



Full wwPDB EM Validation Report ⓘ

Aug 22, 2026 – 07:57 am BST

PDB ID : 5LUF / pdb_00005luf
EMDB ID : EMD-4107
Title : Cryo-EM of bovine respirasome
Authors : Sousa, J.S.; Mills, D.J.; Vonck, J.; Kuehlbrandt, W.
Deposited on : 2016-09-08
Resolution : 9.10 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 : 1.8.4, 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

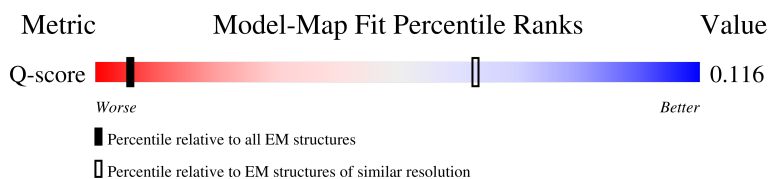
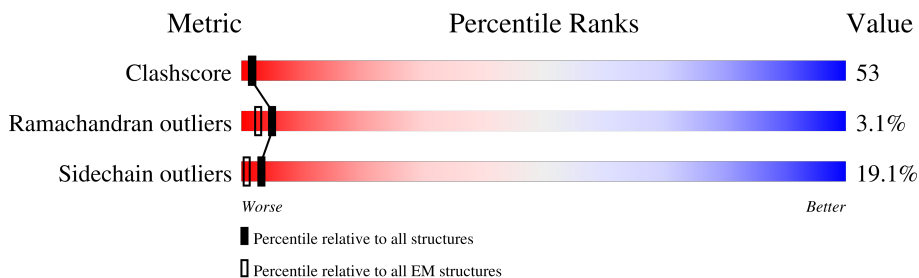
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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	244 (8.60 - 9.60)

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	c	446	
1	l	446	
2	m	439	
2	n	439	

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Mol	Chain	Length	Quality of chain
3	b	379	
3	o	379	
4	d	241	
4	p	241	
5	e	196	
5	q	196	
6	f	110	
6	r	110	
7	g	81	
7	s	81	
8	h	78	
8	t	78	
9	i	78	
9	u	78	
10	j	62	
10	v	62	
11	k	56	
11	w	56	
12	x	514	
13	y	227	
14	z	261	
15	1	147	
16	2	109	
17	3	98	
18	4	84	

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Mol	Chain	Length	Quality of chain
19	5	85	
20	6	73	
21	7	59	
22	8	56	
23	9	47	
24	0	46	
25	A	111	
26	B	143	
27	C	154	
28	D	384	
29	E	159	
30	F	411	
31	G	538	
32	H	313	
33	I	162	
34	J	171	
35	K	84	
36	L	601	
37	M	453	
38	N	345	
39	O	220	
40	P	303	
41	Q	85	
42	R	47	
43	S	80	

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Mol	Chain	Length	Quality of chain
44	T	75	
45	V	71	
46	W	72	
47	X	330	
48	Y	106	
49	a	142	
50	U	828	
51	Z	625	

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
54	FES	G	803	-	-	X	-
59	SF4	B	201	-	-	X	-
59	SF4	I	201	-	-	X	-
59	SF4	I	202	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 74493 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		
1	l	446	Total	C	N	O	S	0	0
			3458	2161	609	668	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		
2	n	419	Total	C	N	O	S	0	0
			3141	1972	556	606	7		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		
3	o	379	Total	C	N	O	S	0	0
			3011	2018	472	502	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		
4	p	241	Total	C	N	O	S	0	0
			1919	1225	330	349	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	75	Total	C	N	O	S	0	0
			566	352	94	118	2		
5	q	196	Total	C	N	O	S	0	0
			1518	956	263	291	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	106	Total	C	N	O	S	0	0
			916	579	166	169	2		
6	r	106	Total	C	N	O	S	0	0
			916	579	166	169	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	56	ASP	ASN	conflict	UNP P00129
r	56	ASP	ASN	conflict	UNP P00129

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	81	Total	C	N	O	S	0	0
			682	441	128	112	1		
7	s	81	Total	C	N	O	S	0	0
			682	441	128	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	64	Total	C	N	O	S	0	0
			524	316	96	107	5		
8	t	64	Total	C	N	O	S	0	0
			524	316	96	107	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	33	Total	C	N	O	S	0	0
			248	152	51	44	1		
9	u	33	Total	C	N	O	S	0	0
			248	152	51	44	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	62	Total	C	N	O	0	0
			512	335	89	88		
10	v	62	Total	C	N	O	0	0
			512	335	89	88		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	22	Total	C	N	O	0	0
			159	103	29	27		
11	w	22	Total	C	N	O	0	0
			159	103	29	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	22	GLN	SER	conflict	UNP P07552
k	34	SER	TRP	conflict	UNP P07552
k	38	SER	TRP	conflict	UNP P07552
w	22	GLN	SER	conflict	UNP P07552
w	34	SER	TRP	conflict	UNP P07552
w	38	SER	TRP	conflict	UNP P07552

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	238	GLY	ALA	conflict	UNP P00415

- Molecule 15 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	8	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 25 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	A	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 26 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	143	Total	C	N	O	S	0	0
			719	429	143	143	4		

- Molecule 27 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	154	Total	C	N	O	0	0
			770	462	154	154		

- Molecule 28 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	D	384	Total	C	N	O	0	0
			1920	1152	384	384		

- Molecule 29 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	159	Total	C	N	O	S	0	0
			799	477	159	159	4		

- Molecule 30 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	411	Total	C	N	O	S	0	0
			2059	1233	411	411	4		

- Molecule 31 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	527	Total	C	N	O	S	0	0
			2651	1584	529	527	11		

- Molecule 32 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	H	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 33 is a protein called complex I.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	162	Total	C	N	O	S	0	0
			818	486	162	162	8		

- Molecule 34 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	J	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 35 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	K	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 36 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	558	Total	C	N	O	0	0
			2790	1674	558	558		

- Molecule 37 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	439	Total	C	N	O	0	0
			2195	1317	439	439		

- Molecule 38 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	326	Total	C	N	O	0	0
			1630	978	326	326		

- Molecule 39 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	O	181	Total	C	N	O	0	0
			905	543	181	181		

- Molecule 40 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	P	252	Total	C	N	O	0	0
			1260	756	252	252		

- Molecule 41 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Q	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 42 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	R	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 43 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	S	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 44 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 45 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	V	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 46 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 47 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	X	329	Total	C	N	O	0	0
			1645	987	329	329		

- Molecule 48 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Y	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 49 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	a	71	Total	C	N	O	0	0
			355	213	71	71		

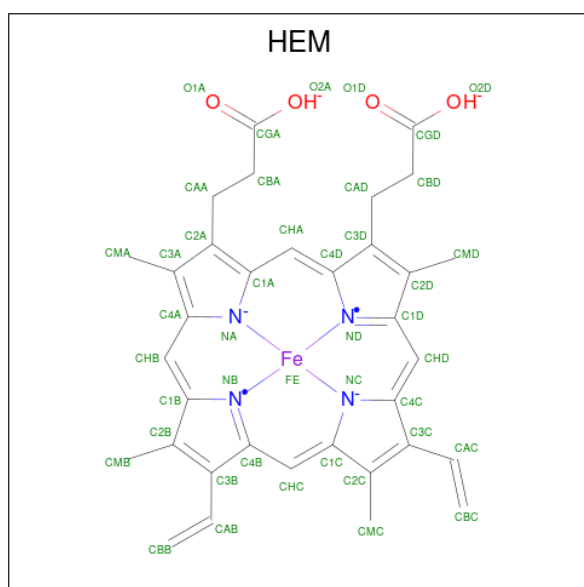
- Molecule 50 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	U	250	Total	C	N	O	0	0
			1250	750	250	250		

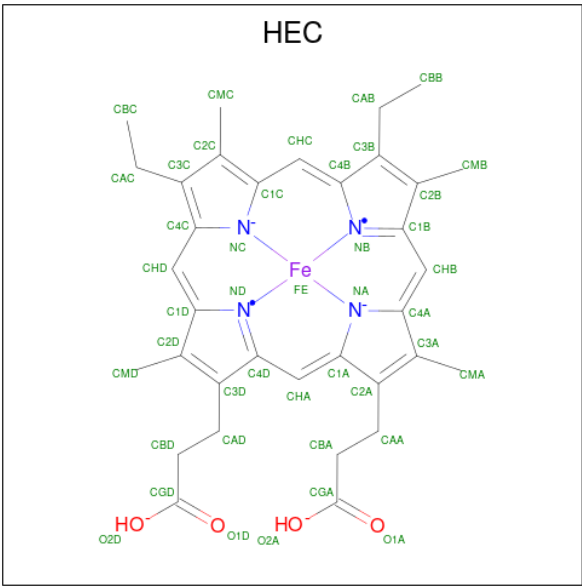
- Molecule 51 is a protein called complex I.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Z	266	Total	C	N	O	0	0
			1329	798	265	266		

- Molecule 52 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

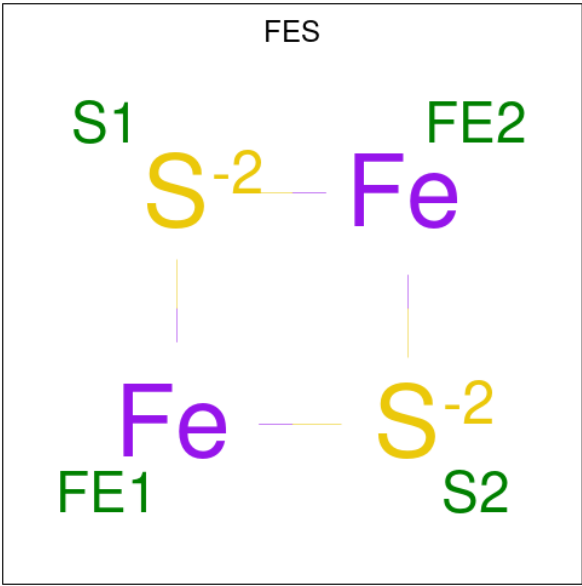


- Molecule 53 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
53	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
53	p	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
54	q	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
54	E	1	Total	Fe	S	0
			4	2	2	
54	G	1	Total	Fe	S	0
			4	2	2	

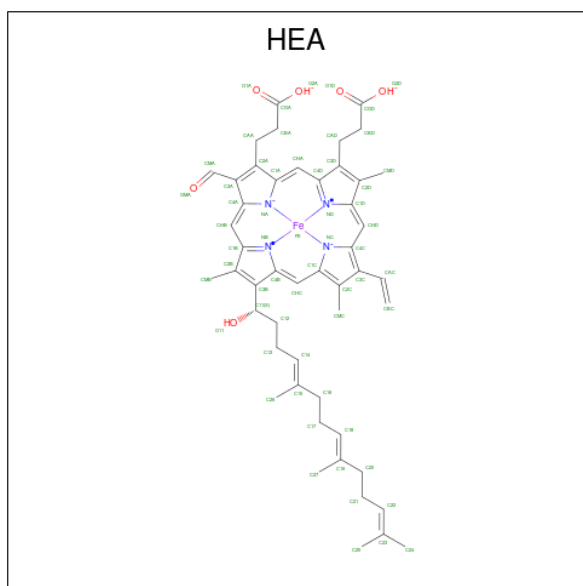
- Molecule 55 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
55	x	1	Total	Cu	0
			1	1	
55	y	2	Total	Cu	0
			2	2	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	x	1	Total	Mg	0
			1	1	

- Molecule 57 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

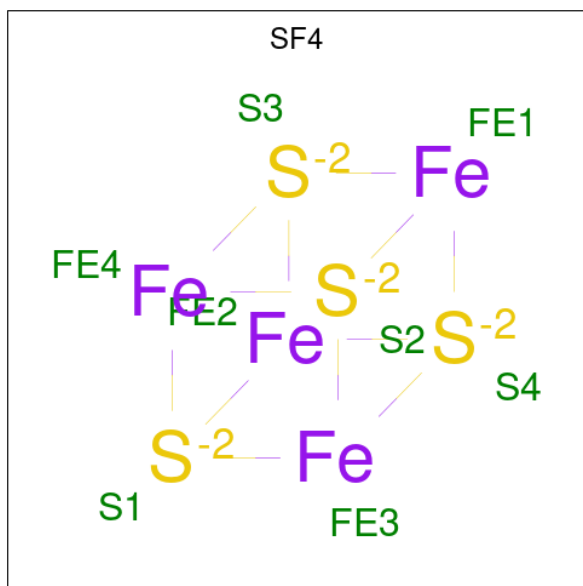


Mol	Chain	Residues	Atoms					AltConf
57	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
57	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	Zn	0
			1	1	

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

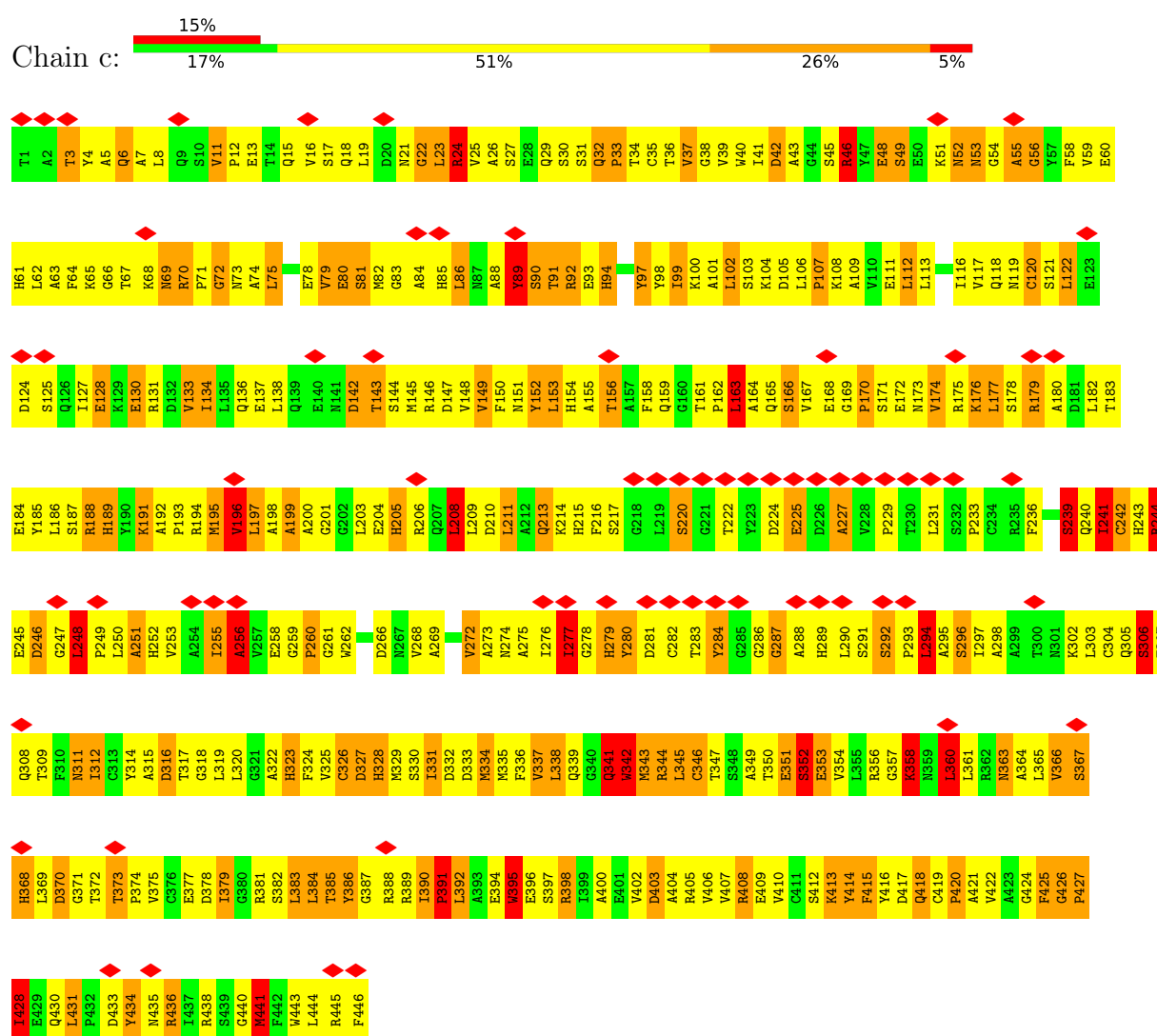


Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	F	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	

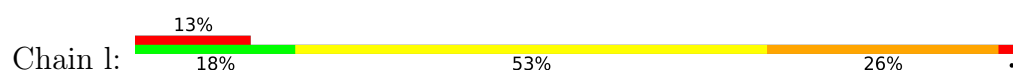
3 Residue-property plots [i](#)

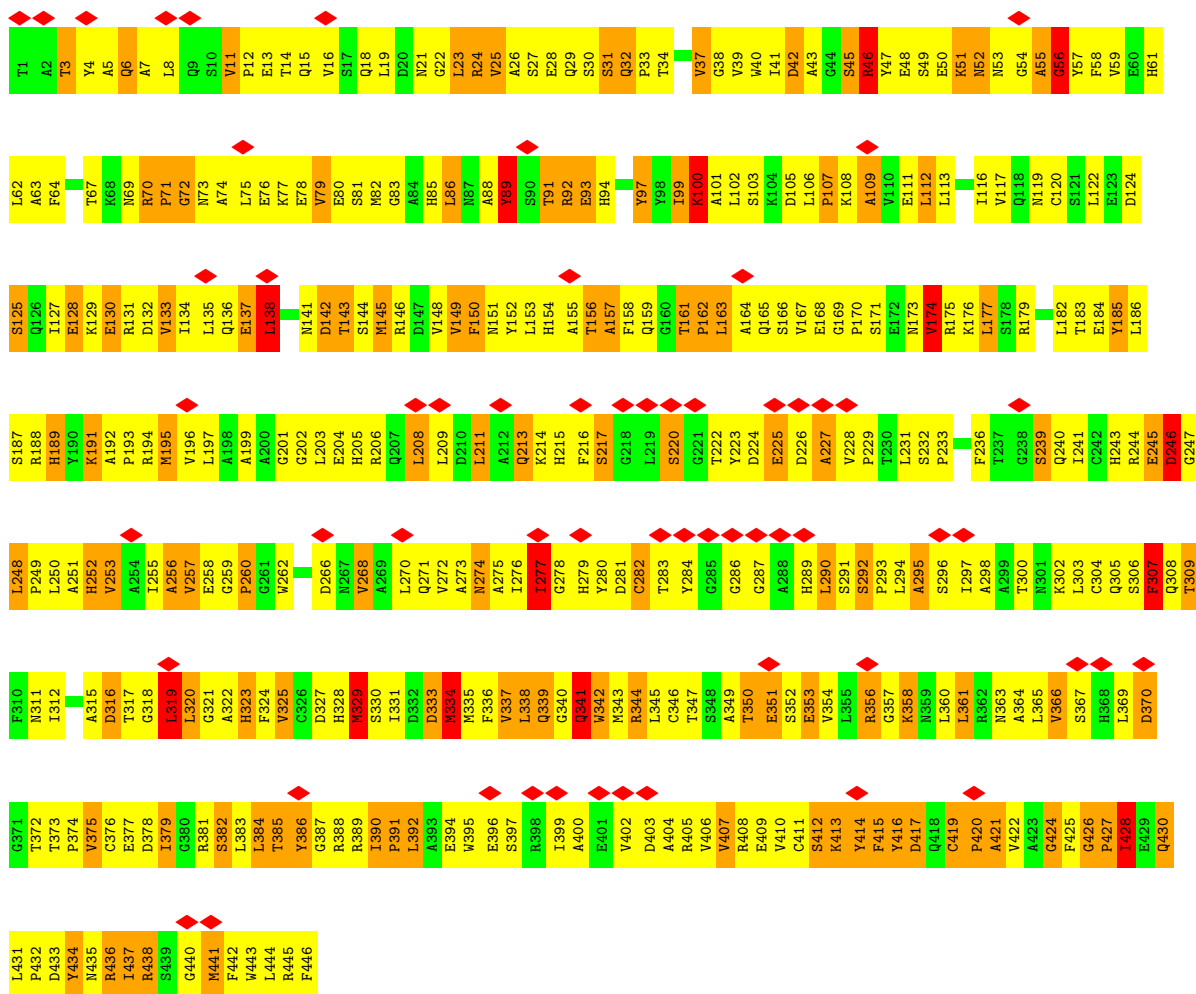
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

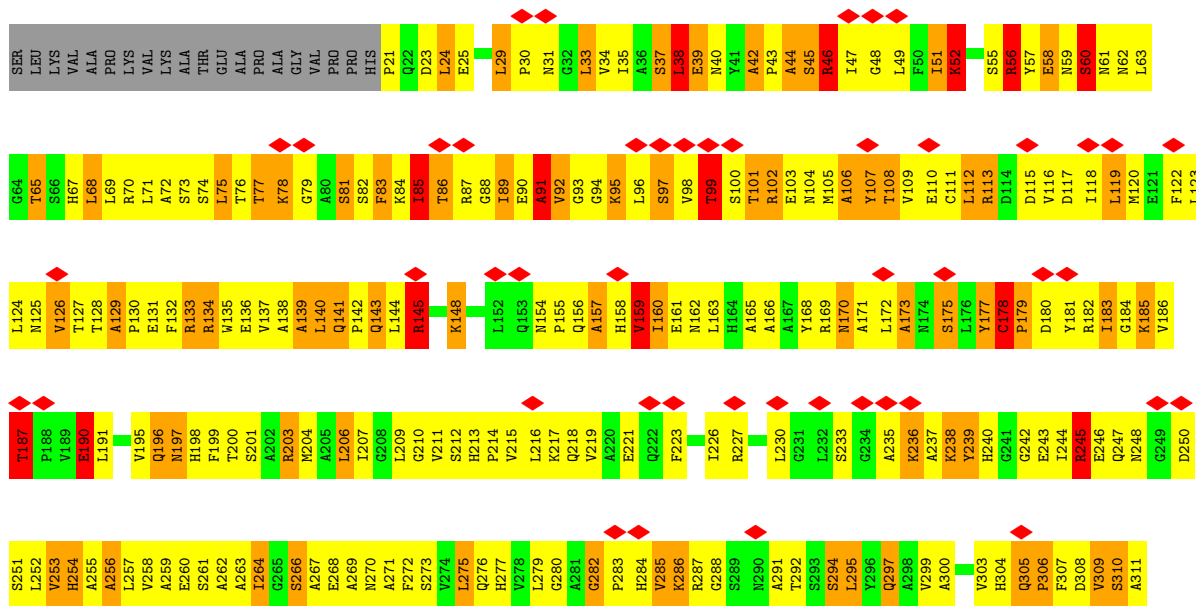
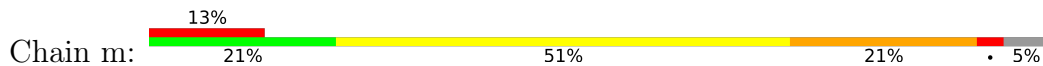


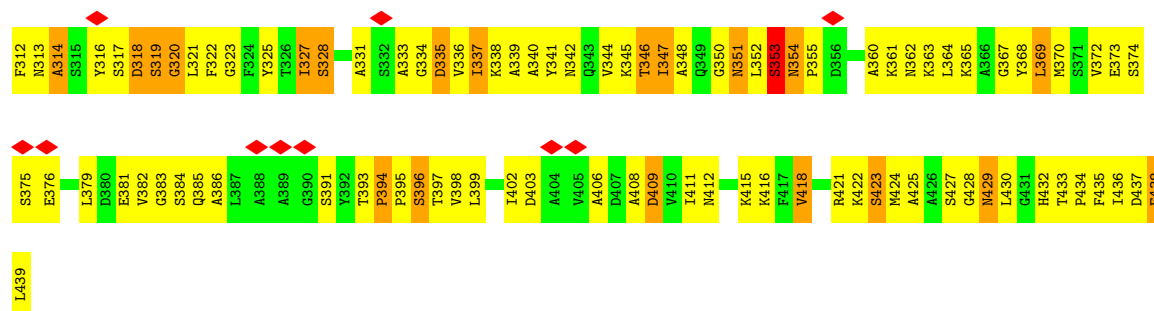
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



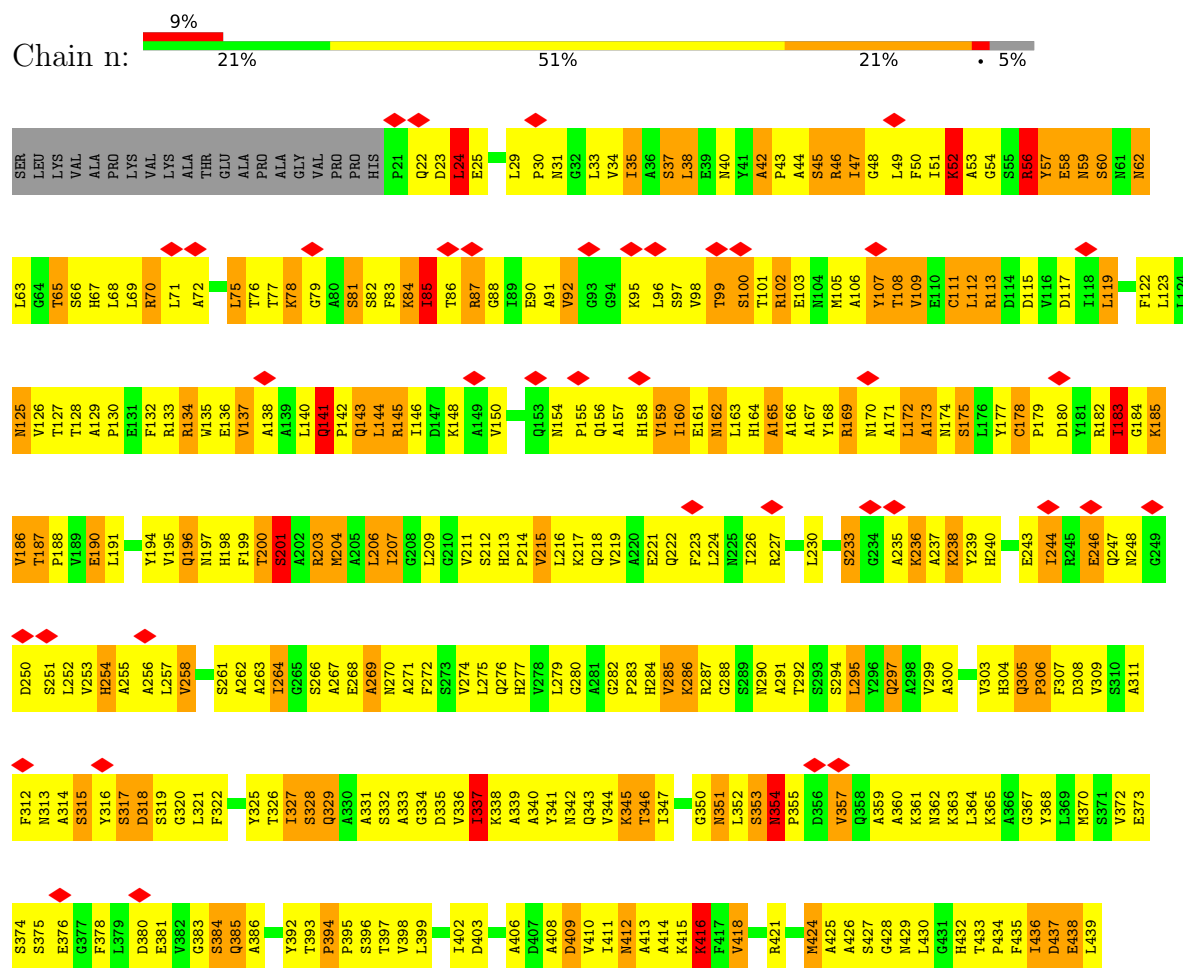


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

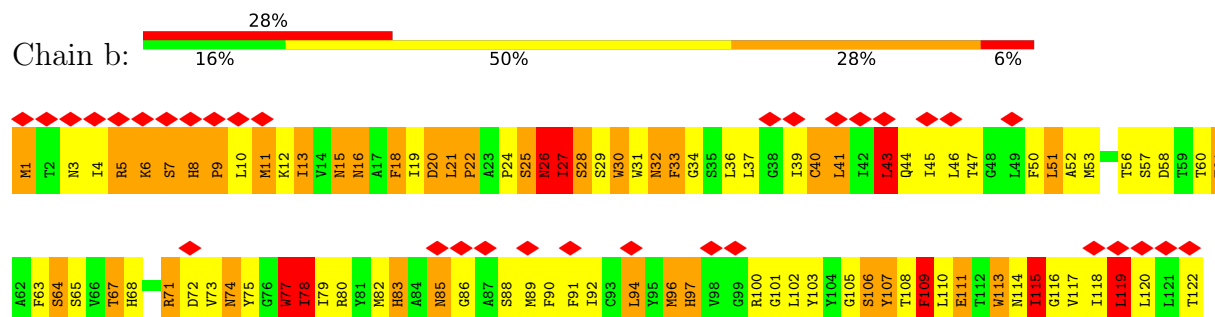


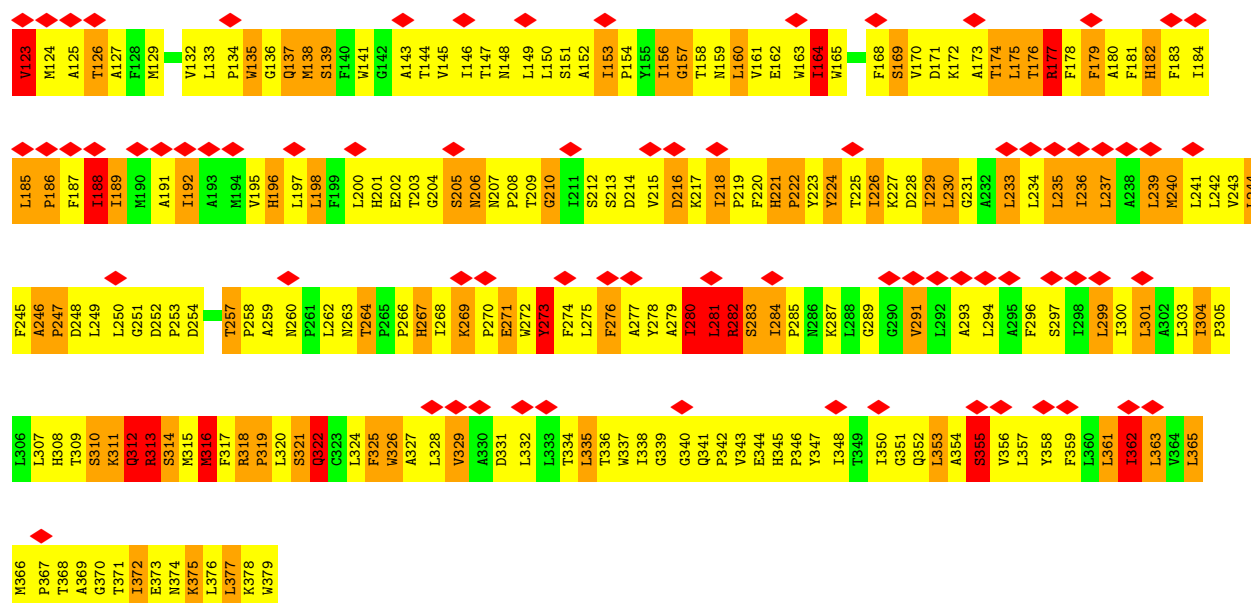


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

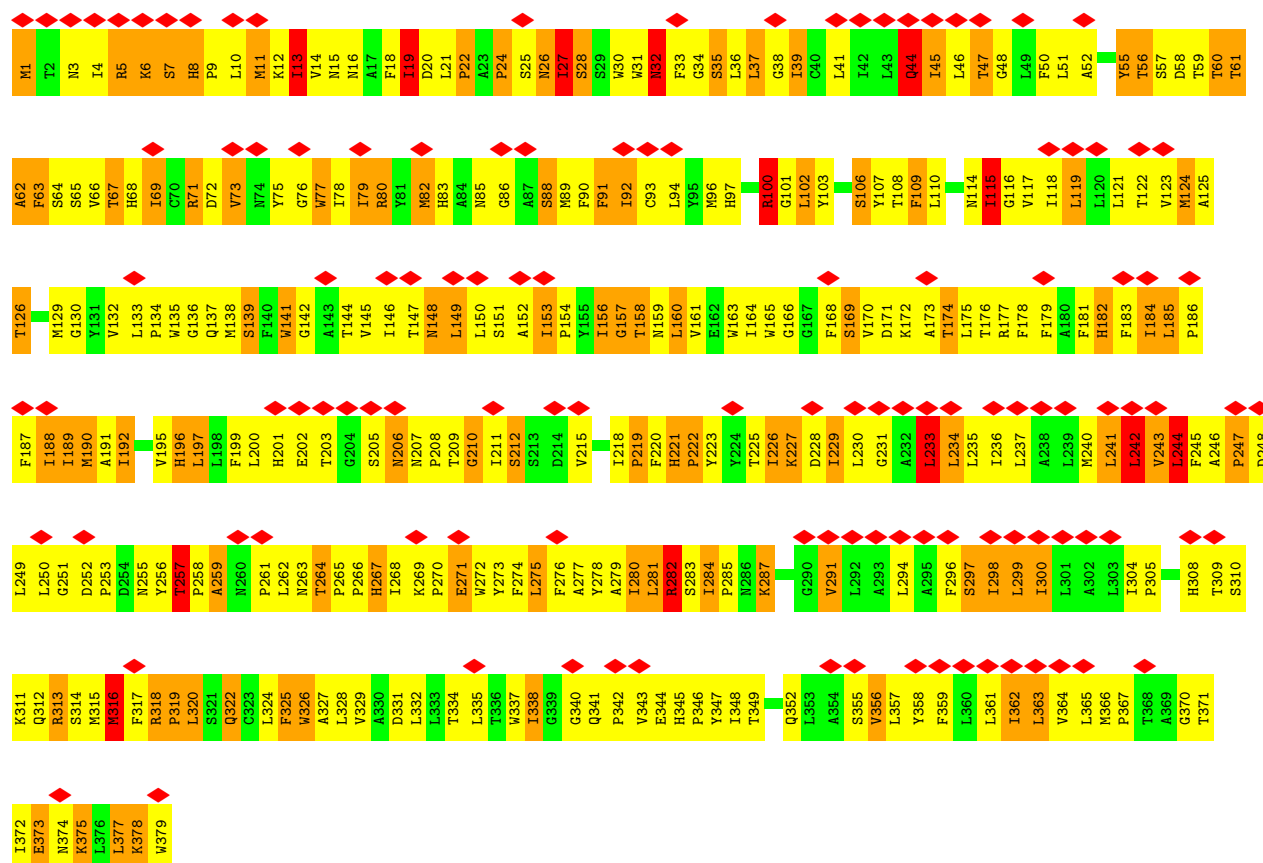
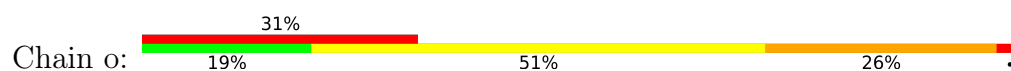


• Molecule 3: Cytochrome b

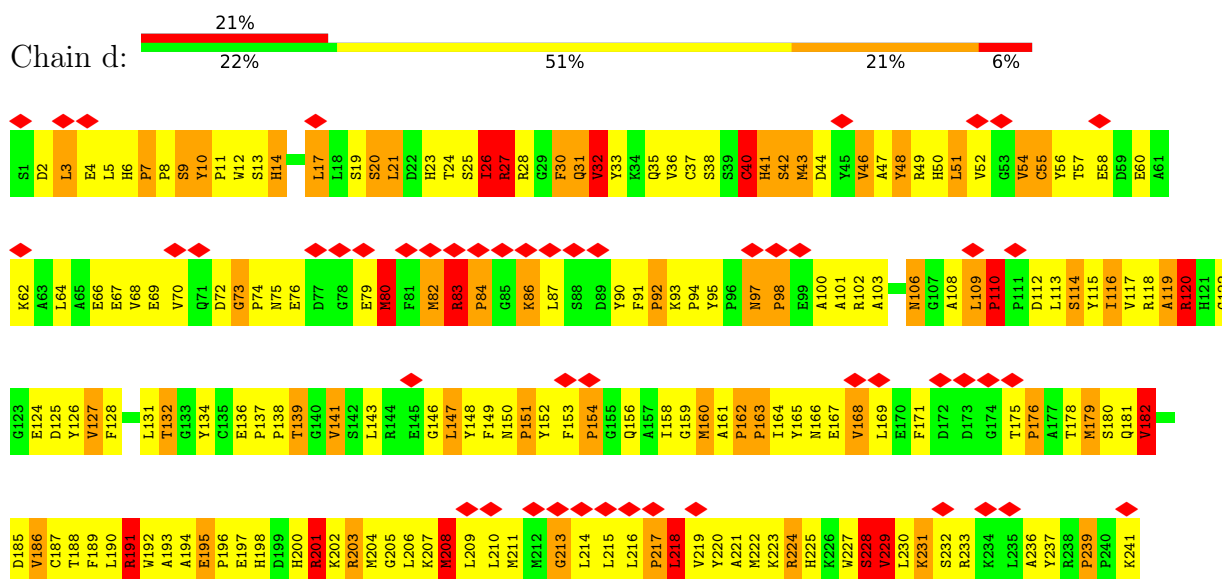




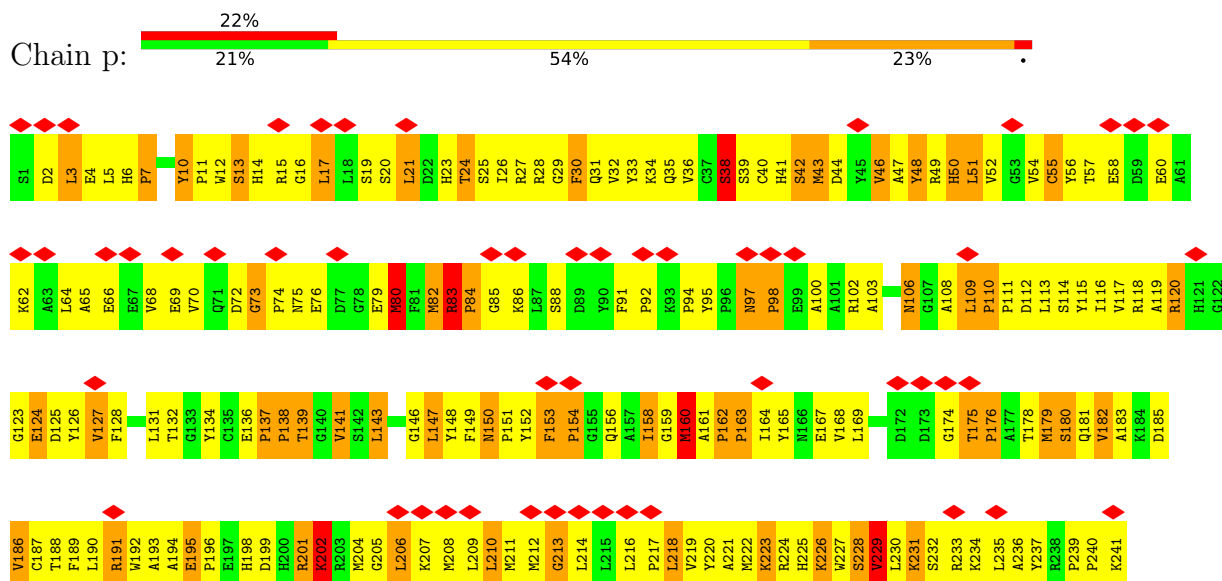
• Molecule 3: Cytochrome b



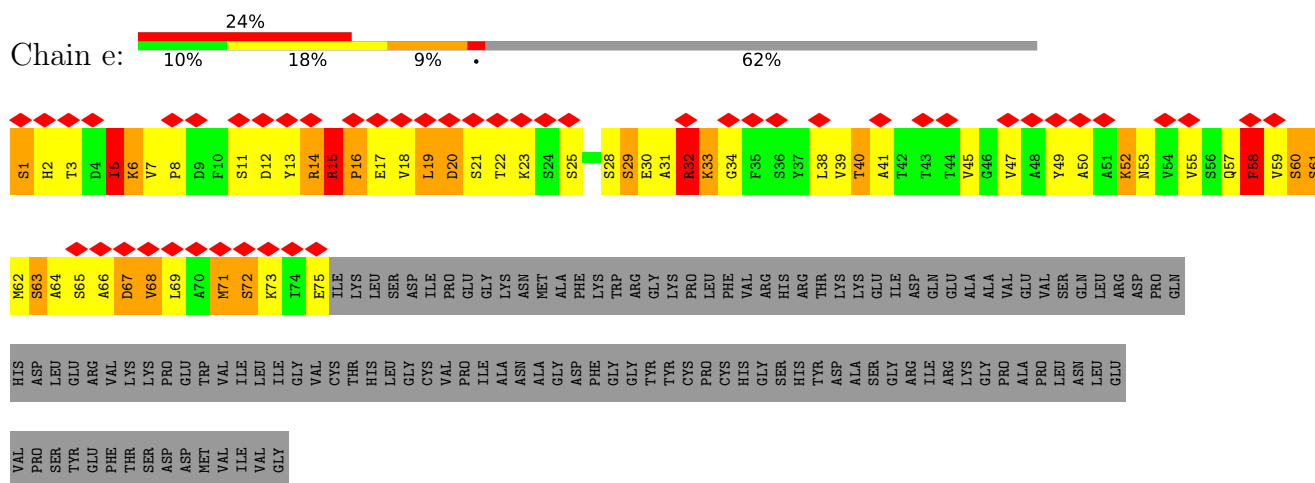
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



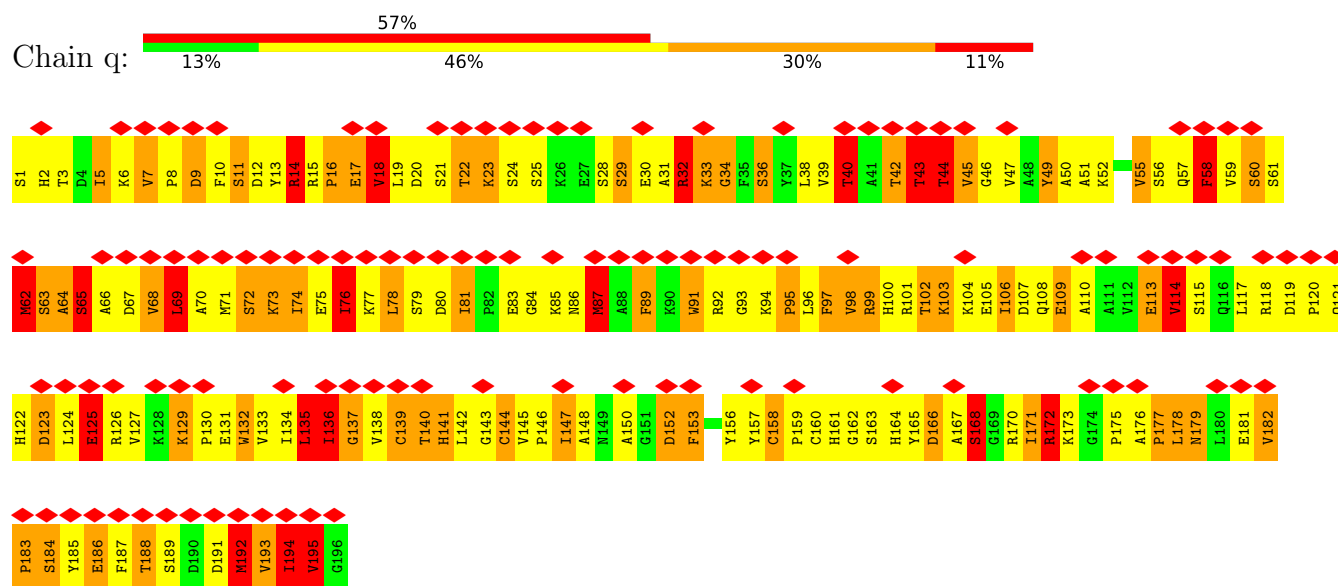
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



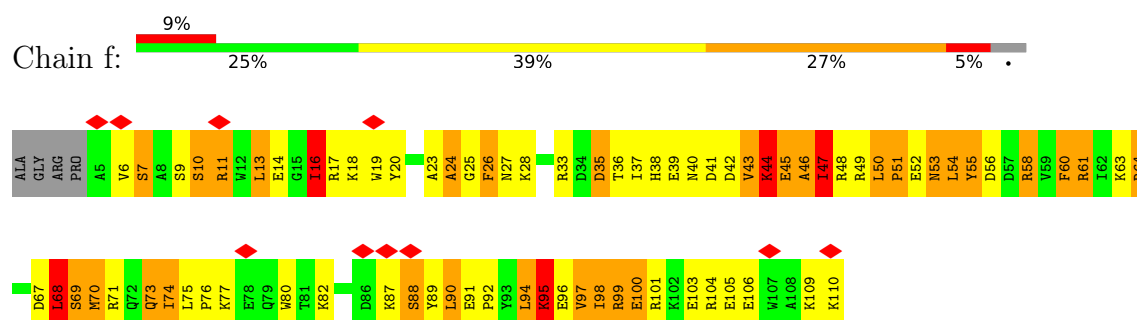
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



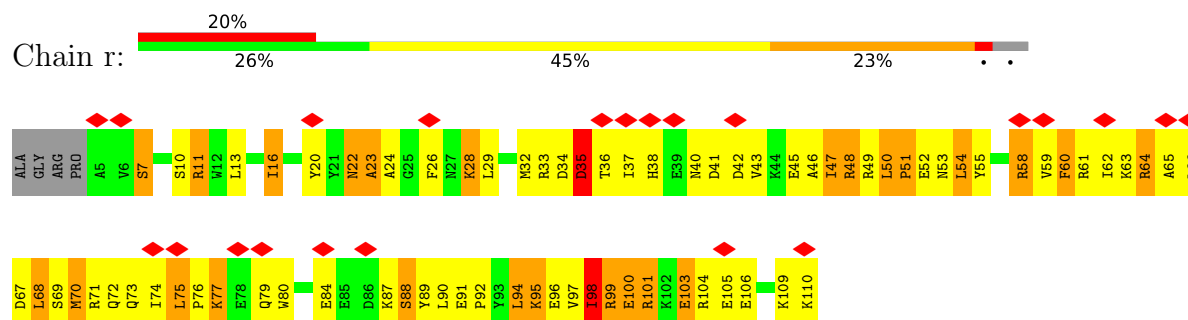
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



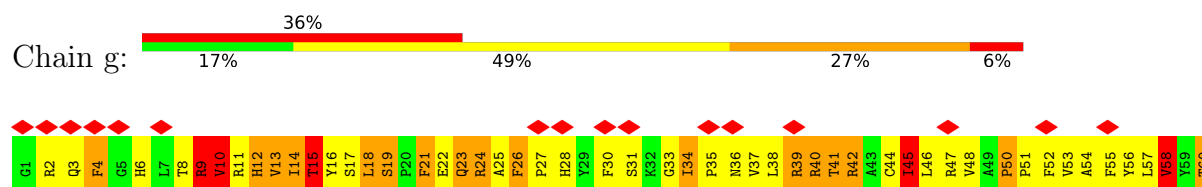
- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 6: Cytochrome b-c1 complex subunit 7

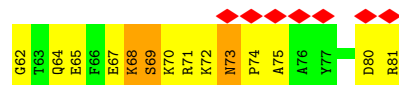
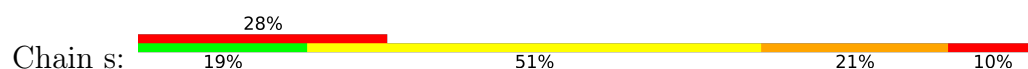


- Molecule 7: Cytochrome b-c1 complex subunit 8





• Molecule 7: Cytochrome b-c1 complex subunit 8



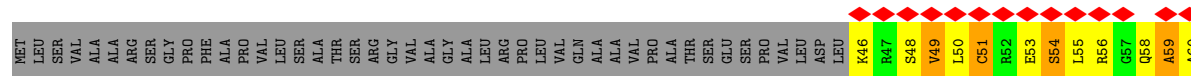
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



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

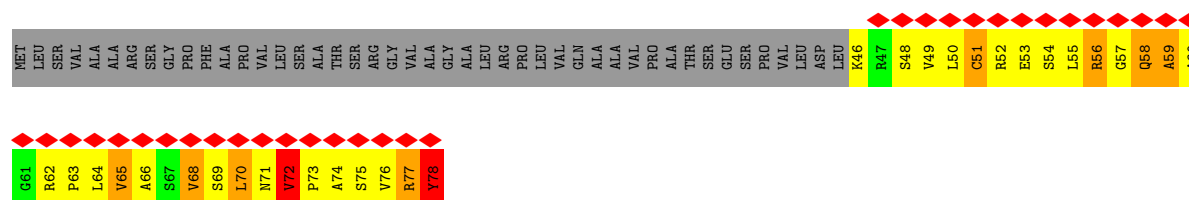


• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

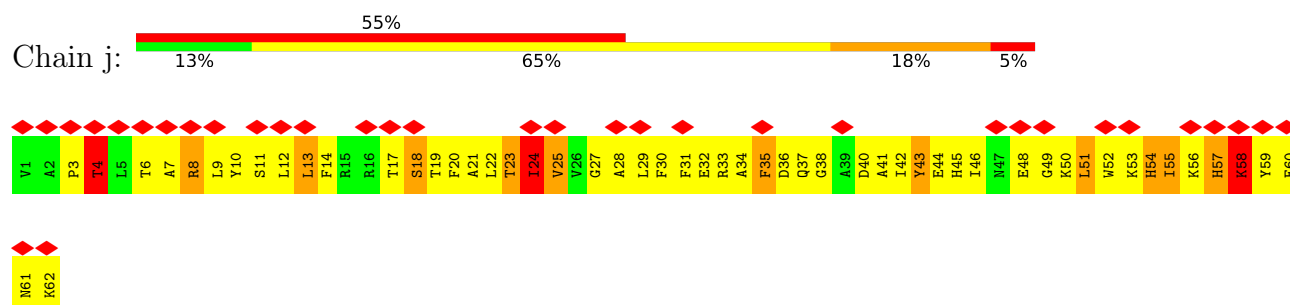


• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

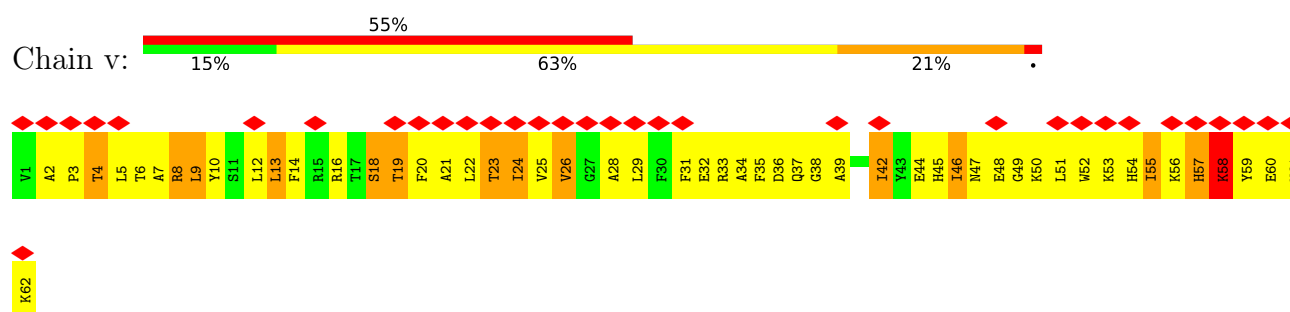




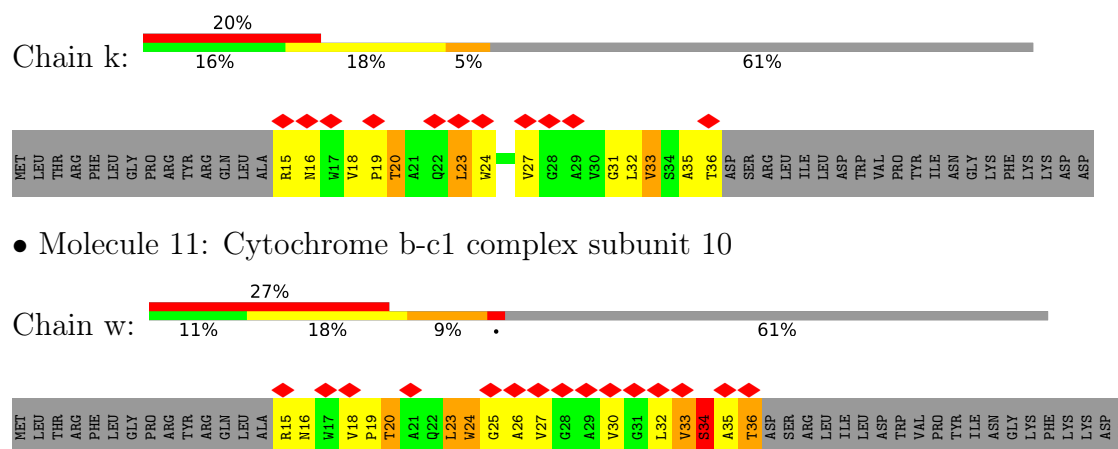
• Molecule 10: Cytochrome b-c1 complex subunit 9



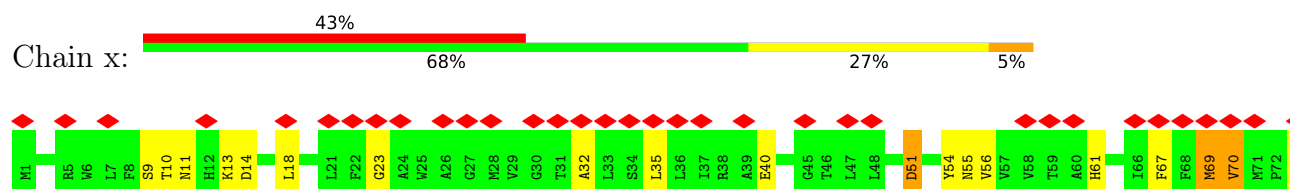
• Molecule 10: Cytochrome b-c1 complex subunit 9

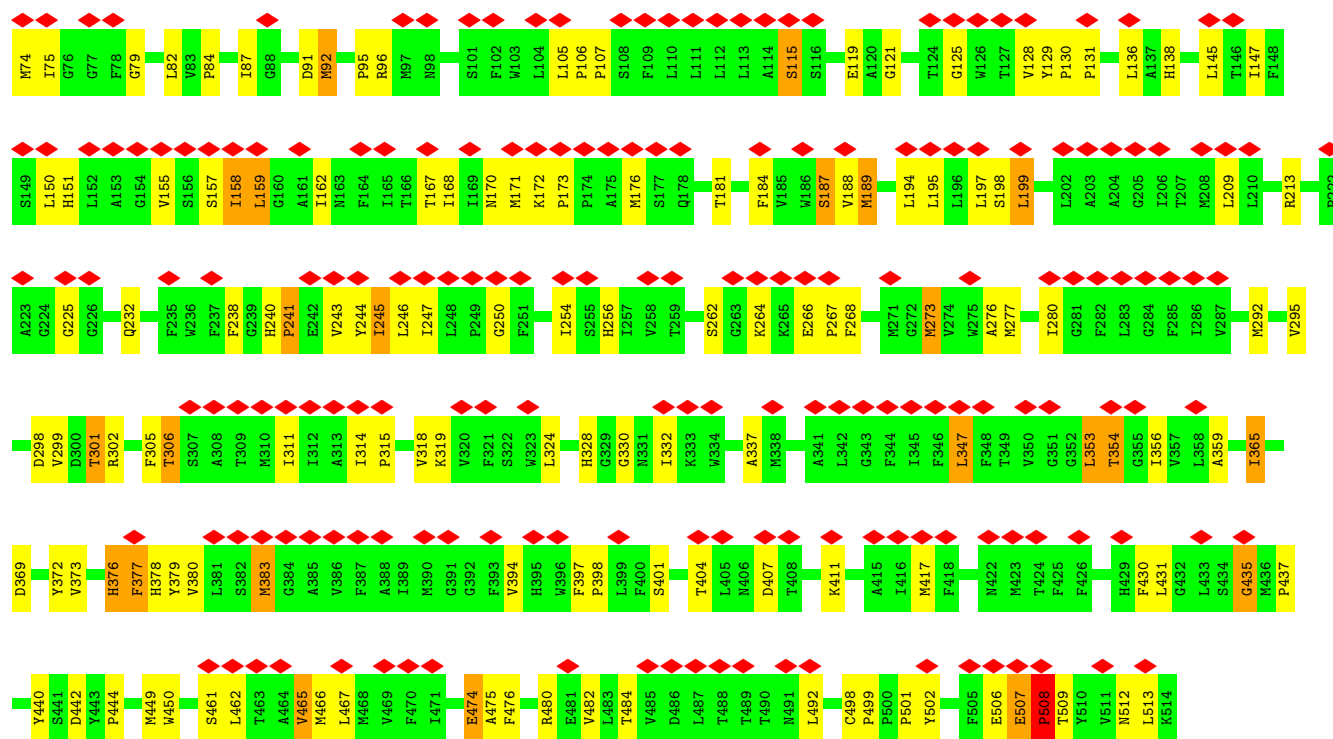


• Molecule 11: Cytochrome b-c1 complex subunit 10

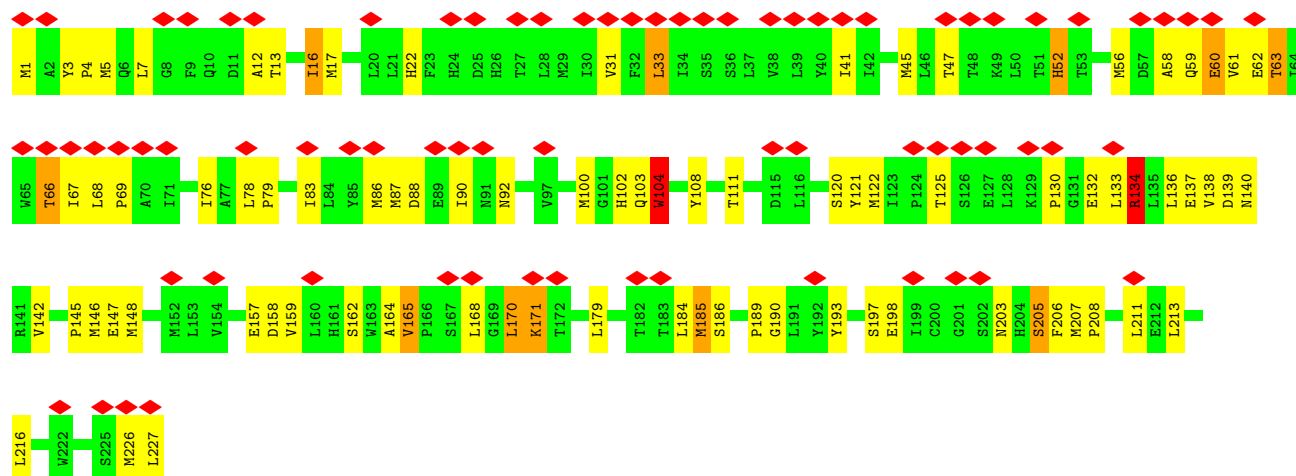


• Molecule 12: Cytochrome c oxidase subunit 1

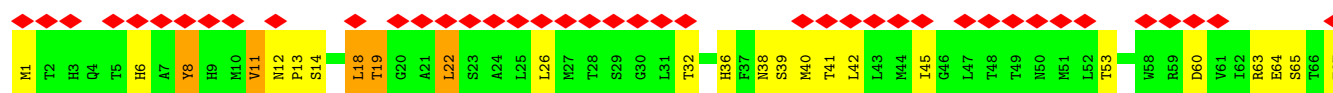


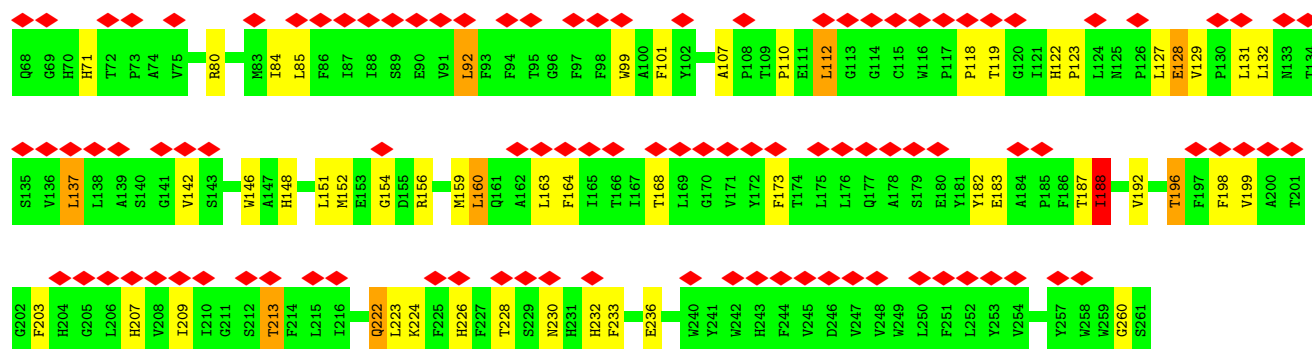


• Molecule 13: Cytochrome c oxidase subunit 2

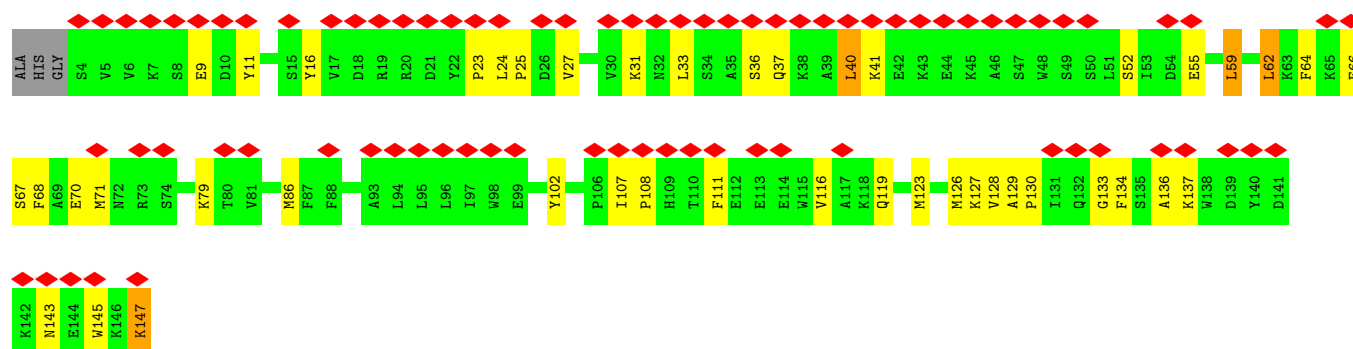


• Molecule 14: Cytochrome c oxidase subunit 3

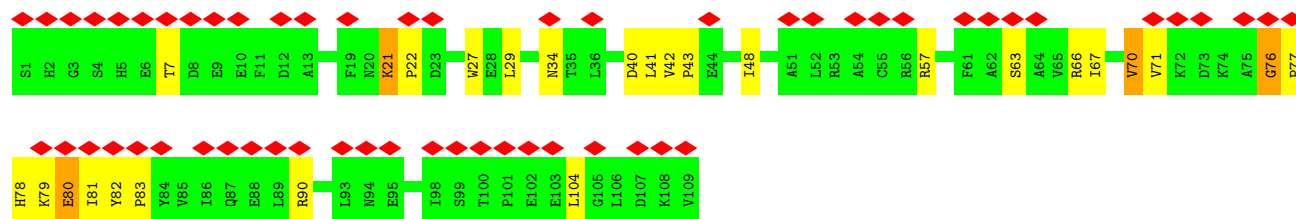




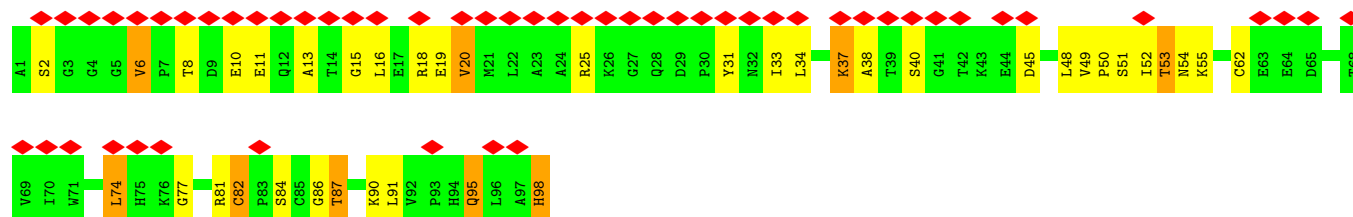
- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



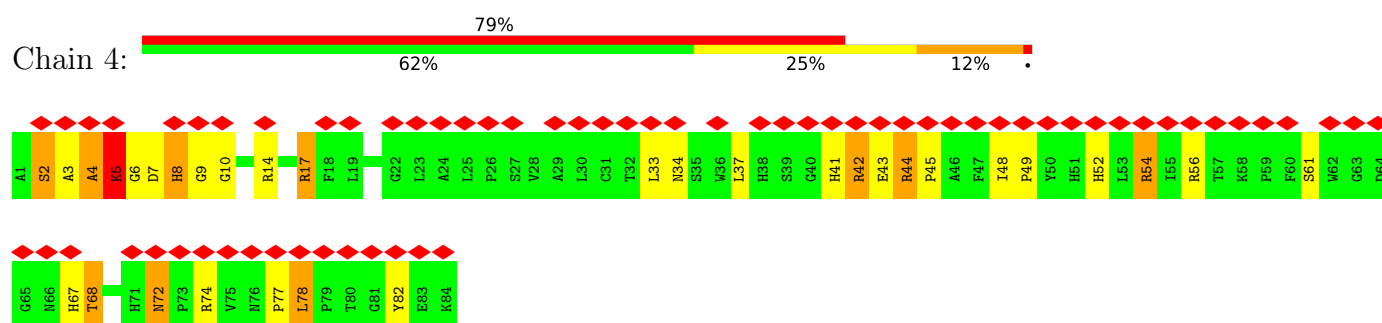
- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial



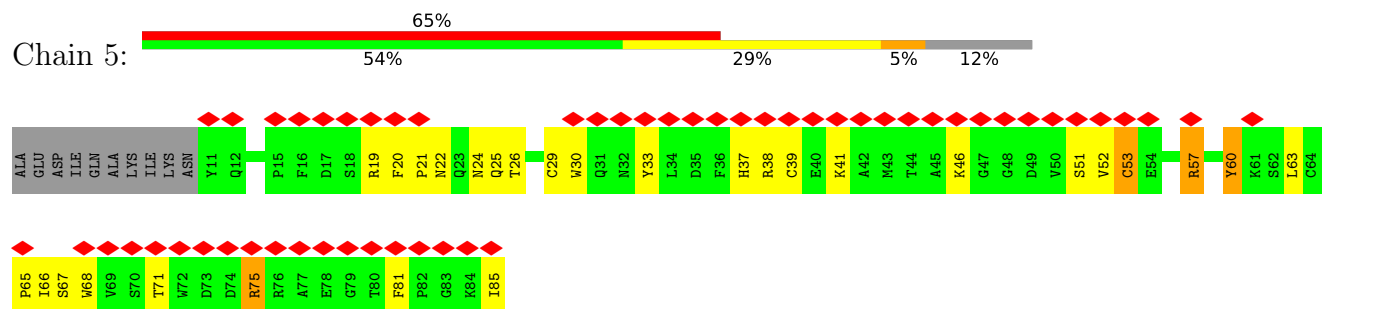
- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial



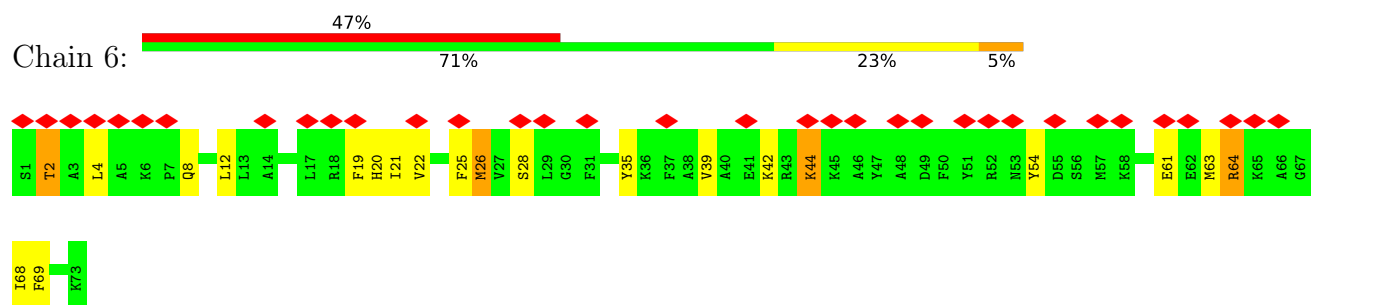
- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial



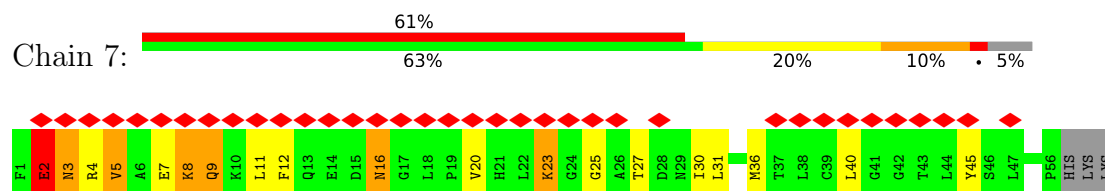
• Molecule 19: Cytochrome c oxidase subunit 6B1



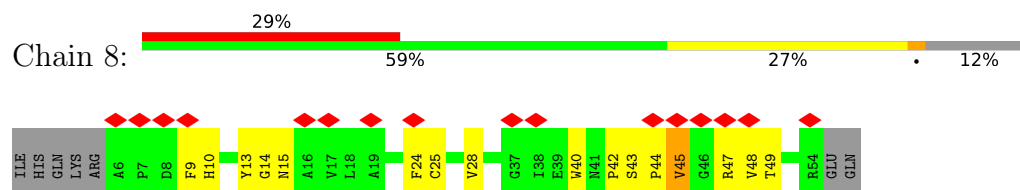
• Molecule 20: Cytochrome c oxidase subunit 6C



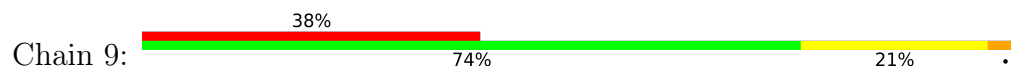
• Molecule 21: Cytochrome c oxidase subunit 7A1, mitochondrial

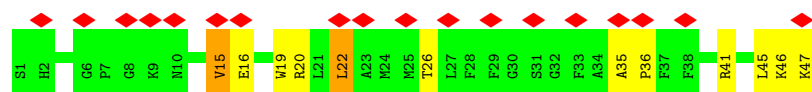


• Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

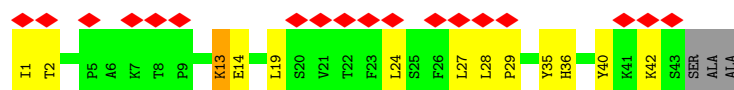
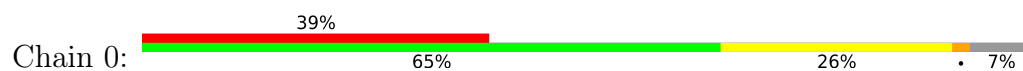


• Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

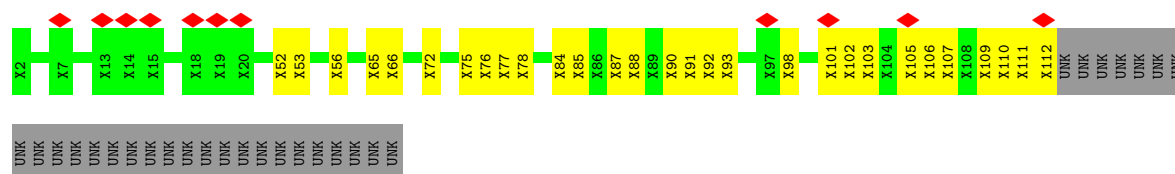




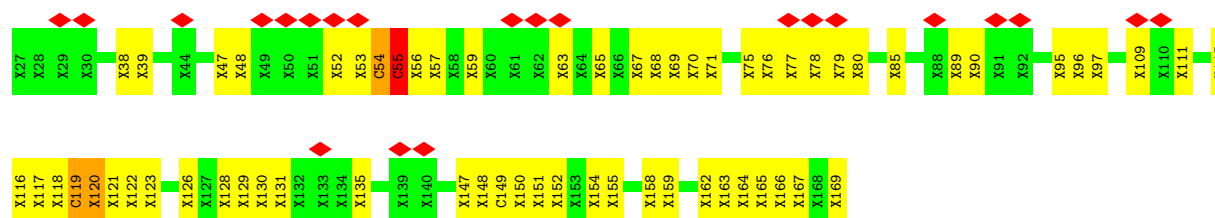
- Molecule 24: Cytochrome c oxidase subunit 8B, mitochondrial



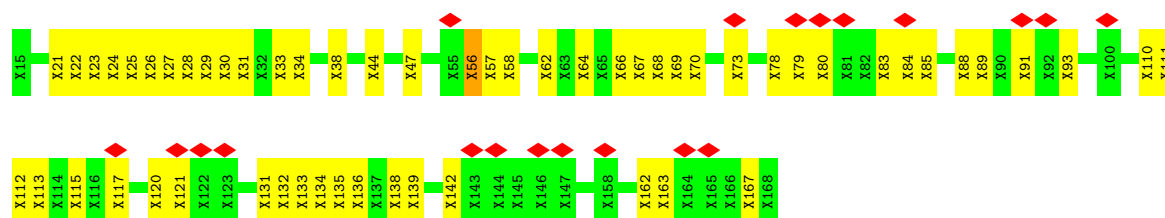
- Molecule 25: complex I



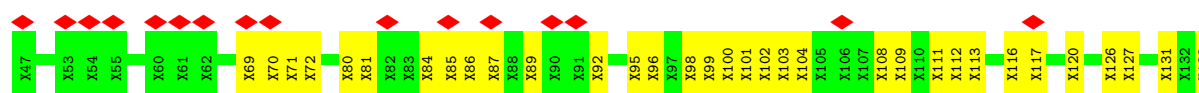
- Molecule 26: complex I

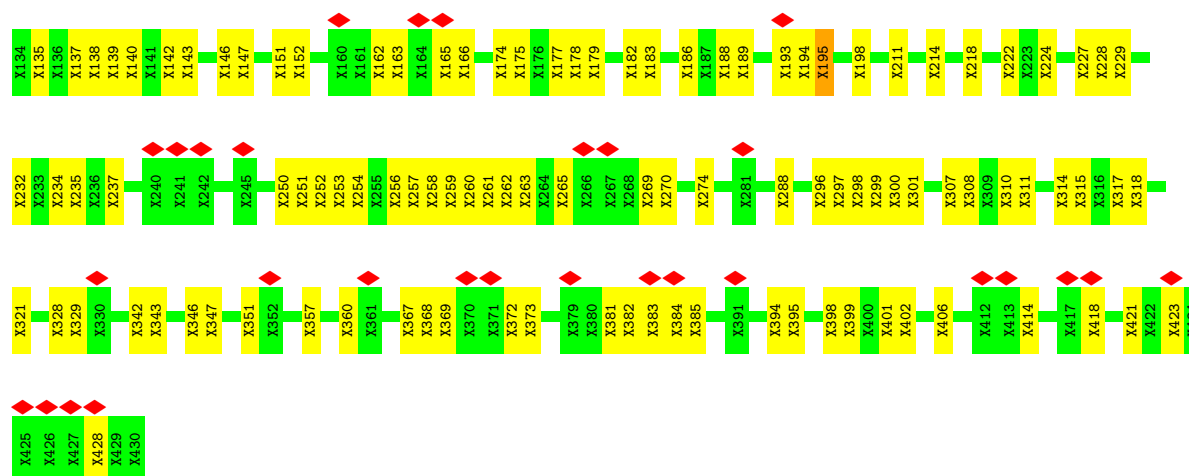


- Molecule 27: complex I

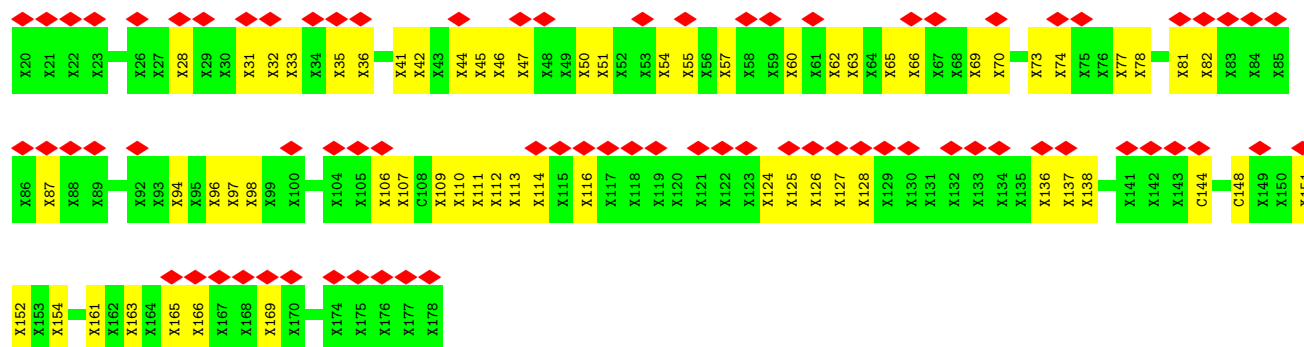


- Molecule 28: complex I



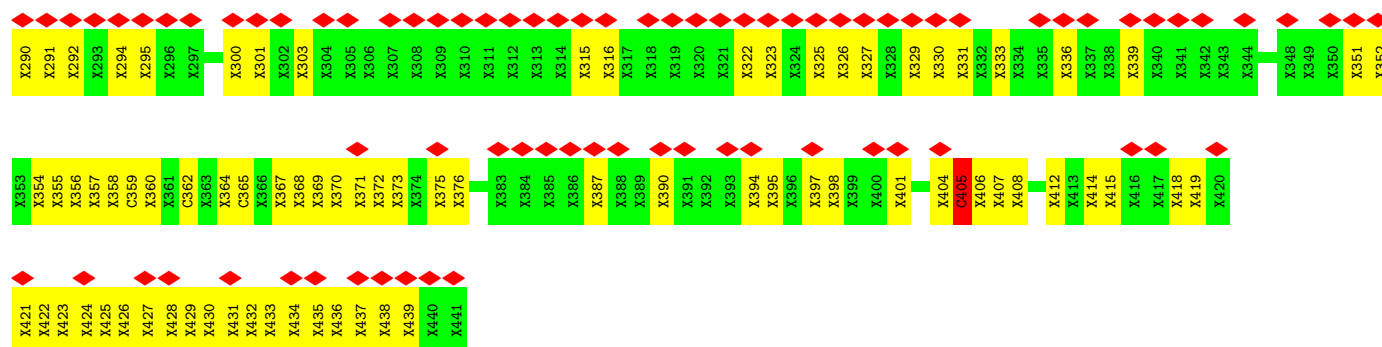


• Molecule 29: complex I

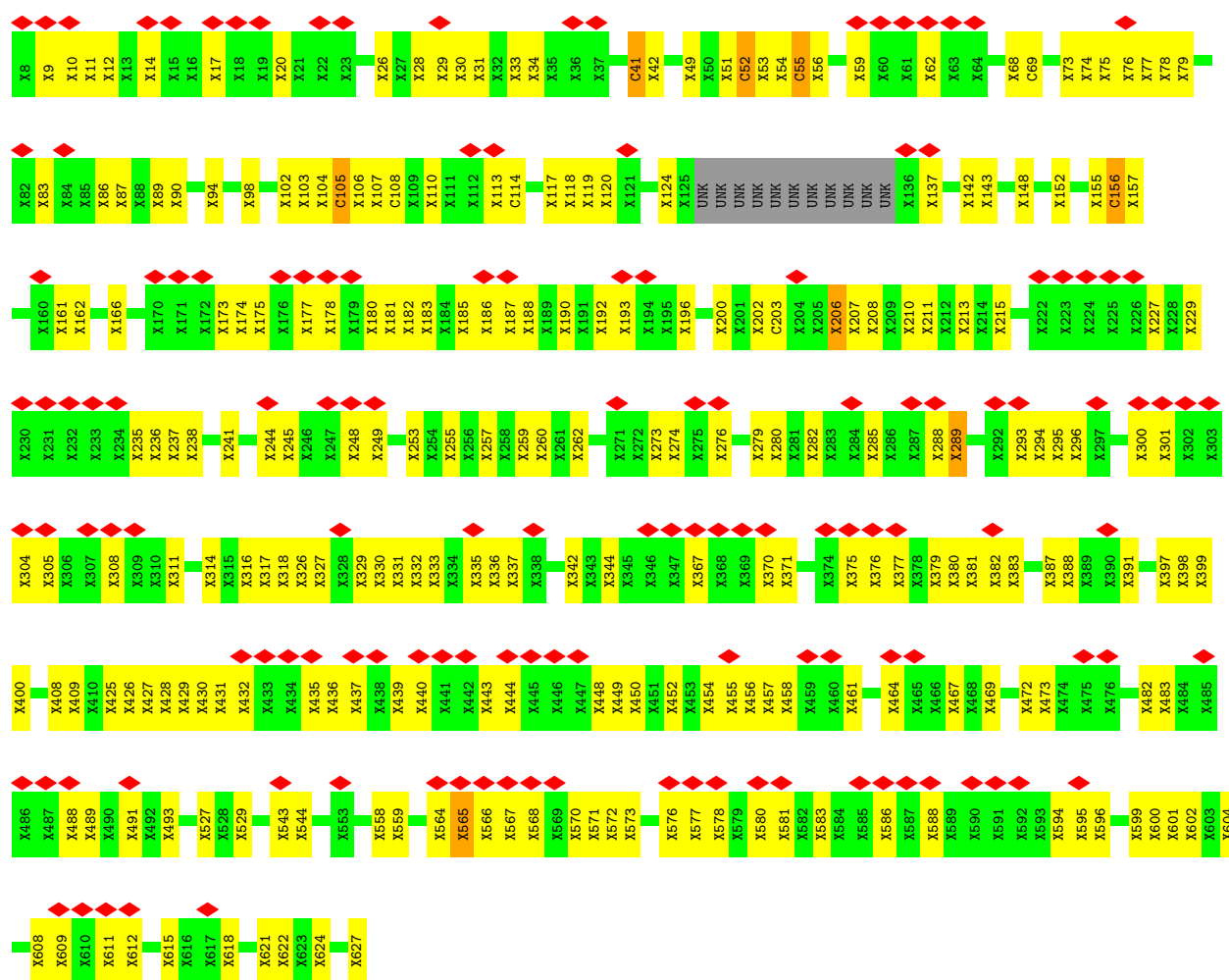


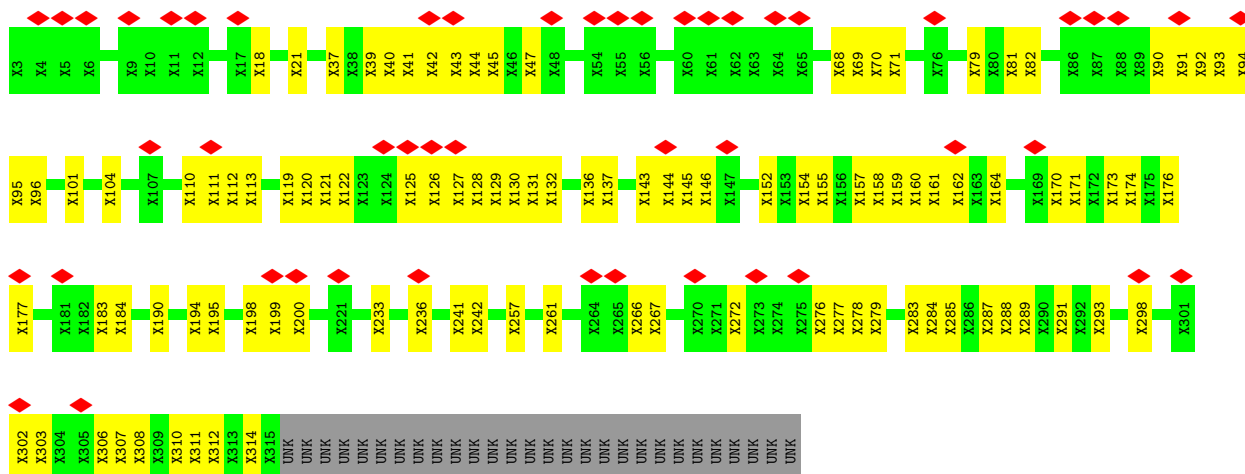
• Molecule 30: complex I



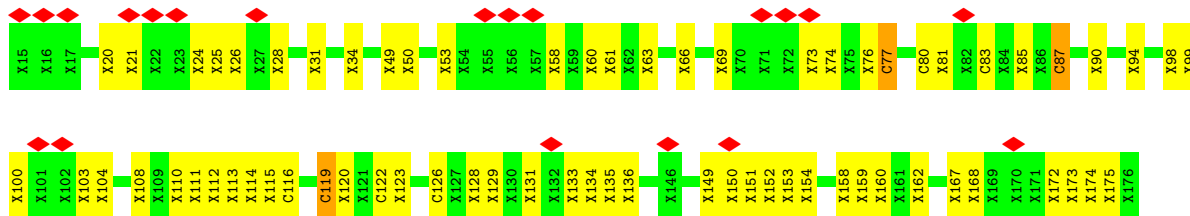


• Molecule 31: complex I

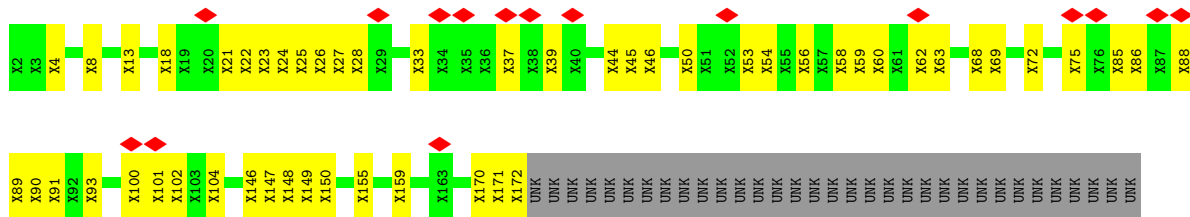




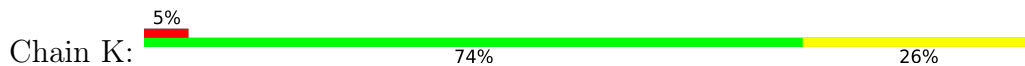
- Molecule 33: complex I



- Molecule 34: complex I

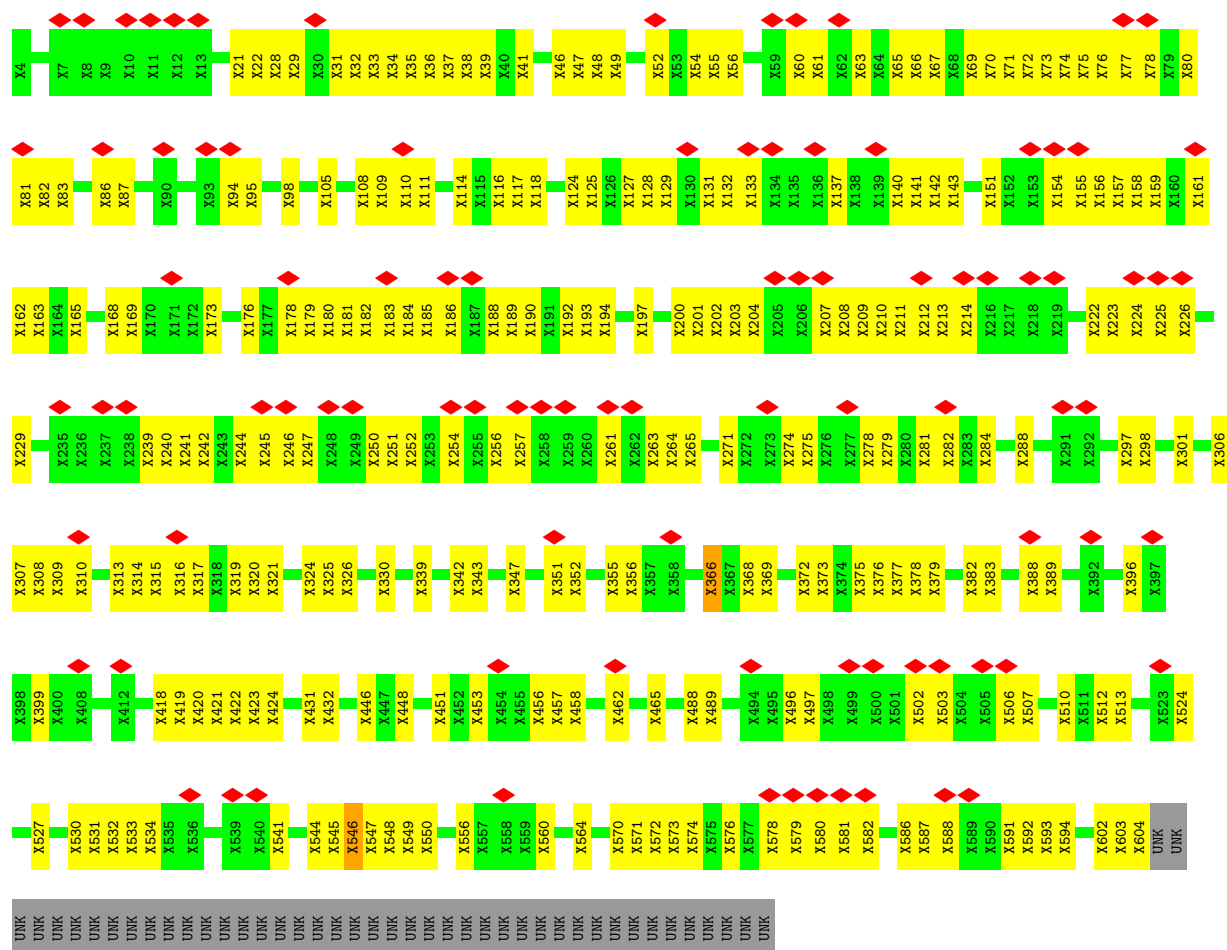


- Molecule 35: complex I

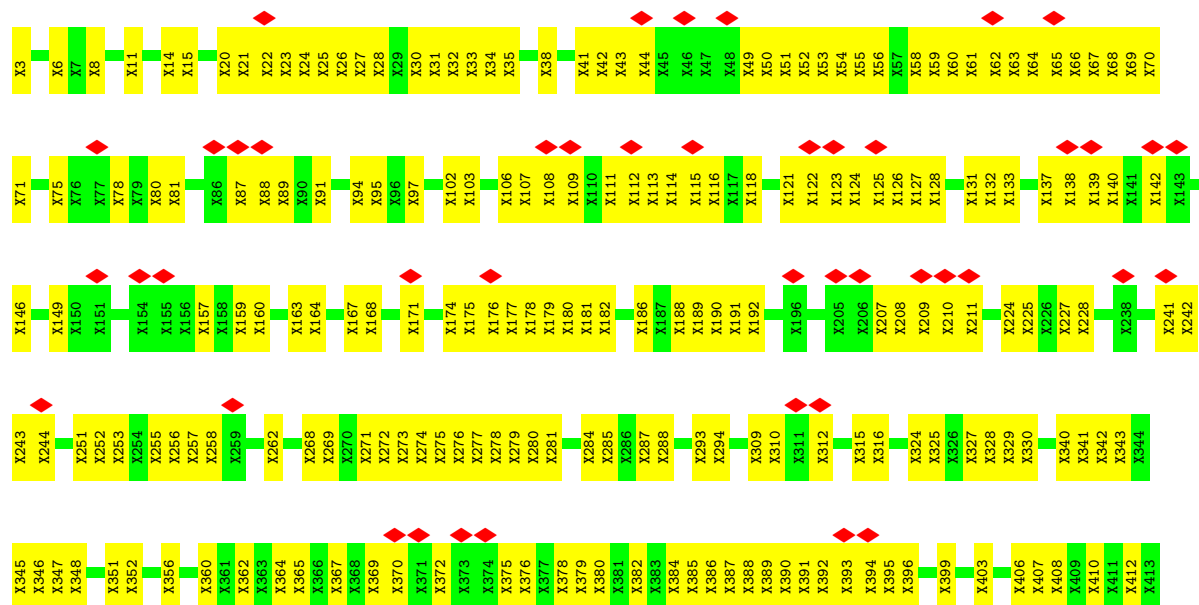


- Molecule 36: complex I

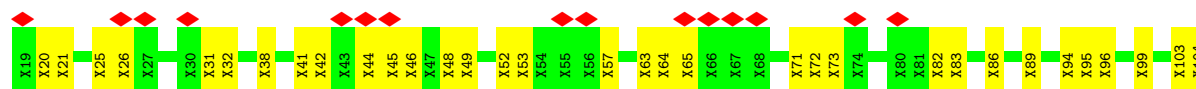
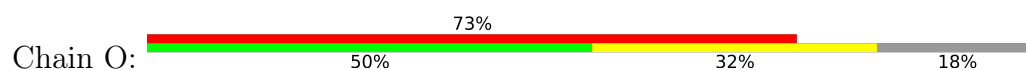




• Molecule 37: complex I

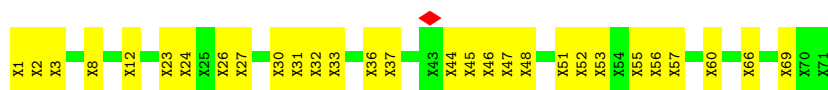


Chain N: 9% 50% 43% 6%



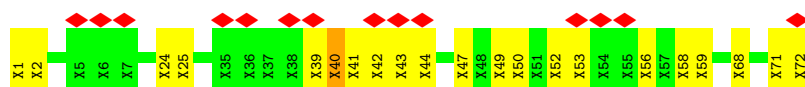
- Molecule 45: complex I

Chain V: 



- Molecule 46: complex I

Chain W: 



- Molecule 47: complex I

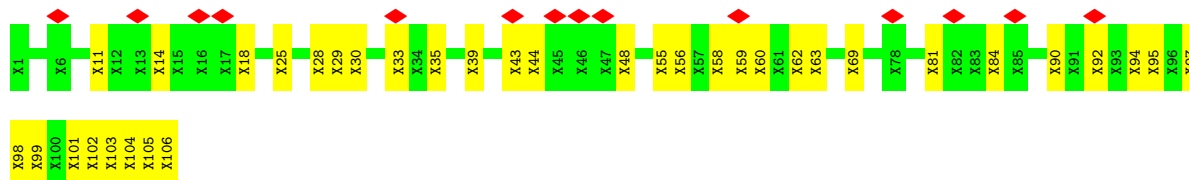
Chain X: 



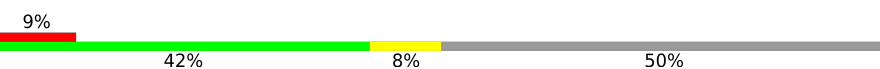
UNK

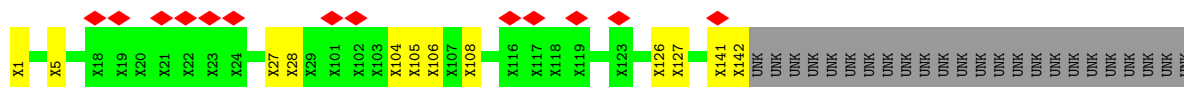
- Molecule 48: complex I

Chain Y: 

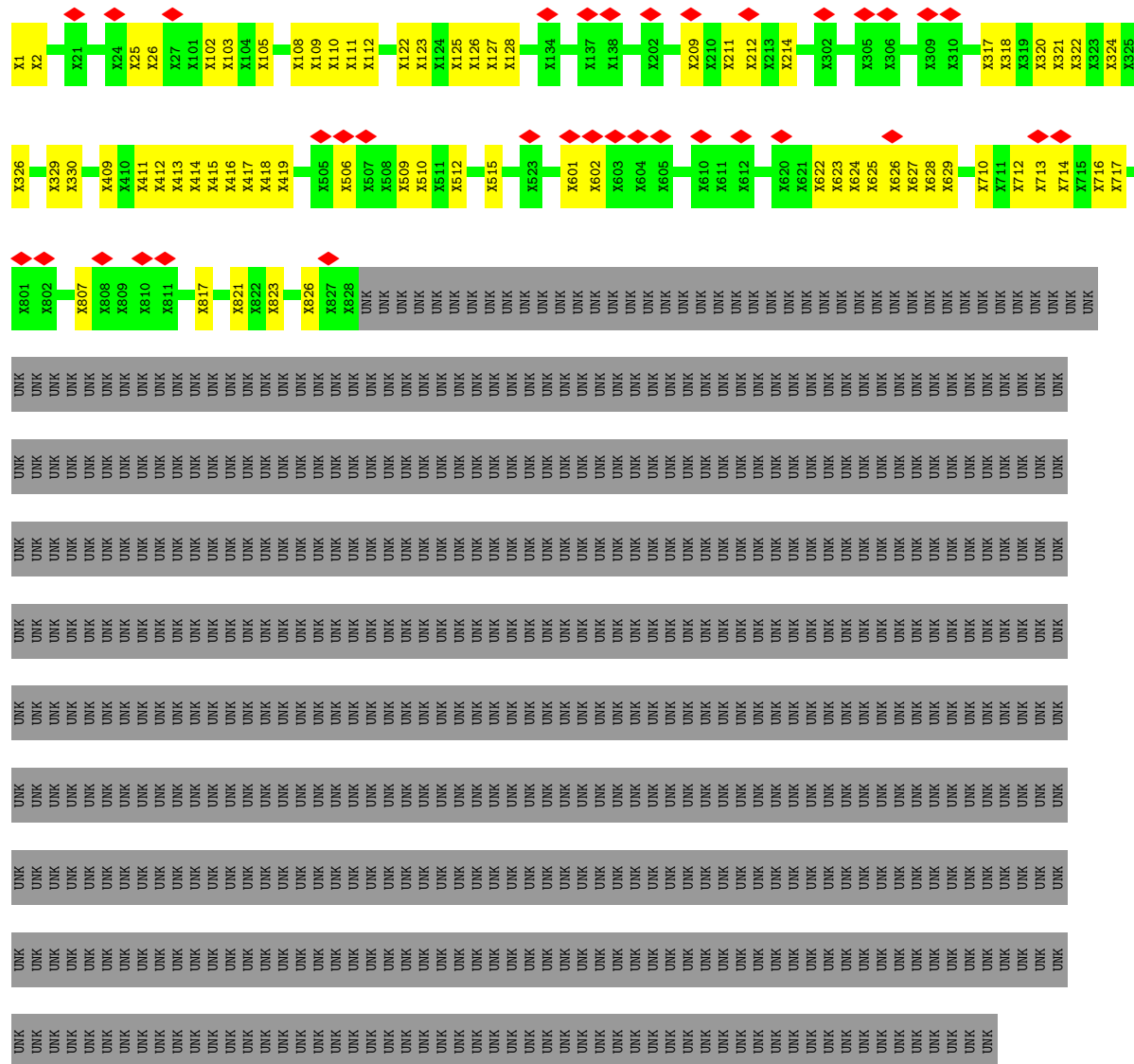


- Molecule 49: complex I

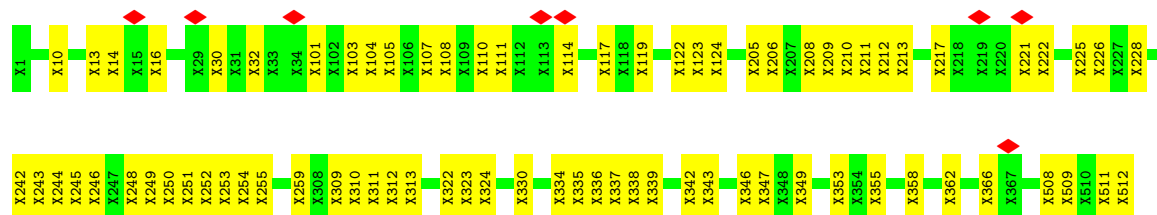
Chain a: 



Chain U: 22% 8% 70%



Chain Z: 



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	57797	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.368	Depositor
Minimum map value	-0.164	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.081	Depositor
Map size (Å)	509.76, 509.76, 509.76	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.77, 1.77, 1.77	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	c	0.77	3/3531 (0.1%)	2.02	137/4792 (2.9%)
1	l	0.82	4/3531 (0.1%)	2.03	115/4792 (2.4%)
2	m	0.67	2/3198 (0.1%)	1.89	85/4336 (2.0%)
2	n	0.65	0/3198	1.81	68/4336 (1.6%)
3	b	0.92	2/3108 (0.1%)	2.20	135/4252 (3.2%)
3	o	0.93	6/3108 (0.2%)	2.07	107/4252 (2.5%)
4	d	0.68	0/1978	1.88	55/2684 (2.0%)
4	p	0.70	2/1978 (0.1%)	1.83	54/2684 (2.0%)
5	e	0.76	0/574	2.02	15/775 (1.9%)
5	q	0.80	1/1551 (0.1%)	2.16	63/2097 (3.0%)
6	f	0.74	1/935 (0.1%)	1.84	23/1253 (1.8%)
6	r	0.74	0/935	1.94	23/1253 (1.8%)
7	g	0.73	0/704	1.89	25/951 (2.6%)
7	s	0.74	0/704	1.77	23/951 (2.4%)
8	h	0.57	0/529	1.61	10/708 (1.4%)
8	t	0.49	0/529	1.51	4/708 (0.6%)
9	i	0.61	0/250	1.88	5/335 (1.5%)
9	u	0.63	0/250	1.85	7/335 (2.1%)
10	j	0.61	0/525	1.61	8/707 (1.1%)
10	v	0.63	0/525	1.71	7/707 (1.0%)
11	k	0.54	0/163	1.34	0/225
11	w	0.59	0/163	1.52	1/225 (0.4%)
12	x	0.86	7/4164 (0.2%)	1.16	34/5688 (0.6%)
13	y	0.77	0/1868	1.12	10/2544 (0.4%)
14	z	0.74	0/2211	1.02	7/3023 (0.2%)
15	1	0.67	0/1229	0.96	3/1658 (0.2%)
16	2	0.64	0/898	1.02	6/1218 (0.5%)
17	3	0.72	0/765	1.13	4/1038 (0.4%)
18	4	0.69	0/699	1.10	6/950 (0.6%)
19	5	0.68	0/648	1.17	5/877 (0.6%)
20	6	0.71	0/611	0.94	2/810 (0.2%)
21	7	0.70	0/451	1.04	3/610 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	8	0.75	0/398	1.01	0/546
23	9	0.77	0/399	0.98	2/534 (0.4%)
24	0	0.68	0/345	0.99	1/470 (0.2%)
26	B	1.75	1/21 (4.8%)	2.41	2/23 (8.7%)
29	E	0.78	0/20	1.47	0/20
30	F	2.61	1/20 (5.0%)	2.17	0/20
31	G	0.93	0/65	1.50	0/67
33	I	2.41	2/40 (5.0%)	1.45	0/40
All	All	0.77	32/46819 (0.1%)	1.73	1055/63494 (1.7%)

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	c	0	13
1	l	0	3
2	m	0	9
2	n	0	5
3	b	0	14
3	o	0	6
4	d	0	5
4	p	0	4
5	e	0	1
5	q	0	9
6	f	0	2
7	g	0	2
7	s	0	3
8	t	0	1
9	i	0	1
9	u	0	1
10	j	0	1
11	w	0	1
26	B	0	2
27	C	0	1
28	D	0	1
30	F	0	2
31	G	0	6
33	I	0	1
36	L	0	4
38	N	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
39	O	0	2
40	P	0	3
41	Q	0	1
43	S	0	1
46	W	0	1
47	X	0	1
All	All	0	109

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	l	253	VAL	C-O	11.10	1.36	1.24
30	F	405	CYS	CA-CB	-9.65	1.34	1.53
33	I	87	CYS	CA-CB	8.98	1.71	1.53
3	o	37	LEU	C-N	-8.20	1.24	1.33
33	I	77	CYS	CA-CB	7.92	1.69	1.53
12	x	61	HIS	CG-CD2	7.60	1.44	1.35
12	x	378	HIS	ND1-CE1	7.22	1.39	1.32
3	o	221	HIS	CD2-NE2	-7.11	1.30	1.37
12	x	378	HIS	CE1-NE2	-6.53	1.26	1.32
3	o	19	ILE	CA-C	-6.43	1.44	1.52
4	p	202	LYS	C-O	6.41	1.31	1.24
3	o	44	GLN	C-N	-6.36	1.26	1.33
12	x	69	MET	SD-CE	-6.20	1.64	1.79
1	l	169	GLY	N-CA	-6.17	1.36	1.44
26	B	55	CYS	CA-CB	6.16	1.65	1.53
1	c	153	LEU	N-CA	-6.13	1.39	1.46
3	o	185	LEU	CA-CB	-6.10	1.45	1.53
3	o	328	LEU	C-N	5.94	1.41	1.33
1	l	340	GLY	C-O	-5.85	1.16	1.23
2	m	148	LYS	C-N	-5.82	1.26	1.33
12	x	61	HIS	ND1-CE1	5.63	1.38	1.32
5	q	55	VAL	C-O	-5.54	1.17	1.24
3	b	97	HIS	C-O	-5.53	1.17	1.24
1	c	373	THR	C-O	5.52	1.29	1.24
12	x	378	HIS	CG-CD2	5.51	1.42	1.35
12	x	376	HIS	ND1-CE1	5.50	1.38	1.32
6	f	68	LEU	C-O	-5.49	1.17	1.24
3	b	126	THR	N-CA	-5.48	1.39	1.46
4	p	228	SER	C-N	-5.21	1.27	1.33
1	l	333	ASP	C-O	-5.21	1.18	1.24
2	m	173	ALA	CA-CB	-5.11	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	104	LYS	CD-CE	5.06	1.67	1.52

All (1055) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	253	VAL	O-C-N	-23.32	98.92	123.18
1	l	253	VAL	CA-C-O	16.92	137.36	120.27
3	b	196	HIS	CA-CB-CG	16.15	129.95	113.80
3	o	196	HIS	CA-CB-CG	15.64	129.44	113.80
3	o	44	GLN	CA-C-N	15.25	139.76	120.70
3	o	44	GLN	C-N-CA	15.25	139.76	120.70
1	l	168	GLU	CA-C-N	14.25	144.25	121.87
1	l	168	GLU	C-N-CA	14.25	144.25	121.87
3	b	204	GLY	CA-C-N	14.23	142.08	121.02
3	b	204	GLY	C-N-CA	14.23	142.08	121.02
1	l	435	ASN	OD1-CG-ND2	13.88	136.48	122.60
1	c	168	GLU	CA-C-O	13.47	135.32	120.10
6	r	65	ALA	CA-C-O	12.87	134.16	120.90
1	c	419	CYS	CA-CB-SG	12.52	143.19	114.40
6	r	77	LYS	CG-CD-CE	11.34	137.38	111.30
1	c	251	ALA	CA-C-O	11.29	132.56	120.36
4	p	235	LEU	CA-C-O	11.29	133.87	121.11
1	l	307	PHE	CA-C-O	11.29	135.45	120.21
3	b	267	HIS	CA-CB-CG	-11.09	102.71	113.80
2	m	178	CYS	O-C-N	10.80	131.75	121.27
2	m	177	TYR	O-C-N	10.60	135.80	123.29
8	t	74	PHE	CA-CB-CG	-10.36	103.44	113.80
12	x	376	HIS	ND1-CE1-NE2	10.32	118.72	108.40
2	m	70	ARG	NE-CZ-NH2	10.27	128.45	119.20
3	o	267	HIS	CA-CB-CG	-10.25	103.55	113.80
3	o	47	THR	O-C-N	-10.23	111.54	122.07
1	l	437	ILE	N-CA-C	-10.22	100.75	111.58
1	l	334	MET	O-C-N	-10.17	110.55	122.15
1	c	294	LEU	CA-C-N	10.13	134.67	120.29
1	c	294	LEU	C-N-CA	10.13	134.67	120.29
5	e	58	PHE	CA-CB-CG	10.04	123.84	113.80
7	g	13	VAL	CA-C-O	9.95	130.83	120.39
3	b	196	HIS	CA-C-O	-9.94	110.56	121.00
8	h	74	PHE	CA-CB-CG	-9.94	103.86	113.80
9	i	75	SER	N-CA-C	9.90	121.00	107.73
4	p	228	SER	CA-C-N	9.87	133.33	120.60
4	p	228	SER	C-N-CA	9.87	133.33	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	19	ILE	O-C-N	-9.61	110.56	122.57
4	d	14	HIS	CA-CB-CG	9.54	123.34	113.80
2	m	245	ARG	NE-CZ-NH2	9.52	127.77	119.20
1	l	46	ARG	NE-CZ-NH2	-9.51	110.64	119.20
3	b	185	LEU	O-C-N	-9.47	112.90	120.38
10	v	26	VAL	CA-CB-CG1	9.45	126.47	110.40
10	v	39	ALA	O-C-N	9.43	132.12	122.12
2	n	56	ARG	CD-NE-CZ	9.20	137.28	124.40
1	l	259	GLY	CA-C-N	9.19	129.75	119.92
1	l	259	GLY	C-N-CA	9.19	129.75	119.92
3	b	41	LEU	N-CA-CB	9.17	123.74	110.16
1	c	373	THR	CA-C-O	9.17	127.06	118.44
9	u	75	SER	N-CA-C	9.08	119.90	107.73
3	b	115	ILE	CA-C-N	-9.05	109.76	119.99
3	b	115	ILE	C-N-CA	-9.05	109.76	119.99
5	q	7	VAL	CA-C-N	9.02	129.09	119.89
5	q	7	VAL	C-N-CA	9.02	129.09	119.89
2	m	178	CYS	CA-C-O	-9.02	111.27	120.02
2	m	42	ALA	CA-C-N	9.00	128.64	119.82
2	m	42	ALA	C-N-CA	9.00	128.64	119.82
3	o	47	THR	CA-C-O	8.98	130.25	120.82
2	m	254	HIS	CA-CB-CG	8.95	122.75	113.80
19	5	52	VAL	N-CA-C	8.94	121.22	108.17
5	q	166	ASP	CA-CB-CG	8.91	121.51	112.60
3	o	221	HIS	N-CA-CB	8.88	118.83	110.39
4	d	195	GLU	CA-C-N	8.82	129.70	119.47
4	d	195	GLU	C-N-CA	8.82	129.70	119.47
3	b	206	ASN	OD1-CG-ND2	8.82	131.42	122.60
19	5	81	PHE	CA-C-N	8.77	128.42	119.56
19	5	81	PHE	C-N-CA	8.77	128.42	119.56
4	d	206	LEU	CB-CA-C	-8.75	96.32	110.84
1	c	256	ALA	N-CA-C	8.70	123.24	109.50
10	v	14	PHE	CA-CB-CG	8.70	122.50	113.80
5	q	47	VAL	CA-C-O	8.66	130.06	121.05
1	c	341	GLN	O-C-N	8.64	131.42	122.09
3	b	196	HIS	O-C-N	8.63	131.01	122.03
1	l	320	LEU	CA-C-O	8.62	130.01	120.70
3	b	43	LEU	O-C-N	-8.59	112.81	122.09
5	q	192	MET	CA-C-O	8.55	129.30	120.24
3	b	175	LEU	N-CA-CB	8.51	123.41	110.30
1	c	292	SER	CA-C-O	8.47	125.59	119.32
2	m	85	ILE	CB-CA-C	-8.45	101.07	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	434	TYR	CA-C-O	-8.43	111.52	120.63
2	m	92	VAL	O-C-N	-8.43	114.49	122.16
5	q	183	PRO	CA-C-O	-8.43	110.18	122.31
6	f	60	PHE	CA-CB-CG	-8.42	105.38	113.80
3	b	182	HIS	CA-CB-CG	8.38	122.18	113.80
3	b	246	ALA	N-CA-CB	-8.36	101.26	110.71
3	o	322	GLN	OE1-CD-NE2	8.25	130.85	122.60
2	m	369	LEU	CA-C-O	8.25	129.19	120.70
3	o	182	HIS	CA-CB-CG	8.24	122.04	113.80
3	o	242	LEU	CB-CA-C	-8.24	98.18	110.95
6	f	43	VAL	CA-C-O	8.23	131.07	120.78
7	g	13	VAL	O-C-N	-8.21	114.39	123.26
2	m	148	LYS	CA-C-N	8.16	131.05	120.44
2	m	148	LYS	C-N-CA	8.16	131.05	120.44
6	f	64	ARG	CD-NE-CZ	-8.16	112.98	124.40
1	l	419	CYS	CA-C-N	8.16	128.21	119.89
1	l	419	CYS	C-N-CA	8.16	128.21	119.89
5	q	58	PHE	CA-CB-CG	8.15	121.95	113.80
6	r	63	LYS	CB-CA-C	8.14	123.66	110.88
23	9	20	ARG	N-CA-C	-8.11	102.52	111.36
3	b	216	ASP	CA-CB-CG	8.11	120.71	112.60
5	e	60	SER	N-CA-C	-8.09	103.42	113.28
1	c	294	LEU	O-C-N	-8.04	113.60	122.12
2	n	141	GLN	OE1-CD-NE2	-8.03	114.57	122.60
12	x	82	LEU	N-CA-C	8.01	122.32	112.23
5	q	55	VAL	CA-CB-CG1	8.01	124.01	110.40
3	b	43	LEU	CA-C-O	8.00	128.94	120.70
6	f	27	ASN	CA-C-O	8.00	129.46	120.90
1	l	323	HIS	CA-CB-CG	7.99	121.79	113.80
1	c	341	GLN	CA-C-O	-7.97	112.49	120.70
1	c	431	LEU	CA-C-N	7.96	129.79	119.84
1	c	431	LEU	C-N-CA	7.96	129.79	119.84
4	p	202	LYS	CA-C-O	-7.96	112.47	120.82
3	b	13	ILE	CB-CA-C	-7.95	101.40	112.14
12	x	378	HIS	ND1-CE1-NE2	7.95	116.35	108.40
2	n	162	ASN	CA-CB-CG	-7.94	104.66	112.60
12	x	56	VAL	N-CA-C	-7.86	103.14	110.53
2	m	320	GLY	O-C-N	-7.86	117.90	123.95
5	q	183	PRO	O-C-N	7.86	132.14	122.71
1	c	168	GLU	O-C-N	-7.84	113.04	122.22
3	o	257	THR	N-CA-CB	7.84	121.46	110.01
4	p	7	PRO	N-CA-C	7.84	120.26	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	30	TRP	CA-C-O	7.84	129.09	120.63
5	q	7	VAL	O-C-N	7.82	130.01	121.10
5	q	135	LEU	O-C-N	-7.81	113.63	123.24
4	d	97	ASN	CA-C-N	7.80	129.59	119.84
4	d	97	ASN	C-N-CA	7.80	129.59	119.84
1	l	325	VAL	O-C-N	-7.80	114.38	123.03
4	d	120	ARG	NE-CZ-NH2	-7.78	112.20	119.20
3	b	33	PHE	CG-CD2-CE2	7.74	133.85	120.70
3	b	321	SER	CA-C-N	7.73	131.41	120.28
3	b	321	SER	C-N-CA	7.73	131.41	120.28
3	b	303	LEU	N-CA-CB	7.73	121.59	110.16
1	c	438	ARG	NE-CZ-NH2	7.72	126.15	119.20
3	b	195	VAL	CA-C-O	-7.71	112.93	120.95
2	n	412	ASN	OD1-CG-ND2	7.71	130.31	122.60
26	B	55	CYS	CA-CB-SG	-7.69	96.70	114.40
7	s	15	THR	CA-CB-CG2	-7.67	97.46	110.50
3	o	82	MET	CA-C-O	7.67	128.54	120.42
1	l	420	PRO	N-CA-CB	7.66	109.76	103.32
12	x	435	GLY	N-CA-C	7.66	126.07	115.27
1	l	392	LEU	N-CA-C	7.64	120.28	111.11
5	q	168	SER	N-CA-C	-7.63	103.97	113.28
3	b	185	LEU	CA-C-O	7.63	126.33	119.08
1	c	242	CYS	CA-C-O	7.62	128.74	120.43
3	b	123	VAL	CA-C-O	7.61	129.24	120.03
2	n	145	ARG	O-C-N	7.61	129.91	122.07
2	m	179	PRO	N-CA-CB	7.60	110.41	103.34
5	q	56	SER	CA-C-O	7.58	128.78	120.82
1	c	441	MET	CA-CB-CG	-7.56	98.98	114.10
10	v	39	ALA	CA-C-O	-7.56	112.54	120.55
3	o	149	LEU	CA-C-O	7.55	128.86	119.05
3	b	85	ASN	CA-CB-CG	-7.55	105.05	112.60
2	m	56	ARG	CD-NE-CZ	7.53	134.94	124.40
3	b	273	TYR	CA-C-N	-7.50	110.33	122.26
3	b	273	TYR	C-N-CA	-7.50	110.33	122.26
1	l	434	TYR	O-C-N	-7.50	114.29	122.09
3	o	242	LEU	N-CA-CB	7.49	120.84	109.98
1	c	323	HIS	CA-CB-CG	7.49	121.29	113.80
3	o	71	ARG	NE-CZ-NH1	-7.49	114.01	121.50
3	b	303	LEU	N-CA-C	7.49	119.52	111.36
1	c	244	ARG	NE-CZ-NH2	7.46	125.92	119.20
5	q	179	ASN	CA-CB-CG	7.45	120.05	112.60
6	r	65	ALA	O-C-N	-7.44	113.99	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	26	PHE	CA-C-N	7.44	129.14	119.84
7	g	26	PHE	C-N-CA	7.44	129.14	119.84
4	d	201	ARG	NE-CZ-NH1	-7.41	114.09	121.50
7	g	13	VAL	CA-C-N	-7.41	110.72	122.64
7	g	13	VAL	C-N-CA	-7.41	110.72	122.64
3	b	106	SER	CA-C-O	7.40	128.52	119.79
4	p	235	LEU	O-C-N	-7.39	113.59	123.19
1	c	364	ALA	O-C-N	7.38	129.94	122.12
24	0	27	LEU	N-CA-C	7.38	119.41	111.36
4	d	160	MET	N-CA-C	7.37	120.43	108.41
3	o	80	ARG	CD-NE-CZ	-7.37	114.08	124.40
3	b	205	SER	O-C-N	-7.36	113.22	123.01
1	l	275	ALA	N-CA-C	-7.36	103.19	111.07
12	x	330	GLY	N-CA-C	7.36	120.42	112.33
1	l	442	PHE	CA-CB-CG	7.35	121.15	113.80
3	b	221	HIS	CA-CB-CG	-7.34	106.45	113.80
3	b	313	ARG	NE-CZ-NH2	7.34	125.81	119.20
3	b	195	VAL	O-C-N	7.31	128.96	121.87
2	m	92	VAL	CA-C-O	7.30	127.02	119.35
3	b	30	TRP	O-C-N	-7.30	114.38	122.12
3	o	222	PRO	CA-C-N	7.29	131.83	120.89
3	o	222	PRO	C-N-CA	7.29	131.83	120.89
1	c	435	ASN	CA-C-O	7.28	128.34	119.97
1	l	256	ALA	CB-CA-C	-7.24	93.48	109.56
2	n	188	PRO	O-C-N	-7.24	112.86	122.64
3	b	113	TRP	O-C-N	-7.23	114.57	122.09
1	l	424	GLY	CA-C-O	-7.23	113.60	121.48
5	q	5	ILE	CB-CA-C	-7.22	101.09	111.34
1	c	419	CYS	N-CA-CB	7.21	119.68	110.23
3	o	88	SER	N-CA-C	-7.21	103.35	111.07
6	f	73	GLN	CB-CA-C	7.21	122.36	109.38
4	d	215	LEU	CA-C-O	7.21	128.50	119.78
1	c	281	ASP	CA-C-N	7.20	130.25	120.38
1	c	281	ASP	C-N-CA	7.20	130.25	120.38
2	n	385	GLN	CA-C-O	7.20	128.05	120.42
12	x	9	SER	N-CA-C	7.17	119.83	110.43
3	b	106	SER	N-CA-C	-7.17	103.20	112.23
3	o	256	TYR	N-CA-C	-7.16	104.48	112.57
1	l	417	ASP	CA-C-N	-7.15	109.73	122.74
1	l	417	ASP	C-N-CA	-7.15	109.73	122.74
5	q	193	VAL	CG1-CB-CG2	7.14	126.51	110.80
5	e	14	ARG	CA-C-N	-7.13	113.69	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	14	ARG	C-N-CA	-7.13	113.69	123.96
4	p	199	ASP	CA-C-O	-7.13	113.33	120.82
4	d	175	THR	CA-C-O	7.12	125.78	119.59
1	c	343	MET	CA-CB-CG	-7.12	99.87	114.10
3	o	37	LEU	CA-C-N	7.11	127.83	120.00
3	o	37	LEU	C-N-CA	7.11	127.83	120.00
6	r	60	PHE	CA-CB-CG	-7.11	106.69	113.80
16	2	76	GLY	CA-C-N	7.11	128.34	120.45
16	2	76	GLY	C-N-CA	7.11	128.34	120.45
3	b	264	THR	CB-CA-C	-7.10	100.42	109.65
16	2	42	VAL	N-CA-C	-7.10	99.68	108.05
12	x	376	HIS	CE1-NE2-CD2	-7.09	101.91	109.00
7	s	21	PHE	CA-CB-CG	-7.09	106.71	113.80
1	c	242	CYS	O-C-N	-7.08	115.27	123.27
2	n	291	ALA	N-CA-C	-7.08	104.77	113.41
12	x	332	ILE	N-CA-C	7.08	118.92	109.37
1	l	138	LEU	CA-C-O	-7.07	112.75	121.02
1	l	443	TRP	N-CA-C	7.07	121.69	107.41
3	o	231	GLY	CA-C-O	7.07	128.07	120.30
5	q	72	SER	CA-C-O	-7.05	113.26	121.16
3	o	244	LEU	O-C-N	7.04	131.54	122.10
3	b	40	CYS	N-CA-C	-7.04	103.36	112.23
2	m	108	THR	N-CA-C	7.03	119.92	110.35
3	o	196	HIS	CE1-NE2-CD2	-7.01	101.99	109.00
6	r	50	LEU	CA-C-N	7.00	128.59	119.84
6	r	50	LEU	C-N-CA	7.00	128.59	119.84
5	q	135	LEU	CA-C-N	7.00	133.59	122.33
5	q	135	LEU	C-N-CA	7.00	133.59	122.33
5	q	182	VAL	CA-C-O	-6.97	116.14	120.88
1	l	414	TYR	N-CA-C	6.96	121.01	112.23
4	p	83	ARG	CA-C-N	6.96	126.99	119.89
4	p	83	ARG	C-N-CA	6.96	126.99	119.89
3	o	230	LEU	CA-C-N	6.96	129.05	120.22
3	o	230	LEU	C-N-CA	6.96	129.05	120.22
6	f	45	GLU	CA-C-N	-6.94	111.49	120.65
6	f	45	GLU	C-N-CA	-6.94	111.49	120.65
3	b	201	HIS	CA-CB-CG	-6.94	106.86	113.80
14	z	36	HIS	N-CA-C	6.94	122.17	113.43
2	m	97	SER	N-CA-C	6.93	120.97	109.46
3	o	284	ILE	CA-C-O	6.93	123.69	119.19
7	g	12	HIS	CA-C-N	-6.91	114.08	123.14
7	g	12	HIS	C-N-CA	-6.91	114.08	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	187	THR	N-CA-C	6.91	118.78	110.07
12	x	130	PRO	N-CA-C	-6.90	102.28	110.70
1	c	283	THR	N-CA-C	6.89	121.29	113.02
6	f	61	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	c	415	PHE	O-C-N	-6.88	111.81	122.13
2	m	70	ARG	NE-CZ-NH1	-6.88	114.62	121.50
5	q	87	MET	CA-C-O	6.87	127.81	120.46
2	n	186	VAL	N-CA-CB	6.87	119.32	111.90
5	e	61	SER	CA-CB-OG	-6.84	97.41	111.10
5	q	25	SER	CA-C-O	6.83	126.94	119.15
2	m	346	THR	CA-CB-OG1	6.82	119.84	109.60
4	p	218	LEU	N-CA-CB	6.82	119.87	109.91
3	b	135	TRP	CA-C-O	-6.80	113.69	121.65
5	q	14	ARG	NE-CZ-NH1	-6.80	114.70	121.50
3	o	241	LEU	O-C-N	6.79	129.89	122.15
1	c	338	LEU	CA-C-O	6.78	128.12	121.00
2	m	173	ALA	CA-C-O	6.78	128.00	119.12
3	o	298	ILE	N-CA-C	6.78	116.90	110.53
1	c	436	ARG	O-C-N	6.78	129.41	122.09
1	l	320	LEU	O-C-N	-6.78	114.42	123.23
5	q	34	GLY	N-CA-C	-6.77	104.30	112.49
4	p	97	ASN	CA-C-N	6.77	128.30	119.84
4	p	97	ASN	C-N-CA	6.77	128.30	119.84
12	x	507	GLU	N-CA-C	-6.76	97.87	109.15
2	n	258	VAL	N-CA-C	6.75	117.26	108.35
5	q	194	ILE	N-CA-CB	-6.74	103.40	111.90
15	l	133	GLY	N-CA-C	6.74	129.16	113.18
10	j	14	PHE	CA-CB-CG	6.74	120.54	113.80
1	l	334	MET	N-CA-CB	-6.74	100.18	110.16
3	o	13	ILE	CB-CA-C	-6.73	103.20	112.02
3	o	328	LEU	CA-C-N	-6.73	112.08	120.56
3	o	328	LEU	C-N-CA	-6.73	112.08	120.56
1	c	259	GLY	CA-C-N	6.70	128.21	119.84
1	c	259	GLY	C-N-CA	6.70	128.21	119.84
2	n	141	GLN	CA-C-N	6.69	128.21	119.84
2	n	141	GLN	C-N-CA	6.69	128.21	119.84
5	q	192	MET	N-CA-C	6.68	119.30	108.34
3	b	143	ALA	N-CA-C	-6.68	104.08	111.36
2	m	102	ARG	NE-CZ-NH2	6.68	125.21	119.20
18	4	5	LYS	N-CA-C	6.67	125.01	110.80
1	l	334	MET	CA-C-O	6.67	127.49	120.42
4	d	7	PRO	N-CA-C	6.66	118.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	177	TYR	CA-C-O	-6.66	113.12	120.38
6	r	35	ASP	CA-C-O	6.65	127.56	119.31
2	m	143	GLN	OE1-CD-NE2	-6.65	115.95	122.60
3	b	218	ILE	O-C-N	6.65	128.68	121.10
2	n	173	ALA	CA-C-O	6.64	127.61	119.11
16	2	81	ILE	N-CA-C	6.64	116.77	110.53
3	b	109	PHE	CA-CB-CG	6.64	120.44	113.80
12	x	74	MET	N-CA-C	6.62	118.16	111.07
3	b	186	PRO	O-C-N	-6.61	114.64	122.24
3	o	222	PRO	CB-CA-C	6.61	122.47	111.56
4	d	32	VAL	N-CA-CB	6.61	117.84	110.51
1	c	169	GLY	CA-C-N	6.59	128.08	119.84
1	c	169	GLY	C-N-CA	6.59	128.08	119.84
9	i	68	VAL	CB-CA-C	-6.59	101.69	110.98
6	r	79	GLN	N-CA-C	6.59	120.31	112.93
1	l	268	VAL	N-CA-C	-6.58	106.38	112.96
3	b	246	ALA	O-C-N	6.58	125.99	121.19
3	o	19	ILE	CA-C-N	6.57	134.28	122.06
3	o	19	ILE	C-N-CA	6.57	134.28	122.06
3	o	299	LEU	CA-C-O	6.57	127.44	119.49
1	c	331	ILE	N-CA-C	6.57	117.25	110.36
4	d	92	PRO	N-CA-CB	6.57	107.63	103.23
5	e	14	ARG	CD-NE-CZ	-6.57	115.21	124.40
1	c	436	ARG	N-CA-CB	6.56	119.59	110.07
5	q	129	LYS	CA-C-N	6.56	128.04	119.84
5	q	129	LYS	C-N-CA	6.56	128.04	119.84
12	x	61	HIS	CB-CG-CD2	-6.56	122.67	131.20
3	o	93	CYS	N-CA-CB	6.55	119.85	110.16
2	n	62	ASN	CA-CB-CG	6.55	119.15	112.60
3	b	322	GLN	OE1-CD-NE2	6.54	129.14	122.60
1	l	307	PHE	O-C-N	-6.54	115.40	123.44
4	d	83	ARG	CA-C-N	6.53	126.55	119.89
4	d	83	ARG	C-N-CA	6.53	126.55	119.89
1	c	199	ALA	CA-C-N	-6.52	112.35	122.59
1	c	199	ALA	C-N-CA	-6.52	112.35	122.59
5	q	24	SER	N-CA-C	6.52	119.68	110.23
8	h	67	HIS	CA-CB-CG	6.52	120.32	113.80
3	o	244	LEU	CA-C-O	-6.50	111.90	119.64
2	m	75	LEU	CA-C-O	-6.50	114.47	121.94
4	d	229	VAL	CB-CA-C	-6.49	103.66	111.97
12	x	506	GLU	N-CA-C	-6.49	104.21	111.28
3	b	312	GLN	O-C-N	-6.48	114.72	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	187	THR	CA-C-N	6.48	127.94	119.84
2	m	187	THR	C-N-CA	6.48	127.94	119.84
2	m	91	ALA	CA-C-N	6.47	132.33	122.69
2	m	91	ALA	C-N-CA	6.47	132.33	122.69
5	q	70	ALA	CA-C-O	6.46	127.27	120.42
1	c	189	HIS	CA-CB-CG	6.46	120.26	113.80
3	b	230	LEU	CA-C-N	6.46	127.28	119.99
3	b	230	LEU	C-N-CA	6.46	127.28	119.99
2	m	29	LEU	CA-C-N	6.45	126.21	119.05
2	m	29	LEU	C-N-CA	6.45	126.21	119.05
7	s	26	PHE	CA-C-N	6.45	127.91	119.84
7	s	26	PHE	C-N-CA	6.45	127.91	119.84
3	b	293	ALA	CA-C-N	-6.45	111.13	120.29
3	b	293	ALA	C-N-CA	-6.45	111.13	120.29
3	o	80	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	l	100	LYS	CA-C-O	-6.45	113.41	120.43
12	x	61	HIS	ND1-CE1-NE2	6.45	114.85	108.40
6	r	36	THR	CA-CB-CG2	6.44	121.44	110.50
1	c	435	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	c	438	ARG	NE-CZ-NH1	-6.43	115.07	121.50
5	e	6	LYS	O-C-N	-6.42	115.43	123.27
1	c	420	PRO	N-CA-CB	6.42	109.43	103.39
3	b	224	TYR	N-CA-C	6.41	120.37	112.54
1	l	174	VAL	CA-CB-CG1	6.40	121.28	110.40
1	c	280	TYR	O-C-N	-6.40	116.10	123.33
1	c	147	ASP	CA-C-O	6.39	127.33	120.24
5	e	5	ILE	CB-CA-C	-6.39	102.45	111.21
2	n	178	CYS	CA-C-N	6.38	126.14	119.76
2	n	178	CYS	C-N-CA	6.38	126.14	119.76
7	g	4	PHE	CA-CB-CG	-6.37	107.43	113.80
2	n	204	MET	N-CA-C	6.37	120.42	110.17
3	b	109	PHE	O-C-N	-6.37	114.12	122.59
5	q	29	SER	N-CA-C	6.36	120.76	113.19
2	m	73	SER	CA-C-O	-6.36	111.42	120.51
3	b	107	TYR	CA-C-N	-6.35	111.68	120.38
3	b	107	TYR	C-N-CA	-6.35	111.68	120.38
6	f	14	GLU	CA-C-N	6.35	126.98	120.00
6	f	14	GLU	C-N-CA	6.35	126.98	120.00
1	l	150	PHE	CA-CB-CG	6.34	120.14	113.80
1	c	436	ARG	CA-C-O	-6.34	114.17	120.70
1	l	239	SER	CA-C-O	-6.33	114.23	121.58
1	c	11	VAL	CA-C-N	6.33	127.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	11	VAL	C-N-CA	6.33	127.75	119.84
3	o	256	TYR	O-C-N	6.33	130.36	122.19
1	c	24	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	c	150	PHE	CA-CB-CG	6.32	120.12	113.80
1	c	251	ALA	CA-C-N	-6.31	114.38	122.77
1	c	251	ALA	C-N-CA	-6.31	114.38	122.77
6	r	24	ALA	CA-C-O	6.30	129.52	120.51
2	n	254	HIS	CA-C-O	-6.29	113.90	120.70
4	d	168	VAL	CB-CA-C	-6.29	103.81	112.24
2	m	145	ARG	CA-C-O	-6.29	114.17	120.90
1	c	434	TYR	O-C-N	6.29	128.78	122.12
1	c	32	GLN	CA-C-N	6.29	127.70	119.84
1	c	32	GLN	C-N-CA	6.29	127.70	119.84
3	b	301	LEU	N-CA-C	6.29	118.65	111.11
2	m	89	ILE	CA-CB-CG2	6.28	121.17	110.50
2	m	291	ALA	N-CA-C	-6.28	105.75	113.41
12	x	10	THR	N-CA-C	-6.27	103.81	112.03
16	2	21	LYS	CA-C-N	6.26	126.46	119.32
16	2	21	LYS	C-N-CA	6.26	126.46	119.32
3	o	325	PHE	O-C-N	6.26	128.54	122.03
7	g	14	ILE	CA-C-N	6.26	132.01	122.93
7	g	14	ILE	C-N-CA	6.26	132.01	122.93
3	b	231	GLY	CA-C-O	6.25	127.48	121.05
1	l	319	LEU	N-CA-CB	-6.24	100.76	110.55
1	c	196	VAL	CA-C-O	-6.24	113.90	120.76
2	n	167	ALA	CA-C-O	6.24	127.14	119.97
3	b	78	ILE	CA-C-N	-6.24	111.56	120.42
3	b	78	ILE	C-N-CA	-6.24	111.56	120.42
7	s	34	ILE	CA-C-N	6.23	125.72	119.24
7	s	34	ILE	C-N-CA	6.23	125.72	119.24
18	4	2	SER	N-CA-C	6.23	119.52	109.79
1	c	69	ASN	O-C-N	-6.23	115.55	122.03
1	l	342	TRP	CA-C-N	6.22	128.94	120.54
1	l	342	TRP	C-N-CA	6.22	128.94	120.54
4	p	110	PRO	CA-C-N	6.22	126.16	119.76
4	p	110	PRO	C-N-CA	6.22	126.16	119.76
5	q	14	ARG	CD-NE-CZ	-6.21	115.70	124.40
1	l	416	TYR	N-CA-C	6.20	118.28	108.67
5	q	123	ASP	CA-CB-CG	-6.20	106.40	112.60
1	c	343	MET	CA-C-N	-6.20	111.88	120.38
1	c	343	MET	C-N-CA	-6.20	111.88	120.38
5	q	153	PHE	CA-CB-CG	6.19	119.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	s	58	VAL	N-CA-CB	6.19	117.38	110.51
1	l	161	THR	CA-C-N	6.19	126.65	119.47
1	l	161	THR	C-N-CA	6.19	126.65	119.47
3	o	233	LEU	O-C-N	6.18	128.52	122.09
7	g	21	PHE	CA-CB-CG	-6.17	107.63	113.80
1	l	277	ILE	CA-C-O	-6.17	114.85	121.27
1	c	392	LEU	N-CA-CB	6.17	119.14	109.94
2	m	306	PRO	N-CA-CB	6.17	108.24	103.30
10	j	8	ARG	CA-C-N	6.17	128.87	120.54
10	j	8	ARG	C-N-CA	6.17	128.87	120.54
5	e	29	SER	N-CA-C	6.17	120.27	112.87
6	r	98	ILE	CA-C-O	6.15	127.67	121.27
1	c	408	ARG	NH1-CZ-NH2	6.15	127.30	119.30
3	b	180	ALA	N-CA-CB	6.14	119.22	110.13
1	c	440	GLY	CA-C-N	-6.13	112.01	122.56
1	c	440	GLY	C-N-CA	-6.13	112.01	122.56
4	p	160	MET	N-CA-C	6.13	118.74	108.02
1	l	142	ASP	N-CA-C	-6.12	105.77	113.18
2	n	66	SER	N-CA-CB	6.12	118.88	110.01
2	m	46	ARG	N-CA-C	6.11	118.37	107.80
5	q	66	ALA	CA-C-O	6.11	127.12	119.12
12	x	170	ASN	N-CA-C	6.09	120.78	113.23
2	n	412	ASN	CB-CG-ND2	-6.09	107.27	116.40
6	r	58	ARG	NE-CZ-NH2	6.08	124.67	119.20
12	x	157	SER	N-CA-C	6.08	118.87	111.82
3	o	221	HIS	CB-CA-C	-6.07	104.03	113.57
1	c	338	LEU	O-C-N	-6.07	115.72	122.03
1	c	153	LEU	N-CA-CB	6.07	119.05	109.82
2	n	87	ARG	O-C-N	6.07	129.32	122.22
1	c	418	GLN	CA-C-N	-6.06	113.18	121.61
1	c	418	GLN	C-N-CA	-6.06	113.18	121.61
1	l	292	SER	CA-C-N	6.06	127.42	119.84
1	l	292	SER	C-N-CA	6.06	127.42	119.84
3	o	196	HIS	ND1-CE1-NE2	6.06	114.46	108.40
19	5	63	LEU	N-CA-C	6.06	119.14	111.69
3	b	13	ILE	CA-CB-CG1	6.05	120.68	110.40
13	y	47	THR	N-CA-C	6.05	119.97	112.59
7	s	10	VAL	CA-C-O	-6.04	114.17	120.27
5	e	32	ARG	NE-CZ-NH1	-6.03	115.47	121.50
3	b	186	PRO	CA-C-O	6.03	130.03	119.84
3	b	280	ILE	N-CA-CB	6.03	118.00	110.47
1	l	205	HIS	CA-CB-CG	-6.02	107.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	292	SER	O-C-N	-6.01	115.82	121.35
2	n	143	GLN	OE1-CD-NE2	-6.01	116.59	122.60
2	m	409	ASP	CA-C-N	6.01	128.65	120.77
2	m	409	ASP	C-N-CA	6.01	128.65	120.77
1	l	54	GLY	O-C-N	6.01	127.68	121.97
1	c	277	ILE	CB-CA-C	-6.01	104.03	112.14
2	m	102	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	l	416	TYR	CA-C-O	-6.01	113.81	120.60
2	n	85	ILE	O-C-N	6.00	130.08	122.57
3	b	179	PHE	CA-CB-CG	6.00	119.80	113.80
3	o	320	LEU	CA-C-N	-6.00	111.20	120.31
3	o	320	LEU	C-N-CA	-6.00	111.20	120.31
2	m	187	THR	CA-C-O	-5.99	115.21	120.60
10	j	22	LEU	N-CA-C	-5.99	104.67	111.07
12	x	125	GLY	N-CA-C	-5.98	104.16	112.18
2	n	306	PRO	N-CA-CB	5.98	108.08	103.30
18	4	44	ARG	CA-C-N	5.98	126.00	119.90
18	4	44	ARG	C-N-CA	5.98	126.00	119.90
4	d	86	LYS	N-CA-C	5.97	118.47	110.35
1	l	438	ARG	CA-CB-CG	-5.97	102.17	114.10
7	s	4	PHE	CA-CB-CG	-5.97	107.83	113.80
1	c	220	SER	CA-C-N	5.96	126.94	120.44
1	c	220	SER	C-N-CA	5.96	126.94	120.44
3	b	257	THR	CA-C-O	5.96	123.73	119.32
1	c	440	GLY	N-CA-C	-5.96	107.51	115.32
3	b	19	ILE	CA-C-O	-5.96	113.87	120.96
1	c	166	SER	CA-C-O	5.96	127.83	121.16
1	c	425	PHE	N-CA-CB	5.96	121.09	110.79
7	s	50	PRO	N-CA-C	5.96	117.97	110.70
4	d	110	PRO	CA-C-N	5.94	125.88	119.76
4	d	110	PRO	C-N-CA	5.94	125.88	119.76
12	x	67	PHE	N-CA-C	5.94	119.72	112.23
14	z	8	TYR	N-CA-C	5.94	118.20	110.53
5	q	80	ASP	CA-CB-CG	-5.94	106.66	112.60
1	c	248	LEU	CA-C-N	5.94	125.81	119.28
1	c	248	LEU	C-N-CA	5.94	125.81	119.28
1	c	284	TYR	O-C-N	-5.94	115.63	122.93
8	h	55	THR	CA-C-O	5.93	127.05	120.82
1	l	274	ASN	OD1-CG-ND2	5.93	128.53	122.60
3	b	22	PRO	CB-CA-C	-5.92	101.79	111.56
1	l	342	TRP	CH2-CZ2-CE2	5.92	125.20	117.50
2	n	167	ALA	O-C-N	-5.92	114.99	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	x	171	MET	N-CA-C	5.92	120.22	111.87
3	b	143	ALA	CA-C-O	5.92	126.69	120.42
1	l	46	ARG	NH1-CZ-NH2	5.92	126.99	119.30
3	b	127	ALA	CA-C-O	5.91	126.77	119.97
3	b	282	ARG	CD-NE-CZ	-5.91	116.12	124.40
1	l	89	TYR	CA-CB-CG	5.91	124.54	113.90
3	o	206	ASN	O-C-N	-5.91	115.71	122.68
4	p	138	PRO	N-CD-CG	-5.91	94.34	103.20
13	y	207	MET	CA-C-N	5.91	127.22	119.84
13	y	207	MET	C-N-CA	5.91	127.22	119.84
5	q	99	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	n	285	VAL	N-CA-C	5.90	116.79	108.17
2	m	145	ARG	O-C-N	5.90	128.22	122.09
5	q	132	TRP	N-CA-C	5.90	119.43	109.76
2	n	75	LEU	N-CA-CB	5.90	118.87	110.44
3	b	91	PHE	CB-CG-CD2	-5.89	110.68	120.70
3	b	160	LEU	N-CA-C	5.89	118.46	111.33
5	e	15	ARG	O-C-N	5.89	126.33	121.32
3	o	102	LEU	O-C-N	5.89	130.58	122.46
1	l	364	ALA	CA-C-O	5.88	126.78	120.55
4	d	92	PRO	CB-CA-C	5.88	116.75	111.40
13	y	134	ARG	N-CA-C	5.88	123.32	110.80
3	o	210	GLY	N-CA-C	-5.88	107.28	114.92
12	x	119	GLU	CB-CA-C	-5.87	109.79	116.54
7	s	15	THR	CB-CA-C	-5.87	98.96	109.71
3	b	71	ARG	NE-CZ-NH1	-5.86	115.64	121.50
4	p	229	VAL	N-CA-CB	5.86	117.01	110.51
2	m	94	GLY	CA-C-O	-5.85	114.26	122.51
3	b	320	LEU	CA-C-N	-5.84	111.43	120.31
3	b	320	LEU	C-N-CA	-5.84	111.43	120.31
3	b	176	THR	CA-CB-OG1	-5.84	100.84	109.60
2	n	47	ILE	CB-CG1-CD1	5.84	126.06	113.80
2	n	157	ALA	N-CA-C	5.84	117.31	111.07
3	o	126	THR	O-C-N	5.83	128.08	122.07
1	c	311	ASN	OD1-CG-ND2	5.83	128.43	122.60
3	b	177	ARG	CB-CA-C	-5.83	101.98	110.96
3	o	227	LYS	O-C-N	5.83	128.07	122.07
2	n	42	ALA	CA-C-N	5.83	127.12	119.84
2	n	42	ALA	C-N-CA	5.83	127.12	119.84
1	c	281	ASP	CA-CB-CG	5.83	118.42	112.60
4	d	182	VAL	N-CA-CB	5.83	119.32	110.58
4	d	151	PRO	N-CA-CB	5.82	108.88	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	157	ALA	N-CA-CB	5.81	118.44	110.01
2	m	138	ALA	CA-C-O	-5.80	114.27	120.42
3	b	205	SER	CA-C-O	5.80	127.37	120.70
3	b	282	ARG	NE-CZ-NH1	-5.80	115.70	121.50
2	m	245	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	c	352	SER	CA-CB-OG	5.79	122.69	111.10
14	z	198	PHE	N-CA-C	5.79	117.59	111.28
3	o	280	ILE	CB-CG1-CD1	5.79	125.95	113.80
5	q	18	VAL	CB-CA-C	-5.79	101.80	111.29
2	n	85	ILE	CA-C-O	-5.79	113.55	120.78
2	n	167	ALA	CA-C-N	-5.79	112.40	122.64
2	n	167	ALA	C-N-CA	-5.79	112.40	122.64
3	o	50	PHE	CA-CB-CG	-5.78	108.02	113.80
1	c	241	ILE	CA-CB-CG1	-5.78	100.58	110.40
1	l	220	SER	CA-C-N	5.78	126.74	120.44
1	l	220	SER	C-N-CA	5.78	126.74	120.44
6	r	28	LYS	CA-C-O	5.78	126.61	119.97
1	l	339	GLN	O-C-N	5.77	130.26	122.59
3	b	189	ILE	CB-CA-C	-5.76	104.49	112.04
2	m	310	SER	N-CA-C	5.76	118.85	109.06
3	o	38	GLY	O-C-N	-5.75	116.61	122.19
5	q	32	ARG	CB-CA-C	5.75	120.46	110.68
3	b	75	TYR	N-CA-C	-5.75	106.21	113.23
13	y	190	GLY	N-CA-C	5.75	117.73	110.38
3	b	153	ILE	CA-C-N	5.74	127.01	119.84
3	b	153	ILE	C-N-CA	5.74	127.01	119.84
7	g	58	VAL	N-CA-CB	5.74	117.64	110.47
4	p	50	HIS	N-CA-C	-5.74	106.11	113.23
4	d	201	ARG	CA-CB-CG	5.73	125.56	114.10
3	o	185	LEU	CA-C-O	-5.73	113.29	118.79
3	o	201	HIS	CA-C-O	5.73	126.00	119.18
5	q	184	SER	CA-C-O	-5.72	114.52	121.05
1	c	434	TYR	CB-CG-CD1	5.72	129.38	120.80
4	d	9	SER	N-CA-C	-5.72	101.04	109.62
3	o	22	PRO	N-CA-CB	5.72	108.26	103.17
3	o	63	PHE	O-C-N	5.72	129.12	122.20
6	r	22	ASN	N-CA-C	-5.72	106.14	113.23
6	f	24	ALA	CA-C-O	5.71	126.97	120.80
3	o	256	TYR	CA-C-O	-5.71	112.78	120.15
1	l	56	GLY	O-C-N	-5.71	115.28	122.70
1	c	23	LEU	CA-C-N	-5.71	114.84	122.72
1	c	23	LEU	C-N-CA	-5.71	114.84	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	25	GLY	N-CA-C	5.71	118.94	110.60
2	n	254	HIS	CA-CB-CG	5.71	119.51	113.80
2	m	157	ALA	N-CA-C	5.71	117.18	111.07
15	1	129	ALA	CA-C-N	5.70	126.97	119.84
15	1	129	ALA	C-N-CA	5.70	126.97	119.84
3	o	46	LEU	N-CA-C	-5.70	104.98	111.14
1	c	368	HIS	CA-CB-CG	-5.70	108.10	113.80
1	l	93	GLU	CA-CB-CG	-5.69	102.71	114.10
9	u	51	CYS	CA-C-N	5.69	128.48	120.28
9	u	51	CYS	C-N-CA	5.69	128.48	120.28
3	b	97	HIS	CB-CG-ND1	5.69	131.24	122.70
2	m	139	ALA	CA-C-O	5.69	126.79	120.82
1	l	292	SER	CA-C-O	5.69	124.14	119.36
1	l	436	ARG	CA-C-N	-5.69	112.13	121.34
1	l	436	ARG	C-N-CA	-5.69	112.13	121.34
2	n	108	THR	N-CA-C	5.68	118.08	110.35
4	p	109	LEU	CA-C-N	5.68	126.23	120.38
4	p	109	LEU	C-N-CA	5.68	126.23	120.38
12	x	129	TYR	CB-CA-C	-5.68	100.50	109.42
3	b	77	TRP	CD2-CE3-CZ3	-5.68	111.22	118.60
1	c	11	VAL	N-CA-C	5.68	114.30	109.02
4	p	195	GLU	CA-C-N	5.67	125.52	119.28
4	p	195	GLU	C-N-CA	5.67	125.52	119.28
6	r	23	ALA	N-CA-C	-5.67	104.79	110.97
1	l	47	TYR	N-CA-C	-5.67	106.53	113.50
2	n	187	THR	CA-C-N	5.67	126.93	119.84
2	n	187	THR	C-N-CA	5.67	126.93	119.84
3	b	96	MET	N-CA-C	-5.67	105.18	111.36
1	c	392	LEU	N-CA-C	5.66	117.91	111.11
2	m	102	ARG	CD-NE-CZ	-5.66	116.47	124.40
4	d	203	ARG	CA-C-O	5.66	127.30	121.07
1	l	138	LEU	O-C-N	5.66	129.05	122.20
1	l	428	ILE	O-C-N	-5.66	116.28	122.05
2	n	165	ALA	CA-C-O	5.66	126.33	119.31
3	b	15	ASN	OD1-CG-ND2	5.66	128.26	122.60
1	l	32	GLN	CA-C-N	5.66	126.91	119.84
1	l	32	GLN	C-N-CA	5.66	126.91	119.84
1	c	193	PRO	N-CA-CB	5.65	108.82	102.60
2	m	65	THR	OG1-CB-CG2	5.65	120.60	109.30
1	c	418	GLN	OE1-CD-NE2	5.65	128.25	122.60
4	p	38	SER	CA-C-N	5.65	128.41	120.28
4	p	38	SER	C-N-CA	5.65	128.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	257	THR	CB-CA-C	-5.64	103.41	109.85
3	o	264	THR	CB-CA-C	-5.64	102.31	109.65
3	b	111	GLU	CA-C-O	-5.63	114.88	120.90
9	u	56	ARG	CA-C-N	5.63	128.70	121.27
9	u	56	ARG	C-N-CA	5.63	128.70	121.27
4	p	30	PHE	CA-CB-CG	-5.63	108.17	113.80
6	f	43	VAL	O-C-N	-5.63	115.54	122.57
3	b	22	PRO	N-CA-CB	5.62	109.15	103.25
3	b	191	ALA	N-CA-C	-5.62	105.06	111.07
1	c	242	CYS	N-CA-C	5.62	118.40	109.24
3	b	16	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	c	279	HIS	O-C-N	-5.62	117.19	123.48
2	n	201	SER	N-CA-C	5.62	117.09	110.97
5	q	47	VAL	N-CA-C	5.61	117.02	110.62
5	q	76	ILE	CA-C-O	-5.61	115.41	121.19
3	o	100	ARG	N-CA-C	-5.61	105.16	112.23
1	l	376	CYS	CA-CB-SG	-5.61	101.50	114.40
3	o	45	ILE	CB-CA-C	-5.60	104.81	111.81
17	3	82	CYS	CA-C-N	5.60	125.44	119.28
17	3	82	CYS	C-N-CA	5.60	125.44	119.28
2	m	61	ASN	OD1-CG-ND2	-5.60	117.00	122.60
8	h	63	HIS	CA-CB-CG	-5.60	108.20	113.80
2	n	45	SER	O-C-N	-5.60	116.64	123.19
13	y	104	TRP	N-CA-C	5.60	122.72	110.80
1	c	205	HIS	CA-CB-CG	-5.59	108.20	113.80
2	m	403	ASP	CA-CB-CG	-5.59	107.01	112.60
14	z	188	ILE	CB-CA-C	-5.58	104.60	112.14
1	c	414	TYR	N-CA-C	5.58	120.21	112.90
3	b	143	ALA	CA-C-N	-5.58	113.19	120.44
3	b	143	ALA	C-N-CA	-5.58	113.19	120.44
1	l	154	HIS	CA-CB-CG	5.58	119.38	113.80
3	o	199	PHE	CB-CG-CD2	5.58	130.19	120.70
4	d	31	GLN	CA-C-O	-5.58	114.93	120.90
3	o	35	SER	CA-C-N	5.57	128.01	120.38
3	o	35	SER	C-N-CA	5.57	128.01	120.38
8	h	54	CYS	CA-C-N	5.57	127.68	120.44
8	h	54	CYS	C-N-CA	5.57	127.68	120.44
20	6	20	HIS	N-CA-C	5.57	118.11	111.71
6	r	99	ARG	CA-C-N	-5.57	112.82	120.28
6	r	99	ARG	C-N-CA	-5.57	112.82	120.28
3	b	21	LEU	N-CA-C	5.56	116.70	109.64
3	o	56	THR	O-C-N	-5.56	116.40	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	196	HIS	N-CA-C	-5.56	105.12	111.07
7	s	19	SER	CA-C-N	5.56	125.02	119.24
7	s	19	SER	C-N-CA	5.56	125.02	119.24
23	9	16	GLU	N-CA-C	5.56	117.42	111.36
1	l	189	HIS	CA-CB-CG	5.55	119.35	113.80
3	b	182	HIS	N-CA-C	-5.55	105.23	111.28
1	c	22	GLY	N-CA-C	-5.55	107.12	114.95
2	m	190	GLU	CA-C-O	-5.55	114.96	120.90
5	q	91	TRP	CB-CG-CD2	5.55	134.57	126.80
1	l	415	PHE	CA-CB-CG	5.55	119.35	113.80
1	l	217	SER	N-CA-CB	-5.55	102.49	110.87
3	o	282	ARG	CD-NE-CZ	-5.55	116.63	124.40
1	l	341	GLN	CA-C-O	-5.54	114.54	120.42
2	m	197	ASN	N-CA-C	5.54	117.40	111.36
3	b	123	VAL	CA-C-N	-5.54	111.26	120.68
3	b	123	VAL	C-N-CA	-5.54	111.26	120.68
1	l	300	THR	CA-CB-OG1	5.54	117.91	109.60
1	l	252	HIS	CA-CB-CG	-5.54	108.27	113.80
18	4	72	ASN	CA-C-N	5.54	125.89	119.47
18	4	72	ASN	C-N-CA	5.54	125.89	119.47
4	d	206	LEU	N-CA-CB	5.53	119.13	109.72
3	o	126	THR	CA-C-O	-5.53	115.01	120.82
5	q	29	SER	CA-C-N	5.53	127.69	120.28
5	q	29	SER	C-N-CA	5.53	127.69	120.28
4	p	16	GLY	N-CA-C	5.53	120.11	112.37
3	o	185	LEU	O-C-N	5.52	124.74	120.38
1	c	360	LEU	N-CA-C	-5.52	105.34	111.36
3	b	120	LEU	CA-C-O	5.52	126.80	120.90
4	d	114	SER	CA-CB-OG	5.52	122.14	111.10
3	b	205	SER	N-CA-C	5.51	118.18	109.96
5	e	49	TYR	N-CA-C	-5.51	104.30	111.02
5	q	40	THR	CA-CB-CG2	5.51	119.87	110.50
8	t	63	HIS	CA-CB-CG	-5.50	108.30	113.80
1	c	69	ASN	CA-C-O	5.50	126.78	121.00
2	m	320	GLY	CA-C-O	5.50	126.48	121.47
1	c	149	VAL	N-CA-CB	5.50	116.98	110.55
2	m	46	ARG	CB-CA-C	-5.50	102.59	110.62
3	b	269	LYS	CA-C-N	5.50	125.80	119.92
3	b	269	LYS	C-N-CA	5.50	125.80	119.92
1	c	395	TRP	CD2-CE2-CZ2	5.50	127.90	122.40
4	d	182	VAL	CA-CB-CG1	5.50	119.75	110.40
7	g	15	THR	N-CA-C	5.50	118.44	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	2	GLU	N-CA-C	5.50	122.51	110.80
4	d	40	CYS	CB-CA-C	5.49	116.25	109.16
7	s	12	HIS	CA-CB-CG	-5.49	108.31	113.80
5	q	10	PHE	CA-CB-CG	-5.49	108.31	113.80
3	b	164	ILE	CA-C-O	-5.49	115.56	121.27
2	m	85	ILE	N-CA-C	5.48	116.11	110.36
10	v	8	ARG	CA-C-N	5.48	127.94	120.54
10	v	8	ARG	C-N-CA	5.48	127.94	120.54
3	b	18	PHE	CA-C-N	5.48	128.57	120.74
3	b	18	PHE	C-N-CA	5.48	128.57	120.74
3	b	26	ASN	O-C-N	-5.47	116.56	123.12
1	c	208	LEU	N-CA-C	-5.47	105.01	110.97
6	r	98	ILE	O-C-N	-5.47	116.47	121.94
6	r	32	MET	N-CA-CB	-5.47	102.04	111.55
9	u	58	GLN	N-CA-C	5.47	118.39	109.59
2	n	329	GLN	CB-CA-C	5.46	119.90	110.45
4	d	208	MET	CA-CB-CG	5.46	125.02	114.10
5	q	69	LEU	CA-C-N	5.46	128.04	120.29
5	q	69	LEU	C-N-CA	5.46	128.04	120.29
3	b	19	ILE	N-CA-C	5.46	116.11	110.82
12	x	245	ILE	N-CA-C	-5.46	104.23	111.05
1	l	375	VAL	O-C-N	5.45	127.23	121.89
4	d	191	ARG	CA-C-O	-5.45	114.64	121.02
3	b	188	ILE	N-CA-CB	5.45	117.55	110.57
6	r	16	ILE	N-CA-C	-5.45	105.54	110.82
3	o	234	LEU	N-CA-C	-5.45	105.42	111.36
3	o	261	PRO	N-CA-CB	5.44	108.97	103.25
4	d	213	GLY	CA-C-O	5.44	125.87	119.45
3	b	195	VAL	CA-C-N	5.43	127.82	120.65
3	b	195	VAL	C-N-CA	5.43	127.82	120.65
1	c	46	ARG	NE-CZ-NH2	-5.43	114.31	119.20
12	x	305	PHE	N-CA-C	5.42	119.00	112.38
1	l	421	ALA	CB-CA-C	5.42	119.62	110.79
3	o	201	HIS	CA-CB-CG	-5.42	108.38	113.80
3	b	74	ASN	N-CA-C	5.42	116.95	109.15
6	f	97	VAL	N-CA-CB	-5.42	102.30	111.23
5	e	71	MET	CA-C-O	-5.41	114.68	120.42
2	m	44	ALA	N-CA-C	5.41	117.34	108.52
1	c	395	TRP	NE1-CE2-CZ2	-5.41	121.99	130.10
2	m	309	VAL	N-CA-C	5.41	114.98	108.06
6	r	36	THR	CA-C-O	5.41	126.20	119.12
4	d	109	LEU	CA-C-N	5.41	125.95	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	109	LEU	C-N-CA	5.41	125.95	120.38
6	f	90	LEU	O-C-N	5.41	129.57	122.33
1	c	443	TRP	N-CA-C	5.40	119.16	107.49
4	p	48	TYR	CA-C-N	5.40	130.12	122.24
4	p	48	TYR	C-N-CA	5.40	130.12	122.24
7	s	12	HIS	CA-C-N	-5.40	115.92	123.10
7	s	12	HIS	C-N-CA	-5.40	115.92	123.10
7	g	18	LEU	O-C-N	-5.39	115.55	122.94
7	g	10	VAL	CA-C-O	5.39	125.59	120.25
1	c	94	HIS	CB-CA-C	-5.39	104.04	110.94
6	f	76	PRO	N-CA-CB	5.39	108.04	103.35
1	l	435	ASN	CB-CG-OD1	-5.39	110.03	120.80
4	p	84	PRO	N-CA-CB	5.39	107.84	103.32
3	b	239	LEU	CD1-CG-CD2	-5.38	98.96	110.80
9	i	51	CYS	N-CA-C	5.38	118.39	109.94
4	d	32	VAL	CB-CA-C	-5.38	105.00	111.88
3	o	32	ASN	CA-CB-CG	-5.38	107.22	112.60
1	c	142	ASP	CA-C-O	5.38	126.00	119.49
5	e	75	GLU	CA-C-O	-5.38	111.66	120.80
1	c	343	MET	O-C-N	-5.37	115.44	122.59
2	n	92	VAL	N-CA-CB	-5.37	105.33	112.26
1	l	419	CYS	CA-CB-SG	5.37	126.75	114.40
1	c	153	LEU	O-C-N	5.37	127.82	122.08
3	b	15	ASN	CA-CB-CG	-5.37	107.23	112.60
1	l	390	ILE	N-CA-CB	5.37	118.72	111.21
3	o	45	ILE	O-C-N	5.37	127.47	121.94
12	x	159	LEU	N-CA-C	-5.37	105.51	111.36
1	c	428	ILE	CA-CB-CG1	5.36	119.52	110.40
1	c	373	THR	O-C-N	-5.36	115.52	120.51
10	v	19	THR	CA-CB-OG1	-5.36	101.56	109.60
1	c	170	PRO	N-CA-CB	5.36	108.87	103.25
2	m	107	TYR	CA-C-N	5.35	128.83	120.75
2	m	107	TYR	C-N-CA	5.35	128.83	120.75
1	c	436	ARG	CD-NE-CZ	-5.35	116.91	124.40
4	d	191	ARG	CA-C-N	5.35	127.71	120.38
4	d	191	ARG	C-N-CA	5.35	127.71	120.38
1	l	315	ALA	CA-C-O	5.35	126.44	120.82
3	o	141	TRP	CA-C-N	5.34	125.87	119.94
3	o	141	TRP	C-N-CA	5.34	125.87	119.94
9	u	78	TYR	CA-CB-CG	5.34	123.51	113.90
1	c	161	THR	CA-C-N	5.33	125.15	119.28
1	c	161	THR	C-N-CA	5.33	125.15	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	50	PRO	N-CA-CB	5.33	108.25	103.08
1	l	392	LEU	N-CA-CB	5.33	117.88	109.94
2	m	60	SER	CA-CB-OG	-5.33	100.44	111.10
3	o	259	ALA	CA-C-O	-5.33	114.68	120.81
7	g	19	SER	CA-C-N	5.33	125.39	119.32
7	g	19	SER	C-N-CA	5.33	125.39	119.32
2	m	133	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	l	260	PRO	N-CA-CB	5.32	108.39	103.39
3	o	106	SER	CA-C-O	5.32	125.92	119.38
10	j	55	ILE	N-CA-C	5.31	118.91	112.80
2	m	33	LEU	O-C-N	5.31	129.32	123.16
1	l	415	PHE	CA-C-O	5.31	126.20	119.78
2	m	89	ILE	O-C-N	-5.30	116.72	121.87
1	l	25	VAL	CA-C-N	-5.30	114.26	122.59
1	l	25	VAL	C-N-CA	-5.30	114.26	122.59
5	q	172	ARG	CA-C-N	5.30	129.77	121.76
5	q	172	ARG	C-N-CA	5.30	129.77	121.76
1	l	145	MET	CA-C-N	-5.30	113.12	120.38
1	l	145	MET	C-N-CA	-5.30	113.12	120.38
5	q	65	SER	O-C-N	-5.30	116.61	122.86
3	b	260	ASN	CA-CB-CG	5.30	117.90	112.60
2	n	394	PRO	CA-C-N	5.30	126.46	119.84
2	n	394	PRO	C-N-CA	5.30	126.46	119.84
3	b	175	LEU	CA-C-O	5.29	126.04	119.79
3	o	199	PHE	CD1-CG-CD2	-5.29	110.66	118.60
12	x	372	TYR	N-CA-C	-5.29	105.41	111.07
2	m	75	LEU	O-C-N	5.29	129.16	122.65
3	b	210	GLY	CA-C-N	5.29	132.01	122.43
3	b	210	GLY	C-N-CA	5.29	132.01	122.43
1	l	428	ILE	CA-C-O	5.29	125.43	120.14
5	q	39	VAL	N-CA-C	-5.29	105.56	110.53
1	l	440	GLY	N-CA-C	-5.29	107.76	114.16
26	B	55	CYS	CB-CA-C	-5.29	100.05	110.10
3	b	135	TRP	O-C-N	5.29	128.92	122.58
4	d	201	ARG	CD-NE-CZ	-5.28	117.00	124.40
4	p	209	LEU	O-C-N	-5.28	115.78	122.17
2	n	70	ARG	NE-CZ-NH2	-5.28	114.45	119.20
3	o	115	ILE	CA-CB-CG1	5.28	119.37	110.40
2	m	94	GLY	CA-C-N	5.27	131.44	122.37
2	m	94	GLY	C-N-CA	5.27	131.44	122.37
2	n	162	ASN	CB-CA-C	5.27	119.49	110.74
3	b	361	LEU	CA-C-O	-5.27	114.94	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	q	91	TRP	CB-CG-CD1	-5.27	119.00	126.90
6	f	99	ARG	O-C-N	-5.26	116.06	122.11
5	q	136	ILE	N-CA-CB	-5.26	106.22	111.90
4	d	46	VAL	CA-C-O	5.26	126.81	120.65
8	h	55	THR	CA-CB-OG1	5.26	117.49	109.60
3	o	226	ILE	CA-C-O	5.26	126.43	120.85
3	b	126	THR	N-CA-CB	5.26	118.36	109.78
2	n	107	TYR	CA-C-N	5.26	128.69	120.75
2	n	107	TYR	C-N-CA	5.26	128.69	120.75
6	f	55	TYR	CA-C-O	-5.26	114.97	120.55
3	b	356	VAL	O-C-N	-5.26	116.77	121.87
1	c	247	GLY	O-C-N	-5.25	117.09	122.19
4	d	46	VAL	N-CA-CB	5.25	116.99	111.00
1	c	342	TRP	CD2-CE2-CZ2	5.25	127.65	122.40
1	c	358	LYS	CA-C-N	5.25	127.58	120.38
1	c	358	LYS	C-N-CA	5.25	127.58	120.38
1	l	162	PRO	CB-CA-C	-5.25	103.49	112.26
3	o	160	LEU	N-CA-C	5.25	117.41	111.11
7	s	17	SER	CA-C-O	-5.25	115.29	121.44
1	c	391	PRO	CA-C-N	5.25	127.63	120.54
1	c	391	PRO	C-N-CA	5.25	127.63	120.54
9	i	69	SER	CA-C-O	-5.25	114.66	120.33
5	q	182	VAL	O-C-N	5.25	126.00	120.96
2	m	353	SER	CA-C-N	5.24	129.85	121.62
2	m	353	SER	C-N-CA	5.24	129.85	121.62
1	c	425	PHE	CA-C-N	5.24	130.10	121.87
1	c	425	PHE	C-N-CA	5.24	130.10	121.87
2	n	274	VAL	O-C-N	5.24	127.23	121.83
3	o	219	PRO	CA-C-O	5.24	126.84	121.23
1	c	357	GLY	N-CA-C	-5.24	106.07	112.77
12	x	262	SER	N-CA-C	-5.23	106.58	113.17
3	b	355	SER	O-C-N	-5.23	116.57	122.12
4	p	137	PRO	CA-C-N	5.23	126.04	120.13
4	p	137	PRO	C-N-CA	5.23	126.04	120.13
4	p	175	THR	CA-C-O	5.22	124.14	119.59
1	c	167	VAL	N-CA-C	-5.22	105.29	110.62
4	d	239	PRO	CA-C-N	5.22	126.37	119.84
4	d	239	PRO	C-N-CA	5.22	126.37	119.84
17	3	38	ALA	N-CA-C	5.22	117.86	110.50
3	b	233	LEU	CA-C-O	-5.22	115.31	120.90
6	f	19	TRP	CA-C-N	5.22	127.58	120.54
6	f	19	TRP	C-N-CA	5.22	127.58	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	416	LYS	N-CA-C	5.21	117.71	111.71
3	o	39	ILE	CB-CG1-CD1	5.21	124.74	113.80
2	n	138	ALA	N-CA-C	5.21	117.36	111.11
6	f	26	PHE	CA-CB-CG	5.21	119.01	113.80
1	l	329	MET	CA-C-N	-5.21	114.35	122.37
1	l	329	MET	C-N-CA	-5.21	114.35	122.37
10	j	54	HIS	CA-C-N	5.21	129.01	121.52
10	j	54	HIS	C-N-CA	5.21	129.01	121.52
1	c	390	ILE	N-CA-CB	5.20	118.49	111.21
1	c	403	ASP	CA-C-N	-5.20	112.40	120.31
1	c	403	ASP	C-N-CA	-5.20	112.40	120.31
4	p	191	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	l	416	TYR	N-CA-CB	5.20	118.26	109.94
1	l	350	THR	CA-C-O	-5.20	115.23	121.11
1	c	311	ASN	CA-C-N	-5.20	115.87	122.37
1	c	311	ASN	C-N-CA	-5.20	115.87	122.37
1	l	277	ILE	CB-CA-C	-5.20	105.23	111.88
1	l	319	LEU	CA-C-O	5.20	126.04	120.32
4	p	195	GLU	CA-C-O	5.20	127.29	120.74
2	n	430	LEU	N-CA-C	5.19	119.29	111.81
7	s	33	GLY	O-C-N	5.19	127.17	122.18
3	b	196	HIS	N-CA-CB	5.19	117.48	109.91
4	p	33	TYR	CA-C-O	-5.19	115.36	121.07
5	e	39	VAL	CB-CA-C	-5.18	105.25	111.88
5	q	40	THR	O-C-N	-5.18	116.70	122.09
2	m	256	ALA	CA-C-O	-5.18	115.26	121.11
3	o	124	MET	N-CA-C	5.18	116.93	111.28
2	m	282	GLY	CA-C-N	5.18	126.31	119.84
2	m	282	GLY	C-N-CA	5.18	126.31	119.84
4	p	85	GLY	CA-C-N	5.18	128.57	120.75
4	p	85	GLY	C-N-CA	5.18	128.57	120.75
3	o	35	SER	O-C-N	-5.17	115.71	122.59
12	x	353	LEU	N-CA-C	-5.17	105.72	111.36
4	p	195	GLU	O-C-N	-5.17	116.62	121.32
3	b	289	GLY	CA-C-O	-5.17	114.82	120.40
6	f	61	ARG	NE-CZ-NH1	-5.17	116.33	121.50
4	d	41	HIS	CA-CB-CG	5.17	118.97	113.80
2	n	57	TYR	CA-C-N	-5.17	114.13	122.81
2	n	57	TYR	C-N-CA	-5.17	114.13	122.81
2	n	246	GLU	N-CA-C	5.17	117.80	107.62
3	b	9	PRO	N-CA-CB	5.16	107.79	103.25
1	c	363	ASN	OD1-CG-ND2	5.16	127.76	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	79	ILE	N-CA-CB	5.16	116.24	110.51
2	n	169	ARG	N-CA-C	-5.16	106.11	112.72
3	o	60	THR	CB-CA-C	-5.16	102.55	110.81
8	h	60	ASP	N-CA-C	-5.16	106.67	113.12
3	o	91	PHE	CA-CB-CG	-5.16	108.64	113.80
14	z	99	TRP	N-CA-C	-5.16	105.55	111.07
3	b	276	PHE	N-CA-CB	5.15	119.20	110.49
3	b	230	LEU	CA-C-O	-5.15	115.41	120.82
2	n	165	ALA	O-C-N	-5.15	115.35	122.46
1	c	188	ARG	CA-C-N	-5.15	113.67	122.11
1	c	188	ARG	C-N-CA	-5.15	113.67	122.11
8	t	55	THR	CA-CB-OG1	5.15	117.32	109.60
3	o	275	LEU	CA-C-O	-5.14	115.00	121.02
4	d	228	SER	CA-C-O	5.14	126.18	120.63
1	l	157	ALA	CA-C-O	5.14	125.30	119.18
1	l	169	GLY	CA-C-N	5.14	125.14	119.90
1	l	169	GLY	C-N-CA	5.14	125.14	119.90
19	5	22	ASN	N-CA-C	5.14	117.67	109.81
2	m	394	PRO	N-CA-CB	5.13	108.06	103.08
1	l	138	LEU	CA-C-N	5.13	127.41	120.38
1	l	138	LEU	C-N-CA	5.13	127.41	120.38
2	m	173	ALA	O-C-N	-5.13	114.80	122.39
2	m	314	ALA	CA-C-O	-5.13	115.16	120.70
7	g	9	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	n	59	ASN	OD1-CG-ND2	-5.13	117.47	122.60
4	d	38	SER	CA-C-N	5.13	127.67	120.28
4	d	38	SER	C-N-CA	5.13	127.67	120.28
4	d	132	THR	CA-CB-OG1	-5.13	101.91	109.60
1	l	295	ALA	CA-C-O	5.13	125.98	120.70
1	l	361	LEU	O-C-N	5.13	127.42	122.09
2	n	66	SER	N-CA-C	-5.13	105.58	111.07
3	b	119	LEU	CA-C-O	5.13	126.71	121.07
2	n	125	ASN	OD1-CG-ND2	5.13	127.73	122.60
4	p	143	LEU	N-CA-C	5.12	116.53	107.61
2	m	429	ASN	CA-CB-CG	-5.12	107.48	112.60
2	m	83	PHE	CA-CB-CG	-5.12	108.68	113.80
1	l	100	LYS	N-CA-C	-5.12	100.89	109.24
7	g	12	HIS	N-CA-C	5.12	118.45	111.39
3	o	26	ASN	CA-C-O	-5.12	115.52	121.15
4	p	195	GLU	CB-CG-CD	5.11	121.29	112.60
1	c	306	SER	O-C-N	-5.11	115.79	122.59
8	t	55	THR	CA-C-O	5.11	125.97	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	y	66	THR	N-CA-C	-5.11	107.70	114.04
11	w	36	THR	CA-C-O	5.11	129.48	120.80
13	y	165	VAL	CA-C-N	5.11	126.22	119.84
13	y	165	VAL	C-N-CA	5.11	126.22	119.84
21	7	9	GLN	N-CA-C	-5.11	105.61	111.07
3	b	281	LEU	O-C-N	-5.11	116.72	122.03
12	x	401	SER	N-CA-C	5.11	119.64	113.41
2	n	337	ILE	CA-C-O	-5.10	115.76	121.17
12	x	377	PHE	N-CA-C	5.09	119.34	113.18
8	h	47	ARG	CA-CB-CG	5.09	124.28	114.10
1	l	11	VAL	CA-C-O	5.09	124.44	119.71
2	n	172	LEU	N-CA-CB	5.09	119.29	110.39
7	s	36	ASN	OD1-CG-ND2	-5.09	117.51	122.60
14	z	107	ALA	CA-C-N	5.09	125.88	119.98
14	z	107	ALA	C-N-CA	5.09	125.88	119.98
4	p	206	LEU	CA-C-N	-5.09	113.19	120.82
4	p	206	LEU	C-N-CA	-5.09	113.19	120.82
2	m	170	ASN	N-CA-C	5.08	119.10	112.13
7	s	5	GLY	CA-C-N	5.08	130.20	122.37
7	s	5	GLY	C-N-CA	5.08	130.20	122.37
1	c	326	CYS	N-CA-C	5.08	117.73	109.24
3	b	325	PHE	CB-CA-C	-5.08	102.87	110.90
1	l	414	TYR	CA-C-O	-5.08	113.79	119.79
3	o	197	LEU	N-CA-CB	5.08	117.59	110.12
5	q	44	THR	OG1-CB-CG2	5.08	119.46	109.30
4	d	30	PHE	CA-CB-CG	-5.08	108.72	113.80
2	m	266	SER	CA-C-O	-5.08	115.52	121.46
4	p	143	LEU	CB-CA-C	-5.08	103.73	110.79
5	q	62	MET	CA-C-N	5.08	131.24	121.54
5	q	62	MET	C-N-CA	5.08	131.24	121.54
20	6	2	THR	N-CA-C	5.08	116.12	108.46
7	g	34	ILE	CA-C-N	5.07	124.68	119.05
7	g	34	ILE	C-N-CA	5.07	124.68	119.05
9	i	78	TYR	CA-CB-CG	5.07	123.03	113.90
4	p	153	PHE	CA-C-N	5.07	126.18	119.84
4	p	153	PHE	C-N-CA	5.07	126.18	119.84
13	y	12	ALA	N-CA-C	5.07	117.52	109.96
2	m	21	PRO	N-CA-CB	5.07	108.58	103.00
2	m	275	LEU	CB-CA-C	-5.07	102.90	110.90
3	o	358	TYR	N-CA-C	5.07	117.19	111.11
3	o	373	GLU	CA-C-O	5.06	126.10	120.63
6	r	34	ASP	CA-CB-CG	-5.06	107.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	111	PRO	N-CA-CB	5.06	107.81	103.31
3	b	361	LEU	O-C-N	5.06	127.48	122.12
4	d	122	GLY	O-C-N	5.06	128.25	122.33
2	n	354	ASN	CA-C-N	5.06	125.08	119.32
2	n	354	ASN	C-N-CA	5.06	125.08	119.32
3	o	221	HIS	CA-C-O	5.06	123.78	119.13
4	p	150	ASN	CA-C-N	5.06	124.72	119.56
4	p	150	ASN	C-N-CA	5.06	124.72	119.56
7	g	15	THR	CA-C-O	-5.05	115.35	120.71
3	b	329	VAL	CA-C-O	-5.05	114.47	120.78
7	s	73	ASN	CA-C-N	5.05	126.05	120.45
7	s	73	ASN	C-N-CA	5.05	126.05	120.45
1	c	328	HIS	CA-C-O	5.04	125.58	119.38
1	c	436	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	l	23	LEU	CA-C-N	-5.04	115.77	122.72
1	l	23	LEU	C-N-CA	-5.04	115.77	122.72
6	f	47	ILE	CB-CG1-CD1	5.04	124.38	113.80
17	3	81	ARG	N-CA-C	5.04	117.66	109.24
6	f	44	LYS	CA-C-O	5.04	126.29	120.90
8	h	55	THR	CB-CA-C	-5.04	102.97	110.88
7	g	19	SER	CA-C-O	-5.03	116.07	120.60
3	o	197	LEU	N-CA-C	-5.03	105.79	111.28
1	c	163	LEU	CA-C-O	5.03	125.57	119.38
2	m	126	VAL	CB-CA-C	-5.03	104.36	112.16
1	l	101	ALA	N-CA-C	5.03	116.17	108.52
12	x	70	VAL	N-CA-C	5.03	115.46	110.23
12	x	378	HIS	CB-CG-CD2	-5.03	124.67	131.20
2	m	38	LEU	CB-CA-C	-5.02	104.89	111.82
4	p	44	ASP	N-CA-C	5.02	116.83	111.36
3	o	82	MET	N-CA-C	-5.02	105.89	111.36
3	o	325	PHE	CG-CD2-CE2	5.02	129.24	120.70
4	d	84	PRO	N-CA-CB	5.02	107.54	103.32
3	o	326	TRP	CA-C-O	-5.02	115.21	120.63
1	l	420	PRO	N-CA-C	5.02	119.08	111.11
1	c	89	TYR	CA-CB-CG	5.01	122.93	113.90
10	j	51	LEU	N-CA-C	5.01	117.98	109.76
3	o	185	LEU	CA-CB-CG	5.01	133.85	116.30
3	o	227	LYS	CA-C-O	-5.01	115.56	120.82
1	l	342	TRP	CD2-CE2-CZ2	-5.01	117.39	122.40
3	b	64	SER	N-CA-C	-5.01	105.71	111.07
4	p	213	GLY	N-CA-C	-5.01	108.76	115.32
5	q	89	PHE	CA-C-N	-5.01	114.34	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	q	89	PHE	C-N-CA	-5.01	114.34	121.50
4	p	229	VAL	N-CA-C	-5.01	105.10	110.36
4	p	15	ARG	CA-C-N	5.01	125.66	120.60
4	p	15	ARG	C-N-CA	5.01	125.66	120.60
12	x	378	HIS	N-CA-C	-5.00	106.34	112.90
4	d	48	TYR	CA-C-N	5.00	129.54	122.24
4	d	48	TYR	C-N-CA	5.00	129.54	122.24
3	o	190	MET	N-CA-CB	5.00	117.47	110.12
1	c	371	GLY	CA-C-O	-5.00	118.97	122.22
1	l	430	GLN	CG-CD-NE2	5.00	123.90	116.40

There are no chirality outliers.

All (109) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	B	120	UNK	Peptide
26	B	130	UNK	Peptide
27	C	56	UNK	Peptide
28	D	195	UNK	Peptide
30	F	166	UNK	Mainchain
30	F	96	UNK	Peptide
31	G	177	UNK	Peptide
31	G	178	UNK	Mainchain
31	G	206	UNK	Peptide
31	G	289	UNK	Peptide
31	G	399	UNK	Mainchain
31	G	565	UNK	Mainchain
33	I	160	UNK	Mainchain
36	L	133	UNK	Peptide
36	L	366	UNK	Peptide
36	L	446	UNK	Peptide
36	L	546	UNK	Mainchain
38	N	276	UNK	Peptide
38	N	91	UNK	Peptide
39	O	229	UNK	Peptide
39	O	92	UNK	Peptide
40	P	223	UNK	Peptide
40	P	225	UNK	Peptide
40	P	42	UNK	Peptide
41	Q	40	UNK	Peptide
43	S	75	UNK	Mainchain
46	W	40	UNK	Peptide

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Mol	Chain	Res	Type	Group
47	X	56	UNK	Peptide
3	b	134	PRO	Mainchain
3	b	164	ILE	Mainchain
3	b	20	ASP	Mainchain
3	b	21	LEU	Mainchain
3	b	222	PRO	Mainchain
3	b	235	LEU	Mainchain
3	b	281	LEU	Mainchain
3	b	322	GLN	Mainchain
3	b	326	TRP	Mainchain
3	b	335	LEU	Mainchain
3	b	355	SER	Mainchain
3	b	362	ILE	Mainchain
3	b	77	TRP	Mainchain
3	b	83	HIS	Mainchain
1	c	118	GLN	Mainchain
1	c	122	LEU	Mainchain
1	c	196	VAL	Mainchain
1	c	210	ASP	Mainchain
1	c	239	SER	Mainchain
1	c	242	CYS	Mainchain
1	c	244	ARG	Mainchain
1	c	256	ALA	Mainchain
1	c	294	LEU	Mainchain
1	c	306	SER	Mainchain
1	c	345	LEU	Mainchain
1	c	383	LEU	Mainchain
1	c	53	ASN	Mainchain
4	d	191	ARG	Mainchain
4	d	217	PRO	Mainchain
4	d	224	ARG	Mainchain
4	d	229	VAL	Mainchain
4	d	54	VAL	Mainchain
5	e	20	ASP	Mainchain
6	f	16	ILE	Mainchain
6	f	46	ALA	Mainchain
7	g	15	THR	Mainchain
7	g	73	ASN	Mainchain
9	i	69	SER	Mainchain
10	j	43	TYR	Mainchain
1	l	100	LYS	Mainchain
1	l	141	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	l	290	LEU	Mainchain
2	m	106	ALA	Mainchain
2	m	159	VAL	Mainchain
2	m	178	CYS	Mainchain
2	m	239	TYR	Mainchain
2	m	285	VAL	Mainchain
2	m	335	ASP	Mainchain
2	m	353	SER	Mainchain
2	m	68	LEU	Mainchain
2	m	99	THR	Mainchain
2	n	137	VAL	Mainchain
2	n	144	LEU	Mainchain
2	n	200	THR	Mainchain
2	n	290	ASN	Mainchain
2	n	353	SER	Mainchain
3	o	148	ASN	Mainchain
3	o	159	ASN	Mainchain
3	o	19	ILE	Mainchain
3	o	355	SER	Mainchain
3	o	55	TYR	Mainchain
3	o	77	TRP	Mainchain
4	p	202	LYS	Mainchain
4	p	229	VAL	Mainchain
4	p	24	THR	Mainchain
4	p	46	VAL	Mainchain
5	q	125	GLU	Mainchain
5	q	135	LEU	Mainchain
5	q	186	GLU	Mainchain
5	q	195	VAL	Mainchain
5	q	32	ARG	Mainchain
5	q	36	SER	Mainchain
5	q	49	TYR	Mainchain
5	q	9	ASP	Mainchain
5	q	97	PHE	Mainchain
7	s	17	SER	Mainchain
7	s	18	LEU	Mainchain
7	s	34	ILE	Mainchain
8	t	40	CYS	Mainchain
9	u	72	VAL	Mainchain
11	w	24	TRP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	3458	0	3356	486	0
1	l	3458	0	3354	500	0
2	m	3141	0	3123	416	0
2	n	3141	0	3123	430	0
3	b	3011	0	3077	464	0
3	o	3011	0	3077	434	0
4	d	1919	0	1868	303	0
4	p	1919	0	1868	295	0
5	e	566	0	564	64	0
5	q	1518	0	1499	275	0
6	f	916	0	909	94	0
6	r	916	0	909	96	0
7	g	682	0	679	108	0
7	s	682	0	679	103	0
8	h	524	0	504	72	0
8	t	524	0	504	78	0
9	i	248	0	265	54	0
9	u	248	0	265	63	0
10	j	512	0	518	72	0
10	v	512	0	518	78	0
11	k	159	0	159	26	0
11	w	159	0	159	27	0
12	x	4025	0	4003	90	0
13	y	1822	0	1834	71	0
14	z	2124	0	2044	53	0
15	1	1195	0	1183	33	0
16	2	878	0	868	21	0
17	3	748	0	728	24	0
18	4	672	0	645	30	0
19	5	628	0	582	20	0
20	6	598	0	612	14	0
21	7	441	0	437	26	0
22	8	384	0	366	12	0
23	9	386	0	388	9	0
24	0	335	0	352	13	0
25	A	415	0	88	25	0
26	B	719	0	161	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	770	0	163	63	0
28	D	1920	0	402	126	0
29	E	799	0	176	56	0
30	F	2059	0	444	263	0
31	G	2651	0	607	226	0
32	H	1425	0	295	99	0
33	I	818	0	195	65	0
34	J	655	0	138	44	0
35	K	420	0	89	14	0
36	L	2790	0	583	255	0
37	M	2195	0	455	208	0
38	N	1630	0	340	147	0
39	O	905	0	197	65	0
40	P	1260	0	271	144	0
41	Q	345	0	80	14	0
42	R	235	0	54	22	0
43	S	400	0	86	46	0
44	T	355	0	76	12	0
45	V	355	0	77	23	0
46	W	360	0	75	18	0
47	X	1645	0	351	102	0
48	Y	530	0	111	30	0
49	a	355	0	75	7	0
50	U	1250	0	272	63	0
51	Z	1329	0	280	74	0
52	b	86	0	60	18	0
52	o	86	0	60	25	0
53	d	43	0	30	4	0
53	p	43	0	30	4	0
54	E	4	0	0	0	0
54	G	4	0	0	3	0
54	q	4	0	0	0	0
55	x	1	0	0	0	0
55	y	2	0	0	0	0
56	x	1	0	0	0	0
57	x	120	0	108	4	0
58	3	1	0	0	0	0
59	B	8	0	0	5	0
59	F	8	0	0	1	0
59	G	16	0	0	0	0
59	I	16	0	0	5	0
All	All	74493	0	51448	6633	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 53.

All (6633) 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)
26:B:148:UNK:CB	26:B:151:UNK:CA	1.77	1.59
30:F:405:CYS:CB	30:F:406:UNK:CB	1.78	1.56
30:F:405:CYS:HB2	30:F:406:UNK:CB	1.04	1.48
36:L:321:UNK:CB	36:L:324:UNK:CB	1.92	1.45
29:E:148:CYS:SG	30:F:103:UNK:CB	2.04	1.44
26:B:119:CYS:N	26:B:122:UNK:CB	1.81	1.44
31:G:55:CYS:HB2	31:G:68:UNK:CB	1.49	1.40
36:L:247:UNK:HA	36:L:251:UNK:CB	1.52	1.37
29:E:148:CYS:CB	30:F:103:UNK:CB	2.07	1.32
29:E:148:CYS:HB2	30:F:103:UNK:CB	1.59	1.30
30:F:405:CYS:CA	30:F:406:UNK:CB	2.07	1.29
30:F:100:UNK:O	30:F:102:UNK:N	1.67	1.27
31:G:10:UNK:O	31:G:76:UNK:HA	1.33	1.27
29:E:148:CYS:SG	30:F:102:UNK:O	1.91	1.27
31:G:376:UNK:N	31:G:449:UNK:N	1.83	1.27
43:S:25:UNK:CA	43:S:57:UNK:CB	2.13	1.26
36:L:65:UNK:CB	36:L:67:UNK:N	1.98	1.26
1:l:405:ARG:NH1	21:7:2:GLU:OE2	1.69	1.25
26:B:119:CYS:CA	26:B:122:UNK:CB	2.18	1.21
36:L:161:UNK:HA	36:L:162:UNK:C	1.65	1.21
30:F:408:UNK:CB	59:F:501:SF4:S4	2.29	1.20
31:G:55:CYS:CB	31:G:68:UNK:CB	2.19	1.20
40:P:170:UNK:CB	40:P:204:UNK:HA	1.70	1.20
1:l:405:ARG:HH12	21:7:2:GLU:CD	1.49	1.19
5:q:15:ARG:HB2	5:q:16:PRO:HD2	1.19	1.18
33:I:151:UNK:O	33:I:154:UNK:N	1.75	1.18
43:S:25:UNK:N	43:S:57:UNK:CB	2.06	1.18
36:L:161:UNK:HA	36:L:163:UNK:N	1.59	1.17
32:H:158:UNK:CB	32:H:314:UNK:O	1.93	1.17
31:G:152:UNK:CB	31:G:206:UNK:CB	2.23	1.16
36:L:225:UNK:HA	36:L:229:UNK:CB	1.73	1.16
7:g:72:LYS:HB3	7:g:75:ALA:HB2	1.20	1.16
37:M:58:UNK:HA	37:M:59:UNK:CB	1.71	1.15
1:l:428:ILE:HG22	1:l:431:LEU:HB2	1.19	1.15
1:c:428:ILE:HG22	1:c:431:LEU:HB2	1.29	1.14
3:b:129:MET:HG2	3:b:178:PHE:HD2	1.03	1.14
37:M:347:UNK:O	37:M:351:UNK:N	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:50:PRO:HB2	7:s:51:PRO:HD3	1.25	1.14
4:d:224:ARG:HB2	7:g:25:ALA:HB1	1.27	1.14
1:l:426:GLY:CA	1:l:428:ILE:HG13	1.78	1.13
5:q:114:VAL:HA	5:q:117:LEU:HD12	1.24	1.13
9:i:72:VAL:HB	9:i:73:PRO:HD3	1.20	1.13
4:p:181:GLN:HG2	8:t:77:LEU:HD22	1.29	1.12
30:F:405:CYS:HA	30:F:406:UNK:CB	1.69	1.12
38:N:103:UNK:O	38:N:107:UNK:N	1.83	1.12
3:o:26:ASN:HD21	3:o:207:ASN:HB2	1.15	1.11
31:G:10:UNK:O	31:G:76:UNK:CA	1.99	1.11
32:H:40:UNK:C	32:H:47:UNK:CB	2.28	1.10
1:l:405:ARG:CD	21:7:4:ARG:NH1	1.99	1.10
2:m:429:ASN:HD21	2:n:60:SER:HB3	1.15	1.10
4:p:83:ARG:HB3	4:p:84:PRO:CD	1.81	1.10
31:G:41:CYS:N	54:G:803:FES:S2	2.23	1.10
40:P:103:UNK:O	40:P:107:UNK:N	1.84	1.10
2:m:60:SER:HB3	2:n:429:ASN:HD21	0.96	1.09
3:b:310:SER:HA	3:b:374:ASN:HD21	1.12	1.09
26:B:119:CYS:HA	26:B:122:UNK:CB	1.80	1.09
1:l:67:THR:HG23	1:l:70:ARG:H	1.13	1.09
47:X:77:UNK:O	47:X:79:UNK:N	1.84	1.09
3:b:77:TRP:CZ3	3:b:78:ILE:HG23	1.88	1.08
31:G:377:UNK:H	31:G:449:UNK:HA	0.99	1.08
4:p:83:ARG:HB3	4:p:84:PRO:HD2	1.14	1.08
3:o:206:ASN:HB2	3:o:313:ARG:NH2	1.68	1.08
26:B:118:UNK:O	26:B:122:UNK:N	1.85	1.08
32:H:143:UNK:O	32:H:146:UNK:N	1.86	1.08
2:n:305:GLN:HB2	2:n:306:PRO:HD3	1.34	1.08
5:q:76:ILE:CG2	5:q:194:ILE:HG12	1.84	1.08
30:F:423:UNK:O	30:F:427:UNK:N	1.87	1.08
2:m:77:THR:HG22	2:m:130:PRO:HA	1.25	1.08
2:n:200:THR:HG22	2:n:203:ARG:HD2	1.36	1.08
36:L:32:UNK:O	36:L:36:UNK:N	1.87	1.08
39:O:229:UNK:CB	39:O:231:UNK:CA	2.32	1.07
40:P:203:UNK:HA	40:P:234:UNK:HA	1.34	1.07
48:Y:102:UNK:O	48:Y:105:UNK:CB	2.01	1.07
3:b:206:ASN:HB2	3:b:313:ARG:NH2	1.69	1.07
1:l:403:ASP:HB3	1:l:406:VAL:HG23	1.34	1.07
40:P:105:UNK:O	40:P:109:UNK:N	1.87	1.07
3:b:170:VAL:HG13	3:b:174:THR:HG21	1.34	1.07
31:G:175:UNK:N	31:G:182:UNK:O	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:101:UNK:O	34:J:104:UNK:N	1.86	1.07
1:c:41:ILE:HG13	1:c:195:MET:HE3	1.36	1.07
1:c:64:PHE:CE1	1:c:86:LEU:HG	1.90	1.07
48:Y:11:UNK:HA	48:Y:48:UNK:CB	1.84	1.06
50:U:506:UNK:O	50:U:510:UNK:CB	2.02	1.06
27:C:34:UNK:O	27:C:38:UNK:N	1.88	1.06
36:L:209:UNK:O	36:L:212:UNK:N	1.88	1.06
40:P:106:UNK:O	40:P:110:UNK:N	1.87	1.06
9:i:72:VAL:HB	9:i:73:PRO:CD	1.86	1.06
31:G:227:UNK:O	31:G:238:UNK:O	1.72	1.06
34:J:68:UNK:O	34:J:72:UNK:N	1.87	1.06
36:L:29:UNK:O	36:L:33:UNK:N	1.88	1.06
43:S:40:UNK:O	43:S:44:UNK:N	1.88	1.06
1:c:67:THR:HG23	1:c:70:ARG:H	0.94	1.06
31:G:435:UNK:C	31:G:437:UNK:HA	1.86	1.06
32:H:177:UNK:HA	47:X:146:UNK:CB	1.86	1.06
51:Z:104:UNK:O	51:Z:108:UNK:N	1.88	1.06
5:q:109:GLU:HG2	5:q:167:ALA:HB3	1.37	1.05
40:P:21:UNK:N	40:P:44:UNK:O	1.88	1.05
31:G:376:UNK:N	31:G:448:UNK:C	2.17	1.05
39:O:229:UNK:CB	39:O:231:UNK:N	2.19	1.05
7:g:34:ILE:HB	7:g:35:PRO:HD3	1.39	1.05
29:E:70:UNK:O	29:E:74:UNK:N	1.89	1.04
30:F:261:UNK:O	30:F:286:UNK:O	1.75	1.04
36:L:33:UNK:O	36:L:37:UNK:N	1.90	1.04
31:G:241:UNK:O	31:G:248:UNK:N	1.88	1.04
1:c:426:GLY:CA	1:c:428:ILE:HG13	1.87	1.04
4:d:83:ARG:HB3	4:d:84:PRO:CD	1.86	1.04
2:n:166:ALA:HB2	2:n:244:ILE:HG13	1.39	1.04
9:u:72:VAL:HB	9:u:73:PRO:HD3	1.36	1.04
1:c:18:GLN:HE21	1:c:22:GLY:HA2	1.19	1.03
3:b:129:MET:HG2	3:b:178:PHE:CD2	1.93	1.03
40:P:133:UNK:N	40:P:166:UNK:O	1.91	1.03
31:G:142:UNK:O	31:G:190:UNK:HA	1.59	1.03
9:u:70:LEU:HD21	9:u:73:PRO:HD2	1.40	1.03
30:F:262:UNK:CB	30:F:286:UNK:N	2.21	1.03
43:S:25:UNK:CB	43:S:57:UNK:CB	2.36	1.03
2:m:165:ALA:HA	2:m:173:ALA:HB1	1.39	1.03
1:l:143:THR:HG21	9:u:48:SER:H	1.24	1.03
29:E:148:CYS:SG	30:F:102:UNK:C	2.45	1.03
36:L:28:UNK:O	36:L:32:UNK:N	1.92	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:96:LEU:HD21	5:q:195:VAL:HG21	1.38	1.02
3:b:202:GLU:OE2	3:o:10:LEU:HB2	1.59	1.02
30:F:294:UNK:N	30:F:339:UNK:CB	2.23	1.02
1:l:428:ILE:HG21	1:l:431:LEU:HD22	1.35	1.02
5:q:75:GLU:O	5:q:194:ILE:HA	1.57	1.02
30:F:422:UNK:O	30:F:426:UNK:N	1.92	1.02
47:X:302:UNK:O	47:X:305:UNK:N	1.92	1.02
2:m:52:LYS:HB2	2:m:203:ARG:HB3	1.39	1.02
2:m:60:SER:CB	2:n:429:ASN:HD21	1.72	1.02
2:m:95:LYS:HE3	9:i:70:LEU:HD22	1.41	1.02
3:b:221:HIS:HB3	3:b:222:PRO:HD3	1.42	1.02
2:m:283:PRO:HG3	9:i:55:LEU:HD22	1.39	1.02
3:o:174:THR:HG23	3:o:178:PHE:HE2	1.25	1.02
36:L:181:UNK:O	36:L:184:UNK:N	1.92	1.02
2:m:24:LEU:HG	2:m:38:LEU:HD11	1.42	1.01
3:b:179:PHE:HE2	3:o:179:PHE:HE2	1.05	1.01
2:m:24:LEU:H	2:m:24:LEU:HD12	1.23	1.01
1:l:24:ARG:HB2	1:l:196:VAL:HG22	1.37	1.01
28:D:133:UNK:CB	28:D:321:UNK:CB	2.39	1.01
30:F:51:UNK:HA	30:F:52:UNK:CB	1.90	1.01
48:Y:103:UNK:O	48:Y:106:UNK:N	1.92	1.01
6:r:28:LYS:HD2	6:r:74:ILE:HD11	1.42	1.01
26:B:148:UNK:CB	26:B:151:UNK:C	2.38	1.01
40:P:170:UNK:O	40:P:205:UNK:N	1.94	1.01
48:Y:55:UNK:O	48:Y:58:UNK:CB	2.08	1.01
3:b:10:LEU:HB2	3:o:202:GLU:OE2	1.59	1.01
4:d:74:PRO:HB2	4:d:79:GLU:HB2	1.43	1.01
3:o:310:SER:HA	3:o:374:ASN:HD21	1.21	1.01
4:p:224:ARG:HB2	7:s:25:ALA:HB1	1.40	1.01
5:q:134:ILE:HD11	5:q:185:TYR:CD2	1.94	1.01
31:G:435:UNK:CB	31:G:440:UNK:CB	2.38	1.01
40:P:300:UNK:HA	40:P:302:UNK:CB	1.90	1.01
42:R:77:UNK:O	42:R:78:UNK:C	2.09	1.01
7:s:72:LYS:HB3	7:s:75:ALA:HB2	1.39	1.01
40:P:172:UNK:N	40:P:205:UNK:O	1.93	1.01
3:b:16:ASN:ND2	3:b:20:ASP:OD2	1.94	1.00
40:P:108:UNK:O	40:P:112:UNK:N	1.94	1.00
6:f:51:PRO:HG2	6:f:54:LEU:HD23	1.44	1.00
30:F:74:UNK:CB	30:F:77:UNK:CB	2.38	1.00
3:b:26:ASN:HB2	6:f:69:SER:OG	1.62	1.00
4:d:181:GLN:HG2	8:h:77:LEU:HD22	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:239:UNK:O	36:L:240:UNK:C	2.07	1.00
1:l:428:ILE:HG22	1:l:431:LEU:CB	1.91	1.00
30:F:369:UNK:O	30:F:370:UNK:O	1.77	1.00
1:l:18:GLN:HE21	1:l:22:GLY:HA2	1.23	1.00
4:d:83:ARG:HB3	4:d:84:PRO:HD2	1.00	1.00
31:G:380:UNK:CB	31:G:408:UNK:CB	2.39	1.00
31:G:604:UNK:CB	31:G:609:UNK:O	2.08	1.00
3:b:100:ARG:HH21	52:b:402:HEM:HBD1	1.26	0.99
26:B:118:UNK:C	26:B:122:UNK:CB	2.40	0.99
36:L:131:UNK:HA	36:L:143:UNK:CB	1.92	0.99
3:o:100:ARG:HH21	52:o:402:HEM:HBD1	1.23	0.99
30:F:288:UNK:CB	30:F:291:UNK:CB	2.41	0.99
30:F:423:UNK:HA	30:F:426:UNK:CB	1.92	0.99
1:c:343:MET:HE1	1:c:416:TYR:CD2	1.98	0.99
43:S:63:UNK:C	43:S:78:UNK:CB	2.40	0.99
36:L:247:UNK:O	36:L:252:UNK:N	1.95	0.99
3:b:264:THR:HG21	5:q:144:CYS:HB3	1.44	0.99
36:L:82:UNK:O	36:L:87:UNK:N	1.96	0.99
8:t:21:ARG:HB3	8:t:65:ARG:HH21	1.26	0.99
47:X:93:UNK:CB	47:X:94:UNK:CB	2.39	0.99
31:G:55:CYS:SG	31:G:68:UNK:CB	2.50	0.99
1:c:24:ARG:HB2	1:c:196:VAL:HG22	1.43	0.98
32:H:40:UNK:O	32:H:47:UNK:CA	2.12	0.98
37:M:387:UNK:C	37:M:389:UNK:HA	1.93	0.98
2:m:429:ASN:HD21	2:n:60:SER:CB	1.75	0.98
1:l:417:ASP:OD2	10:v:10:TYR:OH	1.82	0.98
34:J:147:UNK:O	34:J:149:UNK:N	1.95	0.98
3:b:174:THR:HG23	3:b:178:PHE:CE1	1.98	0.98
29:E:144:CYS:SG	30:F:102:UNK:HA	2.03	0.98
4:d:83:ARG:CB	4:d:84:PRO:HD2	1.90	0.98
4:p:178:THR:HB	4:p:181:GLN:HG3	1.46	0.98
36:L:246:UNK:O	36:L:251:UNK:N	1.96	0.98
1:l:64:PHE:CE1	1:l:86:LEU:HG	1.98	0.98
26:B:118:UNK:O	26:B:121:UNK:N	1.97	0.98
2:n:24:LEU:HG	2:n:38:LEU:HD11	1.43	0.98
29:E:87:UNK:CB	30:F:181:UNK:CB	2.40	0.98
41:Q:99:UNK:HA	41:Q:100:UNK:CB	1.90	0.98
3:b:26:ASN:HD21	3:b:207:ASN:HB2	1.28	0.98
3:o:345:HIS:HB3	3:o:346:PRO:HD3	1.42	0.98
5:q:86:ASN:HB2	5:q:99:ARG:HD2	1.45	0.97
10:j:18:SER:HB3	11:k:23:LEU:HD12	1.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:40:UNK:O	32:H:47:UNK:CB	2.12	0.97
7:g:36:ASN:HA	7:g:39:ARG:HD3	1.46	0.97
8:h:50:THR:HG22	8:h:52:GLU:H	1.28	0.97
4:p:158:ILE:CD1	4:p:160:MET:HB2	1.94	0.97
1:c:304:CYS:HB3	1:c:334:MET:SD	2.04	0.97
3:b:206:ASN:HB2	3:b:313:ARG:HH21	1.24	0.97
3:o:210:GLY:HA3	3:o:314:SER:HB2	1.47	0.97
6:f:50:LEU:HB2	6:f:55:TYR:HB2	1.45	0.97
1:c:408:ARG:HH22	11:k:15:ARG:NE	1.61	0.97
50:U:509:UNK:O	50:U:512:UNK:CB	2.13	0.97
1:l:408:ARG:HH22	11:w:15:ARG:NE	1.61	0.97
36:L:189:UNK:O	36:L:194:UNK:N	1.98	0.97
38:N:293:UNK:O	38:N:294:UNK:C	2.09	0.97
2:m:200:THR:HG22	2:m:203:ARG:HD2	1.44	0.96
2:n:111:CYS:HB3	2:n:119:LEU:HD22	1.46	0.96
3:o:77:TRP:CZ3	3:o:78:ILE:HG23	1.98	0.96
2:n:67:HIS:HD2	2:n:144:LEU:HD22	1.30	0.96
3:o:16:ASN:ND2	3:o:20:ASP:OD2	1.96	0.96
27:C:64:UNK:O	27:C:70:UNK:CB	2.13	0.96
39:O:188:UNK:O	39:O:192:UNK:N	1.99	0.96
31:G:377:UNK:N	31:G:449:UNK:HA	1.80	0.96
2:n:77:THR:HG22	2:n:130:PRO:HA	1.46	0.96
7:s:31:SER:O	7:s:35:PRO:HD2	1.65	0.96
39:O:87:UNK:CB	39:O:88:UNK:HA	1.96	0.96
42:R:63:UNK:O	42:R:64:UNK:C	2.14	0.96
1:l:224:ASP:OD2	51:Z:217:UNK:CB	2.13	0.95
1:l:392:LEU:HA	1:l:395:TRP:CD1	2.00	0.95
30:F:166:UNK:O	30:F:169:UNK:N	1.99	0.95
45:V:55:UNK:O	45:V:57:UNK:N	1.98	0.95
3:o:108:THR:HB	3:o:313:ARG:HH11	1.31	0.95
38:N:276:UNK:O	38:N:279:UNK:N	1.98	0.95
39:O:129:UNK:O	39:O:132:UNK:CB	2.14	0.95
43:S:25:UNK:HA	43:S:57:UNK:CB	1.93	0.95
1:c:67:THR:HG23	1:c:70:ARG:N	1.79	0.95
3:b:174:THR:HG23	3:b:178:PHE:HE1	1.31	0.95
37:M:58:UNK:CA	37:M:59:UNK:CB	2.42	0.95
3:b:240:MET:HA	3:b:243:VAL:HG12	1.49	0.95
4:d:165:TYR:O	4:d:168:VAL:HG23	1.67	0.95
28:D:162:UNK:HA	32:H:279:UNK:CB	1.95	0.95
31:G:14:UNK:N	31:G:79:UNK:O	1.99	0.95
26:B:48:UNK:CB	26:B:80:UNK:HA	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:142:UNK:O	31:G:190:UNK:CB	2.14	0.95
38:N:100:UNK:O	38:N:104:UNK:N	2.00	0.95
2:n:283:PRO:HG3	9:u:55:LEU:HD22	1.47	0.95
53:p:301:HEC:HHD	53:p:301:HEC:HBC2	1.45	0.95
37:M:388:UNK:N	37:M:389:UNK:HA	1.79	0.95
3:o:174:THR:HG23	3:o:178:PHE:CE2	2.00	0.95
31:G:435:UNK:HA	31:G:440:UNK:CB	1.96	0.95
31:G:483:UNK:HA	31:G:576:UNK:CB	1.96	0.95
36:L:161:UNK:CA	36:L:162:UNK:C	2.41	0.95
1:c:133:VAL:HG12	1:c:134:ILE:HD13	1.48	0.94
1:c:403:ASP:HB3	1:c:406:VAL:HG23	1.46	0.94
2:n:316:TYR:OH	9:u:64:LEU:HD23	1.67	0.94
30:F:51:UNK:CA	30:F:52:UNK:CB	2.46	0.94
30:F:190:UNK:CB	30:F:203:UNK:HA	1.96	0.94
34:J:58:UNK:O	34:J:62:UNK:N	2.00	0.94
47:X:90:UNK:O	47:X:92:UNK:N	2.01	0.94
3:b:115:ILE:HG21	3:b:196:HIS:HB2	1.48	0.94
1:l:61:HIS:NE2	1:l:134:ILE:HD11	1.82	0.94
1:c:383:LEU:HD22	1:c:388:ARG:HA	1.45	0.94
2:m:304:HIS:CD2	2:m:306:PRO:HD2	2.01	0.94
4:p:23:HIS:HA	4:p:26:ILE:HD12	1.50	0.94
30:F:289:UNK:HA	30:F:290:UNK:C	1.93	0.94
1:l:21:ASN:HB3	1:l:217:SER:HB3	1.46	0.94
26:B:52:UNK:CB	26:B:89:UNK:O	2.15	0.94
4:d:118:ARG:HG3	4:d:194:ALA:HB1	1.44	0.94
1:l:42:ASP:HB3	1:l:384:LEU:HD22	1.45	0.94
1:c:61:HIS:CD2	1:c:134:ILE:HD11	2.03	0.94
1:c:346:CYS:HB3	1:c:412:SER:OG	1.68	0.94
2:m:67:HIS:HD2	2:m:144:LEU:HD22	1.28	0.94
3:o:206:ASN:HB2	3:o:313:ARG:HH21	1.28	0.94
31:G:52:CYS:O	31:G:53:UNK:C	2.13	0.94
2:n:51:ILE:HG21	2:n:199:PHE:HA	1.48	0.94
39:O:49:UNK:HA	39:O:50:UNK:CB	1.98	0.94
1:c:143:THR:HG21	9:i:48:SER:H	1.33	0.94
2:m:111:CYS:HB3	2:m:119:LEU:HD22	1.49	0.94
2:n:248:ASN:HB2	2:n:428:GLY:HA2	1.47	0.94
9:u:72:VAL:HB	9:u:73:PRO:CD	1.98	0.94
36:L:319:UNK:O	36:L:320:UNK:CB	2.13	0.94
2:m:305:GLN:HB2	2:m:306:PRO:HD3	1.46	0.93
7:g:9:ARG:NH2	7:g:11:ARG:HD2	1.83	0.93
3:o:106:SER:HB3	52:o:402:HEM:HBD2	1.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:155:UNK:O	30:F:159:UNK:N	2.00	0.93
2:m:60:SER:HB3	2:n:429:ASN:ND2	1.81	0.93
1:c:67:THR:CG2	1:c:70:ARG:H	1.81	0.93
2:n:132:PHE:CD2	2:n:191:LEU:HD13	2.04	0.93
4:p:74:PRO:HB2	4:p:79:GLU:HB2	1.46	0.93
4:p:158:ILE:HD13	4:p:160:MET:HB2	1.49	0.93
2:m:159:VAL:HG12	2:m:160:ILE:HD13	1.48	0.93
36:L:83:UNK:HA	36:L:87:UNK:CB	1.97	0.93
9:i:70:LEU:HD21	9:i:73:PRO:HD2	1.48	0.93
12:x:365:ILE:HD12	13:y:87:MET:HE1	1.48	0.93
36:L:55:UNK:N	36:L:56:UNK:O	2.02	0.93
45:V:45:UNK:O	45:V:48:UNK:N	2.02	0.93
27:C:21:UNK:O	27:C:24:UNK:N	2.02	0.93
31:G:237:UNK:O	31:G:253:UNK:N	2.02	0.93
30:F:34:UNK:O	30:F:38:UNK:N	2.02	0.93
36:L:210:UNK:O	36:L:214:UNK:N	2.01	0.93
51:Z:243:UNK:O	51:Z:246:UNK:N	2.01	0.93
1:c:144:SER:O	1:c:148:VAL:HG23	1.69	0.92
1:c:69:ASN:O	1:c:71:PRO:HD3	1.70	0.92
2:m:51:ILE:HG21	2:m:199:PHE:HA	1.49	0.92
2:m:77:THR:HG22	2:m:130:PRO:CA	1.99	0.92
3:o:122:THR:HG22	3:o:189:ILE:HD11	1.51	0.92
12:x:449:MET:SD	13:y:5:MET:HE2	2.09	0.92
18:4:5:LYS:HZ3	18:4:6:GLY:H	1.01	0.92
2:n:29:LEU:HB3	2:n:30:PRO:HD2	1.48	0.92
30:F:426:UNK:HA	30:F:429:UNK:CB	2.00	0.92
37:M:103:UNK:O	37:M:107:UNK:N	2.02	0.92
38:N:142:UNK:O	38:N:145:UNK:CB	2.18	0.92
46:W:49:UNK:HA	46:W:52:UNK:CB	2.00	0.92
47:X:426:UNK:O	47:X:428:UNK:O	1.85	0.92
1:l:61:HIS:CE1	1:l:134:ILE:HD11	2.04	0.92
36:L:321:UNK:O	36:L:324:UNK:CB	2.18	0.92
30:F:60:UNK:O	30:F:64:UNK:N	2.02	0.92
37:M:51:UNK:CB	37:M:58:UNK:CB	2.46	0.92
3:b:310:SER:HB3	3:b:318:ARG:NH1	1.82	0.92
27:C:83:UNK:O	27:C:85:UNK:N	2.02	0.92
5:q:15:ARG:HH21	5:q:32:ARG:HG3	1.35	0.92
26:B:148:UNK:CB	26:B:151:UNK:CB	2.48	0.92
31:G:142:UNK:O	31:G:190:UNK:CA	2.18	0.92
1:c:417:ASP:OD2	10:j:10:TYR:OH	1.88	0.92
4:d:74:PRO:HG2	4:d:82:MET:SD	2.10	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:109:UNK:O	40:P:113:UNK:N	2.03	0.92
3:o:221:HIS:HB3	3:o:222:PRO:HD3	1.52	0.92
28:D:101:UNK:O	28:D:102:UNK:C	2.09	0.92
30:F:121:UNK:CB	30:F:229:UNK:HA	1.99	0.92
50:U:25:UNK:O	50:U:26:UNK:O	1.88	0.92
1:c:392:LEU:HA	1:c:395:TRP:CD1	2.05	0.91
3:o:135:TRP:HH2	3:o:170:VAL:HG12	1.32	0.91
30:F:372:UNK:O	30:F:376:UNK:N	2.03	0.91
1:c:343:MET:HE1	1:c:416:TYR:HD2	1.33	0.91
48:Y:102:UNK:O	48:Y:105:UNK:N	2.03	0.91
3:b:252:ASP:HB3	3:b:253:PRO:HD3	1.52	0.91
37:M:189:UNK:N	37:M:191:UNK:O	2.03	0.91
2:m:385:GLN:HG2	9:i:62:ARG:HH12	1.35	0.91
2:n:207:ILE:HD11	2:n:383:GLY:HA2	1.49	0.91
3:o:26:ASN:ND2	3:o:207:ASN:HB2	1.85	0.91
44:T:55:UNK:CB	44:T:60:UNK:O	2.19	0.91
46:W:39:UNK:C	46:W:41:UNK:CB	2.49	0.91
47:X:203:UNK:O	47:X:206:UNK:N	2.03	0.91
1:l:91:THR:HG22	1:l:93:GLU:H	1.32	0.91
5:q:85:LYS:HG2	5:q:86:ASN:H	1.33	0.91
4:d:231:LYS:HD2	6:f:71:ARG:HG2	1.52	0.91
27:C:131:UNK:O	27:C:132:UNK:C	2.18	0.91
40:P:52:UNK:HA	40:P:72:UNK:CB	2.00	0.91
31:G:193:UNK:HA	31:G:196:UNK:CB	2.01	0.91
1:l:45:SER:HB3	1:l:92:ARG:HA	1.53	0.91
3:b:103:TYR:HA	3:b:315:MET:HE3	1.52	0.91
33:I:113:UNK:O	33:I:115:UNK:O	1.89	0.91
31:G:604:UNK:O	31:G:608:UNK:N	2.04	0.90
3:o:252:ASP:HB3	3:o:253:PRO:HD3	1.50	0.90
30:F:287:UNK:O	30:F:291:UNK:O	1.87	0.90
42:R:77:UNK:O	42:R:78:UNK:O	1.89	0.90
2:m:162:ASN:HD22	2:m:244:ILE:CG2	1.83	0.90
36:L:247:UNK:CA	36:L:251:UNK:CB	2.47	0.90
1:c:236:PHE:CE2	1:c:258:GLU:HB3	2.07	0.90
1:c:91:THR:HG22	1:c:93:GLU:H	1.35	0.90
1:l:236:PHE:CE2	1:l:258:GLU:HB3	2.07	0.90
5:q:109:GLU:CG	5:q:167:ALA:HB3	2.01	0.90
5:q:15:ARG:NH2	5:q:32:ARG:HG3	1.87	0.90
1:c:224:ASP:OD1	1:c:227:ALA:HB3	1.72	0.90
2:m:406:ALA:HB3	2:m:409:ASP:HB2	1.53	0.90
4:d:176:PRO:HB2	4:d:181:GLN:HE22	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:52:LYS:HB2	2:n:203:ARG:HB3	1.54	0.90
30:F:33:UNK:O	30:F:37:UNK:N	2.04	0.90
30:F:52:UNK:O	30:F:56:UNK:N	2.05	0.90
3:b:34:GLY:O	3:b:37:LEU:HB2	1.72	0.90
1:c:426:GLY:H	1:c:428:ILE:CG1	1.85	0.89
27:C:83:UNK:O	27:C:84:UNK:C	2.16	0.89
31:G:377:UNK:H	31:G:449:UNK:CA	1.83	0.89
45:V:44:UNK:O	45:V:47:UNK:CB	2.19	0.89
1:c:408:ARG:NH1	11:k:15:ARG:HE	1.71	0.89
6:f:47:ILE:O	6:f:50:LEU:HG	1.72	0.89
7:s:9:ARG:NH2	7:s:11:ARG:HD2	1.87	0.89
27:C:133:UNK:HA	27:C:136:UNK:CB	2.01	0.89
51:Z:205:UNK:O	51:Z:208:UNK:N	2.05	0.89
37:M:348:UNK:HA	37:M:351:UNK:CB	2.03	0.89
39:O:234:UNK:O	39:O:237:UNK:CB	2.20	0.89
40:P:71:UNK:O	40:P:72:UNK:C	2.18	0.89
4:d:178:THR:OG1	4:d:181:GLN:NE2	2.05	0.89
3:b:266:PRO:HB3	5:q:160:CYS:HA	1.54	0.89
36:L:151:UNK:O	36:L:155:UNK:CB	2.21	0.89
2:m:258:VAL:HG11	2:m:321:LEU:HB3	1.53	0.89
1:l:158:PHE:CE1	1:l:317:THR:HG21	2.08	0.89
1:l:383:LEU:HD22	1:l:388:ARG:HA	1.54	0.89
2:m:342:ASN:O	2:m:345:LYS:HB2	1.72	0.89
4:p:118:ARG:HG3	4:p:194:ALA:HB1	1.55	0.89
1:l:426:GLY:HA3	1:l:428:ILE:HG13	1.55	0.88
36:L:263:UNK:O	36:L:265:UNK:N	2.05	0.88
3:b:10:LEU:HD12	3:b:13:ILE:HD11	1.56	0.88
4:p:165:TYR:O	4:p:168:VAL:HG23	1.73	0.88
5:q:15:ARG:HB2	5:q:16:PRO:CD	2.02	0.88
37:M:347:UNK:O	37:M:351:UNK:CB	2.20	0.88
26:B:121:UNK:HA	26:B:135:UNK:CB	2.03	0.88
28:D:96:UNK:N	28:D:385:UNK:CB	2.35	0.88
33:I:111:UNK:O	33:I:113:UNK:N	2.06	0.88
3:b:185:LEU:HB3	3:b:186:PRO:HD3	1.55	0.88
2:n:304:HIS:CD2	2:n:306:PRO:HD2	2.08	0.88
7:s:50:PRO:HB2	7:s:51:PRO:CD	2.03	0.88
31:G:318:UNK:O	31:G:529:UNK:N	2.07	0.88
3:o:108:THR:HB	3:o:313:ARG:NH1	1.89	0.88
31:G:436:UNK:N	31:G:437:UNK:HA	1.82	0.88
3:b:179:PHE:CE2	3:o:179:PHE:HE2	1.92	0.88
8:h:73:LEU:HD23	8:h:74:PHE:N	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:385:GLN:HG2	9:u:62:ARG:HH12	1.38	0.88
14:z:112:LEU:HG	14:z:118:PRO:HB3	1.55	0.88
30:F:212:UNK:HA	30:F:220:UNK:O	1.74	0.88
36:L:29:UNK:HA	36:L:32:UNK:CB	2.03	0.88
1:c:64:PHE:HE1	1:c:86:LEU:HG	1.36	0.87
1:l:408:ARG:HH12	11:w:15:ARG:HE	1.20	0.87
30:F:294:UNK:CA	30:F:339:UNK:CB	2.52	0.87
38:N:33:UNK:O	38:N:36:UNK:N	2.06	0.87
37:M:68:UNK:O	37:M:69:UNK:C	2.19	0.87
27:C:89:UNK:N	27:C:112:UNK:O	2.07	0.87
28:D:395:UNK:O	28:D:399:UNK:N	2.07	0.87
1:l:408:ARG:NH1	11:w:15:ARG:HE	1.73	0.87
3:o:361:LEU:HD23	3:o:365:LEU:HD12	1.54	0.87
30:F:359:CYS:O	30:F:360:UNK:CB	2.22	0.87
2:m:29:LEU:HB3	2:m:30:PRO:HD2	1.54	0.87
3:b:179:PHE:HE2	3:o:179:PHE:CE2	1.92	0.87
2:n:123:LEU:O	2:n:127:THR:HG22	1.74	0.87
31:G:435:UNK:CA	31:G:440:UNK:CB	2.53	0.87
38:N:146:UNK:N	38:N:147:UNK:HA	1.89	0.87
40:P:106:UNK:HA	40:P:109:UNK:CB	2.05	0.87
47:X:177:UNK:O	47:X:180:UNK:N	2.08	0.87
51:Z:323:UNK:CB	51:Z:324:UNK:HA	2.03	0.87
31:G:174:UNK:HA	31:G:183:UNK:HA	1.55	0.87
1:l:343:MET:HE1	1:l:416:TYR:CD2	2.10	0.87
2:n:305:GLN:HB2	2:n:306:PRO:CD	2.05	0.87
1:c:40:TRP:CZ2	1:c:377:GLU:HA	2.08	0.87
1:c:156:THR:HG23	1:c:239:SER:OG	1.73	0.87
31:G:52:CYS:O	31:G:54:UNK:N	2.08	0.87
33:I:123:UNK:CB	33:I:131:UNK:O	2.23	0.87
37:M:176:UNK:N	37:M:177:UNK:HA	1.89	0.87
6:r:75:LEU:HD12	6:r:76:PRO:HD2	1.57	0.87
1:c:260:PRO:HD3	1:c:414:TYR:CE1	2.10	0.86
30:F:323:UNK:O	30:F:326:UNK:N	2.08	0.86
40:P:21:UNK:CB	40:P:45:UNK:HA	2.04	0.86
2:n:209:LEU:HD22	2:n:375:SER:HB2	1.56	0.86
2:n:347:ILE:O	2:n:411:ILE:HG23	1.75	0.86
40:P:21:UNK:O	40:P:46:UNK:N	2.08	0.86
1:c:213:GLN:HB3	1:c:215:HIS:NE2	1.91	0.86
7:s:36:ASN:HA	7:s:39:ARG:HD3	1.57	0.86
37:M:49:UNK:HA	37:M:50:UNK:CB	2.05	0.86
40:P:99:UNK:CB	40:P:103:UNK:CB	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:R:67:UNK:C	42:R:69:UNK:N	2.33	0.86
3:b:170:VAL:HG13	3:b:174:THR:CG2	2.04	0.86
30:F:369:UNK:O	30:F:370:UNK:C	2.21	0.86
31:G:380:UNK:O	31:G:409:UNK:N	2.08	0.86
40:P:301:UNK:HA	40:P:302:UNK:CB	2.06	0.86
37:M:281:UNK:O	37:M:284:UNK:CB	2.24	0.86
2:n:341:TYR:HE2	2:n:345:LYS:HE3	1.41	0.86
3:o:334:THR:O	3:o:338:ILE:HD13	1.75	0.86
36:L:316:UNK:O	36:L:319:UNK:N	2.09	0.86
36:L:321:UNK:O	36:L:324:UNK:N	2.08	0.86
1:c:46:ARG:HH22	1:c:316:ASP:CG	1.83	0.86
1:c:408:ARG:HH12	11:k:15:ARG:HE	1.22	0.86
7:g:73:ASN:N	7:g:74:PRO:HD2	1.91	0.86
10:j:58:LYS:HG2	10:j:59:TYR:H	1.41	0.86
31:G:187:UNK:N	31:G:188:UNK:HA	1.88	0.86
46:W:47:UNK:CB	46:W:50:UNK:CB	2.54	0.86
3:b:6:LYS:HE2	3:b:16:ASN:HD21	1.38	0.85
50:U:320:UNK:O	50:U:324:UNK:N	2.08	0.85
3:o:107:TYR:OH	3:o:308:HIS:ND1	2.09	0.85
13:y:78:LEU:HB2	13:y:79:PRO:HD3	1.58	0.85
39:O:229:UNK:CB	39:O:231:UNK:HA	2.04	0.85
30:F:419:UNK:HA	30:F:423:UNK:CB	2.05	0.85
36:L:67:UNK:CB	36:L:76:UNK:HA	2.05	0.85
1:c:84:ALA:HB2	1:c:101:ALA:HB2	1.59	0.85
9:i:72:VAL:CB	9:i:73:PRO:HD3	2.05	0.85
1:l:52:ASN:HB2	1:l:55:ALA:HB2	1.58	0.85
1:l:106:LEU:HD22	1:l:203:LEU:HD22	1.58	0.85
1:l:213:GLN:HB3	1:l:215:HIS:NE2	1.91	0.85
30:F:60:UNK:O	30:F:63:UNK:CB	2.24	0.85
30:F:300:UNK:CB	30:F:329:UNK:HA	2.06	0.85
1:c:426:GLY:HA3	1:c:428:ILE:HG13	1.59	0.85
38:N:72:UNK:O	38:N:75:UNK:CB	2.24	0.85
9:i:70:LEU:CD2	9:i:73:PRO:HD2	2.07	0.85
10:j:21:ALA:O	10:j:25:VAL:HG23	1.77	0.85
3:o:26:ASN:HD21	3:o:207:ASN:CB	1.90	0.85
5:q:114:VAL:HA	5:q:117:LEU:CD1	2.06	0.85
1:c:61:HIS:NE2	1:c:134:ILE:HD11	1.91	0.85
4:d:70:VAL:HG23	4:d:84:PRO:HD3	1.59	0.85
3:o:30:TRP:O	3:o:33:PHE:HD2	1.59	0.85
5:q:118:ARG:HH11	5:q:171:ILE:CG1	1.88	0.85
5:q:187:PHE:CD2	5:q:193:VAL:HB	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:34:ILE:HB	7:s:35:PRO:HD3	1.58	0.85
25:A:103:UNK:HA	25:A:106:UNK:CB	2.07	0.85
38:N:89:UNK:C	38:N:91:UNK:HA	2.07	0.85
50:U:122:UNK:O	50:U:125:UNK:N	2.10	0.85
31:G:192:UNK:HA	31:G:193:UNK:CB	2.05	0.85
25:A:102:UNK:O	25:A:106:UNK:N	2.10	0.84
36:L:34:UNK:O	36:L:38:UNK:N	2.10	0.84
36:L:46:UNK:O	36:L:49:UNK:CB	2.25	0.84
3:o:245:PHE:CD1	4:p:17:LEU:HD13	2.11	0.84
38:N:128:UNK:CB	38:N:216:UNK:CB	2.55	0.84
2:m:57:TYR:O	2:m:233:SER:HB2	1.77	0.84
2:n:263:ALA:O	2:n:269:ALA:HB2	1.77	0.84
12:x:187:SER:HB2	12:x:277:MET:HE1	1.60	0.84
2:m:286:LYS:HD3	2:m:287:ARG:NH1	1.92	0.84
1:l:428:ILE:CG2	1:l:431:LEU:HD22	2.07	0.84
2:n:126:VAL:O	2:n:130:PRO:HG3	1.77	0.84
37:M:146:UNK:O	37:M:149:UNK:N	2.09	0.84
50:U:712:UNK:HA	50:U:807:UNK:CB	2.07	0.84
1:c:308:GLN:HG3	1:c:308:GLN:O	1.77	0.84
2:m:213:HIS:N	2:m:214:PRO:HD2	1.91	0.84
3:b:213:SER:O	3:b:216:ASP:N	2.10	0.84
1:l:40:TRP:CZ2	1:l:377:GLU:HA	2.13	0.84
5:q:60:SER:HA	5:q:63:SER:OG	1.75	0.84
32:H:43:UNK:N	32:H:44:UNK:HA	1.91	0.84
32:H:120:UNK:CB	32:H:132:UNK:CB	2.54	0.84
36:L:297:UNK:HA	36:L:356:UNK:N	1.92	0.84
5:q:134:ILE:HD11	5:q:185:TYR:CG	2.12	0.84
31:G:594:UNK:HA	31:G:595:UNK:CB	2.07	0.84
43:S:63:UNK:O	43:S:78:UNK:HA	1.78	0.84
2:m:263:ALA:O	2:m:269:ALA:HB2	1.76	0.84
1:l:408:ARG:HH22	11:w:15:ARG:CZ	1.91	0.84
6:f:51:PRO:HD3	2:n:134:ARG:NH1	1.93	0.84
1:l:32:GLN:CG	1:l:33:PRO:HD2	2.08	0.84
30:F:56:UNK:O	30:F:59:UNK:CB	2.26	0.84
43:S:43:UNK:O	43:S:47:UNK:N	2.10	0.84
50:U:326:UNK:O	50:U:329:UNK:CB	2.25	0.84
1:c:408:ARG:HH22	11:k:15:ARG:CZ	1.90	0.84
1:l:406:VAL:HG22	21:7:7:GLU:OE2	1.78	0.84
36:L:288:UNK:CB	36:L:308:UNK:CB	2.55	0.84
40:P:63:UNK:C	40:P:65:UNK:CB	2.55	0.84
1:c:21:ASN:HB3	1:c:217:SER:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:15:ARG:HB2	5:e:16:PRO:HD2	1.57	0.83
44:T:55:UNK:O	44:T:59:UNK:N	2.11	0.83
2:m:198:HIS:CE1	2:m:233:SER:HB3	2.14	0.83
4:d:17:LEU:O	4:d:202:LYS:HD3	1.78	0.83
2:n:279:LEU:HB3	2:n:295:LEU:HD22	1.60	0.83
36:L:197:UNK:O	36:L:201:UNK:N	2.11	0.83
47:X:333:UNK:O	47:X:336:UNK:CB	2.25	0.83
3:o:234:LEU:CD2	4:p:216:LEU:HD21	2.08	0.83
26:B:148:UNK:CB	26:B:152:UNK:N	2.41	0.83
30:F:365:CYS:HA	30:F:368:UNK:CB	2.08	0.83
2:m:198:HIS:HE1	2:m:233:SER:HB3	1.42	0.83
3:b:163:TRP:CZ2	5:q:62:MET:HE2	2.13	0.83
38:N:233:UNK:O	38:N:236:UNK:CB	2.25	0.83
47:X:334:UNK:O	47:X:337:UNK:N	2.11	0.83
10:j:18:SER:OG	11:k:23:LEU:HB2	1.77	0.83
27:C:131:UNK:O	27:C:134:UNK:N	2.12	0.83
43:S:24:UNK:CB	43:S:59:UNK:O	2.27	0.83
1:c:106:LEU:HD22	1:c:203:LEU:HD22	1.60	0.83
6:f:6:VAL:HB	6:f:10:SER:HB2	1.60	0.83
7:g:50:PRO:HB2	7:g:51:PRO:HD3	1.61	0.83
7:s:72:LYS:CB	7:s:75:ALA:HB2	2.09	0.83
31:G:577:UNK:O	31:G:578:UNK:CB	2.25	0.83
43:S:27:UNK:O	43:S:28:UNK:CB	2.24	0.83
1:c:39:VAL:HG12	1:c:41:ILE:HD11	1.59	0.83
1:c:145:MET:SD	1:c:248:LEU:HD12	2.18	0.83
4:d:220:TYR:CE2	7:g:26:PHE:HE1	1.97	0.83
2:n:58:GLU:OE1	2:n:63:LEU:HA	1.77	0.83
3:b:47:THR:HG21	3:b:83:HIS:HB2	1.61	0.83
3:b:119:LEU:HG	52:b:402:HEM:CBB	2.09	0.83
5:e:15:ARG:CB	5:e:16:PRO:HD2	2.08	0.83
27:C:23:UNK:HA	27:C:26:UNK:CB	2.08	0.83
3:b:115:ILE:CG2	3:b:196:HIS:HB2	2.08	0.82
31:G:104:UNK:O	31:G:107:UNK:N	2.12	0.82
3:b:341:GLN:HB3	3:b:347:TYR:CD2	2.15	0.82
1:l:378:ASP:O	1:l:382:SER:HB2	1.77	0.82
3:o:185:LEU:HB3	3:o:186:PRO:HD3	1.61	0.82
30:F:303:UNK:O	30:F:414:UNK:CB	2.26	0.82
28:D:250:UNK:O	28:D:253:UNK:N	2.12	0.82
28:D:258:UNK:O	28:D:262:UNK:N	2.12	0.82
30:F:426:UNK:O	30:F:429:UNK:N	2.12	0.82
33:I:98:UNK:O	33:I:103:UNK:O	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:229:UNK:CB	39:O:231:UNK:CB	2.57	0.82
1:l:383:LEU:HA	1:l:387:GLY:O	1.78	0.82
3:o:297:SER:O	3:o:300:ILE:HG22	1.79	0.82
51:Z:210:UNK:O	51:Z:213:UNK:N	2.12	0.82
31:G:595:UNK:O	31:G:599:UNK:N	2.12	0.82
40:P:172:UNK:O	40:P:206:UNK:HA	1.80	0.82
41:Q:109:UNK:HA	41:Q:110:UNK:CB	2.09	0.82
2:m:185:LYS:HG3	2:m:185:LYS:O	1.79	0.82
5:q:118:ARG:NH1	5:q:171:ILE:HG13	1.95	0.82
50:U:622:UNK:O	50:U:625:UNK:N	2.13	0.82
7:g:30:PHE:O	7:g:34:ILE:HG13	1.79	0.82
8:h:21:ARG:HB3	8:h:65:ARG:HH21	1.45	0.82
4:p:176:PRO:HB2	4:p:181:GLN:HE22	1.44	0.82
1:c:379:ILE:HD12	1:c:390:ILE:HD12	1.62	0.82
2:m:207:ILE:HD11	2:m:383:GLY:HA2	1.62	0.82
1:l:67:THR:HG22	1:l:70:ARG:HB2	1.61	0.82
4:p:220:TYR:CE2	7:s:26:PHE:HE1	1.98	0.82
1:l:67:THR:HG23	1:l:70:ARG:N	1.92	0.82
4:p:41:HIS:CD2	4:p:113:LEU:HD11	2.15	0.82
37:M:210:UNK:HA	37:M:268:UNK:CB	2.10	0.82
40:P:131:UNK:O	40:P:165:UNK:HA	1.80	0.82
1:c:241:ILE:HG13	7:g:16:TYR:CE1	2.15	0.81
3:o:106:SER:O	3:o:109:PHE:HD2	1.63	0.81
5:q:15:ARG:CB	5:q:16:PRO:HD2	2.06	0.81
6:r:37:ILE:HG12	6:r:43:VAL:HG21	1.59	0.81
30:F:44:UNK:O	30:F:47:UNK:N	2.13	0.81
36:L:321:UNK:O	36:L:325:UNK:N	2.12	0.81
2:n:56:ARG:NH2	2:n:318:ASP:OD1	2.12	0.81
2:n:331:ALA:HA	2:n:432:HIS:ND1	1.96	0.81
3:o:234:LEU:HD23	4:p:216:LEU:HD21	1.59	0.81
1:c:53:ASN:OD1	1:c:165:GLN:HB2	1.80	0.81
9:i:78:TYR:OXT	9:i:78:TYR:HD1	1.64	0.81
8:t:21:ARG:HB3	8:t:65:ARG:NH2	1.95	0.81
30:F:405:CYS:SG	30:F:407:UNK:N	2.53	0.81
3:b:27:ILE:HG22	3:b:27:ILE:O	1.79	0.81
3:o:218:ILE:CG2	3:o:223:TYR:CD2	2.63	0.81
36:L:77:UNK:HA	36:L:78:UNK:CB	2.09	0.81
37:M:281:UNK:O	37:M:285:UNK:N	2.13	0.81
1:l:445:ARG:O	1:l:446:PHE:HB2	1.79	0.81
5:q:91:TRP:HB3	5:q:96:LEU:HB2	1.62	0.81
2:n:217:LYS:HZ2	2:n:221:GLU:CD	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:4:5:LYS:NZ	18:4:6:GLY:H	1.78	0.81
1:c:18:GLN:NE2	1:c:22:GLY:HA2	1.94	0.81
5:e:31:ALA:HB2	10:j:7:ALA:HB2	1.63	0.81
26:B:78:UNK:N	26:B:79:UNK:HA	1.94	0.81
30:F:265:UNK:O	30:F:266:UNK:CB	2.29	0.81
37:M:118:UNK:O	37:M:122:UNK:N	2.13	0.81
1:c:42:ASP:HB3	1:c:384:LEU:HD22	1.62	0.81
2:m:305:GLN:HB2	2:m:306:PRO:CD	2.11	0.81
3:b:266:PRO:HA	5:q:160:CYS:SG	2.21	0.81
5:q:99:ARG:HD3	5:q:156:TYR:OH	1.80	0.81
29:E:98:UNK:O	29:E:137:UNK:HA	1.80	0.81
30:F:264:UNK:CB	30:F:283:UNK:O	2.29	0.81
40:P:103:UNK:O	40:P:106:UNK:N	2.13	0.81
3:b:275:LEU:O	3:b:276:PHE:C	2.23	0.81
1:l:224:ASP:OD1	1:l:227:ALA:HB3	1.80	0.81
4:p:10:TYR:HE1	8:t:73:LEU:CD2	1.94	0.81
31:G:10:UNK:O	31:G:76:UNK:N	2.14	0.81
1:c:426:GLY:CA	1:c:428:ILE:CG1	2.59	0.81
6:r:33:ARG:NH2	6:r:91:GLU:OE2	2.14	0.81
3:b:33:PHE:CE1	3:b:96:MET:HG3	2.16	0.80
4:d:178:THR:HB	4:d:181:GLN:HG3	1.60	0.80
5:q:76:ILE:HG23	5:q:194:ILE:HG12	1.61	0.80
2:m:169:ARG:NH2	2:n:438:GLU:OE2	2.14	0.80
47:X:182:UNK:O	47:X:186:UNK:N	2.14	0.80
51:Z:103:UNK:O	51:Z:107:UNK:N	2.14	0.80
1:c:408:ARG:NH2	11:k:15:ARG:NE	2.28	0.80
2:m:394:PRO:O	2:m:398:VAL:HG23	1.80	0.80
3:b:218:ILE:CG2	3:b:223:TYR:CD2	2.65	0.80
2:n:309:VAL:HG22	2:n:326:THR:HA	1.63	0.80
30:F:294:UNK:C	30:F:339:UNK:CB	2.52	0.80
40:P:223:UNK:HA	40:P:224:UNK:CB	2.10	0.80
1:l:297:ILE:HG22	1:l:303:LEU:HD12	1.63	0.80
40:P:139:UNK:HA	40:P:140:UNK:CB	2.12	0.80
42:R:87:UNK:O	42:R:89:UNK:N	2.14	0.80
43:S:84:UNK:O	43:S:88:UNK:N	2.14	0.80
1:c:102:LEU:HB2	1:c:105:ASP:OD2	1.81	0.80
3:b:111:GLU:O	3:b:115:ILE:HD13	1.81	0.80
3:o:102:LEU:HD21	3:o:304:ILE:CD1	2.12	0.80
33:I:128:UNK:O	33:I:129:UNK:C	2.29	0.80
37:M:108:UNK:HA	37:M:111:UNK:CB	2.12	0.80
43:S:41:UNK:HA	43:S:44:UNK:CB	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:50:HIS:HB3	4:d:54:VAL:HB	1.62	0.80
4:p:27:ARG:HH12	10:v:58:LYS:HG3	1.46	0.80
30:F:133:UNK:CB	30:F:174:UNK:CB	2.60	0.80
40:P:145:UNK:O	40:P:148:UNK:CB	2.30	0.80
52:o:401:HEM:HBC2	52:o:401:HEM:HMC1	1.61	0.80
26:B:154:UNK:O	26:B:158:UNK:N	2.15	0.80
31:G:381:UNK:HA	31:G:409:UNK:O	1.82	0.80
31:G:428:UNK:O	31:G:432:UNK:N	2.14	0.80
40:P:170:UNK:CB	40:P:204:UNK:CA	2.57	0.80
4:p:10:TYR:HE1	8:t:73:LEU:HD21	1.46	0.80
6:r:51:PRO:HG2	6:r:54:LEU:CD2	2.12	0.80
29:E:165:UNK:O	29:E:169:UNK:N	2.14	0.80
36:L:225:UNK:CA	36:L:229:UNK:CB	2.58	0.80
40:P:64:UNK:N	40:P:65:UNK:CB	2.43	0.80
3:b:51:LEU:HD11	3:b:80:ARG:HA	1.62	0.80
51:Z:335:UNK:CB	51:Z:338:UNK:CB	2.60	0.80
1:l:260:PRO:HD3	1:l:414:TYR:CE1	2.17	0.80
3:o:316:MET:HE2	3:o:317:PHE:CE1	2.17	0.80
10:v:3:PRO:HG2	10:v:8:ARG:HG2	1.63	0.80
19:5:39:CYS:SG	19:5:53:CYS:CB	2.70	0.80
30:F:212:UNK:O	30:F:220:UNK:N	2.15	0.80
31:G:41:CYS:HB2	54:G:803:FES:S2	2.20	0.80
36:L:321:UNK:O	36:L:324:UNK:CA	2.30	0.80
2:m:248:ASN:HB2	2:m:428:GLY:HA2	1.63	0.79
3:b:5:ARG:O	3:b:9:PRO:HD2	1.82	0.79
37:M:241:UNK:O	37:M:244:UNK:N	2.15	0.79
46:W:49:UNK:O	46:W:53:UNK:N	2.15	0.79
1:c:155:ALA:HA	1:c:164:ALA:HB1	1.63	0.79
1:l:182:LEU:O	1:l:186:LEU:HD12	1.82	0.79
3:o:246:ALA:HB1	3:o:249:LEU:HB2	1.65	0.79
40:P:53:UNK:CB	40:P:57:UNK:CB	2.60	0.79
43:S:83:UNK:O	43:S:87:UNK:N	2.15	0.79
10:v:58:LYS:HG2	10:v:59:TYR:N	1.97	0.79
33:I:94:UNK:HA	33:I:108:UNK:O	1.82	0.79
38:N:163:UNK:O	38:N:166:UNK:N	2.15	0.79
40:P:146:UNK:O	40:P:149:UNK:N	2.15	0.79
2:m:209:LEU:HD22	2:m:375:SER:HB2	1.64	0.79
2:n:200:THR:CG2	2:n:203:ARG:HD2	2.10	0.79
2:n:261:SER:OG	2:n:320:GLY:HA3	1.83	0.79
47:X:203:UNK:O	47:X:204:UNK:C	2.31	0.79
2:m:42:ALA:HB1	2:m:43:PRO:HD2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:115:TYR:HD1	4:p:119:ALA:HB2	1.47	0.79
7:s:50:PRO:CB	7:s:51:PRO:HD3	2.09	0.79
8:t:73:LEU:HD23	8:t:74:PHE:N	1.98	0.79
30:F:61:UNK:O	30:F:64:UNK:N	2.16	0.79
40:P:203:UNK:HA	40:P:234:UNK:CA	2.12	0.79
3:b:310:SER:HB3	3:b:318:ARG:HH11	1.47	0.79
10:j:58:LYS:HG2	10:j:59:TYR:N	1.96	0.79
2:n:24:LEU:HD12	2:n:24:LEU:H	1.47	0.79
2:n:286:LYS:HD3	2:n:287:ARG:NH1	1.98	0.79
4:p:178:THR:OG1	4:p:181:GLN:NE2	2.14	0.79
2:n:68:LEU:HD23	2:n:186:VAL:CG1	2.12	0.79
4:p:138:PRO:HG2	8:t:55:THR:OG1	1.82	0.79
26:B:95:UNK:O	26:B:97:UNK:N	2.16	0.79
26:B:121:UNK:C	26:B:135:UNK:HA	2.12	0.79
45:V:1:UNK:O	45:V:2:UNK:C	2.30	0.79
2:m:101:THR:HG23	2:m:104:ASN:H	1.48	0.79
2:m:168:TYR:HB2	2:m:173:ALA:HB2	1.63	0.79
7:s:9:ARG:HH21	7:s:11:ARG:HD2	1.44	0.79
34:J:24:UNK:O	34:J:25:UNK:CB	2.31	0.79
40:P:136:UNK:HA	40:P:137:UNK:CB	2.11	0.79
40:P:311:UNK:O	40:P:314:UNK:N	2.16	0.79
44:T:62:UNK:CB	44:T:66:UNK:CB	2.60	0.79
1:c:426:GLY:N	1:c:428:ILE:CG1	2.45	0.79
2:m:304:HIS:HD2	2:m:306:PRO:HD2	1.48	0.79
3:b:3:ASN:N	3:b:8:HIS:NE2	2.30	0.79
7:g:31:SER:O	7:g:35:PRO:HD2	1.83	0.79
2:n:297:GLN:OE1	2:n:297:GLN:HA	1.83	0.79
19:5:39:CYS:SG	19:5:53:CYS:HB3	2.22	0.79
51:Z:101:UNK:O	51:Z:105:UNK:N	2.15	0.79
4:d:10:TYR:CZ	4:d:128:PHE:HE2	2.01	0.79
1:l:75:LEU:O	1:l:79:VAL:HG23	1.82	0.79
2:n:159:VAL:HG12	2:n:160:ILE:HD13	1.65	0.79
3:o:126:THR:OG1	3:o:185:LEU:HD23	1.82	0.79
3:o:135:TRP:CH2	3:o:170:VAL:HG12	2.17	0.79
31:G:120:UNK:O	31:G:124:UNK:O	2.01	0.79
40:P:203:UNK:HA	40:P:233:UNK:CB	2.13	0.79
36:L:578:UNK:O	36:L:579:UNK:C	2.28	0.78
40:P:135:UNK:HA	40:P:168:UNK:N	1.98	0.78
2:m:347:ILE:O	2:m:411:ILE:HG23	1.83	0.78
3:b:51:LEU:HD21	3:b:79:ILE:HG22	1.63	0.78
3:b:106:SER:O	3:b:109:PHE:HD1	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:169:SER:HB2	5:q:93:GLY:HA3	1.64	0.78
3:o:1:MET:SD	3:o:7:SER:HB2	2.23	0.78
9:u:64:LEU:HG	9:u:65:VAL:HG23	1.65	0.78
30:F:262:UNK:CB	30:F:285:UNK:HA	2.13	0.78
31:G:311:UNK:CB	31:G:314:UNK:CB	2.61	0.78
37:M:207:UNK:O	37:M:208:UNK:CB	2.30	0.78
7:g:44:CYS:SG	7:g:48:VAL:HG21	2.22	0.78
1:l:262:TRP:CD2	1:l:385:THR:HG23	2.18	0.78
4:p:10:TYR:CZ	4:p:128:PHE:HE2	2.01	0.78
28:D:174:UNK:O	28:D:177:UNK:N	2.15	0.78
1:c:21:ASN:HB3	1:c:217:SER:OG	1.84	0.78
2:m:438:GLU:OE2	2:n:169:ARG:NH2	2.16	0.78
6:f:28:LYS:CD	6:f:74:ILE:HD11	2.14	0.78
32:H:68:UNK:O	32:H:69:UNK:C	2.24	0.78
42:R:81:UNK:CB	42:R:91:UNK:O	2.31	0.78
30:F:65:UNK:O	30:F:75:UNK:N	2.16	0.78
2:m:297:GLN:OE1	2:m:297:GLN:HA	1.82	0.78
2:m:385:GLN:CG	9:i:62:ARG:HH12	1.96	0.78
1:l:92:ARG:HD2	1:l:163:LEU:HD12	1.65	0.78
26:B:116:UNK:O	26:B:117:UNK:CB	2.31	0.78
31:G:52:CYS:C	31:G:54:UNK:N	2.41	0.78
32:H:101:UNK:N	32:H:161:UNK:HA	1.99	0.78
1:c:86:LEU:HD13	1:c:99:ILE:HG12	1.64	0.78
3:o:341:GLN:HB3	3:o:347:TYR:CD2	2.19	0.78
50:U:416:UNK:O	50:U:419:UNK:N	2.17	0.78
1:c:46:ARG:NH2	1:c:316:ASP:OD2	2.17	0.78
2:n:341:TYR:CE2	2:n:345:LYS:HE3	2.19	0.78
37:M:113:UNK:HA	37:M:114:UNK:CB	2.13	0.78
37:M:191:UNK:CB	37:M:192:UNK:HA	2.14	0.78
41:Q:95:UNK:O	41:Q:99:UNK:N	2.17	0.78
1:c:146:ARG:NH2	1:c:308:GLN:HE22	1.82	0.78
4:d:74:PRO:CB	4:d:79:GLU:HB2	2.13	0.78
1:l:24:ARG:CB	1:l:196:VAL:HG22	2.14	0.78
1:l:408:ARG:NH2	11:w:15:ARG:NE	2.30	0.78
36:L:223:UNK:CB	36:L:256:UNK:CB	2.62	0.78
50:U:713:UNK:O	50:U:716:UNK:N	2.17	0.78
5:e:41:ALA:O	5:e:45:VAL:HG23	1.81	0.77
1:l:405:ARG:HD3	21:7:4:ARG:NH1	1.96	0.77
3:o:3:ASN:N	3:o:8:HIS:NE2	2.32	0.77
3:o:170:VAL:HG13	3:o:174:THR:HG21	1.66	0.77
8:t:50:THR:HG22	8:t:52:GLU:H	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:163:UNK:CA	32:H:278:UNK:HA	2.14	0.77
1:c:39:VAL:HG12	1:c:41:ILE:CD1	2.13	0.77
1:l:21:ASN:HB3	1:l:217:SER:CB	2.13	0.77
1:l:405:ARG:NH1	21:7:2:GLU:CD	2.12	0.77
10:v:58:LYS:HG2	10:v:59:TYR:H	1.48	0.77
3:b:280:ILE:HD11	3:b:335:LEU:HD13	1.64	0.77
4:d:3:LEU:HD11	7:g:71:ARG:HB2	1.64	0.77
2:n:308:ASP:OD1	2:n:309:VAL:N	2.17	0.77
31:G:11:UNK:CB	31:G:77:UNK:O	2.32	0.77
36:L:142:UNK:HA	37:M:370:UNK:CB	2.14	0.77
4:d:228:SER:HB2	7:g:23:GLN:NE2	1.97	0.77
7:g:9:ARG:HH21	7:g:11:ARG:HD2	1.49	0.77
1:l:32:GLN:HG3	1:l:33:PRO:HD2	1.67	0.77
4:p:50:HIS:HB3	4:p:54:VAL:HB	1.64	0.77
4:p:220:TYR:HE2	7:s:26:PHE:HE1	1.29	0.77
25:A:84:UNK:O	25:A:85:UNK:C	2.32	0.77
36:L:67:UNK:CB	36:L:76:UNK:CB	2.63	0.77
1:l:331:ILE:HD11	1:l:427:PRO:O	1.85	0.77
3:o:309:THR:CG2	3:o:370:GLY:HA3	2.14	0.77
5:q:65:SER:OG	5:q:67:ASP:HB3	1.85	0.77
19:5:75:ARG:HG2	19:5:75:ARG:HH11	1.48	0.77
31:G:316:UNK:HA	31:G:342:UNK:O	1.85	0.77
2:m:331:ALA:HA	2:m:432:HIS:ND1	2.00	0.77
4:d:229:VAL:HG12	4:d:233:ARG:HE	1.49	0.77
31:G:227:UNK:O	31:G:238:UNK:C	2.33	0.77
37:M:258:UNK:O	37:M:262:UNK:N	2.17	0.77
2:m:362:ASN:HA	2:m:365:LYS:HD3	1.65	0.77
3:b:264:THR:HG21	5:q:144:CYS:CB	2.13	0.77
3:b:338:ILE:N	3:b:338:ILE:HD12	1.98	0.77
2:n:29:LEU:HB3	2:n:30:PRO:CD	2.14	0.77
36:L:580:UNK:N	36:L:581:UNK:HA	1.98	0.77
37:M:25:UNK:O	37:M:28:UNK:N	2.18	0.77
38:N:257:UNK:O	38:N:259:UNK:N	2.18	0.77
1:c:428:ILE:HG22	1:c:431:LEU:CB	2.12	0.77
4:p:181:GLN:HA	8:t:77:LEU:HD13	1.67	0.77
30:F:426:UNK:O	30:F:430:UNK:N	2.18	0.77
50:U:109:UNK:O	50:U:110:UNK:C	2.31	0.77
1:c:45:SER:HB3	1:c:92:ARG:HA	1.66	0.77
1:c:92:ARG:HD2	1:c:163:LEU:HD12	1.67	0.77
1:c:386:TYR:HD1	1:c:386:TYR:H	1.32	0.77
4:p:198:HIS:NE2	4:p:202:LYS:NZ	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:382:UNK:CB	31:G:454:UNK:HA	2.15	0.77
1:l:41:ILE:HD12	1:l:41:ILE:H	1.50	0.77
38:N:204:UNK:O	38:N:208:UNK:N	2.18	0.77
3:b:26:ASN:ND2	3:b:207:ASN:HB2	1.99	0.76
3:b:187:PHE:CZ	3:o:184:ILE:HG13	2.20	0.76
2:n:49:LEU:HD11	2:n:204:MET:SD	2.26	0.76
5:q:157:TYR:OH	5:q:162:GLY:HA2	1.85	0.76
30:F:61:UNK:O	30:F:64:UNK:CA	2.33	0.76
47:X:171:UNK:O	47:X:175:UNK:CB	2.33	0.76
4:d:14:HIS:HA	4:d:19:SER:HB3	1.66	0.76
4:d:182:VAL:O	4:d:186:VAL:HG23	1.84	0.76
26:B:147:UNK:O	26:B:148:UNK:CB	2.33	0.76
36:L:453:UNK:O	36:L:456:UNK:N	2.19	0.76
51:Z:114:UNK:O	51:Z:117:UNK:CB	2.32	0.76
1:l:39:VAL:HG12	1:l:41:ILE:HD11	1.65	0.76
6:r:50:LEU:HB2	6:r:55:TYR:HB2	1.67	0.76
27:C:21:UNK:O	27:C:24:UNK:CB	2.33	0.76
32:H:194:UNK:O	32:H:195:UNK:CB	2.34	0.76
40:P:203:UNK:CA	40:P:234:UNK:HA	2.15	0.76
6:r:73:GLN:NE2	7:s:32:LYS:NZ	2.33	0.76
13:y:5:MET:HE3	22:8:42:PRO:HA	1.67	0.76
1:l:102:LEU:HB2	1:l:105:ASP:OD2	1.85	0.76
4:p:55:CYS:SG	10:v:52:TRP:HB2	2.25	0.76
36:L:181:UNK:O	36:L:182:UNK:C	2.32	0.76
38:N:165:UNK:CB	38:N:185:UNK:CB	2.63	0.76
51:Z:111:UNK:O	51:Z:114:UNK:N	2.19	0.76
1:c:249:PRO:O	1:c:250:LEU:HD23	1.85	0.76
2:m:59:ASN:O	2:m:63:LEU:HG	1.84	0.76
3:b:108:THR:HB	3:b:313:ARG:NH1	2.00	0.76
7:g:72:LYS:CB	7:g:75:ALA:HB2	2.09	0.76
27:C:62:UNK:O	27:C:66:UNK:N	2.18	0.76
30:F:352:UNK:O	30:F:355:UNK:N	2.19	0.76
36:L:190:UNK:HA	36:L:194:UNK:HA	1.68	0.76
37:M:62:UNK:N	37:M:63:UNK:HA	2.00	0.76
40:P:223:UNK:CA	40:P:224:UNK:CB	2.63	0.76
47:X:426:UNK:O	47:X:427:UNK:C	2.29	0.76
3:b:310:SER:CB	3:b:318:ARG:HH11	1.99	0.76
2:n:200:THR:HG22	2:n:203:ARG:CD	2.15	0.76
13:y:59:GLN:H	13:y:62:GLU:HG3	1.51	0.76
1:c:27:SER:HA	1:c:199:ALA:O	1.86	0.76
2:m:129:ALA:N	2:m:130:PRO:HD2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:234:UNK:O	28:D:237:UNK:N	2.18	0.76
40:P:53:UNK:CA	40:P:57:UNK:CB	2.64	0.76
2:m:148:LYS:HE2	2:m:180:ASP:OD1	1.85	0.76
5:e:55:VAL:O	5:e:59:VAL:HG23	1.85	0.76
2:n:305:GLN:CB	2:n:306:PRO:HD3	2.15	0.76
26:B:155:UNK:O	26:B:159:UNK:N	2.19	0.76
38:N:175:UNK:CB	38:N:225:UNK:O	2.33	0.76
4:d:127:VAL:HG12	4:d:187:CYS:SG	2.26	0.75
3:o:47:THR:CG2	3:o:83:HIS:HB2	2.16	0.75
28:D:193:UNK:O	28:D:194:UNK:CB	2.34	0.75
37:M:447:UNK:O	37:M:450:UNK:O	2.04	0.75
2:n:68:LEU:HD23	2:n:186:VAL:HG12	1.69	0.75
3:o:310:SER:OG	3:o:318:ARG:NH1	2.18	0.75
28:D:218:UNK:O	28:D:222:UNK:CB	2.34	0.75
31:G:148:UNK:CB	31:G:207:UNK:O	2.34	0.75
46:W:41:UNK:O	46:W:42:UNK:CB	2.33	0.75
1:c:72:GLY:O	1:c:73:ASN:OD1	2.04	0.75
1:l:39:VAL:HG23	1:l:113:LEU:HD23	1.68	0.75
27:C:111:UNK:CB	27:C:113:UNK:CB	2.64	0.75
3:b:9:PRO:HG2	3:b:12:LYS:HB2	1.68	0.75
2:n:314:ALA:CB	9:u:64:LEU:HD22	2.16	0.75
29:E:28:UNK:O	29:E:32:UNK:N	2.20	0.75
37:M:347:UNK:O	37:M:351:UNK:CA	2.34	0.75
3:b:345:HIS:HB3	3:b:346:PRO:CD	2.17	0.75
4:d:220:TYR:HE2	7:g:26:PHE:HE1	1.30	0.75
6:f:94:LEU:O	6:f:98:ILE:HG13	1.86	0.75
1:l:386:TYR:HD1	1:l:386:TYR:H	1.33	0.75
3:o:129:MET:HG2	3:o:178:PHE:HD1	1.49	0.75
30:F:322:UNK:O	30:F:327:UNK:N	2.19	0.75
32:H:195:UNK:O	32:H:198:UNK:CB	2.34	0.75
10:j:51:LEU:HD22	10:j:52:TRP:HZ3	1.50	0.75
1:l:405:ARG:HH11	21:7:4:ARG:HD2	1.51	0.75
1:c:236:PHE:CD2	1:c:258:GLU:HG2	2.22	0.75
3:b:47:THR:CG2	3:b:83:HIS:HB2	2.16	0.75
3:b:210:GLY:HA3	3:b:314:SER:HB2	1.68	0.75
3:o:177:ARG:O	3:o:181:PHE:HD2	1.69	0.75
26:B:119:CYS:H	26:B:122:UNK:CB	1.94	0.75
2:m:141:GLN:HB2	2:m:142:PRO:HD3	1.68	0.75
3:b:7:SER:HA	3:b:13:ILE:HG12	1.69	0.75
5:q:171:ILE:CD1	5:q:176:ALA:HB3	2.16	0.75
28:D:139:UNK:O	28:D:143:UNK:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:405:CYS:SG	30:F:408:UNK:N	2.60	0.75
37:M:372:UNK:O	37:M:376:UNK:N	2.20	0.75
42:R:60:UNK:O	42:R:61:UNK:C	2.35	0.75
3:o:122:THR:CG2	3:o:189:ILE:HD11	2.17	0.75
4:p:143:LEU:HD22	4:p:147:LEU:O	1.86	0.75
5:q:77:LYS:HG3	5:q:89:PHE:CE2	2.22	0.75
5:q:134:ILE:HD11	5:q:185:TYR:CE2	2.21	0.75
30:F:352:UNK:O	30:F:355:UNK:CB	2.35	0.75
31:G:317:UNK:HA	31:G:527:UNK:O	1.87	0.75
2:m:328:SER:HB3	2:m:336:VAL:HG21	1.69	0.74
3:o:310:SER:CB	3:o:318:ARG:HH11	2.00	0.74
5:q:153:PHE:HE1	5:q:173:LYS:HG3	1.50	0.74
29:E:106:UNK:O	29:E:110:UNK:N	2.20	0.74
31:G:210:UNK:O	31:G:213:UNK:N	2.20	0.74
37:M:275:UNK:O	37:M:278:UNK:CB	2.35	0.74
3:b:169:SER:OG	3:b:170:VAL:N	2.18	0.74
3:o:22:PRO:HG2	7:s:3:GLN:HB3	1.69	0.74
31:G:185:UNK:O	31:G:188:UNK:CB	2.35	0.74
40:P:38:UNK:O	40:P:41:UNK:O	2.05	0.74
43:S:63:UNK:CB	43:S:78:UNK:CB	2.66	0.74
2:m:207:ILE:HD12	2:m:382:VAL:HG12	1.69	0.74
2:n:59:ASN:O	2:n:63:LEU:HG	1.86	0.74
2:n:213:HIS:N	2:n:214:PRO:HD2	2.01	0.74
13:y:184:LEU:HD11	13:y:211:LEU:HD21	1.69	0.74
36:L:503:UNK:O	36:L:507:UNK:N	2.19	0.74
1:c:292:SER:O	1:c:295:ALA:HB3	1.88	0.74
2:n:257:LEU:HD13	2:n:424:MET:HB2	1.68	0.74
30:F:421:UNK:O	30:F:425:UNK:N	2.20	0.74
33:I:73:UNK:O	33:I:74:UNK:CB	2.34	0.74
36:L:165:UNK:O	36:L:169:UNK:N	2.20	0.74
36:L:224:UNK:N	36:L:256:UNK:CB	2.51	0.74
37:M:23:UNK:O	37:M:25:UNK:N	2.20	0.74
38:N:90:UNK:N	38:N:91:UNK:HA	2.01	0.74
1:l:363:ASN:OD1	2:n:112:LEU:HD23	1.88	0.74
2:n:95:LYS:HE3	9:u:70:LEU:HD22	1.70	0.74
2:n:237:ALA:HB2	2:n:318:ASP:OD2	1.87	0.74
2:n:304:HIS:HD2	2:n:306:PRO:HD2	1.51	0.74
3:o:51:LEU:HD11	3:o:80:ARG:HA	1.69	0.74
1:c:236:PHE:HE2	1:c:258:GLU:HB3	1.50	0.74
5:q:157:TYR:HE2	5:q:159:PRO:HA	1.51	0.74
14:z:187:THR:HG21	18:4:68:THR:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:207:UNK:HA	36:L:208:UNK:CB	2.18	0.74
37:M:241:UNK:O	37:M:242:UNK:C	2.35	0.74
1:c:75:LEU:O	1:c:79:VAL:HG23	1.88	0.74
1:c:316:ASP:N	1:c:316:ASP:OD1	2.21	0.74
36:L:71:UNK:O	36:L:72:UNK:CB	2.36	0.74
1:c:145:MET:HE3	1:c:252:HIS:CE1	2.21	0.74
1:c:236:PHE:HD2	1:c:258:GLU:HG2	1.52	0.74
2:m:162:ASN:HD22	2:m:244:ILE:HG21	1.51	0.74
2:m:395:PRO:O	2:m:398:VAL:HB	1.88	0.74
29:E:152:UNK:O	29:E:163:UNK:N	2.21	0.74
2:m:429:ASN:ND2	2:n:60:SER:HB3	1.98	0.74
3:b:361:LEU:HD23	3:b:365:LEU:HD12	1.69	0.74
3:o:61:THR:O	3:o:62:ALA:C	2.29	0.74
5:q:114:VAL:CA	5:q:117:LEU:HD12	2.12	0.74
5:q:118:ARG:HD2	5:q:171:ILE:HG12	1.70	0.74
31:G:12:UNK:O	31:G:78:UNK:HA	1.87	0.74
42:R:78:UNK:O	42:R:79:UNK:C	2.36	0.74
48:Y:35:UNK:O	48:Y:39:UNK:N	2.21	0.74
2:m:337:ILE:HG21	2:m:434:PRO:HG2	1.68	0.74
8:h:15:ASP:N	8:h:16:PRO:HD2	2.03	0.74
3:o:184:ILE:O	3:o:188:ILE:HD12	1.88	0.74
6:r:28:LYS:CD	6:r:74:ILE:HD11	2.15	0.74
30:F:82:UNK:O	30:F:83:UNK:C	2.34	0.74
30:F:300:UNK:CA	30:F:329:UNK:HA	2.18	0.74
45:V:66:UNK:O	45:V:69:UNK:CB	2.36	0.74
1:c:84:ALA:CB	1:c:101:ALA:HB2	2.18	0.73
3:b:184:ILE:HG13	3:o:187:PHE:CZ	2.23	0.73
1:l:236:PHE:HE2	1:l:258:GLU:HB3	1.51	0.73
3:b:252:ASP:HB3	3:b:253:PRO:CD	2.18	0.73
4:d:5:LEU:HB3	4:d:152:TYR:CD1	2.22	0.73
4:d:11:PRO:O	8:h:74:PHE:CE2	2.41	0.73
1:l:53:ASN:OD1	1:l:165:GLN:HB2	1.87	0.73
1:l:426:GLY:CA	1:l:428:ILE:CG1	2.64	0.73
5:q:98:VAL:HA	5:q:134:ILE:HG22	1.70	0.73
32:H:40:UNK:O	32:H:47:UNK:HA	1.88	0.73
41:Q:40:UNK:CB	41:Q:41:UNK:HA	2.17	0.73
1:c:408:ARG:CZ	11:k:15:ARG:HE	2.01	0.73
3:b:126:THR:OG1	3:b:185:LEU:HD23	1.87	0.73
2:n:385:GLN:CG	9:u:62:ARG:HH12	2.00	0.73
30:F:163:UNK:O	30:F:165:UNK:O	2.06	0.73
1:c:383:LEU:HA	1:c:387:GLY:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:352:LEU:HB3	2:m:411:ILE:HD11	1.70	0.73
3:b:26:ASN:HD21	3:b:207:ASN:CB	2.01	0.73
1:l:255:ILE:HG13	1:l:422:VAL:HG22	1.71	0.73
1:l:408:ARG:HH12	11:w:15:ARG:NE	1.85	0.73
37:M:87:UNK:CB	37:M:88:UNK:HA	2.17	0.73
50:U:329:UNK:O	50:U:330:UNK:CB	2.37	0.73
2:m:279:LEU:CD2	2:m:295:LEU:HD13	2.19	0.73
2:n:34:VAL:HG11	2:n:386:ALA:HB1	1.70	0.73
3:o:90:PHE:CE1	3:o:123:VAL:HG21	2.23	0.73
5:q:188:THR:N	5:q:192:MET:O	2.21	0.73
45:V:45:UNK:C	45:V:47:UNK:N	2.50	0.73
3:b:206:ASN:ND2	3:b:207:ASN:H	1.85	0.73
4:p:10:TYR:CE1	8:t:73:LEU:HD21	2.23	0.73
5:q:134:ILE:O	5:q:135:LEU:HD23	1.89	0.73
18:4:54:ARG:HD3	18:4:54:ARG:N	2.04	0.73
25:A:103:UNK:O	25:A:107:UNK:N	2.21	0.73
26:B:128:UNK:O	26:B:131:UNK:CB	2.36	0.73
1:c:163:LEU:HD12	1:c:163:LEU:O	1.88	0.73
1:c:262:TRP:CD2	1:c:385:THR:HG23	2.24	0.73
3:o:147:THR:HG21	3:o:165:TRP:NE1	2.03	0.73
26:B:121:UNK:HA	26:B:135:UNK:CA	2.18	0.73
36:L:530:UNK:O	36:L:534:UNK:N	2.21	0.73
2:m:384:SER:HB2	9:i:62:ARG:HG2	1.71	0.73
1:l:426:GLY:N	1:l:428:ILE:HG13	2.02	0.73
3:o:361:LEU:CD2	3:o:365:LEU:HD12	2.18	0.73
30:F:61:UNK:C	30:F:64:UNK:N	2.51	0.73
31:G:565:UNK:O	31:G:568:UNK:N	2.22	0.73
2:m:67:HIS:CD2	2:m:144:LEU:HD22	2.18	0.73
2:m:347:ILE:H	2:m:347:ILE:HD12	1.54	0.73
4:d:43:MET:HG2	4:d:46:VAL:HG23	1.70	0.73
1:l:99:ILE:HG13	1:l:113:LEU:HD13	1.69	0.73
4:d:41:HIS:CD2	4:d:113:LEU:HD11	2.24	0.73
27:C:111:UNK:C	27:C:113:UNK:CB	2.67	0.73
30:F:140:UNK:CB	30:F:182:UNK:HA	2.18	0.73
34:J:58:UNK:O	34:J:62:UNK:CB	2.37	0.73
36:L:209:UNK:O	36:L:212:UNK:CB	2.37	0.73
36:L:239:UNK:O	36:L:240:UNK:O	2.06	0.73
46:W:68:UNK:O	46:W:72:UNK:CB	2.37	0.73
50:U:713:UNK:O	50:U:714:UNK:C	2.35	0.73
6:f:28:LYS:HB3	6:f:74:ILE:HD11	1.69	0.72
5:q:55:VAL:O	5:q:59:VAL:HG23	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:469:UNK:O	31:G:473:UNK:N	2.21	0.72
32:H:177:UNK:CA	47:X:146:UNK:CB	2.67	0.72
34:J:22:UNK:CB	34:J:24:UNK:O	2.37	0.72
37:M:27:UNK:O	37:M:30:UNK:N	2.22	0.72
47:X:188:UNK:O	47:X:191:UNK:N	2.22	0.72
3:b:30:TRP:O	3:b:33:PHE:HD2	1.71	0.72
4:d:54:VAL:HG12	4:d:54:VAL:O	1.89	0.72
2:n:68:LEU:HD11	2:n:140:LEU:HD23	1.71	0.72
4:p:27:ARG:NH1	10:v:58:LYS:HZ2	1.87	0.72
6:r:96:GLU:O	6:r:97:VAL:C	2.32	0.72
30:F:74:UNK:O	30:F:78:UNK:N	2.22	0.72
43:S:23:UNK:O	43:S:56:UNK:O	2.07	0.72
1:c:100:LYS:NZ	1:c:373:THR:OG1	2.18	0.72
1:c:408:ARG:HH12	11:k:15:ARG:CG	2.02	0.72
2:n:46:ARG:HH12	2:n:376:GLU:HG3	1.55	0.72
28:D:360:UNK:CB	28:D:381:UNK:HA	2.19	0.72
29:E:98:UNK:N	29:E:136:UNK:O	2.23	0.72
36:L:223:UNK:C	36:L:256:UNK:CB	2.66	0.72
2:m:56:ARG:NH2	2:m:318:ASP:OD1	2.22	0.72
2:m:182:ARG:NH1	2:m:185:LYS:HG2	2.03	0.72
5:e:19:LEU:O	5:e:19:LEU:HD12	1.90	0.72
1:l:335:MET:HE2	1:l:339:GLN:HG3	1.72	0.72
3:o:206:ASN:CB	3:o:313:ARG:HH21	1.99	0.72
15:1:23:PRO:O	16:2:66:ARG:HD3	1.89	0.72
33:I:149:UNK:HA	33:I:150:UNK:CB	2.19	0.72
40:P:236:UNK:O	40:P:237:UNK:CB	2.36	0.72
43:S:84:UNK:O	43:S:87:UNK:N	2.22	0.72
2:m:140:LEU:O	2:m:141:GLN:C	2.30	0.72
6:f:33:ARG:NH2	6:f:91:GLU:OE2	2.22	0.72
9:u:72:VAL:CB	9:u:73:PRO:HD3	2.15	0.72
1:c:408:ARG:HH12	11:k:15:ARG:NE	1.86	0.72
3:b:280:ILE:CD1	3:b:335:LEU:HD13	2.19	0.72
4:d:10:TYR:HE1	8:h:73:LEU:CD2	2.03	0.72
9:i:70:LEU:HD12	9:i:71:ASN:N	2.04	0.72
1:l:262:TRP:CG	1:l:385:THR:HG23	2.24	0.72
4:p:74:PRO:CB	4:p:79:GLU:HB2	2.19	0.72
5:q:118:ARG:HH11	5:q:171:ILE:HG13	1.50	0.72
27:C:113:UNK:O	27:C:115:UNK:N	2.22	0.72
31:G:375:UNK:CB	31:G:376:UNK:HA	2.18	0.72
39:O:130:UNK:O	39:O:131:UNK:C	2.35	0.72
4:d:27:ARG:HH12	10:j:58:LYS:HG3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:67:THR:CG2	1:l:70:ARG:HB2	2.20	0.72
5:q:109:GLU:CD	5:q:167:ALA:HB3	2.15	0.72
36:L:580:UNK:N	36:L:581:UNK:CA	2.51	0.72
40:P:137:UNK:CB	40:P:138:UNK:HA	2.19	0.72
2:m:283:PRO:HG3	9:i:55:LEU:CD2	2.18	0.72
15:l:147:LYS:HA	15:l:147:LYS:HE3	1.72	0.72
38:N:223:UNK:HA	38:N:224:UNK:C	2.19	0.72
1:c:273:ALA:HA	1:c:276:ILE:HD12	1.71	0.72
1:c:274:ASN:HB3	1:c:309:THR:OG1	1.89	0.72
2:m:78:LYS:HB3	2:m:129:ALA:HB1	1.70	0.72
3:o:309:THR:HG21	3:o:370:GLY:HA3	1.70	0.72
4:d:150:ASN:OD1	4:d:151:PRO:HD2	1.90	0.72
1:l:256:ALA:HA	1:l:320:LEU:O	1.89	0.72
2:n:314:ALA:HB2	9:u:64:LEU:HD22	1.70	0.72
31:G:332:UNK:O	31:G:336:UNK:N	2.23	0.72
10:j:49:GLY:HA2	10:j:54:HIS:CB	2.20	0.71
3:o:5:ARG:O	3:o:9:PRO:HD2	1.90	0.71
30:F:362:CYS:SG	30:F:404:UNK:CB	2.78	0.71
38:N:61:UNK:O	38:N:64:UNK:N	2.23	0.71
45:V:27:UNK:O	45:V:31:UNK:N	2.23	0.71
1:c:233:PRO:HG2	5:e:23:LYS:CD	2.20	0.71
45:V:45:UNK:O	45:V:46:UNK:C	2.38	0.71
5:q:121:GLN:O	5:q:170:ARG:NH1	2.18	0.71
9:u:70:LEU:CD2	9:u:73:PRO:HD2	2.17	0.71
30:F:398:UNK:O	30:F:401:UNK:CB	2.39	0.71
31:G:12:UNK:O	31:G:79:UNK:N	2.23	0.71
40:P:104:UNK:O	40:P:108:UNK:N	2.22	0.71
1:c:39:VAL:HG11	1:c:117:VAL:HG21	1.73	0.71
3:b:297:SER:O	3:b:300:ILE:HG22	1.90	0.71
4:d:7:PRO:HG3	4:d:126:TYR:HA	1.71	0.71
1:l:8:LEU:O	1:l:11:VAL:HG23	1.90	0.71
2:n:78:LYS:HB3	2:n:129:ALA:HB1	1.73	0.71
5:q:121:GLN:HB2	5:q:170:ARG:HD3	1.71	0.71
26:B:166:UNK:HA	26:B:169:UNK:O	1.90	0.71
30:F:214:UNK:HA	30:F:218:UNK:O	1.90	0.71
33:I:151:UNK:O	33:I:154:UNK:CB	2.38	0.71
37:M:31:UNK:O	37:M:32:UNK:C	2.37	0.71
38:N:123:UNK:HA	38:N:124:UNK:CB	2.18	0.71
45:V:44:UNK:O	45:V:47:UNK:N	2.24	0.71
48:Y:102:UNK:O	48:Y:105:UNK:CA	2.39	0.71
3:b:100:ARG:NH2	52:b:402:HEM:HBD1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:174:THR:CG2	3:b:178:PHE:HE1	2.03	0.71
52:b:401:HEM:HBC2	52:b:401:HEM:HMC1	1.73	0.71
1:l:45:SER:OG	1:l:92:ARG:HG3	1.91	0.71
2:n:165:ALA:HA	2:n:173:ALA:HB1	1.72	0.71
6:r:73:GLN:HE21	7:s:32:LYS:NZ	1.89	0.71
43:S:41:UNK:O	43:S:45:UNK:N	2.23	0.71
4:p:164:ILE:HD13	4:p:182:VAL:HG12	1.70	0.71
26:B:122:UNK:HA	26:B:123:UNK:CB	2.21	0.71
38:N:33:UNK:O	38:N:34:UNK:C	2.38	0.71
40:P:52:UNK:CA	40:P:72:UNK:CB	2.68	0.71
43:S:44:UNK:O	43:S:48:UNK:N	2.24	0.71
48:Y:103:UNK:O	48:Y:104:UNK:C	2.36	0.71
2:m:162:ASN:O	2:m:244:ILE:HD12	1.89	0.71
3:b:147:THR:HG21	3:b:165:TRP:NE1	2.06	0.71
1:l:274:ASN:HB3	1:l:309:THR:OG1	1.91	0.71
36:L:182:UNK:O	36:L:186:UNK:N	2.24	0.71
37:M:32:UNK:O	37:M:35:UNK:N	2.23	0.71
40:P:146:UNK:O	40:P:150:UNK:N	2.24	0.71
2:n:338:LYS:HG2	2:n:439:LEU:HD21	1.73	0.71
47:X:353:UNK:O	47:X:356:UNK:O	2.07	0.71
1:c:21:ASN:HB3	1:c:217:SER:HB3	1.72	0.71
1:c:334:MET:HA	1:c:334:MET:HE3	1.70	0.71
2:m:29:LEU:HB3	2:m:30:PRO:CD	2.20	0.71
2:m:300:ALA:HA	2:m:307:PHE:CZ	2.26	0.71
2:n:182:ARG:NH1	2:n:185:LYS:HG2	2.06	0.71
12:x:176:MET:HE3	12:x:181:THR:HG22	1.71	0.71
31:G:59:UNK:CB	31:G:62:UNK:CB	2.69	0.71
38:N:158:UNK:O	38:N:161:UNK:CB	2.39	0.71
3:b:156:ILE:HG12	3:b:157:GLY:H	1.56	0.71
1:c:41:ILE:H	1:c:41:ILE:HD12	1.54	0.70
3:b:122:THR:HG22	3:b:189:ILE:HD11	1.72	0.70
5:e:13:TYR:O	7:g:23:GLN:HB3	1.91	0.70
9:i:78:TYR:OXT	9:i:78:TYR:CD1	2.43	0.70
4:p:74:PRO:HG2	4:p:82:MET:SD	2.30	0.70
6:r:59:VAL:HG11	7:s:10:VAL:HG22	1.73	0.70
18:4:5:LYS:HZ3	18:4:5:LYS:HB3	1.55	0.70
30:F:70:UNK:CB	30:F:330:UNK:CB	2.69	0.70
30:F:370:UNK:O	30:F:372:UNK:N	2.24	0.70
31:G:367:UNK:O	31:G:370:UNK:N	2.24	0.70
51:Z:13:UNK:O	51:Z:16:UNK:CB	2.39	0.70
2:m:162:ASN:ND2	2:m:244:ILE:HG21	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:329:MET:SD	7:s:5:GLY:HA3	2.31	0.70
38:N:158:UNK:O	38:N:162:UNK:N	2.24	0.70
2:m:251:SER:OG	2:m:252:LEU:N	2.22	0.70
4:d:51:LEU:HA	4:d:56:TYR:O	1.91	0.70
2:n:100:SER:HB3	2:n:105:MET:HG3	1.73	0.70
11:w:18:VAL:HB	11:w:19:PRO:HD3	1.71	0.70
30:F:351:UNK:O	30:F:354:UNK:N	2.23	0.70
31:G:367:UNK:O	31:G:370:UNK:CB	2.40	0.70
36:L:67:UNK:CB	36:L:76:UNK:CA	2.68	0.70
38:N:258:UNK:CB	38:N:330:UNK:O	2.39	0.70
5:q:118:ARG:HH11	5:q:171:ILE:HG12	1.55	0.70
31:G:73:UNK:O	31:G:74:UNK:CB	2.39	0.70
36:L:34:UNK:HA	36:L:37:UNK:CB	2.22	0.70
37:M:279:UNK:CB	37:M:280:UNK:HA	2.20	0.70
39:O:24:UNK:HA	39:O:122:UNK:O	1.90	0.70
40:P:64:UNK:N	40:P:65:UNK:CA	2.54	0.70
5:q:139:CYS:HB2	5:q:165:TYR:HE2	1.54	0.70
7:s:15:THR:HG22	7:s:16:TYR:N	1.97	0.70
30:F:323:UNK:HA	30:F:327:UNK:O	1.92	0.70
33:I:100:UNK:N	33:I:103:UNK:O	2.24	0.70
36:L:530:UNK:O	36:L:533:UNK:N	2.23	0.70
38:N:142:UNK:O	38:N:145:UNK:N	2.24	0.70
39:O:130:UNK:O	39:O:133:UNK:N	2.24	0.70
3:b:110:LEU:HG	3:b:114:ASN:HD21	1.55	0.70
31:G:288:UNK:HA	31:G:289:UNK:C	2.20	0.70
39:O:50:UNK:CB	39:O:123:UNK:O	2.39	0.70
47:X:177:UNK:O	47:X:180:UNK:CB	2.40	0.70
1:c:379:ILE:HD12	1:c:390:ILE:CD1	2.22	0.70
27:C:132:UNK:O	27:C:136:UNK:N	2.25	0.70
31:G:367:UNK:O	31:G:371:UNK:N	2.25	0.70
38:N:190:UNK:CB	38:N:204:UNK:CB	2.69	0.70
1:c:286:GLY:O	1:c:287:GLY:C	2.33	0.70
4:d:165:TYR:CZ	4:d:168:VAL:HG22	2.27	0.70
1:l:316:ASP:OD1	1:l:316:ASP:N	2.24	0.70
2:n:51:ILE:HD13	2:n:199:PHE:CG	2.26	0.70
2:n:277:HIS:NE2	2:n:364:LEU:HD13	2.05	0.70
3:o:280:ILE:HD13	3:o:335:LEU:HD22	1.72	0.70
4:p:10:TYR:CE1	8:t:73:LEU:CD2	2.75	0.70
5:e:15:ARG:HB2	5:e:16:PRO:CD	2.21	0.70
1:l:351:GLU:OE2	1:l:403:ASP:OD1	2.10	0.70
14:z:156:ARG:HG3	14:z:156:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:58:UNK:O	34:J:62:UNK:CA	2.40	0.70
3:b:18:PHE:O	3:b:220:PHE:CD2	2.45	0.70
1:l:245:GLU:OE1	1:l:248:LEU:HD23	1.92	0.70
1:l:403:ASP:CB	1:l:406:VAL:HG23	2.19	0.70
4:p:11:PRO:O	8:t:74:PHE:CE2	2.45	0.70
5:q:34:GLY:HA2	10:v:10:TYR:HD1	1.57	0.70
28:D:182:UNK:O	28:D:186:UNK:N	2.25	0.70
30:F:150:UNK:O	30:F:154:UNK:N	2.25	0.70
2:m:34:VAL:HG11	2:m:386:ALA:HB1	1.74	0.69
2:m:277:HIS:NE2	2:m:364:LEU:HD13	2.07	0.69
3:b:132:VAL:HA	3:b:139:SER:HB3	1.74	0.69
2:n:352:LEU:HB3	2:n:411:ILE:HD11	1.73	0.69
4:p:158:ILE:HD11	4:p:160:MET:HB2	1.73	0.69
36:L:161:UNK:CA	36:L:163:UNK:N	2.46	0.69
3:b:234:LEU:HD23	4:d:216:LEU:HD21	1.74	0.69
3:o:15:ASN:ND2	3:o:18:PHE:CE2	2.60	0.69
5:q:171:ILE:HG22	5:q:179:ASN:OD1	1.92	0.69
5:q:185:TYR:HB3	5:q:195:VAL:HG13	1.74	0.69
36:L:321:UNK:CA	36:L:324:UNK:CB	2.70	0.69
1:c:298:ALA:HA	1:c:303:LEU:HB2	1.73	0.69
4:d:176:PRO:HB2	4:d:181:GLN:NE2	2.06	0.69
1:l:18:GLN:NE2	1:l:22:GLY:HA2	2.01	0.69
3:o:237:LEU:HD13	4:p:212:MET:HG2	1.73	0.69
5:q:158:CYS:O	5:q:158:CYS:SG	2.50	0.69
14:z:12:ASN:HD22	21:7:20:VAL:H	1.39	0.69
34:J:85:UNK:O	34:J:88:UNK:N	2.25	0.69
35:K:32:UNK:O	35:K:35:UNK:CB	2.39	0.69
1:c:60:GLU:OE2	1:c:88:ALA:O	2.09	0.69
1:c:171:SER:OG	1:c:172:GLU:N	2.19	0.69
2:m:129:ALA:N	2:m:130:PRO:CD	2.55	0.69
7:g:73:ASN:N	7:g:74:PRO:CD	2.55	0.69
1:l:365:LEU:HD21	1:l:395:TRP:CD1	2.27	0.69
3:o:225:THR:O	3:o:229:ILE:HD12	1.92	0.69
4:p:102:ARG:HA	4:p:108:ALA:O	1.92	0.69
26:B:121:UNK:CA	26:B:135:UNK:HA	2.22	0.69
42:R:81:UNK:CB	42:R:92:UNK:HA	2.22	0.69
3:b:177:ARG:NH2	5:q:62:MET:O	2.23	0.69
4:d:102:ARG:HA	4:d:108:ALA:O	1.91	0.69
4:d:134:TYR:HE2	4:d:163:PRO:HG2	1.58	0.69
2:n:140:LEU:O	2:n:141:GLN:C	2.35	0.69
2:n:319:SER:OG	2:n:320:GLY:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:244:LEU:HD11	4:p:204:MET:HE2	1.75	0.69
4:p:97:ASN:OD1	4:p:98:PRO:HD2	1.92	0.69
51:Z:511:UNK:O	51:Z:514:UNK:N	2.25	0.69
2:m:83:PHE:CE2	2:m:87:ARG:HG3	2.27	0.69
2:m:237:ALA:HB2	2:m:318:ASP:OD2	1.92	0.69
4:d:82:MET:SD	4:d:86:LYS:HD2	2.32	0.69
6:f:51:PRO:HD3	2:n:134:ARG:HH12	1.57	0.69
2:n:212:SER:OG	2:n:215:VAL:HB	1.92	0.69
4:p:5:LEU:HB3	4:p:152:TYR:CD1	2.28	0.69
4:p:220:TYR:CE2	7:s:26:PHE:CE1	2.81	0.69
31:G:94:UNK:O	31:G:98:UNK:N	2.25	0.69
36:L:151:UNK:O	36:L:155:UNK:N	2.26	0.69
37:M:274:UNK:O	37:M:278:UNK:CB	2.40	0.69
47:X:156:UNK:O	47:X:159:UNK:CB	2.41	0.69
1:c:351:GLU:OE2	1:c:403:ASP:OD1	2.10	0.69
4:d:97:ASN:OD1	4:d:98:PRO:HD2	1.92	0.69
4:d:224:ARG:CB	7:g:25:ALA:HB1	2.14	0.69
1:l:4:TYR:CZ	1:l:8:LEU:HD11	2.28	0.69
2:n:300:ALA:HA	2:n:307:PHE:CZ	2.28	0.69
3:o:218:ILE:HD13	4:p:230:LEU:CD1	2.22	0.69
36:L:180:UNK:O	36:L:181:UNK:C	2.37	0.69
37:M:21:UNK:O	37:M:22:UNK:C	2.41	0.69
38:N:73:UNK:O	38:N:74:UNK:C	2.38	0.69
1:c:162:PRO:O	1:c:165:GLN:HG2	1.93	0.69
2:m:166:ALA:HB2	2:m:244:ILE:HG13	1.74	0.69
4:d:94:PRO:HB2	4:d:95:TYR:CD1	2.27	0.69
2:n:47:ILE:HG22	2:n:48:GLY:N	2.08	0.69
2:n:248:ASN:HB2	2:n:428:GLY:CA	2.22	0.69
3:o:47:THR:HG21	3:o:83:HIS:HB2	1.73	0.69
3:o:156:ILE:HG13	3:o:157:GLY:H	1.58	0.69
4:p:27:ARG:NH1	10:v:58:LYS:NZ	2.41	0.69
12:x:11:ASN:HD22	12:x:14:ASP:H	1.39	0.69
32:H:127:UNK:O	32:H:131:UNK:CB	2.41	0.69
36:L:35:UNK:O	36:L:39:UNK:N	2.25	0.69
50:U:416:UNK:O	50:U:417:UNK:C	2.38	0.69
1:c:32:GLN:CG	1:c:33:PRO:HD2	2.22	0.69
2:m:46:ARG:HH12	2:m:376:GLU:HG3	1.57	0.69
36:L:314:UNK:O	36:L:317:UNK:CB	2.41	0.69
47:X:703:UNK:C	47:X:705:UNK:N	2.54	0.69
2:m:247:GLN:HE22	2:m:429:ASN:ND2	1.91	0.69
4:d:50:HIS:HB3	4:d:54:VAL:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:5:ALA:O	1:l:8:LEU:HB2	1.93	0.69
1:l:21:ASN:CB	1:l:217:SER:HB3	2.22	0.69
13:y:13:THR:HB	13:y:168:LEU:HD23	1.74	0.69
25:A:109:UNK:O	25:A:110:UNK:CB	2.38	0.69
38:N:77:UNK:O	38:N:80:UNK:O	2.11	0.69
38:N:108:UNK:O	38:N:109:UNK:C	2.41	0.69
40:P:112:UNK:O	40:P:116:UNK:N	2.26	0.69
2:m:62:ASN:ND2	2:m:65:THR:OG1	2.26	0.68
2:m:308:ASP:OD1	2:m:309:VAL:N	2.26	0.68
1:l:145:MET:SD	1:l:248:LEU:HD12	2.32	0.68
3:o:27:ILE:HG22	3:o:27:ILE:O	1.92	0.68
30:F:92:UNK:O	30:F:220:UNK:HA	1.92	0.68
31:G:229:UNK:N	31:G:238:UNK:CB	2.56	0.68
33:I:113:UNK:O	33:I:114:UNK:C	2.37	0.68
38:N:158:UNK:O	38:N:161:UNK:N	2.26	0.68
1:c:341:GLN:OE1	1:c:344:ARG:NH1	2.25	0.68
3:b:245:PHE:CD1	4:d:17:LEU:HD13	2.27	0.68
3:b:310:SER:HA	3:b:374:ASN:ND2	1.97	0.68
1:l:278:GLY:O	1:l:309:THR:HG23	1.92	0.68
4:p:7:PRO:HG3	4:p:126:TYR:HA	1.73	0.68
30:F:34:UNK:O	30:F:38:UNK:CB	2.41	0.68
36:L:369:UNK:O	36:L:373:UNK:N	2.26	0.68
38:N:204:UNK:O	38:N:208:UNK:CB	2.41	0.68
1:l:86:LEU:HD13	1:l:99:ILE:HG12	1.75	0.68
1:l:343:MET:HE1	1:l:416:TYR:HD2	1.57	0.68
1:l:389:ARG:O	1:l:390:ILE:HD13	1.93	0.68
3:o:119:LEU:HD23	52:o:402:HEM:C4B	2.28	0.68
4:p:211:MET:HE1	10:v:31:PHE:CZ	2.28	0.68
5:q:114:VAL:HG12	5:q:115:SER:N	2.08	0.68
5:q:136:ILE:O	5:q:136:ILE:HG22	1.93	0.68
14:z:154:GLY:HA2	17:3:6:VAL:HG22	1.76	0.68
27:C:131:UNK:C	27:C:133:UNK:N	2.54	0.68
1:c:151:ASN:ND2	5:e:2:HIS:NE2	2.42	0.68
3:o:129:MET:HG2	3:o:178:PHE:CD1	2.27	0.68
4:p:158:ILE:HD13	4:p:160:MET:CB	2.22	0.68
6:r:75:LEU:O	6:r:80:TRP:NE1	2.27	0.68
32:H:285:UNK:O	32:H:289:UNK:N	2.26	0.68
38:N:108:UNK:O	38:N:112:UNK:N	2.26	0.68
39:O:41:UNK:O	39:O:44:UNK:CB	2.42	0.68
40:P:160:UNK:N	40:P:162:UNK:N	2.42	0.68
40:P:311:UNK:O	40:P:314:UNK:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:77:UNK:C	47:X:79:UNK:N	2.56	0.68
2:m:77:THR:CG2	2:m:130:PRO:HA	2.13	0.68
3:b:135:TRP:HH2	3:b:170:VAL:HG12	1.57	0.68
1:l:304:CYS:HB3	1:l:334:MET:SD	2.33	0.68
29:E:96:UNK:O	29:E:98:UNK:O	2.10	0.68
30:F:294:UNK:CB	30:F:339:UNK:CB	2.72	0.68
37:M:167:UNK:O	37:M:171:UNK:N	2.26	0.68
38:N:52:UNK:O	38:N:55:UNK:N	2.27	0.68
2:m:135:TRP:CD2	6:r:49:ARG:HD3	2.29	0.68
3:b:169:SER:CB	5:q:93:GLY:HA3	2.24	0.68
1:l:236:PHE:CD2	1:l:258:GLU:HG2	2.28	0.68
1:l:426:GLY:HA2	1:l:428:ILE:HG13	1.72	0.68
2:n:132:PHE:HB3	2:n:137:VAL:HG21	1.76	0.68
2:n:394:PRO:O	2:n:398:VAL:HG23	1.94	0.68
3:o:100:ARG:NH2	52:o:402:HEM:HBD1	2.04	0.68
5:q:95:PRO:HG2	5:q:145:VAL:HG22	1.74	0.68
5:q:121:GLN:HB2	5:q:170:ARG:CD	2.24	0.68
6:r:75:LEU:HD12	6:r:76:PRO:CD	2.23	0.68
23:9:19:TRP:HZ2	24:0:14:GLU:HG2	1.58	0.68
30:F:51:UNK:CB	30:F:52:UNK:CB	2.72	0.68
37:M:24:UNK:O	37:M:27:UNK:CB	2.42	0.68
1:c:408:ARG:NH1	11:k:15:ARG:HG2	2.08	0.68
3:b:244:LEU:HD23	4:d:205:GLY:HA2	1.76	0.68
2:n:148:LYS:HG3	2:n:177:TYR:HB3	1.76	0.68
5:q:171:ILE:HG23	5:q:171:ILE:O	1.94	0.68
32:H:143:UNK:O	32:H:144:UNK:C	2.42	0.68
36:L:419:UNK:O	36:L:422:UNK:CB	2.42	0.68
47:X:334:UNK:O	47:X:335:UNK:C	2.41	0.68
48:Y:11:UNK:CA	48:Y:48:UNK:CB	2.69	0.68
51:Z:343:UNK:O	51:Z:347:UNK:N	2.26	0.68
1:c:80:GLU:O	1:c:83:GLY:N	2.26	0.68
1:c:244:ARG:HG2	7:g:10:VAL:HG12	1.74	0.68
3:b:79:ILE:HG12	5:e:58:PHE:HE1	1.57	0.68
2:n:264:ILE:CG2	2:n:317:SER:HA	2.23	0.68
3:o:345:HIS:HB3	3:o:346:PRO:CD	2.21	0.68
40:P:134:UNK:O	40:P:167:UNK:HA	1.93	0.68
1:c:426:GLY:HA2	1:c:428:ILE:N	2.08	0.68
3:b:22:PRO:HG2	7:g:3:GLN:HB3	1.76	0.68
3:b:56:THR:HG21	3:o:58:ASP:OD2	1.94	0.68
50:U:626:UNK:O	50:U:628:UNK:O	2.12	0.68
1:c:426:GLY:HA2	1:c:427:PRO:C	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:445:ARG:O	1:c:446:PHE:HB2	1.93	0.68
2:m:279:LEU:HD22	2:m:295:LEU:HD13	1.76	0.68
5:q:68:VAL:HG12	5:q:69:LEU:N	2.08	0.68
5:q:83:GLU:HG3	5:q:100:HIS:NE2	2.08	0.68
7:s:51:PRO:O	7:s:54:ALA:HB3	1.94	0.68
10:v:22:LEU:O	10:v:26:VAL:HG23	1.93	0.68
10:v:35:PHE:O	10:v:36:ASP:C	2.37	0.68
26:B:117:UNK:O	26:B:120:UNK:N	2.27	0.68
36:L:46:UNK:O	36:L:49:UNK:N	2.27	0.68
39:O:28:UNK:O	39:O:172:UNK:CB	2.41	0.68
48:Y:103:UNK:C	48:Y:105:UNK:N	2.56	0.68
4:d:237:TYR:CE2	4:d:239:PRO:HG3	2.29	0.67
8:h:22:GLU:O	8:h:25:GLU:HG2	1.94	0.67
18:4:5:LYS:HZ3	18:4:6:GLY:N	1.85	0.67
33:I:173:UNK:HA	33:I:174:UNK:C	2.23	0.67
37:M:60:UNK:C	37:M:63:UNK:N	2.57	0.67
1:c:158:PHE:CE1	1:c:317:THR:HG21	2.28	0.67
3:b:244:LEU:O	4:d:201:ARG:HD3	1.95	0.67
9:i:53:GLU:O	9:i:55:LEU:HG	1.94	0.67
3:o:103:TYR:O	3:o:315:MET:HB2	1.93	0.67
3:o:244:LEU:O	4:p:201:ARG:HD3	1.95	0.67
4:p:138:PRO:HB3	8:t:55:THR:N	2.10	0.67
28:D:357:UNK:HA	28:D:384:UNK:CB	2.25	0.67
34:J:50:UNK:O	34:J:54:UNK:N	2.27	0.67
37:M:60:UNK:C	37:M:62:UNK:C	2.72	0.67
50:U:25:UNK:C	50:U:26:UNK:O	2.42	0.67
1:c:350:THR:HB	1:c:353:GLU:CG	2.24	0.67
1:l:27:SER:HA	1:l:199:ALA:O	1.94	0.67
1:l:39:VAL:HG12	1:l:41:ILE:CD1	2.23	0.67
1:l:46:ARG:HH22	1:l:316:ASP:CG	2.02	0.67
36:L:281:UNK:CB	36:L:315:UNK:HA	2.25	0.67
47:X:93:UNK:CA	47:X:94:UNK:CB	2.71	0.67
4:d:208:MET:HE2	4:d:208:MET:O	1.95	0.67
2:n:159:VAL:HG23	2:n:427:SER:OG	1.95	0.67
3:o:177:ARG:O	3:o:181:PHE:CD2	2.47	0.67
7:s:15:THR:CG2	7:s:16:TYR:N	2.51	0.67
12:x:69:MET:HE2	12:x:70:VAL:HG23	1.74	0.67
26:B:148:UNK:CA	26:B:151:UNK:CA	2.58	0.67
38:N:293:UNK:O	38:N:296:UNK:N	2.27	0.67
30:F:194:UNK:O	30:F:197:UNK:CB	2.42	0.67
36:L:178:UNK:CB	36:L:222:UNK:CB	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:241:ILE:HG13	7:g:16:TYR:CD1	2.30	0.67
1:c:408:ARG:NH1	11:k:15:ARG:CG	2.57	0.67
1:c:426:GLY:N	1:c:428:ILE:HG13	2.06	0.67
3:b:234:LEU:CD2	4:d:216:LEU:HD21	2.24	0.67
3:b:332:LEU:HD21	3:b:358:TYR:HE1	1.60	0.67
5:e:60:SER:HA	5:e:63:SER:OG	1.94	0.67
6:f:42:ASP:OD2	6:f:101:ARG:NH1	2.28	0.67
3:o:8:HIS:HB3	3:o:9:PRO:HD3	1.76	0.67
8:t:65:ARG:HG3	8:t:66:ASP:N	2.09	0.67
27:C:131:UNK:O	27:C:133:UNK:N	2.27	0.67
36:L:297:UNK:HA	36:L:355:UNK:HA	1.77	0.67
1:c:365:LEU:HD21	1:c:395:TRP:CD1	2.29	0.67
2:m:24:LEU:HD12	2:m:24:LEU:N	2.04	0.67
2:n:24:LEU:CG	2:n:38:LEU:HD11	2.19	0.67
2:n:191:LEU:O	2:n:195:VAL:HG23	1.94	0.67
5:q:76:ILE:HG22	5:q:193:VAL:C	2.19	0.67
30:F:289:UNK:CA	30:F:290:UNK:C	2.66	0.67
36:L:226:UNK:HA	36:L:284:UNK:CB	2.24	0.67
38:N:224:UNK:N	38:N:225:UNK:HA	2.08	0.67
39:O:87:UNK:CB	39:O:88:UNK:CA	2.73	0.67
2:m:257:LEU:HD13	2:m:424:MET:HB2	1.77	0.67
5:e:18:VAL:HG11	5:e:32:ARG:NH1	2.09	0.67
8:h:73:LEU:HD21	8:h:74:PHE:HD1	1.58	0.67
5:q:101:ARG:HD3	5:q:133:VAL:HG11	1.76	0.67
10:v:9:LEU:HD12	10:v:13:LEU:HD12	1.77	0.67
28:D:234:UNK:O	28:D:237:UNK:CB	2.43	0.67
42:R:51:UNK:HA	42:R:92:UNK:O	1.95	0.67
50:U:411:UNK:O	50:U:412:UNK:C	2.43	0.67
1:c:67:THR:HG22	1:c:70:ARG:HB2	1.76	0.67
1:c:251:ALA:O	1:c:325:VAL:HA	1.95	0.67
3:b:311:LYS:HD2	3:b:379:TRP:HB3	1.76	0.67
5:e:15:ARG:HH21	5:e:32:ARG:HB2	1.60	0.67
2:n:129:ALA:N	2:n:130:PRO:CD	2.58	0.67
3:o:267:HIS:NE2	3:o:269:LYS:HD3	2.10	0.67
19:5:38:ARG:HG2	19:5:85:ILE:HG23	1.77	0.67
26:B:65:UNK:HA	26:B:68:UNK:CB	2.25	0.67
36:L:207:UNK:CB	36:L:209:UNK:HA	2.25	0.67
38:N:135:UNK:O	38:N:136:UNK:C	2.43	0.67
2:m:109:VAL:HG22	2:m:119:LEU:HD23	1.77	0.67
2:m:200:THR:CG2	2:m:203:ARG:HD2	2.23	0.67
3:b:206:ASN:CB	3:b:313:ARG:HH21	2.05	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:75:ASN:ND2	4:d:80:MET:O	2.28	0.67
7:s:71:ARG:HH21	8:t:60:ASP:CG	2.02	0.67
1:c:351:GLU:HA	1:c:404:ALA:HB2	1.77	0.66
2:m:348:ALA:HB1	2:m:415:LYS:HA	1.76	0.66
3:b:108:THR:HB	3:b:313:ARG:HH11	1.59	0.66
5:e:68:VAL:HG12	5:e:69:LEU:N	2.10	0.66
10:j:36:ASP:O	10:j:37:GLN:C	2.35	0.66
1:l:405:ARG:O	1:l:409:GLU:HG3	1.95	0.66
3:o:102:LEU:HD21	3:o:304:ILE:HD13	1.77	0.66
30:F:291:UNK:O	30:F:292:UNK:C	2.43	0.66
1:c:53:ASN:OD1	1:c:170:PRO:HD3	1.95	0.66
4:d:11:PRO:O	8:h:74:PHE:CZ	2.49	0.66
4:d:241:LYS:HG2	4:d:241:LYS:OXT	1.95	0.66
1:l:163:LEU:HD12	1:l:163:LEU:O	1.95	0.66
2:n:71:LEU:HD13	2:n:143:GLN:HG3	1.78	0.66
2:n:258:VAL:HG11	2:n:321:LEU:HB3	1.74	0.66
2:n:395:PRO:O	2:n:398:VAL:HB	1.94	0.66
4:p:82:MET:SD	4:p:86:LYS:HD2	2.35	0.66
2:m:319:SER:OG	2:m:320:GLY:N	2.27	0.66
3:b:174:THR:O	3:b:178:PHE:HD1	1.77	0.66
7:g:2:ARG:HB2	7:g:6:HIS:HD2	1.59	0.66
1:l:408:ARG:HH12	11:w:15:ARG:CG	2.07	0.66
3:o:79:ILE:HG12	5:q:58:PHE:HE1	1.58	0.66
5:q:89:PHE:HB2	5:q:96:LEU:HB3	1.76	0.66
6:r:51:PRO:HG2	6:r:54:LEU:HD22	1.74	0.66
12:x:298:ASP:HB2	12:x:301:THR:HG23	1.77	0.66
25:A:76:UNK:O	25:A:77:UNK:C	2.38	0.66
31:G:380:UNK:O	31:G:409:UNK:O	2.13	0.66
46:W:47:UNK:O	46:W:50:UNK:CB	2.42	0.66
47:X:703:UNK:O	47:X:704:UNK:C	2.41	0.66
1:c:324:PHE:CD1	1:c:334:MET:HG2	2.30	0.66
10:j:34:ALA:O	10:j:35:PHE:C	2.38	0.66
1:l:408:ARG:CZ	11:w:15:ARG:HE	2.08	0.66
2:n:327:ILE:HG22	2:n:327:ILE:O	1.95	0.66
34:J:101:UNK:O	34:J:102:UNK:C	2.44	0.66
37:M:32:UNK:O	37:M:33:UNK:C	2.42	0.66
2:n:180:ASP:O	2:n:183:ILE:HD12	1.95	0.66
2:n:283:PRO:HG3	9:u:55:LEU:CD2	2.24	0.66
3:o:200:LEU:O	3:o:200:LEU:HG	1.95	0.66
3:o:359:PHE:O	3:o:363:LEU:HB2	1.95	0.66
4:p:32:VAL:HG11	4:p:186:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:2:ARG:HB2	7:s:6:HIS:HD2	1.59	0.66
12:x:151:HIS:O	12:x:155:VAL:HG23	1.95	0.66
13:y:186:SER:HB3	13:y:213:LEU:HD22	1.75	0.66
15:l:24:LEU:H	16:2:34:ASN:HD21	1.44	0.66
30:F:429:UNK:O	30:F:432:UNK:CB	2.44	0.66
33:I:172:UNK:O	33:I:175:UNK:HA	1.95	0.66
37:M:102:UNK:O	37:M:106:UNK:CB	2.43	0.66
40:P:134:UNK:O	40:P:167:UNK:CB	2.43	0.66
51:Z:511:UNK:O	51:Z:512:UNK:C	2.44	0.66
1:c:426:GLY:N	1:c:428:ILE:HG12	2.10	0.66
3:o:32:ASN:O	3:o:36:LEU:HG	1.95	0.66
4:p:236:ALA:HB3	7:s:14:ILE:HB	1.76	0.66
14:z:209:ILE:O	14:z:213:THR:HG23	1.95	0.66
30:F:262:UNK:CB	30:F:285:UNK:CA	2.74	0.66
31:G:12:UNK:HA	31:G:17:UNK:HA	1.77	0.66
31:G:388:UNK:CB	31:G:391:UNK:CB	2.74	0.66
31:G:426:UNK:O	31:G:430:UNK:N	2.29	0.66
1:c:75:LEU:HD21	1:c:116:ILE:HG12	1.78	0.66
2:m:134:ARG:NH1	6:r:51:PRO:HD3	2.11	0.66
1:l:236:PHE:CD2	1:l:258:GLU:HB3	2.30	0.66
1:l:236:PHE:HD2	1:l:258:GLU:HG2	1.60	0.66
2:n:98:VAL:HG22	2:n:107:TYR:CD2	2.31	0.66
2:n:156:GLN:HE22	9:u:56:ARG:HD3	1.58	0.66
3:o:22:PRO:CG	7:s:3:GLN:HB3	2.25	0.66
3:o:156:ILE:O	3:o:157:GLY:C	2.39	0.66
3:o:315:MET:HE2	3:o:318:ARG:HH21	1.60	0.66
28:D:296:UNK:O	28:D:299:UNK:N	2.28	0.66
28:D:383:UNK:CB	28:D:385:UNK:O	2.44	0.66
32:H:152:UNK:O	32:H:155:UNK:N	2.29	0.66
1:c:143:THR:HG23	1:c:143:THR:O	1.94	0.66
1:c:331:ILE:HD11	1:c:427:PRO:O	1.96	0.66
1:l:161:THR:HB	1:l:162:PRO:HD2	1.77	0.66
1:l:298:ALA:HA	1:l:303:LEU:HB2	1.77	0.66
7:s:73:ASN:N	7:s:74:PRO:CD	2.58	0.66
8:t:22:GLU:O	8:t:25:GLU:HG2	1.95	0.66
28:D:218:UNK:O	28:D:222:UNK:N	2.28	0.66
30:F:101:UNK:O	30:F:102:UNK:CB	2.43	0.66
38:N:24:UNK:O	38:N:28:UNK:N	2.28	0.66
38:N:142:UNK:O	38:N:145:UNK:CA	2.43	0.66
39:O:130:UNK:C	39:O:132:UNK:N	2.59	0.66
47:X:187:UNK:O	47:X:190:UNK:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:243:UNK:O	51:Z:244:UNK:C	2.42	0.66
1:c:106:LEU:N	1:c:107:PRO:HD2	2.11	0.66
3:b:109:PHE:O	3:b:110:LEU:C	2.36	0.66
1:l:6:GLN:O	1:l:7:ALA:C	2.39	0.66
1:l:91:THR:HG23	1:l:92:ARG:H	1.60	0.66
5:q:1:SER:CA	5:q:1:SER:OG	2.44	0.66
14:z:101:PHE:HZ	14:z:260:GLY:HA3	1.61	0.66
26:B:48:UNK:HA	26:B:78:UNK:CB	2.26	0.66
31:G:311:UNK:O	31:G:314:UNK:CB	2.43	0.66
36:L:61:UNK:HA	36:L:80:UNK:CB	2.26	0.66
3:b:240:MET:HA	3:b:243:VAL:CG1	2.24	0.66
5:q:102:THR:O	5:q:106:ILE:HG13	1.96	0.66
16:2:43:PRO:HB2	16:2:48:ILE:HD11	1.76	0.66
28:D:229:UNK:O	28:D:232:UNK:N	2.29	0.66
37:M:271:UNK:O	37:M:272:UNK:C	2.44	0.66
1:c:262:TRP:CG	1:c:385:THR:HG23	2.31	0.65
1:l:80:GLU:O	1:l:83:GLY:N	2.28	0.65
3:o:26:ASN:ND2	3:o:208:PRO:HD2	2.11	0.65
3:o:207:ASN:OD1	3:o:210:GLY:N	2.26	0.65
3:o:296:PHE:HD1	3:o:359:PHE:HE1	1.43	0.65
14:z:160:LEU:HD13	14:z:222:GLN:HG2	1.78	0.65
38:N:45:UNK:O	38:N:46:UNK:C	2.45	0.65
49:a:126:UNK:O	49:a:127:UNK:CB	2.44	0.65
2:m:253:VAL:HG23	2:m:427:SER:O	1.96	0.65
3:b:32:ASN:HD21	3:b:228:ASP:HA	1.61	0.65
3:b:156:ILE:O	3:b:157:GLY:C	2.39	0.65
6:f:28:LYS:CB	6:f:74:ILE:HD11	2.26	0.65
7:g:50:PRO:CB	7:g:51:PRO:HD3	2.24	0.65
9:i:70:LEU:CD1	9:i:72:VAL:H	2.09	0.65
3:o:218:ILE:HD13	4:p:230:LEU:HD11	1.78	0.65
9:u:70:LEU:CD1	9:u:72:VAL:H	2.08	0.65
27:C:31:UNK:O	27:C:33:UNK:N	2.30	0.65
31:G:114:CYS:O	31:G:118:UNK:N	2.30	0.65
31:G:375:UNK:C	31:G:449:UNK:N	2.58	0.65
37:M:278:UNK:O	37:M:279:UNK:CB	2.43	0.65
2:m:31:ASN:HB3	2:m:201:SER:HB3	1.78	0.65
4:d:236:ALA:HB3	7:g:14:ILE:HB	1.78	0.65
4:p:50:HIS:HB3	4:p:54:VAL:CB	2.26	0.65
4:p:233:ARG:HG3	7:s:17:SER:HB2	1.77	0.65
31:G:26:UNK:O	31:G:29:UNK:CB	2.45	0.65
37:M:281:UNK:O	37:M:284:UNK:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:34:ILE:HB	7:g:35:PRO:CD	2.21	0.65
1:l:45:SER:OG	1:l:92:ARG:CG	2.44	0.65
1:l:351:GLU:OE2	1:l:404:ALA:HB3	1.96	0.65
1:l:405:ARG:HD2	21:7:4:ARG:NH1	1.42	0.65
6:r:42:ASP:OD2	6:r:101:ARG:NH1	2.30	0.65
25:A:111:UNK:O	25:A:112:UNK:CB	2.43	0.65
38:N:227:UNK:O	38:N:228:UNK:C	2.39	0.65
1:c:78:GLU:HG2	1:c:112:LEU:HD21	1.78	0.65
3:b:310:SER:CB	3:b:318:ARG:NH1	2.58	0.65
2:n:247:GLN:HE22	2:n:429:ASN:ND2	1.95	0.65
4:p:51:LEU:HA	4:p:56:TYR:O	1.97	0.65
4:p:54:VAL:O	4:p:54:VAL:HG12	1.96	0.65
26:B:95:UNK:C	26:B:97:UNK:N	2.55	0.65
31:G:26:UNK:O	31:G:29:UNK:N	2.30	0.65
34:J:4:UNK:O	34:J:8:UNK:N	2.30	0.65
3:b:170:VAL:HG12	3:b:170:VAL:O	1.97	0.65
10:j:55:ILE:HG23	10:j:58:LYS:HE2	1.79	0.65
1:l:279:HIS:HA	1:l:307:PHE:O	1.97	0.65
3:o:90:PHE:HE1	3:o:123:VAL:HG21	1.60	0.65
3:o:311:LYS:HD2	3:o:379:TRP:HB3	1.79	0.65
5:q:188:THR:OG1	5:q:192:MET:HB2	1.96	0.65
13:y:120:SER:OG	13:y:138:VAL:HG21	1.97	0.65
51:Z:244:UNK:O	51:Z:248:UNK:N	2.29	0.65
2:m:354:ASN:N	2:m:355:PRO:HD2	2.11	0.65
4:d:178:THR:HG21	8:h:16:PRO:HG2	1.79	0.65
10:j:12:LEU:HD23	10:j:13:LEU:HD21	1.79	0.65
1:l:335:MET:HE1	1:l:338:LEU:HD23	1.79	0.65
1:l:426:GLY:N	1:l:428:ILE:CG1	2.60	0.65
3:o:102:LEU:HD21	3:o:304:ILE:HD12	1.78	0.65
3:o:122:THR:CG2	3:o:189:ILE:CD1	2.74	0.65
5:q:117:LEU:O	5:q:118:ARG:C	2.39	0.65
6:r:73:GLN:NE2	7:s:32:LYS:HZ1	1.94	0.65
7:s:34:ILE:HB	7:s:35:PRO:CD	2.27	0.65
10:v:51:LEU:HB3	10:v:52:TRP:CZ3	2.32	0.65
30:F:121:UNK:HA	30:F:232:UNK:CB	2.26	0.65
31:G:615:UNK:O	31:G:618:UNK:N	2.30	0.65
33:I:21:UNK:O	33:I:25:UNK:N	2.29	0.65
36:L:579:UNK:CB	36:L:581:UNK:CB	2.74	0.65
1:c:106:LEU:CD2	1:c:203:LEU:HD13	2.26	0.65
3:o:44:GLN:OE1	3:o:83:HIS:ND1	2.30	0.65
23:9:45:LEU:HD21	24:0:40:TYR:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:S:84:UNK:HA	43:S:87:UNK:CB	2.27	0.65
3:b:183:PHE:CE1	3:o:183:PHE:CD1	2.84	0.65
2:n:67:HIS:CD2	2:n:144:LEU:HD22	2.21	0.65
2:n:133:ARG:HD3	2:n:135:TRP:CZ2	2.32	0.65
2:n:436:ILE:HD12	2:n:437:ASP:OD1	1.96	0.65
3:o:122:THR:HG21	3:o:189:ILE:HG12	1.78	0.65
3:o:124:MET:HE1	3:o:298:ILE:HG21	1.77	0.65
30:F:166:UNK:O	30:F:167:UNK:C	2.45	0.65
31:G:155:UNK:C	31:G:156:CYS:O	2.41	0.65
37:M:432:UNK:O	37:M:435:UNK:CB	2.45	0.65
38:N:99:UNK:O	38:N:103:UNK:N	2.30	0.65
38:N:124:UNK:O	38:N:127:UNK:N	2.29	0.65
1:c:41:ILE:CG1	1:c:195:MET:HE3	2.22	0.65
2:m:56:ARG:NH2	2:m:172:LEU:HD21	2.12	0.65
2:m:341:TYR:HE2	2:m:345:LYS:HE3	1.61	0.65
3:b:44:GLN:OE1	3:b:83:HIS:ND1	2.30	0.65
5:e:53:ASN:N	5:e:53:ASN:OD1	2.27	0.65
12:x:273:MET:HG3	12:x:319:LYS:HZ1	1.61	0.65
36:L:321:UNK:C	36:L:324:UNK:CB	2.73	0.65
37:M:180:UNK:O	37:M:181:UNK:C	2.44	0.65
37:M:375:UNK:O	37:M:379:UNK:N	2.30	0.65
50:U:411:UNK:O	50:U:414:UNK:N	2.30	0.65
1:c:236:PHE:CD2	1:c:258:GLU:HB3	2.31	0.64
2:m:155:PRO:HB2	2:m:254:HIS:CE1	2.32	0.64
2:m:333:ALA:O	2:m:337:ILE:HD12	1.97	0.64
3:b:174:THR:O	3:b:178:PHE:CD1	2.50	0.64
3:b:243:VAL:HG13	3:b:244:LEU:HD13	1.77	0.64
3:b:345:HIS:HB3	3:b:346:PRO:HD3	1.79	0.64
2:n:156:GLN:NE2	9:u:56:ARG:HD3	2.12	0.64
3:o:115:ILE:CG2	3:o:196:HIS:HB2	2.27	0.64
27:C:133:UNK:O	27:C:136:UNK:N	2.30	0.64
31:G:241:UNK:O	31:G:248:UNK:CB	2.44	0.64
38:N:328:UNK:CB	50:U:209:UNK:HA	2.27	0.64
3:b:240:MET:O	3:b:244:LEU:HB2	1.96	0.64
3:b:346:PRO:HG2	7:g:66:PHE:HD1	1.63	0.64
4:d:229:VAL:HG22	7:g:18:LEU:O	1.97	0.64
1:l:158:PHE:CZ	1:l:317:THR:HG21	2.31	0.64
2:n:134:ARG:HG2	2:n:135:TRP:N	2.11	0.64
3:o:102:LEU:HB3	3:o:325:PHE:HE1	1.62	0.64
3:o:153:ILE:HG23	3:o:154:PRO:HD2	1.79	0.64
6:r:73:GLN:HA	7:s:39:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:163:UNK:N	32:H:278:UNK:HA	2.12	0.64
40:P:147:UNK:O	40:P:151:UNK:N	2.29	0.64
47:X:306:UNK:O	47:X:307:UNK:C	2.44	0.64
3:b:270:PRO:HB2	3:b:274:PHE:HB2	1.78	0.64
1:l:15:GLN:O	1:l:26:ALA:HA	1.98	0.64
3:o:72:ASP:OD1	4:p:49:ARG:NH1	2.25	0.64
3:o:310:SER:CB	3:o:318:ARG:NH1	2.59	0.64
4:p:120:ARG:HG2	4:p:120:ARG:HH11	1.62	0.64
27:C:68:UNK:O	27:C:69:UNK:CB	2.45	0.64
27:C:112:UNK:N	27:C:113:UNK:CB	2.61	0.64
1:c:385:THR:HG22	1:c:386:TYR:N	2.12	0.64
2:m:347:ILE:HD12	2:m:347:ILE:N	2.13	0.64
4:d:10:TYR:HE1	8:h:73:LEU:HD21	1.60	0.64
1:l:436:ARG:HE	3:o:222:PRO:HD3	1.62	0.64
2:n:279:LEU:HD22	2:n:344:VAL:HG22	1.80	0.64
2:n:303:VAL:HG12	2:n:304:HIS:N	2.11	0.64
28:D:347:UNK:O	28:D:351:UNK:N	2.31	0.64
31:G:55:CYS:O	31:G:56:UNK:C	2.45	0.64
31:G:543:UNK:O	31:G:558:UNK:O	2.16	0.64
33:I:26:UNK:O	33:I:28:UNK:N	2.29	0.64
36:L:116:UNK:O	36:L:117:UNK:C	2.45	0.64
37:M:271:UNK:O	37:M:274:UNK:N	2.30	0.64
37:M:342:UNK:O	37:M:343:UNK:CB	2.45	0.64
1:c:198:ALA:O	1:c:199:ALA:HB2	1.95	0.64
1:l:155:ALA:HA	1:l:164:ALA:HB1	1.80	0.64
1:l:391:PRO:HB2	1:l:395:TRP:CZ2	2.32	0.64
4:p:27:ARG:NH1	10:v:58:LYS:HG3	2.11	0.64
5:q:85:LYS:HG2	5:q:86:ASN:N	2.11	0.64
8:t:67:HIS:CE1	8:t:71:HIS:HE2	2.16	0.64
31:G:102:UNK:O	31:G:103:UNK:CB	2.43	0.64
37:M:382:UNK:O	37:M:385:UNK:N	2.30	0.64
47:X:321:UNK:O	47:X:323:UNK:N	2.30	0.64
1:c:358:LYS:HD2	1:c:402:VAL:CG1	2.28	0.64
3:b:230:LEU:HD12	4:d:219:VAL:HG12	1.80	0.64
3:b:296:PHE:HD1	3:b:359:PHE:HE1	1.45	0.64
3:b:311:LYS:O	6:f:38:HIS:HB2	1.98	0.64
4:d:138:PRO:HB3	8:h:55:THR:N	2.12	0.64
6:f:96:GLU:OE1	6:f:99:ARG:HD2	1.98	0.64
4:p:26:ILE:HG22	4:p:54:VAL:HG13	1.78	0.64
36:L:420:UNK:O	36:L:424:UNK:N	2.31	0.64
41:Q:42:UNK:O	41:Q:45:UNK:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:385:GLN:HG2	9:i:62:ARG:NH1	2.10	0.64
3:b:119:LEU:HD13	3:b:192:ILE:HG22	1.80	0.64
5:q:15:ARG:HH21	5:q:32:ARG:CG	2.08	0.64
7:s:50:PRO:CB	7:s:51:PRO:CD	2.70	0.64
12:x:172:LYS:HB2	12:x:172:LYS:NZ	2.12	0.64
26:B:56:UNK:O	26:B:59:UNK:N	2.31	0.64
30:F:39:UNK:O	30:F:40:UNK:CB	2.45	0.64
30:F:103:UNK:CB	30:F:104:UNK:HA	2.27	0.64
36:L:326:UNK:O	36:L:330:UNK:N	2.29	0.64
47:X:157:UNK:O	47:X:160:UNK:N	2.30	0.64
2:m:109:VAL:HG22	2:m:119:LEU:CD2	2.28	0.64
4:d:10:TYR:O	4:d:12:TRP:CD1	2.51	0.64
4:d:178:THR:HG23	8:h:15:ASP:N	2.11	0.64
1:l:38:GLY:HA3	1:l:40:TRP:HZ3	1.62	0.64
1:l:408:ARG:NH1	11:w:15:ARG:HG2	2.13	0.64
3:o:79:ILE:HG12	5:q:58:PHE:CE1	2.33	0.64
30:F:188:UNK:O	30:F:192:UNK:N	2.31	0.64
30:F:289:UNK:HA	30:F:291:UNK:N	2.11	0.64
36:L:375:UNK:O	36:L:376:UNK:C	2.43	0.64
37:M:60:UNK:O	37:M:62:UNK:O	2.15	0.64
38:N:157:UNK:O	38:N:161:UNK:CB	2.46	0.64
51:Z:604:UNK:O	51:Z:608:UNK:N	2.31	0.64
1:c:158:PHE:HB2	1:c:164:ALA:HB2	1.79	0.64
1:c:342:TRP:O	1:c:343:MET:C	2.38	0.64
2:m:128:THR:HG23	2:m:226:ILE:HD11	1.80	0.64
3:b:27:ILE:O	3:b:27:ILE:CG2	2.46	0.64
1:l:151:ASN:ND2	5:q:2:HIS:NE2	2.46	0.64
1:l:350:THR:HB	1:l:353:GLU:CG	2.28	0.64
2:n:384:SER:HB2	9:u:62:ARG:HG2	1.79	0.64
3:o:207:ASN:HB2	3:o:208:PRO:HD2	1.80	0.64
5:q:76:ILE:HD12	5:q:192:MET:CE	2.28	0.64
28:D:382:UNK:C	28:D:384:UNK:HA	2.28	0.64
34:J:85:UNK:O	34:J:88:UNK:CB	2.46	0.64
37:M:32:UNK:O	37:M:34:UNK:N	2.30	0.64
4:d:32:VAL:HG21	4:d:186:VAL:HG22	1.79	0.64
2:n:209:LEU:CD2	2:n:375:SER:HB2	2.25	0.64
3:o:141:TRP:O	3:o:145:VAL:HG23	1.98	0.64
3:o:160:LEU:HD11	3:o:164:ILE:HD11	1.80	0.64
5:q:76:ILE:HG22	5:q:194:ILE:HG12	1.78	0.64
5:q:126:ARG:NH2	5:q:168:SER:O	2.23	0.64
7:s:25:ALA:C	7:s:27:PRO:HD3	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:187:SER:CB	12:x:277:MET:HE1	2.28	0.64
29:E:151:UNK:HA	29:E:152:UNK:C	2.28	0.64
36:L:571:UNK:O	36:L:574:UNK:N	2.31	0.64
40:P:167:UNK:O	40:P:230:UNK:N	2.31	0.64
2:m:434:PRO:HB3	2:m:438:GLU:HB3	1.80	0.63
4:d:55:CYS:SG	10:j:55:ILE:HG22	2.37	0.63
2:n:207:ILE:CD1	2:n:383:GLY:HA2	2.25	0.63
32:H:40:UNK:O	32:H:47:UNK:N	2.31	0.63
36:L:210:UNK:O	36:L:211:UNK:C	2.45	0.63
47:X:156:UNK:O	47:X:159:UNK:N	2.31	0.63
1:c:38:GLY:HA3	1:c:40:TRP:HZ3	1.62	0.63
3:b:183:PHE:CD1	3:o:183:PHE:CE1	2.86	0.63
3:b:338:ILE:N	3:b:338:ILE:CD1	2.61	0.63
4:d:220:TYR:CE2	7:g:26:PHE:CE1	2.83	0.63
1:l:91:THR:CG2	1:l:92:ARG:N	2.60	0.63
4:p:75:ASN:ND2	4:p:80:MET:O	2.32	0.63
37:M:281:UNK:O	37:M:284:UNK:CA	2.46	0.63
1:c:240:GLN:HG3	1:c:422:VAL:O	1.98	0.63
2:m:384:SER:CB	9:i:62:ARG:HG2	2.28	0.63
3:b:47:THR:HG21	3:b:83:HIS:CB	2.27	0.63
1:l:365:LEU:HG	1:l:365:LEU:O	1.99	0.63
1:l:408:ARG:NH1	11:w:15:ARG:CG	2.61	0.63
3:o:33:PHE:CE1	3:o:96:MET:HG3	2.34	0.63
3:o:172:LYS:O	3:o:173:ALA:C	2.41	0.63
3:o:252:ASP:HB3	3:o:253:PRO:CD	2.23	0.63
6:r:96:GLU:OE1	6:r:99:ARG:HD2	1.98	0.63
1:c:158:PHE:CB	1:c:164:ALA:HB2	2.28	0.63
3:b:78:ILE:HD11	5:e:57:GLN:NE2	2.12	0.63
3:b:119:LEU:HD13	3:b:192:ILE:CG2	2.29	0.63
1:l:385:THR:HG22	1:l:386:TYR:N	2.13	0.63
4:p:62:LYS:O	4:p:66:GLU:HG3	1.99	0.63
12:x:195:LEU:HD23	12:x:245:ILE:HD13	1.79	0.63
40:P:134:UNK:C	40:P:136:UNK:H2	2.11	0.63
51:Z:10:UNK:O	51:Z:14:UNK:N	2.32	0.63
1:c:224:ASP:O	1:c:227:ALA:N	2.31	0.63
4:d:138:PRO:O	4:d:139:THR:C	2.40	0.63
2:n:56:ARG:NH2	2:n:172:LEU:HD21	2.14	0.63
3:o:119:LEU:HD13	3:o:192:ILE:HG22	1.80	0.63
4:p:70:VAL:HG23	4:p:84:PRO:HD3	1.79	0.63
26:B:71:UNK:C	32:H:37:UNK:CB	2.77	0.63
29:E:124:UNK:O	29:E:125:UNK:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:370:UNK:O	30:F:371:UNK:C	2.45	0.63
37:M:68:UNK:O	37:M:70:UNK:N	2.32	0.63
1:c:92:ARG:HD2	1:c:163:LEU:CD1	2.29	0.63
1:c:145:MET:SD	1:c:248:LEU:CD1	2.86	0.63
1:c:351:GLU:O	1:c:352:SER:C	2.42	0.63
1:c:370:ASP:OD1	2:m:375:SER:HB3	1.99	0.63
2:m:42:ALA:CB	2:m:43:PRO:HD2	2.28	0.63
2:m:59:ASN:CG	2:m:60:SER:H	2.07	0.63
4:d:94:PRO:HB2	4:d:95:TYR:CE1	2.33	0.63
31:G:332:UNK:O	31:G:336:UNK:CB	2.46	0.63
1:c:236:PHE:HD2	1:c:258:GLU:CG	2.12	0.63
3:b:296:PHE:CD1	3:b:359:PHE:HE1	2.17	0.63
4:d:233:ARG:HG3	7:g:17:SER:HB2	1.80	0.63
10:j:3:PRO:HG2	10:j:8:ARG:HG2	1.81	0.63
1:l:143:THR:HG23	1:l:143:THR:O	1.98	0.63
1:l:199:ALA:HB3	1:l:208:LEU:HD21	1.79	0.63
1:l:373:THR:HB	1:l:374:PRO:HD3	1.81	0.63
2:n:129:ALA:N	2:n:130:PRO:HD3	2.14	0.63
6:r:73:GLN:HE21	7:s:32:LYS:CE	2.12	0.63
35:K:14:UNK:CB	35:K:36:UNK:CB	2.76	0.63
36:L:376:UNK:O	36:L:377:UNK:C	2.46	0.63
39:O:87:UNK:N	39:O:88:UNK:CB	2.62	0.63
1:c:333:ASP:O	1:c:337:VAL:HG23	1.98	0.63
3:b:25:SER:HA	3:b:218:ILE:CD1	2.29	0.63
3:b:329:VAL:HA	3:b:332:LEU:HD12	1.80	0.63
1:l:309:THR:HA	1:l:322:ALA:HA	1.81	0.63
1:l:426:GLY:CA	1:l:428:ILE:N	2.61	0.63
2:n:255:ALA:HB2	2:n:426:ALA:HB2	1.81	0.63
2:n:257:LEU:HD13	2:n:424:MET:HE2	1.80	0.63
2:n:352:LEU:O	2:n:352:LEU:HG	1.96	0.63
4:p:13:SER:O	4:p:19:SER:HB3	1.99	0.63
10:v:51:LEU:HD22	10:v:52:TRP:HZ3	1.64	0.63
28:D:99:UNK:O	28:D:100:UNK:C	2.44	0.63
30:F:434:UNK:O	30:F:437:UNK:N	2.32	0.63
31:G:330:UNK:CB	31:G:600:UNK:CB	2.77	0.63
36:L:209:UNK:O	36:L:212:UNK:CA	2.46	0.63
37:M:123:UNK:O	37:M:126:UNK:N	2.31	0.63
37:M:441:UNK:O	37:M:445:UNK:N	2.32	0.63
40:P:167:UNK:CB	40:P:229:UNK:HA	2.29	0.63
1:c:64:PHE:CE2	1:c:88:ALA:HB2	2.33	0.63
1:c:269:ALA:HB3	1:c:410:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:308:GLN:O	1:c:308:GLN:CG	2.46	0.63
1:c:436:ARG:HE	3:b:222:PRO:CG	2.12	0.63
2:m:352:LEU:HB3	2:m:411:ILE:CD1	2.29	0.63
1:l:404:ALA:O	1:l:408:ARG:HG3	1.98	0.63
2:n:385:GLN:HG2	9:u:62:ARG:NH1	2.13	0.63
4:p:79:GLU:OE1	4:p:82:MET:HG3	1.98	0.63
4:p:127:VAL:HG12	4:p:187:CYS:SG	2.39	0.63
4:p:164:ILE:HD11	4:p:186:VAL:HG21	1.79	0.63
5:q:63:SER:O	5:q:64:ALA:HB2	1.98	0.63
13:y:122:MET:HB2	13:y:208:PRO:HD2	1.81	0.63
33:I:99:UNK:HA	33:I:104:UNK:HA	1.79	0.63
38:N:77:UNK:O	38:N:78:UNK:C	2.44	0.63
49:a:1:UNK:O	49:a:5:UNK:CB	2.47	0.63
1:c:417:ASP:O	1:c:417:ASP:OD1	2.17	0.62
3:b:116:GLY:HA3	52:b:402:HEM:C3C	2.34	0.62
3:b:313:ARG:HB3	6:f:38:HIS:CD2	2.34	0.62
4:d:50:HIS:HB3	4:d:54:VAL:CG2	2.29	0.62
5:e:29:SER:HA	5:e:32:ARG:HD3	1.81	0.62
1:l:144:SER:O	1:l:148:VAL:HG23	1.99	0.62
1:l:403:ASP:OD1	1:l:404:ALA:N	2.32	0.62
2:n:83:PHE:CE2	2:n:87:ARG:HG3	2.34	0.62
3:o:8:HIS:CB	3:o:9:PRO:HD3	2.29	0.62
4:p:50:HIS:O	4:p:51:LEU:C	2.40	0.62
4:p:176:PRO:HB2	4:p:181:GLN:NE2	2.14	0.62
4:p:229:VAL:HG12	4:p:233:ARG:HE	1.63	0.62
33:I:126:CYS:HA	59:I:202:SF4:S3	2.39	0.62
33:I:151:UNK:O	33:I:154:UNK:CA	2.47	0.62
39:O:160:UNK:O	39:O:163:UNK:N	2.32	0.62
1:l:45:SER:CB	1:l:167:VAL:HG22	2.29	0.62
1:l:86:LEU:HB3	2:n:285:VAL:HG22	1.81	0.62
2:n:352:LEU:HB3	2:n:411:ILE:CD1	2.29	0.62
3:o:115:ILE:HG21	3:o:196:HIS:HB2	1.81	0.62
5:q:76:ILE:HG23	5:q:194:ILE:CG1	2.29	0.62
6:r:43:VAL:HG22	6:r:94:LEU:HD21	1.80	0.62
26:B:163:UNK:O	26:B:164:UNK:C	2.47	0.62
30:F:288:UNK:O	30:F:289:UNK:CB	2.45	0.62
30:F:434:UNK:O	30:F:438:UNK:N	2.32	0.62
2:m:47:ILE:HD12	2:m:120:MET:SD	2.40	0.62
2:m:303:VAL:HG12	2:m:304:HIS:N	2.14	0.62
2:m:341:TYR:CE2	2:m:345:LYS:HE3	2.34	0.62
2:m:434:PRO:HB2	2:m:439:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:72:GLY:O	1:l:73:ASN:OD1	2.17	0.62
1:l:162:PRO:O	1:l:165:GLN:HG2	1.99	0.62
3:o:30:TRP:O	3:o:33:PHE:CD2	2.47	0.62
5:q:157:TYR:CE2	5:q:159:PRO:HA	2.33	0.62
6:r:28:LYS:HD2	6:r:74:ILE:CD1	2.24	0.62
12:x:128:VAL:O	12:x:128:VAL:HG22	1.99	0.62
40:P:64:UNK:N	40:P:65:UNK:HA	2.14	0.62
2:m:95:LYS:HE3	9:i:70:LEU:CD2	2.24	0.62
2:m:155:PRO:O	2:m:156:GLN:C	2.43	0.62
2:m:169:ARG:CZ	2:n:438:GLU:OE2	2.47	0.62
8:h:67:HIS:CE1	8:h:71:HIS:HE2	2.16	0.62
5:q:118:ARG:HB3	5:q:171:ILE:HG23	1.80	0.62
5:q:193:VAL:O	5:q:193:VAL:HG13	1.97	0.62
8:t:34:ARG:O	8:t:38:GLU:HG2	1.99	0.62
12:x:11:ASN:HD21	12:x:13:LYS:HB2	1.64	0.62
12:x:92:MET:HE2	12:x:167:THR:HG21	1.82	0.62
28:D:360:UNK:CB	28:D:381:UNK:CA	2.77	0.62
30:F:428:UNK:O	30:F:431:UNK:CB	2.47	0.62
38:N:262:UNK:O	38:N:265:UNK:N	2.32	0.62
1:c:297:ILE:HG22	1:c:303:LEU:HD12	1.80	0.62
3:b:207:ASN:OD1	3:b:210:GLY:N	2.32	0.62
1:l:134:ILE:HG21	1:l:174:VAL:HG21	1.82	0.62
1:l:358:LYS:HE3	1:l:402:VAL:HB	1.82	0.62
3:o:28:SER:HB3	3:o:30:TRP:HD1	1.63	0.62
3:o:137:GLN:OE1	3:o:259:ALA:HA	1.99	0.62
40:P:53:UNK:HA	40:P:57:UNK:CB	2.28	0.62
1:c:91:THR:CG2	1:c:92:ARG:N	2.62	0.62
1:c:336:PHE:HE2	1:c:446:PHE:HD2	1.47	0.62
1:c:351:GLU:OE2	1:c:404:ALA:HB3	2.00	0.62
1:c:426:GLY:H	1:c:428:ILE:HG13	1.63	0.62
2:m:187:THR:O	2:m:190:GLU:HB2	1.99	0.62
2:m:247:GLN:NE2	2:m:429:ASN:HA	2.14	0.62
3:b:207:ASN:ND2	3:b:209:THR:OG1	2.32	0.62
6:f:75:LEU:O	6:f:80:TRP:NE1	2.30	0.62
7:g:71:ARG:HH21	8:h:60:ASP:CG	2.07	0.62
5:q:103:LYS:HA	5:q:106:ILE:HD12	1.82	0.62
5:q:141:HIS:NE2	5:q:175:PRO:HB2	2.15	0.62
19:5:57:ARG:HB3	19:5:57:ARG:HH11	1.64	0.62
25:A:52:UNK:O	25:A:56:UNK:N	2.31	0.62
26:B:118:UNK:CB	59:B:201:SF4:S3	2.88	0.62
27:C:112:UNK:N	27:C:113:UNK:CA	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:60:UNK:CB	29:E:94:UNK:HA	2.30	0.62
48:Y:92:UNK:O	48:Y:95:UNK:CB	2.48	0.62
51:Z:362:UNK:CB	51:Z:366:UNK:CB	2.77	0.62
1:c:346:CYS:CB	1:c:412:SER:OG	2.44	0.62
2:m:318:ASP:OD1	2:m:318:ASP:N	2.28	0.62
3:b:15:ASN:ND2	3:b:18:PHE:CE1	2.67	0.62
1:l:39:VAL:HG11	1:l:117:VAL:HG21	1.81	0.62
2:n:195:VAL:HG13	2:n:199:PHE:CD2	2.34	0.62
3:o:52:ALA:HB2	52:o:401:HEM:HMD1	1.81	0.62
4:p:3:LEU:HD11	7:s:71:ARG:HB2	1.81	0.62
5:q:91:TRP:O	5:q:92:ARG:HB2	1.97	0.62
10:v:51:LEU:HB3	10:v:52:TRP:CE3	2.35	0.62
31:G:464:UNK:O	31:G:467:UNK:N	2.33	0.62
40:P:113:UNK:O	40:P:117:UNK:N	2.33	0.62
50:U:509:UNK:O	50:U:512:UNK:N	2.32	0.62
2:m:47:ILE:HG22	2:m:48:GLY:N	2.15	0.62
2:m:156:GLN:NE2	9:i:56:ARG:HD3	2.14	0.62
3:b:78:ILE:O	3:b:82:MET:HB2	1.98	0.62
8:h:25:GLU:HA	8:h:30:CYS:SG	2.39	0.62
2:n:95:LYS:CE	9:u:70:LEU:HD22	2.29	0.62
3:o:331:ASP:O	3:o:334:THR:HB	2.00	0.62
7:s:73:ASN:HD22	8:t:56:GLU:CD	2.08	0.62
12:x:84:PRO:HG3	12:x:92:MET:HE3	1.80	0.62
21:7:3:ASN:C	21:7:3:ASN:HD22	2.08	0.62
28:D:80:UNK:O	28:D:81:UNK:CB	2.47	0.62
30:F:116:UNK:O	30:F:119:UNK:N	2.31	0.62
1:c:5:ALA:O	1:c:8:LEU:HB2	2.00	0.62
1:c:24:ARG:CB	1:c:196:VAL:HG22	2.25	0.62
1:c:204:GLU:HG2	1:c:206:ARG:HB3	1.80	0.62
3:b:72:ASP:OD1	4:d:49:ARG:NH1	2.28	0.62
3:b:79:ILE:HG12	5:e:58:PHE:CE1	2.35	0.62
4:d:27:ARG:NH2	4:d:60:GLU:OE2	2.33	0.62
1:l:37:VAL:HG13	1:l:199:ALA:HB2	1.82	0.62
4:p:50:HIS:HB3	4:p:54:VAL:CG2	2.28	0.62
5:q:78:LEU:HD23	5:q:79:SER:H	1.64	0.62
9:u:53:GLU:O	9:u:55:LEU:HG	2.00	0.62
28:D:126:UNK:O	28:D:127:UNK:CB	2.45	0.62
31:G:624:UNK:O	31:G:627:UNK:N	2.32	0.62
40:P:103:UNK:HA	40:P:106:UNK:CB	2.29	0.62
40:P:135:UNK:O	40:P:136:UNK:C	2.48	0.62
43:S:84:UNK:O	43:S:87:UNK:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:59:ASN:OD1	2:m:60:SER:N	2.32	0.62
3:b:183:PHE:CD1	3:b:183:PHE:O	2.52	0.62
3:b:267:HIS:NE2	3:b:269:LYS:HD3	2.15	0.62
4:d:72:ASP:O	4:d:73:GLY:O	2.18	0.62
2:n:37:SER:OG	2:n:213:HIS:HB2	2.00	0.62
3:o:7:SER:HA	3:o:13:ILE:HG12	1.81	0.62
4:p:68:VAL:HG12	4:p:92:PRO:HG2	1.82	0.62
15:1:16:TYR:CE1	15:1:25:PRO:HG3	2.34	0.62
30:F:44:UNK:O	30:F:47:UNK:CB	2.48	0.62
30:F:103:UNK:HA	30:F:104:UNK:C	2.30	0.62
30:F:325:UNK:O	30:F:326:UNK:CB	2.45	0.62
1:c:154:HIS:O	1:c:158:PHE:HB2	2.01	0.61
1:c:428:ILE:HG21	1:c:431:LEU:HD22	1.82	0.61
2:m:101:THR:OG1	2:m:102:ARG:N	2.32	0.61
2:m:163:LEU:HD22	2:m:256:ALA:CB	2.29	0.61
3:b:153:ILE:HG23	3:b:154:PRO:HD2	1.82	0.61
3:o:8:HIS:CB	3:o:9:PRO:CD	2.78	0.61
3:o:304:ILE:N	3:o:305:PRO:HD2	2.14	0.61
4:p:27:ARG:HH11	10:v:58:LYS:NZ	1.98	0.61
17:3:13:ALA:O	17:3:18:ARG:HD2	2.00	0.61
30:F:294:UNK:CB	30:F:295:UNK:HA	2.30	0.61
31:G:296:UNK:O	31:G:300:UNK:CB	2.48	0.61
31:G:367:UNK:O	31:G:370:UNK:CA	2.47	0.61
33:I:87:CYS:SG	33:I:90:UNK:N	2.73	0.61
36:L:376:UNK:O	36:L:378:UNK:N	2.33	0.61
46:W:1:UNK:O	46:W:2:UNK:CB	2.46	0.61
3:b:26:ASN:O	3:b:27:ILE:HG13	2.00	0.61
4:d:165:TYR:CE1	4:d:168:VAL:HG22	2.34	0.61
9:u:62:ARG:N	9:u:63:PRO:HD2	2.15	0.61
14:z:154:GLY:HA2	17:3:6:VAL:CG2	2.30	0.61
30:F:60:UNK:O	30:F:63:UNK:CA	2.48	0.61
31:G:202:UNK:O	31:G:203:CYS:C	2.43	0.61
1:c:6:GLN:O	1:c:7:ALA:C	2.41	0.61
2:m:58:GLU:HB2	2:m:63:LEU:HD23	1.82	0.61
2:m:156:GLN:HE22	9:i:56:ARG:HD3	1.65	0.61
4:d:57:THR:HG22	4:d:58:GLU:H	1.65	0.61
4:d:236:ALA:O	7:g:14:ILE:N	2.27	0.61
4:p:32:VAL:HG11	4:p:186:VAL:CG2	2.31	0.61
13:y:16:ILE:HD12	13:y:17:MET:N	2.15	0.61
14:z:148:HIS:O	14:z:152:MET:HG3	2.01	0.61
25:A:103:UNK:O	25:A:106:UNK:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:154:UNK:O	32:H:157:UNK:O	2.18	0.61
37:M:26:UNK:O	37:M:27:UNK:C	2.47	0.61
38:N:100:UNK:HA	38:N:103:UNK:CB	2.30	0.61
40:P:155:UNK:O	40:P:158:UNK:CB	2.48	0.61
3:b:309:THR:HG23	3:b:370:GLY:HA3	1.80	0.61
6:f:106:GLU:HA	6:f:109:LYS:HZ3	1.66	0.61
2:n:154:ASN:O	2:n:155:PRO:C	2.43	0.61
2:n:362:ASN:HA	2:n:365:LYS:HD3	1.82	0.61
2:n:412:ASN:O	2:n:415:LYS:HB2	2.01	0.61
3:o:126:THR:HG21	52:o:401:HEM:C3B	2.36	0.61
5:q:121:GLN:HB3	5:q:126:ARG:HD3	1.83	0.61
5:q:187:PHE:CE2	5:q:193:VAL:HB	2.34	0.61
26:B:89:UNK:O	26:B:90:UNK:CB	2.47	0.61
27:C:23:UNK:O	27:C:26:UNK:N	2.33	0.61
27:C:27:UNK:O	27:C:30:UNK:N	2.34	0.61
28:D:70:UNK:O	28:D:71:UNK:C	2.48	0.61
30:F:166:UNK:O	30:F:168:UNK:N	2.33	0.61
30:F:262:UNK:HA	30:F:286:UNK:CB	2.31	0.61
1:c:43:ALA:CB	1:c:189:HIS:HB3	2.30	0.61
1:c:338:LEU:O	1:c:339:GLN:C	2.41	0.61
1:c:403:ASP:OD1	1:c:404:ALA:N	2.33	0.61
1:c:433:ASP:HB2	3:b:219:PRO:HG2	1.82	0.61
2:m:200:THR:HG22	2:m:203:ARG:CD	2.25	0.61
3:b:78:ILE:HG21	4:d:204:MET:HE1	1.81	0.61
4:d:10:TYR:CE1	8:h:73:LEU:CD2	2.84	0.61
7:g:34:ILE:CB	7:g:35:PRO:HD3	2.18	0.61
5:q:153:PHE:CE1	5:q:173:LYS:HG3	2.34	0.61
5:q:188:THR:OG1	5:q:189:SER:N	2.33	0.61
6:r:73:GLN:HG2	7:s:36:ASN:HD21	1.65	0.61
30:F:44:UNK:O	30:F:48:UNK:N	2.34	0.61
30:F:370:UNK:O	30:F:373:UNK:N	2.32	0.61
31:G:331:UNK:O	31:G:335:UNK:N	2.33	0.61
36:L:383:UNK:O	36:L:389:UNK:CB	2.48	0.61
3:o:171:ASP:O	3:o:172:LYS:C	2.44	0.61
4:p:231:LYS:HD2	6:r:71:ARG:HG2	1.81	0.61
7:s:54:ALA:O	7:s:58:VAL:HG23	2.01	0.61
27:C:79:UNK:O	27:C:93:UNK:N	2.33	0.61
30:F:428:UNK:O	30:F:431:UNK:N	2.33	0.61
47:X:203:UNK:O	47:X:205:UNK:N	2.32	0.61
2:m:123:LEU:O	2:m:127:THR:HG22	2.00	0.61
3:b:106:SER:HB3	52:b:402:HEM:HBD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:218:ILE:HG22	3:b:223:TYR:CD2	2.35	0.61
5:e:62:MET:O	3:o:177:ARG:NH2	2.30	0.61
6:f:106:GLU:HA	6:f:109:LYS:NZ	2.16	0.61
2:n:203:ARG:NE	2:n:230:LEU:HD23	2.15	0.61
3:o:196:HIS:HE1	52:o:402:HEM:C1D	2.19	0.61
10:v:13:LEU:O	10:v:19:THR:OG1	2.17	0.61
27:C:44:UNK:O	27:C:47:UNK:N	2.33	0.61
30:F:272:UNK:O	30:F:273:UNK:CB	2.49	0.61
32:H:128:UNK:O	32:H:132:UNK:N	2.34	0.61
37:M:168:UNK:CB	37:M:174:UNK:HA	2.30	0.61
47:X:503:UNK:O	47:X:506:UNK:N	2.33	0.61
2:m:58:GLU:OE1	2:m:63:LEU:HA	2.00	0.61
2:m:86:THR:HG23	9:i:71:ASN:HD21	1.66	0.61
10:j:51:LEU:HB3	10:j:52:TRP:CZ3	2.36	0.61
1:l:53:ASN:OD1	1:l:170:PRO:HD3	1.99	0.61
4:p:178:THR:CB	4:p:181:GLN:HG3	2.28	0.61
36:L:546:UNK:O	36:L:549:UNK:N	2.34	0.61
51:Z:252:UNK:O	51:Z:255:UNK:N	2.34	0.61
1:c:327:ASP:OD1	1:c:328:HIS:N	2.32	0.61
2:m:256:ALA:O	2:m:424:MET:HG3	2.01	0.61
2:m:338:LYS:HD3	2:m:439:LEU:HD23	1.81	0.61
3:b:146:ILE:O	3:b:149:LEU:HB3	2.00	0.61
3:b:315:MET:HA	3:b:318:ARG:HG3	1.82	0.61
4:d:204:MET:O	4:d:205:GLY:C	2.42	0.61
7:g:25:ALA:C	7:g:27:PRO:HD3	2.26	0.61
1:l:4:TYR:CE2	1:l:396:GLU:HG3	2.36	0.61
3:o:4:ILE:HG22	3:o:4:ILE:O	2.00	0.61
3:o:244:LEU:HD23	4:p:205:GLY:HA2	1.83	0.61
4:p:214:LEU:O	4:p:218:LEU:HG	2.01	0.61
12:x:92:MET:CE	12:x:167:THR:HG21	2.31	0.61
13:y:59:GLN:HA	13:y:62:GLU:HB2	1.83	0.61
28:D:211:UNK:O	28:D:214:UNK:N	2.34	0.61
31:G:104:UNK:O	31:G:106:UNK:N	2.33	0.61
31:G:565:UNK:O	31:G:566:UNK:C	2.48	0.61
47:X:423:UNK:O	47:X:426:UNK:CB	2.49	0.61
4:d:28:ARG:HD2	4:d:185:ASP:OD2	2.01	0.61
3:o:132:VAL:HA	3:o:139:SER:HB3	1.81	0.61
5:q:13:TYR:O	7:s:23:GLN:HB3	2.00	0.61
11:w:26:ALA:O	11:w:30:VAL:HG23	2.00	0.61
16:2:82:TYR:HB3	16:2:83:PRO:HD3	1.81	0.61
39:O:225:UNK:C	39:O:227:UNK:O	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:108:UNK:O	47:X:111:UNK:CB	2.49	0.61
51:Z:119:UNK:O	51:Z:122:UNK:O	2.19	0.61
2:m:60:SER:CB	2:n:429:ASN:ND2	2.53	0.60
2:m:140:LEU:HD12	2:m:143:GLN:HB3	1.83	0.60
2:m:435:PHE:HB2	2:m:438:GLU:OE1	2.00	0.60
1:l:91:THR:HG23	1:l:92:ARG:N	2.16	0.60
4:p:27:ARG:NH2	4:p:60:GLU:OE2	2.34	0.60
4:p:138:PRO:HG2	8:t:55:THR:CB	2.30	0.60
28:D:360:UNK:HA	28:D:381:UNK:HA	1.81	0.60
39:O:229:UNK:C	39:O:231:UNK:N	2.55	0.60
1:c:32:GLN:HG3	1:c:33:PRO:HD2	1.80	0.60
2:m:299:VAL:O	2:m:303:VAL:HG23	2.01	0.60
3:b:22:PRO:CG	7:g:3:GLN:HB3	2.31	0.60
3:b:163:TRP:O	3:b:177:ARG:NH1	2.32	0.60
4:d:27:ARG:O	4:d:28:ARG:C	2.41	0.60
4:d:164:ILE:HD11	53:d:301:HEC:HBB2	1.83	0.60
9:i:58:GLN:HA	9:i:78:TYR:CD2	2.37	0.60
3:o:296:PHE:CD1	3:o:359:PHE:HE1	2.19	0.60
4:p:11:PRO:O	8:t:74:PHE:CZ	2.54	0.60
4:p:237:TYR:CD2	4:p:239:PRO:HD3	2.36	0.60
10:v:55:ILE:HG23	10:v:58:LYS:HE2	1.83	0.60
24:0:13:LYS:H	24:0:13:LYS:HD3	1.65	0.60
28:D:383:UNK:CB	28:D:385:UNK:C	2.79	0.60
37:M:113:UNK:HA	37:M:114:UNK:C	2.31	0.60
51:Z:225:UNK:O	51:Z:226:UNK:C	2.45	0.60
1:c:86:LEU:HD13	1:c:99:ILE:CG1	2.31	0.60
1:c:151:ASN:O	1:c:152:TYR:C	2.43	0.60
1:c:394:GLU:O	1:c:395:TRP:C	2.44	0.60
2:m:337:ILE:CG2	2:m:434:PRO:HG2	2.30	0.60
9:i:62:ARG:HB3	9:i:63:PRO:HD3	1.83	0.60
1:l:366:VAL:HG12	1:l:367:SER:N	2.16	0.60
5:q:101:ARG:HD3	5:q:133:VAL:CG1	2.30	0.60
51:Z:221:UNK:O	51:Z:222:UNK:CB	2.48	0.60
1:c:80:GLU:O	1:c:82:MET:N	2.34	0.60
1:c:244:ARG:CZ	7:g:10:VAL:HB	2.31	0.60
8:h:73:LEU:HD21	8:h:74:PHE:CD1	2.35	0.60
1:l:354:VAL:CG1	1:l:407:VAL:HG21	2.31	0.60
2:n:384:SER:CB	9:u:62:ARG:HG2	2.32	0.60
3:o:221:HIS:HB3	3:o:222:PRO:CD	2.29	0.60
4:p:139:THR:HB	8:t:44:VAL:HB	1.84	0.60
31:G:425:UNK:O	31:G:428:UNK:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:280:TYR:O	1:c:306:SER:HA	2.00	0.60
3:o:242:LEU:HD21	3:o:250:LEU:HD22	1.83	0.60
8:t:15:ASP:HB2	8:t:16:PRO:HD3	1.83	0.60
17:3:62:CYS:SG	17:3:84:SER:OG	2.60	0.60
42:R:77:UNK:C	42:R:78:UNK:O	2.45	0.60
1:c:61:HIS:NE2	1:c:134:ILE:CD1	2.62	0.60
2:m:111:CYS:CB	2:m:119:LEU:HD22	2.28	0.60
3:b:10:LEU:HD12	3:b:13:ILE:CD1	2.28	0.60
3:b:52:ALA:HB2	52:b:401:HEM:HMD2	1.83	0.60
3:b:372:ILE:O	3:b:375:LYS:N	2.32	0.60
1:l:64:PHE:CE2	1:l:88:ALA:HB2	2.37	0.60
4:p:72:ASP:O	4:p:73:GLY:O	2.20	0.60
4:p:134:TYR:HE2	4:p:163:PRO:HG2	1.66	0.60
5:q:97:PHE:CE1	5:q:137:GLY:HA3	2.37	0.60
9:u:78:TYR:HD1	9:u:78:TYR:OXT	1.83	0.60
31:G:333:UNK:O	31:G:337:UNK:N	2.33	0.60
36:L:321:UNK:C	36:L:324:UNK:N	2.64	0.60
36:L:502:UNK:O	36:L:506:UNK:N	2.35	0.60
1:c:408:ARG:CZ	11:k:15:ARG:NE	2.63	0.60
2:m:209:LEU:CD2	2:m:375:SER:HB2	2.30	0.60
7:g:73:ASN:H	7:g:74:PRO:HD2	1.67	0.60
8:h:40:CYS:HB2	8:h:57:GLU:HG2	1.83	0.60
1:l:312:ILE:HB	1:l:319:LEU:HB2	1.83	0.60
1:l:408:ARG:NH1	11:w:15:ARG:NE	2.47	0.60
2:n:269:ALA:O	2:n:272:PHE:N	2.35	0.60
14:z:6:HIS:HD2	14:z:8:TYR:H	1.49	0.60
26:B:67:UNK:N	26:B:68:UNK:HA	2.17	0.60
27:C:138:UNK:O	27:C:139:UNK:CB	2.50	0.60
43:S:83:UNK:O	43:S:86:UNK:CB	2.50	0.60
45:V:52:UNK:O	45:V:53:UNK:CB	2.50	0.60
1:c:5:ALA:O	1:c:6:GLN:C	2.43	0.60
3:b:28:SER:HB3	3:b:30:TRP:HD1	1.67	0.60
9:i:62:ARG:N	9:i:63:PRO:HD2	2.17	0.60
1:l:146:ARG:NH2	1:l:308:GLN:HE22	2.00	0.60
1:l:184:GLU:O	1:l:188:ARG:HG3	2.02	0.60
4:p:42:SER:O	4:p:112:ASP:OD1	2.20	0.60
19:5:39:CYS:HG	19:5:53:CYS:HG	0.64	0.60
27:C:56:UNK:O	27:C:57:UNK:C	2.49	0.60
28:D:165:UNK:O	28:D:166:UNK:CB	2.49	0.60
36:L:128:UNK:O	36:L:131:UNK:N	2.35	0.60
37:M:68:UNK:O	37:M:71:UNK:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:209:UNK:O	51:Z:212:UNK:N	2.35	0.60
1:c:413:LYS:HB2	1:c:414:TYR:CD2	2.36	0.60
3:b:301:LEU:O	3:b:304:ILE:HD12	2.02	0.60
4:d:168:VAL:O	4:d:169:LEU:HD23	2.01	0.60
3:o:129:MET:CG	3:o:178:PHE:HD1	2.14	0.60
5:q:29:SER:HA	5:q:32:ARG:HD3	1.83	0.60
5:q:118:ARG:HH22	5:q:173:LYS:HA	1.66	0.60
7:s:71:ARG:O	8:t:56:GLU:OE2	2.19	0.60
37:M:137:UNK:O	37:M:138:UNK:CB	2.50	0.60
1:c:317:THR:HG22	1:c:318:GLY:H	1.67	0.60
1:c:350:THR:HB	1:c:353:GLU:HG3	1.84	0.60
2:m:111:CYS:HB3	2:m:119:LEU:CD2	2.29	0.60
4:d:26:ILE:HG22	4:d:54:VAL:HG13	1.84	0.60
1:l:352:SER:OG	1:l:353:GLU:N	2.31	0.60
1:l:426:GLY:HA2	1:l:428:ILE:N	2.17	0.60
9:u:58:GLN:HA	9:u:78:TYR:CD2	2.37	0.60
14:z:192:VAL:O	14:z:196:THR:HB	2.01	0.60
23:9:46:LYS:O	23:9:47:LYS:HB2	2.02	0.60
30:F:129:UNK:O	30:F:130:UNK:CB	2.48	0.60
31:G:119:UNK:O	31:G:120:UNK:C	2.48	0.60
33:I:99:UNK:O	33:I:104:UNK:CB	2.50	0.60
38:N:144:UNK:O	38:N:145:UNK:C	2.46	0.60
38:N:298:UNK:O	38:N:300:UNK:N	2.35	0.60
43:S:84:UNK:O	43:S:87:UNK:CA	2.50	0.60
1:c:426:GLY:HA2	1:c:428:ILE:CG1	2.32	0.59
2:m:217:LYS:O	2:m:218:GLN:C	2.45	0.59
3:b:239:LEU:HD12	3:b:239:LEU:O	2.02	0.59
4:d:30:PHE:HD1	4:d:189:PHE:CE1	2.19	0.59
4:d:57:THR:HG22	4:d:58:GLU:N	2.17	0.59
6:f:42:ASP:O	6:f:43:VAL:C	2.43	0.59
1:l:55:ALA:O	1:l:56:GLY:C	2.43	0.59
2:n:100:SER:HB3	2:n:105:MET:CG	2.32	0.59
2:n:352:LEU:HD21	2:n:357:VAL:HG23	1.82	0.59
3:o:348:ILE:O	3:o:352:GLN:HG3	2.02	0.59
14:z:119:THR:O	18:4:52:HIS:HE1	1.84	0.59
26:B:121:UNK:HA	26:B:135:UNK:HA	1.82	0.59
26:B:166:UNK:O	26:B:169:UNK:O	2.19	0.59
27:C:80:UNK:HA	27:C:91:UNK:O	2.01	0.59
31:G:186:UNK:HA	31:G:187:UNK:C	2.31	0.59
37:M:324:UNK:O	37:M:328:UNK:CB	2.50	0.59
2:m:196:GLN:HG2	2:m:197:ASN:OD1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:165:TYR:CE2	4:d:168:VAL:HG22	2.37	0.59
6:f:96:GLU:OE2	6:f:99:ARG:NH1	2.34	0.59
7:g:71:ARG:O	8:h:56:GLU:OE2	2.20	0.59
1:l:106:LEU:N	1:l:107:PRO:HD2	2.18	0.59
2:n:69:LEU:HD21	2:n:199:PHE:CZ	2.37	0.59
2:n:255:ALA:HA	2:n:425:ALA:O	2.01	0.59
3:o:32:ASN:HD21	3:o:228:ASP:HA	1.67	0.59
5:q:101:ARG:HA	5:q:105:GLU:OE1	2.02	0.59
5:q:121:GLN:HG3	5:q:179:ASN:HD22	1.67	0.59
31:G:383:UNK:O	31:G:387:UNK:CB	2.49	0.59
36:L:211:UNK:O	36:L:214:UNK:CB	2.50	0.59
39:O:25:UNK:O	39:O:123:UNK:HA	2.02	0.59
40:P:143:UNK:C	40:P:145:UNK:N	2.65	0.59
41:Q:32:UNK:CB	41:Q:59:UNK:C	2.80	0.59
2:m:98:VAL:HG22	2:m:107:TYR:CD2	2.37	0.59
3:b:115:ILE:N	3:b:115:ILE:CD1	2.66	0.59
3:b:122:THR:HG23	3:b:185:LEU:HD11	1.83	0.59
4:d:50:HIS:O	4:d:54:VAL:N	2.28	0.59
4:p:36:VAL:HG23	4:p:169:LEU:HD11	1.84	0.59
9:u:62:ARG:HB3	9:u:63:PRO:HD3	1.84	0.59
47:X:172:UNK:O	47:X:176:UNK:CB	2.51	0.59
50:U:623:UNK:O	50:U:626:UNK:CB	2.50	0.59
1:c:106:LEU:HD22	1:c:203:LEU:CD2	2.31	0.59
1:c:395:TRP:O	1:c:396:GLU:C	2.43	0.59
2:m:438:GLU:OE2	2:n:169:ARG:CZ	2.51	0.59
4:d:10:TYR:CE1	8:h:73:LEU:HD21	2.37	0.59
3:o:78:ILE:O	3:o:82:MET:HB2	2.02	0.59
9:u:70:LEU:HD12	9:u:71:ASN:N	2.16	0.59
37:M:356:UNK:O	37:M:360:UNK:N	2.35	0.59
1:c:15:GLN:O	1:c:26:ALA:HA	2.03	0.59
1:c:182:LEU:O	1:c:186:LEU:HD12	2.01	0.59
3:b:359:PHE:O	3:b:363:LEU:HB2	2.03	0.59
6:f:96:GLU:O	6:f:97:VAL:C	2.45	0.59
1:l:272:VAL:HG21	1:l:402:VAL:HG21	1.85	0.59
2:n:354:ASN:N	2:n:355:PRO:HD2	2.16	0.59
5:q:45:VAL:HG23	10:v:24:ILE:HA	1.83	0.59
5:q:164:HIS:H	5:q:173:LYS:HB2	1.67	0.59
7:s:25:ALA:O	7:s:27:PRO:HD3	2.02	0.59
8:t:73:LEU:HD21	8:t:74:PHE:HD1	1.68	0.59
10:v:9:LEU:HD12	10:v:13:LEU:CD1	2.32	0.59
26:B:122:UNK:CA	26:B:123:UNK:CB	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:U:823:UNK:O	50:U:826:UNK:CB	2.51	0.59
51:Z:309:UNK:O	51:Z:312:UNK:CB	2.51	0.59
2:m:162:ASN:HB3	2:m:244:ILE:HG21	1.84	0.59
3:b:25:SER:O	3:b:26:ASN:C	2.45	0.59
3:b:160:LEU:HD12	3:b:160:LEU:O	2.03	0.59
4:d:40:CYS:HB3	4:d:95:TYR:OH	2.02	0.59
7:g:44:CYS:SG	7:g:48:VAL:CG2	2.91	0.59
2:n:76:THR:HG21	2:n:133:ARG:NH2	2.18	0.59
2:n:183:ILE:HG22	2:n:184:GLY:N	2.16	0.59
5:q:76:ILE:HA	5:q:193:VAL:O	2.03	0.59
30:F:212:UNK:C	30:F:220:UNK:H	2.16	0.59
31:G:33:UNK:O	31:G:34:UNK:CB	2.50	0.59
50:U:122:UNK:O	50:U:123:UNK:C	2.47	0.59
3:b:8:HIS:CB	3:b:9:PRO:CD	2.81	0.59
3:b:296:PHE:O	3:b:300:ILE:HB	2.02	0.59
1:l:233:PRO:HG2	5:q:23:LYS:CD	2.32	0.59
1:l:239:SER:HB2	7:s:18:LEU:HD23	1.85	0.59
10:v:20:PHE:O	10:v:23:THR:HB	2.02	0.59
30:F:352:UNK:HA	30:F:355:UNK:CB	2.33	0.59
32:H:79:UNK:O	32:H:81:UNK:N	2.36	0.59
47:X:720:UNK:O	47:X:724:UNK:N	2.35	0.59
1:c:373:THR:HB	1:c:374:PRO:HD3	1.84	0.59
2:m:248:ASN:HB2	2:m:428:GLY:CA	2.33	0.59
3:b:4:ILE:O	3:b:4:ILE:HG22	2.02	0.59
3:b:115:ILE:O	3:b:116:GLY:C	2.46	0.59
4:d:23:HIS:CD2	10:j:51:LEU:HA	2.37	0.59
6:f:28:LYS:HD3	6:f:74:ILE:HD11	1.84	0.59
1:l:363:ASN:CG	2:n:112:LEU:HD23	2.27	0.59
30:F:163:UNK:H	30:F:166:UNK:CB	2.16	0.59
36:L:576:UNK:CB	38:N:167:UNK:CB	2.80	0.59
38:N:45:UNK:O	38:N:47:UNK:N	2.35	0.59
2:m:203:ARG:CZ	2:m:230:LEU:HD23	2.32	0.59
3:b:264:THR:CG2	5:q:144:CYS:HB3	2.25	0.59
3:b:332:LEU:HD21	3:b:358:TYR:CE1	2.38	0.59
11:k:32:LEU:O	11:k:33:VAL:C	2.45	0.59
5:q:104:LYS:O	5:q:104:LYS:HG2	2.01	0.59
10:v:18:SER:HB3	11:w:23:LEU:HD12	1.84	0.59
10:v:45:HIS:O	10:v:48:GLU:HG2	2.02	0.59
10:v:57:HIS:O	10:v:58:LYS:C	2.46	0.59
36:L:547:UNK:O	36:L:550:UNK:N	2.35	0.59
37:M:42:UNK:O	37:M:44:UNK:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:R:64:UNK:O	42:R:65:UNK:C	2.51	0.59
1:c:426:GLY:CA	1:c:428:ILE:N	2.66	0.59
3:b:327:ALA:O	3:b:331:ASP:N	2.32	0.59
4:d:223:LYS:HZ2	4:d:227:TRP:CD1	2.21	0.59
5:e:34:GLY:HA2	10:j:10:TYR:HD2	1.67	0.59
1:l:46:ARG:NH2	1:l:316:ASP:OD2	2.35	0.59
1:l:308:GLN:HG3	1:l:308:GLN:O	2.02	0.59
3:o:275:LEU:O	3:o:276:PHE:C	2.45	0.59
4:p:23:HIS:CD2	10:v:51:LEU:HA	2.38	0.59
19:5:57:ARG:HG3	19:5:60:TYR:CE2	2.38	0.59
37:M:80:UNK:O	37:M:81:UNK:C	2.48	0.59
2:m:132:PHE:HB3	2:m:137:VAL:HG21	1.85	0.58
3:b:372:ILE:O	3:b:373:GLU:C	2.46	0.58
7:g:73:ASN:HD22	8:h:56:GLU:CD	2.10	0.58
9:i:58:GLN:O	9:i:59:ALA:HB2	2.01	0.58
1:l:428:ILE:HG22	1:l:431:LEU:CG	2.32	0.58
2:n:206:LEU:HD13	2:n:224:LEU:HD11	1.84	0.58
3:o:153:ILE:HD12	3:o:153:ILE:N	2.18	0.58
4:p:113:LEU:O	4:p:114:SER:C	2.46	0.58
5:q:78:LEU:HD23	5:q:79:SER:N	2.17	0.58
13:y:226:MET:O	13:y:227:LEU:HB2	2.01	0.58
36:L:316:UNK:O	36:L:319:UNK:CB	2.51	0.58
38:N:91:UNK:H	38:N:92:UNK:C	2.16	0.58
43:S:63:UNK:O	43:S:78:UNK:CA	2.49	0.58
1:c:11:VAL:HG13	1:c:12:PRO:HD2	1.84	0.58
2:m:90:GLU:O	2:m:91:ALA:C	2.44	0.58
2:m:258:VAL:CG1	2:m:321:LEU:HB3	2.29	0.58
3:b:312:GLN:HE22	3:b:317:PHE:HB2	1.67	0.58
4:d:79:GLU:OE1	4:d:82:MET:HG3	2.03	0.58
8:h:65:ARG:CG	8:h:66:ASP:N	2.66	0.58
1:l:43:ALA:CB	1:l:189:HIS:HB3	2.32	0.58
2:n:203:ARG:CZ	2:n:230:LEU:HD23	2.33	0.58
3:o:110:LEU:HG	3:o:114:ASN:HD21	1.67	0.58
4:p:46:VAL:HG12	4:p:47:ALA:O	2.02	0.58
6:r:58:ARG:HG2	6:r:58:ARG:HH11	1.68	0.58
7:s:2:ARG:HB2	7:s:6:HIS:CD2	2.37	0.58
7:s:34:ILE:CB	7:s:35:PRO:HD3	2.32	0.58
13:y:145:PRO:CG	13:y:148:MET:HE2	2.32	0.58
13:y:179:LEU:HD21	19:5:65:PRO:HD3	1.85	0.58
30:F:212:UNK:HA	30:F:220:UNK:C	2.33	0.58
31:G:377:UNK:N	31:G:449:UNK:CA	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:143:UNK:O	38:N:145:UNK:O	2.21	0.58
39:O:26:UNK:HA	39:O:124:UNK:O	2.03	0.58
50:U:714:UNK:O	50:U:717:UNK:CB	2.51	0.58
1:c:64:PHE:HE1	1:c:86:LEU:CG	2.12	0.58
1:c:156:THR:OG1	1:c:241:ILE:HB	2.03	0.58
3:b:137:GLN:OE1	3:b:259:ALA:HA	2.02	0.58
4:p:240:PRO:CD	4:p:241:LYS:H	2.16	0.58
5:q:20:ASP:O	5:q:21:SER:C	2.46	0.58
6:r:47:ILE:O	6:r:50:LEU:HG	2.04	0.58
7:s:68:LYS:O	7:s:72:LYS:N	2.31	0.58
22:8:43:SER:OG	22:8:45:VAL:HG12	2.03	0.58
24:0:28:LEU:HB2	24:0:29:PRO:HD3	1.83	0.58
27:C:83:UNK:C	27:C:85:UNK:N	2.64	0.58
31:G:114:CYS:O	31:G:118:UNK:CB	2.52	0.58
34:J:101:UNK:O	34:J:104:UNK:CA	2.51	0.58
37:M:340:UNK:O	37:M:342:UNK:N	2.36	0.58
47:X:309:UNK:O	47:X:312:UNK:N	2.36	0.58
2:m:52:LYS:HB2	2:m:203:ARG:CB	2.25	0.58
3:b:213:SER:O	3:b:215:VAL:N	2.36	0.58
1:l:236:PHE:HD2	1:l:258:GLU:CG	2.15	0.58
1:l:397:SER:O	1:l:400:ALA:HB3	2.03	0.58
2:n:304:HIS:CG	2:n:305:GLN:H	2.22	0.58
3:o:1:MET:SD	3:o:4:ILE:HB	2.43	0.58
8:t:37:LEU:HD21	8:t:58:LEU:HA	1.83	0.58
16:2:80:GLU:H	16:2:80:GLU:CD	2.10	0.58
29:E:96:UNK:C	29:E:98:UNK:O	2.52	0.58
31:G:379:UNK:O	31:G:452:UNK:N	2.37	0.58
38:N:276:UNK:O	38:N:279:UNK:CB	2.51	0.58
51:Z:205:UNK:O	51:Z:206:UNK:C	2.48	0.58
1:c:408:ARG:NH1	11:k:15:ARG:NE	2.45	0.58
1:c:436:ARG:HE	3:b:222:PRO:HD3	1.68	0.58
3:b:377:LEU:HB3	6:f:33:ARG:HD2	1.85	0.58
4:d:138:PRO:CB	8:h:55:THR:N	2.66	0.58
5:e:33:LYS:HB3	7:g:21:PHE:CE2	2.38	0.58
10:j:57:HIS:O	10:j:58:LYS:C	2.46	0.58
1:l:91:THR:HG22	1:l:94:HIS:H	1.67	0.58
1:l:91:THR:CG2	1:l:93:GLU:H	2.10	0.58
2:n:280:GLY:HA2	2:n:311:ALA:HB3	1.85	0.58
3:o:92:ILE:O	3:o:96:MET:HG2	2.02	0.58
4:p:120:ARG:HH11	4:p:120:ARG:CG	2.16	0.58
5:q:40:THR:HG22	10:v:20:PHE:HZ	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:147:ILE:N	5:q:157:TYR:O	2.36	0.58
9:u:70:LEU:HD21	9:u:73:PRO:CD	2.26	0.58
31:G:439:UNK:O	31:G:443:UNK:N	2.37	0.58
36:L:38:UNK:O	36:L:41:UNK:N	2.37	0.58
38:N:59:UNK:O	38:N:62:UNK:N	2.37	0.58
39:O:119:UNK:C	39:O:121:UNK:H	2.16	0.58
44:T:55:UNK:CA	44:T:60:UNK:O	2.51	0.58
1:c:408:ARG:NH2	11:k:15:ARG:CZ	2.64	0.58
4:d:3:LEU:HD22	7:g:70:LYS:NZ	2.19	0.58
4:d:100:ALA:O	4:d:103:ALA:N	2.37	0.58
4:d:138:PRO:HG2	8:h:55:THR:OG1	2.04	0.58
1:l:351:GLU:HA	1:l:404:ALA:HB2	1.85	0.58
4:p:161:ALA:HB1	4:p:162:PRO:HD2	1.86	0.58
5:q:69:LEU:HG	5:q:69:LEU:O	2.02	0.58
30:F:60:UNK:O	30:F:63:UNK:C	2.52	0.58
30:F:352:UNK:O	30:F:355:UNK:CA	2.51	0.58
30:F:387:UNK:O	30:F:390:UNK:N	2.37	0.58
32:H:136:UNK:O	32:H:137:UNK:C	2.50	0.58
51:Z:243:UNK:C	51:Z:245:UNK:N	2.59	0.58
51:Z:323:UNK:CB	51:Z:324:UNK:CA	2.81	0.58
1:c:4:TYR:CE2	1:c:396:GLU:HG3	2.38	0.58
1:c:36:THR:OG1	1:c:372:THR:HG22	2.03	0.58
2:m:134:ARG:HH12	6:r:51:PRO:HD3	1.69	0.58
4:d:32:VAL:HG11	4:d:182:VAL:HG13	1.84	0.58
9:i:58:GLN:HG2	9:i:78:TYR:CD2	2.38	0.58
2:n:109:VAL:HG13	2:n:109:VAL:O	2.04	0.58
2:n:264:ILE:HD12	2:n:315:SER:O	2.03	0.58
3:o:320:LEU:HB2	3:o:373:GLU:OE2	2.04	0.58
8:t:73:LEU:O	8:t:73:LEU:HG	2.02	0.58
26:B:77:UNK:CB	26:B:78:UNK:C	2.82	0.58
31:G:210:UNK:O	31:G:211:UNK:C	2.52	0.58
47:X:302:UNK:O	47:X:303:UNK:C	2.52	0.58
51:Z:322:UNK:O	51:Z:323:UNK:CB	2.52	0.58
1:c:145:MET:HE3	1:c:252:HIS:HE1	1.67	0.58
1:c:311:ASN:OD1	1:c:320:LEU:CD2	2.52	0.58
2:m:49:LEU:HD21	2:m:204:MET:SD	2.44	0.58
2:m:68:LEU:HD11	2:m:140:LEU:HD23	1.85	0.58
3:b:309:THR:HG21	3:b:367:PRO:O	2.03	0.58
1:l:64:PHE:HE1	1:l:86:LEU:HG	1.61	0.58
1:l:161:THR:CB	1:l:162:PRO:HD2	2.34	0.58
1:l:270:LEU:O	1:l:273:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:341:GLN:OE1	1:l:344:ARG:HD3	2.03	0.58
1:l:350:THR:HB	1:l:353:GLU:HG3	1.85	0.58
2:n:299:VAL:HG13	2:n:303:VAL:HG21	1.86	0.58
3:o:211:ILE:HG21	6:r:62:ILE:HD13	1.86	0.58
3:o:240:MET:HA	3:o:243:VAL:HG12	1.86	0.58
3:o:270:PRO:HB2	3:o:274:PHE:HB2	1.85	0.58
4:p:138:PRO:CB	8:t:55:THR:N	2.67	0.58
13:y:193:TYR:HE1	15:l:126:MET:HE1	1.68	0.58
26:B:71:UNK:CB	32:H:37:UNK:CB	2.82	0.58
26:B:166:UNK:O	26:B:169:UNK:C	2.52	0.58
29:E:97:UNK:N	29:E:136:UNK:O	2.37	0.58
33:I:159:UNK:O	33:I:162:UNK:CB	2.52	0.58
36:L:604:UNK:CB	38:N:93:UNK:N	2.67	0.58
37:M:75:UNK:O	37:M:78:UNK:N	2.37	0.58
38:N:32:UNK:O	38:N:35:UNK:CB	2.51	0.58
51:Z:209:UNK:O	51:Z:212:UNK:CB	2.52	0.58
1:c:32:GLN:HG2	1:c:33:PRO:CD	2.33	0.58
2:m:169:ARG:HG2	2:n:435:PHE:CE1	2.39	0.58
2:m:238:LYS:HE3	2:m:239:TYR:O	2.04	0.58
2:m:247:GLN:HG3	2:m:248:ASN:N	2.19	0.58
3:b:67:THR:O	3:b:71:ARG:HG3	2.04	0.58
7:g:68:LYS:O	7:g:72:LYS:N	2.34	0.58
10:j:32:GLU:CG	10:j:33:ARG:N	2.67	0.58
2:n:56:ARG:NE	2:n:103:GLU:OE1	2.19	0.58
2:n:141:GLN:HB2	2:n:142:PRO:HD3	1.86	0.58
2:n:328:SER:HB3	2:n:336:VAL:HG21	1.86	0.58
3:o:149:LEU:HD21	3:o:281:LEU:HD22	1.86	0.58
26:B:54:CYS:O	26:B:57:UNK:N	2.37	0.58
30:F:183:UNK:O	30:F:186:UNK:N	2.37	0.58
30:F:209:UNK:CA	30:F:210:UNK:C	2.82	0.58
31:G:180:UNK:O	31:G:181:UNK:C	2.47	0.58
1:c:233:PRO:HG2	5:e:23:LYS:HD2	1.84	0.58
1:c:338:LEU:O	1:c:341:GLN:N	2.35	0.58
1:c:417:ASP:OD1	5:e:33:LYS:HD2	2.04	0.58
1:l:268:VAL:O	1:l:272:VAL:HG23	2.04	0.58
2:n:146:ILE:O	2:n:150:VAL:HG13	2.03	0.58
2:n:262:ALA:HB2	2:n:272:PHE:HE2	1.69	0.58
3:o:240:MET:O	3:o:244:LEU:HB2	2.03	0.58
5:q:153:PHE:CE1	5:q:172:ARG:HB2	2.39	0.58
6:r:73:GLN:HE21	7:s:32:LYS:HZ1	1.48	0.58
10:v:29:LEU:HD13	11:w:34:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:103:UNK:O	40:P:106:UNK:CA	2.51	0.58
50:U:624:UNK:O	50:U:627:UNK:CB	2.52	0.58
2:m:72:ALA:O	2:m:75:LEU:HG	2.04	0.57
5:e:33:LYS:HA	7:g:21:PHE:CE2	2.38	0.57
7:g:33:GLY:O	7:g:37:VAL:N	2.36	0.57
8:h:58:LEU:HD11	8:h:62:LEU:CD1	2.34	0.57
2:n:148:LYS:HD2	2:n:178:CYS:O	2.04	0.57
5:q:185:TYR:HA	5:q:194:ILE:O	2.04	0.57
8:t:58:LEU:HD11	8:t:62:LEU:CD1	2.32	0.57
37:M:108:UNK:CA	37:M:111:UNK:CB	2.80	0.57
1:c:48:GLU:OE1	1:c:53:ASN:O	2.20	0.57
1:c:106:LEU:HB3	1:c:107:PRO:HD3	1.85	0.57
1:c:142:ASP:OD1	5:e:2:HIS:ND1	2.36	0.57
1:c:248:LEU:N	1:c:248:LEU:HD23	2.19	0.57
4:d:21:LEU:HD11	4:d:192:TRP:HB2	1.84	0.57
4:d:115:TYR:HD2	4:d:119:ALA:HB2	1.69	0.57
8:h:35:GLU:O	8:h:39:LEU:HG	2.04	0.57
1:l:354:VAL:HG13	1:l:407:VAL:HG21	1.86	0.57
2:n:59:ASN:CG	2:n:60:SER:H	2.11	0.57
2:n:303:VAL:CG1	2:n:304:HIS:N	2.67	0.57
3:o:234:LEU:HD21	4:p:216:LEU:HD21	1.86	0.57
10:v:51:LEU:H	10:v:54:HIS:HD2	1.49	0.57
28:D:163:UNK:HA	32:H:278:UNK:HA	1.87	0.57
28:D:269:UNK:CB	28:D:368:UNK:CB	2.82	0.57
30:F:435:UNK:O	30:F:439:UNK:N	2.36	0.57
31:G:594:UNK:CB	31:G:595:UNK:C	2.82	0.57
38:N:85:UNK:O	38:N:86:UNK:CB	2.51	0.57
40:P:170:UNK:CB	40:P:203:UNK:O	2.52	0.57
3:b:51:LEU:CD2	3:b:79:ILE:HG22	2.34	0.57
4:d:43:MET:HG2	4:d:46:VAL:CG2	2.33	0.57
7:g:2:ARG:HB2	7:g:6:HIS:CD2	2.38	0.57
1:l:233:PRO:HG2	5:q:23:LYS:NZ	2.19	0.57
3:o:165:TRP:HA	3:o:174:THR:OG1	2.04	0.57
4:p:10:TYR:O	4:p:12:TRP:CD1	2.58	0.57
5:q:114:VAL:O	5:q:117:LEU:HB2	2.04	0.57
5:q:121:GLN:HG3	5:q:179:ASN:ND2	2.20	0.57
6:r:51:PRO:HG2	6:r:54:LEU:HD23	1.84	0.57
14:z:203:PHE:O	14:z:207:HIS:HD2	1.88	0.57
30:F:371:UNK:O	30:F:375:UNK:CB	2.52	0.57
36:L:419:UNK:O	36:L:422:UNK:N	2.37	0.57
6:f:91:GLU:HB2	6:f:92:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:38:GLY:O	10:j:42:ILE:HG13	2.04	0.57
2:n:34:VAL:HG11	2:n:386:ALA:CB	2.32	0.57
2:n:97:SER:OG	9:u:70:LEU:HB2	2.04	0.57
5:q:188:THR:CG2	5:q:194:ILE:HG13	2.34	0.57
37:M:31:UNK:O	37:M:32:UNK:O	2.23	0.57
39:O:43:UNK:O	39:O:46:UNK:N	2.38	0.57
40:P:25:UNK:CB	40:P:95:UNK:CB	2.82	0.57
40:P:147:UNK:O	40:P:150:UNK:CB	2.52	0.57
42:R:63:UNK:O	42:R:64:UNK:O	2.22	0.57
1:c:268:VAL:O	1:c:272:VAL:HG23	2.03	0.57
2:n:79:GLY:CA	2:n:125:ASN:HD21	2.17	0.57
13:y:145:PRO:HG3	13:y:148:MET:HE2	1.87	0.57
31:G:604:UNK:O	31:G:608:UNK:CA	2.51	0.57
33:I:69:UNK:CB	33:I:74:UNK:O	2.53	0.57
34:J:170:UNK:O	34:J:171:UNK:C	2.53	0.57
36:L:137:UNK:O	36:L:140:UNK:N	2.38	0.57
36:L:579:UNK:C	36:L:581:UNK:CB	2.83	0.57
37:M:94:UNK:O	37:M:95:UNK:C	2.48	0.57
40:P:103:UNK:O	40:P:104:UNK:C	2.52	0.57
40:P:136:UNK:HA	40:P:137:UNK:C	2.33	0.57
1:c:86:LEU:HD13	1:c:99:ILE:CD1	2.35	0.57
1:c:120:CYS:O	1:c:122:LEU:HG	2.04	0.57
3:b:218:ILE:HG21	3:b:223:TYR:CD2	2.38	0.57
1:l:224:ASP:CG	51:Z:217:UNK:CB	2.77	0.57
1:l:317:THR:HG22	1:l:318:GLY:N	2.19	0.57
1:l:334:MET:HA	1:l:334:MET:HE3	1.86	0.57
1:l:349:ALA:HB3	1:l:408:ARG:CG	2.35	0.57
1:l:417:ASP:OD1	5:q:33:LYS:HD2	2.05	0.57
2:n:304:HIS:CG	2:n:305:GLN:N	2.72	0.57
3:o:28:SER:HB3	3:o:30:TRP:CD1	2.39	0.57
3:o:68:HIS:NE2	5:q:67:ASP:HB2	2.18	0.57
3:o:218:ILE:HG23	3:o:219:PRO:HD2	1.86	0.57
4:p:158:ILE:HG12	4:p:159:GLY:N	2.19	0.57
27:C:23:UNK:CA	27:C:26:UNK:CB	2.81	0.57
30:F:150:UNK:O	30:F:153:UNK:CB	2.52	0.57
31:G:333:UNK:O	31:G:337:UNK:CB	2.53	0.57
35:K:13:UNK:O	35:K:16:UNK:CB	2.52	0.57
40:P:133:UNK:CA	40:P:166:UNK:O	2.52	0.57
3:b:88:SER:O	3:b:89:MET:C	2.47	0.57
3:b:221:HIS:HB3	3:b:222:PRO:CD	2.27	0.57
8:h:34:ARG:O	8:h:38:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:53:GLU:O	9:i:54:SER:C	2.47	0.57
2:n:275:LEU:HD22	2:n:414:ALA:HB2	1.85	0.57
7:s:31:SER:O	7:s:35:PRO:CD	2.47	0.57
13:y:193:TYR:CE1	15:l:126:MET:HE1	2.39	0.57
28:D:188:UNK:O	28:D:189:UNK:CB	2.52	0.57
31:G:318:UNK:HA	31:G:344:UNK:O	2.03	0.57
31:G:425:UNK:O	31:G:428:UNK:N	2.38	0.57
32:H:176:UNK:O	47:X:146:UNK:CB	2.53	0.57
36:L:368:UNK:O	36:L:372:UNK:N	2.37	0.57
36:L:382:UNK:CB	36:L:389:UNK:HA	2.34	0.57
1:c:436:ARG:HE	3:b:222:PRO:CD	2.18	0.57
2:n:264:ILE:HG21	2:n:317:SER:HA	1.85	0.57
5:q:77:LYS:HG3	5:q:89:PHE:HE2	1.68	0.57
26:B:54:CYS:C	26:B:56:UNK:N	2.61	0.57
40:P:111:UNK:HA	40:P:151:UNK:CB	2.35	0.57
50:U:817:UNK:O	50:U:821:UNK:N	2.38	0.57
1:c:394:GLU:O	1:c:397:SER:N	2.38	0.57
3:b:215:VAL:O	6:f:63:LYS:NZ	2.37	0.57
3:b:225:THR:O	3:b:229:ILE:HD12	2.05	0.57
4:d:229:VAL:CG1	4:d:233:ARG:HE	2.18	0.57
1:l:18:GLN:HG2	1:l:19:LEU:O	2.04	0.57
2:n:206:LEU:HD13	2:n:224:LEU:CD1	2.34	0.57
3:o:67:THR:O	3:o:71:ARG:HG3	2.04	0.57
5:q:87:MET:HG2	5:q:89:PHE:CE1	2.40	0.57
19:5:71:THR:O	19:5:75:ARG:HD3	2.05	0.57
28:D:369:UNK:N	28:D:372:UNK:O	2.38	0.57
30:F:315:UNK:HA	30:F:316:UNK:O	2.04	0.57
31:G:11:UNK:CB	31:G:77:UNK:N	2.67	0.57
32:H:41:UNK:CB	32:H:44:UNK:CB	2.82	0.57
34:J:59:UNK:O	34:J:63:UNK:CB	2.52	0.57
36:L:207:UNK:CA	36:L:208:UNK:C	2.82	0.57
37:M:180:UNK:C	37:M:182:UNK:N	2.65	0.57
45:V:30:UNK:O	45:V:33:UNK:N	2.38	0.57
1:c:278:GLY:O	1:c:309:THR:HG23	2.05	0.57
2:m:203:ARG:NE	2:m:230:LEU:HD23	2.20	0.57
3:b:18:PHE:O	3:b:220:PHE:HD2	1.84	0.57
3:b:71:ARG:NH2	4:d:193:ALA:O	2.38	0.57
2:n:217:LYS:O	2:n:221:GLU:HG3	2.05	0.57
2:n:352:LEU:HD12	2:n:353:SER:N	2.20	0.57
3:o:377:LEU:O	3:o:378:LYS:HB3	2.03	0.57
6:r:28:LYS:CB	6:r:74:ILE:HD11	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:t:25:GLU:HA	8:t:30:CYS:SG	2.44	0.57
9:u:58:GLN:HG2	9:u:78:TYR:CD2	2.40	0.57
12:x:95:PRO:HB2	14:z:11:VAL:HG13	1.87	0.57
36:L:21:UNK:O	36:L:22:UNK:C	2.52	0.57
47:X:320:UNK:O	47:X:321:UNK:CB	2.50	0.57
2:m:47:ILE:CD1	2:m:120:MET:SD	2.93	0.56
1:l:45:SER:HB3	1:l:167:VAL:HG22	1.86	0.56
1:l:64:PHE:HA	1:l:75:LEU:CD2	2.35	0.56
1:l:134:ILE:HA	1:l:137:GLU:HG3	1.87	0.56
1:l:270:LEU:O	1:l:273:ALA:N	2.38	0.56
2:n:92:VAL:O	2:n:92:VAL:HG12	2.06	0.56
3:o:163:TRP:O	3:o:177:ARG:NH1	2.34	0.56
3:o:310:SER:HB3	3:o:318:ARG:NH1	2.18	0.56
28:D:224:UNK:O	28:D:227:UNK:N	2.38	0.56
32:H:93:UNK:N	32:H:94:UNK:HA	2.20	0.56
33:I:81:UNK:N	59:I:202:SF4:S1	2.77	0.56
35:K:9:UNK:O	35:K:12:UNK:N	2.38	0.56
37:M:91:UNK:O	37:M:94:UNK:N	2.38	0.56
37:M:328:UNK:O	37:M:329:UNK:C	2.52	0.56
1:c:25:VAL:HG21	1:c:209:LEU:HD12	1.87	0.56
2:m:99:THR:O	2:m:106:ALA:N	2.37	0.56
3:b:51:LEU:HD21	3:b:79:ILE:CG2	2.33	0.56
3:b:316:MET:HE2	3:b:317:PHE:CE1	2.40	0.56
4:d:27:ARG:NH1	10:j:58:LYS:HG3	2.18	0.56
4:d:150:ASN:OD1	4:d:151:PRO:CD	2.53	0.56
1:l:32:GLN:HG2	1:l:33:PRO:HD2	1.85	0.56
1:l:438:ARG:HH11	1:l:438:ARG:HG3	1.70	0.56
3:o:18:PHE:O	3:o:220:PHE:CD2	2.58	0.56
4:p:26:ILE:O	4:p:27:ARG:C	2.47	0.56
12:x:404:THR:O	12:x:480:ARG:NH1	2.37	0.56
30:F:315:UNK:HA	30:F:316:UNK:CB	2.34	0.56
48:Y:25:UNK:O	48:Y:28:UNK:O	2.23	0.56
1:c:30:SER:N	1:c:201:GLY:O	2.38	0.56
1:c:309:THR:HA	1:c:322:ALA:HA	1.86	0.56
1:c:343:MET:O	1:c:344:ARG:C	2.41	0.56
1:c:425:PHE:O	1:c:426:GLY:O	2.23	0.56
2:m:264:ILE:CG2	2:m:317:SER:HA	2.36	0.56
4:d:35:GLN:HB2	4:d:169:LEU:CD1	2.35	0.56
4:d:224:ARG:O	4:d:225:HIS:C	2.47	0.56
6:f:75:LEU:C	6:f:80:TRP:HE1	2.12	0.56
1:l:32:GLN:HG2	1:l:33:PRO:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:240:GLN:HG3	1:l:422:VAL:O	2.05	0.56
1:l:342:TRP:O	1:l:345:LEU:HB2	2.04	0.56
2:n:187:THR:O	2:n:190:GLU:HB2	2.05	0.56
2:n:294:SER:HB3	2:n:343:GLN:HE21	1.70	0.56
3:o:34:GLY:O	3:o:37:LEU:HB2	2.05	0.56
3:o:309:THR:HG23	3:o:370:GLY:HA3	1.86	0.56
3:o:313:ARG:HB3	6:r:38:HIS:CD2	2.40	0.56
4:p:21:LEU:HD11	4:p:192:TRP:HB2	1.88	0.56
13:y:132:GLU:HB3	13:y:137:GLU:HG3	1.87	0.56
13:y:189:PRO:HD2	20:6:54:TYR:OH	2.05	0.56
16:2:78:HIS:ND1	20:6:12:LEU:HD22	2.21	0.56
19:5:75:ARG:HG2	19:5:75:ARG:NH1	2.19	0.56
23:9:41:ARG:HG3	24:0:40:TYR:CE2	2.40	0.56
28:D:234:UNK:HA	28:D:237:UNK:CB	2.35	0.56
28:D:383:UNK:N	28:D:384:UNK:HA	2.21	0.56
28:D:394:UNK:O	28:D:398:UNK:N	2.38	0.56
30:F:275:UNK:CB	30:F:278:UNK:CB	2.83	0.56
32:H:79:UNK:O	32:H:82:UNK:N	2.38	0.56
35:K:50:UNK:O	35:K:51:UNK:C	2.52	0.56
36:L:546:UNK:O	36:L:547:UNK:C	2.52	0.56
37:M:410:UNK:O	37:M:414:UNK:N	2.38	0.56
38:N:122:UNK:O	38:N:124:UNK:HA	2.05	0.56
39:O:109:UNK:O	39:O:112:UNK:N	2.38	0.56
40:P:103:UNK:O	40:P:106:UNK:C	2.53	0.56
43:S:28:UNK:C	43:S:30:UNK:N	2.62	0.56
43:S:66:UNK:HA	43:S:75:UNK:O	2.04	0.56
47:X:72:UNK:O	47:X:73:UNK:CB	2.53	0.56
50:U:506:UNK:O	50:U:510:UNK:N	2.38	0.56
51:Z:349:UNK:O	51:Z:353:UNK:N	2.39	0.56
1:c:272:VAL:HG13	1:c:358:LYS:HA	1.88	0.56
2:m:237:ALA:HB2	2:m:318:ASP:CG	2.31	0.56
3:b:28:SER:HB3	3:b:30:TRP:CD1	2.40	0.56
4:d:113:LEU:O	4:d:114:SER:C	2.48	0.56
5:e:29:SER:CB	5:e:32:ARG:HD3	2.35	0.56
1:l:134:ILE:CG2	1:l:174:VAL:HG21	2.35	0.56
1:l:245:GLU:O	1:l:247:GLY:N	2.38	0.56
1:l:408:ARG:NH2	11:w:15:ARG:CZ	2.65	0.56
2:n:264:ILE:HG22	2:n:317:SER:HA	1.88	0.56
3:o:15:ASN:O	3:o:18:PHE:HD2	1.87	0.56
5:q:86:ASN:HD21	5:q:97:PHE:HD2	1.54	0.56
28:D:117:UNK:CB	28:D:367:UNK:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:65:UNK:CB	36:L:66:UNK:CA	2.83	0.56
36:L:512:UNK:O	36:L:513:UNK:C	2.53	0.56
2:m:261:SER:OG	2:m:262:ALA:N	2.39	0.56
2:m:277:HIS:CD2	2:m:364:LEU:HD13	2.40	0.56
3:b:171:ASP:O	3:b:172:LYS:C	2.47	0.56
4:d:50:HIS:O	4:d:51:LEU:C	2.48	0.56
2:n:155:PRO:O	2:n:156:GLN:C	2.49	0.56
4:p:50:HIS:HE1	4:p:91:PHE:HZ	1.54	0.56
4:p:117:VAL:HG11	4:p:191:ARG:HH11	1.70	0.56
4:p:138:PRO:O	4:p:141:VAL:HB	2.06	0.56
10:v:47:ASN:HB3	10:v:50:LYS:HD2	1.88	0.56
30:F:100:UNK:O	30:F:101:UNK:C	2.48	0.56
36:L:457:UNK:O	36:L:458:UNK:C	2.51	0.56
42:R:75:UNK:O	42:R:76:UNK:CB	2.53	0.56
1:c:62:LEU:O	1:c:63:ALA:C	2.46	0.56
2:m:86:THR:CG2	9:i:71:ASN:HD21	2.19	0.56
3:b:300:ILE:CD1	3:b:362:ILE:HG21	2.36	0.56
4:d:178:THR:CB	4:d:181:GLN:HG3	2.32	0.56
10:j:60:GLU:HG3	10:j:60:GLU:O	2.06	0.56
1:l:279:HIS:CE1	1:l:284:TYR:HH	2.23	0.56
2:n:79:GLY:HA3	2:n:125:ASN:HD21	1.69	0.56
2:n:198:HIS:HE1	2:n:233:SER:OG	1.89	0.56
3:o:26:ASN:HD22	3:o:208:PRO:HD2	1.70	0.56
3:o:300:ILE:O	3:o:300:ILE:HG12	2.05	0.56
6:r:28:LYS:HB3	6:r:74:ILE:HD11	1.86	0.56
25:A:65:UNK:O	25:A:66:UNK:C	2.52	0.56
28:D:402:UNK:O	28:D:406:UNK:N	2.38	0.56
37:M:121:UNK:O	37:M:124:UNK:CB	2.53	0.56
40:P:169:UNK:CB	40:P:231:UNK:CB	2.83	0.56
1:c:162:PRO:O	1:c:165:GLN:NE2	2.38	0.56
1:c:335:MET:HE2	1:c:339:GLN:HG3	1.88	0.56
2:m:55:SER:OG	2:m:102:ARG:HG2	2.06	0.56
3:b:135:TRP:HH2	3:b:170:VAL:O	1.89	0.56
3:b:338:ILE:CD1	3:b:338:ILE:H	2.19	0.56
3:o:44:GLN:HE22	3:o:86:GLY:HA3	1.70	0.56
3:o:132:VAL:HA	3:o:139:SER:CB	2.36	0.56
12:x:184:PHE:H	12:x:256:HIS:HE1	1.52	0.56
28:D:163:UNK:CB	32:H:278:UNK:CB	2.83	0.56
28:D:357:UNK:CA	28:D:384:UNK:CB	2.84	0.56
30:F:69:UNK:O	30:F:70:UNK:CB	2.53	0.56
33:I:149:UNK:CA	33:I:150:UNK:CB	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:160:ILE:HD11	2:m:325:TYR:CE2	2.40	0.56
2:m:239:TYR:OH	2:m:421:ARG:O	2.19	0.56
2:m:273:SER:O	2:m:276:GLN:HB3	2.06	0.56
3:b:115:ILE:N	3:b:115:ILE:HD12	2.21	0.56
3:b:264:THR:O	3:b:266:PRO:HD3	2.06	0.56
3:b:337:TRP:O	3:b:338:ILE:C	2.48	0.56
4:d:11:PRO:HB2	8:h:74:PHE:CG	2.41	0.56
4:d:79:GLU:O	4:d:80:MET:C	2.49	0.56
6:f:49:ARG:HD3	2:n:135:TRP:CD2	2.41	0.56
1:l:240:GLN:HA	1:l:422:VAL:O	2.06	0.56
2:n:141:GLN:HE22	2:n:186:VAL:HB	1.70	0.56
2:n:155:PRO:HB2	2:n:254:HIS:CE1	2.40	0.56
3:o:274:PHE:O	3:o:275:LEU:C	2.47	0.56
3:o:310:SER:HB3	3:o:318:ARG:HH11	1.69	0.56
4:p:43:MET:HE3	4:p:91:PHE:CD2	2.41	0.56
4:p:139:THR:HG21	8:t:41:ASP:O	2.06	0.56
5:q:76:ILE:CG2	5:q:194:ILE:CG1	2.74	0.56
30:F:44:UNK:O	30:F:47:UNK:CA	2.54	0.56
30:F:214:UNK:HA	30:F:218:UNK:C	2.36	0.56
30:F:215:UNK:C	30:F:217:UNK:N	2.63	0.56
30:F:303:UNK:HA	30:F:414:UNK:CB	2.36	0.56
36:L:156:UNK:O	36:L:157:UNK:CB	2.54	0.56
37:M:42:UNK:O	37:M:43:UNK:C	2.53	0.56
43:S:62:UNK:O	43:S:78:UNK:CB	2.54	0.56
51:Z:310:UNK:O	51:Z:313:UNK:CB	2.54	0.56
1:c:354:VAL:HG21	1:c:404:ALA:HA	1.87	0.56
3:b:26:ASN:ND2	3:b:26:ASN:C	2.63	0.56
3:b:182:HIS:O	3:b:186:PRO:HD2	2.06	0.56
3:b:218:ILE:HG22	3:b:219:PRO:N	2.20	0.56
4:d:139:THR:HB	8:h:44:VAL:HB	1.87	0.56
6:f:73:GLN:HA	7:g:39:ARG:HH21	1.71	0.56
10:j:12:LEU:HD23	10:j:13:LEU:CD2	2.36	0.56
1:l:136:GLN:HE21	9:u:50:LEU:HB3	1.70	0.56
2:n:133:ARG:O	2:n:134:ARG:C	2.49	0.56
2:n:213:HIS:N	2:n:214:PRO:CD	2.69	0.56
3:o:315:MET:HA	3:o:318:ARG:HG3	1.87	0.56
34:J:101:UNK:O	34:J:104:UNK:CB	2.54	0.56
36:L:366:UNK:O	36:L:369:UNK:N	2.39	0.56
37:M:176:UNK:CB	37:M:179:UNK:N	2.69	0.56
38:N:26:UNK:CB	38:N:27:UNK:CB	2.84	0.56
2:m:280:GLY:HA2	2:m:311:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:69:GLU:HA	4:d:73:GLY:HA2	1.88	0.56
8:h:21:ARG:CB	8:h:65:ARG:HH21	2.17	0.56
3:o:206:ASN:CB	3:o:313:ARG:NH2	2.55	0.56
5:q:76:ILE:O	5:q:77:LYS:HG2	2.06	0.56
5:q:118:ARG:HB3	5:q:171:ILE:CG2	2.36	0.56
5:q:187:PHE:HA	5:q:193:VAL:HA	1.88	0.56
26:B:123:UNK:N	26:B:126:UNK:O	2.40	0.56
28:D:259:UNK:O	28:D:261:UNK:N	2.39	0.56
30:F:212:UNK:O	30:F:219:UNK:HA	2.05	0.56
31:G:273:UNK:O	31:G:276:UNK:N	2.39	0.56
38:N:55:UNK:CB	38:N:121:UNK:CB	2.84	0.56
38:N:158:UNK:O	38:N:161:UNK:CA	2.53	0.56
39:O:234:UNK:O	39:O:237:UNK:N	2.39	0.56
1:c:136:GLN:HE21	9:i:50:LEU:HB3	1.70	0.55
3:b:41:LEU:O	3:b:45:ILE:HG13	2.06	0.55
3:b:244:LEU:HD11	4:d:204:MET:CE	2.36	0.55
4:d:51:LEU:HD22	4:d:58:GLU:HA	1.89	0.55
5:e:31:ALA:HB1	10:j:6:THR:OG1	2.05	0.55
5:e:72:SER:O	5:e:73:LYS:HG2	2.05	0.55
1:l:233:PRO:HG2	5:q:23:LYS:CE	2.36	0.55
1:l:408:ARG:CZ	11:w:15:ARG:NE	2.67	0.55
3:o:88:SER:HA	3:o:272:TRP:HZ2	1.70	0.55
3:o:169:SER:OG	3:o:170:VAL:N	2.37	0.55
3:o:296:PHE:O	3:o:300:ILE:HB	2.05	0.55
8:t:40:CYS:HB2	8:t:57:GLU:HG2	1.89	0.55
10:v:34:ALA:O	10:v:35:PHE:C	2.45	0.55
27:C:135:UNK:O	27:C:139:UNK:HA	2.06	0.55
31:G:456:UNK:CB	31:G:457:UNK:CA	2.83	0.55
36:L:510:UNK:O	36:L:513:UNK:CB	2.54	0.55
45:V:45:UNK:O	45:V:47:UNK:N	2.39	0.55
48:Y:56:UNK:C	48:Y:58:UNK:N	2.66	0.55
1:c:272:VAL:HG21	1:c:402:VAL:HG21	1.87	0.55
1:c:385:THR:CG2	1:c:386:TYR:CD1	2.89	0.55
4:d:21:LEU:CD1	4:d:192:TRP:HB2	2.36	0.55
4:d:69:GLU:O	4:d:73:GLY:HA3	2.05	0.55
4:d:219:VAL:HA	4:d:222:MET:HG3	1.88	0.55
5:q:139:CYS:HB2	5:q:165:TYR:CE2	2.39	0.55
14:z:42:LEU:HD13	21:7:45:TYR:CD2	2.41	0.55
30:F:214:UNK:CB	30:F:218:UNK:HA	2.36	0.55
30:F:300:UNK:O	30:F:333:UNK:N	2.39	0.55
30:F:367:UNK:O	30:F:371:UNK:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:66:UNK:HA	33:I:158:UNK:CB	2.36	0.55
36:L:181:UNK:O	36:L:183:UNK:N	2.39	0.55
36:L:207:UNK:CB	36:L:208:UNK:C	2.84	0.55
38:N:253:UNK:HA	38:N:259:UNK:CB	2.36	0.55
39:O:84:UNK:O	39:O:85:UNK:C	2.53	0.55
50:U:710:UNK:O	50:U:713:UNK:N	2.39	0.55
1:c:55:ALA:O	1:c:56:GLY:C	2.48	0.55
2:m:33:LEU:HB2	2:m:204:MET:O	2.07	0.55
3:b:378:LYS:HD3	6:f:33:ARG:HH12	1.72	0.55
6:f:74:ILE:HD13	6:f:80:TRP:CZ2	2.40	0.55
1:l:266:ASP:O	1:l:270:LEU:HG	2.06	0.55
2:n:62:ASN:O	2:n:62:ASN:ND2	2.40	0.55
2:n:342:ASN:O	2:n:345:LYS:HB2	2.06	0.55
2:n:435:PHE:HB2	2:n:438:GLU:OE1	2.05	0.55
3:o:24:PRO:HG2	3:o:205:SER:O	2.06	0.55
3:o:244:LEU:HD11	4:p:204:MET:CE	2.36	0.55
4:p:182:VAL:O	4:p:186:VAL:HG23	2.06	0.55
31:G:527:UNK:HA	31:G:544:UNK:O	2.06	0.55
36:L:351:UNK:O	36:L:352:UNK:CB	2.53	0.55
38:N:108:UNK:O	38:N:111:UNK:N	2.39	0.55
38:N:293:UNK:C	38:N:295:UNK:N	2.63	0.55
40:P:82:UNK:O	40:P:86:UNK:N	2.39	0.55
3:b:71:ARG:HE	4:d:196:PRO:HG3	1.72	0.55
3:b:124:MET:HG2	3:b:274:PHE:HE1	1.71	0.55
3:b:192:ILE:HD13	3:b:192:ILE:N	2.21	0.55
3:b:353:LEU:N	3:b:353:LEU:HD23	2.21	0.55
4:d:33:TYR:HA	4:d:37:CYS:HB2	1.89	0.55
5:e:45:VAL:HG13	10:j:28:ALA:N	2.21	0.55
6:f:10:SER:OG	6:f:13:LEU:HD11	2.07	0.55
6:f:39:GLU:HB3	6:f:44:LYS:HE2	1.87	0.55
1:l:386:TYR:N	1:l:386:TYR:CD1	2.74	0.55
1:l:434:TYR:HA	1:l:437:ILE:HD12	1.87	0.55
2:n:318:ASP:OD1	2:n:318:ASP:N	2.39	0.55
3:o:170:VAL:HG13	3:o:174:THR:CG2	2.34	0.55
6:r:106:GLU:OE1	6:r:109:LYS:HE2	2.06	0.55
30:F:322:UNK:CB	30:F:327:UNK:CB	2.85	0.55
30:F:433:UNK:O	30:F:436:UNK:N	2.40	0.55
33:I:80:CYS:N	59:I:202:SF4:S1	2.79	0.55
33:I:150:UNK:CB	33:I:154:UNK:CB	2.83	0.55
36:L:383:UNK:C	36:L:389:UNK:CB	2.84	0.55
38:N:32:UNK:O	38:N:35:UNK:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:160:UNK:N	40:P:161:UNK:C	2.70	0.55
2:m:102:ARG:HH12	2:m:175:SER:HA	1.71	0.55
3:b:133:LEU:HD21	3:b:179:PHE:HA	1.88	0.55
4:d:74:PRO:HG2	4:d:82:MET:HB3	1.89	0.55
4:d:181:GLN:HA	8:h:77:LEU:HD13	1.87	0.55
5:e:15:ARG:NH2	5:e:32:ARG:HG3	2.22	0.55
6:f:101:ARG:HG2	6:f:105:GLU:OE2	2.06	0.55
1:l:106:LEU:HD22	1:l:203:LEU:CD2	2.35	0.55
5:q:140:THR:HG21	5:q:178:LEU:HB2	1.88	0.55
25:A:72:UNK:O	25:A:75:UNK:N	2.40	0.55
29:E:154:UNK:N	29:E:161:UNK:O	2.39	0.55
30:F:52:UNK:O	30:F:55:UNK:CB	2.54	0.55
31:G:215:UNK:CB	33:I:99:UNK:CB	2.85	0.55
37:M:61:UNK:CA	37:M:62:UNK:C	2.85	0.55
37:M:188:UNK:CB	37:M:189:UNK:CB	2.84	0.55
51:Z:245:UNK:O	51:Z:249:UNK:N	2.38	0.55
1:c:173:ASN:O	1:c:177:LEU:HB2	2.07	0.55
1:c:426:GLY:H	1:c:428:ILE:HG12	1.66	0.55
3:b:102:LEU:HB3	3:b:325:PHE:HE1	1.71	0.55
3:b:106:SER:O	3:b:109:PHE:CD1	2.55	0.55
3:b:312:GLN:O	3:b:314:SER:N	2.40	0.55
4:d:178:THR:O	4:d:179:MET:C	2.50	0.55
8:h:21:ARG:HB3	8:h:65:ARG:NH2	2.17	0.55
1:l:111:GLU:HG2	1:l:213:GLN:HE22	1.71	0.55
2:n:261:SER:HG	2:n:320:GLY:HA3	1.70	0.55
2:n:264:ILE:HB	2:n:316:TYR:O	2.06	0.55
3:o:371:THR:O	3:o:372:ILE:C	2.49	0.55
5:q:50:ALA:O	5:q:51:ALA:C	2.49	0.55
5:q:118:ARG:HH22	5:q:173:LYS:CA	2.20	0.55
5:q:142:LEU:HD12	5:q:161:HIS:HE1	1.71	0.55
26:B:118:UNK:C	26:B:120:UNK:N	2.69	0.55
28:D:137:UNK:O	28:D:140:UNK:N	2.39	0.55
30:F:260:UNK:CB	30:F:336:UNK:CB	2.85	0.55
32:H:173:UNK:O	32:H:174:UNK:C	2.54	0.55
36:L:61:UNK:CB	36:L:80:UNK:CB	2.85	0.55
36:L:593:UNK:O	36:L:594:UNK:C	2.52	0.55
37:M:209:UNK:O	37:M:211:UNK:O	2.25	0.55
37:M:227:UNK:CA	37:M:228:UNK:CB	2.85	0.55
38:N:107:UNK:CB	38:N:108:UNK:HA	2.35	0.55
50:U:622:UNK:O	50:U:623:UNK:C	2.54	0.55
1:c:143:THR:HG21	9:i:48:SER:N	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:146:ARG:CZ	1:c:308:GLN:HE22	2.19	0.55
1:c:256:ALA:HA	1:c:320:LEU:O	2.06	0.55
4:d:213:GLY:O	4:d:217:PRO:HG3	2.07	0.55
4:d:229:VAL:O	4:d:233:ARG:HG3	2.05	0.55
1:l:224:ASP:O	1:l:227:ALA:N	2.39	0.55
2:n:168:TYR:HB2	2:n:173:ALA:HB2	1.88	0.55
4:p:138:PRO:O	4:p:139:THR:C	2.50	0.55
5:q:32:ARG:HH12	7:s:22:GLU:CD	2.15	0.55
5:q:136:ILE:O	5:q:136:ILE:CG2	2.55	0.55
15:1:108:PRO:HG2	15:1:111:PHE:CE2	2.42	0.55
20:6:63:MET:HB3	20:6:68:ILE:HD11	1.89	0.55
26:B:65:UNK:C	26:B:68:UNK:CB	2.85	0.55
29:E:96:UNK:N	29:E:138:UNK:CB	2.70	0.55
30:F:209:UNK:CB	30:F:210:UNK:C	2.85	0.55
30:F:351:UNK:O	30:F:352:UNK:C	2.54	0.55
31:G:9:UNK:N	31:G:20:UNK:O	2.40	0.55
33:I:63:UNK:CB	33:I:133:UNK:CB	2.84	0.55
36:L:77:UNK:CA	36:L:78:UNK:CB	2.84	0.55
37:M:94:UNK:O	37:M:97:UNK:N	2.40	0.55
42:R:68:UNK:CB	42:R:86:UNK:CB	2.84	0.55
43:S:64:UNK:HA	43:S:78:UNK:CA	2.37	0.55
51:Z:330:UNK:CB	51:Z:334:UNK:CB	2.85	0.55
3:b:68:HIS:NE2	5:e:67:ASP:HB2	2.22	0.55
10:j:51:LEU:HB3	10:j:52:TRP:CE3	2.42	0.55
1:l:331:ILE:CD1	1:l:427:PRO:O	2.55	0.55
1:l:394:GLU:O	1:l:395:TRP:C	2.47	0.55
2:n:33:LEU:HD23	2:n:33:LEU:O	2.07	0.55
2:n:308:ASP:OD2	9:u:55:LEU:HA	2.06	0.55
3:o:265:PRO:O	3:o:268:ILE:HG13	2.07	0.55
6:r:98:ILE:O	6:r:99:ARG:C	2.48	0.55
31:G:200:UNK:CB	31:G:208:UNK:CB	2.85	0.55
36:L:488:UNK:O	36:L:489:UNK:C	2.50	0.55
1:c:317:THR:HG22	1:c:318:GLY:N	2.21	0.55
2:m:276:GLN:O	2:m:280:GLY:N	2.40	0.55
3:b:135:TRP:CH2	3:b:170:VAL:HG12	2.41	0.55
3:b:240:MET:CA	3:b:243:VAL:HG12	2.28	0.55
1:l:112:LEU:O	1:l:116:ILE:HG13	2.07	0.55
1:l:335:MET:CE	1:l:339:GLN:HG3	2.35	0.55
3:o:109:PHE:O	3:o:110:LEU:C	2.49	0.55
3:o:122:THR:HG22	3:o:189:ILE:CD1	2.27	0.55
3:o:206:ASN:ND2	3:o:207:ASN:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:234:LEU:HD21	4:p:216:LEU:CD2	2.37	0.55
18:4:5:LYS:HD2	18:4:5:LYS:C	2.32	0.55
18:4:5:LYS:HD2	18:4:6:GLY:N	2.21	0.55
29:E:46:UNK:O	29:E:47:UNK:C	2.55	0.55
30:F:31:UNK:N	30:F:35:UNK:CB	2.70	0.55
30:F:209:UNK:HA	30:F:210:UNK:C	2.36	0.55
32:H:42:UNK:C	32:H:44:UNK:HA	2.37	0.55
36:L:65:UNK:CB	36:L:66:UNK:C	2.83	0.55
36:L:242:UNK:O	36:L:245:UNK:N	2.39	0.55
37:M:372:UNK:CB	37:M:375:UNK:CB	2.85	0.55
38:N:70:UNK:O	38:N:71:UNK:C	2.52	0.55
1:c:18:GLN:HG2	1:c:19:LEU:O	2.07	0.55
1:c:386:TYR:N	1:c:386:TYR:CD1	2.72	0.55
2:m:100:SER:HB3	2:m:105:MET:HG3	1.89	0.55
3:b:15:ASN:O	3:b:18:PHE:HD1	1.90	0.55
3:b:25:SER:HA	3:b:218:ILE:HD12	1.89	0.55
3:b:72:ASP:HB3	5:e:67:ASP:H	1.71	0.55
4:d:164:ILE:HD11	53:d:301:HEC:CBB	2.37	0.55
9:i:58:GLN:HG2	9:i:78:TYR:HD2	1.72	0.55
1:l:324:PHE:CD1	1:l:334:MET:HG2	2.42	0.55
3:o:148:ASN:O	3:o:151:SER:OG	2.24	0.55
4:p:42:SER:HB3	4:p:94:PRO:HD2	1.89	0.55
4:p:128:PHE:HB2	4:p:187:CYS:SG	2.46	0.55
7:s:33:GLY:O	7:s:37:VAL:N	2.35	0.55
13:y:111:THR:HG21	19:5:66:ILE:HD11	1.88	0.55
30:F:31:UNK:H	30:F:35:UNK:CB	2.20	0.55
30:F:125:UNK:O	30:F:128:UNK:N	2.40	0.55
31:G:436:UNK:N	31:G:437:UNK:CA	2.62	0.55
32:H:159:UNK:CB	32:H:164:UNK:CB	2.85	0.55
38:N:107:UNK:CB	38:N:108:UNK:CA	2.85	0.55
40:P:138:UNK:CB	40:P:149:UNK:CB	2.85	0.55
40:P:233:UNK:CB	40:P:234:UNK:HA	2.37	0.55
44:T:55:UNK:HA	44:T:60:UNK:O	2.07	0.55
51:Z:250:UNK:O	51:Z:251:UNK:C	2.52	0.55
1:c:61:HIS:CB	1:c:130:GLU:HG3	2.37	0.54
1:c:89:TYR:C	1:c:89:TYR:CD1	2.85	0.54
1:c:93:GLU:O	1:c:94:HIS:ND1	2.40	0.54
4:d:50:HIS:HE1	4:d:91:PHE:HZ	1.53	0.54
1:l:53:ASN:HB3	1:l:170:PRO:HD2	1.89	0.54
1:l:426:GLY:HA3	1:l:428:ILE:H	1.71	0.54
2:n:68:LEU:HD23	2:n:186:VAL:HG11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:159:VAL:HG12	2:n:160:ILE:N	2.21	0.54
3:o:174:THR:O	3:o:178:PHE:HD2	1.90	0.54
4:p:180:SER:HB3	8:t:17:LEU:HB2	1.88	0.54
5:q:102:THR:OG1	5:q:105:GLU:HB2	2.06	0.54
5:q:118:ARG:NH1	5:q:171:ILE:CG1	2.57	0.54
8:t:35:GLU:O	8:t:39:LEU:HG	2.07	0.54
8:t:70:ALA:HA	8:t:73:LEU:HD22	1.89	0.54
12:x:407:ASP:O	12:x:411:LYS:HG3	2.07	0.54
28:D:360:UNK:CB	28:D:381:UNK:CB	2.85	0.54
32:H:92:UNK:C	32:H:94:UNK:CB	2.85	0.54
32:H:183:UNK:O	32:H:184:UNK:C	2.51	0.54
37:M:25:UNK:O	37:M:26:UNK:C	2.55	0.54
37:M:113:UNK:CA	37:M:114:UNK:C	2.85	0.54
37:M:133:UNK:CA	37:M:224:UNK:CB	2.85	0.54
40:P:20:UNK:CB	40:P:89:UNK:CB	2.85	0.54
43:S:48:UNK:CB	43:S:51:UNK:CB	2.85	0.54
1:c:397:SER:O	1:c:400:ALA:HB3	2.07	0.54
2:m:213:HIS:N	2:m:214:PRO:CD	2.66	0.54
1:l:55:ALA:O	1:l:58:PHE:N	2.39	0.54
1:l:64:PHE:CE1	1:l:86:LEU:CG	2.81	0.54
1:l:256:ALA:HB3	1:l:421:ALA:HB3	1.89	0.54
1:l:413:LYS:HB2	1:l:414:TYR:CD2	2.42	0.54
2:n:359:ALA:O	2:n:360:ALA:C	2.50	0.54
2:n:372:VAL:O	2:n:372:VAL:HG12	2.08	0.54
3:o:327:ALA:O	3:o:331:ASP:N	2.35	0.54
3:o:377:LEU:HB3	6:r:33:ARG:HD2	1.88	0.54
4:p:94:PRO:HB2	4:p:95:TYR:CE1	2.42	0.54
28:D:186:UNK:CB	33:I:60:UNK:C	2.85	0.54
30:F:398:UNK:O	30:F:401:UNK:N	2.40	0.54
32:H:101:UNK:O	32:H:104:UNK:N	2.40	0.54
33:I:113:UNK:C	33:I:115:UNK:N	2.65	0.54
36:L:28:UNK:CB	36:L:31:UNK:CB	2.86	0.54
36:L:38:UNK:O	36:L:39:UNK:C	2.55	0.54
40:P:203:UNK:CA	40:P:234:UNK:C	2.85	0.54
40:P:215:UNK:O	40:P:219:UNK:N	2.40	0.54
40:P:301:UNK:CB	40:P:303:UNK:CB	2.86	0.54
51:Z:210:UNK:C	51:Z:212:UNK:N	2.66	0.54
2:m:185:LYS:O	2:m:185:LYS:CG	2.54	0.54
3:b:30:TRP:HA	3:b:33:PHE:HE2	1.73	0.54
4:d:82:MET:HE2	4:d:86:LYS:NZ	2.23	0.54
5:e:20:ASP:O	5:e:21:SER:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:73:LEU:HD23	8:h:73:LEU:C	2.31	0.54
1:l:270:LEU:O	1:l:271:GLN:C	2.47	0.54
3:o:218:ILE:CG2	3:o:223:TYR:HD2	2.19	0.54
3:o:218:ILE:HG21	3:o:223:TYR:CD2	2.43	0.54
4:p:7:PRO:CB	4:p:125:ASP:HB3	2.37	0.54
4:p:216:LEU:N	4:p:217:PRO:HD2	2.22	0.54
5:q:89:PHE:O	5:q:96:LEU:N	2.23	0.54
5:q:188:THR:HG21	5:q:194:ILE:HD11	1.87	0.54
9:u:62:ARG:H	9:u:63:PRO:HD2	1.71	0.54
12:x:69:MET:HE2	12:x:70:VAL:CG2	2.35	0.54
26:B:47:UNK:CB	26:B:85:UNK:CB	2.85	0.54
29:E:60:UNK:CB	29:E:94:UNK:CA	2.85	0.54
30:F:195:UNK:O	30:F:198:UNK:N	2.40	0.54
30:F:397:UNK:O	30:F:401:UNK:N	2.41	0.54
31:G:137:UNK:CB	42:R:75:UNK:O	2.55	0.54
36:L:310:UNK:O	36:L:313:UNK:CB	2.55	0.54
36:L:448:UNK:CB	36:L:451:UNK:CB	2.85	0.54
36:L:531:UNK:O	36:L:532:UNK:C	2.53	0.54
37:M:176:UNK:O	47:X:418:UNK:CB	2.55	0.54
37:M:279:UNK:CB	37:M:280:UNK:CA	2.85	0.54
40:P:140:UNK:N	40:P:141:UNK:HA	2.20	0.54
44:T:43:UNK:CB	44:T:46:UNK:CB	2.86	0.54
2:m:266:SER:O	2:m:269:ALA:HB3	2.07	0.54
2:m:303:VAL:CG1	2:m:304:HIS:N	2.70	0.54
3:b:61:THR:O	3:b:64:SER:N	2.41	0.54
3:b:88:SER:CB	3:b:250:LEU:HD23	2.37	0.54
3:b:137:GLN:HB2	3:b:257:THR:OG1	2.07	0.54
3:b:236:ILE:O	3:b:237:LEU:C	2.48	0.54
7:g:15:THR:O	7:g:15:THR:HG22	2.07	0.54
2:n:88:GLY:O	2:n:91:ALA:HB3	2.07	0.54
52:o:401:HEM:HBC2	52:o:401:HEM:CMC	2.35	0.54
4:p:4:GLU:HG3	4:p:6:HIS:CE1	2.42	0.54
5:q:78:LEU:HD21	5:q:132:TRP:CZ2	2.43	0.54
8:t:66:ASP:O	8:t:67:HIS:C	2.49	0.54
30:F:103:UNK:CB	30:F:104:UNK:CA	2.85	0.54
30:F:301:UNK:CB	30:F:331:UNK:CB	2.85	0.54
31:G:104:UNK:O	31:G:105:CYS:C	2.49	0.54
32:H:40:UNK:CB	32:H:47:UNK:CB	2.86	0.54
32:H:143:UNK:C	32:H:145:UNK:N	2.66	0.54
36:L:197:UNK:CB	36:L:200:UNK:CB	2.85	0.54
38:N:24:UNK:C	38:N:28:UNK:CB	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:137:UNK:CB	40:P:138:UNK:CA	2.84	0.54
2:m:100:SER:CB	2:m:105:MET:HG3	2.37	0.54
2:m:203:ARG:NH2	2:m:230:LEU:HD23	2.22	0.54
3:b:88:SER:HB3	3:b:250:LEU:CD2	2.38	0.54
4:d:74:PRO:O	4:d:79:GLU:N	2.36	0.54
4:d:131:LEU:CD2	4:d:163:PRO:HB3	2.38	0.54
1:l:106:LEU:O	1:l:107:PRO:C	2.51	0.54
1:l:249:PRO:O	1:l:250:LEU:HD23	2.06	0.54
26:B:78:UNK:N	26:B:79:UNK:CA	2.70	0.54
28:D:178:UNK:O	28:D:182:UNK:N	2.41	0.54
28:D:395:UNK:CB	28:D:428:UNK:CB	2.85	0.54
31:G:210:UNK:CB	31:G:213:UNK:CB	2.85	0.54
31:G:464:UNK:O	31:G:467:UNK:CB	2.56	0.54
36:L:176:UNK:O	36:L:179:UNK:CB	2.56	0.54
38:N:24:UNK:CB	38:N:28:UNK:CB	2.86	0.54
38:N:91:UNK:CB	38:N:92:UNK:CB	2.85	0.54
38:N:134:UNK:O	38:N:137:UNK:CB	2.56	0.54
39:O:43:UNK:C	39:O:45:UNK:N	2.65	0.54
39:O:102:UNK:O	39:O:106:UNK:CB	2.55	0.54
1:c:342:TRP:O	1:c:345:LEU:N	2.40	0.54
2:m:62:ASN:ND2	2:m:62:ASN:O	2.41	0.54
2:m:132:PHE:CD2	2:m:191:LEU:HD13	2.43	0.54
2:m:160:ILE:CD1	2:m:325:TYR:HE2	2.21	0.54
2:m:162:ASN:ND2	2:m:244:ILE:CG2	2.61	0.54
3:b:251:GLY:O	3:b:252:ASP:C	2.50	0.54
3:b:310:SER:HB3	3:b:318:ARG:HH12	1.70	0.54
1:l:51:LYS:O	1:l:53:ASN:N	2.38	0.54
1:l:433:ASP:CG	3:o:223:TYR:HH	2.10	0.54
3:o:147:THR:O	3:o:150:LEU:HB2	2.07	0.54
3:o:251:GLY:O	3:o:252:ASP:C	2.51	0.54
4:p:7:PRO:HG3	4:p:126:TYR:CA	2.36	0.54
4:p:168:VAL:O	4:p:169:LEU:HD23	2.08	0.54
28:D:163:UNK:CB	32:H:278:UNK:CA	2.85	0.54
30:F:53:UNK:O	30:F:54:UNK:C	2.55	0.54
30:F:100:UNK:C	30:F:102:UNK:N	2.57	0.54
30:F:242:UNK:O	30:F:252:UNK:HA	2.07	0.54
31:G:375:UNK:CB	31:G:376:UNK:CA	2.85	0.54
31:G:456:UNK:CB	31:G:457:UNK:HA	2.37	0.54
36:L:188:UNK:CB	36:L:211:UNK:CB	2.84	0.54
36:L:376:UNK:C	36:L:378:UNK:N	2.68	0.54
38:N:25:UNK:C	38:N:27:UNK:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:253:UNK:CB	38:N:259:UNK:CB	2.85	0.54
41:Q:50:UNK:CB	41:Q:51:UNK:C	2.85	0.54
1:c:255:ILE:HG13	1:c:422:VAL:CG2	2.37	0.54
2:m:262:ALA:HB2	2:m:272:PHE:HE2	1.72	0.54
3:b:58:ASP:OD2	3:o:56:THR:HG21	2.08	0.54
2:n:408:ALA:O	2:n:411:ILE:N	2.40	0.54
3:o:207:ASN:ND2	3:o:209:THR:OG1	2.41	0.54
5:q:150:ALA:HB3	5:q:157:TYR:CB	2.36	0.54
8:t:15:ASP:HB2	8:t:16:PRO:CD	2.37	0.54
27:C:34:UNK:CB	27:C:38:UNK:CB	2.85	0.54
36:L:111:UNK:CB	36:L:114:UNK:CB	2.85	0.54
37:M:293:UNK:O	37:M:294:UNK:C	2.52	0.54
39:O:32:UNK:C	39:O:34:UNK:N	2.67	0.54
50:U:122:UNK:O	50:U:125:UNK:CB	2.55	0.54
1:c:61:HIS:CD2	2:m:287:ARG:HD3	2.43	0.54
1:c:111:GLU:HG2	1:c:213:GLN:HE22	1.73	0.54
1:c:241:ILE:O	1:c:241:ILE:HG23	2.07	0.54
2:m:396:SER:O	2:m:399:LEU:HB2	2.08	0.54
6:f:28:LYS:HD2	6:f:74:ILE:HD11	1.88	0.54
6:f:40:ASN:CG	6:f:41:ASP:H	2.16	0.54
1:l:191:LYS:NZ	1:l:220:SER:OG	2.41	0.54
3:o:76:GLY:HA2	3:o:79:ILE:HD12	1.90	0.54
10:v:18:SER:HB3	11:w:23:LEU:HB2	1.90	0.54
36:L:55:UNK:CB	36:L:56:UNK:CB	2.86	0.54
50:U:416:UNK:C	50:U:418:UNK:N	2.67	0.54
50:U:601:UNK:O	50:U:602:UNK:C	2.56	0.54
51:Z:343:UNK:CB	51:Z:346:UNK:CB	2.85	0.54
1:c:39:VAL:CG2	1:c:197:LEU:HD22	2.37	0.54
1:c:53:ASN:C	1:c:53:ASN:HD22	2.16	0.54
5:e:29:SER:CA	5:e:32:ARG:HD3	2.37	0.54
6:f:7:SER:HA	6:f:11:ARG:HE	1.73	0.54
1:l:22:GLY:O	1:l:24:ARG:HG2	2.08	0.54
1:l:405:ARG:NH1	21:7:4:ARG:HD2	2.21	0.54
3:o:106:SER:O	3:o:109:PHE:CD2	2.54	0.54
3:o:170:VAL:HG12	3:o:170:VAL:O	2.08	0.54
5:q:139:CYS:O	5:q:143:GLY:HA2	2.08	0.54
30:F:294:UNK:CB	30:F:295:UNK:CA	2.85	0.54
37:M:343:UNK:C	37:M:345:UNK:N	2.70	0.54
38:N:135:UNK:O	38:N:138:UNK:N	2.41	0.54
39:O:103:UNK:O	39:O:107:UNK:CB	2.56	0.54
41:Q:113:UNK:O	41:Q:114:UNK:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Y:98:UNK:O	48:Y:101:UNK:N	2.41	0.54
1:c:112:LEU:O	1:c:116:ILE:HD12	2.07	0.54
1:c:397:SER:OG	1:c:398:ARG:N	2.41	0.54
1:c:418:GLN:O	1:c:420:PRO:HD3	2.08	0.54
3:b:88:SER:HA	3:b:272:TRP:HZ2	1.73	0.54
3:b:218:ILE:HG22	3:b:223:TYR:HD2	1.72	0.54
8:h:73:LEU:HG	8:h:73:LEU:O	2.08	0.54
1:l:88:ALA:O	2:n:286:LYS:HE2	2.08	0.54
1:l:223:TYR:CZ	51:Z:259:UNK:CB	2.91	0.54
1:l:336:PHE:HE2	1:l:446:PHE:HD2	1.55	0.54
2:n:255:ALA:HB2	2:n:426:ALA:CB	2.37	0.54
3:o:119:LEU:HD13	3:o:192:ILE:CG2	2.37	0.54
3:o:245:PHE:CG	4:p:17:LEU:HD13	2.43	0.54
4:p:11:PRO:HB2	8:t:74:PHE:CG	2.43	0.54
4:p:51:LEU:HD22	4:p:58:GLU:HA	1.90	0.54
4:p:149:PHE:HZ	8:t:55:THR:HG23	1.71	0.54
4:p:160:MET:HE3	4:p:163:PRO:HG3	1.90	0.54
9:u:58:GLN:HG2	9:u:78:TYR:HD2	1.72	0.54
13:y:165:VAL:HB	13:y:170:LEU:HD12	1.90	0.54
26:B:78:UNK:CB	26:B:79:UNK:C	2.86	0.54
28:D:96:UNK:O	28:D:99:UNK:CB	2.55	0.54
32:H:93:UNK:CA	32:H:94:UNK:CB	2.86	0.54
34:J:86:UNK:O	34:J:89:UNK:N	2.41	0.54
36:L:587:UNK:O	36:L:591:UNK:N	2.41	0.54
40:P:94:UNK:O	40:P:95:UNK:CB	2.54	0.54
43:S:36:UNK:CB	43:S:84:UNK:CB	2.85	0.54
1:c:109:ALA:O	1:c:112:LEU:N	2.40	0.53
3:b:183:PHE:CE1	3:b:187:PHE:CE2	2.96	0.53
6:f:55:TYR:C	6:f:55:TYR:CD1	2.86	0.53
10:j:32:GLU:HG2	10:j:33:ARG:N	2.22	0.53
1:l:61:HIS:CB	1:l:130:GLU:HG3	2.38	0.53
1:l:143:THR:HG21	9:u:48:SER:N	2.08	0.53
2:n:132:PHE:HD2	2:n:191:LEU:HD13	1.67	0.53
4:p:69:GLU:HG3	4:p:84:PRO:HA	1.89	0.53
4:p:219:VAL:HA	4:p:222:MET:HG3	1.89	0.53
8:t:68:CYS:O	8:t:69:VAL:C	2.51	0.53
17:3:82:CYS:N	17:3:86:GLY:O	2.40	0.53
27:C:73:UNK:O	28:D:252:UNK:HA	2.07	0.53
31:G:285:UNK:CB	31:G:288:UNK:CB	2.86	0.53
34:J:13:UNK:CB	34:J:39:UNK:CB	2.87	0.53
36:L:127:UNK:O	36:L:131:UNK:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:M:241:UNK:O	37:M:243:UNK:N	2.40	0.53
38:N:66:UNK:O	38:N:67:UNK:C	2.55	0.53
38:N:72:UNK:O	38:N:76:UNK:N	2.41	0.53
38:N:292:UNK:O	38:N:295:UNK:CB	2.55	0.53
43:S:83:UNK:O	43:S:86:UNK:N	2.41	0.53
1:c:106:LEU:HD21	1:c:203:LEU:HD13	1.89	0.53
1:c:134:ILE:HD13	1:c:134:ILE:N	2.23	0.53
3:b:141:TRP:HB3	3:b:268:ILE:HD13	1.90	0.53
10:j:52:TRP:CE3	10:j:52:TRP:N	2.76	0.53
2:n:111:CYS:CB	2:n:119:LEU:HD22	2.31	0.53
2:n:168:TYR:HD2	2:n:238:LYS:O	1.92	0.53
2:n:262:ALA:HB2	2:n:268:GLU:HB3	1.90	0.53
2:n:280:GLY:HA2	2:n:311:ALA:CB	2.38	0.53
3:o:7:SER:O	3:o:8:HIS:O	2.26	0.53
3:o:174:THR:O	3:o:178:PHE:CD2	2.61	0.53
4:p:3:LEU:HD21	7:s:71:ARG:HA	1.90	0.53
5:q:12:ASP:O	7:s:24:ARG:NH2	2.32	0.53
6:r:7:SER:HA	6:r:11:ARG:HE	1.73	0.53
12:x:398:PRO:O	12:x:498:CYS:HB3	2.08	0.53
13:y:136:LEU:HB3	13:y:193:TYR:HD2	1.73	0.53
14:z:151:LEU:HB2	14:z:159:MET:HG3	1.89	0.53
27:C:21:UNK:O	27:C:24:UNK:CA	2.56	0.53
30:F:183:UNK:CB	30:F:186:UNK:CB	2.86	0.53
31:G:108:CYS:SG	31:G:110:UNK:CB	2.96	0.53
31:G:570:UNK:HA	31:G:583:UNK:O	2.07	0.53
36:L:210:UNK:O	36:L:213:UNK:N	2.41	0.53
37:M:364:UNK:O	37:M:367:UNK:N	2.42	0.53
39:O:188:UNK:CB	39:O:191:UNK:CB	2.85	0.53
1:c:49:SER:N	1:c:52:ASN:OD1	2.35	0.53
2:m:69:LEU:HD21	2:m:199:PHE:CZ	2.44	0.53
2:m:161:GLU:OE1	2:m:175:SER:HB2	2.07	0.53
2:m:304:HIS:CG	2:m:305:GLN:N	2.76	0.53
3:b:1:MET:SD	3:b:4:ILE:HB	2.48	0.53
3:b:219:PRO:CB	3:b:222:PRO:HD2	2.39	0.53
4:d:4:GLU:HG3	4:d:6:HIS:CE1	2.43	0.53
1:l:317:THR:HG22	1:l:318:GLY:H	1.73	0.53
3:o:37:LEU:HD11	3:o:97:HIS:CG	2.43	0.53
3:o:219:PRO:HB2	3:o:222:PRO:HD2	1.89	0.53
4:p:138:PRO:HB3	8:t:55:THR:HA	1.90	0.53
5:q:171:ILE:HD12	5:q:176:ALA:HB3	1.90	0.53
8:t:73:LEU:HD21	8:t:74:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:z:222:GLN:HA	14:z:222:GLN:HE21	1.72	0.53
16:2:41:LEU:O	16:2:41:LEU:HD12	2.08	0.53
29:E:96:UNK:O	29:E:98:UNK:C	2.56	0.53
30:F:300:UNK:CB	30:F:329:UNK:CA	2.84	0.53
31:G:10:UNK:C	31:G:76:UNK:HA	2.28	0.53
33:I:135:UNK:O	33:I:136:UNK:C	2.56	0.53
36:L:117:UNK:O	36:L:118:UNK:C	2.53	0.53
37:M:364:UNK:O	37:M:367:UNK:CB	2.56	0.53
47:X:302:UNK:O	47:X:305:UNK:CB	2.57	0.53
50:U:411:UNK:C	50:U:413:UNK:N	2.69	0.53
1:c:32:GLN:CG	1:c:33:PRO:CD	2.86	0.53
1:c:236:PHE:CD2	1:c:258:GLU:CB	2.91	0.53
4:d:138:PRO:HG2	8:h:55:THR:CB	2.38	0.53
6:f:35:ASP:OD2	6:f:61:ARG:HD2	2.07	0.53
6:f:51:PRO:CD	2:n:134:ARG:NH1	2.68	0.53
7:g:25:ALA:O	7:g:27:PRO:HD3	2.08	0.53
8:h:65:ARG:HG3	8:h:66:ASP:N	2.23	0.53
8:h:73:LEU:CD2	8:h:74:PHE:HD1	2.21	0.53
1:l:236:PHE:CD2	1:l:258:GLU:CB	2.91	0.53
1:l:241:ILE:HG13	7:s:16:TYR:CE2	2.43	0.53
2:n:217:LYS:O	2:n:218:GLN:C	2.51	0.53
3:o:133:LEU:HB2	3:o:134:PRO:HD3	1.89	0.53
53:p:301:HEC:HBC2	53:p:301:HEC:CHD	2.26	0.53
5:q:34:GLY:CA	10:v:10:TYR:HD1	2.22	0.53
5:q:45:VAL:CG2	10:v:24:ILE:HA	2.39	0.53
15:1:67:SER:OG	15:1:70:GLU:HG3	2.08	0.53
36:L:31:UNK:O	36:L:35:UNK:N	2.41	0.53
47:X:334:UNK:C	47:X:336:UNK:N	2.68	0.53
50:U:317:UNK:O	50:U:321:UNK:N	2.42	0.53
1:c:33:PRO:O	1:c:103:SER:N	2.36	0.53
1:c:143:THR:O	1:c:143:THR:CG2	2.56	0.53
2:m:79:GLY:H	2:m:125:ASN:ND2	2.07	0.53
2:m:90:GLU:O	2:m:92:VAL:N	2.41	0.53
3:b:148:ASN:O	3:b:151:SER:OG	2.26	0.53
4:d:211:MET:HA	4:d:211:MET:HE3	1.89	0.53
7:g:64:GLN:O	7:g:65:GLU:C	2.50	0.53
1:l:25:VAL:HG21	1:l:209:LEU:CD1	2.39	0.53
3:o:108:THR:CB	3:o:313:ARG:HH11	2.12	0.53
3:o:210:GLY:CA	3:o:314:SER:HB2	2.31	0.53
6:r:91:GLU:N	6:r:92:PRO:HD2	2.22	0.53
15:1:128:VAL:O	15:1:134:PHE:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:51:SER:HB2	17:3:91:LEU:HD11	1.90	0.53
26:B:77:UNK:N	26:B:78:UNK:HA	2.23	0.53
27:C:113:UNK:C	27:C:115:UNK:N	2.66	0.53
30:F:426:UNK:C	30:F:429:UNK:N	2.72	0.53
31:G:235:UNK:O	31:G:236:UNK:CB	2.56	0.53
32:H:307:UNK:O	32:H:310:UNK:CB	2.56	0.53
33:I:63:UNK:CB	33:I:134:UNK:N	2.71	0.53
36:L:181:UNK:C	36:L:183:UNK:N	2.71	0.53
36:L:201:UNK:O	36:L:202:UNK:C	2.54	0.53
45:V:8:UNK:O	45:V:12:UNK:N	2.42	0.53
49:a:27:UNK:O	49:a:28:UNK:C	2.55	0.53
1:c:85:HIS:HA	2:m:284:HIS:O	2.09	0.53
1:c:279:HIS:ND1	1:c:284:TYR:OH	2.42	0.53
3:b:183:PHE:CD1	3:o:183:PHE:CD1	2.97	0.53
4:d:64:LEU:O	4:d:68:VAL:HG23	2.09	0.53
4:d:190:LEU:O	4:d:191:ARG:C	2.52	0.53
5:e:52:LYS:NZ	10:j:32:GLU:OE1	2.40	0.53
1:l:33:PRO:O	1:l:103:SER:N	2.34	0.53
1:l:152:TYR:O	1:l:153:LEU:C	2.47	0.53
2:n:95:LYS:HE3	2:n:97:SER:OG	2.08	0.53
3:o:6:LYS:HE2	3:o:16:ASN:HD21	1.74	0.53
4:p:79:GLU:O	4:p:80:MET:C	2.52	0.53
4:p:237:TYR:HD1	7:s:13:VAL:HG22	1.73	0.53
15:1:23:PRO:HD2	16:2:34:ASN:HD22	1.74	0.53
15:1:52:SER:OG	15:1:55:GLU:HG3	2.09	0.53
17:3:48:LEU:O	17:3:50:PRO:HD3	2.08	0.53
30:F:140:UNK:CB	30:F:182:UNK:CA	2.86	0.53
31:G:114:CYS:SG	31:G:117:UNK:CB	2.97	0.53
31:G:329:UNK:O	31:G:333:UNK:N	2.42	0.53
31:G:440:UNK:O	31:G:444:UNK:N	2.41	0.53
36:L:55:UNK:N	36:L:56:UNK:C	2.71	0.53
39:O:102:UNK:O	39:O:106:UNK:N	2.41	0.53
40:P:203:UNK:N	40:P:234:UNK:O	2.41	0.53
47:X:187:UNK:O	47:X:190:UNK:CB	2.56	0.53
50:U:211:UNK:O	50:U:214:UNK:N	2.41	0.53
1:c:394:GLU:O	1:c:397:SER:OG	2.26	0.53
3:b:309:THR:CG2	3:b:370:GLY:HA3	2.38	0.53
5:e:15:ARG:HH21	5:e:32:ARG:HG3	1.74	0.53
6:f:45:GLU:O	6:f:49:ARG:HG3	2.08	0.53
1:l:204:GLU:HG2	1:l:206:ARG:HB3	1.90	0.53
12:x:268:PHE:CZ	13:y:58:ALA:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:z:156:ARG:HG3	14:z:156:ARG:NH1	2.22	0.53
18:4:8:HIS:O	18:4:10:GLY:N	2.42	0.53
28:D:383:UNK:N	28:D:384:UNK:CA	2.72	0.53
30:F:60:UNK:O	30:F:63:UNK:N	2.41	0.53
37:M:391:UNK:O	37:M:392:UNK:CB	2.56	0.53
40:P:49:UNK:N	40:P:73:UNK:CB	2.71	0.53
2:m:89:ILE:O	2:m:90:GLU:C	2.47	0.53
2:m:279:LEU:HD22	2:m:344:VAL:HG22	1.91	0.53
3:b:80:ARG:O	3:b:80:ARG:HD3	2.09	0.53
1:l:241:ILE:CD1	7:s:16:TYR:CE2	2.92	0.53
4:p:69:GLU:O	4:p:73:GLY:HA3	2.09	0.53
29:E:154:UNK:O	29:E:161:UNK:N	2.42	0.53
30:F:94:UNK:CB	30:F:135:UNK:O	2.57	0.53
30:F:433:UNK:O	30:F:434:UNK:C	2.55	0.53
40:P:95:UNK:O	40:P:96:UNK:CB	2.57	0.53
40:P:203:UNK:HA	40:P:234:UNK:C	2.39	0.53
51:Z:337:UNK:HA	51:Z:342:UNK:CB	2.39	0.53
4:d:79:GLU:HB3	4:d:82:MET:HB2	1.91	0.53
5:e:12:ASP:O	7:g:24:ARG:NH2	2.35	0.53
5:e:31:ALA:O	5:e:34:GLY:N	2.42	0.53
5:e:63:SER:O	5:e:64:ALA:HB2	2.08	0.53
1:l:338:LEU:O	1:l:341:GLN:N	2.38	0.53
1:l:417:ASP:CG	10:v:10:TYR:OH	2.51	0.53
2:n:164:HIS:O	2:n:173:ALA:HA	2.09	0.53
2:n:277:HIS:CD2	2:n:364:LEU:HD13	2.43	0.53
2:n:285:VAL:HG12	2:n:288:GLY:HA3	1.91	0.53
2:n:294:SER:O	2:n:295:LEU:C	2.51	0.53
3:o:200:LEU:HD13	52:o:402:HEM:HAD2	1.90	0.53
7:s:27:PRO:O	7:s:28:HIS:C	2.48	0.53
13:y:203:ASN:HD22	13:y:206:PHE:HD2	1.55	0.53
26:B:95:UNK:O	26:B:96:UNK:C	2.57	0.53
28:D:163:UNK:N	32:H:278:UNK:CB	2.72	0.53
29:E:109:UNK:O	29:E:112:UNK:N	2.42	0.53
30:F:209:UNK:CB	30:F:211:UNK:HA	2.39	0.53
31:G:31:UNK:O	31:G:34:UNK:N	2.42	0.53
37:M:3:UNK:H	37:M:6:UNK:CB	2.22	0.53
40:P:143:UNK:O	40:P:145:UNK:N	2.42	0.53
40:P:216:UNK:O	40:P:220:UNK:N	2.42	0.53
44:T:70:UNK:HA	44:T:75:UNK:CB	2.39	0.53
46:W:56:UNK:O	46:W:59:UNK:CB	2.56	0.53
48:Y:59:UNK:O	48:Y:60:UNK:C	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:381:ARG:HA	1:c:384:LEU:HD12	1.91	0.53
1:c:426:GLY:H	1:c:428:ILE:CD1	2.22	0.53
2:m:191:LEU:O	2:m:195:VAL:HG23	2.09	0.53
2:m:300:ALA:HA	2:m:307:PHE:HZ	1.74	0.53
2:m:308:ASP:OD2	9:i:55:LEU:HA	2.09	0.53
2:m:316:TYR:OH	9:i:64:LEU:HD23	2.09	0.53
3:b:103:TYR:O	3:b:315:MET:CB	2.57	0.53
3:b:277:ALA:O	3:b:278:TYR:C	2.52	0.53
3:b:301:LEU:HA	3:b:304:ILE:HD12	1.91	0.53
3:b:348:ILE:O	3:b:352:GLN:HG3	2.08	0.53
6:f:16:ILE:O	6:f:17:ARG:C	2.50	0.53
8:h:66:ASP:O	8:h:67:HIS:C	2.50	0.53
1:l:32:GLN:CG	1:l:33:PRO:CD	2.86	0.53
2:n:25:GLU:O	2:n:213:HIS:CE1	2.62	0.53
6:r:49:ARG:NH2	6:r:100:GLU:OE2	2.37	0.53
10:v:49:GLY:HA2	10:v:54:HIS:CB	2.39	0.53
12:x:11:ASN:ND2	12:x:14:ASP:H	2.07	0.53
12:x:302:ARG:O	12:x:306:THR:HG23	2.09	0.53
13:y:33:LEU:HD23	20:6:28:SER:HB2	1.91	0.53
17:3:55:LYS:HA	17:3:74:LEU:O	2.08	0.53
27:C:133:UNK:CA	27:C:136:UNK:CB	2.82	0.53
28:D:95:UNK:N	28:D:98:UNK:CB	2.72	0.53
28:D:360:UNK:CA	28:D:381:UNK:HA	2.39	0.53
47:X:414:UNK:O	47:X:418:UNK:N	2.41	0.53
51:Z:101:UNK:N	51:Z:104:UNK:CB	2.72	0.53
1:c:11:VAL:CG1	1:c:12:PRO:HD2	2.39	0.52
1:c:239:SER:OG	1:c:240:GLN:N	2.39	0.52
1:c:433:ASP:CG	3:b:223:TYR:HH	2.15	0.52
2:m:340:ALA:O	2:m:344:VAL:HG23	2.08	0.52
2:m:435:PHE:CE1	2:n:169:ARG:HG2	2.44	0.52
4:d:48:TYR:OH	4:d:68:VAL:HG11	2.09	0.52
4:d:82:MET:CE	4:d:86:LYS:HZ2	2.22	0.52
6:f:96:GLU:OE1	6:f:96:GLU:HA	2.09	0.52
1:l:92:ARG:HD2	1:l:163:LEU:CD1	2.37	0.52
1:l:244:ARG:CZ	7:s:10:VAL:HB	2.38	0.52
2:n:262:ALA:HB3	2:n:269:ALA:HA	1.91	0.52
3:o:218:ILE:HG23	3:o:223:TYR:CD2	2.43	0.52
4:p:27:ARG:NH1	10:v:58:LYS:CE	2.72	0.52
4:p:237:TYR:CE2	4:p:239:PRO:HD3	2.44	0.52
5:q:81:ILE:H	5:q:81:ILE:HD12	1.75	0.52
8:t:21:ARG:CB	8:t:65:ARG:HH21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:v:4:THR:HG22	10:v:6:THR:OG1	2.09	0.52
10:v:36:ASP:O	10:v:37:GLN:C	2.52	0.52
18:4:42:ARG:HH11	18:4:42:ARG:HG3	1.74	0.52
27:C:88:UNK:HA	27:C:112:UNK:HA	1.91	0.52
31:G:110:UNK:O	31:G:113:UNK:O	2.26	0.52
33:I:110:UNK:HA	33:I:150:UNK:O	2.10	0.52
34:J:21:UNK:O	34:J:22:UNK:C	2.55	0.52
34:J:59:UNK:HA	34:J:63:UNK:CB	2.39	0.52
36:L:67:UNK:CB	36:L:75:UNK:O	2.57	0.52
37:M:114:UNK:N	37:M:177:UNK:CB	2.72	0.52
37:M:325:UNK:O	37:M:329:UNK:N	2.41	0.52
38:N:26:UNK:CA	38:N:27:UNK:CB	2.87	0.52
43:S:34:UNK:O	43:S:38:UNK:N	2.42	0.52
46:W:49:UNK:CA	46:W:52:UNK:CB	2.81	0.52
1:c:260:PRO:HD3	1:c:414:TYR:CD1	2.44	0.52
2:m:92:VAL:O	2:m:92:VAL:HG12	2.08	0.52
3:b:92:ILE:O	3:b:96:MET:HG2	2.09	0.52
6:f:25:GLY:O	6:f:28:LYS:HG3	2.09	0.52
10:j:45:HIS:O	10:j:48:GLU:HG2	2.08	0.52
1:l:134:ILE:HD13	1:l:137:GLU:HG3	1.91	0.52
1:l:277:ILE:CG2	1:l:294:LEU:HD12	2.39	0.52
2:n:51:ILE:CG2	2:n:199:PHE:HA	2.33	0.52
2:n:258:VAL:HG12	2:n:321:LEU:HD22	1.89	0.52
2:n:395:PRO:O	2:n:396:SER:C	2.53	0.52
2:n:435:PHE:H	2:n:438:GLU:HB2	1.75	0.52
3:o:304:ILE:N	3:o:305:PRO:CD	2.73	0.52
4:p:55:CYS:SG	10:v:52:TRP:CB	2.97	0.52
4:p:195:GLU:HG3	4:p:198:HIS:HB2	1.92	0.52
4:p:237:TYR:CE2	4:p:239:PRO:HG3	2.44	0.52
30:F:262:UNK:CB	30:F:285:UNK:C	2.87	0.52
33:I:151:UNK:C	33:I:153:UNK:N	2.68	0.52
36:L:207:UNK:CB	36:L:209:UNK:N	2.72	0.52
37:M:362:UNK:O	37:M:365:UNK:N	2.42	0.52
38:N:293:UNK:O	38:N:295:UNK:N	2.41	0.52
40:P:140:UNK:N	40:P:141:UNK:CA	2.72	0.52
51:Z:244:UNK:O	51:Z:245:UNK:C	2.55	0.52
1:c:91:THR:HG23	1:c:92:ARG:H	1.74	0.52
1:c:252:HIS:CD2	1:c:325:VAL:CG2	2.92	0.52
1:c:436:ARG:HE	3:b:222:PRO:HG3	1.73	0.52
2:m:160:ILE:HD11	2:m:325:TYR:HE2	1.74	0.52
2:m:429:ASN:ND2	2:n:60:SER:CB	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:143:LEU:HD22	4:d:147:LEU:O	2.09	0.52
10:j:35:PHE:O	10:j:36:ASP:C	2.50	0.52
10:j:56:LYS:HE2	10:j:60:GLU:OE1	2.09	0.52
3:o:71:ARG:NH2	4:p:193:ALA:O	2.42	0.52
4:p:106:ASN:C	4:p:106:ASN:HD22	2.17	0.52
5:q:85:LYS:CG	5:q:86:ASN:H	2.12	0.52
5:q:102:THR:H	5:q:105:GLU:HB2	1.74	0.52
6:r:51:PRO:HG2	6:r:54:LEU:HB2	1.89	0.52
9:u:53:GLU:O	9:u:54:SER:C	2.51	0.52
13:y:104:TRP:CG	13:y:203:ASN:HB2	2.44	0.52
31:G:282:UNK:O	31:G:293:UNK:HA	2.09	0.52
32:H:101:UNK:N	32:H:161:UNK:CB	2.72	0.52
36:L:383:UNK:N	36:L:389:UNK:CB	2.72	0.52
37:M:378:UNK:C	37:M:380:UNK:N	2.72	0.52
38:N:91:UNK:N	38:N:92:UNK:CB	2.73	0.52
1:c:34:THR:HB	2:m:373:GLU:OE1	2.09	0.52
1:c:53:ASN:CG	1:c:165:GLN:HB2	2.34	0.52
1:c:334:MET:HA	1:c:334:MET:CE	2.37	0.52
2:m:140:LEU:HD12	2:m:143:GLN:CB	2.38	0.52
2:m:280:GLY:HA2	2:m:311:ALA:CB	2.40	0.52
2:m:350:GLY:HA2	2:m:411:ILE:HG21	1.92	0.52
3:b:90:PHE:CE1	3:b:123:VAL:HG21	2.44	0.52
3:b:184:ILE:O	3:b:188:ILE:HD12	2.10	0.52
4:d:68:VAL:HG12	4:d:92:PRO:HG2	1.91	0.52
1:l:111:GLU:HG2	1:l:213:GLN:NE2	2.25	0.52
1:l:334:MET:O	1:l:335:MET:C	2.48	0.52
1:l:445:ARG:O	1:l:446:PHE:CB	2.55	0.52
3:o:200:LEU:CD1	52:o:402:HEM:HAD2	2.40	0.52
6:r:75:LEU:C	6:r:80:TRP:HE1	2.17	0.52
6:r:95:LYS:O	6:r:96:GLU:C	2.53	0.52
10:v:52:TRP:O	10:v:53:LYS:C	2.53	0.52
15:1:40:LEU:HD13	15:1:59:LEU:HD13	1.90	0.52
25:A:90:UNK:O	25:A:93:UNK:CB	2.58	0.52
28:D:163:UNK:N	32:H:278:UNK:CA	2.72	0.52
28:D:258:UNK:N	28:D:261:UNK:CB	2.72	0.52
30:F:290:UNK:O	30:F:291:UNK:CB	2.57	0.52
30:F:421:UNK:N	30:F:424:UNK:CB	2.73	0.52
37:M:190:UNK:N	37:M:191:UNK:C	2.73	0.52
37:M:309:UNK:O	37:M:312:UNK:N	2.43	0.52
47:X:503:UNK:O	47:X:504:UNK:C	2.56	0.52
47:X:721:UNK:O	47:X:725:UNK:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:111:UNK:O	51:Z:114:UNK:CB	2.57	0.52
1:c:134:ILE:HA	1:c:137:GLU:HG3	1.91	0.52
2:m:135:TRP:CD1	2:m:136:GLU:HG3	2.44	0.52
3:b:85:ASN:O	3:b:86:GLY:C	2.50	0.52
4:d:233:ARG:HG3	7:g:17:SER:CB	2.40	0.52
1:l:29:GLN:HG3	1:l:203:LEU:O	2.09	0.52
1:l:53:ASN:HB3	1:l:170:PRO:CD	2.39	0.52
1:l:277:ILE:HB	1:l:309:THR:HG21	1.91	0.52
1:l:426:GLY:HA2	1:l:428:ILE:CG1	2.37	0.52
2:n:24:LEU:HD12	2:n:24:LEU:N	2.22	0.52
2:n:304:HIS:CD2	2:n:305:GLN:N	2.78	0.52
3:o:196:HIS:CE1	52:o:402:HEM:C1D	2.97	0.52
5:q:95:PRO:HG2	5:q:145:VAL:CG2	2.38	0.52
5:q:119:ASP:OD1	5:q:120:PRO:HD2	2.09	0.52
30:F:300:UNK:CB	30:F:330:UNK:N	2.73	0.52
34:J:147:UNK:C	34:J:149:UNK:N	2.71	0.52
36:L:69:UNK:CB	36:L:74:UNK:HA	2.39	0.52
36:L:161:UNK:CB	36:L:162:UNK:HA	2.40	0.52
36:L:241:UNK:O	36:L:244:UNK:CB	2.57	0.52
36:L:279:UNK:O	36:L:282:UNK:N	2.43	0.52
39:O:141:UNK:O	39:O:142:UNK:CB	2.58	0.52
40:P:223:UNK:N	40:P:224:UNK:CB	2.73	0.52
2:m:122:PHE:O	2:m:123:LEU:C	2.53	0.52
2:m:141:GLN:OE1	2:m:183:ILE:O	2.27	0.52
3:b:103:TYR:O	3:b:315:MET:HB2	2.10	0.52
4:d:10:TYR:CZ	4:d:128:PHE:CE2	2.92	0.52
9:i:58:GLN:HB3	9:i:78:TYR:HB2	1.91	0.52
1:l:262:TRP:CE3	1:l:385:THR:CG2	2.93	0.52
3:o:275:LEU:O	3:o:278:TYR:N	2.42	0.52
5:q:42:THR:O	5:q:43:THR:C	2.53	0.52
30:F:276:UNK:O	30:F:280:UNK:N	2.43	0.52
33:I:21:UNK:O	33:I:24:UNK:CB	2.58	0.52
33:I:21:UNK:HA	33:I:24:UNK:CB	2.40	0.52
36:L:82:UNK:N	36:L:86:UNK:CB	2.73	0.52
37:M:393:UNK:O	37:M:394:UNK:C	2.57	0.52
38:N:26:UNK:N	38:N:27:UNK:C	2.73	0.52
38:N:276:UNK:O	38:N:277:UNK:C	2.57	0.52
1:c:41:ILE:HD12	1:c:41:ILE:N	2.24	0.52
1:c:55:ALA:O	1:c:58:PHE:N	2.35	0.52
1:c:329:MET:HA	1:c:430:GLN:OE1	2.10	0.52
2:m:25:GLU:O	2:m:213:HIS:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:286:LYS:O	2:m:287:ARG:HB2	2.09	0.52
3:b:119:LEU:HD23	52:b:402:HEM:C4B	2.45	0.52
3:b:282:ARG:O	3:b:284:ILE:N	2.43	0.52
4:d:46:VAL:HG12	4:d:47:ALA:O	2.10	0.52
5:e:47:VAL:O	5:e:50:ALA:HB3	2.10	0.52
1:l:292:SER:O	1:l:295:ALA:HB3	2.09	0.52
6:r:73:GLN:HE21	7:s:32:LYS:HE3	1.74	0.52
8:t:58:LEU:O	8:t:58:LEU:HD12	2.10	0.52
31:G:227:UNK:O	31:G:238:UNK:CA	2.58	0.52
31:G:282:UNK:N	31:G:293:UNK:CB	2.73	0.52
37:M:115:UNK:N	37:M:175:UNK:CB	2.73	0.52
38:N:26:UNK:N	38:N:27:UNK:CB	2.73	0.52
40:P:114:UNK:O	40:P:118:UNK:N	2.43	0.52
40:P:134:UNK:O	40:P:167:UNK:CA	2.57	0.52
1:c:53:ASN:HB3	1:c:170:PRO:HD2	1.91	0.52
1:c:279:HIS:CE1	1:c:284:TYR:OH	2.63	0.52
2:m:79:GLY:HA3	2:m:125:ASN:HD21	1.75	0.52
2:m:257:LEU:HD13	2:m:424:MET:HE2	1.91	0.52
2:m:268:GLU:O	2:m:271:ALA:HB3	2.10	0.52
3:b:135:TRP:CH2	3:b:170:VAL:O	2.62	0.52
3:b:300:ILE:HD13	3:b:362:ILE:HG21	1.92	0.52
3:b:350:ILE:O	3:b:351:GLY:C	2.53	0.52
5:e:2:HIS:O	5:e:5:ILE:HG12	2.09	0.52
1:l:19:LEU:HD13	1:l:214:LYS:HG2	1.92	0.52
1:l:25:VAL:HG21	1:l:209:LEU:HD13	1.91	0.52
1:l:106:LEU:HB3	1:l:107:PRO:HD3	1.91	0.52
1:l:408:ARG:O	1:l:412:SER:OG	2.28	0.52
2:n:279:LEU:CD2	2:n:344:VAL:HG22	2.40	0.52
3:o:252:ASP:CB	3:o:253:PRO:HD3	2.34	0.52
28:D:229:UNK:HA	28:D:232:UNK:CB	2.40	0.52
30:F:257:UNK:O	30:F:333:UNK:HA	2.09	0.52
31:G:448:UNK:O	31:G:449:UNK:CB	2.58	0.52
32:H:190:UNK:O	32:H:194:UNK:CB	2.57	0.52
37:M:392:UNK:C	37:M:394:UNK:N	2.68	0.52
41:Q:50:UNK:N	41:Q:51:UNK:HA	2.25	0.52
1:c:346:CYS:HB3	1:c:412:SER:HG	1.74	0.52
1:c:433:ASP:CB	3:b:219:PRO:HG2	2.40	0.52
2:m:383:GLY:O	2:m:386:ALA:HB3	2.10	0.52
3:b:377:LEU:O	3:b:378:LYS:HB3	2.09	0.52
7:g:80:ASP:O	7:g:81:ARG:HB2	2.10	0.52
1:l:106:LEU:HB3	1:l:107:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:247:GLN:NE2	2:n:429:ASN:HA	2.25	0.52
4:p:27:ARG:O	4:p:28:ARG:C	2.52	0.52
8:t:50:THR:HG22	8:t:51:GLU:N	2.25	0.52
13:y:102:HIS:O	13:y:104:TRP:N	2.42	0.52
28:D:307:UNK:O	28:D:308:UNK:C	2.57	0.52
29:E:46:UNK:O	29:E:50:UNK:N	2.43	0.52
30:F:121:UNK:CB	30:F:232:UNK:CB	2.88	0.52
30:F:300:UNK:N	30:F:329:UNK:HA	2.25	0.52
38:N:25:UNK:C	38:N:28:UNK:N	2.72	0.52
40:P:203:UNK:C	40:P:233:UNK:CB	2.88	0.52
47:X:353:UNK:O	47:X:354:UNK:C	2.58	0.52
1:c:37:VAL:HG13	1:c:199:ALA:CB	2.40	0.52
1:c:111:GLU:HG2	1:c:213:GLN:NE2	2.25	0.52
1:c:331:ILE:CD1	1:c:427:PRO:O	2.58	0.52
2:m:85:ILE:O	2:m:89:ILE:HG13	2.10	0.52
2:m:97:SER:OG	9:i:70:LEU:HB2	2.10	0.52
2:m:115:ASP:HA	2:m:118:ILE:HD12	1.92	0.52
2:m:347:ILE:H	2:m:347:ILE:CD1	2.21	0.52
4:d:7:PRO:HB2	4:d:125:ASP:HB3	1.92	0.52
4:d:62:LYS:O	4:d:66:GLU:HG3	2.10	0.52
4:d:139:THR:HG21	8:h:41:ASP:O	2.09	0.52
5:e:18:VAL:HG11	5:e:32:ARG:HH11	1.73	0.52
6:f:7:SER:O	6:f:11:ARG:HD2	2.10	0.52
1:l:131:ARG:O	1:l:132:ASP:C	2.53	0.52
2:n:247:GLN:HG3	2:n:248:ASN:N	2.24	0.52
3:o:52:ALA:HB2	52:o:401:HEM:CMD	2.40	0.52
3:o:117:VAL:N	52:o:402:HEM:HBC2	2.25	0.52
3:o:196:HIS:CE1	52:o:402:HEM:ND	2.78	0.52
3:o:246:ALA:N	3:o:247:PRO:CD	2.73	0.52
7:s:67:GLU:O	7:s:71:ARG:HB3	2.10	0.52
8:t:62:LEU:O	8:t:65:ARG:HG2	2.09	0.52
16:2:63:SER:O	16:2:67:ILE:HG13	2.10	0.52
28:D:211:UNK:O	28:D:214:UNK:CB	2.58	0.52
33:I:119:CYS:O	33:I:120:UNK:CB	2.58	0.52
36:L:580:UNK:N	36:L:581:UNK:CB	2.73	0.52
37:M:22:UNK:HA	37:M:23:UNK:CB	2.40	0.52
37:M:61:UNK:N	37:M:62:UNK:C	2.73	0.52
37:M:62:UNK:CB	37:M:64:UNK:N	2.73	0.52
37:M:68:UNK:C	37:M:70:UNK:N	2.66	0.52
40:P:117:UNK:O	40:P:120:UNK:N	2.43	0.52
47:X:88:UNK:O	47:X:91:UNK:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:85:HIS:CD2	2:m:370:MET:HE1	2.45	0.51
1:c:211:LEU:HD12	1:c:211:LEU:O	2.10	0.51
1:c:326:CYS:SG	1:c:331:ILE:HA	2.50	0.51
10:j:51:LEU:H	10:j:54:HIS:HD2	1.57	0.51
1:l:40:TRP:HZ2	1:l:377:GLU:HB2	1.75	0.51
2:n:393:THR:HG22	2:n:394:PRO:O	2.10	0.51
3:o:153:ILE:HD12	3:o:153:ILE:H	1.74	0.51
4:p:83:ARG:CB	4:p:84:PRO:CD	2.63	0.51
8:t:65:ARG:CG	8:t:66:ASP:N	2.72	0.51
13:y:68:LEU:HB3	13:y:69:PRO:HD3	1.91	0.51
28:D:162:UNK:CB	32:H:279:UNK:N	2.73	0.51
28:D:174:UNK:O	28:D:175:UNK:C	2.57	0.51
28:D:259:UNK:C	28:D:261:UNK:N	2.71	0.51
30:F:322:UNK:CA	30:F:327:UNK:CB	2.87	0.51
36:L:207:UNK:CB	36:L:209:UNK:CA	2.89	0.51
1:c:67:THR:OG1	1:c:119:ASN:HB2	2.09	0.51
2:m:77:THR:HG22	2:m:130:PRO:N	2.24	0.51
2:m:162:ASN:HB3	2:m:244:ILE:CG2	2.40	0.51
2:m:166:ALA:HB2	2:m:244:ILE:CD1	2.41	0.51
3:b:240:MET:SD	3:b:243:VAL:HG11	2.51	0.51
4:d:229:VAL:HG12	4:d:233:ARG:NE	2.23	0.51
10:j:49:GLY:HA2	10:j:54:HIS:HB2	1.91	0.51
1:l:67:THR:CG2	1:l:70:ARG:H	2.03	0.51
1:l:426:GLY:HA3	1:l:428:ILE:N	2.25	0.51
5:q:135:LEU:HD22	5:q:182:VAL:HG22	1.92	0.51
12:x:240:HIS:HB3	12:x:241:PRO:HD3	1.92	0.51
13:y:1:MET:SD	13:y:133:LEU:CD1	2.98	0.51
15:1:40:LEU:HD22	15:1:59:LEU:HD13	1.92	0.51
19:5:60:TYR:CD1	19:5:60:TYR:C	2.88	0.51
31:G:565:UNK:O	31:G:567:UNK:N	2.43	0.51
36:L:47:UNK:O	36:L:48:UNK:C	2.53	0.51
36:L:524:UNK:HA	36:L:527:UNK:CB	2.40	0.51
36:L:602:UNK:C	36:L:604:UNK:N	2.72	0.51
43:S:25:UNK:N	43:S:57:UNK:CA	2.73	0.51
47:X:605:UNK:O	47:X:608:UNK:N	2.43	0.51
51:Z:225:UNK:O	51:Z:228:UNK:N	2.43	0.51
51:Z:310:UNK:O	51:Z:313:UNK:N	2.43	0.51
1:c:19:LEU:HB2	1:c:23:LEU:HB3	1.92	0.51
1:c:347:THR:O	11:k:16:ASN:ND2	2.43	0.51
2:m:45:SER:HB2	2:m:210:GLY:HA3	1.93	0.51
2:m:148:LYS:HD2	2:m:178:CYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:261:SER:HB3	2:m:321:LEU:N	2.25	0.51
2:m:304:HIS:CG	2:m:305:GLN:H	2.29	0.51
4:d:30:PHE:O	4:d:31:GLN:C	2.53	0.51
5:e:38:LEU:HD13	10:j:9:LEU:HD23	1.92	0.51
1:l:389:ARG:C	1:l:391:PRO:HD3	2.36	0.51
2:n:67:HIS:CE1	2:n:177:TYR:HD1	2.28	0.51
2:n:141:GLN:OE1	2:n:183:ILE:O	2.28	0.51
2:n:198:HIS:CE1	2:n:233:SER:HB3	2.45	0.51
2:n:206:LEU:CD1	2:n:224:LEU:HD11	2.41	0.51
4:p:7:PRO:HB2	4:p:125:ASP:HB3	1.93	0.51
4:p:48:TYR:OH	4:p:68:VAL:HG11	2.08	0.51
4:p:138:PRO:HB3	8:t:55:THR:CA	2.40	0.51
6:r:96:GLU:OE2	6:r:99:ARG:NH1	2.43	0.51
28:D:163:UNK:CB	32:H:278:UNK:HA	2.41	0.51
29:E:113:UNK:O	29:E:114:UNK:C	2.57	0.51
32:H:93:UNK:N	32:H:94:UNK:CA	2.73	0.51
33:I:111:UNK:C	33:I:113:UNK:N	2.72	0.51
35:K:42:UNK:O	35:K:45:UNK:CB	2.58	0.51
37:M:227:UNK:N	37:M:228:UNK:CB	2.72	0.51
38:N:163:UNK:O	38:N:166:UNK:CB	2.58	0.51
39:O:33:UNK:CB	39:O:36:UNK:CB	2.89	0.51
39:O:43:UNK:O	39:O:45:UNK:N	2.43	0.51
44:T:63:UNK:O	44:T:66:UNK:N	2.43	0.51
47:X:333:UNK:O	47:X:336:UNK:N	2.44	0.51
1:c:34:THR:CB	2:m:373:GLU:OE1	2.59	0.51
1:c:106:LEU:HB3	1:c:107:PRO:CD	2.41	0.51
1:c:166:SER:CB	5:e:3:THR:HG22	2.39	0.51
2:m:68:LEU:C	2:m:68:LEU:HD12	2.34	0.51
2:m:163:LEU:HD22	2:m:256:ALA:HB1	1.90	0.51
4:d:10:TYR:HD1	8:h:74:PHE:CE1	2.28	0.51
4:d:42:SER:O	4:d:112:ASP:OD1	2.29	0.51
4:d:149:PHE:HZ	8:h:55:THR:HG23	1.73	0.51
1:l:3:THR:O	1:l:4:TYR:C	2.54	0.51
2:n:102:ARG:HH12	2:n:175:SER:HA	1.75	0.51
2:n:209:LEU:O	2:n:209:LEU:HG	2.09	0.51
3:o:357:LEU:O	3:o:361:LEU:HG	2.11	0.51
4:p:10:TYR:HD1	8:t:74:PHE:CE1	2.29	0.51
5:q:150:ALA:HB3	5:q:157:TYR:HB3	1.90	0.51
6:r:58:ARG:HG2	6:r:58:ARG:NH1	2.25	0.51
13:y:186:SER:CB	13:y:213:LEU:HD22	2.40	0.51
18:4:2:SER:OG	18:4:3:ALA:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:94:UNK:O	36:L:95:UNK:C	2.56	0.51
38:N:224:UNK:N	38:N:225:UNK:CA	2.73	0.51
3:b:200:LEU:HD13	52:b:402:HEM:HAD2	1.92	0.51
3:b:221:HIS:HA	3:b:225:THR:HG23	1.92	0.51
4:d:32:VAL:HG11	4:d:186:VAL:CG2	2.41	0.51
5:e:15:ARG:HH21	5:e:32:ARG:CB	2.24	0.51
1:l:411:CYS:O	1:l:415:PHE:HD1	1.92	0.51
2:n:198:HIS:HE1	2:n:233:SER:CB	2.23	0.51
2:n:258:VAL:CG1	2:n:321:LEU:HD22	2.40	0.51
2:n:262:ALA:HB3	2:n:269:ALA:N	2.24	0.51
3:o:152:ALA:N	3:o:287:LYS:NZ	2.59	0.51
3:o:200:LEU:HD13	52:o:402:HEM:CAD	2.40	0.51
3:o:276:PHE:O	3:o:277:ALA:C	2.52	0.51
4:p:213:GLY:O	4:p:217:PRO:HG3	2.11	0.51
4:p:220:TYR:O	4:p:221:ALA:C	2.53	0.51
5:q:51:ALA:O	5:q:55:VAL:HG23	2.11	0.51
10:v:32:GLU:CG	10:v:33:ARG:N	2.74	0.51
17:3:8:THR:OG1	17:3:11:GLU:HG2	2.09	0.51
28:D:195:UNK:O	28:D:198:UNK:O	2.28	0.51
30:F:103:UNK:CA	30:F:104:UNK:C	2.89	0.51
36:L:47:UNK:C	36:L:49:UNK:N	2.71	0.51
36:L:60:UNK:O	36:L:81:UNK:N	2.43	0.51
37:M:347:UNK:HA	37:M:415:UNK:HA	1.92	0.51
40:P:170:UNK:O	40:P:172:UNK:N	2.43	0.51
44:T:62:UNK:C	44:T:63:UNK:O	2.56	0.51
1:c:236:PHE:HB2	5:e:25:SER:HB2	1.93	0.51
2:m:197:ASN:HB2	2:m:198:HIS:CD2	2.46	0.51
2:m:352:LEU:HD23	2:m:411:ILE:HD11	1.92	0.51
2:m:372:VAL:O	2:m:372:VAL:HG12	2.11	0.51
3:b:106:SER:CB	52:b:402:HEM:HBD2	2.41	0.51
3:b:368:THR:O	3:b:371:THR:HB	2.10	0.51
6:f:23:ALA:O	6:f:24:ALA:C	2.52	0.51
1:l:46:ARG:NH1	1:l:316:ASP:OD1	2.40	0.51
3:o:10:LEU:HD12	3:o:13:ILE:HD11	1.92	0.51
3:o:218:ILE:HD13	4:p:230:LEU:HD13	1.91	0.51
4:p:30:PHE:HD1	4:p:189:PHE:CE1	2.29	0.51
5:q:119:ASP:HB3	5:q:179:ASN:ND2	2.26	0.51
5:q:191:ASP:OD1	5:q:191:ASP:N	2.42	0.51
13:y:100:MET:CE	13:y:157:GLU:HG3	2.40	0.51
28:D:108:UNK:O	28:D:109:UNK:C	2.58	0.51
30:F:102:UNK:O	30:F:103:UNK:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:594:UNK:CA	31:G:595:UNK:C	2.87	0.51
34:J:90:UNK:O	34:J:93:UNK:N	2.44	0.51
36:L:190:UNK:HA	36:L:194:UNK:CA	2.40	0.51
36:L:321:UNK:O	36:L:324:UNK:C	2.58	0.51
37:M:341:UNK:O	37:M:342:UNK:C	2.56	0.51
37:M:348:UNK:N	37:M:415:UNK:CB	2.74	0.51
38:N:33:UNK:C	38:N:35:UNK:N	2.67	0.51
40:P:135:UNK:HA	40:P:167:UNK:C	2.41	0.51
40:P:139:UNK:CB	40:P:140:UNK:C	2.88	0.51
50:U:623:UNK:O	50:U:626:UNK:N	2.44	0.51
1:c:291:SER:HB3	2:m:87:ARG:HD3	1.93	0.51
2:m:198:HIS:HE1	2:m:233:SER:CB	2.19	0.51
3:b:153:ILE:HD12	3:b:153:ILE:N	2.25	0.51
3:b:175:LEU:O	3:b:175:LEU:HG	2.11	0.51
3:b:341:GLN:O	3:b:342:PRO:C	2.52	0.51
1:l:5:ALA:O	1:l:6:GLN:C	2.53	0.51
2:n:112:LEU:O	2:n:113:ARG:C	2.54	0.51
3:o:30:TRP:HA	3:o:33:PHE:HE2	1.75	0.51
3:o:166:GLY:HA3	3:o:177:ARG:NH2	2.26	0.51
4:p:11:PRO:HG2	8:t:74:PHE:HB2	1.92	0.51
13:y:139:ASP:OD1	13:y:140:ASN:N	2.44	0.51
26:B:129:UNK:O	26:B:131:UNK:N	2.43	0.51
32:H:93:UNK:HA	32:H:94:UNK:CB	2.40	0.51
33:I:100:UNK:CB	33:I:103:UNK:N	2.74	0.51
36:L:70:UNK:O	36:L:73:UNK:O	2.28	0.51
37:M:241:UNK:C	37:M:243:UNK:N	2.71	0.51
44:T:40:UNK:O	44:T:41:UNK:CB	2.58	0.51
47:X:703:UNK:O	47:X:705:UNK:N	2.43	0.51
2:m:88:GLY:O	2:m:91:ALA:HB3	2.11	0.51
2:m:200:THR:OG1	2:m:201:SER:N	2.44	0.51
2:m:275:LEU:HD11	2:m:279:LEU:CD1	2.41	0.51
3:b:164:ILE:O	3:b:177:ARG:NH1	2.42	0.51
4:d:228:SER:HB2	7:g:23:GLN:HE22	1.71	0.51
5:e:71:MET:O	5:e:72:SER:C	2.54	0.51
6:f:13:LEU:O	6:f:16:ILE:N	2.42	0.51
6:f:104:ARG:O	6:f:105:GLU:C	2.53	0.51
1:l:51:LYS:C	1:l:53:ASN:H	2.19	0.51
1:l:327:ASP:OD1	1:l:328:HIS:N	2.44	0.51
3:o:147:THR:HG21	3:o:165:TRP:CD1	2.46	0.51
3:o:152:ALA:HB2	3:o:287:LYS:NZ	2.26	0.51
4:p:50:HIS:O	4:p:54:VAL:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:347:LEU:HG	12:x:383:MET:HE3	1.93	0.51
29:E:112:UNK:C	29:E:114:UNK:N	2.72	0.51
36:L:556:UNK:O	36:L:560:UNK:N	2.43	0.51
38:N:145:UNK:CB	38:N:147:UNK:CB	2.88	0.51
38:N:234:UNK:O	38:N:237:UNK:O	2.28	0.51
40:P:248:UNK:CB	40:P:317:UNK:CB	2.89	0.51
48:Y:94:UNK:O	48:Y:97:UNK:N	2.43	0.51
51:Z:253:UNK:O	51:Z:254:UNK:C	2.59	0.51
1:c:48:GLU:HB3	1:c:52:ASN:O	2.10	0.51
1:c:343:MET:CE	1:c:416:TYR:HD2	2.17	0.51
2:m:178:CYS:SG	2:m:179:PRO:HD2	2.51	0.51
2:m:375:SER:OG	2:m:376:GLU:N	2.42	0.51
3:b:183:PHE:CD1	3:b:183:PHE:C	2.88	0.51
4:d:26:ILE:HG21	4:d:54:VAL:HG22	1.92	0.51
6:f:35:ASP:OD1	6:f:89:TYR:OH	2.21	0.51
8:h:15:ASP:N	8:h:16:PRO:CD	2.73	0.51
8:h:27:LEU:O	8:h:30:CYS:N	2.38	0.51
1:l:428:ILE:CG2	1:l:431:LEU:CD2	2.85	0.51
2:n:350:GLY:HA2	2:n:411:ILE:HG21	1.93	0.51
3:o:19:ILE:HG23	3:o:221:HIS:HB2	1.92	0.51
4:p:24:THR:O	4:p:25:SER:C	2.54	0.51
4:p:48:TYR:CD2	4:p:65:ALA:HB2	2.46	0.51
4:p:153:PHE:O	4:p:156:GLN:N	2.36	0.51
6:r:37:ILE:HG23	6:r:37:ILE:O	2.11	0.51
29:E:62:UNK:O	29:E:63:UNK:C	2.58	0.51
30:F:370:UNK:C	30:F:372:UNK:N	2.74	0.51
36:L:246:UNK:O	36:L:250:UNK:N	2.44	0.51
37:M:139:UNK:HA	37:M:140:UNK:CB	2.39	0.51
40:P:203:UNK:CA	40:P:233:UNK:CB	2.87	0.51
47:X:183:UNK:O	47:X:184:UNK:C	2.54	0.51
47:X:702:UNK:O	47:X:705:UNK:CB	2.59	0.51
48:Y:29:UNK:O	48:Y:30:UNK:CB	2.58	0.51
1:c:113:LEU:HA	1:c:116:ILE:HD12	1.92	0.51
1:c:124:ASP:O	1:c:128:GLU:HG2	2.11	0.51
1:c:142:ASP:OD2	5:e:1:SER:HB3	2.11	0.51
3:b:119:LEU:HG	52:b:402:HEM:HBB2	1.90	0.51
3:b:331:ASP:OD1	3:b:354:ALA:HB1	2.11	0.51
4:d:30:PHE:CE1	4:d:50:HIS:CE1	2.99	0.51
7:g:52:PHE:O	7:g:53:VAL:C	2.54	0.51
8:h:70:ALA:HA	8:h:73:LEU:HD22	1.92	0.51
1:l:30:SER:N	1:l:201:GLY:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:124:ASP:O	1:l:128:GLU:HG2	2.11	0.51
2:n:68:LEU:CD1	2:n:140:LEU:HD23	2.39	0.51
2:n:239:TYR:OH	2:n:421:ARG:O	2.29	0.51
2:n:275:LEU:HB2	2:n:410:VAL:HG13	1.92	0.51
3:o:344:GLU:O	3:o:348:ILE:HG13	2.11	0.51
3:o:378:LYS:O	3:o:378:LYS:HD3	2.11	0.51
26:B:129:UNK:C	26:B:131:UNK:N	2.73	0.51
28:D:357:UNK:N	28:D:384:UNK:CB	2.74	0.51
31:G:227:UNK:O	31:G:238:UNK:CB	2.59	0.51
34:J:26:UNK:O	34:J:27:UNK:CB	2.59	0.51
37:M:341:UNK:C	37:M:342:UNK:O	2.56	0.51
39:O:125:UNK:O	39:O:126:UNK:CB	2.59	0.51
40:P:49:UNK:O	40:P:73:UNK:N	2.44	0.51
40:P:155:UNK:O	40:P:158:UNK:N	2.44	0.51
40:P:203:UNK:N	40:P:234:UNK:C	2.73	0.51
45:V:1:UNK:C	45:V:3:UNK:N	2.67	0.51
45:V:23:UNK:O	45:V:24:UNK:CB	2.58	0.51
45:V:55:UNK:C	45:V:57:UNK:N	2.74	0.51
1:c:26:ALA:O	1:c:27:SER:HB3	2.11	0.50
1:c:426:GLY:HA2	1:c:428:ILE:HG13	1.84	0.50
4:d:27:ARG:NH1	10:j:58:LYS:HE3	2.26	0.50
4:d:153:PHE:O	4:d:154:PRO:C	2.54	0.50
4:d:161:ALA:HB1	4:d:162:PRO:HD2	1.93	0.50
1:l:53:ASN:CG	1:l:165:GLN:HB2	2.35	0.50
1:l:151:ASN:O	1:l:152:TYR:C	2.53	0.50
1:l:213:GLN:CB	1:l:215:HIS:NE2	2.70	0.50
4:p:232:SER:CB	7:s:23:GLN:OE1	2.59	0.50
5:q:45:VAL:HG22	10:v:28:ALA:N	2.26	0.50
12:x:40:GLU:HG2	12:x:54:TYR:CD1	2.47	0.50
12:x:145:LEU:HD21	14:z:32:THR:HG21	1.93	0.50
12:x:232:GLN:HB2	12:x:292:MET:HE3	1.93	0.50
28:D:101:UNK:O	28:D:103:UNK:N	2.42	0.50
31:G:573:UNK:O	31:G:580:UNK:HA	2.11	0.50
36:L:263:UNK:O	36:L:264:UNK:C	2.59	0.50
49:a:1:UNK:O	49:a:5:UNK:N	2.44	0.50
2:m:412:ASN:O	2:m:415:LYS:HB2	2.11	0.50
3:b:46:LEU:O	3:b:50:PHE:HD1	1.94	0.50
3:b:177:ARG:O	3:b:181:PHE:HD2	1.93	0.50
3:b:183:PHE:O	3:b:183:PHE:HD1	1.94	0.50
3:b:185:LEU:HB3	3:b:186:PRO:CD	2.36	0.50
3:b:312:GLN:NE2	3:b:317:PHE:HB2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:33:GLY:O	7:g:37:VAL:HB	2.11	0.50
2:n:109:VAL:HG22	2:n:119:LEU:CD2	2.41	0.50
3:o:91:PHE:O	3:o:92:ILE:C	2.52	0.50
3:o:160:LEU:O	3:o:164:ILE:HD12	2.11	0.50
4:p:14:HIS:HA	4:p:19:SER:HB3	1.93	0.50
4:p:72:ASP:OD1	4:p:76:GLU:OE1	2.29	0.50
4:p:146:GLY:O	4:p:148:TYR:N	2.42	0.50
4:p:146:GLY:O	4:p:148:TYR:CD1	2.65	0.50
5:q:18:VAL:HG11	5:q:32:ARG:NH1	2.27	0.50
5:q:119:ASP:HB3	5:q:179:ASN:HD21	1.76	0.50
27:C:23:UNK:O	27:C:27:UNK:N	2.44	0.50
29:E:112:UNK:O	29:E:113:UNK:C	2.57	0.50
30:F:419:UNK:CA	30:F:423:UNK:CB	2.84	0.50
39:O:33:UNK:O	39:O:36:UNK:N	2.44	0.50
40:P:25:UNK:CB	40:P:95:UNK:CA	2.89	0.50
40:P:170:UNK:O	40:P:205:UNK:CA	2.59	0.50
1:c:200:ALA:HB2	1:c:375:VAL:HG12	1.92	0.50
1:c:378:ASP:O	1:c:382:SER:HB2	2.11	0.50
1:c:417:ASP:CG	10:j:10:TYR:OH	2.55	0.50
2:m:322:PHE:CD1	2:m:322:PHE:C	2.90	0.50
3:b:105:GLY:HA2	3:b:107:TYR:CD1	2.46	0.50
3:b:280:ILE:N	3:b:280:ILE:HD13	2.27	0.50
4:d:13:SER:O	4:d:19:SER:HB3	2.11	0.50
4:d:120:ARG:CG	4:d:120:ARG:HH11	2.24	0.50
1:l:291:SER:HB3	2:n:87:ARG:HD3	1.93	0.50
2:n:262:ALA:CB	2:n:268:GLU:HB3	2.41	0.50
3:o:317:PHE:CD1	6:r:26:PHE:HB3	2.47	0.50
4:p:82:MET:HE2	4:p:86:LYS:NZ	2.25	0.50
32:H:110:UNK:O	32:H:113:UNK:N	2.44	0.50
32:H:284:UNK:O	32:H:288:UNK:N	2.45	0.50
35:K:9:UNK:O	35:K:12:UNK:CB	2.60	0.50
37:M:63:UNK:O	37:M:67:UNK:N	2.44	0.50
39:O:129:UNK:O	39:O:132:UNK:N	2.44	0.50
47:X:69:UNK:O	47:X:70:UNK:C	2.59	0.50
47:X:526:UNK:O	47:X:527:UNK:C	2.57	0.50
1:c:37:VAL:HG13	1:c:199:ALA:HB2	1.93	0.50
2:m:34:VAL:HG11	2:m:386:ALA:CB	2.40	0.50
3:b:276:PHE:HE2	3:b:297:SER:OG	1.95	0.50
4:d:138:PRO:CB	8:h:55:THR:CA	2.90	0.50
1:l:329:MET:HA	1:l:430:GLN:OE1	2.11	0.50
1:l:343:MET:HE1	1:l:416:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:261:SER:HB3	2:n:321:LEU:N	2.25	0.50
2:n:406:ALA:HB3	2:n:409:ASP:HB2	1.92	0.50
3:o:142:GLY:O	3:o:146:ILE:HG12	2.12	0.50
10:v:60:GLU:HG3	10:v:60:GLU:O	2.11	0.50
14:z:18:LEU:HD22	14:z:22:LEU:HD22	1.92	0.50
26:B:71:UNK:O	32:H:37:UNK:CB	2.60	0.50
30:F:234:UNK:O	30:F:237:UNK:O	2.30	0.50
32:H:79:UNK:C	32:H:81:UNK:N	2.73	0.50
36:L:257:UNK:O	36:L:261:UNK:N	2.43	0.50
36:L:547:UNK:O	36:L:550:UNK:CB	2.60	0.50
38:N:297:UNK:C	38:N:299:UNK:N	2.72	0.50
40:P:203:UNK:H2	40:P:234:UNK:C	2.23	0.50
43:S:63:UNK:O	43:S:78:UNK:CB	2.58	0.50
47:X:714:UNK:O	47:X:717:UNK:CB	2.59	0.50
51:Z:13:UNK:O	51:Z:16:UNK:N	2.45	0.50
51:Z:30:UNK:C	51:Z:32:UNK:N	2.73	0.50
2:m:258:VAL:CG1	2:m:321:LEU:HD22	2.42	0.50
2:m:429:ASN:ND2	2:n:60:SER:OG	2.45	0.50
3:b:100:ARG:NH2	52:b:402:HEM:O2A	2.44	0.50
3:b:163:TRP:CE2	5:q:62:MET:HE2	2.46	0.50
6:f:96:GLU:O	6:f:99:ARG:N	2.44	0.50
10:j:52:TRP:H	10:j:52:TRP:HE3	1.57	0.50
1:l:120:CYS:O	1:l:122:LEU:HG	2.12	0.50
1:l:426:GLY:HA2	1:l:427:PRO:C	2.36	0.50
2:n:47:ILE:CG2	2:n:48:GLY:N	2.72	0.50
2:n:129:ALA:H	2:n:130:PRO:HD3	1.76	0.50
3:o:4:ILE:O	3:o:5:ARG:C	2.55	0.50
3:o:242:LEU:HD21	3:o:250:LEU:CD2	2.41	0.50
3:o:296:PHE:O	3:o:297:SER:C	2.52	0.50
4:p:165:TYR:H	4:p:168:VAL:CG2	2.24	0.50
7:s:80:ASP:O	7:s:81:ARG:HB2	2.11	0.50
9:u:58:GLN:HB3	9:u:78:TYR:HB2	1.92	0.50
12:x:250:GLY:O	12:x:254:ILE:HG12	2.11	0.50
17:3:37:LYS:HD3	17:3:37:LYS:N	2.27	0.50
37:M:256:UNK:O	37:M:257:UNK:C	2.56	0.50
38:N:184:UNK:O	38:N:188:UNK:N	2.44	0.50
51:Z:110:UNK:O	51:Z:111:UNK:C	2.59	0.50
2:m:207:ILE:CD1	2:m:383:GLY:HA2	2.37	0.50
3:b:26:ASN:ND2	3:b:208:PRO:HD2	2.27	0.50
3:b:74:ASN:O	5:e:61:SER:HA	2.12	0.50
3:b:147:THR:O	3:b:150:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:33:TYR:O	4:d:37:CYS:HB2	2.12	0.50
4:d:164:ILE:HG21	4:d:182:VAL:HG12	1.92	0.50
1:l:294:LEU:CD2	1:l:337:VAL:HG12	2.41	0.50
2:n:47:ILE:HG22	2:n:48:GLY:H	1.76	0.50
3:o:27:ILE:O	3:o:27:ILE:CG2	2.58	0.50
3:o:47:THR:HG22	3:o:83:HIS:HB2	1.91	0.50
3:o:329:VAL:HA	3:o:332:LEU:HD12	1.94	0.50
6:r:75:LEU:CD1	6:r:76:PRO:HD2	2.36	0.50
15:l:64:PHE:CE1	16:2:66:ARG:HD2	2.47	0.50
28:D:270:UNK:O	28:D:274:UNK:HA	2.11	0.50
33:I:120:UNK:N	59:I:201:SF4:S4	2.85	0.50
37:M:106:UNK:O	37:M:109:UNK:N	2.45	0.50
38:N:194:UNK:O	38:N:195:UNK:C	2.58	0.50
1:c:252:HIS:CD2	1:c:325:VAL:HG22	2.47	0.50
1:c:286:GLY:O	1:c:287:GLY:O	2.30	0.50
1:c:408:ARG:HH12	11:k:15:ARG:CD	2.25	0.50
2:m:170:ASN:CG	2:m:171:ALA:N	2.70	0.50
2:m:348:ALA:HB3	2:m:418:VAL:HG21	1.94	0.50
3:b:43:LEU:O	3:b:44:GLN:C	2.51	0.50
3:b:122:THR:HG21	3:b:189:ILE:CG1	2.42	0.50
1:l:370:ASP:OD1	2:n:375:SER:HB3	2.12	0.50
2:n:185:LYS:HG3	2:n:185:LYS:O	2.11	0.50
2:n:255:ALA:CB	2:n:426:ALA:HB2	2.42	0.50
4:p:43:MET:HA	4:p:112:ASP:OD1	2.10	0.50
4:p:190:LEU:O	4:p:191:ARG:C	2.55	0.50
4:p:224:ARG:NH2	7:s:27:PRO:HD2	2.26	0.50
6:r:10:SER:HA	6:r:13:LEU:CD1	2.42	0.50
12:x:225:GLY:HA3	14:z:112:LEU:HD13	1.92	0.50
26:B:119:CYS:HG	59:B:201:SF4:FE1	1.29	0.50
26:B:129:UNK:CB	27:C:167:UNK:O	2.59	0.50
28:D:86:UNK:O	28:D:87:UNK:C	2.59	0.50
30:F:91:UNK:HA	30:F:219:UNK:O	2.12	0.50
36:L:241:UNK:O	36:L:244:UNK:N	2.45	0.50
37:M:23:UNK:C	37:M:25:UNK:N	2.73	0.50
37:M:27:UNK:O	37:M:28:UNK:C	2.58	0.50
1:c:22:GLY:O	1:c:24:ARG:HG2	2.11	0.50
9:i:62:ARG:N	9:i:63:PRO:CD	2.75	0.50
10:j:4:THR:HG22	10:j:6:THR:H	1.77	0.50
2:n:196:GLN:HG2	2:n:197:ASN:OD1	2.11	0.50
2:n:300:ALA:HA	2:n:307:PHE:HZ	1.77	0.50
3:o:130:GLY:O	52:o:401:HEM:HAA1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:35:GLN:HB2	4:p:169:LEU:CD1	2.42	0.50
4:p:168:VAL:HG12	4:p:169:LEU:HD23	1.93	0.50
4:p:178:THR:HB	4:p:181:GLN:CG	2.32	0.50
5:q:152:ASP:N	5:q:164:HIS:ND1	2.59	0.50
7:s:48:VAL:O	7:s:51:PRO:HD2	2.12	0.50
10:v:21:ALA:O	10:v:22:LEU:C	2.53	0.50
12:x:377:PHE:HA	12:x:380:VAL:HG22	1.93	0.50
12:x:508:PRO:HG3	14:z:6:HIS:HB3	1.94	0.50
13:y:136:LEU:HB3	13:y:193:TYR:CD2	2.46	0.50
26:B:150:UNK:HA	59:B:201:SF4:S1	2.51	0.50
30:F:95:UNK:O	30:F:96:UNK:C	2.57	0.50
38:N:26:UNK:N	38:N:27:UNK:CA	2.74	0.50
1:c:53:ASN:C	1:c:53:ASN:ND2	2.69	0.50
2:m:247:GLN:NE2	2:m:429:ASN:ND2	2.59	0.50
2:m:275:LEU:HD12	2:m:275:LEU:O	2.12	0.50
3:b:344:GLU:O	3:b:348:ILE:HG13	2.11	0.50
4:d:102:ARG:HG2	4:d:109:LEU:HB2	1.93	0.50
4:d:138:PRO:HB3	8:h:55:THR:HA	1.94	0.50
7:g:54:ALA:O	7:g:58:VAL:HG23	2.12	0.50
1:l:170:PRO:O	1:l:171:SER:C	2.55	0.50
1:l:392:LEU:HA	1:l:395:TRP:NE1	2.25	0.50
2:n:97:SER:HA	9:u:70:LEU:HB2	1.94	0.50
2:n:308:ASP:OD2	9:u:54:SER:O	2.29	0.50
3:o:25:SER:HB3	6:r:70:MET:HE2	1.94	0.50
12:x:75:ILE:O	12:x:79:GLY:HA3	2.11	0.50
14:z:42:LEU:HD13	21:7:45:TYR:HD2	1.77	0.50
18:4:44:ARG:HD2	18:4:74:ARG:O	2.12	0.50
29:E:111:UNK:C	29:E:113:UNK:N	2.72	0.50
31:G:469:UNK:HA	31:G:472:UNK:CB	2.42	0.50
34:J:50:UNK:O	34:J:54:UNK:CB	2.60	0.50
36:L:105:UNK:O	36:L:109:UNK:N	2.45	0.50
47:X:411:UNK:O	47:X:414:UNK:CB	2.60	0.50
51:Z:252:UNK:O	51:Z:255:UNK:CB	2.60	0.50
1:c:395:TRP:O	1:c:398:ARG:N	2.45	0.49
2:m:38:LEU:O	2:m:40:ASN:N	2.45	0.49
2:m:79:GLY:CA	2:m:125:ASN:HD21	2.25	0.49
2:m:255:ALA:HA	2:m:425:ALA:O	2.12	0.49
2:n:76:THR:HG21	2:n:133:ARG:CZ	2.42	0.49
2:n:92:VAL:O	2:n:92:VAL:CG1	2.60	0.49
4:p:117:VAL:CG1	4:p:191:ARG:HH11	2.25	0.49
7:s:64:GLN:O	7:s:65:GLU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:z:119:THR:O	18:4:52:HIS:CE1	2.63	0.49
26:B:121:UNK:CA	26:B:135:UNK:CB	2.85	0.49
33:I:20:UNK:O	33:I:24:UNK:N	2.45	0.49
36:L:137:UNK:O	36:L:140:UNK:CB	2.60	0.49
36:L:288:UNK:CB	36:L:308:UNK:CA	2.89	0.49
37:M:189:UNK:N	37:M:191:UNK:C	2.75	0.49
37:M:227:UNK:CB	37:M:228:UNK:CB	2.90	0.49
38:N:123:UNK:CA	38:N:124:UNK:CB	2.90	0.49
40:P:53:UNK:C	40:P:57:UNK:CB	2.89	0.49
48:Y:103:UNK:O	48:Y:106:UNK:CA	2.60	0.49
51:Z:205:UNK:O	51:Z:208:UNK:CB	2.60	0.49
3:b:103:TYR:OH	3:b:322:GLN:HG3	2.12	0.49
3:b:125:ALA:O	3:b:126:THR:C	2.53	0.49
4:d:2:ASP:HB3	4:d:156:GLN:NE2	2.26	0.49
4:d:26:ILE:HG22	4:d:27:ARG:N	2.27	0.49
4:d:237:TYR:CD2	4:d:239:PRO:HD3	2.47	0.49
10:j:18:SER:CB	11:k:23:LEU:HD12	2.30	0.49
1:l:307:PHE:HA	1:l:323:HIS:O	2.12	0.49
3:o:26:ASN:HA	6:r:70:MET:HA	1.94	0.49
3:o:164:ILE:O	3:o:177:ARG:NH1	2.44	0.49
4:p:138:PRO:HB3	8:t:54:CYS:C	2.37	0.49
4:p:138:PRO:CB	8:t:55:THR:CA	2.90	0.49
9:u:51:CYS:SG	9:u:53:GLU:HB3	2.52	0.49
12:x:168:ILE:HG21	12:x:189:MET:HG3	1.94	0.49
50:U:109:UNK:O	50:U:112:UNK:N	2.46	0.49
1:c:15:GLN:O	1:c:205:HIS:CE1	2.66	0.49
1:c:64:PHE:HA	1:c:75:LEU:CD2	2.42	0.49
1:c:158:PHE:O	1:c:164:ALA:HB2	2.12	0.49
1:c:296:SER:O	1:c:297:ILE:C	2.55	0.49
2:m:429:ASN:C	2:m:429:ASN:HD22	2.19	0.49
3:b:373:GLU:HB3	6:f:20:TYR:OH	2.12	0.49
10:j:49:GLY:HA2	10:j:54:HIS:HB3	1.92	0.49
1:l:256:ALA:CA	1:l:320:LEU:O	2.59	0.49
2:n:170:ASN:CG	2:n:171:ALA:N	2.69	0.49
3:o:191:ALA:O	3:o:195:VAL:HG23	2.12	0.49
4:p:69:GLU:HA	4:p:73:GLY:HA2	1.93	0.49
28:D:257:UNK:O	28:D:259:UNK:N	2.45	0.49
29:E:126:UNK:O	29:E:127:UNK:C	2.55	0.49
30:F:92:UNK:N	30:F:219:UNK:O	2.45	0.49
30:F:365:CYS:O	30:F:368:UNK:N	2.45	0.49
31:G:28:UNK:O	31:G:29:UNK:C	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:143:UNK:O	32:H:145:UNK:N	2.46	0.49
33:I:98:UNK:C	33:I:103:UNK:O	2.60	0.49
37:M:396:UNK:O	37:M:399:UNK:N	2.45	0.49
38:N:169:UNK:CB	38:N:292:UNK:CB	2.90	0.49
39:O:119:UNK:C	39:O:121:UNK:N	2.73	0.49
2:m:166:ALA:HB2	2:m:244:ILE:CG1	2.39	0.49
3:b:37:LEU:HD21	3:b:94:LEU:HD13	1.93	0.49
3:b:246:ALA:HB1	3:b:249:LEU:HB2	1.94	0.49
3:b:357:LEU:O	3:b:361:LEU:HG	2.13	0.49
4:d:72:ASP:OD1	4:d:76:GLU:OE1	2.30	0.49
4:d:138:PRO:HB3	8:h:54:CYS:C	2.37	0.49
1:l:4:TYR:CE1	2:n:43:PRO:HB3	2.48	0.49
2:n:130:PRO:HB2	2:n:132:PHE:CE1	2.46	0.49
5:q:9:ASP:OD1	5:q:11:SER:OG	2.30	0.49
5:q:76:ILE:HG22	5:q:193:VAL:O	2.12	0.49
9:u:62:ARG:N	9:u:63:PRO:CD	2.75	0.49
25:A:91:UNK:O	25:A:92:UNK:C	2.61	0.49
26:B:166:UNK:O	26:B:167:UNK:C	2.60	0.49
30:F:352:UNK:O	30:F:356:UNK:N	2.45	0.49
31:G:236:UNK:CB	31:G:259:UNK:CB	2.90	0.49
31:G:611:UNK:O	31:G:612:UNK:CB	2.60	0.49
33:I:49:UNK:O	33:I:53:UNK:N	2.45	0.49
47:X:179:UNK:O	47:X:180:UNK:C	2.56	0.49
1:c:106:LEU:HD22	1:c:203:LEU:HD13	1.93	0.49
2:m:112:LEU:O	2:m:113:ARG:C	2.54	0.49
4:d:161:ALA:O	4:d:163:PRO:N	2.45	0.49
1:l:82:MET:SD	1:l:105:ASP:HB3	2.51	0.49
2:n:303:VAL:CG1	2:n:304:HIS:H	2.24	0.49
2:n:340:ALA:O	2:n:344:VAL:HG23	2.12	0.49
3:o:85:ASN:O	3:o:86:GLY:C	2.53	0.49
3:o:115:ILE:HD13	3:o:115:ILE:N	2.27	0.49
3:o:221:HIS:CB	3:o:222:PRO:HD3	2.34	0.49
4:p:100:ALA:O	4:p:103:ALA:N	2.45	0.49
5:q:142:LEU:HD12	5:q:161:HIS:CE1	2.46	0.49
9:u:78:TYR:OXT	9:u:78:TYR:CD1	2.64	0.49
12:x:87:ILE:O	12:x:173:PRO:HD3	2.13	0.49
13:y:16:ILE:HD12	13:y:17:MET:H	1.78	0.49
13:y:90:ILE:H	13:y:90:ILE:HD12	1.77	0.49
18:4:42:ARG:HD2	18:4:42:ARG:O	2.12	0.49
33:I:85:UNK:C	33:I:87:CYS:H	2.24	0.49
47:X:714:UNK:O	47:X:718:UNK:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Z:107:UNK:O	51:Z:108:UNK:C	2.60	0.49
1:c:39:VAL:CG1	1:c:41:ILE:HD11	2.36	0.49
1:c:272:VAL:O	1:c:275:ALA:HB3	2.12	0.49
2:m:130:PRO:HB2	2:m:132:PHE:CE1	2.48	0.49
2:m:132:PHE:HB3	2:m:137:VAL:CG2	2.42	0.49
2:m:141:GLN:OE1	2:m:141:GLN:HA	2.13	0.49
2:m:352:LEU:HD23	2:m:411:ILE:CD1	2.43	0.49
4:d:138:PRO:O	4:d:141:VAL:HB	2.12	0.49
6:f:50:LEU:CB	6:f:55:TYR:HB2	2.29	0.49
8:h:68:CYS:O	8:h:69:VAL:C	2.55	0.49
1:l:286:GLY:O	1:l:287:GLY:C	2.56	0.49
1:l:349:ALA:O	1:l:408:ARG:NH2	2.45	0.49
2:n:24:LEU:HD13	2:n:392:TYR:CD2	2.48	0.49
2:n:194:TYR:O	2:n:195:VAL:C	2.54	0.49
4:p:23:HIS:CD2	10:v:50:LYS:O	2.65	0.49
4:p:79:GLU:HB3	4:p:82:MET:HB2	1.93	0.49
5:q:51:ALA:O	5:q:52:LYS:C	2.54	0.49
5:q:188:THR:HG21	5:q:194:ILE:CD1	2.43	0.49
9:u:58:GLN:O	9:u:59:ALA:HB2	2.11	0.49
13:y:13:THR:O	13:y:13:THR:HG22	2.12	0.49
31:G:193:UNK:CA	31:G:196:UNK:CB	2.85	0.49
32:H:39:UNK:C	32:H:41:UNK:N	2.72	0.49
36:L:161:UNK:HA	36:L:163:UNK:CA	2.37	0.49
36:L:163:UNK:C	36:L:165:UNK:N	2.69	0.49
36:L:239:UNK:C	36:L:240:UNK:O	2.60	0.49
36:L:602:UNK:O	36:L:604:UNK:N	2.45	0.49
39:O:191:UNK:O	39:O:192:UNK:C	2.60	0.49
40:P:82:UNK:O	40:P:83:UNK:C	2.60	0.49
47:X:187:UNK:O	47:X:188:UNK:C	2.60	0.49
1:c:63:ALA:HB2	1:c:97:TYR:HE2	1.76	0.49
1:c:315:ALA:HB3	1:c:316:ASP:OD1	2.13	0.49
1:c:415:PHE:O	1:c:441:MET:HE2	2.13	0.49
2:m:126:VAL:O	2:m:126:VAL:HG12	2.11	0.49
2:m:294:SER:O	2:m:295:LEU:C	2.55	0.49
2:m:299:VAL:HG13	2:m:303:VAL:HG21	1.94	0.49
3:b:282:ARG:O	3:b:283:SER:C	2.55	0.49
4:d:3:LEU:HD21	7:g:71:ARG:HA	1.95	0.49
7:g:40:ARG:O	7:g:41:THR:C	2.55	0.49
9:i:60:ALA:HB3	9:i:63:PRO:O	2.12	0.49
1:l:243:HIS:CD2	1:l:425:PHE:CE1	3.01	0.49
1:l:446:PHE:HE2	3:o:6:LYS:HZ1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:118:ARG:HH12	5:q:173:LYS:N	2.11	0.49
8:t:73:LEU:HD23	8:t:73:LEU:C	2.37	0.49
30:F:194:UNK:O	30:F:198:UNK:N	2.45	0.49
30:F:423:UNK:O	30:F:426:UNK:N	2.46	0.49
31:G:301:UNK:O	31:G:304:UNK:CB	2.61	0.49
36:L:580:UNK:CB	36:L:581:UNK:HA	2.43	0.49
38:N:61:UNK:O	38:N:62:UNK:C	2.60	0.49
40:P:204:UNK:N	40:P:233:UNK:CB	2.75	0.49
1:c:37:VAL:CG1	1:c:199:ALA:HB2	2.43	0.49
1:c:171:SER:O	1:c:174:VAL:HB	2.12	0.49
3:b:4:ILE:O	3:b:5:ARG:C	2.53	0.49
4:d:134:TYR:HE2	4:d:163:PRO:CG	2.24	0.49
4:d:139:THR:CG2	8:h:44:VAL:HB	2.43	0.49
7:g:50:PRO:HB2	7:g:51:PRO:CD	2.38	0.49
1:l:162:PRO:O	1:l:165:GLN:NE2	2.42	0.49
2:n:283:PRO:HG3	9:u:55:LEU:HB3	1.95	0.49
2:n:381:GLU:OE1	2:n:381:GLU:HA	2.13	0.49
3:o:28:SER:CB	3:o:30:TRP:HD1	2.26	0.49
3:o:150:LEU:O	3:o:153:ILE:HD13	2.13	0.49
5:q:38:LEU:O	5:q:42:THR:OG1	2.30	0.49
5:q:87:MET:HG2	5:q:89:PHE:HE1	1.78	0.49
31:G:570:UNK:O	31:G:571:UNK:CB	2.61	0.49
37:M:384:UNK:C	37:M:386:UNK:N	2.72	0.49
1:c:349:ALA:HB3	1:c:408:ARG:HG2	1.95	0.49
2:m:207:ILE:HG22	2:m:379:LEU:HD12	1.95	0.49
3:b:88:SER:HB3	3:b:250:LEU:HD21	1.95	0.49
6:f:51:PRO:HG3	2:n:134:ARG:HH12	1.78	0.49
2:n:227:ARG:HD2	2:n:227:ARG:N	2.27	0.49
3:o:284:ILE:CG2	3:o:285:PRO:HD2	2.43	0.49
3:o:341:GLN:O	3:o:342:PRO:C	2.55	0.49
27:C:117:UNK:O	27:C:142:UNK:HA	2.13	0.49
29:E:109:UNK:C	29:E:111:UNK:N	2.73	0.49
30:F:300:UNK:CA	30:F:329:UNK:CA	2.90	0.49
31:G:425:UNK:O	31:G:429:UNK:N	2.45	0.49
32:H:257:UNK:O	32:H:261:UNK:N	2.46	0.49
36:L:281:UNK:CB	36:L:315:UNK:CA	2.91	0.49
47:X:46:UNK:C	47:X:48:UNK:N	2.72	0.49
53:d:301:HEC:HHA	53:d:301:HEC:HBD1	1.95	0.49
1:l:80:GLU:O	1:l:82:MET:N	2.46	0.49
1:l:349:ALA:HB3	1:l:408:ARG:HE	1.78	0.49
3:o:278:TYR:O	3:o:279:ALA:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:134:TYR:HE2	4:p:163:PRO:CG	2.25	0.49
5:q:103:LYS:HA	5:q:106:ILE:CD1	2.43	0.49
6:r:7:SER:O	6:r:11:ARG:HD2	2.13	0.49
7:s:71:ARG:O	7:s:73:ASN:N	2.46	0.49
12:x:397:PHE:HB3	12:x:398:PRO:HD3	1.95	0.49
13:y:186:SER:HB3	13:y:213:LEU:CD2	2.42	0.49
27:C:31:UNK:C	27:C:33:UNK:N	2.75	0.49
30:F:191:UNK:O	30:F:195:UNK:N	2.46	0.49
47:X:41:UNK:O	47:X:44:UNK:N	2.46	0.49
3:b:103:TYR:HA	3:b:315:MET:CE	2.32	0.48
3:b:312:GLN:O	3:b:313:ARG:C	2.53	0.48
1:l:62:LEU:HB3	1:l:122:LEU:HD22	1.94	0.48
1:l:100:LYS:HD2	1:l:373:THR:OG1	2.13	0.48
1:l:161:THR:HB	1:l:162:PRO:CD	2.41	0.48
1:l:385:THR:CG2	1:l:386:TYR:CD1	2.96	0.48
2:n:72:ALA:HB2	2:n:140:LEU:CD2	2.43	0.48
2:n:254:HIS:O	2:n:426:ALA:HA	2.13	0.48
3:o:192:ILE:HD13	3:o:192:ILE:N	2.28	0.48
5:q:15:ARG:CB	5:q:16:PRO:CD	2.74	0.48
17:3:49:VAL:HG21	17:3:74:LEU:HD12	1.95	0.48
19:5:24:ASN:ND2	19:5:26:THR:H	2.11	0.48
27:C:112:UNK:N	27:C:113:UNK:HA	2.27	0.48
28:D:116:UNK:O	28:D:120:UNK:N	2.46	0.48
31:G:75:UNK:C	31:G:77:UNK:N	2.73	0.48
31:G:173:UNK:O	31:G:183:UNK:O	2.30	0.48
35:K:40:UNK:O	35:K:43:UNK:CB	2.61	0.48
38:N:267:UNK:O	38:N:271:UNK:N	2.45	0.48
47:X:40:UNK:O	47:X:44:UNK:N	2.46	0.48
1:c:43:ALA:HB2	1:c:189:HIS:HB3	1.94	0.48
1:c:106:LEU:O	1:c:107:PRO:C	2.56	0.48
4:d:7:PRO:CB	4:d:125:ASP:HB3	2.43	0.48
4:d:24:THR:O	4:d:25:SER:C	2.53	0.48
4:d:82:MET:SD	4:d:86:LYS:NZ	2.83	0.48
4:d:138:PRO:HB3	8:h:55:THR:CA	2.43	0.48
4:d:224:ARG:NH2	7:g:27:PRO:HD2	2.28	0.48
4:d:230:LEU:O	4:d:233:ARG:HB2	2.12	0.48
6:f:73:GLN:HA	7:g:39:ARG:NH2	2.28	0.48
1:l:431:LEU:HD12	1:l:432:PRO:HD2	1.95	0.48
2:n:79:GLY:H	2:n:125:ASN:ND2	2.11	0.48
2:n:237:ALA:HB2	2:n:318:ASP:CG	2.37	0.48
2:n:257:LEU:CD1	2:n:424:MET:HB2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:2:ASP:HB3	4:p:156:GLN:NE2	2.27	0.48
4:p:10:TYR:CE1	8:t:73:LEU:HD22	2.47	0.48
5:q:102:THR:O	5:q:105:GLU:N	2.46	0.48
12:x:476:PHE:CD1	23:9:15:VAL:HG21	2.48	0.48
18:4:42:ARG:NH1	18:4:74:ARG:HH21	2.10	0.48
27:C:56:UNK:O	27:C:58:UNK:N	2.47	0.48
29:E:62:UNK:O	29:E:65:UNK:N	2.46	0.48
30:F:150:UNK:O	30:F:153:UNK:N	2.47	0.48
31:G:30:UNK:O	31:G:33:UNK:CB	2.61	0.48
35:K:11:UNK:O	35:K:12:UNK:C	2.61	0.48
36:L:161:UNK:CB	36:L:162:UNK:CA	2.90	0.48
36:L:306:UNK:O	36:L:307:UNK:C	2.60	0.48
37:M:275:UNK:C	37:M:278:UNK:CB	2.91	0.48
40:P:203:UNK:CA	40:P:234:UNK:CA	2.86	0.48
41:Q:115:UNK:O	41:Q:116:UNK:C	2.61	0.48
1:c:335:MET:CE	1:c:339:GLN:HG3	2.42	0.48
2:m:187:THR:HG23	2:m:190:GLU:OE1	2.13	0.48
2:m:303:VAL:CG1	2:m:304:HIS:H	2.26	0.48
3:b:44:GLN:HE22	3:b:86:GLY:HA3	1.78	0.48
3:b:269:LYS:CD	3:b:340:GLY:HA2	2.43	0.48
3:b:338:ILE:HA	3:b:341:GLN:CG	2.43	0.48
4:d:32:VAL:CB	4:d:186:VAL:HG22	2.43	0.48
4:d:131:LEU:HD22	4:d:163:PRO:HB3	1.95	0.48
4:d:224:ARG:HH21	7:g:27:PRO:HD2	1.78	0.48
8:h:40:CYS:O	8:h:44:VAL:HG23	2.12	0.48
1:l:158:PHE:HE1	1:l:317:THR:HG21	1.72	0.48
1:l:262:TRP:CE3	1:l:385:THR:HG21	2.48	0.48
4:p:31:GLN:O	4:p:32:VAL:C	2.56	0.48
4:p:168:VAL:HG12	4:p:169:LEU:CD2	2.42	0.48
5:q:65:SER:HG	5:q:67:ASP:HB3	1.79	0.48
5:q:158:CYS:SG	5:q:160:CYS:HB2	2.54	0.48
8:t:15:ASP:CB	8:t:16:PRO:CD	2.91	0.48
10:v:32:GLU:HG2	10:v:33:ARG:N	2.28	0.48
12:x:197:LEU:O	14:z:92:LEU:HD22	2.13	0.48
14:z:65:SER:HB3	14:z:71:HIS:CE1	2.48	0.48
27:C:28:UNK:O	27:C:31:UNK:N	2.46	0.48
28:D:183:UNK:HA	33:I:58:UNK:CB	2.43	0.48
32:H:241:UNK:O	32:H:242:UNK:CB	2.61	0.48
46:W:24:UNK:O	46:W:25:UNK:CB	2.56	0.48
47:X:90:UNK:C	47:X:92:UNK:N	2.76	0.48
1:c:261:GLY:HA2	1:c:314:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:381:GLU:O	2:m:384:SER:OG	2.24	0.48
4:d:158:ILE:HG13	53:d:301:HEC:HBD2	1.95	0.48
4:d:160:MET:HE2	4:d:163:PRO:HG3	1.95	0.48
4:d:217:PRO:HG2	4:d:218:LEU:H	1.78	0.48
5:e:72:SER:HB2	3:o:168:PHE:CE2	2.48	0.48
7:g:34:ILE:O	7:g:38:LEU:HG	2.14	0.48
1:l:406:VAL:O	1:l:410:VAL:HG23	2.13	0.48
1:l:436:ARG:HE	3:o:222:PRO:CD	2.26	0.48
2:n:267:ALA:O	2:n:268:GLU:C	2.56	0.48
2:n:360:ALA:O	2:n:363:LYS:N	2.47	0.48
3:o:345:HIS:CB	3:o:346:PRO:HD3	2.26	0.48
5:q:107:ASP:O	5:q:108:GLN:C	2.55	0.48
5:q:193:VAL:O	5:q:193:VAL:CG1	2.61	0.48
10:v:38:GLY:O	10:v:42:ILE:HG13	2.14	0.48
12:x:115:SER:O	12:x:121:GLY:HA2	2.14	0.48
13:y:59:GLN:O	13:y:62:GLU:HB2	2.13	0.48
29:E:33:UNK:O	29:E:36:UNK:N	2.47	0.48
30:F:45:UNK:O	30:F:48:UNK:CB	2.61	0.48
30:F:315:UNK:HA	30:F:316:UNK:C	2.42	0.48
38:N:201:UNK:O	38:N:202:UNK:C	2.57	0.48
1:c:43:ALA:HB1	1:c:189:HIS:HB3	1.94	0.48
1:c:426:GLY:CA	1:c:427:PRO:C	2.86	0.48
2:m:252:LEU:HD11	9:i:49:VAL:HB	1.95	0.48
2:m:381:GLU:OE1	2:m:381:GLU:HA	2.13	0.48
3:b:345:HIS:CB	3:b:346:PRO:CD	2.85	0.48
4:d:23:HIS:O	4:d:24:THR:C	2.55	0.48
4:d:116:ILE:HD11	4:d:120:ARG:HH11	1.78	0.48
4:d:237:TYR:HB2	6:f:60:PHE:CE1	2.47	0.48
6:f:51:PRO:CD	2:n:134:ARG:HH12	2.24	0.48
7:g:67:GLU:O	7:g:71:ARG:HB3	2.14	0.48
1:l:34:THR:HB	2:n:373:GLU:OE1	2.14	0.48
1:l:89:TYR:CD1	1:l:89:TYR:C	2.90	0.48
1:l:329:MET:CA	1:l:329:MET:HE3	2.44	0.48
2:n:197:ASN:HB2	2:n:198:HIS:CD2	2.49	0.48
3:o:248:ASP:CG	4:p:118:ARG:HH21	2.22	0.48
4:p:178:THR:O	4:p:179:MET:C	2.55	0.48
5:q:29:SER:CA	5:q:32:ARG:HD3	2.44	0.48
6:r:40:ASN:CG	6:r:41:ASP:H	2.20	0.48
13:y:59:GLN:N	13:y:62:GLU:HG3	2.24	0.48
28:D:84:UNK:O	28:D:85:UNK:CB	2.62	0.48
28:D:234:UNK:O	28:D:237:UNK:CA	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:190:UNK:CB	30:F:203:UNK:CA	2.83	0.48
30:F:262:UNK:CA	30:F:286:UNK:N	2.76	0.48
30:F:412:UNK:O	30:F:415:UNK:CB	2.61	0.48
30:F:426:UNK:C	30:F:428:UNK:N	2.70	0.48
31:G:49:UNK:C	31:G:51:UNK:N	2.76	0.48
33:I:76:UNK:O	33:I:77:CYS:C	2.54	0.48
40:P:145:UNK:O	40:P:149:UNK:N	2.47	0.48
50:U:415:UNK:O	50:U:418:UNK:CB	2.60	0.48
2:m:141:GLN:CB	2:m:142:PRO:HD3	2.41	0.48
3:b:26:ASN:N	6:f:70:MET:HB2	2.29	0.48
4:d:50:HIS:CE1	4:d:91:PHE:HZ	2.31	0.48
4:d:228:SER:HB2	7:g:23:GLN:HE21	1.74	0.48
5:e:40:THR:HG22	10:j:20:PHE:HZ	1.79	0.48
7:g:56:TYR:O	7:g:57:LEU:C	2.56	0.48
8:h:50:THR:HG22	8:h:51:GLU:N	2.29	0.48
1:l:255:ILE:O	1:l:321:GLY:HA3	2.14	0.48
1:l:280:TYR:O	1:l:306:SER:HA	2.14	0.48
2:n:362:ASN:O	2:n:363:LYS:C	2.57	0.48
3:o:51:LEU:HD21	3:o:79:ILE:HG22	1.95	0.48
3:o:64:SER:O	3:o:65:SER:C	2.55	0.48
3:o:322:GLN:HE21	3:o:326:TRP:HE1	1.62	0.48
4:p:66:GLU:O	4:p:69:GLU:HG2	2.13	0.48
5:q:153:PHE:HE1	5:q:173:LYS:CG	2.25	0.48
6:r:45:GLU:O	6:r:49:ARG:HG3	2.14	0.48
7:s:80:ASP:CG	8:t:47:ARG:HH22	2.22	0.48
11:w:34:SER:OG	11:w:35:ALA:N	2.46	0.48
20:6:39:VAL:O	20:6:42:LYS:HE2	2.14	0.48
30:F:431:UNK:O	30:F:434:UNK:CB	2.60	0.48
36:L:297:UNK:CA	36:L:356:UNK:N	2.73	0.48
37:M:287:UNK:O	37:M:288:UNK:C	2.57	0.48
38:N:16:UNK:O	38:N:19:UNK:N	2.45	0.48
38:N:137:UNK:O	38:N:138:UNK:C	2.56	0.48
39:O:229:UNK:CA	39:O:231:UNK:N	2.75	0.48
50:U:512:UNK:O	50:U:515:UNK:CB	2.62	0.48
1:c:61:HIS:CE1	1:c:134:ILE:HD11	2.49	0.48
1:c:84:ALA:HB1	1:c:100:LYS:O	2.14	0.48
1:c:385:THR:HB	1:c:386:TYR:CD1	2.48	0.48
2:m:213:HIS:O	2:m:213:HIS:HD2	1.96	0.48
3:b:218:ILE:CG2	3:b:223:TYR:CE2	2.97	0.48
6:f:45:GLU:O	6:f:46:ALA:O	2.31	0.48
9:i:70:LEU:HG	9:i:72:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:329:MET:HA	1:l:329:MET:HE3	1.95	0.48
3:o:107:TYR:HE1	3:o:305:PRO:HA	1.78	0.48
3:o:122:THR:CG2	3:o:189:ILE:HG12	2.44	0.48
3:o:218:ILE:HG23	3:o:223:TYR:CE2	2.49	0.48
3:o:233:LEU:CD2	4:p:219:VAL:HG21	2.44	0.48
5:q:33:LYS:HB2	10:v:10:TYR:CE1	2.49	0.48
5:q:122:HIS:ND1	5:q:124:LEU:HB2	2.29	0.48
12:x:266:GLU:HB2	12:x:267:PRO:HD2	1.94	0.48
18:4:5:LYS:NZ	18:4:5:LYS:HB3	2.27	0.48
25:A:90:UNK:O	25:A:93:UNK:N	2.47	0.48
27:C:28:UNK:O	27:C:31:UNK:CB	2.61	0.48
34:J:171:UNK:O	34:J:172:UNK:C	2.62	0.48
37:M:63:UNK:O	37:M:66:UNK:N	2.46	0.48
38:N:72:UNK:C	38:N:75:UNK:CB	2.92	0.48
38:N:168:UNK:O	38:N:169:UNK:C	2.61	0.48
40:P:206:UNK:O	40:P:209:UNK:N	2.47	0.48
47:X:72:UNK:CB	47:X:75:UNK:HA	2.43	0.48
3:b:110:LEU:HG	3:b:114:ASN:ND2	2.27	0.48
3:b:215:VAL:O	6:f:63:LYS:CE	2.62	0.48
3:b:284:ILE:CG2	3:b:285:PRO:HD2	2.44	0.48
4:d:69:GLU:HG3	4:d:84:PRO:HA	1.95	0.48
7:g:33:GLY:O	7:g:34:ILE:C	2.56	0.48
1:l:41:ILE:HD12	1:l:41:ILE:N	2.24	0.48
1:l:53:ASN:ND2	1:l:165:GLN:HG3	2.29	0.48
2:n:111:CYS:HB3	2:n:119:LEU:CD2	2.32	0.48
2:n:128:THR:HG23	2:n:226:ILE:HD11	1.96	0.48
2:n:304:HIS:CD2	2:n:305:GLN:H	2.30	0.48
2:n:312:PHE:HD1	9:u:58:GLN:O	1.97	0.48
3:o:126:THR:HG21	52:o:401:HEM:CAB	2.43	0.48
4:p:49:ARG:HG3	4:p:49:ARG:O	2.13	0.48
5:q:42:THR:O	5:q:45:VAL:N	2.45	0.48
5:q:163:SER:HA	5:q:173:LYS:O	2.14	0.48
28:D:310:UNK:O	28:D:314:UNK:N	2.46	0.48
31:G:285:UNK:HA	31:G:289:UNK:O	2.13	0.48
36:L:52:UNK:C	36:L:54:UNK:N	2.73	0.48
2:m:207:ILE:CG2	2:m:379:LEU:HD12	2.43	0.48
3:b:192:ILE:N	3:b:192:ILE:CD1	2.77	0.48
3:b:210:GLY:HA3	3:b:314:SER:CB	2.41	0.48
3:b:221:HIS:CB	3:b:222:PRO:CD	2.90	0.48
4:d:23:HIS:NE2	10:j:51:LEU:HA	2.29	0.48
4:d:36:VAL:HG23	4:d:169:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:18:VAL:HB	11:k:19:PRO:HD3	1.95	0.48
1:l:62:LEU:O	1:l:63:ALA:C	2.57	0.48
1:l:307:PHE:CD1	1:l:307:PHE:C	2.91	0.48
1:l:335:MET:O	1:l:335:MET:HE3	2.14	0.48
2:n:132:PHE:CE2	2:n:191:LEU:HD22	2.49	0.48
3:o:221:HIS:N	3:o:222:PRO:HD2	2.28	0.48
53:p:301:HEC:HHD	53:p:301:HEC:CBC	2.30	0.48
5:q:114:VAL:CG1	5:q:115:SER:N	2.73	0.48
6:r:46:ALA:O	6:r:47:ILE:C	2.53	0.48
21:7:8:LYS:NZ	21:7:8:LYS:HB3	2.29	0.48
30:F:322:UNK:HA	30:F:327:UNK:CB	2.43	0.48
30:F:364:UNK:O	30:F:367:UNK:CB	2.62	0.48
36:L:571:UNK:C	36:L:573:UNK:N	2.76	0.48
38:N:223:UNK:CB	38:N:224:UNK:HA	2.43	0.48
1:c:40:TRP:CZ2	1:c:377:GLU:CA	2.89	0.48
1:c:260:PRO:CD	1:c:414:TYR:CE1	2.92	0.48
2:m:360:ALA:O	2:m:363:LYS:HB2	2.14	0.48
3:b:132:VAL:HA	3:b:139:SER:CB	2.42	0.48
1:l:251:ALA:O	1:l:325:VAL:HA	2.14	0.48
1:l:379:ILE:O	1:l:383:LEU:HG	2.13	0.48
3:o:122:THR:HB	3:o:189:ILE:HD13	1.95	0.48
4:p:10:TYR:HD1	8:t:74:PHE:CD1	2.32	0.48
4:p:120:ARG:HG2	4:p:120:ARG:NH1	2.24	0.48
4:p:146:GLY:O	4:p:148:TYR:HD1	1.97	0.48
5:q:105:GLU:O	5:q:108:GLN:HB3	2.14	0.48
7:s:56:TYR:HD1	7:s:57:LEU:HD23	1.78	0.48
12:x:11:ASN:ND2	12:x:13:LYS:HB2	2.28	0.48
26:B:150:UNK:CA	59:B:201:SF4:S1	3.02	0.48
32:H:195:UNK:HA	32:H:198:UNK:HA	1.96	0.48
37:M:386:UNK:HA	37:M:390:UNK:HA	1.96	0.48
38:N:133:UNK:O	38:N:136:UNK:CB	2.62	0.48
38:N:149:UNK:O	38:N:150:UNK:C	2.61	0.48
43:S:19:UNK:HA	43:S:66:UNK:O	2.13	0.48
1:c:39:VAL:HG23	1:c:113:LEU:HD23	1.95	0.47
1:c:85:HIS:CE1	2:m:284:HIS:ND1	2.82	0.47
1:c:277:ILE:CG2	1:c:294:LEU:HD12	2.44	0.47
1:c:343:MET:H	1:c:343:MET:HG2	1.34	0.47
1:c:403:ASP:CB	1:c:406:VAL:HG23	2.33	0.47
2:m:38:LEU:O	2:m:39:GLU:C	2.56	0.47
2:m:47:ILE:CG2	2:m:48:GLY:N	2.77	0.47
2:m:76:THR:HG21	2:m:133:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:115:ILE:HG21	3:b:196:HIS:CB	2.33	0.47
3:b:147:THR:HG21	3:b:165:TRP:CD1	2.48	0.47
3:b:297:SER:O	3:b:300:ILE:CG2	2.62	0.47
4:d:7:PRO:HG3	4:d:126:TYR:CA	2.43	0.47
5:e:32:ARG:HH12	7:g:22:GLU:CD	2.21	0.47
1:l:33:PRO:O	1:l:103:SER:HB3	2.14	0.47
1:l:134:ILE:O	1:l:137:GLU:N	2.47	0.47
2:n:56:ARG:HH22	2:n:318:ASP:CG	2.18	0.47
3:o:119:LEU:HD23	52:o:402:HEM:C3B	2.49	0.47
4:p:10:TYR:CZ	4:p:128:PHE:CE2	2.92	0.47
4:p:131:LEU:HD22	4:p:163:PRO:HB2	1.96	0.47
4:p:220:TYR:CD2	7:s:26:PHE:CE1	3.02	0.47
5:q:141:HIS:HE2	5:q:175:PRO:HB2	1.78	0.47
10:v:52:TRP:CE3	10:v:52:TRP:N	2.82	0.47
10:v:61:ASN:O	10:v:62:LYS:HB2	2.13	0.47
12:x:184:PHE:H	12:x:256:HIS:CE1	2.29	0.47
13:y:22:HIS:CE1	20:6:44:LYS:HD3	2.49	0.47
36:L:48:UNK:O	36:L:52:UNK:N	2.46	0.47
36:L:111:UNK:O	36:L:114:UNK:N	2.47	0.47
36:L:604:UNK:CB	38:N:92:UNK:C	2.92	0.47
37:M:133:UNK:HA	37:M:224:UNK:CB	2.44	0.47
37:M:351:UNK:O	37:M:352:UNK:CB	2.62	0.47
38:N:157:UNK:O	38:N:158:UNK:C	2.60	0.47
38:N:255:UNK:HA	38:N:256:UNK:HA	1.66	0.47
50:U:318:UNK:O	50:U:322:UNK:N	2.47	0.47
1:c:239:SER:HB2	7:g:18:LEU:HD23	1.95	0.47
1:c:260:PRO:HG3	1:c:414:TYR:CZ	2.49	0.47
2:m:24:LEU:H	2:m:24:LEU:CD1	2.03	0.47
2:m:99:THR:O	2:m:99:THR:HG22	2.14	0.47
2:m:183:ILE:HG22	2:m:184:GLY:N	2.28	0.47
2:m:305:GLN:CB	2:m:306:PRO:HD3	2.31	0.47
2:m:341:TYR:O	2:m:342:ASN:C	2.57	0.47
3:b:24:PRO:O	3:b:224:TYR:OH	2.19	0.47
4:d:93:LYS:O	4:d:94:PRO:C	2.56	0.47
11:k:19:PRO:O	11:k:23:LEU:HG	2.14	0.47
1:l:34:THR:CB	2:n:373:GLU:OE1	2.62	0.47
3:o:21:LEU:HD12	3:o:22:PRO:HD2	1.94	0.47
3:o:147:THR:CG2	3:o:165:TRP:NE1	2.75	0.47
3:o:227:LYS:HG2	4:p:223:LYS:HZ3	1.78	0.47
5:q:46:GLY:O	5:q:49:TYR:HB3	2.14	0.47
5:q:96:LEU:CD2	5:q:195:VAL:HG21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:22:ASN:O	6:r:23:ALA:C	2.57	0.47
26:B:115:UNK:CB	26:B:120:UNK:CB	2.91	0.47
26:B:119:CYS:SG	59:B:201:SF4:S4	3.09	0.47
28:D:367:UNK:O	28:D:373:UNK:HA	2.14	0.47
30:F:125:UNK:O	30:F:128:UNK:CB	2.62	0.47
31:G:87:UNK:O	31:G:90:UNK:N	2.48	0.47
40:P:135:UNK:CA	40:P:168:UNK:N	2.72	0.47
42:R:59:UNK:O	42:R:70:UNK:HA	2.13	0.47
1:c:131:ARG:NH2	1:c:177:LEU:O	2.47	0.47
1:c:365:LEU:O	1:c:365:LEU:HG	2.15	0.47
2:m:76:THR:HG21	2:m:133:ARG:CZ	2.44	0.47
2:m:235:ALA:O	2:m:236:LYS:CB	2.61	0.47
4:d:82:MET:HE2	4:d:86:LYS:HZ2	1.76	0.47
4:d:102:ARG:HE	4:d:109:LEU:HB2	1.78	0.47
8:h:22:GLU:O	8:h:23:GLN:C	2.57	0.47
10:j:32:GLU:HG2	10:j:33:ARG:H	1.79	0.47
10:j:51:LEU:O	10:j:54:HIS:N	2.46	0.47
2:n:84:LYS:O	2:n:85:ILE:C	2.57	0.47
3:o:276:PHE:CG	3:o:277:ALA:N	2.82	0.47
5:q:18:VAL:HG21	7:s:22:GLU:OE1	2.14	0.47
5:q:127:VAL:CG1	5:q:133:VAL:HG23	2.44	0.47
6:r:35:ASP:OD1	6:r:89:TYR:OH	2.22	0.47
10:v:4:THR:HG22	10:v:6:THR:H	1.80	0.47
12:x:513:LEU:HD12	12:x:513:LEU:HA	1.65	0.47
26:B:123:UNK:N	26:B:126:UNK:C	2.72	0.47
35:K:41:UNK:O	35:K:42:UNK:C	2.58	0.47
36:L:339:UNK:O	36:L:342:UNK:N	2.47	0.47
37:M:133:UNK:C	37:M:224:UNK:CB	2.92	0.47
38:N:163:UNK:O	38:N:164:UNK:C	2.62	0.47
47:X:165:UNK:O	47:X:166:UNK:C	2.57	0.47
3:b:6:LYS:HG2	3:b:16:ASN:OD1	2.15	0.47
8:h:62:LEU:O	8:h:65:ARG:HG2	2.14	0.47
2:n:250:ASP:OD1	2:n:251:SER:N	2.47	0.47
2:n:286:LYS:O	2:n:287:ARG:HB2	2.14	0.47
3:o:221:HIS:N	3:o:222:PRO:CD	2.77	0.47
4:p:211:MET:O	4:p:214:LEU:N	2.41	0.47
5:q:94:LYS:HD2	5:q:138:VAL:HG21	1.97	0.47
6:r:103:GLU:O	6:r:104:ARG:C	2.55	0.47
15:1:68:PHE:HA	15:1:71:MET:HG2	1.95	0.47
30:F:163:UNK:N	30:F:166:UNK:CB	2.77	0.47
34:J:22:UNK:C	34:J:24:UNK:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:64:PHE:HE2	1:c:88:ALA:HB2	1.75	0.47
2:m:276:GLN:OE1	2:m:313:ASN:HB3	2.14	0.47
3:b:107:TYR:OH	3:b:308:HIS:ND1	2.09	0.47
6:f:49:ARG:NH2	6:f:100:GLU:OE2	2.47	0.47
7:g:44:CYS:O	7:g:45:ILE:C	2.57	0.47
3:o:47:THR:HG21	3:o:83:HIS:CB	2.43	0.47
3:o:130:GLY:HA3	3:o:182:HIS:CE1	2.49	0.47
3:o:269:LYS:CD	3:o:340:GLY:HA2	2.45	0.47
4:p:224:ARG:HH21	7:s:27:PRO:HD2	1.79	0.47
5:q:43:THR:HG22	5:q:44:THR:N	2.30	0.47
5:q:147:ILE:O	5:q:148:ALA:C	2.57	0.47
29:E:77:UNK:O	29:E:81:UNK:N	2.48	0.47
30:F:433:UNK:O	30:F:436:UNK:CB	2.63	0.47
31:G:377:UNK:N	31:G:449:UNK:CB	2.77	0.47
31:G:382:UNK:CB	31:G:454:UNK:CA	2.90	0.47
38:N:134:UNK:O	38:N:137:UNK:N	2.47	0.47
47:X:516:UNK:O	47:X:520:UNK:N	2.47	0.47
1:c:51:LYS:O	1:c:53:ASN:N	2.46	0.47
1:c:61:HIS:HB3	1:c:130:GLU:HG3	1.97	0.47
1:c:372:THR:O	1:c:373:THR:C	2.58	0.47
2:m:139:ALA:O	2:m:142:PRO:HD2	2.14	0.47
2:m:159:VAL:HG12	2:m:160:ILE:N	2.30	0.47
2:m:216:LEU:O	2:m:217:LYS:C	2.58	0.47
3:b:326:TRP:NE1	7:g:48:VAL:HG22	2.30	0.47
4:d:26:ILE:O	4:d:27:ARG:C	2.56	0.47
4:d:165:TYR:H	4:d:168:VAL:CG2	2.26	0.47
8:h:15:ASP:HB2	8:h:16:PRO:CD	2.45	0.47
1:l:436:ARG:HE	3:o:222:PRO:HG3	1.79	0.47
3:o:41:LEU:HD23	3:o:190:MET:HG3	1.96	0.47
3:o:277:ALA:O	3:o:278:TYR:C	2.57	0.47
3:o:341:GLN:HA	3:o:341:GLN:NE2	2.29	0.47
3:o:361:LEU:HD23	3:o:365:LEU:CD1	2.36	0.47
5:q:121:GLN:CG	5:q:179:ASN:ND2	2.77	0.47
5:q:170:ARG:O	5:q:172:ARG:HG2	2.15	0.47
5:q:182:VAL:C	5:q:183:PRO:O	2.57	0.47
13:y:63:THR:O	13:y:66:THR:HG22	2.15	0.47
15:1:33:LEU:HD13	15:1:41:LYS:HG3	1.97	0.47
30:F:209:UNK:CB	30:F:211:UNK:N	2.77	0.47
30:F:212:UNK:C	30:F:219:UNK:HA	2.44	0.47
32:H:126:UNK:O	32:H:130:UNK:CB	2.63	0.47
38:N:328:UNK:CB	50:U:209:UNK:CB	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:21:UNK:CB	40:P:45:UNK:CA	2.86	0.47
48:Y:62:UNK:O	48:Y:63:UNK:CB	2.63	0.47
1:c:52:ASN:HB2	1:c:55:ALA:HB2	1.97	0.47
1:c:60:GLU:OE1	1:c:90:SER:HB2	2.15	0.47
1:c:84:ALA:HB2	1:c:101:ALA:CB	2.37	0.47
1:c:89:TYR:C	1:c:89:TYR:HD1	2.21	0.47
1:c:277:ILE:HG22	1:c:294:LEU:HD12	1.96	0.47
1:c:379:ILE:CD1	1:c:390:ILE:HD12	2.41	0.47
2:m:140:LEU:O	2:m:142:PRO:N	2.47	0.47
2:m:207:ILE:HG22	2:m:379:LEU:CD1	2.44	0.47
3:b:105:GLY:HA2	3:b:107:TYR:CE1	2.50	0.47
4:d:232:SER:CB	7:g:23:GLN:OE1	2.63	0.47
5:e:65:SER:OG	5:e:67:ASP:HB3	2.15	0.47
6:f:36:THR:O	6:f:36:THR:HG22	2.14	0.47
7:g:11:ARG:HB3	7:g:12:HIS:CD2	2.50	0.47
7:g:50:PRO:CB	7:g:51:PRO:CD	2.92	0.47
1:l:43:ALA:HB1	1:l:189:HIS:HB3	1.97	0.47
1:l:61:HIS:CD2	2:n:287:ARG:HD3	2.49	0.47
1:l:64:PHE:HE1	1:l:86:LEU:CG	2.21	0.47
1:l:276:ILE:O	1:l:277:ILE:C	2.57	0.47
1:l:279:HIS:CE1	1:l:284:TYR:OH	2.68	0.47
1:l:361:LEU:HG	1:l:399:ILE:HD11	1.96	0.47
2:n:38:LEU:HD13	2:n:378:PHE:CE2	2.50	0.47
2:n:276:GLN:O	2:n:280:GLY:N	2.40	0.47
2:n:279:LEU:CD2	2:n:295:LEU:HD13	2.45	0.47
3:o:309:THR:HG23	3:o:310:SER:N	2.30	0.47
4:p:233:ARG:HG3	7:s:17:SER:CB	2.42	0.47
7:s:34:ILE:O	7:s:38:LEU:HG	2.14	0.47
8:t:73:LEU:CD2	8:t:74:PHE:HD1	2.28	0.47
12:x:172:LYS:HB2	12:x:172:LYS:HZ3	1.80	0.47
13:y:83:ILE:O	13:y:87:MET:HG3	2.14	0.47
14:z:137:LEU:HD12	14:z:137:LEU:HA	1.69	0.47
14:z:173:PHE:CD1	14:z:173:PHE:C	2.92	0.47
21:7:16:ASN:H	21:7:16:ASN:ND2	2.12	0.47
27:C:67:UNK:O	27:C:68:UNK:C	2.59	0.47
31:G:305:UNK:O	31:G:308:UNK:CB	2.63	0.47
31:G:564:UNK:CB	31:G:568:UNK:CB	2.93	0.47
32:H:199:UNK:O	32:H:200:UNK:CB	2.63	0.47
33:I:119:CYS:N	59:I:201:SF4:S4	2.88	0.47
37:M:168:UNK:CB	37:M:174:UNK:CB	2.93	0.47
38:N:73:UNK:C	38:N:75:UNK:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:26:UNK:O	45:V:30:UNK:N	2.48	0.47
50:U:25:UNK:O	50:U:26:UNK:C	2.55	0.47
50:U:622:UNK:C	50:U:624:UNK:N	2.71	0.47
1:c:21:ASN:CB	1:c:217:SER:CB	2.89	0.47
1:c:41:ILE:CD1	1:c:41:ILE:H	2.25	0.47
1:c:70:ARG:HB3	1:c:74:ALA:HB3	1.97	0.47
1:c:312:ILE:HB	1:c:319:LEU:HB2	1.97	0.47
2:m:141:GLN:HE22	2:m:186:VAL:HB	1.79	0.47
3:b:26:ASN:ND2	3:b:26:ASN:O	2.48	0.47
4:d:76:GLU:OE2	4:d:93:LYS:O	2.33	0.47
4:d:195:GLU:HG3	4:d:195:GLU:O	2.14	0.47
4:d:241:LYS:HE3	6:f:53:ASN:HB3	1.96	0.47
7:g:80:ASP:CG	8:h:47:ARG:HH22	2.22	0.47
1:l:61:HIS:HB3	1:l:130:GLU:HG3	1.97	0.47
1:l:75:LEU:HD12	1:l:112:LEU:HD11	1.96	0.47
1:l:260:PRO:HG3	1:l:414:TYR:CZ	2.50	0.47
2:n:262:ALA:HB3	2:n:269:ALA:CA	2.44	0.47
2:n:299:VAL:O	2:n:303:VAL:HG23	2.14	0.47
3:o:26:ASN:O	3:o:27:ILE:HG13	2.14	0.47
3:o:300:ILE:HD13	3:o:362:ILE:HG21	1.95	0.47
7:s:39:ARG:HA	7:s:42:ARG:HD2	1.96	0.47
10:v:56:LYS:HE2	10:v:60:GLU:OE1	2.15	0.47
14:z:164:PHE:O	14:z:168:THR:HG23	2.14	0.47
15:1:41:LYS:HD3	15:1:62:LEU:HD23	1.97	0.47
28:D:85:UNK:O	28:D:86:UNK:C	2.63	0.47
30:F:63:UNK:O	30:F:64:UNK:C	2.62	0.47
30:F:212:UNK:CA	30:F:220:UNK:H	2.28	0.47
33:I:99:UNK:C	33:I:104:UNK:CB	2.93	0.47
34:J:33:UNK:O	34:J:37:UNK:N	2.48	0.47
34:J:155:UNK:O	34:J:159:UNK:N	2.47	0.47
37:M:273:UNK:O	37:M:277:UNK:N	2.48	0.47
50:U:627:UNK:C	50:U:628:UNK:O	2.56	0.47
51:Z:511:UNK:C	51:Z:513:UNK:N	2.76	0.47
1:c:36:THR:CB	1:c:372:THR:HG22	2.44	0.47
1:c:64:PHE:HE2	1:c:88:ALA:CB	2.27	0.47
1:c:106:LEU:N	1:c:107:PRO:CD	2.77	0.47
3:b:278:TYR:O	3:b:279:ALA:C	2.55	0.47
3:b:376:LEU:HD13	6:f:20:TYR:CD2	2.50	0.47
6:f:73:GLN:HG2	7:g:36:ASN:HD21	1.78	0.47
1:l:40:TRP:HZ2	1:l:377:GLU:CB	2.28	0.47
2:n:269:ALA:O	2:n:270:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:338:LYS:O	2:n:339:ALA:C	2.58	0.47
3:o:9:PRO:HB2	3:o:12:LYS:HB2	1.96	0.47
3:o:107:TYR:CE1	3:o:305:PRO:HA	2.50	0.47
3:o:185:LEU:HB3	3:o:186:PRO:CD	2.35	0.47
3:o:372:ILE:O	3:o:375:LYS:N	2.45	0.47
4:p:218:LEU:HD23	4:p:218:LEU:HA	1.73	0.47
15:1:33:LEU:HD22	15:1:37:GLN:HB3	1.97	0.47
36:L:396:UNK:O	36:L:399:UNK:N	2.48	0.47
1:c:32:GLN:HG2	1:c:33:PRO:N	2.30	0.47
1:c:236:PHE:CD2	1:c:258:GLU:CG	2.92	0.47
1:c:433:ASP:O	1:c:434:TYR:C	2.56	0.47
2:m:37:SER:HB3	2:m:213:HIS:HB2	1.97	0.47
2:m:135:TRP:NE1	2:m:136:GLU:HG3	2.30	0.47
3:b:334:THR:O	3:b:337:TRP:HB3	2.15	0.47
3:b:378:LYS:NZ	6:f:91:GLU:OE1	2.47	0.47
4:d:220:TYR:O	4:d:221:ALA:C	2.56	0.47
1:l:37:VAL:HG13	1:l:199:ALA:CB	2.45	0.47
1:l:46:ARG:HB3	1:l:92:ARG:O	2.16	0.47
1:l:277:ILE:H	1:l:277:ILE:HG12	1.41	0.47
3:o:61:THR:O	3:o:64:SER:N	2.48	0.47
5:q:99:ARG:NH1	5:q:156:TYR:CZ	2.83	0.47
5:q:188:THR:HG21	5:q:194:ILE:HG13	1.96	0.47
12:x:306:THR:HB	12:x:359:ALA:O	2.15	0.47
12:x:484:THR:HB	24:0:2:THR:OG1	2.15	0.47
12:x:507:GLU:O	12:x:508:PRO:O	2.32	0.47
15:1:102:TYR:CD2	24:0:35:TYR:HE1	2.34	0.47
25:A:76:UNK:C	25:A:78:UNK:N	2.71	0.47
31:G:248:UNK:O	31:G:249:UNK:CB	2.63	0.47
37:M:49:UNK:CA	37:M:50:UNK:CB	2.84	0.47
37:M:106:UNK:HA	37:M:109:UNK:CB	2.45	0.47
37:M:131:UNK:O	37:M:132:UNK:C	2.63	0.47
42:R:50:UNK:O	42:R:91:UNK:HA	2.15	0.47
51:Z:210:UNK:O	51:Z:213:UNK:CB	2.63	0.47
1:c:360:LEU:HD22	2:m:93:GLY:HA2	1.97	0.46
1:c:405:ARG:O	1:c:409:GLU:HG3	2.15	0.46
2:m:145:ARG:HG3	2:m:183:ILE:HD13	1.97	0.46
2:m:218:GLN:O	2:m:221:GLU:HB2	2.15	0.46
3:b:136:GLY:O	3:b:139:SER:N	2.49	0.46
4:d:161:ALA:O	4:d:163:PRO:HD3	2.14	0.46
4:d:168:VAL:HG12	4:d:169:LEU:HD23	1.97	0.46
5:e:65:SER:O	5:e:66:ALA:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:95:LYS:O	6:f:96:GLU:C	2.57	0.46
1:l:57:TYR:HE2	1:l:134:ILE:HD12	1.80	0.46
1:l:64:PHE:HA	1:l:75:LEU:HD23	1.96	0.46
1:l:70:ARG:HB3	1:l:74:ALA:HB3	1.97	0.46
1:l:130:GLU:O	1:l:131:ARG:C	2.57	0.46
2:n:262:ALA:HB2	2:n:272:PHE:CE2	2.48	0.46
3:o:153:ILE:CG2	3:o:154:PRO:HD2	2.45	0.46
3:o:218:ILE:CD1	4:p:230:LEU:HD13	2.45	0.46
5:q:15:ARG:HH21	5:q:32:ARG:CB	2.27	0.46
5:q:122:HIS:CE1	5:q:124:LEU:HD12	2.50	0.46
5:q:134:ILE:HD11	5:q:185:TYR:CD1	2.48	0.46
15:1:108:PRO:HG2	15:1:111:PHE:CD2	2.50	0.46
17:3:31:TYR:HE1	17:3:98:HIS:HE1	1.62	0.46
28:D:89:UNK:O	28:D:92:UNK:N	2.48	0.46
28:D:234:UNK:O	28:D:235:UNK:C	2.63	0.46
28:D:328:UNK:O	28:D:329:UNK:C	2.58	0.46
30:F:423:UNK:C	30:F:425:UNK:N	2.72	0.46
31:G:455:UNK:O	31:G:456:UNK:CB	2.62	0.46
31:G:488:UNK:O	31:G:489:UNK:C	2.61	0.46
36:L:225:UNK:C	36:L:229:UNK:CB	2.93	0.46
37:M:157:UNK:O	37:M:160:UNK:N	2.48	0.46
37:M:188:UNK:CB	37:M:189:UNK:CA	2.93	0.46
39:O:25:UNK:O	39:O:124:UNK:N	2.48	0.46
39:O:114:UNK:O	39:O:117:UNK:O	2.33	0.46
43:S:24:UNK:C	43:S:57:UNK:CB	2.87	0.46
45:V:32:UNK:O	45:V:36:UNK:N	2.48	0.46
1:c:67:THR:CG2	1:c:70:ARG:HB2	2.43	0.46
2:m:71:LEU:HD13	2:m:143:GLN:HG3	1.97	0.46
2:m:128:THR:C	2:m:130:PRO:HD2	2.39	0.46
3:b:63:PHE:O	3:b:67:THR:OG1	2.33	0.46
3:b:149:LEU:O	3:b:291:VAL:HG21	2.15	0.46
3:b:213:SER:O	3:b:214:ASP:C	2.56	0.46
4:d:220:TYR:CD2	7:g:26:PHE:CE1	3.03	0.46
7:g:36:ASN:O	7:g:37:VAL:C	2.56	0.46
10:j:52:TRP:N	10:j:52:TRP:HE3	2.14	0.46
1:l:4:TYR:O	1:l:5:ALA:C	2.56	0.46
1:l:45:SER:OG	1:l:92:ARG:HG2	2.15	0.46
1:l:236:PHE:HD2	1:l:258:GLU:CB	2.29	0.46
2:n:163:LEU:HD22	2:n:256:ALA:CB	2.45	0.46
3:o:208:PRO:O	3:o:314:SER:OG	2.30	0.46
3:o:313:ARG:CB	6:r:38:HIS:CD2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:30:PHE:CE1	4:p:50:HIS:CE1	3.03	0.46
4:p:64:LEU:O	4:p:68:VAL:HG23	2.15	0.46
5:q:40:THR:CG2	10:v:20:PHE:HZ	2.28	0.46
5:q:49:TYR:O	5:q:50:ALA:C	2.56	0.46
8:t:40:CYS:O	8:t:44:VAL:HG23	2.15	0.46
18:4:67:HIS:CD2	18:4:78:LEU:HD11	2.50	0.46
28:D:250:UNK:C	28:D:252:UNK:N	2.73	0.46
32:H:101:UNK:N	32:H:161:UNK:CA	2.73	0.46
34:J:45:UNK:O	34:J:46:UNK:CB	2.63	0.46
34:J:147:UNK:O	34:J:148:UNK:C	2.57	0.46
36:L:95:UNK:O	36:L:98:UNK:N	2.48	0.46
37:M:133:UNK:CB	37:M:224:UNK:CB	2.92	0.46
37:M:273:UNK:O	37:M:276:UNK:N	2.48	0.46
43:S:64:UNK:HA	43:S:77:UNK:C	2.44	0.46
50:U:411:UNK:O	50:U:413:UNK:N	2.48	0.46
2:m:308:ASP:OD2	9:i:54:SER:O	2.32	0.46
4:d:117:VAL:CG1	4:d:191:ARG:HH11	2.27	0.46
4:d:165:TYR:CD1	4:d:168:VAL:HG22	2.51	0.46
5:e:7:VAL:HG13	7:g:16:TYR:CD1	2.51	0.46
6:f:10:SER:HA	6:f:13:LEU:CD1	2.45	0.46
10:j:61:ASN:O	10:j:62:LYS:HB2	2.15	0.46
1:l:184:GLU:O	1:l:185:TYR:C	2.56	0.46
1:l:241:ILE:HG13	7:s:16:TYR:CD2	2.50	0.46
1:l:287:GLY:O	1:l:289:HIS:N	2.48	0.46
1:l:290:LEU:HD13	1:l:295:ALA:HB1	1.95	0.46
2:n:24:LEU:HD13	2:n:392:TYR:HD2	1.78	0.46
2:n:239:TYR:HE2	2:n:421:ARG:HB3	1.80	0.46
3:o:116:GLY:O	3:o:119:LEU:HB2	2.16	0.46
5:q:114:VAL:O	5:q:117:LEU:CB	2.62	0.46
5:q:122:HIS:ND1	5:q:124:LEU:N	2.57	0.46
5:q:171:ILE:O	5:q:171:ILE:CG2	2.62	0.46
12:x:172:LYS:HB3	12:x:176:MET:HE2	1.96	0.46
15:1:23:PRO:HB3	16:2:70:VAL:CG2	2.45	0.46
24:0:1:ILE:HG23	24:0:1:ILE:O	2.15	0.46
25:A:88:UNK:O	25:A:91:UNK:N	2.48	0.46
29:E:28:UNK:HA	29:E:31:UNK:CB	2.46	0.46
31:G:155:UNK:O	31:G:156:CYS:O	2.33	0.46
34:J:85:UNK:O	34:J:86:UNK:C	2.61	0.46
1:c:39:VAL:CG1	1:c:195:MET:CE	2.93	0.46
1:c:184:GLU:O	1:c:188:ARG:HG3	2.16	0.46
1:c:240:GLN:HE21	1:c:431:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:29:LEU:HD12	2:m:33:LEU:HD21	1.98	0.46
2:m:83:PHE:CZ	2:m:87:ARG:HG3	2.49	0.46
2:m:113:ARG:O	2:m:116:VAL:HG23	2.15	0.46
3:b:109:PHE:HD2	3:b:203:THR:HG1	1.59	0.46
1:l:28:GLU:OE1	1:l:375:VAL:HG11	2.15	0.46
1:l:245:GLU:C	1:l:247:GLY:H	2.24	0.46
2:n:327:ILE:O	2:n:327:ILE:CG2	2.62	0.46
2:n:396:SER:O	2:n:399:LEU:HB2	2.15	0.46
3:o:137:GLN:HE22	3:o:263:ASN:HB3	1.80	0.46
4:p:220:TYR:CD2	7:s:26:PHE:CZ	3.04	0.46
13:y:108:TYR:N	13:y:108:TYR:CD1	2.83	0.46
37:M:281:UNK:O	37:M:284:UNK:C	2.64	0.46
38:N:25:UNK:O	38:N:28:UNK:N	2.48	0.46
38:N:45:UNK:O	38:N:48:UNK:N	2.48	0.46
40:P:136:UNK:CA	40:P:137:UNK:C	2.93	0.46
40:P:301:UNK:CB	40:P:303:UNK:N	2.78	0.46
42:R:63:UNK:C	42:R:65:UNK:N	2.72	0.46
47:X:157:UNK:O	47:X:160:UNK:CB	2.64	0.46
1:c:243:HIS:CD2	1:c:425:PHE:CE2	3.04	0.46
3:b:51:LEU:CD2	3:b:79:ILE:CG2	2.93	0.46
3:b:80:ARG:HD3	3:b:80:ARG:C	2.39	0.46
3:b:125:ALA:HB3	3:b:185:LEU:HD21	1.98	0.46
3:b:299:LEU:HD22	3:b:299:LEU:HA	1.79	0.46
4:d:10:TYR:CE1	8:h:73:LEU:HD22	2.51	0.46
4:d:82:MET:CG	4:d:86:LYS:HZ2	2.28	0.46
1:l:43:ALA:CB	1:l:189:HIS:CB	2.94	0.46
1:l:223:TYR:CE1	51:Z:259:UNK:CB	2.98	0.46
2:n:62:ASN:HD21	2:n:65:THR:CB	2.28	0.46
2:n:198:HIS:HE1	2:n:233:SER:HB3	1.81	0.46
2:n:352:LEU:HD21	2:n:357:VAL:CG2	2.46	0.46
3:o:63:PHE:O	3:o:67:THR:OG1	2.33	0.46
4:p:115:TYR:O	4:p:119:ALA:N	2.47	0.46
5:q:141:HIS:HA	5:q:177:PRO:HD3	1.96	0.46
6:r:88:SER:O	6:r:92:PRO:HD2	2.15	0.46
13:y:58:ALA:O	13:y:60:GLU:HG3	2.16	0.46
27:C:89:UNK:CA	27:C:112:UNK:O	2.63	0.46
28:D:70:UNK:C	28:D:72:UNK:N	2.74	0.46
30:F:352:UNK:C	30:F:355:UNK:N	2.79	0.46
31:G:427:UNK:O	31:G:431:UNK:N	2.48	0.46
43:S:64:UNK:HA	43:S:78:UNK:CB	2.45	0.46
1:c:289:HIS:O	1:c:290:LEU:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:324:PHE:CG	1:c:334:MET:HG2	2.50	0.46
3:b:156:ILE:HG12	3:b:157:GLY:N	2.29	0.46
4:d:233:ARG:CG	7:g:17:SER:CB	2.94	0.46
5:e:33:LYS:HA	7:g:21:PHE:CD2	2.50	0.46
10:j:55:ILE:CG2	10:j:58:LYS:HE2	2.44	0.46
2:n:345:LYS:HG2	2:n:418:VAL:CG1	2.46	0.46
2:n:346:THR:HG23	2:n:351:ASN:HB3	1.96	0.46
3:o:44:GLN:OE1	3:o:83:HIS:CE1	2.69	0.46
3:o:116:GLY:HA3	52:o:402:HEM:C3C	2.51	0.46
3:o:183:PHE:CE1	3:o:187:PHE:CE2	3.03	0.46
5:q:14:ARG:H	5:q:14:ARG:HG2	1.53	0.46
5:q:99:ARG:HD3	5:q:156:TYR:HH	1.78	0.46
5:q:109:GLU:HG2	5:q:167:ALA:CB	2.25	0.46
12:x:299:VAL:HA	12:x:302:ARG:NH1	2.31	0.46
21:7:11:LEU:O	21:7:11:LEU:HD23	2.15	0.46
28:D:101:UNK:O	28:D:104:UNK:N	2.48	0.46
36:L:545:UNK:O	36:L:548:UNK:N	2.49	0.46
38:N:40:UNK:O	38:N:41:UNK:C	2.61	0.46
47:X:719:UNK:O	47:X:723:UNK:N	2.49	0.46
48:Y:43:UNK:O	48:Y:44:UNK:C	2.57	0.46
50:U:1:UNK:O	50:U:2:UNK:C	2.64	0.46
1:c:64:PHE:CE1	1:c:86:LEU:CG	2.81	0.46
1:c:120:CYS:HB2	1:c:122:LEU:HD21	1.96	0.46
1:c:192:ALA:HA	1:c:194:ARG:N	2.31	0.46
1:c:332:ASP:OD1	1:c:332:ASP:O	2.34	0.46
2:m:160:ILE:HD13	2:m:160:ILE:N	2.31	0.46
2:m:242:GLY:H	2:m:423:SER:HB3	1.79	0.46
2:m:262:ALA:HB3	2:m:269:ALA:N	2.31	0.46
2:m:279:LEU:HD23	2:m:295:LEU:HD13	1.94	0.46
3:b:8:HIS:O	3:b:9:PRO:C	2.57	0.46
3:b:31:TRP:CD2	3:b:100:ARG:HD2	2.50	0.46
3:b:108:THR:CB	3:b:313:ARG:HH11	2.27	0.46
3:b:373:GLU:HA	3:b:376:LEU:HD12	1.97	0.46
5:e:15:ARG:HH21	5:e:32:ARG:CG	2.29	0.46
6:f:46:ALA:O	6:f:47:ILE:C	2.56	0.46
1:l:24:ARG:CG	1:l:196:VAL:HG22	2.45	0.46
2:n:276:GLN:OE1	2:n:313:ASN:HB3	2.15	0.46
2:n:308:ASP:OD1	2:n:308:ASP:C	2.57	0.46
3:o:26:ASN:ND2	3:o:26:ASN:O	2.48	0.46
3:o:115:ILE:HG22	3:o:196:HIS:HB2	1.98	0.46
3:o:269:LYS:HA	3:o:270:PRO:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:312:GLN:NE2	3:o:317:PHE:HB2	2.30	0.46
4:p:143:LEU:HD11	4:p:149:PHE:HB2	1.98	0.46
6:r:7:SER:O	6:r:11:ARG:HB2	2.16	0.46
12:x:195:LEU:CD2	12:x:245:ILE:HD13	2.45	0.46
13:y:1:MET:SD	13:y:133:LEU:HD11	2.56	0.46
13:y:76:ILE:O	13:y:79:PRO:HD2	2.16	0.46
15:l:66:GLU:O	16:2:66:ARG:NH2	2.49	0.46
17:3:40:SER:OG	17:3:45:ASP:HB3	2.16	0.46
26:B:90:UNK:C	26:B:119:CYS:HB3	2.46	0.46
33:I:26:UNK:C	33:I:28:UNK:N	2.78	0.46
36:L:169:UNK:O	36:L:173:UNK:N	2.49	0.46
37:M:127:UNK:O	37:M:128:UNK:C	2.60	0.46
37:M:140:UNK:C	37:M:142:UNK:N	2.74	0.46
37:M:255:UNK:O	37:M:258:UNK:CB	2.63	0.46
38:N:72:UNK:HA	38:N:75:UNK:CB	2.46	0.46
45:V:56:UNK:O	45:V:60:UNK:N	2.49	0.46
47:X:423:UNK:O	47:X:426:UNK:N	2.49	0.46
51:Z:605:UNK:C	51:Z:607:UNK:N	2.78	0.46
2:m:227:ARG:N	2:m:227:ARG:HD2	2.30	0.46
2:m:312:PHE:N	2:m:323:GLY:O	2.47	0.46
3:b:28:SER:CB	3:b:30:TRP:HD1	2.28	0.46
3:b:108:THR:O	3:b:110:LEU:N	2.46	0.46
3:b:246:ALA:N	3:b:247:PRO:HD3	2.31	0.46
4:d:74:PRO:CG	4:d:82:MET:HB3	2.46	0.46
6:f:28:LYS:HB3	6:f:74:ILE:CD1	2.44	0.46
9:i:62:ARG:H	9:i:63:PRO:HD2	1.76	0.46
10:j:55:ILE:O	10:j:58:LYS:HD2	2.14	0.46
1:l:236:PHE:CD2	1:l:258:GLU:CG	2.94	0.46
1:l:252:HIS:O	1:l:424:GLY:HA2	2.16	0.46
1:l:408:ARG:HH12	11:w:15:ARG:CD	2.28	0.46
2:n:35:ILE:HD11	2:n:213:HIS:CD2	2.50	0.46
4:p:183:ALA:HA	4:p:186:VAL:HG23	1.97	0.46
5:q:63:SER:O	5:q:64:ALA:CB	2.60	0.46
5:q:120:PRO:O	5:q:121:GLN:NE2	2.49	0.46
5:q:122:HIS:HB3	5:q:125:GLU:HG3	1.97	0.46
6:r:64:ARG:O	6:r:68:LEU:HD12	2.16	0.46
12:x:32:ALA:HB3	23:9:36:PRO:HG2	1.98	0.46
14:z:80:ARG:O	14:z:84:ILE:HG12	2.14	0.46
17:3:31:TYR:HE1	17:3:98:HIS:CE1	2.34	0.46
25:A:103:UNK:C	25:A:106:UNK:N	2.79	0.46
32:H:125:UNK:O	32:H:129:UNK:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:K:19:UNK:O	35:K:20:UNK:CB	2.61	0.46
36:L:108:UNK:O	36:L:111:UNK:N	2.49	0.46
36:L:316:UNK:O	36:L:319:UNK:CA	2.64	0.46
40:P:161:UNK:O	40:P:162:UNK:O	2.34	0.46
40:P:173:UNK:O	40:P:176:UNK:CB	2.63	0.46
1:c:146:ARG:NH2	1:c:308:GLN:NE2	2.58	0.46
2:m:56:ARG:HH22	2:m:318:ASP:CG	2.22	0.46
3:b:40:CYS:HB3	3:b:90:PHE:HD2	1.81	0.46
3:b:200:LEU:O	3:b:200:LEU:HG	2.15	0.46
3:b:310:SER:OG	3:b:311:LYS:N	2.48	0.46
4:d:35:GLN:HB2	4:d:169:LEU:HD11	1.98	0.46
6:f:50:LEU:HA	6:f:51:PRO:HD2	1.74	0.46
1:l:39:VAL:CG1	1:l:41:ILE:HD11	2.40	0.46
1:l:192:ALA:HA	1:l:194:ARG:N	2.31	0.46
1:l:430:GLN:CG	1:l:430:GLN:O	2.63	0.46
2:n:159:VAL:CG1	2:n:160:ILE:HD13	2.40	0.46
2:n:360:ALA:O	2:n:361:LYS:C	2.58	0.46
3:o:248:ASP:O	3:o:249:LEU:C	2.58	0.46
3:o:316:MET:HE2	3:o:317:PHE:CZ	2.51	0.46
4:p:161:ALA:O	4:p:163:PRO:N	2.49	0.46
10:v:52:TRP:HE3	10:v:52:TRP:H	1.62	0.46
26:B:147:UNK:O	26:B:151:UNK:CB	2.64	0.46
32:H:43:UNK:N	32:H:44:UNK:CA	2.70	0.46
36:L:128:UNK:O	36:L:129:UNK:C	2.61	0.46
36:L:314:UNK:O	36:L:317:UNK:N	2.49	0.46
37:M:432:UNK:O	37:M:435:UNK:N	2.49	0.46
40:P:233:UNK:N	40:P:234:UNK:HA	2.31	0.46
42:R:82:UNK:O	42:R:90:UNK:HA	2.16	0.46
47:X:93:UNK:HA	47:X:94:UNK:CB	2.46	0.46
47:X:111:UNK:O	47:X:112:UNK:C	2.63	0.46
48:Y:98:UNK:O	48:Y:99:UNK:C	2.64	0.46
1:c:91:THR:HG22	1:c:92:ARG:N	2.31	0.46
1:c:184:GLU:O	1:c:185:TYR:C	2.59	0.46
1:c:277:ILE:H	1:c:277:ILE:HG12	1.53	0.46
2:m:84:LYS:HG3	2:m:122:PHE:HZ	1.80	0.46
2:m:161:GLU:CD	2:m:175:SER:HB2	2.40	0.46
2:m:299:VAL:CG1	2:m:303:VAL:HG21	2.46	0.46
2:m:338:LYS:HD3	2:m:439:LEU:CD2	2.46	0.46
3:b:136:GLY:O	3:b:138:MET:N	2.49	0.46
3:b:221:HIS:CB	3:b:222:PRO:HD3	2.22	0.46
4:d:25:SER:O	4:d:26:ILE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:44:CYS:O	7:g:47:ARG:N	2.47	0.46
8:h:50:THR:HG22	8:h:52:GLU:N	2.13	0.46
1:l:49:SER:N	1:l:52:ASN:OD1	2.41	0.46
2:n:141:GLN:CB	2:n:142:PRO:HD3	2.46	0.46
3:o:183:PHE:CD1	3:o:183:PHE:C	2.94	0.46
3:o:264:THR:O	3:o:266:PRO:HD3	2.16	0.46
5:q:138:VAL:O	5:q:139:CYS:C	2.59	0.46
6:r:48:ARG:HD3	6:r:48:ARG:HA	1.51	0.46
13:y:185:MET:SD	13:y:185:MET:C	2.98	0.46
22:8:9:PHE:HD1	22:8:10:HIS:HD2	1.64	0.46
28:D:146:UNK:O	28:D:147:UNK:C	2.62	0.46
30:F:61:UNK:O	30:F:64:UNK:CB	2.64	0.46
31:G:260:UNK:C	31:G:262:UNK:N	2.78	0.46
34:J:56:UNK:O	34:J:60:UNK:CB	2.64	0.46
37:M:38:UNK:O	37:M:41:UNK:N	2.49	0.46
38:N:91:UNK:CA	38:N:92:UNK:CB	2.94	0.46
47:X:710:UNK:O	47:X:713:UNK:N	2.49	0.46
48:Y:69:UNK:CB	48:Y:98:UNK:CB	2.93	0.46
1:c:255:ILE:HG13	1:c:422:VAL:HG22	1.98	0.45
2:m:264:ILE:HG21	2:m:317:SER:HA	1.97	0.45
2:m:285:VAL:O	2:m:285:VAL:HG12	2.16	0.45
2:m:334:GLY:O	2:m:335:ASP:C	2.59	0.45
3:b:280:ILE:HD13	3:b:280:ILE:H	1.80	0.45
3:b:347:TYR:O	3:b:348:ILE:C	2.59	0.45
4:d:116:ILE:HD11	4:d:120:ARG:HG3	1.97	0.45
6:f:37:ILE:CD1	6:f:43:VAL:HG22	2.47	0.45
1:l:11:VAL:CG1	1:l:12:PRO:HD2	2.46	0.45
1:l:50:GLU:O	1:l:173:ASN:ND2	2.49	0.45
1:l:392:LEU:O	1:l:392:LEU:HG	2.09	0.45
1:l:394:GLU:O	1:l:397:SER:N	2.49	0.45
2:n:129:ALA:O	2:n:130:PRO:C	2.58	0.45
4:p:137:PRO:HA	4:p:138:PRO:HD3	1.58	0.45
4:p:240:PRO:CG	4:p:241:LYS:N	2.79	0.45
5:q:133:VAL:HG13	5:q:133:VAL:O	2.15	0.45
12:x:147:ILE:HD11	12:x:209:LEU:HD23	1.98	0.45
12:x:498:CYS:HA	12:x:499:PRO:HA	1.78	0.45
26:B:65:UNK:CA	26:B:68:UNK:CB	2.94	0.45
28:D:179:UNK:O	28:D:183:UNK:N	2.50	0.45
30:F:178:UNK:C	30:F:179:UNK:O	2.58	0.45
31:G:162:UNK:O	31:G:166:UNK:N	2.49	0.45
31:G:229:UNK:O	31:G:235:UNK:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:61:UNK:CA	36:L:80:UNK:CB	2.93	0.45
36:L:544:UNK:O	36:L:545:UNK:C	2.61	0.45
37:M:113:UNK:CA	37:M:114:UNK:CB	2.89	0.45
40:P:139:UNK:CA	40:P:140:UNK:CB	2.88	0.45
41:Q:99:UNK:CA	41:Q:100:UNK:CB	2.76	0.45
47:X:309:UNK:O	47:X:310:UNK:C	2.62	0.45
49:a:106:UNK:O	49:a:108:UNK:N	2.49	0.45
50:U:320:UNK:O	50:U:324:UNK:CB	2.64	0.45
1:c:39:VAL:HG22	1:c:197:LEU:HD22	1.98	0.45
2:m:56:ARG:HH21	2:m:103:GLU:CD	2.25	0.45
2:m:262:ALA:HB2	2:m:268:GLU:HB3	1.98	0.45
3:b:152:ALA:CA	3:b:287:LYS:HZ2	2.30	0.45
3:b:345:HIS:N	3:b:346:PRO:HD2	2.29	0.45
4:d:10:TYR:CE1	4:d:128:PHE:HE2	2.34	0.45
4:d:116:ILE:HD12	4:d:116:ILE:HA	1.69	0.45
2:n:50:PHE:CE1	2:n:207:ILE:HG13	2.52	0.45
2:n:159:VAL:CG1	2:n:160:ILE:N	2.79	0.45
2:n:235:ALA:O	2:n:236:LYS:CB	2.65	0.45
4:p:82:MET:HE2	4:p:86:LYS:HZ2	1.82	0.45
5:q:186:GLU:HG3	5:q:186:GLU:O	2.16	0.45
13:y:4:PRO:HB2	22:8:43:SER:HA	1.96	0.45
18:4:42:ARG:HG3	18:4:42:ARG:NH1	2.32	0.45
28:D:117:UNK:O	28:D:120:UNK:N	2.49	0.45
39:O:185:UNK:O	39:O:186:UNK:C	2.55	0.45
44:T:62:UNK:O	44:T:63:UNK:C	2.64	0.45
50:U:125:UNK:O	50:U:128:UNK:CB	2.64	0.45
2:m:83:PHE:CZ	6:r:104:ARG:HG2	2.52	0.45
2:m:304:HIS:CD2	2:m:305:GLN:N	2.85	0.45
3:b:90:PHE:CE1	3:b:123:VAL:HG11	2.52	0.45
4:d:23:HIS:CD2	10:j:50:LYS:O	2.70	0.45
4:d:80:MET:H	4:d:80:MET:HG2	1.47	0.45
4:d:98:PRO:O	4:d:101:ALA:HB3	2.16	0.45
6:f:67:ASP:HA	6:f:70:MET:HE2	1.99	0.45
7:g:48:VAL:O	7:g:51:PRO:HD2	2.16	0.45
7:g:71:ARG:O	7:g:73:ASN:N	2.50	0.45
1:l:16:VAL:HG11	1:l:388:ARG:HB2	1.98	0.45
1:l:279:HIS:ND1	1:l:284:TYR:OH	2.39	0.45
1:l:430:GLN:O	1:l:430:GLN:HG2	2.16	0.45
2:n:203:ARG:NH2	2:n:230:LEU:HD23	2.31	0.45
2:n:271:ALA:O	2:n:272:PHE:C	2.57	0.45
3:o:102:LEU:HA	3:o:102:LEU:HD23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:277:ALA:HB1	3:o:294:LEU:HD11	1.98	0.45
4:p:138:PRO:CB	8:t:55:THR:HA	2.46	0.45
18:4:44:ARG:HA	18:4:45:PRO:HD2	1.75	0.45
28:D:101:UNK:C	28:D:103:UNK:N	2.75	0.45
39:O:85:UNK:O	39:O:86:UNK:C	2.61	0.45
40:P:136:UNK:CA	40:P:137:UNK:CB	2.85	0.45
40:P:145:UNK:O	40:P:148:UNK:CA	2.64	0.45
40:P:145:UNK:O	40:P:148:UNK:N	2.49	0.45
43:S:64:UNK:N	43:S:78:UNK:CB	2.78	0.45
51:Z:205:UNK:O	51:Z:208:UNK:CA	2.65	0.45
1:c:17:SER:HB2	1:c:25:VAL:HB	1.99	0.45
1:c:389:ARG:C	1:c:391:PRO:HD3	2.41	0.45
2:m:395:PRO:O	2:m:396:SER:C	2.59	0.45
3:b:61:THR:O	3:b:64:SER:HB3	2.16	0.45
3:b:165:TRP:HA	3:b:174:THR:OG1	2.16	0.45
4:d:28:ARG:HB2	4:d:185:ASP:HB3	1.99	0.45
1:l:243:HIS:O	1:l:425:PHE:HA	2.16	0.45
3:o:252:ASP:CB	3:o:253:PRO:CD	2.90	0.45
7:s:68:LYS:O	7:s:69:SER:C	2.58	0.45
28:D:300:UNK:O	28:D:301:UNK:C	2.63	0.45
30:F:351:UNK:O	30:F:354:UNK:CB	2.63	0.45
35:K:44:UNK:O	35:K:45:UNK:C	2.61	0.45
36:L:203:UNK:HA	36:L:204:UNK:HA	1.87	0.45
36:L:207:UNK:HA	36:L:208:UNK:C	2.45	0.45
37:M:87:UNK:HA	37:M:89:UNK:HA	1.98	0.45
37:M:225:UNK:CB	37:M:228:UNK:CB	2.95	0.45
37:M:448:UNK:O	37:M:449:UNK:C	2.61	0.45
38:N:135:UNK:C	38:N:137:UNK:N	2.78	0.45
39:O:138:UNK:O	39:O:141:UNK:N	2.49	0.45
48:Y:94:UNK:O	48:Y:97:UNK:CB	2.65	0.45
49:a:141:UNK:O	49:a:142:UNK:C	2.64	0.45
50:U:409:UNK:O	50:U:412:UNK:CB	2.64	0.45
1:c:369:LEU:HD21	1:c:378:ASP:OD2	2.16	0.45
4:d:168:VAL:HG12	4:d:169:LEU:CD2	2.47	0.45
7:g:34:ILE:CB	7:g:35:PRO:CD	2.89	0.45
7:g:75:ALA:O	7:g:76:ALA:C	2.60	0.45
1:l:125:SER:O	1:l:129:LYS:HG3	2.16	0.45
1:l:253:VAL:O	1:l:323:HIS:HA	2.16	0.45
1:l:294:LEU:HD23	1:l:337:VAL:HG12	1.98	0.45
2:n:68:LEU:HG	2:n:191:LEU:HD21	1.98	0.45
2:n:261:SER:HB3	2:n:321:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:308:ASP:O	2:n:309:VAL:HG23	2.17	0.45
3:o:174:THR:CG2	3:o:178:PHE:HE2	2.11	0.45
3:o:373:GLU:O	3:o:377:LEU:HD12	2.16	0.45
4:p:23:HIS:CD2	10:v:52:TRP:N	2.85	0.45
4:p:65:ALA:O	4:p:69:GLU:OE2	2.35	0.45
4:p:188:THR:O	4:p:189:PHE:C	2.55	0.45
5:q:7:VAL:HG13	5:q:8:PRO:HD2	1.98	0.45
13:y:60:GLU:CD	13:y:61:VAL:H	2.24	0.45
16:2:70:VAL:HG12	16:2:71:VAL:N	2.31	0.45
17:3:98:HIS:ND1	17:3:98:HIS:N	2.64	0.45
28:D:109:UNK:O	28:D:111:UNK:N	2.50	0.45
31:G:601:UNK:O	31:G:602:UNK:C	2.63	0.45
34:J:44:UNK:CB	34:J:53:UNK:CB	2.94	0.45
36:L:316:UNK:O	36:L:317:UNK:C	2.63	0.45
37:M:42:UNK:C	37:M:44:UNK:N	2.76	0.45
37:M:327:UNK:O	37:M:330:UNK:N	2.49	0.45
43:S:84:UNK:O	43:S:85:UNK:C	2.64	0.45
47:X:94:UNK:O	47:X:95:UNK:C	2.64	0.45
2:m:243:GLU:HA	2:m:424:MET:O	2.17	0.45
2:m:267:ALA:O	2:m:268:GLU:C	2.59	0.45
4:d:5:LEU:HG	4:d:152:TYR:CE1	2.51	0.45
4:d:32:VAL:HG11	4:d:186:VAL:HG22	1.97	0.45
4:d:138:PRO:CB	8:h:55:THR:HA	2.46	0.45
4:d:221:ALA:O	4:d:222:MET:C	2.57	0.45
1:l:142:ASP:OD1	5:q:2:HIS:ND1	2.45	0.45
2:n:161:GLU:O	2:n:162:ASN:C	2.60	0.45
3:o:26:ASN:HB2	6:r:69:SER:OG	2.16	0.45
3:o:327:ALA:HA	7:s:51:PRO:HB3	1.99	0.45
4:p:28:ARG:HD2	4:p:185:ASP:OD2	2.17	0.45
4:p:228:SER:HB2	7:s:23:GLN:NE2	2.32	0.45
5:q:131:GLU:HG2	5:q:132:TRP:CD1	2.51	0.45
31:G:491:UNK:C	31:G:493:UNK:N	2.78	0.45
34:J:72:UNK:HA	34:J:75:UNK:CB	2.46	0.45
36:L:151:UNK:O	36:L:155:UNK:CA	2.64	0.45
36:L:271:UNK:O	36:L:274:UNK:N	2.49	0.45
47:X:304:UNK:O	47:X:307:UNK:N	2.49	0.45
47:X:603:UNK:C	47:X:605:UNK:N	2.79	0.45
48:Y:81:UNK:O	48:Y:84:UNK:O	2.34	0.45
1:c:51:LYS:C	1:c:53:ASN:H	2.25	0.45
1:c:248:LEU:HA	1:c:249:PRO:HD3	1.59	0.45
2:m:270:ASN:O	2:m:271:ALA:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:285:VAL:HG12	2:m:288:GLY:HA3	1.98	0.45
3:b:11:MET:HE3	3:b:11:MET:HB3	1.67	0.45
3:b:152:ALA:N	3:b:287:LYS:NZ	2.64	0.45
3:b:182:HIS:O	3:b:186:PRO:CD	2.64	0.45
3:b:281:LEU:HD12	3:b:281:LEU:O	2.16	0.45
3:b:341:GLN:NE2	3:b:341:GLN:HA	2.31	0.45
4:d:35:GLN:OE1	4:d:35:GLN:HA	2.15	0.45
4:d:91:PHE:HA	4:d:92:PRO:HD3	1.58	0.45
4:d:180:SER:HB3	8:h:17:LEU:HB2	1.98	0.45
7:g:60:THR:O	7:g:61:TRP:C	2.59	0.45
1:l:392:LEU:HA	1:l:395:TRP:HD1	1.72	0.45
3:o:8:HIS:HB3	3:o:9:PRO:CD	2.44	0.45
3:o:278:TYR:O	3:o:281:LEU:N	2.48	0.45
4:p:102:ARG:O	4:p:106:ASN:N	2.49	0.45
4:p:241:LYS:NZ	6:r:53:ASN:HB2	2.31	0.45
5:q:29:SER:OG	5:q:32:ARG:HD3	2.17	0.45
5:q:40:THR:HG22	10:v:20:PHE:CZ	2.51	0.45
13:y:162:SER:HB2	13:y:198:GLU:HB2	1.99	0.45
18:4:3:ALA:O	18:4:4:ALA:HB2	2.17	0.45
28:D:228:UNK:O	28:D:232:UNK:CB	2.65	0.45
43:S:64:UNK:CA	43:S:78:UNK:CB	2.94	0.45
51:Z:355:UNK:O	51:Z:358:UNK:O	2.34	0.45
1:c:75:LEU:O	1:c:79:VAL:CG2	2.63	0.45
1:c:236:PHE:HD2	1:c:258:GLU:CB	2.28	0.45
2:m:211:VAL:HG12	2:m:212:SER:N	2.32	0.45
2:m:245:ARG:HH11	2:m:245:ARG:HD3	1.53	0.45
2:m:346:THR:O	2:m:347:ILE:C	2.60	0.45
2:m:360:ALA:O	2:m:361:LYS:C	2.60	0.45
3:b:25:SER:HA	3:b:218:ILE:HD11	1.98	0.45
3:b:361:LEU:CD2	3:b:365:LEU:HD12	2.42	0.45
7:g:36:ASN:HA	7:g:39:ARG:CD	2.32	0.45
1:l:272:VAL:HG13	1:l:358:LYS:HA	1.98	0.45
1:l:366:VAL:HG11	2:n:44:ALA:HB2	1.99	0.45
1:l:381:ARG:HA	1:l:384:LEU:HD12	1.99	0.45
2:n:134:ARG:HE	2:n:134:ARG:HB3	1.48	0.45
2:n:207:ILE:CD1	2:n:383:GLY:CA	2.93	0.45
3:o:345:HIS:CB	3:o:346:PRO:CD	2.88	0.45
3:o:347:TYR:O	3:o:348:ILE:C	2.58	0.45
8:t:65:ARG:O	8:t:69:VAL:HG23	2.16	0.45
12:x:240:HIS:O	12:x:243:VAL:HG22	2.16	0.45
12:x:431:LEU:HD21	12:x:450:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:435:GLY:O	12:x:437:PRO:HD3	2.16	0.45
21:7:2:GLU:CG	21:7:3:ASN:H	2.30	0.45
37:M:14:UNK:O	37:M:15:UNK:C	2.60	0.45
37:M:61:UNK:N	37:M:63:UNK:N	2.65	0.45
39:O:26:UNK:CB	39:O:124:UNK:O	2.65	0.45
47:X:188:UNK:O	47:X:191:UNK:CB	2.65	0.45
1:c:64:PHE:CZ	1:c:88:ALA:HB2	2.51	0.45
1:c:345:LEU:HD23	1:c:345:LEU:HA	1.68	0.45
1:c:349:ALA:O	1:c:408:ARG:NH2	2.50	0.45
3:b:177:ARG:HG2	3:b:181:PHE:HE2	1.82	0.45
4:d:31:GLN:HA	4:d:31:GLN:OE1	2.17	0.45
4:d:120:ARG:HH11	4:d:120:ARG:HG2	1.82	0.45
4:d:165:TYR:CD2	4:d:168:VAL:HG22	2.52	0.45
9:i:51:CYS:SG	9:i:53:GLU:HB3	2.57	0.45
1:l:246:ASP:HA	1:l:427:PRO:HD3	1.97	0.45
1:l:324:PHE:CG	1:l:334:MET:HG2	2.52	0.45
1:l:405:ARG:HH11	21:7:4:ARG:CD	2.27	0.45
3:o:30:TRP:HA	3:o:33:PHE:CE2	2.52	0.45
3:o:48:GLY:HA3	52:o:401:HEM:C3C	2.52	0.45
3:o:352:GLN:O	3:o:356:VAL:HG23	2.17	0.45
4:p:136:GLU:O	4:p:137:PRO:C	2.60	0.45
4:p:210:LEU:O	4:p:211:MET:C	2.60	0.45
10:v:4:THR:O	10:v:5:LEU:C	2.57	0.45
11:w:18:VAL:CB	11:w:19:PRO:HD3	2.41	0.45
11:w:23:LEU:N	11:w:23:LEU:HD23	2.32	0.45
12:x:449:MET:HE3	22:8:40:TRP:HB3	1.98	0.45
16:2:78:HIS:CE1	20:6:12:LEU:HD22	2.52	0.45
26:B:163:UNK:C	26:B:165:UNK:N	2.78	0.45
29:E:33:UNK:C	29:E:35:UNK:N	2.74	0.45
30:F:405:CYS:SG	30:F:406:UNK:CB	2.98	0.45
30:F:430:UNK:O	30:F:433:UNK:N	2.50	0.45
31:G:41:CYS:SG	31:G:49:UNK:O	2.74	0.45
31:G:621:UNK:O	31:G:622:UNK:C	2.64	0.45
36:L:545:UNK:C	36:L:547:UNK:N	2.74	0.45
37:M:114:UNK:CA	37:M:177:UNK:CB	2.95	0.45
40:P:180:UNK:O	40:P:181:UNK:C	2.65	0.45
2:m:201:SER:HG	2:m:226:ILE:H	1.61	0.45
2:m:275:LEU:HD11	2:m:279:LEU:HD12	1.99	0.45
3:b:47:THR:HG23	3:b:79:ILE:HG23	1.99	0.45
3:b:235:LEU:HG	3:b:236:ILE:N	2.32	0.45
3:b:242:LEU:HD21	3:b:250:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:338:ILE:HA	3:b:341:GLN:HG3	1.99	0.45
4:d:20:SER:OG	4:d:21:LEU:N	2.46	0.45
4:d:32:VAL:CG2	4:d:186:VAL:HG22	2.44	0.45
6:f:43:VAL:O	6:f:44:LYS:C	2.58	0.45
1:l:11:VAL:HA	1:l:12:PRO:HD3	1.87	0.45
1:l:14:THR:HG21	1:l:390:ILE:HG13	1.98	0.45
1:l:329:MET:HG3	7:s:2:ARG:HH11	1.82	0.45
1:l:426:GLY:CA	1:l:427:PRO:C	2.90	0.45
3:o:90:PHE:CE1	3:o:123:VAL:HG11	2.52	0.45
3:o:276:PHE:HE2	3:o:297:SER:OG	2.00	0.45
3:o:364:VAL:O	3:o:367:PRO:HG2	2.17	0.45
4:p:23:HIS:NE2	10:v:51:LEU:HA	2.31	0.45
5:q:171:ILE:HB	5:q:178:LEU:O	2.17	0.45
6:r:43:VAL:HG22	6:r:94:LEU:CD2	2.45	0.45
10:v:49:GLY:HA2	10:v:54:HIS:HB3	1.98	0.45
12:x:158:ILE:O	12:x:162:ILE:HG13	2.17	0.45
57:x:604:HEA:O11	57:x:604:HEA:HHC	2.17	0.45
13:y:59:GLN:CA	13:y:62:GLU:HB2	2.46	0.45
30:F:247:UNK:O	30:F:250:UNK:O	2.35	0.45
37:M:347:UNK:C	37:M:351:UNK:CB	2.92	0.45
1:c:46:ARG:NH1	1:c:316:ASP:OD1	2.50	0.44
1:c:152:TYR:OH	1:c:243:HIS:CD2	2.70	0.44
1:c:358:LYS:HD2	1:c:402:VAL:HB	1.98	0.44
1:c:428:ILE:CG2	1:c:431:LEU:HD22	2.47	0.44
2:m:282:GLY:HA2	2:m:283:PRO:HD2	1.78	0.44
3:b:77:TRP:CE3	3:b:78:ILE:HG23	2.44	0.44
4:d:10:TYR:HD1	8:h:74:PHE:CD1	2.36	0.44
4:d:167:GLU:HG2	4:d:167:GLU:O	2.17	0.44
1:l:395:TRP:O	1:l:396:GLU:C	2.57	0.44
1:l:405:ARG:CD	21:7:4:ARG:HH12	2.16	0.44
2:n:314:ALA:HB1	9:u:64:LEU:HD22	1.97	0.44
3:o:107:TYR:OH	3:o:308:HIS:HB2	2.17	0.44
3:o:123:VAL:O	3:o:123:VAL:CG1	2.65	0.44
3:o:236:ILE:O	3:o:237:LEU:C	2.57	0.44
5:q:81:ILE:HD11	5:q:132:TRP:HH2	1.82	0.44
5:q:134:ILE:C	5:q:135:LEU:HD23	2.42	0.44
5:q:186:GLU:O	5:q:186:GLU:CG	2.66	0.44
7:s:26:PHE:N	7:s:27:PRO:HD3	2.32	0.44
7:s:44:CYS:O	7:s:45:ILE:C	2.59	0.44
13:y:41:ILE:O	13:y:45:MET:HG2	2.16	0.44
14:z:183:GLU:O	18:4:42:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:78:UNK:CB	34:J:146:UNK:O	2.65	0.44
25:A:106:UNK:O	25:A:107:UNK:C	2.63	0.44
28:D:296:UNK:O	28:D:299:UNK:CB	2.64	0.44
28:D:298:UNK:O	28:D:299:UNK:C	2.65	0.44
29:E:113:UNK:O	29:E:116:UNK:N	2.50	0.44
31:G:11:UNK:CB	31:G:76:UNK:C	2.95	0.44
31:G:311:UNK:O	31:G:314:UNK:N	2.50	0.44
37:M:52:UNK:HA	37:M:53:UNK:HA	1.71	0.44
43:S:63:UNK:CA	43:S:78:UNK:CB	2.94	0.44
50:U:326:UNK:O	50:U:329:UNK:N	2.50	0.44
1:c:197:LEU:HD11	1:c:208:LEU:HD11	1.98	0.44
1:c:293:PRO:HA	1:c:296:SER:OG	2.18	0.44
2:m:271:ALA:O	2:m:272:PHE:C	2.58	0.44
4:d:67:GLU:O	4:d:70:VAL:HG12	2.17	0.44
5:e:15:ARG:O	5:e:16:PRO:C	2.61	0.44
5:e:33:LYS:HA	7:g:21:PHE:HE2	1.82	0.44
1:l:43:ALA:HB2	1:l:189:HIS:HB3	1.99	0.44
1:l:64:PHE:HE1	1:l:86:LEU:CD1	2.31	0.44
3:o:10:LEU:O	3:o:13:ILE:HG13	2.17	0.44
3:o:58:ASP:O	3:o:59:THR:C	2.60	0.44
3:o:101:GLY:O	3:o:107:TYR:HD2	2.01	0.44
3:o:310:SER:HA	3:o:374:ASN:ND2	2.07	0.44
4:p:74:PRO:O	4:p:79:GLU:N	2.42	0.44
4:p:227:TRP:CE3	4:p:230:LEU:HD12	2.51	0.44
5:q:99:ARG:NH1	5:q:148:ALA:HB1	2.32	0.44
9:u:57:GLY:O	9:u:78:TYR:CE2	2.70	0.44
10:v:23:THR:O	10:v:24:ILE:C	2.58	0.44
10:v:52:TRP:CG	10:v:53:LYS:N	2.85	0.44
27:C:133:UNK:O	27:C:136:UNK:CB	2.65	0.44
28:D:95:UNK:CB	28:D:98:UNK:CB	2.96	0.44
28:D:342:UNK:O	28:D:343:UNK:C	2.65	0.44
29:E:165:UNK:O	29:E:166:UNK:C	2.65	0.44
30:F:426:UNK:CA	30:F:429:UNK:CB	2.83	0.44
31:G:89:UNK:O	31:G:90:UNK:C	2.64	0.44
31:G:305:UNK:O	31:G:308:UNK:N	2.51	0.44
35:K:21:UNK:O	35:K:22:UNK:C	2.64	0.44
36:L:29:UNK:CA	36:L:32:UNK:CB	2.85	0.44
36:L:288:UNK:CB	36:L:308:UNK:HA	2.47	0.44
37:M:123:UNK:CB	38:N:255:UNK:CB	2.96	0.44
50:U:108:UNK:O	50:U:111:UNK:CB	2.66	0.44
1:c:16:VAL:HG11	1:c:388:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:341:GLN:OE1	1:c:344:ARG:HD3	2.16	0.44
2:m:178:CYS:HA	2:m:179:PRO:HD3	1.80	0.44
2:m:181:TYR:CD1	2:m:181:TYR:C	2.96	0.44
2:m:201:SER:OG	2:m:226:ILE:N	2.44	0.44
3:b:9:PRO:CG	3:b:12:LYS:HB2	2.45	0.44
3:b:53:MET:SD	3:o:181:PHE:CZ	3.10	0.44
3:b:153:ILE:HD12	3:b:153:ILE:H	1.82	0.44
3:b:294:LEU:O	3:b:297:SER:HB3	2.17	0.44
3:b:357:LEU:HG	3:b:361:LEU:HD11	1.98	0.44
4:d:150:ASN:OD1	4:d:151:PRO:N	2.49	0.44
4:d:187:CYS:O	4:d:188:THR:C	2.60	0.44
1:l:19:LEU:HB2	1:l:23:LEU:HB3	1.99	0.44
1:l:64:PHE:HE2	1:l:88:ALA:HB2	1.81	0.44
1:l:438:ARG:HG3	1:l:438:ARG:NH1	2.31	0.44
2:n:53:ALA:O	2:n:105:MET:HB2	2.17	0.44
2:n:81:SER:O	2:n:84:LYS:N	2.50	0.44
2:n:222:GLN:HB3	2:n:223:PHE:CD2	2.53	0.44
2:n:338:LYS:O	2:n:341:TYR:N	2.50	0.44
4:p:55:CYS:SG	10:v:52:TRP:HA	2.56	0.44
4:p:181:GLN:HG2	8:t:77:LEU:CD2	2.21	0.44
21:7:3:ASN:ND2	21:7:5:VAL:HG13	2.33	0.44
27:C:120:UNK:O	27:C:121:UNK:C	2.64	0.44
29:E:107:UNK:O	29:E:110:UNK:N	2.50	0.44
30:F:275:UNK:O	30:F:279:UNK:N	2.50	0.44
31:G:175:UNK:CB	31:G:182:UNK:N	2.80	0.44
31:G:572:UNK:HA	31:G:581:UNK:O	2.17	0.44
36:L:155:UNK:O	36:L:239:UNK:CB	2.65	0.44
37:M:32:UNK:C	37:M:34:UNK:N	2.79	0.44
37:M:406:UNK:O	37:M:407:UNK:C	2.64	0.44
38:N:91:UNK:O	38:N:95:UNK:CB	2.65	0.44
38:N:146:UNK:N	38:N:147:UNK:CA	2.72	0.44
40:P:106:UNK:CA	40:P:109:UNK:CB	2.85	0.44
46:W:71:UNK:O	46:W:72:UNK:C	2.65	0.44
47:X:203:UNK:C	47:X:205:UNK:N	2.73	0.44
1:c:255:ILE:HD12	1:c:335:MET:CE	2.47	0.44
2:m:59:ASN:CG	2:m:60:SER:N	2.74	0.44
2:m:124:LEU:HD13	2:m:223:PHE:CG	2.52	0.44
3:b:26:ASN:CA	6:f:70:MET:HB2	2.48	0.44
3:b:334:THR:HG1	7:g:55:PHE:HD1	1.64	0.44
3:b:346:PRO:CG	7:g:66:PHE:HD1	2.28	0.44
4:d:137:PRO:HA	4:d:138:PRO:HD3	1.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:150:ASN:OD1	4:d:150:ASN:C	2.59	0.44
2:n:357:VAL:O	2:n:360:ALA:HB3	2.18	0.44
2:n:380:ASP:O	2:n:381:GLU:C	2.61	0.44
3:o:156:ILE:HG13	3:o:157:GLY:N	2.29	0.44
3:o:218:ILE:CG2	3:o:219:PRO:HD2	2.46	0.44
4:p:28:ARG:O	4:p:29:GLY:C	2.60	0.44
4:p:165:TYR:CZ	4:p:168:VAL:HG22	2.53	0.44
12:x:51:ASP:O	12:x:55:ASN:HB2	2.17	0.44
17:3:33:ILE:HG22	17:3:34:LEU:HD12	1.98	0.44
28:D:70:UNK:O	28:D:72:UNK:N	2.50	0.44
28:D:137:UNK:O	28:D:138:UNK:C	2.63	0.44
30:F:351:UNK:O	30:F:355:UNK:N	2.51	0.44
31:G:482:UNK:O	31:G:576:UNK:CB	2.66	0.44
32:H:298:UNK:O	32:H:302:UNK:N	2.50	0.44
33:I:50:UNK:HA	33:I:53:UNK:O	2.18	0.44
36:L:124:UNK:O	36:L:125:UNK:C	2.63	0.44
37:M:118:UNK:O	37:M:121:UNK:N	2.49	0.44
47:X:172:UNK:O	47:X:176:UNK:N	2.51	0.44
47:X:503:UNK:O	47:X:506:UNK:CB	2.65	0.44
50:U:102:UNK:O	50:U:103:UNK:C	2.59	0.44
50:U:714:UNK:O	50:U:717:UNK:N	2.50	0.44
1:c:46:ARG:NH2	1:c:316:ASP:CG	2.62	0.44
1:c:385:THR:HG22	1:c:386:TYR:CD1	2.52	0.44
2:m:264:ILE:HG22	2:m:317:SER:HA	1.99	0.44
4:d:229:VAL:HG12	4:d:229:VAL:O	2.18	0.44
5:e:45:VAL:HG13	10:j:28:ALA:CA	2.46	0.44
1:l:82:MET:HE2	1:l:82:MET:HB2	1.93	0.44
2:n:135:TRP:CD1	2:n:136:GLU:HG3	2.52	0.44
6:r:28:LYS:HB3	6:r:74:ILE:CD1	2.47	0.44
9:u:64:LEU:CG	9:u:65:VAL:HG23	2.42	0.44
12:x:70:VAL:HG11	12:x:246:LEU:HD22	2.00	0.44
14:z:41:THR:O	14:z:45:ILE:HG13	2.18	0.44
20:6:19:PHE:CD1	20:6:19:PHE:C	2.94	0.44
27:C:21:UNK:O	27:C:22:UNK:C	2.66	0.44
28:D:383:UNK:CB	28:D:384:UNK:C	2.95	0.44
30:F:76:UNK:O	30:F:80:UNK:CB	2.66	0.44
30:F:300:UNK:CB	30:F:329:UNK:C	2.95	0.44
30:F:423:UNK:C	30:F:426:UNK:N	2.81	0.44
35:K:10:UNK:O	35:K:13:UNK:N	2.51	0.44
37:M:159:UNK:O	37:M:160:UNK:C	2.64	0.44
38:N:320:UNK:O	38:N:321:UNK:C	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:337:UNK:O	38:N:341:UNK:N	2.51	0.44
47:X:704:UNK:O	47:X:705:UNK:C	2.65	0.44
1:c:199:ALA:HB3	1:c:208:LEU:HD21	1.99	0.44
1:c:252:HIS:NE2	1:c:325:VAL:HG21	2.32	0.44
1:c:392:LEU:HA	1:c:395:TRP:NE1	2.30	0.44
1:c:426:GLY:H	1:c:428:ILE:HD11	1.83	0.44
2:m:46:ARG:NH1	2:m:376:GLU:HG3	2.30	0.44
3:b:15:ASN:ND2	3:b:18:PHE:HE1	2.12	0.44
3:b:202:GLU:OE2	3:o:10:LEU:CB	2.48	0.44
3:b:276:PHE:CE2	3:b:297:SER:OG	2.68	0.44
3:b:328:LEU:O	3:b:329:VAL:C	2.56	0.44
4:d:197:GLU:O	4:d:198:HIS:C	2.59	0.44
4:d:233:ARG:CG	7:g:17:SER:HB3	2.48	0.44
6:f:58:ARG:HG2	6:f:58:ARG:HH11	1.82	0.44
6:f:106:GLU:OE1	6:f:109:LYS:HE2	2.17	0.44
10:j:57:HIS:O	10:j:60:GLU:HG2	2.17	0.44
1:l:75:LEU:HD21	1:l:116:ILE:HG12	2.00	0.44
1:l:143:THR:O	1:l:143:THR:CG2	2.66	0.44
1:l:149:VAL:CG1	1:l:150:PHE:N	2.81	0.44
1:l:157:ALA:HB2	1:l:421:ALA:HB1	2.00	0.44
1:l:339:GLN:O	1:l:343:MET:HG2	2.17	0.44
1:l:426:GLY:H	1:l:428:ILE:HD11	1.82	0.44
3:o:185:LEU:N	3:o:186:PRO:CD	2.80	0.44
9:u:70:LEU:CD2	9:u:73:PRO:CD	2.92	0.44
12:x:273:MET:HG3	12:x:319:LYS:NZ	2.31	0.44
15:1:79:LYS:NZ	22:8:15:ASN:HD21	2.15	0.44
26:B:118:UNK:C	26:B:122:UNK:N	2.73	0.44
27:C:132:UNK:O	27:C:133:UNK:C	2.63	0.44
27:C:162:UNK:O	27:C:163:UNK:C	2.65	0.44
32:H:41:UNK:CB	32:H:44:UNK:C	2.96	0.44
33:I:112:UNK:O	33:I:115:UNK:CB	2.66	0.44
33:I:112:UNK:O	33:I:115:UNK:N	2.50	0.44
36:L:211:UNK:HA	36:L:214:UNK:CB	2.47	0.44
36:L:246:UNK:O	36:L:250:UNK:CA	2.65	0.44
36:L:541:UNK:O	36:L:545:UNK:N	2.50	0.44
37:M:30:UNK:O	37:M:33:UNK:N	2.50	0.44
37:M:91:UNK:O	37:M:94:UNK:CB	2.66	0.44
39:O:130:UNK:O	39:O:132:UNK:N	2.50	0.44
47:X:42:UNK:O	47:X:45:UNK:CB	2.66	0.44
2:m:52:LYS:CB	2:m:203:ARG:HB3	2.28	0.44
2:m:177:TYR:C	2:m:178:CYS:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:314:ALA:CB	9:i:64:LEU:HD22	2.48	0.44
3:b:7:SER:O	3:b:8:HIS:O	2.36	0.44
3:b:26:ASN:HA	6:f:70:MET:HA	1.98	0.44
3:b:32:ASN:O	3:b:36:LEU:HG	2.18	0.44
3:b:192:ILE:HD13	3:b:192:ILE:H	1.82	0.44
3:b:357:LEU:HD12	3:b:361:LEU:HG	2.00	0.44
10:j:52:TRP:CG	10:j:53:LYS:N	2.86	0.44
1:l:8:LEU:HD11	1:l:396:GLU:HG3	2.00	0.44
1:l:76:GLU:O	1:l:77:LYS:C	2.60	0.44
1:l:245:GLU:C	1:l:247:GLY:N	2.76	0.44
2:n:258:VAL:HG21	2:n:312:PHE:HD2	1.82	0.44
2:n:279:LEU:HD23	2:n:295:LEU:HD13	2.00	0.44
2:n:322:PHE:CD1	2:n:322:PHE:C	2.96	0.44
3:o:119:LEU:CD1	3:o:192:ILE:HG22	2.45	0.44
13:y:1:MET:SD	13:y:133:LEU:HD13	2.58	0.44
20:6:61:GLU:OE1	20:6:64:ARG:NH1	2.51	0.44
27:C:23:UNK:O	27:C:26:UNK:CB	2.65	0.44
28:D:254:UNK:O	28:D:256:UNK:N	2.50	0.44
28:D:421:UNK:C	28:D:423:UNK:N	2.79	0.44
30:F:52:UNK:O	30:F:55:UNK:CA	2.66	0.44
31:G:30:UNK:O	31:G:34:UNK:N	2.51	0.44
47:X:421:UNK:O	47:X:422:UNK:C	2.61	0.44
1:c:152:TYR:O	1:c:153:LEU:C	2.57	0.44
2:m:211:VAL:CG1	2:m:212:SER:N	2.81	0.44
4:d:83:ARG:CB	4:d:84:PRO:CD	2.66	0.44
9:i:64:LEU:HG	9:i:65:VAL:HG23	1.99	0.44
1:l:53:ASN:CG	1:l:170:PRO:HD3	2.42	0.44
1:l:252:HIS:CD2	1:l:325:VAL:HG22	2.53	0.44
1:l:281:ASP:HB3	1:l:284:TYR:CD1	2.53	0.44
2:n:53:ALA:HB2	2:n:198:HIS:HB3	1.99	0.44
2:n:162:ASN:ND2	2:n:244:ILE:HG21	2.33	0.44
2:n:182:ARG:O	2:n:185:LYS:HB3	2.17	0.44
2:n:216:LEU:HD12	2:n:216:LEU:HA	1.81	0.44
3:o:31:TRP:CD2	3:o:100:ARG:HD2	2.53	0.44
4:p:131:LEU:HD22	4:p:163:PRO:CB	2.48	0.44
5:q:121:GLN:O	5:q:170:ARG:HD3	2.18	0.44
5:q:145:VAL:HA	5:q:146:PRO:HD3	1.75	0.44
7:s:40:ARG:O	7:s:44:CYS:SG	2.71	0.44
15:1:40:LEU:HD22	15:1:59:LEU:CD1	2.47	0.44
21:7:36:MET:O	21:7:40:LEU:HG	2.18	0.44
31:G:567:UNK:O	31:G:586:UNK:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:18:UNK:O	32:H:21:UNK:N	2.50	0.44
33:I:31:UNK:O	33:I:34:UNK:CB	2.66	0.44
36:L:165:UNK:HA	36:L:168:UNK:CB	2.47	0.44
39:O:105:UNK:O	39:O:108:UNK:N	2.50	0.44
40:P:64:UNK:CB	40:P:65:UNK:HA	2.46	0.44
47:X:46:UNK:O	47:X:49:UNK:N	2.51	0.44
51:Z:104:UNK:HA	51:Z:107:UNK:CB	2.47	0.44
1:c:191:LYS:NZ	1:c:220:SER:OG	2.45	0.44
1:c:197:LEU:CD1	1:c:208:LEU:HD11	2.47	0.44
3:b:126:THR:HG21	52:b:401:HEM:C3B	2.53	0.44
3:b:254:ASP:HB3	4:d:119:ALA:O	2.18	0.44
4:d:223:LYS:NZ	4:d:227:TRP:CD1	2.86	0.44
10:j:31:PHE:CD1	10:j:31:PHE:C	2.96	0.44
1:l:19:LEU:CD1	1:l:214:LYS:HG2	2.48	0.44
1:l:271:GLN:O	1:l:272:VAL:C	2.59	0.44
2:n:51:ILE:HD13	2:n:199:PHE:CD2	2.53	0.44
2:n:109:VAL:O	2:n:109:VAL:CG1	2.66	0.44
2:n:109:VAL:HG22	2:n:119:LEU:HD23	1.98	0.44
2:n:433:THR:HA	2:n:434:PRO:HD2	1.58	0.44
2:n:436:ILE:H	2:n:436:ILE:HG13	1.41	0.44
3:o:337:TRP:O	3:o:341:GLN:HG2	2.17	0.44
4:p:226:LYS:HD3	4:p:226:LYS:HA	1.76	0.44
5:q:76:ILE:HD12	5:q:192:MET:HE1	1.97	0.44
12:x:379:TYR:CE2	12:x:383:MET:HE2	2.52	0.44
14:z:19:THR:CG2	14:z:53:THR:OG1	2.66	0.44
16:2:76:GLY:HA3	16:2:77:PRO:HD2	1.85	0.44
21:7:30:ILE:HG13	21:7:31:LEU:N	2.32	0.44
26:B:162:UNK:O	26:B:165:UNK:CB	2.65	0.44
31:G:86:UNK:O	31:G:87:UNK:C	2.65	0.44
33:I:151:UNK:O	33:I:152:UNK:C	2.66	0.44
39:O:38:UNK:O	39:O:41:UNK:N	2.51	0.44
39:O:101:UNK:O	39:O:105:UNK:N	2.50	0.44
40:P:48:UNK:CB	40:P:73:UNK:CB	2.95	0.44
40:P:158:UNK:O	40:P:161:UNK:N	2.51	0.44
43:S:84:UNK:C	43:S:87:UNK:N	2.80	0.44
47:X:306:UNK:C	47:X:308:UNK:N	2.79	0.44
50:U:512:UNK:O	50:U:515:UNK:N	2.51	0.44
50:U:622:UNK:O	50:U:624:UNK:N	2.51	0.44
51:Z:309:UNK:O	51:Z:312:UNK:N	2.50	0.44
1:c:213:GLN:HB3	1:c:215:HIS:CD2	2.53	0.43
1:c:311:ASN:OD1	1:c:320:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:71:LEU:HA	2:m:71:LEU:HD23	1.72	0.43
3:b:113:TRP:O	3:b:117:VAL:HG23	2.17	0.43
3:b:245:PHE:CE1	4:d:17:LEU:HB3	2.53	0.43
4:d:153:PHE:HA	4:d:154:PRO:HD2	1.70	0.43
6:f:75:LEU:HD12	6:f:75:LEU:HA	1.80	0.43
10:j:13:LEU:O	10:j:19:THR:OG1	2.16	0.43
10:j:49:GLY:H	10:j:54:HIS:CD2	2.36	0.43
1:l:64:PHE:CZ	1:l:88:ALA:HB2	2.51	0.43
1:l:152:TYR:OH	1:l:243:HIS:CD2	2.71	0.43
1:l:277:ILE:HG22	1:l:294:LEU:HD12	1.99	0.43
1:l:349:ALA:O	1:l:408:ARG:CZ	2.65	0.43
2:n:62:ASN:ND2	2:n:65:THR:CB	2.81	0.43
2:n:160:ILE:HD11	2:n:325:TYR:CE2	2.53	0.43
2:n:275:LEU:O	2:n:276:GLN:C	2.60	0.43
2:n:363:LYS:O	2:n:364:LEU:C	2.61	0.43
3:o:160:LEU:O	3:o:160:LEU:HD12	2.18	0.43
3:o:221:HIS:CB	3:o:222:PRO:CD	2.92	0.43
4:p:237:TYR:HB2	6:r:60:PHE:CE1	2.53	0.43
8:t:58:LEU:CD1	8:t:62:LEU:HG	2.48	0.43
13:y:121:TYR:C	13:y:138:VAL:HG23	2.42	0.43
13:y:122:MET:HB2	13:y:208:PRO:CD	2.47	0.43
14:z:63:ARG:HA	14:z:67:PHE:CD2	2.53	0.43
23:9:35:ALA:HB3	23:9:36:PRO:HD3	1.99	0.43
30:F:315:UNK:CA	30:F:316:UNK:C	2.95	0.43
31:G:185:UNK:C	31:G:188:UNK:CB	2.96	0.43
32:H:283:UNK:O	32:H:287:UNK:N	2.51	0.43
40:P:129:UNK:O	40:P:163:UNK:CB	2.66	0.43
1:c:179:ARG:HG3	1:c:180:ALA:N	2.31	0.43
1:c:311:ASN:CG	1:c:320:LEU:CD2	2.91	0.43
2:m:110:GLU:O	2:m:111:CYS:HB3	2.18	0.43
2:m:154:ASN:O	2:m:155:PRO:C	2.60	0.43
2:m:262:ALA:HB2	2:m:272:PHE:CE2	2.53	0.43
2:m:262:ALA:CB	2:m:268:GLU:HB3	2.47	0.43
3:b:26:ASN:HD22	3:b:208:PRO:HD2	1.82	0.43
3:b:30:TRP:HA	3:b:33:PHE:CE2	2.51	0.43
3:b:183:PHE:HZ	3:o:184:ILE:HB	1.82	0.43
3:b:365:LEU:O	3:b:366:MET:C	2.61	0.43
4:d:158:ILE:CG1	4:d:159:GLY:N	2.82	0.43
6:f:87:LYS:HG3	6:f:89:TYR:HB3	2.00	0.43
6:f:88:SER:O	6:f:92:PRO:HD3	2.18	0.43
8:h:69:VAL:O	8:h:73:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:385:THR:HB	1:l:386:TYR:CD1	2.52	0.43
2:n:332:SER:O	2:n:333:ALA:C	2.60	0.43
3:o:103:TYR:CE1	3:o:322:GLN:HG3	2.53	0.43
3:o:366:MET:N	3:o:367:PRO:HD2	2.33	0.43
4:p:94:PRO:HB2	4:p:95:TYR:CD1	2.53	0.43
5:q:22:THR:O	5:q:22:THR:OG1	2.34	0.43
5:q:122:HIS:HB3	5:q:125:GLU:CG	2.48	0.43
7:s:68:LYS:HD3	7:s:72:LYS:HE3	2.01	0.43
10:v:55:ILE:CG2	10:v:58:LYS:HE2	2.46	0.43
25:A:53:UNK:O	25:A:56:UNK:N	2.50	0.43
26:B:117:UNK:O	26:B:118:UNK:C	2.62	0.43
30:F:56:UNK:C	30:F:59:UNK:CB	2.96	0.43
30:F:433:UNK:O	30:F:437:UNK:N	2.51	0.43
32:H:110:UNK:C	32:H:112:UNK:N	2.78	0.43
36:L:343:UNK:O	36:L:347:UNK:N	2.51	0.43
1:c:21:ASN:CB	1:c:217:SER:HB3	2.45	0.43
1:c:349:ALA:HB3	1:c:408:ARG:CG	2.48	0.43
2:m:51:ILE:CG2	2:m:199:PHE:HA	2.34	0.43
2:m:182:ARG:NH1	2:m:185:LYS:CG	2.77	0.43
2:m:258:VAL:HG11	2:m:321:LEU:HD22	2.00	0.43
3:b:107:TYR:CE2	3:b:305:PRO:HA	2.53	0.43
1:l:226:ASP:O	1:l:228:VAL:N	2.51	0.43
1:l:262:TRP:CE3	1:l:385:THR:HG23	2.52	0.43
1:l:426:GLY:H	1:l:428:ILE:CG1	2.30	0.43
2:n:47:ILE:CG2	2:n:48:GLY:H	2.31	0.43
3:o:55:TYR:CE2	3:o:56:THR:O	2.71	0.43
3:o:227:LYS:CG	4:p:223:LYS:NZ	2.82	0.43
3:o:271:GLU:H	3:o:271:GLU:HG2	1.54	0.43
3:o:341:GLN:HA	3:o:341:GLN:HE21	1.82	0.43
3:o:373:GLU:HB3	6:r:20:TYR:OH	2.18	0.43
4:p:50:HIS:CE1	4:p:91:PHE:HZ	2.33	0.43
4:p:68:VAL:CG1	4:p:92:PRO:HG2	2.47	0.43
4:p:165:TYR:CE1	4:p:168:VAL:HA	2.54	0.43
5:q:150:ALA:CB	5:q:157:TYR:HB2	2.48	0.43
10:v:4:THR:CG2	10:v:6:THR:OG1	2.66	0.43
11:w:24:TRP:O	11:w:25:GLY:C	2.58	0.43
11:w:32:LEU:O	11:w:33:VAL:C	2.61	0.43
27:C:22:UNK:O	27:C:26:UNK:CB	2.66	0.43
29:E:69:UNK:O	29:E:73:UNK:N	2.51	0.43
29:E:96:UNK:C	29:E:136:UNK:O	2.67	0.43
30:F:58:UNK:O	30:F:61:UNK:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:586:UNK:C	31:G:588:UNK:N	2.80	0.43
36:L:309:UNK:O	36:L:313:UNK:N	2.50	0.43
38:N:65:UNK:O	38:N:68:UNK:N	2.51	0.43
46:W:58:UNK:O	46:W:59:UNK:C	2.66	0.43
48:Y:103:UNK:O	48:Y:105:UNK:N	2.51	0.43
50:U:510:UNK:C	50:U:512:UNK:N	2.77	0.43
1:c:33:PRO:O	1:c:103:SER:HB3	2.17	0.43
1:c:260:PRO:HG3	1:c:414:TYR:OH	2.19	0.43
1:c:444:LEU:HD12	1:c:444:LEU:HA	1.82	0.43
2:m:135:TRP:CE2	6:r:49:ARG:HD3	2.53	0.43
3:b:37:LEU:CD1	3:b:97:HIS:CD2	3.01	0.43
3:b:243:VAL:HG22	3:b:243:VAL:O	2.17	0.43
4:d:116:ILE:CD1	4:d:120:ARG:HH11	2.32	0.43
6:f:52:GLU:HG3	6:f:56:ASP:OD2	2.18	0.43
1:l:4:TYR:CD1	2:n:43:PRO:HB3	2.53	0.43
1:l:64:PHE:CD1	1:l:86:LEU:HG	2.51	0.43
1:l:153:LEU:CD2	1:l:319:LEU:HD13	2.48	0.43
1:l:233:PRO:HG2	5:q:23:LYS:HD3	1.98	0.43
1:l:287:GLY:O	1:l:290:LEU:HG	2.18	0.43
1:l:444:LEU:HD12	1:l:444:LEU:HA	1.73	0.43
2:n:182:ARG:NH1	2:n:185:LYS:CG	2.79	0.43
3:o:146:ILE:O	3:o:147:THR:C	2.62	0.43
3:o:338:ILE:HA	3:o:341:GLN:HG3	1.99	0.43
4:p:116:ILE:HD12	4:p:116:ILE:HA	1.74	0.43
6:r:37:ILE:CG1	6:r:43:VAL:HG21	2.40	0.43
12:x:377:PHE:CD2	57:x:604:HEA:HAD1	2.53	0.43
13:y:3:TYR:CD1	13:y:3:TYR:N	2.87	0.43
20:6:26:MET:N	20:6:26:MET:SD	2.91	0.43
27:C:110:UNK:O	27:C:111:UNK:C	2.65	0.43
30:F:115:UNK:O	30:F:116:UNK:C	2.67	0.43
30:F:150:UNK:O	30:F:153:UNK:CA	2.67	0.43
31:G:380:UNK:O	31:G:409:UNK:C	2.67	0.43
34:J:18:UNK:HA	34:J:21:UNK:CB	2.49	0.43
34:J:149:UNK:O	34:J:150:UNK:C	2.65	0.43
40:P:203:UNK:CB	40:P:234:UNK:HA	2.48	0.43
50:U:126:UNK:O	50:U:127:UNK:C	2.67	0.43
51:Z:335:UNK:CB	51:Z:339:UNK:N	2.82	0.43
1:c:143:THR:CG2	9:i:48:SER:H	2.18	0.43
2:m:112:LEU:HD22	2:m:112:LEU:HA	1.79	0.43
2:m:122:PHE:O	2:m:126:VAL:HG23	2.18	0.43
3:b:8:HIS:HB2	3:b:9:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:103:TYR:CE1	3:b:322:GLN:HG3	2.53	0.43
3:b:147:THR:CG2	3:b:165:TRP:NE1	2.78	0.43
3:b:226:ILE:O	3:b:227:LYS:C	2.61	0.43
3:b:336:THR:O	3:b:336:THR:HG22	2.18	0.43
4:d:10:TYR:CE1	4:d:128:PHE:CE2	3.07	0.43
4:d:161:ALA:O	4:d:163:PRO:CD	2.66	0.43
6:f:99:ARG:O	6:f:100:GLU:C	2.57	0.43
10:j:4:THR:HG22	10:j:6:THR:N	2.33	0.43
1:l:73:ASN:O	1:l:77:LYS:CD	2.66	0.43
1:l:297:ILE:CG2	1:l:303:LEU:HD12	2.42	0.43
2:n:204:MET:HE1	2:n:224:LEU:HB3	2.00	0.43
3:o:136:GLY:O	3:o:137:GLN:C	2.60	0.43
3:o:280:ILE:HD13	3:o:335:LEU:CD2	2.44	0.43
4:p:26:ILE:HG21	4:p:54:VAL:HG22	1.99	0.43
5:q:136:ILE:O	5:q:138:VAL:N	2.49	0.43
10:v:57:HIS:O	10:v:60:GLU:HG2	2.18	0.43
14:z:80:ARG:HG2	14:z:233:PHE:CE1	2.54	0.43
15:1:37:GLN:O	15:1:41:LYS:HG2	2.18	0.43
23:9:22:LEU:HD23	23:9:22:LEU:HA	1.83	0.43
28:D:297:UNK:O	28:D:298:UNK:C	2.63	0.43
30:F:74:UNK:O	30:F:77:UNK:N	2.52	0.43
39:O:43:UNK:O	39:O:44:UNK:C	2.67	0.43
48:Y:14:UNK:CB	48:Y:44:UNK:O	2.66	0.43
50:U:625:UNK:O	50:U:628:UNK:CB	2.66	0.43
1:c:66:GLY:O	1:c:121:SER:N	2.50	0.43
3:b:307:LEU:O	3:b:308:HIS:C	2.62	0.43
3:b:342:PRO:HG2	7:g:66:PHE:CZ	2.53	0.43
6:f:68:LEU:HD11	6:f:75:LEU:HD13	2.01	0.43
8:h:15:ASP:HB2	8:h:16:PRO:HD3	2.01	0.43
11:k:31:GLY:O	11:k:35:ALA:N	2.46	0.43
1:l:40:TRP:CZ2	1:l:377:GLU:CA	2.95	0.43
1:l:145:MET:CE	1:l:248:LEU:HD12	2.48	0.43
1:l:211:LEU:HD12	1:l:211:LEU:O	2.18	0.43
3:o:207:ASN:OD1	3:o:207:ASN:O	2.37	0.43
3:o:282:ARG:O	3:o:283:SER:C	2.59	0.43
4:p:26:ILE:CG2	4:p:54:VAL:HG13	2.47	0.43
4:p:102:ARG:HE	4:p:109:LEU:HB2	1.83	0.43
4:p:161:ALA:O	4:p:163:PRO:HD3	2.18	0.43
8:t:22:GLU:O	8:t:23:GLN:C	2.60	0.43
13:y:162:SER:HB3	13:y:197:SER:C	2.44	0.43
23:9:41:ARG:HD2	24:0:40:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E:54:UNK:O	29:E:57:UNK:N	2.51	0.43
31:G:41:CYS:CA	54:G:803:FES:S2	3.01	0.43
31:G:187:UNK:N	31:G:188:UNK:CA	2.73	0.43
38:N:253:UNK:CA	38:N:259:UNK:CB	2.96	0.43
39:O:42:UNK:C	39:O:44:UNK:N	2.76	0.43
40:P:48:UNK:C	40:P:73:UNK:CB	2.97	0.43
47:X:331:UNK:O	47:X:332:UNK:C	2.65	0.43
51:Z:508:UNK:O	51:Z:509:UNK:C	2.64	0.43
1:c:29:GLN:HA	1:c:201:GLY:O	2.18	0.43
1:c:86:LEU:HD12	1:c:98:TYR:O	2.18	0.43
3:b:71:ARG:HB3	4:d:49:ARG:HH22	1.84	0.43
3:b:90:PHE:CZ	3:b:123:VAL:HG21	2.54	0.43
4:d:69:GLU:O	4:d:73:GLY:CA	2.67	0.43
6:f:45:GLU:O	6:f:46:ALA:C	2.56	0.43
10:j:27:GLY:O	10:j:28:ALA:C	2.59	0.43
1:l:292:SER:O	1:l:295:ALA:N	2.52	0.43
2:n:140:LEU:O	2:n:142:PRO:N	2.51	0.43
2:n:213:HIS:HD2	2:n:213:HIS:O	2.02	0.43
3:o:183:PHE:CD1	3:o:183:PHE:O	2.72	0.43
3:o:235:LEU:HD12	3:o:235:LEU:O	2.19	0.43
4:p:34:LYS:O	4:p:34:LYS:HG2	2.18	0.43
4:p:131:LEU:CD2	4:p:163:PRO:HB3	2.48	0.43
7:s:73:ASN:N	7:s:74:PRO:HD2	2.31	0.43
12:x:131:PRO:HB2	13:y:159:VAL:HA	1.99	0.43
13:y:63:THR:HA	13:y:66:THR:HG22	2.00	0.43
26:B:55:CYS:SG	26:B:117:UNK:CB	3.06	0.43
29:E:96:UNK:CB	29:E:98:UNK:O	2.66	0.43
30:F:73:UNK:O	30:F:74:UNK:C	2.67	0.43
31:G:31:UNK:O	31:G:34:UNK:HA	2.18	0.43
31:G:259:UNK:C	31:G:260:UNK:O	2.58	0.43
31:G:558:UNK:O	31:G:559:UNK:CB	2.67	0.43
32:H:195:UNK:HA	32:H:198:UNK:CA	2.48	0.43
36:L:209:UNK:O	36:L:210:UNK:C	2.66	0.43
37:M:393:UNK:C	37:M:395:UNK:N	2.79	0.43
40:P:313:UNK:O	40:P:314:UNK:C	2.67	0.43
1:c:61:HIS:HB2	1:c:130:GLU:HG3	2.00	0.43
2:m:42:ALA:HB1	2:m:43:PRO:CD	2.40	0.43
2:m:239:TYR:OH	2:m:423:SER:OG	2.37	0.43
3:b:157:GLY:O	3:b:160:LEU:N	2.51	0.43
3:b:177:ARG:O	3:b:181:PHE:CD2	2.72	0.43
3:b:196:HIS:HE1	52:b:402:HEM:C1D	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:145:MET:HE3	1:l:145:MET:HB2	1.87	0.43
1:l:248:LEU:HA	1:l:249:PRO:HD3	1.78	0.43
1:l:349:ALA:HB3	1:l:408:ARG:NE	2.34	0.43
3:o:119:LEU:CD1	3:o:192:ILE:CG2	2.97	0.43
3:o:211:ILE:HG22	3:o:212:SER:N	2.34	0.43
3:o:319:PRO:O	3:o:320:LEU:C	2.61	0.43
4:p:139:THR:HB	8:t:54:CYS:SG	2.58	0.43
5:q:114:VAL:O	5:q:117:LEU:N	2.48	0.43
6:r:73:GLN:HA	7:s:39:ARG:NH2	2.29	0.43
6:r:101:ARG:HG2	6:r:105:GLU:OE2	2.19	0.43
7:s:71:ARG:NH2	8:t:60:ASP:OD1	2.38	0.43
12:x:247:ILE:HB	57:x:604:HEA:HBC1	2.01	0.43
20:6:21:ILE:O	20:6:25:PHE:HD2	2.02	0.43
20:6:68:ILE:HG13	20:6:69:PHE:N	2.33	0.43
26:B:63:UNK:HA	26:B:69:UNK:CB	2.48	0.43
29:E:106:UNK:O	29:E:109:UNK:N	2.51	0.43
32:H:272:UNK:O	32:H:276:UNK:CB	2.67	0.43
36:L:63:UNK:CB	36:L:78:UNK:CB	2.97	0.43
36:L:379:UNK:O	36:L:388:UNK:CB	2.66	0.43
37:M:348:UNK:CA	37:M:351:UNK:CB	2.85	0.43
39:O:25:UNK:O	39:O:123:UNK:CA	2.66	0.43
41:Q:50:UNK:N	41:Q:51:UNK:CA	2.82	0.43
1:c:347:THR:HA	11:k:16:ASN:HD22	1.83	0.43
3:b:183:PHE:CE1	3:b:187:PHE:HE2	2.35	0.43
3:b:200:LEU:HD13	52:b:402:HEM:CAD	2.49	0.43
3:b:235:LEU:O	3:b:235:LEU:HD12	2.19	0.43
4:d:7:PRO:HB2	4:d:125:ASP:CB	2.49	0.43
1:l:158:PHE:O	1:l:164:ALA:HB2	2.18	0.43
2:n:367:GLY:O	2:n:368:TYR:C	2.61	0.43
3:o:133:LEU:HA	3:o:175:LEU:HD11	2.01	0.43
4:p:25:SER:O	4:p:26:ILE:C	2.61	0.43
4:p:229:VAL:HG12	4:p:233:ARG:NE	2.32	0.43
5:q:20:ASP:O	5:q:22:THR:N	2.52	0.43
6:r:67:ASP:HA	6:r:70:MET:HE3	2.01	0.43
10:v:51:LEU:O	10:v:52:TRP:C	2.61	0.43
14:z:110:PRO:HB3	19:5:30:TRP:CD2	2.54	0.43
26:B:166:UNK:O	26:B:169:UNK:N	2.52	0.43
28:D:151:UNK:O	28:D:152:UNK:C	2.66	0.43
28:D:311:UNK:O	28:D:315:UNK:N	2.52	0.43
30:F:303:UNK:O	30:F:414:UNK:CA	2.67	0.43
37:M:62:UNK:CB	37:M:65:UNK:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Y:18:UNK:CB	48:Y:44:UNK:CB	2.97	0.43
51:Z:30:UNK:O	51:Z:32:UNK:N	2.51	0.43
1:c:106:LEU:HD12	1:c:106:LEU:HA	1.74	0.43
2:m:170:ASN:OD1	2:m:171:ALA:N	2.52	0.43
2:m:257:LEU:HD22	2:m:424:MET:HE2	1.99	0.43
3:b:239:LEU:O	3:b:243:VAL:HB	2.19	0.43
3:b:319:PRO:O	3:b:322:GLN:N	2.52	0.43
7:g:26:PHE:N	7:g:27:PRO:HD3	2.33	0.43
7:g:36:ASN:OD1	7:g:39:ARG:NE	2.52	0.43
7:g:39:ARG:HA	7:g:42:ARG:HD2	2.00	0.43
11:k:20:THR:HG23	11:k:24:TRP:CD1	2.54	0.43
1:l:85:HIS:HA	2:n:284:HIS:O	2.18	0.43
1:l:136:GLN:HE21	9:u:50:LEU:HG	1.84	0.43
2:n:99:THR:OG1	9:u:68:VAL:HG13	2.19	0.43
2:n:372:VAL:O	2:n:372:VAL:CG1	2.67	0.43
5:q:185:TYR:HB3	5:q:195:VAL:HA	2.00	0.43
9:u:77:ARG:HB2	9:u:78:TYR:H	1.74	0.43
12:x:106:PRO:HB2	12:x:107:PRO:HD3	2.01	0.43
12:x:240:HIS:NE2	12:x:244:TYR:CE2	2.81	0.43
16:2:27:TRP:CH2	17:3:86:GLY:HA2	2.54	0.43
20:6:42:LYS:HE2	20:6:42:LYS:HB3	1.83	0.43
26:B:149:CYS:CA	26:B:150:UNK:C	2.93	0.43
32:H:291:UNK:C	32:H:293:UNK:N	2.81	0.43
36:L:544:UNK:O	36:L:547:UNK:CB	2.67	0.43
39:O:209:UNK:O	39:O:210:UNK:C	2.66	0.43
40:P:71:UNK:O	40:P:73:UNK:N	2.50	0.43
40:P:134:UNK:C	40:P:136:UNK:N	2.74	0.43
43:S:83:UNK:O	43:S:86:UNK:CA	2.67	0.43
51:Z:311:UNK:O	51:Z:312:UNK:C	2.67	0.43
1:c:7:ALA:O	1:c:8:LEU:C	2.60	0.42
1:c:80:GLU:C	1:c:82:MET:N	2.77	0.42
2:m:129:ALA:O	2:m:130:PRO:C	2.62	0.42
2:m:259:ALA:O	2:m:260:GLU:C	2.61	0.42
3:b:92:ILE:HG12	3:b:272:TRP:CH2	2.54	0.42
3:b:122:THR:CG2	3:b:189:ILE:CG1	2.96	0.42
3:b:218:ILE:CG2	3:b:219:PRO:N	2.82	0.42
3:b:248:ASP:CG	4:d:118:ARG:HH21	2.28	0.42
3:b:284:ILE:HA	3:b:285:PRO:HD2	1.82	0.42
4:d:72:ASP:OD2	4:d:92:PRO:HB2	2.18	0.42
4:d:220:TYR:CD2	7:g:26:PHE:CZ	3.06	0.42
1:l:106:LEU:HA	1:l:109:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:83:PHE:CZ	2:n:87:ARG:HG3	2.53	0.42
2:n:257:LEU:HA	2:n:257:LEU:HD12	1.67	0.42
2:n:286:LYS:HZ2	2:n:286:LYS:HG3	1.69	0.42
2:n:334:GLY:O	2:n:335:ASP:C	2.60	0.42
3:o:41:LEU:HD12	52:o:401:HEM:HBB1	2.00	0.42
3:o:56:THR:HG22	3:o:57:SER:N	2.34	0.42
4:p:12:TRP:O	4:p:13:SER:C	2.61	0.42
4:p:27:ARG:NH1	10:v:58:LYS:HE3	2.33	0.42
4:p:233:ARG:O	4:p:234:LYS:HE2	2.19	0.42
5:q:29:SER:CB	5:q:32:ARG:HD3	2.49	0.42
5:q:102:THR:H	5:q:105:GLU:CB	2.32	0.42
6:r:51:PRO:O	6:r:52:GLU:C	2.62	0.42
14:z:19:THR:HG22	14:z:53:THR:OG1	2.19	0.42
25:A:98:UNK:O	25:A:101:UNK:N	2.52	0.42
31:G:192:UNK:CA	31:G:193:UNK:CB	2.83	0.42
31:G:398:UNK:C	31:G:400:UNK:N	2.77	0.42
31:G:425:UNK:O	31:G:428:UNK:CA	2.66	0.42
32:H:68:UNK:O	32:H:71:UNK:N	2.52	0.42
32:H:170:UNK:O	32:H:171:UNK:C	2.65	0.42
34:J:100:UNK:O	34:J:101:UNK:C	2.63	0.42
36:L:250:UNK:O	36:L:254:UNK:CB	2.67	0.42
1:c:33:PRO:O	1:c:103:SER:CB	2.67	0.42
1:c:366:VAL:HG11	2:m:44:ALA:HB2	2.01	0.42
2:m:79:GLY:H	2:m:125:ASN:HD22	1.67	0.42
2:m:369:LEU:O	2:m:370:MET:C	2.61	0.42
3:b:373:GLU:O	3:b:377:LEU:HD12	2.18	0.42
4:d:35:GLN:HB2	4:d:169:LEU:HD13	2.02	0.42
4:d:138:PRO:CG	8:h:55:THR:HA	2.48	0.42
6:f:103:GLU:O	6:f:104:ARG:C	2.62	0.42
7:g:45:ILE:HD12	7:g:45:ILE:HA	1.67	0.42
8:h:59:LEU:HD23	8:h:59:LEU:HA	1.76	0.42
1:l:213:GLN:HB2	1:l:215:HIS:CD2	2.54	0.42
2:n:72:ALA:HB1	2:n:75:LEU:CD1	2.49	0.42
2:n:294:SER:O	2:n:297:GLN:N	2.52	0.42
3:o:88:SER:O	3:o:89:MET:C	2.61	0.42
3:o:126:THR:CG2	52:o:401:HEM:C3B	3.01	0.42
3:o:207:ASN:O	3:o:208:PRO:C	2.62	0.42
4:p:7:PRO:HB3	4:p:125:ASP:HB3	2.01	0.42
4:p:178:THR:HG23	8:t:15:ASP:N	2.34	0.42
4:p:240:PRO:CG	4:p:241:LYS:H	2.33	0.42
4:p:240:PRO:HG2	4:p:241:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:114:VAL:HG13	5:q:120:PRO:HB3	2.01	0.42
6:r:94:LEU:O	6:r:98:ILE:HG13	2.19	0.42
7:s:33:GLY:O	7:s:37:VAL:HB	2.20	0.42
21:7:11:LEU:HD23	21:7:11:LEU:C	2.44	0.42
25:A:103:UNK:O	25:A:106:UNK:CA	2.67	0.42
27:C:112:UNK:CB	27:C:113:UNK:HA	2.49	0.42
28:D:296:UNK:O	28:D:297:UNK:C	2.66	0.42
29:E:50:UNK:O	29:E:51:UNK:C	2.67	0.42
31:G:12:UNK:HA	31:G:17:UNK:CA	2.47	0.42
31:G:426:UNK:HA	31:G:429:UNK:CB	2.50	0.42
36:L:141:UNK:O	36:L:142:UNK:C	2.67	0.42
37:M:168:UNK:CB	37:M:174:UNK:CA	2.97	0.42
1:c:255:ILE:HD12	1:c:335:MET:HE1	2.01	0.42
2:m:279:LEU:CD2	2:m:344:VAL:HG22	2.49	0.42
3:b:34:GLY:O	3:b:37:LEU:N	2.52	0.42
3:b:174:THR:CG2	3:b:178:PHE:CE1	2.83	0.42
3:b:234:LEU:HD21	4:d:216:LEU:HD21	2.01	0.42
3:b:338:ILE:O	3:b:341:GLN:N	2.51	0.42
4:d:3:LEU:HD22	7:g:70:LYS:HZ1	1.81	0.42
4:d:8:PRO:O	4:d:125:ASP:CG	2.62	0.42
4:d:21:LEU:CD1	4:d:26:ILE:HD11	2.49	0.42
4:d:109:LEU:HA	4:d:110:PRO:HD2	1.74	0.42
4:d:165:TYR:O	4:d:166:ASN:C	2.61	0.42
1:l:283:THR:OG1	9:u:74:ALA:HB3	2.20	0.42
2:n:122:PHE:HD1	2:n:122:PHE:HA	1.74	0.42
2:n:178:CYS:HA	2:n:179:PRO:HD3	1.63	0.42
3:o:192:ILE:N	3:o:192:ILE:CD1	2.82	0.42
3:o:233:LEU:HD12	3:o:233:LEU:HA	1.74	0.42
3:o:315:MET:O	3:o:318:ARG:N	2.40	0.42
4:p:35:GLN:OE1	4:p:35:GLN:HA	2.18	0.42
4:p:204:MET:O	4:p:205:GLY:C	2.60	0.42
14:z:60:ASP:O	14:z:64:GLU:HG3	2.19	0.42
14:z:148:HIS:CE1	14:z:152:MET:HE3	2.54	0.42
19:5:24:ASN:HD22	19:5:25:GLN:N	2.18	0.42
21:7:31:LEU:HA	21:7:31:LEU:HD23	1.83	0.42
30:F:394:UNK:O	30:F:395:UNK:C	2.66	0.42
36:L:108:UNK:O	36:L:111:UNK:CB	2.67	0.42
36:L:140:UNK:O	36:L:143:UNK:N	2.53	0.42
36:L:241:UNK:O	36:L:242:UNK:C	2.68	0.42
36:L:462:UNK:O	36:L:465:UNK:N	2.52	0.42
37:M:408:UNK:O	37:M:412:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:160:UNK:N	40:P:161:UNK:CA	2.83	0.42
1:c:277:ILE:HB	1:c:309:THR:HG21	2.00	0.42
3:b:107:TYR:HE2	3:b:305:PRO:HA	1.83	0.42
4:d:131:LEU:HD13	4:d:164:ILE:CD1	2.48	0.42
4:d:214:LEU:O	4:d:218:LEU:HG	2.19	0.42
1:l:441:MET:HE3	1:l:441:MET:HB3	1.74	0.42
2:n:29:LEU:HG	2:n:33:LEU:CD2	2.50	0.42
2:n:264:ILE:HB	2:n:316:TYR:C	2.44	0.42
2:n:282:GLY:HA2	2:n:283:PRO:HD2	1.78	0.42
3:o:109:PHE:HE1	3:o:203:THR:HG1	1.61	0.42
3:o:122:THR:HB	3:o:189:ILE:CD1	2.49	0.42
3:o:257:THR:O	3:o:258:PRO:C	2.62	0.42
3:o:282:ARG:CZ	3:o:343:VAL:HG22	2.49	0.42
4:p:115:TYR:O	4:p:116:ILE:C	2.60	0.42
5:q:97:PHE:CD1	5:q:137:GLY:HA3	2.54	0.42
6:r:70:MET:HE3	6:r:70:MET:HB3	1.65	0.42
12:x:462:LEU:O	12:x:466:MET:HG3	2.20	0.42
27:C:78:UNK:HA	27:C:93:UNK:O	2.18	0.42
30:F:215:UNK:O	30:F:216:UNK:C	2.64	0.42
33:I:113:UNK:O	33:I:115:UNK:N	2.53	0.42
36:L:32:UNK:HA	36:L:35:UNK:CB	2.48	0.42
37:M:22:UNK:CA	37:M:23:UNK:CB	2.97	0.42
48:Y:92:UNK:O	48:Y:95:UNK:N	2.52	0.42
1:c:134:ILE:HA	1:c:134:ILE:HD12	1.93	0.42
1:c:136:GLN:HE21	9:i:50:LEU:HG	1.84	0.42
1:c:154:HIS:HE1	1:c:314:TYR:OH	2.02	0.42
1:c:262:TRP:CE3	1:c:385:THR:CG2	3.02	0.42
1:c:280:TYR:CD1	1:c:280:TYR:C	2.98	0.42
2:m:83:PHE:CE1	6:r:104:ARG:HG2	2.54	0.42
2:m:158:HIS:ND1	2:m:246:GLU:OE1	2.53	0.42
3:b:368:THR:O	3:b:369:ALA:C	2.62	0.42
4:d:70:VAL:HG23	4:d:84:PRO:CD	2.41	0.42
4:d:171:PHE:HZ	4:d:182:VAL:HG22	1.85	0.42
1:l:100:LYS:HG2	2:n:370:MET:SD	2.59	0.42
2:n:31:ASN:HB3	2:n:201:SER:CB	2.50	0.42
2:n:99:THR:O	2:n:106:ALA:N	2.51	0.42
3:o:26:ASN:O	3:o:26:ASN:CG	2.63	0.42
3:o:271:GLU:OE2	3:o:273:TYR:OH	2.38	0.42
4:p:58:GLU:O	4:p:62:LYS:HB2	2.19	0.42
4:p:116:ILE:O	4:p:117:VAL:C	2.60	0.42
4:p:206:LEU:O	4:p:207:LYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:14:ARG:HA	7:s:23:GLN:HA	2.01	0.42
5:q:185:TYR:HD2	5:q:193:VAL:HG21	1.84	0.42
8:t:59:LEU:HD23	8:t:59:LEU:HA	1.71	0.42
13:y:52:HIS:CD2	16:2:40:ASP:HB2	2.54	0.42
17:3:86:GLY:O	17:3:87:THR:O	2.37	0.42
18:4:77:PRO:HA	18:4:82:TYR:HA	2.02	0.42
39:O:22:UNK:CB	39:O:23:UNK:CA	2.97	0.42
47:X:331:UNK:O	47:X:334:UNK:N	2.52	0.42
1:c:32:GLN:HE22	2:m:373:GLU:HA	1.83	0.42
1:c:56:GLY:O	1:c:59:VAL:HB	2.19	0.42
1:c:227:ALA:O	1:c:229:PRO:HD3	2.19	0.42
1:c:381:ARG:O	1:c:382:SER:C	2.62	0.42
2:m:295:LEU:O	2:m:299:VAL:HG23	2.19	0.42
3:b:3:ASN:HA	3:b:8:HIS:CD2	2.55	0.42
3:b:257:THR:O	3:b:258:PRO:C	2.61	0.42
3:b:371:THR:O	3:b:372:ILE:C	2.61	0.42
6:f:91:GLU:O	6:f:92:PRO:C	2.62	0.42
7:g:27:PRO:O	7:g:28:HIS:C	2.62	0.42
10:j:20:PHE:O	10:j:23:THR:HB	2.20	0.42
11:k:20:THR:HG23	11:k:24:TRP:HD1	1.83	0.42
1:l:61:HIS:HB2	1:l:130:GLU:HG3	2.02	0.42
2:n:47:ILE:HB	2:n:109:VAL:CG1	2.49	0.42
3:o:183:PHE:CE1	3:o:187:PHE:HE2	2.37	0.42
3:o:316:MET:HE2	3:o:317:PHE:HE1	1.77	0.42
3:o:338:ILE:HA	3:o:341:GLN:CG	2.49	0.42
4:p:5:LEU:HG	4:p:152:TYR:CE1	2.54	0.42
4:p:120:ARG:HD2	53:p:301:HEC:CGA	2.50	0.42
4:p:192:TRP:CE3	4:p:193:ALA:N	2.88	0.42
4:p:220:TYR:HE2	7:s:26:PHE:CE1	2.19	0.42
4:p:220:TYR:O	4:p:223:LYS:N	2.52	0.42
4:p:224:ARG:O	4:p:225:HIS:C	2.62	0.42
8:t:15:ASP:CB	8:t:16:PRO:HD3	2.49	0.42
18:4:5:LYS:CD	18:4:6:GLY:N	2.81	0.42
19:5:57:ARG:HA	19:5:60:TYR:CD2	2.55	0.42
22:8:44:PRO:HA	22:8:47:ARG:NH1	2.34	0.42
24:0:19:LEU:C	24:0:19:LEU:HD23	2.45	0.42
26:B:75:UNK:O	26:B:76:UNK:CB	2.68	0.42
26:B:166:UNK:CA	26:B:169:UNK:O	2.63	0.42
30:F:34:UNK:O	30:F:38:UNK:CA	2.67	0.42
30:F:286:UNK:HA	30:F:287:UNK:HA	1.55	0.42
31:G:456:UNK:CB	31:G:457:UNK:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:H:95:UNK:HA	32:H:96:UNK:HA	1.81	0.42
33:I:83:CYS:HB2	33:I:122:CYS:HB2	2.02	0.42
36:L:582:UNK:O	36:L:586:UNK:N	2.53	0.42
37:M:315:UNK:O	37:M:316:UNK:C	2.64	0.42
50:U:627:UNK:O	50:U:628:UNK:C	2.65	0.42
1:c:3:THR:O	1:c:4:TYR:C	2.62	0.42
1:c:19:LEU:HD22	1:c:214:LYS:NZ	2.34	0.42
1:c:54:GLY:O	1:c:55:ALA:O	2.37	0.42
1:c:62:LEU:HB3	1:c:122:LEU:HD22	2.02	0.42
1:c:136:GLN:NE2	9:i:50:LEU:HG	2.35	0.42
2:m:433:THR:HA	2:m:434:PRO:HD2	1.90	0.42
3:b:53:MET:SD	3:o:181:PHE:HZ	2.43	0.42
4:d:116:ILE:CD1	4:d:120:ARG:HG3	2.49	0.42
8:h:15:ASP:CB	8:h:16:PRO:CD	2.97	0.42
2:n:49:LEU:HD21	2:n:204:MET:SD	2.60	0.42
2:n:283:PRO:HG3	9:u:55:LEU:CG	2.49	0.42
2:n:312:PHE:CD1	9:u:58:GLN:O	2.73	0.42
3:o:25:SER:HA	3:o:218:ILE:HD12	2.02	0.42
3:o:44:GLN:OE1	3:o:44:GLN:HA	2.19	0.42
3:o:277:ALA:HB1	3:o:294:LEU:CD1	2.50	0.42
4:p:50:HIS:HB3	4:p:54:VAL:HG21	2.01	0.42
5:q:109:GLU:OE2	5:q:166:ASP:OD2	2.37	0.42
5:q:150:ALA:CB	5:q:157:TYR:CB	2.98	0.42
6:r:50:LEU:HA	6:r:51:PRO:HD2	1.71	0.42
6:r:71:ARG:O	6:r:72:GLN:HB2	2.19	0.42
8:t:67:HIS:O	8:t:68:CYS:C	2.63	0.42
13:y:78:LEU:HB2	13:y:79:PRO:CD	2.38	0.42
13:y:146:MET:SD	13:y:189:PRO:HB3	2.60	0.42
14:z:40:MET:O	14:z:41:THR:C	2.62	0.42
26:B:117:UNK:O	26:B:120:UNK:CA	2.67	0.42
30:F:56:UNK:O	30:F:59:UNK:N	2.53	0.42
34:J:58:UNK:O	34:J:63:UNK:N	2.52	0.42
34:J:69:UNK:HA	34:J:72:UNK:CB	2.50	0.42
34:J:88:UNK:O	34:J:91:UNK:CB	2.67	0.42
36:L:82:UNK:O	36:L:86:UNK:N	2.52	0.42
36:L:128:UNK:O	36:L:132:UNK:N	2.53	0.42
36:L:369:UNK:O	36:L:372:UNK:N	2.53	0.42
37:M:168:UNK:HA	37:M:174:UNK:HA	2.02	0.42
37:M:175:UNK:C	37:M:177:UNK:HA	2.47	0.42
38:N:76:UNK:O	38:N:80:UNK:N	2.52	0.42
40:P:301:UNK:C	40:P:303:UNK:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:303:UNK:O	47:X:304:UNK:C	2.68	0.42
1:c:80:GLU:O	1:c:81:SER:C	2.63	0.42
1:c:224:ASP:O	1:c:225:GLU:C	2.61	0.42
1:c:255:ILE:CD1	1:c:335:MET:HE1	2.49	0.42
1:c:385:THR:CG2	1:c:386:TYR:N	2.77	0.42
1:c:385:THR:HB	1:c:386:TYR:HD1	1.83	0.42
2:m:68:LEU:HB2	2:m:144:LEU:HD21	2.02	0.42
2:m:92:VAL:HG11	2:m:115:ASP:HB3	2.02	0.42
2:m:213:HIS:H	2:m:214:PRO:HD2	1.77	0.42
2:m:367:GLY:O	2:m:368:TYR:C	2.59	0.42
3:b:36:LEU:HD22	3:b:235:LEU:HB2	2.02	0.42
3:b:89:MET:O	3:b:90:PHE:C	2.62	0.42
3:b:316:MET:HG2	3:b:317:PHE:CD1	2.54	0.42
52:b:401:HEM:HBB2	52:b:401:HEM:CMB	2.48	0.42
1:l:67:THR:OG1	1:l:119:ASN:HB2	2.20	0.42
1:l:88:ALA:O	2:n:286:LYS:HD2	2.20	0.42
1:l:134:ILE:HA	1:l:134:ILE:HD13	1.53	0.42
1:l:224:ASP:OD1	1:l:224:ASP:O	2.37	0.42
1:l:224:ASP:O	1:l:225:GLU:C	2.60	0.42
1:l:372:THR:O	1:l:373:THR:C	2.62	0.42
2:n:34:VAL:O	2:n:35:ILE:HG22	2.19	0.42
2:n:211:VAL:HG12	2:n:212:SER:N	2.34	0.42
3:o:7:SER:O	3:o:8:HIS:C	2.61	0.42
5:q:141:HIS:CE1	5:q:175:PRO:HG2	2.54	0.42
12:x:311:ILE:HG21	12:x:311:ILE:HD13	1.75	0.42
12:x:474:GLU:HG3	12:x:475:ALA:N	2.34	0.42
15:1:126:MET:HG3	15:1:128:VAL:HG23	2.00	0.42
17:3:53:THR:HG22	17:3:54:ASN:OD1	2.19	0.42
25:A:84:UNK:O	25:A:87:UNK:N	2.52	0.42
28:D:317:UNK:O	28:D:318:UNK:C	2.68	0.42
30:F:185:UNK:C	30:F:187:UNK:N	2.81	0.42
31:G:326:UNK:O	31:G:327:UNK:C	2.67	0.42
34:J:25:UNK:O	34:J:28:UNK:CB	2.68	0.42
36:L:158:UNK:O	36:L:159:UNK:C	2.64	0.42
37:M:164:UNK:O	37:M:167:UNK:N	2.52	0.42
37:M:369:UNK:O	37:M:372:UNK:CB	2.68	0.42
39:O:80:UNK:O	39:O:83:UNK:N	2.53	0.42
39:O:231:UNK:O	39:O:234:UNK:N	2.53	0.42
45:V:30:UNK:O	45:V:31:UNK:C	2.67	0.42
2:m:57:TYR:HB3	2:m:198:HIS:CE1	2.55	0.42
2:m:283:PRO:HG3	9:i:55:LEU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:335:LEU:HD23	3:b:335:LEU:HA	1.70	0.42
6:f:10:SER:HA	6:f:13:LEU:HG	2.01	0.42
6:f:64:ARG:O	6:f:68:LEU:HD12	2.20	0.42
6:f:94:LEU:O	6:f:94:LEU:HD12	2.20	0.42
1:l:85:HIS:CD2	2:n:370:MET:HE1	2.54	0.42
1:l:152:TYR:CE2	1:l:243:HIS:HD2	2.38	0.42
1:l:213:GLN:CB	1:l:215:HIS:CD2	3.02	0.42
1:l:228:VAL:HA	1:l:229:PRO:HD2	1.94	0.42
2:n:206:LEU:C	2:n:207:ILE:HG12	2.43	0.42
3:o:184:ILE:O	3:o:184:ILE:HG12	2.20	0.42
3:o:234:LEU:O	3:o:237:LEU:HB3	2.19	0.42
3:o:314:SER:OG	3:o:316:MET:HB3	2.19	0.42
4:p:43:MET:HE3	4:p:91:PHE:CE2	2.54	0.42
4:p:150:ASN:OD1	4:p:151:PRO:HD2	2.19	0.42
4:p:165:TYR:CE2	4:p:168:VAL:HG22	2.55	0.42
5:q:33:LYS:HA	7:s:21:PHE:CE1	2.55	0.42
6:r:84:GLU:CD	6:r:84:GLU:H	2.28	0.42
31:G:12:UNK:N	31:G:77:UNK:O	2.53	0.42
31:G:565:UNK:C	31:G:567:UNK:N	2.78	0.42
31:G:604:UNK:O	31:G:609:UNK:N	2.53	0.42
32:H:110:UNK:O	32:H:111:UNK:C	2.68	0.42
32:H:277:UNK:O	32:H:278:UNK:CB	2.66	0.42
45:V:33:UNK:O	45:V:37:UNK:N	2.53	0.42
45:V:51:UNK:O	45:V:52:UNK:CB	2.68	0.42
47:X:322:UNK:HA	47:X:325:UNK:CB	2.50	0.42
1:c:185:TYR:O	1:c:186:LEU:C	2.62	0.42
1:c:244:ARG:NH1	7:g:10:VAL:HG21	2.35	0.42
1:c:280:TYR:HB3	1:c:307:PHE:CD2	2.55	0.42
2:m:24:LEU:CG	2:m:38:LEU:HD11	2.31	0.42
2:m:55:SER:HG	2:m:102:ARG:HG2	1.85	0.42
2:m:72:ALA:HB2	2:m:140:LEU:CD2	2.50	0.42
2:m:92:VAL:O	2:m:92:VAL:CG1	2.68	0.42
2:m:283:PRO:CG	9:i:55:LEU:HD13	2.50	0.42
2:m:342:ASN:O	2:m:345:LYS:N	2.52	0.42
2:m:434:PRO:HB2	2:m:439:LEU:CD1	2.49	0.42
3:b:16:ASN:HD22	3:b:20:ASP:CG	2.08	0.42
3:b:101:GLY:HA2	3:b:106:SER:HB2	2.02	0.42
3:b:163:TRP:CD1	5:q:63:SER:HA	2.55	0.42
7:g:3:GLN:HA	7:g:3:GLN:OE1	2.20	0.42
1:l:31:SER:N	1:l:202:GLY:HA2	2.35	0.42
1:l:333:ASP:O	1:l:334:MET:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:385:THR:HG22	1:l:386:TYR:CD1	2.55	0.42
2:n:24:LEU:HG	2:n:38:LEU:CD1	2.31	0.42
2:n:90:GLU:O	2:n:91:ALA:C	2.62	0.42
2:n:135:TRP:NE1	2:n:136:GLU:HG3	2.35	0.42
3:o:150:LEU:HD12	3:o:150:LEU:HA	1.82	0.42
3:o:300:ILE:CD1	3:o:362:ILE:HG21	2.50	0.42
4:p:10:TYR:CE1	4:p:128:PHE:HE2	2.37	0.42
6:r:35:ASP:OD2	6:r:61:ARG:HD2	2.20	0.42
7:s:34:ILE:CB	7:s:35:PRO:CD	2.91	0.42
8:t:65:ARG:HH11	8:t:65:ARG:HD2	1.65	0.42
9:u:66:ALA:O	9:u:77:ARG:HG3	2.20	0.42
22:8:13:TYR:O	22:8:14:GLY:C	2.63	0.42
26:B:109:UNK:O	26:B:111:UNK:N	2.53	0.42
26:B:149:CYS:HA	26:B:150:UNK:HA	1.94	0.42
28:D:182:UNK:O	28:D:186:UNK:HA	2.20	0.42
30:F:183:UNK:CB	30:F:186:UNK:N	2.82	0.42
31:G:143:UNK:CB	31:G:190:UNK:CB	2.98	0.42
31:G:273:UNK:O	31:G:274:UNK:C	2.67	0.42
31:G:288:UNK:CA	31:G:289:UNK:C	2.89	0.42
31:G:491:UNK:O	31:G:493:UNK:N	2.53	0.42
36:L:34:UNK:O	36:L:37:UNK:N	2.52	0.42
36:L:297:UNK:HA	36:L:355:UNK:CA	2.48	0.42
37:M:139:UNK:CA	37:M:140:UNK:CB	2.98	0.42
38:N:12:UNK:O	38:N:16:UNK:N	2.52	0.42
38:N:124:UNK:C	38:N:126:UNK:N	2.78	0.42
47:X:212:UNK:O	47:X:213:UNK:C	2.68	0.42
51:Z:245:UNK:O	51:Z:249:UNK:CB	2.68	0.42
1:c:97:TYR:CD1	1:c:97:TYR:N	2.88	0.41
1:c:151:ASN:O	1:c:154:HIS:N	2.53	0.41
1:c:297:ILE:HG22	1:c:303:LEU:CD1	2.49	0.41
1:c:328:HIS:NE2	1:c:329:MET:HG2	2.35	0.41
2:m:81:SER:O	2:m:82:SER:C	2.62	0.41
2:m:348:ALA:CB	2:m:418:VAL:HG21	2.49	0.41
3:b:310:SER:OG	3:b:312:GLN:N	2.48	0.41
4:d:55:CYS:SG	10:j:52:TRP:HB2	2.60	0.41
1:l:38:GLY:HA3	1:l:40:TRP:CZ3	2.50	0.41
1:l:227:ALA:O	1:l:229:PRO:HD3	2.20	0.41
2:n:160:ILE:CD1	2:n:325:TYR:HE2	2.33	0.41
2:n:200:THR:OG1	2:n:201:SER:N	2.53	0.41
2:n:286:LYS:HD3	2:n:287:ARG:HH12	1.80	0.41
3:o:10:LEU:HD12	3:o:13:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:15:ASN:ND2	3:o:18:PHE:CD2	2.88	0.41
3:o:18:PHE:O	3:o:220:PHE:HD2	2.03	0.41
3:o:63:PHE:CD1	3:o:63:PHE:C	2.98	0.41
3:o:218:ILE:HG22	3:o:223:TYR:HD2	1.84	0.41
3:o:244:LEU:O	4:p:201:ARG:HG2	2.20	0.41
5:q:177:PRO:HB2	5:q:178:LEU:HG	2.02	0.41
6:r:87:LYS:HE2	6:r:89:TYR:HB3	2.01	0.41
10:v:44:GLU:O	10:v:45:HIS:C	2.62	0.41
14:z:122:HIS:HA	14:z:123:PRO:HD2	1.91	0.41
22:8:9:PHE:CD1	22:8:9:PHE:C	2.97	0.41
25:A:105:UNK:O	25:A:109:UNK:HA	2.20	0.41
29:E:54:UNK:O	29:E:55:UNK:C	2.65	0.41
31:G:594:UNK:CB	31:G:596:UNK:N	2.83	0.41
36:L:274:UNK:O	36:L:275:UNK:C	2.67	0.41
37:M:54:UNK:HA	37:M:55:UNK:HA	1.65	0.41
37:M:178:UNK:O	37:M:179:UNK:C	2.62	0.41
37:M:179:UNK:O	37:M:180:UNK:C	2.68	0.41
40:P:53:UNK:O	40:P:57:UNK:N	2.53	0.41
40:P:120:UNK:O	40:P:121:UNK:C	2.67	0.41
40:P:229:UNK:N	40:P:299:UNK:CB	2.83	0.41
50:U:103:UNK:C	50:U:105:UNK:N	2.82	0.41
1:c:361:LEU:O	1:c:361:LEU:HD12	2.19	0.41
1:c:436:ARG:NE	3:b:222:PRO:HG3	2.33	0.41
3:b:170:VAL:O	3:b:170:VAL:CG1	2.68	0.41
3:b:313:ARG:HH11	3:b:313:ARG:HD2	1.59	0.41
3:b:317:PHE:CD1	6:f:26:PHE:HB3	2.55	0.41
4:d:43:MET:HA	4:d:112:ASP:OD1	2.20	0.41
10:j:43:TYR:O	10:j:43:TYR:CG	2.73	0.41
1:l:78:GLU:HG2	1:l:112:LEU:HD21	2.02	0.41
1:l:369:LEU:HD21	1:l:378:ASP:OD2	2.20	0.41
2:n:54:GLY:H	2:n:57:TYR:HD1	1.65	0.41
2:n:56:ARG:HH21	2:n:103:GLU:CD	2.29	0.41
2:n:201:SER:OG	2:n:226:ILE:N	2.51	0.41
2:n:255:ALA:HA	2:n:426:ALA:HA	2.02	0.41
4:p:139:THR:CG2	8:t:44:VAL:HB	2.50	0.41
5:q:13:TYR:O	7:s:24:ARG:HG3	2.20	0.41
7:s:36:ASN:OD1	7:s:39:ARG:NE	2.53	0.41
10:v:24:ILE:O	10:v:25:VAL:C	2.61	0.41
12:x:501:PRO:O	12:x:502:TYR:C	2.63	0.41
19:5:57:ARG:HB3	19:5:57:ARG:NH1	2.31	0.41
26:B:71:UNK:CB	32:H:37:UNK:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:95:UNK:O	28:D:98:UNK:N	2.54	0.41
30:F:181:UNK:O	30:F:182:UNK:CB	2.69	0.41
30:F:213:UNK:HA	30:F:214:UNK:HA	1.67	0.41
33:I:100:UNK:O	33:I:103:UNK:C	2.69	0.41
36:L:109:UNK:O	36:L:110:UNK:CB	2.67	0.41
36:L:161:UNK:CB	36:L:163:UNK:N	2.84	0.41
36:L:184:UNK:O	36:L:188:UNK:N	2.54	0.41
37:M:124:UNK:O	37:M:125:UNK:C	2.64	0.41
37:M:433:UNK:O	37:M:434:UNK:C	2.63	0.41
38:N:11:UNK:O	38:N:15:UNK:N	2.53	0.41
38:N:124:UNK:O	38:N:127:UNK:CB	2.68	0.41
1:c:64:PHE:HA	1:c:75:LEU:HD22	2.02	0.41
1:c:252:HIS:O	1:c:424:GLY:HA2	2.21	0.41
2:m:24:LEU:HG	2:m:38:LEU:CD1	2.31	0.41
2:m:335:ASP:O	2:m:336:VAL:C	2.64	0.41
3:b:152:ALA:HB2	3:b:287:LYS:HZ3	1.85	0.41
4:d:44:ASP:OD1	4:d:93:LYS:HE3	2.20	0.41
4:d:237:TYR:HD1	7:g:13:VAL:HG22	1.85	0.41
9:i:62:ARG:HB3	9:i:63:PRO:CD	2.50	0.41
1:l:28:GLU:OE1	1:l:375:VAL:CG1	2.68	0.41
1:l:156:THR:OG1	1:l:241:ILE:HB	2.21	0.41
1:l:166:SER:HB2	5:q:3:THR:HG22	2.02	0.41
2:n:70:ARG:HD2	9:u:69:SER:HB3	2.01	0.41
2:n:168:TYR:CZ	2:n:172:LEU:HD12	2.56	0.41
2:n:333:ALA:O	2:n:337:ILE:HD12	2.20	0.41
2:n:341:TYR:O	2:n:342:ASN:C	2.64	0.41
2:n:435:PHE:N	2:n:438:GLU:HB2	2.35	0.41
3:o:378:LYS:CD	6:r:33:ARG:HH12	2.32	0.41
4:p:167:GLU:O	4:p:167:GLU:HG2	2.20	0.41
5:q:75:GLU:O	5:q:194:ILE:CA	2.47	0.41
5:q:184:SER:O	5:q:195:VAL:HA	2.20	0.41
11:w:15:ARG:HB3	11:w:16:ASN:H	1.66	0.41
14:z:146:TRP:NE1	18:4:17:ARG:HB2	2.35	0.41
15:1:130:PRO:O	15:1:136:ALA:HB2	2.20	0.41
26:B:38:UNK:O	26:B:39:UNK:C	2.68	0.41
26:B:118:UNK:O	26:B:122:UNK:CA	2.63	0.41
28:D:250:UNK:O	28:D:251:UNK:C	2.68	0.41
29:E:78:UNK:HA	29:E:81:UNK:CB	2.50	0.41
32:H:266:UNK:O	32:H:267:UNK:C	2.69	0.41
38:N:290:UNK:O	38:N:294:UNK:N	2.54	0.41
46:W:56:UNK:O	46:W:59:UNK:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:X:156:UNK:O	47:X:157:UNK:C	2.66	0.41
47:X:413:UNK:O	47:X:417:UNK:N	2.54	0.41
1:c:134:ILE:O	1:c:137:GLU:N	2.53	0.41
2:m:134:ARG:HG2	2:m:135:TRP:N	2.35	0.41
4:d:146:GLY:O	4:d:148:TYR:HD1	2.04	0.41
10:j:29:LEU:HD12	10:j:32:GLU:OE2	2.21	0.41
1:l:59:VAL:CG2	1:l:186:LEU:HD11	2.50	0.41
1:l:69:ASN:C	1:l:71:PRO:HD3	2.45	0.41
1:l:91:THR:HG22	1:l:94:HIS:N	2.33	0.41
1:l:158:PHE:HB2	1:l:164:ALA:HB2	2.02	0.41
1:l:241:ILE:HD11	7:s:16:TYR:CE2	2.56	0.41
1:l:241:ILE:HG21	1:l:241:ILE:HD13	1.64	0.41
1:l:282:CYS:SG	1:l:305:GLN:CD	3.03	0.41
2:n:134:ARG:HG2	2:n:135:TRP:H	1.84	0.41
2:n:237:ALA:O	2:n:238:LYS:HB2	2.20	0.41
2:n:285:VAL:HG12	2:n:285:VAL:O	2.20	0.41
2:n:309:VAL:CG2	2:n:326:THR:HG22	2.50	0.41
3:o:47:THR:HG23	3:o:79:ILE:HG23	2.01	0.41
3:o:47:THR:O	3:o:48:GLY:C	2.64	0.41
4:p:138:PRO:CG	8:t:55:THR:OG1	2.61	0.41
4:p:164:ILE:CD1	4:p:186:VAL:HG21	2.50	0.41
4:p:174:GLY:O	4:p:175:THR:C	2.61	0.41
5:q:119:ASP:OD1	5:q:120:PRO:CD	2.67	0.41
10:v:52:TRP:N	10:v:52:TRP:HE3	2.18	0.41
11:w:20:THR:HG23	11:w:24:TRP:HD1	1.85	0.41
14:z:6:HIS:CD2	14:z:8:TYR:HB2	2.55	0.41
14:z:233:PHE:HA	14:z:236:GLU:HG3	2.03	0.41
18:4:5:LYS:NZ	18:4:6:GLY:N	2.54	0.41
21:7:5:VAL:O	21:7:9:GLN:HG3	2.21	0.41
30:F:365:CYS:CA	30:F:368:UNK:CB	2.91	0.41
33:I:100:UNK:O	33:I:104:UNK:N	2.52	0.41
36:L:182:UNK:O	36:L:185:UNK:N	2.54	0.41
36:L:418:UNK:O	36:L:421:UNK:CB	2.69	0.41
36:L:431:UNK:O	36:L:432:UNK:CB	2.67	0.41
36:L:588:UNK:O	36:L:592:UNK:N	2.53	0.41
37:M:111:UNK:O	37:M:112:UNK:CB	2.68	0.41
37:M:209:UNK:O	37:M:210:UNK:C	2.69	0.41
37:M:327:UNK:O	37:M:330:UNK:CB	2.69	0.41
47:X:426:UNK:O	47:X:428:UNK:N	2.52	0.41
51:Z:624:UNK:O	51:Z:625:UNK:C	2.66	0.41
1:c:29:GLN:HG3	1:c:203:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:43:ALA:HB1	1:c:189:HIS:CB	2.50	0.41
1:c:224:ASP:OD1	1:c:224:ASP:O	2.38	0.41
2:m:55:SER:OG	2:m:102:ARG:HA	2.20	0.41
2:m:68:LEU:HD12	2:m:68:LEU:O	2.21	0.41
2:m:154:ASN:O	2:m:157:ALA:N	2.54	0.41
2:m:338:LYS:O	2:m:339:ALA:C	2.64	0.41
3:b:119:LEU:HD12	3:b:119:LEU:HA	1.85	0.41
4:d:208:MET:HE2	4:d:208:MET:C	2.44	0.41
4:d:209:LEU:O	4:d:210:LEU:C	2.62	0.41
8:h:50:THR:CG2	8:h:51:GLU:N	2.83	0.41
1:l:85:HIS:HE2	2:n:370:MET:HE1	1.86	0.41
1:l:420:PRO:HG3	1:l:441:MET:SD	2.60	0.41
2:n:223:PHE:O	2:n:224:LEU:HD23	2.21	0.41
2:n:346:THR:O	2:n:347:ILE:C	2.62	0.41
2:n:396:SER:HA	2:n:399:LEU:HD12	2.02	0.41
3:o:115:ILE:N	3:o:115:ILE:CD1	2.83	0.41
3:o:170:VAL:O	3:o:170:VAL:CG1	2.68	0.41
5:q:7:VAL:HA	5:q:8:PRO:HD2	1.77	0.41
14:z:182:TYR:O	18:4:72:ASN:HB2	2.21	0.41
15:1:86:MET:O	22:8:25:CYS:HB2	2.20	0.41
15:1:137:LYS:O	15:1:145:TRP:HE3	2.03	0.41
16:2:21:LYS:O	16:2:57:ARG:NH1	2.53	0.41
16:2:21:LYS:HA	16:2:22:PRO:HD2	1.84	0.41
17:3:77:GLY:O	17:3:90:LYS:NZ	2.54	0.41
18:4:78:LEU:HD12	18:4:78:LEU:HA	1.75	0.41
21:7:12:PHE:O	21:7:23:LYS:HE2	2.21	0.41
26:B:48:UNK:CB	26:B:80:UNK:CA	2.84	0.41
26:B:121:UNK:C	26:B:135:UNK:CA	2.92	0.41
27:C:23:UNK:C	27:C:26:UNK:CB	2.98	0.41
30:F:322:UNK:CB	30:F:327:UNK:C	2.98	0.41
31:G:41:CYS:O	31:G:42:UNK:CB	2.69	0.41
32:H:94:UNK:O	32:H:95:UNK:C	2.68	0.41
36:L:420:UNK:O	36:L:423:UNK:N	2.53	0.41
36:L:530:UNK:C	36:L:532:UNK:N	2.78	0.41
36:L:570:UNK:O	36:L:573:UNK:N	2.53	0.41
38:N:200:UNK:O	38:N:201:UNK:C	2.68	0.41
39:O:50:UNK:O	39:O:51:UNK:CB	2.68	0.41
48:Y:33:UNK:C	48:Y:35:UNK:N	2.81	0.41
1:c:43:ALA:CB	1:c:189:HIS:CB	2.97	0.41
1:c:253:VAL:O	1:c:323:HIS:HA	2.20	0.41
3:b:16:ASN:ND2	3:b:20:ASP:CG	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:103:TYR:O	3:b:315:MET:HB3	2.20	0.41
3:b:159:ASN:O	3:b:162:GLU:HB2	2.20	0.41
3:b:198:LEU:HD22	3:o:11:MET:HG2	2.02	0.41
3:b:263:ASN:OD1	3:b:264:THR:N	2.54	0.41
3:b:264:THR:HG21	5:q:144:CYS:SG	2.60	0.41
4:d:146:GLY:O	4:d:148:TYR:CD1	2.73	0.41
4:d:204:MET:O	4:d:207:LYS:N	2.53	0.41
1:l:195:MET:HE3	1:l:195:MET:HB3	1.61	0.41
1:l:257:VAL:O	1:l:320:LEU:HB2	2.21	0.41
1:l:354:VAL:HG11	1:l:407:VAL:HG21	2.02	0.41
2:n:33:LEU:HB2	2:n:204:MET:O	2.20	0.41
3:o:45:ILE:CD1	3:o:190:MET:HE2	2.51	0.41
3:o:227:LYS:HG3	4:p:223:LYS:NZ	2.36	0.41
3:o:276:PHE:CE2	3:o:297:SER:OG	2.74	0.41
3:o:282:ARG:NH1	3:o:343:VAL:HG22	2.36	0.41
4:p:70:VAL:HB	4:p:84:PRO:HG3	2.03	0.41
4:p:230:LEU:O	4:p:233:ARG:HB2	2.19	0.41
5:q:31:ALA:HB2	10:v:7:ALA:HB2	2.02	0.41
5:q:107:ASP:O	5:q:110:ALA:N	2.51	0.41
5:q:113:GLU:O	5:q:114:VAL:C	2.63	0.41
12:x:240:HIS:O	12:x:241:PRO:C	2.64	0.41
12:x:314:ILE:HB	12:x:315:PRO:CD	2.50	0.41
12:x:430:PHE:O	12:x:431:LEU:C	2.64	0.41
13:y:193:TYR:CD1	13:y:193:TYR:N	2.88	0.41
14:z:146:TRP:CE2	18:4:17:ARG:HB2	2.55	0.41
17:3:16:LEU:O	17:3:20:VAL:HG13	2.21	0.41
27:C:25:UNK:O	27:C:28:UNK:N	2.54	0.41
30:F:87:UNK:O	30:F:88:UNK:C	2.68	0.41
30:F:183:UNK:O	30:F:186:UNK:CB	2.69	0.41
30:F:315:UNK:CA	30:F:316:UNK:O	2.69	0.41
31:G:157:UNK:O	31:G:161:UNK:CB	2.69	0.41
31:G:461:UNK:O	31:G:464:UNK:N	2.54	0.41
37:M:50:UNK:O	37:M:51:UNK:CB	2.68	0.41
45:V:44:UNK:O	45:V:47:UNK:CA	2.68	0.41
47:X:177:UNK:O	47:X:178:UNK:C	2.69	0.41
51:Z:101:UNK:H	51:Z:104:UNK:CB	2.34	0.41
1:c:53:ASN:CG	1:c:170:PRO:HD3	2.44	0.41
1:c:256:ALA:HB3	1:c:421:ALA:HB3	2.02	0.41
1:c:260:PRO:HG3	1:c:414:TYR:CE1	2.55	0.41
2:m:327:ILE:O	2:m:327:ILE:HG22	2.20	0.41
3:b:107:TYR:HH	3:b:308:HIS:HD1	0.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:145:VAL:O	3:b:145:VAL:HG12	2.20	0.41
3:b:271:GLU:CD	3:b:273:TYR:HH	2.27	0.41
3:b:280:ILE:HA	3:b:355:SER:OG	2.20	0.41
4:d:57:THR:CG2	4:d:58:GLU:H	2.32	0.41
4:d:143:LEU:HD11	4:d:149:PHE:HB2	2.02	0.41
4:d:153:PHE:O	4:d:156:GLN:N	2.35	0.41
4:d:195:GLU:HA	4:d:196:PRO:HD2	1.80	0.41
6:f:51:PRO:HG2	6:f:54:LEU:CD2	2.33	0.41
9:i:70:LEU:CG	9:i:72:VAL:H	2.34	0.41
1:l:177:LEU:HD12	1:l:177:LEU:HA	1.74	0.41
1:l:402:VAL:HG13	1:l:407:VAL:HG23	2.03	0.41
2:n:38:LEU:O	2:n:40:ASN:N	2.54	0.41
2:n:54:GLY:HA3	2:n:102:ARG:O	2.20	0.41
2:n:243:GLU:HA	2:n:424:MET:O	2.20	0.41
2:n:276:GLN:OE1	9:u:59:ALA:HB1	2.20	0.41
2:n:343:GLN:O	2:n:343:GLN:HG3	2.20	0.41
3:o:66:VAL:O	3:o:69:ILE:HB	2.21	0.41
3:o:75:TYR:CG	5:q:57:GLN:HG2	2.56	0.41
3:o:149:LEU:O	3:o:291:VAL:HG21	2.21	0.41
4:p:138:PRO:CG	8:t:55:THR:HA	2.50	0.41
5:q:14:ARG:HB2	5:q:15:ARG:H	1.70	0.41
5:q:15:ARG:HH21	5:q:32:ARG:HB2	1.86	0.41
5:q:141:HIS:HB3	5:q:142:LEU:H	1.49	0.41
6:r:74:ILE:HG23	6:r:75:LEU:O	2.21	0.41
12:x:23:GLY:HA3	12:x:73:ILE:HG13	2.03	0.41
12:x:264:LYS:NZ	13:y:56:MET:HE2	2.35	0.41
12:x:276:ALA:O	12:x:280:ILE:HG13	2.21	0.41
12:x:356:ILE:HD13	12:x:356:ILE:HA	1.90	0.41
12:x:461:SER:O	12:x:465:VAL:HG13	2.21	0.41
14:z:188:ILE:H	14:z:188:ILE:HG13	1.62	0.41
18:4:42:ARG:NH1	18:4:74:ARG:NH2	2.68	0.41
28:D:263:UNK:HA	28:D:288:UNK:CB	2.51	0.41
28:D:342:UNK:O	28:D:346:UNK:N	2.54	0.41
30:F:225:UNK:O	30:F:228:UNK:N	2.54	0.41
30:F:428:UNK:O	30:F:429:UNK:C	2.68	0.41
31:G:377:UNK:O	31:G:450:UNK:N	2.53	0.41
32:H:41:UNK:CB	32:H:45:UNK:N	2.84	0.41
40:P:31:UNK:O	40:P:32:UNK:C	2.68	0.41
43:S:36:UNK:O	43:S:40:UNK:N	2.54	0.41
47:X:302:UNK:O	47:X:305:UNK:CA	2.65	0.41
1:c:8:LEU:HD11	1:c:396:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:266:ASP:OD1	1:c:266:ASP:N	2.54	0.41
1:c:314:TYR:HB2	1:c:317:THR:O	2.20	0.41
2:m:408:ALA:O	2:m:411:ILE:N	2.54	0.41
3:b:341:GLN:OE1	3:b:347:TYR:CZ	2.74	0.41
4:d:207:LYS:HB3	10:j:35:PHE:HE2	1.85	0.41
1:l:34:THR:OG1	2:n:373:GLU:OE1	2.37	0.41
1:l:329:MET:HA	1:l:329:MET:CE	2.50	0.41
1:l:426:GLY:H	1:l:428:ILE:HG13	1.83	0.41
2:n:170:ASN:OD1	2:n:171:ALA:N	2.50	0.41
3:o:51:LEU:HD12	52:o:401:HEM:O1D	2.21	0.41
3:o:246:ALA:N	3:o:247:PRO:HD3	2.36	0.41
4:p:7:PRO:HB3	4:p:125:ASP:C	2.46	0.41
4:p:57:THR:HB	4:p:60:GLU:H	1.86	0.41
5:q:73:LYS:O	5:q:74:ILE:HD13	2.20	0.41
5:q:109:GLU:OE2	5:q:166:ASP:CG	2.63	0.41
5:q:118:ARG:HH11	5:q:118:ARG:HD2	1.69	0.41
6:r:91:GLU:O	6:r:95:LYS:HG3	2.21	0.41
10:v:31:PHE:CD2	10:v:31:PHE:C	2.98	0.41
13:y:86:MET:HB2	13:y:86:MET:HE3	1.80	0.41
14:z:223:LEU:HD23	14:z:223:LEU:HA	1.79	0.41
28:D:95:UNK:HA	28:D:385:UNK:CB	2.51	0.41
28:D:414:UNK:O	28:D:418:UNK:N	2.54	0.41
31:G:244:UNK:O	31:G:245:UNK:CB	2.65	0.41
31:G:255:UNK:C	31:G:257:UNK:N	2.79	0.41
31:G:567:UNK:O	31:G:586:UNK:N	2.54	0.41
32:H:160:UNK:O	32:H:161:UNK:CB	2.69	0.41
32:H:233:UNK:O	32:H:236:UNK:N	2.54	0.41
36:L:297:UNK:CA	36:L:355:UNK:HA	2.49	0.41
37:M:115:UNK:O	37:M:116:UNK:CB	2.69	0.41
37:M:189:UNK:C	37:M:191:UNK:O	2.69	0.41
37:M:225:UNK:O	37:M:228:UNK:C	2.69	0.41
37:M:399:UNK:O	37:M:403:UNK:N	2.53	0.41
42:R:60:UNK:O	42:R:62:UNK:N	2.54	0.41
1:c:5:ALA:O	1:c:6:GLN:O	2.38	0.41
1:c:39:VAL:HG12	1:c:41:ILE:HD12	1.95	0.41
1:c:39:VAL:HG13	1:c:195:MET:CE	2.51	0.41
1:c:46:ARG:NE	1:c:163:LEU:HD22	2.36	0.41
1:c:48:GLU:HB2	1:c:53:ASN:HA	2.03	0.41
1:c:176:LYS:O	1:c:177:LEU:C	2.64	0.41
1:c:367:SER:O	1:c:368:HIS:C	2.63	0.41
2:m:133:ARG:O	2:m:134:ARG:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:206:LEU:HD12	2:m:206:LEU:HA	1.85	0.41
2:m:211:VAL:HG11	2:m:216:LEU:HD13	2.02	0.41
2:m:312:PHE:HB3	2:m:323:GLY:O	2.20	0.41
3:b:88:SER:CB	3:b:250:LEU:CD2	2.99	0.41
3:b:163:TRP:HD1	5:q:63:SER:HA	1.86	0.41
3:b:257:THR:OG1	3:b:257:THR:O	2.38	0.41
3:b:275:LEU:O	3:b:276:PHE:O	2.39	0.41
3:b:300:ILE:HD11	3:b:362:ILE:CG2	2.50	0.41
3:b:315:MET:O	3:b:318:ARG:N	2.35	0.41
3:b:345:HIS:HB3	3:b:346:PRO:HD2	2.02	0.41
4:d:56:TYR:HD1	4:d:60:GLU:CD	2.29	0.41
4:d:106:ASN:HD22	4:d:106:ASN:C	2.28	0.41
5:e:20:ASP:O	5:e:22:THR:N	2.54	0.41
10:j:24:ILE:O	10:j:25:VAL:C	2.62	0.41
10:j:44:GLU:O	10:j:45:HIS:C	2.62	0.41
1:l:43:ALA:HB1	1:l:189:HIS:CB	2.50	0.41
1:l:71:PRO:O	1:l:72:GLY:C	2.64	0.41
1:l:166:SER:CB	5:q:3:THR:HG22	2.51	0.41
1:l:194:ARG:H	1:l:194:ARG:HG2	1.67	0.41
1:l:245:GLU:OE1	1:l:248:LEU:CD2	2.65	0.41
2:n:22:GLN:OE1	2:n:22:GLN:HA	2.21	0.41
2:n:163:LEU:HD22	2:n:256:ALA:HB1	2.01	0.41
2:n:217:LYS:NZ	2:n:221:GLU:CD	2.70	0.41
2:n:264:ILE:HD12	2:n:315:SER:OG	2.20	0.41
2:n:275:LEU:HD11	2:n:279:LEU:HD11	2.03	0.41
2:n:413:ALA:O	2:n:416:LYS:HB2	2.21	0.41
3:o:11:MET:O	3:o:14:VAL:HB	2.21	0.41
3:o:14:VAL:O	3:o:14:VAL:HG12	2.20	0.41
3:o:73:VAL:O	3:o:73:VAL:HG12	2.21	0.41
3:o:135:TRP:HH2	3:o:170:VAL:O	2.04	0.41
3:o:156:ILE:O	3:o:158:THR:N	2.54	0.41
3:o:196:HIS:HE1	52:o:402:HEM:CHD	2.32	0.41
3:o:272:TRP:CE2	3:o:273:TYR:HD1	2.39	0.41
3:o:284:ILE:HG23	3:o:285:PRO:HD2	2.02	0.41
4:p:34:LYS:O	4:p:38:SER:HB3	2.21	0.41
4:p:48:TYR:OH	4:p:68:VAL:HG21	2.21	0.41
4:p:220:TYR:HD2	7:s:26:PHE:CZ	2.39	0.41
5:q:122:HIS:HE1	5:q:124:LEU:HD12	1.85	0.41
6:r:55:TYR:CD1	6:r:55:TYR:C	2.99	0.41
6:r:62:ILE:O	6:r:66:LEU:HG	2.21	0.41
6:r:73:GLN:HG2	7:s:36:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:74:ILE:H	7:s:39:ARG:NH2	2.19	0.41
9:u:60:ALA:HB3	9:u:63:PRO:O	2.21	0.41
10:v:46:ILE:H	10:v:46:ILE:HG12	1.39	0.41
11:w:24:TRP:CE3	11:w:24:TRP:HA	2.55	0.41
12:x:442:ASP:OD2	13:y:134:ARG:NH2	2.54	0.41
15:1:102:TYR:HD2	24:0:35:TYR:HE1	1.68	0.41
15:1:127:LYS:O	15:1:130:PRO:HD3	2.20	0.41
19:5:20:PHE:N	19:5:21:PRO:HD3	2.35	0.41
19:5:65:PRO:HG2	19:5:68:TRP:CG	2.55	0.41
22:8:24:PHE:CE1	22:8:28:VAL:HG21	2.56	0.41
24:0:13:LYS:HD3	24:0:13:LYS:N	2.35	0.41
24:0:35:TYR:HD2	24:0:36:HIS:CE1	2.39	0.41
26:B:47:UNK:HA	26:B:85:UNK:O	2.20	0.41
26:B:53:UNK:N	26:B:90:UNK:CB	2.82	0.41
26:B:68:UNK:O	26:B:70:UNK:N	2.54	0.41
27:C:28:UNK:O	27:C:29:UNK:C	2.69	0.41
28:D:131:UNK:O	28:D:135:UNK:N	2.54	0.41
30:F:61:UNK:O	30:F:64:UNK:HA	2.15	0.41
30:F:71:UNK:O	30:F:72:UNK:CB	2.69	0.41
30:F:72:UNK:O	30:F:73:UNK:C	2.65	0.41
30:F:90:UNK:O	30:F:218:UNK:CB	2.68	0.41
30:F:303:UNK:C	30:F:414:UNK:CB	2.99	0.41
31:G:83:UNK:O	31:G:86:UNK:N	2.54	0.41
31:G:210:UNK:O	31:G:213:UNK:C	2.69	0.41
31:G:241:UNK:O	31:G:248:UNK:CA	2.65	0.41
31:G:279:UNK:O	31:G:280:UNK:CB	2.69	0.41
32:H:101:UNK:CB	32:H:162:UNK:N	2.84	0.41
32:H:101:UNK:CA	32:H:161:UNK:HA	2.51	0.41
33:I:63:UNK:CB	33:I:134:UNK:O	2.69	0.41
36:L:275:UNK:O	36:L:278:UNK:N	2.54	0.41
36:L:298:UNK:O	36:L:301:UNK:CB	2.69	0.41
36:L:496:UNK:O	36:L:497:UNK:C	2.68	0.41
36:L:560:UNK:O	36:L:564:UNK:N	2.54	0.41
37:M:108:UNK:O	37:M:111:UNK:CB	2.69	0.41
37:M:133:UNK:O	37:M:224:UNK:CB	2.69	0.41
37:M:163:UNK:O	37:M:164:UNK:C	2.69	0.41
37:M:390:UNK:O	37:M:391:UNK:C	2.69	0.41
38:N:72:UNK:O	38:N:75:UNK:N	2.54	0.41
38:N:126:UNK:O	38:N:127:UNK:C	2.67	0.41
38:N:276:UNK:O	38:N:279:UNK:CA	2.68	0.41
39:O:114:UNK:O	39:O:117:UNK:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:P:143:UNK:O	40:P:144:UNK:CB	2.68	0.41
41:Q:42:UNK:O	41:Q:43:UNK:C	2.69	0.41
43:S:83:UNK:O	43:S:84:UNK:C	2.68	0.41
46:W:71:UNK:O	46:W:72:UNK:O	2.38	0.41
49:a:104:UNK:O	49:a:105:UNK:C	2.69	0.41
50:U:628:UNK:O	50:U:629:UNK:CB	2.69	0.41
51:Z:605:UNK:O	51:Z:606:UNK:C	2.69	0.41
1:c:282:CYS:SG	1:c:305:GLN:CD	3.04	0.41
1:c:291:SER:OG	2:m:90:GLU:OE1	2.26	0.41
2:m:346:THR:HG23	2:m:351:ASN:HB3	2.03	0.41
3:b:163:TRP:CH2	5:q:62:MET:HE2	2.56	0.41
3:b:301:LEU:HA	3:b:304:ILE:CD1	2.51	0.41
4:d:136:GLU:O	4:d:137:PRO:C	2.62	0.41
4:d:165:TYR:CE1	4:d:168:VAL:HA	2.56	0.41
11:k:24:TRP:HA	11:k:24:TRP:CE3	2.56	0.41
1:l:32:GLN:HG2	1:l:33:PRO:N	2.36	0.41
1:l:97:TYR:CD1	1:l:97:TYR:N	2.89	0.41
1:l:130:GLU:OE2	9:u:52:ARG:NH2	2.54	0.41
1:l:137:GLU:O	1:l:138:LEU:C	2.63	0.41
1:l:239:SER:CB	7:s:18:LEU:HD23	2.49	0.41
4:p:23:HIS:O	4:p:26:ILE:HB	2.20	0.41
6:r:29:LEU:HD22	6:r:68:LEU:HB2	2.03	0.41
10:v:2:ALA:HB1	10:v:3:PRO:HD2	2.03	0.41
12:x:337:ALA:HB2	12:x:394:VAL:HG23	2.03	0.41
17:3:10:GLU:HG2	17:3:25:ARG:HH22	1.86	0.41
29:E:41:UNK:O	29:E:42:UNK:CB	2.69	0.41
30:F:52:UNK:O	30:F:55:UNK:C	2.68	0.41
30:F:62:UNK:C	30:F:64:UNK:N	2.79	0.41
30:F:262:UNK:HA	30:F:286:UNK:N	2.36	0.41
32:H:152:UNK:O	32:H:155:UNK:CB	2.69	0.41
33:I:167:UNK:O	33:I:168:UNK:C	2.69	0.41
37:M:186:UNK:O	37:M:253:UNK:CB	2.69	0.41
38:N:291:UNK:O	38:N:292:UNK:C	2.69	0.41
47:X:605:UNK:O	47:X:608:UNK:CB	2.69	0.41
51:Z:208:UNK:O	51:Z:211:UNK:CB	2.69	0.41
1:c:292:SER:O	1:c:293:PRO:C	2.63	0.40
2:m:102:ARG:NH1	2:m:175:SER:HA	2.35	0.40
2:m:159:VAL:CG1	2:m:160:ILE:N	2.84	0.40
3:b:133:LEU:HA	3:b:175:LEU:HD11	2.04	0.40
3:b:152:ALA:HB2	3:b:287:LYS:NZ	2.36	0.40
3:b:269:LYS:HA	3:b:270:PRO:HD3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:274:PHE:O	3:b:275:LEU:C	2.62	0.40
4:d:50:HIS:HB3	4:d:54:VAL:HG21	2.01	0.40
7:g:31:SER:O	7:g:35:PRO:CD	2.62	0.40
7:g:68:LYS:O	7:g:69:SER:C	2.64	0.40
1:l:56:GLY:O	1:l:57:TYR:C	2.59	0.40
1:l:185:TYR:O	1:l:186:LEU:C	2.64	0.40
1:l:244:ARG:NH1	7:s:10:VAL:HB	2.36	0.40
1:l:356:ARG:HG2	1:l:357:GLY:N	2.36	0.40
2:n:59:ASN:OD1	2:n:60:SER:N	2.43	0.40
2:n:81:SER:O	2:n:82:SER:C	2.63	0.40
2:n:95:LYS:HG3	9:u:70:LEU:HD13	2.02	0.40
2:n:254:HIS:ND1	2:n:325:TYR:OH	2.43	0.40
3:o:337:TRP:NE1	3:o:341:GLN:OE1	2.54	0.40
4:p:195:GLU:HA	4:p:196:PRO:HD2	1.73	0.40
5:q:181:GLU:HG2	5:q:182:VAL:N	2.36	0.40
7:s:50:PRO:O	7:s:53:VAL:HB	2.21	0.40
7:s:54:ALA:O	7:s:55:PHE:C	2.64	0.40
7:s:61:TRP:O	7:s:62:GLY:C	2.64	0.40
10:v:23:THR:HG22	10:v:24:ILE:N	2.36	0.40
10:v:42:ILE:O	10:v:46:ILE:HG12	2.21	0.40
12:x:128:VAL:O	12:x:128:VAL:CG2	2.69	0.40
12:x:198:SER:HB2	12:x:238:PHE:HA	2.03	0.40
57:x:603:HEA:HHC	57:x:603:HEA:H122	2.02	0.40
13:y:5:MET:CE	22:8:42:PRO:HA	2.45	0.40
14:z:128:GLU:HB3	14:z:129:VAL:H	1.56	0.40
14:z:228:THR:O	14:z:232:HIS:HD2	2.04	0.40
17:3:19:GLU:HB3	17:3:98:HIS:CE1	2.57	0.40
27:C:27:UNK:O	27:C:30:UNK:CB	2.69	0.40
28:D:138:UNK:O	28:D:142:UNK:CB	2.69	0.40
28:D:250:UNK:O	28:D:253:UNK:CB	2.69	0.40
29:E:78:UNK:O	29:E:82:UNK:N	2.54	0.40
29:E:127:UNK:O	29:E:128:UNK:C	2.70	0.40
30:F:276:UNK:N	30:F:315:UNK:O	2.54	0.40
31:G:49:UNK:O	31:G:51:UNK:N	2.54	0.40
32:H:68:UNK:C	32:H:70:UNK:N	2.79	0.40
36:L:34:UNK:O	36:L:37:UNK:CB	2.69	0.40
47:X:43:UNK:HA	47:X:59:UNK:CB	2.51	0.40
1:c:146:ARG:HH21	1:c:308:GLN:HE22	1.62	0.40
1:c:163:LEU:HD21	1:c:314:TYR:CD2	2.57	0.40
1:c:363:ASN:OD1	2:m:112:LEU:HD23	2.21	0.40
2:m:163:LEU:HD21	2:m:258:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:68:HIS:NE2	5:e:67:ASP:CB	2.85	0.40
3:b:184:ILE:O	3:b:184:ILE:HG12	2.19	0.40
3:b:200:LEU:CD1	52:b:402:HEM:HAD2	2.50	0.40
4:d:158:ILE:HG12	4:d:160:MET:N	2.36	0.40
4:d:161:ALA:O	4:d:162:PRO:C	2.63	0.40
4:d:200:HIS:O	4:d:203:ARG:HB3	2.20	0.40
6:f:98:ILE:O	6:f:99:ARG:C	2.63	0.40
8:h:61:PHE:O	8:h:62:LEU:C	2.64	0.40
10:j:29:LEU:O	10:j:30:PHE:C	2.64	0.40
10:j:49:GLY:N	10:j:54:HIS:CD2	2.89	0.40
1:l:349:ALA:O	1:l:408:ARG:NE	2.54	0.40
1:l:438:ARG:NH1	1:l:438:ARG:CG	2.82	0.40
2:n:180:ASP:HA	2:n:183:ILE:HD12	2.03	0.40
4:p:21:LEU:CD1	4:p:192:TRP:HB2	2.50	0.40
4:p:153:PHE:O	4:p:154:PRO:C	2.64	0.40
4:p:206:LEU:O	4:p:210:LEU:HD12	2.22	0.40
5:q:78:LEU:CD2	5:q:132:TRP:CZ2	3.05	0.40
5:q:87:MET:O	5:q:89:PHE:HD1	2.04	0.40
5:q:122:HIS:O	5:q:123:ASP:C	2.62	0.40
6:r:10:SER:HA	6:r:13:LEU:HG	2.03	0.40
7:s:45:ILE:HD12	7:s:45:ILE:HA	1.88	0.40
12:x:354:THR:HG21	12:x:376:HIS:HA	2.03	0.40
12:x:398:PRO:HB3	12:x:482:VAL:HG21	2.03	0.40
12:x:440:TYR:CG	13:y:205:SER:HB3	2.56	0.40
13:y:164:ALA:HB2	13:y:171:LYS:HD3	2.03	0.40
14:z:22:LEU:HD12	14:z:22:LEU:HA	1.87	0.40
14:z:224:LYS:NZ	14:z:226:HIS:HE2	2.18	0.40
15:1:11:TYR:CD1	15:1:11:TYR:C	2.99	0.40
16:2:43:PRO:HB2	16:2:48:ILE:CD1	2.48	0.40
16:2:104:LEU:HD23	16:2:104:LEU:HA	1.87	0.40
20:6:35:TYR:O	20:6:39:VAL:HB	2.19	0.40
26:B:54:CYS:O	26:B:55:CYS:C	2.64	0.40
29:E:44:UNK:O	29:E:45:UNK:C	2.69	0.40
30:F:242:UNK:O	30:F:252:UNK:CB	2.69	0.40
31:G:12:UNK:O	31:G:78:UNK:CA	2.65	0.40
31:G:294:UNK:O	31:G:295:UNK:C	2.69	0.40
31:G:397:UNK:O	31:G:400:UNK:CB	2.69	0.40
32:H:283:UNK:O	32:H:284:UNK:C	2.70	0.40
32:H:308:UNK:HA	32:H:312:UNK:CB	2.51	0.40
32:H:310:UNK:O	32:H:311:UNK:CB	2.68	0.40
33:I:60:UNK:O	33:I:61:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:192:UNK:O	36:L:193:UNK:C	2.69	0.40
37:M:345:UNK:O	37:M:346:UNK:CB	2.69	0.40
38:N:18:UNK:O	38:N:21:UNK:N	2.54	0.40
38:N:90:UNK:HA	38:N:91:UNK:CB	2.50	0.40
38:N:115:UNK:O	38:N:116:UNK:C	2.70	0.40
38:N:182:UNK:O	38:N:183:UNK:C	2.69	0.40
38:N:266:UNK:O	38:N:270:UNK:N	2.54	0.40
40:P:145:UNK:O	40:P:146:UNK:C	2.70	0.40
43:S:28:UNK:O	43:S:29:UNK:CB	2.69	0.40
46:W:53:UNK:O	46:W:56:UNK:N	2.54	0.40
47:X:604:UNK:C	47:X:606:UNK:N	2.82	0.40
48:Y:90:UNK:C	48:Y:92:UNK:N	2.84	0.40
1:c:241:ILE:O	1:c:241:ILE:CG2	2.69	0.40
2:m:168:TYR:HD2	2:m:238:LYS:O	2.04	0.40
2:m:250:ASP:OD1	2:m:251:SER:N	2.54	0.40
3:b:25:SER:HB2	3:b:26:ASN:H	1.53	0.40
3:b:40:CYS:CB	3:b:90:PHE:HD2	2.34	0.40
3:b:168:PHE:CE2	5:q:72:SER:HB2	2.56	0.40
3:b:243:VAL:HG13	3:b:244:LEU:CD1	2.48	0.40
4:d:90:TYR:O	4:d:91:PHE:C	2.62	0.40
4:d:165:TYR:HD1	4:d:166:ASN:O	2.04	0.40
4:d:220:TYR:HD2	7:g:26:PHE:CZ	2.40	0.40
5:e:7:VAL:HA	5:e:8:PRO:HD3	1.84	0.40
1:l:42:ASP:O	1:l:42:ASP:CG	2.63	0.40
1:l:64:PHE:HE2	1:l:88:ALA:CB	2.34	0.40
1:l:333:ASP:O	1:l:337:VAL:HG23	2.21	0.40
1:l:428:ILE:CG2	1:l:431:LEU:CG	2.97	0.40
2:n:102:ARG:NH1	2:n:174:ASN:O	2.52	0.40
2:n:250:ASP:OD1	2:n:252:LEU:N	2.50	0.40
3:o:26:ASN:ND2	3:o:26:ASN:C	2.78	0.40
3:o:211:ILE:CG2	6:r:62:ILE:HD13	2.50	0.40
4:p:102:ARG:HG2	4:p:109:LEU:HB2	2.02	0.40
4:p:124:GLU:H	4:p:124:GLU:HG2	1.46	0.40
4:p:139:THR:CB	8:t:44:VAL:HB	2.49	0.40
4:p:139:THR:O	8:t:44:VAL:HG11	2.20	0.40
4:p:178:THR:OG1	8:t:16:PRO:HD2	2.22	0.40
7:s:44:CYS:O	7:s:47:ARG:N	2.54	0.40
8:t:37:LEU:HD21	8:t:58:LEU:CA	2.49	0.40
12:x:199:LEU:HD12	12:x:199:LEU:HA	1.91	0.40
13:y:100:MET:HE3	13:y:157:GLU:HG3	2.01	0.40
17:3:49:VAL:O	17:3:91:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:67:UNK:N	26:B:68:UNK:CA	2.83	0.40
28:D:112:UNK:O	28:D:113:UNK:C	2.69	0.40
30:F:35:UNK:O	30:F:39:UNK:N	2.55	0.40
30:F:121:UNK:CA	30:F:232:UNK:CB	2.97	0.40
30:F:135:UNK:HA	30:F:176:UNK:O	2.21	0.40
30:F:418:UNK:O	30:F:423:UNK:CB	2.68	0.40
31:G:142:UNK:O	31:G:143:UNK:CB	2.69	0.40
31:G:624:UNK:O	31:G:627:UNK:CA	2.68	0.40
36:L:570:UNK:O	36:L:571:UNK:C	2.70	0.40
36:L:571:UNK:O	36:L:572:UNK:C	2.69	0.40
36:L:603:UNK:O	36:L:604:UNK:CB	2.70	0.40
37:M:8:UNK:O	37:M:11:UNK:N	2.55	0.40
37:M:55:UNK:HA	37:M:56:UNK:HA	1.82	0.40
37:M:66:UNK:O	37:M:67:UNK:C	2.70	0.40
37:M:174:UNK:O	37:M:175:UNK:C	2.69	0.40
38:N:29:UNK:O	38:N:32:UNK:N	2.54	0.40
40:P:146:UNK:O	40:P:149:UNK:CA	2.69	0.40
42:R:87:UNK:C	42:R:89:UNK:N	2.84	0.40
46:W:43:UNK:O	46:W:44:UNK:CB	2.69	0.40
51:Z:123:UNK:O	51:Z:124:UNK:C	2.69	0.40
51:Z:242:UNK:O	51:Z:243:UNK:CB	2.69	0.40
1:c:38:GLY:HA3	1:c:40:TRP:CZ3	2.50	0.40
1:c:198:ALA:O	1:c:199:ALA:CB	2.63	0.40
2:m:140:LEU:O	2:m:143:GLN:N	2.40	0.40
2:m:304:HIS:CD2	2:m:305:GLN:H	2.40	0.40
2:m:312:PHE:HD1	9:i:58:GLN:O	2.05	0.40
2:m:397:THR:O	2:m:398:VAL:C	2.63	0.40
3:b:97:HIS:HD2	52:b:402:HEM:C1C	2.39	0.40
3:b:172:LYS:O	3:b:173:ALA:C	2.60	0.40
6:f:70:MET:HE2	6:f:70:MET:HB3	1.60	0.40
10:j:40:ASP:O	10:j:41:ALA:C	2.65	0.40
1:l:133:VAL:HG12	1:l:134:ILE:N	2.35	0.40
1:l:134:ILE:O	1:l:135:LEU:C	2.65	0.40
1:l:311:ASN:CG	1:l:320:LEU:CD2	2.95	0.40
1:l:338:LEU:O	1:l:339:GLN:C	2.65	0.40
2:n:42:ALA:HB1	2:n:43:PRO:HD2	2.03	0.40
2:n:92:VAL:HG11	2:n:115:ASP:CB	2.51	0.40
2:n:95:LYS:NZ	9:u:70:LEU:CD2	2.85	0.40
2:n:257:LEU:CD1	2:n:424:MET:HE2	2.49	0.40
2:n:374:SER:O	2:n:375:SER:C	2.64	0.40
2:n:397:THR:O	2:n:398:VAL:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:121:LEU:HA	3:o:124:MET:SD	2.62	0.40
4:p:206:LEU:HG	4:p:210:LEU:HD11	2.02	0.40
5:q:16:PRO:O	5:q:17:GLU:C	2.63	0.40
5:q:115:SER:C	5:q:117:LEU:H	2.28	0.40
5:q:157:TYR:HE1	5:q:164:HIS:CD2	2.40	0.40
28:D:182:UNK:O	28:D:186:UNK:CA	2.69	0.40
28:D:253:UNK:O	28:D:254:UNK:CB	2.70	0.40
28:D:260:UNK:O	28:D:265:UNK:CB	2.70	0.40
28:D:401:UNK:O	28:D:402:UNK:C	2.69	0.40
29:E:65:UNK:O	29:E:66:UNK:C	2.63	0.40
30:F:82:UNK:O	30:F:84:UNK:N	2.54	0.40
30:F:357:UNK:O	30:F:358:UNK:C	2.70	0.40
31:G:435:UNK:CB	31:G:437:UNK:HA	2.51	0.40
32:H:90:UNK:CB	32:H:95:UNK:O	2.70	0.40
33:I:110:UNK:CB	33:I:150:UNK:O	2.70	0.40
36:L:65:UNK:CB	36:L:66:UNK:HA	2.50	0.40
37:M:268:UNK:O	37:M:269:UNK:C	2.70	0.40
38:N:12:UNK:O	38:N:15:UNK:CB	2.69	0.40
39:O:187:UNK:O	39:O:188:UNK:C	2.70	0.40
40:P:26:UNK:O	40:P:31:UNK:CB	2.70	0.40
41:Q:40:UNK:CB	41:Q:41:UNK:CA	2.93	0.40
44:T:63:UNK:O	44:T:64:UNK:C	2.66	0.40
46:W:40:UNK:N	46:W:41:UNK:CB	2.82	0.40
50:U:211:UNK:O	50:U:212:UNK:C	2.69	0.40
50:U:622:UNK:O	50:U:625:UNK:CB	2.69	0.40
51:Z:336:UNK:O	51:Z:342:UNK:CB	2.70	0.40
1:c:4:TYR:O	1:c:5:ALA:C	2.63	0.40
1:c:67:THR:CG2	1:c:70:ARG:N	2.60	0.40
2:m:162:ASN:CB	2:m:244:ILE:HG21	2.50	0.40
3:b:341:GLN:HA	3:b:341:GLN:HE21	1.86	0.40
4:d:27:ARG:NH1	10:j:58:LYS:CE	2.84	0.40
4:d:149:PHE:CZ	8:h:55:THR:HG23	2.54	0.40
8:h:57:GLU:OE1	8:h:57:GLU:N	2.55	0.40
10:j:3:PRO:O	10:j:4:THR:C	2.63	0.40
1:l:257:VAL:N	1:l:320:LEU:O	2.47	0.40
2:n:102:ARG:NH1	2:n:175:SER:HA	2.37	0.40
2:n:158:HIS:ND1	2:n:246:GLU:OE1	2.54	0.40
2:n:345:LYS:HG2	2:n:418:VAL:HG11	2.03	0.40
3:o:103:TYR:OH	3:o:322:GLN:HG3	2.22	0.40
3:o:125:ALA:HB3	3:o:185:LEU:HD21	2.03	0.40
3:o:219:PRO:HB2	3:o:222:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:6:HIS:HA	4:p:7:PRO:HD3	1.87	0.40
4:p:206:LEU:HG	4:p:210:LEU:CD1	2.52	0.40
4:p:216:LEU:N	4:p:217:PRO:CD	2.85	0.40
5:q:29:SER:O	5:q:33:LYS:HG3	2.22	0.40
5:q:83:GLU:HA	5:q:100:HIS:CG	2.57	0.40
6:r:96:GLU:O	6:r:99:ARG:N	2.55	0.40
15:1:119:GLN:O	15:1:123:MET:HG3	2.22	0.40
19:5:33:TYR:O	19:5:37:HIS:HD2	2.05	0.40
25:A:76:UNK:O	25:A:78:UNK:N	2.55	0.40
28:D:69:UNK:O	28:D:70:UNK:CB	2.70	0.40
28:D:262:UNK:O	28:D:263:UNK:C	2.69	0.40
28:D:394:UNK:O	28:D:398:UNK:CB	2.70	0.40
30:F:44:UNK:O	30:F:45:UNK:C	2.70	0.40
30:F:322:UNK:O	30:F:327:UNK:CA	2.70	0.40
31:G:457:UNK:O	31:G:458:UNK:CB	2.68	0.40
32:H:90:UNK:O	32:H:91:UNK:CB	2.70	0.40
32:H:119:UNK:O	32:H:120:UNK:C	2.70	0.40
32:H:119:UNK:O	32:H:122:UNK:CB	2.69	0.40
32:H:120:UNK:O	32:H:121:UNK:C	2.70	0.40
32:H:303:UNK:O	32:H:306:UNK:N	2.54	0.40
33:I:63:UNK:CB	33:I:133:UNK:CA	3.00	0.40
34:J:22:UNK:O	34:J:23:UNK:CB	2.69	0.40
36:L:111:UNK:O	36:L:114:UNK:CB	2.70	0.40
36:L:154:UNK:O	36:L:155:UNK:C	2.70	0.40
36:L:182:UNK:O	36:L:183:UNK:C	2.69	0.40
37:M:20:UNK:O	37:M:21:UNK:CB	2.70	0.40
37:M:251:UNK:O	37:M:252:UNK:CB	2.69	0.40
37:M:309:UNK:O	37:M:310:UNK:C	2.70	0.40
38:N:74:UNK:O	38:N:75:UNK:C	2.70	0.40
38:N:106:UNK:O	38:N:107:UNK:CB	2.68	0.40
39:O:129:UNK:O	39:O:132:UNK:CA	2.67	0.40
39:O:234:UNK:O	39:O:237:UNK:CA	2.69	0.40
40:P:146:UNK:O	40:P:149:UNK:CB	2.69	0.40
47:X:177:UNK:O	47:X:180:UNK:CA	2.69	0.40
47:X:204:UNK:O	47:X:205:UNK:C	2.70	0.40
51:Z:243:UNK:O	51:Z:245:UNK:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	c	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	1	15
1	l	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	2	17
2	m	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	5	29
2	n	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	4	25
3	b	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	2	20
3	o	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3	23
4	d	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	1	13
4	p	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	1	16
5	e	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	4	25
5	q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	1	14
6	f	104/110 (94%)	89 (86%)	13 (12%)	2 (2%)	6	32
6	r	104/110 (94%)	87 (84%)	15 (14%)	2 (2%)	6	32
7	g	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	2	19
7	s	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	2	19
8	h	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	t	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	7	38
9	i	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	12
9	u	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	7
10	j	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0	7
10	v	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	12
11	k	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	1	16
11	w	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	7
12	x	512/514 (100%)	480 (94%)	28 (6%)	4 (1%)	16	54
13	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
14	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	1	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
16	2	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
17	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
18	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
19	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	40
20	6	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
21	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	20
22	8	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
23	9	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
24	0	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
26	B	4/143 (3%)	3 (75%)	0	1 (25%)	0	1
29	E	4/159 (2%)	3 (75%)	1 (25%)	0	100	100
30	F	4/411 (1%)	4 (100%)	0	0	100	100
31	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0	2
33	I	8/162 (5%)	7 (88%)	0	1 (12%)	0	4
All	All	5719/7551 (76%)	4821 (84%)	718 (13%)	180 (3%)	5	22

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	327	ASP
1	c	426	GLY
1	c	427	PRO
2	m	141	GLN
2	m	183	ILE
2	m	305	GLN
3	b	8	HIS
3	b	27	ILE
3	b	109	PHE
4	d	51	LEU
4	d	73	GLY
4	d	98	PRO
9	i	72	VAL
1	l	55	ALA
1	l	427	PRO
2	n	141	GLN
2	n	183	ILE

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Mol	Chain	Res	Type
2	n	351	ASN
3	o	8	HIS
3	o	27	ILE
3	o	157	GLY
4	p	51	LEU
4	p	73	GLY
5	q	114	VAL
5	q	141	HIS
9	u	72	VAL
10	v	58	LYS
12	x	328	HIS
12	x	508	PRO
17	3	2	SER
17	3	87	THR
17	3	95	GLN
18	4	4	ALA
18	4	9	GLY
19	5	46	LYS
21	7	2	GLU
26	B	119	CYS
31	G	105	CYS
1	c	55	ALA
1	c	56	GLY
1	c	72	GLY
1	c	80	GLU
1	c	81	SER
1	c	227	ALA
1	c	287	GLY
1	c	288	ALA
1	c	342	TRP
2	m	236	LYS
2	m	351	ASN
3	b	28	SER
3	b	137	GLN
3	b	157	GLY
3	b	313	ARG
4	d	119	ALA
4	d	154	PRO
7	g	68	LYS
9	i	59	ALA
10	j	58	LYS
1	l	52	ASN

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Mol	Chain	Res	Type
1	l	72	GLY
1	l	227	ALA
1	l	246	ASP
1	l	282	CYS
1	l	385	THR
2	n	236	LYS
5	q	137	GLY
9	u	59	ALA
10	v	23	THR
10	v	24	ILE
18	4	5	LYS
33	I	116	CYS
1	c	52	ASN
1	c	352	SER
1	c	385	THR
1	c	395	TRP
2	m	91	ALA
3	b	283	SER
3	b	319	PRO
4	d	27	ARG
4	d	162	PRO
4	d	218	LEU
5	e	16	PRO
5	e	72	SER
10	j	23	THR
10	j	35	PHE
1	l	81	SER
1	l	107	PRO
1	l	426	GLY
2	n	24	LEU
2	n	305	GLN
3	o	28	SER
3	o	62	ALA
3	o	316	MET
3	o	319	PRO
4	p	80	MET
4	p	162	PRO
5	q	64	ALA
5	q	177	PRO
7	s	68	LYS
10	v	57	HIS
11	w	33	VAL

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Mol	Chain	Res	Type
13	y	104	TRP
18	4	61	SER
31	G	156	CYS
1	c	107	PRO
1	c	246	ASP
1	c	391	PRO
3	b	236	ILE
3	b	365	LEU
4	d	80	MET
4	d	147	LEU
6	f	95	LYS
10	j	4	THR
10	j	57	HIS
1	l	6	GLN
1	l	109	ALA
2	n	269	ALA
2	n	409	ASP
3	o	24	PRO
3	o	109	PHE
4	p	147	LEU
5	q	130	PRO
6	r	95	LYS
12	x	51	ASP
1	c	6	GLN
1	c	152	TYR
2	m	39	GLU
3	b	316	MET
7	g	72	LYS
1	l	338	LEU
1	l	391	PRO
3	o	247	PRO
3	o	255	ASN
4	p	83	ARG
4	p	98	PRO
4	p	110	PRO
4	p	154	PRO
5	q	16	PRO
5	q	69	LEU
5	q	188	THR
7	s	50	PRO
11	w	34	SER
13	y	103	GLN

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Mol	Chain	Res	Type
21	7	3	ASN
1	c	33	PRO
2	m	52	LYS
4	d	110	PRO
4	d	163	PRO
4	d	176	PRO
7	g	45	ILE
1	l	185	TYR
2	n	52	LYS
4	p	176	PRO
5	q	43	THR
12	x	91	ASP
13	y	158	ASP
18	4	49	PRO
2	m	129	ALA
6	f	51	PRO
1	l	56	GLY
1	l	293	PRO
3	b	339	GLY
4	d	83	ARG
2	n	85	ILE
2	n	109	VAL
4	p	123	GLY
5	q	84	GLY
8	t	69	VAL
17	3	15	GLY
10	j	24	ILE
6	r	51	PRO
7	s	45	ILE
1	c	260	PRO
11	k	33	VAL
4	p	163	PRO
9	u	65	VAL
3	b	372	ILE
4	d	26	ILE
1	l	71	PRO
1	l	193	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	c	370/370 (100%)	278 (75%)	92 (25%)	0	4
1	l	370/370 (100%)	284 (77%)	86 (23%)	1	5
2	m	328/343 (96%)	254 (77%)	74 (23%)	1	6
2	n	328/343 (96%)	254 (77%)	74 (23%)	1	6
3	b	327/327 (100%)	252 (77%)	75 (23%)	1	6
3	o	327/327 (100%)	259 (79%)	68 (21%)	1	6
4	d	206/206 (100%)	172 (84%)	34 (16%)	2	10
4	p	206/206 (100%)	170 (82%)	36 (18%)	2	9
5	e	65/168 (39%)	47 (72%)	18 (28%)	0	3
5	q	167/168 (99%)	110 (66%)	57 (34%)	0	1
6	f	96/98 (98%)	68 (71%)	28 (29%)	0	2
6	r	96/98 (98%)	76 (79%)	20 (21%)	1	6
7	g	71/71 (100%)	53 (75%)	18 (25%)	0	3
7	s	71/71 (100%)	51 (72%)	20 (28%)	0	3
8	h	61/74 (82%)	50 (82%)	11 (18%)	2	9
8	t	61/74 (82%)	50 (82%)	11 (18%)	2	9
9	i	27/60 (45%)	19 (70%)	8 (30%)	0	2
9	u	27/60 (45%)	19 (70%)	8 (30%)	0	2
10	j	52/52 (100%)	43 (83%)	9 (17%)	2	9
10	v	52/52 (100%)	42 (81%)	10 (19%)	1	8
11	k	15/46 (33%)	11 (73%)	4 (27%)	0	3
11	w	15/46 (33%)	10 (67%)	5 (33%)	0	2
12	x	427/427 (100%)	387 (91%)	40 (9%)	8	26
13	y	211/211 (100%)	191 (90%)	20 (10%)	8	25
14	z	226/226 (100%)	199 (88%)	27 (12%)	5	18
15	1	128/129 (99%)	117 (91%)	11 (9%)	10	29
16	2	95/95 (100%)	89 (94%)	6 (6%)	16	37
17	3	81/81 (100%)	73 (90%)	8 (10%)	7	24
18	4	68/68 (100%)	52 (76%)	16 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	5	67/75 (89%)	58 (87%)	9 (13%)	4	14
20	6	58/58 (100%)	51 (88%)	7 (12%)	5	17
21	7	47/50 (94%)	41 (87%)	6 (13%)	4	15
22	8	39/46 (85%)	36 (92%)	3 (8%)	12	32
23	9	40/40 (100%)	37 (92%)	3 (8%)	12	33
24	0	37/38 (97%)	34 (92%)	3 (8%)	11	31
26	B	4/4 (100%)	2 (50%)	2 (50%)	0	0
29	E	4/4 (100%)	4 (100%)	0	100	100
30	F	4/4 (100%)	3 (75%)	1 (25%)	0	4
31	G	12/12 (100%)	8 (67%)	4 (33%)	0	2
33	I	8/8 (100%)	7 (88%)	1 (12%)	4	16
All	All	4894/5206 (94%)	3961 (81%)	933 (19%)	3	8

All (933) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	3	THR
1	c	13	GLU
1	c	24	ARG
1	c	31	SER
1	c	35	CYS
1	c	37	VAL
1	c	42	ASP
1	c	46	ARG
1	c	48	GLU
1	c	49	SER
1	c	65	LYS
1	c	68	LYS
1	c	70	ARG
1	c	75	LEU
1	c	79	VAL
1	c	86	LEU
1	c	89	TYR
1	c	90	SER
1	c	91	THR
1	c	92	ARG
1	c	97	TYR
1	c	99	ILE

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Mol	Chain	Res	Type
1	c	102	LEU
1	c	108	LYS
1	c	112	LEU
1	c	120	CYS
1	c	125	SER
1	c	127	ILE
1	c	128	GLU
1	c	130	GLU
1	c	133	VAL
1	c	134	ILE
1	c	138	LEU
1	c	143	THR
1	c	149	VAL
1	c	156	THR
1	c	159	GLN
1	c	163	LEU
1	c	174	VAL
1	c	175	ARG
1	c	176	LYS
1	c	177	LEU
1	c	178	SER
1	c	179	ARG
1	c	183	THR
1	c	187	SER
1	c	191	LYS
1	c	195	MET
1	c	196	VAL
1	c	197	LEU
1	c	208	LEU
1	c	211	LEU
1	c	213	GLN
1	c	216	PHE
1	c	222	THR
1	c	225	GLU
1	c	231	LEU
1	c	239	SER
1	c	241	ILE
1	c	245	GLU
1	c	246	ASP
1	c	248	LEU
1	c	255	ILE
1	c	272	VAL

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Mol	Chain	Res	Type
1	c	277	ILE
1	c	296	SER
1	c	302	LYS
1	c	312	ILE
1	c	316	ASP
1	c	330	SER
1	c	334	MET
1	c	337	VAL
1	c	341	GLN
1	c	344	ARG
1	c	346	CYS
1	c	351	GLU
1	c	352	SER
1	c	353	GLU
1	c	356	ARG
1	c	358	LYS
1	c	360	LEU
1	c	366	VAL
1	c	367	SER
1	c	370	ASP
1	c	379	ILE
1	c	384	LEU
1	c	386	TYR
1	c	398	ARG
1	c	407	VAL
1	c	413	LYS
1	c	428	ILE
1	c	441	MET
2	m	23	ASP
2	m	24	LEU
2	m	35	ILE
2	m	37	SER
2	m	38	LEU
2	m	45	SER
2	m	46	ARG
2	m	51	ILE
2	m	52	LYS
2	m	56	ARG
2	m	58	GLU
2	m	60	SER
2	m	74	SER
2	m	77	THR

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Mol	Chain	Res	Type
2	m	78	LYS
2	m	81	SER
2	m	85	ILE
2	m	86	THR
2	m	95	LYS
2	m	96	LEU
2	m	99	THR
2	m	101	THR
2	m	108	THR
2	m	112	LEU
2	m	113	ARG
2	m	117	ASP
2	m	119	LEU
2	m	131	GLU
2	m	134	ARG
2	m	140	LEU
2	m	145	ARG
2	m	159	VAL
2	m	160	ILE
2	m	175	SER
2	m	185	LYS
2	m	187	THR
2	m	190	GLU
2	m	196	GLN
2	m	203	ARG
2	m	206	LEU
2	m	215	VAL
2	m	219	VAL
2	m	238	LYS
2	m	240	HIS
2	m	245	ARG
2	m	253	VAL
2	m	264	ILE
2	m	286	LYS
2	m	292	THR
2	m	294	SER
2	m	295	LEU
2	m	297	GLN
2	m	310	SER
2	m	318	ASP
2	m	319	SER
2	m	327	ILE

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Mol	Chain	Res	Type
2	m	328	SER
2	m	337	ILE
2	m	347	ILE
2	m	353	SER
2	m	354	ASN
2	m	374	SER
2	m	391	SER
2	m	393	THR
2	m	396	SER
2	m	402	ILE
2	m	416	LYS
2	m	418	VAL
2	m	422	LYS
2	m	423	SER
2	m	430	LEU
2	m	436	ILE
2	m	437	ASP
2	m	438	GLU
3	b	1	MET
3	b	5	ARG
3	b	6	LYS
3	b	7	SER
3	b	11	MET
3	b	25	SER
3	b	26	ASN
3	b	27	ILE
3	b	29	SER
3	b	32	ASN
3	b	39	ILE
3	b	43	LEU
3	b	51	LEU
3	b	57	SER
3	b	60	THR
3	b	61	THR
3	b	65	SER
3	b	67	THR
3	b	73	VAL
3	b	78	ILE
3	b	94	LEU
3	b	115	ILE
3	b	118	ILE
3	b	119	LEU

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Mol	Chain	Res	Type
3	b	123	VAL
3	b	138	MET
3	b	139	SER
3	b	144	THR
3	b	156	ILE
3	b	158	THR
3	b	161	VAL
3	b	169	SER
3	b	174	THR
3	b	176	THR
3	b	177	ARG
3	b	188	ILE
3	b	192	ILE
3	b	197	LEU
3	b	198	LEU
3	b	205	SER
3	b	212	SER
3	b	217	LYS
3	b	226	ILE
3	b	229	ILE
3	b	233	LEU
3	b	237	LEU
3	b	240	MET
3	b	241	LEU
3	b	244	LEU
3	b	247	PRO
3	b	262	LEU
3	b	271	GLU
3	b	273	TYR
3	b	280	ILE
3	b	281	LEU
3	b	282	ARG
3	b	284	ILE
3	b	291	VAL
3	b	299	LEU
3	b	304	ILE
3	b	310	SER
3	b	311	LYS
3	b	312	GLN
3	b	313	ARG
3	b	314	SER
3	b	316	MET

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Mol	Chain	Res	Type
3	b	318	ARG
3	b	321	SER
3	b	324	LEU
3	b	343	VAL
3	b	353	LEU
3	b	362	ILE
3	b	363	LEU
3	b	375	LYS
3	b	377	LEU
4	d	3	LEU
4	d	9	SER
4	d	10	TYR
4	d	17	LEU
4	d	20	SER
4	d	21	LEU
4	d	26	ILE
4	d	27	ARG
4	d	32	VAL
4	d	40	CYS
4	d	42	SER
4	d	43	MET
4	d	52	VAL
4	d	55	CYS
4	d	80	MET
4	d	82	MET
4	d	83	ARG
4	d	87	LEU
4	d	106	ASN
4	d	116	ILE
4	d	120	ARG
4	d	124	GLU
4	d	127	VAL
4	d	132	THR
4	d	139	THR
4	d	141	VAL
4	d	179	MET
4	d	182	VAL
4	d	186	VAL
4	d	201	ARG
4	d	208	MET
4	d	218	LEU
4	d	228	SER

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Mol	Chain	Res	Type
4	d	231	LYS
5	e	1	SER
5	e	5	ILE
5	e	6	LYS
5	e	11	SER
5	e	14	ARG
5	e	15	ARG
5	e	17	GLU
5	e	19	LEU
5	e	28	SER
5	e	30	GLU
5	e	32	ARG
5	e	33	LYS
5	e	40	THR
5	e	52	LYS
5	e	58	PHE
5	e	63	SER
5	e	67	ASP
5	e	68	VAL
6	f	7	SER
6	f	9	SER
6	f	10	SER
6	f	11	ARG
6	f	13	LEU
6	f	16	ILE
6	f	18	LYS
6	f	35	ASP
6	f	44	LYS
6	f	47	ILE
6	f	48	ARG
6	f	50	LEU
6	f	53	ASN
6	f	54	LEU
6	f	58	ARG
6	f	68	LEU
6	f	69	SER
6	f	70	MET
6	f	74	ILE
6	f	77	LYS
6	f	82	LYS
6	f	88	SER
6	f	90	LEU

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Mol	Chain	Res	Type
6	f	94	LEU
6	f	95	LYS
6	f	98	ILE
6	f	100	GLU
6	f	110	LYS
7	g	4	PHE
7	g	8	THR
7	g	9	ARG
7	g	10	VAL
7	g	15	THR
7	g	19	SER
7	g	23	GLN
7	g	24	ARG
7	g	39	ARG
7	g	40	ARG
7	g	41	THR
7	g	42	ARG
7	g	45	ILE
7	g	46	LEU
7	g	58	VAL
7	g	60	THR
7	g	69	SER
7	g	70	LYS
8	h	20	VAL
8	h	29	LYS
8	h	30	CYS
8	h	31	VAL
8	h	54	CYS
8	h	57	GLU
8	h	58	LEU
8	h	59	LEU
8	h	73	LEU
8	h	74	PHE
8	h	76	SER
9	i	46	LYS
9	i	49	VAL
9	i	54	SER
9	i	69	SER
9	i	70	LEU
9	i	72	VAL
9	i	77	ARG
9	i	78	TYR

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Mol	Chain	Res	Type
10	j	4	THR
10	j	11	SER
10	j	13	LEU
10	j	17	THR
10	j	18	SER
10	j	24	ILE
10	j	25	VAL
10	j	46	ILE
10	j	58	LYS
11	k	20	THR
11	k	23	LEU
11	k	27	VAL
11	k	36	THR
1	l	3	THR
1	l	13	GLU
1	l	24	ARG
1	l	31	SER
1	l	37	VAL
1	l	42	ASP
1	l	45	SER
1	l	46	ARG
1	l	48	GLU
1	l	51	LYS
1	l	70	ARG
1	l	79	VAL
1	l	86	LEU
1	l	89	TYR
1	l	91	THR
1	l	92	ARG
1	l	97	TYR
1	l	99	ILE
1	l	108	LYS
1	l	112	LEU
1	l	125	SER
1	l	127	ILE
1	l	128	GLU
1	l	130	GLU
1	l	133	VAL
1	l	137	GLU
1	l	138	LEU
1	l	143	THR
1	l	149	VAL

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Mol	Chain	Res	Type
1	1	156	THR
1	1	159	GLN
1	1	163	LEU
1	1	174	VAL
1	1	175	ARG
1	1	176	LYS
1	1	177	LEU
1	1	179	ARG
1	1	183	THR
1	1	187	SER
1	1	191	LYS
1	1	195	MET
1	1	197	LEU
1	1	208	LEU
1	1	211	LEU
1	1	213	GLN
1	1	216	PHE
1	1	222	THR
1	1	225	GLU
1	1	231	LEU
1	1	232	SER
1	1	245	GLU
1	1	246	ASP
1	1	248	LEU
1	1	257	VAL
1	1	277	ILE
1	1	296	SER
1	1	302	LYS
1	1	307	PHE
1	1	309	THR
1	1	316	ASP
1	1	319	LEU
1	1	329	MET
1	1	330	SER
1	1	334	MET
1	1	337	VAL
1	1	341	GLN
1	1	344	ARG
1	1	346	CYS
1	1	347	THR
1	1	351	GLU
1	1	353	GLU

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Mol	Chain	Res	Type
1	l	356	ARG
1	l	358	LYS
1	l	360	LEU
1	l	366	VAL
1	l	370	ASP
1	l	379	ILE
1	l	382	SER
1	l	384	LEU
1	l	386	TYR
1	l	407	VAL
1	l	412	SER
1	l	413	LYS
1	l	419	CYS
1	l	428	ILE
1	l	441	MET
2	n	23	ASP
2	n	24	LEU
2	n	35	ILE
2	n	37	SER
2	n	38	LEU
2	n	45	SER
2	n	46	ARG
2	n	52	LYS
2	n	56	ARG
2	n	58	GLU
2	n	60	SER
2	n	65	THR
2	n	78	LYS
2	n	81	SER
2	n	84	LYS
2	n	85	ILE
2	n	86	THR
2	n	96	LEU
2	n	99	THR
2	n	100	SER
2	n	101	THR
2	n	102	ARG
2	n	108	THR
2	n	111	CYS
2	n	112	LEU
2	n	113	ARG
2	n	117	ASP

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Mol	Chain	Res	Type
2	n	119	LEU
2	n	134	ARG
2	n	145	ARG
2	n	159	VAL
2	n	160	ILE
2	n	175	SER
2	n	183	ILE
2	n	185	LYS
2	n	190	GLU
2	n	196	GLN
2	n	201	SER
2	n	203	ARG
2	n	206	LEU
2	n	207	ILE
2	n	215	VAL
2	n	219	VAL
2	n	233	SER
2	n	238	LYS
2	n	240	HIS
2	n	244	ILE
2	n	253	VAL
2	n	264	ILE
2	n	266	SER
2	n	286	LYS
2	n	292	THR
2	n	295	LEU
2	n	297	GLN
2	n	315	SER
2	n	317	SER
2	n	318	ASP
2	n	327	ILE
2	n	328	SER
2	n	329	GLN
2	n	337	ILE
2	n	345	LYS
2	n	346	THR
2	n	354	ASN
2	n	357	VAL
2	n	384	SER
2	n	402	ILE
2	n	403	ASP
2	n	416	LYS

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Mol	Chain	Res	Type
2	n	418	VAL
2	n	424	MET
2	n	436	ILE
2	n	437	ASP
2	n	438	GLU
3	o	1	MET
3	o	5	ARG
3	o	6	LYS
3	o	7	SER
3	o	11	MET
3	o	13	ILE
3	o	27	ILE
3	o	32	ASN
3	o	35	SER
3	o	39	ILE
3	o	44	GLN
3	o	60	THR
3	o	61	THR
3	o	67	THR
3	o	69	ILE
3	o	73	VAL
3	o	92	ILE
3	o	94	LEU
3	o	100	ARG
3	o	115	ILE
3	o	118	ILE
3	o	119	LEU
3	o	138	MET
3	o	139	SER
3	o	144	THR
3	o	153	ILE
3	o	156	ILE
3	o	158	THR
3	o	161	VAL
3	o	169	SER
3	o	174	THR
3	o	176	THR
3	o	184	ILE
3	o	188	ILE
3	o	189	ILE
3	o	192	ILE
3	o	197	LEU

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Mol	Chain	Res	Type
3	o	212	SER
3	o	215	VAL
3	o	226	ILE
3	o	229	ILE
3	o	233	LEU
3	o	241	LEU
3	o	242	LEU
3	o	243	VAL
3	o	244	LEU
3	o	257	THR
3	o	262	LEU
3	o	271	GLU
3	o	281	LEU
3	o	282	ARG
3	o	287	LYS
3	o	291	VAL
3	o	297	SER
3	o	299	LEU
3	o	300	ILE
3	o	313	ARG
3	o	316	MET
3	o	318	ARG
3	o	324	LEU
3	o	338	ILE
3	o	349	THR
3	o	356	VAL
3	o	362	ILE
3	o	363	LEU
3	o	375	LYS
3	o	377	LEU
3	o	378	LYS
4	p	3	LEU
4	p	10	TYR
4	p	13	SER
4	p	17	LEU
4	p	20	SER
4	p	21	LEU
4	p	38	SER
4	p	39	SER
4	p	40	CYS
4	p	42	SER
4	p	43	MET

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Mol	Chain	Res	Type
4	p	52	VAL
4	p	55	CYS
4	p	80	MET
4	p	82	MET
4	p	83	ARG
4	p	88	SER
4	p	106	ASN
4	p	120	ARG
4	p	124	GLU
4	p	127	VAL
4	p	132	THR
4	p	139	THR
4	p	141	VAL
4	p	158	ILE
4	p	160	MET
4	p	179	MET
4	p	180	SER
4	p	182	VAL
4	p	186	VAL
4	p	201	ARG
4	p	208	MET
4	p	210	LEU
4	p	223	LYS
4	p	226	LYS
4	p	231	LYS
5	q	5	ILE
5	q	6	LYS
5	q	11	SER
5	q	14	ARG
5	q	17	GLU
5	q	18	VAL
5	q	19	LEU
5	q	22	THR
5	q	23	LYS
5	q	28	SER
5	q	30	GLU
5	q	32	ARG
5	q	33	LYS
5	q	36	SER
5	q	40	THR
5	q	42	THR
5	q	43	THR

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Mol	Chain	Res	Type
5	q	44	THR
5	q	45	VAL
5	q	58	PHE
5	q	60	SER
5	q	61	SER
5	q	62	MET
5	q	63	SER
5	q	65	SER
5	q	68	VAL
5	q	71	MET
5	q	73	LYS
5	q	74	ILE
5	q	76	ILE
5	q	78	LEU
5	q	81	ILE
5	q	87	MET
5	q	95	PRO
5	q	98	VAL
5	q	102	THR
5	q	103	LYS
5	q	106	ILE
5	q	109	GLU
5	q	113	GLU
5	q	114	VAL
5	q	125	GLU
5	q	129	LYS
5	q	136	ILE
5	q	139	CYS
5	q	140	THR
5	q	144	CYS
5	q	147	ILE
5	q	152	ASP
5	q	158	CYS
5	q	168	SER
5	q	171	ILE
5	q	172	ARG
5	q	178	LEU
5	q	192	MET
5	q	194	ILE
5	q	195	VAL
6	r	7	SER
6	r	11	ARG

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Mol	Chain	Res	Type
6	r	16	ILE
6	r	35	ASP
6	r	47	ILE
6	r	48	ARG
6	r	54	LEU
6	r	64	ARG
6	r	68	LEU
6	r	70	MET
6	r	75	LEU
6	r	77	LYS
6	r	88	SER
6	r	90	LEU
6	r	94	LEU
6	r	98	ILE
6	r	100	GLU
6	r	101	ARG
6	r	103	GLU
6	r	110	LYS
7	s	4	PHE
7	s	7	LEU
7	s	8	THR
7	s	9	ARG
7	s	10	VAL
7	s	15	THR
7	s	18	LEU
7	s	19	SER
7	s	23	GLN
7	s	24	ARG
7	s	31	SER
7	s	39	ARG
7	s	40	ARG
7	s	41	THR
7	s	42	ARG
7	s	45	ILE
7	s	46	LEU
7	s	58	VAL
7	s	69	SER
7	s	70	LYS
8	t	20	VAL
8	t	29	LYS
8	t	30	CYS
8	t	31	VAL

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Mol	Chain	Res	Type
8	t	46	SER
8	t	48	SER
8	t	54	CYS
8	t	57	GLU
8	t	58	LEU
8	t	73	LEU
8	t	74	PHE
9	u	46	LYS
9	u	49	VAL
9	u	68	VAL
9	u	70	LEU
9	u	72	VAL
9	u	76	VAL
9	u	77	ARG
9	u	78	TYR
10	v	4	THR
10	v	9	LEU
10	v	12	LEU
10	v	13	LEU
10	v	16	ARG
10	v	18	SER
10	v	42	ILE
10	v	46	ILE
10	v	55	ILE
10	v	58	LYS
11	w	20	THR
11	w	23	LEU
11	w	27	VAL
11	w	34	SER
11	w	36	THR
12	x	18	LEU
12	x	35	LEU
12	x	92	MET
12	x	96	ARG
12	x	105	LEU
12	x	115	SER
12	x	136	LEU
12	x	138	HIS
12	x	150	LEU
12	x	158	ILE
12	x	159	LEU
12	x	187	SER

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Mol	Chain	Res	Type
12	x	188	VAL
12	x	189	MET
12	x	194	LEU
12	x	199	LEU
12	x	213	ARG
12	x	241	PRO
12	x	273	MET
12	x	295	VAL
12	x	301	THR
12	x	306	THR
12	x	318	VAL
12	x	324	LEU
12	x	347	LEU
12	x	353	LEU
12	x	354	THR
12	x	365	ILE
12	x	369	ASP
12	x	373	VAL
12	x	383	MET
12	x	417	MET
12	x	444	PRO
12	x	465	VAL
12	x	467	LEU
12	x	474	GLU
12	x	492	LEU
12	x	508	PRO
12	x	509	THR
12	x	512	ASN
13	y	7	LEU
13	y	16	ILE
13	y	31	VAL
13	y	33	LEU
13	y	52	HIS
13	y	60	GLU
13	y	63	THR
13	y	67	ILE
13	y	88	ASP
13	y	92	ASN
13	y	125	THR
13	y	130	PRO
13	y	134	ARG
13	y	142	VAL

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Mol	Chain	Res	Type
13	y	147	GLU
13	y	170	LEU
13	y	171	LYS
13	y	185	MET
13	y	205	SER
13	y	216	LEU
14	z	1	MET
14	z	11	VAL
14	z	13	PRO
14	z	14	SER
14	z	18	LEU
14	z	19	THR
14	z	22	LEU
14	z	26	LEU
14	z	38	ASN
14	z	39	SER
14	z	85	LEU
14	z	92	LEU
14	z	112	LEU
14	z	127	LEU
14	z	128	GLU
14	z	131	LEU
14	z	132	LEU
14	z	137	LEU
14	z	142	VAL
14	z	160	LEU
14	z	163	LEU
14	z	188	ILE
14	z	196	THR
14	z	199	VAL
14	z	213	THR
14	z	222	GLN
14	z	230	ASN
15	1	9	GLU
15	1	27	VAL
15	1	31	LYS
15	1	36	SER
15	1	40	LEU
15	1	59	LEU
15	1	62	LEU
15	1	107	ILE
15	1	116	VAL

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Mol	Chain	Res	Type
15	1	143	ASN
15	1	147	LYS
16	2	7	THR
16	2	29	LEU
16	2	70	VAL
16	2	79	LYS
16	2	80	GLU
16	2	90	ARG
17	3	6	VAL
17	3	20	VAL
17	3	37	LYS
17	3	52	ILE
17	3	53	THR
17	3	74	LEU
17	3	95	GLN
17	3	98	HIS
18	4	5	LYS
18	4	7	ASP
18	4	8	HIS
18	4	14	ARG
18	4	17	ARG
18	4	33	LEU
18	4	34	ASN
18	4	37	LEU
18	4	41	HIS
18	4	42	ARG
18	4	43	GLU
18	4	48	ILE
18	4	54	ARG
18	4	56	ARG
18	4	68	THR
18	4	78	LEU
19	5	19	ARG
19	5	29	CYS
19	5	41	LYS
19	5	51	SER
19	5	53	CYS
19	5	57	ARG
19	5	60	TYR
19	5	67	SER
19	5	75	ARG
20	6	2	THR

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Mol	Chain	Res	Type
20	6	4	LEU
20	6	8	GLN
20	6	22	VAL
20	6	26	MET
20	6	44	LYS
20	6	64	ARG
21	7	2	GLU
21	7	5	VAL
21	7	8	LYS
21	7	16	ASN
21	7	23	LYS
21	7	27	THR
22	8	45	VAL
22	8	48	VAL
22	8	49	THR
23	9	15	VAL
23	9	22	LEU
23	9	26	THR
24	0	13	LYS
24	0	24	LEU
24	0	42	LYS
26	B	54	CYS
26	B	55	CYS
30	F	405	CYS
31	G	41	CYS
31	G	52	CYS
31	G	55	CYS
31	G	69	CYS
33	I	119	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	18	GLN
1	c	21	ASN
1	c	32	GLN
1	c	73	ASN
1	c	85	HIS
1	c	136	GLN
1	c	151	ASN
1	c	154	HIS
1	c	189	HIS

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Mol	Chain	Res	Type
1	c	240	GLN
1	c	243	HIS
1	c	252	HIS
1	c	289	HIS
1	c	308	GLN
1	c	435	ASN
2	m	62	ASN
2	m	67	HIS
2	m	125	ASN
2	m	162	ASN
2	m	198	HIS
2	m	247	GLN
2	m	304	HIS
2	m	429	ASN
3	b	15	ASN
3	b	26	ASN
3	b	32	ASN
3	b	114	ASN
3	b	206	ASN
3	b	312	GLN
3	b	374	ASN
4	d	6	HIS
4	d	50	HIS
4	d	75	ASN
4	d	106	ASN
4	d	181	GLN
4	d	225	HIS
5	e	57	GLN
6	f	38	HIS
7	g	6	HIS
7	g	12	HIS
9	i	71	ASN
10	j	54	HIS
1	l	18	GLN
1	l	32	GLN
1	l	85	HIS
1	l	136	GLN
1	l	151	ASN
1	l	154	HIS
1	l	159	GLN
1	l	189	HIS
1	l	213	GLN

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Mol	Chain	Res	Type
1	l	240	GLN
1	l	243	HIS
1	l	308	GLN
1	l	323	HIS
1	l	339	GLN
1	l	435	ASN
2	n	62	ASN
2	n	67	HIS
2	n	125	ASN
2	n	141	GLN
2	n	156	GLN
2	n	198	HIS
2	n	247	GLN
2	n	304	HIS
2	n	429	ASN
3	o	15	ASN
3	o	26	ASN
3	o	32	ASN
3	o	114	ASN
3	o	206	ASN
3	o	374	ASN
4	p	6	HIS
4	p	50	HIS
4	p	106	ASN
4	p	181	GLN
4	p	225	HIS
5	q	53	ASN
5	q	121	GLN
6	r	38	HIS
6	r	73	GLN
7	s	6	HIS
9	u	58	GLN
10	v	54	HIS
11	w	16	ASN
12	x	4	ASN
12	x	11	ASN
12	x	12	HIS
12	x	55	ASN
12	x	99	ASN
12	x	170	ASN
12	x	256	HIS
12	x	360	ASN

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Mol	Chain	Res	Type
12	x	368	HIS
12	x	413	HIS
12	x	503	HIS
12	x	512	ASN
13	y	52	HIS
13	y	91	ASN
13	y	102	HIS
13	y	195	GLN
13	y	203	ASN
14	z	3	HIS
14	z	6	HIS
14	z	12	ASN
14	z	133	ASN
14	z	148	HIS
14	z	158	HIS
14	z	204	HIS
14	z	207	HIS
14	z	222	GLN
14	z	232	HIS
15	1	32	ASN
15	1	109	HIS
16	2	34	ASN
17	3	66	ASN
18	4	51	HIS
18	4	52	HIS
19	5	23	GLN
19	5	24	ASN
19	5	25	GLN
19	5	28	ASN
19	5	37	HIS
21	7	3	ASN
21	7	16	ASN
21	7	21	HIS
22	8	10	HIS
22	8	15	ASN
22	8	35	GLN
22	8	41	ASN
23	9	42	HIS
24	0	39	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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
52	HEM	o	401	3	50,50,50	1.40	7 (14%)	66,82,82	1.92	18 (27%)
53	HEC	p	301	4	50,50,50	1.31	5 (10%)	68,82,82	1.05	4 (5%)
53	HEC	d	301	4	50,50,50	1.29	3 (6%)	68,82,82	1.14	5 (7%)
52	HEM	b	401	3	50,50,50	1.30	6 (12%)	66,82,82	1.53	9 (13%)
59	SF4	I	201	33	0,12,12	-	-	-	-	-
54	FES	E	201	29	0,4,4	-	-	-	-	-
57	HEA	x	603	12	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
59	SF4	B	201	26	0,12,12	-	-	-	-	-
59	SF4	G	801	31	0,12,12	-	-	-	-	-
52	HEM	o	402	3	50,50,50	1.34	7 (14%)	66,82,82	1.77	15 (22%)
52	HEM	b	402	3	50,50,50	1.26	6 (12%)	66,82,82	1.85	18 (27%)
54	FES	q	201	5	0,4,4	-	-	-	-	-
59	SF4	F	501	30	0,12,12	-	-	-	-	-
59	SF4	I	202	33	0,12,12	-	-	-	-	-
59	SF4	G	802	31	0,12,12	-	-	-	-	-
54	FES	G	803	31	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	HEA	x	604	12	66,67,67	1.22	8 (12%)	78,103,103	1.37	12 (15%)

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
52	HEM	o	401	3	-	6/14/54/54	-
53	HEC	p	301	4	-	8/14/54/54	-
53	HEC	d	301	4	-	8/14/54/54	-
52	HEM	b	401	3	-	4/14/54/54	-
59	SF4	I	201	33	-	-	0/6/5/5
54	FES	E	201	29	-	-	0/1/1/1
57	HEA	x	603	12	-	9/36/76/76	-
59	SF4	B	201	26	-	-	0/6/5/5
59	SF4	G	801	31	-	-	0/6/5/5
52	HEM	o	402	3	-	4/14/54/54	-
52	HEM	b	402	3	-	6/14/54/54	-
54	FES	q	201	5	-	-	0/1/1/1
59	SF4	F	501	30	-	-	0/6/5/5
59	SF4	I	202	33	-	-	0/6/5/5
59	SF4	G	802	31	-	-	0/6/5/5
54	FES	G	803	31	-	-	0/1/1/1
57	HEA	x	604	12	-	7/36/76/76	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	x	604	HEA	CMA-C3A	-3.80	1.37	1.45
53	d	301	HEC	CBB-CAB	-3.54	1.35	1.51
53	p	301	HEC	CBC-CAC	-3.49	1.35	1.51
53	d	301	HEC	CBC-CAC	-3.37	1.36	1.51
53	p	301	HEC	CBB-CAB	-3.34	1.36	1.51
52	o	402	HEM	FE-NA	3.34	2.06	1.95
52	b	401	HEM	CAB-C3B	3.33	1.56	1.47
52	o	401	HEM	CAB-C3B	3.29	1.56	1.47
52	o	402	HEM	FE-NC	3.26	2.06	1.95
52	b	401	HEM	FE-NB	3.19	2.04	1.94
52	o	401	HEM	FE-NB	3.12	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	b	401	HEM	C3B-C2B	-3.08	1.31	1.37
52	b	402	HEM	CHB-C4A	-3.08	1.32	1.39
57	x	604	HEA	FE-NA	2.86	2.04	1.95
52	o	401	HEM	C1B-C2B	2.83	1.50	1.44
57	x	604	HEA	C1D-C2D	2.70	1.49	1.44
57	x	604	HEA	C1D-ND	-2.68	1.35	1.40
57	x	603	HEA	C1A-C2A	-2.67	1.40	1.45
57	x	603	HEA	CMA-C3A	-2.67	1.39	1.45
52	o	402	HEM	CAC-C3C	2.66	1.54	1.47
52	o	401	HEM	CAC-C3C	2.56	1.54	1.47
57	x	604	HEA	C3A-C2A	-2.55	1.31	1.36
52	b	401	HEM	FE-ND	2.49	2.02	1.94
52	o	402	HEM	C1A-NA	2.39	1.44	1.39
52	o	402	HEM	FE-NB	2.39	2.02	1.94
52	b	401	HEM	CAC-C3C	2.37	1.53	1.47
53	p	301	HEC	FE-ND	2.37	2.02	1.94
57	x	603	HEA	C3A-C4A	-2.36	1.41	1.46
57	x	604	HEA	CMD-C2D	2.30	1.55	1.50
52	b	402	HEM	FE-ND	2.29	2.01	1.94
52	o	401	HEM	C3D-C2D	-2.25	1.31	1.36
52	b	402	HEM	FE-NC	2.23	2.02	1.95
52	b	402	HEM	FE-NB	2.19	2.01	1.94
52	o	401	HEM	C2A-C3A	-2.18	1.33	1.38
52	o	402	HEM	CAB-C3B	2.17	1.53	1.47
53	p	301	HEC	CAB-C3B	2.15	1.56	1.51
52	b	401	HEM	C2A-C3A	-2.15	1.33	1.38
52	o	402	HEM	C2A-C3A	-2.13	1.33	1.38
52	b	402	HEM	CAB-C3B	2.13	1.53	1.47
52	o	401	HEM	FE-NA	2.11	2.02	1.95
53	p	301	HEC	C3C-C2C	-2.10	1.33	1.38
57	x	604	HEA	FE-NC	2.07	2.02	1.95
53	d	301	HEC	FE-ND	2.03	2.01	1.94
57	x	604	HEA	CHB-C4A	2.00	1.42	1.38
52	b	402	HEM	C1C-C2C	2.00	1.49	1.45

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	o	401	HEM	C3B-C2B-C1B	-5.58	102.35	106.49
52	o	402	HEM	C3B-C2B-C1B	4.93	110.15	106.49
52	o	401	HEM	CMA-C3A-C4A	-4.87	117.95	125.37
52	b	402	HEM	CAA-CBA-CGA	4.76	123.86	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	401	HEM	CBD-CAD-C3D	4.72	125.74	112.63
52	o	401	HEM	C4B-C3B-C2B	4.45	110.64	107.11
52	o	402	HEM	C2A-C1A-NA	-4.16	105.49	110.15
52	o	402	HEM	CHC-C4B-NB	4.08	128.85	124.42
52	b	401	HEM	O1D-CGD-CBD	-4.01	110.19	123.08
57	x	603	HEA	C17-C18-C19	-3.97	118.11	127.66
52	b	401	HEM	CBB-CAB-C3B	-3.90	108.23	127.62
52	o	402	HEM	CHA-C1A-C2A	3.88	133.83	125.36
52	o	402	HEM	CHB-C1B-NB	-3.82	119.66	124.37
52	b	402	HEM	C4D-ND-C1D	3.69	108.89	105.07
52	o	401	HEM	C2B-C1B-NB	3.62	114.13	109.84
52	o	401	HEM	O1D-CGD-CBD	-3.57	111.61	123.08
52	o	401	HEM	CHB-C1B-NB	-3.55	119.99	124.37
52	o	401	HEM	O2D-CGD-O1D	3.54	132.13	123.30
52	b	402	HEM	C4C-NC-C1C	-3.53	101.89	105.35
52	b	402	HEM	CMA-C3A-C4A	-3.44	120.13	125.37
52	b	402	HEM	C3C-C2C-C1C	-3.43	103.80	107.08
57	x	604	HEA	CHA-C1A-NA	-3.37	120.80	124.44
52	b	402	HEM	CHD-C1D-ND	3.36	128.07	124.42
52	b	402	HEM	CAD-CBD-CGD	3.29	120.68	113.60
52	o	401	HEM	CMA-C3A-C2A	3.22	132.57	125.61
57	x	603	HEA	C13-C14-C15	-3.17	120.03	127.66
52	o	402	HEM	O1D-CGD-CBD	-3.04	113.32	123.08
52	b	402	HEM	O2A-CGA-CBA	3.00	123.66	114.03
52	b	402	HEM	O2A-CGA-O1A	-2.92	116.01	123.30
52	b	401	HEM	O2A-CGA-O1A	2.92	130.58	123.30
52	b	402	HEM	CHC-C1C-NC	-2.91	121.29	124.44
52	b	402	HEM	C4A-CHB-C1B	2.91	133.25	126.34
52	b	402	HEM	CHB-C1B-NB	-2.86	120.85	124.37
57	x	603	HEA	C1B-C2B-C3B	2.83	110.19	106.80
52	b	401	HEM	CMB-C2B-C1B	-2.83	120.73	125.04
52	o	401	HEM	C1B-NB-C4B	-2.81	102.17	105.07
52	b	402	HEM	CMA-C3A-C2A	2.81	131.68	125.61
52	b	402	HEM	C4A-NA-C1A	2.79	108.08	105.35
52	o	401	HEM	CMD-C2D-C1D	-2.79	120.79	125.04
52	o	402	HEM	CAA-C2A-C1A	-2.71	119.56	124.89
53	p	301	HEC	O1D-CGD-CBD	-2.67	114.50	123.08
52	o	401	HEM	CAB-C3B-C2B	-2.61	119.99	128.60
57	x	603	HEA	C3C-C4C-NC	2.61	111.85	110.25
57	x	604	HEA	C4A-C3A-C2A	2.60	108.89	106.75
57	x	604	HEA	CMD-C2D-C1D	2.59	128.98	125.04
52	b	402	HEM	CBD-CAD-C3D	2.55	119.72	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	d	301	HEC	O1A-CGA-CBA	-2.51	115.01	123.08
53	d	301	HEC	O2D-CGD-O1D	2.51	129.54	123.30
52	o	402	HEM	C4B-C3B-C2B	-2.49	105.14	107.11
52	o	401	HEM	CMB-C2B-C3B	2.48	134.36	128.30
52	b	401	HEM	O2D-CGD-CBD	2.47	121.96	114.03
52	o	401	HEM	CBD-CAD-C3D	2.45	119.43	112.63
52	b	402	HEM	CAA-C2A-C1A	-2.44	120.09	124.89
52	o	401	HEM	CHA-C4D-ND	-2.44	121.37	124.37
57	x	604	HEA	C1D-C2D-C3D	-2.43	104.40	106.96
57	x	603	HEA	C17-C16-C15	-2.42	105.03	112.98
57	x	604	HEA	CAA-C2A-C1A	2.41	129.44	124.89
53	p	301	HEC	CAD-CBD-CGD	2.40	118.77	113.60
52	o	402	HEM	C4A-NA-C1A	2.38	107.68	105.35
52	b	401	HEM	CMA-C3A-C4A	-2.37	121.75	125.37
52	b	401	HEM	C4B-C3B-C2B	2.37	109.00	107.11
52	o	402	HEM	CMB-C2B-C3B	-2.37	122.50	128.30
57	x	603	HEA	C16-C17-C18	-2.36	104.14	111.88
57	x	603	HEA	C20-C19-C18	2.36	125.88	121.12
57	x	604	HEA	CMB-C2B-C3B	-2.34	125.89	130.34
57	x	603	HEA	CAD-C3D-C4D	2.31	128.69	124.66
57	x	604	HEA	C25-C23-C24	2.30	119.69	114.60
53	d	301	HEC	CAD-C3D-C2D	2.28	132.12	127.88
53	d	301	HEC	O1D-CGD-CBD	-2.27	115.78	123.08
52	b	402	HEM	C3D-C4D-ND	-2.27	107.64	110.17
57	x	604	HEA	C13-C14-C15	-2.27	122.19	127.66
52	o	401	HEM	CAA-CBA-CGA	2.25	118.45	113.60
52	b	401	HEM	CHC-C1C-NC	2.23	126.86	124.44
52	o	402	HEM	CMD-C2D-C1D	-2.23	121.64	125.04
52	o	402	HEM	O2D-CGD-CBD	2.22	121.15	114.03
52	o	401	HEM	C4A-C3A-C2A	2.21	109.41	106.83
57	x	603	HEA	C12-C13-C14	-2.19	106.46	112.23
52	b	402	HEM	C2A-C1A-NA	-2.18	107.72	110.15
57	x	604	HEA	C26-C15-C16	2.17	118.92	115.27
52	o	401	HEM	C3C-C2C-C1C	2.16	109.13	107.08
57	x	603	HEA	C4B-C3B-C2B	-2.14	103.75	107.41
53	d	301	HEC	CAD-C3D-C4D	-2.13	120.93	124.66
52	o	402	HEM	CMC-C2C-C1C	-2.12	120.98	124.71
53	p	301	HEC	CAC-C3C-C4C	-2.12	121.97	124.92
52	o	402	HEM	CHA-C1A-NA	-2.11	119.97	123.85
57	x	604	HEA	C3A-C2A-C1A	-2.08	105.09	107.08
57	x	603	HEA	C27-C19-C18	-2.08	118.35	123.68
52	o	401	HEM	O1A-CGA-CBA	-2.07	116.44	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	x	604	HEA	CBD-CAD-C3D	2.04	118.30	112.63
57	x	604	HEA	C3C-C4C-NC	2.04	111.50	110.25
52	o	402	HEM	CAA-CBA-CGA	2.03	117.97	113.60
53	p	301	HEC	O1A-CGA-CBA	-2.01	116.62	123.08

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	o	401	HEM	C2B-C3B-CAB-CBB
57	x	603	HEA	C2A-C3A-CMA-OMA
57	x	603	HEA	C4A-C3A-CMA-OMA
57	x	603	HEA	C12-C11-C3B-C2B
57	x	604	HEA	C2A-C3A-CMA-OMA
57	x	604	HEA	C4A-C3A-CMA-OMA
53	p	301	HEC	C2C-C3C-CAC-CBC
53	d	301	HEC	C2B-C3B-CAB-CBB
53	d	301	HEC	C4B-C3B-CAB-CBB
57	x	603	HEA	C15-C16-C17-C18
53	p	301	HEC	C4C-C3C-CAC-CBC
53	d	301	HEC	C2C-C3C-CAC-CBC
52	o	401	HEM	C4B-C3B-CAB-CBB
53	p	301	HEC	C1A-C2A-CAA-CBA
53	d	301	HEC	C4C-C3C-CAC-CBC
53	p	301	HEC	C3A-C2A-CAA-CBA
52	b	402	HEM	C2B-C3B-CAB-CBB
53	d	301	HEC	C1A-C2A-CAA-CBA
53	d	301	HEC	C3A-C2A-CAA-CBA
52	o	401	HEM	CAD-CBD-CGD-O2D
52	b	402	HEM	CAA-CBA-CGA-O2A
52	o	401	HEM	CAD-CBD-CGD-O1D
57	x	603	HEA	CAD-CBD-CGD-O1D
52	o	402	HEM	CAA-CBA-CGA-O1A
52	b	401	HEM	CAD-CBD-CGD-O2D
53	d	301	HEC	CAA-CBA-CGA-O1A
53	p	301	HEC	CAA-CBA-CGA-O1A
52	b	401	HEM	CAD-CBD-CGD-O1D
52	b	402	HEM	CAA-CBA-CGA-O1A
57	x	604	HEA	CAD-CBD-CGD-O1D
53	p	301	HEC	C2A-CAA-CBA-CGA
53	d	301	HEC	CAA-CBA-CGA-O2A
52	b	402	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
57	x	604	HEA	CAD-CBD-CGD-O2D
52	o	402	HEM	CAA-CBA-CGA-O2A
53	p	301	HEC	CAA-CBA-CGA-O2A
57	x	603	HEA	CAA-CBA-CGA-O1A
52	o	401	HEM	CAA-CBA-CGA-O2A
52	o	402	HEM	CAD-CBD-CGD-O2D
57	x	603	HEA	CAD-CBD-CGD-O2D
52	b	402	HEM	CAD-CBD-CGD-O2D
52	o	402	HEM	CAD-CBD-CGD-O1D
52	b	401	HEM	CAA-CBA-CGA-O2A
52	o	401	HEM	CAA-CBA-CGA-O1A
52	b	402	HEM	C4B-C3B-CAB-CBB
57	x	604	HEA	CAA-CBA-CGA-O2A
52	b	401	HEM	CAA-CBA-CGA-O1A
57	x	604	HEA	CAA-CBA-CGA-O1A
57	x	603	HEA	CAA-CBA-CGA-O2A
53	p	301	HEC	CAD-CBD-CGD-O2D
57	x	604	HEA	C26-C15-C16-C17
57	x	603	HEA	O11-C11-C3B-C2B

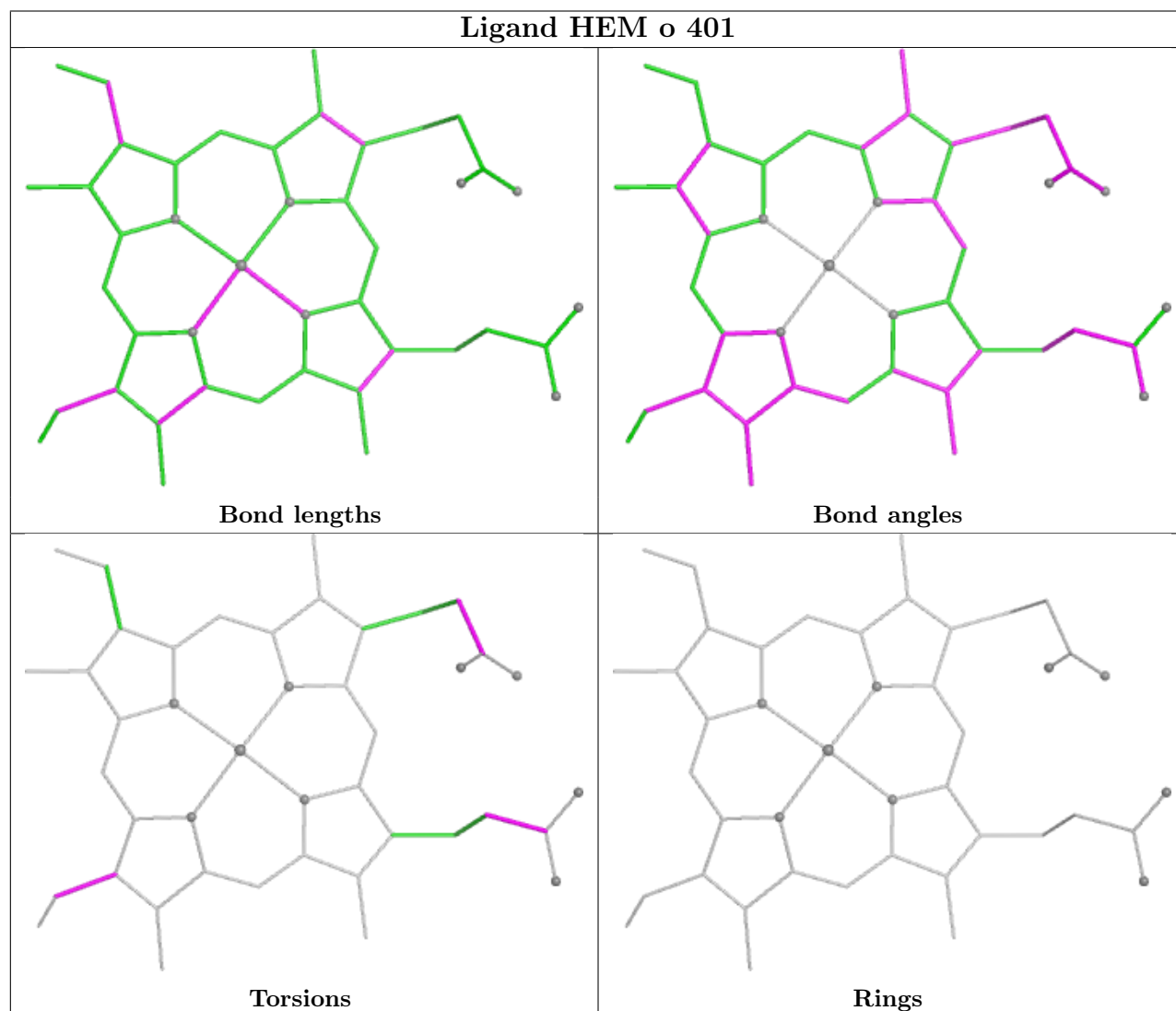
There are no ring outliers.

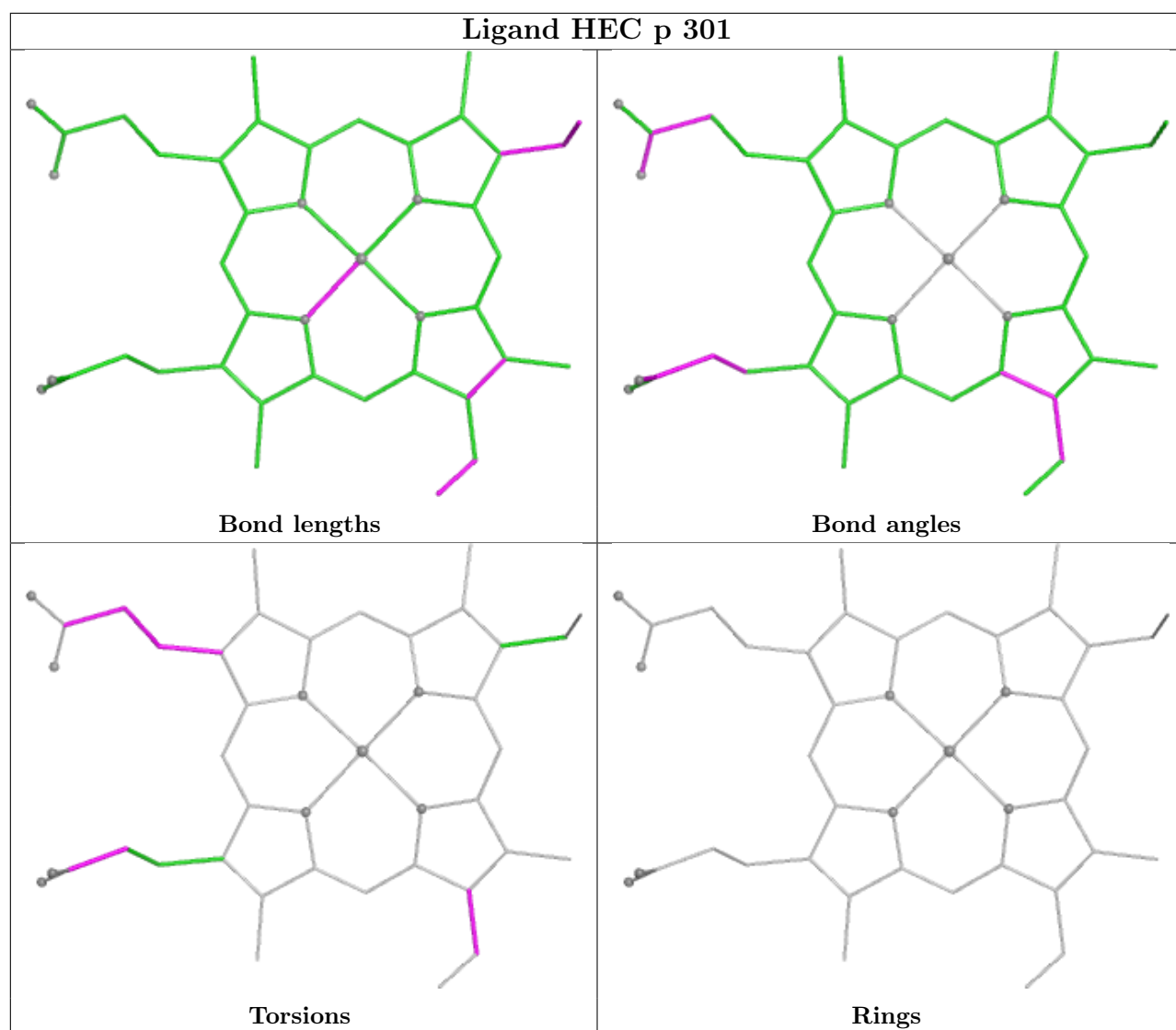
13 monomers are involved in 69 short contacts:

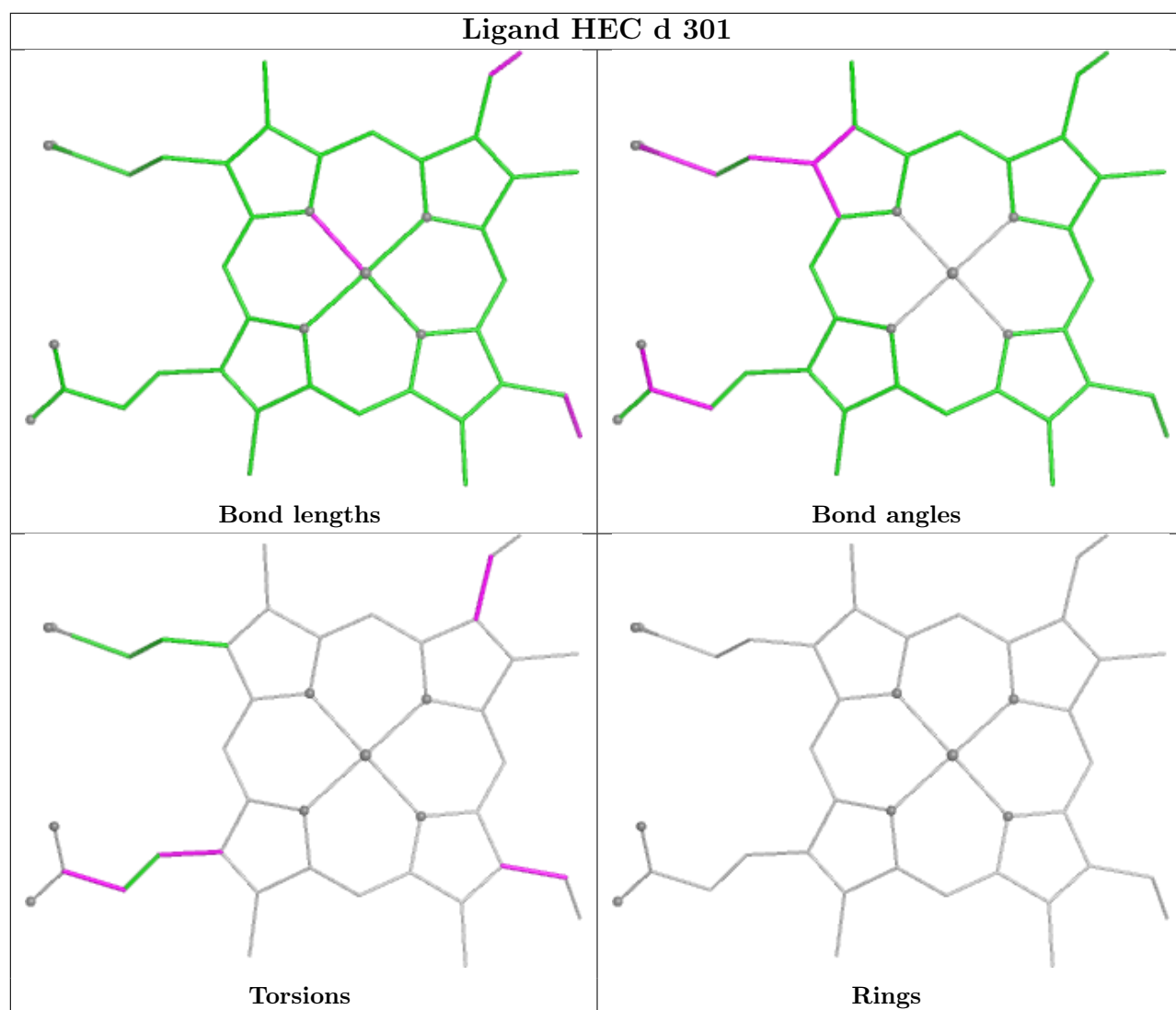
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	o	401	HEM	11	0
53	p	301	HEC	4	0
53	d	301	HEC	4	0
52	b	401	HEM	4	0
59	I	201	SF4	2	0
57	x	603	HEA	1	0
59	B	201	SF4	5	0
52	o	402	HEM	14	0
52	b	402	HEM	14	0
59	F	501	SF4	1	0
59	I	202	SF4	3	0
54	G	803	FES	3	0
57	x	604	HEA	3	0

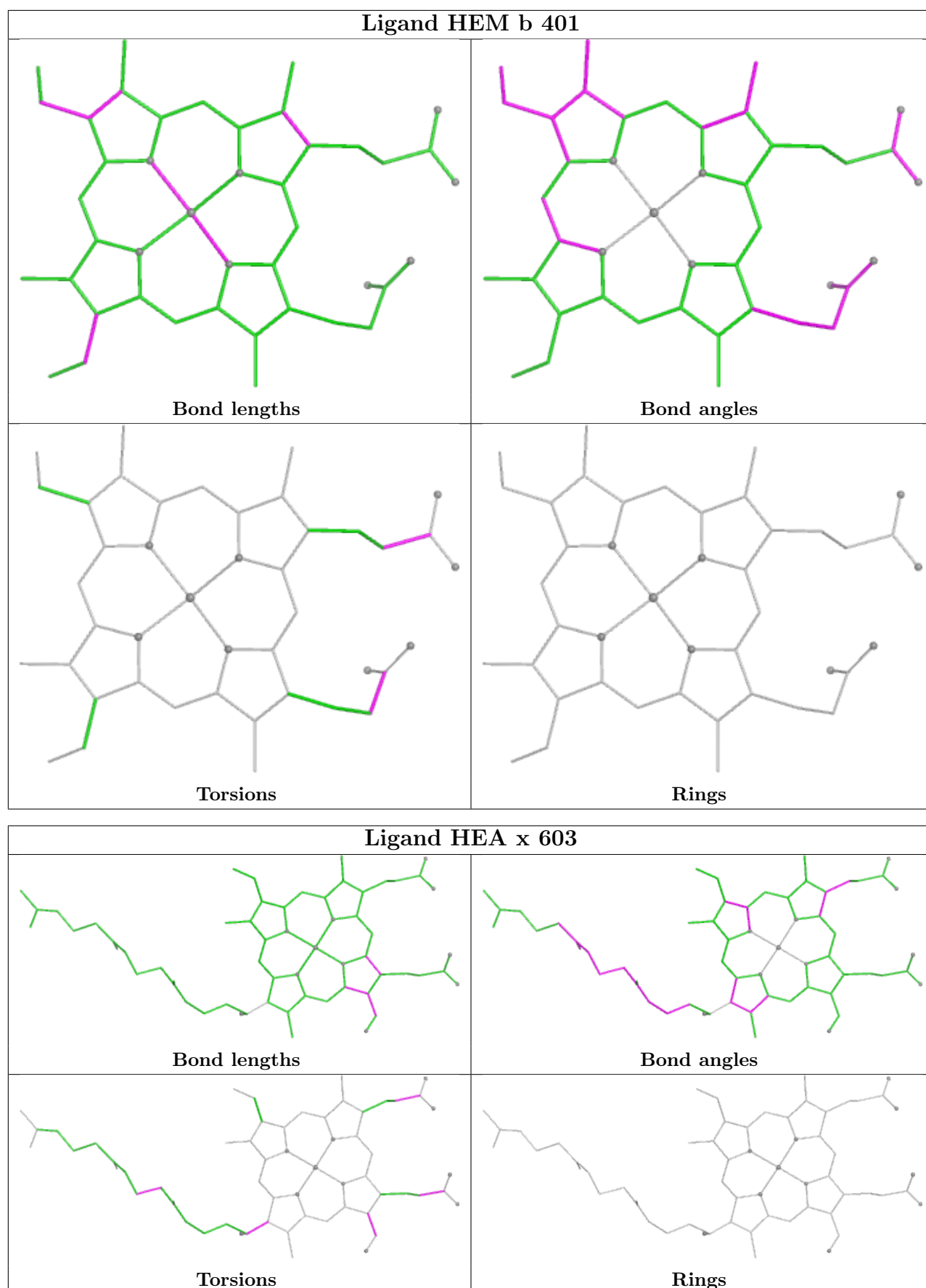
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

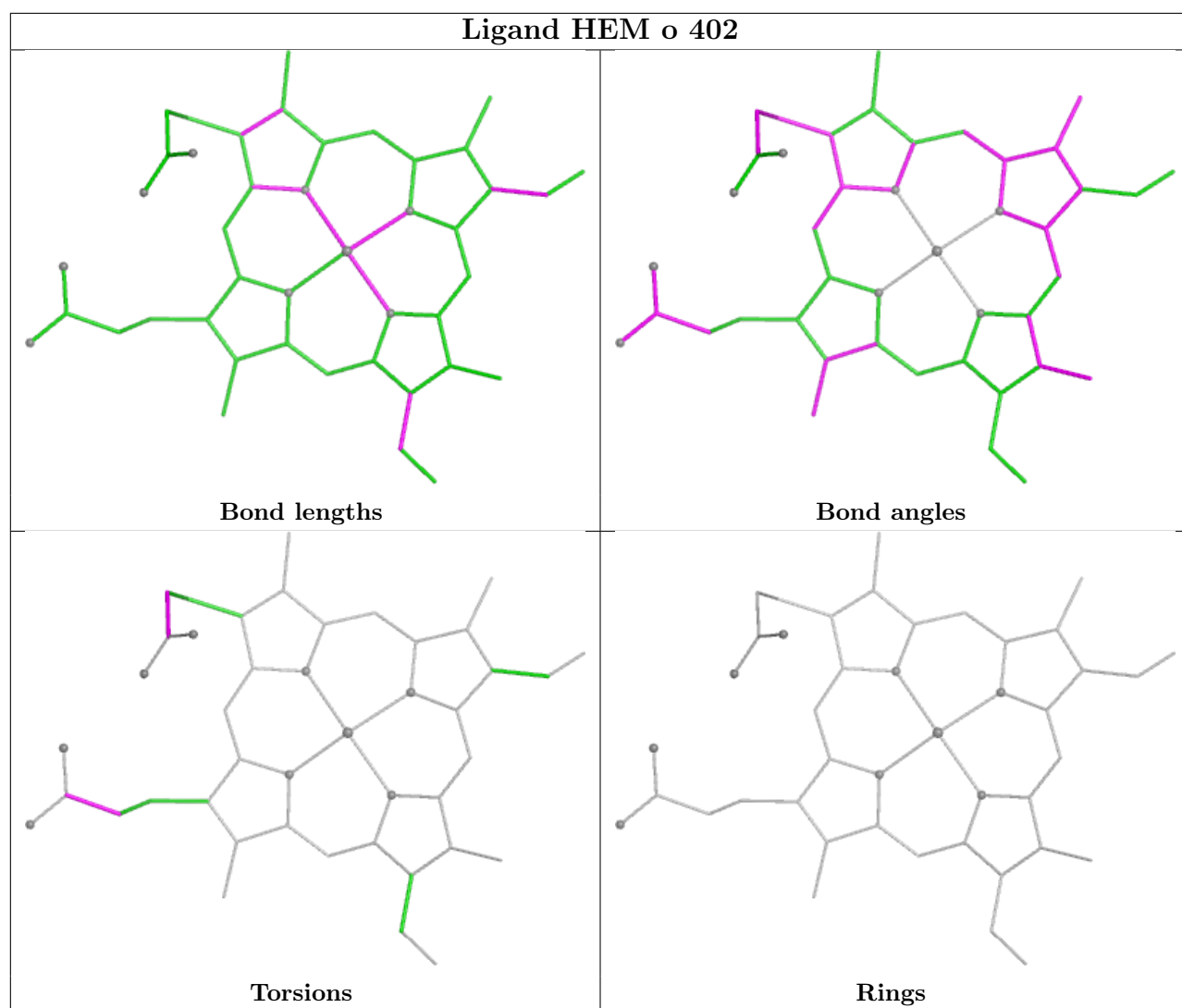
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

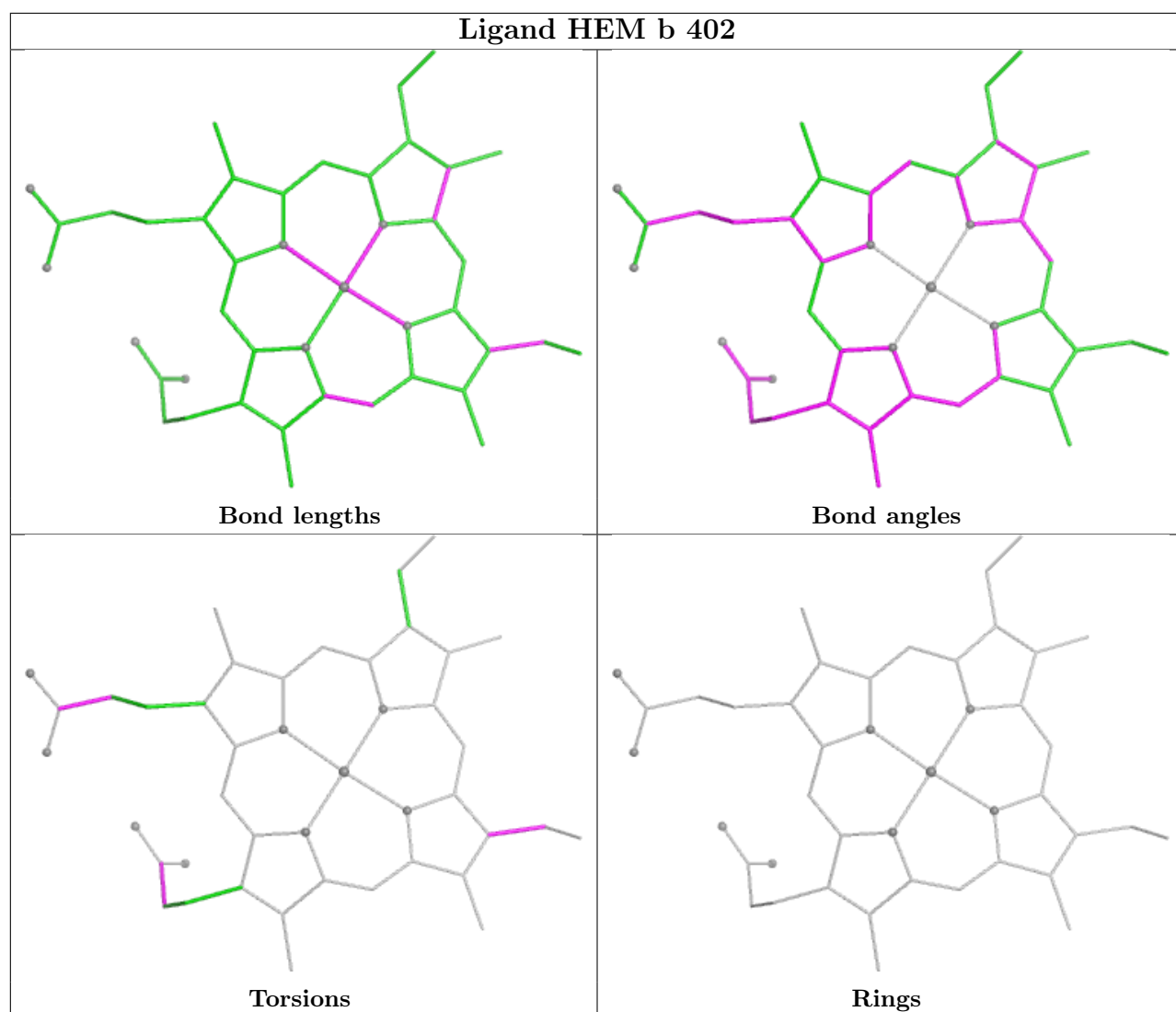


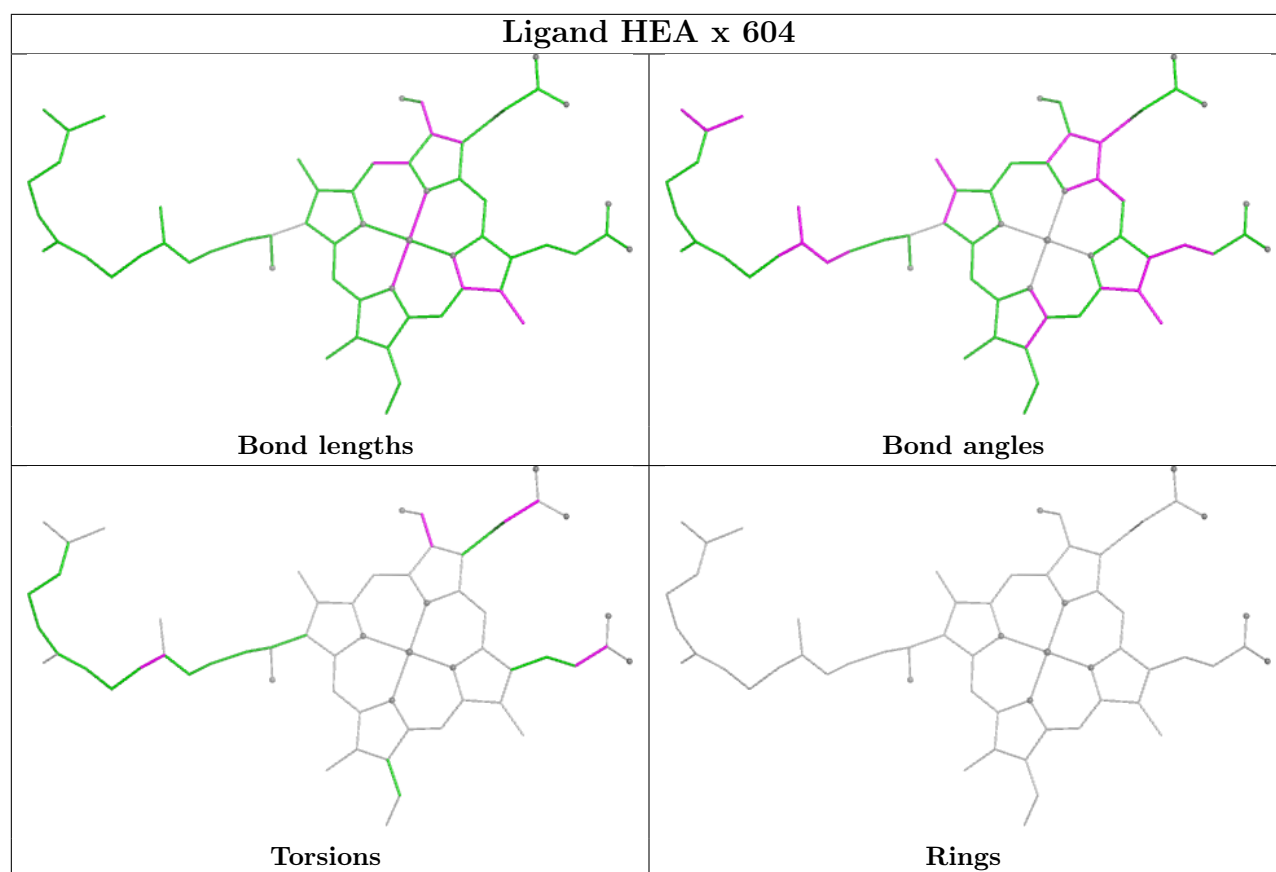












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
50	U	8
47	X	7
51	Z	6
31	G	6
36	L	5
39	O	3
34	J	2
40	P	2
32	H	2
44	T	2
49	a	1

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Mol	Chain	Number of breaks
25	A	1
38	N	1
37	M	1
41	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	226:UNK	C	301:UNK	N	71.67
1	X	113:UNK	C	133:UNK	N	66.39
1	U	27:UNK	C	101:UNK	N	63.89
1	a	29:UNK	C	101:UNK	N	61.67
1	U	630:UNK	C	701:UNK	N	57.60
1	Z	34:UNK	C	101:UNK	N	53.76
1	U	330:UNK	C	401:UNK	N	52.64
1	Z	124:UNK	C	201:UNK	N	45.23
1	U	530:UNK	C	601:UNK	N	42.27
1	A	23:UNK	C	52:UNK	N	39.81
1	X	615:UNK	C	701:UNK	N	36.95
1	U	220:UNK	C	301:UNK	N	35.63
1	Z	259:UNK	C	308:UNK	N	35.43
1	X	428:UNK	C	501:UNK	N	35.30
1	U	724:UNK	C	801:UNK	N	31.76
1	J	107:UNK	C	140:UNK	N	30.90
1	X	357:UNK	C	401:UNK	N	28.19
1	N	300:UNK	C	320:UNK	N	26.56
1	P	250:UNK	C	285:UNK	N	26.49
1	L	466:UNK	C	487:UNK	N	23.59
1	G	347:UNK	C	367:UNK	N	22.81
1	M	415:UNK	C	430:UNK	N	22.06
1	P	185:UNK	C	203:UNK	N	21.21
1	H	200:UNK	C	219:UNK	N	20.56
1	Z	421:UNK	C	501:UNK	N	20.30
1	J	76:UNK	C	85:UNK	N	19.66
1	Z	528:UNK	C	601:UNK	N	19.36
1	Z	382:UNK	C	401:UNK	N	19.30
1	H	242:UNK	C	253:UNK	N	18.95
1	U	139:UNK	C	201:UNK	N	18.89
1	G	495:UNK	C	525:UNK	N	18.00
1	L	513:UNK	C	520:UNK	N	17.41
1	G	530:UNK	C	542:UNK	N	16.15
1	U	422:UNK	C	501:UNK	N	15.81
1	L	400:UNK	C	408:UNK	N	14.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	59:UNK	C	76:UNK	N	13.52
1	O	54:UNK	C	79:UNK	N	12.62
1	G	318:UNK	C	326:UNK	N	12.59
1	L	22:UNK	C	28:UNK	N	11.17
1	O	167:UNK	C	172:UNK	N	11.07
1	X	197:UNK	C	201:UNK	N	10.95
1	O	210:UNK	C	222:UNK	N	10.93
1	T	23:UNK	C	28:UNK	N	9.73
1	L	358:UNK	C	363:UNK	N	8.92
1	G	410:UNK	C	425:UNK	N	7.46
1	G	400:UNK	C	404:UNK	N	6.25
1	X	527:UNK	C	601:UNK	N	5.18
1	T	8:UNK	C	9:UNK	N	1.65

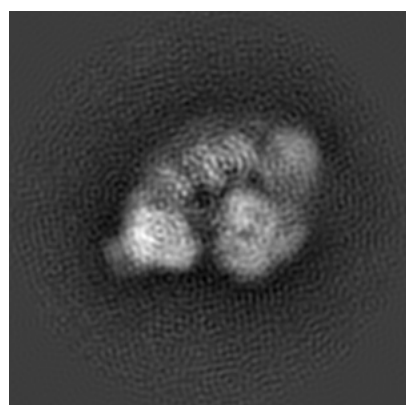
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4107. These allow visual inspection of the internal detail of the map and identification of artifacts.

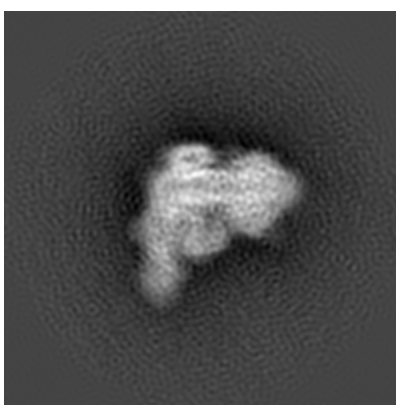
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

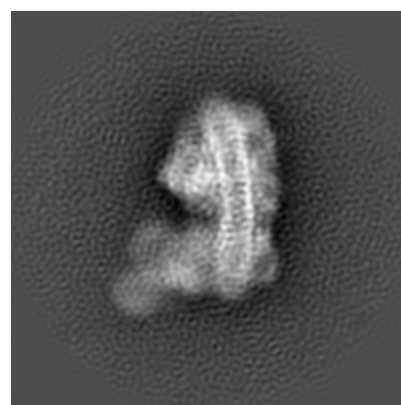
6.1.1 Primary map



X



Y

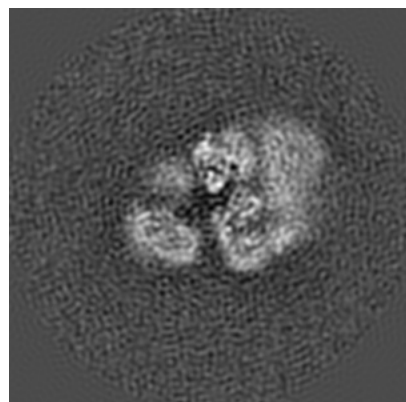


Z

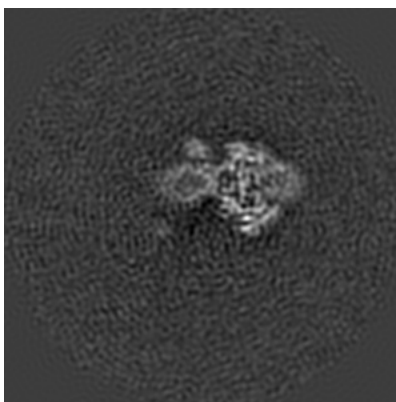
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

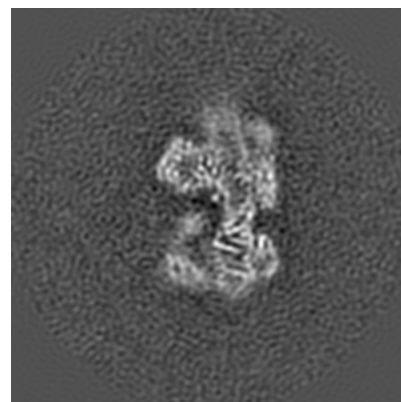
6.2.1 Primary map



X Index: 144



Y Index: 144

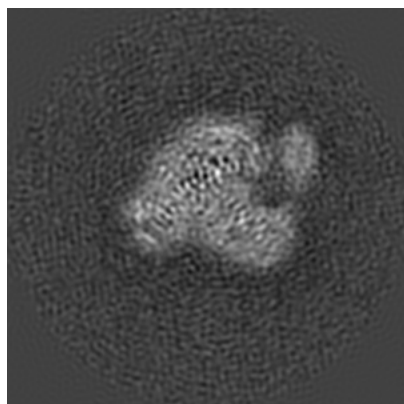


Z Index: 144

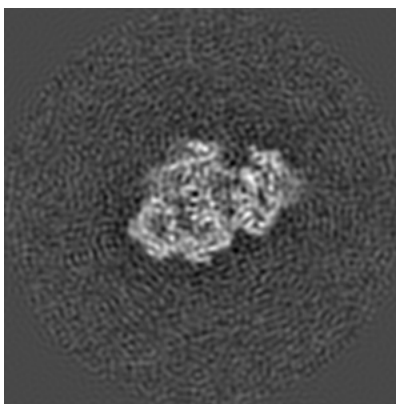
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

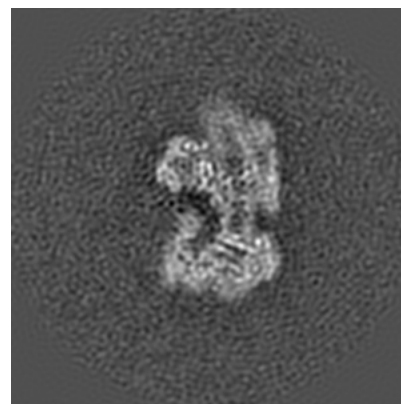
6.3.1 Primary map



X Index: 170



Y Index: 166

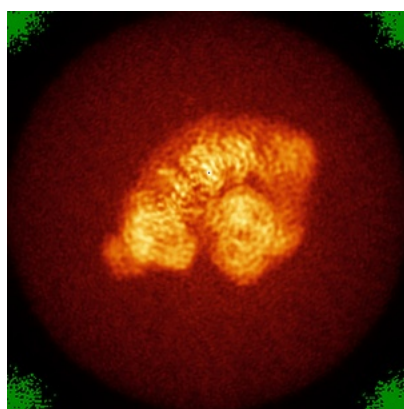


Z Index: 139

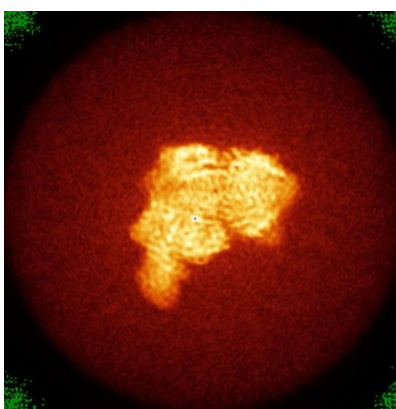
The images above show the largest variance slices of the map in three orthogonal directions.

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

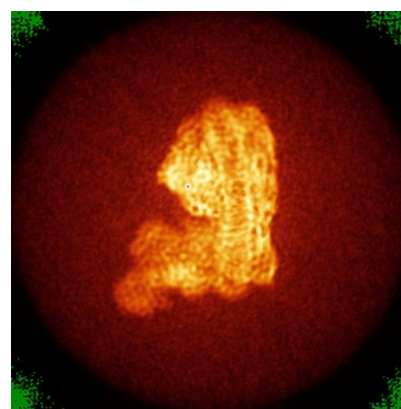
6.4.1 Primary map



X



Y

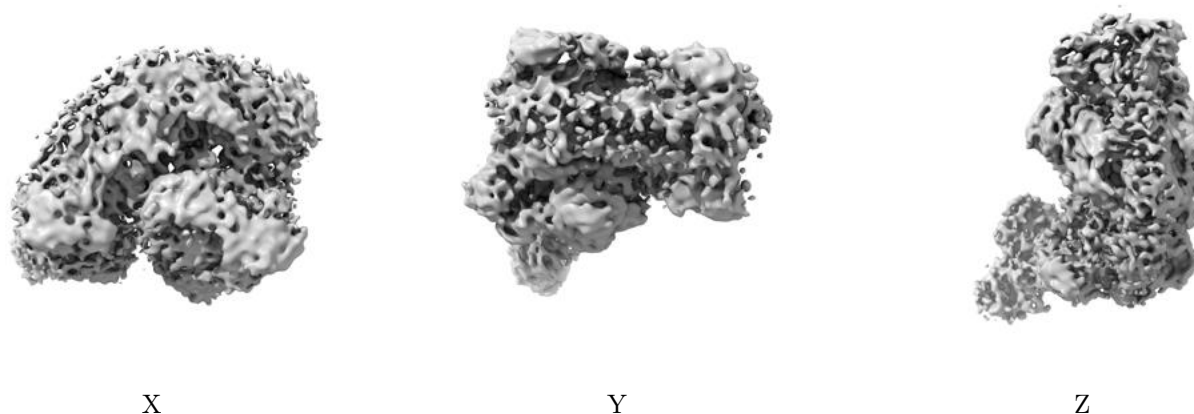


Z

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

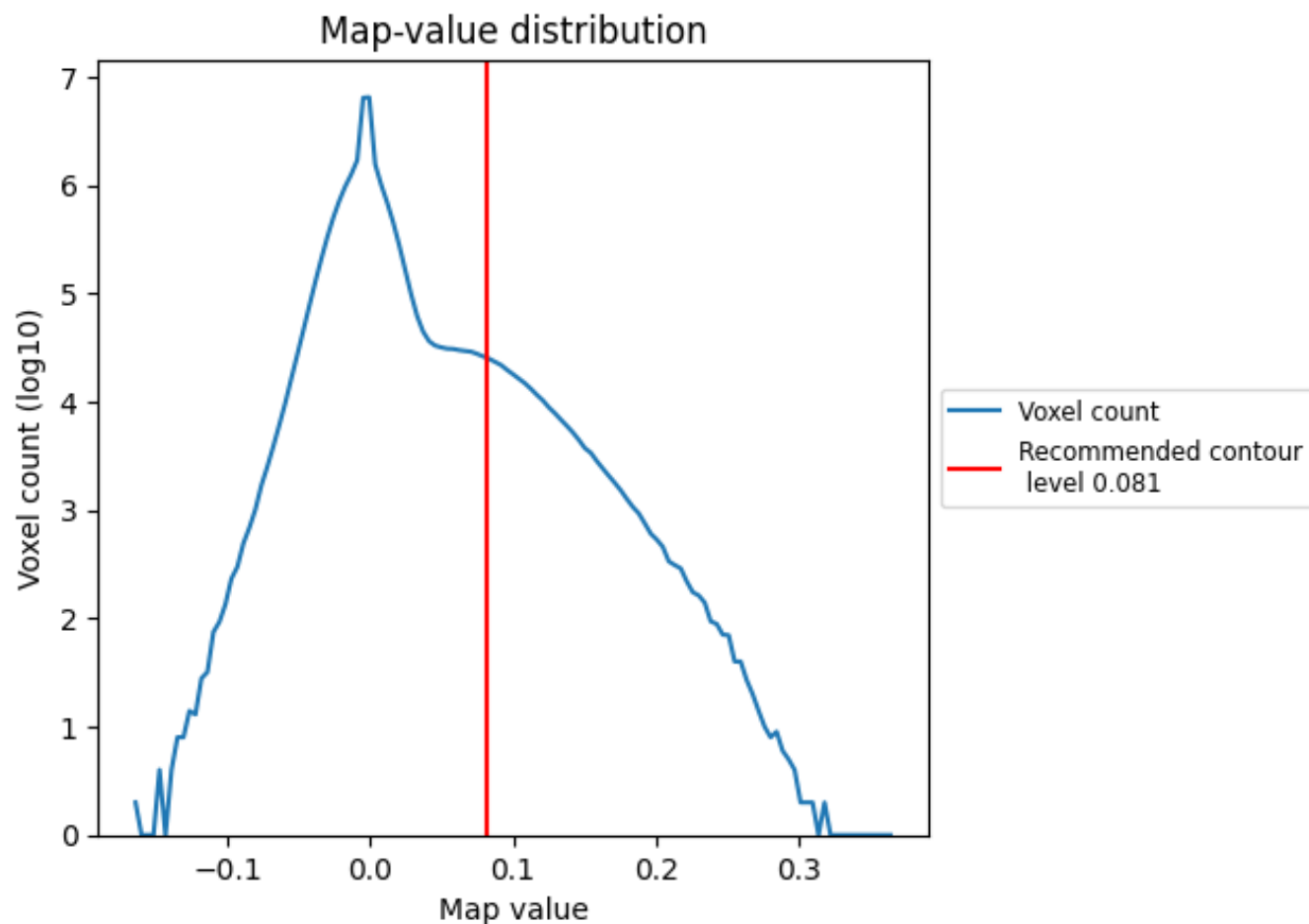
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

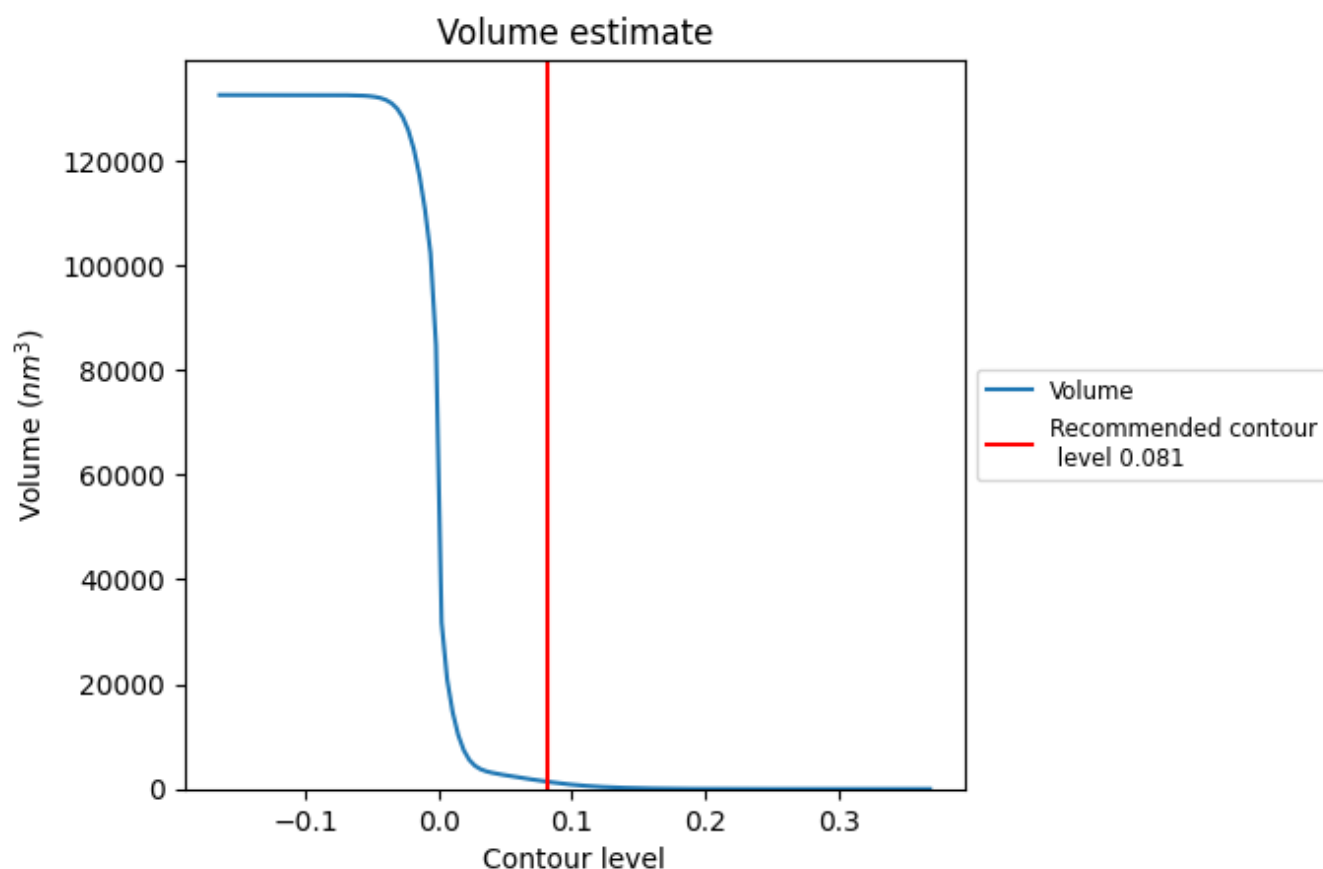
This section contains the results of statistical analysis of the map.

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.

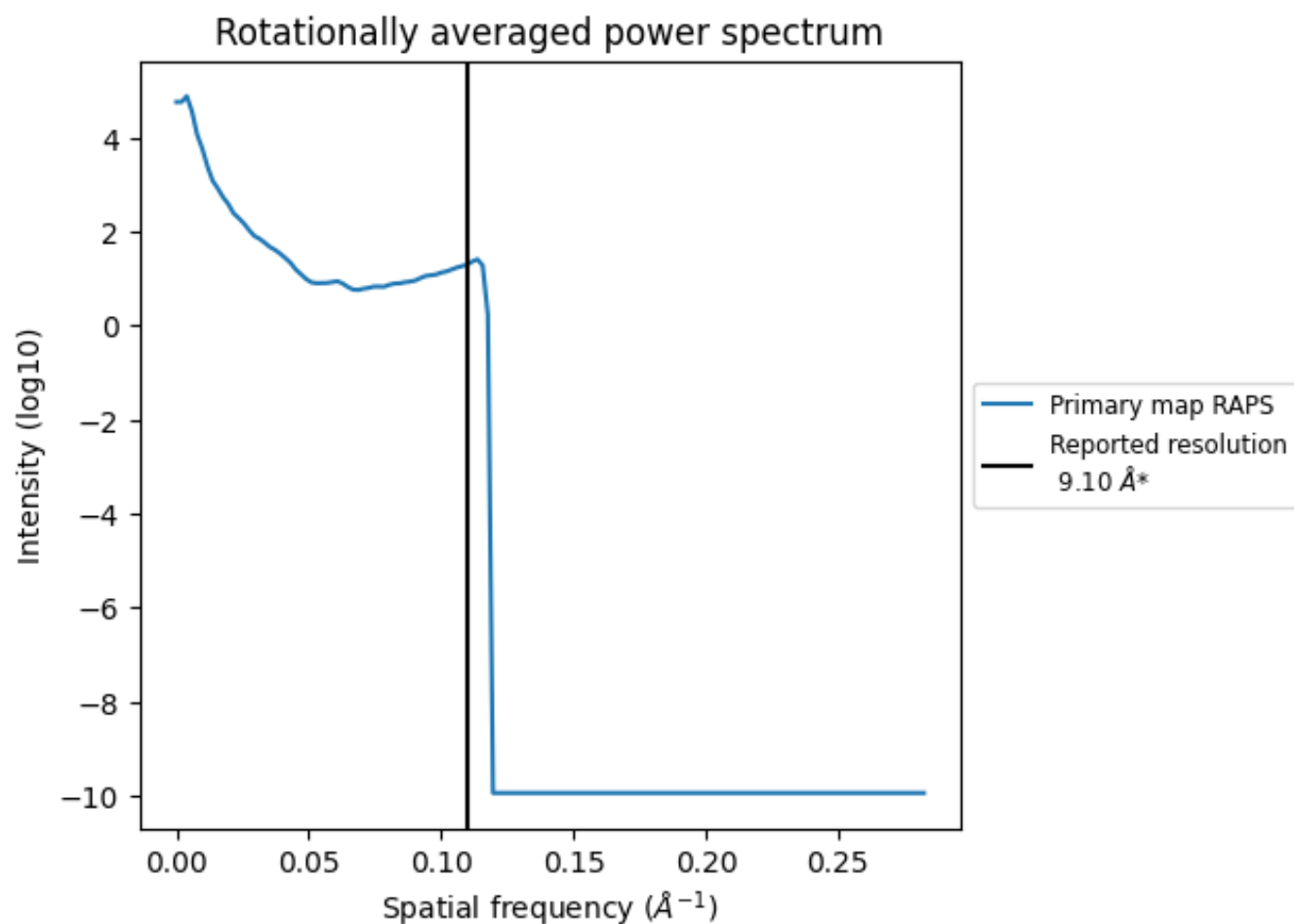
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1405 nm^3 ; this corresponds to an approximate mass of 1269 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 0.110 Å⁻¹

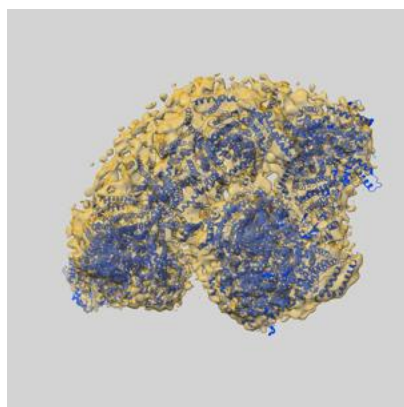
8 Fourier-Shell correlation

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

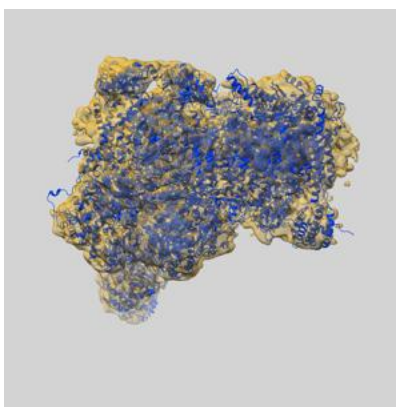
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4107 and PDB model 5LUF. Per-residue inclusion information can be found in section 3 on page 18.

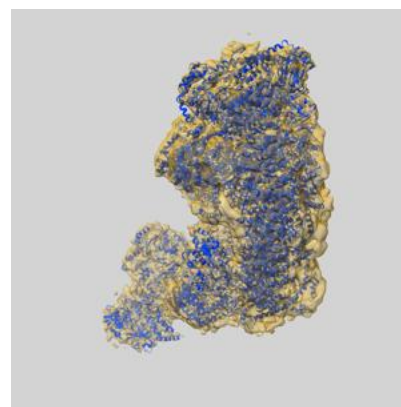
9.1 Map-model overlay [i](#)



X



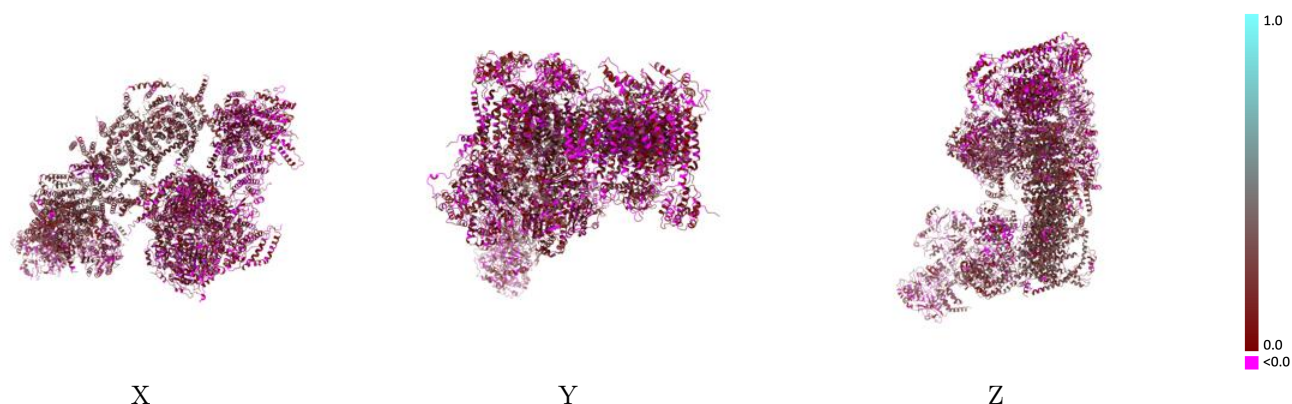
Y



Z

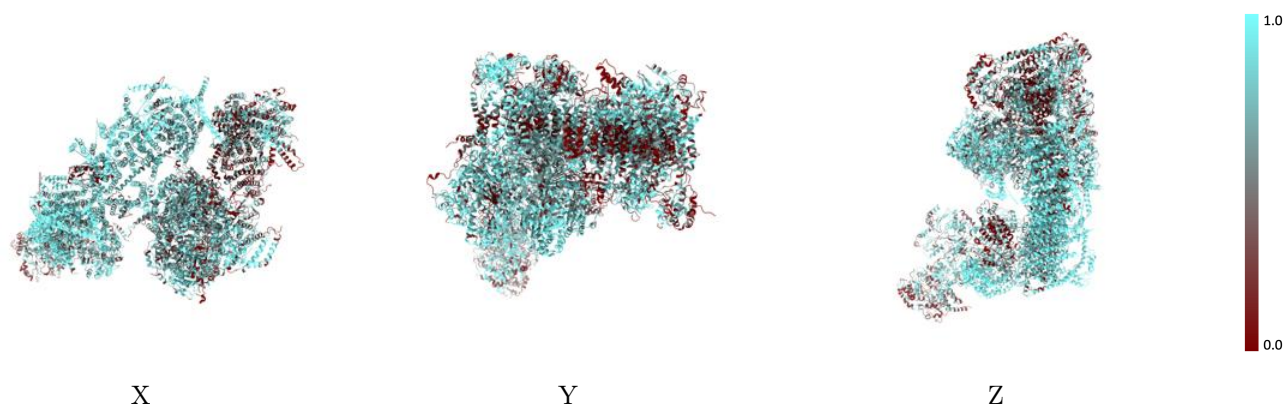
The images above show the 3D surface view of the map at the recommended contour level 0.081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



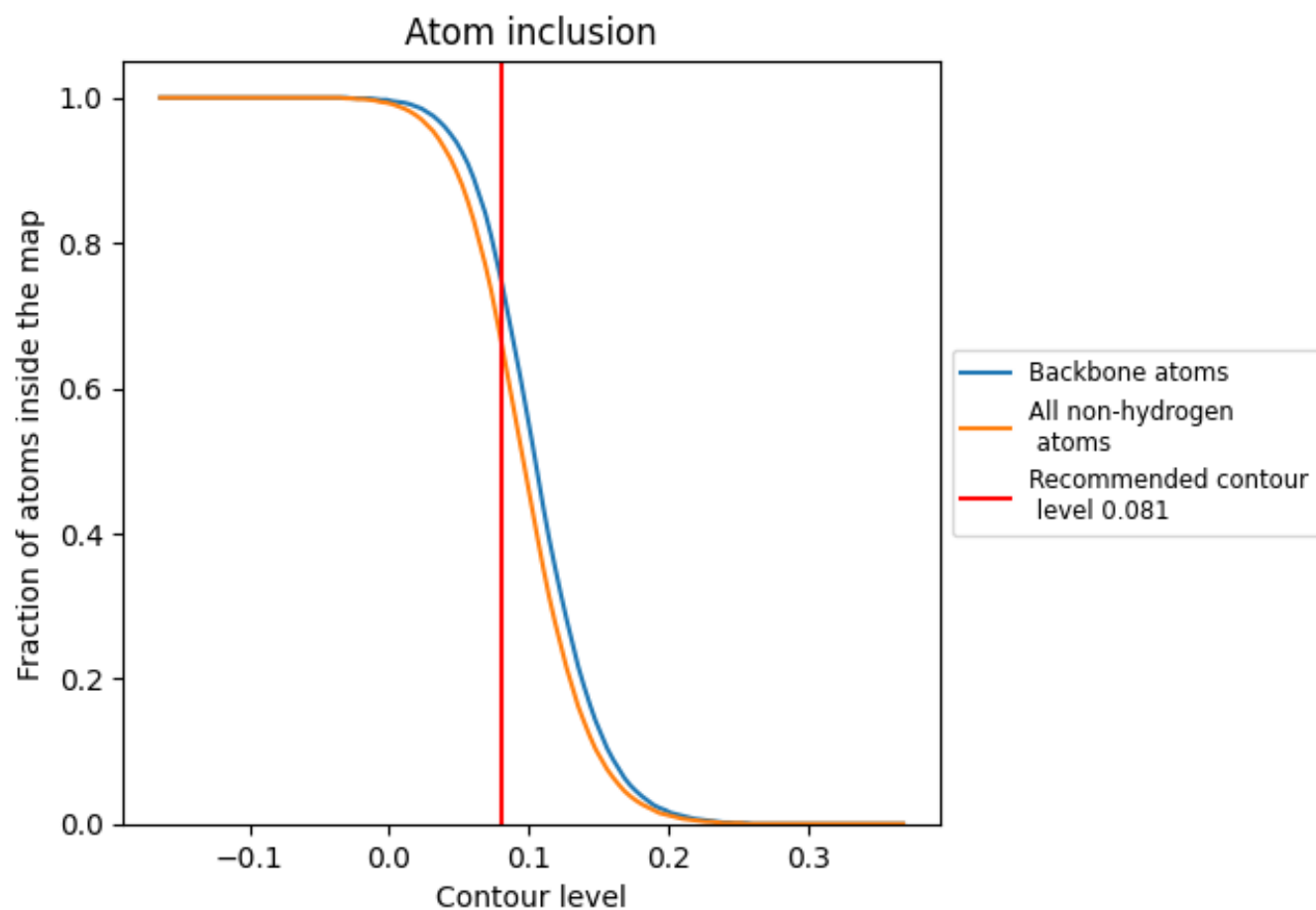
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.081).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.1160
0	 0.5210	 0.1040
1	 0.4150	 0.0580
2	 0.4350	 0.0580
3	 0.4020	 0.0310
4	 0.2190	 -0.0020
5	 0.2610	 0.0540
6	 0.4550	 0.0650
7	 0.2790	 0.0510
8	 0.5330	 0.0780
9	 0.5000	 0.0550
A	 0.8100	 0.2640
B	 0.8170	 0.1760
C	 0.8440	 0.1700
D	 0.8540	 0.1700
E	 0.5040	 0.0580
F	 0.4690	 0.0870
G	 0.7290	 0.1010
H	 0.7990	 0.2150
I	 0.8670	 0.1290
J	 0.7830	 0.2180
K	 0.8570	 0.2430
L	 0.7950	 0.2180
M	 0.8390	 0.2470
N	 0.8620	 0.2510
O	 0.1380	 0.0250
P	 0.7630	 0.1270
Q	 0.5390	 0.1060
R	 0.3150	 0.0480
S	 0.6200	 0.1160
T	 0.5580	 0.1320
U	 0.8300	 0.2110
V	 0.9630	 0.2470
W	 0.7810	 0.1910
X	 0.9630	 0.2400



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Chain	Atom inclusion	Q-score
Y	 0.8400	 0.2070
Z	 0.9310	 0.2490
a	 0.8060	 0.2040
b	 0.6240	 0.1050
c	 0.7550	 0.0740
d	 0.7180	 0.0810
e	 0.3200	 0.0120
f	 0.7370	 0.1280
g	 0.5550	 0.0720
h	 0.7500	 0.0750
i	 0.0290	 -0.0600
j	 0.3780	 0.0430
k	 0.4450	 0.1510
l	 0.7210	 0.1030
m	 0.7670	 0.1000
n	 0.8220	 0.1160
o	 0.5950	 0.1030
p	 0.6710	 0.0830
q	 0.3810	 0.0600
r	 0.6440	 0.1280
s	 0.5880	 0.0990
t	 0.6740	 0.0770
u	 0.0550	 -0.0640
v	 0.4060	 0.0980
w	 0.3030	 0.0900
x	 0.5070	 0.0580
y	 0.6130	 0.0520
z	 0.4050	 0.0220