYS:HZ3	1.76	0.49
58:C2:42:LEU:HD13	65:C3:45:TYR:HD2	1.77	0.49
62:A4:42:ARG:HD2	62:A4:42:ARG:O	2.13	0.49
1:9:110:MET:HE1	10:A:209:TYR:H	1.77	0.49
7:3:38:GLU:OE1	8:1:64:ALA:N	2.44	0.49
9:8:244:ASN:O	9:8:248:VAL:HG22	2.11	0.49
10:A:81:GLU:HG3	10:A:108:LYS:HB3	1.94	0.49
11:B:215:GLU:CD	14:E:97:PHE:HD1	2.20	0.49
11:B:215:GLU:CG	14:E:97:PHE:HD1	2.24	0.49
11:B:229:PRO:HG2	11:B:389:TYR:OH	2.12	0.49
11:B:320:ILE:CD1	14:E:39:LYS:O	2.33	0.49
12:C:207:SER:CB	13:D:171:ARG:HH21	2.23	0.49
12:C:218:VAL:C	12:C:219:LYS:CG	2.77	0.49
18:I:80:VAL:HG11	18:I:85:ILE:HD11	1.94	0.49
21:L:8:PHE:HD2	21:L:9:LEU:HD12	1.78	0.49
23:O:33:ARG:CZ	31:M:48:VAL:HG21	2.42	0.49
25:Q:88:CYS:SG	25:Q:89:ILE:N	2.86	0.49
26:R:317:ASP:O	26:R:321:ARG:N	2.42	0.49
28:T:10:TRP:C	28:T:12:ILE:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:139:PRO:HB3	36:b:158:ARG:HG3	1.93	0.49
31:M:18:VAL:HG21	31:M:54:MET:SD	2.52	0.49
46:x:438:GLU:OE1	46:x:438:GLU:N	2.43	0.49
56:A9:145:LEU:HD21	58:C2:32:THR:HG21	1.94	0.49
56:A9:377:PHE:HA	56:A9:380:VAL:HG22	1.93	0.49
2:4:449:LEU:HD12	71:4:502:CDL:H331	1.93	0.49
5:6:101:MET:HE2	5:6:121:LEU:HD22	1.94	0.49
5:6:161:ARG:O	5:6:164:ALA:N	2.39	0.49
5:6:286:LEU:HD22	5:6:411:MET:SD	2.52	0.49
5:6:353:GLU:O	5:6:354:GLN:HG2	2.12	0.49
5:6:353:GLU:OE2	5:6:358:LYS:HB2	2.12	0.49
6:5:26:LEU:O	6:5:29:SER:OG	2.25	0.49
8:1:288:LEU:O	8:1:292:ASN:HB2	2.13	0.49
9:8:273:THR:HA	9:8:291:GLU:HA	1.93	0.49
10:A:380:ASP:C	10:A:382:ARG:H	2.20	0.49
11:B:141:TYR:HH	11:B:458:PHE:C	2.14	0.49
12:C:240:PRO:CD	16:G:88:GLN:HE22	2.25	0.49
13:D:101:ALA:HB1	13:D:102:PRO:HD2	1.94	0.49
13:D:138:ARG:CZ	13:D:141:TYR:CD2	2.84	0.49
13:D:191:GLU:CG	14:E:173:PHE:CD1	2.95	0.49
26:R:192:ARG:HH21	26:R:200:ILE:HG22	1.77	0.49
28:T:101:LEU:HD11	28:T:111:GLY:N	2.27	0.49
34:Z:79:VAL:O	34:Z:82:ILE:N	2.42	0.49
40:h:149:LEU:HD11	43:g:167:ARG:HA	1.89	0.49
41:i:68:GLU:HB3	42:j:19:ARG:CG	2.42	0.49
42:j:107:LYS:HD2	42:j:111:GLU:HG2	1.94	0.49
43:g:30:ILE:O	43:g:34:THR:HG22	2.12	0.49
47:m:312:GLN:HE21	47:m:318:ARG:HG3	1.78	0.49
50:q:35:ASP:OD2	50:q:61:ARG:NH2	2.35	0.49
62:A4:44:ARG:HD2	62:A4:74:ARG:O	2.12	0.49
2:4:22:MET:SD	40:h:82:VAL:HG21	2.52	0.49
3:2:258:SER:OG	3:2:330:VAL:O	2.29	0.49
5:6:592:LEU:HD12	6:5:17:VAL:HG23	1.94	0.49
6:5:6:MET:O	6:5:7:ASN:ND2	2.46	0.49
10:A:223:ILE:HD12	10:A:233:SER:HB2	1.93	0.49
10:A:504:SER:N	10:A:505:GLY:HA2	2.23	0.49
12:C:185:ASP:OD1	12:C:186:LEU:N	2.45	0.49
12:C:209:TYR:CE1	16:G:120:PRO:HG3	2.48	0.49
13:D:189:THR:C	13:D:191:GLU:H	2.19	0.49
16:G:82:PRO:HG3	16:G:98:LYS:NZ	2.28	0.49
18:I:51:TYR:HE1	26:R:55:VAL:HG22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:143:ASP:C	26:R:146:VAL:H	2.18	0.49
29:U:49:TYR:HD2	29:U:61:TRP:CH2	2.29	0.49
37:c:95:TYR:CE2	43:g:10:TYR:CD1	2.99	0.49
42:j:116:PHE:CE2	43:g:161:GLN:HG3	2.48	0.49
47:y:271:GLU:CD	47:y:273:TYR:HH	2.16	0.49
57:C4:13:THR:O	57:C4:13:THR:HG22	2.12	0.49
62:A4:42:ARG:NH1	62:A4:74:ARG:HH21	2.10	0.49
2:4:82:HIS:CE1	2:4:432:ARG:HH12	2.30	0.49
2:4:294:MET:O	2:4:297:VAL:HG22	2.13	0.49
2:4:360:LEU:HD13	71:6:701:CDL:C52	2.42	0.49
5:6:63:ILE:HD13	5:6:65:ASN:ND2	2.27	0.49
5:6:102:GLU:O	5:6:105:MET:HB3	2.13	0.49
5:6:335:PHE:CZ	5:6:383:MET:HE1	2.48	0.49
5:6:454:ILE:HG22	5:6:458:LEU:HD23	1.94	0.49
8:1:172:MET:HE2	8:1:176:LEU:CB	2.42	0.49
9:8:270:ASN:HD21	9:8:338:ASP:CB	2.25	0.49
9:8:362:ASP:O	9:8:366:ALA:N	2.46	0.49
10:A:287:SER:OG	10:A:288:ASP:N	2.45	0.49
13:D:203:LYS:HG2	13:D:203:LYS:O	2.13	0.49
16:G:163:ASN:HB3	16:G:172:VAL:HG22	1.94	0.49
17:H:37:GLU:O	17:H:40:TRP:N	2.44	0.49
25:Q:53:PRO:HG3	36:b:188:ASP:OD2	2.12	0.49
27:S:335:VAL:C	42:j:52:PRO:CD	2.69	0.49
29:U:46:ASN:HD21	29:U:83:PRO:HD3	1.78	0.49
35:a:47:TYR:CG	44:e:105:MET:CB	2.56	0.49
48:o:178:THR:HB	48:o:181:GLN:HB2	1.94	0.49
49:p:85:LYS:HA	49:p:86:ASN:C	2.37	0.49
50:q:15:GLY:C	50:q:19:TRP:HB3	2.28	0.49
51:r:74:PRO:HA	51:r:77:TYR:O	2.11	0.49
45:w:17:SER:OG	45:w:205:HIS:NE2	2.44	0.49
45:w:211:LEU:O	45:w:213:GLN:HB2	2.12	0.49
46:x:155:PRO:HB2	46:x:254:HIS:HE1	1.73	0.49
1:9:168:LEU:HD12	1:9:169:PHE:CG	2.48	0.49
2:4:12:MET:HG2	2:4:16:TRP:CH2	2.48	0.49
2:4:15:THR:OG1	2:4:16:TRP:N	2.45	0.49
2:4:16:TRP:CZ2	70:4:501:3PE:C2G	2.87	0.49
4:7:73:ALA:C	4:7:74:MET:HE2	2.38	0.49
8:1:101:GLY:O	8:1:104:PHE:HB3	2.13	0.49
12:C:214:TYR:CE2	13:D:138:ARG:HD3	2.47	0.49
13:D:86:THR:H	13:D:114:ARG:HH21	1.59	0.49
14:E:189:LYS:NZ	14:E:193:ASN:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:80:VAL:HG13	18:I:82:SER:H	1.76	0.49
26:R:85:ARG:NH2	76:R:601:NAP:N1A	2.59	0.49
26:R:178:SER:O	26:R:181:LEU:N	2.45	0.49
27:S:117:TYR:HB2	27:S:167:ILE:CD1	2.43	0.49
72:S:401:PC1:O14	72:S:401:PC1:H342	2.13	0.49
32:X:38:ARG:HA	32:X:56:TRP:CZ3	2.48	0.49
38:d:63:LEU:HD22	38:d:87:TRP:HE1	1.78	0.49
46:l:121:GLU:O	46:l:125:ASN:ND2	2.46	0.49
46:l:281:ALA:HB1	46:l:290:ASN:HD22	1.78	0.49
47:m:320:LEU:O	47:m:323:CYS:N	2.46	0.49
47:m:377:LEU:HD11	50:q:20:TYR:CE2	2.47	0.49
45:w:132:ASP:O	45:w:136:GLN:N	2.44	0.49
45:w:392:LEU:HA	45:w:395:TRP:HD1	1.78	0.49
77:y:402:HEM:HBC2	77:y:402:HEM:CMC	2.42	0.49
56:A9:266:GLU:HB2	56:A9:267:PRO:HD2	1.95	0.49
62:A4:5:LYS:NZ	62:A4:5:LYS:HB3	2.27	0.49
10:A:567:VAL:HG13	10:A:582:VAL:O	2.13	0.49
12:C:123:THR:CB	16:G:128:PHE:HA	2.43	0.49
13:D:146:GLU:CB	13:D:147:PRO:HD3	2.42	0.49
20:K:94:VAL:O	20:K:97:SER:OG	2.27	0.49
25:Q:69:GLU:O	25:Q:73:GLN:N	2.42	0.49
27:S:335:VAL:HG21	42:j:50:ARG:O	2.12	0.49
28:T:77:SER:CB	28:T:80:VAL:HG21	2.42	0.49
42:j:88:HIS:CD2	42:j:89:ASP:OD1	2.66	0.49
44:e:48:ARG:HA	44:e:49:ALA:HA	1.47	0.49
45:k:252:HIS:CD2	45:k:323:HIS:HE1	2.10	0.49
46:l:72:ALA:HB1	46:l:75:LEU:HD12	1.95	0.49
54:u:52:TRP:C	54:u:56:LYS:H	2.18	0.49
45:w:270:LEU:HD13	45:w:320:LEU:HD11	1.95	0.49
50:A1:75:LEU:HD12	50:A1:76:PRO:HD2	1.94	0.49
54:B2:55:ILE:O	54:B2:58:LYS:HG2	2.12	0.49
57:C4:186:SER:CB	57:C4:213:LEU:HD22	2.40	0.49
2:4:16:TRP:CD1	2:4:17:LEU:N	2.80	0.49
3:2:113:PHE:HE2	28:T:43:LEU:CD2	2.26	0.49
3:2:171:ASN:O	11:B:51:VAL:O	2.31	0.49
3:2:278:LEU:CD1	28:T:136:PHE:CE1	2.96	0.49
5:6:272:TYR:O	5:6:275:SER:OG	2.24	0.49
9:8:244:ASN:CG	9:8:245:VAL:H	2.21	0.49
9:8:306:GLY:O	9:8:308:THR:N	2.46	0.49
16:G:94:THR:HG22	16:G:95:LYS:N	2.28	0.49
19:J:3:PHE:HA	19:J:6:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:6:LEU:C	28:T:6:LEU:CD2	2.86	0.49
28:T:77:SER:CA	28:T:80:VAL:HG13	2.36	0.49
28:T:101:LEU:HG	28:T:110:ILE:HG22	1.93	0.49
45:k:191:LYS:O	45:k:194:ARG:HB2	2.13	0.49
45:k:392:LEU:HA	45:k:395:TRP:HD1	1.78	0.49
48:o:33:TYR:CD1	48:o:37:CYS:HB2	2.48	0.49
50:q:75:LEU:HD12	50:q:76:PRO:HD2	1.93	0.49
46:x:305:GLN:HG2	46:x:306:PRO:HD2	1.95	0.49
53:A3:39:ARG:HG3	53:A3:39:ARG:NH1	2.24	0.49
1:9:149:LEU:CD2	1:9:150:GLU:H	2.22	0.49
1:9:155:LYS:HZ1	1:9:205:ILE:HG21	1.78	0.49
4:7:156:VAL:O	4:7:160:SER:N	2.41	0.49
5:6:175:ASN:O	5:6:179:ASP:N	2.45	0.49
5:6:556:ILE:HD13	35:a:77:TYR:HB2	1.95	0.49
11:B:123:LEU:HD21	13:D:162:TYR:CE2	2.48	0.49
13:D:86:THR:H	13:D:114:ARG:NH2	2.11	0.49
13:D:195:TYR:CE2	29:U:116:ASN:CG	2.89	0.49
18:I:109:THR:CB	18:I:120:ARG:N	2.74	0.49
19:J:2:TRP:HE3	19:J:3:PHE:CD1	2.30	0.49
21:L:23:PHE:CZ	72:L:200:PC1:C27	2.93	0.49
43:g:107:GLN:O	43:g:110:LEU:HB3	2.12	0.49
45:k:292:SER:O	45:k:295:ALA:N	2.41	0.49
77:m:402:HEM:HBC2	77:m:402:HEM:CMC	2.42	0.49
48:o:144:ARG:HB2	48:o:147:LEU:HD12	1.95	0.49
50:q:16:ILE:HG23	50:q:17:ARG:N	2.28	0.49
47:y:59:THR:OG1	47:y:172:LYS:HG2	2.13	0.49
48:z:144:ARG:HB2	48:z:147:LEU:HD12	1.95	0.49
49:A0:10:PHE:O	49:A0:13:TYR:N	2.42	0.49
51:A2:50:PRO:HB2	51:A2:51:PRO:HD3	1.95	0.49
56:A9:476:PHE:CD1	67:C1:15:VAL:HG21	2.48	0.49
58:C2:119:THR:O	62:A4:52:HIS:CE1	2.63	0.49
61:A6:49:VAL:HG21	61:A6:74:LEU:HD12	1.95	0.49
63:A5:24:ASN:ND2	63:A5:26:THR:H	2.11	0.49
1:9:164:THR:HG22	1:9:169:PHE:H	1.78	0.48
2:4:1:MET:CG	2:4:2:LEU:H	2.18	0.48
2:4:421:TYR:OH	35:a:59:VAL:CG1	2.61	0.48
72:2:402:PC1:H241	72:2:402:PC1:H321	1.95	0.48
4:7:125:TRP:HB3	4:7:128:TYR:CB	2.43	0.48
6:5:15:SER:O	6:5:20:LEU:HB2	2.13	0.48
8:1:105:MET:O	8:1:108:MET:N	2.46	0.48
9:8:228:PRO:HB2	9:8:229:PHE:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:103:LEU:HD21	10:A:106:SER:HB3	1.93	0.48
10:A:663:ASN:CG	10:A:664:TYR:H	2.21	0.48
11:B:446:ASP:O	11:B:449:ALA:N	2.44	0.48
12:C:126:ASN:HB3	12:C:149:THR:O	2.13	0.48
13:D:158:ASN:HB3	14:E:150:THR:HG21	1.94	0.48
14:E:105:ARG:HD3	14:E:109:GLY:CA	2.41	0.48
14:E:146:ASP:OD1	14:E:186:ASN:HA	2.13	0.48
25:Q:51:LYS:HZ1	36:b:189:ASN:ND2	2.08	0.48
25:Q:162:ARG:HD3	36:b:149:LEU:CD2	2.43	0.48
45:k:148:VAL:O	45:k:151:ASN:N	2.46	0.48
49:p:147:ILE:N	49:p:148:ALA:HB3	2.28	0.48
54:u:55:ILE:O	54:u:58:LYS:HG2	2.12	0.48
45:w:267:ASN:O	45:w:271:GLN:HG2	2.13	0.48
47:y:78:ILE:HG13	47:y:79:ILE:N	2.27	0.48
48:z:33:TYR:CD1	48:z:37:CYS:HB2	2.48	0.48
3:2:144:GLN:HE21	17:H:3:PHE:HB2	1.78	0.48
5:6:467:ILE:HD13	38:d:77:PHE:CZ	2.46	0.48
8:1:253:GLU:HG2	8:1:254:LEU:N	2.29	0.48
9:8:98:LYS:HA	9:8:101:PHE:CB	2.43	0.48
10:A:50:LEU:HD12	10:A:60:ILE:HD11	1.95	0.48
10:A:121:LEU:CD1	11:B:376:GLU:OE2	2.61	0.48
11:B:88:HIS:HB2	11:B:89:PRO:HD3	1.95	0.48
11:B:216:ARG:HA	14:E:94:SER:HB2	1.93	0.48
11:B:263:THR:OG1	11:B:264:ASN:N	2.47	0.48
11:B:360:ASP:OD1	11:B:360:ASP:N	2.45	0.48
12:C:230:GLN:NE2	12:C:233:ARG:NH1	2.61	0.48
20:K:14:LEU:N	20:K:70:ALA:H	2.10	0.48
23:O:25:MET:HB3	23:O:29:LYS:NZ	2.28	0.48
26:R:143:ASP:O	26:R:146:VAL:N	2.43	0.48
36:b:66:ARG:HH12	36:b:70:LEU:HD11	1.78	0.48
31:M:35:HIS:HB3	31:M:38:LYS:NZ	2.28	0.48
45:k:152:TYR:HD1	45:k:241:ILE:HD13	1.78	0.48
45:k:370:ASP:OD1	45:k:371:GLY:N	2.46	0.48
48:o:228:SER:O	51:r:23:GLN:NE2	2.46	0.48
49:p:75:GLU:HG2	49:p:76:ILE:HA	1.94	0.48
46:x:56:ARG:NE	46:x:103:GLU:OE1	2.46	0.48
46:x:281:ALA:HB1	46:x:290:ASN:HD22	1.78	0.48
49:A0:155:GLY:C	49:A0:157:TYR:N	2.71	0.48
58:C2:65:SER:HB3	58:C2:71:HIS:CE1	2.48	0.48
59:A7:68:PHE:HA	59:A7:71:MET:HG2	1.95	0.48
1:9:41:HIS:HE1	18:I:83:ARG:NH2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:183:ALA:CB	1:9:195:ASP:HA	2.43	0.48
2:4:57:PHE:CE2	2:4:113:MET:HA	2.49	0.48
3:2:321:LYS:HG2	72:2:402:PC1:H251	1.93	0.48
5:6:119:LYS:HD3	71:6:701:CDL:H312	1.94	0.48
5:6:550:SER:OG	5:6:551:SER:N	2.44	0.48
5:6:578:THR:CB	11:B:58:THR:OG1	2.62	0.48
7:3:7:LEU:HD11	7:3:11:PHE:HE2	1.78	0.48
7:3:35:SER:HB2	7:3:37:TYR:HD2	1.78	0.48
10:A:140:GLN:NE2	11:B:382:PHE:CD2	2.81	0.48
10:A:359:ASN:HD21	20:K:68:ARG:NH2	2.12	0.48
11:B:241:MET:CE	11:B:351:MET:HE1	2.42	0.48
13:D:155:SER:OG	13:D:161:GLY:HA2	2.14	0.48
23:O:24:ASP:O	23:O:26:ASN:N	2.47	0.48
47:m:58:ASP:HB2	47:m:61:THR:HB	1.95	0.48
49:p:75:GLU:OE1	49:p:75:GLU:N	2.43	0.48
45:w:370:ASP:OD1	45:w:371:GLY:N	2.46	0.48
47:y:216:ASP:O	47:y:217:LYS:HD2	2.13	0.48
57:C4:59:GLN:O	57:C4:62:GLU:HB2	2.13	0.48
64:B4:39:VAL:O	64:B4:42:LYS:HE2	2.14	0.48
3:2:45:MET:O	3:2:47:ASN:N	2.46	0.48
5:6:578:THR:CG2	11:B:58:THR:OG1	2.61	0.48
6:5:17:VAL:C	6:5:20:LEU:H	2.22	0.48
8:1:136:VAL:O	8:1:139:THR:OG1	2.28	0.48
10:A:403:VAL:HG12	10:A:432:ILE:HD12	1.96	0.48
11:B:253:LEU:HB3	11:B:254:ARG:HH12	1.76	0.48
12:C:232:PHE:HA	13:D:165:TYR:OH	2.13	0.48
13:D:185:GLY:HA3	14:E:154:TYR:HE2	1.78	0.48
13:D:199:GLN:HG3	14:E:178:GLU:HG3	1.93	0.48
18:I:59:ARG:HB3	29:U:125:VAL:HG21	1.94	0.48
19:J:48:MET:O	19:J:51:ASP:N	2.45	0.48
22:N:62:GLU:OE2	22:N:71:ARG:NH1	2.46	0.48
27:S:158:LEU:O	27:S:162:TYR:N	2.37	0.48
27:S:232:THR:O	27:S:235:PRO:HD2	2.13	0.48
28:T:101:LEU:HD11	28:T:110:ILE:C	2.38	0.48
44:e:119:THR:HG1	44:e:120:SER:H	1.54	0.48
45:k:259:GLY:N	45:k:318:GLY:O	2.39	0.48
49:p:20:ASP:OD1	49:p:21:SER:N	2.46	0.48
49:p:62:MET:O	47:y:177:ARG:NH2	2.46	0.48
45:w:148:VAL:O	45:w:151:ASN:N	2.46	0.48
56:A9:197:LEU:O	58:C2:92:LEU:HD22	2.13	0.48
1:9:62:ARG:NE	15:F:86:LEU:CA	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:110:PHE:CD1	2:4:241:TYR:CE2	3.02	0.48
3:2:278:LEU:CD1	28:T:136:PHE:HE1	2.27	0.48
4:7:55:MET:O	4:7:58:LEU:N	2.47	0.48
71:6:701:CDL:H561	71:6:701:CDL:H742	1.95	0.48
8:1:75:PRO:C	8:1:77:MET:N	2.69	0.48
9:8:177:TYR:CD1	9:8:182:ILE:HB	2.46	0.48
11:B:65:PRO:HG2	11:B:71:PRO:HD3	1.95	0.48
20:K:20:ARG:HG2	20:K:54:LEU:HB2	1.95	0.48
26:R:333:PRO:HB3	26:R:337:ASP:OD2	2.14	0.48
36:b:67:PHE:CG	36:b:68:LEU:N	2.81	0.48
42:j:108:THR:CB	43:g:78:GLN:O	2.61	0.48
43:g:8:ASP:HA	43:g:11:PRO:HG3	1.95	0.48
46:l:56:ARG:NE	46:l:103:GLU:OE1	2.46	0.48
46:l:78:LYS:HE3	46:l:129:ALA:HB1	1.95	0.48
51:r:50:PRO:HB2	51:r:51:PRO:HD3	1.95	0.48
47:y:136:GLY:O	47:y:139:SER:OG	2.22	0.48
47:y:320:LEU:O	47:y:323:CYS:N	2.46	0.48
57:C4:16:ILE:HD12	57:C4:17:MET:H	1.77	0.48
5:6:364:LYS:O	5:6:366:MET:HG2	2.14	0.48
8:1:210:GLY:O	8:1:212:ASN:N	2.45	0.48
8:1:237:PHE:HD1	8:1:240:ILE:HD11	1.75	0.48
8:1:256:THR:HA	8:1:259:PHE:HB3	1.96	0.48
9:8:362:ASP:OD1	9:8:449:ARG:NH2	2.46	0.48
10:A:270:VAL:C	10:A:271:MET:HE2	2.39	0.48
11:B:217:VAL:HG13	11:B:218:SER:N	2.28	0.48
11:B:301:ASP:OD1	11:B:301:ASP:C	2.56	0.48
11:B:390:GLN:O	24:P:60:ARG:CD	2.62	0.48
12:C:101:PHE:HE1	12:C:105:HIS:CD2	2.32	0.48
13:D:193:LEU:HD23	13:D:193:LEU:C	2.39	0.48
21:L:59:ASP:HB2	21:L:63:MET:HE3	1.95	0.48
23:O:33:ARG:NH1	31:M:45:LEU:CA	2.76	0.48
26:R:283:VAL:O	26:R:285:HIS:ND1	2.33	0.48
27:S:204:SER:HA	27:S:207:GLN:HB3	1.94	0.48
32:X:20:PHE:O	32:X:23:GLY:N	2.47	0.48
35:a:128:SER:HA	35:a:129:TYR:HB3	1.93	0.48
36:b:70:LEU:HD13	40:h:91:PHE:CE2	2.49	0.48
48:o:23:HIS:HA	48:o:26:ILE:HD12	1.96	0.48
51:r:72:LYS:HA	52:s:56:GLU:OE2	2.14	0.48
45:w:191:LYS:O	45:w:194:ARG:HB2	2.13	0.48
46:x:72:ALA:HB1	46:x:75:LEU:HD12	1.95	0.48
48:z:23:HIS:ND1	48:z:53:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:87:ILE:O	56:A9:173:PRO:HD3	2.13	0.48
57:C4:22:HIS:CE1	64:B4:44:LYS:HD3	2.49	0.48
57:C4:90:ILE:H	57:C4:90:ILE:HD12	1.77	0.48
2:4:14:LEU:O	2:4:14:LEU:HD23	2.14	0.48
2:4:278:ARG:HE	35:a:72:ARG:HH22	1.62	0.48
3:2:30:TRP:HZ3	3:2:67:SER:HB3	1.74	0.48
5:6:556:ILE:HD11	35:a:76:ILE:HD12	0.60	0.48
9:8:281:HIS:CD2	9:8:357:MET:HA	2.47	0.48
9:8:398:ARG:HG3	9:8:403:ASP:CB	2.39	0.48
11:B:238:LEU:HA	30:V:10:MET:HE1	1.96	0.48
12:C:91:HIS:CG	12:C:92:PRO:HD2	2.49	0.48
17:H:43:CYS:HB2	17:H:59:GLU:OE1	2.14	0.48
28:T:18:CYS:C	28:T:75:CYS:HG	2.13	0.48
35:a:121:LEU:HD12	35:a:122:ASP:N	2.28	0.48
36:b:128:GLY:O	36:b:130:GLU:N	2.46	0.48
48:o:33:TYR:CE1	48:o:43:MET:HE2	2.49	0.48
45:w:259:GLY:N	45:w:318:GLY:O	2.39	0.48
46:x:121:GLU:O	46:x:125:ASN:ND2	2.46	0.48
4:7:140:ALA:C	4:7:142:GLY:N	2.72	0.48
6:5:17:VAL:HA	6:5:20:LEU:CB	2.43	0.48
6:5:37:MET:HE3	6:5:67:ALA:HB2	1.96	0.48
6:5:93:LEU:HD12	6:5:94:ASN:HA	1.96	0.48
8:1:169:GLN:NE2	8:1:174:LEU:CB	2.77	0.48
9:8:204:TYR:HB3	9:8:377:GLU:CG	2.43	0.48
10:A:154:LEU:HD12	10:A:155:GLU:HB3	1.96	0.48
10:A:248:THR:O	10:A:248:THR:OG1	2.28	0.48
11:B:178:THR:HG22	11:B:214:TYR:OH	2.14	0.48
16:G:165:SER:CB	16:G:168:LYS:HB2	2.43	0.48
20:K:14:LEU:HG	20:K:17:ARG:NH2	2.29	0.48
23:O:37:ARG:HA	23:O:40:TYR:HB3	1.95	0.48
26:R:167:ILE:HA	26:R:201:ILE:HG22	1.96	0.48
28:T:26:THR:HA	28:T:68:ALA:N	2.29	0.48
36:b:94:GLY:O	43:g:61:TYR:CD2	2.63	0.48
40:h:142:PHE:CE2	43:g:162:ARG:NH2	2.82	0.48
45:k:267:ASN:O	45:k:271:GLN:HG2	2.13	0.48
45:k:270:LEU:HD13	45:k:320:LEU:HD11	1.95	0.48
47:m:216:ASP:O	47:m:217:LYS:HD2	2.13	0.48
46:x:228:GLY:O	46:x:230:LEU:N	2.46	0.48
47:y:58:ASP:HB2	47:y:61:THR:HB	1.95	0.48
53:A3:43:ASP:O	53:A3:47:TYR:HE2	1.86	0.48
56:A9:11:ASN:ND2	56:A9:13:LYS:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:180:CYS:SG	9:8:123:GLY:HA2	2.53	0.48
1:9:206:ASP:HA	1:9:209:LYS:HE2	1.95	0.48
2:4:289:SER:HB3	2:4:406:TYR:OH	2.14	0.48
2:4:360:LEU:CD2	71:6:701:CDL:H532	2.43	0.48
2:4:424:ASN:HA	35:a:57:ARG:CZ	2.35	0.48
2:4:429:SER:HA	2:4:433:GLU:HG3	1.95	0.48
3:2:25:HIS:HB2	17:H:15:ASP:OD2	2.13	0.48
3:2:234:TRP:HZ3	27:S:327:TYR:CE2	2.29	0.48
5:6:298:ILE:O	5:6:302:ILE:HG12	2.14	0.48
5:6:408:ALA:O	5:6:412:THR:N	2.37	0.48
5:6:467:ILE:HD13	38:d:77:PHE:CE1	2.49	0.48
8:1:169:GLN:O	8:1:170:GLU:C	2.55	0.48
8:1:173:TRP:C	8:1:175:ILE:H	2.19	0.48
8:1:312:SER:OG	30:V:55:ARG:CZ	2.62	0.48
10:A:139:LEU:O	11:B:379:ILE:HD13	2.13	0.48
10:A:449:PRO:HD3	10:A:682:ASP:O	2.14	0.48
10:A:643:ARG:HA	10:A:646:LEU:HB2	1.95	0.48
11:B:320:ILE:CD1	14:E:39:LYS:H	2.26	0.48
11:B:322:SER:HB2	14:E:42:ASN:O	2.13	0.48
13:D:191:GLU:C	13:D:193:LEU:N	2.72	0.48
14:E:166:ALA:O	14:E:168:VAL:HG23	2.14	0.48
26:R:329:LEU:HD11	26:R:331:HIS:HD2	1.78	0.48
33:Y:69:TRP:O	33:Y:72:ILE:HG22	2.13	0.48
36:b:93:ILE:HG23	43:g:61:TYR:CZ	2.48	0.48
46:l:354:ASN:N	46:l:355:PRO:HD2	2.29	0.48
47:m:319:PRO:O	47:m:323:CYS:N	2.43	0.48
48:o:186:VAL:O	48:o:189:PHE:N	2.46	0.48
48:z:186:VAL:O	48:z:189:PHE:N	2.46	0.48
2:4:383:MET:HE1	5:6:187:ALA:HB2	1.96	0.48
3:2:114:TRP:CD1	3:2:114:TRP:C	2.90	0.48
3:2:218:MET:HE1	3:2:240:MET:SD	2.54	0.48
4:7:59:ILE:HD12	7:3:70:ALA:CB	2.43	0.48
5:6:68:TRP:CD1	5:6:69:LEU:H	2.32	0.48
5:6:114:ILE:HD11	5:6:118:PHE:CE2	2.48	0.48
5:6:306:THR:HB	5:6:336:LYS:HE3	1.95	0.48
6:5:12:PHE:O	6:5:12:PHE:CG	2.67	0.48
8:1:61:LEU:HD21	13:D:118:ARG:HD2	1.96	0.48
11:B:359:ASP:HB2	24:P:45:PRO:HG2	1.95	0.48
25:Q:111:VAL:HG13	25:Q:115:LEU:HD11	1.95	0.48
27:S:298:ILE:O	27:S:300:VAL:N	2.44	0.48
28:T:114:ALA:O	28:T:118:MET:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:36:PHE:O	42:j:39:TYR:N	2.47	0.48
50:q:19:TRP:O	50:q:22:ASN:HB2	2.14	0.48
45:w:106:LEU:HD22	45:w:203:LEU:HD11	1.96	0.48
46:x:78:LYS:HE3	46:x:129:ALA:HB1	1.95	0.48
47:y:133:LEU:HD11	47:y:182:HIS:HD2	1.79	0.48
47:y:313:ARG:HB2	50:A1:38:HIS:HD2	1.79	0.48
48:z:134:TYR:CE1	48:z:162:PRO:HG3	2.49	0.48
49:A0:7:VAL:HG21	49:A0:10:PHE:CZ	2.48	0.48
56:A9:115:SER:O	56:A9:121:GLY:HA2	2.14	0.48
65:C3:8:LYS:NZ	65:C3:8:LYS:HB3	2.28	0.48
2:4:187:HIS:CG	2:4:188:ASN:H	2.31	0.47
2:4:208:PRO:HB3	2:4:213:HIS:CB	2.42	0.47
3:2:113:PHE:CE2	28:T:43:LEU:HD22	2.49	0.47
6:5:38:LEU:HA	6:5:41:PHE:HB3	1.95	0.47
11:B:118:ARG:HD3	13:D:163:TYR:CE2	2.48	0.47
11:B:261:MET:HE3	11:B:261:MET:HB3	1.64	0.47
12:C:66:TYR:OH	24:P:95:VAL:O	2.27	0.47
13:D:195:TYR:HE2	29:U:116:ASN:CG	2.21	0.47
13:D:199:GLN:HG2	14:E:178:GLU:HG3	1.96	0.47
15:F:86:LEU:O	15:F:90:LEU:N	2.25	0.47
16:G:131:LYS:HZ1	16:G:147:VAL:HG11	1.79	0.47
21:L:23:PHE:HE1	72:L:200:PC1:C2B	2.26	0.47
26:R:205:GLU:O	26:R:239:PRO:HA	2.14	0.47
27:S:175:TYR:HA	27:S:178:VAL:HB	1.96	0.47
27:S:187:LEU:HD13	27:S:277:ARG:HB2	1.96	0.47
27:S:196:ASP:OD2	27:S:250:GLU:C	2.57	0.47
29:U:3:LEU:HD12	29:U:4:LEU:N	2.29	0.47
33:Y:77:TRP:HA	33:Y:78:HIS:HA	1.50	0.47
42:j:114:GLU:HB2	43:g:160:LYS:HD2	1.79	0.47
48:z:41:HIS:HB3	48:z:113:LEU:HG	1.94	0.47
48:z:66:GLU:HA	48:z:84:PRO:HD2	1.96	0.47
53:A3:24:TRP:NE1	54:B2:18:SER:OG	2.47	0.47
53:A3:43:ASP:OD1	53:A3:47:TYR:CD2	2.67	0.47
54:B2:52:TRP:C	54:B2:56:LYS:H	2.18	0.47
56:A9:507:GLU:O	56:A9:508:PRO:O	2.32	0.47
57:C4:148:MET:HE3	57:C4:148:MET:HB3	1.77	0.47
3:2:14:MET:HE2	3:2:133:TRP:CZ2	2.49	0.47
3:2:122:ILE:HG22	3:2:124:LEU:H	1.78	0.47
5:6:246:LEU:O	5:6:251:THR:OG1	2.31	0.47
5:6:362:LEU:HA	5:6:431:LEU:HD22	1.96	0.47
8:1:171:GLN:H	8:1:171:GLN:NE2	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:171:GLN:NE2	8:1:171:GLN:C	2.72	0.47
10:A:343:GLY:HA3	10:A:369:GLU:H	1.79	0.47
10:A:373:PRO:HD2	10:A:481:LEU:HG	1.95	0.47
10:A:522:GLN:O	10:A:525:ALA:N	2.47	0.47
10:A:607:LYS:HE2	16:G:78:ARG:NE	2.28	0.47
10:A:643:ARG:O	10:A:647:GLU:N	2.47	0.47
11:B:123:LEU:CD1	12:C:206:LEU:CD2	2.87	0.47
12:C:95:VAL:N	12:C:97:PRO:HD2	2.29	0.47
12:C:242:GLU:CA	16:G:92:ASN:ND2	2.77	0.47
13:D:173:CYS:O	13:D:173:CYS:SG	2.71	0.47
22:N:86:ASN:OD1	22:N:86:ASN:N	2.46	0.47
26:R:64:PHE:CZ	26:R:208:GLY:HA3	2.49	0.47
28:T:90:TYR:CD1	28:T:126:LYS:HE3	2.49	0.47
29:U:26:VAL:O	29:U:29:ARG:HG2	2.14	0.47
29:U:47:LYS:O	29:U:86:TRP:HH2	1.97	0.47
40:h:149:LEU:HD21	43:g:167:ARG:CA	2.43	0.47
45:k:424:GLY:C	45:k:428:ILE:HD11	2.39	0.47
47:m:59:THR:OG1	47:m:172:LYS:HG2	2.13	0.47
47:m:133:LEU:HD11	47:m:182:HIS:HD2	1.79	0.47
48:o:5:LEU:CD1	52:s:63:HIS:HB2	2.44	0.47
48:o:134:TYR:CE1	48:o:162:PRO:HG3	2.49	0.47
47:y:312:GLN:HE21	47:y:318:ARG:HG3	1.78	0.47
2:4:31:SER:OG	2:4:74:PRO:HB3	2.15	0.47
2:4:278:ARG:HH21	35:a:72:ARG:NH2	2.10	0.47
3:2:112:HIS:HE2	3:2:164:ILE:HD13	1.79	0.47
5:6:19:ILE:HG23	71:6:701:CDL:H372	1.94	0.47
5:6:128:MET:HE2	5:6:251:THR:HA	1.97	0.47
10:A:454:ASP:HB2	10:A:460:HIS:CE1	2.49	0.47
11:B:61:TRP:CZ3	11:B:64:PRO:HG3	2.42	0.47
11:B:205:GLU:OE2	14:E:82:ALA:CB	2.62	0.47
20:K:39:LYS:HG3	20:K:84:ALA:HB1	1.96	0.47
21:L:9:LEU:HD21	72:L:200:PC1:C38	2.41	0.47
27:S:335:VAL:HB	42:j:52:PRO:N	2.29	0.47
34:Z:64:VAL:O	34:Z:67:LEU:N	2.47	0.47
37:c:75:VAL:O	37:c:78:PRO:HD2	2.15	0.47
40:h:86:ASN:HA	40:h:89:VAL:HG12	1.96	0.47
45:k:292:SER:HB3	45:k:295:ALA:HB3	1.94	0.47
46:l:156:GLN:O	46:l:160:ILE:HG12	2.14	0.47
46:x:50:PHE:CE2	46:x:383:GLY:HA3	2.50	0.47
46:x:156:GLN:O	46:x:160:ILE:HG12	2.14	0.47
57:C4:83:ILE:O	57:C4:87:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:153:GLN:HG3	1:9:158:ILE:O	2.14	0.47
2:4:423:ILE:HD12	35:a:57:ARG:CB	2.44	0.47
3:2:234:TRP:CZ3	27:S:327:TYR:CD2	3.02	0.47
4:7:151:THR:O	4:7:155:ILE:HG22	2.15	0.47
5:6:463:PHE:O	5:6:467:ILE:HG12	2.14	0.47
8:1:11:ILE:HB	8:1:12:PRO:HD3	1.95	0.47
9:8:93:PHE:HE2	9:8:98:LYS:HD3	1.79	0.47
9:8:207:GLY:O	73:8:501:FMN:C8	2.61	0.47
10:A:359:ASN:HD21	20:K:68:ARG:HH22	1.61	0.47
10:A:405:THR:OG1	10:A:410:GLU:OE2	2.30	0.47
13:D:181:ILE:HD13	13:D:200:LEU:HD13	1.96	0.47
14:E:197:TRP:O	14:E:197:TRP:CD1	2.67	0.47
22:N:40:LYS:HB2	22:N:45:ARG:NH1	2.29	0.47
23:O:83:VAL:O	23:O:87:LYS:N	2.39	0.47
28:T:33:GLY:O	28:T:36:VAL:HG12	2.14	0.47
31:W:140:CYS:HB3	31:W:143:GLU:CB	2.43	0.47
40:h:95:PHE:O	40:h:96:SER:OG	2.20	0.47
46:l:33:LEU:HB3	46:l:201:SER:O	2.15	0.47
53:t:28:GLY:O	53:t:32:LEU:N	2.35	0.47
46:x:354:ASN:N	46:x:355:PRO:HD2	2.29	0.47
47:y:207:ASN:HB2	47:y:208:PRO:HD2	1.96	0.47
54:B2:58:LYS:HG3	54:B2:59:TYR:H	1.80	0.47
2:4:447:LEU:HA	71:4:502:CDL:H351	1.97	0.47
3:2:60:PHE:CZ	6:5:70:GLU:OE2	2.67	0.47
9:8:330:SER:O	9:8:332:CYS:N	2.48	0.47
10:A:61:PRO:HG3	10:A:146:PHE:HE2	1.76	0.47
10:A:217:GLU:C	10:A:219:SER:H	2.22	0.47
10:A:257:VAL:HG23	10:A:258:GLY:O	2.15	0.47
11:B:177:ILE:HG23	11:B:210:MET:HE3	1.96	0.47
11:B:205:GLU:CD	14:E:82:ALA:HB3	2.40	0.47
27:S:333:GLU:O	27:S:335:VAL:N	2.40	0.47
28:T:6:LEU:HD23	28:T:6:LEU:O	2.15	0.47
38:d:18:ASP:O	38:d:20:LEU:N	2.47	0.47
38:d:34:ARG:HA	38:d:35:LYS:HA	1.53	0.47
39:f:163:LEU:H	39:f:166:LEU:HB2	1.78	0.47
48:o:66:GLU:HA	48:o:84:PRO:HD2	1.96	0.47
54:u:58:LYS:HG3	54:u:59:TYR:H	1.80	0.47
48:z:239:PRO:HG2	48:z:241:LYS:OXT	2.15	0.47
52:B3:36:ARG:HA	52:B3:39:LEU:HD12	1.97	0.47
58:C2:80:ARG:O	58:C2:84:ILE:HG12	2.14	0.47
59:A7:79:LYS:HZ3	66:B0:15:ASN:HD21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:54:ASP:OD1	1:9:60:TYR:OH	2.33	0.47
2:4:166:TYR:CB	70:4:503:3PE:O22	2.57	0.47
3:2:255:PRO:N	3:2:256:PRO:HD2	2.30	0.47
5:6:321:GLN:OE1	5:6:324:LEU:HD12	2.14	0.47
5:6:349:SER:OG	5:6:443:ILE:HA	2.14	0.47
5:6:536:LEU:O	5:6:539:TYR:N	2.47	0.47
5:6:556:ILE:O	5:6:560:ALA:N	2.45	0.47
7:3:52:SER:O	7:3:55:PHE:HB2	2.14	0.47
9:8:101:PHE:CG	9:8:102:MET:N	2.82	0.47
9:8:346:GLN:NE2	9:8:440:ARG:HD3	2.30	0.47
11:B:421:ARG:NH2	11:B:423:LYS:HD3	2.29	0.47
12:C:95:VAL:HG13	12:C:96:ILE:H	1.80	0.47
13:D:83:TRP:CD1	13:D:112:VAL:HG12	2.49	0.47
13:D:199:GLN:HG3	14:E:178:GLU:CD	2.38	0.47
22:N:42:ALA:HB2	22:N:100:TRP:CB	2.45	0.47
22:N:59:VAL:O	22:N:61:ALA:HA	2.14	0.47
23:O:115:PRO:C	23:O:117:ASP:H	2.22	0.47
25:Q:81:PRO:HA	25:Q:84:GLU:OE2	2.14	0.47
27:S:26:TYR:O	27:S:30:ALA:HB3	2.14	0.47
35:a:22:GLU:H	35:a:22:GLU:CD	2.22	0.47
45:k:106:LEU:HD22	45:k:203:LEU:HD11	1.96	0.47
46:l:304:HIS:CD2	46:l:305:GLN:H	2.33	0.47
48:o:23:HIS:ND1	48:o:53:GLY:O	2.47	0.47
48:o:239:PRO:HG2	48:o:241:LYS:OXT	2.14	0.47
49:p:71:MET:HG3	49:p:72:SER:N	2.23	0.47
52:s:36:ARG:HA	52:s:39:LEU:HD12	1.97	0.47
45:w:61:HIS:HB3	45:w:65:LYS:NZ	2.29	0.47
45:w:152:TYR:HD1	45:w:241:ILE:HD13	1.78	0.47
46:x:233:SER:O	46:x:235:ALA:N	2.48	0.47
46:x:312:PHE:HB2	55:B1:57:GLY:HA2	1.97	0.47
1:9:149:LEU:HD23	1:9:150:GLU:N	2.24	0.47
2:4:114:GLU:HB3	2:4:175:ASN:O	2.15	0.47
2:4:190:TRP:CB	28:T:127:MET:CG	2.84	0.47
2:4:419:TYR:CD1	2:4:420:THR:HA	2.50	0.47
2:4:431:THR:HG21	40:h:91:PHE:HZ	1.79	0.47
70:4:501:3PE:H331	70:4:501:3PE:H362	1.56	0.47
3:2:113:PHE:HE2	28:T:43:LEU:HD21	1.78	0.47
3:2:219:PHE:O	3:2:223:SER:OG	2.29	0.47
4:7:77:GLU:H	4:7:77:GLU:CD	2.23	0.47
5:6:89:PHE:O	5:6:92:VAL:N	2.48	0.47
5:6:96:VAL:O	5:6:99:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:116:LYS:HE2	71:6:701:CDL:OA8	2.15	0.47
5:6:435:PRO:CG	34:Z:57:PHE:CD2	2.92	0.47
5:6:489:THR:HA	5:6:492:ILE:HD12	1.96	0.47
5:6:584:ILE:HG23	6:5:90:VAL:HG22	1.96	0.47
6:5:15:SER:O	6:5:16:LEU:C	2.58	0.47
7:3:64:LEU:HD23	7:3:64:LEU:HA	1.70	0.47
8:1:311:THR:CG2	30:V:51:MET:HG3	2.45	0.47
10:A:77:MET:HG3	10:A:77:MET:O	2.15	0.47
10:A:401:LEU:O	10:A:474:VAL:HA	2.14	0.47
11:B:266:ARG:NH2	14:E:66:LEU:CB	2.78	0.47
11:B:288:PHE:CD2	11:B:292:MET:HE3	2.49	0.47
11:B:431:HIS:HB3	11:B:454:GLN:HB3	1.97	0.47
13:D:138:ARG:NH2	13:D:142:ASP:N	2.62	0.47
18:I:105:LYS:O	18:I:106:GLU:HG3	2.13	0.47
25:Q:121:ASP:CG	25:Q:122:LEU:H	2.22	0.47
26:R:163:LYS:O	26:R:165:ILE:HG13	2.15	0.47
26:R:271:TYR:OH	26:R:325:THR:HG21	2.14	0.47
26:R:309:PRO:C	26:R:310:PHE:CD2	2.92	0.47
27:S:102:LEU:HD23	27:S:105:PHE:CE2	2.50	0.47
28:T:26:THR:HA	28:T:67:GLY:C	2.40	0.47
32:X:43:LEU:HA	32:X:44:TYR:C	2.40	0.47
34:Z:41:LEU:N	34:Z:42:ARG:HA	2.26	0.47
34:Z:79:VAL:C	34:Z:82:ILE:H	2.23	0.47
43:g:34:THR:HG23	43:g:35:LYS:HD2	1.96	0.47
48:o:49:ARG:O	48:o:51:LEU:N	2.46	0.47
49:p:30:GLU:OE2	54:u:10:TYR:HD2	1.97	0.47
45:w:251:ALA:HB3	45:w:331:ILE:HD11	1.97	0.47
48:z:33:TYR:CE1	48:z:43:MET:HE2	2.49	0.47
50:A1:88:SER:O	50:A1:90:LEU:N	2.48	0.47
52:B3:22:GLU:HA	52:B3:25:GLU:HG2	1.97	0.47
53:A3:15:ARG:HG3	53:A3:16:ASN:N	2.27	0.47
53:A3:39:ARG:CG	53:A3:39:ARG:NH1	2.77	0.47
56:A9:172:LYS:HB3	56:A9:176:MET:HE2	1.96	0.47
56:A9:195:LEU:CD2	56:A9:245:ILE:HD13	2.45	0.47
56:A9:397:PHE:HB3	56:A9:398:PRO:HD3	1.95	0.47
57:C4:63:THR:O	57:C4:66:THR:HG22	2.15	0.47
57:C4:108:TYR:N	57:C4:108:TYR:CD1	2.83	0.47
59:A7:41:LYS:HD3	59:A7:62:LEU:HD23	1.97	0.47
2:4:95[B]:PHE:CE2	2:4:136:TRP:CD1	3.03	0.47
3:2:234:TRP:CE3	27:S:327:TYR:CE2	3.03	0.47
72:2:402:PC1:H261	72:2:402:PC1:H292	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:303:ALA:O	5:6:306:THR:HG22	2.14	0.47
10:A:168:LEU:HD13	10:A:292:PHE:HE2	1.79	0.47
10:A:246:ARG:HB2	10:A:265:THR:HG23	1.97	0.47
10:A:385:TYR:CZ	10:A:526:LEU:HD22	2.49	0.47
12:C:192:ASP:CB	13:D:132:LYS:HG3	2.44	0.47
12:C:211:GLU:HB2	12:C:226:VAL:HG23	1.97	0.47
19:J:16:LEU:C	19:J:19:PRO:HD2	2.39	0.47
23:O:54:ILE:HB	23:O:58:GLN:OE1	2.14	0.47
27:S:124:TYR:CE1	27:S:151:ILE:HD11	2.50	0.47
56:A9:11:ASN:ND2	56:A9:14:ASP:H	2.07	0.47
58:C2:173:PHE:CD1	58:C2:173:PHE:C	2.92	0.47
61:A6:31:TYR:HE1	61:A6:98:HIS:HE1	1.62	0.47
2:4:139:GLN:H	2:4:222:GLU:CD	2.14	0.47
2:4:227:GLY:CA	2:4:230:VAL:HB	2.43	0.47
9:8:61:ASP:HA	9:8:256:ARG:HH12	1.80	0.47
9:8:103:ASN:ND2	9:8:149:MET:HE1	2.29	0.47
11:B:266:ARG:NH1	70:B:501:3PE:H231	2.25	0.47
11:B:297:GLY:O	11:B:298:ILE:C	2.58	0.47
22:N:35:LEU:CD2	22:N:45:ARG:HG3	2.45	0.47
22:N:80:VAL:O	22:N:83:GLN:HB2	2.15	0.47
25:Q:165:SER:OG	42:j:83:TYR:CG	2.51	0.47
26:R:355:ARG:O	26:R:357:ARG:N	2.47	0.47
37:c:115:GLU:HA	38:d:65:ARG:HH12	1.80	0.47
31:M:64:ASP:OD1	31:M:65:ILE:N	2.45	0.47
46:l:50:PHE:CE2	46:l:383:GLY:HA3	2.50	0.47
50:q:28:LYS:CB	50:q:74:ILE:HD11	2.40	0.47
48:z:23:HIS:HA	48:z:26:ILE:HD12	1.96	0.47
48:z:165:TYR:CZ	48:z:168:VAL:HA	2.50	0.47
55:B1:66:ALA:HB2	55:B1:77:ARG:NH2	2.30	0.47
56:A9:306:THR:HB	56:A9:359:ALA:O	2.15	0.47
57:C4:4:PRO:HB2	66:B0:43:SER:HA	1.96	0.47
58:C2:164:PHE:O	58:C2:168:THR:HG23	2.14	0.47
59:A7:23:PRO:HB3	60:C0:70:VAL:CG2	2.45	0.47
5:6:437:PHE:CD1	5:6:441:VAL:HG21	2.49	0.47
8:1:172:MET:CE	8:1:176:LEU:CB	2.93	0.47
10:A:688:GLN:O	10:A:689:LEU:HD12	2.14	0.47
11:B:61:TRP:CD1	11:B:61:TRP:C	2.88	0.47
12:C:214:TYR:H	13:D:176:ILE:HD13	1.80	0.47
14:E:89:GLU:HG2	29:U:61:TRP:HB3	1.97	0.47
16:G:121:LEU:C	16:G:123:ASN:H	2.19	0.47
20:K:28:PRO:HA	20:K:34:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:147:LYS:O	26:R:151:ALA:N	2.38	0.47
38:d:63:LEU:HD13	38:d:87:TRP:NE1	2.30	0.47
72:j:201:PC1:O32	72:j:201:PC1:H132	2.15	0.47
44:e:132:HIS:C	44:e:135:GLY:H	2.23	0.47
45:k:61:HIS:HB3	45:k:65:LYS:NZ	2.29	0.47
46:l:233:SER:O	46:l:235:ALA:N	2.48	0.47
50:q:88:SER:O	50:q:90:LEU:N	2.48	0.47
52:s:22:GLU:HA	52:s:25:GLU:HG2	1.97	0.47
46:x:78:LYS:CB	46:x:129:ALA:HB1	2.45	0.47
59:A7:33:LEU:HD13	59:A7:41:LYS:HG3	1.97	0.47
59:A7:108:PRO:HG2	59:A7:111:PHE:CD2	2.50	0.47
2:4:163:ALA:CB	70:4:503:3PE:H241	2.45	0.46
3:2:5:ILE:HG13	3:2:6:PHE:N	2.30	0.46
3:2:169:GLY:CA	3:2:292:PHE:HE1	2.28	0.46
4:7:125:TRP:CE3	4:7:125:TRP:HA	2.49	0.46
5:6:477:ILE:HD12	38:d:87:TRP:CZ2	2.50	0.46
8:1:237:PHE:O	8:1:240:ILE:N	2.36	0.46
10:A:163:LYS:HZ1	10:A:207:GLY:HA3	1.79	0.46
10:A:319:TRP:CG	23:O:122:PHE:CE2	3.03	0.46
10:A:430:ALA:HB2	10:A:462:PHE:HZ	1.79	0.46
11:B:179:ARG:O	11:B:183:HIS:CD2	2.69	0.46
22:N:70:GLU:C	22:N:72:LEU:H	2.23	0.46
26:R:43:HIS:HB2	26:R:51:VAL:CG2	2.45	0.46
27:S:335:VAL:H	42:j:52:PRO:CD	2.27	0.46
28:T:30:GLY:HA2	28:T:64:ALA:CA	2.45	0.46
36:b:153:GLU:O	36:b:157:ARG:N	2.48	0.46
45:k:383:LEU:HD23	45:k:388:ARG:HA	1.97	0.46
45:k:436:ARG:NH2	47:m:221:HIS:HB3	2.27	0.46
47:m:207:ASN:HB2	47:m:208:PRO:HD2	1.96	0.46
47:m:376:LEU:O	50:q:17:ARG:HD3	2.15	0.46
54:u:58:LYS:HG3	54:u:59:TYR:N	2.31	0.46
45:w:424:GLY:C	45:w:428:ILE:HD11	2.39	0.46
46:x:230:LEU:HD12	46:x:230:LEU:O	2.15	0.46
47:y:35:SER:O	47:y:38:GLY:N	2.49	0.46
53:A3:40:LEU:CD1	53:A3:47:TYR:CD1	2.97	0.46
68:A8:1:ILE:HG23	68:A8:1:ILE:O	2.15	0.46
1:9:110:MET:HG2	10:A:194:ASP:O	2.16	0.46
1:9:137:THR:O	1:9:141:MET:N	2.44	0.46
3:2:33:PHE:CE1	3:2:105:LYS:HE3	2.51	0.46
4:7:12:ILE:O	4:7:16:GLY:N	2.48	0.46
5:6:385:PHE:HB3	33:Y:72:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:437:PHE:O	34:Z:52:ARG:CZ	2.62	0.46
7:3:112:GLU:OE1	8:1:290:TRP:CD1	2.68	0.46
8:1:178:ALA:C	8:1:180:PRO:HD2	2.40	0.46
8:1:221:ALA:O	8:1:225:MET:N	2.48	0.46
9:8:390:ASP:OD2	10:A:202:ASN:HB2	2.16	0.46
11:B:137:ASP:HB2	11:B:148:GLU:OE2	2.14	0.46
12:C:150:ASP:CG	12:C:151:GLU:H	2.17	0.46
13:D:180:ASP:HB3	13:D:181:ILE:HD12	1.96	0.46
14:E:106:TYR:CE1	14:E:112:ARG:NH1	2.83	0.46
17:H:65:GLU:OE2	17:H:71:LYS:HD3	2.15	0.46
18:I:108:LYS:CE	18:I:108:LYS:CA	2.85	0.46
23:O:55:SER:OG	23:O:58:GLN:HG3	2.15	0.46
25:Q:81:PRO:O	25:Q:84:GLU:HG2	2.15	0.46
26:R:228:LEU:HA	26:R:229:ILE:HA	1.53	0.46
27:S:73:HIS:CD2	27:S:74:PHE:N	2.84	0.46
72:S:401:PC1:O14	72:S:401:PC1:H321	2.16	0.46
36:b:159:LEU:HD12	36:b:161:ARG:HB2	1.96	0.46
45:k:217:SER:N	45:k:218:GLY:CA	2.78	0.46
45:k:251:ALA:HB3	45:k:331:ILE:HD11	1.97	0.46
46:l:203:ARG:HD2	46:l:231:GLY:HA2	1.97	0.46
45:w:64:PHE:CD1	45:w:86:LEU:HD21	2.51	0.46
50:A1:13:LEU:C	50:A1:14:GLU:CG	2.68	0.46
56:A9:240:HIS:NE2	56:A9:244:TYR:CE2	2.81	0.46
59:A7:102:TYR:CD2	68:A8:35:TYR:HE1	2.33	0.46
70:4:503:3PE:H361	3:2:277:ILE:HD13	1.98	0.46
3:2:110:PRO:HD2	3:2:157:LEU:CD2	2.46	0.46
5:6:116:LYS:HG2	5:6:119:LYS:HZ3	1.76	0.46
5:6:285:THR:HG22	5:6:311:GLY:HA3	1.96	0.46
8:1:71:PHE:C	8:1:72:ILE:HG13	2.40	0.46
9:8:52:ARG:HH12	9:8:168:ASN:ND2	2.14	0.46
9:8:97:LEU:O	9:8:101:PHE:N	2.48	0.46
9:8:99:TRP:CD1	9:8:99:TRP:N	2.79	0.46
9:8:230:PRO:O	9:8:232:ASP:N	2.49	0.46
11:B:101:LEU:HA	11:B:106:VAL:O	2.16	0.46
14:E:111:GLU:O	14:E:113:CYS:N	2.49	0.46
18:I:85:ILE:HG22	18:I:86:SER:N	2.30	0.46
21:L:19:LEU:HD21	72:L:200:PC1:H153	1.98	0.46
25:Q:83:THR:HA	25:Q:86:TRP:HE1	1.80	0.46
26:R:171:ASN:OD1	26:R:326:ASP:HB3	2.15	0.46
45:k:92:ARG:NH1	45:k:154:HIS:CG	2.83	0.46
46:l:276:GLN:HG3	46:l:277:HIS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:344:GLU:O	47:m:348:ILE:HG13	2.16	0.46
45:w:343:MET:HE1	45:w:416:TYR:CD2	2.50	0.46
49:A0:156:TYR:N	49:A0:165:TYR:CB	2.78	0.46
52:B3:21:ARG:HH11	52:B3:65:ARG:NH2	2.13	0.46
65:C3:16:ASN:ND2	65:C3:16:ASN:H	2.12	0.46
2:4:80:SER:HA	2:4:226:ALA:HB2	1.96	0.46
2:4:112:ALA:O	2:4:114:GLU:N	2.49	0.46
2:4:158:LEU:HB2	2:4:159:PRO:HD3	1.97	0.46
2:4:368:ALA:HB1	2:4:375:LEU:HG	1.97	0.46
3:2:33:PHE:CD1	3:2:105:LYS:HE3	2.50	0.46
70:2:401:3PE:O14	42:j:63:LEU:HD22	2.15	0.46
8:1:205:SER:H	8:1:279:ARG:NH1	2.13	0.46
9:8:416:SER:O	9:8:420:GLU:OE2	2.33	0.46
10:A:366:LEU:O	10:A:531:LYS:HG2	2.15	0.46
13:D:106:MET:SD	13:D:194:LEU:HD21	2.56	0.46
13:D:215:ARG:HD3	76:R:601:NAP:O1X	2.13	0.46
14:E:38:TYR:CE1	24:P:104:TRP:HB2	2.50	0.46
23:O:48:HIS:C	26:R:359:TYR:HE1	2.24	0.46
25:Q:8:PRO:C	30:V:88:ARG:NH2	2.73	0.46
25:Q:81:PRO:HB2	25:Q:107:PHE:HA	1.97	0.46
30:V:48:TRP:CZ2	30:V:52:LYS:HE3	2.51	0.46
37:c:94:PRO:HB2	43:g:10:TYR:CE1	2.51	0.46
43:g:48:VAL:O	43:g:51:PHE:HB3	2.16	0.46
45:k:17:SER:OG	45:k:205:HIS:NE2	2.44	0.46
46:l:312:PHE:N	46:l:323:GLY:O	2.39	0.46
46:x:276:GLN:HG3	46:x:277:HIS:N	2.31	0.46
48:z:49:ARG:O	48:z:51:LEU:N	2.46	0.46
57:C4:58:ALA:O	57:C4:60:GLU:HG3	2.16	0.46
2:4:48:ASN:OD1	43:g:90:MET:SD	2.74	0.46
3:2:150:ASN:HD22	5:6:604:PHE:HA	1.81	0.46
4:7:152:TRP:HA	4:7:155:ILE:HG22	1.96	0.46
5:6:119:LYS:HZ2	71:6:701:CDL:C31	2.28	0.46
5:6:264:TYR:HA	5:6:267:THR:HG22	1.97	0.46
5:6:577:VAL:HG13	6:5:97:GLN:CD	2.40	0.46
10:A:140:GLN:NE2	11:B:382:PHE:HD2	2.14	0.46
11:B:292:MET:HG3	11:B:329:ARG:HE	1.81	0.46
13:D:199:GLN:HG2	14:E:178:GLU:CG	2.45	0.46
14:E:65:GLU:O	14:E:66:LEU:HB3	2.15	0.46
16:G:147:VAL:HG12	16:G:148:GLU:O	2.16	0.46
23:O:126:HIS:C	23:O:128:PRO:HD3	2.40	0.46
35:a:51:TYR:HA	35:a:56:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:M:64:ASP:C	31:M:66:ASP:H	2.23	0.46
49:A0:122:HIS:CB	49:A0:168:SER:N	2.79	0.46
55:B1:62:ARG:HG2	55:B1:63:PRO:HD2	1.98	0.46
57:C4:185:MET:SD	57:C4:185:MET:C	2.99	0.46
2:4:437:MET:HE2	2:4:437:MET:HB2	1.80	0.46
3:2:109:ALA:CB	3:2:110:PRO:HD3	2.46	0.46
3:2:137:ALA:HB3	3:2:138:PRO:HD3	1.97	0.46
5:6:439:THR:HG23	31:W:82:ARG:HH12	1.81	0.46
8:1:185:TRP:NE1	8:1:238:THR:OG1	2.46	0.46
10:A:253:VAL:HG23	10:A:253:VAL:O	2.15	0.46
10:A:272:ARG:NH1	10:A:274:LEU:HD21	2.31	0.46
10:A:312:GLY:N	29:U:144:TYR:CE1	2.79	0.46
10:A:357:LEU:HD23	10:A:358:LEU:HD12	1.97	0.46
11:B:238:LEU:HD11	24:P:37:PRO:O	2.15	0.46
13:D:215:ARG:NE	76:R:601:NAP:O1X	2.49	0.46
22:N:77:ILE:O	22:N:80:VAL:N	2.48	0.46
25:Q:93:GLY:C	25:Q:95:GLN:H	2.22	0.46
25:Q:162:ARG:HD3	36:b:149:LEU:HD22	1.97	0.46
26:R:196:PRO:HG2	26:R:197:GLU:OE1	2.16	0.46
39:f:28:GLU:HA	39:f:31:CYS:SG	2.56	0.46
40:h:120:ARG:HH22	43:g:66:ARG:N	1.97	0.46
43:g:125:CYS:HB3	43:g:128:GLU:OE1	2.15	0.46
62:A4:67:HIS:CD2	62:A4:78:LEU:HD11	2.50	0.46
2:4:2:LEU:HD23	2:4:6:ILE:HD11	1.97	0.46
2:4:353:PRO:O	71:6:701:CDL:HA22	2.14	0.46
3:2:67:SER:O	3:2:70:LEU:HB3	2.15	0.46
3:2:291:TYR:CG	3:2:291:TYR:O	2.69	0.46
5:6:15:LEU:C	5:6:18:PRO:HD2	2.40	0.46
5:6:548:SER:O	5:6:552:LEU:HB3	2.15	0.46
8:1:184:MET:HE2	8:1:293:PHE:CD1	2.51	0.46
10:A:121:LEU:HA	10:A:121:LEU:HD23	1.62	0.46
11:B:208:GLU:O	11:B:210:MET:N	2.49	0.46
13:D:134:ALA:HB3	13:D:135:PRO:HD3	1.98	0.46
14:E:116:CYS:SG	74:E:302:SF4:S2	3.13	0.46
22:N:106:GLU:HG3	22:N:107:PRO:HD2	1.96	0.46
25:Q:89:ILE:N	25:Q:100:CYS:SG	2.88	0.46
25:Q:158:LEU:CG	25:Q:159:LYS:N	2.26	0.46
26:R:70:VAL:HG13	26:R:80:VAL:HG11	1.97	0.46
26:R:309:PRO:O	26:R:310:PHE:CD2	2.69	0.46
72:S:401:PC1:H372	72:S:401:PC1:H341	1.67	0.46
43:g:151:SER:C	43:g:153:ARG:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:153:ILE:HG23	47:m:154:PRO:HD2	1.97	0.46
49:A0:2:HIS:C	49:A0:4:ASP:H	2.22	0.46
50:A1:10:SER:HB3	50:A1:11:ARG:H	1.57	0.46
56:A9:435:GLY:O	56:A9:437:PRO:HD3	2.16	0.46
59:A7:33:LEU:HD22	59:A7:37:GLN:HB3	1.97	0.46
65:C3:11:LEU:HD23	65:C3:11:LEU:O	2.15	0.46
1:9:155:LYS:NZ	1:9:205:ILE:HG21	2.31	0.46
2:4:208:PRO:HG2	2:4:216:LEU:HD22	1.98	0.46
71:4:502:CDL:H151	71:4:502:CDL:H122	1.48	0.46
3:2:72:MET:O	3:2:76:ILE:HG12	2.16	0.46
5:6:1:MET:HA	5:6:4:PHE:HB2	1.97	0.46
5:6:150:MET:CE	71:6:701:CDL:C58	2.92	0.46
9:8:52:ARG:HH22	9:8:168:ASN:ND2	2.14	0.46
9:8:174:ARG:NH2	15:F:92:LEU:CB	2.79	0.46
9:8:295:PRO:HD2	9:8:298:GLU:OE2	2.15	0.46
10:A:381:LEU:HD21	10:A:664:TYR:O	2.15	0.46
11:B:173:LEU:HD11	11:B:244:ILE:HD13	1.98	0.46
14:E:189:LYS:HZ2	14:E:193:ASN:HB2	1.79	0.46
17:H:77:HIS:ND1	17:H:77:HIS:O	2.48	0.46
23:O:45:ASN:OD1	23:O:48:HIS:NE2	2.48	0.46
24:P:33:LYS:O	24:P:34:ARG:HD3	2.15	0.46
27:S:45:SER:O	27:S:144:GLY:HA2	2.15	0.46
27:S:117:TYR:HE1	27:S:175:TYR:CD2	2.33	0.46
29:U:64:TYR:HE1	29:U:81:MET:HB2	1.81	0.46
30:V:80:ASP:OD1	30:V:81:ARG:N	2.49	0.46
33:Y:47:TYR:HE2	34:Z:16:LEU:HD12	1.78	0.46
35:a:67:ARG:HH11	44:e:79:PRO:CD	2.27	0.46
48:o:165:TYR:CZ	48:o:168:VAL:HA	2.50	0.46
50:q:49:ARG:HD3	46:x:135:TRP:CD2	2.51	0.46
52:s:21:ARG:HH11	52:s:65:ARG:NH2	2.13	0.46
45:w:57:TYR:OH	45:w:137:GLU:OE1	2.30	0.46
46:x:33:LEU:HB3	46:x:201:SER:O	2.15	0.46
57:C4:41:ILE:O	57:C4:45:MET:HG2	2.16	0.46
3:2:51:ARG:HG3	11:B:69:VAL:HG21	1.98	0.46
3:2:326:LEU:HD11	72:2:402:PC1:C2B	2.37	0.46
4:7:14:VAL:HG21	6:5:7:ASN:CG	2.41	0.46
4:7:100:GLU:HA	4:7:103:MET:HB3	1.97	0.46
4:7:107:VAL:HG13	4:7:108:LEU:N	2.25	0.46
5:6:120:TYR:HB3	5:6:154:LEU:HD21	1.97	0.46
5:6:484:TYR:C	5:6:486:LEU:H	2.24	0.46
6:5:24:SER:CB	6:5:89:TYR:HA	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:6:ILE:O	8:1:8:MET:N	2.49	0.46
10:A:139:LEU:HD23	10:A:139:LEU:HA	1.33	0.46
10:A:409:PHE:CD1	10:A:694:PHE:HB2	2.51	0.46
11:B:317:ASP:O	11:B:319:PRO:HD3	2.16	0.46
12:C:192:ASP:OD2	13:D:131:ASN:HB3	2.16	0.46
14:E:61:LEU:CG	21:L:17:PRO:O	2.64	0.46
14:E:78:PHE:HB2	24:P:12:ARG:HG2	1.97	0.46
20:K:76:ASN:OD1	20:K:76:ASN:N	2.49	0.46
26:R:201:ILE:HG23	26:R:203:PRO:HD3	1.98	0.46
27:S:191:VAL:O	27:S:191:VAL:HG12	2.15	0.46
36:b:145:GLU:OE1	36:b:145:GLU:N	2.49	0.46
46:l:438:GLU:OE1	46:l:438:GLU:N	2.43	0.46
48:o:141:VAL:HB	52:s:53:ASP:OD2	2.15	0.46
50:q:16:ILE:HG23	50:q:17:ARG:H	1.81	0.46
45:w:383:LEU:HD23	45:w:388:ARG:HA	1.97	0.46
56:A9:147:ILE:HD11	56:A9:209:LEU:HD23	1.98	0.46
57:C4:59:GLN:CA	57:C4:62:GLU:HB2	2.46	0.46
58:C2:137:LEU:HD12	58:C2:137:LEU:HA	1.69	0.46
2:4:187:HIS:CD2	2:4:188:ASN:H	2.34	0.46
2:4:449:LEU:HB3	71:4:502:CDL:CA7	2.44	0.46
3:2:26:TRP:HH2	3:2:145:ILE:HD11	1.81	0.46
3:2:196:TYR:CD1	28:T:138:GLU:OE2	2.68	0.46
4:7:98:LEU:O	4:7:102:PHE:N	2.39	0.46
5:6:68:TRP:CD1	5:6:76:LEU:HD11	2.51	0.46
5:6:556:ILE:CG1	35:a:76:ILE:HD11	2.23	0.46
9:8:210:THR:CG2	9:8:224:ARG:HB2	2.46	0.46
9:8:420:GLU:H	9:8:422:HIS:CD2	2.30	0.46
10:A:131:CYS:O	10:A:134:GLY:N	2.48	0.46
10:A:439:THR:HG1	10:A:440:TYR:HD2	1.64	0.46
11:B:293:LEU:O	11:B:294:ARG:C	2.59	0.46
70:B:501:3PE:O32	21:L:18:VAL:HG21	2.16	0.46
70:B:501:3PE:H3I3	21:L:28:LEU:HD21	1.98	0.46
25:Q:40:ASN:OD1	25:Q:41:LYS:N	2.41	0.46
37:c:12:LEU:O	37:c:16:ARG:HG2	2.15	0.46
42:j:17:GLU:OE1	42:j:81:TYR:HE1	1.99	0.46
45:k:64:PHE:CD1	45:k:86:LEU:HD21	2.51	0.46
45:k:291:SER:OG	46:l:90:GLU:OE1	2.25	0.46
48:o:81:PHE:CD1	48:o:84:PRO:HA	2.51	0.46
50:q:98:ILE:O	50:q:102:LYS:HG2	2.16	0.46
45:w:210:ASP:N	45:w:210:ASP:OD1	2.49	0.46
54:B2:58:LYS:HG3	54:B2:59:TYR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:180:GLN:O	2:4:183:VAL:HG23	2.16	0.45
9:8:326:LEU:HD11	9:8:363:ILE:HG21	1.98	0.45
11:B:61:TRP:NE1	11:B:62:LYS:O	2.49	0.45
11:B:80:LEU:HD23	11:B:81:THR:H	1.81	0.45
13:D:172:GLY:C	13:D:174:ASP:H	2.24	0.45
14:E:106:TYR:C	14:E:107:PRO:O	2.59	0.45
21:L:56:PRO:HB2	25:Q:130:LYS:HA	1.99	0.45
24:P:40:LYS:C	30:V:7:LYS:N	2.75	0.45
25:Q:47:ARG:HH12	30:V:76:GLN:NE2	2.14	0.45
27:S:236:GLU:HA	27:S:239:GLU:CB	2.46	0.45
39:f:139:GLN:O	39:f:143:GLU:N	2.42	0.45
45:k:78:GLU:O	45:k:81:SER:HB2	2.16	0.45
54:u:52:TRP:O	54:u:53:LYS:C	2.60	0.45
46:x:98:VAL:O	55:B1:68:VAL:HG13	2.16	0.45
46:x:366:ALA:HB1	46:x:370:MET:HE2	1.98	0.45
47:y:26:ASN:OD1	47:y:26:ASN:N	2.48	0.45
47:y:153:ILE:HG23	47:y:154:PRO:HD2	1.97	0.45
52:B3:29:LYS:HA	52:B3:32:LYS:HB3	1.98	0.45
57:C4:76:ILE:O	57:C4:79:PRO:HD2	2.16	0.45
60:C0:70:VAL:HG12	60:C0:71:VAL:N	2.31	0.45
61:A6:40:SER:OG	61:A6:45:ASP:HB3	2.16	0.45
1:9:187:GLN:HG3	1:9:191:ASN:O	2.15	0.45
2:4:111:THR:C	2:4:113:MET:H	2.21	0.45
2:4:166:TYR:CE2	70:4:503:3PE:O22	2.60	0.45
2:4:329:LEU:HD13	2:4:359:TRP:CE3	2.51	0.45
5:6:40:ILE:HD11	5:6:101:MET:CE	2.46	0.45
5:6:127:THR:O	5:6:130:ILE:HG22	2.15	0.45
5:6:230:HIS:O	5:6:232:TRP:N	2.49	0.45
5:6:362:LEU:HD12	5:6:363:PHE:HB2	1.98	0.45
8:1:107:ALA:O	8:1:111:LEU:HD13	2.16	0.45
8:1:172:MET:CE	8:1:176:LEU:HB2	2.47	0.45
10:A:382:ARG:CG	10:A:383:SER:H	2.26	0.45
11:B:262:LEU:O	11:B:263:THR:C	2.59	0.45
12:C:67:VAL:O	12:C:67:VAL:HG12	2.16	0.45
17:H:44:ALA:HB1	36:b:173:THR:HG21	1.97	0.45
17:H:91:LYS:HB3	17:H:93:THR:HG23	1.99	0.45
21:L:27:GLY:O	21:L:28:LEU:HB3	2.15	0.45
27:S:161:MET:O	27:S:167:ILE:HG22	2.15	0.45
27:S:334:ASP:CB	42:j:50:ARG:HB3	2.46	0.45
28:T:30:GLY:HA2	28:T:64:ALA:N	2.31	0.45
35:a:64:ALA:CB	44:e:108:ASP:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:69:TYR:CD1	42:j:20:SER:CB	3.00	0.45
45:k:329:MET:SD	51:r:5:GLY:HA3	2.56	0.45
45:w:350:THR:N	45:w:353:GLU:OE2	2.50	0.45
46:x:182:ARG:CD	46:x:185:LYS:HD3	2.46	0.45
46:x:203:ARG:HD2	46:x:231:GLY:HA2	1.97	0.45
47:y:87:ALA:O	47:y:90:PHE:HB3	2.16	0.45
48:z:112:ASP:OD1	48:z:113:LEU:N	2.50	0.45
48:z:215:LEU:HD21	49:A0:46:GLY:HA3	1.98	0.45
61:A6:31:TYR:HE1	61:A6:98:HIS:CE1	2.34	0.45
66:B0:9:PHE:HD1	66:B0:10:HIS:HD2	1.64	0.45
2:4:115:LEU:HD23	2:4:115:LEU:HA	1.68	0.45
2:4:193:VAL:O	2:4:197:LEU:N	2.44	0.45
3:2:234:TRP:HE1	3:2:303:THR:CB	2.29	0.45
5:6:460:GLY:O	5:6:464:ALA:HB2	2.17	0.45
6:5:88:ASP:N	6:5:88:ASP:OD1	2.48	0.45
8:1:29:GLY:HA2	13:D:108:ARG:HH21	1.81	0.45
8:1:73:LEU:HA	8:1:76:ILE:HD13	1.24	0.45
8:1:101:GLY:O	8:1:102:VAL:C	2.59	0.45
8:1:283:ASP:C	8:1:285:LEU:N	2.73	0.45
9:8:118:ASP:HB3	9:8:206:CYS:CB	2.46	0.45
9:8:203:ALA:HB1	9:8:205:ILE:H	1.81	0.45
9:8:362:ASP:CG	9:8:449:ARG:HH22	2.25	0.45
10:A:126:LEU:HD21	11:B:373:THR:O	2.16	0.45
10:A:259:SER:HA	10:A:282:ASN:HD21	1.80	0.45
10:A:355:LYS:HB2	10:A:530:TYR:CE1	2.50	0.45
10:A:360:ARG:HD2	10:A:632:MET:SD	2.57	0.45
11:B:163:PRO:HB2	11:B:167:ALA:CB	2.45	0.45
13:D:82:LEU:O	13:D:83:TRP:HD1	1.98	0.45
14:E:177:THR:HG21	14:E:182:GLU:OE2	2.15	0.45
16:G:139:GLU:O	16:G:142:GLY:N	2.49	0.45
18:I:111:THR:HG22	18:I:119:PHE:HB3	1.99	0.45
21:L:23:PHE:CE1	72:L:200:PC1:H2A2	2.52	0.45
23:O:123:TYR:O	26:R:42:PRO:HG3	2.15	0.45
26:R:269:SER:HA	26:R:270:ARG:HA	1.51	0.45
27:S:126:SER:O	27:S:129:LEU:N	2.50	0.45
27:S:158:LEU:HA	27:S:161:MET:HE2	1.98	0.45
39:f:166:LEU:HA	39:f:167:TRP:HA	1.47	0.45
31:M:62:ILE:HG21	31:M:67:ALA:HB2	1.96	0.45
45:k:350:THR:O	45:k:354:VAL:HG23	2.16	0.45
47:m:35:SER:O	47:m:38:GLY:N	2.49	0.45
47:m:87:ALA:O	47:m:90:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:m:98:VAL:O	47:m:101:GLY:N	2.49	0.45
51:r:8:THR:HG22	51:r:9:ARG:N	2.31	0.45
45:w:78:GLU:O	45:w:81:SER:HB2	2.16	0.45
47:y:98:VAL:O	47:y:101:GLY:N	2.49	0.45
55:B1:62:ARG:CG	55:B1:63:PRO:HD2	2.46	0.45
57:C4:60:GLU:CD	57:C4:61:VAL:H	2.24	0.45
59:A7:66:GLU:O	60:C0:66:ARG:NH2	2.49	0.45
1:9:164:THR:N	1:9:169:PHE:O	2.29	0.45
2:4:2:LEU:HA	2:4:5:ILE:HG12	1.98	0.45
2:4:112:ALA:C	2:4:114:GLU:H	2.24	0.45
8:1:71:PHE:O	8:1:72:ILE:HG13	2.17	0.45
10:A:382:ARG:HH22	10:A:652:ASN:ND2	2.13	0.45
11:B:272:THR:HG23	11:B:326:CYS:HB2	1.98	0.45
70:B:501:3PE:H341	14:E:61:LEU:HD12	1.99	0.45
22:N:27:LEU:O	22:N:31:ILE:N	2.47	0.45
24:P:52:ASN:HB3	24:P:57:ARG:HH12	1.82	0.45
26:R:156:SER:O	26:R:161:VAL:HG22	2.17	0.45
27:S:72:LYS:HE3	27:S:74:PHE:CE1	2.51	0.45
27:S:75:PRO:O	27:S:130:GLN:NE2	2.50	0.45
39:f:104:LEU:C	39:f:107:TRP:HE1	2.24	0.45
40:h:69:LYS:O	40:h:70:ASN:ND2	2.50	0.45
46:l:78:LYS:CB	46:l:129:ALA:HB1	2.45	0.45
47:m:293:ALA:O	47:m:297:SER:N	2.50	0.45
49:A0:155:GLY:O	49:A0:157:TYR:N	2.49	0.45
50:A1:40:ASN:O	50:A1:44:LYS:HG2	2.16	0.45
56:A9:449:MET:HE3	66:B0:40:TRP:HB3	1.98	0.45
56:A9:484:THR:HB	68:A8:2:THR:OG1	2.15	0.45
56:A9:498:CYS:HA	56:A9:499:PRO:HA	1.78	0.45
57:C4:1:MET:SD	57:C4:133:LEU:HD11	2.56	0.45
62:A4:5:LYS:NZ	62:A4:6:GLY:N	2.54	0.45
63:A5:57:ARG:HB3	63:A5:57:ARG:NH1	2.31	0.45
1:9:68:LYS:HG2	15:F:100:PRO:HD3	1.99	0.45
2:4:60:SER:C	2:4:62:SER:H	2.21	0.45
2:4:375:LEU:HD23	2:4:375:LEU:HA	1.83	0.45
8:1:243:LEU:O	8:1:262:LYS:NZ	2.40	0.45
10:A:217:GLU:O	10:A:218:LEU:HB2	2.16	0.45
10:A:485:ASP:HB3	10:A:680:LEU:HG	1.99	0.45
10:A:562:LYS:O	10:A:564:CYS:N	2.49	0.45
11:B:62:LYS:O	11:B:64:PRO:CD	2.64	0.45
18:I:93:ALA:O	18:I:94:LEU:HD12	2.16	0.45
18:I:105:LYS:O	18:I:106:GLU:CG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:114:TRP:C	22:N:116:ILE:H	2.24	0.45
23:O:63:VAL:O	23:O:67:PHE:HD2	1.99	0.45
25:Q:28:ALA:C	25:Q:30:HIS:H	2.24	0.45
26:R:195:PHE:O	26:R:195:PHE:CD1	2.70	0.45
27:S:67:GLU:HA	27:S:68:LYS:C	2.42	0.45
28:T:128:GLY:HA2	28:T:133:TRP:CE3	2.50	0.45
37:c:83:HIS:HE1	37:c:87:LYS:HB2	1.80	0.45
39:f:136:GLU:O	39:f:139:GLN:HG2	2.16	0.45
40:h:106:VAL:HA	40:h:109:LEU:CB	2.46	0.45
42:j:119:VAL:CG2	43:g:147:GLY:C	2.89	0.45
45:k:350:THR:N	45:k:353:GLU:OE2	2.50	0.45
46:l:182:ARG:CD	46:l:185:LYS:HD3	2.46	0.45
48:o:138:PRO:HG3	52:s:58:LEU:HD22	1.99	0.45
50:q:13:LEU:O	50:q:17:ARG:N	2.43	0.45
46:x:116:VAL:O	46:x:120:MET:N	2.36	0.45
49:A0:76:ILE:O	49:A0:77:LYS:CB	2.64	0.45
49:A0:110:ALA:HB1	49:A0:122:HIS:O	2.02	0.45
56:A9:299:VAL:HA	56:A9:302:ARG:NH1	2.31	0.45
56:A9:431:LEU:HD21	56:A9:450:TRP:HB2	1.99	0.45
61:A6:33:ILE:HG22	61:A6:34:LEU:HD12	1.98	0.45
64:B4:19:PHE:CD1	64:B4:19:PHE:C	2.94	0.45
3:2:30:TRP:CH2	3:2:67:SER:HB3	2.51	0.45
3:2:326:LEU:HD21	72:2:402:PC1:C2C	2.40	0.45
4:7:17:PHE:HD1	4:7:20:PHE:CE2	2.35	0.45
5:6:27:TYR:HD1	5:6:28:LYS:O	1.99	0.45
5:6:190:LEU:HD11	5:6:196:TRP:CE3	2.51	0.45
5:6:437:PHE:O	34:Z:52:ARG:NH1	2.50	0.45
10:A:76:ARG:HD3	10:A:76:ARG:HA	1.71	0.45
11:B:221:ARG:HA	11:B:221:ARG:HD3	1.60	0.45
12:C:192:ASP:CG	12:C:193:TYR:H	2.23	0.45
13:D:184:PRO:CG	14:E:183:LEU:HD13	2.46	0.45
71:J:101:CDL:H161	24:P:7:PHE:CG	2.52	0.45
26:R:199:THR:OG1	26:R:259:ARG:HA	2.17	0.45
26:R:333:PRO:HB2	26:R:334:GLY:HA2	1.97	0.45
28:T:34:LEU:HD22	28:T:34:LEU:O	2.17	0.45
29:U:18:GLY:HA3	29:U:22:GLY:HA3	1.97	0.45
45:k:215:HIS:HA	45:k:216:PHE:HA	1.39	0.45
47:m:136:GLY:O	47:m:139:SER:OG	2.22	0.45
79:A9:602:HEA:HHC	79:A9:602:HEA:O11	2.17	0.45
59:A7:79:LYS:NZ	66:B0:15:ASN:HD21	2.15	0.45
1:9:227:PRO:CD	9:8:48:ARG:NH2	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:120:TYR:CE1	71:6:701:CDL:H541	2.51	0.45
5:6:295:GLN:O	5:6:301:ILE:HD11	2.17	0.45
7:3:23:TRP:CZ2	7:3:27:LEU:HD22	2.52	0.45
7:3:68:GLU:H	7:3:68:GLU:HG2	1.57	0.45
8:1:45:LEU:HD11	19:J:7:PRO:HB3	1.99	0.45
8:1:118:TRP:O	8:1:122:ALA:N	2.42	0.45
9:8:53:LEU:O	9:8:136:HIS:NE2	2.46	0.45
10:A:259:SER:CA	10:A:282:ASN:HD21	2.29	0.45
10:A:639:LEU:HD21	10:A:643:ARG:NE	2.32	0.45
11:B:208:GLU:O	11:B:211:PHE:N	2.49	0.45
11:B:216:ARG:CG	14:E:94:SER:HB2	2.46	0.45
11:B:390:GLN:O	24:P:60:ARG:NE	2.49	0.45
12:C:123:THR:HG21	16:G:128:PHE:C	2.41	0.45
14:E:37:THR:N	24:P:104:TRP:HD1	2.14	0.45
16:G:105:GLU:OE1	16:G:105:GLU:N	2.36	0.45
21:L:19:LEU:O	21:L:22:SER:OG	2.13	0.45
21:L:23:PHE:CD1	72:L:200:PC1:H281	2.37	0.45
22:N:24:LEU:O	22:N:27:LEU:N	2.49	0.45
27:S:49:THR:HG22	27:S:192:VAL:HG22	1.99	0.45
28:T:72:LEU:C	28:T:72:LEU:CD1	2.86	0.45
45:k:210:ASP:OD1	45:k:210:ASP:N	2.49	0.45
46:l:128:THR:C	46:l:130:PRO:HD3	2.41	0.45
46:l:135:TRP:CE2	50:A1:49:ARG:HD3	2.51	0.45
47:m:334:THR:O	47:m:338:ILE:HG12	2.17	0.45
48:o:191:ARG:NH2	48:o:195:GLU:OE2	2.49	0.45
50:q:40:ASN:O	50:q:44:LYS:HG2	2.16	0.45
53:t:43:ASP:CA	54:u:33:ARG:HH22	2.26	0.45
45:w:235:ARG:CD	49:A0:14:ARG:HH22	2.30	0.45
47:y:22:PRO:HG3	51:A2:4:PHE:CE2	2.51	0.45
48:z:167:GLU:HG3	48:z:177:ALA:HB3	1.99	0.45
48:z:191:ARG:NH2	48:z:195:GLU:OE2	2.49	0.45
50:A1:91:GLU:HB3	50:A1:95:LYS:NZ	2.32	0.45
51:A2:8:THR:HG22	51:A2:9:ARG:N	2.31	0.45
52:B3:15:ASP:OD2	52:B3:18:THR:HG23	2.17	0.45
56:A9:32:ALA:HB3	67:C1:36:PRO:HG2	1.98	0.45
1:9:143:ARG:HH11	9:8:285:PRO:CG	2.27	0.45
71:4:502:CDL:H161	71:4:502:CDL:H561	1.98	0.45
3:2:211:MET:HE1	3:2:259:GLY:HA2	1.99	0.45
5:6:13:LEU:O	5:6:16:THR:OG1	2.30	0.45
5:6:177:ILE:O	5:6:180:ILE:HG22	2.17	0.45
5:6:596:LEU:HD12	5:6:597:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:233:MET:HE2	8:1:233:MET:HB3	1.75	0.45
10:A:272:ARG:HH12	10:A:274:LEU:HD11	1.80	0.45
11:B:237:PRO:N	14:E:96:ARG:HH22	2.11	0.45
11:B:304:LYS:HB3	11:B:304:LYS:HE2	1.77	0.45
12:C:120:ASP:N	12:C:120:ASP:OD1	2.49	0.45
13:D:138:ARG:NH2	13:D:141:TYR:CD2	2.84	0.45
27:S:284:MET:CB	72:S:401:PC1:C13	2.94	0.45
36:b:61:GLY:O	36:b:65:LYS:HG2	2.16	0.45
40:h:125:LEU:HG	40:h:129:ARG:HH12	1.81	0.45
31:M:44:SER:O	31:M:48:VAL:HG23	2.17	0.45
31:M:64:ASP:CG	31:M:65:ILE:H	2.25	0.45
45:k:186:LEU:HD23	45:k:190:TYR:CE2	2.51	0.45
51:r:44:CYS:O	51:r:47:ARG:N	2.45	0.45
52:s:15:ASP:OD2	52:s:18:THR:HG23	2.17	0.45
53:t:33:VAL:O	53:t:37:ASP:CB	2.54	0.45
46:x:128:THR:C	46:x:130:PRO:HD3	2.41	0.45
50:A1:98:ILE:O	50:A1:102:LYS:HG2	2.16	0.45
56:A9:273:MET:HG3	56:A9:319:LYS:NZ	2.30	0.45
60:C0:78:HIS:CE1	64:B4:12:LEU:HD22	2.52	0.45
61:A6:98:HIS:ND1	61:A6:98:HIS:N	2.64	0.45
1:9:155:LYS:HD3	1:9:202:GLU:OE1	2.17	0.45
70:2:401:3PE:H2H2	70:2:401:3PE:H2E1	1.79	0.45
4:7:136:PHE:C	4:7:138:GLU:N	2.75	0.45
5:6:101:MET:HE2	5:6:121:LEU:CD2	2.46	0.45
6:5:7:ASN:HA	6:5:8:ILE:HA	1.68	0.45
6:5:57:SER:O	6:5:60:PRO:HD2	2.17	0.45
7:3:67:LEU:HA	7:3:67:LEU:HD23	1.75	0.45
8:1:178:ALA:O	8:1:181:LEU:N	2.49	0.45
8:1:248:ASN:O	8:1:250:HIS:N	2.49	0.45
11:B:420:TYR:O	11:B:421:ARG:C	2.58	0.45
12:C:199:PRO:HG3	13:D:167:TYR:CZ	2.52	0.45
14:E:133:GLU:CG	14:E:134:PRO:HD2	2.47	0.45
20:K:92:GLU:HA	20:K:95:LEU:HB3	1.98	0.45
23:O:47:VAL:HG11	23:O:56:VAL:HG22	1.98	0.45
27:S:109:PRO:HB2	27:S:112:ASN:CB	2.40	0.45
27:S:167:ILE:HD11	27:S:171:CYS:HB2	1.98	0.45
29:U:29:ARG:NH2	29:U:61:TRP:HZ3	2.15	0.45
31:M:57:GLU:C	31:M:59:GLY:H	2.25	0.45
45:k:67:THR:OG1	45:k:68:LYS:N	2.50	0.45
47:m:26:ASN:OD1	47:m:26:ASN:N	2.48	0.45
52:s:29:LYS:HA	52:s:32:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:191:LYS:HA	45:w:218:GLY:HA3	1.99	0.45
56:A9:240:HIS:O	56:A9:243:VAL:HG22	2.16	0.45
1:9:179:ALA:CB	9:8:125:CYS:SG	3.04	0.45
1:9:215:LYS:O	1:9:217:GLY:N	2.49	0.45
2:4:62:SER:HB3	2:4:457:PRO:CD	2.47	0.45
2:4:317:ILE:HD11	2:4:454:ILE:HG23	1.98	0.45
3:2:268:GLN:NE2	3:2:272:LYS:HE2	2.31	0.45
5:6:316:THR:O	5:6:321:GLN:HB2	2.16	0.45
5:6:353:GLU:OE1	5:6:358:LYS:HB2	2.17	0.45
8:1:30:TYR:OH	19:J:4:GLU:HB2	2.17	0.45
12:C:57:HIS:CE1	12:C:80:VAL:HG11	2.52	0.45
12:C:192:ASP:CG	13:D:132:LYS:HG2	2.41	0.45
21:L:36:SER:HA	21:L:37:PRO:HD3	1.82	0.45
23:O:128:PRO:HG3	26:R:45:LYS:CE	2.29	0.45
36:b:93:ILE:HG23	43:g:61:TYR:OH	2.17	0.45
36:b:100:GLU:CB	36:b:101:ILE:HA	2.47	0.45
41:i:69:TYR:CG	42:j:20:SER:HA	2.50	0.45
42:j:116:PHE:CG	43:g:160:LYS:C	2.95	0.45
77:m:402:HEM:O2A	77:m:402:HEM:HHA	2.17	0.45
49:p:127:VAL:CB	49:p:132:TRP:H	2.30	0.45
45:w:333:ASP:OD2	47:y:1:MET:N	2.38	0.45
45:w:389:ARG:O	45:w:390:ILE:HD13	2.17	0.45
46:x:289:SER:HB2	46:x:296:TYR:HE2	1.82	0.45
47:y:293:ALA:O	47:y:297:SER:N	2.50	0.45
77:y:402:HEM:O2A	77:y:402:HEM:HHA	2.17	0.45
49:A0:162:GLY:O	49:A0:163:SER:CB	2.65	0.45
59:A7:40:LEU:HD22	59:A7:59:LEU:CD1	2.47	0.45
65:C3:30:ILE:HG13	65:C3:31:LEU:N	2.32	0.45
2:4:151:PHE:O	2:4:155:ALA:HB2	2.17	0.44
2:4:317:ILE:HD11	2:4:454:ILE:CG2	2.47	0.44
70:4:501:3PE:O14	3:2:238:PRO:HG2	2.17	0.44
5:6:207:SER:OG	5:6:208:ASP:N	2.50	0.44
5:6:251:THR:O	5:6:253:VAL:N	2.48	0.44
5:6:606:GLU:N	5:6:606:GLU:OE1	2.50	0.44
71:6:701:CDL:H111	36:b:68:LEU:CD2	2.46	0.44
9:8:204:TYR:O	9:8:207:GLY:N	2.38	0.44
9:8:451:GLN:HA	9:8:454:ALA:HB3	1.99	0.44
10:A:140:GLN:HG3	11:B:379:ILE:HG23	2.00	0.44
11:B:180:LEU:HA	11:B:180:LEU:HD23	1.66	0.44
11:B:431:HIS:HB3	11:B:454:GLN:HG2	1.98	0.44
12:C:179:PHE:CE1	23:O:84:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:107:ASP:C	13:D:109:PHE:H	2.25	0.44
17:H:2:PRO:HG2	17:H:4:PHE:HE1	1.82	0.44
21:L:19:LEU:HD12	21:L:20:VAL:N	2.32	0.44
23:O:95:LYS:HB2	23:O:95:LYS:HE3	1.72	0.44
25:Q:48:TRP:CH2	36:b:185:ALA:HA	2.52	0.44
26:R:60:GLY:HA3	26:R:129:LEU:HD11	1.99	0.44
27:S:114:GLY:HA3	27:S:115:ASN:HA	1.59	0.44
28:T:10:TRP:CE3	28:T:10:TRP:CA	2.94	0.44
28:T:98:GLY:CA	28:T:111:GLY:O	2.62	0.44
30:V:71:LEU:C	30:V:73:PRO:HD2	2.42	0.44
38:d:25:PHE:CE2	38:d:41:ALA:O	2.70	0.44
40:h:113:ARG:O	40:h:114:MET:C	2.60	0.44
31:M:12:LYS:NZ	31:M:77:VAL:HG21	2.33	0.44
47:m:91:PHE:HD2	47:m:273:TYR:CD2	2.35	0.44
48:o:112:ASP:OD1	48:o:113:LEU:N	2.49	0.44
56:A9:158:ILE:O	56:A9:162:ILE:HG13	2.17	0.44
65:C3:2:GLU:CG	65:C3:3:ASN:H	2.30	0.44
1:9:243:PHE:HD2	9:8:257:ARG:HB2	1.81	0.44
2:4:5:ILE:HA	2:4:8:THR:HG22	1.99	0.44
2:4:52:PHE:HZ	2:4:58:SER:OG	2.00	0.44
8:1:316:PRO:HG3	30:V:57:ARG:CG	2.48	0.44
10:A:360:ARG:HB3	10:A:632:MET:SD	2.57	0.44
11:B:266:ARG:NH1	14:E:66:LEU:HD23	2.31	0.44
11:B:359:ASP:CG	24:P:45:PRO:HG2	2.43	0.44
11:B:421:ARG:CG	12:C:119:VAL:HG22	2.47	0.44
23:O:33:ARG:HH21	31:M:44:SER:HB2	1.60	0.44
25:Q:106:GLN:OE1	25:Q:106:GLN:N	2.42	0.44
28:T:106:ARG:HH11	28:T:106:ARG:CA	2.13	0.44
28:T:108:TYR:O	28:T:108:TYR:CD1	2.70	0.44
36:b:96:ALA:HA	36:b:97:GLU:HA	1.66	0.44
45:k:389:ARG:O	45:k:390:ILE:HD13	2.17	0.44
46:l:366:ALA:HB1	46:l:370:MET:HE2	1.98	0.44
48:z:138:PRO:HD2	48:z:141:VAL:HG11	2.00	0.44
56:A9:131:PRO:HB2	57:C4:159:VAL:HA	2.00	0.44
57:C4:121:TYR:C	57:C4:138:VAL:HG23	2.42	0.44
57:C4:162:SER:HB2	57:C4:198:GLU:HB2	1.99	0.44
62:A4:42:ARG:HG3	62:A4:42:ARG:NH1	2.32	0.44
1:9:183:ALA:HB1	1:9:184:PRO:HD2	1.99	0.44
2:4:305:THR:OG1	2:4:305:THR:O	2.29	0.44
3:2:67:SER:O	3:2:70:LEU:N	2.51	0.44
8:1:146:LEU:HD12	8:1:146:LEU:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:210:GLY:C	8:1:212:ASN:H	2.26	0.44
8:1:249:PRO:O	25:Q:91:TYR:HE2	2.00	0.44
8:1:311:THR:CG2	30:V:51:MET:CG	2.96	0.44
9:8:399:PHE:HE2	9:8:412:LEU:HD13	1.83	0.44
9:8:451:GLN:O	9:8:455:GLN:HG2	2.18	0.44
10:A:117:MET:SD	10:A:143:SER:HB2	2.56	0.44
10:A:380:ASP:OD1	10:A:380:ASP:N	2.49	0.44
11:B:378:LEU:O	11:B:380:HIS:N	2.50	0.44
11:B:427:PRO:HB3	11:B:431:HIS:ND1	2.33	0.44
15:F:92:LEU:O	15:F:96:ARG:HB2	2.17	0.44
21:L:27:GLY:C	21:L:29:ALA:H	2.26	0.44
25:Q:132:LYS:HE3	25:Q:134:ASP:CG	2.42	0.44
25:Q:158:LEU:CA	42:j:88:HIS:ND1	2.79	0.44
45:k:403:ASP:OD1	45:k:404:ALA:N	2.44	0.44
48:o:97:ASN:OD1	48:o:98:PRO:HD2	2.18	0.44
48:o:167:GLU:HG3	48:o:177:ALA:HB3	1.99	0.44
50:q:57:ASP:O	50:q:61:ARG:NH1	2.51	0.44
45:w:92:ARG:NH1	45:w:154:HIS:CG	2.84	0.44
45:w:251:ALA:HB2	45:w:427:PRO:HD2	1.99	0.44
45:w:252:HIS:CD2	45:w:323:HIS:HE1	2.10	0.44
45:w:350:THR:O	45:w:354:VAL:HG23	2.16	0.44
45:w:436:ARG:HH21	47:y:221:HIS:HB3	1.82	0.44
57:C4:1:MET:SD	57:C4:133:LEU:HD13	2.58	0.44
62:A4:3:ALA:O	62:A4:4:ALA:HB2	2.17	0.44
1:9:87:GLN:NE2	1:9:123:ASN:OD1	2.50	0.44
2:4:314:ALA:O	2:4:318:ALA:HB2	2.17	0.44
70:2:401:3PE:H352	42:j:67:SER:HB2	2.00	0.44
4:7:160:SER:O	4:7:163:ILE:HG22	2.17	0.44
5:6:120:TYR:OH	71:6:701:CDL:OB6	2.33	0.44
7:3:77:TRP:NE1	8:1:318:THR:O	2.49	0.44
9:8:379:CYS:HB2	74:8:502:SF4:S1	2.50	0.44
10:A:643:ARG:HG2	10:A:646:LEU:HD12	1.99	0.44
11:B:213:PHE:O	11:B:217:VAL:HG12	2.16	0.44
11:B:421:ARG:HH21	11:B:423:LYS:HD3	1.83	0.44
12:C:70:ILE:HG13	12:C:71:LEU:CD1	2.47	0.44
12:C:123:THR:CG2	16:G:128:PHE:HB3	2.47	0.44
14:E:118:LEU:HD23	14:E:118:LEU:HA	1.61	0.44
14:E:172:ASN:OD1	29:U:87:HIS:ND1	2.51	0.44
20:K:59:SER:O	20:K:61:VAL:N	2.51	0.44
24:P:19:ASP:O	24:P:21:GLN:N	2.50	0.44
26:R:154:GLN:HG3	26:R:155:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:178:SER:O	26:R:182:ARG:N	2.30	0.44
28:T:61:PHE:CD2	28:T:61:PHE:O	2.70	0.44
28:T:66:ILE:C	28:T:69:ILE:CG2	2.90	0.44
28:T:70:PHE:HZ	28:T:90:TYR:CE1	2.36	0.44
29:U:81:MET:HG2	29:U:115:PHE:HE1	1.83	0.44
32:X:38:ARG:HA	32:X:56:TRP:HZ3	1.83	0.44
32:X:55:THR:CG2	36:b:131:LYS:HD2	2.45	0.44
34:Z:33:GLN:HA	34:Z:36:LEU:HG	2.00	0.44
39:f:55:LYS:CB	39:f:59:LYS:HB3	2.48	0.44
31:M:52:MET:HA	31:M:55:GLU:OE1	2.18	0.44
47:m:241:LEU:HD12	47:m:245:PHE:HD2	1.83	0.44
48:o:76:GLU:O	48:o:78:GLY:N	2.50	0.44
48:o:237:TYR:CD2	48:o:239:PRO:HD3	2.53	0.44
45:w:389:ARG:C	45:w:391:PRO:HD3	2.43	0.44
46:x:191:LEU:O	46:x:195:VAL:HG23	2.18	0.44
47:y:31:TRP:HA	47:y:100:ARG:HH11	1.83	0.44
47:y:91:PHE:HD2	47:y:273:TYR:CD2	2.35	0.44
47:y:334:THR:O	47:y:338:ILE:HG12	2.17	0.44
56:A9:51:ASP:O	56:A9:55:ASN:HB2	2.17	0.44
1:9:134:VAL:HG11	1:9:149:LEU:HD12	1.99	0.44
2:4:121:LEU:HA	2:4:124:ALA:CB	2.48	0.44
2:4:298:ILE:O	2:4:302:LEU:HD13	2.18	0.44
8:1:200:LEU:HD12	8:1:206:GLU:HG2	2.00	0.44
8:1:307:LEU:HD23	30:V:47:TYR:CZ	2.52	0.44
10:A:79:LEU:HD12	10:A:112:ALA:HB1	1.99	0.44
10:A:311:LYS:C	29:U:144:TYR:HE1	2.17	0.44
10:A:359:ASN:ND2	20:K:68:ARG:CZ	2.80	0.44
11:B:102:SER:C	11:B:104:GLU:H	2.25	0.44
11:B:404:LYS:HE2	11:B:404:LYS:HB3	1.80	0.44
12:C:167:TRP:O	12:C:169:GLU:N	2.50	0.44
12:C:210:VAL:HG23	12:C:210:VAL:O	2.17	0.44
26:R:273:LEU:N	26:R:367:GLU:OE2	2.51	0.44
28:T:139:PRO:CB	36:b:158:ARG:HG3	2.48	0.44
32:X:14:VAL:C	32:X:17:PRO:HD2	2.42	0.44
35:a:53:ASP:OD1	35:a:53:ASP:N	2.51	0.44
39:f:57:MET:O	39:f:59:LYS:N	2.51	0.44
45:k:163:LEU:HD21	45:k:314:TYR:CD2	2.52	0.44
45:k:389:ARG:C	45:k:391:PRO:HD3	2.42	0.44
46:l:67:HIS:ND1	46:l:70:ARG:NH2	2.66	0.44
46:l:155:PRO:O	46:l:158:HIS:N	2.51	0.44
54:u:17:THR:HA	54:u:20:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A0:2:HIS:O	49:A0:4:ASP:N	2.50	0.44
49:A0:158:CYS:O	49:A0:163:SER:CB	2.66	0.44
56:A9:379:TYR:CE2	56:A9:383:MET:HE2	2.52	0.44
58:C2:19:THR:CG2	58:C2:53:THR:OG1	2.66	0.44
59:A7:37:GLN:O	59:A7:41:LYS:HG2	2.18	0.44
1:9:227:PRO:CD	9:8:48:ARG:HH12	2.24	0.44
1:9:238:PRO:HG2	1:9:241:PRO:CG	2.47	0.44
2:4:177:LEU:HD21	2:4:245:ARG:HB3	1.98	0.44
3:2:112:HIS:CD2	3:2:112:HIS:H	2.36	0.44
3:2:169:GLY:C	3:2:171:ASN:N	2.75	0.44
5:6:441:VAL:HG12	5:6:443:ILE:HG23	2.00	0.44
6:5:89:TYR:O	6:5:91:GLN:N	2.51	0.44
8:1:5:ASN:ND2	19:J:23:THR:HG23	2.27	0.44
8:1:80:GLY:O	8:1:83:LEU:N	2.50	0.44
9:8:46:TYR:HE2	9:8:51:TRP:HE1	1.65	0.44
10:A:305:PRO:CB	10:A:319:TRP:CZ3	2.93	0.44
11:B:404:LYS:CE	11:B:455:ASP:OD2	2.66	0.44
12:C:214:TYR:HB3	13:D:176:ILE:CA	2.37	0.44
12:C:218:VAL:HG22	12:C:219:LYS:HG3	2.00	0.44
13:D:186:CYS:HA	74:D:301:SF4:S4	2.58	0.44
14:E:54:THR:O	14:E:58:ALA:N	2.47	0.44
14:E:196:LYS:HD2	14:E:197:TRP:CZ3	2.52	0.44
26:R:249:ILE:O	26:R:252:ALA:N	2.51	0.44
27:S:333:GLU:OE2	42:j:53:VAL:HA	2.17	0.44
35:a:108:ASP:O	35:a:109:ARG:HB3	2.17	0.44
55:B1:77:ARG:HG2	55:B1:78:TYR:N	2.32	0.44
58:C2:183:GLU:O	62:A4:42:ARG:NH2	2.50	0.44
1:9:53:PHE:HE2	1:9:55:PHE:CE1	2.36	0.44
1:9:54:ASP:O	1:9:89:GLN:NE2	2.51	0.44
2:4:72:LEU:O	2:4:76:MET:HE3	2.18	0.44
2:4:268:GLY:HA2	2:4:271:MET:HB3	1.99	0.44
3:2:245:LEU:HD22	3:2:301:THR:HG21	2.00	0.44
5:6:353:GLU:CD	5:6:358:LYS:HB2	2.43	0.44
5:6:385:PHE:O	5:6:466:TYR:OH	2.27	0.44
7:3:9:THR:O	7:3:12:THR:HG22	2.17	0.44
8:1:150:LEU:O	8:1:154:LEU:HD13	2.18	0.44
12:C:96:ILE:O	12:C:100:THR:OG1	2.25	0.44
13:D:160:GLY:O	13:D:161:GLY:C	2.60	0.44
14:E:60:THR:CG2	21:L:17:PRO:HD2	2.42	0.44
22:N:56:LEU:HD12	22:N:59:VAL:HB	1.98	0.44
27:S:128:LEU:HD11	27:S:186:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:34:LEU:CD1	28:T:34:LEU:C	2.86	0.44
45:k:217:SER:N	45:k:218:GLY:HA3	2.33	0.44
46:l:435:PHE:HE2	46:x:169:ARG:HG2	1.82	0.44
50:q:91:GLU:HB3	50:q:95:LYS:NZ	2.32	0.44
46:x:155:PRO:O	46:x:158:HIS:N	2.51	0.44
50:A1:43:VAL:HA	50:A1:46:ALA:HB3	2.00	0.44
53:A3:40:LEU:HG	53:A3:47:TYR:CD1	2.53	0.44
57:C4:63:THR:HA	57:C4:66:THR:HG22	2.00	0.44
63:A5:84:LYS:HD2	63:A5:84:LYS:HA	1.82	0.44
67:C1:35:ALA:HB3	67:C1:36:PRO:HD3	1.99	0.44
1:9:57:PRO:HA	1:9:60:TYR:HD2	1.83	0.44
2:4:2:LEU:HB3	2:4:6:ILE:CD1	2.48	0.44
2:4:39:LEU:HD21	40:h:105:PHE:CD2	2.53	0.44
2:4:423:ILE:HG22	35:a:57:ARG:CD	2.47	0.44
4:7:60:TYR:O	4:7:64:MET:HB3	2.18	0.44
5:6:116:LYS:HG2	5:6:119:LYS:NZ	2.29	0.44
5:6:173:LEU:O	5:6:177:ILE:HD12	2.18	0.44
5:6:350:LEU:O	5:6:350:LEU:HD23	2.18	0.44
8:1:47:GLN:HB3	8:1:48:PRO:HD3	2.00	0.44
10:A:281:ILE:H	10:A:281:ILE:HG12	1.51	0.44
10:A:330:LEU:HA	10:A:544:MET:HE1	2.00	0.44
10:A:488:ALA:O	10:A:492:ALA:N	2.47	0.44
10:A:619:ASP:O	10:A:622:ILE:HG22	2.17	0.44
11:B:155:VAL:O	11:B:156:GLU:C	2.61	0.44
11:B:393:PRO:CG	12:C:247:TYR:CE1	2.96	0.44
13:D:138:ARG:C	13:D:138:ARG:HE	2.26	0.44
14:E:74:LEU:HA	14:E:74:LEU:HD12	1.61	0.44
14:E:149:MET:HE3	14:E:149:MET:HB3	1.68	0.44
22:N:35:LEU:HD21	22:N:45:ARG:HG3	2.00	0.44
26:R:43:HIS:H	26:R:51:VAL:HG23	1.83	0.44
26:R:143:ASP:O	26:R:147:LYS:HG2	2.18	0.44
27:S:201:GLU:O	27:S:204:SER:N	2.50	0.44
28:T:34:LEU:C	28:T:34:LEU:CD2	2.85	0.44
33:Y:70:PHE:O	33:Y:73:LEU:HB2	2.16	0.44
37:c:32:GLU:C	37:c:34:VAL:H	2.26	0.44
37:c:83:HIS:CE1	37:c:87:LYS:HE2	2.53	0.44
31:M:56:ASP:OD1	31:M:56:ASP:N	2.48	0.44
45:k:343:MET:HE1	45:k:416:TYR:CD2	2.50	0.44
48:o:150:ASN:OD1	48:o:151:PRO:HD2	2.18	0.44
49:p:63:SER:HA	47:y:163:TRP:CD1	2.53	0.44
47:y:128:PHE:O	47:y:129:MET:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B3:66:ASP:HA	52:B3:69:VAL:HB	1.99	0.44
53:A3:20:THR:O	53:A3:24:TRP:HD1	2.01	0.44
3:2:302:LEU:O	11:B:39:PRO:HB3	2.17	0.44
3:2:326:LEU:HD12	72:2:402:PC1:H2A2	1.85	0.44
8:1:79:LEU:HD11	8:1:222:LEU:HD23	1.91	0.44
8:1:126:LYS:HA	8:1:129:LEU:HB3	2.00	0.44
9:8:203:ALA:CB	9:8:205:ILE:HD12	2.48	0.44
10:A:126:LEU:HD12	10:A:126:LEU:N	2.32	0.44
10:A:356:ASP:CG	10:A:645:ARG:HH21	2.26	0.44
10:A:591:GLU:HG3	10:A:610:VAL:O	2.18	0.44
12:C:77:GLN:O	12:C:89:CYS:N	2.47	0.44
12:C:150:ASP:CG	12:C:151:GLU:N	2.75	0.44
12:C:169:GLU:OE1	12:C:183:HIS:HD2	2.00	0.44
12:C:174:ASP:OD2	12:C:189:ILE:O	2.36	0.44
13:D:158:ASN:HB2	14:E:150:THR:HB	1.99	0.44
14:E:104:ARG:HD2	14:E:168:VAL:HG21	2.00	0.44
28:T:30:GLY:HA2	28:T:64:ALA:HB2	1.98	0.44
28:T:96:ALA:CA	28:T:99:LEU:HD13	2.46	0.44
28:T:101:LEU:HG	28:T:110:ILE:HG21	1.95	0.44
29:U:83:PRO:O	29:U:85:GLU:N	2.45	0.44
35:a:47:TYR:O	35:a:50:GLN:HB3	2.17	0.44
36:b:137:MET:HE1	43:g:87:GLU:HG3	1.99	0.44
37:c:36:PRO:HG2	37:c:37:PRO:O	2.18	0.44
38:d:82:HIS:O	38:d:86:ASP:N	2.34	0.44
40:h:149:LEU:HD13	43:g:166:GLU:HB3	1.99	0.44
42:j:108:THR:CB	43:g:79:GLU:CA	2.94	0.44
31:M:36:PHE:N	31:M:39:ASP:HB3	2.33	0.44
45:k:228:VAL:HA	45:k:229:PRO:HA	1.79	0.44
49:p:41:ALA:HB2	54:u:20:PHE:HE1	1.83	0.44
45:w:64:PHE:CE1	45:w:86:LEU:HD21	2.52	0.44
45:w:163:LEU:HD21	45:w:314:TYR:CD2	2.52	0.44
47:y:319:PRO:O	47:y:323:CYS:N	2.43	0.44
48:z:97:ASN:OD1	48:z:98:PRO:HD2	2.18	0.44
57:C4:122:MET:HB2	57:C4:208:PRO:CD	2.47	0.44
65:C3:3:ASN:ND2	65:C3:5:VAL:HG13	2.33	0.44
68:A8:37:LEU:HD23	68:A8:37:LEU:HA	1.83	0.44
1:9:130:TYR:HA	1:9:189:ASN:ND2	2.29	0.43
1:9:179:ALA:HB1	9:8:125:CYS:SG	2.57	0.43
2:4:23:ILE:HG13	2:4:24:TRP:N	2.33	0.43
2:4:30:HIS:O	2:4:33:LEU:N	2.51	0.43
2:4:62:SER:HB2	40:h:113:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:96:ILE:O	2:4:100:ILE:HG13	2.17	0.43
2:4:278:ARG:NH2	35:a:72:ARG:HH22	2.12	0.43
5:6:136:ASN:O	5:6:139:GLN:N	2.51	0.43
5:6:264:TYR:CD2	5:6:265:PRO:HD3	2.52	0.43
6:5:49:LEU:HD12	6:5:49:LEU:HA	1.68	0.43
8:1:1:MET:HB2	8:1:4:ILE:HG22	2.00	0.43
8:1:281:ARG:HG3	11:B:445:ALA:HB3	2.00	0.43
10:A:81:GLU:CG	10:A:108:LYS:HD3	2.48	0.43
11:B:363:VAL:O	11:B:363:VAL:HG12	2.18	0.43
12:C:221:VAL:HG13	13:D:176:ILE:HD12	1.99	0.43
71:J:101:CDL:H541	71:J:101:CDL:H571	1.66	0.43
27:S:87:GLY:HA3	27:S:88:ASP:C	2.43	0.43
29:U:42:ASP:HA	29:U:43:LYS:HA	1.74	0.43
33:Y:41:ALA:O	33:Y:43:ILE:N	2.51	0.43
35:a:47:TYR:CE1	44:e:105:MET:N	2.85	0.43
42:j:116:PHE:CB	43:g:160:LYS:HB3	2.43	0.43
31:M:29:LYS:HE2	31:M:39:ASP:CG	2.43	0.43
46:l:247:GLN:HG3	46:x:181:TYR:OH	2.18	0.43
46:l:289:SER:HB2	46:l:296:TYR:HE2	1.82	0.43
49:p:78:LEU:HA	49:p:79:SER:HA	1.75	0.43
45:w:211:LEU:C	45:w:213:GLN:N	2.75	0.43
46:x:67:HIS:ND1	46:x:70:ARG:NH2	2.66	0.43
48:z:11:PRO:HB2	52:B3:74:PHE:CE2	2.53	0.43
48:z:78:GLY:O	48:z:79:GLU:HB3	2.17	0.43
48:z:237:TYR:CD2	48:z:239:PRO:HD3	2.53	0.43
2:4:237:LYS:HE2	2:4:237:LYS:HB3	1.85	0.43
3:2:129:ILE:HG21	72:2:402:PC1:H372	1.99	0.43
5:6:154:LEU:HD23	5:6:154:LEU:HA	1.82	0.43
5:6:432:LEU:O	34:Z:60:ASN:CG	2.61	0.43
8:1:63:PRO:HG3	8:1:214:GLU:CD	2.43	0.43
8:1:107:ALA:C	8:1:108:MET:HE2	2.43	0.43
9:8:103:ASN:ND2	9:8:232:ASP:OD2	2.51	0.43
9:8:206:CYS:CB	73:8:501:FMN:C4	2.96	0.43
9:8:318:ILE:HG22	9:8:320:GLY:O	2.18	0.43
10:A:159:ALA:O	18:I:102:ASN:HB2	2.17	0.43
10:A:171:THR:HG23	10:A:173:MET:HE2	1.99	0.43
11:B:238:LEU:HB2	24:P:35:THR:OG1	2.18	0.43
11:B:381:HIS:O	11:B:381:HIS:CG	2.71	0.43
13:D:168:SER:O	13:D:168:SER:OG	2.29	0.43
17:H:80:ARG:HG2	17:H:81:ARG:HH12	1.82	0.43
19:J:38:VAL:HA	30:V:144:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:8:PRO:C	30:V:88:ARG:HH22	2.25	0.43
25:Q:32:TYR:HH	30:V:74:LEU:HD22	1.78	0.43
27:S:68:LYS:HB3	27:S:69:LEU:HD12	1.99	0.43
35:a:27:SER:HA	35:a:28:GLU:HA	1.69	0.43
36:b:66:ARG:HG2	40:h:74:HIS:NE2	2.33	0.43
39:f:162:ASP:HA	39:f:163:LEU:HA	1.83	0.43
40:h:115:GLN:O	40:h:118:ALA:N	2.51	0.43
42:j:116:PHE:CD2	43:g:160:LYS:C	2.96	0.43
45:k:3:THR:H	45:k:6:GLN:HB2	1.83	0.43
46:l:191:LEU:O	46:l:195:VAL:HG23	2.18	0.43
47:m:180:ALA:O	47:m:184:ILE:HG22	2.19	0.43
77:m:401:HEM:HBB2	77:m:401:HEM:CMB	2.48	0.43
48:o:48:TYR:O	48:o:87:LEU:HD23	2.18	0.43
52:s:66:ASP:HA	52:s:69:VAL:HB	1.99	0.43
45:w:262:TRP:HD1	45:w:315:ALA:HA	1.83	0.43
46:x:97:SER:HA	55:B1:70:LEU:HB3	1.99	0.43
48:z:48:TYR:O	48:z:87:LEU:HD23	2.18	0.43
50:A1:57:ASP:O	50:A1:61:ARG:NH1	2.51	0.43
1:9:188:ILE:H	1:9:188:ILE:HG13	1.63	0.43
2:4:182:TRP:O	2:4:182:TRP:CD1	2.72	0.43
3:2:131:LEU:HA	3:2:131:LEU:HD23	1.57	0.43
8:1:316:PRO:HD2	30:V:57:ARG:HH21	1.83	0.43
9:8:52:ARG:HH12	9:8:168:ASN:HD21	1.66	0.43
9:8:128:ARG:O	9:8:132:ARG:HB2	2.18	0.43
10:A:320:GLU:H	23:O:123:TYR:HE1	1.66	0.43
11:B:65:PRO:HD2	11:B:69:VAL:HG12	2.00	0.43
12:C:192:ASP:CG	13:D:132:LYS:CG	2.91	0.43
13:D:197:ILE:C	13:D:199:GLN:N	2.76	0.43
14:E:211:TYR:CZ	24:P:39:PRO:HG3	2.53	0.43
20:K:25:GLN:HG2	20:K:57:GLU:OE2	2.19	0.43
21:L:45:ILE:HD12	21:L:81:LEU:HD22	2.00	0.43
23:O:33:ARG:CZ	31:M:48:VAL:CG2	2.92	0.43
26:R:179:LYS:HB3	26:R:317:ASP:CG	2.44	0.43
26:R:235:THR:HA	26:R:236:VAL:HA	1.66	0.43
34:Z:44:PRO:HA	34:Z:45:TRP:HA	1.71	0.43
35:a:47:TYR:HE1	44:e:105:MET:HA	1.71	0.43
39:f:24:LEU:O	39:f:27:LEU:HB3	2.19	0.43
45:k:251:ALA:HB2	45:k:427:PRO:HD2	1.99	0.43
46:l:51:ILE:HG22	46:l:53:ALA:H	1.83	0.43
50:q:19:TRP:CE3	50:q:19:TRP:C	2.97	0.43
52:s:18:THR:HA	52:s:21:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:t:38:TRP:HB3	53:t:39:ARG:H	1.63	0.43
45:w:235:ARG:HD2	49:A0:14:ARG:HH22	1.81	0.43
58:C2:63:ARG:HA	58:C2:67:PHE:CD2	2.53	0.43
1:9:222:ARG:HH22	9:8:284:ASN:HB2	1.83	0.43
2:4:52:PHE:CZ	2:4:58:SER:OG	2.71	0.43
2:4:62:SER:HB3	2:4:457:PRO:HD3	1.99	0.43
2:4:62:SER:HB3	2:4:457:PRO:HG3	2.00	0.43
2:4:108:MET:HB3	2:4:121:LEU:HD13	1.99	0.43
2:4:156:GLY:C	2:4:159:PRO:HD2	2.43	0.43
2:4:303:ILE:HG22	2:4:304:GLN:O	2.19	0.43
4:7:13:PHE:C	4:7:16:GLY:H	2.21	0.43
4:7:57:PHE:CD1	4:7:61:LEU:HD22	2.54	0.43
5:6:161:ARG:NH1	5:6:238:GLU:O	2.51	0.43
5:6:237:MET:HE1	5:6:248:HIS:CD2	2.54	0.43
7:3:11:PHE:O	7:3:14:ALA:N	2.52	0.43
9:8:242:VAL:HG12	73:8:501:FMN:C5'	2.45	0.43
11:B:62:LYS:CG	11:B:63:PRO:CD	2.67	0.43
11:B:223:HIS:CE1	13:D:91:CYS:HB3	2.52	0.43
12:C:230:GLN:NE2	12:C:233:ARG:HH12	2.16	0.43
14:E:135:ARG:HG2	14:E:136:ALA:N	2.33	0.43
17:H:86:LEU:O	17:H:89:GLU:N	2.48	0.43
22:N:107:PRO:C	22:N:109:ALA:H	2.26	0.43
25:Q:158:LEU:CD1	42:j:88:HIS:HB3	2.34	0.43
27:S:71:LEU:HD23	27:S:146:VAL:HG13	2.00	0.43
72:S:401:PC1:H132	72:S:401:PC1:H111	1.56	0.43
31:W:104:PHE:O	31:W:107:ASP:C	2.61	0.43
31:W:144:ILE:O	31:W:148:ILE:HG12	2.19	0.43
36:b:67:PHE:C	36:b:69:LYS:H	2.26	0.43
43:g:82:VAL:O	43:g:86:PHE:N	2.51	0.43
43:g:87:GLU:O	43:g:90:MET:N	2.51	0.43
45:k:64:PHE:CE1	45:k:86:LEU:HD21	2.52	0.43
45:k:443:TRP:HB3	45:k:445:ARG:H	1.83	0.43
47:y:345:HIS:N	47:y:346:PRO:HD2	2.34	0.43
56:A9:377:PHE:CD2	79:A9:602:HEA:HAD1	2.53	0.43
57:C4:162:SER:HB3	57:C4:197:SER:C	2.44	0.43
58:C2:148:HIS:CE1	58:C2:152:MET:HE3	2.54	0.43
65:C3:36:MET:O	65:C3:40:LEU:HG	2.18	0.43
2:4:214:LEU:HD11	5:6:558:LEU:HD13	2.00	0.43
3:2:60:PHE:CZ	6:5:74:GLY:HA3	2.54	0.43
3:2:221:ALA:HB3	3:2:236:LYS:NZ	2.34	0.43
3:2:323:MET:HE1	3:2:327:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:116:ASN:ND2	73:8:501:FMN:N1	2.67	0.43
10:A:140:GLN:HA	11:B:379:ILE:HG21	1.99	0.43
10:A:145:MET:C	10:A:146:PHE:HD1	2.26	0.43
11:B:169:TRP:HE3	11:B:347:CYS:SG	2.42	0.43
11:B:406:GLU:O	11:B:427:PRO:HD3	2.19	0.43
25:Q:25:LEU:O	25:Q:29:ALA:HB2	2.19	0.43
25:Q:52:ASP:O	25:Q:54:ARG:N	2.42	0.43
26:R:203:PRO:HB3	26:R:265:PHE:CD2	2.47	0.43
35:a:90:GLY:O	35:a:94:GLY:N	2.45	0.43
39:f:25:ARG:O	39:f:28:GLU:HG2	2.19	0.43
42:j:116:PHE:CE1	43:g:157:ALA:HA	2.53	0.43
45:k:57:TYR:OH	45:k:137:GLU:OE1	2.30	0.43
45:k:182:LEU:O	45:k:186:LEU:N	2.29	0.43
45:k:229:PRO:C	45:k:231:LEU:H	2.25	0.43
45:k:262:TRP:HD1	45:k:315:ALA:HA	1.83	0.43
46:l:169:ARG:HH11	46:l:238:LYS:NZ	2.17	0.43
47:m:128:PHE:O	47:m:129:MET:C	2.61	0.43
47:m:345:HIS:N	47:m:346:PRO:HD2	2.34	0.43
45:w:57:TYR:HE2	45:w:134:ILE:HD12	1.83	0.43
45:w:61:HIS:HB3	45:w:65:LYS:HZ1	1.83	0.43
45:w:186:LEU:HD23	45:w:190:TYR:CE2	2.51	0.43
47:y:337:TRP:O	47:y:341:GLN:HG2	2.19	0.43
48:z:150:ASN:OD1	48:z:151:PRO:HD2	2.18	0.43
53:A3:47:TYR:CG	54:B2:33:ARG:NH2	2.69	0.43
56:A9:247:ILE:HB	79:A9:602:HEA:HBC1	2.01	0.43
56:A9:513:LEU:HD12	56:A9:513:LEU:HA	1.65	0.43
57:C4:52:HIS:CD2	60:C0:40:ASP:HB2	2.54	0.43
58:C2:80:ARG:HG2	58:C2:233:PHE:CE1	2.54	0.43
2:4:241:TYR:O	2:4:244:LEU:N	2.24	0.43
2:4:339:SER:OG	2:4:344:LEU:HD23	2.17	0.43
70:4:501:3PE:O14	3:2:238:PRO:CB	2.64	0.43
4:7:100:GLU:O	4:7:103:MET:HB3	2.19	0.43
4:7:125:TRP:HH2	6:5:4:VAL:HG23	1.83	0.43
5:6:340:PHE:O	5:6:343:SER:N	2.51	0.43
5:6:437:PHE:CE1	5:6:441:VAL:HG21	2.54	0.43
8:1:169:GLN:HE21	8:1:174:LEU:HD12	1.84	0.43
8:1:205:SER:H	8:1:279:ARG:HH12	1.65	0.43
8:1:234:MET:O	8:1:237:PHE:HB3	2.19	0.43
8:1:282:TYR:O	8:1:285:LEU:HB3	2.18	0.43
9:8:48:ARG:HG3	9:8:133:HIS:NE2	2.33	0.43
10:A:234:LYS:O	10:A:237:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:286:ILE:HG23	10:A:287:SER:O	2.18	0.43
10:A:364:ASP:CG	10:A:365:THR:H	2.26	0.43
11:B:255:ILE:HD12	11:B:255:ILE:HA	1.81	0.43
11:B:429:PHE:HD1	11:B:429:PHE:HA	1.59	0.43
12:C:86:LEU:HB2	12:C:143:ILE:HG13	2.01	0.43
12:C:96:ILE:HB	12:C:97:PRO:HD3	2.00	0.43
26:R:198:ALA:H	26:R:260:GLY:H	1.67	0.43
26:R:238:GLN:NE2	26:R:271:TYR:HA	2.33	0.43
29:U:64:TYR:CE1	29:U:81:MET:HB2	2.54	0.43
29:U:83:PRO:C	29:U:85:GLU:H	2.27	0.43
37:c:32:GLU:O	37:c:34:VAL:N	2.51	0.43
44:e:92:TRP:O	44:e:94:HIS:HB2	2.18	0.43
45:w:3:THR:H	45:w:6:GLN:HB2	1.83	0.43
45:w:86:LEU:HD13	45:w:99:ILE:HG12	2.01	0.43
45:w:329:MET:CE	51:A2:2:ARG:HH21	2.32	0.43
46:x:304:HIS:CG	46:x:305:GLN:N	2.85	0.43
47:y:207:ASN:ND2	47:y:213:SER:HB3	2.34	0.43
47:y:241:LEU:HD12	47:y:245:PHE:HD2	1.83	0.43
48:z:165:TYR:CE2	48:z:168:VAL:HG22	2.54	0.43
56:A9:70:VAL:HG11	56:A9:246:LEU:HD22	1.99	0.43
60:C0:27:TRP:CH2	61:A6:86:GLY:HA2	2.54	0.43
67:C1:41:ARG:HD2	68:A8:40:TYR:CZ	2.54	0.43
2:4:109:THR:HG22	2:4:110:PHE:N	2.33	0.43
2:4:423:ILE:CG2	35:a:57:ARG:CD	2.96	0.43
70:4:503:3PE:H2E1	70:4:503:3PE:H2B1	1.68	0.43
3:2:320:MET:O	3:2:321:LYS:C	2.60	0.43
4:7:127:ILE:O	4:7:129:ASP:N	2.52	0.43
5:6:557:TRP:CH2	35:a:80:PHE:CE2	3.06	0.43
9:8:98:LYS:O	9:8:101:PHE:HB3	2.18	0.43
9:8:155:TYR:CE1	9:8:196:PHE:HD2	2.36	0.43
10:A:63:PHE:HB2	10:A:75:CYS:HB2	2.01	0.43
10:A:259:SER:HA	10:A:282:ASN:ND2	2.33	0.43
10:A:273:ILE:HD11	10:A:290:THR:O	2.18	0.43
10:A:379:THR:HG22	20:K:54:LEU:HD22	2.01	0.43
14:E:170:GLY:HA2	14:E:171:PRO:HD3	1.67	0.43
21:L:38:TYR:O	21:L:41:TYR:HB2	2.19	0.43
25:Q:51:LYS:HZ3	36:b:189:ASN:ND2	2.14	0.43
25:Q:158:LEU:CD1	25:Q:159:LYS:H	2.26	0.43
26:R:271:TYR:O	26:R:272:LEU:HB2	2.18	0.43
26:R:339:GLY:HA3	26:R:340:VAL:HA	1.65	0.43
27:S:56:SER:OG	27:S:57:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:108:ASP:O	27:S:110:LYS:N	2.51	0.43
28:T:70:PHE:CD1	28:T:70:PHE:O	2.72	0.43
30:V:28:ARG:HA	30:V:29:GLY:HA3	1.76	0.43
40:h:79:ASP:O	40:h:83:ASP:OD2	2.37	0.43
46:x:169:ARG:HH11	46:x:238:LYS:NZ	2.17	0.43
46:x:170:ASN:OD1	46:x:170:ASN:N	2.48	0.43
54:B2:57:HIS:ND1	54:B2:60:GLU:OE2	2.52	0.43
66:B0:44:PRO:HA	66:B0:47:ARG:NH1	2.34	0.43
3:2:21:MET:HG2	3:2:140:SER:CB	2.49	0.43
3:2:60:PHE:CE1	6:5:70:GLU:OE2	2.71	0.43
4:7:161:LEU:O	4:7:164:GLY:N	2.45	0.43
9:8:127:ASP:O	9:8:128:ARG:HB3	2.18	0.43
10:A:81:GLU:HG3	10:A:108:LYS:HD3	2.00	0.43
10:A:82:ILE:HD11	10:A:100:TRP:HB3	2.00	0.43
10:A:415:ASN:O	10:A:418:ILE:N	2.43	0.43
11:B:141:TYR:O	11:B:144:MET:HE2	2.18	0.43
14:E:118:LEU:C	14:E:120:GLU:H	2.27	0.43
26:R:182:ARG:C	26:R:184:LYS:H	2.26	0.43
26:R:309:PRO:O	26:R:310:PHE:CG	2.72	0.43
30:V:9:ASP:C	30:V:10:MET:HE2	2.44	0.43
35:a:70:TYR:O	35:a:75:ASN:ND2	2.52	0.43
36:b:149:LEU:HD23	42:j:90:MET:CE	2.37	0.43
42:j:119:VAL:CA	43:g:147:GLY:H	2.27	0.43
48:o:241:LYS:NZ	50:q:57:ASP:OD2	2.46	0.43
49:p:125:GLU:O	49:p:128:LYS:N	2.51	0.43
52:s:12:GLU:HG2	52:s:13:LEU:N	2.34	0.43
45:w:443:TRP:HB3	45:w:445:ARG:H	1.83	0.43
46:x:83:PHE:CZ	46:x:87:ARG:HG3	2.54	0.43
51:A2:44:CYS:O	51:A2:47:ARG:N	2.45	0.43
54:B2:17:THR:HA	54:B2:20:PHE:HB3	2.00	0.43
54:B2:52:TRP:O	54:B2:53:LYS:C	2.59	0.43
56:A9:106:PRO:HB2	56:A9:107:PRO:HD3	2.01	0.43
58:C2:60:ASP:O	58:C2:64:GLU:HG3	2.18	0.43
64:B4:26:MET:N	64:B4:26:MET:SD	2.91	0.43
2:4:239:GLY:C	2:4:241:TYR:H	2.27	0.43
3:2:47:ASN:HD21	3:2:123:PRO:HB2	1.83	0.43
3:2:100:MET:HE1	5:6:598:SER:CB	2.49	0.43
3:2:158:SER:O	3:2:161:SER:HB3	2.18	0.43
5:6:90:ILE:HB	5:6:91:PRO:HD3	2.01	0.43
5:6:106:TRP:CD1	5:6:447:ASN:HD21	2.37	0.43
5:6:359:MET:CB	5:6:430:ALA:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:32:GLN:O	8:1:33:LEU:HB2	2.18	0.43
8:1:149:ILE:HD11	8:1:185:TRP:HE3	1.83	0.43
8:1:278:PRO:HB2	11:B:194:ILE:HG22	2.00	0.43
9:8:54:LYS:HA	9:8:136:HIS:NE2	2.34	0.43
10:A:140:GLN:HA	11:B:379:ILE:CG2	2.49	0.43
10:A:385:TYR:O	10:A:385:TYR:CG	2.72	0.43
11:B:106:VAL:HG23	11:B:107:ARG:N	2.28	0.43
11:B:138:ARG:CD	14:E:153:ILE:HD11	2.48	0.43
11:B:182:ASN:N	11:B:182:ASN:OD1	2.48	0.43
11:B:371:MET:HB2	11:B:371:MET:HE3	1.74	0.43
14:E:104:ARG:HH12	14:E:112:ARG:HH21	1.66	0.43
16:G:154:LYS:HB3	16:G:155:PRO:CD	2.49	0.43
21:L:61:GLY:O	21:L:63:MET:HB3	2.19	0.43
25:Q:30:HIS:CE1	30:V:63:GLU:OE2	2.72	0.43
27:S:52:GLY:O	27:S:149:ARG:NH2	2.52	0.43
27:S:284:MET:CA	72:S:401:PC1:H112	2.39	0.43
39:f:92:GLU:OE1	39:f:92:GLU:N	2.52	0.43
31:M:18:VAL:O	31:M:21:LEU:N	2.46	0.43
45:k:235:ARG:CZ	49:p:14:ARG:HH12	2.30	0.43
47:m:31:TRP:HA	47:m:100:ARG:HH11	1.83	0.43
48:o:138:PRO:HD2	48:o:141:VAL:HG11	2.00	0.43
52:s:43:ARG:NH2	52:s:52:GLU:OE2	2.52	0.43
45:w:205:HIS:O	45:w:208:LEU:HB3	2.19	0.43
45:w:329:MET:HE3	51:A2:2:ARG:NE	2.31	0.43
64:B4:68:ILE:HG13	64:B4:69:PHE:N	2.33	0.43
65:C3:3:ASN:C	65:C3:3:ASN:ND2	2.77	0.43
65:C3:11:LEU:HD23	65:C3:11:LEU:C	2.44	0.43
3:2:265:MET:HE1	25:Q:167:LEU:HD11	2.01	0.43
5:6:189:PHE:O	5:6:193:LEU:N	2.49	0.43
5:6:527:GLY:C	5:6:529:PHE:H	2.27	0.43
5:6:577:VAL:HG13	6:5:97:GLN:OE1	2.19	0.43
8:1:159:SER:HB3	8:1:317:GLN:HG2	2.01	0.43
8:1:159:SER:HB3	8:1:317:GLN:HG3	2.01	0.43
8:1:251:MET:HB3	8:1:251:MET:HE3	1.48	0.43
73:8:501:FMN:H9	73:8:501:FMN:H1'1	1.59	0.43
10:A:223:ILE:H	10:A:223:ILE:HG12	1.52	0.43
11:B:78:SER:O	11:B:79:ASN:ND2	2.52	0.43
11:B:237:PRO:HA	14:E:211:TYR:CZ	2.54	0.43
12:C:110:PHE:CG	12:C:136:SER:HB3	2.53	0.43
13:D:97:MET:O	13:D:100:ALA:N	2.50	0.43
13:D:202:LYS:NZ	29:U:117:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:52:ASN:HB3	24:P:57:ARG:NH1	2.34	0.43
25:Q:109:GLU:CG	25:Q:110:CYS:H	2.29	0.43
26:R:131:GLY:O	76:R:601:NAP:C3D	2.65	0.43
27:S:100:CYS:CB	27:S:119:LEU:HB2	2.48	0.43
36:b:174:ILE:HD12	36:b:174:ILE:HA	1.87	0.43
39:f:109:PRO:HA	39:f:112:LYS:H	1.84	0.43
31:M:32:VAL:C	31:M:73:PRO:HG2	2.44	0.43
47:m:55:TYR:CG	47:m:56:THR:N	2.87	0.43
47:m:110:LEU:HD12	47:m:110:LEU:HA	1.72	0.43
48:o:5:LEU:HD23	48:o:152:TYR:CE1	2.54	0.43
48:o:54:VAL:HG12	48:o:54:VAL:O	2.19	0.43
54:u:57:HIS:ND1	54:u:60:GLU:OE2	2.52	0.43
46:x:228:GLY:C	46:x:230:LEU:H	2.25	0.43
50:A1:12:TRP:CE3	50:A1:12:TRP:C	2.97	0.43
57:C4:78:LEU:HB2	57:C4:79:PRO:CD	2.38	0.43
58:C2:41:THR:O	58:C2:45:ILE:HG13	2.18	0.43
58:C2:110:PRO:HB3	63:A5:30:TRP:CD2	2.54	0.43
2:4:12:MET:HB3	2:4:13:PRO:HD3	2.01	0.42
2:4:184:GLN:OE1	2:4:184:GLN:N	2.52	0.42
2:4:360:LEU:HD13	71:6:701:CDL:C53	2.49	0.42
2:4:446:LEU:CG	71:4:502:CDL:H342	2.48	0.42
3:2:89:LEU:O	3:2:91:ASN:N	2.52	0.42
3:2:146:PHE:HE1	3:2:195:PRO:HA	1.84	0.42
5:6:4:PHE:CD2	5:6:61:LEU:HD12	2.48	0.42
71:6:701:CDL:H731	71:6:701:CDL:H762	1.83	0.42
8:1:290:TRP:O	8:1:295:PRO:HD3	2.19	0.42
10:A:310:GLU:HG2	10:A:311:LYS:N	2.34	0.42
10:A:359:ASN:CG	20:K:68:ARG:NH1	2.78	0.42
10:A:691:ILE:HG23	10:A:692:LYS:N	2.34	0.42
11:B:203:MET:HE2	11:B:203:MET:HA	2.00	0.42
11:B:412:VAL:HG12	11:B:413:SER:N	2.33	0.42
11:B:456:ILE:HA	11:B:456:ILE:HD13	1.69	0.42
70:B:501:3PE:H232	14:E:63:TRP:NE1	2.33	0.42
13:D:186:CYS:HB3	74:D:301:SF4:S4	2.59	0.42
25:Q:28:ALA:C	25:Q:30:HIS:N	2.76	0.42
26:R:261:LYS:HG2	26:R:263:PHE:HE1	1.83	0.42
27:S:196:ASP:OD2	27:S:250:GLU:HA	2.19	0.42
27:S:235:PRO:O	27:S:239:GLU:N	2.51	0.42
31:W:109:GLY:HA2	31:W:110:LEU:HA	1.75	0.42
31:W:156:GLU:OE2	37:c:24:LYS:CA	2.31	0.42
34:Z:63:PHE:CZ	34:Z:64:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Z:64:VAL:HA	34:Z:67:LEU:HG	2.01	0.42
42:j:97:HIS:N	42:j:98:PRO:HD3	2.34	0.42
43:g:174:ALA:HA	43:g:175:ALA:HA	1.68	0.42
44:e:88:PRO:HD2	44:e:114:ARG:HG3	1.99	0.42
45:k:205:HIS:O	45:k:208:LEU:HB3	2.19	0.42
47:m:50:PHE:CE2	49:p:58:PHE:HB3	2.54	0.42
48:o:81:PHE:HZ	48:o:89:ASP:OD1	2.01	0.42
49:p:31:ALA:HB2	54:u:7:ALA:HB2	2.00	0.42
49:p:60:SER:HA	49:p:63:SER:OG	2.18	0.42
50:q:8:ALA:O	50:q:12:TRP:N	2.51	0.42
45:w:67:THR:OG1	45:w:68:LYS:N	2.50	0.42
46:x:51:ILE:HG22	46:x:53:ALA:H	1.84	0.42
47:y:55:TYR:CG	47:y:56:THR:N	2.87	0.42
48:z:3:LEU:HD12	52:B3:59:LEU:HD12	2.00	0.42
52:B3:18:THR:HA	52:B3:21:ARG:HD2	2.00	0.42
60:C0:93:LEU:HD23	60:C0:93:LEU:HA	1.88	0.42
1:9:133:GLN:HG3	1:9:172:ILE:HD11	2.01	0.42
2:4:408:LEU:CD2	5:6:172:ILE:HG21	2.49	0.42
2:4:448:THR:O	5:6:68:TRP:CZ3	2.73	0.42
3:2:260:PHE:HE2	3:2:264:TRP:CE3	2.37	0.42
4:7:70:TYR:OH	7:3:55:PHE:O	2.23	0.42
4:7:140:ALA:C	4:7:142:GLY:H	2.26	0.42
5:6:17:MET:HB3	5:6:18:PRO:HD3	2.01	0.42
5:6:389:PHE:O	5:6:393:ASP:HB3	2.19	0.42
8:1:303:TRP:CE2	8:1:307:LEU:HD21	2.53	0.42
8:1:316:PRO:HG3	30:V:57:ARG:HG2	2.00	0.42
9:8:369:ARG:HD2	9:8:369:ARG:HA	1.82	0.42
10:A:455:ILE:HB	10:A:460:HIS:NE2	2.34	0.42
11:B:65:PRO:HB2	11:B:69:VAL:HA	2.00	0.42
11:B:106:VAL:C	11:B:108:LYS:H	2.26	0.42
11:B:211:PHE:HD1	11:B:211:PHE:HA	1.68	0.42
12:C:127:ARG:NH1	16:G:137:PHE:HZ	2.16	0.42
12:C:188:ARG:HD3	12:C:192:ASP:O	2.19	0.42
13:D:86:THR:C	13:D:87:PHE:HD1	2.27	0.42
14:E:206:GLN:HA	14:E:209:TYR:CD2	2.54	0.42
14:E:206:GLN:HA	14:E:209:TYR:HD2	1.84	0.42
21:L:23:PHE:HZ	72:L:200:PC1:H261	1.82	0.42
26:R:134:TRP:CZ2	26:R:311:GLU:HG3	2.54	0.42
27:S:225:ILE:HG13	27:S:226:GLU:N	2.35	0.42
29:U:124:TYR:O	29:U:125:VAL:C	2.62	0.42
30:V:142:TRP:C	30:V:143:TYR:CD2	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:137:LYS:HE3	37:c:8:GLU:HG3	2.01	0.42
33:Y:66:ALA:O	33:Y:70:PHE:N	2.29	0.42
35:a:84:THR:OG1	35:a:86:THR:HG22	2.20	0.42
31:M:77:VAL:O	31:M:81:ALA:N	2.45	0.42
46:l:182:ARG:HH11	46:l:185:LYS:CD	2.32	0.42
47:m:91:PHE:HE2	47:m:273:TYR:CZ	2.38	0.42
47:m:256:TYR:HB2	48:o:115:TYR:CE1	2.53	0.42
47:m:278:TYR:HE2	47:m:282:ARG:HH21	1.67	0.42
48:o:41:HIS:HD2	78:o:301:HEC:NB	2.17	0.42
48:o:44:ASP:OD1	48:o:93:LYS:HE2	2.18	0.42
48:o:65:ALA:O	48:o:67:GLU:N	2.52	0.42
48:o:165:TYR:CE2	48:o:168:VAL:HG22	2.54	0.42
50:q:43:VAL:HA	50:q:46:ALA:HB3	2.01	0.42
47:y:91:PHE:CD2	47:y:273:TYR:CG	3.07	0.42
58:C2:19:THR:HG22	58:C2:53:THR:OG1	2.18	0.42
1:9:110:MET:HE1	10:A:209:TYR:N	2.34	0.42
2:4:259:TYR:CD2	35:a:102:TYR:HE1	2.37	0.42
5:6:237:MET:HB3	5:6:299:LYS:CD	2.46	0.42
5:6:477:ILE:HD12	38:d:87:TRP:HZ2	1.84	0.42
6:5:37:MET:HG3	6:5:67:ALA:HB1	2.01	0.42
8:1:233:MET:C	8:1:236:ILE:HG23	2.44	0.42
8:1:235:ASN:ND2	8:1:270:PHE:CZ	2.73	0.42
10:A:246:ARG:HB2	10:A:265:THR:CG2	2.50	0.42
10:A:355:LYS:HA	10:A:530:TYR:OH	2.18	0.42
11:B:331:LEU:HA	11:B:331:LEU:HD23	1.56	0.42
11:B:340:SER:O	11:B:343:ILE:N	2.50	0.42
70:B:501:3PE:H3I3	21:L:28:LEU:CD2	2.49	0.42
18:I:71:LEU:HD23	18:I:71:LEU:O	2.20	0.42
22:N:6:LYS:O	22:N:16:VAL:HG21	2.19	0.42
24:P:108:GLN:HG2	24:P:108:GLN:O	2.19	0.42
26:R:171:ASN:O	26:R:181:LEU:HD21	2.18	0.42
26:R:217:PHE:C	26:R:219:ASN:H	2.26	0.42
27:S:117:TYR:HB2	27:S:167:ILE:HD11	2.02	0.42
27:S:206:ILE:HD11	27:S:214:GLU:CB	2.47	0.42
27:S:282:LEU:O	27:S:284:MET:N	2.52	0.42
28:T:69:ILE:HG21	28:T:100:ILE:CG1	2.49	0.42
44:e:91:ASP:O	44:e:92:TRP:C	2.62	0.42
31:M:14:ARG:HA	31:M:17:TYR:HE2	1.83	0.42
48:o:69:GLU:OE1	48:o:84:PRO:HD3	2.19	0.42
49:p:73:LYS:HD3	49:p:94:LYS:CA	2.44	0.42
45:w:118:GLN:HE22	45:w:217:SER:C	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:76:THR:HG22	46:x:77:THR:O	2.20	0.42
46:x:182:ARG:HH11	46:x:185:LYS:CD	2.32	0.42
46:x:253:VAL:HG11	46:x:333:ALA:HB2	2.01	0.42
47:y:180:ALA:O	47:y:184:ILE:HG22	2.19	0.42
52:B3:43:ARG:NH2	52:B3:52:GLU:OE2	2.52	0.42
53:A3:15:ARG:O	53:A3:17:TRP:N	2.51	0.42
55:B1:70:LEU:CD1	55:B1:71:ASN:H	2.24	0.42
1:9:112:VAL:O	1:9:113:TYR:C	2.62	0.42
1:9:119:TYR:HB3	9:8:201:ALA:HB3	2.02	0.42
1:9:177:LEU:HA	9:8:159:ARG:HH11	1.81	0.42
2:4:278:ARG:HG3	5:6:546:GLN:OE1	2.19	0.42
3:2:96:MET:O	3:2:100:MET:HG2	2.19	0.42
3:2:150:ASN:C	3:2:152:ASN:H	2.28	0.42
3:2:234:TRP:CE3	27:S:327:TYR:CD2	3.08	0.42
4:7:135:PHE:O	4:7:135:PHE:CG	2.72	0.42
4:7:145:ALA:O	4:7:146:LEU:HD23	2.19	0.42
5:6:95:PHE:O	5:6:98:TRP:HB3	2.19	0.42
5:6:310:LEU:HD23	5:6:313:MET:CE	2.49	0.42
5:6:590:SER:HB2	28:T:42:ALA:HB1	2.01	0.42
8:1:28:LEU:O	8:1:32:GLN:HG2	2.20	0.42
8:1:96:ILE:HG21	8:1:98:MET:HE3	2.01	0.42
8:1:184:MET:HE2	8:1:293:PHE:HD1	1.83	0.42
9:8:249:ALA:O	9:8:252:PRO:HD2	2.19	0.42
10:A:74:ASN:OD1	10:A:74:ASN:N	2.35	0.42
10:A:125:PRO:HG3	10:A:174:THR:CG2	2.50	0.42
10:A:657:ASP:OD1	10:A:657:ASP:O	2.36	0.42
11:B:266:ARG:HB2	14:E:66:LEU:HD22	2.01	0.42
11:B:461:VAL:O	11:B:461:VAL:HG12	2.20	0.42
13:D:123:MET:HE3	13:D:123:MET:HB2	1.93	0.42
13:D:156:CYS:HB2	74:D:301:SF4:S1	2.60	0.42
17:H:80:ARG:HG2	17:H:81:ARG:NH1	2.35	0.42
26:R:187:GLY:HA2	26:R:191:VAL:HG23	2.01	0.42
26:R:306:GLU:C	26:R:307:ILE:HG23	2.44	0.42
27:S:53:ASN:O	27:S:149:ARG:NH2	2.53	0.42
27:S:103:GLU:HA	27:S:106:TYR:CD2	2.54	0.42
29:U:67:GLU:HA	29:U:71:LYS:HB3	2.02	0.42
45:k:86:LEU:HD13	45:k:99:ILE:HG12	2.01	0.42
46:l:31:ASN:ND2	46:l:225:ASN:OD1	2.52	0.42
46:l:253:VAL:HG11	46:l:333:ALA:HB2	2.01	0.42
46:l:354:ASN:ND2	46:l:407:ASP:OD2	2.52	0.42
48:z:20:SER:OG	48:z:21:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:41:HIS:HD2	78:z:301:HEC:NB	2.17	0.42
48:z:44:ASP:OD1	48:z:93:LYS:HE2	2.18	0.42
48:z:65:ALA:O	48:z:67:GLU:N	2.52	0.42
64:B4:61:GLU:OE1	64:B4:64:ARG:NH1	2.51	0.42
2:4:112:ALA:C	2:4:114:GLU:N	2.78	0.42
2:4:150:LEU:C	2:4:152:TYR:N	2.77	0.42
2:4:350:THR:OG1	2:4:351:LEU:HG	2.19	0.42
4:7:17:PHE:HD1	4:7:20:PHE:HE2	1.68	0.42
5:6:576:LEU:HD23	5:6:576:LEU:O	2.20	0.42
9:8:183:GLY:HA2	9:8:184:LYS:HA	1.61	0.42
10:A:116:VAL:O	10:A:119:PHE:N	2.37	0.42
10:A:117:MET:SD	10:A:142:GLN:HB2	2.60	0.42
12:C:171:GLU:O	12:C:174:ASP:N	2.51	0.42
13:D:153:MET:HE1	13:D:193:LEU:HD11	2.01	0.42
13:D:209:ARG:HG2	13:D:210:LEU:N	2.35	0.42
18:I:85:ILE:HG22	18:I:86:SER:H	1.83	0.42
21:L:58:ARG:HH22	25:Q:137:LEU:HD13	1.84	0.42
23:O:103:VAL:O	23:O:105:ARG:N	2.51	0.42
25:Q:53:PRO:CD	36:b:188:ASP:OD2	2.68	0.42
26:R:197:GLU:HG2	26:R:259:ARG:HE	1.84	0.42
27:S:53:ASN:CG	27:S:54:ILE:H	2.27	0.42
27:S:102:LEU:HA	27:S:105:PHE:HE2	1.85	0.42
28:T:20:ARG:CZ	28:T:20:ARG:CB	2.86	0.42
28:T:69:ILE:CB	28:T:100:ILE:HD11	2.49	0.42
35:a:76:ILE:O	35:a:79:ASN:N	2.52	0.42
39:f:18:ARG:O	39:f:22:ARG:NE	2.52	0.42
31:M:60:PHE:HE2	31:M:62:ILE:HG13	1.84	0.42
45:k:215:HIS:H	45:k:217:SER:H	1.66	0.42
45:k:243:HIS:O	45:k:426:GLY:N	2.52	0.42
48:o:165:TYR:CD2	48:o:168:VAL:HG22	2.55	0.42
45:w:243:HIS:O	45:w:426:GLY:N	2.52	0.42
47:y:71:ARG:HB3	48:z:49:ARG:HH22	1.83	0.42
77:y:401:HEM:HBB2	77:y:401:HEM:CMB	2.48	0.42
56:A9:365:ILE:HD12	57:C4:87:MET:CE	2.34	0.42
56:A9:462:LEU:O	56:A9:466:MET:HG3	2.20	0.42
62:A4:5:LYS:CD	62:A4:6:GLY:N	2.81	0.42
62:A4:77:PRO:HA	62:A4:82:TYR:HA	2.02	0.42
2:4:95[B]:PHE:CE2	2:4:136:TRP:HD1	2.38	0.42
2:4:143:LEU:HA	2:4:143:LEU:HD23	1.68	0.42
2:4:423:ILE:CB	35:a:57:ARG:CG	2.57	0.42
3:2:52:ALA:HB2	3:2:123:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:78:LEU:HD23	3:2:78:LEU:O	2.18	0.42
3:2:202:LEU:O	3:2:205:LEU:N	2.52	0.42
3:2:337:LEU:HD12	3:2:337:LEU:O	2.20	0.42
7:3:3:LEU:O	7:3:6:ALA:N	2.46	0.42
7:3:99:ALA:HB2	8:1:298:LEU:HD23	2.00	0.42
8:1:5:ASN:HD21	19:J:23:THR:CG2	2.28	0.42
9:8:207:GLY:O	73:8:501:FMN:C8M	2.67	0.42
9:8:406:PRO:C	9:8:408:GLU:H	2.26	0.42
73:8:501:FMN:C2	73:8:501:FMN:HO3'	2.16	0.42
10:A:55:LYS:HE2	10:A:55:LYS:HB2	1.80	0.42
10:A:175:ARG:O	10:A:176:CYS:C	2.59	0.42
10:A:302:LEU:HG	10:A:571:HIS:O	2.19	0.42
14:E:197:TRP:HB3	29:U:84:PRO:CB	2.41	0.42
23:O:25:MET:HB3	23:O:29:LYS:HZ1	1.84	0.42
26:R:207:PHE:CZ	26:R:241:TYR:HB2	2.54	0.42
27:S:335:VAL:H	42:j:52:PRO:HD3	1.84	0.42
31:W:128:PHE:O	31:W:130:ILE:N	2.37	0.42
35:a:67:ARG:NH1	44:e:79:PRO:CG	2.82	0.42
36:b:121:ILE:HG23	36:b:122:ALA:N	2.35	0.42
37:c:40:VAL:HA	37:c:41:SER:HA	1.91	0.42
38:d:66:PHE:O	38:d:70:LYS:HG2	2.19	0.42
40:h:111:ASP:N	40:h:111:ASP:OD1	2.52	0.42
46:l:231:GLY:O	46:l:232:LEU:C	2.62	0.42
47:m:192:ILE:O	47:m:195:VAL:N	2.52	0.42
47:m:248:ASP:CG	48:o:118:ARG:HH21	2.28	0.42
45:w:329:MET:HE3	51:A2:2:ARG:HH21	1.84	0.42
46:x:200:THR:C	46:x:204:MET:HE2	2.45	0.42
46:x:354:ASN:ND2	46:x:407:ASP:OD2	2.52	0.42
47:y:91:PHE:HE2	47:y:273:TYR:CZ	2.37	0.42
52:B3:17:LEU:HD21	52:B3:21:ARG:HH21	1.85	0.42
53:A3:15:ARG:C	53:A3:17:TRP:N	2.77	0.42
64:B4:21:ILE:O	64:B4:25:PHE:HD2	2.02	0.42
1:9:133:GLN:O	1:9:186:VAL:HG23	2.19	0.42
2:4:52:PHE:HZ	2:4:58:SER:HG	1.60	0.42
2:4:89:LEU:HD13	2:4:93:LYS:NZ	2.35	0.42
2:4:176:PHE:CE2	36:b:143:GLU:OE1	2.72	0.42
2:4:408:LEU:O	2:4:412:ILE:HG22	2.20	0.42
2:4:440:HIS:C	2:4:443:PRO:HD2	2.44	0.42
3:2:150:ASN:O	3:2:152:ASN:N	2.51	0.42
3:2:325:PHE:CE2	70:2:401:3PE:C2H	3.03	0.42
3:2:342:MET:O	42:j:82:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:5:ILE:HA	4:7:8:ILE:HG22	2.01	0.42
4:7:9:LEU:HD23	4:7:9:LEU:HA	1.82	0.42
4:7:113:VAL:HA	4:7:114:GLU:HA	1.62	0.42
4:7:152:TRP:HA	4:7:155:ILE:CG2	2.50	0.42
8:1:140:ILE:HA	8:1:143:GLU:OE1	2.20	0.42
9:8:149:MET:HE3	9:8:149:MET:HB3	1.80	0.42
10:A:89:VAL:HB	10:A:94:MET:SD	2.60	0.42
10:A:312:GLY:CA	29:U:144:TYR:CE1	2.98	0.42
10:A:337:ASP:O	10:A:543:LYS:N	2.52	0.42
10:A:431:LEU:HD23	10:A:432:ILE:C	2.45	0.42
10:A:534:VAL:O	10:A:534:VAL:HG13	2.19	0.42
12:C:214:TYR:CD1	13:D:138:ARG:HD3	2.55	0.42
13:D:76:TRP:O	13:D:76:TRP:CG	2.72	0.42
13:D:103:ARG:HD2	14:E:84:ILE:HD13	2.02	0.42
19:J:55:SER:OG	19:J:56:GLY:N	2.52	0.42
20:K:56:ARG:HD3	20:K:56:ARG:HA	1.79	0.42
22:N:38:ILE:HG22	22:N:39:PRO:O	2.19	0.42
27:S:124:TYR:CZ	27:S:151:ILE:HD11	2.55	0.42
28:T:77:SER:CA	28:T:80:VAL:CG2	2.98	0.42
37:c:18:LEU:O	37:c:21:ARG:HB3	2.19	0.42
41:i:69:TYR:CD1	42:j:20:SER:HB2	2.54	0.42
42:j:25:LYS:HE2	42:j:25:LYS:HB3	1.79	0.42
48:o:72:ASP:OD1	48:o:73:GLY:N	2.52	0.42
46:x:31:ASN:ND2	46:x:225:ASN:OD1	2.52	0.42
50:A1:12:TRP:CE3	50:A1:13:LEU:CA	3.03	0.42
56:A9:173:PRO:HA	56:A9:174:PRO:HD3	1.96	0.42
1:9:143:ARG:HH12	9:8:285:PRO:CD	2.33	0.42
2:4:74:PRO:O	2:4:78:MET:HE2	2.20	0.42
2:4:121:LEU:HA	2:4:124:ALA:HB2	2.02	0.42
2:4:125:THR:O	2:4:126:LEU:HB2	2.20	0.42
3:2:87:MET:CE	3:2:90:PHE:HZ	2.23	0.42
3:2:222:ASN:ND2	27:S:304:GLU:O	2.53	0.42
3:2:248:LEU:HD13	3:2:296:LEU:HD23	2.01	0.42
4:7:71:THR:C	4:7:73:ALA:H	2.28	0.42
5:6:261:ILE:HD13	5:6:326:PHE:HB2	2.01	0.42
5:6:329:ILE:H	5:6:329:ILE:HD12	1.84	0.42
10:A:253:VAL:HG11	10:A:596:TYR:CG	2.55	0.42
10:A:275:PRO:HB3	10:A:286:ILE:HB	2.01	0.42
10:A:423:LEU:C	10:A:425:ASN:N	2.76	0.42
10:A:541:PRO:CB	10:A:561:PRO:HG3	2.50	0.42
13:D:90:ALA:O	13:D:91:CYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:130:ILE:HG12	14:E:145:TYR:CD1	2.55	0.42
21:L:16:GLU:OE1	21:L:16:GLU:N	2.53	0.42
21:L:54:PRO:HB2	25:Q:128:VAL:HB	2.02	0.42
25:Q:96:LEU:HD23	25:Q:98:ARG:HG2	2.01	0.42
30:V:141:ILE:HD12	30:V:141:ILE:HG23	1.84	0.42
37:c:100:LYS:HA	43:g:115:GLN:O	2.20	0.42
38:d:63:LEU:HD12	38:d:66:PHE:HB3	2.01	0.42
40:h:82:VAL:O	40:h:83:ASP:C	2.62	0.42
40:h:118:ALA:HB3	43:g:101:GLU:OE2	2.20	0.42
44:e:63:GLU:C	44:e:65:TYR:H	2.21	0.42
46:l:83:PHE:CZ	46:l:87:ARG:HG3	2.54	0.42
46:l:383:GLY:O	46:l:386:ALA:N	2.53	0.42
46:l:398:VAL:O	46:l:402:ILE:HG13	2.20	0.42
47:m:207:ASN:ND2	47:m:213:SER:HB3	2.34	0.42
47:m:271:GLU:CD	47:m:273:TYR:HH	2.19	0.42
47:m:274:PHE:O	47:m:275:LEU:C	2.63	0.42
49:p:75:GLU:HG2	49:p:76:ILE:O	2.20	0.42
52:s:17:LEU:HD21	52:s:21:ARG:HH21	1.85	0.42
52:s:66:ASP:O	52:s:70:ALA:N	2.53	0.42
46:x:212:SER:HB2	46:x:214:PRO:HD2	2.02	0.42
48:z:54:VAL:O	48:z:54:VAL:HG12	2.19	0.42
59:A7:127:LYS:O	59:A7:130:PRO:HD3	2.20	0.42
61:A6:86:GLY:O	61:A6:87:THR:O	2.37	0.42
63:A5:20:PHE:N	63:A5:21:PRO:HD3	2.35	0.42
2:4:59:ASP:OD2	2:4:64:PRO:HA	2.19	0.42
2:4:423:ILE:HG22	35:a:57:ARG:HD2	2.01	0.42
3:2:139:MET:HE3	3:2:190:MET:SD	2.60	0.42
3:2:144:GLN:C	3:2:146:PHE:H	2.27	0.42
3:2:169:GLY:O	3:2:170:LEU:C	2.63	0.42
4:7:19:GLY:O	4:7:24:PRO:HG3	2.19	0.42
5:6:150:MET:HA	5:6:150:MET:HE2	2.02	0.42
5:6:254:VAL:O	5:6:258:PHE:N	2.50	0.42
8:1:97:ASN:ND2	19:J:38:VAL:HG12	2.35	0.42
9:8:77:LEU:HD23	9:8:100:SER:HA	2.02	0.42
9:8:325:PRO:HD2	9:8:347:THR:CG2	2.48	0.42
10:A:140:GLN:HG2	11:B:383:LYS:HD3	2.02	0.42
10:A:436:VAL:O	10:A:442:TYR:OH	2.34	0.42
10:A:447:ASP:O	10:A:448:SER:HB3	2.20	0.42
11:B:122:LYS:HB2	12:C:200:PHE:CD1	2.55	0.42
11:B:138:ARG:CZ	14:E:153:ILE:HG12	2.50	0.42
11:B:238:LEU:HD21	30:V:8:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:330:TYR:O	11:B:333:ARG:N	2.49	0.42
11:B:378:LEU:HD12	11:B:378:LEU:N	2.35	0.42
11:B:382:PHE:O	11:B:382:PHE:CG	2.73	0.42
11:B:397:TYR:CD2	11:B:398:THR:N	2.88	0.42
12:C:183:HIS:O	12:C:184:PRO:C	2.61	0.42
15:F:85:PHE:O	15:F:88:LEU:HB2	2.20	0.42
22:N:103:LEU:HD23	22:N:104:VAL:N	2.35	0.42
23:O:69:LYS:HE3	23:O:70:ASN:OD1	2.20	0.42
23:O:76:PRO:C	23:O:78:VAL:H	2.27	0.42
27:S:167:ILE:HD12	27:S:167:ILE:HA	1.82	0.42
28:T:15:GLY:O	28:T:78:ALA:HB1	2.20	0.42
37:c:8:GLU:OE1	37:c:8:GLU:N	2.38	0.42
38:d:105:GLU:CD	44:e:165:ASN:N	2.62	0.42
43:g:120:SER:C	43:g:122:ARG:N	2.78	0.42
31:M:35:HIS:H	31:M:39:ASP:CG	2.28	0.42
45:k:57:TYR:HE2	45:k:134:ILE:HD12	1.83	0.42
46:l:200:THR:C	46:l:204:MET:HE2	2.45	0.42
48:o:121:HIS:CG	48:o:122:GLY:N	2.88	0.42
45:w:394:GLU:CD	45:w:398:ARG:HE	2.28	0.42
45:w:408:ARG:O	45:w:412:SER:OG	2.26	0.42
45:w:445:ARG:HA	45:w:445:ARG:HD3	1.83	0.42
46:x:283:PRO:HA	46:x:290:ASN:HD21	1.85	0.42
59:A7:126:MET:HG3	59:A7:128:VAL:HG23	2.01	0.42
63:A5:24:ASN:HD22	63:A5:25:GLN:N	2.18	0.42
2:4:82:HIS:CE1	2:4:432:ARG:NH1	2.88	0.42
3:2:230:LEU:C	3:2:232:HIS:H	2.27	0.42
3:2:311:MET:HE1	27:S:98:GLY:H	1.85	0.42
4:7:148:SER:O	4:7:150:GLY:N	2.53	0.42
8:1:171:GLN:NE2	8:1:171:GLN:CA	2.83	0.42
8:1:216:ALA:O	8:1:220:PHE:HB3	2.20	0.42
9:8:214:GLU:O	9:8:217:GLU:HB3	2.20	0.42
10:A:435:PRO:HG3	10:A:444:HIS:ND1	2.35	0.42
11:B:218:SER:OG	14:E:98:ARG:NH2	2.45	0.42
12:C:156:GLU:N	12:C:156:GLU:OE1	2.53	0.42
22:N:94:MET:SD	22:N:99:PRO:HG2	2.59	0.42
25:Q:69:GLU:HA	25:Q:72:ARG:HB3	2.01	0.42
26:R:45:LYS:HD3	26:R:45:LYS:HA	1.83	0.42
26:R:128:ASN:ND2	26:R:130:VAL:HG12	2.35	0.42
27:S:272:LEU:HB3	27:S:275:ASN:CB	2.50	0.42
27:S:335:VAL:CG1	42:j:51:ARG:O	2.68	0.42
28:T:80:VAL:HB	28:T:81:ARG:H	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:88:LEU:O	28:T:88:LEU:HD23	2.20	0.42
29:U:26:VAL:HG13	29:U:33:VAL:HG23	2.01	0.42
31:W:119:ILE:HB	31:W:130:ILE:HD13	2.01	0.42
36:b:128:GLY:C	36:b:130:GLU:H	2.27	0.42
38:d:92:HIS:CE1	38:d:96:VAL:HG21	2.55	0.42
39:f:19:LEU:HA	39:f:22:ARG:NH2	2.35	0.42
45:k:229:PRO:C	45:k:231:LEU:N	2.78	0.42
45:k:282:CYS:SG	45:k:305:GLN:HB3	2.60	0.42
46:l:395:PRO:O	46:l:399:LEU:HG	2.19	0.42
47:m:265:PRO:HG2	47:m:268:ILE:CG1	2.50	0.42
48:o:23:HIS:CD2	54:u:51:LEU:HA	2.51	0.42
50:q:77:LYS:HA	50:q:80:TRP:CD1	2.55	0.42
45:w:133:VAL:O	45:w:136:GLN:HB3	2.20	0.42
47:y:172:LYS:O	47:y:174:THR:N	2.53	0.42
48:z:5:LEU:HD23	48:z:152:TYR:CE1	2.54	0.42
57:C4:146:MET:SD	57:C4:189:PRO:HB3	2.60	0.42
59:A7:130:PRO:O	59:A7:136:ALA:HB2	2.20	0.42
61:A6:53:THR:HG22	61:A6:54:ASN:OD1	2.19	0.42
2:4:196:TRP:HB2	2:4:251:ASN:ND2	2.36	0.41
2:4:306:PRO:HD2	43:g:149:HIS:CB	2.49	0.41
2:4:445:LEU:HD12	2:4:446:LEU:N	2.35	0.41
6:5:89:TYR:CD1	6:5:91:GLN:NE2	2.88	0.41
7:3:82:ALA:O	7:3:83:ASN:C	2.62	0.41
8:1:33:LEU:HD23	14:E:82:ALA:H	1.85	0.41
8:1:77:MET:HB3	8:1:77:MET:HE2	1.36	0.41
9:8:225:LEU:O	9:8:228:PRO:HD3	2.19	0.41
10:A:130:ILE:HG22	14:E:140:ARG:CZ	2.50	0.41
10:A:448:SER:OG	10:A:451:ILE:HG12	2.20	0.41
10:A:611:THR:CG2	16:G:105:GLU:HA	2.49	0.41
11:B:339:GLN:O	11:B:342:ARG:HB3	2.20	0.41
12:C:63:PHE:CG	24:P:97:PRO:HG3	2.55	0.41
12:C:138:ARG:O	24:P:101:ILE:HG13	2.19	0.41
12:C:213:ARG:HB2	13:D:175:ARG:HG3	2.02	0.41
12:C:218:VAL:O	12:C:219:LYS:HG3	2.16	0.41
27:S:211:ASN:HB3	27:S:214:GLU:HB2	2.01	0.41
28:T:6:LEU:C	28:T:6:LEU:HD23	2.45	0.41
29:U:62:VAL:HG22	29:U:63:ILE:N	2.35	0.41
42:j:38:GLY:HA2	42:j:41:SER:HB3	2.02	0.41
42:j:116:PHE:CE1	43:g:157:ALA:O	2.73	0.41
43:g:6:ASP:HB2	43:g:9:VAL:HB	2.02	0.41
31:M:25:ILE:HB	31:M:42:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:l:37:SER:C	46:l:38:LEU:HD12	2.45	0.41
47:m:22:PRO:HG3	51:r:4:PHE:CE2	2.55	0.41
47:m:91:PHE:CD2	47:m:273:TYR:CG	3.07	0.41
47:m:337:TRP:O	47:m:341:GLN:HG2	2.19	0.41
48:o:14:HIS:HB3	48:o:21:LEU:HD23	2.01	0.41
46:x:37:SER:C	46:x:38:LEU:HD12	2.45	0.41
47:y:19:ILE:HG23	47:y:221:HIS:HB2	2.01	0.41
47:y:129:MET:HE1	47:y:181:PHE:HB3	2.02	0.41
48:z:70:VAL:HG23	48:z:81:PHE:O	2.20	0.41
55:B1:77:ARG:HG2	55:B1:78:TYR:H	1.85	0.41
56:A9:474:GLU:HG3	56:A9:475:ALA:N	2.34	0.41
58:C2:160:LEU:HD12	58:C2:160:LEU:HA	1.94	0.41
59:A7:102:TYR:HD2	68:A8:35:TYR:HE1	1.68	0.41
62:A4:54:ARG:N	62:A4:54:ARG:CD	2.80	0.41
1:9:244:GLY:O	1:9:246:GLN:HG3	2.19	0.41
2:4:116:ILE:HD12	2:4:116:ILE:HA	1.84	0.41
2:4:197:LEU:HD11	2:4:201:MET:HE2	2.02	0.41
2:4:363:SER:HB3	2:4:411:LEU:HD11	2.01	0.41
2:4:382:VAL:HA	2:4:385:THR:HG22	2.01	0.41
3:2:177:LYS:O	3:2:180:ALA:N	2.53	0.41
8:1:108:MET:HE1	8:1:111:LEU:HD22	2.01	0.41
9:8:346:GLN:CD	9:8:440:ARG:HD3	2.45	0.41
10:A:353:ALA:HB1	10:A:623:ILE:HG21	2.01	0.41
10:A:355:LYS:HB2	10:A:530:TYR:HH	1.73	0.41
10:A:385:TYR:CE1	10:A:526:LEU:HD13	2.54	0.41
11:B:142:VAL:HG12	11:B:182:ASN:OD1	2.20	0.41
13:D:82:LEU:C	13:D:84:PRO:HD3	2.45	0.41
14:E:57:ALA:HB3	21:L:13:TRP:CH2	2.43	0.41
19:J:41:TYR:O	19:J:44:GLN:N	2.53	0.41
26:R:191:VAL:HG12	26:R:195:PHE:CE2	2.55	0.41
28:T:89:ASN:O	28:T:92:ILE:HG13	2.20	0.41
28:T:101:LEU:CD1	28:T:111:GLY:CA	2.98	0.41
28:T:106:ARG:HA	28:T:106:ARG:CZ	2.45	0.41
31:W:123:GLU:CD	31:W:127:GLY:HA2	2.44	0.41
31:W:136:GLU:OE1	31:W:136:GLU:N	2.50	0.41
33:Y:48:ARG:CB	34:Z:51:TRP:HE1	2.33	0.41
39:f:115:TYR:N	39:f:116:PRO:HD3	2.35	0.41
42:j:34:VAL:HG11	42:j:72:GLY:HA3	2.01	0.41
43:g:101:GLU:O	43:g:104:ASN:N	2.53	0.41
31:M:64:ASP:C	31:M:66:ASP:N	2.78	0.41
45:k:242:CYS:O	51:r:14:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:12:GLU:O	52:s:13:LEU:HB2	2.19	0.41
45:w:92:ARG:NH1	45:w:154:HIS:CD2	2.89	0.41
45:w:182:LEU:O	45:w:186:LEU:N	2.29	0.41
45:w:282:CYS:SG	45:w:305:GLN:HB3	2.60	0.41
48:z:165:TYR:CD2	48:z:168:VAL:HG22	2.55	0.41
56:A9:264:LYS:NZ	57:C4:56:MET:HE2	2.35	0.41
57:C4:3:TYR:CD1	57:C4:3:TYR:N	2.87	0.41
58:C2:42:LEU:HD12	58:C2:42:LEU:HA	1.66	0.41
59:A7:86:MET:O	66:B0:25:CYS:HB2	2.20	0.41
2:4:151:PHE:C	2:4:155:ALA:HB2	2.45	0.41
4:7:171:ILE:H	4:7:171:ILE:HG13	1.60	0.41
5:6:233:LEU:O	5:6:236:ALA:N	2.44	0.41
5:6:574:SER:O	5:6:578:THR:OG1	2.31	0.41
6:5:89:TYR:C	6:5:91:GLN:H	2.28	0.41
7:3:62:PHE:O	7:3:63:LEU:C	2.63	0.41
8:1:37:PRO:HD3	13:D:108:ARG:HG2	2.02	0.41
8:1:236:ILE:CD1	8:1:259:PHE:CE2	3.03	0.41
8:1:303:TRP:CH2	8:1:307:LEU:HD11	2.54	0.41
9:8:413:TRP:CZ3	9:8:417:LYS:HG3	2.55	0.41
10:A:58:MET:HE2	10:A:58:MET:HB3	1.92	0.41
10:A:359:ASN:ND2	20:K:68:ARG:HH12	2.18	0.41
12:C:213:ARG:NE	26:R:48:ARG:HH12	2.18	0.41
13:D:92:CYS:N	74:D:301:SF4:S2	2.93	0.41
16:G:98:LYS:HD3	16:G:125:VAL:HG21	2.02	0.41
18:I:80:VAL:HG13	18:I:81:GLY:N	2.36	0.41
20:K:42:VAL:O	20:K:46:LYS:HB2	2.20	0.41
23:O:75:ASP:OD2	23:O:76:PRO:O	2.39	0.41
23:O:101:THR:O	23:O:101:THR:HG22	2.20	0.41
27:S:335:VAL:N	42:j:52:PRO:HG3	2.14	0.41
28:T:66:ILE:N	28:T:66:ILE:CD1	2.83	0.41
29:U:39:VAL:HG12	29:U:49:TYR:HE1	1.84	0.41
29:U:65:THR:O	29:U:74:PHE:HD1	2.02	0.41
35:a:64:ALA:HB1	44:e:108:ASP:N	2.34	0.41
36:b:137:MET:CE	43:g:87:GLU:HG3	2.50	0.41
40:h:87:MET:O	40:h:91:PHE:HD2	2.04	0.41
44:e:47:GLU:CB	44:e:64:PRO:HG2	2.50	0.41
45:k:248:LEU:HA	45:k:249:PRO:HD3	1.92	0.41
47:m:129:MET:HE1	47:m:181:PHE:HB3	2.02	0.41
48:o:8:PRO:HG2	52:s:66:ASP:HB3	2.02	0.41
50:q:77:LYS:HA	50:q:80:TRP:CE2	2.56	0.41
46:x:67:HIS:CD2	46:x:144:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:399:LEU:HA	46:x:402:ILE:HD12	2.03	0.41
47:y:36:LEU:HD23	47:y:36:LEU:HA	1.70	0.41
56:A9:314:ILE:HB	56:A9:315:PRO:CD	2.50	0.41
56:A9:495:LEU:HD23	56:A9:495:LEU:HA	1.68	0.41
63:A5:57:ARG:HA	63:A5:60:TYR:CD2	2.55	0.41
64:B4:35:TYR:O	64:B4:39:VAL:HB	2.19	0.41
1:9:62:ARG:CD	15:F:86:LEU:HA	2.49	0.41
2:4:80:SER:HA	2:4:226:ALA:CB	2.49	0.41
2:4:248:LEU:HD11	43:g:150:TYR:C	2.45	0.41
3:2:286:ALA:O	3:2:289:ASN:HB3	2.20	0.41
5:6:240:PRO:HD2	5:6:243:VAL:HG21	2.02	0.41
5:6:581:LYS:HD2	6:5:96:LEU:CG	2.48	0.41
10:A:50:LEU:CG	10:A:60:ILE:HD11	2.50	0.41
10:A:134:GLY:HA3	10:A:241:ARG:HH21	1.85	0.41
10:A:302:LEU:HD11	10:A:585:PRO:HA	2.01	0.41
10:A:381:LEU:HG	10:A:664:TYR:HB3	2.02	0.41
10:A:493:VAL:O	10:A:496:ILE:HG22	2.20	0.41
11:B:157:LYS:O	11:B:159:LEU:N	2.53	0.41
70:B:501:3PE:H351	70:B:501:3PE:H381	1.61	0.41
12:C:127:ARG:HB3	12:C:128:PHE:CD1	2.56	0.41
12:C:209:TYR:HE1	16:G:120:PRO:HG2	1.85	0.41
14:E:133:GLU:HG3	14:E:134:PRO:HD2	2.02	0.41
17:H:50:ILE:HD13	36:b:171:TYR:HE2	1.85	0.41
21:L:40:LYS:HB3	21:L:40:LYS:HE3	1.76	0.41
23:O:33:ARG:NE	31:M:48:VAL:HG21	2.24	0.41
24:P:110:GLU:O	24:P:112:TYR:N	2.53	0.41
28:T:108:TYR:O	28:T:108:TYR:HD1	2.03	0.41
29:U:62:VAL:HG23	29:U:86:TRP:HZ3	1.85	0.41
36:b:131:LYS:O	36:b:135:ARG:HB3	2.21	0.41
40:h:136:ILE:CD1	43:g:106:ILE:HD11	2.49	0.41
31:M:57:GLU:O	31:M:58:PHE:HB3	2.20	0.41
45:k:133:VAL:O	45:k:136:GLN:HB3	2.20	0.41
46:l:29:LEU:HD12	46:l:33:LEU:HG	2.02	0.41
46:l:341:TYR:CE2	46:l:345:LYS:HE3	2.55	0.41
47:m:37:LEU:HA	47:m:37:LEU:HD23	1.86	0.41
47:m:202:GLU:OE2	47:y:10:LEU:HB2	2.21	0.41
49:p:15:ARG:HB3	51:r:24:ARG:CG	2.50	0.41
50:q:18:LYS:CG	50:q:83:TYR:CE2	2.71	0.41
51:r:7:LEU:HD23	51:r:7:LEU:HA	1.88	0.41
45:w:348:SER:HG	53:A3:17:TRP:HE1	1.60	0.41
46:x:97:SER:HA	55:B1:70:LEU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:x:144:LEU:HD23	46:x:144:LEU:HA	1.83	0.41
46:x:341:TYR:CE2	46:x:345:LYS:HE3	2.55	0.41
46:x:380:ASP:OD2	55:B1:62:ARG:NH2	2.54	0.41
46:x:411:ILE:O	46:x:415:LYS:HG3	2.20	0.41
47:y:274:PHE:O	47:y:275:LEU:C	2.63	0.41
47:y:278:TYR:HE2	47:y:282:ARG:HH21	1.67	0.41
60:C0:21:LYS:O	60:C0:57:ARG:NH1	2.53	0.41
60:C0:43:PRO:HB2	60:C0:48:ILE:CD1	2.48	0.41
61:A6:16:LEU:O	61:A6:20:VAL:HG13	2.21	0.41
66:B0:9:PHE:CD1	66:B0:9:PHE:C	2.97	0.41
1:9:92:TRP:CZ3	1:9:94:PRO:HG3	2.55	0.41
1:9:133:GLN:HB2	1:9:187:GLN:HB3	2.03	0.41
1:9:181:VAL:HG23	1:9:182:ASN:OD1	2.19	0.41
2:4:347:GLY:HA3	2:4:418:LYS:CB	2.50	0.41
2:4:393:ILE:HD11	5:6:183:ILE:HD12	2.02	0.41
3:2:14:MET:HB3	3:2:133:TRP:CH2	2.55	0.41
5:6:159:TYR:O	5:6:160:GLY:C	2.63	0.41
5:6:224:SER:O	5:6:310:LEU:HD13	2.21	0.41
7:3:42:ASP:HB2	8:1:127:TYR:HE2	1.85	0.41
10:A:367:CYS:SG	10:A:531:LYS:O	2.79	0.41
11:B:228:ARG:NH2	11:B:233:HIS:HD2	2.18	0.41
11:B:266:ARG:HB2	11:B:266:ARG:HE	1.52	0.41
12:C:221:VAL:HG22	13:D:138:ARG:CG	2.41	0.41
14:E:192:ASN:O	14:E:196:LYS:N	2.53	0.41
16:G:128:PHE:CD2	16:G:134:ALA:HA	2.52	0.41
23:O:42:GLU:OE1	23:O:45:ASN:HB3	2.19	0.41
26:R:127:ILE:HG22	26:R:165:ILE:HD12	2.02	0.41
43:g:5:TRP:CD1	43:g:10:TYR:HB2	2.55	0.41
31:M:72:CYS:SG	31:M:74:GLN:HB2	2.61	0.41
47:m:19:ILE:HG23	47:m:221:HIS:HB2	2.01	0.41
47:m:97:HIS:CE1	47:m:100:ARG:NH2	2.88	0.41
47:m:345:HIS:HA	47:m:348:ILE:HD12	2.02	0.41
49:p:111:ALA:HA	49:p:112:VAL:HA	1.87	0.41
49:p:127:VAL:CB	49:p:131:GLU:H	2.33	0.41
45:w:236:PHE:CD1	45:w:258:GLU:HG2	2.55	0.41
46:x:50:PHE:N	46:x:50:PHE:CD1	2.88	0.41
47:y:64:SER:O	47:y:67:THR:HB	2.21	0.41
47:y:345:HIS:HA	47:y:348:ILE:HD12	2.02	0.41
49:A0:110:ALA:CB	49:A0:122:HIS:C	2.80	0.41
53:A3:15:ARG:CG	53:A3:16:ASN:N	2.83	0.41
56:A9:430:PHE:O	56:A9:431:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:A7:137:LYS:O	59:A7:145:TRP:HE3	2.03	0.41
62:A4:44:ARG:HA	62:A4:45:PRO:HD2	1.75	0.41
65:C3:5:VAL:O	65:C3:9:GLN:HG3	2.21	0.41
1:9:80:LEU:HA	1:9:80:LEU:HD23	1.76	0.41
1:9:137:THR:HG22	1:9:138:THR:N	2.35	0.41
2:4:25:VAL:HG11	40:h:82:VAL:HG11	2.03	0.41
2:4:119:TYR:O	2:4:122:PHE:N	2.53	0.41
2:4:214:LEU:HD11	5:6:558:LEU:HB3	2.02	0.41
2:4:412:ILE:HD13	2:4:412:ILE:HG21	1.91	0.41
3:2:203:LEU:HD23	3:2:203:LEU:C	2.46	0.41
5:6:75:LYS:HE3	5:6:75:LYS:HB3	1.74	0.41
71:6:701:CDL:H321	71:6:701:CDL:H351	1.63	0.41
7:3:28:ASN:ND2	26:R:306:GLU:O	2.54	0.41
8:1:169:GLN:CG	8:1:174:LEU:HB2	2.48	0.41
10:A:398:ASP:OD1	10:A:399:VAL:N	2.52	0.41
10:A:408:ARG:HD3	10:A:409:PHE:CE2	2.56	0.41
10:A:550:ALA:HB3	10:A:568:TYR:HE1	1.85	0.41
11:B:71:PRO:N	11:B:72:PRO:HD3	2.35	0.41
11:B:317:ASP:OD1	11:B:317:ASP:N	2.52	0.41
13:D:138:ARG:NH2	13:D:141:TYR:HD2	2.12	0.41
25:Q:82:PHE:HD1	25:Q:107:PHE:CE1	2.39	0.41
27:S:191:VAL:O	27:S:193:VAL:HG23	2.21	0.41
27:S:215:MET:O	27:S:217:ILE:N	2.53	0.41
27:S:282:LEU:C	27:S:284:MET:H	2.29	0.41
28:T:26:THR:HG22	28:T:68:ALA:C	2.45	0.41
30:V:130:SER:OG	30:V:131:GLU:N	2.53	0.41
31:W:79:ILE:HD11	31:W:148:ILE:HB	2.03	0.41
40:h:82:VAL:HA	40:h:85:TRP:HD1	1.86	0.41
42:j:51:ARG:HG2	42:j:56:ALA:HB2	2.01	0.41
45:k:51:LYS:HE3	45:k:181:ASP:OD2	2.20	0.41
45:k:414:TYR:O	45:k:418:GLN:HG3	2.20	0.41
46:l:50:PHE:N	46:l:50:PHE:CD1	2.89	0.41
46:l:116:VAL:O	46:l:120:MET:N	2.36	0.41
46:l:250:ASP:OD1	46:l:251:SER:N	2.53	0.41
47:m:64:SER:O	47:m:67:THR:HB	2.21	0.41
47:m:172:LYS:O	47:m:174:THR:N	2.53	0.41
47:m:218:ILE:CG2	47:m:223:TYR:HD2	2.34	0.41
48:o:71:GLN:OE1	48:o:71:GLN:N	2.53	0.41
47:y:126:THR:HG23	47:y:182:HIS:HD1	1.86	0.41
61:A6:74:LEU:HA	61:A6:74:LEU:HD23	1.87	0.41
2:4:187:HIS:CG	2:4:188:ASN:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:343:ILE:O	2:4:346:ARG:HG3	2.21	0.41
5:6:366:MET:N	5:6:367:PRO:HD3	2.35	0.41
5:6:556:ILE:HG13	35:a:76:ILE:HD13	1.96	0.41
71:6:701:CDL:H311	71:6:701:CDL:HA61	1.84	0.41
7:3:102:LEU:O	7:3:103:ALA:C	2.64	0.41
8:1:278:PRO:CB	11:B:194:ILE:HG22	2.50	0.41
9:8:210:THR:HG22	9:8:210:THR:O	2.20	0.41
9:8:297:LYS:HB2	9:8:333:GLU:HB2	2.03	0.41
10:A:154:LEU:H	10:A:154:LEU:HG	1.66	0.41
10:A:259:SER:CB	10:A:282:ASN:HD21	2.33	0.41
11:B:150:ALA:HB2	11:B:400:ILE:CD1	2.48	0.41
11:B:359:ASP:HB2	24:P:45:PRO:CG	2.50	0.41
12:C:46:ARG:CZ	12:C:46:ARG:HB2	2.50	0.41
12:C:110:PHE:H	12:C:136:SER:CB	2.34	0.41
12:C:186:LEU:HD12	12:C:186:LEU:HA	1.91	0.41
13:D:107:ASP:HA	13:D:111:VAL:O	2.21	0.41
17:H:21:GLN:HE21	17:H:31:SER:CB	2.34	0.41
20:K:16:LEU:HA	20:K:69:TYR:HB3	2.02	0.41
23:O:44:PRO:O	23:O:47:VAL:N	2.53	0.41
26:R:92:MET:C	26:R:94:LEU:N	2.76	0.41
26:R:125:VAL:HA	26:R:162:GLU:O	2.21	0.41
26:R:355:ARG:O	26:R:358:THR:N	2.53	0.41
28:T:10:TRP:O	28:T:12:ILE:N	2.52	0.41
28:T:20:ARG:H	28:T:20:ARG:HD3	1.83	0.41
30:V:34:SER:O	30:V:37:ALA:HB3	2.20	0.41
32:X:23:GLY:O	32:X:26:LEU:N	2.53	0.41
39:f:108:HIS:HA	39:f:109:PRO:HD2	1.84	0.41
46:l:144:LEU:HA	46:l:144:LEU:HD23	1.83	0.41
46:l:283:PRO:HA	46:l:290:ASN:HD21	1.85	0.41
52:s:59:LEU:O	52:s:62:LEU:N	2.54	0.41
45:w:213:GLN:O	45:w:215:HIS:N	2.53	0.41
45:w:348:SER:OG	53:A3:17:TRP:NE1	2.26	0.41
46:x:398:VAL:O	46:x:402:ILE:HG13	2.20	0.41
47:y:218:ILE:CG2	47:y:223:TYR:HD2	2.34	0.41
48:z:76:GLU:O	48:z:78:GLY:N	2.50	0.41
49:A0:53:ASN:O	49:A0:57:GLN:N	2.53	0.41
56:A9:276:ALA:O	56:A9:280:ILE:HG13	2.21	0.41
57:C4:193:TYR:N	57:C4:193:TYR:CD1	2.88	0.41
58:C2:6:HIS:CD2	58:C2:8:TYR:HB2	2.55	0.41
58:C2:146:TRP:NE1	62:A4:17:ARG:HB2	2.35	0.41
58:C2:182:TYR:O	62:A4:72:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C2:233:PHE:HA	58:C2:236:GLU:HG3	2.03	0.41
59:A7:11:TYR:CD1	59:A7:11:TYR:C	2.99	0.41
1:9:193:TYR:CD1	1:9:216:PRO:HA	2.56	0.41
2:4:45:PHE:HA	2:4:46:GLY:HA3	1.77	0.41
5:6:277:THR:OG1	5:6:318:GLY:HA2	2.21	0.41
6:5:62:ILE:O	6:5:62:ILE:HG22	2.21	0.41
8:1:34:ARG:CZ	13:D:108:ARG:NH1	2.84	0.41
8:1:79:LEU:HA	8:1:79:LEU:HD23	1.80	0.41
8:1:236:ILE:O	8:1:236:ILE:CG1	2.69	0.41
9:8:259:GLY:HA3	9:8:261:TRP:N	2.26	0.41
10:A:133:GLN:O	10:A:135:GLY:N	2.53	0.41
10:A:334:GLN:HE22	10:A:361:VAL:HG22	1.84	0.41
10:A:352:ILE:HA	10:A:352:ILE:HD13	1.84	0.41
10:A:682:ASP:OD1	10:A:683:PRO:HD2	2.21	0.41
11:B:100:GLU:HB2	11:B:108:LYS:HD3	2.02	0.41
11:B:292:MET:HE2	11:B:431:HIS:CD2	2.56	0.41
13:D:142:ASP:O	13:D:144:MET:N	2.54	0.41
20:K:65:LEU:HD12	20:K:66:TRP:H	1.86	0.41
25:Q:61:LYS:O	25:Q:65:GLN:HB2	2.21	0.41
27:S:103:GLU:HA	27:S:106:TYR:HD2	1.85	0.41
28:T:37:SER:HB3	28:T:60:THR:CB	2.50	0.41
29:U:71:LYS:HG3	29:U:72:ASN:O	2.20	0.41
31:W:103:HIS:C	31:W:105:MET:H	2.28	0.41
40:h:127:LYS:O	40:h:131:ALA:N	2.53	0.41
44:e:37:LEU:H	44:e:77:LYS:CD	2.33	0.41
44:e:92:TRP:O	44:e:93:ASP:C	2.63	0.41
45:k:32:GLN:NE2	46:l:373:GLU:HB2	2.35	0.41
45:k:426:GLY:CA	45:k:428:ILE:HG13	2.48	0.41
46:l:76:THR:HG22	46:l:77:THR:O	2.20	0.41
47:m:61:THR:O	47:m:62:ALA:C	2.64	0.41
49:p:18:VAL:CG1	49:p:32:ARG:HH11	2.34	0.41
49:p:56:SER:O	49:p:60:SER:N	2.36	0.41
50:q:55:TYR:O	50:q:58:ARG:HB3	2.21	0.41
45:w:51:LYS:HE3	45:w:181:ASP:OD2	2.20	0.41
45:w:361:LEU:HD12	45:w:361:LEU:HA	1.89	0.41
46:x:250:ASP:OD1	46:x:251:SER:N	2.53	0.41
52:B3:59:LEU:O	52:B3:62:LEU:N	2.54	0.41
53:A3:23:LEU:O	53:A3:26:ALA:N	2.53	0.41
57:C4:86:MET:HE3	57:C4:86:MET:HB2	1.80	0.41
57:C4:164:ALA:HB2	57:C4:171:LYS:HD3	2.03	0.41
58:C2:40:MET:O	58:C2:41:THR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:B0:13:TYR:O	66:B0:14:GLY:C	2.63	0.41
68:A8:19:LEU:HD23	68:A8:19:LEU:C	2.45	0.41
2:4:6:ILE:HA	2:4:9:ILE:HG22	2.02	0.41
2:4:89:LEU:HD12	2:4:90:THR:HG23	2.02	0.41
2:4:114:GLU:OE2	2:4:117:LEU:HG	2.21	0.41
2:4:129:THR:HG21	2:4:236:LEU:HD11	2.02	0.41
2:4:246:ILE:O	2:4:248:LEU:N	2.54	0.41
2:4:379:LEU:HD23	2:4:379:LEU:HA	1.84	0.41
2:4:446:LEU:HG	71:4:502:CDL:H351	2.00	0.41
72:2:402:PC1:H391	72:2:402:PC1:H362	1.64	0.41
4:7:13:PHE:CD2	6:5:8:ILE:HG21	2.56	0.41
5:6:28:LYS:HD2	5:6:29:PRO:HD2	2.03	0.41
5:6:103:PHE:CD1	5:6:341:MET:HG3	2.56	0.41
5:6:126:ILE:O	5:6:129:LEU:HB3	2.21	0.41
5:6:243:VAL:O	5:6:246:LEU:N	2.53	0.41
5:6:581:LYS:HD2	6:5:96:LEU:CD2	2.51	0.41
5:6:590:SER:CB	28:T:42:ALA:HB1	2.51	0.41
6:5:89:TYR:C	6:5:91:GLN:N	2.79	0.41
8:1:220:PHE:O	8:1:220:PHE:CG	2.74	0.41
8:1:276:SER:OG	14:E:74:LEU:HD22	2.21	0.41
9:8:390:ASP:N	9:8:390:ASP:OD1	2.51	0.41
9:8:398:ARG:CG	9:8:403:ASP:HB3	2.44	0.41
10:A:139:LEU:HD11	10:A:177:ILE:CG2	2.50	0.41
10:A:222:ILE:O	10:A:225:ILE:N	2.37	0.41
11:B:53:TYR:CB	11:B:57:GLU:HG3	2.51	0.41
11:B:80:LEU:CD2	11:B:82:LEU:HG	2.51	0.41
11:B:81:THR:O	11:B:82:LEU:C	2.64	0.41
11:B:117:HIS:O	11:B:119:GLY:N	2.54	0.41
11:B:308:TYR:OH	11:B:400:ILE:HB	2.20	0.41
11:B:379:ILE:HD13	11:B:379:ILE:HG21	1.69	0.41
12:C:62:ALA:O	12:C:64:GLY:N	2.54	0.41
12:C:123:THR:CG2	16:G:128:PHE:CB	2.98	0.41
12:C:181:ALA:O	12:C:182:ASN:C	2.62	0.41
12:C:199:PRO:HB2	13:D:167:TYR:CE2	2.56	0.41
12:C:212:LEU:HD21	12:C:221:VAL:CG1	2.50	0.41
13:D:138:ARG:NE	13:D:138:ARG:C	2.76	0.41
18:I:51:TYR:CE2	18:I:52:ARG:HD3	2.56	0.41
23:O:43:VAL:HG21	23:O:59:GLY:O	2.21	0.41
24:P:19:ASP:OD1	24:P:19:ASP:N	2.53	0.41
25:Q:165:SER:O	25:Q:166:ARG:C	2.63	0.41
27:S:252:GLN:C	27:S:254:ALA:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:3:LYS:HD2	28:T:3:LYS:HA	1.76	0.41
28:T:77:SER:O	28:T:80:VAL:HG13	2.21	0.41
29:U:32:ASP:O	29:U:34:ARG:N	2.54	0.41
29:U:125:VAL:HG23	29:U:125:VAL:O	2.20	0.41
39:f:166:LEU:HD12	39:f:167:TRP:HB3	2.03	0.41
42:j:56:ALA:O	42:j:57:GLY:C	2.61	0.41
44:e:150:TYR:HA	44:e:151:PRO:HA	1.98	0.41
45:k:92:ARG:NH1	45:k:154:HIS:CD2	2.89	0.41
45:k:280:TYR:HA	45:k:284:TYR:HE2	1.86	0.41
46:l:212:SER:HB2	46:l:214:PRO:HD2	2.02	0.41
46:l:236:LYS:HZ1	46:l:238:LYS:HB2	1.85	0.41
46:l:411:ILE:O	46:l:415:LYS:HG3	2.20	0.41
47:m:26:ASN:HD22	50:q:69:SER:HB3	1.86	0.41
49:p:76:ILE:N	49:p:77:LYS:HA	2.36	0.41
49:p:140:THR:HA	49:p:141:HIS:HA	1.83	0.41
50:q:50:LEU:HD23	50:q:50:LEU:HA	1.88	0.41
52:s:15:ASP:OD1	52:s:18:THR:N	2.52	0.41
45:w:408:ARG:HE	53:A3:15:ARG:CZ	2.34	0.41
45:w:414:TYR:O	45:w:418:GLN:HG3	2.20	0.41
46:x:303:VAL:HG12	46:x:304:HIS:N	2.22	0.41
46:x:383:GLY:O	46:x:386:ALA:N	2.53	0.41
46:x:395:PRO:O	46:x:399:LEU:HG	2.19	0.41
47:y:214:ASP:HB3	51:A2:8:THR:OG1	2.21	0.41
47:y:265:PRO:HG2	47:y:268:ILE:CG1	2.50	0.41
48:z:14:HIS:HB3	48:z:21:LEU:HD23	2.02	0.41
48:z:121:HIS:CG	48:z:122:GLY:N	2.88	0.41
48:z:138:PRO:HG3	52:B3:58:LEU:CD2	2.51	0.41
50:A1:8:ALA:O	50:A1:12:TRP:CE3	2.74	0.41
50:A1:55:TYR:O	50:A1:58:ARG:HB3	2.21	0.41
50:A1:77:LYS:HA	50:A1:80:TRP:CD1	2.55	0.41
50:A1:77:LYS:HA	50:A1:80:TRP:CE2	2.56	0.41
51:A2:71:ARG:HH21	52:B3:60:ASP:CG	2.29	0.41
52:B3:12:GLU:N	52:B3:12:GLU:OE1	2.54	0.41
52:B3:66:ASP:O	52:B3:70:ALA:N	2.53	0.41
56:A9:168:ILE:CG2	56:A9:189:MET:HG3	2.51	0.41
56:A9:354:THR:HG21	56:A9:376:HIS:HA	2.03	0.41
56:A9:442:ASP:OD2	57:C4:134:ARG:NH2	2.54	0.41
56:A9:461:SER:O	56:A9:465:VAL:HG13	2.21	0.41
58:C2:146:TRP:CE2	62:A4:17:ARG:HB2	2.55	0.41
58:C2:169:LEU:HD23	58:C2:169:LEU:HA	1.92	0.41
58:C2:228:THR:O	58:C2:232:HIS:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:C0:104:LEU:HD23	60:C0:104:LEU:HA	1.87	0.41
61:A6:49:VAL:O	61:A6:91:LEU:HD12	2.21	0.41
62:A4:42:ARG:NH1	62:A4:74:ARG:NH2	2.68	0.41
65:C3:12:PHE:O	65:C3:23:LYS:HE2	2.21	0.41
2:4:113:MET:O	2:4:113:MET:HG3	2.20	0.41
2:4:179:LEU:HD11	43:g:82:VAL:CG2	2.51	0.41
2:4:179:LEU:CD1	43:g:82:VAL:HG21	2.50	0.41
2:4:351:LEU:O	2:4:352:LEU:HD12	2.21	0.41
2:4:452:LYS:HD2	2:4:455:LEU:HD13	2.02	0.41
3:2:261:MET:N	3:2:262:PRO:HD2	2.36	0.41
3:2:335:MET:HE1	42:j:33:PHE:HZ	1.85	0.41
4:7:24:PRO:O	4:7:25:SER:C	2.64	0.41
5:6:435:PRO:CB	34:Z:52:ARG:HD3	2.50	0.41
8:1:265:LEU:HD22	8:1:265:LEU:HA	1.55	0.41
8:1:294:LEU:O	8:1:295:PRO:C	2.64	0.41
9:8:156:ILE:HD12	9:8:157:TYR:N	2.35	0.41
10:A:41:VAL:CG2	10:A:55:LYS:HD2	2.51	0.41
10:A:438:LEU:HA	10:A:438:LEU:HD23	1.85	0.41
10:A:454:ASP:HB3	10:A:459:SER:OG	2.20	0.41
10:A:544:MET:HA	10:A:565:PHE:O	2.21	0.41
11:B:37:TRP:CD1	11:B:39:PRO:HD3	2.55	0.41
11:B:140:ASP:N	11:B:140:ASP:OD1	2.50	0.41
11:B:335:GLU:O	11:B:339:GLN:HG2	2.21	0.41
14:E:100:GLU:CD	14:E:193:ASN:HD21	2.27	0.41
15:F:96:ARG:O	15:F:98:PRO:HD3	2.21	0.41
17:H:89:GLU:N	17:H:89:GLU:OE1	2.54	0.41
23:O:33:ARG:HH21	31:M:44:SER:CB	2.15	0.41
25:Q:166:ARG:HH22	42:j:86:ARG:NH1	2.12	0.41
26:R:206:ILE:HG22	26:R:240:VAL:HG13	2.03	0.41
28:T:70:PHE:HD1	28:T:93:GLY:CA	2.30	0.41
31:M:43:ASP:OD1	31:M:44:SER:N	2.54	0.41
45:k:61:HIS:CE1	45:k:134:ILE:HD11	2.56	0.41
46:l:286:LYS:C	46:l:288:GLY:H	2.29	0.41
48:o:70:VAL:HG12	48:o:83:ARG:H	1.86	0.41
45:w:67:THR:OG1	45:w:119:ASN:O	2.38	0.41
46:x:129:ALA:N	46:x:130:PRO:HD3	2.36	0.41
47:y:97:HIS:CE1	47:y:100:ARG:NH2	2.88	0.41
47:y:129:MET:O	47:y:130:GLY:C	2.64	0.41
49:A0:53:ASN:O	49:A0:57:GLN:HG3	2.20	0.41
52:B3:18:THR:O	52:B3:21:ARG:HB2	2.21	0.41
56:A9:23:GLY:HA3	56:A9:73:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:A9:501:PRO:O	56:A9:502:TYR:C	2.63	0.41
1:9:178:GLY:N	9:8:162:PHE:CE1	2.89	0.40
1:9:188:ILE:CD1	1:9:189:ASN:H	2.23	0.40
2:4:50:LEU:HD21	2:4:52:PHE:CD2	2.56	0.40
3:2:43:ILE:HD13	3:2:43:ILE:HA	1.91	0.40
3:2:251:MET:HE3	3:2:293:TYR:OH	2.21	0.40
8:1:36:GLY:O	8:1:37:PRO:C	2.63	0.40
10:A:140:GLN:HG3	11:B:379:ILE:CG2	2.51	0.40
10:A:445:LEU:HD21	10:A:460:HIS:HD2	1.86	0.40
11:B:71:PRO:CD	11:B:72:PRO:HD3	2.51	0.40
11:B:99:MET:HE3	11:B:99:MET:HB2	1.88	0.40
11:B:208:GLU:C	11:B:210:MET:N	2.79	0.40
11:B:316:PHE:HA	11:B:342:ARG:NH1	2.36	0.40
12:C:167:TRP:CD1	12:C:170:ARG:HH12	2.39	0.40
13:D:146:GLU:O	13:D:148:ARG:HG2	2.21	0.40
16:G:58:LYS:HB3	16:G:58:LYS:HE2	1.81	0.40
16:G:130:THR:O	16:G:134:ALA:N	2.55	0.40
20:K:75:LYS:HE3	20:K:75:LYS:HB3	1.91	0.40
28:T:37:SER:HB3	28:T:60:THR:CG2	2.48	0.40
28:T:101:LEU:CD2	28:T:101:LEU:C	2.85	0.40
29:U:123:GLN:O	29:U:124:TYR:HB3	2.21	0.40
35:a:39:ILE:CB	44:e:56:ASN:CA	2.94	0.40
35:a:43:LEU:O	35:a:46:GLU:N	2.54	0.40
36:b:152:LYS:HA	36:b:152:LYS:HD2	1.72	0.40
42:j:114:GLU:CA	43:g:160:LYS:CE	2.94	0.40
43:g:75:THR:O	43:g:75:THR:OG1	2.34	0.40
45:k:236:PHE:CD1	45:k:258:GLU:HG2	2.55	0.40
46:l:67:HIS:CD2	46:l:144:LEU:HD22	2.56	0.40
46:l:197:ASN:O	46:l:230:LEU:HB3	2.20	0.40
46:l:303:VAL:HG12	46:l:304:HIS:N	2.22	0.40
47:m:126:THR:HG23	47:m:182:HIS:HD1	1.86	0.40
48:o:5:LEU:HD12	48:o:5:LEU:HA	1.86	0.40
46:x:29:LEU:HD12	46:x:33:LEU:HG	2.02	0.40
48:z:75:ASN:H	48:z:79:GLU:HG2	1.85	0.40
48:z:144:ARG:HA	48:z:144:ARG:HD3	1.87	0.40
56:A9:337:ALA:HB2	56:A9:394:VAL:HG23	2.03	0.40
58:C2:12:ASN:O	58:C2:13:PRO:C	2.65	0.40
65:C3:31:LEU:HD23	65:C3:31:LEU:HA	1.82	0.40
1:9:138:THR:O	1:9:142:LEU:HG	2.21	0.40
2:4:25:VAL:CG2	40:h:89:VAL:HG11	2.41	0.40
3:2:326:LEU:HD11	72:2:402:PC1:C2C	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:74:MET:HB3	7:3:51:PHE:HD1	1.86	0.40
5:6:213:LEU:HD13	5:6:273:ILE:HD13	2.03	0.40
7:3:44:MET:CE	23:O:49:LEU:O	2.58	0.40
8:1:248:ASN:C	8:1:250:HIS:N	2.78	0.40
10:A:497:ALA:CB	10:A:513:MET:HB2	2.50	0.40
10:A:591:GLU:OE1	10:A:591:GLU:N	2.54	0.40
11:B:152:SER:HG	11:B:228:ARG:C	2.23	0.40
11:B:228:ARG:CZ	11:B:233:HIS:HD2	2.34	0.40
11:B:238:LEU:CD1	24:P:37:PRO:HD2	2.36	0.40
11:B:332:CYS:O	11:B:336:GLU:N	2.54	0.40
11:B:335:GLU:O	11:B:335:GLU:HG3	2.21	0.40
12:C:167:TRP:NE1	12:C:170:ARG:HH12	2.18	0.40
14:E:70:LEU:HD23	14:E:70:LEU:HA	1.72	0.40
19:J:51:ASP:OD1	25:Q:21:SER:HA	2.21	0.40
24:P:19:ASP:CG	24:P:20:LEU:H	2.29	0.40
24:P:48:LYS:HB2	24:P:48:LYS:HE2	1.90	0.40
26:R:168:SER:HB3	26:R:201:ILE:O	2.21	0.40
27:S:233:PHE:O	27:S:233:PHE:CG	2.74	0.40
27:S:275:ASN:C	27:S:277:ARG:N	2.71	0.40
31:W:106:LYS:H	31:W:106:LYS:HG2	1.44	0.40
35:a:67:ARG:NE	44:e:52:ALA:HB2	2.35	0.40
35:a:105:PHE:O	35:a:108:ASP:N	2.54	0.40
42:j:51:ARG:HA	42:j:51:ARG:HD3	1.88	0.40
43:g:97:LYS:HB3	43:g:97:LYS:HE3	1.89	0.40
43:g:125:CYS:C	43:g:127:LYS:H	2.29	0.40
45:k:61:HIS:HB3	45:k:65:LYS:HZ1	1.85	0.40
47:m:133:LEU:HD11	47:m:182:HIS:CD2	2.56	0.40
48:o:71:GLN:O	48:o:72:ASP:C	2.64	0.40
52:s:40:CYS:O	52:s:44:VAL:HG23	2.22	0.40
49:A0:7:VAL:HG11	49:A0:10:PHE:CZ	2.56	0.40
50:A1:28:LYS:CB	50:A1:74:ILE:HD11	2.40	0.40
51:A2:79:ASN:O	52:B3:50:THR:HG21	2.21	0.40
56:A9:440:TYR:CG	57:C4:205:SER:HB3	2.57	0.40
61:A6:10:GLU:HG2	61:A6:25:ARG:HH22	1.86	0.40
68:A8:35:TYR:HD2	68:A8:36:HIS:CE1	2.39	0.40
1:9:139:PRO:HG3	9:8:355:ILE:HG21	2.03	0.40
1:9:215:LYS:HD3	1:9:215:LYS:HA	1.85	0.40
2:4:90:THR:HB	70:4:501:3PE:H2	2.02	0.40
2:4:100:ILE:O	2:4:103:GLN:N	2.54	0.40
2:4:269:MET:HE1	2:4:396:MET:HB2	2.03	0.40
2:4:326:LEU:HA	2:4:326:LEU:HD23	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:370:PRO:HG3	5:6:141:PHE:CE2	2.56	0.40
3:2:169:GLY:HA3	3:2:292:PHE:HE1	1.86	0.40
3:2:220:MET:HE3	3:2:220:MET:HB3	1.85	0.40
4:7:148:SER:O	4:7:149:TYR:C	2.64	0.40
5:6:40:ILE:O	5:6:41:SER:C	2.64	0.40
6:5:81:VAL:O	6:5:84:THR:HG22	2.22	0.40
7:3:61:THR:O	7:3:65:PHE:HD2	2.03	0.40
8:1:6:ILE:C	8:1:8:MET:N	2.78	0.40
8:1:181:LEU:HG	8:1:300:LEU:HD22	2.04	0.40
9:8:228:PRO:HB2	9:8:229:PHE:O	2.21	0.40
10:A:50:LEU:O	10:A:50:LEU:HD23	2.21	0.40
10:A:125:PRO:HG3	10:A:174:THR:HG22	2.03	0.40
11:B:133:LEU:O	11:B:134:PRO:C	2.64	0.40
11:B:238:LEU:HG	14:E:211:TYR:OH	2.20	0.40
11:B:438:MET:HE3	11:B:438:MET:HB2	1.96	0.40
11:B:443:MET:HE2	11:B:443:MET:HB3	1.90	0.40
12:C:198:HIS:O	12:C:201:ARG:HG2	2.21	0.40
13:D:82:LEU:HB2	13:D:111:VAL:HG22	2.04	0.40
13:D:215:ARG:NE	76:R:601:NAP:P2B	2.94	0.40
22:N:47:TYR:HE1	24:P:92:LYS:CB	2.33	0.40
26:R:82:VAL:O	26:R:82:VAL:HG13	2.22	0.40
26:R:220:ILE:HD12	26:R:220:ILE:HA	1.98	0.40
26:R:369:VAL:N	26:R:370:GLN:HA	2.36	0.40
27:S:285:LEU:O	72:S:401:PC1:H131	2.21	0.40
48:o:28:ARG:HB3	48:o:171:PHE:CE1	2.56	0.40
48:o:215:LEU:O	48:o:218:LEU:N	2.55	0.40
49:p:109:GLU:N	49:p:110:ALA:HB3	2.37	0.40
45:w:61:HIS:CE1	45:w:134:ILE:HD11	2.56	0.40
46:x:77:THR:HG23	46:x:85:ILE:HD11	2.04	0.40
49:A0:169:GLY:O	49:A0:180:LEU:CB	2.70	0.40
50:A1:25:GLY:O	50:A1:28:LYS:N	2.33	0.40
53:A3:36:THR:HB	53:A3:37:ASP:H	1.70	0.40
57:C4:100:MET:HE3	57:C4:157:GLU:HG3	2.01	0.40
65:C3:21:HIS:CD2	65:C3:22:LEU:HG	2.57	0.40
66:B0:24:PHE:CE1	66:B0:28:VAL:HG21	2.56	0.40
2:4:235:LEU:HD23	2:4:235:LEU:C	2.47	0.40
2:4:259:TYR:N	2:4:260:PRO:HD2	2.37	0.40
2:4:431:THR:HG21	40:h:91:PHE:CZ	2.56	0.40
3:2:120:GLN:HG2	3:2:177:LYS:HE3	2.04	0.40
3:2:217:THR:HG22	72:2:402:PC1:C25	2.49	0.40
3:2:257:LEU:HD22	3:2:331:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:13:PHE:CE2	6:5:8:ILE:HG21	2.57	0.40
4:7:121:GLY:O	4:7:122:LEU:HD12	2.21	0.40
5:6:216:LEU:HD13	5:6:263:PHE:CE2	2.56	0.40
5:6:592:LEU:HD12	6:5:17:VAL:CG2	2.51	0.40
8:1:6:ILE:C	8:1:8:MET:H	2.27	0.40
8:1:178:ALA:O	8:1:180:PRO:N	2.54	0.40
9:8:98:LYS:HA	9:8:101:PHE:HB2	2.04	0.40
10:A:482:GLN:HG2	10:A:482:GLN:O	2.21	0.40
11:B:78:SER:O	11:B:79:ASN:CG	2.63	0.40
11:B:79:ASN:ND2	11:B:102:SER:HA	2.35	0.40
11:B:124:ILE:HG21	11:B:124:ILE:HD13	1.80	0.40
11:B:182:ASN:ND2	11:B:403:PRO:HG2	2.36	0.40
11:B:200:PHE:CE1	11:B:204:PHE:CE2	3.10	0.40
11:B:271:ARG:HA	11:B:271:ARG:HD2	1.75	0.40
12:C:128:PHE:CD1	12:C:128:PHE:N	2.88	0.40
12:C:218:VAL:O	12:C:219:LYS:CG	2.69	0.40
14:E:107:PRO:O	14:E:108:SER:C	2.63	0.40
17:H:74:LYS:HD2	17:H:74:LYS:HA	1.67	0.40
24:P:40:LYS:H	30:V:7:LYS:N	2.20	0.40
26:R:73:LEU:HD23	26:R:73:LEU:HA	1.75	0.40
27:S:192:VAL:HG11	27:S:233:PHE:HZ	1.87	0.40
72:S:401:PC1:H232	72:S:401:PC1:H292	2.03	0.40
28:T:34:LEU:HD13	28:T:35:VAL:HA	1.95	0.40
31:W:106:LYS:HB3	31:W:106:LYS:HE2	1.40	0.40
44:e:111:MET:HG2	44:e:112:TYR:N	2.30	0.40
46:l:129:ALA:N	46:l:130:PRO:HD3	2.36	0.40
47:m:91:PHE:HD2	47:m:273:TYR:CG	2.39	0.40
47:m:245:PHE:O	47:m:247:PRO:HD3	2.21	0.40
48:o:47:ALA:HB2	48:o:90:TYR:CE1	2.57	0.40
50:q:25:GLY:O	50:q:28:LYS:N	2.33	0.40
47:y:245:PHE:O	47:y:247:PRO:HD3	2.21	0.40
47:y:377:LEU:HD11	50:A1:20:TYR:CE2	2.55	0.40
48:z:230:LEU:HD23	48:z:230:LEU:HA	1.87	0.40
49:A0:122:HIS:CB	49:A0:168:SER:H	2.33	0.40
51:A2:7:LEU:HA	51:A2:7:LEU:HD23	1.88	0.40
56:A9:83:VAL:HB	56:A9:84:PRO:HD3	2.04	0.40
57:C4:215:PRO:HD3	64:B4:60:PHE:CD1	2.57	0.40
61:A6:1:ALA:O	61:A6:2:SER:CB	2.70	0.40
61:A6:8:THR:HG1	61:A6:11:GLU:HG2	1.85	0.40
63:A5:33:TYR:O	63:A5:37:HIS:HD2	2.05	0.40
1:9:140:CYS:HB3	1:9:145:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:14:LEU:HD21	2:4:30:HIS:CD2	2.56	0.40
2:4:120:ILE:O	2:4:124:ALA:HB2	2.22	0.40
2:4:430:PHE:O	2:4:433:GLU:N	2.52	0.40
5:6:188:TRP:CD2	5:6:212:PRO:HB3	2.56	0.40
5:6:264:TYR:CG	5:6:265:PRO:HD3	2.56	0.40
9:8:53:LEU:HB3	9:8:54:LYS:H	1.81	0.40
9:8:124:THR:C	9:8:126:LYS:H	2.29	0.40
10:A:364:ASP:N	10:A:364:ASP:OD1	2.49	0.40
13:D:203:LYS:HE3	13:D:203:LYS:HB3	1.89	0.40
14:E:52:SER:O	14:E:54:THR:N	2.55	0.40
14:E:174:GLU:O	14:E:175:PHE:CG	2.74	0.40
15:F:96:ARG:C	15:F:98:PRO:HD3	2.46	0.40
16:G:124:LEU:HD23	16:G:124:LEU:HA	1.94	0.40
16:G:131:LYS:C	16:G:134:ALA:H	2.29	0.40
25:Q:86:TRP:HA	25:Q:89:ILE:HG22	2.03	0.40
25:Q:158:LEU:HD13	42:j:88:HIS:CG	2.52	0.40
26:R:222:TRP:NE1	26:R:223:PHE:CE2	2.90	0.40
27:S:71:LEU:HG	27:S:144:GLY:CA	2.50	0.40
27:S:333:GLU:C	27:S:335:VAL:N	2.79	0.40
28:T:60:THR:O	28:T:60:THR:HG23	2.21	0.40
31:W:108:LEU:O	31:W:109:GLY:C	2.63	0.40
33:Y:91:ASP:N	33:Y:92:PRO:HD2	2.37	0.40
37:c:17:GLU:O	37:c:21:ARG:HB2	2.21	0.40
39:f:95:GLU:O	39:f:95:GLU:HG3	2.22	0.40
43:g:131:GLN:O	43:g:135:VAL:HG23	2.21	0.40
45:k:57:TYR:CE2	45:k:134:ILE:HD12	2.57	0.40
45:k:179:ARG:HA	45:k:182:LEU:HD12	2.04	0.40
45:k:361:LEU:HA	45:k:361:LEU:HD12	1.89	0.40
45:k:394:GLU:CD	45:k:398:ARG:HE	2.28	0.40
46:l:399:LEU:HA	46:l:402:ILE:HD12	2.03	0.40
47:m:129:MET:O	47:m:130:GLY:C	2.64	0.40
48:o:18:LEU:HA	48:o:18:LEU:HD23	1.86	0.40
48:o:20:SER:OG	48:o:21:LEU:N	2.53	0.40
45:w:431:LEU:HD12	45:w:432:PRO:CD	2.52	0.40
46:x:70:ARG:NH1	55:B1:67:SER:HB3	2.37	0.40
46:x:260:GLU:HG2	46:x:261:SER:O	2.22	0.40
47:y:44:GLN:O	47:y:45:ILE:C	2.65	0.40
47:y:61:THR:O	47:y:62:ALA:C	2.64	0.40
47:y:91:PHE:HD2	47:y:273:TYR:CG	2.39	0.40
49:A0:106:ILE:N	49:A0:167:ALA:HA	2.35	0.40
58:C2:224:LYS:NZ	58:C2:226:HIS:HE2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:A7:119:GLN:O	59:A7:123:MET:HG3	2.22	0.40
63:A5:54:GLU:CD	63:A5:57:ARG:HH12	2.30	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%)	167 (82%)	31 (15%)	7 (3%)	3	20
2	4	457/459 (100%)	393 (86%)	56 (12%)	8 (2%)	6	33
3	2	342/347 (99%)	283 (83%)	57 (17%)	2 (1%)	21	58
4	7	170/175 (97%)	138 (81%)	25 (15%)	7 (4%)	2	18
5	6	604/606 (100%)	517 (86%)	84 (14%)	3 (0%)	24	63
6	5	94/98 (96%)	78 (83%)	16 (17%)	0	100	100
7	3	110/115 (96%)	93 (84%)	16 (14%)	1 (1%)	14	49
8	1	316/318 (99%)	255 (81%)	48 (15%)	13 (4%)	2	18
9	8	425/444 (96%)	349 (82%)	69 (16%)	7 (2%)	7	37
10	A	686/704 (97%)	559 (82%)	112 (16%)	15 (2%)	5	29
11	B	428/430 (100%)	343 (80%)	79 (18%)	6 (1%)	9	39
12	C	206/228 (90%)	173 (84%)	30 (15%)	3 (2%)	8	38
13	D	150/179 (84%)	121 (81%)	25 (17%)	4 (3%)	4	25
14	E	174/176 (99%)	148 (85%)	23 (13%)	3 (2%)	7	35
15	F	26/75 (35%)	18 (69%)	7 (27%)	1 (4%)	2	19
16	G	121/133 (91%)	101 (84%)	19 (16%)	1 (1%)	16	53
17	H	94/105 (90%)	70 (74%)	21 (22%)	3 (3%)	3	21
18	I	69/96 (72%)	58 (84%)	8 (12%)	3 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	J	67/70 (96%)	60 (90%)	5 (8%)	2 (3%)	3	22
20	K	82/98 (84%)	65 (79%)	16 (20%)	1 (1%)	10	42
21	L	78/83 (94%)	67 (86%)	11 (14%)	0	100	100
22	N	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
23	O	112/127 (88%)	97 (87%)	12 (11%)	3 (3%)	4	25
24	P	86/112 (77%)	64 (74%)	22 (26%)	0	100	100
25	Q	166/171 (97%)	112 (68%)	51 (31%)	3 (2%)	6	33
26	R	315/345 (91%)	243 (77%)	65 (21%)	7 (2%)	5	29
27	S	317/320 (99%)	240 (76%)	67 (21%)	10 (3%)	3	21
28	T	136/140 (97%)	102 (75%)	15 (11%)	19 (14%)	0	3
29	U	128/145 (88%)	98 (77%)	30 (23%)	0	100	100
30	V	136/143 (95%)	110 (81%)	22 (16%)	4 (3%)	3	23
31	M	78/88 (89%)	56 (72%)	19 (24%)	3 (4%)	2	19
31	W	84/88 (96%)	68 (81%)	15 (18%)	1 (1%)	10	42
32	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	17
33	Y	55/72 (76%)	44 (80%)	10 (18%)	1 (2%)	6	33
34	Z	72/98 (74%)	54 (75%)	16 (22%)	2 (3%)	4	24
35	a	112/128 (88%)	93 (83%)	19 (17%)	0	100	100
36	b	137/143 (96%)	106 (77%)	30 (22%)	1 (1%)	18	55
37	c	86/128 (67%)	66 (77%)	20 (23%)	0	100	100
38	d	105/117 (90%)	87 (83%)	15 (14%)	3 (3%)	3	23
39	f	165/178 (93%)	130 (79%)	33 (20%)	2 (1%)	10	42
40	h	82/125 (66%)	56 (68%)	23 (28%)	3 (4%)	2	19
41	i	36/49 (74%)	33 (92%)	3 (8%)	0	100	100
42	j	111/120 (92%)	94 (85%)	17 (15%)	0	100	100
43	g	171/176 (97%)	141 (82%)	29 (17%)	1 (1%)	21	58
44	e	139/158 (88%)	81 (58%)	45 (32%)	13 (9%)	0	8
45	k	444/480 (92%)	407 (92%)	34 (8%)	3 (1%)	18	55
45	w	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	18	55
46	l	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	43	77
46	x	417/453 (92%)	387 (93%)	29 (7%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	m	377/379 (100%)	348 (92%)	29 (8%)	0	100	100
47	y	377/379 (100%)	349 (93%)	28 (7%)	0	100	100
48	o	239/241 (99%)	213 (89%)	21 (9%)	5 (2%)	5	30
48	z	239/241 (99%)	213 (89%)	20 (8%)	6 (2%)	4	26
49	A0	184/196 (94%)	105 (57%)	48 (26%)	31 (17%)	0	2
49	p	147/196 (75%)	101 (69%)	33 (22%)	13 (9%)	0	9
50	A1	104/111 (94%)	91 (88%)	7 (7%)	6 (6%)	1	14
50	q	104/111 (94%)	96 (92%)	8 (8%)	0	100	100
51	A2	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
51	r	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
52	B3	67/91 (74%)	59 (88%)	6 (9%)	2 (3%)	3	22
52	s	65/91 (71%)	58 (89%)	5 (8%)	2 (3%)	3	22
53	A3	37/56 (66%)	23 (62%)	10 (27%)	4 (11%)	0	6
53	t	31/56 (55%)	23 (74%)	7 (23%)	1 (3%)	3	21
54	B2	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
54	u	60/64 (94%)	55 (92%)	5 (8%)	0	100	100
55	B1	20/78 (26%)	10 (50%)	7 (35%)	3 (15%)	0	3
55	v	16/78 (20%)	8 (50%)	6 (38%)	2 (12%)	0	4
56	A9	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
57	C4	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	41
58	C2	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
59	A7	142/169 (84%)	135 (95%)	7 (5%)	0	100	100
60	C0	107/152 (70%)	104 (97%)	3 (3%)	0	100	100
61	A6	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	39
64	B4	71/74 (96%)	65 (92%)	6 (8%)	0	100	100
65	C3	54/80 (68%)	48 (89%)	4 (7%)	2 (4%)	2	19
66	B0	47/80 (59%)	41 (87%)	6 (13%)	0	100	100
67	C1	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
68	A8	41/70 (59%)	39 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13638/14963 (91%)	11529 (84%)	1839 (14%)	270 (2%)	8	31

All (270) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	84	TRP
4	7	141	MET
4	7	171	ILE
8	1	170	GLU
8	1	174	LEU
8	1	268	MET
10	A	383	SER
10	A	461	PRO
10	A	463	SER
11	B	294	ARG
13	D	146	GLU
18	I	106	GLU
18	I	109	THR
27	S	200	PRO
27	S	276	ASP
28	T	4	THR
28	T	12	ILE
28	T	13	PRO
28	T	45	THR
28	T	46	PRO
28	T	61	PHE
28	T	63	ALA
28	T	80	VAL
28	T	96	ALA
28	T	110	ILE
30	V	143	TYR
34	Z	63	PHE
34	Z	64	VAL
40	h	81	ALA
40	h	82	VAL
44	e	42	PRO
44	e	81	ARG
44	e	82	SER
44	e	115	ASN
49	p	82	PRO
49	p	120	PRO
49	p	129	LYS

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Mol	Chain	Res	Type
49	p	146	PRO
49	p	159	PRO
52	s	14	VAL
48	z	80	MET
49	A0	82	PRO
49	A0	95	PRO
49	A0	118	ARG
49	A0	120	PRO
49	A0	121	GLN
49	A0	150	ALA
49	A0	159	PRO
49	A0	163	SER
49	A0	175	PRO
49	A0	176	ALA
49	A0	183	PRO
50	A1	14	GLU
52	B3	14	VAL
53	A3	39	ARG
53	A3	40	LEU
56	A9	328	HIS
56	A9	508	PRO
61	A6	2	SER
61	A6	87	THR
61	A6	95	GLN
62	A4	4	ALA
62	A4	9	GLY
63	A5	46	LYS
65	C3	2	GLU
1	9	75	LYS
1	9	76	ALA
2	4	21	ASN
2	4	420	THR
3	2	88	LYS
8	1	76	ILE
8	1	78	ALA
8	1	173	TRP
8	1	176	LEU
8	1	282	TYR
10	A	189	ILE
11	B	310	VAL
12	C	219	LYS
13	D	147	PRO

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Mol	Chain	Res	Type
13	D	184	PRO
17	H	16	ARG
23	O	100	ARG
26	R	155	VAL
26	R	272	LEU
26	R	309	PRO
27	S	58	LYS
28	T	3	LYS
28	T	90	TYR
28	T	108	TYR
28	T	109	GLY
32	X	14	VAL
44	e	43	LYS
44	e	71	GLY
46	l	305	GLN
49	p	115	SER
49	p	130	PRO
55	v	65	VAL
48	z	79	GLU
49	A0	77	LYS
49	A0	81	ILE
49	A0	129	LYS
49	A0	156	TYR
49	A0	188	THR
50	A1	13	LEU
55	B1	65	VAL
62	A4	5	LYS
2	4	61	LEU
2	4	65	LEU
4	7	140	ALA
4	7	148	SER
4	7	170	GLU
5	6	352	ASP
7	3	82	ALA
8	1	177	PRO
9	8	235	VAL
9	8	403	ASP
10	A	129	PRO
10	A	283	GLU
10	A	541	PRO
11	B	291	VAL
11	B	293	LEU

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Mol	Chain	Res	Type
20	K	52	PRO
25	Q	94	LEU
25	Q	121	ASP
26	R	99	ASP
27	S	280	HIS
27	S	333	GLU
28	T	78	ALA
31	W	129	GLU
43	g	126	ALA
44	e	70	THR
48	o	50	HIS
49	p	81	ILE
49	p	134	ILE
53	t	38	TRP
48	z	50	HIS
49	A0	91	TRP
49	A0	114	VAL
49	A0	154	GLY
49	A0	181	GLU
50	A1	6	VAL
53	A3	41	ILE
57	C4	104	TRP
62	A4	61	SER
8	1	71	PHE
12	C	127	ARG
13	D	103	ARG
14	E	106	TYR
14	E	107	PRO
16	G	122	SER
17	H	57	LYS
18	I	108	LYS
23	O	25	MET
26	R	325	THR
27	S	216	LYS
27	S	281	LYS
28	T	11	ASP
28	T	62	THR
30	V	26	PRO
38	d	19	PRO
38	d	39	MET
39	f	165	PRO
44	e	76	PRO

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Mol	Chain	Res	Type
31	M	30	LEU
31	M	60	PHE
45	k	229	PRO
45	k	427	PRO
48	o	51	LEU
49	p	116	GLN
55	v	66	ALA
45	w	214	LYS
45	w	427	PRO
48	z	51	LEU
49	A0	79	SER
49	A0	85	LYS
49	A0	115	SER
49	A0	152	ASP
49	A0	178	LEU
49	A0	179	ASN
50	A1	10	SER
50	A1	12	TRP
53	A3	42	LEU
56	A9	51	ASP
1	9	150	GLU
1	9	232	THR
1	9	234	LEU
2	4	58	SER
2	4	112	ALA
8	1	316	PRO
9	8	236	PHE
9	8	282	VAL
9	8	381	GLN
10	A	563	ASP
11	B	78	SER
25	Q	32	TYR
26	R	316	ARG
27	S	334	ASP
28	T	35	VAL
28	T	77	SER
30	V	25	LEU
32	X	13	HIS
36	b	111	GLU
44	e	79	PRO
49	p	136	ILE
46	x	305	GLN

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Mol	Chain	Res	Type
49	A0	2	HIS
49	A0	63	SER
49	A0	171	ILE
57	C4	103	GLN
65	C3	3	ASN
2	4	82	HIS
4	7	137	SER
4	7	149	TYR
5	6	65	ASN
9	8	227	PRO
9	8	387	GLU
10	A	128	CYS
10	A	188	GLU
10	A	242	PRO
15	F	86	LEU
19	J	55	SER
23	O	116	LYS
39	f	149	PRO
44	e	105	MET
48	o	49	ARG
52	s	28	GLU
48	z	49	ARG
50	A1	8	ALA
52	B3	28	GLU
56	A9	91	ASP
57	C4	158	ASP
62	A4	49	PRO
5	6	71	ILE
10	A	561	PRO
11	B	39	PRO
19	J	57	VAL
38	d	40	VAL
44	e	44	THR
49	A0	106	ILE
8	1	249	PRO
26	R	371	PRO
30	V	73	PRO
40	h	80	PRO
48	o	70	VAL
49	p	93	GLY
55	B1	63	PRO
55	B1	72	VAL

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Mol	Chain	Res	Type
8	1	208	VAL
10	A	45	PRO
10	A	210	ILE
12	C	218	VAL
33	Y	90	PRO
45	k	71	PRO
45	w	71	PRO
61	A6	15	GLY
1	9	241	PRO
2	4	306	PRO
10	A	263	VAL
14	E	171	PRO
17	H	25	GLN
48	o	74	PRO
49	p	114	VAL
48	z	74	PRO
49	A0	193	VAL
1	9	216	PRO
27	S	340	ILE
44	e	78	LEU
44	e	87	ASP
31	M	27	PRO
27	S	323	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	169/183 (92%)	166 (98%)	3 (2%)	51	67
2	4	389/413 (94%)	389 (100%)	0	100	100
3	2	304/316 (96%)	302 (99%)	2 (1%)	76	79
4	7	116/142 (82%)	115 (99%)	1 (1%)	70	76
5	6	524/534 (98%)	520 (99%)	4 (1%)	73	77
6	5	80/86 (93%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	3	95/101 (94%)	95 (100%)	0	100	100
8	1	274/275 (100%)	257 (94%)	17 (6%)	16	38
9	8	270/353 (76%)	269 (100%)	1 (0%)	84	82
10	A	560/588 (95%)	556 (99%)	4 (1%)	76	79
11	B	363/371 (98%)	356 (98%)	7 (2%)	50	66
12	C	188/204 (92%)	186 (99%)	2 (1%)	65	74
13	D	127/150 (85%)	122 (96%)	5 (4%)	28	49
14	E	148/151 (98%)	145 (98%)	3 (2%)	48	65
15	F	14/69 (20%)	14 (100%)	0	100	100
16	G	106/119 (89%)	106 (100%)	0	100	100
17	H	80/95 (84%)	80 (100%)	0	100	100
18	I	53/79 (67%)	49 (92%)	4 (8%)	12	33
19	J	50/59 (85%)	49 (98%)	1 (2%)	48	65
20	K	67/81 (83%)	67 (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	73/96 (76%)	72 (99%)	1 (1%)	59	71
25	Q	142/154 (92%)	141 (99%)	1 (1%)	76	79
26	R	232/298 (78%)	230 (99%)	2 (1%)	70	76
27	S	205/283 (72%)	204 (100%)	1 (0%)	81	81
28	T	73/101 (72%)	48 (66%)	25 (34%)	0	2
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%)	55 (96%)	2 (4%)	32	53
32	X	32/54 (59%)	32 (100%)	0	100	100
33	Y	29/62 (47%)	29 (100%)	0	100	100
34	Z	28/76 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	c	45/122 (37%)	45 (100%)	0	100	100
38	d	44/107 (41%)	44 (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	86/106 (81%)	85 (99%)	1 (1%)	63	73
43	g	130/157 (83%)	129 (99%)	1 (1%)	73	77
44	e	44/141 (31%)	41 (93%)	3 (7%)	14	36
45	k	369/394 (94%)	369 (100%)	0	100	100
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%)	326 (100%)	1 (0%)	86	84
47	y	327/327 (100%)	326 (100%)	1 (0%)	86	84
48	o	206/206 (100%)	206 (100%)	0	100	100
48	z	202/206 (98%)	202 (100%)	0	100	100
49	A0	64/168 (38%)	61 (95%)	3 (5%)	23	45
49	p	65/168 (39%)	65 (100%)	0	100	100
50	A1	96/99 (97%)	92 (96%)	4 (4%)	26	48
50	q	96/99 (97%)	96 (100%)	0	100	100
51	A2	70/72 (97%)	69 (99%)	1 (1%)	59	71
51	r	71/72 (99%)	71 (100%)	0	100	100
52	B3	66/85 (78%)	66 (100%)	0	100	100
52	s	64/85 (75%)	64 (100%)	0	100	100
53	A3	31/46 (67%)	28 (90%)	3 (10%)	8	25
53	t	24/46 (52%)	23 (96%)	1 (4%)	26	48
54	B2	52/54 (96%)	50 (96%)	2 (4%)	29	51
54	u	52/54 (96%)	52 (100%)	0	100	100
55	B1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	C4	211/211 (100%)	192 (91%)	19 (9%)	9	28
58	C2	226/226 (100%)	207 (92%)	19 (8%)	10	30
59	A7	128/148 (86%)	119 (93%)	9 (7%)	14	36
60	C0	95/123 (77%)	89 (94%)	6 (6%)	16	38
61	A6	81/103 (79%)	81 (100%)	0	100	100
62	A4	68/79 (86%)	66 (97%)	2 (3%)	37	57
63	A5	67/76 (88%)	64 (96%)	3 (4%)	24	46
64	B4	58/59 (98%)	53 (91%)	5 (9%)	10	29
65	C3	47/68 (69%)	41 (87%)	6 (13%)	4	17
66	B0	39/66 (59%)	36 (92%)	3 (8%)	12	32
67	C1	40/55 (73%)	40 (100%)	0	100	100
68	A8	37/57 (65%)	34 (92%)	3 (8%)	11	31
All	All	10787/12809 (84%)	10565 (98%)	222 (2%)	46	65

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9	68	LYS
1	9	93	LEU
1	9	188	ILE
3	2	7	ILE
3	2	84	TRP
4	7	171	ILE
5	6	116	LYS
5	6	120	TYR
5	6	301	ILE
5	6	427	ILE
8	1	70	MET
8	1	71	PHE
8	1	77	MET
8	1	156	MET
8	1	157	SER
8	1	171	GLN
8	1	172	MET
8	1	174	LEU
8	1	235	ASN
8	1	236	ILE
8	1	250	HIS

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Mol	Chain	Res	Type
8	1	251	MET
8	1	265	LEU
8	1	266	LEU
8	1	309	ILE
8	1	317	GLN
8	1	318	THR
9	8	156	ILE
10	A	146	PHE
10	A	223	ILE
10	A	319	TRP
10	A	381	LEU
11	B	141	TYR
11	B	236	LEU
11	B	254	ARG
11	B	264	ASN
11	B	389	TYR
11	B	429	PHE
11	B	432	LEU
12	C	95	VAL
12	C	219	LYS
13	D	74	ILE
13	D	138	ARG
13	D	146	GLU
13	D	175	ARG
13	D	181	ILE
14	E	41	VAL
14	E	62	LEU
14	E	67	ILE
18	I	101	ILE
18	I	103	LEU
18	I	106	GLU
18	I	108	LYS
19	J	18	ILE
24	P	106	LEU
25	Q	158	LEU
26	R	152	ILE
26	R	206	ILE
27	S	327	TYR
28	T	3	LYS
28	T	5	VAL
28	T	6	LEU
28	T	10	TRP

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Mol	Chain	Res	Type
28	T	14	GLU
28	T	20	ARG
28	T	22	THR
28	T	28	ILE
28	T	34	LEU
28	T	58	ARG
28	T	59	TYR
28	T	60	THR
28	T	66	ILE
28	T	69	ILE
28	T	72	LEU
28	T	73	THR
28	T	76	ILE
28	T	80	VAL
28	T	81	ARG
28	T	88	LEU
28	T	99	LEU
28	T	101	LEU
28	T	106	ARG
28	T	107	SER
28	T	108	TYR
31	W	106	LYS
31	W	108	LEU
42	j	88	HIS
43	g	79	GLU
44	e	114	ARG
44	e	118	ASP
44	e	119	THR
47	m	153	ILE
53	t	39	ARG
47	y	153	ILE
49	A0	72	SER
49	A0	73	LYS
49	A0	74	ILE
50	A1	6	VAL
50	A1	7	SER
50	A1	9	SER
50	A1	12	TRP
51	A2	23	GLN
53	A3	19	PRO
53	A3	39	ARG
53	A3	40	LEU

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Mol	Chain	Res	Type
54	B2	36	ASP
54	B2	54	HIS
56	A9	18	LEU
56	A9	35	LEU
56	A9	92	MET
56	A9	96	ARG
56	A9	105	LEU
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

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Mol	Chain	Res	Type
57	C4	16	ILE
57	C4	31	VAL
57	C4	33	LEU
57	C4	52	HIS
57	C4	60	GLU
57	C4	63	THR
57	C4	67	ILE
57	C4	88	ASP
57	C4	92	ASN
57	C4	125	THR
57	C4	130	PRO
57	C4	134	ARG
57	C4	142	VAL
57	C4	147	GLU
57	C4	170	LEU
57	C4	171	LYS
57	C4	185	MET
57	C4	205	SER
57	C4	216	LEU
58	C2	1	MET
58	C2	19	THR
58	C2	85	LEU
58	C2	92	LEU
58	C2	112	LEU
58	C2	127	LEU
58	C2	128	GLU
58	C2	131	LEU
58	C2	132	LEU
58	C2	137	LEU
58	C2	142	VAL
58	C2	160	LEU
58	C2	163	LEU
58	C2	188	ILE
58	C2	196	THR
58	C2	199	VAL
58	C2	213	THR
58	C2	222	GLN
58	C2	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
60	C0	7	THR
60	C0	29	LEU
60	C0	70	VAL
60	C0	79	LYS
60	C0	80	GLU
60	C0	90	ARG
62	A4	33	LEU
62	A4	56	ARG
63	A5	29	CYS
63	A5	41	LYS
63	A5	53	CYS
64	B4	4	LEU
64	B4	8	GLN
64	B4	26	MET
64	B4	29	LEU
64	B4	64	ARG
65	C3	2	GLU
65	C3	5	VAL
65	C3	8	LYS
65	C3	16	ASN
65	C3	23	LYS
65	C3	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 (212) such sidechains are listed below:

Mol	Chain	Res	Type
1	9	41	HIS
1	9	87	GLN
1	9	187	GLN
2	4	30	HIS
2	4	44	GLN

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Mol	Chain	Res	Type
2	4	331	ASN
2	4	366	ASN
2	4	390	ASN
2	4	422	HIS
2	4	440	HIS
3	2	36	ASN
3	2	48	HIS
3	2	49	ASN
3	2	83	GLN
3	2	268	GLN
5	6	59	GLN
5	6	113	ASN
5	6	226	GLN
5	6	296	ASN
5	6	332	HIS
5	6	447	ASN
5	6	470	ASN
5	6	471	ASN
5	6	546	GLN
5	6	605	HIS
6	5	7	ASN
6	5	97	GLN
8	1	5	ASN
8	1	47	GLN
8	1	169	GLN
8	1	171	GLN
8	1	230	ASN
8	1	287	HIS
8	1	317	GLN
9	8	103	ASN
9	8	164	ASN
9	8	168	ASN
9	8	220	GLN
9	8	281	HIS
9	8	393	ASN
9	8	422	HIS
10	A	142	GLN
10	A	282	ASN
10	A	359	ASN
10	A	424	HIS
10	A	460	HIS
10	A	572	HIS

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Mol	Chain	Res	Type
11	B	46	GLN
11	B	79	ASN
11	B	160	ASN
11	B	182	ASN
11	B	183	HIS
11	B	234	GLN
11	B	346	GLN
11	B	349	ASN
11	B	381	HIS
12	C	230	GLN
12	C	249	GLN
13	D	75	ASN
13	D	164	HIS
14	E	85	ASN
14	E	172	ASN
14	E	204	ASN
16	G	88	GLN
16	G	92	ASN
17	H	7	GLN
17	H	21	GLN
17	H	82	GLN
19	J	40	HIS
20	K	48	ASN
21	L	71	GLN
23	O	102	HIS
24	P	52	ASN
25	Q	143	HIS
26	R	323	HIS
26	R	331	HIS
27	S	120	GLN
27	S	164	GLN
27	S	190	HIS
27	S	211	ASN
29	U	13	GLN
29	U	123	GLN
30	V	76	GLN
31	W	115	GLN
32	X	13	HIS
33	Y	57	GLN
35	a	79	ASN
37	c	74	HIS
37	c	83	HIS

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Mol	Chain	Res	Type
37	c	89	HIS
38	d	92	HIS
40	h	70	ASN
40	h	74	HIS
40	h	86	ASN
40	h	115	GLN
41	i	62	HIS
42	j	97	HIS
43	g	55	GLN
43	g	144	HIS
44	e	94	HIS
44	e	160	GLN
31	M	35	HIS
31	M	74	GLN
45	k	9	GLN
45	k	15	GLN
45	k	61	HIS
45	k	119	ASN
45	k	207	GLN
45	k	252	HIS
45	k	323	HIS
45	k	363	ASN
46	l	31	ASN
46	l	125	ASN
46	l	198	HIS
46	l	254	HIS
46	l	290	ASN
46	l	304	HIS
46	l	354	ASN
47	m	3	ASN
47	m	8	HIS
47	m	16	ASN
47	m	32	ASN
47	m	114	ASN
47	m	201	HIS
47	m	255	ASN
47	m	308	HIS
47	m	341	GLN
47	m	374	ASN
48	o	23	HIS
48	o	198	HIS
48	o	200	HIS

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Mol	Chain	Res	Type
49	p	53	ASN
51	r	79	ASN
54	u	45	HIS
45	w	9	GLN
45	w	15	GLN
45	w	61	HIS
45	w	207	GLN
45	w	252	HIS
45	w	323	HIS
45	w	363	ASN
46	x	31	ASN
46	x	125	ASN
46	x	198	HIS
46	x	254	HIS
46	x	290	ASN
46	x	304	HIS
46	x	354	ASN
47	y	3	ASN
47	y	8	HIS
47	y	16	ASN
47	y	32	ASN
47	y	114	ASN
47	y	201	HIS
47	y	255	ASN
47	y	341	GLN
47	y	374	ASN
48	z	71	GLN
48	z	75	ASN
48	z	198	HIS
48	z	200	HIS
49	A0	53	ASN
51	A2	36	ASN
51	A2	79	ASN
52	B3	63	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

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Mol	Chain	Res	Type
56	A9	360	ASN
56	A9	368	HIS
56	A9	413	HIS
56	A9	503	HIS
56	A9	512	ASN
57	C4	52	HIS
57	C4	91	ASN
57	C4	102	HIS
57	C4	195	GLN
57	C4	203	ASN
58	C2	3	HIS
58	C2	6	HIS
58	C2	12	ASN
58	C2	133	ASN
58	C2	148	HIS
58	C2	149	HIS
58	C2	158	HIS
58	C2	204	HIS
58	C2	207	HIS
58	C2	222	GLN
58	C2	232	HIS
59	A7	109	HIS
60	C0	34	ASN
61	A6	66	ASN
62	A4	52	HIS
63	A5	23	GLN
63	A5	24	ASN
63	A5	25	GLN
63	A5	28	ASN
63	A5	32	ASN
63	A5	37	HIS
65	C3	3	ASN
65	C3	16	ASN
65	C3	21	HIS
66	B0	10	HIS
66	B0	15	ASN
66	B0	35	GLN
66	B0	41	ASN
68	A8	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	401	47	50,50,50	1.69	15 (30%)	66,82,82	1.32	6 (9%)
71	CDL	6	701	-	63,63,99	1.08	7 (11%)	69,75,111	1.26	4 (5%)
72	PC1	4	504	-	45,45,53	1.05	3 (6%)	51,53,61	1.13	2 (3%)
70	3PE	B	501	-	50,50,50	0.87	2 (4%)	53,55,55	1.34	4 (7%)
69	FES	m	403	-	0,4,4	-	-	-	-	-
79	HEA	A9	601	56	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
76	NAP	R	601	-	49,52,52	4.47	20 (40%)	69,80,80	1.98	19 (27%)
78	HEC	z	301	48	50,50,50	1.63	5 (10%)	68,82,82	1.21	5 (7%)
74	SF4	A	801	10	0,12,12	-	-	-	-	-
70	3PE	4	503	-	40,40,50	0.90	3 (7%)	43,45,55	1.38	2 (4%)
78	HEC	o	301	48	50,50,50	1.63	5 (10%)	68,82,82	1.22	5 (7%)
79	HEA	A9	602	56	66,67,67	1.22	7 (10%)	78,103,103	1.36	11 (14%)
72	PC1	2	402	-	45,45,53	1.02	2 (4%)	51,53,61	0.99	2 (3%)
72	PC1	S	401	27	46,46,53	1.03	4 (8%)	52,54,61	1.07	2 (3%)
74	SF4	A	802	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	CDL	J	101	-	57,57,99	1.16	7 (12%)	63,69,111	1.19	5 (7%)
69	FES	A	803	10	0,4,4	-	-	-	-	-
77	HEM	y	401	47	50,50,50	1.69	15 (30%)	66,82,82	1.31	6 (9%)
72	PC1	j	201	-	38,38,53	1.15	6 (15%)	44,46,61	1.06	2 (4%)
74	SF4	8	502	-	0,12,12	-	-	-	-	-
70	3PE	4	501	-	40,40,50	1.03	2 (5%)	43,45,55	1.10	3 (6%)
77	HEM	y	402	47	50,50,50	1.59	12 (24%)	66,82,82	1.14	4 (6%)
74	SF4	E	301	14	0,12,12	-	-	-	-	-
72	PC1	L	200	-	46,46,53	0.98	3 (6%)	52,54,61	1.08	2 (3%)
74	SF4	E	302	14	0,12,12	-	-	-	-	-
77	HEM	m	402	47	50,50,50	1.59	12 (24%)	66,82,82	1.14	4 (6%)
73	FMN	8	501	-	33,33,33	1.19	2 (6%)	48,50,50	1.62	12 (25%)
69	FES	9	301	1	0,4,4	-	-	-	-	-
71	CDL	4	502	-	81,81,99	0.98	6 (7%)	87,93,111	1.15	4 (4%)
70	3PE	2	401	-	45,45,50	0.89	3 (6%)	48,50,55	1.08	2 (4%)
74	SF4	D	301	13	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEM	m	401	47	-	4/14/54/54	-
71	CDL	6	701	-	-	34/74/74/110	-
72	PC1	4	504	-	-	23/49/49/57	-
70	3PE	B	501	-	-	28/54/54/54	-
79	HEA	A9	601	56	-	9/36/76/76	-
69	FES	m	403	-	-	-	0/1/1/1
78	HEC	z	301	48	1/1/3/7	6/14/54/54	-
76	NAP	R	601	-	-	17/35/67/67	0/5/5/5
74	SF4	A	801	10	-	-	0/6/5/5
70	3PE	4	503	-	-	25/44/44/54	-
78	HEC	o	301	48	1/1/3/7	6/14/54/54	-
79	HEA	A9	602	56	-	7/36/76/76	-
72	PC1	2	402	-	-	30/49/49/57	-
72	PC1	S	401	27	-	30/50/50/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	SF4	A	802	-	-	-	0/6/5/5
71	CDL	J	101	-	-	24/68/68/110	-
77	HEM	y	401	47	-	4/14/54/54	-
69	FES	A	803	10	-	-	0/1/1/1
72	PC1	j	201	-	-	21/42/42/57	-
70	3PE	4	501	-	-	29/44/44/54	-
74	SF4	8	502	-	-	-	0/6/5/5
77	HEM	y	402	47	-	2/14/54/54	-
74	SF4	E	301	14	-	-	0/6/5/5
72	PC1	L	200	-	-	23/50/50/57	-
74	SF4	E	302	14	-	-	0/6/5/5
77	HEM	m	402	47	-	2/14/54/54	-
73	FMN	8	501	-	-	9/18/18/18	0/3/3/3
69	FES	9	301	1	-	-	0/1/1/1
71	CDL	4	502	-	-	41/92/92/110	-
70	3PE	2	401	-	-	20/49/49/54	-
74	SF4	D	301	13	-	-	0/6/5/5

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	R	601	NAP	C2D-C1D	-15.67	1.30	1.53
76	R	601	NAP	O4D-C1D	15.38	1.62	1.41
76	R	601	NAP	C2B-C1B	-9.64	1.28	1.53
76	R	601	NAP	O4B-C1B	8.46	1.62	1.42
76	R	601	NAP	O4D-C4D	-7.08	1.29	1.45
78	o	301	HEC	C3D-C2D	6.96	1.51	1.36
78	z	301	HEC	C3D-C2D	6.95	1.51	1.36
76	R	601	NAP	C7N-N7N	6.91	1.46	1.33
76	R	601	NAP	O4B-C4B	-6.15	1.31	1.45
76	R	601	NAP	C3N-C7N	4.72	1.57	1.50
76	R	601	NAP	O3D-C3D	-4.32	1.32	1.43
76	R	601	NAP	C5A-N7A	-4.32	1.30	1.39
70	4	501	3PE	O31-C31	4.26	1.45	1.33
70	4	501	3PE	O21-C21	4.12	1.45	1.34
76	R	601	NAP	C6A-N6A	3.94	1.44	1.34
79	A9	602	HEA	CMA-C3A	-3.69	1.37	1.45
76	R	601	NAP	O7N-C7N	-3.67	1.17	1.24
76	R	601	NAP	O2D-C2D	3.57	1.51	1.43
77	y	401	HEM	C2A-C3A	-3.24	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	m	401	HEM	FE-NC	-3.22	1.84	1.95
77	m	401	HEM	C2A-C3A	-3.20	1.30	1.38
77	y	401	HEM	FE-NC	-3.18	1.84	1.95
76	R	601	NAP	C5A-C4A	-3.18	1.33	1.39
76	R	601	NAP	C4A-N9A	-3.06	1.30	1.37
77	m	402	HEM	C2A-C3A	-3.04	1.30	1.38
77	y	402	HEM	C2A-C3A	-3.03	1.30	1.38
77	y	401	HEM	C3D-C2D	-3.01	1.30	1.36
72	4	504	PC1	O21-C2	-2.98	1.39	1.46
76	R	601	NAP	O3B-C3B	-2.94	1.36	1.43
77	m	402	HEM	C3C-C2C	-2.93	1.31	1.37
70	B	501	3PE	O21-C2	-2.92	1.39	1.46
77	m	401	HEM	C3D-C2D	-2.91	1.30	1.36
77	y	402	HEM	C3C-C2C	-2.91	1.31	1.37
79	A9	602	HEA	FE-NA	2.89	2.04	1.95
71	6	701	CDL	OA6-CA4	-2.78	1.39	1.46
71	J	101	CDL	OB6-CB4	-2.73	1.39	1.46
71	4	502	CDL	OB8-CB7	2.73	1.41	1.33
76	R	601	NAP	C8A-N9A	-2.73	1.32	1.37
73	8	501	FMN	C4A-N5	2.70	1.36	1.30
71	4	502	CDL	OA6-CA4	-2.69	1.39	1.46
77	y	401	HEM	C3C-C2C	-2.68	1.31	1.37
79	A9	601	HEA	CMA-C3A	-2.68	1.39	1.45
77	m	401	HEM	C3C-C2C	-2.67	1.31	1.37
79	A9	601	HEA	C1A-C2A	-2.67	1.40	1.45
79	A9	602	HEA	C3A-C2A	-2.66	1.31	1.36
71	J	101	CDL	OA6-CA4	-2.65	1.40	1.46
78	z	301	HEC	C3C-C2C	-2.65	1.31	1.38
70	2	401	3PE	O21-C2	-2.63	1.40	1.46
77	y	401	HEM	C3B-C2B	-2.62	1.32	1.37
78	o	301	HEC	C3C-C2C	-2.62	1.31	1.38
79	A9	602	HEA	C1D-C2D	2.62	1.49	1.44
79	A9	602	HEA	C1D-ND	-2.61	1.35	1.40
78	z	301	HEC	FE-NB	2.60	2.02	1.94
77	m	401	HEM	C3B-C2B	-2.60	1.32	1.37
78	o	301	HEC	FE-NB	2.59	2.02	1.94
76	R	601	NAP	C4N-C3N	-2.58	1.34	1.39
77	y	401	HEM	CHB-C4A	-2.58	1.33	1.39
70	B	501	3PE	O31-C3	-2.57	1.39	1.45
71	J	101	CDL	OA8-CA7	2.56	1.40	1.33
77	m	401	HEM	C3C-C4C	-2.55	1.41	1.46
78	z	301	HEC	C2A-C3A	-2.55	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	4	502	CDL	OB6-CB5	2.54	1.41	1.34
78	o	301	HEC	C2A-C3A	-2.54	1.31	1.36
77	m	401	HEM	CHB-C4A	-2.53	1.33	1.39
70	4	503	3PE	O31-C3	-2.53	1.39	1.45
77	y	401	HEM	C3C-C4C	-2.53	1.41	1.46
77	m	402	HEM	C3B-C2B	-2.52	1.32	1.37
72	L	200	PC1	O21-C2	-2.51	1.40	1.46
72	2	402	PC1	O21-C21	2.51	1.41	1.34
77	y	402	HEM	CAB-C3B	2.50	1.54	1.47
76	R	601	NAP	PA-O5B	2.49	1.69	1.59
77	y	402	HEM	CHB-C4A	-2.49	1.33	1.39
71	4	502	CDL	OA8-CA7	2.49	1.40	1.33
77	m	402	HEM	CHB-C4A	-2.49	1.33	1.39
77	y	402	HEM	C3B-C2B	-2.48	1.32	1.37
72	S	401	PC1	O21-C2	-2.48	1.40	1.46
72	4	504	PC1	O31-C3	-2.47	1.39	1.45
77	m	402	HEM	CAB-C3B	2.47	1.54	1.47
72	S	401	PC1	O31-C31	2.46	1.40	1.33
72	j	201	PC1	O31-C31	2.46	1.40	1.33
72	2	402	PC1	O31-C31	2.45	1.40	1.33
71	6	701	CDL	OA8-CA6	-2.44	1.39	1.45
71	6	701	CDL	OB6-CB5	2.43	1.41	1.34
77	m	402	HEM	C3D-C2D	-2.43	1.31	1.36
71	6	701	CDL	OB8-CB6	-2.42	1.39	1.45
77	y	402	HEM	C3D-C2D	-2.41	1.31	1.36
77	m	401	HEM	C1B-NB	-2.40	1.36	1.40
79	A9	601	HEA	C3A-C4A	-2.38	1.41	1.46
79	A9	602	HEA	CMD-C2D	2.36	1.55	1.50
77	y	401	HEM	C1B-NB	-2.32	1.36	1.40
71	J	101	CDL	OB8-CB7	2.32	1.40	1.33
77	m	401	HEM	CHA-C1A	-2.32	1.34	1.39
72	j	201	PC1	O21-C21	2.31	1.40	1.34
72	L	200	PC1	O31-C3	-2.30	1.39	1.45
70	2	401	3PE	O31-C31	2.30	1.40	1.33
77	y	401	HEM	CHA-C1A	-2.29	1.34	1.39
77	y	401	HEM	CHD-C4C	-2.28	1.34	1.38
72	j	201	PC1	O21-C2	-2.25	1.41	1.46
77	y	402	HEM	CHB-C1B	-2.24	1.34	1.38
77	m	401	HEM	CHD-C4C	-2.24	1.34	1.38
77	y	401	HEM	CHB-C1B	-2.23	1.34	1.38
77	m	402	HEM	C1B-NB	-2.22	1.36	1.40
77	m	402	HEM	CHC-C1C	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	y	402	HEM	C1B-NB	-2.21	1.36	1.40
77	m	401	HEM	CHD-C1D	-2.21	1.34	1.39
71	J	101	CDL	OB8-CB6	-2.20	1.40	1.45
77	y	401	HEM	CHD-C1D	-2.20	1.34	1.39
77	m	402	HEM	CHB-C1B	-2.19	1.34	1.38
70	4	503	3PE	O21-C21	2.19	1.40	1.34
71	6	701	CDL	OA8-CA7	2.18	1.39	1.33
77	y	402	HEM	CHC-C1C	-2.17	1.34	1.38
71	J	101	CDL	OB6-CB5	2.17	1.40	1.34
71	J	101	CDL	OA6-CA5	2.17	1.40	1.34
72	S	401	PC1	O31-C3	-2.16	1.40	1.45
77	m	401	HEM	CHB-C1B	-2.15	1.34	1.38
73	8	501	FMN	C4A-C10	-2.15	1.37	1.44
77	m	402	HEM	C4D-ND	-2.14	1.36	1.40
72	j	201	PC1	O31-C3	-2.14	1.40	1.45
77	m	402	HEM	CHC-C4B	-2.14	1.34	1.39
77	m	401	HEM	CAB-C3B	2.14	1.53	1.47
78	o	301	HEC	C3B-C2B	-2.13	1.32	1.36
72	S	401	PC1	O21-C21	2.12	1.40	1.34
77	y	401	HEM	CAB-C3B	2.12	1.53	1.47
72	4	504	PC1	O31-C31	2.12	1.39	1.33
76	R	601	NAP	P2B-O2B	2.11	1.63	1.59
70	2	401	3PE	O31-C3	-2.11	1.40	1.45
72	L	200	PC1	O21-C21	2.10	1.40	1.34
77	y	402	HEM	CHC-C4B	-2.10	1.34	1.39
71	4	502	CDL	OA8-CA6	-2.09	1.40	1.45
71	4	502	CDL	OA6-CA5	2.09	1.40	1.34
78	z	301	HEC	C3B-C2B	-2.08	1.32	1.36
72	j	201	PC1	C12-N	-2.07	1.44	1.51
79	A9	602	HEA	FE-NC	2.06	2.02	1.95
77	m	401	HEM	CAC-C3C	2.06	1.53	1.47
77	y	402	HEM	C4D-ND	-2.05	1.36	1.40
72	j	201	PC1	C13-N	-2.04	1.44	1.50
71	6	701	CDL	OB6-CB4	-2.03	1.41	1.46
71	6	701	CDL	OA6-CA5	2.02	1.40	1.34
70	4	503	3PE	O21-C2	-2.02	1.41	1.46
77	y	402	HEM	CAC-C3C	2.02	1.52	1.47
77	m	402	HEM	CAC-C3C	2.02	1.52	1.47
77	y	401	HEM	C4C-NC	-2.02	1.35	1.39
77	y	401	HEM	C4D-ND	-2.02	1.36	1.40
77	m	401	HEM	C4C-NC	-2.01	1.35	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	R	601	NAP	N3A-C2A-N1A	-6.38	118.62	128.60
76	R	601	NAP	N6A-C6A-N1A	-5.56	106.17	118.35
70	B	501	3PE	O21-C21-C22	5.41	123.16	111.50
70	4	503	3PE	O21-C21-C22	5.12	122.53	111.50
76	R	601	NAP	C5A-C4A-N3A	-5.00	120.22	126.75
76	R	601	NAP	N9A-C8A-N7A	-4.95	107.14	113.91
71	6	701	CDL	OB6-CB5-C51	4.63	121.49	111.50
71	J	101	CDL	OA6-CA5-C11	4.43	121.04	111.50
78	o	301	HEC	C1D-ND-C4D	4.29	109.51	105.07
78	z	301	HEC	C1D-ND-C4D	4.26	109.47	105.07
71	4	502	CDL	OA6-CA5-C11	4.15	120.44	111.50
72	S	401	PC1	O21-C21-C22	4.13	120.39	111.50
71	6	701	CDL	OA6-CA5-C11	4.10	120.33	111.50
72	4	504	PC1	O21-C21-C22	4.06	120.25	111.50
70	4	501	3PE	O21-C21-C22	4.02	120.16	111.50
76	R	601	NAP	C2A-N3A-C4A	3.98	121.15	111.75
73	8	501	FMN	C4-N3-C2	-3.98	118.29	125.64
79	A9	601	HEA	C17-C18-C19	-3.97	118.09	127.66
76	R	601	NAP	C5A-C6A-N6A	3.92	131.96	123.43
77	m	401	HEM	CAD-CBD-CGD	-3.89	105.23	113.60
77	m	402	HEM	CAA-CBA-CGA	-3.86	105.30	113.60
77	y	401	HEM	CAD-CBD-CGD	-3.85	105.31	113.60
77	y	402	HEM	CAA-CBA-CGA	-3.85	105.32	113.60
71	4	502	CDL	OB6-CB5-C51	3.81	119.70	111.50
72	L	200	PC1	O21-C21-C22	3.75	119.59	111.50
70	2	401	3PE	O21-C21-C22	3.63	119.32	111.50
76	R	601	NAP	C2B-C1B-N9A	-3.53	107.58	113.53
72	2	402	PC1	O21-C21-C22	3.45	118.94	111.50
71	J	101	CDL	OB6-CB5-C51	3.44	118.92	111.50
72	j	201	PC1	O21-C21-C22	3.37	120.20	110.80
70	B	501	3PE	O31-C31-C32	3.28	122.21	111.91
79	A9	601	HEA	C13-C14-C15	-3.18	120.00	127.66
79	A9	602	HEA	CHA-C1A-NA	-3.18	121.00	124.44
76	R	601	NAP	C5A-N7A-C8A	3.12	107.94	103.51
73	8	501	FMN	C4A-C10-N10	3.10	121.02	116.48
73	8	501	FMN	C4A-C10-N1	-3.09	117.55	124.73
73	8	501	FMN	C5A-C9A-N10	3.09	121.15	117.95
71	4	502	CDL	OB8-CB7-C71	3.05	121.49	111.91
78	o	301	HEC	C1A-CHA-C4D	-3.03	119.52	126.06
73	8	501	FMN	O4-C4-C4A	-3.03	118.56	126.60
77	m	401	HEM	CBD-CAD-C3D	-3.03	104.21	112.63
78	z	301	HEC	C1A-CHA-C4D	-3.02	119.55	126.06
77	y	401	HEM	CBD-CAD-C3D	-3.00	104.28	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	R	601	NAP	PN-O3-PA	-2.90	122.87	132.83
72	4	504	PC1	O31-C31-C32	2.88	120.94	111.91
76	R	601	NAP	C4A-N9A-C1B	-2.88	119.74	126.59
71	4	502	CDL	OA8-CA7-C31	2.88	120.93	111.91
71	J	101	CDL	OA8-CA7-C31	2.87	120.92	111.91
73	8	501	FMN	C4A-C4-N3	2.84	120.41	113.19
79	A9	601	HEA	C1B-C2B-C3B	2.81	110.16	106.80
71	6	701	CDL	OA8-CA7-C31	2.81	120.72	111.91
78	o	301	HEC	CAD-CBD-CGD	-2.80	107.57	113.60
78	z	301	HEC	CAD-CBD-CGD	-2.80	107.57	113.60
79	A9	602	HEA	C4A-C3A-C2A	2.80	109.05	106.75
72	j	201	PC1	O31-C31-C32	2.78	120.65	111.91
77	y	401	HEM	CBA-CAA-C2A	-2.74	105.01	112.63
77	m	401	HEM	CBA-CAA-C2A	-2.73	105.04	112.63
72	S	401	PC1	O31-C31-C32	2.72	120.44	111.91
71	J	101	CDL	OB8-CB7-C71	2.71	120.41	111.91
71	6	701	CDL	OB8-CB7-C71	2.70	120.39	111.91
73	8	501	FMN	C4-C4A-C10	2.67	121.28	116.79
76	R	601	NAP	N3A-C4A-N9A	2.64	131.43	127.08
70	4	501	3PE	O31-C31-C32	2.63	120.17	111.91
70	2	401	3PE	O31-C31-C32	2.61	120.10	111.91
72	2	402	PC1	O31-C31-C32	2.61	120.09	111.91
79	A9	601	HEA	C3C-C4C-NC	2.60	111.85	110.25
79	A9	602	HEA	CMD-C2D-C1D	2.57	128.95	125.04
77	y	402	HEM	CBA-CAA-C2A	-2.52	105.63	112.63
77	m	402	HEM	C4A-CHB-C1B	-2.51	120.38	126.34
77	m	402	HEM	CBA-CAA-C2A	-2.50	105.67	112.63
76	R	601	NAP	C4A-N9A-C8A	2.50	108.44	105.73
77	y	402	HEM	C4A-CHB-C1B	-2.48	120.46	126.34
70	4	501	3PE	C2-O21-C21	-2.45	111.76	117.79
79	A9	602	HEA	C1D-C2D-C3D	-2.42	104.41	106.96
70	4	503	3PE	C23-C22-C21	-2.41	104.84	113.62
79	A9	601	HEA	C17-C16-C15	-2.41	105.06	112.98
79	A9	602	HEA	CAA-C2A-C1A	2.39	129.41	124.89
77	m	401	HEM	C4A-CHB-C1B	-2.39	120.68	126.34
79	A9	601	HEA	C20-C19-C18	2.35	125.88	121.12
79	A9	602	HEA	CMB-C2B-C3B	-2.35	125.86	130.34
79	A9	601	HEA	C16-C17-C18	-2.34	104.19	111.88
77	y	401	HEM	C4A-CHB-C1B	-2.34	120.79	126.34
76	R	601	NAP	C2N-C3N-C4N	2.34	120.91	118.26
73	8	501	FMN	O2'-C2'-C3'	-2.32	103.45	109.10
73	8	501	FMN	C10-N1-C2	2.32	121.55	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	A9	602	HEA	C13-C14-C15	-2.32	122.08	127.66
79	A9	601	HEA	CAD-C3D-C4D	2.31	128.69	124.66
79	A9	602	HEA	C25-C23-C24	2.29	119.67	114.60
77	y	401	HEM	CHD-C4C-NC	2.27	126.90	124.44
77	y	401	HEM	C4C-CHD-C1D	-2.26	121.18	126.06
70	B	501	3PE	O31-C31-O32	-2.26	117.89	123.59
70	B	501	3PE	C23-C22-C21	-2.26	105.42	113.62
73	8	501	FMN	C4'-C3'-C2'	-2.25	108.68	113.36
77	m	401	HEM	C4C-CHD-C1D	-2.24	121.22	126.06
71	J	101	CDL	CA4-OA6-CA5	-2.24	112.27	117.79
77	m	401	HEM	CHD-C4C-NC	2.24	126.86	124.44
77	m	402	HEM	C4C-CHD-C1D	-2.22	121.27	126.06
73	8	501	FMN	C9A-N10-C10	-2.22	117.31	120.77
76	R	601	NAP	C5A-C4A-N9A	2.20	108.34	105.78
79	A9	602	HEA	C26-C15-C16	2.20	118.97	115.27
77	y	402	HEM	C4C-CHD-C1D	-2.19	121.33	126.06
79	A9	601	HEA	C12-C13-C14	-2.18	106.49	112.23
79	A9	601	HEA	C4B-C3B-C2B	-2.16	103.73	107.41
78	o	301	HEC	C1C-CHC-C4B	-2.14	121.26	126.34
76	R	601	NAP	O4B-C1B-N9A	2.12	112.25	108.06
78	z	301	HEC	C1C-CHC-C4B	-2.12	121.30	126.34
73	8	501	FMN	C6-C5A-C9A	2.10	121.90	118.94
79	A9	602	HEA	C3A-C2A-C1A	-2.09	105.08	107.08
76	R	601	NAP	C5A-C6A-N1A	2.09	121.87	117.39
76	R	601	NAP	O3B-C3B-C2B	-2.08	105.27	111.17
76	R	601	NAP	C1B-N9A-C8A	2.08	131.82	127.14
79	A9	601	HEA	C27-C19-C18	-2.07	118.36	123.68
79	A9	602	HEA	CBD-CAD-C3D	2.06	118.34	112.63
72	L	200	PC1	O31-C31-C32	2.04	118.30	111.91
76	R	601	NAP	C4A-C5A-N7A	-2.03	108.14	110.62
78	o	301	HEC	CAA-CBA-CGA	-2.02	109.26	113.60
78	z	301	HEC	CAA-CBA-CGA	-2.00	109.30	113.60

All (2) chirality outliers are listed below:

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

All (394) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	4	501	3PE	C11-O13-P-O11
70	4	501	3PE	C11-O13-P-O12
70	4	501	3PE	C11-O13-P-O14
70	4	501	3PE	O13-C11-C12-N
70	4	501	3PE	C22-C21-O21-C2
70	4	503	3PE	C11-O13-P-O14
70	4	503	3PE	C22-C21-O21-C2
70	2	401	3PE	C11-O13-P-O12
70	2	401	3PE	C11-O13-P-O14
70	2	401	3PE	O13-C11-C12-N
70	B	501	3PE	C1-O11-P-O14
70	B	501	3PE	O22-C21-O21-C2
70	B	501	3PE	C22-C21-O21-C2
71	4	502	CDL	CA2-OA2-PA1-OA3
71	6	701	CDL	CA3-OA5-PA1-OA4
71	6	701	CDL	CB2-OB2-PB2-OB3
71	6	701	CDL	CB2-OB2-PB2-OB4
71	6	701	CDL	CB3-OB5-PB2-OB3
71	J	101	CDL	CA2-OA2-PA1-OA3
71	J	101	CDL	CA2-OA2-PA1-OA5
71	J	101	CDL	C11-CA5-OA6-CA4
71	J	101	CDL	CB2-OB2-PB2-OB3
71	J	101	CDL	CB2-OB2-PB2-OB4
71	J	101	CDL	OB5-CB3-CB4-OB6
72	4	504	PC1	C11-O13-P-O12
72	4	504	PC1	C1-O11-P-O12
72	4	504	PC1	C1-O11-P-O13
72	4	504	PC1	O13-C11-C12-N
72	4	504	PC1	C22-C21-O21-C2
72	2	402	PC1	C1-O11-P-O12
72	2	402	PC1	C1-O11-P-O14
72	L	200	PC1	C22-C21-O21-C2
72	S	401	PC1	C11-O13-P-O12
72	S	401	PC1	C11-O13-P-O14
72	S	401	PC1	O13-C11-C12-N
72	j	201	PC1	C11-O13-P-O12
72	j	201	PC1	C1-O11-P-O13
72	j	201	PC1	O13-C11-C12-N
72	j	201	PC1	O22-C21-O21-C2
72	j	201	PC1	C22-C21-O21-C2
73	8	501	FMN	N10-C1'-C2'-C3'
73	8	501	FMN	O4'-C4'-C5'-O5'
73	8	501	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
73	8	501	FMN	C5'-O5'-P-O2P
73	8	501	FMN	C5'-O5'-P-O3P
76	R	601	NAP	C5B-O5B-PA-O2A
76	R	601	NAP	C5B-O5B-PA-O3
76	R	601	NAP	C1B-C2B-O2B-P2B
76	R	601	NAP	C5D-O5D-PN-O3
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	2	401	3PE	O32-C31-O31-C3
71	4	502	CDL	OA9-CA7-OA8-CA6
71	6	701	CDL	OA9-CA7-OA8-CA6
70	2	401	3PE	C32-C31-O31-C3
71	6	701	CDL	C31-CA7-OA8-CA6
71	4	502	CDL	OB9-CB7-OB8-CB6
70	4	501	3PE	O22-C21-O21-C2
71	J	101	CDL	OA7-CA5-OA6-CA4
72	4	504	PC1	O22-C21-O21-C2
72	2	402	PC1	O22-C21-O21-C2
72	L	200	PC1	O22-C21-O21-C2
71	4	502	CDL	C31-CA7-OA8-CA6
71	J	101	CDL	OA9-CA7-OA8-CA6
71	4	502	CDL	C71-CB7-OB8-CB6
71	J	101	CDL	C71-CB7-OB8-CB6
70	4	503	3PE	O22-C21-O21-C2
71	J	101	CDL	OB9-CB7-OB8-CB6
70	4	501	3PE	C32-C31-O31-C3
72	2	402	PC1	C22-C21-O21-C2
76	R	601	NAP	O4D-C4D-C5D-O5D
71	J	101	CDL	C31-CA7-OA8-CA6
70	4	503	3PE	C2-C1-O11-P
72	2	402	PC1	C36-C37-C38-C39
72	2	402	PC1	C26-C27-C28-C29
79	A9	601	HEA	C15-C16-C17-C18
72	S	401	PC1	C23-C24-C25-C26
70	4	501	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
70	4	501	3PE	O32-C31-O31-C3
72	2	402	PC1	C32-C33-C34-C35
72	4	504	PC1	C32-C31-O31-C3
72	L	200	PC1	C32-C31-O31-C3
72	j	201	PC1	C32-C31-O31-C3
72	L	200	PC1	C34-C35-C36-C37
71	4	502	CDL	C12-C13-C14-C15
72	S	401	PC1	C3B-C3C-C3D-C3E
72	2	402	PC1	C21-C22-C23-C24
72	j	201	PC1	O32-C31-O31-C3
72	L	200	PC1	C21-C22-C23-C24
70	4	503	3PE	C2B-C2C-C2D-C2E
70	4	503	3PE	C31-C32-C33-C34
70	2	401	3PE	C31-C32-C33-C34
72	4	504	PC1	C21-C22-C23-C24
77	m	401	HEM	C3D-CAD-CBD-CGD
77	y	401	HEM	C3D-CAD-CBD-CGD
70	4	501	3PE	C33-C34-C35-C36
72	4	504	PC1	O32-C31-O31-C3
71	6	701	CDL	C32-C33-C34-C35
71	J	101	CDL	CA7-C31-C32-C33
72	4	504	PC1	C24-C25-C26-C27
72	L	200	PC1	O32-C31-O31-C3
70	4	503	3PE	C1-O11-P-O13
70	2	401	3PE	C11-O13-P-O11
70	B	501	3PE	C1-O11-P-O13
71	4	502	CDL	CB2-OB2-PB2-OB5
71	6	701	CDL	CB2-OB2-PB2-OB5
71	6	701	CDL	CB3-OB5-PB2-OB2
71	J	101	CDL	CB2-OB2-PB2-OB5
72	2	402	PC1	C1-O11-P-O13
72	S	401	PC1	C11-O13-P-O11
72	j	201	PC1	C11-O13-P-O11
70	4	503	3PE	C27-C28-C29-C2A
70	4	501	3PE	C21-C22-C23-C24
71	6	701	CDL	OB7-CB5-OB6-CB4
72	S	401	PC1	C34-C35-C36-C37
71	6	701	CDL	C51-CB5-OB6-CB4
72	S	401	PC1	C22-C21-O21-C2
70	4	501	3PE	C2C-C2D-C2E-C2F
70	4	503	3PE	C2E-C2F-C2G-C2H
70	B	501	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
71	4	502	CDL	C60-C61-C62-C63
72	4	504	PC1	C26-C27-C28-C29
72	L	200	PC1	C3C-C3D-C3E-C3F
70	4	501	3PE	C27-C28-C29-C2A
70	B	501	3PE	C2A-C2B-C2C-C2D
72	L	200	PC1	C3B-C3C-C3D-C3E
72	S	401	PC1	C24-C25-C26-C27
72	j	201	PC1	C3B-C3C-C3D-C3E
72	S	401	PC1	O22-C21-O21-C2
72	j	201	PC1	C35-C36-C37-C38
71	J	101	CDL	C14-C15-C16-C17
71	4	502	CDL	O1-C1-CA2-OA2
71	4	502	CDL	C13-C14-C15-C16
71	4	502	CDL	C11-C12-C13-C14
72	j	201	PC1	C3D-C3E-C3F-C3G
72	2	402	PC1	C2C-C2D-C2E-C2F
70	B	501	3PE	C35-C36-C37-C38
72	S	401	PC1	C37-C38-C39-C3A
70	B	501	3PE	C37-C38-C39-C3A
70	4	501	3PE	C32-C33-C34-C35
70	4	503	3PE	C23-C24-C25-C26
70	2	401	3PE	C35-C36-C37-C38
72	S	401	PC1	C32-C31-O31-C3
70	2	401	3PE	C22-C23-C24-C25
70	B	501	3PE	C39-C3A-C3B-C3C
71	J	101	CDL	C15-C16-C17-C18
72	2	402	PC1	C28-C29-C2A-C2B
72	j	201	PC1	C33-C34-C35-C36
70	4	503	3PE	C2A-C2B-C2C-C2D
70	4	503	3PE	C2C-C2D-C2E-C2F
70	4	503	3PE	C32-C31-O31-C3
72	S	401	PC1	C35-C36-C37-C38
71	4	502	CDL	C81-C82-C83-C84
72	L	200	PC1	C3A-C3B-C3C-C3D
72	j	201	PC1	C31-C32-C33-C34
70	2	401	3PE	C28-C29-C2A-C2B
70	B	501	3PE	C28-C29-C2A-C2B
71	4	502	CDL	CA5-C11-C12-C13
70	B	501	3PE	C2D-C2E-C2F-C2G
72	L	200	PC1	C32-C33-C34-C35
72	4	504	PC1	C33-C34-C35-C36
72	2	402	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
72	L	200	PC1	C22-C23-C24-C25
72	L	200	PC1	C11-C12-N-C13
71	6	701	CDL	C11-CA5-OA6-CA4
72	4	504	PC1	C27-C28-C29-C2A
72	2	402	PC1	C22-C23-C24-C25
70	4	501	3PE	C25-C26-C27-C28
70	4	503	3PE	O32-C31-O31-C3
72	S	401	PC1	O32-C31-O31-C3
70	4	503	3PE	C21-C22-C23-C24
71	6	701	CDL	C31-C32-C33-C34
71	J	101	CDL	CB5-C51-C52-C53
70	2	401	3PE	C22-C21-O21-C2
70	B	501	3PE	O11-C1-C2-O21
72	L	200	PC1	O11-C1-C2-O21
70	B	501	3PE	C23-C24-C25-C26
70	2	401	3PE	O22-C21-O21-C2
72	L	200	PC1	C11-C12-N-C14
72	L	200	PC1	C11-C12-N-C15
72	2	402	PC1	C25-C26-C27-C28
71	4	502	CDL	C31-C32-C33-C34
71	6	701	CDL	OA7-CA5-OA6-CA4
71	4	502	CDL	C51-CB5-OB6-CB4
70	2	401	3PE	C2D-C2E-C2F-C2G
71	4	502	CDL	CA2-OA2-PA1-OA5
71	6	701	CDL	CA3-OA5-PA1-OA2
72	4	504	PC1	C11-O13-P-O11
72	2	402	PC1	C11-O13-P-O11
71	4	502	CDL	C76-C77-C78-C79
70	4	501	3PE	C1-C2-C3-O31
71	6	701	CDL	C34-C35-C36-C37
72	4	504	PC1	C1-C2-C3-O31
70	2	401	3PE	C3A-C3B-C3C-C3D
70	B	501	3PE	C3B-C3C-C3D-C3E
72	4	504	PC1	C2A-C2B-C2C-C2D
70	4	503	3PE	C35-C36-C37-C38
70	2	401	3PE	C34-C35-C36-C37
70	4	503	3PE	C33-C34-C35-C36
72	2	402	PC1	C24-C25-C26-C27
70	4	501	3PE	C3-C2-O21-C21
70	2	401	3PE	C36-C37-C38-C39
76	R	601	NAP	C2B-C1B-N9A-C8A
71	J	101	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
71	4	502	CDL	OB6-CB4-CB6-OB8
71	4	502	CDL	C59-C60-C61-C62
71	4	502	CDL	OB7-CB5-OB6-CB4
71	6	701	CDL	C72-C73-C74-C75
70	4	501	3PE	C2F-C2G-C2H-C2I
70	4	501	3PE	O11-C1-C2-C3
70	B	501	3PE	O11-C1-C2-C3
71	J	101	CDL	OB5-CB3-CB4-CB6
72	L	200	PC1	O11-C1-C2-C3
70	B	501	3PE	C38-C39-C3A-C3B
71	4	502	CDL	C57-C58-C59-C60
73	8	501	FMN	C2'-C1'-N10-C10
70	B	501	3PE	C3C-C3D-C3E-C3F
72	L	200	PC1	C1-C2-C3-O31
71	6	701	CDL	CA5-C11-C12-C13
72	2	402	PC1	C39-C3A-C3B-C3C
72	S	401	PC1	C3C-C3D-C3E-C3F
72	L	200	PC1	O31-C31-C32-C33
71	J	101	CDL	OA5-CA3-CA4-OA6
71	4	502	CDL	OA6-CA4-CA6-OA8
72	L	200	PC1	O21-C2-C3-O31
72	S	401	PC1	O21-C2-C3-O31
71	6	701	CDL	C51-C52-C53-C54
71	4	502	CDL	OA7-CA5-OA6-CA4
72	2	402	PC1	C37-C38-C39-C3A
77	m	401	HEM	C2A-CAA-CBA-CGA
77	y	401	HEM	C2A-CAA-CBA-CGA
71	4	502	CDL	C11-CA5-OA6-CA4
76	R	601	NAP	PN-O3-PA-O5B
72	S	401	PC1	O11-C1-C2-C3
72	4	504	PC1	C2B-C2C-C2D-C2E
76	R	601	NAP	C3D-C4D-C5D-O5D
70	4	503	3PE	C24-C25-C26-C27
70	B	501	3PE	C3A-C3B-C3C-C3D
70	4	503	3PE	C1-C2-O21-C21
71	6	701	CDL	C71-C72-C73-C74
72	2	402	PC1	C32-C31-O31-C3
70	4	501	3PE	C26-C27-C28-C29
72	S	401	PC1	O11-C1-C2-O21
72	j	201	PC1	O11-C1-C2-O21
70	4	501	3PE	O21-C2-C3-O31
70	2	401	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
76	R	601	NAP	C2B-O2B-P2B-O3X
71	4	502	CDL	C34-C35-C36-C37
70	4	503	3PE	C11-O13-P-O11
70	2	401	3PE	C2E-C2F-C2G-C2H
71	6	701	CDL	C1-CA2-OA2-PA1
72	4	504	PC1	C2-C1-O11-P
70	4	503	3PE	C1-O11-P-O12
70	4	503	3PE	C1-O11-P-O14
70	B	501	3PE	C1-O11-P-O12
71	4	502	CDL	CA2-OA2-PA1-OA4
71	4	502	CDL	CB2-OB2-PB2-OB3
71	6	701	CDL	CA2-OA2-PA1-OA3
71	6	701	CDL	CA3-OA5-PA1-OA3
71	J	101	CDL	CA3-OA5-PA1-OA4
72	4	504	PC1	C11-O13-P-O14
72	4	504	PC1	C1-O11-P-O14
72	2	402	PC1	C11-O13-P-O12
72	j	201	PC1	C11-O13-P-O14
72	j	201	PC1	C1-O11-P-O12
76	R	601	NAP	C5B-O5B-PA-O1A
71	4	502	CDL	OB5-CB3-CB4-CB6
72	j	201	PC1	C12-C11-O13-P
73	8	501	FMN	C1'-C2'-C3'-O3'
72	2	402	PC1	C38-C39-C3A-C3B
72	L	200	PC1	C26-C27-C28-C29
70	4	501	3PE	O11-C1-C2-O21
70	B	501	3PE	C24-C25-C26-C27
71	4	502	CDL	CB3-CB4-CB6-OB8
72	2	402	PC1	O13-C11-C12-N
72	L	200	PC1	O13-C11-C12-N
72	S	401	PC1	C1-C2-C3-O31
72	4	504	PC1	O21-C2-C3-O31
72	S	401	PC1	C32-C33-C34-C35
70	2	401	3PE	O21-C21-C22-C23
70	B	501	3PE	C2C-C2D-C2E-C2F
72	2	402	PC1	O32-C31-O31-C3
71	4	502	CDL	C63-C64-C65-C66
70	B	501	3PE	C29-C2A-C2B-C2C
71	4	502	CDL	C77-C78-C79-C80
71	J	101	CDL	OA5-CA3-CA4-CA6
72	j	201	PC1	C38-C39-C3A-C3B
70	4	501	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
71	J	101	CDL	CB3-OB5-PB2-OB2
72	S	401	PC1	C1-O11-P-O13
72	j	201	PC1	C3F-C3G-C3H-C3I
71	6	701	CDL	CA4-CA3-OA5-PA1
72	2	402	PC1	C31-C32-C33-C34
70	B	501	3PE	C31-C32-C33-C34
76	R	601	NAP	C2B-C1B-N9A-C4A
71	4	502	CDL	CA2-C1-CB2-OB2
79	A9	601	HEA	CAD-CBD-CGD-O1D
71	4	502	CDL	CB3-CB4-OB6-CB5
71	6	701	CDL	CB3-CB4-OB6-CB5
72	2	402	PC1	C1-C2-O21-C21
72	4	504	PC1	C38-C39-C3A-C3B
71	4	502	CDL	C71-C72-C73-C74
73	8	501	FMN	C3'-C4'-C5'-O5'
70	B	501	3PE	C26-C27-C28-C29
72	j	201	PC1	O11-C1-C2-C3
79	A9	602	HEA	CAD-CBD-CGD-O1D
71	6	701	CDL	O1-C1-CB2-OB2
71	6	701	CDL	OA6-CA4-CA6-OA8
79	A9	602	HEA	CAD-CBD-CGD-O2D
71	4	502	CDL	CB2-C1-CA2-OA2
71	J	101	CDL	CA2-C1-CB2-OB2
79	A9	601	HEA	CAA-CBA-CGA-O1A
79	A9	601	HEA	CAD-CBD-CGD-O2D
70	4	503	3PE	C22-C23-C24-C25
78	o	301	HEC	CAD-CBD-CGD-O2D
78	z	301	HEC	CAD-CBD-CGD-O2D
70	2	401	3PE	C21-C22-C23-C24
72	S	401	PC1	C28-C29-C2A-C2B
72	2	402	PC1	C29-C2A-C2B-C2C
72	S	401	PC1	C21-C22-C23-C24
70	B	501	3PE	C32-C33-C34-C35
70	4	501	3PE	O31-C31-C32-C33
71	6	701	CDL	C72-C71-CB7-OB8
72	L	200	PC1	O32-C31-C32-C33
71	6	701	CDL	C15-C16-C17-C18
78	o	301	HEC	CAA-CBA-CGA-O1A
78	z	301	HEC	CAA-CBA-CGA-O1A
77	m	402	HEM	CAA-CBA-CGA-O1A
77	y	402	HEM	CAA-CBA-CGA-O1A
71	4	502	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
76	R	601	NAP	O4B-C1B-N9A-C8A
71	4	502	CDL	OB5-CB3-CB4-OB6
72	2	402	PC1	C2D-C2E-C2F-C2G
70	B	501	3PE	O31-C31-C32-C33
78	o	301	HEC	CAA-CBA-CGA-O2A
78	z	301	HEC	CAA-CBA-CGA-O2A
79	A9	602	HEA	CAA-CBA-CGA-O2A
71	6	701	CDL	CA7-C31-C32-C33
77	m	402	HEM	CAA-CBA-CGA-O2A
77	y	402	HEM	CAA-CBA-CGA-O2A
72	2	402	PC1	O31-C31-C32-C33
79	A9	602	HEA	CAA-CBA-CGA-O1A
70	4	501	3PE	C35-C36-C37-C38
70	4	501	3PE	C2-C1-O11-P
76	R	601	NAP	O4B-C4B-C5B-O5B
78	o	301	HEC	C3D-CAD-CBD-CGD
78	z	301	HEC	C3D-CAD-CBD-CGD
78	o	301	HEC	CAD-CBD-CGD-O1D
78	z	301	HEC	CAD-CBD-CGD-O1D
70	4	501	3PE	C23-C24-C25-C26
71	4	502	CDL	CA3-CA4-CA6-OA8
71	6	701	CDL	CA3-CA4-CA6-OA8
70	B	501	3PE	C25-C26-C27-C28
72	S	401	PC1	C27-C28-C29-C2A
70	4	501	3PE	O32-C31-C32-C33
71	4	502	CDL	C12-C11-CA5-OA7
78	o	301	HEC	C2D-C3D-CAD-CBD
78	z	301	HEC	C2D-C3D-CAD-CBD
71	J	101	CDL	C55-C56-C57-C58
71	6	701	CDL	C72-C71-CB7-OB9
79	A9	601	HEA	CAA-CBA-CGA-O2A
71	4	502	CDL	CB2-OB2-PB2-OB4
71	4	502	CDL	CB3-OB5-PB2-OB3
72	2	402	PC1	C11-O13-P-O14
70	B	501	3PE	O32-C31-C32-C33
72	2	402	PC1	O32-C31-C32-C33
72	S	401	PC1	O31-C31-C32-C33
72	L	200	PC1	C38-C39-C3A-C3B
70	4	501	3PE	C12-C11-O13-P
70	4	503	3PE	C12-C11-O13-P
72	S	401	PC1	C12-C11-O13-P
72	S	401	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
70	4	503	3PE	C26-C27-C28-C29
72	S	401	PC1	C33-C34-C35-C36
77	m	401	HEM	CAD-CBD-CGD-O1D
77	y	401	HEM	CAD-CBD-CGD-O1D
72	j	201	PC1	C36-C37-C38-C39
79	A9	602	HEA	C26-C15-C16-C17
73	8	501	FMN	N10-C1'-C2'-O2'
79	A9	601	HEA	O11-C11-C3B-C2B
71	6	701	CDL	C32-C31-CA7-OA8
72	4	504	PC1	O31-C31-C32-C33
71	6	701	CDL	C74-C75-C76-C77
77	m	401	HEM	CAD-CBD-CGD-O2D
77	y	401	HEM	CAD-CBD-CGD-O2D
72	S	401	PC1	O32-C31-C32-C33
72	S	401	PC1	C11-C12-N-C13

There are no ring outliers.

27 monomers are involved in 414 short contacts:

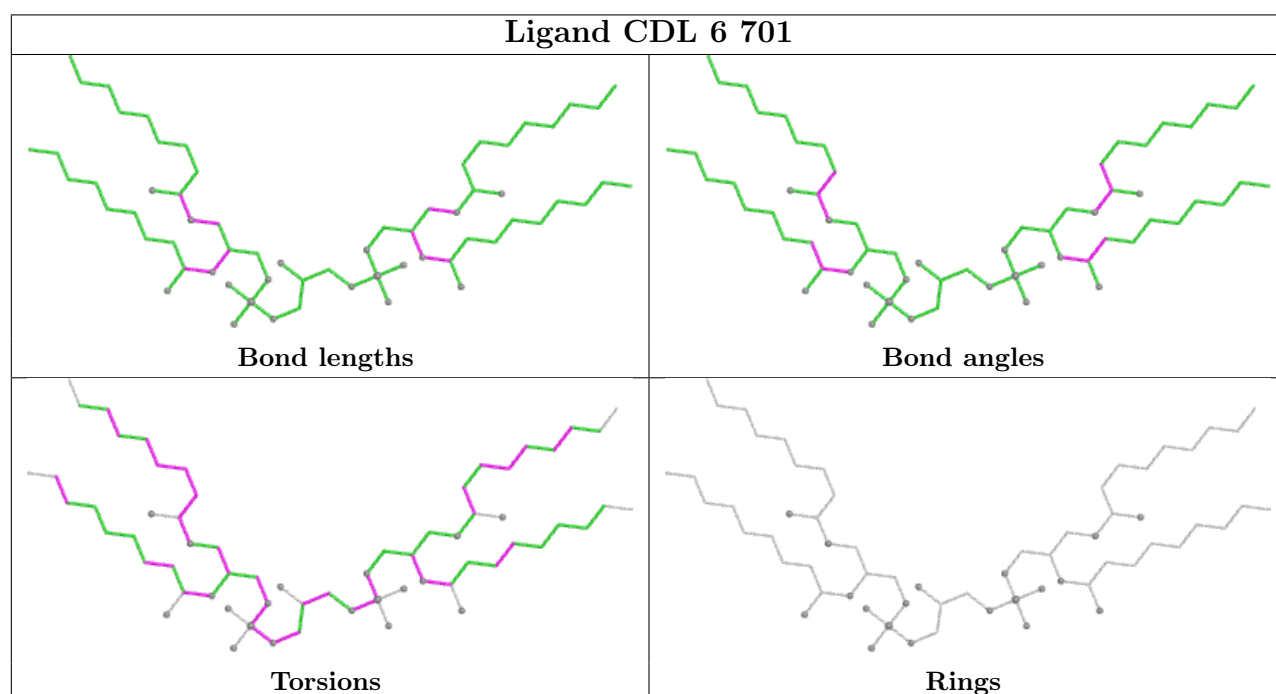
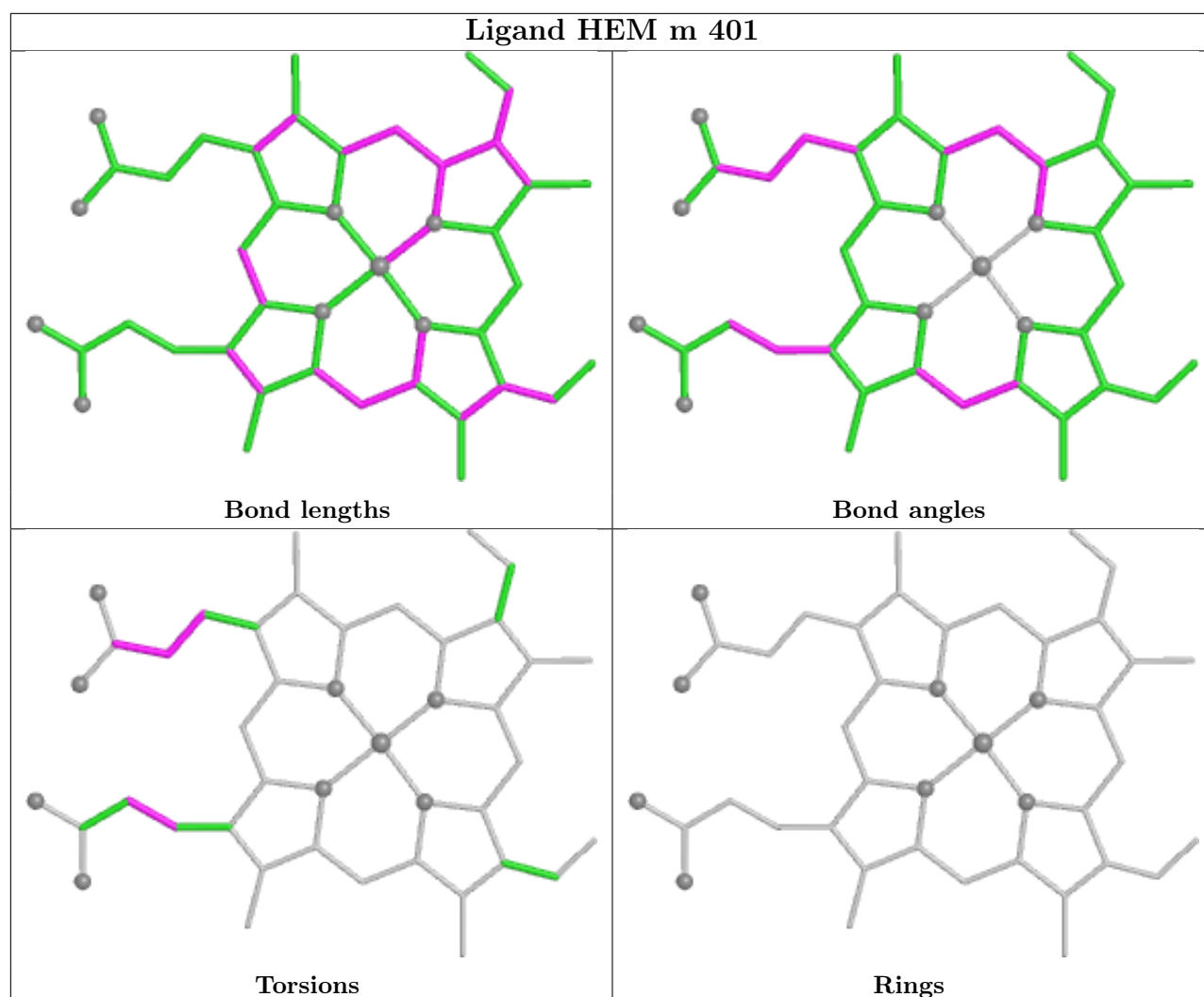
Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	m	401	HEM	4	0
71	6	701	CDL	66	0
72	4	504	PC1	13	0
70	B	501	3PE	27	0
76	R	601	NAP	10	0
78	z	301	HEC	1	0
74	A	801	SF4	6	0
70	4	503	3PE	25	0
78	o	301	HEC	1	0
79	A9	602	HEA	3	0
72	2	402	PC1	32	0
72	S	401	PC1	15	0
74	A	802	SF4	5	0
71	J	101	CDL	14	0
69	A	803	FES	2	0
77	y	401	HEM	4	0
72	j	201	PC1	1	0
74	8	502	SF4	3	0
70	4	501	3PE	27	0
77	y	402	HEM	6	0
72	L	200	PC1	34	0
74	E	302	SF4	1	0

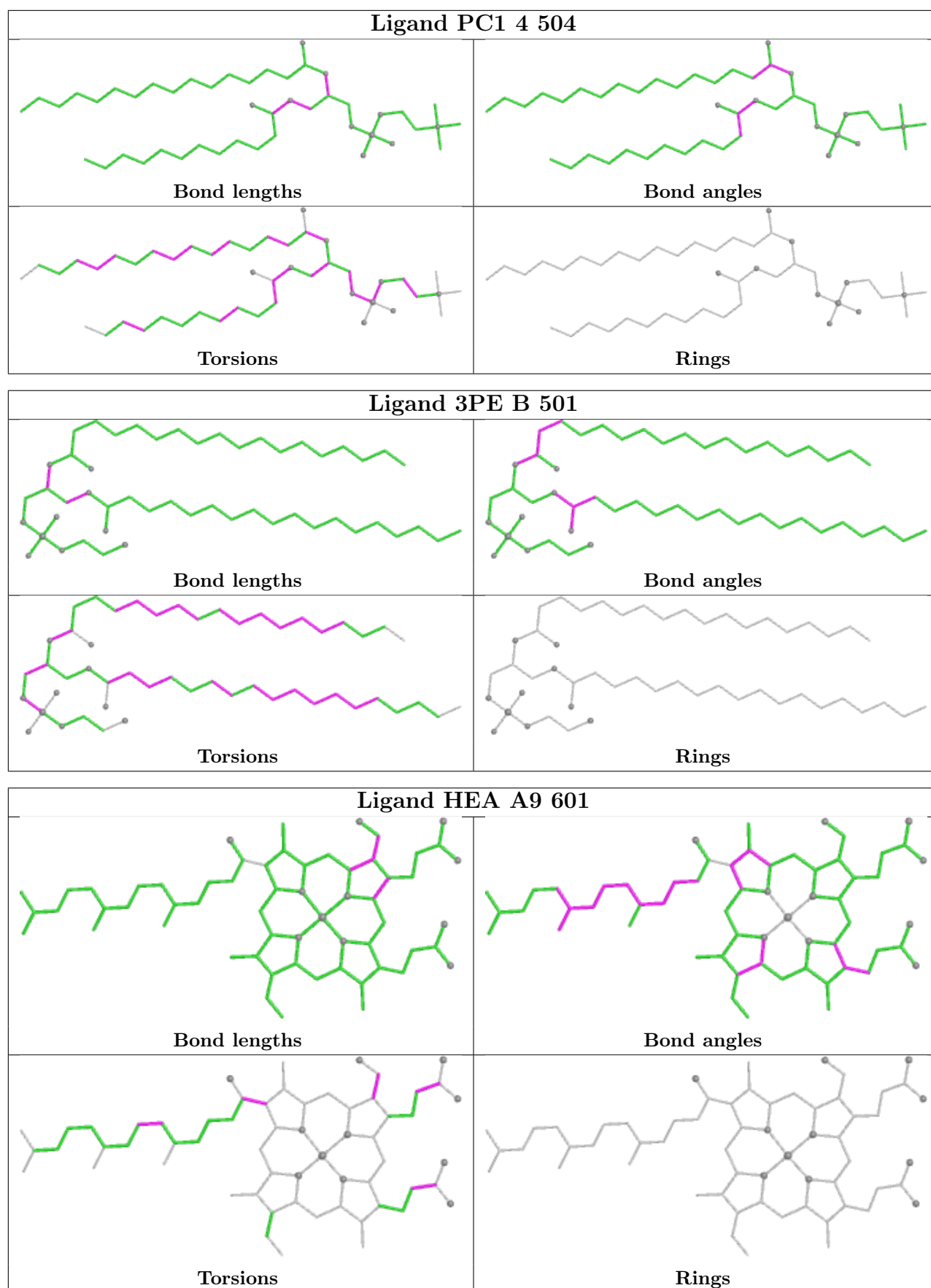
Continued on next page...

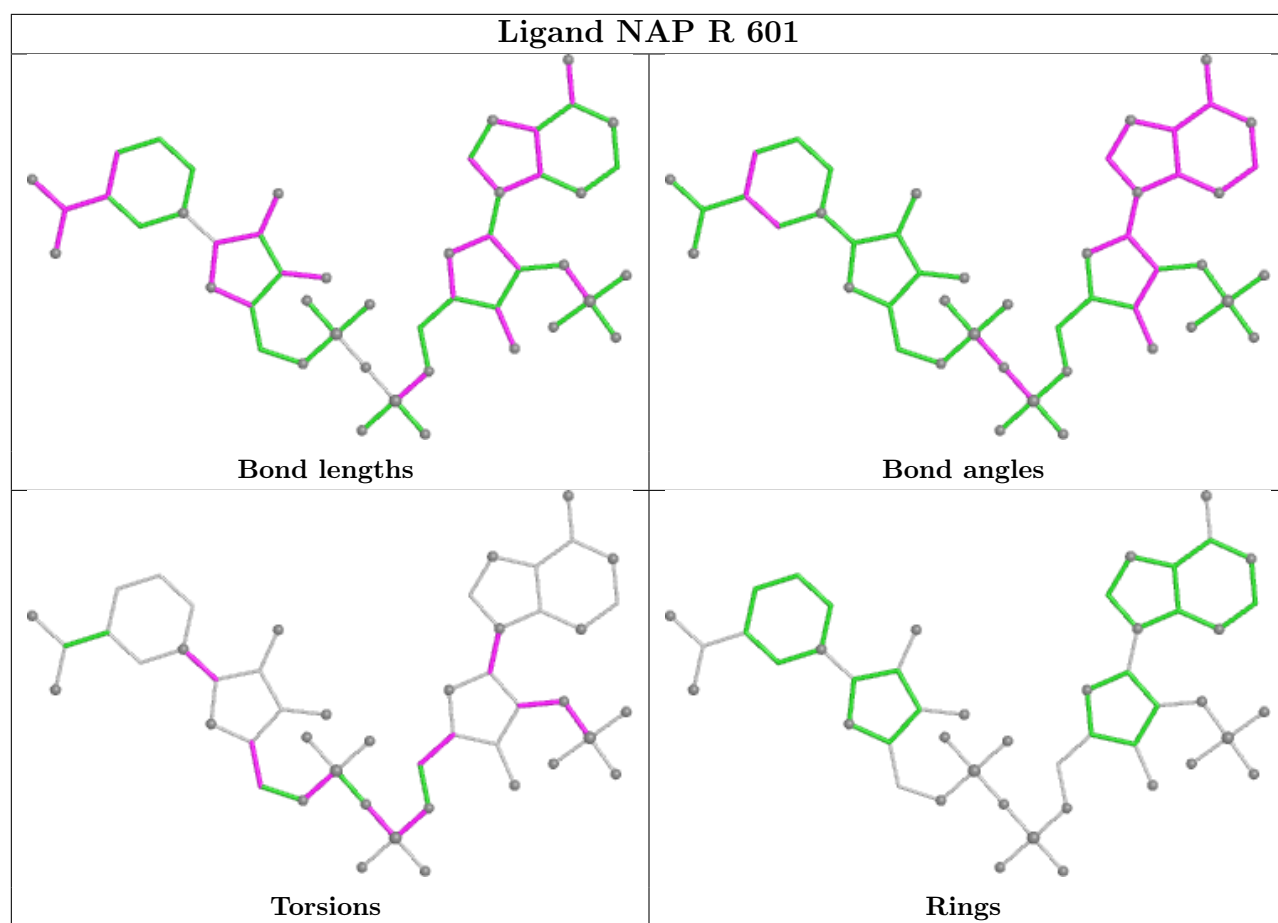
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	m	402	HEM	6	0
73	8	501	FMN	39	0
71	4	502	CDL	44	0
70	2	401	3PE	18	0
74	D	301	SF4	7	0

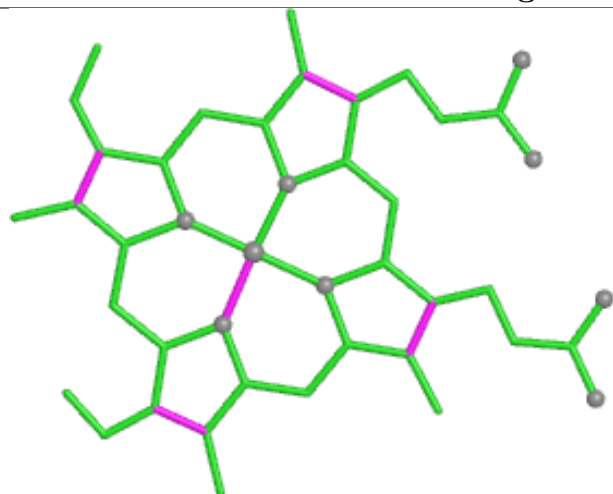
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



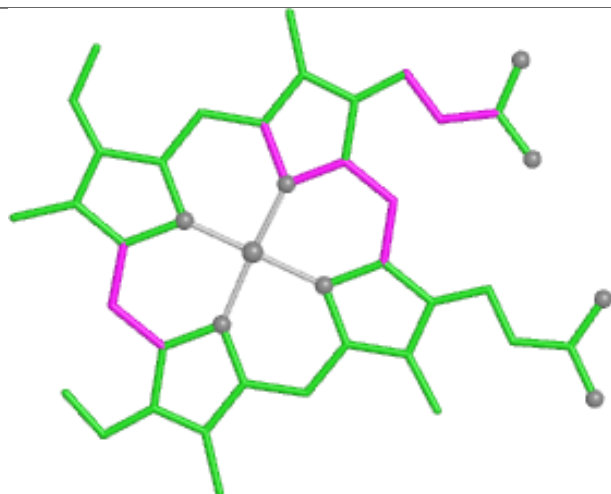




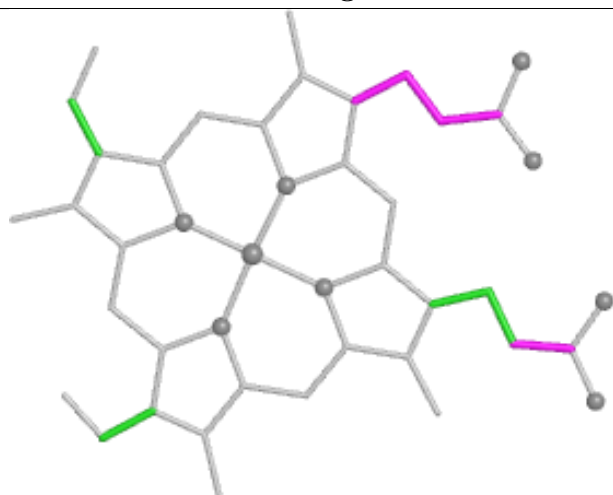
Ligand HEC z 301



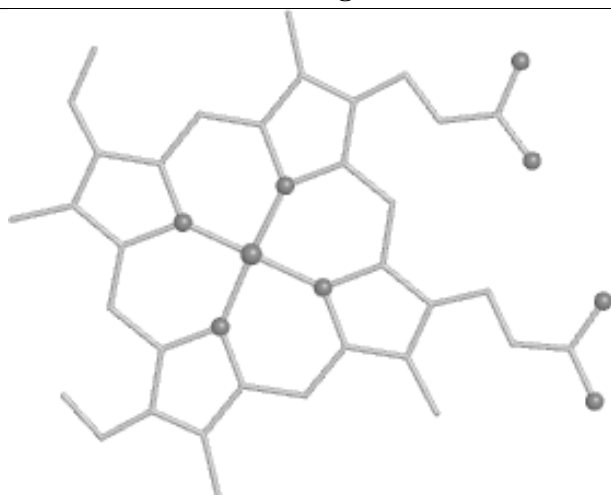
Bond lengths



Bond angles



Torsions



Rings

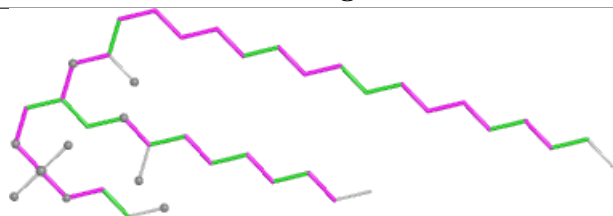
Ligand 3PE 4 503



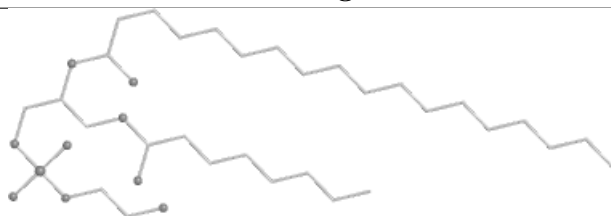
Bond lengths



Bond angles

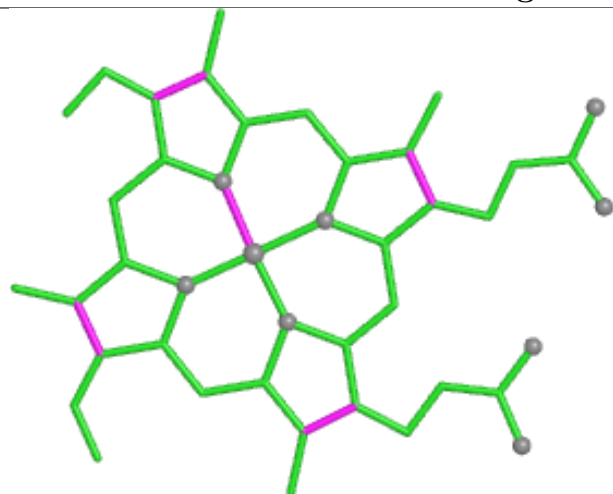


Torsions

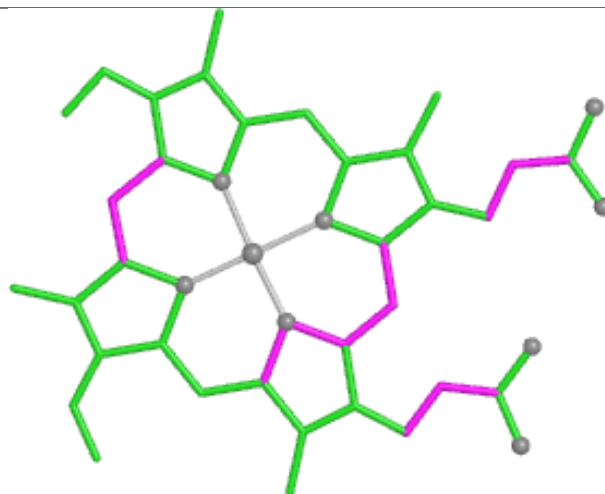


Rings

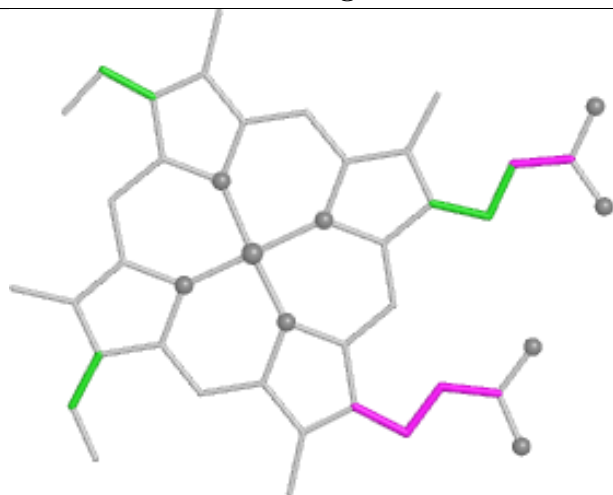
Ligand HEC o 301



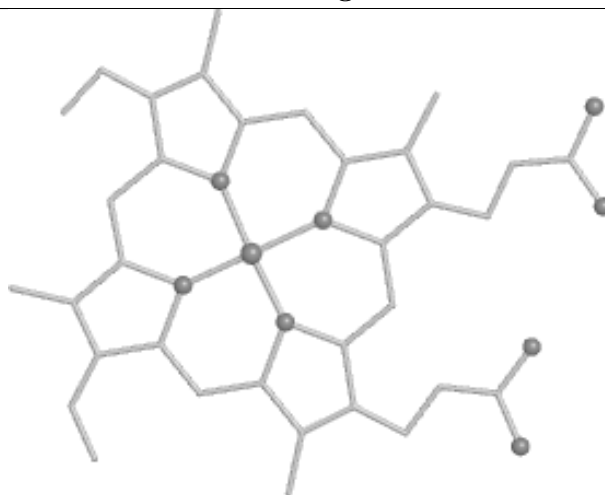
Bond lengths



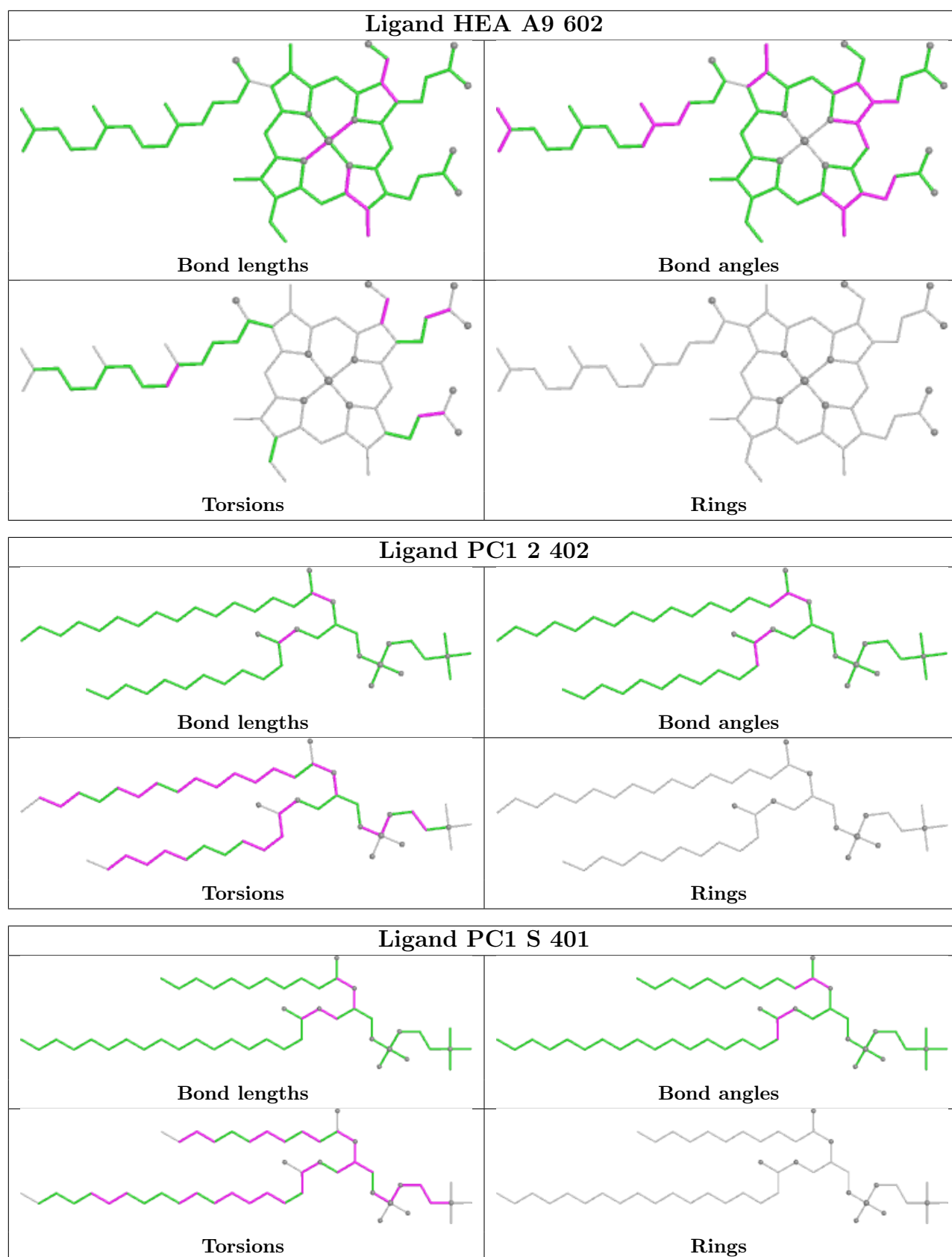
Bond angles

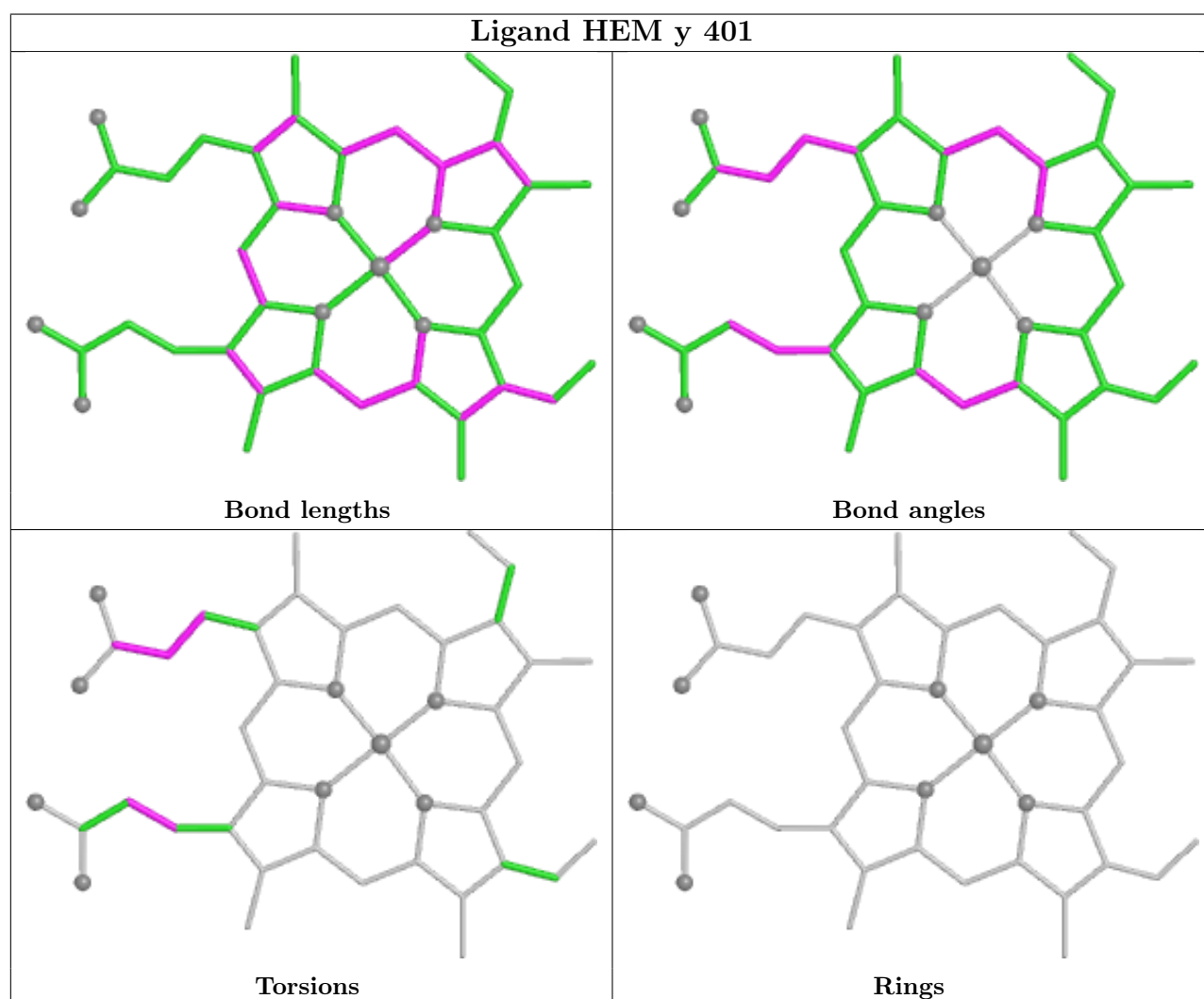
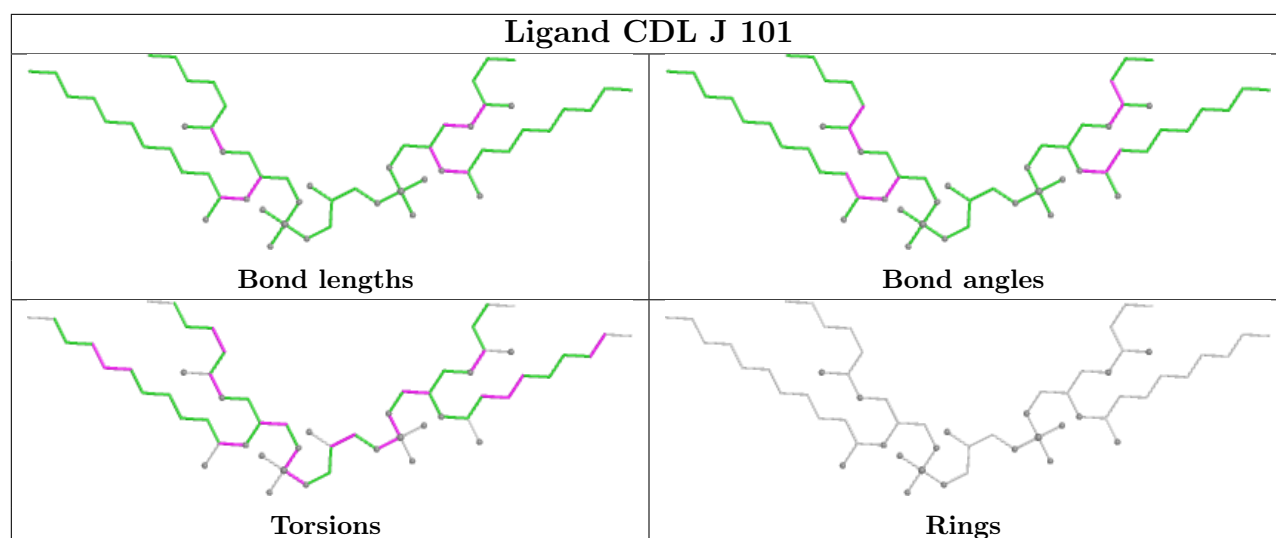


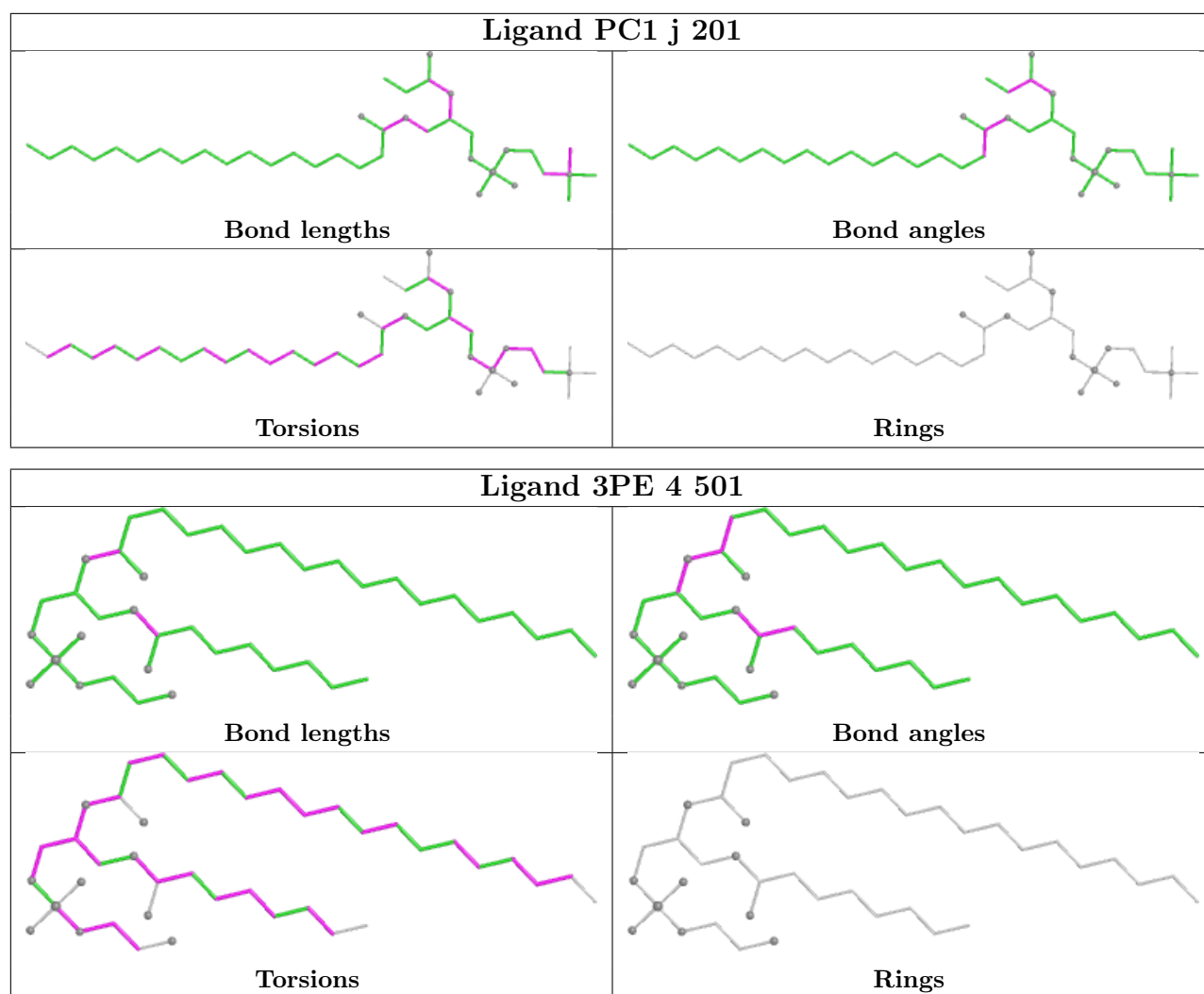
Torsions

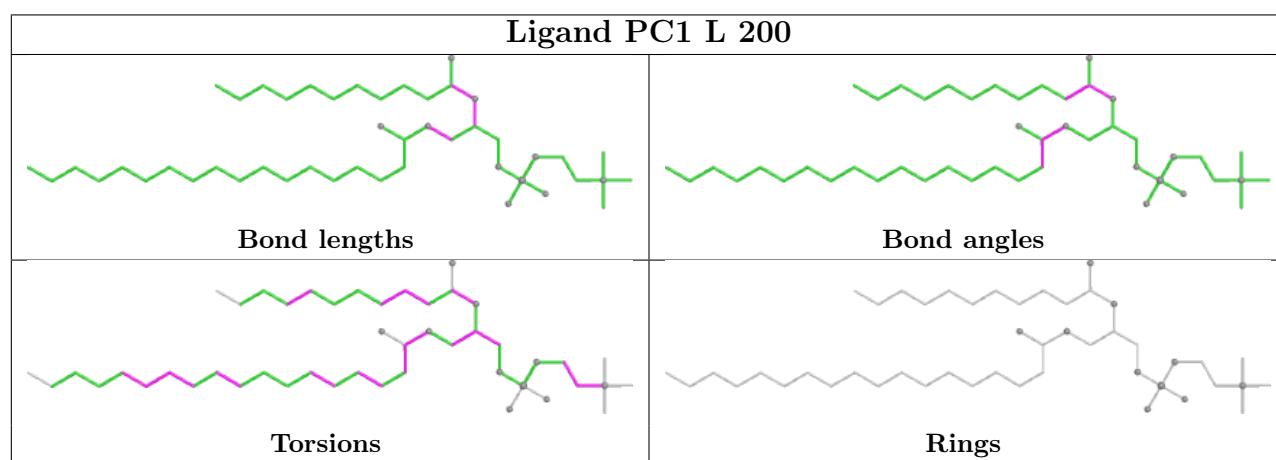
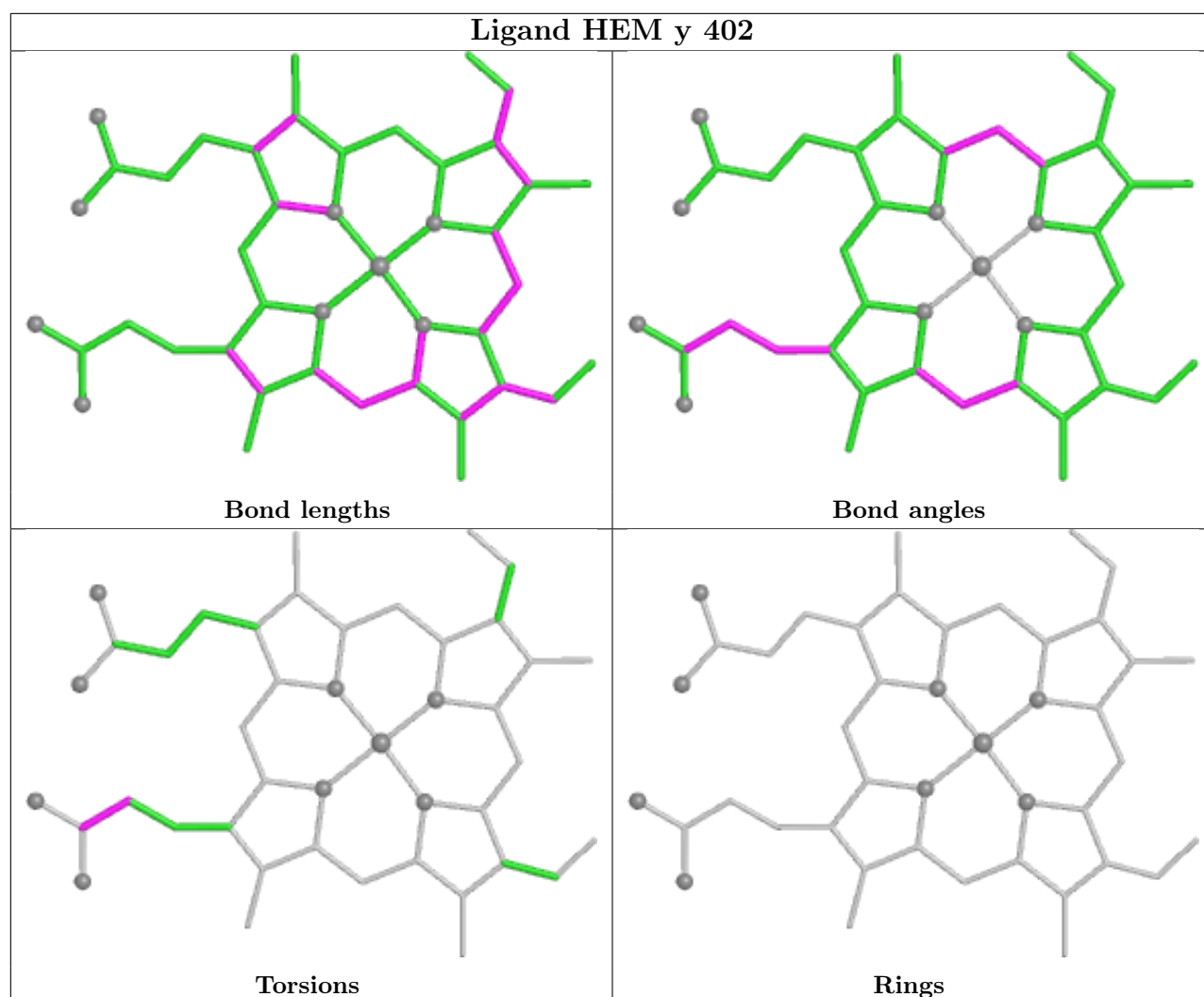


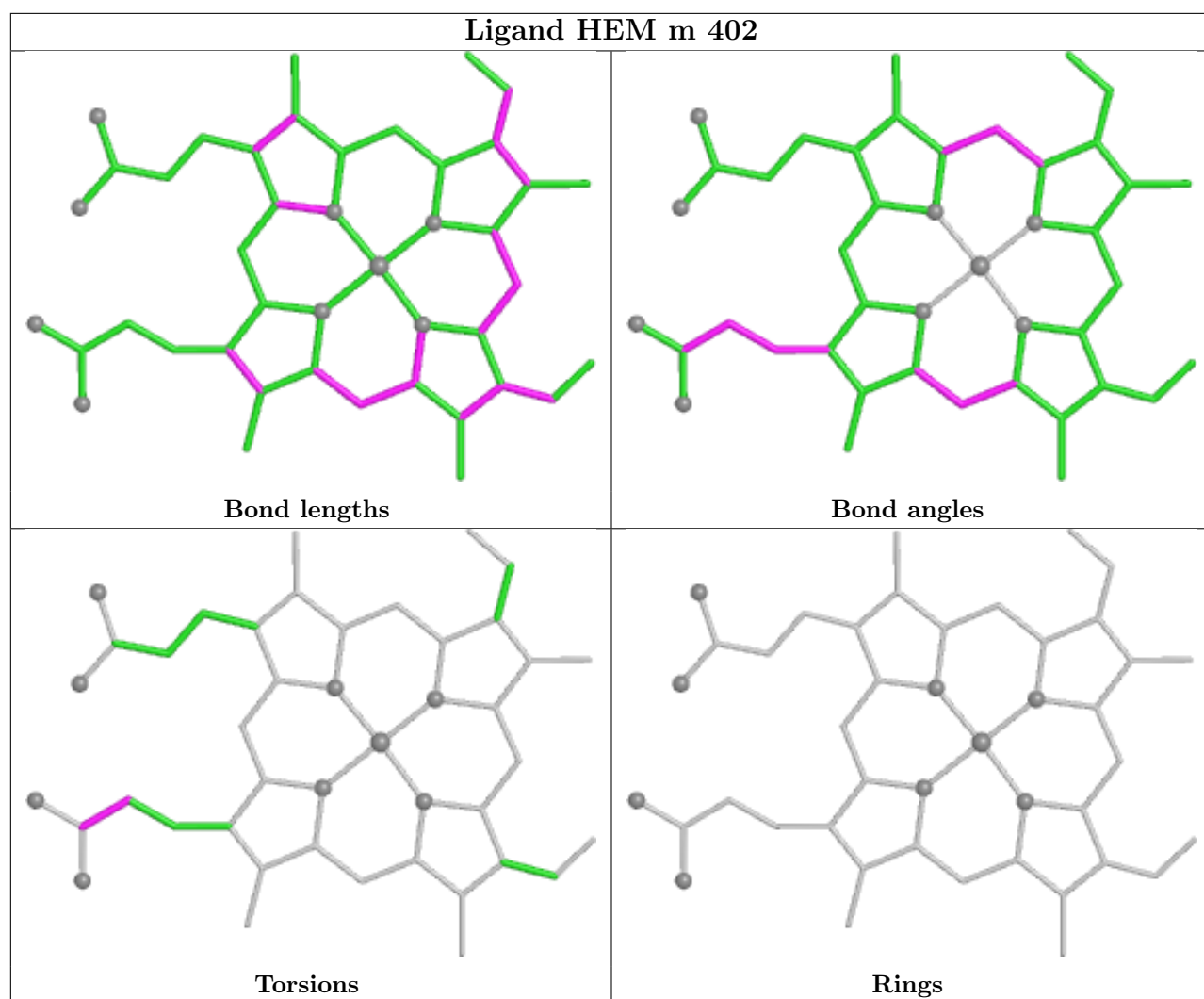
Rings

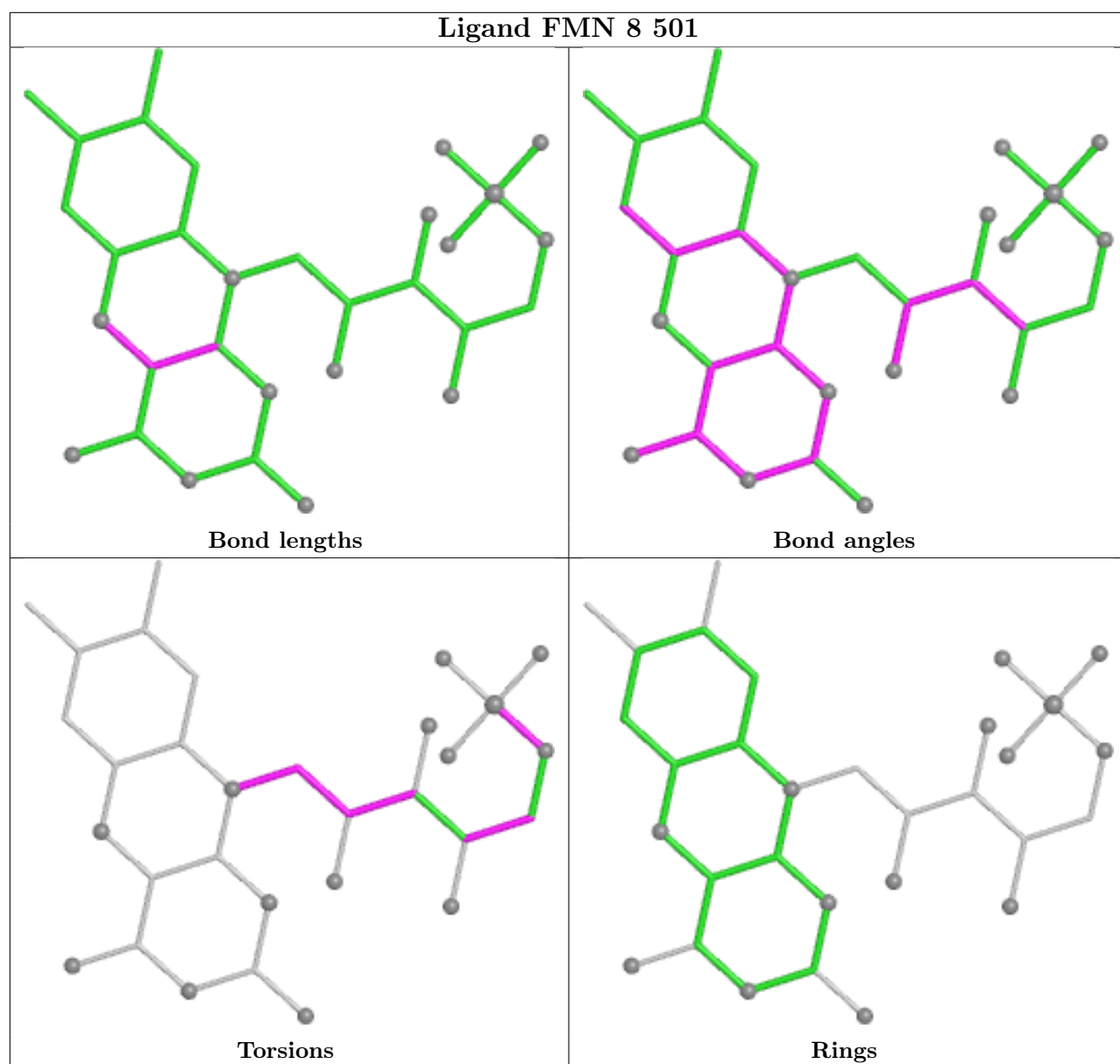


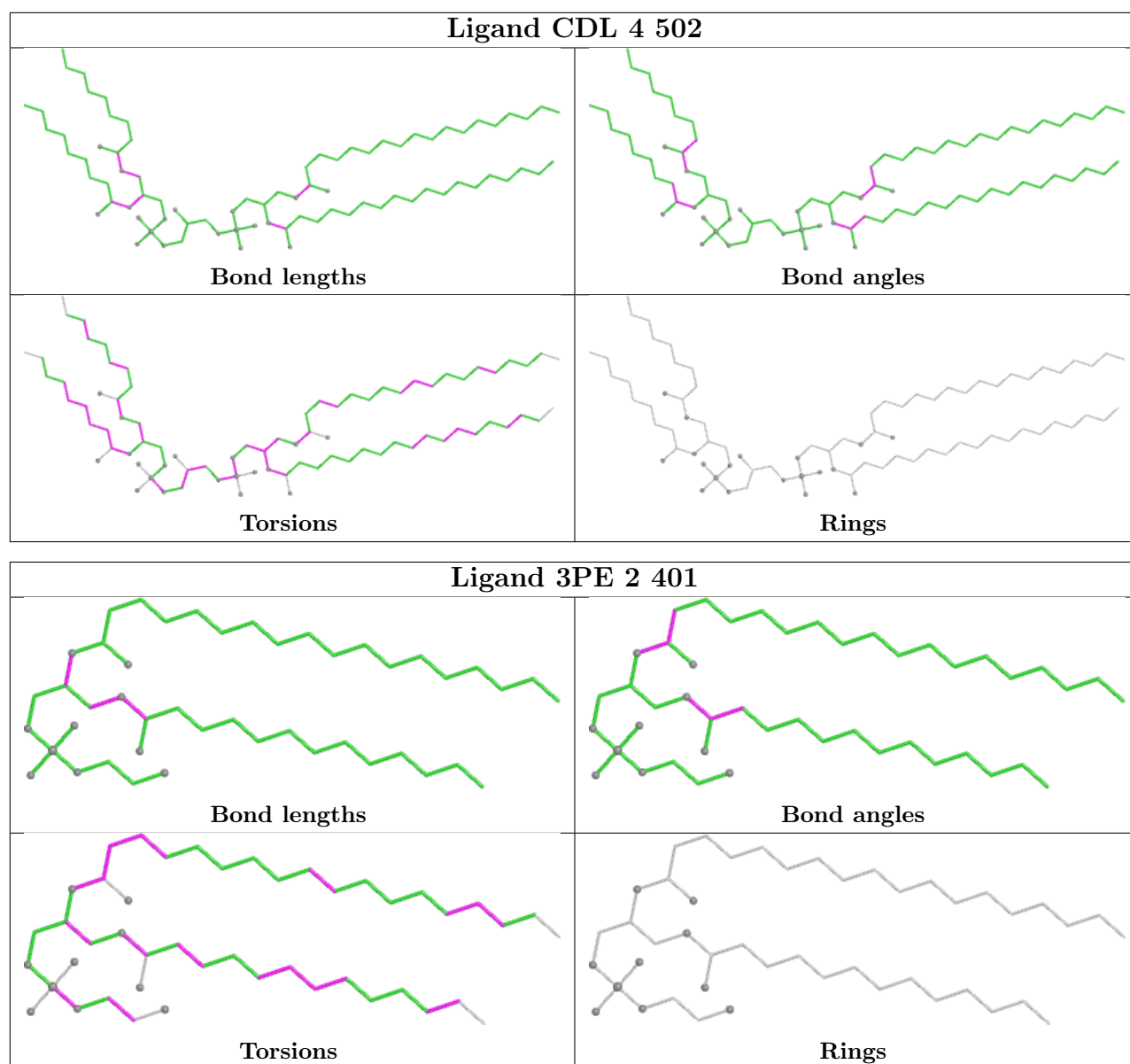












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

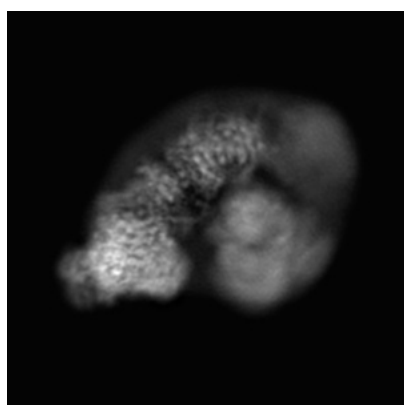
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30674. These allow visual inspection of the internal detail of the map and identification of artifacts.

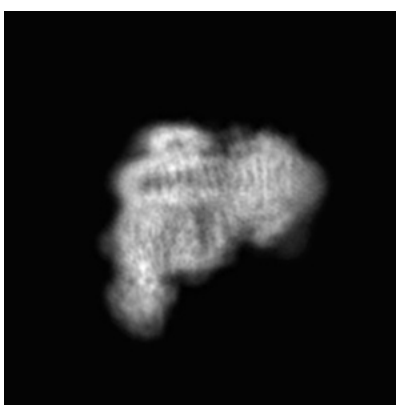
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

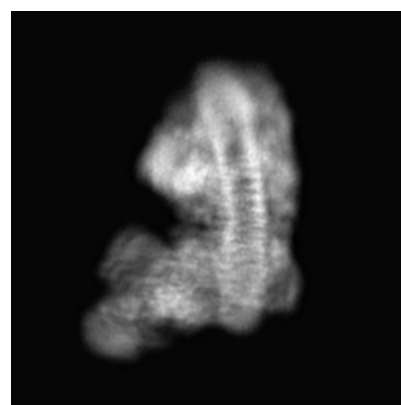
6.1.1 Primary map



X



Y

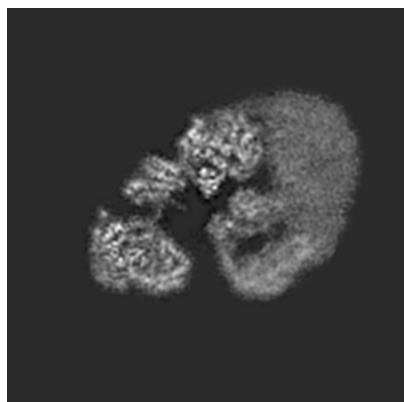


Z

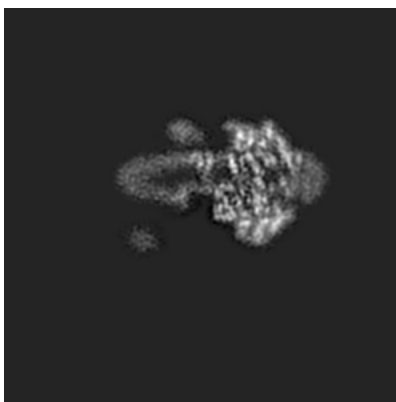
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

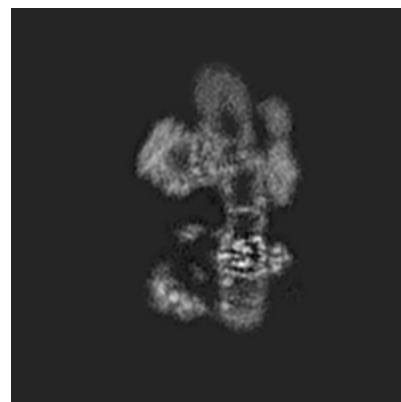
6.2.1 Primary map



X Index: 140



Y Index: 140

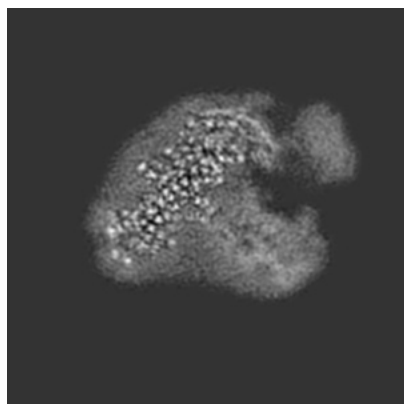


Z Index: 140

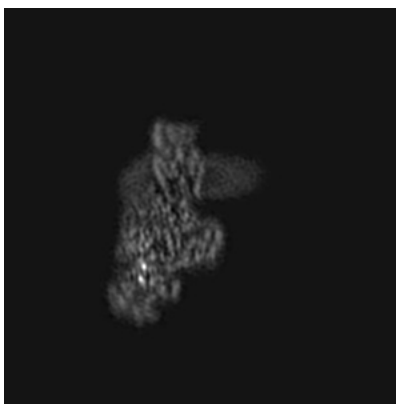
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

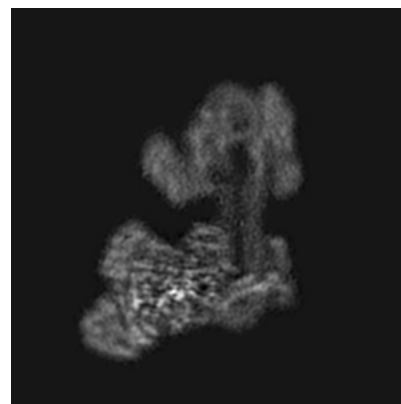
6.3.1 Primary map



X Index: 173



Y Index: 75

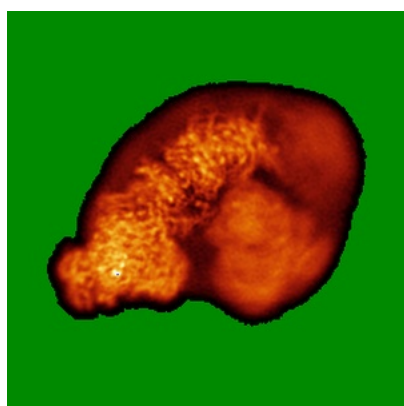


Z Index: 103

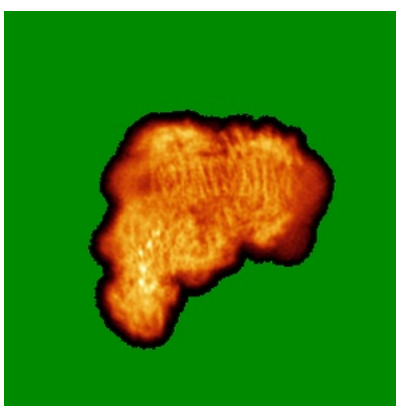
The images above show the largest variance slices of the map in three orthogonal directions.

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

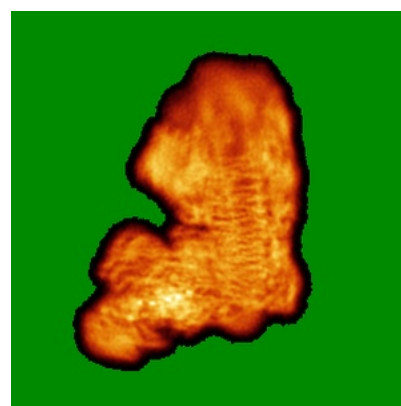
6.4.1 Primary map



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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

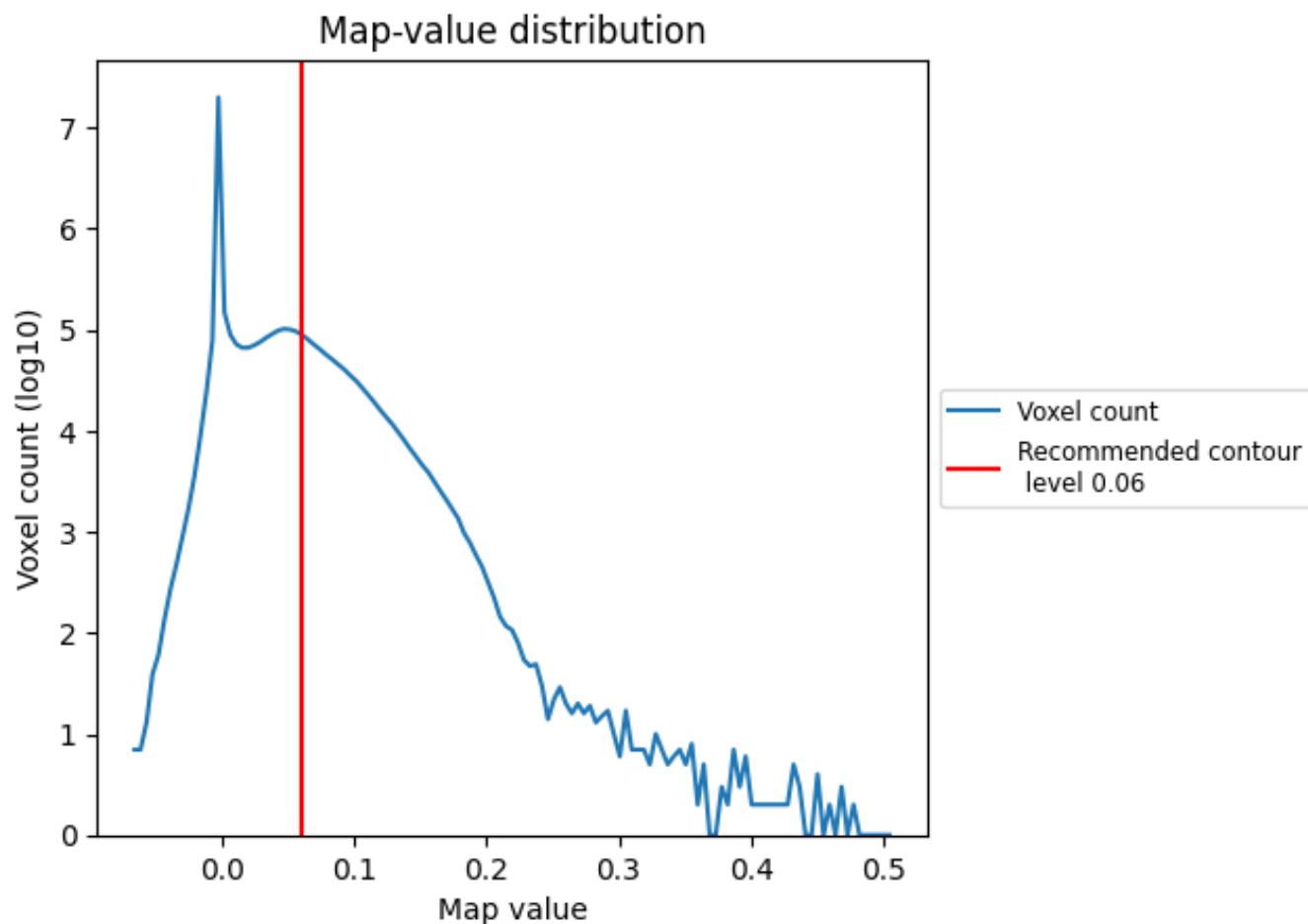
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

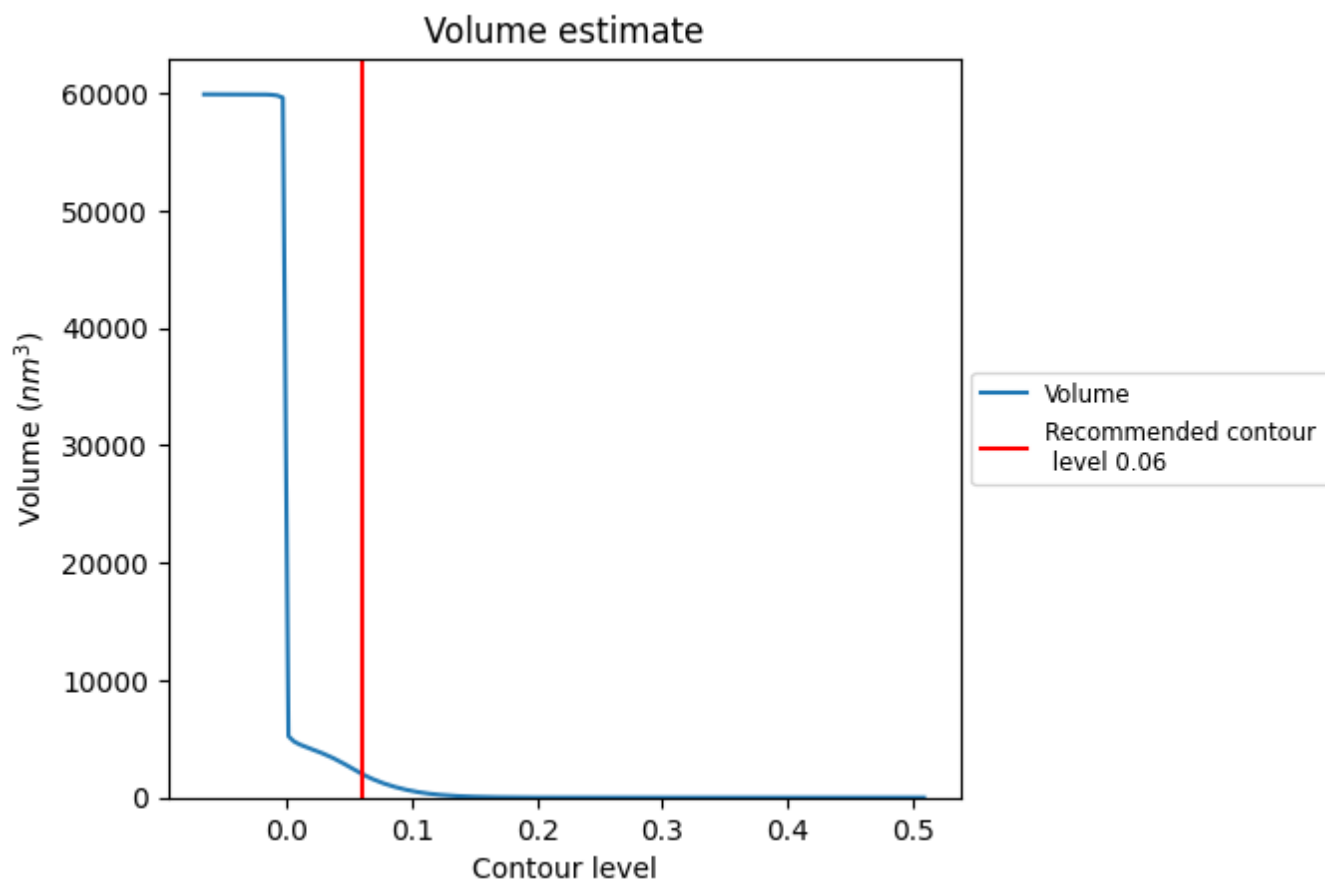
This section contains the results of statistical analysis of the map.

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.

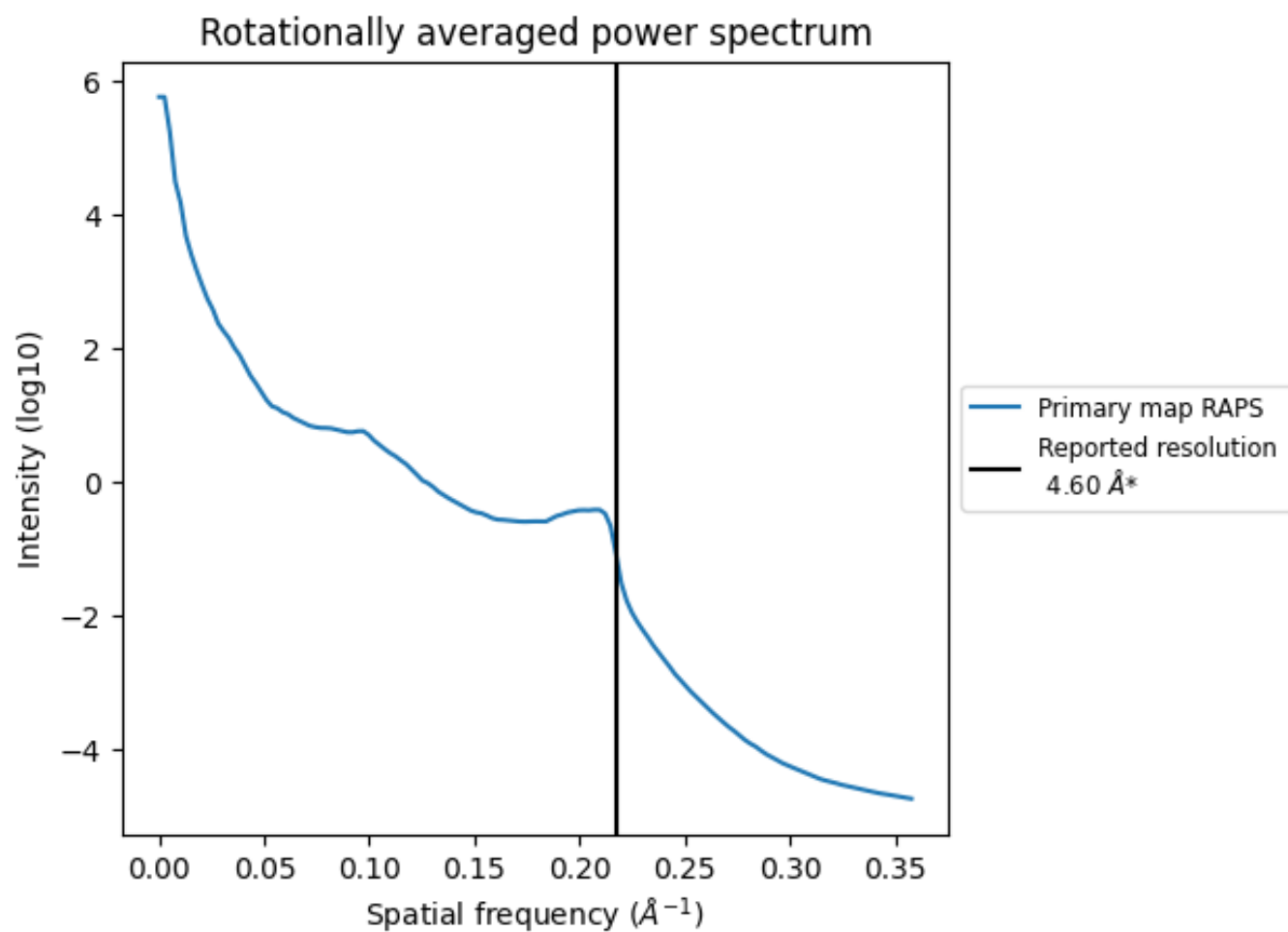
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2007 nm³; this corresponds to an approximate mass of 1813 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 0.217 Å⁻¹

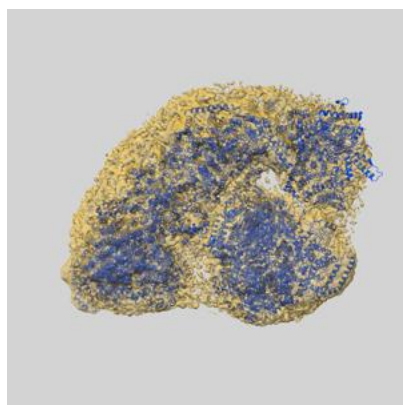
8 Fourier-Shell correlation

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

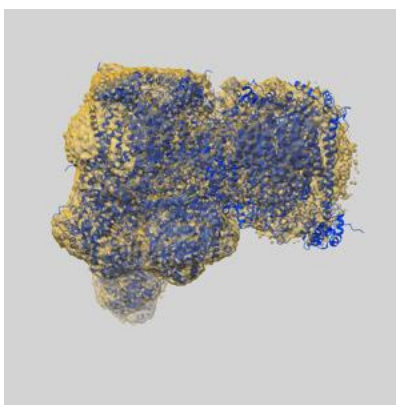
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30674 and PDB model 7DGR. Per-residue inclusion information can be found in section [3](#) on page [25](#).

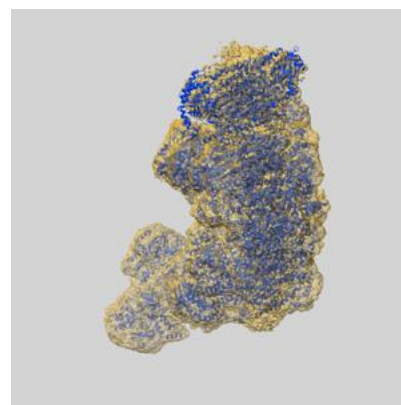
9.1 Map-model overlay [i](#)



X



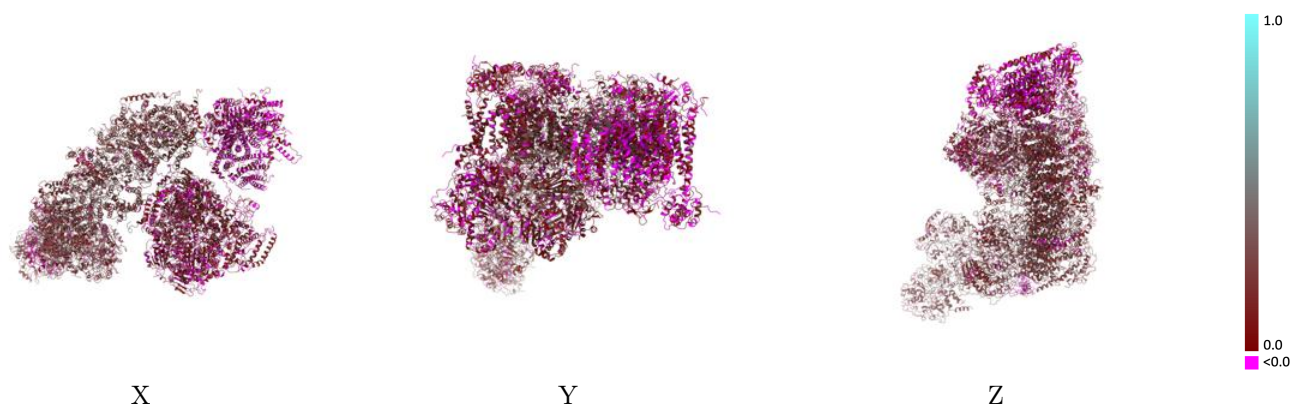
Y



Z

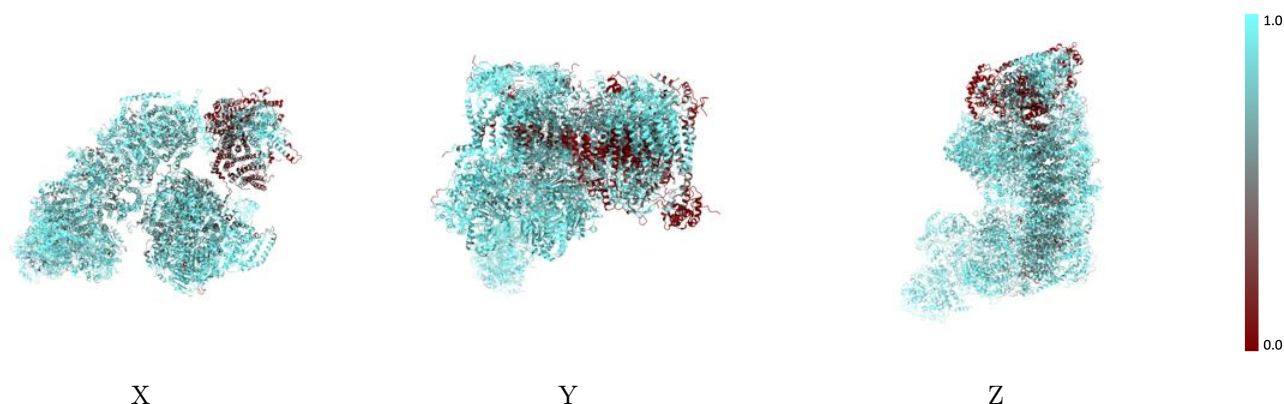
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



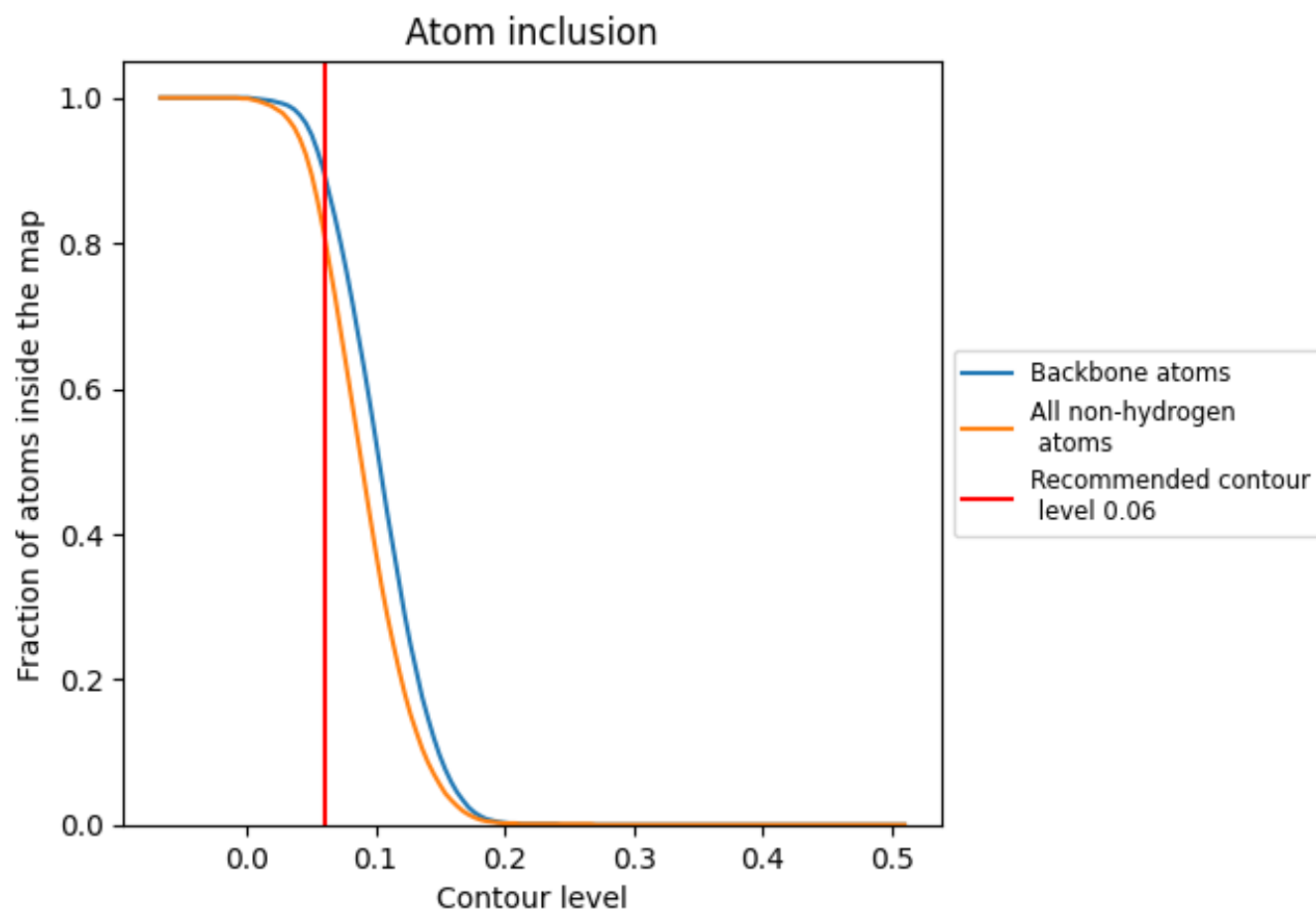
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.1780
1	 0.8290	 0.2630
2	 0.8070	 0.2820
3	 0.7050	 0.2230
4	 0.7840	 0.2760
5	 0.7910	 0.2750
6	 0.7760	 0.2350
7	 0.7750	 0.2410
8	 0.9830	 0.2200
9	 0.9630	 0.2180
A	 0.9670	 0.2460
A0	 0.7870	 0.1230
A1	 0.7440	 0.1590
A2	 0.6870	 0.1430
A3	 0.6470	 0.1640
A4	 0.1930	 0.0300
A5	 0.5640	 0.0450
A6	 0.3280	 0.0150
A7	 0.2770	 0.0260
A8	 0.2680	 0.0780
A9	 0.5820	 0.0150
B	 0.8680	 0.2900
B0	 0.3550	 0.0390
B1	 0.8120	 0.1000
B2	 0.5710	 0.1400
B3	 0.7510	 0.0800
B4	 0.3910	 0.0290
C	 0.9200	 0.2310
C0	 0.1480	 0.0420
C1	 0.3260	 0.0240
C2	 0.4270	 0.0210
C3	 0.1820	 0.0190
C4	 0.7760	 0.0260
D	 0.9030	 0.3030
E	 0.9120	 0.1400



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Chain	Atom inclusion	Q-score
F	 0.9120	 0.1510
G	 0.9280	 0.2900
H	 0.9530	 0.2880
I	 0.8980	 0.2440
J	 0.9350	 0.2190
K	 0.9730	 0.1990
L	 0.8100	 0.2180
M	 0.8680	 0.2270
N	 0.9160	 0.1760
O	 0.8670	 0.1790
P	 0.8340	 0.1560
Q	 0.9570	 0.2550
R	 0.8840	 0.2300
S	 0.9040	 0.2270
T	 0.8080	 0.2450
U	 0.6760	 0.0490
V	 0.9460	 0.2580
W	 0.9800	 0.2310
X	 0.8990	 0.2630
Y	 0.9500	 0.2510
Z	 0.9280	 0.2100
a	 0.7950	 0.1490
b	 0.9460	 0.2950
c	 0.9540	 0.2300
d	 0.9770	 0.1890
e	 0.9170	 0.2890
f	 0.9650	 0.2730
g	 0.9350	 0.2480
h	 0.9230	 0.2550
i	 0.9230	 0.2540
j	 0.7830	 0.1210
k	 0.9270	 0.0920
l	 0.9110	 0.1020
m	 0.7760	 0.1460
o	 0.9360	 0.1160
p	 0.8970	 0.0940
q	 0.8840	 0.1250
r	 0.7960	 0.1150
s	 0.8790	 0.1230
t	 0.7310	 0.0810
u	 0.8400	 0.0760
v	 0.8390	 0.0170

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Chain	Atom inclusion	Q-score
w	 0.8910	 0.1790
x	 0.9430	 0.1400
y	 0.7240	 0.1610
z	 0.8810	 0.1340