



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:05 AM JST

PDB ID : 5XTD / pdb_00005xtd
EMDB ID : EMD-6773
Title : Cryo-EM structure of human respiratory complex I
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

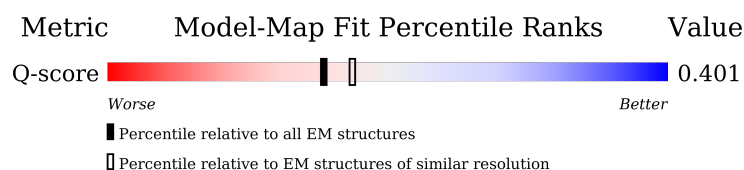
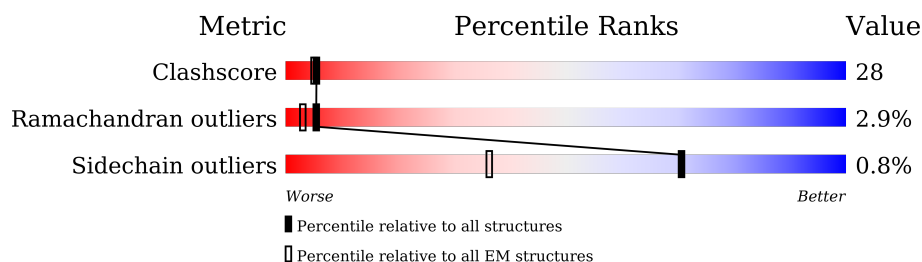
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	113	

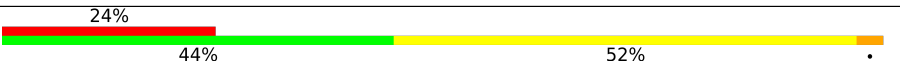
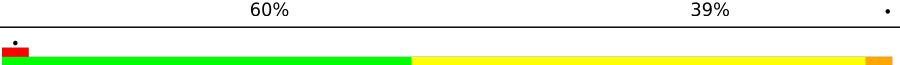
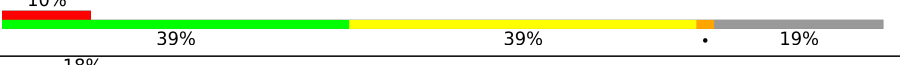
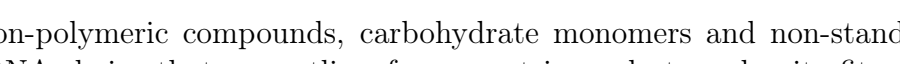
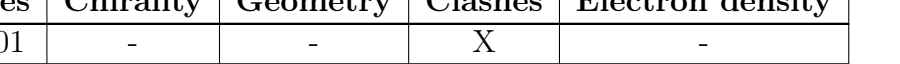
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Mol	Chain	Length	Quality of chain
5	F	83	
6	G	85	
6	X	85	
7	H	112	
8	I	110	
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	128	
26	c	153	
27	d	171	
28	e	97	

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Mol	Chain	Length	Quality of chain
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	137	
44	w	320	

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
45	SF4	A	501	-	-	X	-
45	SF4	B	302	-	-	X	-
45	SF4	M	801	-	-	X	-
46	FMN	A	502	-	-	X	-
47	PLX	b	201	-	-	X	-
49	NDP	J	401	-	-	X	-
50	FES	O	301	-	-	X	-
52	PEE	V	202	-	-	X	-
52	PEE	l	701	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 66789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

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

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

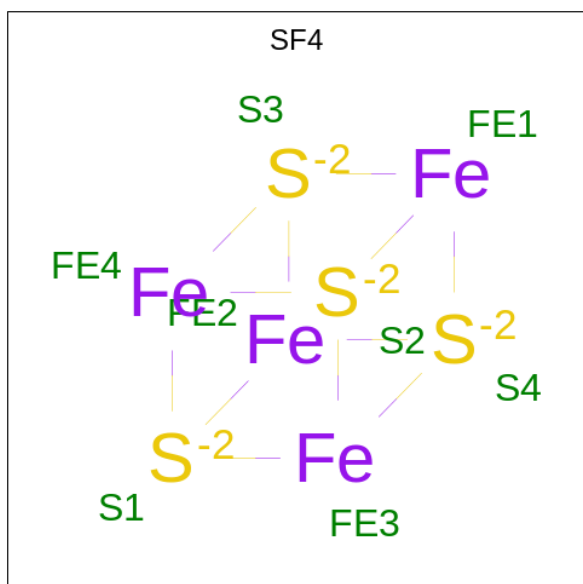
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

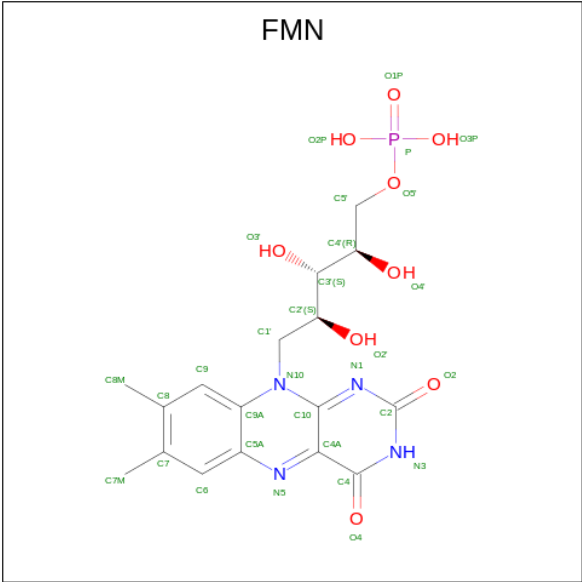
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



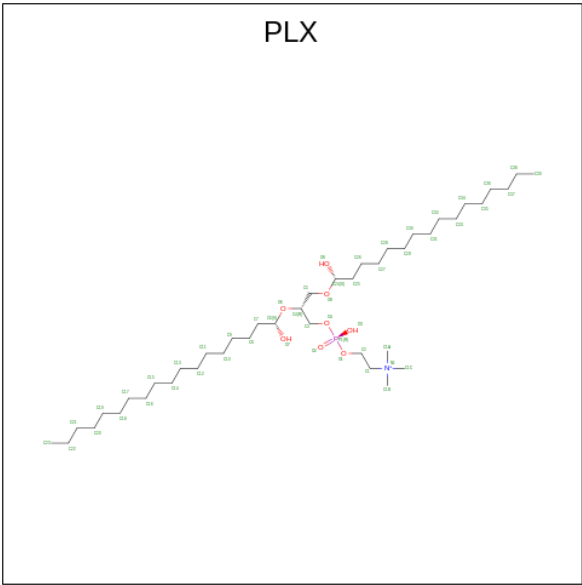
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 47 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



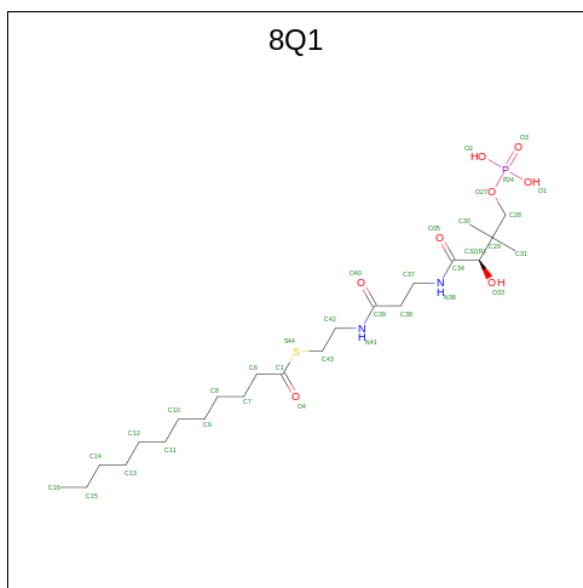
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	U	1	Total	C	N	O	P	0
			52	42	1	8	1	

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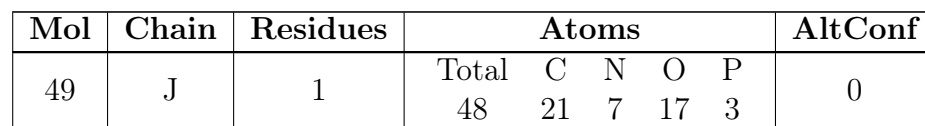
Mol	Chain	Residues	Atoms					AltConf
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

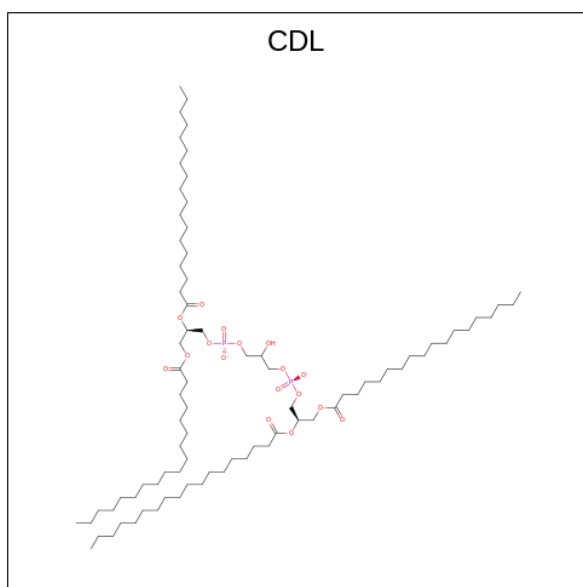
- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



- FES
-
- S1 S⁻² Fe FE2
- Fe S⁻² S2
- FE1

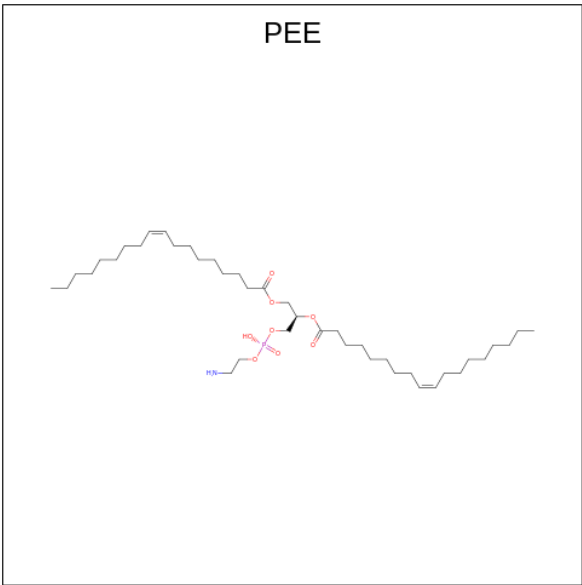
Mol	Chain	Residues	Atoms			AltConf
50	M	1	Total 4	Fe 2	S 2	0
50	O	1	Total 4	Fe 2	S 2	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			63	44	17	2	
51	i	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	l	1	Total	C	O	P	0
			64	45	17	2	
51	n	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 52 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

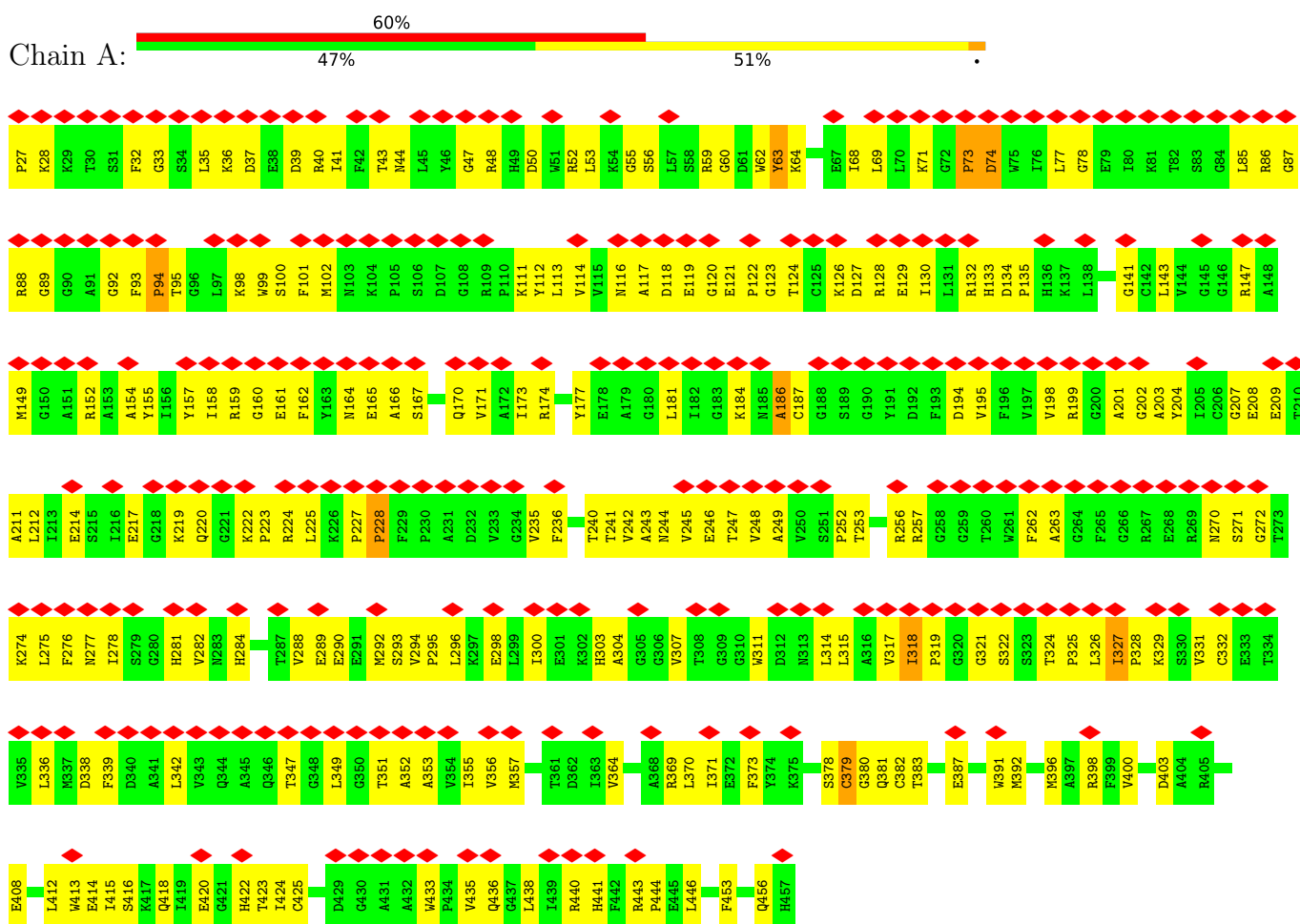


Mol	Chain	Residues	Atoms					AltConf
52	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	1	1	Total	C	N	O	P	0
			51	41	1	8	1	

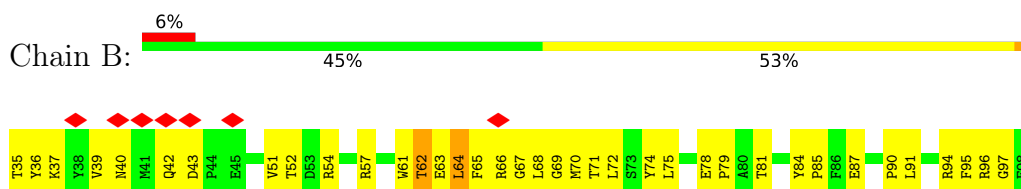
3 Residue-property plots

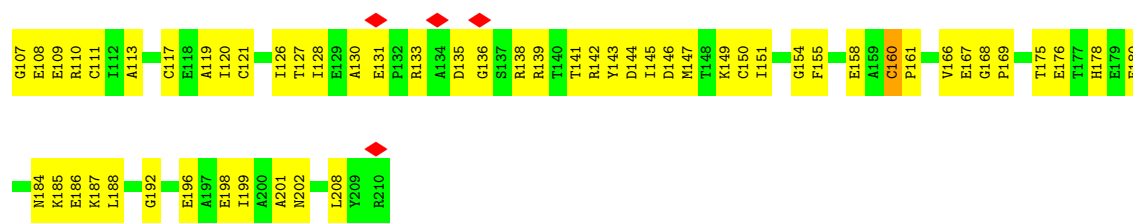
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

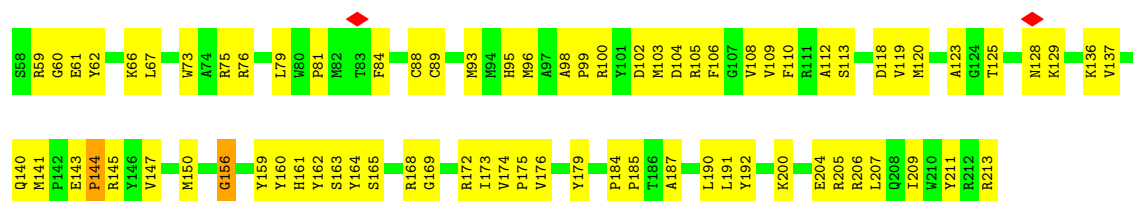


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

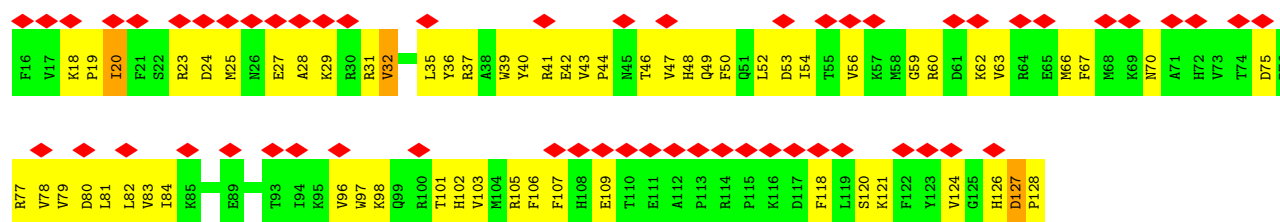




- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial





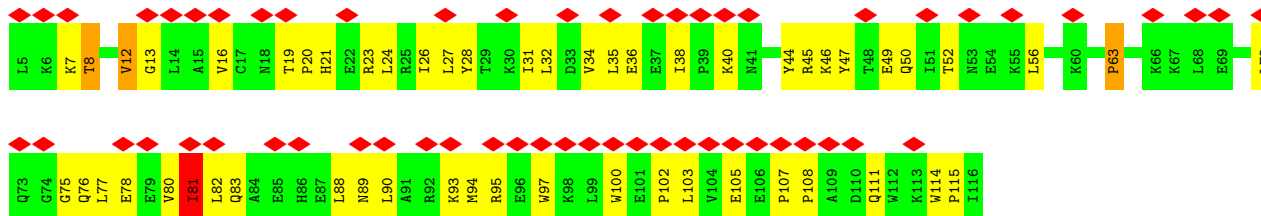
- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 53% 44%



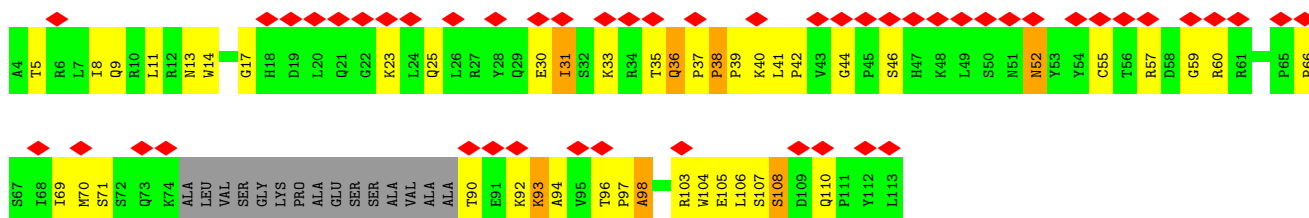
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 51% 52% 45%



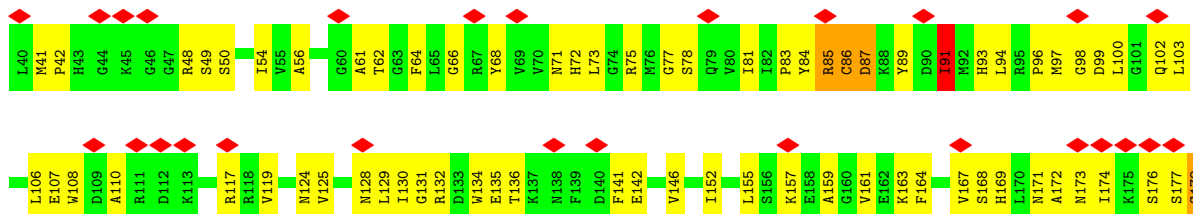
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

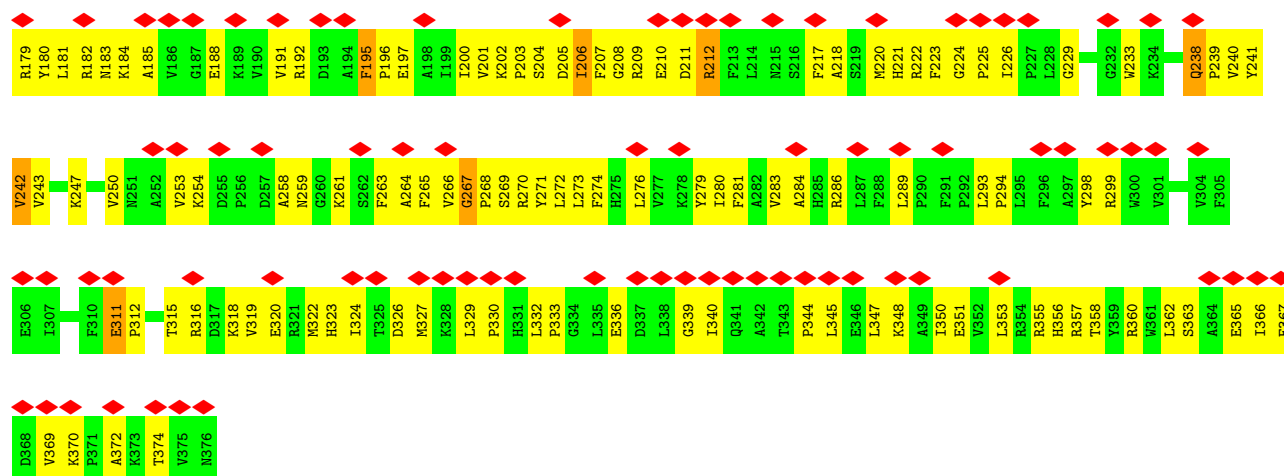
Chain I: 45% 45% 35% 6% 14%



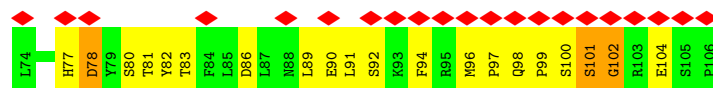
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J: 32% 45% 51%

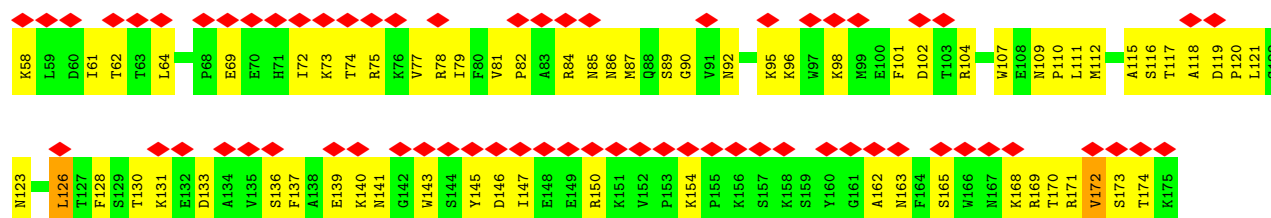




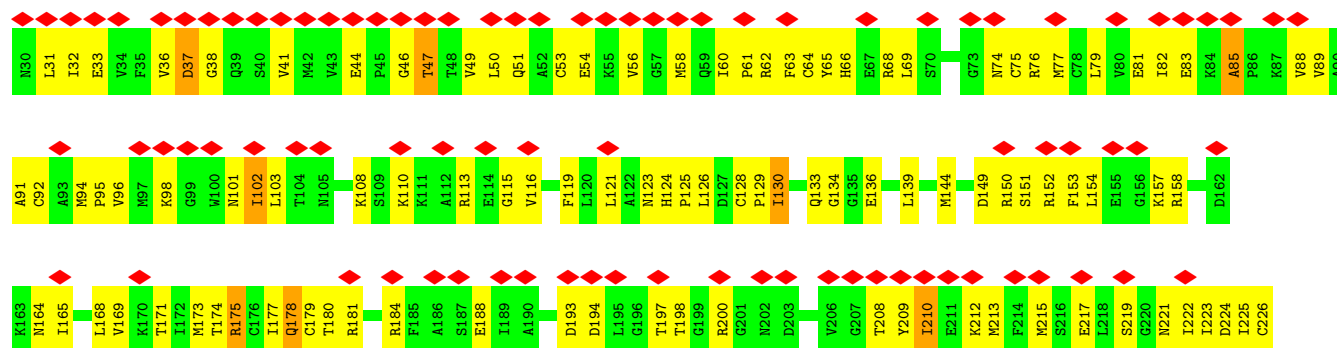
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

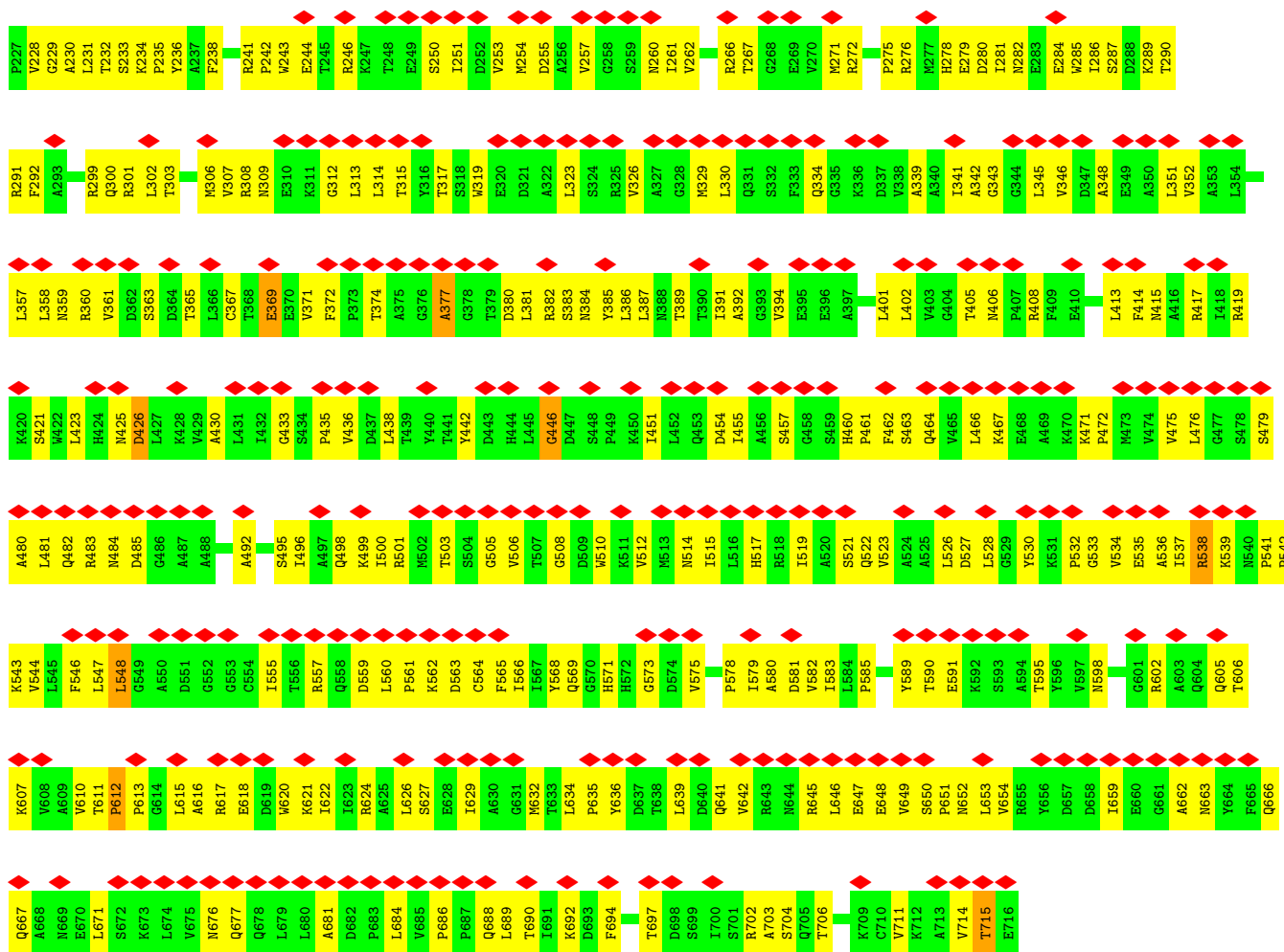


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

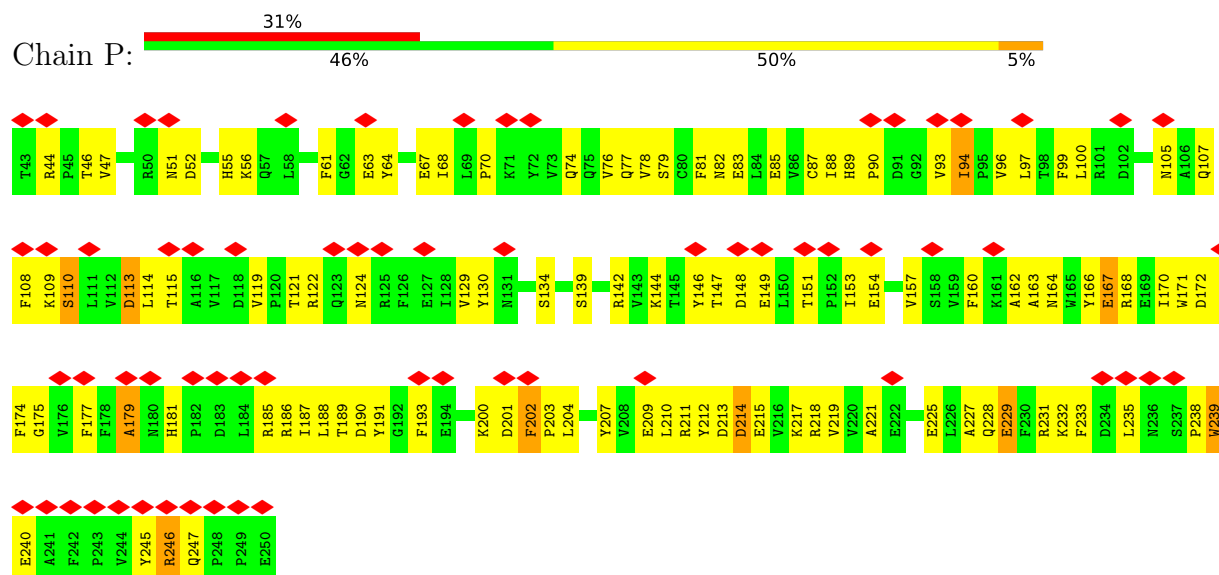


• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

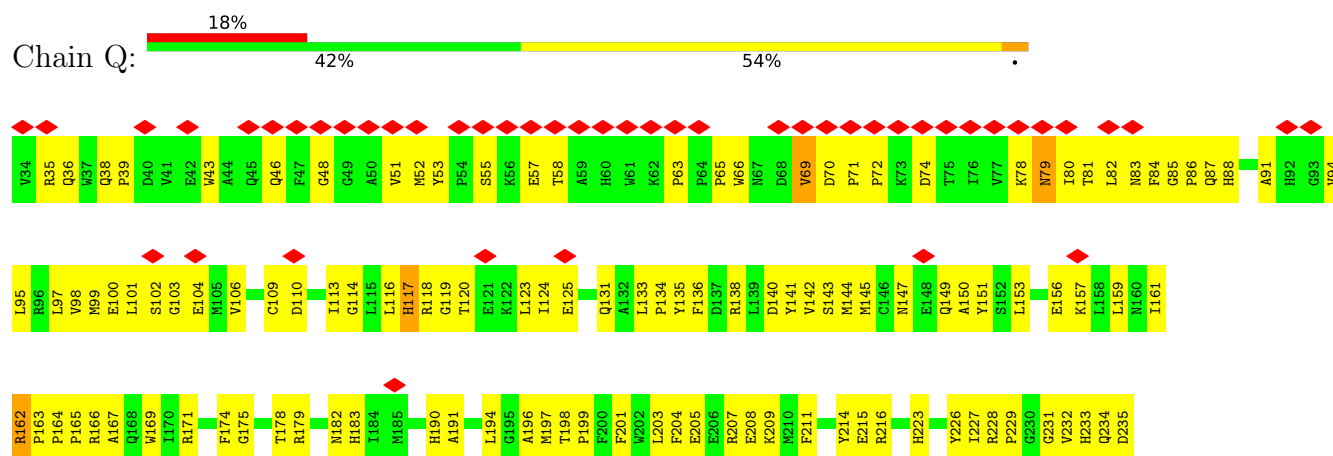


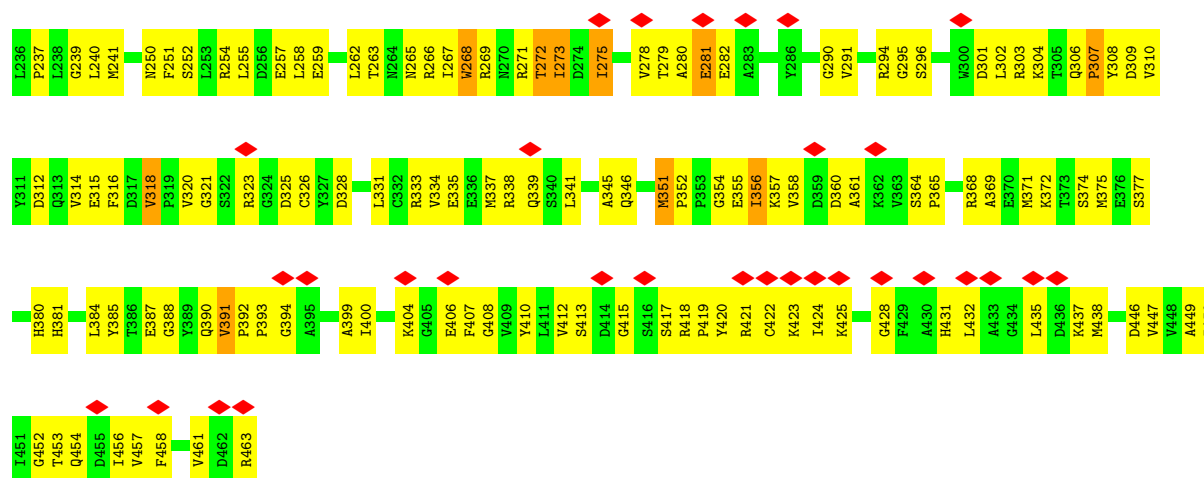


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

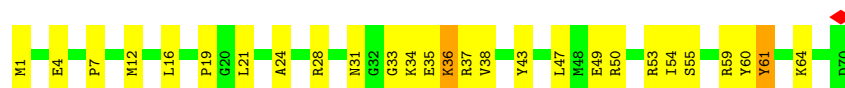


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

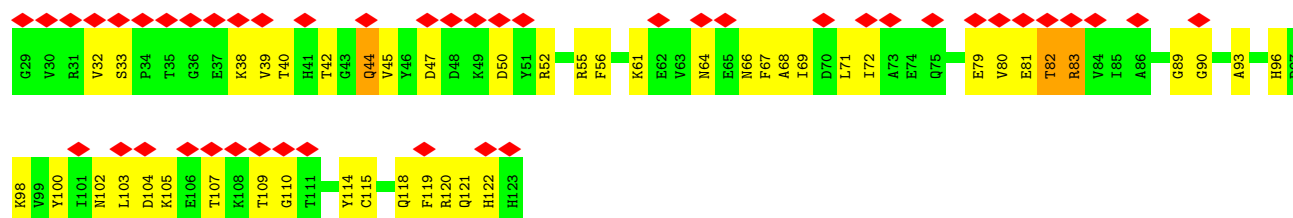




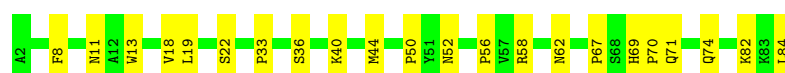
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



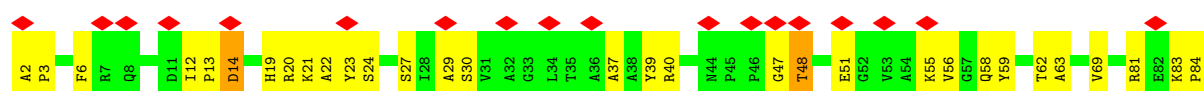
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

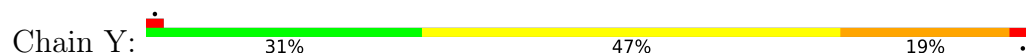




- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



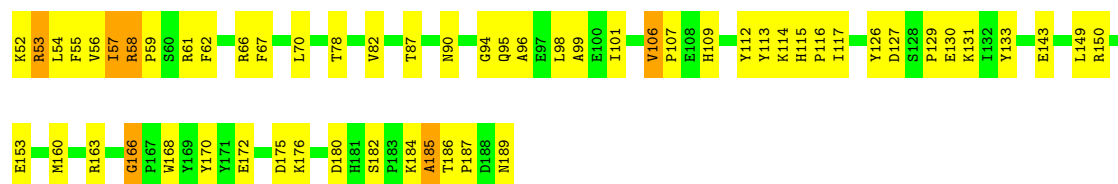
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



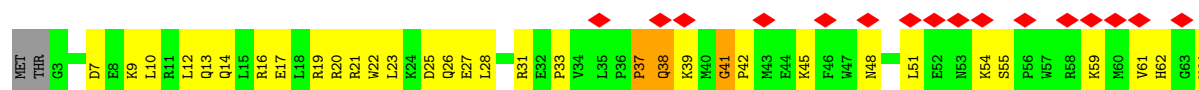
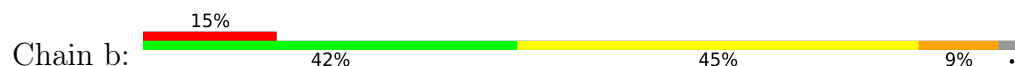
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

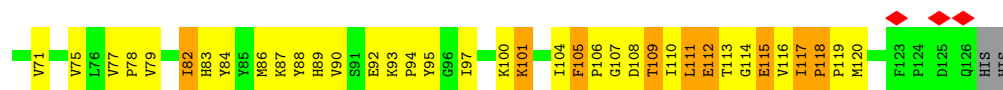


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

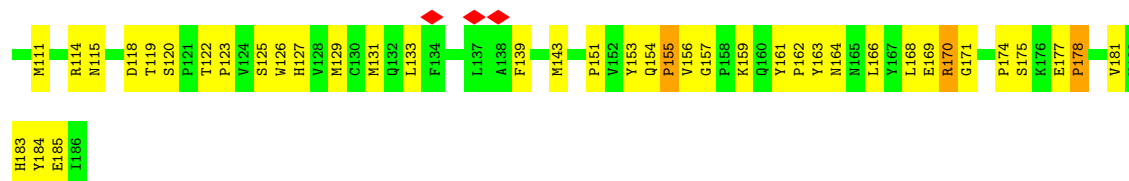
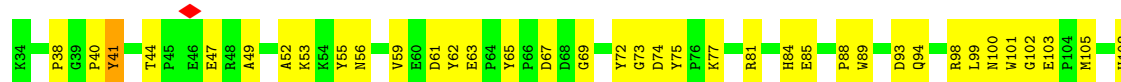


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6





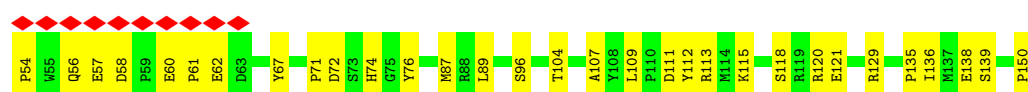
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



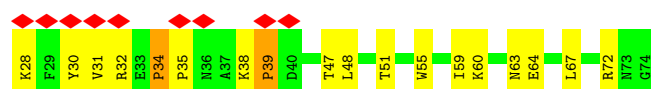
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

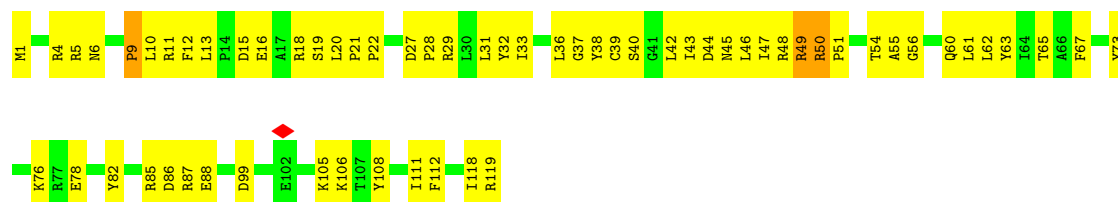


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

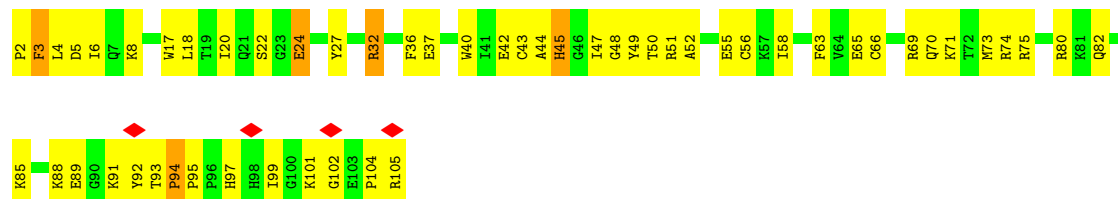


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

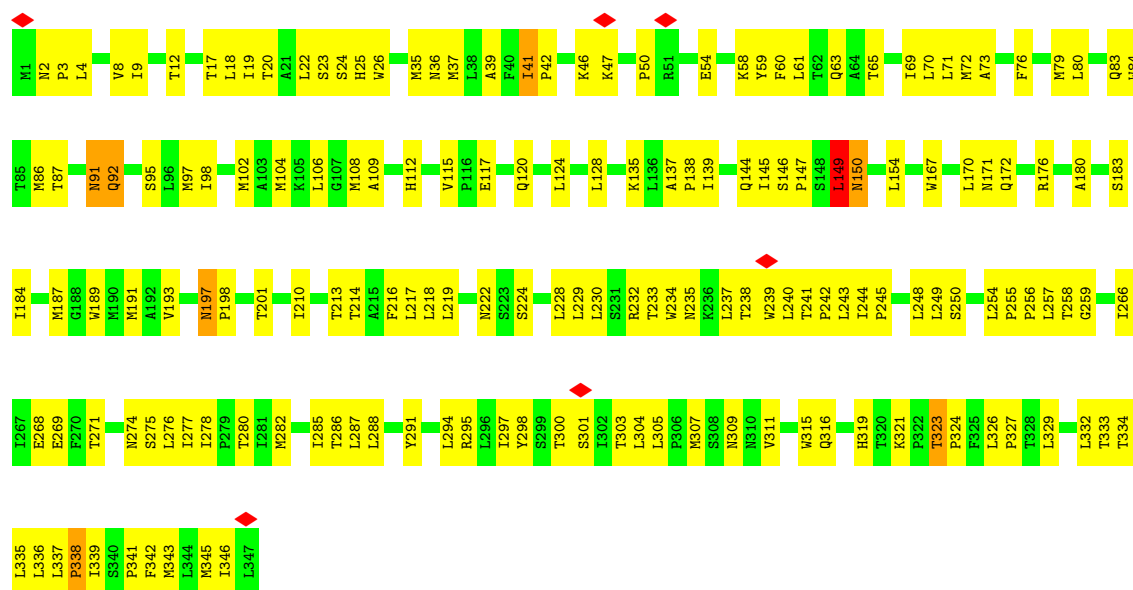




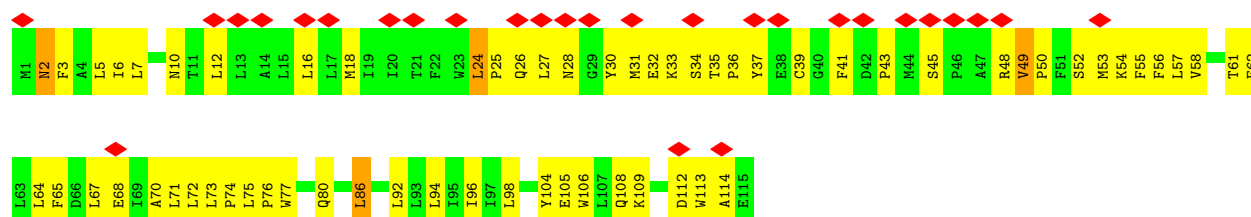
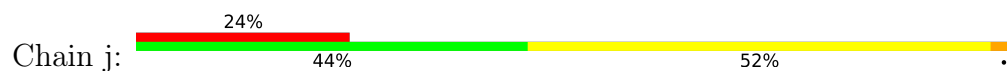
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



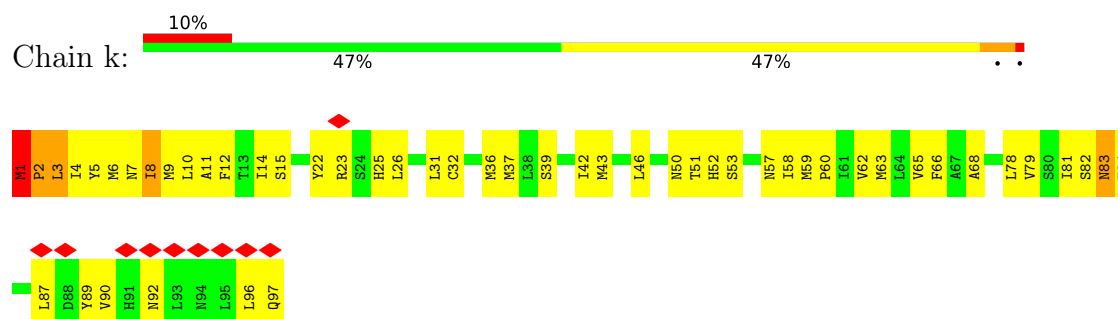
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2



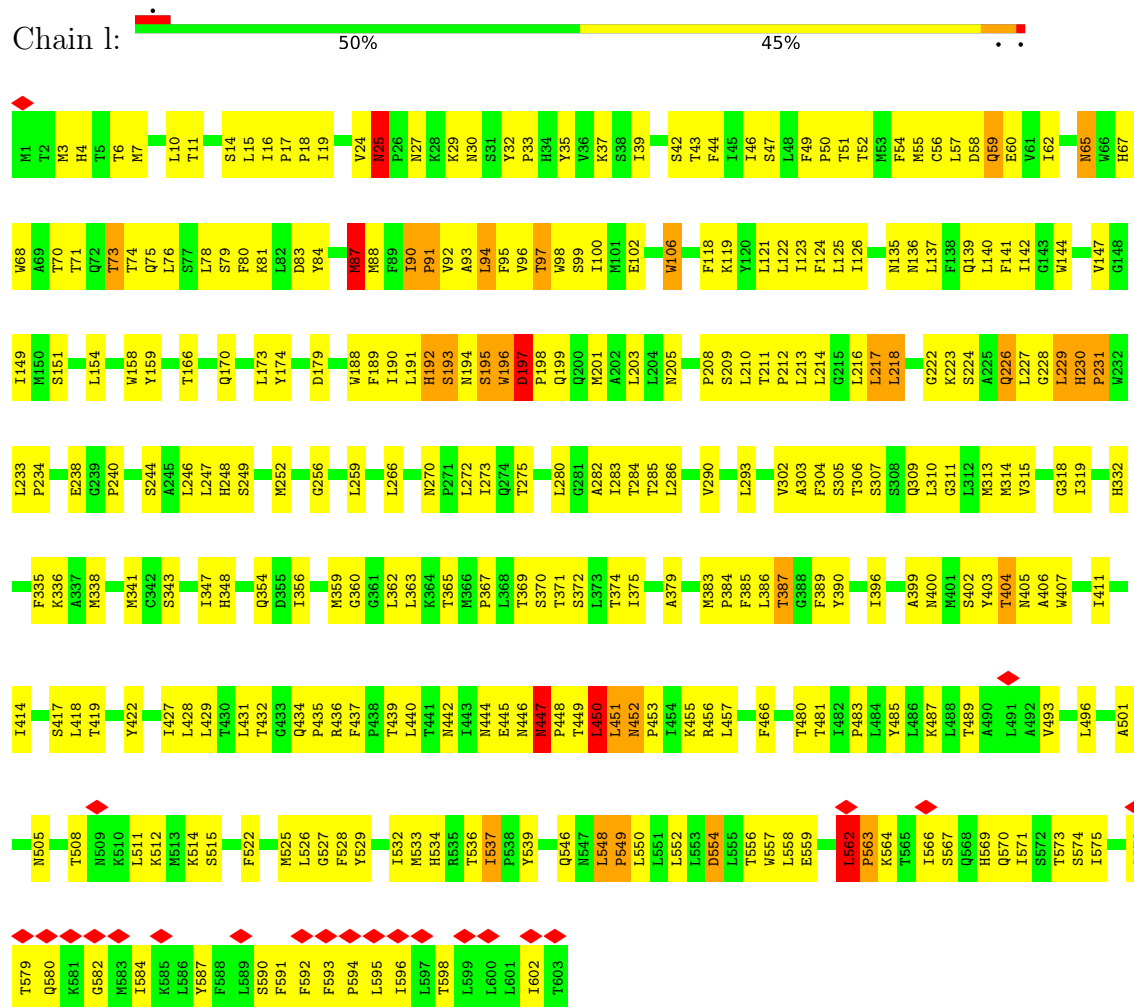
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



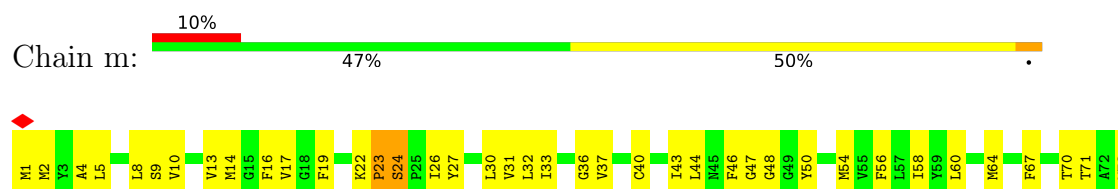
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

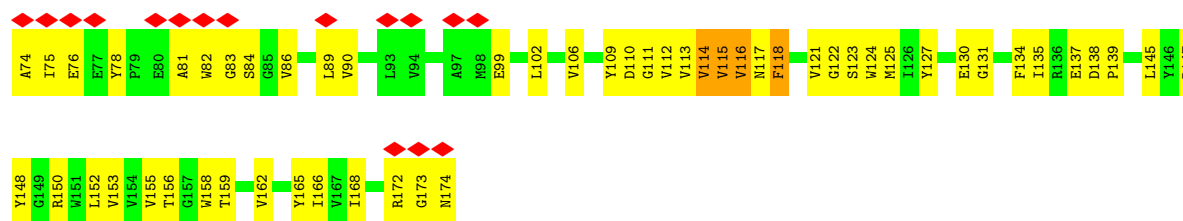


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

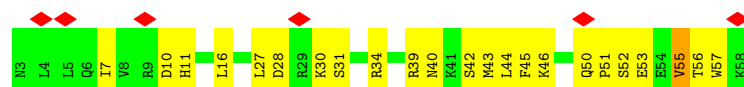


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6





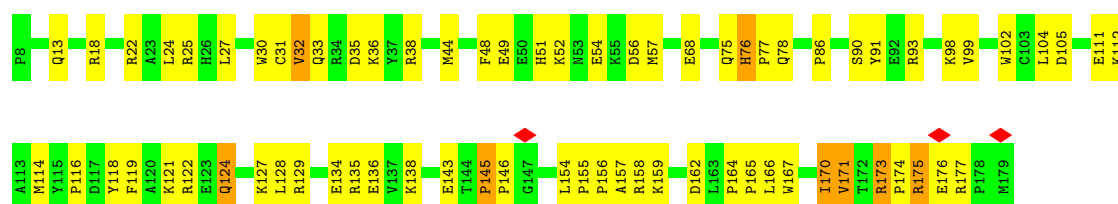
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



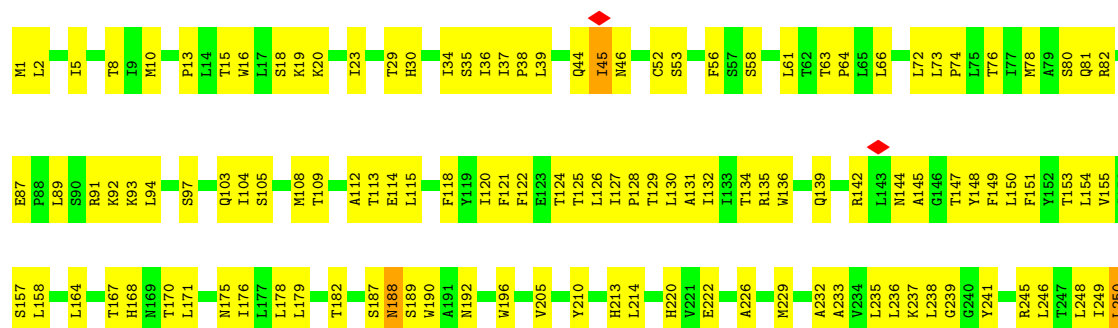
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

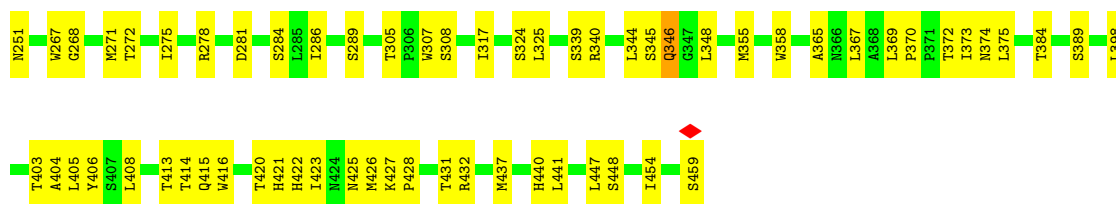


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

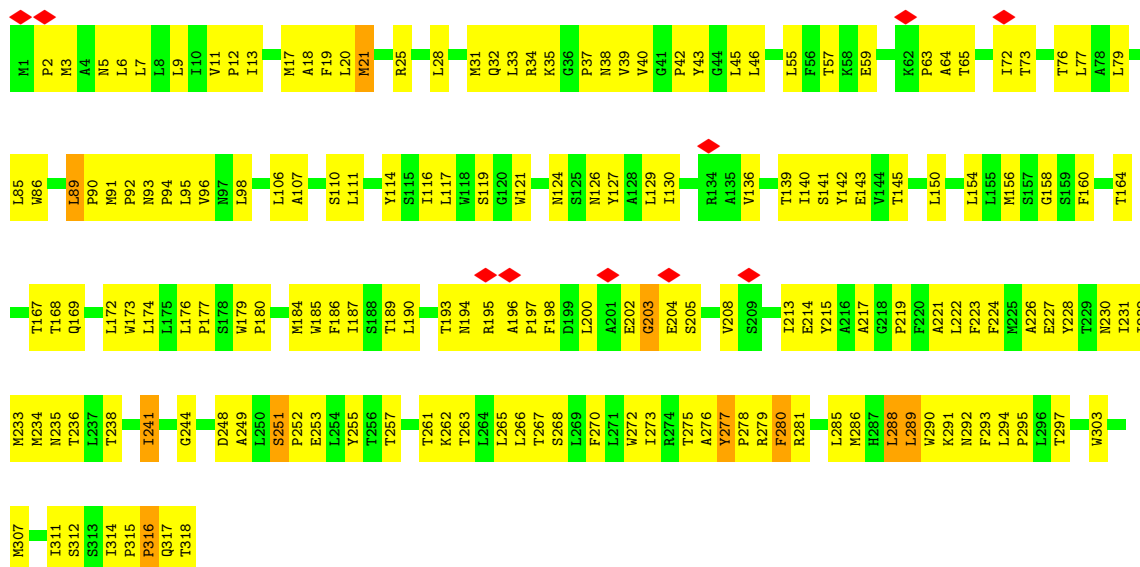


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

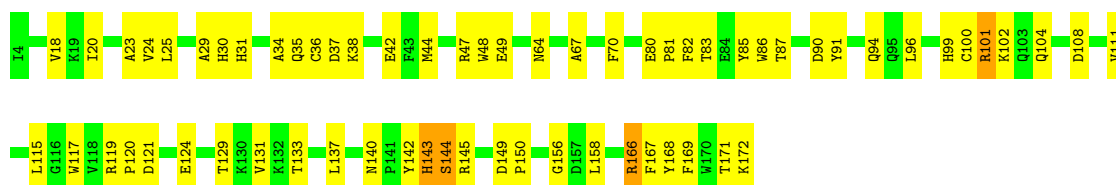




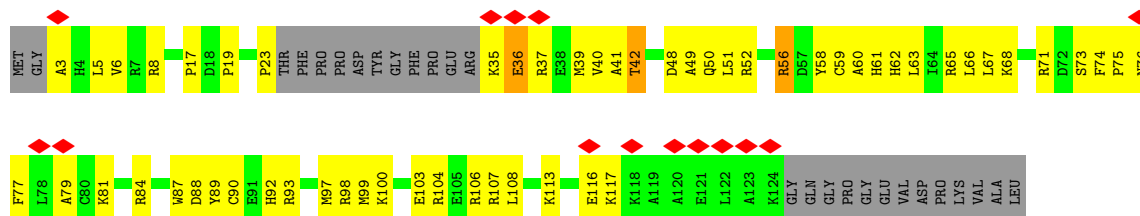
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



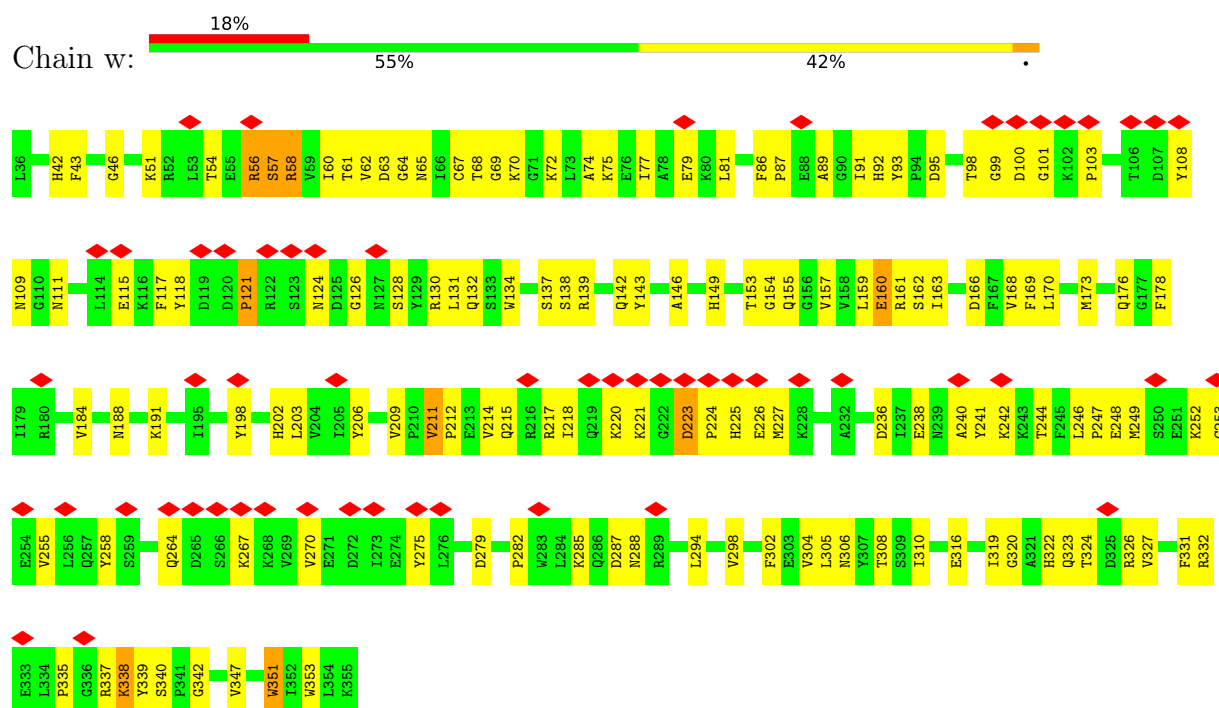
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0525	Depositor
Map size ($\text{\AA}$)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8Q1, PEE, PLX, NDP, SF4, CDL, FMN, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3398	0.87	5/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	F	0.36	0/682	0.87	0/922
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	H	0.45	0/941	0.87	2/1275 (0.2%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	K	0.30	0/282	0.73	0/381
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	N	0.44	0/1236	0.91	7/1681 (0.4%)
14	O	0.39	0/1682	0.87	4/2289 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)
16	Q	0.55	0/3552	1.01	15/4815 (0.3%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	T	0.38	0/755	0.79	0/1017
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	W	0.74	1/1166 (0.1%)	1.05	5/1579 (0.3%)
22	Y	0.61	0/559	1.16	7/763 (0.9%)
23	Z	0.56	0/669	0.82	0/899
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	d	0.78	0/1445	0.97	3/1945 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	l	0.84	4/4840 (0.1%)	1.03	29/6611 (0.4%)
36	m	0.82	0/1346	0.99	5/1832 (0.3%)
37	n	0.63	0/484	0.99	0/652
38	o	0.71	0/1093	0.89	0/1479
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	v	0.63	0/934	1.00	4/1241 (0.3%)
44	w	0.53	1/2533 (0.0%)	0.91	7/3440 (0.2%)
All	All	0.67	12/67276 (0.0%)	0.96	232/91300 (0.3%)

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
44	w	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.58	1.50	1.54
25	b	117	ILE	C-N	6.56	1.41	1.33
21	W	117	VAL	CA-CB	-6.07	1.49	1.54
40	r	37	ILE	CA-CB	-5.94	1.51	1.54
25	b	105	PHE	C-N	5.80	1.41	1.33
44	w	211	VAL	CA-CB	5.58	1.57	1.54
25	b	118	PRO	N-CD	5.25	1.55	1.47
34	k	2	PRO	N-CD	5.21	1.55	1.47
35	l	90	ILE	C-N	5.17	1.41	1.34
35	l	231	PRO	N-CD	5.12	1.54	1.47
35	l	230	HIS	C-N	5.10	1.41	1.34
35	l	91	PRO	N-CD	5.04	1.54	1.47

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	10	MET	CA-C-N	-10.85	109.21	120.38
21	W	10	MET	C-N-CA	-10.85	109.21	120.38
8	I	38	PRO	CA-C-N	10.35	130.66	119.28
8	I	38	PRO	C-N-CA	10.35	130.66	119.28
16	Q	162	ARG	CA-C-N	10.24	127.03	119.66
16	Q	162	ARG	C-N-CA	10.24	127.03	119.66
16	Q	365	PRO	CA-C-N	9.98	129.93	119.85
16	Q	365	PRO	C-N-CA	9.98	129.93	119.85
41	s	314	ILE	CA-C-N	9.76	126.78	119.66
41	s	314	ILE	C-N-CA	9.76	126.78	119.66
4	E	18	LYS	CA-C-N	9.23	129.18	119.85
4	E	18	LYS	C-N-CA	9.23	129.18	119.85
3	C	60	GLY	N-CA-C	8.53	122.81	112.49
32	i	323	THR	CA-C-N	8.51	147.42	127.00
32	i	323	THR	C-N-CA	8.51	147.42	127.00
22	Y	86	TYR	C-N-CD	8.43	139.15	120.60
22	Y	92	TRP	N-CA-C	-8.41	92.10	107.75
22	Y	47	PHE	CA-C-N	8.26	128.29	119.78
22	Y	47	PHE	C-N-CA	8.26	128.29	119.78
13	N	82	VAL	CA-C-N	8.15	125.61	119.66
13	N	82	VAL	C-N-CA	8.15	125.61	119.66
27	d	119	CYS	N-CA-C	8.02	120.02	111.28
9	J	311	GLU	CA-C-N	7.98	128.00	119.78
9	J	311	GLU	C-N-CA	7.98	128.00	119.78
32	i	255	PRO	N-CA-C	7.85	120.27	110.70
27	d	2	PRO	N-CA-CB	7.80	111.44	103.25
43	v	17	PRO	N-CA-CB	7.50	110.42	103.15
16	Q	318	VAL	N-CA-C	7.47	115.31	107.76
43	v	42	THR	CB-CA-C	-7.42	108.02	116.63
41	s	89	LEU	CA-C-N	7.38	129.07	119.84
41	s	89	LEU	C-N-CA	7.38	129.07	119.84
32	i	323	THR	C-N-CD	-7.37	104.38	120.60
3	C	141	MET	CA-C-N	7.33	127.33	119.78
3	C	141	MET	C-N-CA	7.33	127.33	119.78
25	b	117	ILE	CA-C-N	-7.32	112.84	120.38
25	b	117	ILE	C-N-CA	-7.32	112.84	120.38
19	U	33	PRO	N-CA-C	7.28	119.58	110.70
41	s	277	TYR	CA-C-N	7.14	127.06	119.85
41	s	277	TYR	C-N-CA	7.14	127.06	119.85
30	g	21	PRO	CA-C-N	7.12	124.79	119.66
30	g	21	PRO	C-N-CA	7.12	124.79	119.66
35	l	515	SER	CA-C-N	7.11	127.10	119.78
35	l	515	SER	C-N-CA	7.11	127.10	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	351	MET	CA-C-N	7.09	124.84	119.66
16	Q	351	MET	C-N-CA	7.09	124.84	119.66
39	p	173	ARG	CA-C-N	7.08	127.07	119.28
39	p	173	ARG	C-N-CA	7.08	127.07	119.28
14	O	237	PRO	N-CA-C	7.03	119.28	110.70
39	p	171	VAL	N-CA-C	7.00	117.79	110.72
35	l	537	ILE	CA-C-N	-6.98	111.61	119.28
35	l	537	ILE	C-N-CA	-6.98	111.61	119.28
32	i	197	ASN	CA-C-N	6.92	126.89	119.28
32	i	197	ASN	C-N-CA	6.92	126.89	119.28
16	Q	356	ILE	N-CA-C	-6.92	105.79	112.29
22	Y	93	THR	N-CA-C	6.90	120.01	108.20
1	A	318	ILE	CA-C-N	6.87	126.86	119.78
1	A	318	ILE	C-N-CA	6.87	126.86	119.78
9	J	224	GLY	CA-C-N	6.85	126.81	120.03
9	J	224	GLY	C-N-CA	6.85	126.81	120.03
31	h	94	PRO	CA-C-N	-6.84	113.33	120.38
31	h	94	PRO	C-N-CA	-6.84	113.33	120.38
35	l	24	VAL	CA-C-N	-6.80	115.37	122.85
35	l	24	VAL	C-N-CA	-6.80	115.37	122.85
1	A	327	ILE	CA-C-N	6.77	126.76	119.78
1	A	327	ILE	C-N-CA	6.77	126.76	119.78
26	c	157	GLY	CA-C-N	6.74	126.72	119.78
26	c	157	GLY	C-N-CA	6.74	126.72	119.78
25	b	105	PHE	CA-C-N	-6.72	112.84	119.76
25	b	105	PHE	C-N-CA	-6.72	112.84	119.76
43	v	23	PRO	N-CA-CB	6.71	110.38	103.00
26	c	72	TYR	N-CA-C	-6.68	100.14	110.10
15	P	166	TYR	N-CA-C	-6.62	104.06	111.28
17	S	61	TYR	N-CA-C	-6.61	104.08	111.28
2	B	168	GLY	CA-C-N	6.60	126.55	119.28
2	B	168	GLY	C-N-CA	6.60	126.55	119.28
22	Y	87	PRO	CA-N-CD	-6.57	102.30	111.50
35	l	562	LEU	CA-C-N	-6.56	111.64	119.84
35	l	562	LEU	C-N-CA	-6.56	111.64	119.84
16	Q	63	PRO	CA-C-N	6.52	124.42	119.66
16	Q	63	PRO	C-N-CA	6.52	124.42	119.66
36	m	135	ILE	N-CA-C	6.51	117.49	108.12
35	l	548	LEU	CA-C-N	-6.46	111.76	119.84
35	l	548	LEU	C-N-CA	-6.46	111.76	119.84
29	f	34	PRO	N-CA-C	6.40	118.51	110.70
44	w	211	VAL	CA-C-N	-6.37	111.98	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	w	211	VAL	C-N-CA	-6.37	111.98	119.05
9	J	91	ILE	CB-CA-C	-6.36	104.88	112.19
39	p	78	GLN	CA-C-N	6.26	126.23	119.78
39	p	78	GLN	C-N-CA	6.26	126.23	119.78
12	M	505	GLY	N-CA-C	-6.25	107.08	115.21
9	J	238	GLN	CA-C-N	6.25	126.22	119.78
9	J	238	GLN	C-N-CA	6.25	126.22	119.78
15	P	119	VAL	CA-C-N	6.25	126.15	119.28
15	P	119	VAL	C-N-CA	6.25	126.15	119.28
20	V	14	ASP	N-CA-C	6.25	117.75	111.07
8	I	98	ALA	CA-C-N	-6.24	113.95	120.38
8	I	98	ALA	C-N-CA	-6.24	113.95	120.38
43	v	19	PRO	N-CA-CB	6.24	110.13	103.39
41	s	179	TRP	CA-C-N	-6.22	112.44	119.28
41	s	179	TRP	C-N-CA	-6.22	112.44	119.28
44	w	56	ARG	N-CA-C	-6.20	105.65	112.72
31	h	94	PRO	N-CA-C	6.18	118.24	110.70
26	c	155	PRO	CA-C-N	-6.15	116.87	123.08
26	c	155	PRO	C-N-CA	-6.15	116.87	123.08
35	l	447	ASN	N-CA-C	6.11	115.99	108.11
44	w	253	CYS	CB-CA-C	-6.08	109.55	116.54
12	M	175	ARG	N-CA-C	6.06	117.89	111.28
9	J	86	CYS	N-CA-C	6.04	117.53	111.07
41	s	251	SER	CA-C-N	6.03	125.91	119.28
41	s	251	SER	C-N-CA	6.03	125.91	119.28
13	N	64	TYR	N-CA-C	6.02	120.47	113.18
16	Q	391	VAL	CA-C-N	-6.00	115.28	119.66
16	Q	391	VAL	C-N-CA	-6.00	115.28	119.66
2	B	160	CYS	CA-C-N	5.99	125.87	119.28
2	B	160	CYS	C-N-CA	5.99	125.87	119.28
21	W	31	SER	N-CA-C	-5.99	105.73	113.16
35	l	404	THR	N-CA-C	5.97	116.31	108.07
24	a	106	VAL	CA-C-N	5.97	125.88	119.85
24	a	106	VAL	C-N-CA	5.97	125.88	119.85
35	l	106	TRP	N-CA-C	5.95	117.84	111.36
39	p	155	PRO	CA-C-N	5.91	125.82	119.85
39	p	155	PRO	C-N-CA	5.91	125.82	119.85
41	s	158	GLY	N-CA-C	5.89	121.70	114.69
44	w	340	SER	N-CA-C	5.87	117.10	109.64
41	s	315	PRO	CA-C-N	5.86	127.16	119.84
41	s	315	PRO	C-N-CA	5.86	127.16	119.84
35	l	90	ILE	O-C-N	5.85	124.22	120.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	118	PRO	CA-C-N	5.85	125.75	119.85
21	W	118	PRO	C-N-CA	5.85	125.75	119.85
15	P	113	ASP	N-CA-C	5.81	117.94	108.76
20	V	22	ALA	N-CA-C	-5.80	105.04	111.36
2	B	64	LEU	N-CA-C	-5.77	104.90	111.07
25	b	37	PRO	CA-N-CD	-5.76	103.93	112.00
22	Y	85	PRO	N-CA-C	5.75	124.32	112.47
35	l	87	MET	N-CA-C	5.74	117.34	111.14
8	I	36	GLN	CA-C-N	5.74	123.85	119.66
8	I	36	GLN	C-N-CA	5.74	123.85	119.66
1	A	318	ILE	N-CA-C	5.73	114.19	107.77
13	N	65	THR	CB-CA-C	-5.73	108.97	115.79
7	H	81	ILE	N-CA-C	-5.72	104.94	110.72
40	r	427	LYS	CA-C-N	5.71	125.66	119.78
40	r	427	LYS	C-N-CA	5.71	125.66	119.78
42	u	166	ARG	N-CA-C	-5.71	106.54	112.93
33	j	49	VAL	N-CA-C	5.69	114.52	108.95
35	l	197	ASP	CA-C-N	-5.69	112.74	119.05
35	l	197	ASP	C-N-CA	-5.69	112.74	119.05
12	M	612	PRO	CA-C-N	5.68	125.52	119.28
12	M	612	PRO	C-N-CA	5.68	125.52	119.28
33	j	45	SER	CA-C-N	5.67	125.58	119.85
33	j	45	SER	C-N-CA	5.67	125.58	119.85
41	s	21	MET	N-CA-C	-5.67	106.21	113.01
8	I	17	GLY	N-CA-C	-5.65	107.84	115.36
41	s	280	PHE	N-CA-C	5.65	118.38	111.82
25	b	9	LYS	N-CA-C	-5.64	105.04	111.07
24	a	56	VAL	N-CA-C	5.62	117.83	111.88
35	l	450	LEU	N-CA-C	5.61	122.75	110.80
35	l	90	ILE	CA-C-N	-5.60	112.83	119.05
35	l	90	ILE	C-N-CA	-5.60	112.83	119.05
30	g	36	LEU	N-CA-C	-5.59	105.28	111.71
16	Q	272	THR	N-CA-C	5.59	120.38	113.50
14	O	236	GLU	CA-C-N	5.59	126.13	120.38
14	O	236	GLU	C-N-CA	5.59	126.13	120.38
26	c	120	SER	CA-C-N	5.56	125.51	119.78
26	c	120	SER	C-N-CA	5.56	125.51	119.78
12	M	261	ILE	N-CA-C	5.56	116.67	108.45
35	l	25	ASN	N-CA-C	5.55	118.19	108.75
14	O	233	SER	CB-CA-C	-5.52	109.72	117.23
24	a	166	GLY	CA-C-N	5.52	125.35	119.28
24	a	166	GLY	C-N-CA	5.52	125.35	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	149	LEU	N-CA-C	5.51	120.01	113.28
42	u	171	THR	N-CA-C	-5.51	106.61	113.38
36	m	127	TYR	CB-CA-C	-5.50	110.22	116.54
39	p	154	LEU	CA-C-N	5.47	123.60	119.66
39	p	154	LEU	C-N-CA	5.47	123.60	119.66
9	J	267	GLY	CA-C-N	5.43	125.25	119.28
9	J	267	GLY	C-N-CA	5.43	125.25	119.28
26	c	161	TYR	CA-C-N	5.42	125.36	119.78
26	c	161	TYR	C-N-CA	5.42	125.36	119.78
12	M	85	ALA	CA-C-N	5.41	125.23	119.28
12	M	85	ALA	C-N-CA	5.41	125.23	119.28
34	k	89	TYR	CB-CA-C	-5.39	109.38	115.79
16	Q	281	GLU	N-CA-C	5.37	117.13	111.28
2	B	78	GLU	CA-C-N	5.36	125.30	119.78
2	B	78	GLU	C-N-CA	5.36	125.30	119.78
35	l	192	HIS	N-CA-C	5.36	117.20	111.36
26	c	126	TRP	N-CA-C	5.36	116.81	110.97
30	g	22	PRO	O-C-N	5.34	123.66	121.15
35	l	270	ASN	CA-C-N	5.30	125.11	119.28
35	l	270	ASN	C-N-CA	5.30	125.11	119.28
2	B	43	ASP	CA-C-N	5.29	125.23	119.78
2	B	43	ASP	C-N-CA	5.29	125.23	119.78
16	Q	79	ASN	N-CA-C	5.27	116.45	108.07
32	i	172	GLN	N-CA-C	5.27	117.48	110.53
35	l	230	HIS	CA-C-N	-5.26	113.21	119.05
35	l	230	HIS	C-N-CA	-5.26	113.21	119.05
7	H	12	VAL	N-CA-C	5.24	115.91	110.82
13	N	83	PRO	CA-C-N	5.24	125.04	119.28
13	N	83	PRO	C-N-CA	5.24	125.04	119.28
35	l	16	ILE	CB-CA-C	-5.22	108.81	114.35
12	M	102	ILE	N-CA-C	5.20	114.28	106.42
34	k	1	MET	CA-C-N	-5.18	113.30	119.05
34	k	1	MET	C-N-CA	-5.18	113.30	119.05
39	p	145	PRO	CA-C-N	5.18	124.98	119.28
39	p	145	PRO	C-N-CA	5.18	124.98	119.28
35	l	437	PHE	CA-C-N	5.18	125.11	119.78
35	l	437	PHE	C-N-CA	5.18	125.11	119.78
27	d	120	ILE	N-CA-C	5.15	115.87	110.62
11	L	126	LEU	N-CA-C	5.14	116.55	107.61
36	m	114	VAL	CA-C-N	5.13	131.21	121.97
36	m	114	VAL	C-N-CA	5.13	131.21	121.97
32	i	321	LYS	CA-C-N	5.12	124.92	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	321	LYS	C-N-CA	5.12	124.92	119.28
19	U	36	SER	CA-C-N	5.12	124.91	119.28
19	U	36	SER	C-N-CA	5.12	124.91	119.28
36	m	137	GLU	N-CA-C	5.12	116.67	111.14
4	E	32	VAL	N-CA-C	5.12	115.33	110.42
19	U	62	ASN	CB-CA-C	-5.09	109.21	116.34
44	w	223	ASP	CA-C-N	5.07	124.86	119.28
44	w	223	ASP	C-N-CA	5.07	124.86	119.28
20	V	86	ASP	CA-C-N	5.07	124.73	119.56
20	V	86	ASP	C-N-CA	5.07	124.73	119.56
9	J	195	PHE	CA-C-N	5.07	124.85	119.28
9	J	195	PHE	C-N-CA	5.07	124.85	119.28
12	M	681	ALA	N-CA-C	5.07	114.83	108.45
32	i	41	ILE	CB-CA-C	-5.06	107.37	114.00
24	a	106	VAL	N-CA-C	5.05	112.55	107.55
15	P	94	ILE	CB-CA-C	-5.04	107.39	114.00
2	B	67	GLY	N-CA-C	-5.03	106.69	112.73
28	e	58	ASP	CA-C-N	5.02	124.95	119.78
28	e	58	ASP	C-N-CA	5.02	124.95	119.78
9	J	242	VAL	N-CA-C	5.00	116.45	111.00
13	N	61	TRP	N-CA-C	5.00	115.90	108.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	213	0
2	B	1420	0	1371	119	0
3	C	1249	0	1253	82	0
4	E	968	0	982	63	0
5	F	670	0	679	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	H	922	0	950	58	0
8	I	769	0	788	46	0
9	J	2712	0	2757	235	0
10	K	274	0	257	25	0
11	L	964	0	962	63	0
12	M	5274	0	5312	339	0
13	N	1195	0	1155	50	0
14	O	1643	0	1646	113	0
15	P	1730	0	1685	115	0
16	Q	3460	0	3419	310	0
17	S	568	0	567	39	0
18	T	742	0	723	40	0
19	U	647	0	653	17	0
20	V	1038	0	1027	36	0
21	W	1135	0	1129	56	0
22	Y	533	0	475	97	0
23	Z	648	0	627	19	0
24	a	1174	0	1177	105	0
25	b	1059	0	1079	126	0
26	c	1236	0	1092	81	0
27	d	1418	0	1375	120	0
28	e	810	0	772	35	0
29	f	405	0	407	19	0
30	g	1004	0	1008	64	0
31	h	863	0	861	66	0
32	i	2735	0	2893	185	0
33	j	919	0	968	76	0
34	k	740	0	792	89	0
35	l	4717	0	4893	400	0
36	m	1313	0	1330	122	0
37	n	473	0	480	30	0
38	o	1066	0	1086	52	0
39	p	1495	0	1440	94	0
40	r	3629	0	3825	164	0
41	s	2509	0	2617	170	0
42	u	1394	0	1367	60	0
43	v	921	0	892	90	0
44	w	2474	0	2304	116	0
45	A	8	0	0	6	0
45	B	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	0	0
45	M	16	0	0	3	0
46	A	31	0	19	16	0
47	B	52	0	88	4	0
47	U	52	0	88	3	0
47	V	52	0	88	5	0
47	b	52	0	88	38	0
47	g	156	0	264	13	0
47	r	104	0	176	23	0
48	E	35	0	0	4	0
48	p	35	0	0	12	0
49	J	48	0	26	26	0
50	M	4	0	0	1	0
50	O	4	0	0	2	0
51	V	63	0	68	8	0
51	i	64	0	72	3	0
51	l	128	0	144	4	0
51	n	64	0	72	10	0
52	V	51	0	82	21	0
52	W	51	0	82	19	0
52	l	100	0	157	68	0
All	All	66789	0	67204	3729	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 28.

All (3729) 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)
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.65
35:l:533:MET:CE	52:l:702:PEE:H36	1.25	1.58
35:l:37:LYS:HE2	35:l:98:TRP:CD1	1.40	1.57
24:a:55:PHE:HE2	39:p:118:TYR:CE2	1.17	1.56
24:a:55:PHE:CE2	39:p:118:TYR:CD2	1.91	1.55
24:a:98:LEU:HB3	27:d:57:TYR:CE1	1.45	1.52
32:i:288:LEU:CD2	52:l:701:PEE:H58	1.37	1.52
35:l:533:MET:HE1	52:l:702:PEE:C22	1.41	1.51
9:J:130:ILE:HG23	49:J:401:NDP:C8A	1.46	1.46
35:l:571:ILE:CD1	52:l:701:PEE:O5	1.64	1.43
12:M:134:GLY:HA2	45:M:801:SF4:S3	1.57	1.42
35:l:84:TYR:CD1	35:l:88:MET:HE2	1.54	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:84:TYR:CE1	35:l:88:MET:CE	2.05	1.40
24:a:55:PHE:HE2	39:p:118:TYR:CD2	1.32	1.35
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
35:l:84:TYR:CE1	35:l:88:MET:HE2	1.64	1.31
32:i:288:LEU:HD23	52:l:701:PEE:C36	1.60	1.30
16:Q:271:ARG:NH1	41:s:281:ARG:HB2	1.45	1.29
24:a:98:LEU:CB	27:d:57:TYR:HE1	1.46	1.28
9:J:206:ILE:HA	9:J:240:VAL:O	1.35	1.27
24:a:55:PHE:CD2	39:p:118:TYR:CE2	2.22	1.27
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.26
16:Q:82:LEU:O	16:Q:98:VAL:HG13	1.25	1.26
35:l:188:TRP:CE2	35:l:192:HIS:HD2	1.54	1.26
35:l:447:ASN:OD1	35:l:448:PRO:HD2	1.30	1.24
9:J:130:ILE:HG23	49:J:401:NDP:N7A	1.52	1.22
22:Y:84:PHE:CE2	35:l:483:PRO:HG3	1.74	1.20
35:l:37:LYS:CE	35:l:98:TRP:CD1	2.24	1.20
22:Y:87:PRO:HB3	43:v:103:GLU:OE2	1.38	1.19
22:Y:72:ARG:NH1	35:l:390:TYR:OH	1.76	1.19
24:a:55:PHE:CD2	39:p:118:TYR:CZ	2.30	1.19
9:J:206:ILE:O	9:J:211:ASP:OD2	1.61	1.19
9:J:171:ASN:O	9:J:181:LEU:CD2	1.92	1.18
9:J:171:ASN:C	9:J:181:LEU:HD21	1.69	1.18
35:l:226:GLN:HE21	35:l:314:MET:CE	1.56	1.18
25:b:110:ILE:HG23	25:b:111:LEU:HG	1.24	1.17
52:V:202:PEE:C42	52:l:701:PEE:C45	2.23	1.17
24:a:55:PHE:HD2	39:p:118:TYR:CZ	1.62	1.16
52:V:202:PEE:H70	52:l:701:PEE:C45	1.75	1.16
52:W:201:PEE:H75	41:s:77:LEU:CD2	1.75	1.16
35:l:188:TRP:CE2	35:l:192:HIS:CD2	2.33	1.15
1:A:93:PHE:CE2	1:A:98:LYS:HD3	1.80	1.14
16:Q:268:TRP:CZ3	16:Q:272:THR:HG21	1.80	1.14
32:i:291:TYR:CE2	52:l:701:PEE:C31	2.29	1.14
35:l:533:MET:SD	52:l:702:PEE:H36	1.86	1.14
39:p:167:TRP:O	39:p:171:VAL:HG23	1.47	1.14
16:Q:85:GLY:HA3	33:j:39:CYS:SG	1.87	1.13
22:Y:84:PHE:CD1	22:Y:85:PRO:HD3	1.83	1.13
4:E:25:MET:HB3	4:E:29:LYS:CE	1.77	1.13
27:d:59:HIS:CE1	28:e:120:ARG:HB3	1.84	1.12
35:l:84:TYR:CE1	35:l:88:MET:HE3	1.74	1.12
34:k:4:ILE:HD11	36:m:125:MET:SD	1.91	1.11
52:W:201:PEE:H75	41:s:77:LEU:HD21	1.19	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:54:PHE:CE1	35:l:58:ASP:OD1	2.06	1.08
9:J:130:ILE:HG23	49:J:401:NDP:H8A	1.28	1.08
22:Y:71:TRP:CH2	22:Y:75:HIS:CD2	2.42	1.08
16:Q:271:ARG:HH11	41:s:281:ARG:CB	1.66	1.08
22:Y:84:PHE:CZ	35:l:483:PRO:HG3	1.88	1.08
24:a:98:LEU:CB	27:d:57:TYR:CE1	2.25	1.07
35:l:97:THR:HG21	35:l:125:LEU:HD12	1.35	1.07
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
26:c:181:VAL:CB	43:v:37:ARG:HH21	1.66	1.07
35:l:84:TYR:HE1	35:l:88:MET:CE	1.50	1.07
24:a:114:LYS:HB2	27:d:57:TYR:CE2	1.88	1.07
12:M:134:GLY:CA	45:M:801:SF4:S3	2.42	1.06
16:Q:271:ARG:NH1	41:s:281:ARG:CB	2.18	1.06
35:l:54:PHE:CZ	35:l:58:ASP:OD1	2.07	1.06
24:a:55:PHE:HD2	39:p:118:TYR:CE1	1.75	1.05
35:l:227:LEU:O	35:l:230:HIS:ND1	1.88	1.05
27:d:81:GLU:OE1	37:n:43:MET:HE3	1.57	1.05
44:w:332:ARG:O	44:w:338:LYS:HA	1.55	1.05
27:d:105:LYS:CE	35:l:197:ASP:OD2	2.04	1.04
34:k:1:MET:N	34:k:1:MET:SD	2.30	1.04
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.04
22:Y:71:TRP:CH2	22:Y:75:HIS:HD2	1.76	1.04
34:k:7:ASN:HD21	36:m:9:SER:C	1.65	1.04
6:X:112:SER:CA	48:p:201:8Q1:O2	2.06	1.04
16:Q:69:VAL:O	16:Q:72:PRO:HD2	1.58	1.03
16:Q:82:LEU:O	16:Q:98:VAL:CG1	2.06	1.03
35:l:84:TYR:CD1	35:l:88:MET:CE	2.30	1.03
32:i:285:ILE:HG12	52:l:701:PEE:H75	1.34	1.03
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.03
35:l:571:ILE:HD11	52:l:701:PEE:C30	1.89	1.03
24:a:96:ALA:HB3	27:d:55:TYR:HB2	1.33	1.02
35:l:37:LYS:CE	35:l:98:TRP:HD1	1.65	1.02
24:a:96:ALA:CB	27:d:55:TYR:HB2	1.90	1.02
35:l:59:GLN:HA	35:l:59:GLN:HE21	1.23	1.02
47:r:502:PLX:H332	47:r:502:PLX:H372	1.37	1.02
35:l:25:ASN:ND2	35:l:25:ASN:O	1.91	1.02
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.25	1.02
27:d:105:LYS:NZ	35:l:197:ASP:OD2	1.91	1.01
35:l:571:ILE:HD11	52:l:701:PEE:O5	0.84	1.01
9:J:130:ILE:CG2	49:J:401:NDP:N7A	2.24	1.01
35:l:222:GLY:CA	35:l:229:LEU:HD12	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:226:GLN:HG3	35:l:280:LEU:CD2	1.91	1.01
35:l:534:HIS:ND1	52:l:702:PEE:H14	1.74	1.01
39:p:170:ILE:H	39:p:170:ILE:HD12	1.24	1.01
39:p:48:PHE:HE1	48:p:201:8Q1:C8	1.73	1.00
32:i:291:TYR:CZ	52:l:701:PEE:H49	1.97	1.00
52:l:701:PEE:H37	40:r:155:VAL:HB	1.42	1.00
32:i:291:TYR:CE2	52:l:701:PEE:H48	1.95	1.00
35:l:193:SER:OG	35:l:205:ASN:ND2	1.95	1.00
35:l:533:MET:CE	52:l:702:PEE:C22	2.16	1.00
9:J:130:ILE:CG2	49:J:401:NDP:C8A	2.41	0.99
9:J:176:SER:HA	9:J:182:ARG:HH21	1.24	0.99
9:J:141:PHE:CE2	9:J:180:TYR:HA	1.98	0.99
52:V:202:PEE:C25	52:V:202:PEE:H60	1.92	0.99
35:l:533:MET:HE1	52:l:702:PEE:H35	1.44	0.99
34:k:7:ASN:HD22	36:m:9:SER:CB	1.75	0.99
16:Q:53:TYR:HE1	52:l:701:PEE:O1P	1.44	0.98
35:l:84:TYR:HE1	35:l:88:MET:HE3	1.08	0.98
1:A:116:ASN:ND2	46:A:502:FMN:C8	2.25	0.98
9:J:171:ASN:HB3	9:J:181:LEU:HD11	1.46	0.98
35:l:51:THR:HG21	35:l:91:PRO:HG2	1.42	0.98
25:b:107:GLY:N	25:b:115:GLU:OE1	1.96	0.98
34:k:4:ILE:CD1	36:m:125:MET:SD	2.52	0.98
35:l:231:PRO:O	35:l:234:PRO:HD2	1.64	0.98
52:l:701:PEE:C22	40:r:155:VAL:HG11	1.94	0.97
25:b:93:LYS:HE3	35:l:65:ASN:O	1.64	0.97
52:l:701:PEE:H36	40:r:155:VAL:HG11	1.44	0.97
35:l:226:GLN:NE2	35:l:314:MET:CE	2.27	0.97
39:p:44:MET:HE1	48:p:201:8Q1:C10	1.94	0.97
52:l:701:PEE:H37	40:r:155:VAL:CB	1.93	0.97
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.96
52:V:202:PEE:H14	32:i:276:LEU:CD1	1.96	0.96
39:p:48:PHE:CE1	48:p:201:8Q1:C8	2.48	0.96
35:l:84:TYR:HD1	35:l:88:MET:HE2	1.20	0.95
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	0.95
35:l:74:THR:CG2	35:l:194:ASN:OD1	2.14	0.95
52:V:202:PEE:H14	32:i:276:LEU:HD12	1.47	0.95
24:a:55:PHE:CD2	39:p:118:TYR:CD2	2.49	0.95
34:k:1:MET:HB3	36:m:125:MET:HB2	1.43	0.95
24:a:176:LYS:HE2	31:h:42:GLU:HG2	1.49	0.95
3:C:137:VAL:HG21	16:Q:87:GLN:HE21	1.29	0.94
22:Y:86:TYR:OH	43:v:100:LYS:CE	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HD22	46:A:502:FMN:C8M	1.78	0.94
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.47	0.94
47:b:201:PLX:O9	47:r:502:PLX:H1C3	1.67	0.94
26:c:122:THR:OG1	38:o:12:ARG:NH1	1.99	0.94
25:b:88:TYR:CD1	47:b:201:PLX:H1C1	2.02	0.94
14:O:177:LEU:N	50:O:301:FES:S1	2.39	0.94
35:l:226:GLN:CG	35:l:280:LEU:HD21	1.98	0.94
34:k:7:ASN:ND2	36:m:9:SER:CB	2.31	0.93
32:i:291:TYR:CE2	52:l:701:PEE:H49	2.00	0.93
25:b:118:PRO:O	25:b:120:MET:HG2	1.68	0.93
32:i:167:TRP:CZ3	35:l:573:THR:CB	2.52	0.93
22:Y:87:PRO:CB	43:v:103:GLU:OE2	2.17	0.93
27:d:59:HIS:HE1	28:e:120:ARG:HB3	1.24	0.92
1:A:116:ASN:HD22	46:A:502:FMN:C8	1.82	0.92
34:k:3:LEU:CD2	36:m:117:ASN:HD21	1.83	0.92
27:d:59:HIS:CE1	28:e:120:ARG:CB	2.53	0.92
25:b:110:ILE:HG23	25:b:111:LEU:CG	1.99	0.92
22:Y:83:HIS:O	22:Y:84:PHE:HB2	1.67	0.91
4:E:25:MET:O	4:E:29:LYS:HG3	1.69	0.91
47:b:201:PLX:H1C3	47:b:201:PLX:C3	2.01	0.90
22:Y:79:GLU:O	35:l:487:LYS:HE3	1.70	0.90
7:H:45:ARG:NH1	7:H:49:GLU:OE2	2.04	0.90
9:J:141:PHE:CZ	9:J:180:TYR:HA	2.07	0.90
27:d:60:ARG:HG2	27:d:60:ARG:HH11	1.36	0.90
9:J:169:HIS:HD2	49:J:401:NDP:H5N	1.34	0.90
16:Q:271:ARG:HH11	41:s:281:ARG:HB2	1.08	0.90
35:l:226:GLN:CG	35:l:280:LEU:CD2	2.49	0.89
32:i:291:TYR:HE2	52:l:701:PEE:H48	1.32	0.89
34:k:7:ASN:ND2	36:m:9:SER:HB2	1.86	0.89
35:l:51:THR:HG21	35:l:91:PRO:CG	2.02	0.89
35:l:227:LEU:HD12	35:l:230:HIS:ND1	1.85	0.89
27:d:105:LYS:HE2	35:l:197:ASP:OD2	1.70	0.89
40:r:78:MET:O	40:r:432:ARG:NH1	2.05	0.89
22:Y:96:GLU:OE2	26:c:185:GLU:O	1.89	0.89
24:a:114:LYS:HB2	27:d:57:TYR:HE2	1.31	0.89
35:l:78:LEU:HD21	35:l:80:PHE:CE1	2.07	0.89
25:b:110:ILE:C	25:b:111:LEU:HD23	1.98	0.89
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.89
27:d:110:ARG:HG2	27:d:110:ARG:HH11	1.38	0.89
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
27:d:108:GLN:HG2	35:l:199:GLN:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:85:GLY:HA3	33:j:39:CYS:CB	2.02	0.88
9:J:83:PRO:HB2	9:J:108:TRP:NE1	1.88	0.88
16:Q:400:ILE:HB	16:Q:407:PHE:HB3	1.53	0.88
35:l:37:LYS:HE3	35:l:102:GLU:HG3	1.53	0.88
52:l:701:PEE:H37	40:r:155:VAL:CG1	2.02	0.88
35:l:193:SER:HB2	35:l:195:SER:OG	1.74	0.88
35:l:226:GLN:HG3	35:l:280:LEU:HD21	1.53	0.88
26:c:169:GLU:OE2	43:v:56:ARG:NH2	2.05	0.88
3:C:137:VAL:CG2	16:Q:87:GLN:HE21	1.85	0.88
35:l:88:MET:O	35:l:91:PRO:HD2	1.74	0.88
33:j:105:GLU:HG2	36:m:168:ILE:HD11	1.56	0.88
34:k:23:ARG:H	36:m:22:LYS:HE2	1.39	0.88
41:s:185:TRP:HE1	41:s:238:THR:HG22	1.39	0.88
43:v:66:LEU:HD11	43:v:84:ARG:HD2	1.55	0.88
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
32:i:167:TRP:HZ3	35:l:570:GLN:HA	1.37	0.88
32:i:288:LEU:CD2	52:l:701:PEE:C36	2.32	0.88
34:k:2:PRO:HG2	36:m:115:VAL:HG21	1.56	0.88
35:l:78:LEU:HD21	35:l:80:PHE:HE1	1.39	0.88
22:Y:86:TYR:OH	43:v:100:LYS:CG	2.22	0.87
24:a:87:THR:HG22	47:b:201:PLX:C13	2.03	0.87
22:Y:84:PHE:CG	22:Y:85:PRO:CD	2.57	0.87
47:b:201:PLX:H102	47:b:201:PLX:H6	1.56	0.87
32:i:224:SER:HB2	32:i:229:LEU:HB3	1.56	0.87
34:k:1:MET:HB2	34:k:4:ILE:CD1	2.04	0.87
26:c:181:VAL:CB	43:v:37:ARG:NH2	2.37	0.87
35:l:533:MET:SD	52:l:702:PEE:C22	2.62	0.87
35:l:447:ASN:OD1	35:l:448:PRO:CD	2.19	0.87
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.87
52:V:202:PEE:C43	52:l:701:PEE:C45	2.53	0.87
27:d:59:HIS:CE1	28:e:120:ARG:CG	2.58	0.87
9:J:212:ARG:HG2	9:J:212:ARG:HH11	1.37	0.86
12:M:130:ILE:HD13	18:T:114:TYR:CE1	2.11	0.86
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.86
44:w:99:GLY:HA3	44:w:337:ARG:HH12	1.40	0.86
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.86
25:b:110:ILE:O	25:b:111:LEU:HD23	1.75	0.86
22:Y:84:PHE:CD1	22:Y:85:PRO:CD	2.58	0.86
35:l:533:MET:SD	52:l:702:PEE:H37	2.15	0.86
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.86
9:J:169:HIS:HD2	49:J:401:NDP:C5N	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:W:201:PEE:O2P	52:W:201:PEE:N	2.08	0.86
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.40	0.85
16:Q:271:ARG:HH11	41:s:281:ARG:CA	1.88	0.85
24:a:96:ALA:HB3	27:d:55:TYR:CB	2.05	0.85
27:d:114:ASN:O	27:d:114:ASN:ND2	2.09	0.85
34:k:2:PRO:HG2	36:m:115:VAL:CG2	2.05	0.85
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.85
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.85
39:p:167:TRP:HE3	39:p:171:VAL:HG21	1.40	0.85
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.85
27:d:111:GLU:OE2	27:d:119:CYS:N	2.09	0.85
44:w:332:ARG:O	44:w:338:LYS:HG2	1.76	0.85
1:A:244:ASN:N	46:A:502:FMN:O2P	2.09	0.84
16:Q:271:ARG:NH1	41:s:281:ARG:CA	2.40	0.84
32:i:54:GLU:OE2	32:i:58:LYS:NZ	2.10	0.84
9:J:85:ARG:HG3	9:J:85:ARG:HH11	1.41	0.84
9:J:176:SER:CA	9:J:182:ARG:HH21	1.88	0.84
24:a:53:ARG:HD2	25:b:28:LEU:HD11	1.57	0.84
16:Q:53:TYR:CE1	52:l:701:PEE:O1P	2.30	0.84
52:V:202:PEE:H74	52:l:701:PEE:C45	2.08	0.84
30:g:1:MET:HE2	30:g:85:ARG:HD3	1.57	0.84
20:V:84:PRO:O	20:V:89:ASN:ND2	2.10	0.84
26:c:122:THR:HG1	38:o:12:ARG:HH12	1.26	0.84
32:i:12:THR:HG21	36:m:162:VAL:HG21	1.60	0.84
35:l:188:TRP:NE1	35:l:192:HIS:CD2	2.45	0.83
24:a:90:ASN:HD22	47:b:201:PLX:H122	1.43	0.83
4:E:70:ASN:OD1	48:E:201:8Q1:O4	1.95	0.83
30:g:62:LEU:HD22	47:g:203:PLX:H91	1.61	0.83
44:w:160:GLU:HG2	44:w:161:ARG:H	1.43	0.83
41:s:17:MET:HE1	41:s:232:ILE:HD12	1.61	0.82
16:Q:145:MET:HE1	16:Q:226:TYR:HB3	1.61	0.82
24:a:143:GLU:OE1	40:r:175:ASN:ND2	2.11	0.82
27:d:59:HIS:CE1	28:e:120:ARG:HG2	2.14	0.82
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.82
24:a:54:LEU:HD22	25:b:26:GLN:C	2.04	0.82
33:j:6:ILE:O	33:j:10:ASN:ND2	2.12	0.82
16:Q:87:GLN:O	16:Q:88:HIS:C	2.22	0.82
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.82
32:i:235:ASN:ND2	32:i:307:MET:SD	2.53	0.82
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.82
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:124:GLN:O	39:p:128:LEU:HG	1.79	0.82
24:a:87:THR:HG22	47:b:201:PLX:H132	1.61	0.82
9:J:169:HIS:CD2	49:J:401:NDP:H5N	2.15	0.82
6:X:112:SER:N	48:p:201:8Q1:O2	2.14	0.81
22:Y:72:ARG:HH11	35:l:466:PHE:HD1	1.29	0.81
35:l:533:MET:HE1	52:l:702:PEE:H36	0.83	0.81
40:r:365:ALA:O	40:r:374:ASN:ND2	2.13	0.81
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.81
6:X:99:SER:HG	6:X:102:SER:HG	1.25	0.81
26:c:159:LYS:HA	43:v:98:ARG:HH22	1.46	0.81
30:g:49:ARG:HD3	44:w:339:TYR:HA	1.61	0.81
31:h:88:LYS:HG3	31:h:89:GLU:HG3	1.63	0.81
32:i:167:TRP:CZ3	35:l:570:GLN:HA	2.14	0.81
43:v:8:ARG:HH11	43:v:106:ARG:HH22	1.29	0.81
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.80
35:l:188:TRP:NE1	35:l:192:HIS:HD2	1.78	0.80
16:Q:58:THR:HG23	35:l:580:GLN:HE21	1.46	0.80
35:l:188:TRP:CZ2	35:l:192:HIS:CD2	2.69	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80
52:W:201:PEE:C44	41:s:77:LEU:HD21	2.09	0.80
22:Y:74:TRP:HZ3	22:Y:75:HIS:HD1	1.29	0.80
34:k:7:ASN:ND2	36:m:9:SER:C	2.38	0.80
35:l:222:GLY:HA2	35:l:229:LEU:HD12	1.63	0.80
35:l:227:LEU:O	35:l:227:LEU:HD12	1.82	0.80
52:l:701:PEE:C23	40:r:155:VAL:HG11	2.11	0.80
47:r:502:PLX:H372	47:r:502:PLX:C33	2.09	0.80
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.80
44:w:332:ARG:O	44:w:338:LYS:CA	2.29	0.80
32:i:91:ASN:OD1	32:i:92:GLN:N	2.13	0.80
34:k:1:MET:HB2	34:k:4:ILE:HD12	1.63	0.80
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.80
35:l:226:GLN:NE2	35:l:314:MET:SD	2.54	0.79
35:l:224:SER:OG	35:l:256:GLY:HA3	1.80	0.79
47:r:502:PLX:H52	47:r:502:PLX:O3	1.82	0.79
22:Y:74:TRP:CE3	22:Y:75:HIS:HA	2.16	0.79
9:J:217:PHE:HZ	9:J:322:MET:CE	1.95	0.79
22:Y:86:TYR:OH	43:v:100:LYS:HE2	1.82	0.79
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.65	0.79
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.79
25:b:110:ILE:CG2	25:b:111:LEU:HG	2.11	0.79
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:70:ASP:O	16:Q:74:ASP:OD1	2.00	0.79
32:i:12:THR:HG22	36:m:158:TRP:HE1	1.47	0.79
35:l:4:HIS:CE1	35:l:87:MET:CE	2.65	0.79
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.79
25:b:86:MET:O	25:b:90:VAL:HG23	1.83	0.79
32:i:339:ILE:HG22	32:i:342:PHE:HB3	1.64	0.79
26:c:166:LEU:HD21	43:v:56:ARG:HG3	1.65	0.79
27:d:111:GLU:OE1	27:d:115:TYR:HB2	1.82	0.79
33:j:108:GLN:O	36:m:172:ARG:NH2	2.16	0.79
9:J:177:SER:HB2	9:J:320:GLU:HB3	1.64	0.78
9:J:206:ILE:HG12	49:J:401:NDP:N7N	1.99	0.78
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.78
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.65	0.78
5:F:63:PRO:HB2	5:F:79:LEU:HB2	1.65	0.78
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.65	0.78
39:p:143:GLU:OE2	39:p:158:ARG:NH2	2.15	0.78
2:B:133:ARG:HG3	2:B:135:ASP:H	1.48	0.78
32:i:50:PRO:HB3	34:k:84:THR:HG21	1.65	0.78
9:J:86:CYS:O	9:J:87:ASP:HB2	1.83	0.78
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.02	0.78
40:r:355:MET:HE1	40:r:437:MET:HE3	1.65	0.78
22:Y:90:SER:HA	43:v:107:ARG:NH1	1.98	0.78
39:p:13:GLN:NE2	48:p:201:8Q1:O3	2.15	0.78
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.65	0.78
39:p:167:TRP:O	39:p:171:VAL:CG2	2.28	0.78
9:J:176:SER:HA	9:J:182:ARG:NH2	1.98	0.78
32:i:167:TRP:CH2	35:l:570:GLN:HG3	2.19	0.78
34:k:97:GLN:HB2	35:l:579:THR:HG21	1.66	0.78
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.78
37:n:55:VAL:HG12	37:n:56:THR:H	1.48	0.78
34:k:3:LEU:HD23	36:m:117:ASN:HD21	1.48	0.78
36:m:111:GLY:HA2	36:m:116:VAL:HA	1.65	0.78
22:Y:83:HIS:O	22:Y:84:PHE:CB	2.31	0.77
47:b:201:PLX:H6	47:b:201:PLX:C10	2.13	0.77
26:c:155:PRO:HB3	43:v:5:LEU:HD22	1.67	0.77
22:Y:84:PHE:CG	22:Y:85:PRO:HD2	2.19	0.77
22:Y:86:TYR:OH	43:v:100:LYS:HG2	1.84	0.77
9:J:217:PHE:CB	9:J:280:ILE:HD13	2.15	0.77
15:P:187:ILE:HG22	15:P:188:LEU:HG	1.66	0.77
47:b:201:PLX:C6	47:b:201:PLX:H111	2.14	0.77
34:k:23:ARG:N	36:m:22:LYS:HE2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:NZ	8:I:35:THR:O	2.18	0.77
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77
22:Y:81:LEU:HD22	43:v:92:HIS:CD2	2.18	0.77
24:a:54:LEU:CD2	25:b:27:GLU:HA	2.14	0.77
27:d:63:ARG:NH1	37:n:44:LEU:O	2.18	0.77
16:Q:85:GLY:HA3	33:j:39:CYS:HG	1.49	0.77
22:Y:96:GLU:O	22:Y:97:LEU:HD23	1.84	0.77
44:w:64:GLY:O	44:w:161:ARG:NH2	2.17	0.77
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.77
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.17	0.77
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.77
32:i:288:LEU:HD23	52:l:701:PEE:H58	0.77	0.77
35:l:74:THR:HG22	35:l:194:ASN:OD1	1.83	0.77
35:l:90:ILE:O	35:l:94:LEU:HD22	1.84	0.77
16:Q:82:LEU:C	16:Q:98:VAL:HG13	2.10	0.77
35:l:226:GLN:HE21	35:l:314:MET:HE1	1.48	0.77
35:l:226:GLN:NE2	35:l:314:MET:HE3	1.99	0.76
44:w:56:ARG:NH1	44:w:81:LEU:O	2.18	0.76
44:w:60:ILE:HG13	44:w:203:LEU:HD11	1.68	0.76
12:M:68:ARG:HD2	12:M:285:TRP:HE1	1.48	0.76
16:Q:268:TRP:CZ3	16:Q:272:THR:CG2	2.66	0.76
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.19	0.76
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
4:E:79:VAL:HG22	48:E:201:8Q1:C38	2.16	0.76
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.76
35:l:190:ILE:H	35:l:190:ILE:HD12	1.49	0.76
3:C:105:ARG:HA	41:s:37:PRO:HA	1.67	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	0.76
1:A:116:ASN:HD22	46:A:502:FMN:HM81	1.51	0.76
7:H:50:GLN:HE22	8:I:93:LYS:HA	1.50	0.76
11:L:75:ARG:NH1	11:L:119:ASP:OD2	2.16	0.76
12:M:54:GLU:OE2	12:M:62:ARG:NH2	2.19	0.76
9:J:130:ILE:CG2	49:J:401:NDP:H8A	2.10	0.75
12:M:543:LYS:HG3	12:M:565:PHE:HD2	1.51	0.75
36:m:115:VAL:O	36:m:117:ASN:N	2.18	0.75
39:p:54:GLU:OE2	48:p:201:8Q1:C38	2.34	0.75
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.19	0.75
5:F:42:VAL:HG21	12:M:671:LEU:HD12	1.66	0.75
24:a:55:PHE:CD2	39:p:118:TYR:CE1	2.64	0.75
9:J:221:HIS:ND1	9:J:222:ARG:N	2.35	0.75
16:Q:86:PRO:HG2	33:j:41:PHE:HE2	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:54:PHE:CD1	35:l:58:ASP:HA	2.21	0.75
35:l:228:GLY:C	35:l:229:LEU:HD23	2.11	0.75
19:U:82:LYS:NZ	42:u:121:ASP:OD1	2.18	0.75
35:l:190:ILE:HD11	35:l:196:TRP:NE1	2.02	0.75
12:M:128:CYS:HB2	12:M:129:PRO:HD3	1.68	0.75
20:V:40:ARG:HH22	20:V:55:LYS:HD3	1.50	0.75
9:J:77:GLY:O	9:J:102:GLN:NE2	2.19	0.75
16:Q:262:LEU:CD2	16:Q:268:TRP:CD1	2.60	0.75
24:a:189:ASN:ND2	42:u:142:TYR:OH	2.20	0.75
27:d:81:GLU:CD	37:n:43:MET:HE3	2.11	0.75
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	0.75
22:Y:84:PHE:CZ	35:l:483:PRO:CG	2.68	0.75
1:A:174:ARG:HG3	10:K:91:LEU:HD21	1.69	0.74
22:Y:71:TRP:CZ2	22:Y:75:HIS:CD2	2.74	0.74
22:Y:89:PRO:O	43:v:107:ARG:NH2	2.20	0.74
9:J:54:ILE:HB	9:J:78:SER:HB2	1.68	0.74
22:Y:84:PHE:CG	22:Y:85:PRO:HD3	2.22	0.74
47:b:201:PLX:H1C3	47:b:201:PLX:H32	1.68	0.74
35:l:533:MET:SD	52:l:702:PEE:C23	2.75	0.74
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.74
22:Y:45:ARG:HH21	35:l:439:THR:HG21	1.52	0.74
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.68	0.74
44:w:319:ILE:HG23	44:w:323:GLN:HE21	1.53	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	0.74
24:a:163:ARG:NH2	30:g:99:ASP:OD2	2.20	0.74
12:M:50:LEU:HB2	12:M:92:CYS:HA	1.68	0.74
52:V:202:PEE:H60	52:V:202:PEE:H41	1.67	0.74
22:Y:86:TYR:HH	43:v:100:LYS:HE2	1.52	0.74
27:d:154:ARG:NH2	30:g:108:TYR:O	2.19	0.74
35:l:78:LEU:HG	35:l:139:GLN:NE2	2.02	0.74
44:w:98:THR:O	44:w:337:ARG:NH2	2.18	0.74
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.74
24:a:168:TRP:NE1	30:g:88:GLU:OE1	2.20	0.74
39:p:170:ILE:HD12	39:p:170:ILE:N	2.02	0.74
40:r:114:GLU:HG3	42:u:169:PHE:HB3	1.68	0.74
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.74
26:c:123:PRO:HG3	39:p:75:GLN:HE21	1.52	0.74
33:j:6:ILE:HG13	41:s:6:LEU:HD11	1.68	0.74
35:l:135:ASN:OD1	35:l:198:PRO:HG3	1.88	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.73
39:p:27:LEU:HD11	39:p:44:MET:HG3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:289:LEU:HA	41:s:293:PHE:HB3	1.70	0.73
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	0.73
35:l:4:HIS:NE2	35:l:87:MET:HE1	2.02	0.73
9:J:174:ILE:HG13	9:J:182:ARG:HG3	1.70	0.73
12:M:406:ASN:HB2	12:M:438:LEU:HD21	1.68	0.73
52:V:202:PEE:C44	52:l:701:PEE:C45	2.66	0.73
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	0.73
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.73
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73
1:A:98:LYS:HD2	1:A:101:PHE:CE2	2.24	0.73
52:V:202:PEE:H39	52:V:202:PEE:H32	1.70	0.73
16:Q:345:ALA:HB2	21:W:19:ILE:HD11	1.70	0.73
9:J:132:ARG:NH2	49:J:401:NDP:C2B	2.52	0.73
18:T:83:ARG:NH1	18:T:102:ASN:OD1	2.22	0.73
1:A:158:ILE:HG21	1:A:166:ALA:HB2	1.69	0.73
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.22	0.73
31:h:70:GLN:HG2	36:m:115:VAL:HG12	1.71	0.73
44:w:209:VAL:HG13	44:w:214:VAL:HG21	1.70	0.73
27:d:154:ARG:NH1	30:g:111:ILE:O	2.22	0.72
35:l:571:ILE:CG1	52:l:701:PEE:O5	2.36	0.72
2:B:61:TRP:CH2	41:s:187:ILE:HD11	2.24	0.72
9:J:83:PRO:HB2	9:J:108:TRP:HE1	1.53	0.72
9:J:132:ARG:NH2	49:J:401:NDP:O2B	2.22	0.72
12:M:198:THR:HG22	14:O:39:PHE:HB3	1.70	0.72
16:Q:232:VAL:HG12	16:Q:234:GLN:H	1.54	0.72
35:l:227:LEU:HD12	35:l:230:HIS:CE1	2.24	0.72
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.72	0.72
24:a:54:LEU:HD22	25:b:26:GLN:O	1.90	0.72
34:k:3:LEU:HD22	36:m:117:ASN:HD21	1.53	0.72
35:l:451:LEU:H	35:l:453:PRO:HD2	1.54	0.72
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	0.72
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.72
33:j:25:PRO:O	33:j:27:LEU:N	2.22	0.72
35:l:384:PRO:O	35:l:389:PHE:HB2	1.89	0.72
1:A:219:LYS:HA	11:L:174:THR:HG22	1.71	0.72
1:A:381:GLN:HG2	45:A:501:SF4:S2	2.29	0.72
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.54	0.72
9:J:212:ARG:NH2	49:J:401:NDP:O2N	2.22	0.72
27:d:73:GLU:HG2	30:g:111:ILE:HD11	1.72	0.72
35:l:170:GLN:NE2	52:l:702:PEE:O2P	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:116:ALA:O	14:O:124:ARG:NH1	2.22	0.72
16:Q:85:GLY:CA	33:j:39:CYS:CB	2.67	0.72
25:b:109:THR:HB	25:b:113:THR:HA	1.71	0.72
32:i:167:TRP:CE3	35:l:573:THR:CB	2.72	0.72
35:l:59:GLN:HA	35:l:59:GLN:NE2	2.00	0.72
1:A:391:TRP:HH2	12:M:153:PHE:HA	1.55	0.72
3:C:143:GLU:OE2	3:C:145:ARG:NH2	2.23	0.72
11:L:137:PHE:O	11:L:141:ASN:ND2	2.15	0.72
1:A:124:THR:HG23	1:A:126:LYS:HG2	1.72	0.72
16:Q:282:GLU:OE2	16:Q:437:LYS:NZ	2.22	0.72
16:Q:333:ARG:NH2	16:Q:453:THR:O	2.22	0.72
22:Y:43:ARG:HG3	22:Y:46:GLN:HB2	1.72	0.72
24:a:55:PHE:CE2	39:p:118:TYR:HE2	1.96	0.72
35:l:450:LEU:C	35:l:450:LEU:HD22	2.15	0.72
1:A:327:ILE:HG23	1:A:331:VAL:HG13	1.72	0.71
9:J:221:HIS:CE1	9:J:222:ARG:CG	2.72	0.71
16:Q:241:MET:HG3	21:W:11:PRO:HB2	1.72	0.71
1:A:381:GLN:NE2	45:A:501:SF4:S3	2.63	0.71
12:M:374:THR:HB	12:M:377:ALA:HA	1.72	0.71
12:M:543:LYS:NZ	12:M:563:ASP:OD2	2.23	0.71
52:V:202:PEE:H60	52:V:202:PEE:H42	1.73	0.71
5:F:68:ARG:NH1	12:M:359:ASN:OD1	2.23	0.71
35:l:78:LEU:CD2	35:l:80:PHE:HE1	2.02	0.71
14:O:129:LYS:H	14:O:168:LEU:HA	1.53	0.71
16:Q:95:LEU:HD13	16:Q:97:LEU:HD23	1.73	0.71
27:d:136:ARG:NH2	28:e:138:GLU:O	2.23	0.71
12:M:63:PHE:O	12:M:181:ARG:NH2	2.23	0.71
14:O:187:GLN:HE21	14:O:190:ASP:HA	1.56	0.71
21:W:115:ARG:HH11	31:h:36:PHE:HD1	1.36	0.71
22:Y:86:TYR:HB3	22:Y:87:PRO:CA	2.19	0.71
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.71
35:l:379:ALA:HA	35:l:386:LEU:HD11	1.73	0.71
10:K:80:SER:HG	10:K:83:THR:HG1	1.38	0.71
15:P:134:SER:HG	15:P:139:SER:HG	1.25	0.71
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.72	0.71
47:r:502:PLX:H31	47:r:502:PLX:H72	1.73	0.71
12:M:566:ILE:HG13	12:M:580:ALA:HA	1.72	0.71
16:Q:432:LEU:HD12	16:Q:461:VAL:HG11	1.73	0.71
25:b:106:PRO:HA	25:b:115:GLU:OE2	1.89	0.71
35:l:567:SER:O	35:l:571:ILE:CD1	2.39	0.71
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.73	0.71
34:k:7:ASN:HD22	36:m:9:SER:HB2	1.47	0.71
35:l:10:LEU:HD22	35:l:46:ILE:HG21	1.72	0.71
39:p:104:LEU:HD21	39:p:119:PHE:HE1	1.55	0.71
1:A:158:ILE:HB	1:A:199:ARG:HG2	1.73	0.70
1:A:383:THR:HG22	12:M:75:CYS:HA	1.72	0.70
16:Q:281:GLU:N	16:Q:281:GLU:OE1	2.22	0.70
39:p:170:ILE:H	39:p:170:ILE:CD1	2.02	0.70
1:A:116:ASN:ND2	46:A:502:FMN:C8M	2.52	0.70
5:F:39:LYS:HG3	5:F:40:ARG:H	1.56	0.70
22:Y:86:TYR:OH	43:v:100:LYS:HE3	1.89	0.70
25:b:10:LEU:HD22	39:p:156:PRO:HB2	1.71	0.70
33:j:67:LEU:HD21	34:k:68:ALA:HB3	1.72	0.70
35:l:78:LEU:HG	35:l:139:GLN:HE22	1.55	0.70
35:l:135:ASN:HD21	35:l:199:GLN:HE22	1.39	0.70
4:E:25:MET:O	4:E:29:LYS:CG	2.38	0.70
35:l:71:THR:HG21	40:r:307:TRP:HE1	1.54	0.70
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.73	0.70
8:I:106:LEU:O	8:I:108:SER:N	2.19	0.70
12:M:557:ARG:NH1	12:M:579:ILE:O	2.24	0.70
35:l:338:MET:HE3	35:l:372:SER:HB2	1.74	0.70
1:A:116:ASN:O	1:A:245:VAL:HG23	1.91	0.70
15:P:93:VAL:HB	15:P:154:GLU:HB2	1.72	0.70
35:l:190:ILE:HG13	35:l:196:TRP:CD1	2.27	0.70
52:l:701:PEE:H46	40:r:155:VAL:HG12	1.71	0.70
40:r:44:GLN:O	40:r:46:ASN:N	2.24	0.70
2:B:184:ASN:HD21	13:N:127:TYR:H	1.38	0.70
4:E:70:ASN:O	48:E:201:8Q1:O40	2.10	0.70
16:Q:48:GLY:HA2	32:i:228:LEU:HD11	1.74	0.70
22:Y:81:LEU:HD23	22:Y:81:LEU:C	2.15	0.70
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.70
21:W:108:GLU:OE2	31:h:75:ARG:NH1	2.24	0.70
6:X:91:ASP:OD1	23:Z:47:ARG:NH1	2.24	0.70
35:l:78:LEU:CD2	35:l:80:PHE:CE1	2.74	0.70
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.70
25:b:105:PHE:CE2	43:v:68:LYS:HA	2.26	0.70
27:d:59:HIS:HE1	28:e:120:ARG:CB	1.97	0.70
27:d:65:VAL:H	27:d:85:GLN:NE2	1.89	0.70
35:l:100:ILE:HD12	35:l:246:LEU:HG	1.72	0.70
35:l:546:GLN:OE1	40:r:278:ARG:NE	2.22	0.70
35:l:567:SER:O	35:l:571:ILE:HD12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.09	0.70
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.70
21:W:134:LEU:HD11	36:m:2:MET:HB2	1.72	0.70
32:i:298:TYR:O	32:i:303:THR:OG1	2.08	0.70
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	0.69
9:J:210:GLU:O	9:J:210:GLU:HG2	1.92	0.69
22:Y:86:TYR:CB	22:Y:87:PRO:HA	2.22	0.69
9:J:233:TRP:HA	9:J:272:LEU:HD21	1.74	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.25	0.69
15:P:46:THR:O	16:Q:162:ARG:N	2.16	0.69
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
30:g:15:ASP:HB2	30:g:18:ARG:HH21	1.57	0.69
34:k:66:PHE:HE1	36:m:159:THR:HG21	1.57	0.69
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.69
41:s:235:ASN:HD22	41:s:267:THR:HG22	1.56	0.69
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.69
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.69
34:k:2:PRO:CG	36:m:115:VAL:HG21	2.21	0.69
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.74	0.69
25:b:16:ARG:O	25:b:20:ARG:HG2	1.93	0.69
47:b:201:PLX:O3	47:b:201:PLX:O7	2.05	0.69
44:w:67:CYS:N	44:w:70:LYS:HD3	2.07	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.56	0.69
35:l:226:GLN:HG3	35:l:280:LEU:HD23	1.74	0.69
52:W:201:PEE:H24	52:W:201:PEE:H53	1.74	0.69
25:b:54:LYS:HG3	25:b:55:SER:H	1.58	0.69
28:e:76:TYR:O	40:r:82:ARG:NH1	2.21	0.69
28:e:129:ARG:NH1	28:e:136:ILE:O	2.24	0.69
35:l:141:PHE:HE2	40:r:375:LEU:HD21	1.58	0.69
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.69
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.58	0.69
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.69
24:a:98:LEU:HA	27:d:57:TYR:CD1	2.28	0.69
35:l:4:HIS:HE1	35:l:87:MET:HE3	1.57	0.69
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.24	0.69
35:l:4:HIS:CE1	35:l:87:MET:HE1	2.28	0.69
52:l:701:PEE:H37	40:r:155:VAL:HG11	1.70	0.69
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	0.68
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.68
25:b:120:MET:SD	43:v:65:ARG:NH2	2.66	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:4:HIS:CE1	35:l:87:MET:HE3	2.28	0.68
52:l:701:PEE:H36	40:r:155:VAL:CG1	2.21	0.68
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.68
15:P:157:VAL:HG21	15:P:181:HIS:HD2	1.59	0.68
16:Q:190:HIS:HD2	16:Q:452:GLY:HA3	1.58	0.68
25:b:94:PRO:HB3	27:d:5:TRP:HA	1.74	0.68
36:m:121:VAL:O	36:m:123:SER:N	2.26	0.68
44:w:63:ASP:OD2	44:w:241:TYR:OH	2.11	0.68
7:H:12:VAL:HG13	16:Q:280:ALA:N	2.07	0.68
12:M:225:ILE:HD12	12:M:285:TRP:HH2	1.57	0.68
18:T:79:GLU:HG2	18:T:120:ARG:HB3	1.76	0.68
25:b:12:LEU:HB3	25:b:16:ARG:HH12	1.58	0.68
33:j:30:TYR:HB2	33:j:33:LYS:HD2	1.75	0.68
35:l:396:ILE:O	35:l:400:ASN:ND2	2.26	0.68
9:J:171:ASN:O	9:J:181:LEU:CG	2.41	0.68
12:M:144:MET:SD	16:Q:380:HIS:ND1	2.63	0.68
16:Q:80:ILE:O	16:Q:100:GLU:CA	2.42	0.68
20:V:81:ARG:HG2	20:V:83:LYS:HG3	1.75	0.68
3:C:128:ASN:ND2	3:C:164:TYR:O	2.24	0.68
14:O:137:THR:HG21	14:O:176:CYS:HB2	1.74	0.68
24:a:55:PHE:CD2	39:p:118:TYR:CG	2.82	0.68
40:r:144:ASN:O	40:r:147:THR:OG1	2.10	0.68
9:J:203:PRO:HA	9:J:265:PHE:HB2	1.75	0.68
9:J:247:LYS:HD2	9:J:340:ILE:HD12	1.74	0.68
46:A:502:FMN:O4'	46:A:502:FMN:H9	1.94	0.68
3:C:159:TYR:HE1	16:Q:135:TYR:CZ	2.12	0.68
12:M:194:ASP:O	12:M:208:THR:OG1	2.10	0.68
16:Q:262:LEU:HD13	16:Q:268:TRP:NE1	2.08	0.68
32:i:180:ALA:O	32:i:183:SER:OG	2.08	0.68
35:l:222:GLY:HA3	35:l:229:LEU:HD12	1.74	0.68
6:G:105:MET:HG3	6:G:106:LYS:HG3	1.76	0.68
49:J:401:NDP:O2X	49:J:401:NDP:H1B	1.94	0.68
22:Y:86:TYR:HB3	22:Y:87:PRO:HA	1.75	0.68
47:b:201:PLX:H6	47:b:201:PLX:C11	2.24	0.68
47:b:201:PLX:H6	47:b:201:PLX:H111	1.75	0.68
35:l:447:ASN:CG	35:l:448:PRO:HD2	2.16	0.68
41:s:85:LEU:HB3	41:s:233:MET:SD	2.34	0.68
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.67
52:W:201:PEE:H36	33:j:7:LEU:HD22	1.77	0.67
39:p:48:PHE:HE1	48:p:201:8Q1:C7	2.06	0.67
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ILE:HD11	16:Q:385:TYR:HB3	1.74	0.67
12:M:476:LEU:HB3	12:M:515:ILE:HG22	1.74	0.67
24:a:98:LEU:HA	27:d:57:TYR:HD1	1.60	0.67
26:c:122:THR:O	38:o:12:ARG:NH2	2.27	0.67
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.67
42:u:34:ALA:HB2	42:u:120:PRO:HD3	1.75	0.67
2:B:119:ALA:HA	15:P:233:PHE:HE2	1.60	0.67
7:H:114:TRP:HE1	16:Q:394:GLY:HA2	1.59	0.67
9:J:173:ASN:HB2	9:J:327:MET:HE1	1.76	0.67
22:Y:81:LEU:CD2	43:v:92:HIS:CD2	2.78	0.67
25:b:88:TYR:O	25:b:92:GLU:CB	2.42	0.67
26:c:62:TYR:OH	26:c:74:ASP:O	2.11	0.67
34:k:25:HIS:HA	34:k:90:VAL:HG13	1.77	0.67
35:l:188:TRP:CD2	35:l:192:HIS:HD2	2.09	0.67
1:A:295:PRO:HG2	1:A:298:GLU:HB2	1.77	0.67
1:A:379:CYS:HA	12:M:200:ARG:HB2	1.74	0.67
16:Q:87:GLN:OE1	16:Q:87:GLN:N	2.26	0.67
16:Q:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.67
24:a:98:LEU:CB	27:d:57:TYR:CD1	2.77	0.67
34:k:83:ASN:ND2	36:m:173:GLY:O	2.27	0.67
35:l:444:ASN:OD1	35:l:445:GLU:N	2.26	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	0.67
3:C:137:VAL:HG21	16:Q:87:GLN:NE2	2.05	0.67
6:G:145:VAL:HA	6:G:148:ILE:HD12	1.77	0.67
12:M:500:ILE:O	12:M:503:THR:OG1	2.12	0.67
16:Q:80:ILE:O	16:Q:100:GLU:HA	1.94	0.67
22:Y:84:PHE:CD2	22:Y:85:PRO:HD2	2.30	0.67
44:w:132:GLN:HE22	44:w:169:PHE:HD2	1.41	0.67
10:K:100:SER:HA	14:O:72:GLU:HB3	1.77	0.67
14:O:54:ASP:OD1	14:O:60:TYR:OH	2.11	0.67
25:b:51:LEU:HD11	25:b:62:HIS:CD2	2.30	0.67
27:d:49:GLN:OE1	27:d:49:GLN:N	2.27	0.67
33:j:3:PHE:HA	33:j:6:ILE:HD13	1.77	0.67
41:s:265:LEU:O	41:s:268:SER:OG	2.10	0.67
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.67
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.67
32:i:170:LEU:HD12	35:l:574:SER:HB3	1.77	0.67
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.77	0.67
14:O:133:GLN:HB2	14:O:174:VAL:HG21	1.75	0.67
25:b:115:GLU:HG2	25:b:116:VAL:N	2.10	0.67
26:c:184:TYR:CB	43:v:37:ARG:HG3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:5:LEU:HD13	41:s:3:MET:HE1	1.77	0.67
33:j:36:PRO:HG2	33:j:43:PRO:HG3	1.77	0.67
34:k:3:LEU:HD23	36:m:117:ASN:ND2	2.09	0.67
40:r:15:THR:O	40:r:93:LYS:NZ	2.24	0.67
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.59	0.67
10:K:99:PRO:HG2	14:O:71:PRO:HB3	1.76	0.67
11:L:58:LYS:NZ	11:L:139:GLU:OE1	2.27	0.67
12:M:381:LEU:O	12:M:383:SER:N	2.24	0.67
16:Q:338:ARG:HH22	21:W:23:ARG:HB3	1.58	0.67
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.77	0.67
25:b:93:LYS:CE	35:l:65:ASN:O	2.41	0.67
3:C:125:THR:HG21	16:Q:118:ARG:HG2	1.76	0.66
3:C:161:HIS:O	3:C:168:ARG:NH2	2.28	0.66
25:b:38:GLN:OE1	25:b:39:LYS:N	2.28	0.66
27:d:108:GLN:NE2	35:l:199:GLN:O	2.29	0.66
35:l:190:ILE:HG12	35:l:196:TRP:CE2	2.31	0.66
40:r:369:LEU:O	40:r:372:THR:OG1	2.12	0.66
2:B:111:CYS:O	2:B:139:ARG:NH2	2.28	0.66
12:M:173:MET:O	12:M:175:ARG:N	2.24	0.66
40:r:150:LEU:O	40:r:153:THR:OG1	2.12	0.66
41:s:169:GLN:HE21	41:s:174:LEU:H	1.42	0.66
21:W:86:MET:SD	21:W:128:ARG:NH1	2.66	0.66
27:d:108:GLN:NE2	35:l:203:LEU:HG	2.10	0.66
34:k:51:THR:O	34:k:53:SER:N	2.27	0.66
22:Y:90:SER:HA	43:v:107:ARG:HH12	1.59	0.66
35:l:226:GLN:HG2	35:l:280:LEU:CD2	2.25	0.66
35:l:359:MET:O	35:l:436:ARG:NH2	2.29	0.66
41:s:200:LEU:HD12	41:s:285:LEU:HD11	1.77	0.66
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	0.66
24:a:58:ARG:HH21	24:a:61:ARG:HD2	1.60	0.66
40:r:305:THR:O	40:r:308:SER:OG	2.12	0.66
1:A:116:ASN:ND2	46:A:502:FMN:C9	2.59	0.66
4:E:107:PHE:HB3	4:E:109:GLU:HG3	1.78	0.66
25:b:114:GLY:O	25:b:115:GLU:HB3	1.95	0.66
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.66
25:b:105:PHE:CZ	43:v:67:LEU:HB2	2.31	0.66
11:L:81:VAL:HG11	11:L:150:ARG:HA	1.78	0.66
34:k:26:LEU:HD11	34:k:78:LEU:HD21	1.78	0.66
1:A:74:ASP:O	1:A:78:GLY:N	2.27	0.66
12:M:300:GLN:HB2	13:N:137:TRP:HA	1.77	0.66
35:l:453:PRO:HA	35:l:456:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:202:GLU:O	41:s:204:GLU:N	2.29	0.66
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.78	0.65
12:M:254:MET:HB2	12:M:290:THR:HG22	1.78	0.65
22:Y:85:PRO:HG2	43:v:99:MET:HE2	1.78	0.65
43:v:74:PHE:O	43:v:76:ASN:ND2	2.29	0.65
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.65
32:i:12:THR:HG22	36:m:158:TRP:NE1	2.10	0.65
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.65
22:Y:81:LEU:HD12	43:v:88:ASP:HB3	1.78	0.65
16:Q:271:ARG:NH1	41:s:281:ARG:HA	2.10	0.65
41:s:185:TRP:NE1	41:s:238:THR:HG22	2.11	0.65
44:w:58:ARG:NH1	44:w:279:ASP:O	2.29	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	0.65
15:P:173:MET:HE1	15:P:189:THR:HG23	1.77	0.65
34:k:11:ALA:HB1	36:m:16:PHE:CD2	2.31	0.65
44:w:188:ASN:HA	44:w:191:LYS:HE2	1.77	0.65
8:I:66:PRO:HB3	15:P:79:SER:HB3	1.77	0.65
9:J:48:ARG:NH1	9:J:98:GLY:O	2.29	0.65
52:W:201:PEE:H1	41:s:98:LEU:HD22	1.79	0.65
36:m:147:ASP:OD1	36:m:148:TYR:N	2.30	0.65
41:s:20:LEU:HD13	41:s:232:ILE:HD11	1.78	0.65
9:J:132:ARG:NH2	49:J:401:NDP:H2B	2.11	0.65
47:U:101:PLX:HO9	33:j:106:TRP:CD1	2.13	0.65
34:k:1:MET:HB2	34:k:4:ILE:HD13	1.77	0.65
44:w:249:MET:HB3	44:w:255:VAL:HG11	1.79	0.65
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	0.65
25:b:110:ILE:HG23	25:b:111:LEU:CD2	2.26	0.65
32:i:42:PRO:HG3	36:m:166:ILE:HG23	1.78	0.65
1:A:424:ILE:HG22	45:A:501:SF4:S4	2.36	0.65
12:M:169:VAL:HG12	12:M:223:ILE:HD11	1.79	0.65
17:S:53:ARG:NH2	31:h:105:ARG:HD3	2.12	0.65
30:g:27:ASP:OD2	30:g:29:ARG:NH1	2.29	0.65
34:k:4:ILE:HD13	36:m:125:MET:SD	2.34	0.65
7:H:12:VAL:HG11	16:Q:278:VAL:O	1.96	0.65
7:H:72:LEU:HD22	7:H:77:LEU:HD13	1.78	0.65
18:T:40:THR:OG1	18:T:42:THR:O	2.14	0.65
22:Y:79:GLU:O	22:Y:80:VAL:HG13	1.96	0.65
35:l:227:LEU:HD12	35:l:230:HIS:HD1	1.60	0.65
27:d:110:ARG:HG2	27:d:110:ARG:NH1	2.11	0.64
28:e:76:TYR:H	40:r:432:ARG:HD2	1.61	0.64
42:u:31:HIS:CE1	42:u:119:ARG:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:332:ARG:O	44:w:338:LYS:CG	2.45	0.64
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.78	0.64
9:J:205:ASP:HB2	9:J:239:PRO:HA	1.79	0.64
12:M:65:TYR:O	12:M:181:ARG:NH2	2.29	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CZ	2.32	0.64
21:W:68:ARG:HD3	36:m:134:PHE:CE1	2.32	0.64
24:a:94:GLY:O	24:a:96:ALA:N	2.30	0.64
2:B:51:VAL:HG22	2:B:54:ARG:HH11	1.62	0.64
11:L:111:LEU:HG	11:L:112:MET:HG2	1.80	0.64
12:M:618:GLU:OE2	12:M:620:TRP:NE1	2.30	0.64
16:Q:35:ARG:NH1	28:e:60:GLU:OE2	2.28	0.64
52:l:701:PEE:C22	40:r:155:VAL:HG21	2.27	0.64
41:s:228:TYR:HD1	41:s:231:ILE:HD12	1.63	0.64
3:C:93:MET:HG2	3:C:110:PHE:HZ	1.63	0.64
5:F:56:ARG:NH2	12:M:527:ASP:O	2.29	0.64
31:h:91:LYS:HG3	31:h:92:TYR:H	1.62	0.64
35:l:226:GLN:OE1	35:l:226:GLN:HA	1.97	0.64
35:l:307:SER:HA	35:l:310:LEU:HD12	1.80	0.64
2:B:151:ILE:HG21	3:C:159:TYR:HD2	1.62	0.64
16:Q:80:ILE:HB	16:Q:101:LEU:O	1.97	0.64
21:W:39:GLY:O	21:W:42:THR:OG1	2.15	0.64
25:b:112:GLU:N	25:b:112:GLU:OE2	2.31	0.64
32:i:291:TYR:CD2	52:l:701:PEE:H51	2.32	0.64
35:l:97:THR:HG21	35:l:125:LEU:CD1	2.20	0.64
52:l:701:PEE:H36	40:r:155:VAL:HG21	1.79	0.64
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.64
18:T:39:VAL:HG12	18:T:45:VAL:HB	1.79	0.64
32:i:197:ASN:HB3	32:i:269:GLU:OE1	1.98	0.64
35:l:405:ASN:OD1	35:l:406:ALA:N	2.31	0.64
42:u:140:ASN:ND2	42:u:143:HIS:O	2.31	0.64
10:K:81:THR:HB	14:O:88:ARG:HD2	1.78	0.64
12:M:543:LYS:HG3	12:M:565:PHE:CD2	2.33	0.64
12:M:591:GLU:OE1	12:M:591:GLU:N	2.30	0.64
25:b:108:ASP:O	25:b:113:THR:HA	1.98	0.64
26:c:159:LYS:HA	43:v:98:ARG:HH12	1.62	0.64
32:i:288:LEU:HD21	52:l:701:PEE:H64	1.80	0.64
35:l:67:HIS:CE1	35:l:75:GLN:HG3	2.33	0.64
24:a:95:GLN:HA	24:a:116:PRO:HD3	1.79	0.64
35:l:332:HIS:HE1	35:l:336:LYS:HZ1	1.46	0.64
2:B:68:LEU:HG	41:s:272:TRP:HE1	1.62	0.64
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	0.64
24:a:96:ALA:CB	27:d:55:TYR:CB	2.70	0.64
31:h:5:ASP:HB3	31:h:8:LYS:HB3	1.80	0.64
35:l:88:MET:O	35:l:92:VAL:HG23	1.98	0.64
35:l:501:ALA:O	35:l:505:ASN:ND2	2.29	0.64
41:s:280:PHE:HE2	41:s:288:LEU:HD11	1.63	0.64
14:O:245:VAL:O	14:O:247:ALA:N	2.31	0.63
16:Q:145:MET:H	16:Q:178:THR:HG21	1.63	0.63
16:Q:171:ARG:HH21	16:Q:231:GLY:HA2	1.61	0.63
20:V:27:SER:O	20:V:30:SER:OG	2.14	0.63
52:W:201:PEE:H75	41:s:77:LEU:HD23	1.75	0.63
24:a:127:ASP:HB3	24:a:131:LYS:HD3	1.80	0.63
35:l:537:ILE:HD11	52:l:702:PEE:H38	1.80	0.63
40:r:112:ALA:O	40:r:113:THR:OG1	2.14	0.63
1:A:85:LEU:HD21	1:A:247:THR:HG23	1.80	0.63
6:G:120:MET:HA	6:G:123:GLU:HG2	1.79	0.63
8:I:23:LYS:NZ	16:Q:252:SER:OG	2.31	0.63
44:w:89:ALA:N	44:w:160:GLU:OE1	2.27	0.63
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.63
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.63
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	0.63
29:f:38:LYS:HB2	29:f:39:PRO:HD3	1.81	0.63
35:l:190:ILE:HD11	35:l:196:TRP:HE1	1.61	0.63
36:m:116:VAL:O	36:m:118:PHE:N	2.31	0.63
2:B:57:ARG:O	16:Q:266:ARG:NH2	2.30	0.63
3:C:137:VAL:CG2	16:Q:87:GLN:NE2	2.59	0.63
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.63
52:V:202:PEE:H32	52:V:202:PEE:C24	2.24	0.63
27:d:112:GLY:O	27:d:115:TYR:HB3	1.99	0.63
1:A:398:ARG:NH1	1:A:408:GLU:OE1	2.25	0.63
22:Y:74:TRP:HE3	22:Y:75:HIS:HA	1.62	0.63
24:a:87:THR:HG22	47:b:201:PLX:H131	1.81	0.63
33:j:77:TRP:NE1	41:s:318:THR:O	2.31	0.63
42:u:24:VAL:HG22	42:u:86:TRP:NE1	2.12	0.63
1:A:207:GLY:O	46:A:502:FMN:C5A	2.47	0.63
2:B:70:MET:HE2	16:Q:257:GLU:HG2	1.79	0.63
23:Z:32:ILE:HD12	39:p:35:ASP:OD1	1.98	0.63
34:k:92:ASN:ND2	35:l:582:GLY:O	2.31	0.63
38:o:56:ARG:HH12	38:o:59:LEU:C	2.06	0.63
40:r:373:ILE:HG23	40:r:448:SER:HA	1.81	0.63
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:84:PHE:HE2	16:Q:91:ALA:HB2	1.63	0.63
25:b:105:PHE:CE2	43:v:68:LYS:CA	2.81	0.63
32:i:271:THR:HG22	32:i:276:LEU:HD22	1.81	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	0.63
22:Y:73:PHE:HA	35:l:385:PHE:CE2	2.33	0.63
25:b:88:TYR:CD1	47:b:201:PLX:C1C	2.79	0.63
35:l:534:HIS:ND1	52:l:702:PEE:C11	2.59	0.63
40:r:210:TYR:O	40:r:213:HIS:ND1	2.31	0.63
41:s:169:GLN:NE2	41:s:244:GLY:H	1.96	0.63
10:K:82:TYR:HD2	14:O:62:ARG:HH12	1.47	0.63
12:M:467:LYS:HG3	12:M:503:THR:HB	1.81	0.63
16:Q:72:PRO:HB2	32:i:50:PRO:HG3	1.80	0.63
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.63
32:i:72:MET:HE1	34:k:9:MET:HG2	1.81	0.63
36:m:56:PHE:HD2	41:s:107:ALA:HB1	1.64	0.63
43:v:40:VAL:HB	43:v:61:HIS:CE1	2.34	0.63
2:B:99:HIS:NE2	45:B:302:SF4:S1	2.70	0.62
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.81	0.62
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.81	0.62
35:l:229:LEU:HD23	35:l:229:LEU:N	2.13	0.62
41:s:107:ALA:O	41:s:110:SER:OG	2.11	0.62
44:w:117:PHE:HB2	44:w:131:LEU:HD21	1.80	0.62
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
47:b:201:PLX:O4	47:b:201:PLX:H11	1.99	0.62
34:k:82:SER:HB3	34:k:87:LEU:HD23	1.80	0.62
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.62
35:l:124:PHE:HE1	35:l:147:VAL:HG13	1.64	0.62
35:l:450:LEU:O	35:l:450:LEU:HD13	2.00	0.62
13:N:29:ARG:NH2	13:N:65:THR:O	2.23	0.62
14:O:158:ILE:HD11	14:O:164:THR:HB	1.81	0.62
32:i:245:PRO:HB3	32:i:297:ILE:HG12	1.80	0.62
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.81	0.62
12:M:627:SER:OG	12:M:632:MET:O	2.17	0.62
25:b:7:ASP:HB2	39:p:156:PRO:HG3	1.79	0.62
43:v:52:ARG:O	43:v:56:ARG:NH1	2.33	0.62
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	0.62
9:J:48:ARG:HH21	15:P:211:ARG:HD2	1.64	0.62
22:Y:96:GLU:O	22:Y:97:LEU:HB2	1.98	0.62
23:Z:24:ILE:HD11	23:Z:47:ARG:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:30:HIS:CE1	42:u:119:ARG:HH11	2.17	0.62
6:G:80:GLN:HE22	6:G:100:VAL:HG13	1.63	0.62
11:L:75:ARG:HH21	11:L:101:PHE:HB3	1.63	0.62
16:Q:150:ALA:HB1	16:Q:400:ILE:HG13	1.81	0.62
9:J:241:TYR:CE2	9:J:243:VAL:HB	2.35	0.62
15:P:83:GLU:HB3	15:P:142:ARG:HH12	1.65	0.62
35:l:54:PHE:HD2	35:l:55:MET:HE2	1.65	0.62
36:m:56:PHE:CD2	41:s:107:ALA:HB1	2.35	0.62
44:w:60:ILE:O	44:w:159:LEU:N	2.33	0.62
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	0.62
26:c:159:LYS:HA	43:v:98:ARG:NH2	2.13	0.62
35:l:37:LYS:NZ	35:l:98:TRP:NE1	2.47	0.62
2:B:36:TYR:HB3	8:I:104:TRP:CE3	2.34	0.62
15:P:154:GLU:HA	15:P:179:ALA:HB2	1.81	0.62
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.30	0.62
17:S:53:ARG:HB2	31:h:105:ARG:HH12	1.64	0.62
32:i:37:MET:HE1	32:i:60:PHE:HA	1.82	0.62
52:l:701:PEE:H32	40:r:155:VAL:HG21	1.80	0.62
38:o:26:SER:O	38:o:29:THR:OG1	2.15	0.62
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.33	0.61
12:M:387:LEU:HA	12:M:514:ASN:HB2	1.82	0.61
14:O:143:ARG:HB3	14:O:184:PRO:HD3	1.82	0.61
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.81	0.61
24:a:55:PHE:CD2	39:p:118:TYR:CD1	2.88	0.61
27:d:107:CYS:SG	27:d:119:CYS:HA	2.39	0.61
34:k:10:LEU:HD12	36:m:102:LEU:HD12	1.82	0.61
35:l:4:HIS:HE1	35:l:87:MET:CE	2.10	0.61
35:l:216:LEU:HD22	35:l:259:LEU:HD21	1.80	0.61
36:m:118:PHE:CD1	36:m:121:VAL:HB	2.34	0.61
12:M:282:ASN:HA	12:M:413:LEU:HD23	1.82	0.61
12:M:546:PHE:HB2	12:M:568:TYR:HA	1.81	0.61
35:l:303:ALA:O	35:l:306:THR:OG1	2.17	0.61
35:l:450:LEU:HD22	35:l:450:LEU:O	2.00	0.61
47:r:502:PLX:H31	47:r:502:PLX:C7	2.30	0.61
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.61
16:Q:51:VAL:HG13	32:i:171:ASN:OD1	2.00	0.61
41:s:186:PHE:O	41:s:189:THR:OG1	2.16	0.61
3:C:105:ARG:HB3	41:s:39:VAL:HG23	1.81	0.61
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	0.61
27:d:60:ARG:HG2	27:d:60:ARG:NH1	2.12	0.61
35:l:37:LYS:NZ	35:l:98:TRP:CD1	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:61:LEU:HD22	40:r:241:TYR:HD1	1.64	0.61
1:A:161:GLU:O	14:O:192:TYR:OH	2.18	0.61
12:M:177:ILE:HG13	12:M:179:CYS:SG	2.40	0.61
22:Y:81:LEU:HD23	22:Y:82:GLY:N	2.14	0.61
40:r:150:LEU:HD21	40:r:154:LEU:HD12	1.79	0.61
1:A:88:ARG:O	1:A:244:ASN:ND2	2.32	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.33	0.61
12:M:346:VAL:HB	12:M:548:LEU:HD13	1.82	0.61
14:O:87:GLN:O	14:O:91:GLY:N	2.23	0.61
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
25:b:42:PRO:HA	25:b:45:LYS:HB2	1.82	0.61
35:l:194:ASN:HB2	38:o:125:PHE:O	2.01	0.61
36:m:118:PHE:HE1	36:m:124:TRP:HE1	1.47	0.61
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.61
7:H:89:ASN:O	7:H:93:LYS:HG2	2.00	0.61
9:J:226:ILE:HD12	9:J:289:LEU:N	2.16	0.61
9:J:286:ARG:NH2	9:J:356:HIS:O	2.34	0.61
12:M:534:VAL:HG12	12:M:536:ALA:H	1.66	0.61
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
16:Q:38:GLN:HE21	32:i:304:LEU:HB2	1.64	0.61
16:Q:53:TYR:HE1	52:l:701:PEE:P	2.22	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
25:b:12:LEU:HB3	25:b:16:ARG:NH1	2.15	0.61
25:b:14:GLN:NE2	39:p:164:PRO:HD3	2.15	0.61
31:h:37:GLU:HB2	31:h:63:PHE:CE1	2.35	0.61
33:j:32:GLU:O	33:j:37:TYR:OH	2.18	0.61
44:w:67:CYS:H	44:w:70:LYS:HD3	1.65	0.61
44:w:160:GLU:HG2	44:w:161:ARG:N	2.13	0.61
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.61
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.61
13:N:130:THR:N	18:T:44:GLN:OE1	2.34	0.61
35:l:552:LEU:HD13	38:o:90:GLY:HA2	1.83	0.61
1:A:339:PHE:HB3	1:A:349:LEU:HD13	1.81	0.61
11:L:75:ARG:HH11	11:L:104:ARG:HE	1.49	0.61
15:P:212:TYR:HA	15:P:219:VAL:HA	1.83	0.61
22:Y:73:PHE:O	22:Y:73:PHE:HD1	1.84	0.61
3:C:184:PRO:HD3	16:Q:223:HIS:HD2	1.65	0.61
14:O:137:THR:OG1	14:O:176:CYS:N	2.34	0.61
51:V:201:CDL:OA7	51:V:201:CDL:O1	2.16	0.61
32:i:58:LYS:HE3	35:l:584:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:280:PHE:CE2	41:s:288:LEU:HD11	2.36	0.61
12:M:31:LEU:HD22	12:M:44:GLU:HA	1.83	0.60
12:M:483:ARG:O	12:M:485:ASP:N	2.34	0.60
17:S:50:ARG:HA	31:h:105:ARG:CZ	2.30	0.60
27:d:59:HIS:NE2	28:e:121:GLU:HG2	2.16	0.60
30:g:9:PRO:O	30:g:11:ARG:N	2.32	0.60
35:l:427:ILE:HG23	35:l:431:LEU:HD12	1.82	0.60
35:l:508:THR:O	39:p:36:LYS:NZ	2.30	0.60
41:s:28:LEU:O	41:s:32:GLN:HB2	2.01	0.60
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	0.60
11:L:128:PHE:HA	15:P:121:THR:HG22	1.82	0.60
12:M:228:VAL:HG23	12:M:230:ALA:H	1.66	0.60
12:M:339:ALA:HB3	12:M:544:VAL:HG12	1.82	0.60
33:j:55:PHE:O	33:j:58:VAL:HG12	2.01	0.60
40:r:447:LEU:HD13	40:r:454:ILE:HD11	1.83	0.60
40:r:447:LEU:HD11	47:r:502:PLX:H382	1.82	0.60
2:B:103:ARG:NH2	18:T:66:ASN:O	2.35	0.60
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.34	0.60
9:J:171:ASN:HB2	9:J:181:LEU:HD11	1.84	0.60
12:M:345:LEU:HB2	12:M:548:LEU:HD21	1.84	0.60
29:f:55:TRP:O	29:f:59:ILE:HG12	2.00	0.60
35:l:37:LYS:HE2	35:l:98:TRP:HD1	0.69	0.60
43:v:8:ARG:HH11	43:v:106:ARG:NH2	1.97	0.60
3:C:205:ARG:HG3	3:C:205:ARG:O	2.02	0.60
25:b:88:TYR:HD1	25:b:92:GLU:OE2	1.82	0.60
25:b:100:LYS:O	25:b:101:LYS:HG2	2.01	0.60
34:k:3:LEU:CD2	36:m:117:ASN:ND2	2.60	0.60
9:J:272:LEU:HD23	9:J:274:PHE:H	1.65	0.60
12:M:352:VAL:HG21	12:M:646:LEU:HD21	1.82	0.60
21:W:111:PHE:HE2	21:W:117:VAL:HG11	1.66	0.60
6:X:72:PRO:HG3	35:l:442:ASN:HD22	1.65	0.60
30:g:32:TYR:OH	32:i:335:LEU:O	2.13	0.60
9:J:208:GLY:H	9:J:211:ASP:HB2	1.66	0.60
9:J:319:VAL:O	9:J:323:HIS:ND1	2.28	0.60
16:Q:338:ARG:HH12	21:W:23:ARG:HB3	1.65	0.60
25:b:115:GLU:HG2	25:b:116:VAL:H	1.65	0.60
31:h:49:TYR:HA	31:h:52:ALA:HB3	1.82	0.60
37:n:10:ASP:HB3	40:r:19:LYS:HZ3	1.65	0.60
37:n:50:GLN:HG3	37:n:51:PRO:HD2	1.83	0.60
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.82	0.60
16:Q:78:LYS:HE2	33:j:48:ARG:HH21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.14	0.60
52:W:201:PEE:C44	41:s:77:LEU:CD2	2.67	0.60
26:c:84:HIS:CE1	26:c:114:ARG:HA	2.37	0.60
32:i:291:TYR:CE2	52:l:701:PEE:C32	2.85	0.60
4:E:97:TRP:HH2	15:P:185:ARG:HH11	1.49	0.60
9:J:217:PHE:HB2	9:J:280:ILE:HD13	1.83	0.60
12:M:602:ARG:HE	12:M:659:ILE:HD11	1.67	0.60
27:d:54:ARG:HD3	27:d:56:TYR:CE1	2.37	0.60
35:l:575:ILE:O	35:l:578:SER:OG	2.16	0.60
40:r:190:TRP:NE1	47:r:501:PLX:H1A2	2.17	0.60
44:w:65:ASN:HD22	44:w:209:VAL:HG21	1.67	0.60
7:H:77:LEU:O	7:H:80:VAL:HG12	2.02	0.60
9:J:188:GLU:HG3	9:J:200:ILE:HG21	1.83	0.60
13:N:137:TRP:CH2	13:N:140:PRO:HD3	2.36	0.60
16:Q:271:ARG:HD3	41:s:279:ARG:O	2.01	0.60
47:U:101:PLX:H252	33:j:106:TRP:CD1	2.36	0.60
26:c:105:MET:HE2	38:o:65:LEU:HA	1.83	0.60
27:d:108:GLN:HG2	35:l:199:GLN:CB	2.31	0.60
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	0.60
2:B:61:TRP:HH2	41:s:187:ILE:HD11	1.67	0.60
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	0.60
35:l:149:ILE:HD12	40:r:369:LEU:HD21	1.83	0.60
12:M:460:HIS:CD2	12:M:462:PHE:HB3	2.38	0.59
13:N:129:THR:HA	18:T:44:GLN:HE22	1.67	0.59
39:p:121:LYS:O	39:p:124:GLN:HG2	2.02	0.59
3:C:62:TYR:OH	3:C:66:LYS:NZ	2.29	0.59
12:M:69:LEU:HD21	12:M:184:ARG:HB2	1.83	0.59
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.83	0.59
16:Q:86:PRO:CG	33:j:41:PHE:HE2	2.14	0.59
24:a:176:LYS:HB2	31:h:45:HIS:CD2	2.36	0.59
26:c:169:GLU:O	26:c:169:GLU:HG2	2.02	0.59
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	0.59
13:N:34:LYS:HZ1	13:N:58:ARG:HG2	1.66	0.59
32:i:193:VAL:HG21	32:i:266:ILE:HG12	1.82	0.59
34:k:97:GLN:HG2	35:l:582:GLY:HA2	1.84	0.59
36:m:83:GLY:HA2	36:m:89:LEU:HD21	1.83	0.59
41:s:172:LEU:HD21	41:s:176:LEU:HB2	1.84	0.59
1:A:35:LEU:HD22	1:A:290:GLU:HA	1.82	0.59
2:B:208:LEU:HD22	8:I:39:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.59
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.67	0.59
22:Y:45:ARG:HG3	23:Z:52:ARG:HB2	1.84	0.59
25:b:79:VAL:HG11	27:d:35:VAL:HG11	1.84	0.59
32:i:8:VAL:HG11	36:m:165:TYR:CE2	2.37	0.59
32:i:58:LYS:NZ	34:k:92:ASN:OD1	2.35	0.59
35:l:367:PRO:O	35:l:370:SER:OG	2.17	0.59
1:A:263:ALA:HA	1:A:271:SER:HB3	1.83	0.59
9:J:172:ALA:O	9:J:185:ALA:HB2	2.03	0.59
12:M:519:ILE:HG12	12:M:521:SER:H	1.67	0.59
27:d:54:ARG:HD3	27:d:56:TYR:CZ	2.37	0.59
32:i:24:SER:O	32:i:86:MET:HG2	2.02	0.59
44:w:304:VAL:HG23	44:w:305:LEU:HG	1.84	0.59
1:A:412:LEU:HA	1:A:415:ILE:HD12	1.84	0.59
4:E:127:ASP:HB3	4:E:128:PRO:HD2	1.84	0.59
9:J:207:PHE:HE2	9:J:348:LYS:HB2	1.67	0.59
20:V:40:ARG:HA	51:V:201:CDL:OB3	2.02	0.59
52:V:202:PEE:H71	52:l:701:PEE:C45	2.27	0.59
21:W:81:ARG:HH22	42:u:64:ASN:ND2	2.00	0.59
23:Z:66:VAL:HG22	35:l:363:LEU:HD22	1.85	0.59
25:b:51:LEU:HD21	25:b:62:HIS:HB2	1.83	0.59
35:l:227:LEU:HB2	35:l:284:THR:HG22	1.84	0.59
37:n:31:SER:O	37:n:34:ARG:HG2	2.02	0.59
40:r:30:HIS:O	40:r:34:ILE:HD12	2.01	0.59
1:A:220:GLN:NE2	14:O:114:GLU:O	2.35	0.59
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.84	0.59
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.59
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.59
25:b:88:TYR:CG	47:b:201:PLX:C1C	2.86	0.59
31:h:94:PRO:HG2	31:h:95:PRO:HD3	1.85	0.59
33:j:54:LYS:HE3	33:j:113:TRP:CD1	2.38	0.59
35:l:247:LEU:O	35:l:252:MET:HB3	2.03	0.59
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.59
25:b:100:LYS:HB2	35:l:60:GLU:HB2	1.84	0.59
35:l:174:TYR:OH	52:l:702:PEE:H19	2.02	0.59
39:p:112:LYS:HA	39:p:119:PHE:CE2	2.38	0.59
2:B:64:LEU:O	2:B:68:LEU:N	2.30	0.59
17:S:53:ARG:HB2	31:h:105:ARG:NH1	2.18	0.59
31:h:44:ALA:HA	31:h:47:ILE:HD12	1.85	0.59
31:h:51:ARG:NH1	31:h:55:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:37:LYS:CE	35:l:98:TRP:NE1	2.65	0.59
44:w:132:GLN:HG2	44:w:170:LEU:HD12	1.85	0.59
1:A:123:GLY:HA3	1:A:355:ILE:HD11	1.83	0.59
12:M:624:ARG:NE	12:M:636:TYR:O	2.36	0.59
52:V:202:PEE:C11	32:i:276:LEU:HD12	2.28	0.59
23:Z:25:GLU:HA	23:Z:30:GLU:HG3	1.84	0.59
26:c:93:ASP:OD2	26:c:101:TRP:N	2.36	0.59
35:l:456:ARG:CB	35:l:456:ARG:HH21	2.16	0.59
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
25:b:88:TYR:O	25:b:92:GLU:HB2	2.03	0.58
47:b:201:PLX:P1	47:b:201:PLX:H72	2.43	0.58
26:c:94:GLN:O	26:c:98:ARG:N	2.30	0.58
33:j:2:ASN:O	33:j:5:LEU:HG	2.03	0.58
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	0.58
2:B:186:GLU:OE2	18:T:64:ASN:N	2.36	0.58
3:C:89:CYS:HB2	3:C:123:ALA:HB1	1.86	0.58
9:J:192:ARG:O	9:J:196:PRO:HA	2.02	0.58
9:J:212:ARG:HG2	9:J:212:ARG:NH1	2.15	0.58
12:M:126:LEU:HD12	18:T:98:LYS:O	2.04	0.58
14:O:138:THR:HA	14:O:141:MET:HB3	1.85	0.58
52:W:201:PEE:H8	41:s:98:LEU:HD22	1.84	0.58
25:b:105:PHE:HE2	43:v:68:LYS:N	2.01	0.58
27:d:134:GLN:NE2	38:o:123:ARG:O	2.35	0.58
33:j:7:LEU:HA	33:j:10:ASN:HD22	1.67	0.58
38:o:25:ILE:HD12	38:o:30:ARG:HD3	1.85	0.58
44:w:170:LEU:HD21	44:w:184:VAL:HG22	1.84	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
16:Q:438:MET:HE1	16:Q:454:GLN:NE2	2.18	0.58
24:a:53:ARG:HH21	25:b:28:LEU:HD11	1.66	0.58
32:i:145:ILE:HD12	32:i:149:LEU:HD11	1.84	0.58
33:j:32:GLU:HA	33:j:35:THR:HG23	1.84	0.58
39:p:98:LYS:HE2	39:p:176:GLU:HA	1.83	0.58
42:u:38:LYS:O	42:u:42:GLU:HB2	2.03	0.58
1:A:93:PHE:HE2	1:A:98:LYS:CD	2.05	0.58
14:O:48:ASN:HD22	14:O:94:PRO:HA	1.68	0.58
24:a:67:PHE:HD1	40:r:431:THR:HG23	1.68	0.58
21:W:61:GLN:HE22	41:s:317:GLN:HA	1.68	0.58
27:d:153:GLN:O	27:d:157:MET:HG2	2.03	0.58
32:i:249:LEU:HB3	32:i:254:LEU:HD12	1.85	0.58
33:j:72:LEU:HD21	33:j:94:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:37:MET:HE1	34:k:63:MET:HB3	1.86	0.58
35:l:88:MET:C	35:l:91:PRO:HD2	2.28	0.58
35:l:227:LEU:CD1	35:l:230:HIS:CE1	2.86	0.58
37:n:10:ASP:HB3	40:r:19:LYS:NZ	2.18	0.58
41:s:294:LEU:O	41:s:297:THR:OG1	2.15	0.58
42:u:96:LEU:HD11	42:u:99:HIS:CD2	2.38	0.58
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	0.58
2:B:198:GLU:OE1	13:N:88:ARG:HB2	2.04	0.58
4:E:32:VAL:O	4:E:35:LEU:HB3	2.03	0.58
12:M:330:LEU:HD22	12:M:626:LEU:HD21	1.84	0.58
15:P:147:THR:HG21	15:P:153:ILE:HB	1.85	0.58
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.69	0.58
44:w:149:HIS:O	44:w:153:THR:OG1	2.15	0.58
8:I:23:LYS:HD3	16:Q:250:ASN:HA	1.85	0.58
8:I:69:ILE:HB	15:P:76:VAL:HB	1.85	0.58
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
27:d:21:PRO:HG2	27:d:24:ILE:HD12	1.85	0.58
32:i:277:ILE:O	32:i:280:THR:OG1	2.21	0.58
35:l:96:VAL:O	35:l:100:ILE:HG13	2.04	0.58
12:M:308:ARG:HA	12:M:314:LEU:HA	1.86	0.58
12:M:501:ARG:NH1	12:M:666:GLN:HB2	2.18	0.58
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.69	0.58
1:A:307:VAL:HG11	1:A:314:LEU:HD21	1.86	0.58
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.58
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58
17:S:49:GLU:O	31:h:105:ARG:NH2	2.37	0.58
42:u:124:GLU:OE1	42:u:124:GLU:N	2.37	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	0.58
24:a:52:LYS:O	24:a:53:ARG:HG2	2.03	0.58
35:l:310:LEU:HA	35:l:313:MET:HE3	1.86	0.58
52:l:701:PEE:C23	40:r:155:VAL:CB	2.77	0.58
41:s:85:LEU:HD13	41:s:233:MET:HE1	1.85	0.58
2:B:36:TYR:HB3	8:I:104:TRP:HE3	1.68	0.57
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.84	0.57
4:E:118:PHE:HA	4:E:121:LYS:HD3	1.86	0.57
14:O:160:VAL:HA	14:O:171:LEU:HD23	1.86	0.57
19:U:67:PRO:HB3	19:U:74:GLN:HB2	1.86	0.57
27:d:135:ASP:HB3	27:d:156:ARG:NH2	2.19	0.57
40:r:126:LEU:O	40:r:129:THR:OG1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:169:GLN:NE2	41:s:174:LEU:H	2.02	0.57
44:w:332:ARG:O	44:w:338:LYS:CB	2.52	0.57
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	0.57
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
1:A:243:ALA:HA	46:A:502:FMN:O2P	2.04	0.57
9:J:204:SER:O	9:J:240:VAL:HG23	2.04	0.57
9:J:329:LEU:HD13	9:J:332:LEU:HB2	1.84	0.57
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.57
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	1.86	0.57
32:i:245:PRO:HA	32:i:248:LEU:HD12	1.85	0.57
35:l:286:LEU:HD12	35:l:411:ILE:HG23	1.86	0.57
38:o:54:PRO:HA	39:p:129:ARG:HH21	1.67	0.57
43:v:113:LYS:HE2	43:v:117:LYS:HE3	1.85	0.57
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.57
1:A:438:LEU:HD21	1:A:446:LEU:HD21	1.86	0.57
3:C:67:LEU:HD22	3:C:207:LEU:CD2	2.34	0.57
8:I:36:GLN:HE22	16:Q:239:GLY:HA2	1.68	0.57
10:K:89:LEU:HD11	14:O:61:LYS:HE3	1.86	0.57
12:M:210:ILE:HG23	12:M:212:LYS:H	1.69	0.57
52:W:201:PEE:H1	41:s:98:LEU:CD2	2.34	0.57
22:Y:72:ARG:NH1	35:l:466:PHE:HD1	2.02	0.57
32:i:120:GLN:O	32:i:176:ARG:NH2	2.38	0.57
35:l:453:PRO:HA	35:l:456:ARG:HH22	1.69	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
12:M:222:ILE:O	12:M:225:ILE:HG22	2.05	0.57
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.57
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.57
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.57
16:Q:78:LYS:O	16:Q:79:ASN:HB3	2.04	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
20:V:40:ARG:HD3	20:V:59:TYR:HE2	1.68	0.57
21:W:47:HIS:CE1	41:s:307:MET:HE1	2.40	0.57
21:W:78:GLU:HB3	31:h:105:ARG:HB3	1.86	0.57
25:b:105:PHE:CD2	43:v:68:LYS:HA	2.39	0.57
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.87	0.57
35:l:556:THR:OG1	35:l:557:TRP:N	2.37	0.57
47:r:502:PLX:H72	47:r:502:PLX:C3	2.31	0.57
1:A:118:ASP:OD1	1:A:120:GLY:N	2.35	0.57
5:F:63:PRO:HB2	5:F:79:LEU:CB	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:177:ILE:HG13	12:M:177:ILE:O	2.04	0.57
25:b:88:TYR:CG	47:b:201:PLX:H1C1	2.38	0.57
26:c:156:VAL:O	43:v:98:ARG:HG2	2.05	0.57
30:g:1:MET:SD	32:i:345:MET:HE1	2.44	0.57
34:k:2:PRO:HG2	36:m:115:VAL:HG23	1.86	0.57
35:l:27:ASN:HB3	35:l:29:LYS:HG2	1.84	0.57
37:n:56:THR:HG1	37:n:57:TRP:CD1	2.22	0.57
1:A:209:GLU:HB3	46:A:502:FMN:H3'	1.85	0.57
2:B:97:GLY:H	2:B:167:GLU:HG3	1.70	0.57
6:G:134:ASP:O	6:G:138:LEU:N	2.38	0.57
9:J:220:MET:HB2	9:J:281:PHE:HZ	1.68	0.57
12:M:636:TYR:CE1	12:M:642:VAL:HB	2.39	0.57
22:Y:39:HIS:ND1	22:Y:40:ILE:HG13	2.20	0.57
32:i:258:THR:HG22	32:i:336:LEU:HB3	1.87	0.57
35:l:272:LEU:O	35:l:275:THR:OG1	2.18	0.57
39:p:176:GLU:HG2	39:p:177:ARG:HG3	1.85	0.57
2:B:68:LEU:CG	41:s:272:TRP:HE1	2.17	0.57
12:M:306:MET:HB3	12:M:314:LEU:HD13	1.86	0.57
16:Q:81:THR:HA	16:Q:100:GLU:HA	1.86	0.57
22:Y:44:TYR:CD1	35:l:440:LEU:HB2	2.40	0.57
22:Y:73:PHE:HA	35:l:385:PHE:HE2	1.70	0.57
1:A:235:VAL:HG22	1:A:240:THR:HG21	1.87	0.57
1:A:382:CYS:SG	45:A:501:SF4:S4	3.03	0.57
2:B:66:ARG:NH2	21:W:26:PRO:O	2.38	0.57
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	0.57
9:J:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.57
21:W:111:PHE:HE1	31:h:65:GLU:OE1	1.88	0.57
33:j:57:LEU:O	33:j:61:THR:HG23	2.04	0.57
35:l:35:TYR:CZ	35:l:39:ILE:HD11	2.40	0.57
44:w:124:ASN:HB3	44:w:316:GLU:HG2	1.85	0.57
3:C:147:VAL:HG23	3:C:176:VAL:HA	1.86	0.57
12:M:358:LEU:O	12:M:363:SER:N	2.35	0.57
16:Q:306:GLN:O	16:Q:308:TYR:N	2.38	0.57
16:Q:390:GLN:HE22	16:Q:417:SER:HB3	1.68	0.57
25:b:88:TYR:CD1	25:b:92:GLU:OE2	2.57	0.57
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.33	0.57
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	0.57
8:I:41:LEU:C	21:W:8:GLN:HE22	2.13	0.57
12:M:391:ILE:O	12:M:417:ARG:NH2	2.38	0.57
14:O:148:ILE:HG23	14:O:201:ILE:HD11	1.87	0.57
20:V:139:PRO:O	20:V:141:VAL:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:132:ASP:OD2	39:p:18:ARG:HG2	2.05	0.57
24:a:53:ARG:O	24:a:54:LEU:HD23	2.04	0.57
25:b:111:LEU:O	25:b:112:GLU:HB2	2.05	0.57
35:l:37:LYS:HZ3	35:l:98:TRP:NE1	2.02	0.57
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.56
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.56
16:Q:267:ILE:HG23	41:s:280:PHE:HD1	1.70	0.56
52:V:202:PEE:H57	52:V:202:PEE:H40	1.87	0.56
24:a:114:LYS:CB	27:d:57:TYR:CE2	2.77	0.56
47:g:203:PLX:H251	32:i:324:PRO:HB2	1.85	0.56
33:j:114:ALA:HB1	41:s:286:MET:HB2	1.87	0.56
40:r:178:LEU:O	40:r:182:THR:OG1	2.16	0.56
40:r:210:TYR:HB2	40:r:268:GLY:HA3	1.85	0.56
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	0.56
9:J:217:PHE:HB3	9:J:280:ILE:HD13	1.87	0.56
12:M:454:ASP:HB3	12:M:460:HIS:HB2	1.85	0.56
29:f:72:ARG:HH11	30:g:19:SER:HB3	1.70	0.56
35:l:332:HIS:HE1	35:l:336:LYS:NZ	2.02	0.56
35:l:452:ASN:HB2	35:l:453:PRO:HD3	1.87	0.56
2:B:74:TYR:OH	16:Q:257:GLU:OE1	2.20	0.56
8:I:46:SER:OG	12:M:150:ARG:NH2	2.38	0.56
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.56
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.39	0.56
22:Y:86:TYR:OH	43:v:100:LYS:HG3	2.03	0.56
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.70	0.56
32:i:230:LEU:HD11	32:i:244:ILE:HG21	1.86	0.56
34:k:7:ASN:ND2	36:m:9:SER:OG	2.31	0.56
35:l:51:THR:HG21	35:l:91:PRO:HG3	1.86	0.56
35:l:564:LYS:O	35:l:567:SER:OG	2.22	0.56
44:w:115:GLU:OE2	44:w:225:HIS:ND1	2.39	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.56
16:Q:84:PHE:CE2	16:Q:91:ALA:HB2	2.40	0.56
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.39	0.56
17:S:59:ARG:O	17:S:61:TYR:N	2.36	0.56
23:Z:51:TRP:O	23:Z:53:TYR:N	2.37	0.56
25:b:110:ILE:HG13	25:b:111:LEU:HD21	1.87	0.56
32:i:237:LEU:HD13	32:i:240:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:702:PEE:O4	52:l:702:PEE:H7	2.05	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.56
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.56
2:B:72:LEU:HB2	41:s:272:TRP:CH2	2.41	0.56
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.44	0.56
20:V:40:ARG:NH2	20:V:55:LYS:HD3	2.20	0.56
25:b:88:TYR:O	25:b:92:GLU:HB3	2.05	0.56
26:c:127:HIS:O	26:c:131:MET:HG2	2.04	0.56
35:l:452:ASN:N	35:l:453:PRO:CD	2.68	0.56
41:s:190:LEU:HD22	41:s:195:ARG:HG2	1.86	0.56
41:s:280:PHE:O	41:s:281:ARG:HB3	2.05	0.56
42:u:35:GLN:O	42:u:37:ASP:N	2.34	0.56
2:B:151:ILE:HG21	3:C:159:TYR:CD2	2.41	0.56
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.86	0.56
23:Z:22:TRP:CE3	23:Z:51:TRP:HA	2.41	0.56
25:b:105:PHE:HE2	43:v:68:LYS:HA	1.70	0.56
27:d:59:HIS:ND1	28:e:120:ARG:HG2	2.21	0.56
27:d:107:CYS:HG	27:d:119:CYS:HA	1.70	0.56
47:g:203:PLX:H1A2	47:g:203:PLX:H72	1.87	0.56
32:i:250:SER:O	32:i:259:GLY:HA3	2.04	0.56
41:s:156:MET:HE1	41:s:177:PRO:HB2	1.88	0.56
5:F:16:LEU:HD11	5:F:19:ILE:HB	1.87	0.56
9:J:141:PHE:CZ	9:J:180:TYR:CD1	2.93	0.56
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.88	0.56
20:V:62:THR:HG22	20:V:104:ARG:HE	1.69	0.56
6:X:99:SER:OG	6:X:102:SER:OG	2.11	0.56
36:m:156:THR:O	36:m:159:THR:OG1	2.22	0.56
39:p:30:TRP:CE2	39:p:76:HIS:HB2	2.40	0.56
5:F:16:LEU:HB3	5:F:51:LEU:HD13	1.88	0.56
11:L:82:PRO:HD3	11:L:98:LYS:HG2	1.87	0.56
12:M:225:ILE:HD12	12:M:285:TRP:CH2	2.39	0.56
22:Y:85:PRO:CG	43:v:99:MET:HE2	2.36	0.56
24:a:98:LEU:CA	27:d:57:TYR:CE1	2.89	0.56
36:m:16:PHE:HA	36:m:19:PHE:CE1	2.40	0.56
38:o:8:PRO:HB3	38:o:14:LEU:HG	1.88	0.56
39:p:56:ASP:OD1	39:p:57:MET:N	2.38	0.56
40:r:346:GLN:HB2	40:r:420:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:44:MET:HE3	42:u:48:TRP:CZ3	2.41	0.56
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	0.56
25:b:105:PHE:CE2	43:v:68:LYS:N	2.74	0.56
27:d:60:ARG:HH11	27:d:60:ARG:CG	2.12	0.56
31:h:70:GLN:HG2	36:m:115:VAL:CG1	2.36	0.56
35:l:73:THR:OG1	35:l:74:THR:N	2.39	0.56
35:l:407:TRP:NE1	35:l:411:ILE:HD11	2.21	0.56
36:m:81:ALA:HB3	36:m:84:SER:HB3	1.87	0.56
43:v:40:VAL:H	43:v:61:HIS:HE1	1.53	0.56
5:F:17:ARG:HB3	5:F:68:ARG:HH21	1.71	0.56
12:M:221:ASN:HB3	12:M:285:TRP:CE3	2.40	0.56
1:A:381:GLN:CG	45:A:501:SF4:S2	2.94	0.55
4:E:66:MET:HE3	4:E:106:PHE:HD1	1.71	0.55
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	0.55
12:M:173:MET:C	12:M:175:ARG:N	2.60	0.55
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.70	0.55
20:V:3:PRO:HA	20:V:6:PHE:HB3	1.88	0.55
25:b:75:VAL:O	25:b:79:VAL:HG23	2.06	0.55
47:g:201:PLX:H261	32:i:346:ILE:HG23	1.87	0.55
32:i:106:LEU:HD21	32:i:138:PRO:HB2	1.87	0.55
40:r:164:LEU:O	40:r:167:THR:OG1	2.18	0.55
44:w:287:ASP:OD1	44:w:288:ASN:N	2.34	0.55
4:E:75:ASP:HB3	4:E:78:VAL:HG23	1.89	0.55
9:J:132:ARG:HD2	9:J:134:TRP:NE1	2.20	0.55
12:M:476:LEU:HD11	12:M:480:ALA:HB3	1.87	0.55
12:M:481:LEU:HD11	12:M:515:ILE:HD12	1.88	0.55
20:V:47:GLY:O	20:V:48:THR:OG1	2.25	0.55
31:h:2:PRO:O	31:h:4:LEU:N	2.39	0.55
31:h:74:ARG:HA	36:m:116:VAL:HG21	1.88	0.55
32:i:287:LEU:HD21	40:r:158:LEU:HD11	1.87	0.55
1:A:342:LEU:HB3	1:A:347:THR:HB	1.87	0.55
2:B:103:ARG:HH12	18:T:68:ALA:HB2	1.69	0.55
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.89	0.55
4:E:36:TYR:HD1	4:E:67:PHE:CE2	2.25	0.55
12:M:128:CYS:N	12:M:129:PRO:HD2	2.21	0.55
12:M:598:ASN:HB3	12:M:602:ARG:HB3	1.89	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.55
14:O:41:HIS:ND1	14:O:41:HIS:O	2.39	0.55
16:Q:66:TRP:NE1	44:w:310:ILE:HD11	2.20	0.55
16:Q:103:GLY:HA2	33:j:50:PRO:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:50:ARG:HA	31:h:105:ARG:NE	2.21	0.55
21:W:122:GLY:HA3	36:m:124:TRP:CE3	2.41	0.55
25:b:84:TYR:HE1	27:d:43:ARG:HD3	1.71	0.55
30:g:47:ILE:HD12	32:i:327:PRO:HG3	1.88	0.55
30:g:51:PRO:HG2	30:g:55:ALA:HB2	1.87	0.55
32:i:124:LEU:HD23	32:i:176:ARG:HD3	1.88	0.55
39:p:86:PRO:HA	39:p:91:TYR:CD1	2.41	0.55
40:r:232:ALA:O	40:r:237:LYS:NZ	2.39	0.55
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.55
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.55
12:M:50:LEU:N	12:M:91:ALA:O	2.38	0.55
35:l:456:ARG:NH2	35:l:456:ARG:HB2	2.21	0.55
36:m:16:PHE:CD1	36:m:19:PHE:HE1	2.25	0.55
39:p:102:TRP:HZ2	40:r:422:HIS:HA	1.70	0.55
42:u:115:LEU:HB3	42:u:117:TRP:CZ3	2.42	0.55
1:A:418:GLN:O	1:A:422:HIS:ND1	2.39	0.55
11:L:61:ILE:HB	11:L:64:LEU:HB2	1.89	0.55
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.55
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.55
20:V:40:ARG:HD3	20:V:59:TYR:CE2	2.41	0.55
52:V:202:PEE:H60	52:V:202:PEE:C24	2.37	0.55
22:Y:74:TRP:HE3	22:Y:75:HIS:CA	2.19	0.55
33:j:80:GLN:NE2	41:s:316:PRO:O	2.39	0.55
33:j:92:LEU:O	33:j:96:ILE:HG12	2.06	0.55
42:u:100:CYS:SG	42:u:101:ARG:N	2.78	0.55
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	0.55
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.55
12:M:408:ARG:HB3	12:M:415:ASN:ND2	2.21	0.55
19:U:67:PRO:HA	19:U:74:GLN:OE1	2.07	0.55
22:Y:81:LEU:CD1	43:v:88:ASP:HB3	2.37	0.55
24:a:59:PRO:HD3	39:p:99:VAL:HG21	1.89	0.55
25:b:83:HIS:CD2	35:l:6:THR:HG21	2.42	0.55
26:c:56:ASN:ND2	38:o:43:LEU:HD11	2.22	0.55
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.55
52:W:201:PEE:H4	52:W:201:PEE:P	2.28	0.55
27:d:109:GLN:HG2	35:l:62:ILE:HD13	1.88	0.55
34:k:57:ASN:O	34:k:60:PRO:HD2	2.06	0.55
37:n:30:LYS:NZ	51:n:101:CDL:HA31	2.22	0.55
38:o:28:GLU:HA	38:o:31:ARG:HD3	1.88	0.55
40:r:403:THR:HA	40:r:406:TYR:CE2	2.42	0.55
41:s:117:LEU:HD12	41:s:136:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:GLN:HG2	33:j:37:TYR:CD2	2.42	0.55
7:H:16:VAL:HA	7:H:78:GLU:OE2	2.06	0.55
13:N:57:GLY:H	13:N:59:HIS:CE1	2.24	0.55
25:b:87:LYS:HE3	27:d:43:ARG:HG2	1.89	0.55
27:d:134:GLN:O	27:d:138:GLN:HB2	2.06	0.55
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	0.55
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
11:L:133:ASP:O	11:L:136:SER:OG	2.21	0.55
15:P:235:LEU:HD22	16:Q:387:GLU:HG2	1.87	0.55
25:b:110:ILE:HG13	25:b:111:LEU:CD2	2.37	0.55
26:c:184:TYR:O	43:v:35:LYS:O	2.25	0.55
27:d:81:GLU:OE1	37:n:43:MET:CE	2.43	0.55
32:i:288:LEU:HD21	52:l:701:PEE:H58	1.70	0.55
35:l:102:GLU:OE1	35:l:453:PRO:HG3	2.07	0.55
35:l:546:GLN:O	35:l:550:LEU:HB2	2.07	0.55
40:r:73:LEU:HD12	40:r:103:GLN:HG2	1.89	0.55
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.55
11:L:162:ALA:HA	11:L:168:LYS:NZ	2.22	0.55
12:M:329:MET:HG3	12:M:565:PHE:CE2	2.41	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	0.55
15:P:94:ILE:N	15:P:154:GLU:OE1	2.28	0.55
22:Y:74:TRP:CE3	22:Y:74:TRP:C	2.85	0.55
33:j:24:LEU:H	33:j:25:PRO:HD2	1.72	0.55
34:k:1:MET:CB	34:k:4:ILE:HD13	2.36	0.55
36:m:138:ASP:HB2	36:m:139:PRO:HD3	1.89	0.55
37:n:7:ILE:O	37:n:11:HIS:N	2.37	0.55
4:E:56:VAL:HG23	9:J:367:GLU:OE2	2.07	0.54
5:F:68:ARG:HD2	5:F:72:GLY:HA2	1.87	0.54
12:M:124:HIS:ND1	12:M:125:PRO:HD2	2.22	0.54
12:M:510:TRP:CD1	12:M:512:VAL:HG22	2.42	0.54
16:Q:291:VAL:HA	16:Q:294:ARG:HB2	1.89	0.54
4:E:25:MET:HE3	4:E:29:LYS:HE2	1.88	0.54
11:L:170:THR:O	11:L:172:VAL:N	2.35	0.54
12:M:241:ARG:HG2	12:M:243:TRP:CZ2	2.42	0.54
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.54
25:b:45:LYS:HA	25:b:48:ASN:HB2	1.87	0.54
30:g:44:ASP:OD2	30:g:63:TYR:OH	2.16	0.54
32:i:167:TRP:HH2	35:l:570:GLN:HG3	1.70	0.54
35:l:3:MET:O	35:l:7:MET:HG2	2.08	0.54
35:l:238:GLU:N	35:l:238:GLU:OE1	2.40	0.54
35:l:452:ASN:N	35:l:452:ASN:OD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:91:ARG:HG2	40:r:136:TRP:HH2	1.72	0.54
3:C:106:PHE:CD1	41:s:39:VAL:HG21	2.41	0.54
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.54
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.71	0.54
12:M:308:ARG:HD2	12:M:312:GLY:O	2.08	0.54
12:M:341:ILE:HD12	12:M:555:ILE:HG13	1.89	0.54
12:M:380:ASP:OD1	12:M:381:LEU:N	2.40	0.54
25:b:105:PHE:HE2	43:v:67:LEU:C	2.15	0.54
27:d:114:ASN:OD1	43:v:50:GLN:HG2	2.07	0.54
32:i:17:THR:OG1	32:i:36:ASN:ND2	2.39	0.54
35:l:190:ILE:O	35:l:194:ASN:HA	2.08	0.54
36:m:48:GLY:HA2	36:m:138:ASP:OD2	2.08	0.54
40:r:1:MET:HG3	40:r:2:LEU:H	1.71	0.54
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.54
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	0.54
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.54
15:P:55:HIS:CD2	15:P:78:VAL:HG12	2.42	0.54
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54
27:d:115:TYR:CD1	27:d:115:TYR:C	2.85	0.54
36:m:155:VAL:O	36:m:159:THR:HG23	2.08	0.54
40:r:358:TRP:CE3	40:r:441:LEU:HD12	2.42	0.54
1:A:207:GLY:O	46:A:502:FMN:C9A	2.56	0.54
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
10:K:92:SER:HB2	14:O:68:LYS:HD2	1.90	0.54
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.40	0.54
15:P:107:GLN:HB3	15:P:109:LYS:HE3	1.89	0.54
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.89	0.54
30:g:46:LEU:HD11	32:i:239:TRP:HB3	1.88	0.54
40:r:236:LEU:O	40:r:239:GLY:N	2.40	0.54
40:r:317:ILE:HD12	40:r:454:ILE:HG23	1.88	0.54
41:s:145:THR:HG21	41:s:289:LEU:HD22	1.90	0.54
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.90	0.54
9:J:172:ALA:HA	9:J:181:LEU:CD2	2.38	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.89	0.54
12:M:697:THR:O	12:M:702:ARG:NH2	2.40	0.54
16:Q:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CB	2.55	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CD2	2.54	0.54
24:a:133:TYR:OH	27:d:81:GLU:HG2	2.08	0.54
35:l:293:LEU:HD23	35:l:422:TYR:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:32:LEU:HD13	36:m:64:MET:HE1	1.88	0.54
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.90	0.54
9:J:167:VAL:HA	9:J:201:VAL:HB	1.88	0.54
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	0.54
9:J:203:PRO:HG2	49:J:401:NDP:C5N	2.37	0.54
15:P:85:GLU:HG3	15:P:142:ARG:HB2	1.88	0.54
16:Q:262:LEU:HD22	16:Q:268:TRP:NE1	2.18	0.54
35:l:197:ASP:O	35:l:201:MET:HG3	2.08	0.54
44:w:206:TYR:OH	44:w:238:GLU:OE2	2.25	0.54
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	0.54
21:W:81:ARG:HH22	42:u:64:ASN:HD21	1.56	0.54
22:Y:81:LEU:HD22	43:v:92:HIS:HD2	1.70	0.54
34:k:87:LEU:HD11	36:m:73:MET:O	2.08	0.54
35:l:95:PHE:CD1	35:l:95:PHE:C	2.86	0.54
36:m:16:PHE:HD1	36:m:19:PHE:HE1	1.54	0.54
1:A:33:GLY:H	1:A:294:VAL:HG12	1.72	0.54
1:A:41:ILE:HG23	1:A:253:THR:HG21	1.90	0.54
6:G:99:SER:HG	6:G:102:SER:HG	1.54	0.54
8:I:42:PRO:HB3	21:W:10:MET:HE1	1.90	0.54
9:J:168:SER:O	49:J:401:NDP:H6N	2.08	0.54
12:M:358:LEU:HB3	12:M:363:SER:O	2.07	0.54
24:a:54:LEU:HD23	25:b:27:GLU:HA	1.89	0.54
28:e:74:HIS:ND1	28:e:87:MET:HG3	2.23	0.54
35:l:98:TRP:CD1	35:l:98:TRP:C	2.86	0.54
44:w:61:THR:HG22	44:w:159:LEU:HD23	1.90	0.54
44:w:128:SER:O	44:w:131:LEU:HG	2.08	0.54
2:B:61:TRP:CD1	16:Q:266:ARG:HH12	2.26	0.54
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.90	0.54
13:N:84:PRO:HA	13:N:87:HIS:HB3	1.90	0.54
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.54
16:Q:391:VAL:HG12	16:Q:392:PRO:O	2.09	0.54
12:M:402:LEU:HA	12:M:475:VAL:HB	1.88	0.53
12:M:405:THR:HA	12:M:686:PRO:HG3	1.90	0.53
15:P:235:LEU:HB3	16:Q:387:GLU:HG2	1.90	0.53
16:Q:43:TRP:HZ3	32:i:305:LEU:HD21	1.74	0.53
17:S:12:MET:HE1	41:s:20:LEU:HD12	1.91	0.53
2:B:66:ARG:HH22	21:W:28:ARG:HB2	1.74	0.53
7:H:111:GLN:NE2	15:P:124:ASN:HB2	2.22	0.53
8:I:59:GLY:HA2	15:P:47:VAL:HG22	1.90	0.53
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.90	0.53
16:Q:267:ILE:HG21	41:s:278:PRO:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.73	0.53
16:Q:449:ALA:O	16:Q:453:THR:HG23	2.08	0.53
41:s:127:TYR:HA	41:s:130:ILE:HD12	1.89	0.53
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.53
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
9:J:178:SER:OG	9:J:181:LEU:CB	2.57	0.53
9:J:207:PHE:CZ	9:J:345:LEU:HA	2.44	0.53
12:M:47:THR:OG1	12:M:51:GLN:OE1	2.23	0.53
12:M:565:PHE:HA	12:M:581:ASP:OD2	2.08	0.53
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	0.53
24:a:98:LEU:HB3	27:d:57:TYR:HE1	0.54	0.53
32:i:217:LEU:HB3	32:i:326:LEU:HD12	1.89	0.53
33:j:104:TYR:CG	36:m:165:TYR:HE1	2.26	0.53
39:p:102:TRP:NE1	40:r:426:MET:HE1	2.23	0.53
2:B:61:TRP:O	2:B:63:GLU:N	2.41	0.53
4:E:128:PRO:HB3	11:L:104:ARG:HH22	1.73	0.53
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.53
12:M:82:ILE:HB	12:M:85:ALA:HB2	1.91	0.53
16:Q:265:ASN:OD1	16:Q:266:ARG:N	2.41	0.53
52:V:202:PEE:C24	52:V:202:PEE:H57	2.39	0.53
52:W:201:PEE:C3	41:s:98:LEU:HD22	2.38	0.53
23:Z:24:ILE:HG22	23:Z:30:GLU:HB2	1.90	0.53
25:b:78:PRO:O	25:b:82:ILE:HD12	2.08	0.53
26:c:84:HIS:CD2	26:c:118:ASP:HB3	2.43	0.53
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.90	0.53
40:r:414:THR:O	40:r:415:GLN:NE2	2.41	0.53
41:s:126:ASN:HA	41:s:129:LEU:HD12	1.91	0.53
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.90	0.53
1:A:382:CYS:HA	12:M:74:ASN:HA	1.91	0.53
4:E:24:ASP:OD1	4:E:25:MET:N	2.41	0.53
9:J:172:ALA:HA	9:J:181:LEU:HD23	1.90	0.53
12:M:53:CYS:SG	12:M:102:ILE:HD12	2.48	0.53
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.20	0.53
12:M:124:HIS:CD2	16:Q:375:MET:HE2	2.43	0.53
12:M:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.53
17:S:28:ARG:NH1	42:u:91:TYR:OH	2.42	0.53
24:a:98:LEU:CA	27:d:57:TYR:CD1	2.91	0.53
24:a:112:TYR:HD1	27:d:58:TYR:O	1.92	0.53
31:h:48:GLY:O	31:h:50:THR:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:66:PHE:CE1	36:m:159:THR:HG21	2.40	0.53
42:u:83:THR:O	42:u:86:TRP:HB3	2.08	0.53
44:w:138:SER:O	44:w:142:GLN:HG2	2.07	0.53
44:w:149:HIS:CE1	44:w:155:GLN:HB3	2.43	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.53
2:B:65:PHE:O	2:B:69:GLY:N	2.41	0.53
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.35	0.53
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.89	0.53
9:J:64:PHE:CE1	9:J:68:TYR:HE2	2.27	0.53
12:M:394:VAL:HG21	12:M:414:PHE:HE1	1.73	0.53
13:N:94:THR:HG22	13:N:96:ASP:H	1.73	0.53
14:O:129:LYS:HB3	14:O:168:LEU:HG	1.91	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
16:Q:80:ILE:O	16:Q:100:GLU:C	2.52	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
22:Y:84:PHE:CE2	35:l:483:PRO:CG	2.69	0.53
32:i:311:VAL:HG12	32:i:315:TRP:HE1	1.73	0.53
35:l:51:THR:CG2	35:l:91:PRO:HG2	2.30	0.53
35:l:282:ALA:O	35:l:285:THR:OG1	2.27	0.53
41:s:195:ARG:NH1	41:s:270:PHE:HB3	2.24	0.53
6:G:75:THR:O	6:G:79:ILE:HG12	2.09	0.53
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.44	0.53
12:M:215:MET:HE1	12:M:714:VAL:HG23	1.90	0.53
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	0.53
25:b:95:TYR:HE2	27:d:10:TYR:CD1	2.27	0.53
41:s:32:GLN:HB3	41:s:34:ARG:HG2	1.91	0.53
44:w:137:SER:O	44:w:139:ARG:N	2.37	0.53
1:A:117:ALA:HB3	1:A:157:TYR:O	2.08	0.53
1:A:121:GLU:HA	1:A:204:TYR:HE1	1.74	0.53
1:A:293:SER:HB2	1:A:336:LEU:HD23	1.91	0.53
7:H:97:TRP:HB3	7:H:100:TRP:CH2	2.43	0.53
25:b:110:ILE:N	27:d:17:THR:O	2.41	0.53
31:h:99:ILE:HD12	31:h:101:LYS:HD2	1.91	0.53
32:i:291:TYR:HB2	40:r:151:PHE:CZ	2.44	0.53
40:r:272:THR:HA	40:r:275:ILE:HD12	1.90	0.53
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	0.53
1:A:164:ASN:HB3	10:K:77:HIS:HB2	1.91	0.53
1:A:317:VAL:HG13	1:A:356:VAL:HA	1.91	0.53
2:B:90:PRO:HD2	3:C:100:ARG:HH11	1.74	0.53
11:L:120:PRO:HB2	15:P:203:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	0.53
25:b:105:PHE:HD2	43:v:68:LYS:HG3	1.74	0.53
35:l:293:LEU:HD11	35:l:418:LEU:HD22	1.90	0.53
40:r:73:LEU:O	40:r:76:THR:OG1	2.18	0.53
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.91	0.53
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.91	0.53
6:G:105:MET:HE2	6:G:138:LEU:HD23	1.89	0.53
12:M:308:ARG:NH1	12:M:578:PRO:O	2.42	0.53
12:M:519:ILE:HD13	12:M:522:GLN:HB2	1.90	0.53
15:P:115:THR:HG22	16:Q:423:LYS:HD3	1.91	0.53
16:Q:435:LEU:HA	16:Q:438:MET:HE3	1.91	0.53
18:T:52:ARG:HB3	18:T:55:ARG:HH12	1.74	0.53
19:U:69:HIS:ND1	19:U:70:PRO:HA	2.24	0.53
22:Y:71:TRP:CE3	22:Y:71:TRP:C	2.87	0.53
25:b:105:PHE:HE2	43:v:68:LYS:CA	2.19	0.53
31:h:40:TRP:HH2	32:i:83:GLN:HE21	1.57	0.53
32:i:300:THR:OG1	32:i:301:SER:N	2.38	0.53
34:k:11:ALA:HB1	36:m:16:PHE:HD2	1.72	0.53
34:k:62:VAL:HG21	36:m:152:LEU:HD21	1.91	0.53
36:m:19:PHE:CZ	36:m:32:LEU:HD21	2.43	0.53
40:r:286:ILE:O	40:r:289:SER:OG	2.23	0.53
1:A:116:ASN:HD22	46:A:502:FMN:C9	2.22	0.52
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.52
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.52
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.52
17:S:54:ILE:HG13	31:h:105:ARG:HH11	1.72	0.52
27:d:57:TYR:HD1	27:d:57:TYR:O	1.91	0.52
27:d:73:GLU:HG3	30:g:106:LYS:O	2.08	0.52
32:i:229:LEU:HD22	32:i:232:ARG:NH1	2.24	0.52
34:k:7:ASN:OD1	36:m:13:VAL:CG2	2.57	0.52
43:v:56:ARG:O	43:v:60:ALA:HB2	2.10	0.52
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.52
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.52
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.24	0.52
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.52
33:j:24:LEU:H	33:j:25:PRO:CD	2.22	0.52
34:k:15:SER:OG	34:k:36:MET:HG2	2.08	0.52
34:k:58:ILE:HG23	36:m:145:LEU:HD12	1.92	0.52
36:m:23:PRO:O	36:m:24:SER:OG	2.24	0.52
47:r:501:PLX:H262	47:r:501:PLX:H6	1.91	0.52
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
9:J:223:PHE:O	9:J:225:PRO:HD2	2.09	0.52
12:M:613:PRO:HB3	13:N:134:ILE:HG21	1.91	0.52
24:a:90:ASN:ND2	47:b:201:PLX:H122	2.19	0.52
26:c:101:TRP:NE1	38:o:61:GLU:O	2.43	0.52
35:l:144:TRP:NE1	35:l:179:ASP:OD1	2.42	0.52
35:l:566:ILE:HA	35:l:569:HIS:HD2	1.73	0.52
1:A:68:ILE:HD11	1:A:256:ARG:HG2	1.91	0.52
3:C:75:ARG:NH2	3:C:144:PRO:HG3	2.24	0.52
12:M:314:LEU:HD11	13:N:140:PRO:HD2	1.92	0.52
17:S:12:MET:CE	41:s:20:LEU:HD12	2.39	0.52
22:Y:61:PHE:CE2	35:l:455:LYS:HG2	2.44	0.52
34:k:4:ILE:O	34:k:8:ILE:HD13	2.09	0.52
35:l:106:TRP:HB2	35:l:449:THR:OG1	2.09	0.52
35:l:194:ASN:HD22	38:o:127:LEU:HD12	1.74	0.52
35:l:195:SER:O	35:l:196:TRP:HB2	2.08	0.52
36:m:36:GLY:HA3	36:m:60:LEU:HD21	1.90	0.52
36:m:50:TYR:O	36:m:54:MET:HG2	2.10	0.52
40:r:131:ALA:O	40:r:135:ARG:HB3	2.09	0.52
44:w:58:ARG:HB3	44:w:202:HIS:CE1	2.44	0.52
6:G:123:GLU:HB2	6:G:128:PHE:O	2.09	0.52
9:J:64:PHE:CD1	9:J:210:GLU:HB3	2.44	0.52
15:P:113:ASP:HB3	15:P:115:THR:HG23	1.91	0.52
15:P:186:ARG:NH2	15:P:193:PHE:O	2.40	0.52
16:Q:66:TRP:CE2	44:w:310:ILE:HD11	2.45	0.52
16:Q:338:ARG:NH2	21:W:23:ARG:HB3	2.24	0.52
20:V:124:LEU:HD23	20:V:127:MET:HE3	1.91	0.52
27:d:57:TYR:CD1	27:d:57:TYR:C	2.85	0.52
30:g:27:ASP:OD1	42:u:172:LYS:NZ	2.42	0.52
36:m:106:VAL:HG11	36:m:117:ASN:HD22	1.75	0.52
37:n:40:ASN:ND2	37:n:56:THR:HG23	2.25	0.52
42:u:24:VAL:HG13	42:u:86:TRP:CD1	2.45	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.92	0.52
11:L:61:ILE:HG22	11:L:64:LEU:HD12	1.91	0.52
12:M:253:VAL:HG23	12:M:345:LEU:HD22	1.90	0.52
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
16:Q:99:MET:HE2	16:Q:109:CYS:SG	2.49	0.52
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.88	0.52
25:b:22:TRP:O	25:b:25:ASP:HB3	2.10	0.52
32:i:239:TRP:HA	51:i:401:CDL:HB32	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:285:ILE:CG1	52:l:701:PEE:H75	2.25	0.52
35:l:59:GLN:HE21	35:l:59:GLN:CA	2.09	0.52
41:s:139:THR:O	41:s:143:GLU:HG3	2.09	0.52
42:u:111:VAL:HG12	42:u:117:TRP:O	2.09	0.52
44:w:294:LEU:O	44:w:298:VAL:HG23	2.09	0.52
6:G:137:LYS:O	6:G:139:MET:N	2.42	0.52
7:H:24:LEU:HD21	7:H:81:ILE:HG22	1.92	0.52
9:J:168:SER:HA	9:J:184:LYS:CE	2.40	0.52
12:M:319:TRP:HZ2	12:M:615:LEU:O	1.92	0.52
12:M:645:ARG:O	12:M:648:GLU:HG2	2.10	0.52
15:P:238:PRO:O	15:P:239:TRP:HB2	2.08	0.52
16:Q:39:PRO:HB3	16:Q:43:TRP:CE3	2.45	0.52
21:W:33:TYR:CG	21:W:34:SER:N	2.77	0.52
21:W:35:MET:HA	21:W:38:ILE:HD12	1.91	0.52
25:b:105:PHE:CD2	43:v:68:LYS:CB	2.93	0.52
27:d:110:ARG:NH1	27:d:110:ARG:CG	2.73	0.52
32:i:222:ASN:HD21	32:i:233:THR:HG22	1.75	0.52
40:r:187:SER:O	40:r:192:ASN:ND2	2.43	0.52
41:s:13:ILE:HG23	41:s:17:MET:HE3	1.92	0.52
1:A:181:LEU:HA	1:A:187:CYS:HB3	1.91	0.52
1:A:236:PHE:HZ	14:O:77:ALA:HB2	1.73	0.52
1:A:423:THR:OG1	45:A:501:SF4:S4	2.68	0.52
17:S:37:ARG:O	21:W:143:TYR:OH	2.27	0.52
20:V:58:GLN:O	20:V:62:THR:HG23	2.10	0.52
24:a:153:GLU:OE2	42:u:166:ARG:NH1	2.33	0.52
26:c:69:GLY:CA	38:o:81:ARG:H	2.23	0.52
33:j:18:MET:SD	41:s:72:ILE:HA	2.50	0.52
36:m:130:GLU:HG2	36:m:131:GLY:O	2.10	0.52
40:r:20:LYS:HA	40:r:89:LEU:HD13	1.92	0.52
44:w:198:TYR:OH	44:w:304:VAL:HG12	2.10	0.52
12:M:89:VAL:HB	12:M:94:MET:HG3	1.91	0.52
14:O:152:ILE:HG21	14:O:171:LEU:HD13	1.92	0.52
16:Q:55:SER:OG	35:l:580:GLN:NE2	2.42	0.52
25:b:39:LYS:HG3	25:b:41:GLY:H	1.74	0.52
25:b:105:PHE:CD2	43:v:68:LYS:HB2	2.45	0.52
35:l:190:ILE:CG1	35:l:196:TRP:CD1	2.93	0.52
35:l:190:ILE:CG1	35:l:196:TRP:NE1	2.73	0.52
40:r:130:LEU:HD11	40:r:150:LEU:HD12	1.92	0.52
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.52
2:B:66:ARG:HH12	21:W:28:ARG:HB3	1.74	0.52
48:E:201:8Q1:C30	48:E:201:8Q1:N36	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:143:GLU:HA	6:G:146:ASP:HB3	1.92	0.52
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.25	0.52
17:S:34:LYS:NZ	42:u:90:ASP:HB3	2.25	0.52
24:a:129:PRO:HG2	27:d:60:ARG:HH22	1.75	0.52
27:d:110:ARG:HH11	27:d:110:ARG:CG	2.14	0.52
32:i:336:LEU:HD21	32:i:343:MET:SD	2.50	0.52
35:l:244:SER:HA	35:l:248:HIS:HD2	1.73	0.52
35:l:371:THR:O	35:l:374:THR:OG1	2.28	0.52
40:r:5:ILE:O	40:r:8:THR:OG1	2.26	0.52
41:s:17:MET:CE	41:s:232:ILE:HD12	2.37	0.52
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	0.51
2:B:72:LEU:HA	41:s:31:MET:HE1	1.92	0.51
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.91	0.51
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.51
11:L:84:ARG:HG3	11:L:90:GLY:O	2.10	0.51
16:Q:304:LYS:HE3	16:Q:316:PHE:CE1	2.46	0.51
19:U:84:LEU:O	21:W:59:ARG:NH1	2.41	0.51
25:b:105:PHE:HZ	43:v:67:LEU:CB	2.23	0.51
47:b:201:PLX:O3	47:b:201:PLX:H72	2.10	0.51
47:r:502:PLX:C7	47:r:502:PLX:C3	2.88	0.51
41:s:173:TRP:CZ3	41:s:262:LYS:HE2	2.45	0.51
42:u:31:HIS:CE1	42:u:111:VAL:HG11	2.44	0.51
5:F:72:GLY:HA3	12:M:359:ASN:HB3	1.92	0.51
12:M:278:HIS:CD2	12:M:280:ASP:HB2	2.44	0.51
12:M:634:LEU:HD23	12:M:636:TYR:CZ	2.45	0.51
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.51
16:Q:228:ARG:CZ	16:Q:233:HIS:HB2	2.40	0.51
18:T:56:PHE:CD1	18:T:61:LYS:HB2	2.45	0.51
24:a:87:THR:CG2	47:b:201:PLX:H131	2.40	0.51
33:j:70:ALA:HB1	36:m:58:ILE:HD11	1.92	0.51
35:l:332:HIS:CE1	35:l:336:LYS:HG3	2.46	0.51
35:l:567:SER:O	35:l:571:ILE:HD13	2.09	0.51
1:A:300:ILE:HA	1:A:304:ALA:HB3	1.93	0.51
6:G:147:TYR:O	6:G:151:LYS:N	2.43	0.51
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	0.51
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
26:c:159:LYS:HA	43:v:98:ARG:NH1	2.24	0.51
44:w:98:THR:HG23	44:w:337:ARG:NH2	2.25	0.51
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.45	0.51
2:B:127:THR:HB	2:B:144:ASP:OD1	2.10	0.51
3:C:75:ARG:HH11	41:s:57:THR:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:ILE:HG21	9:J:86:CYS:O	2.11	0.51
4:E:50:PHE:HB2	4:E:52:LEU:CD1	2.40	0.51
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.51
12:M:61:PRO:HG2	12:M:113:ARG:HE	1.74	0.51
12:M:464:GLN:HE22	12:M:467:LYS:HE2	1.75	0.51
20:V:12:ILE:HG22	20:V:13:PRO:O	2.11	0.51
27:d:135:ASP:C	27:d:156:ARG:HH21	2.18	0.51
32:i:137:ALA:HB3	32:i:138:PRO:HD3	1.93	0.51
34:k:7:ASN:OD1	36:m:13:VAL:HG23	2.10	0.51
35:l:135:ASN:OD1	35:l:198:PRO:CG	2.57	0.51
35:l:226:GLN:HG2	35:l:280:LEU:HD21	1.85	0.51
35:l:227:LEU:HD12	35:l:227:LEU:C	2.35	0.51
35:l:592:PHE:CE2	35:l:596:ILE:HD11	2.45	0.51
36:m:27:TYR:HB3	36:m:82:TRP:CZ2	2.45	0.51
36:m:114:VAL:O	36:m:115:VAL:HG13	2.11	0.51
1:A:86:ARG:NE	1:A:92:GLY:O	2.41	0.51
11:L:169:ARG:NH1	12:M:426:ASP:HA	2.25	0.51
12:M:430:ALA:HA	12:M:442:TYR:HB2	1.93	0.51
16:Q:203:LEU:HD11	16:Q:258:LEU:HD11	1.93	0.51
27:d:76:ILE:O	27:d:80:TYR:N	2.40	0.51
32:i:37:MET:HE3	32:i:41:ILE:HD11	1.93	0.51
35:l:119:LYS:O	35:l:123:ILE:HG12	2.11	0.51
35:l:419:THR:HA	35:l:422:TYR:CE2	2.45	0.51
40:r:145:ALA:HA	40:r:148:TYR:HB3	1.91	0.51
41:s:167:THR:C	41:s:169:GLN:H	2.18	0.51
42:u:142:TYR:O	42:u:144:SER:N	2.44	0.51
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	0.51
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.51
15:P:168:ARG:NH1	15:P:185:ARG:HG3	2.26	0.51
18:T:83:ARG:NH1	18:T:103:LEU:H	2.08	0.51
6:X:77:GLU:HB2	23:Z:13:LYS:HE2	1.93	0.51
24:a:160:MET:HE2	24:a:168:TRP:HB2	1.92	0.51
25:b:108:ASP:O	25:b:109:THR:HB	2.10	0.51
28:e:56:GLN:HG2	44:w:320:GLY:HA3	1.93	0.51
28:e:87:MET:HE1	40:r:431:THR:HG21	1.92	0.51
35:l:485:TYR:O	35:l:489:THR:HG23	2.10	0.51
35:l:563:PRO:HG3	40:r:148:TYR:OH	2.10	0.51
44:w:54:THR:C	44:w:56:ARG:H	2.19	0.51
44:w:115:GLU:HA	44:w:118:TYR:HD2	1.76	0.51
2:B:109:GLU:OE2	2:B:139:ARG:HD2	2.10	0.51
3:C:112:ALA:O	3:C:113:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.51
9:J:168:SER:N	9:J:201:VAL:O	2.40	0.51
12:M:76:ARG:HE	12:M:79:LEU:HD21	1.75	0.51
16:Q:271:ARG:HH12	41:s:281:ARG:HA	1.76	0.51
35:l:87:MET:O	35:l:91:PRO:HD3	2.11	0.51
38:o:17:THR:O	38:o:23:TYR:OH	2.21	0.51
40:r:281:ASP:HB2	40:r:284:SER:OG	2.10	0.51
44:w:128:SER:OG	44:w:173:MET:SD	2.69	0.51
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.51
11:L:107:TRP:HZ3	11:L:118:ALA:HB2	1.76	0.51
12:M:372:PHE:CD1	12:M:481:LEU:HD13	2.46	0.51
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.51
13:N:18:GLY:O	13:N:20:LEU:N	2.44	0.51
16:Q:381:HIS:O	16:Q:385:TYR:HD2	1.93	0.51
47:g:202:PLX:H1C2	47:g:202:PLX:H31	1.93	0.51
32:i:128:LEU:HD11	32:i:213:THR:HG22	1.93	0.51
34:k:8:ILE:CD1	34:k:8:ILE:N	2.73	0.51
35:l:343:SER:O	35:l:347:ILE:HD12	2.11	0.51
40:r:104:ILE:O	40:r:108:MET:HG2	2.10	0.51
41:s:154:LEU:HD13	41:s:160:PHE:CD1	2.46	0.51
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.51
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	0.51
3:C:162:TYR:O	16:Q:123:LEU:HD21	2.10	0.51
9:J:84:TYR:HB2	9:J:91:ILE:HD11	1.92	0.51
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	0.51
12:M:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.51
6:X:85:TYR:HE2	22:Y:45:ARG:NH1	2.09	0.51
6:X:155:TYR:CD1	25:b:23:LEU:HB3	2.46	0.51
25:b:19:ARG:NH2	39:p:173:ARG:HB2	2.26	0.51
25:b:86:MET:HA	25:b:89:HIS:HB3	1.92	0.51
27:d:111:GLU:HB3	27:d:115:TYR:CB	2.41	0.51
32:i:234:TRP:O	32:i:238:THR:HG22	2.11	0.51
35:l:593:PHE:HB2	35:l:594:PRO:HD3	1.93	0.51
40:r:271:MET:O	40:r:275:ILE:HG13	2.11	0.51
41:s:223:PHE:O	41:s:227:GLU:HG3	2.11	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.51
18:T:80:VAL:HG12	18:T:82:THR:H	1.76	0.51
19:U:58:ARG:NH2	42:u:49:GLU:OE1	2.43	0.51
47:V:203:PLX:H151	38:o:91:ALA:HB2	1.93	0.51
25:b:92:GLU:HG2	25:b:93:LYS:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:113:THR:OG1	25:b:114:GLY:N	2.44	0.51
32:i:268:GLU:OE2	42:u:168:TYR:OH	2.24	0.51
33:j:65:PHE:HA	33:j:68:GLU:HB2	1.93	0.51
44:w:121:PRO:HG2	44:w:178:PHE:HB3	1.93	0.51
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.46	0.50
1:A:87:GLY:N	1:A:93:PHE:O	2.44	0.50
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
2:B:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.50
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	0.50
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.50
11:L:61:ILE:HG12	11:L:140:LYS:O	2.10	0.50
12:M:506:VAL:HG12	12:M:508:GLY:N	2.24	0.50
15:P:74:GLN:HB2	15:P:87:CYS:HB2	1.93	0.50
17:S:24:ALA:HA	41:s:93:ASN:HD22	1.76	0.50
29:f:55:TRP:CE2	30:g:65:THR:HG22	2.46	0.50
31:h:99:ILE:HD12	31:h:101:LYS:HB2	1.93	0.50
32:i:139:ILE:HD11	32:i:187:MET:HE1	1.92	0.50
32:i:243:LEU:HD21	51:i:401:CDL:H752	1.92	0.50
34:k:81:ILE:HG22	34:k:87:LEU:HA	1.92	0.50
35:l:42:SER:O	35:l:46:ILE:HG12	2.11	0.50
36:m:67:PHE:O	36:m:71:THR:HG23	2.11	0.50
39:p:104:LEU:HD21	39:p:119:PHE:CE1	2.41	0.50
12:M:302:LEU:HB3	12:M:585:PRO:HB3	1.93	0.50
13:N:30:THR:HG21	13:N:63:VAL:HG22	1.91	0.50
14:O:63:ILE:HA	14:O:66:ILE:HD12	1.92	0.50
16:Q:85:GLY:H	16:Q:88:HIS:HE2	1.58	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:HB3	1.93	0.50
23:Z:29:LEU:HD23	39:p:35:ASP:OD1	2.12	0.50
47:b:201:PLX:H21	27:d:43:ARG:HH22	1.77	0.50
30:g:29:ARG:HH21	42:u:172:LYS:HB3	1.76	0.50
31:h:80:ARG:NH1	36:m:121:VAL:HG22	2.26	0.50
40:r:120:ILE:O	40:r:124:THR:HG23	2.11	0.50
40:r:134:THR:O	40:r:142:ARG:NE	2.33	0.50
40:r:144:ASN:OD1	40:r:145:ALA:N	2.45	0.50
2:B:37:LYS:O	16:Q:320:VAL:N	2.37	0.50
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.33	0.50
9:J:142:GLU:OE2	9:J:146:VAL:HG21	2.11	0.50
12:M:569:GLN:NE2	12:M:622:ILE:HD12	2.26	0.50
13:N:40:GLY:HA3	13:N:48:TYR:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.50
15:P:202:PHE:HB2	15:P:203:PRO:HD2	1.93	0.50
16:Q:394:GLY:O	16:Q:413:SER:OG	2.23	0.50
22:Y:51:THR:HG21	35:l:446:ASN:HD21	1.76	0.50
24:a:184:LYS:O	24:a:186:THR:N	2.45	0.50
29:f:47:THR:HG22	47:g:203:PLX:H1A1	1.94	0.50
31:h:6:ILE:HB	32:i:22:LEU:HD22	1.93	0.50
35:l:15:LEU:O	35:l:18:PRO:HD2	2.11	0.50
40:r:423:ILE:HD12	40:r:425:ASN:H	1.75	0.50
43:v:5:LEU:O	43:v:8:ARG:HG2	2.11	0.50
2:B:108:GLU:OE1	18:T:68:ALA:HB1	2.12	0.50
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.50
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.50
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	0.50
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.50
12:M:213:MET:HG3	12:M:215:MET:HG3	1.93	0.50
13:N:137:TRP:HH2	13:N:140:PRO:HD3	1.75	0.50
24:a:54:LEU:CD2	25:b:27:GLU:CA	2.89	0.50
27:d:156:ARG:NH1	28:e:139:SER:O	2.37	0.50
32:i:150:ASN:HD21	35:l:602:ILE:HD13	1.76	0.50
35:l:68:TRP:HB2	35:l:76:LEU:CD1	2.41	0.50
35:l:428:LEU:HD23	35:l:432:THR:HG21	1.93	0.50
37:n:50:GLN:OE1	37:n:51:PRO:HD2	2.11	0.50
38:o:6:TYR:OH	38:o:12:ARG:HG2	2.11	0.50
44:w:218:ILE:HD11	44:w:226:GLU:HB3	1.93	0.50
5:F:30:SER:OG	5:F:63:PRO:HG3	2.11	0.50
9:J:206:ILE:HB	9:J:242:VAL:HG23	1.90	0.50
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	0.50
12:M:151:SER:OG	16:Q:374:SER:HB2	2.11	0.50
12:M:307:VAL:HB	12:M:317:THR:HG21	1.93	0.50
12:M:405:THR:HG1	12:M:479:SER:HG	1.55	0.50
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	0.50
16:Q:69:VAL:HG12	16:Q:72:PRO:CD	2.41	0.50
16:Q:82:LEU:N	16:Q:99:MET:O	2.41	0.50
47:V:203:PLX:H201	38:o:95:PHE:CZ	2.47	0.50
31:h:101:LYS:C	31:h:104:PRO:HD2	2.37	0.50
32:i:315:TRP:HZ3	44:w:327:VAL:HG12	1.76	0.50
35:l:594:PRO:O	35:l:598:THR:HG23	2.12	0.50
39:p:170:ILE:O	39:p:173:ARG:HG3	2.11	0.50
47:r:502:PLX:C33	47:r:502:PLX:C37	2.85	0.50
41:s:303:TRP:NE1	41:s:307:MET:SD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:139:ARG:HD2	44:w:166:ASP:OD2	2.12	0.50
44:w:331:PHE:CZ	44:w:337:ARG:HB3	2.46	0.50
1:A:112:TYR:CD1	1:A:155:TYR:HE2	2.29	0.50
9:J:159:ALA:HB3	9:J:161:VAL:HG23	1.93	0.50
16:Q:291:VAL:N	16:Q:294:ARG:HH21	2.09	0.50
27:d:60:ARG:NH1	27:d:60:ARG:CG	2.73	0.50
28:e:112:TYR:O	40:r:45:ILE:HG23	2.11	0.50
29:f:30:TYR:HD2	44:w:98:THR:HA	1.77	0.50
32:i:98:ILE:O	32:i:102:MET:HG2	2.12	0.50
32:i:309:ASN:OD1	44:w:319:ILE:HD11	2.11	0.50
35:l:49:PHE:O	35:l:52:THR:OG1	2.22	0.50
35:l:136:ASN:OD1	35:l:137:LEU:N	2.44	0.50
41:s:230:ASN:O	41:s:234:MET:HG2	2.11	0.50
44:w:248:GLU:OE1	44:w:252:LYS:NZ	2.45	0.50
1:A:443:ARG:HB3	1:A:444:PRO:HD3	1.94	0.50
2:B:36:TYR:HD2	8:I:104:TRP:HB2	1.77	0.50
2:B:72:LEU:HB2	41:s:272:TRP:HH2	1.76	0.50
2:B:81:THR:HG23	41:s:35:LYS:H	1.77	0.50
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.50
12:M:92:CYS:SG	50:M:803:FES:S2	3.10	0.50
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.50
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.50
6:X:88:LYS:HZ1	6:X:98:LEU:HD22	1.76	0.50
22:Y:86:TYR:HB3	22:Y:87:PRO:CB	2.41	0.50
32:i:244:ILE:HB	32:i:245:PRO:HD3	1.93	0.50
35:l:44:PHE:O	35:l:47:SER:OG	2.24	0.50
35:l:306:THR:HA	35:l:336:LYS:NZ	2.27	0.50
40:r:355:MET:HA	40:r:358:TRP:HD1	1.77	0.50
41:s:180:PRO:O	41:s:184:MET:HG2	2.11	0.50
16:Q:65:PRO:HG2	16:Q:69:VAL:HG22	1.94	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.50
25:b:89:HIS:C	25:b:89:HIS:CD2	2.90	0.50
35:l:190:ILE:CD1	35:l:196:TRP:NE1	2.73	0.50
51:n:101:CDL:HB62	42:u:172:LYS:HB2	1.93	0.50
41:s:203:GLY:O	41:s:205:SER:N	2.43	0.50
1:A:118:ASP:O	1:A:159:ARG:CD	2.60	0.50
4:E:50:PHE:HE1	4:E:96:VAL:HG13	1.76	0.50
9:J:268:PRO:HG3	9:J:344:PRO:HA	1.94	0.50
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.50
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
24:a:99:ALA:O	27:d:58:TYR:HD1	1.95	0.50
26:c:69:GLY:HA3	38:o:81:ARG:O	2.12	0.50
30:g:38:TYR:CE2	30:g:42:LEU:HD11	2.47	0.50
35:l:70:THR:HG23	35:l:75:GLN:HB3	1.94	0.50
35:l:74:THR:HG23	35:l:194:ASN:OD1	2.08	0.50
40:r:220:HIS:HE1	40:r:232:ALA:HB2	1.77	0.50
41:s:9:LEU:HD13	41:s:95:LEU:HD12	1.94	0.50
43:v:39:MET:SD	43:v:58:TYR:HD1	2.34	0.50
44:w:57:SER:OG	44:w:154:GLY:O	2.28	0.50
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.49
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.49
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.49
9:J:62:THR:HB	49:J:401:NDP:HO3A	1.76	0.49
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.49
16:Q:85:GLY:CA	33:j:39:CYS:HB2	2.42	0.49
16:Q:87:GLN:O	16:Q:88:HIS:O	2.30	0.49
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.49
16:Q:271:ARG:HH11	41:s:281:ARG:N	2.09	0.49
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.45	0.49
18:T:89:GLY:HA2	18:T:115:CYS:SG	2.52	0.49
25:b:33:PRO:HD2	39:p:114:MET:O	2.12	0.49
25:b:61:VAL:HA	25:b:64:VAL:HG12	1.93	0.49
26:c:55:TYR:OH	26:c:74:ASP:OD2	2.24	0.49
33:j:109:LYS:HA	33:j:112:ASP:HB2	1.94	0.49
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.46	0.49
35:l:566:ILE:HA	35:l:569:HIS:CD2	2.47	0.49
36:m:33:ILE:HA	36:m:60:LEU:HD22	1.94	0.49
39:p:167:TRP:CE3	39:p:171:VAL:HG21	2.32	0.49
44:w:149:HIS:HE1	44:w:155:GLN:HB3	1.76	0.49
1:A:63:TYR:HD2	1:A:256:ARG:HD2	1.76	0.49
3:C:79:LEU:HB2	3:C:108:VAL:HG12	1.94	0.49
6:G:112:SER:O	6:G:115:GLN:HB3	2.11	0.49
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
7:H:115:PRO:HG3	16:Q:393:PRO:HB2	1.94	0.49
9:J:179:ARG:HB3	9:J:179:ARG:NH1	2.27	0.49
9:J:201:VAL:HG13	9:J:265:PHE:CE2	2.47	0.49
12:M:61:PRO:HG2	12:M:113:ARG:NE	2.26	0.49
12:M:209:TYR:O	12:M:210:ILE:HG22	2.12	0.49
12:M:381:LEU:HB2	12:M:384:ASN:OD1	2.12	0.49
13:N:87:HIS:O	13:N:91:HIS:HD2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:V:202:PEE:H40	52:V:202:PEE:C35	2.42	0.49
25:b:77:VAL:HB	25:b:78:PRO:HD3	1.94	0.49
30:g:4:ARG:NH1	30:g:6:ASN:HB3	2.28	0.49
35:l:188:TRP:CD2	35:l:212:PRO:HG3	2.48	0.49
41:s:195:ARG:HG3	41:s:197:PRO:HD2	1.93	0.49
44:w:335:PRO:HA	44:w:338:LYS:HG3	1.94	0.49
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.77	0.49
5:F:41:TYR:OH	12:M:380:ASP:OD2	2.20	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
9:J:212:ARG:HH11	9:J:212:ARG:CG	2.12	0.49
10:K:104:GLU:OE1	10:K:104:GLU:N	2.46	0.49
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	0.49
12:M:168:LEU:HD23	12:M:292:PHE:CD2	2.47	0.49
26:c:111:MET:HG3	40:r:278:ARG:HH12	1.77	0.49
32:i:9:ILE:O	32:i:12:THR:OG1	2.30	0.49
32:i:234:TRP:C	32:i:238:THR:HG22	2.37	0.49
35:l:450:LEU:C	35:l:450:LEU:CD2	2.85	0.49
3:C:73:TRP:HD1	3:C:76:ARG:NH2	2.10	0.49
4:E:25:MET:CB	4:E:29:LYS:CE	2.59	0.49
12:M:385:TYR:O	12:M:517:HIS:NE2	2.43	0.49
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.49
24:a:115:HIS:HE1	24:a:117:ILE:HD12	1.77	0.49
30:g:27:ASP:OD1	30:g:28:PRO:HD2	2.13	0.49
32:i:329:LEU:O	32:i:333:THR:HG23	2.11	0.49
38:o:8:PRO:HD3	38:o:14:LEU:HD21	1.95	0.49
41:s:228:TYR:CD1	41:s:231:ILE:HD12	2.43	0.49
44:w:305:LEU:O	44:w:308:THR:HG22	2.12	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.49
9:J:238:GLN:NE2	9:J:267:GLY:O	2.43	0.49
12:M:300:GLN:HA	13:N:135:GLN:O	2.12	0.49
12:M:348:ALA:O	12:M:352:VAL:HG23	2.12	0.49
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
25:b:13:GLN:O	25:b:17:GLU:HG2	2.12	0.49
33:j:28:ASN:HB2	33:j:30:TYR:CZ	2.47	0.49
35:l:189:PHE:CD1	35:l:201:MET:HE3	2.48	0.49
36:m:130:GLU:OE1	36:m:130:GLU:N	2.39	0.49
1:A:71:LYS:HA	1:A:147:ARG:HH21	1.77	0.49
6:G:123:GLU:OE1	6:G:130:ILE:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:350:ILE:HG21	9:J:366:ILE:HG12	1.95	0.49
12:M:711:VAL:HA	12:M:714:VAL:HG12	1.94	0.49
16:Q:323:ARG:N	16:Q:328:ASP:OD2	2.46	0.49
16:Q:424:ILE:O	16:Q:463:ARG:NE	2.45	0.49
20:V:62:THR:HG22	20:V:104:ARG:NE	2.27	0.49
22:Y:78:GLU:HG2	35:l:385:PHE:HE1	1.78	0.49
22:Y:86:TYR:HH	43:v:100:LYS:HG2	1.78	0.49
26:c:108:HIS:HE1	35:l:546:GLN:HG2	1.77	0.49
30:g:29:ARG:NH2	42:u:172:LYS:HD2	2.28	0.49
32:i:232:ARG:NH2	44:w:306:ASN:OD1	2.29	0.49
34:k:60:PRO:O	34:k:63:MET:HB2	2.12	0.49
35:l:286:LEU:HB2	35:l:411:ILE:HG23	1.95	0.49
42:u:131:VAL:HG12	42:u:133:THR:HG23	1.95	0.49
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.49
3:C:140:GLN:HG2	33:j:37:TYR:CG	2.47	0.49
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.49
9:J:85:ARG:CG	9:J:85:ARG:NH1	2.72	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
9:J:212:ARG:NH1	9:J:212:ARG:CG	2.73	0.49
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.49
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.49
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.49
20:V:39:TYR:HD2	51:V:201:CDL:H721	1.76	0.49
21:W:101:VAL:HG21	31:h:82:GLN:NE2	2.28	0.49
24:a:101:ILE:HG13	27:d:58:TYR:HB3	1.94	0.49
52:l:701:PEE:C23	40:r:155:VAL:HB	2.29	0.49
36:m:22:LYS:N	36:m:23:PRO:HD3	2.28	0.49
41:s:79:LEU:HD11	41:s:222:LEU:HD22	1.94	0.49
1:A:160:GLY:HA2	1:A:199:ARG:NH1	2.27	0.49
11:L:75:ARG:HH11	11:L:104:ARG:NE	2.10	0.49
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
15:P:190:ASP:OD1	15:P:191:TYR:N	2.45	0.49
16:Q:175:GLY:O	16:Q:178:THR:OG1	2.29	0.49
16:Q:358:VAL:HG12	16:Q:360:ASP:H	1.78	0.49
26:c:52:ALA:CB	26:c:59:VAL:HA	2.42	0.49
32:i:41:ILE:HD11	32:i:60:PHE:HD1	1.78	0.49
35:l:75:GLN:HG2	35:l:75:GLN:O	2.13	0.49
39:p:136:GLU:HG2	39:p:165:PRO:HA	1.94	0.49
40:r:113:THR:O	40:r:176:ILE:HG13	2.12	0.49
41:s:141:SER:HB2	41:s:290:TRP:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:62:THR:HB	49:J:401:NDP:O2X	2.12	0.49
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.77	0.49
13:N:11:LEU:HA	13:N:14:ILE:HD12	1.94	0.49
14:O:193:TYR:HB3	14:O:196:LEU:HD11	1.94	0.49
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.49
52:V:202:PEE:H41	52:V:202:PEE:C37	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
35:l:47:SER:O	35:l:50:PRO:HD2	2.12	0.49
35:l:100:ILE:HD12	35:l:246:LEU:CG	2.39	0.49
35:l:386:LEU:HD12	35:l:387:THR:N	2.28	0.49
36:m:118:PHE:HZ	36:m:124:TRP:HZ2	1.61	0.49
40:r:220:HIS:CE1	40:r:232:ALA:HB2	2.47	0.49
44:w:217:ARG:HA	44:w:220:LYS:HD2	1.95	0.49
1:A:202:GLY:O	12:M:200:ARG:NH2	2.42	0.49
7:H:46:LYS:HE3	8:I:90:THR:OG1	2.13	0.49
8:I:96:THR:OG1	8:I:98:ALA:O	2.19	0.49
9:J:217:PHE:CZ	9:J:322:MET:CE	2.86	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
22:Y:44:TYR:HD1	35:l:440:LEU:HB2	1.78	0.49
26:c:111:MET:HG3	40:r:278:ARG:NH1	2.27	0.49
32:i:334:THR:OG1	32:i:335:LEU:N	2.45	0.49
32:i:337:LEU:O	32:i:339:ILE:N	2.46	0.49
34:k:81:ILE:CG2	34:k:87:LEU:HA	2.43	0.49
35:l:51:THR:CG2	35:l:91:PRO:CG	2.84	0.49
40:r:18:SER:OG	40:r:23:ILE:HG12	2.13	0.49
43:v:113:LYS:HA	43:v:116:GLU:OE1	2.13	0.49
44:w:242:LYS:HA	44:w:246:LEU:HG	1.95	0.49
1:A:274:LYS:HB2	1:A:292:MET:SD	2.53	0.48
2:B:51:VAL:HG22	2:B:54:ARG:NH1	2.26	0.48
9:J:152:ILE:HG22	9:J:164:PHE:HE1	1.77	0.48
12:M:372:PHE:CE1	12:M:481:LEU:HD13	2.48	0.48
16:Q:86:PRO:HG2	33:j:41:PHE:CE2	2.37	0.48
16:Q:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.48
16:Q:438:MET:HE1	16:Q:454:GLN:HE22	1.78	0.48
20:V:62:THR:HG22	20:V:104:ARG:HD3	1.95	0.48
30:g:38:TYR:O	30:g:42:LEU:HG	2.13	0.48
31:h:32:ARG:NH2	34:k:50:ASN:O	2.42	0.48
35:l:119:LYS:HD2	51:l:703:CDL:HB32	1.95	0.48
47:r:502:PLX:H52	47:r:502:PLX:P1	2.53	0.48
41:s:106:LEU:HD21	41:s:150:LEU:HD12	1.94	0.48
43:v:41:ALA:O	43:v:42:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:323:GLN:O	44:w:326:ARG:HB3	2.13	0.48
1:A:256:ARG:O	14:O:246:GLN:HB3	2.13	0.48
1:A:378:SER:O	1:A:380:GLY:N	2.45	0.48
3:C:109:VAL:HG21	41:s:25:ARG:HH12	1.78	0.48
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.48
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.96	0.48
12:M:136:GLU:OE1	12:M:136:GLU:N	2.46	0.48
12:M:171:THR:HB	12:M:173:MET:HE3	1.94	0.48
12:M:200:ARG:HH21	14:O:120:THR:HG23	1.78	0.48
16:Q:149:GLN:HG3	16:Q:171:ARG:HD3	1.94	0.48
17:S:50:ARG:CZ	17:S:54:ILE:HD11	2.43	0.48
21:W:141:MET:SD	36:m:47:GLY:HA2	2.53	0.48
23:Z:28:PRO:O	23:Z:31:THR:OG1	2.22	0.48
32:i:18:LEU:O	32:i:22:LEU:HG	2.14	0.48
32:i:115:VAL:HG12	32:i:180:ALA:HB1	1.95	0.48
35:l:383:MET:SD	35:l:384:PRO:HD2	2.52	0.48
37:n:55:VAL:HG12	37:n:56:THR:N	2.24	0.48
41:s:73:THR:O	41:s:76:THR:OG1	2.20	0.48
1:A:318:ILE:HD11	1:A:355:ILE:HD13	1.94	0.48
14:O:115:VAL:O	14:O:119:TYR:HD2	1.96	0.48
19:U:58:ARG:HH12	42:u:137:LEU:N	2.10	0.48
20:V:29:ALA:O	20:V:63:ALA:HB1	2.13	0.48
24:a:54:LEU:HD21	25:b:27:GLU:HA	1.90	0.48
25:b:39:LYS:O	25:b:42:PRO:HD2	2.13	0.48
28:e:107:ALA:O	47:r:502:PLX:H1B3	2.13	0.48
32:i:59:TYR:CZ	32:i:63:GLN:OE1	2.67	0.48
35:l:37:LYS:HZ3	35:l:98:TRP:CD1	2.31	0.48
35:l:173:LEU:HD21	40:r:405:LEU:HD21	1.96	0.48
35:l:347:ILE:HG12	35:l:354:GLN:HG2	1.95	0.48
40:r:188:ASN:CG	40:r:189:SER:H	2.21	0.48
44:w:109:ASN:HD21	44:w:111:ASN:HD22	1.61	0.48
44:w:335:PRO:HA	44:w:338:LYS:NZ	2.29	0.48
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
9:J:197:GLU:OE1	9:J:197:GLU:N	2.45	0.48
9:J:360:ARG:HA	36:m:78:TYR:CE1	2.48	0.48
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.48
21:W:47:HIS:O	21:W:51:MET:HG3	2.13	0.48
24:a:114:LYS:CA	27:d:57:TYR:CD2	2.97	0.48
30:g:119:ARG:HD3	38:o:116:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.95	0.48
9:J:93:HIS:O	9:J:96:PRO:HD2	2.14	0.48
11:L:75:ARG:NH2	11:L:101:PHE:HB3	2.29	0.48
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	0.48
12:M:365:THR:HG22	12:M:537:ILE:HD11	1.95	0.48
12:M:610:VAL:O	12:M:611:THR:OG1	2.25	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
17:S:53:ARG:HH21	31:h:105:ARG:HD3	1.77	0.48
24:a:160:MET:HE3	24:a:166:GLY:HA3	1.96	0.48
32:i:117:GLU:OE1	32:i:117:GLU:N	2.41	0.48
35:l:224:SER:OG	35:l:256:GLY:CA	2.59	0.48
35:l:302:VAL:O	35:l:305:SER:OG	2.24	0.48
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.48
2:B:74:TYR:HD2	41:s:33:LEU:HG	1.79	0.48
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	0.48
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.48
11:L:98:LYS:HA	11:L:126:LEU:O	2.13	0.48
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.48	0.48
14:O:233:SER:OG	14:O:234:LEU:N	2.47	0.48
17:S:28:ARG:O	17:S:33:GLY:N	2.47	0.48
27:d:34:ILE:HG13	27:d:35:VAL:HG13	1.95	0.48
32:i:282:MET:O	32:i:286:THR:HG23	2.14	0.48
40:r:61:LEU:HD22	40:r:241:TYR:CD1	2.45	0.48
41:s:226:ALA:O	41:s:230:ASN:ND2	2.40	0.48
44:w:139:ARG:HH12	44:w:160:GLU:CD	2.22	0.48
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.48
2:B:62:THR:HG22	21:W:35:MET:HE1	1.95	0.48
4:E:128:PRO:HG3	11:L:74:THR:OG1	2.14	0.48
8:I:11:LEU:O	8:I:14:TRP:HB3	2.13	0.48
9:J:357:ARG:HG3	9:J:362:LEU:HA	1.94	0.48
12:M:392:ALA:HA	12:M:417:ARG:HH22	1.78	0.48
12:M:564:CYS:O	12:M:566:ILE:HG12	2.14	0.48
12:M:636:TYR:HB2	12:M:641:GLN:HB3	1.96	0.48
13:N:129:THR:HA	18:T:44:GLN:NE2	2.28	0.48
32:i:128:LEU:HD13	32:i:216:PHE:HD2	1.78	0.48
40:r:127:ILE:HB	40:r:128:PRO:HD3	1.94	0.48
42:u:24:VAL:HG22	42:u:86:TRP:HE1	1.76	0.48
1:A:132:ARG:HG2	1:A:165:GLU:OE1	2.13	0.48
3:C:156:GLY:HA2	3:C:169:GLY:CA	2.41	0.48
4:E:20:ILE:H	4:E:77:ARG:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:52:LEU:HB3	4:E:54:ILE:HG13	1.96	0.48
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.94	0.48
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.48
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.48
24:a:55:PHE:CE2	39:p:118:TYR:CG	2.82	0.48
25:b:108:ASP:CG	25:b:109:THR:H	2.20	0.48
32:i:106:LEU:HB3	32:i:187:MET:HE2	1.95	0.48
33:j:54:LYS:HB3	33:j:113:TRP:NE1	2.29	0.48
35:l:591:PHE:O	35:l:594:PRO:HD2	2.13	0.48
1:A:114:VAL:O	1:A:242:VAL:HA	2.13	0.48
1:A:370:LEU:O	1:A:373:PHE:HB3	2.14	0.48
9:J:250:VAL:O	9:J:254:LYS:HG2	2.13	0.48
10:K:96:MET:HE3	10:K:97:PRO:HD2	1.96	0.48
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.95	0.48
16:Q:124:ILE:HG22	16:Q:419:PRO:HG3	1.96	0.48
21:W:30:LEU:HB2	21:W:32:GLY:H	1.78	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
24:a:95:GLN:OE1	24:a:114:LYS:NZ	2.46	0.48
32:i:37:MET:CE	32:i:60:PHE:HA	2.44	0.48
38:o:73:THR:OG1	38:o:74:ILE:N	2.47	0.48
40:r:1:MET:HG3	40:r:2:LEU:N	2.29	0.48
41:s:42:PRO:HD2	41:s:45:LEU:HD12	1.95	0.48
44:w:258:TYR:CE1	44:w:267:LYS:HA	2.49	0.48
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.48
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.48
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.48
9:J:176:SER:CA	9:J:182:ARG:NH2	2.67	0.48
9:J:203:PRO:O	49:J:401:NDP:H5N	2.14	0.48
12:M:37:ASP:OD1	12:M:38:GLY:N	2.41	0.48
12:M:383:SER:HA	12:M:386:LEU:HD12	1.96	0.48
16:Q:301:ASP:OD1	16:Q:302:LEU:N	2.47	0.48
19:U:52:ASN:HD21	31:h:27:TYR:C	2.20	0.48
22:Y:41:GLU:HG2	35:l:442:ASN:HB2	1.96	0.48
31:h:91:LYS:HG3	31:h:92:TYR:N	2.28	0.48
35:l:213:LEU:HB3	35:l:273:ILE:HD13	1.96	0.48
40:r:94:LEU:O	40:r:97:SER:OG	2.21	0.48
41:s:205:SER:OG	41:s:279:ARG:NH1	2.47	0.48
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.47
20:V:37:ALA:HB1	20:V:56:VAL:HG22	1.95	0.47
20:V:40:ARG:HG3	51:V:201:CDL:HB22	1.96	0.47
25:b:109:THR:HG22	25:b:111:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:b:201:PLX:H111	47:b:201:PLX:C7	2.43	0.47
47:b:201:PLX:O7	47:b:201:PLX:H31	2.13	0.47
47:b:201:PLX:H171	47:b:201:PLX:H141	1.69	0.47
30:g:20:LEU:HD21	42:u:158:LEU:HB3	1.96	0.47
32:i:237:LEU:HD22	32:i:240:LEU:HD12	1.96	0.47
32:i:288:LEU:HD22	52:l:701:PEE:H58	1.69	0.47
33:j:67:LEU:HD23	34:k:65:VAL:HG13	1.95	0.47
34:k:97:GLN:HG2	35:l:587:TYR:OH	2.14	0.47
35:l:19:ILE:HD11	35:l:126:ILE:HD11	1.96	0.47
35:l:306:THR:HA	35:l:336:LYS:HZ3	1.77	0.47
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.96	0.47
40:r:44:GLN:O	40:r:46:ASN:ND2	2.47	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
1:A:123:GLY:N	14:O:180:CYS:SG	2.71	0.47
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47
5:F:35:ASP:O	5:F:39:LYS:HG2	2.14	0.47
5:F:68:ARG:HA	5:F:74:GLU:HG2	1.95	0.47
7:H:35:LEU:O	7:H:45:ARG:NE	2.43	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
11:L:115:ALA:O	15:P:228:GLN:N	2.44	0.47
13:N:38:LEU:HD22	13:N:50:GLU:HB2	1.96	0.47
51:V:201:CDL:H552	51:V:201:CDL:H522	1.69	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
27:d:18:PRO:HG2	43:v:71:ARG:NH1	2.29	0.47
32:i:149:LEU:HD23	32:i:154:LEU:HD13	1.96	0.47
52:l:701:PEE:H65	52:l:701:PEE:H71	1.79	0.47
40:r:132:ILE:O	40:r:136:TRP:HB2	2.14	0.47
41:s:253:GLU:O	41:s:257:THR:HG23	2.13	0.47
42:u:85:TYR:OH	42:u:104:GLN:NE2	2.45	0.47
2:B:40:ASN:O	2:B:42:GLN:N	2.43	0.47
2:B:84:TYR:CE2	2:B:85:PRO:HB3	2.49	0.47
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	0.47
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
10:K:91:LEU:HA	10:K:94:PHE:HD2	1.79	0.47
12:M:236:TYR:CZ	12:M:272:ARG:HD3	2.49	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
24:a:114:LYS:N	27:d:57:TYR:HD2	2.12	0.47
25:b:42:PRO:HA	25:b:45:LYS:HD2	1.96	0.47
25:b:105:PHE:CZ	43:v:67:LEU:CB	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.95	0.47
27:d:20:GLN:OE1	43:v:71:ARG:NH1	2.48	0.47
28:e:89:LEU:HD13	40:r:29:THR:HG21	1.95	0.47
31:h:18:LEU:HD21	34:k:59:MET:HE3	1.96	0.47
32:i:17:THR:HG23	32:i:137:ALA:HB2	1.96	0.47
32:i:135:LYS:O	32:i:139:ILE:HG12	2.14	0.47
32:i:198:PRO:O	32:i:201:THR:OG1	2.23	0.47
39:p:157:ALA:HB2	39:p:164:PRO:N	2.30	0.47
44:w:332:ARG:HA	44:w:332:ARG:HD3	1.61	0.47
1:A:208:GLU:OE1	1:A:211:ALA:N	2.38	0.47
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.47
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.47
9:J:221:HIS:ND1	9:J:221:HIS:C	2.73	0.47
12:M:287:SER:HB3	12:M:290:THR:HG23	1.96	0.47
12:M:360:ARG:NH1	12:M:635:PRO:HD3	2.29	0.47
12:M:704:SER:OG	12:M:706:THR:HG22	2.14	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.47
17:S:21:LEU:HD21	41:s:253:GLU:HA	1.97	0.47
17:S:53:ARG:HB2	31:h:105:ARG:NH2	2.30	0.47
20:V:96:ALA:HA	20:V:99:LEU:HD12	1.95	0.47
24:a:126:TYR:OH	28:e:109:LEU:HD22	2.14	0.47
29:f:31:VAL:O	29:f:34:PRO:HD2	2.15	0.47
30:g:67:PHE:CE1	47:g:203:PLX:H172	2.49	0.47
32:i:319:HIS:CE1	44:w:302:PHE:HD2	2.32	0.47
34:k:83:ASN:HD21	36:m:174:ASN:HA	1.78	0.47
35:l:95:PHE:C	35:l:95:PHE:HD1	2.23	0.47
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.96	0.47
35:l:549:PRO:HG3	40:r:271:MET:HE3	1.96	0.47
39:p:54:GLU:OE2	48:p:201:8Q1:C37	2.61	0.47
9:J:41:MET:HE3	9:J:42:PRO:HD2	1.96	0.47
11:L:92:ASN:O	11:L:95:LYS:HG2	2.15	0.47
16:Q:136:PHE:CE2	16:Q:151:TYR:HB2	2.49	0.47
16:Q:205:GLU:HG3	16:Q:209:LYS:NZ	2.29	0.47
17:S:50:ARG:HD3	31:h:105:ARG:HG2	1.97	0.47
22:Y:50:LEU:O	22:Y:51:THR:OG1	2.27	0.47
26:c:156:VAL:HG12	43:v:98:ARG:CD	2.44	0.47
31:h:22:SER:HB3	31:h:37:GLU:OE1	2.13	0.47
35:l:159:TYR:HB2	40:r:416:TRP:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:194:ASN:ND2	38:o:127:LEU:HB2	2.29	0.47
51:n:101:CDL:H312	51:n:101:CDL:H341	1.56	0.47
41:s:126:ASN:O	41:s:130:ILE:HG13	2.14	0.47
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.48	0.47
5:F:48:ASN:HD21	5:F:53:ILE:HD11	1.77	0.47
8:I:69:ILE:O	8:I:71:SER:N	2.48	0.47
10:K:89:LEU:HD13	14:O:65:ALA:HB2	1.95	0.47
11:L:121:LEU:HA	15:P:203:PRO:HB3	1.97	0.47
12:M:303:THR:O	12:M:615:LEU:HB2	2.15	0.47
18:T:109:THR:HB	18:T:118:GLN:HB3	1.95	0.47
24:a:113:TYR:C	27:d:57:TYR:HD2	2.23	0.47
26:c:184:TYR:HA	43:v:36:GLU:C	2.39	0.47
32:i:241:THR:OG1	32:i:242:PRO:HD3	2.15	0.47
32:i:256:PRO:HG2	32:i:257:LEU:HG	1.96	0.47
32:i:319:HIS:CE1	44:w:302:PHE:CD2	3.02	0.47
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.50	0.47
41:s:65:THR:O	41:s:124:ASN:ND2	2.46	0.47
1:A:276:PHE:CE2	1:A:290:GLU:HB3	2.50	0.47
2:B:151:ILE:HD13	3:C:159:TYR:CD2	2.50	0.47
47:B:303:PLX:H272	41:s:280:PHE:HZ	1.79	0.47
7:H:32:LEU:HG	7:H:52:THR:HG21	1.97	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.47
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.29	0.47
16:Q:57:GLU:HB2	35:l:580:GLN:CD	2.39	0.47
20:V:14:ASP:O	20:V:21:LYS:NZ	2.45	0.47
21:W:101:VAL:HG13	21:W:102:PRO:HD2	1.96	0.47
52:W:201:PEE:H28	52:W:201:PEE:H22	1.50	0.47
24:a:114:LYS:HA	27:d:57:TYR:CD2	2.50	0.47
24:a:168:TRP:HZ2	30:g:85:ARG:HG3	1.80	0.47
24:a:182:SER:O	24:a:184:LYS:HG3	2.15	0.47
47:b:201:PLX:H72	47:b:201:PLX:O2	2.14	0.47
28:e:71:PRO:O	28:e:72:ASP:HB2	2.15	0.47
29:f:60:LYS:O	29:f:64:GLU:HG3	2.14	0.47
47:g:203:PLX:H72	47:g:203:PLX:H11	1.96	0.47
35:l:190:ILE:CG1	35:l:196:TRP:CE2	2.96	0.47
35:l:315:VAL:O	35:l:318:GLY:N	2.48	0.47
40:r:61:LEU:O	40:r:64:PRO:HD2	2.15	0.47
41:s:142:TYR:CE1	41:s:289:LEU:HD21	2.49	0.47
41:s:231:ILE:HG23	41:s:270:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	0.47
3:C:140:GLN:HG2	33:j:37:TYR:CE2	2.50	0.47
7:H:28:TYR:HD1	7:H:52:THR:HG23	1.80	0.47
9:J:281:PHE:HA	9:J:284:ALA:HB3	1.97	0.47
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
12:M:535:GLU:O	12:M:538:ARG:HG2	2.15	0.47
12:M:546:PHE:CE2	12:M:566:ILE:HD12	2.50	0.47
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.47
16:Q:103:GLY:HA3	33:j:52:SER:HB3	1.97	0.47
17:S:34:LYS:HZ1	42:u:90:ASP:HB3	1.80	0.47
17:S:35:GLU:HG2	17:S:35:GLU:O	2.14	0.47
21:W:48:TRP:O	21:W:51:MET:HB2	2.15	0.47
22:Y:88:ASP:N	22:Y:89:PRO:CD	2.78	0.47
25:b:108:ASP:CG	25:b:109:THR:N	2.73	0.47
26:c:159:LYS:CA	43:v:98:ARG:HH12	2.27	0.47
32:i:274:ASN:O	32:i:275:SER:OG	2.30	0.47
40:r:66:LEU:HA	40:r:66:LEU:HD23	1.76	0.47
44:w:46:GLY:HA2	44:w:51:LYS:HE3	1.97	0.47
1:A:69:LEU:HD11	1:A:143:LEU:HD21	1.96	0.47
3:C:59:ARG:HH22	3:C:61:GLU:CB	2.25	0.47
6:G:104:PHE:CD1	6:G:108:LEU:HD22	2.49	0.47
9:J:238:GLN:HG3	9:J:269:SER:O	2.15	0.47
11:L:77:VAL:HG22	11:L:78:ARG:H	1.80	0.47
16:Q:46:GLN:NE2	52:l:701:PEE:H11	2.29	0.47
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.97	0.47
16:Q:338:ARG:NH1	21:W:23:ARG:HB3	2.29	0.47
27:d:141:GLY:HA3	30:g:118:ILE:HD12	1.97	0.47
35:l:189:PHE:CG	35:l:201:MET:HE3	2.50	0.47
2:B:75:LEU:HB2	41:s:31:MET:SD	2.55	0.47
9:J:229:GLY:HA2	9:J:293:LEU:O	2.15	0.47
12:M:69:LEU:HD22	12:M:181:ARG:HG3	1.95	0.47
14:O:138:THR:OG1	14:O:139:PRO:HD3	2.15	0.47
16:Q:57:GLU:HB2	35:l:580:GLN:NE2	2.29	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.15	0.47
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.47
16:Q:281:GLU:N	16:Q:281:GLU:CD	2.73	0.47
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.97	0.47
17:S:4:GLU:O	17:S:7:PRO:HD2	2.15	0.47
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.96	0.47
26:c:163:TYR:OH	43:v:42:THR:O	2.11	0.47
29:f:28:LYS:HE2	44:w:100:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:3:PHE:O	33:j:6:ILE:HB	2.14	0.47
35:l:527:GLY:C	35:l:529:TYR:H	2.22	0.47
35:l:548:LEU:HB2	35:l:549:PRO:HD3	1.95	0.47
40:r:80:SER:HB3	40:r:226:ALA:HB2	1.97	0.47
40:r:130:LEU:O	40:r:134:THR:OG1	2.25	0.47
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
9:J:365:GLU:N	9:J:365:GLU:OE1	2.45	0.46
12:M:68:ARG:NH2	12:M:284:GLU:OE1	2.33	0.46
14:O:54:ASP:OD1	14:O:55:PHE:N	2.47	0.46
16:Q:71:PRO:N	16:Q:72:PRO:CD	2.78	0.46
17:S:53:ARG:HB2	31:h:105:ARG:HH22	1.80	0.46
22:Y:74:TRP:CE3	22:Y:75:HIS:CA	2.91	0.46
47:b:201:PLX:C3	47:b:201:PLX:C1C	2.86	0.46
29:f:28:LYS:HB3	29:f:31:VAL:HB	1.96	0.46
32:i:332:LEU:HD22	32:i:336:LEU:HD12	1.96	0.46
34:k:12:PHE:O	34:k:15:SER:OG	2.25	0.46
35:l:140:LEU:O	35:l:144:TRP:HB2	2.15	0.46
40:r:58:SER:HB2	40:r:63:THR:HG22	1.97	0.46
1:A:203:ALA:HB2	14:O:119:TYR:CE1	2.50	0.46
2:B:91:LEU:HG	16:Q:215:GLU:OE2	2.15	0.46
2:B:94:ARG:NH2	16:Q:237:PRO:HG3	2.30	0.46
3:C:147:VAL:CG2	3:C:176:VAL:HA	2.46	0.46
9:J:355:ARG:HB3	33:j:31:MET:SD	2.56	0.46
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.46
16:Q:97:LEU:HD12	16:Q:97:LEU:O	2.15	0.46
21:W:77:ALA:O	21:W:80:ASP:HB3	2.16	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.46
25:b:106:PRO:HG2	25:b:118:PRO:HD3	1.96	0.46
27:d:120:ILE:O	27:d:123:VAL:N	2.48	0.46
37:n:34:ARG:CZ	51:n:101:CDL:HB22	2.45	0.46
41:s:236:THR:HG22	41:s:263:THR:HG21	1.96	0.46
43:v:104:ARG:O	43:v:108:LEU:HG	2.15	0.46
9:J:299:ARG:HE	9:J:316:ARG:HH11	1.62	0.46
12:M:620:TRP:NE1	12:M:639:LEU:HD13	2.30	0.46
14:O:84:ASP:O	14:O:88:ARG:N	2.47	0.46
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.46
14:O:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46
15:P:83:GLU:HB3	15:P:142:ARG:NH1	2.29	0.46
16:Q:156:GLU:OE2	16:Q:163:PRO:HG3	2.15	0.46
25:b:111:LEU:HB2	25:b:112:GLU:OE1	2.14	0.46
27:d:133:TYR:O	27:d:136:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:33:ILE:HG22	30:g:67:PHE:HB3	1.97	0.46
35:l:100:ILE:CD1	35:l:246:LEU:HG	2.40	0.46
35:l:559:GLU:O	35:l:564:LYS:HG2	2.15	0.46
40:r:35:SER:O	40:r:38:PRO:HD2	2.15	0.46
40:r:63:THR:OG1	40:r:64:PRO:HD3	2.15	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.46
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.46
7:H:36:GLU:HA	7:H:45:ARG:NH2	2.19	0.46
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
11:L:69:GLU:HB2	11:L:73:LYS:HZ2	1.79	0.46
11:L:69:GLU:HB2	11:L:73:LYS:NZ	2.30	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	0.46
12:M:299:ARG:O	12:M:301:ARG:HG2	2.15	0.46
12:M:645:ARG:HG3	12:M:648:GLU:OE2	2.16	0.46
16:Q:131:GLN:O	16:Q:134:PRO:HD2	2.16	0.46
16:Q:159:LEU:O	16:Q:161:ILE:HG13	2.16	0.46
16:Q:241:MET:HE3	21:W:16:TYR:OH	2.15	0.46
17:S:47:LEU:HA	17:S:50:ARG:HB3	1.98	0.46
20:V:121:ALA:O	20:V:125:VAL:HG23	2.16	0.46
24:a:168:TRP:CZ2	30:g:85:ARG:HG3	2.50	0.46
24:a:170:TYR:HE2	24:a:172:GLU:HG2	1.80	0.46
27:d:120:ILE:O	27:d:121:LYS:C	2.56	0.46
47:g:202:PLX:H101	47:g:202:PLX:H132	1.44	0.46
33:j:56:PHE:CE1	36:m:70:THR:HG21	2.51	0.46
34:k:2:PRO:CG	36:m:115:VAL:CG2	2.84	0.46
35:l:508:THR:HG22	35:l:514:LYS:HE3	1.96	0.46
36:m:10:VAL:O	36:m:14:MET:HG2	2.16	0.46
37:n:42:SER:O	37:n:46:LYS:HB2	2.16	0.46
40:r:73:LEU:HB3	40:r:74:PRO:HD3	1.97	0.46
3:C:106:PHE:CE2	3:C:191:LEU:HD11	2.51	0.46
6:G:84:LEU:HD23	6:G:87:LEU:HD12	1.96	0.46
9:J:207:PHE:CE2	9:J:348:LYS:HB2	2.49	0.46
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.46
25:b:38:GLN:OE1	25:b:38:GLN:HA	2.14	0.46
25:b:105:PHE:CD2	43:v:68:LYS:CA	2.98	0.46
27:d:65:VAL:HG11	27:d:81:GLU:HB3	1.96	0.46
27:d:121:LYS:O	27:d:125:GLN:HG3	2.15	0.46
29:f:55:TRP:CZ2	30:g:65:THR:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:62:PHE:CG	41:s:140:ILE:HG23	2.50	0.46
37:n:34:ARG:HH22	51:n:101:CDL:PA1	2.38	0.46
51:n:101:CDL:H342	51:n:101:CDL:HA62	1.97	0.46
40:r:367:LEU:HD13	40:r:404:ALA:HA	1.97	0.46
44:w:270:VAL:O	44:w:275:TYR:N	2.47	0.46
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.46
1:A:116:ASN:HD21	46:A:502:FMN:C8	2.22	0.46
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.46
1:A:174:ARG:HB2	10:K:91:LEU:HD11	1.96	0.46
1:A:369:ARG:NH2	14:O:175:GLU:OE2	2.33	0.46
2:B:151:ILE:HD13	3:C:159:TYR:CE2	2.51	0.46
3:C:81:PRO:HA	3:C:119:VAL:O	2.15	0.46
5:F:14:LEU:N	5:F:17:ARG:HH22	2.13	0.46
14:O:78:ALA:O	14:O:82:VAL:HG23	2.15	0.46
16:Q:205:GLU:O	16:Q:209:LYS:HG3	2.16	0.46
23:Z:49:GLU:OE2	39:p:38:ARG:NH2	2.33	0.46
24:a:66:ARG:NH1	28:e:74:HIS:NE2	2.63	0.46
26:c:44:THR:HB	26:c:47:GLU:HG2	1.97	0.46
26:c:168:LEU:HD12	26:c:169:GLU:HB3	1.98	0.46
30:g:32:TYR:HB2	51:n:101:CDL:H732	1.97	0.46
34:k:37:MET:HE1	34:k:63:MET:HE3	1.96	0.46
35:l:32:TYR:HB3	35:l:33:PRO:HD3	1.96	0.46
35:l:211:THR:HG21	51:l:704:CDL:HA4	1.96	0.46
36:m:19:PHE:HB3	36:m:31:VAL:HB	1.98	0.46
38:o:52:ASN:HD22	39:p:166:LEU:HG	1.81	0.46
38:o:52:ASN:O	39:p:129:ARG:NH2	2.49	0.46
41:s:248:ASP:OD1	41:s:249:ALA:N	2.49	0.46
41:s:294:LEU:HB3	41:s:295:PRO:HD3	1.97	0.46
44:w:137:SER:C	44:w:139:ARG:H	2.18	0.46
2:B:192:GLY:O	2:B:196:GLU:HB2	2.15	0.46
8:I:33:LYS:NZ	8:I:36:GLN:HA	2.30	0.46
11:L:107:TRP:O	11:L:116:SER:HB2	2.16	0.46
12:M:292:PHE:HB3	12:M:706:THR:HG21	1.96	0.46
13:N:83:PRO:HG2	13:N:86:TRP:HB2	1.98	0.46
14:O:58:GLU:O	14:O:62:ARG:HG3	2.15	0.46
16:Q:255:LEU:HD11	16:Q:337:MET:HG2	1.98	0.46
17:S:43:TYR:CZ	21:W:68:ARG:HD2	2.50	0.46
24:a:187:PRO:HB3	42:u:47:ARG:HG3	1.96	0.46
25:b:89:HIS:CE1	25:b:97:ILE:HG13	2.51	0.46
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.98	0.46
25:b:111:LEU:HB2	25:b:112:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:123:PRO:HG3	39:p:75:GLN:NE2	2.25	0.46
32:i:39:ALA:O	32:i:42:PRO:HD2	2.16	0.46
32:i:335:LEU:O	32:i:338:PRO:HD2	2.16	0.46
35:l:79:SER:OG	35:l:135:ASN:HB3	2.16	0.46
35:l:370:SER:O	35:l:374:THR:HG23	2.16	0.46
40:r:267:TRP:O	40:r:271:MET:HG2	2.15	0.46
41:s:7:LEU:HD23	41:s:7:LEU:HA	1.78	0.46
44:w:86:PHE:CE2	44:w:157:VAL:HG11	2.50	0.46
44:w:91:ILE:HG23	44:w:134:TRP:CD1	2.51	0.46
44:w:212:PRO:O	44:w:215:GLN:HB2	2.14	0.46
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	0.46
4:E:62:LYS:HE3	4:E:66:MET:HE2	1.98	0.46
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.51	0.46
9:J:220:MET:O	9:J:223:PHE:HB2	2.16	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	0.46
11:L:162:ALA:HA	11:L:168:LYS:HZ2	1.80	0.46
12:M:164:ASN:OD1	12:M:165:ILE:N	2.49	0.46
16:Q:216:ARG:HE	16:Q:240:LEU:HD23	1.80	0.46
47:V:203:PLX:H221	38:o:95:PHE:CE1	2.50	0.46
21:W:115:ARG:NH1	31:h:36:PHE:HD1	2.08	0.46
22:Y:89:PRO:O	43:v:107:ARG:NH1	2.49	0.46
25:b:112:GLU:N	25:b:112:GLU:CD	2.74	0.46
28:e:113:ARG:HH21	40:r:459:SER:HB2	1.80	0.46
32:i:92:GLN:O	32:i:95:SER:OG	2.21	0.46
32:i:146:SER:O	32:i:149:LEU:HD13	2.16	0.46
35:l:367:PRO:O	35:l:371:THR:HG23	2.16	0.46
35:l:369:THR:O	35:l:372:SER:OG	2.27	0.46
40:r:1:MET:HE1	40:r:53:SER:HB3	1.98	0.46
4:E:40:TYR:CE1	4:E:60:ARG:HD3	2.51	0.46
5:F:36:PHE:CE1	5:F:40:ARG:HB2	2.51	0.46
7:H:35:LEU:HA	7:H:38:ILE:HD12	1.96	0.46
12:M:457:SER:O	12:M:499:LYS:NZ	2.49	0.46
12:M:589:TYR:CE2	12:M:590:THR:HG23	2.50	0.46
13:N:49:TYR:HD2	13:N:61:TRP:CZ3	2.33	0.46
14:O:236:GLU:C	14:O:238:PRO:HD2	2.41	0.46
17:S:38:VAL:HG21	42:u:94:GLN:HG2	1.97	0.46
23:Z:31:THR:O	23:Z:34:LYS:HB3	2.16	0.46
25:b:106:PRO:HA	25:b:115:GLU:CD	2.41	0.46
26:c:101:TRP:CD1	38:o:62:ASN:ND2	2.84	0.46
32:i:291:TYR:CZ	52:l:701:PEE:C31	2.71	0.46
32:i:339:ILE:HG22	32:i:342:PHE:CB	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:86:LEU:HD21	36:m:150:ARG:HD3	1.96	0.46
35:l:587:TYR:O	35:l:590:SER:OG	2.27	0.46
36:m:118:PHE:HD1	36:m:121:VAL:HB	1.79	0.46
39:p:51:HIS:O	48:p:201:8Q1:C38	2.64	0.46
1:A:128:ARG:O	1:A:132:ARG:HG3	2.15	0.46
1:A:321:GLY:HA2	1:A:353:ALA:HB3	1.97	0.46
1:A:392:MET:O	1:A:396:MET:HG2	2.16	0.46
6:G:133:ILE:O	6:G:136:GLU:HB2	2.15	0.46
14:O:218:PRO:HG2	14:O:222:ARG:O	2.16	0.46
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.80	0.46
16:Q:412:VAL:O	16:Q:420:TYR:N	2.43	0.46
16:Q:446:ASP:O	16:Q:450:ILE:HG13	2.16	0.46
22:Y:42:PRO:HD2	23:Z:14:MET:HG3	1.98	0.46
26:c:41:TYR:CE1	26:c:67:ASP:HB3	2.51	0.46
26:c:153:TYR:HB3	35:l:403:TYR:CD1	2.48	0.46
47:g:202:PLX:H1B3	47:g:202:PLX:H22	1.58	0.46
32:i:46:LYS:O	32:i:47:LYS:HB2	2.16	0.46
35:l:319:ILE:HG22	35:l:319:ILE:O	2.17	0.46
36:m:109:TYR:O	36:m:112:VAL:HG23	2.16	0.46
40:r:339:SER:O	40:r:340:ARG:HB2	2.16	0.46
44:w:124:ASN:O	44:w:126:GLY:N	2.41	0.46
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.45
6:G:77:GLU:OE1	6:G:77:GLU:N	2.38	0.45
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.45
25:b:88:TYR:CG	47:b:201:PLX:H1C2	2.51	0.45
25:b:109:THR:HA	27:d:18:PRO:HA	1.97	0.45
26:c:174:PRO:O	26:c:175:SER:OG	2.26	0.45
27:d:20:GLN:NE2	35:l:57:LEU:HD21	2.30	0.45
27:d:43:ARG:O	27:d:47:GLU:HG2	2.15	0.45
29:f:47:THR:OG1	29:f:48:LEU:N	2.48	0.45
29:f:47:THR:O	29:f:51:THR:HG23	2.16	0.45
30:g:48:ARG:O	30:g:50:ARG:HG3	2.16	0.45
32:i:102:MET:HE3	32:i:138:PRO:HB3	1.98	0.45
35:l:302:VAL:O	35:l:306:THR:HG23	2.16	0.45
37:n:50:GLN:CG	37:n:51:PRO:HD2	2.46	0.45
40:r:405:LEU:HA	40:r:405:LEU:HD23	1.73	0.45
42:u:25:LEU:O	42:u:29:ALA:HB2	2.16	0.45
43:v:62:HIS:CD2	43:v:90:CYS:HG	2.33	0.45
9:J:220:MET:SD	9:J:223:PHE:HD2	2.39	0.45
9:J:311:GLU:HA	9:J:312:PRO:HD3	1.79	0.45
12:M:221:ASN:OD1	12:M:291:ARG:NH2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:692:LYS:HG3	12:M:714:VAL:HG13	1.98	0.45
16:Q:136:PHE:CD2	16:Q:151:TYR:HB2	2.52	0.45
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.98	0.45
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.98	0.45
29:f:32:ARG:O	29:f:35:PRO:HD2	2.16	0.45
30:g:32:TYR:CD2	32:i:339:ILE:HD11	2.51	0.45
52:l:701:PEE:H33	52:l:701:PEE:H27	1.62	0.45
36:m:32:LEU:HB3	36:m:64:MET:HE3	1.99	0.45
38:o:17:THR:HG21	39:p:22:ARG:HH12	1.82	0.45
43:v:60:ALA:O	43:v:61:HIS:C	2.59	0.45
2:B:138:ARG:HD3	12:M:130:ILE:HG22	1.98	0.45
12:M:64:CYS:SG	12:M:75:CYS:HB3	2.56	0.45
13:N:48:TYR:HB3	13:N:89:TRP:HZ3	1.80	0.45
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.45
16:Q:94:VAL:HG21	16:Q:458:PHE:HB2	1.99	0.45
17:S:16:LEU:O	17:S:19:PRO:HD2	2.16	0.45
17:S:53:ARG:HB3	31:h:102:GLY:HA2	1.99	0.45
17:S:54:ILE:HG13	31:h:105:ARG:NH1	2.32	0.45
18:T:68:ALA:O	18:T:72:ILE:HG13	2.16	0.45
21:W:57:ARG:CZ	41:s:168:THR:HG22	2.47	0.45
21:W:111:PHE:CD2	21:W:117:VAL:HG21	2.51	0.45
29:f:34:PRO:O	29:f:38:LYS:HG3	2.16	0.45
32:i:25:HIS:CE1	32:i:84:TRP:CE3	3.04	0.45
35:l:286:LEU:O	35:l:290:VAL:HG23	2.17	0.45
42:u:23:ALA:HB1	42:u:90:ASP:OD1	2.16	0.45
44:w:79:GLU:OE1	44:w:79:GLU:N	2.43	0.45
44:w:139:ARG:O	44:w:142:GLN:HB2	2.16	0.45
44:w:168:VAL:HG11	44:w:241:TYR:HA	1.97	0.45
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.45
1:A:371:ILE:HD11	1:A:435:VAL:HB	1.97	0.45
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	0.45
3:C:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.45
4:E:43:VAL:HB	4:E:44:PRO:HD3	1.98	0.45
9:J:169:HIS:CD2	49:J:401:NDP:C5N	2.79	0.45
12:M:158:ARG:HH21	12:M:178:GLN:HE22	1.64	0.45
12:M:602:ARG:NE	12:M:659:ILE:HD11	2.30	0.45
15:P:170:ILE:HG23	15:P:174:PHE:CD2	2.52	0.45
16:Q:70:ASP:N	16:Q:71:PRO:CD	2.80	0.45
24:a:175:ASP:OD1	24:a:176:LYS:N	2.50	0.45
26:c:69:GLY:HA2	38:o:81:ARG:H	1.80	0.45
27:d:59:HIS:HD2	28:e:121:GLU:OE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:g:203:PLX:H101	47:g:203:PLX:H291	1.98	0.45
35:l:173:LEU:HA	35:l:173:LEU:HD23	1.73	0.45
35:l:558:LEU:HD23	35:l:558:LEU:HA	1.71	0.45
37:n:7:ILE:HG23	37:n:11:HIS:HB2	1.98	0.45
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.65	0.45
44:w:108:TYR:HD1	44:w:327:VAL:HG13	1.82	0.45
1:A:44:ASN:HD22	1:A:59:ARG:NH2	2.14	0.45
2:B:160:CYS:O	16:Q:368:ARG:NH1	2.41	0.45
4:E:120:SER:O	4:E:124:VAL:HG23	2.17	0.45
7:H:31:ILE:HG12	7:H:88:LEU:HA	1.99	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.17	0.45
12:M:323:LEU:HG	12:M:629:ILE:HD12	1.98	0.45
12:M:688:GLN:O	12:M:690:THR:N	2.50	0.45
14:O:196:LEU:HD21	14:O:204:ILE:HG13	1.98	0.45
15:P:164:ASN:HA	15:P:181:HIS:HE2	1.82	0.45
15:P:214:ASP:O	15:P:217:LYS:HD2	2.16	0.45
18:T:52:ARG:HB3	18:T:55:ARG:NH1	2.31	0.45
30:g:39:CYS:O	30:g:43:ILE:HG13	2.17	0.45
31:h:36:PHE:HD2	31:h:66:CYS:HB2	1.82	0.45
32:i:2:ASN:HD21	32:i:4:LEU:HB2	1.81	0.45
32:i:337:LEU:C	32:i:339:ILE:H	2.23	0.45
34:k:22:TYR:CG	34:k:22:TYR:O	2.69	0.45
35:l:30:ASN:O	35:l:33:PRO:HD2	2.17	0.45
35:l:166:THR:CG2	52:l:702:PEE:H2	2.46	0.45
35:l:533:MET:HE3	52:l:702:PEE:H32	1.97	0.45
36:m:13:VAL:HG11	36:m:99:GLU:HG2	1.99	0.45
36:m:118:PHE:HZ	36:m:124:TRP:CZ2	2.34	0.45
44:w:211:VAL:HG13	44:w:212:PRO:HD3	1.98	0.45
1:A:319:PRO:HB2	1:A:347:THR:HG21	1.98	0.45
2:B:94:ARG:HE	16:Q:234:GLN:NE2	2.15	0.45
3:C:161:HIS:CE1	3:C:168:ARG:HD2	2.51	0.45
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	0.45
7:H:28:TYR:CD2	7:H:56:LEU:HD13	2.52	0.45
8:I:30:GLU:HG2	8:I:31:ILE:N	2.32	0.45
12:M:446:GLY:N	12:M:451:ILE:HD11	2.32	0.45
12:M:541:PRO:HA	12:M:542:PRO:HD2	1.77	0.45
12:M:546:PHE:CZ	12:M:566:ILE:HD12	2.52	0.45
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	0.45
16:Q:145:MET:HG3	16:Q:174:PHE:HB3	1.99	0.45
16:Q:304:LYS:HE3	16:Q:316:PHE:CZ	2.51	0.45
24:a:55:PHE:HE2	39:p:118:TYR:HE2	1.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:90:VAL:HG22	25:b:97:ILE:HD12	1.98	0.45
47:b:201:PLX:H1C3	47:b:201:PLX:H31	1.94	0.45
26:c:56:ASN:HD21	38:o:43:LEU:HD11	1.81	0.45
35:l:18:PRO:HG3	35:l:39:ILE:HD12	1.98	0.45
35:l:304:PHE:HZ	35:l:526:LEU:HD22	1.81	0.45
35:l:595:LEU:O	35:l:598:THR:OG1	2.31	0.45
40:r:13:PRO:HA	40:r:16:TRP:HB2	1.99	0.45
5:F:22:HIS:HB2	5:F:64:LYS:HB3	1.97	0.45
6:G:123:GLU:O	6:G:127:GLY:N	2.50	0.45
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	0.45
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
12:M:471:LYS:HB3	12:M:510:TRP:CH2	2.52	0.45
14:O:80:LEU:HB2	14:O:81:PRO:HD3	1.99	0.45
16:Q:259:GLU:O	16:Q:263:THR:OG1	2.34	0.45
16:Q:316:PHE:HD1	16:Q:339:GLN:NE2	2.14	0.45
19:U:18:VAL:HG11	41:s:292:ASN:O	2.17	0.45
25:b:116:VAL:HG12	25:b:117:ILE:N	2.32	0.45
32:i:324:PRO:C	32:i:326:LEU:H	2.24	0.45
35:l:194:ASN:ND2	38:o:127:LEU:HD12	2.32	0.45
35:l:434:GLN:HB3	35:l:435:PRO:HD2	1.99	0.45
40:r:145:ALA:HB3	40:r:222:GLU:OE2	2.17	0.45
41:s:288:LEU:O	41:s:293:PHE:N	2.50	0.45
9:J:163:LYS:HE2	9:J:253:VAL:HA	1.98	0.45
9:J:273:LEU:O	9:J:276:LEU:HB3	2.17	0.45
11:L:102:ASP:OD1	11:L:102:ASP:N	2.50	0.45
14:O:207:GLU:HG2	14:O:213:ILE:HG13	1.99	0.45
15:P:167:GLU:HG2	15:P:181:HIS:CD2	2.52	0.45
16:Q:235:ASP:OD1	16:Q:356:ILE:HD12	2.17	0.45
51:V:201:CDL:H541	51:V:201:CDL:H572	1.46	0.45
22:Y:73:PHE:HD1	22:Y:73:PHE:C	2.24	0.45
26:c:177:GLU:O	26:c:178:PRO:C	2.59	0.45
32:i:146:SER:OG	32:i:147:PRO:HD3	2.17	0.45
33:j:75:LEU:N	33:j:76:PRO:HD2	2.32	0.45
40:r:56:PHE:HZ	40:r:108:MET:HE1	1.82	0.45
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	0.45
1:A:440:ARG:HE	1:A:441:HIS:CE1	2.35	0.45
2:B:90:PRO:HG2	13:N:56:PHE:CE2	2.52	0.45
7:H:50:GLN:NE2	8:I:93:LYS:HD2	2.32	0.45
9:J:178:SER:OG	9:J:181:LEU:HB2	2.17	0.45
12:M:382:ARG:O	12:M:386:LEU:HG	2.16	0.45
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:498:GLN:HE22	12:M:501:ARG:HD2	1.82	0.45
16:Q:369:ALA:HA	18:T:93:ALA:HB2	1.99	0.45
20:V:2:ALA:O	20:V:6:PHE:N	2.45	0.45
21:W:27:ARG:C	21:W:29:GLY:N	2.75	0.45
22:Y:74:TRP:HE3	22:Y:75:HIS:N	2.15	0.45
22:Y:78:GLU:CG	35:l:385:PHE:HE1	2.30	0.45
32:i:4:LEU:HG	44:w:43:PHE:HE2	1.82	0.45
32:i:20:THR:O	32:i:23:SER:OG	2.34	0.45
34:k:42:ILE:O	34:k:46:LEU:HG	2.17	0.45
35:l:33:PRO:HA	35:l:118:PHE:HD2	1.82	0.45
35:l:399:ALA:O	35:l:402:SER:OG	2.33	0.45
35:l:481:THR:HG22	43:v:92:HIS:CD2	2.52	0.45
38:o:6:TYR:HE1	38:o:12:ARG:NH2	2.15	0.45
41:s:234:MET:O	41:s:238:THR:HG23	2.17	0.45
42:u:82:PHE:CE2	42:u:86:TRP:HD1	2.35	0.45
44:w:58:ARG:HB3	44:w:202:HIS:HE1	1.82	0.45
3:C:88:CYS:SG	16:Q:223:HIS:CE1	3.10	0.45
9:J:108:TRP:HZ3	9:J:110:ALA:HA	1.82	0.45
12:M:421:SER:O	12:M:425:ASN:N	2.49	0.45
14:O:198:ALA:HA	14:O:201:ILE:HD12	1.99	0.45
18:T:96:HIS:NE2	18:T:115:CYS:SG	2.90	0.45
34:k:31:LEU:HD23	34:k:31:LEU:HA	1.75	0.45
44:w:92:HIS:HB3	44:w:103:PRO:HB3	1.99	0.45
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
9:J:319:VAL:C	9:J:323:HIS:HD1	2.22	0.44
12:M:157:LYS:HB2	18:T:100:TYR:CD2	2.52	0.44
12:M:255:ASP:HB3	12:M:257:VAL:HG23	1.98	0.44
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	0.44
12:M:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.18	0.44
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	0.44
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.44
22:Y:81:LEU:HD12	43:v:88:ASP:CB	2.45	0.44
22:Y:81:LEU:HD11	43:v:89:TYR:HA	1.98	0.44
32:i:291:TYR:CE2	52:l:701:PEE:H51	2.52	0.44
44:w:351:TRP:HA	44:w:353:TRP:CZ3	2.52	0.44
7:H:32:LEU:HA	7:H:35:LEU:HG	1.97	0.44
9:J:130:ILE:HG21	49:J:401:NDP:N7A	2.23	0.44
11:L:136:SER:O	11:L:140:LYS:HG3	2.16	0.44
12:M:221:ASN:HB3	12:M:285:TRP:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:307:VAL:HG22	12:M:582:VAL:HG13	2.00	0.44
17:S:31:ASN:HD21	17:S:36:LYS:HD3	1.82	0.44
18:T:81:GLU:HA	18:T:122:HIS:O	2.17	0.44
52:V:202:PEE:H60	52:V:202:PEE:H40	1.99	0.44
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.44
22:Y:55:VAL:O	22:Y:58:SER:OG	2.33	0.44
22:Y:72:ARG:NH1	35:l:390:TYR:CZ	2.79	0.44
26:c:52:ALA:HB2	26:c:62:TYR:HB2	1.99	0.44
31:h:80:ARG:NH1	36:m:1:MET:SD	2.89	0.44
34:k:59:MET:HB2	34:k:60:PRO:HD3	1.99	0.44
41:s:40:VAL:CG1	41:s:46:LEU:HB2	2.47	0.44
41:s:257:THR:O	41:s:261:THR:HG23	2.17	0.44
42:u:100:CYS:O	42:u:102:LYS:N	2.50	0.44
1:A:317:VAL:HG22	1:A:356:VAL:HA	1.99	0.44
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.44
16:Q:201:PHE:CB	41:s:32:GLN:HG3	2.48	0.44
20:V:40:ARG:HE	51:V:201:CDL:CA2	2.30	0.44
20:V:69:VAL:HG21	20:V:100:THR:HG21	1.98	0.44
21:W:111:PHE:CE2	21:W:117:VAL:HG11	2.50	0.44
22:Y:85:PRO:O	22:Y:86:TYR:CD1	2.70	0.44
30:g:45:ASN:HD21	30:g:60:GLN:HE21	1.65	0.44
30:g:78:GLU:OE1	32:i:342:PHE:HD1	2.01	0.44
40:r:109:THR:HG22	40:r:121:PHE:HB2	2.00	0.44
40:r:246:LEU:HD23	40:r:246:LEU:HA	1.81	0.44
47:r:501:PLX:H101	47:r:501:PLX:H132	1.59	0.44
43:v:49:ALA:O	43:v:51:LEU:N	2.46	0.44
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	0.44
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.44
9:J:168:SER:CA	9:J:184:LYS:HE3	2.47	0.44
11:L:72:ILE:HA	11:L:143:TRP:NE1	2.33	0.44
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.99	0.44
12:M:309:ASN:N	12:M:313:LEU:O	2.46	0.44
12:M:371:VAL:HG12	12:M:533:GLY:O	2.17	0.44
18:T:67:PHE:O	18:T:71:LEU:HD13	2.17	0.44
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.44
25:b:105:PHE:HZ	43:v:67:LEU:HB2	1.75	0.44
26:c:101:TRP:CD1	38:o:47:TYR:CD1	3.06	0.44
26:c:166:LEU:HB2	26:c:170:ARG:NH2	2.32	0.44
27:d:107:CYS:HG	27:d:119:CYS:CA	2.31	0.44
32:i:2:ASN:HA	32:i:3:PRO:HD2	1.87	0.44
35:l:567:SER:C	35:l:571:ILE:HD13	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:701:PEE:H51	52:l:701:PEE:H56	1.56	0.44
38:o:6:TYR:CD2	38:o:14:LEU:HD23	2.53	0.44
40:r:339:SER:HB2	40:r:344:LEU:HD12	2.00	0.44
41:s:142:TYR:CD2	41:s:289:LEU:HD11	2.52	0.44
44:w:238:GLU:O	44:w:242:LYS:HG3	2.17	0.44
1:A:99:TRP:HA	1:A:149:MET:HE1	2.00	0.44
1:A:173:ILE:HG22	1:A:177:TYR:CE2	2.52	0.44
1:A:194:ASP:OD2	10:K:96:MET:N	2.41	0.44
2:B:69:GLY:O	2:B:72:LEU:HB3	2.17	0.44
2:B:91:LEU:HD23	2:B:95:PHE:CD2	2.52	0.44
2:B:169:PRO:HG3	2:B:198:GLU:HG2	2.00	0.44
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.82	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.44
9:J:141:PHE:CD2	9:J:183:ASN:ND2	2.86	0.44
9:J:329:LEU:HD12	9:J:329:LEU:O	2.17	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.44
12:M:229:GLY:O	12:M:232:THR:HG23	2.18	0.44
12:M:306:MET:HA	12:M:315:THR:O	2.18	0.44
12:M:612:PRO:HB3	12:M:616:ALA:HB3	1.99	0.44
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.44
14:O:195:ASP:HB2	14:O:219:ARG:H	1.83	0.44
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.98	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
16:Q:85:GLY:CA	33:j:39:CYS:HB3	2.47	0.44
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.66	0.44
26:c:63:GLU:O	26:c:77:LYS:N	2.43	0.44
31:h:3:PHE:HB2	32:i:144:GLN:HE21	1.83	0.44
35:l:37:LYS:HE3	35:l:102:GLU:CG	2.37	0.44
39:p:173:ARG:HA	39:p:174:PRO:HD3	1.83	0.44
40:r:325:LEU:HD12	40:r:440:HIS:HB3	1.99	0.44
47:r:502:PLX:H192	47:r:502:PLX:H162	1.44	0.44
41:s:89:LEU:HD12	41:s:91:MET:HE2	1.98	0.44
41:s:215:TYR:HD1	41:s:219:PRO:HB2	1.83	0.44
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.44
2:B:79:PRO:HD2	17:S:1:MET:SD	2.57	0.44
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.44
4:E:35:LEU:HD11	4:E:39:TRP:HE1	1.82	0.44
7:H:12:VAL:HG13	7:H:13:GLY:N	2.33	0.44
7:H:23:ARG:O	7:H:26:ILE:HB	2.18	0.44
9:J:71:ASN:ND2	15:P:214:ASP:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	0.44
52:W:201:PEE:N	52:W:201:PEE:P	2.87	0.44
29:f:32:ARG:C	29:f:35:PRO:HD2	2.42	0.44
32:i:8:VAL:O	32:i:12:THR:HG23	2.18	0.44
33:j:34:SER:HB2	41:s:63:PRO:HA	2.00	0.44
33:j:48:ARG:HD2	33:j:49:VAL:H	1.83	0.44
35:l:98:TRP:CD1	35:l:98:TRP:O	2.71	0.44
40:r:36:ILE:O	40:r:39:LEU:HB3	2.18	0.44
41:s:266:LEU:HA	41:s:266:LEU:HD23	1.73	0.44
44:w:246:LEU:HB2	44:w:247:PRO:HD3	1.99	0.44
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	0.44
9:J:220:MET:HA	9:J:223:PHE:CD2	2.53	0.44
12:M:37:ASP:HA	12:M:103:LEU:HD23	1.98	0.44
16:Q:82:LEU:HD23	16:Q:82:LEU:HA	1.78	0.44
16:Q:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.44
16:Q:190:HIS:HD2	16:Q:452:GLY:CA	2.26	0.44
16:Q:265:ASN:OD1	16:Q:267:ILE:HD12	2.17	0.44
52:W:201:PEE:C2	41:s:98:LEU:HD22	2.47	0.44
28:e:54:PRO:O	28:e:56:GLN:HG3	2.18	0.44
32:i:197:ASN:HA	32:i:198:PRO:HD3	1.79	0.44
33:j:30:TYR:HB2	33:j:33:LYS:CD	2.47	0.44
34:k:46:LEU:HD22	36:m:46:PHE:CD2	2.53	0.44
35:l:122:LEU:HD23	35:l:122:LEU:HA	1.85	0.44
36:m:2:MET:N	36:m:123:SER:OG	2.50	0.44
37:n:27:LEU:HD12	40:r:2:LEU:HD21	1.99	0.44
41:s:92:PRO:HB3	41:s:255:TYR:CD2	2.53	0.44
1:A:167:SER:O	1:A:171:VAL:HG23	2.18	0.44
1:A:225:LEU:HB2	1:A:424:ILE:HD11	1.99	0.44
2:B:72:LEU:HD13	41:s:272:TRP:CH2	2.53	0.44
2:B:128:ILE:HG12	2:B:143:TYR:HD1	1.83	0.44
2:B:131:GLU:OE1	2:B:141:THR:HG21	2.18	0.44
12:M:278:HIS:NE2	12:M:280:ASP:HB2	2.32	0.44
12:M:385:TYR:HB2	12:M:517:HIS:CE1	2.53	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.18	0.44
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.78	0.44
14:O:132:ILE:O	14:O:172:ILE:HG22	2.18	0.44
21:W:120:LEU:HG	31:h:69:ARG:NH1	2.32	0.44
52:W:201:PEE:H51	52:W:201:PEE:H56	1.33	0.44
26:c:108:HIS:CE1	35:l:546:GLN:HG2	2.53	0.44
47:g:201:PLX:H1B1	31:h:2:PRO:HG2	1.99	0.44
38:o:100:PHE:CZ	38:o:104:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:25:ARG:HA	39:p:25:ARG:HD3	1.80	0.44
40:r:72:LEU:O	40:r:76:THR:HG23	2.18	0.44
42:u:104:GLN:O	42:u:108:ASP:N	2.41	0.44
43:v:63:LEU:O	43:v:67:LEU:HG	2.18	0.44
44:w:86:PHE:HD2	44:w:159:LEU:HD13	1.83	0.44
8:I:37:PRO:HA	8:I:38:PRO:HD3	1.81	0.44
12:M:358:LEU:HD22	12:M:363:SER:HB2	1.99	0.44
12:M:510:TRP:HD1	12:M:512:VAL:HG22	1.82	0.44
16:Q:55:SER:N	16:Q:58:THR:OG1	2.51	0.44
30:g:87:ARG:HD2	42:u:156:GLY:C	2.42	0.44
32:i:79:MET:SD	34:k:43:MET:HE1	2.58	0.44
47:r:502:PLX:H151	47:r:502:PLX:H122	1.83	0.44
41:s:224:PHE:CZ	41:s:228:TYR:HE2	2.36	0.44
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	0.43
3:C:211:TYR:CD1	3:C:211:TYR:C	2.96	0.43
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.43
12:M:646:LEU:HD13	12:M:653:LEU:HB3	2.00	0.43
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	0.43
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.49	0.43
16:Q:391:VAL:O	16:Q:415:GLY:HA2	2.18	0.43
17:S:12:MET:HE1	41:s:19:PHE:C	2.43	0.43
20:V:51:GLU:HB3	20:V:55:LYS:NZ	2.33	0.43
24:a:150:ARG:NH1	40:r:168:HIS:CE1	2.86	0.43
25:b:79:VAL:HG22	35:l:10:LEU:CD1	2.48	0.43
26:c:139:PHE:O	26:c:143:MET:HG2	2.18	0.43
27:d:111:GLU:OE1	27:d:119:CYS:HB2	2.18	0.43
32:i:309:ASN:HD21	44:w:130:ARG:HD3	1.82	0.43
33:j:49:VAL:HG12	36:m:75:ILE:H	1.82	0.43
35:l:208:PRO:HG2	35:l:266:LEU:HB3	1.99	0.43
35:l:356:ILE:CG2	35:l:429:LEU:HB3	2.48	0.43
40:r:237:LYS:HD2	40:r:237:LYS:N	2.33	0.43
47:r:501:PLX:H211	47:r:501:PLX:H182	1.66	0.43
43:v:93:ARG:O	43:v:97:MET:HG2	2.18	0.43
1:A:88:ARG:C	1:A:244:ASN:HD22	2.26	0.43
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	0.43
4:E:53:ASP:HA	9:J:366:ILE:HD11	2.00	0.43
9:J:81:ILE:HG22	9:J:83:PRO:HD3	2.00	0.43
9:J:83:PRO:HA	9:J:106:LEU:O	2.18	0.43
9:J:168:SER:O	9:J:203:PRO:HD2	2.18	0.43
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43
14:O:236:GLU:HB3	14:O:238:PRO:HD2	2.00	0.43
15:P:55:HIS:NE2	15:P:78:VAL:HG12	2.33	0.43
16:Q:147:ASN:O	16:Q:150:ALA:HB3	2.17	0.43
16:Q:307:PRO:HB2	16:Q:312:ASP:HB3	2.00	0.43
25:b:111:LEU:C	25:b:112:GLU:CD	2.85	0.43
31:h:82:GLN:HA	31:h:85:LYS:HE3	1.99	0.43
33:j:34:SER:HB2	41:s:64:ALA:H	1.82	0.43
34:k:8:ILE:N	34:k:8:ILE:HD12	2.33	0.43
38:o:9:SER:OG	38:o:12:ARG:HB3	2.18	0.43
39:p:30:TRP:O	39:p:32:VAL:HG23	2.18	0.43
40:r:345:SER:O	40:r:348:LEU:HG	2.18	0.43
42:u:121:ASP:HB3	42:u:124:GLU:OE2	2.18	0.43
2:B:166:VAL:HG11	2:B:199:ILE:HG23	2.00	0.43
3:C:88:CYS:HB3	16:Q:141:TYR:CG	2.54	0.43
6:G:138:LEU:O	6:G:143:GLU:HB2	2.18	0.43
12:M:566:ILE:HD11	12:M:579:ILE:HG22	1.99	0.43
15:P:55:HIS:HD2	15:P:79:SER:O	2.01	0.43
17:S:43:TYR:CE2	21:W:68:ARG:HD2	2.53	0.43
18:T:47:ASP:N	18:T:50:ASP:OD2	2.47	0.43
19:U:52:ASN:ND2	31:h:27:TYR:O	2.42	0.43
21:W:110:VAL:HG11	31:h:71:LYS:HB2	2.01	0.43
24:a:150:ARG:NH1	40:r:168:HIS:HE1	2.16	0.43
26:c:41:TYR:CZ	26:c:67:ASP:HB3	2.54	0.43
27:d:57:TYR:CD1	27:d:57:TYR:O	2.70	0.43
28:e:115:LYS:O	28:e:118:SER:OG	2.30	0.43
31:h:56:CYS:HA	42:u:145:ARG:NH1	2.33	0.43
32:i:232:ARG:NH1	44:w:306:ASN:O	2.50	0.43
32:i:237:LEU:HB3	32:i:240:LEU:HB2	2.00	0.43
35:l:81:LYS:HD3	35:l:83:ASP:OD2	2.18	0.43
35:l:533:MET:CE	52:l:702:PEE:H32	2.48	0.43
40:r:115:LEU:O	40:r:118:PHE:HB3	2.19	0.43
41:s:59:GLU:OE1	41:s:59:GLU:N	2.52	0.43
44:w:217:ARG:O	44:w:221:LYS:HG2	2.18	0.43
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.83	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	0.43
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	0.43
5:F:39:LYS:HG3	5:F:40:ARG:N	2.29	0.43
5:F:65:LEU:O	5:F:76:ASN:HA	2.18	0.43
10:K:78:ASP:HA	14:O:215:LYS:HD3	2.00	0.43
10:K:86:ASP:O	10:K:90:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:221:ASN:HB3	12:M:285:TRP:CZ3	2.53	0.43
12:M:323:LEU:HA	12:M:326:VAL:HG22	1.99	0.43
12:M:455:ILE:HG12	12:M:463:SER:HB3	1.99	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
23:Z:65:ASP:O	23:Z:69:LYS:HB2	2.19	0.43
28:e:57:GLU:HB2	44:w:323:GLN:HB3	1.99	0.43
30:g:15:ASP:OD1	30:g:16:GLU:N	2.52	0.43
34:k:87:LEU:HD13	36:m:74:ALA:HB2	2.00	0.43
35:l:151:SER:HA	35:l:247:LEU:HD13	2.01	0.43
35:l:210:LEU:HD21	35:l:214:LEU:HD13	2.01	0.43
35:l:227:LEU:HA	35:l:230:HIS:HB3	2.00	0.43
40:r:408:LEU:HD23	40:r:408:LEU:HA	1.70	0.43
42:u:18:VAL:HG12	42:u:20:ILE:H	1.83	0.43
43:v:50:GLN:O	43:v:56:ARG:NH1	2.41	0.43
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.43
46:A:502:FMN:H4'	46:A:502:FMN:H1'2	1.63	0.43
6:G:115:GLN:NE2	6:G:135:ALA:HB1	2.34	0.43
8:I:38:PRO:HA	8:I:39:PRO:HD3	1.58	0.43
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	0.43
12:M:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.43
13:N:5:GLN:O	13:N:9:ARG:HG2	2.17	0.43
14:O:104:VAL:HG12	14:O:105:LEU:HD12	2.00	0.43
17:S:53:ARG:HH21	31:h:105:ARG:HA	1.83	0.43
25:b:71:VAL:O	25:b:75:VAL:HB	2.18	0.43
25:b:115:GLU:CG	25:b:116:VAL:N	2.81	0.43
33:j:53:MET:HG3	34:k:79:VAL:HG13	1.99	0.43
33:j:64:LEU:O	33:j:68:GLU:HG2	2.18	0.43
34:k:32:CYS:O	34:k:36:MET:HG3	2.18	0.43
39:p:54:GLU:OE1	39:p:54:GLU:N	2.51	0.43
41:s:289:LEU:HA	41:s:289:LEU:HD23	1.82	0.43
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	0.43
3:C:150:MET:HE3	3:C:185:PRO:HG2	2.00	0.43
5:F:67:ALA:HB3	5:F:75:THR:OG1	2.18	0.43
9:J:56:ALA:HA	9:J:125:VAL:HG23	2.01	0.43
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.00	0.43
11:L:72:ILE:HA	11:L:143:TRP:CD1	2.53	0.43
11:L:77:VAL:HG22	11:L:78:ARG:N	2.33	0.43
12:M:136:GLU:HB3	12:M:242:PRO:HG2	2.00	0.43
12:M:200:ARG:HB3	14:O:118:PHE:CD1	2.54	0.43
22:Y:58:SER:HB2	35:l:371:THR:HG21	2.01	0.43
30:g:82:TYR:OH	32:i:341:PRO:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:218:LEU:HD23	32:i:218:LEU:HA	1.81	0.43
33:j:106:TRP:HZ3	41:s:291:LYS:HA	1.83	0.43
35:l:222:GLY:N	35:l:229:LEU:HD12	2.31	0.43
40:r:87:GLU:O	40:r:92:LYS:HE3	2.18	0.43
40:r:105:SER:O	40:r:109:THR:HG23	2.18	0.43
41:s:142:TYR:CE2	41:s:289:LEU:HD11	2.54	0.43
42:u:80:GLU:N	42:u:81:PRO:HD2	2.33	0.43
42:u:149:ASP:HA	42:u:150:PRO:HD3	1.88	0.43
1:A:418:GLN:CD	12:M:115:GLY:HA2	2.44	0.43
2:B:99:HIS:ND1	2:B:147:MET:HE1	2.34	0.43
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	0.43
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
8:I:5:THR:HB	8:I:8:ILE:HD12	2.00	0.43
9:J:167:VAL:HG22	9:J:201:VAL:HB	2.00	0.43
9:J:283:VAL:O	9:J:357:ARG:NH2	2.51	0.43
15:P:163:ALA:O	15:P:167:GLU:HB2	2.17	0.43
47:V:203:PLX:H332	47:V:203:PLX:H141	2.01	0.43
24:a:185:ALA:O	42:u:48:TRP:HZ2	2.01	0.43
26:c:154:GLN:C	26:c:156:VAL:HG23	2.44	0.43
29:f:28:LYS:HE3	44:w:101:GLY:H	1.83	0.43
35:l:222:GLY:HA2	35:l:229:LEU:CD1	2.43	0.43
37:n:39:ARG:HB2	37:n:57:TRP:CZ2	2.53	0.43
9:J:141:PHE:HE2	9:J:180:TYR:HA	1.75	0.43
12:M:133:GLN:HA	12:M:136:GLU:OE2	2.17	0.43
13:N:106:ARG:O	13:N:109:ILE:HG12	2.18	0.43
15:P:171:TRP:CZ3	15:P:177:PHE:HA	2.54	0.43
15:P:188:LEU:HA	16:Q:114:GLY:HA3	2.00	0.43
16:Q:119:GLY:H	16:Q:463:ARG:C	2.27	0.43
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.54	0.43
32:i:76:PHE:CZ	32:i:80:LEU:HD11	2.54	0.43
33:j:68:GLU:HG3	33:j:98:LEU:HD21	2.01	0.43
34:k:97:GLN:CD	35:l:587:TYR:HE1	2.27	0.43
35:l:209:SER:O	35:l:212:PRO:HD2	2.19	0.43
35:l:217:LEU:O	35:l:217:LEU:HD23	2.19	0.43
51:n:101:CDL:H741	51:n:101:CDL:H711	1.60	0.43
41:s:251:SER:HA	41:s:252:PRO:HD2	1.85	0.43
44:w:163:ILE:HD12	44:w:166:ASP:OD2	2.19	0.43
1:A:73:PRO:HB2	1:A:74:ASP:H	1.58	0.43
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.43
2:B:175:THR:HB	2:B:180:GLU:OE1	2.19	0.43
3:C:156:GLY:O	3:C:161:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	0.43
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.43
9:J:124:ASN:OD1	9:J:125:VAL:N	2.51	0.43
12:M:243:TRP:CD1	12:M:244:GLU:HG3	2.54	0.43
13:N:27:PHE:HZ	41:s:43:TYR:CE1	2.37	0.43
15:P:129:VAL:HG22	15:P:144:LYS:HB3	2.01	0.43
16:Q:144:MET:HA	16:Q:147:ASN:HD22	1.84	0.43
16:Q:410:TYR:O	16:Q:422:CYS:HA	2.19	0.43
21:W:33:TYR:O	21:W:34:SER:OG	2.27	0.43
24:a:66:ARG:O	24:a:70:LEU:HG	2.19	0.43
24:a:170:TYR:CD1	30:g:5:ARG:HD3	2.54	0.43
31:h:73:MET:HG2	36:m:124:TRP:CH2	2.54	0.43
32:i:71:LEU:HA	32:i:71:LEU:HD23	1.73	0.43
34:k:39:SER:HB3	36:m:16:PHE:HE2	1.84	0.43
35:l:67:HIS:ND1	35:l:75:GLN:HG3	2.33	0.43
35:l:68:TRP:HB2	35:l:76:LEU:HD12	2.01	0.43
35:l:280:LEU:O	35:l:284:THR:HG23	2.19	0.43
36:m:26:ILE:HD13	41:s:121:TRP:CE2	2.54	0.43
36:m:56:PHE:CZ	41:s:111:LEU:HD11	2.54	0.43
39:p:49:GLU:O	39:p:52:LYS:HG2	2.19	0.43
39:p:104:LEU:HD22	39:p:122:ARG:NH2	2.34	0.43
40:r:45:ILE:O	40:r:45:ILE:HG22	2.19	0.43
40:r:122:PHE:CE1	40:r:238:LEU:HD21	2.54	0.43
41:s:150:LEU:O	41:s:154:LEU:HG	2.19	0.43
1:A:129:GLU:OE1	1:A:132:ARG:NH1	2.49	0.43
1:A:403:ASP:HA	1:A:453:PHE:CE2	2.54	0.43
5:F:87:VAL:O	5:F:91:LEU:HG	2.18	0.43
8:I:42:PRO:HG3	16:Q:354:GLY:O	2.19	0.43
9:J:125:VAL:HG12	9:J:163:LYS:HB2	2.00	0.43
12:M:153:PHE:C	12:M:154:LEU:HD12	2.44	0.43
12:M:307:VAL:HA	12:M:582:VAL:HA	2.01	0.43
15:P:90:PRO:O	15:P:93:VAL:HG23	2.18	0.43
16:Q:372:LYS:HD2	18:T:93:ALA:HA	2.00	0.43
20:V:95:CYS:O	20:V:99:LEU:HG	2.19	0.43
22:Y:74:TRP:C	22:Y:74:TRP:CD2	2.97	0.43
26:c:44:THR:HB	26:c:47:GLU:CG	2.49	0.43
30:g:32:TYR:CE2	32:i:339:ILE:HD11	2.54	0.43
30:g:51:PRO:HG2	30:g:55:ALA:CA	2.49	0.43
32:i:214:THR:HG22	32:i:329:LEU:HB3	2.01	0.43
32:i:258:THR:CG2	32:i:336:LEU:HB3	2.48	0.43
33:j:64:LEU:HD23	33:j:64:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:227:LEU:HD22	35:l:283:ILE:HG22	2.00	0.43
35:l:550:LEU:HA	35:l:554:ASP:HB3	2.01	0.43
39:p:48:PHE:CZ	48:p:201:8Q1:C8	2.99	0.43
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.43
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	0.42
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.42
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.42
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.42
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.42
11:L:170:THR:HG22	12:M:423:LEU:O	2.18	0.42
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.54	0.42
16:Q:85:GLY:HA2	33:j:39:CYS:HB2	2.01	0.42
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	2.01	0.42
20:V:62:THR:HG22	20:V:104:ARG:CD	2.49	0.42
47:b:201:PLX:C2	27:d:43:ARG:HH22	2.31	0.42
30:g:15:ASP:HB2	30:g:18:ARG:NH2	2.29	0.42
32:i:298:TYR:HE2	40:r:147:THR:HG23	1.83	0.42
34:k:7:ASN:ND2	36:m:9:SER:CA	2.82	0.42
35:l:95:PHE:HZ	35:l:456:ARG:HG2	1.83	0.42
35:l:548:LEU:O	35:l:552:LEU:HB2	2.18	0.42
52:l:701:PEE:H36	40:r:155:VAL:CG2	2.46	0.42
40:r:308:SER:HB3	40:r:384:THR:HG21	2.01	0.42
41:s:195:ARG:O	41:s:198:PHE:N	2.52	0.42
1:A:220:GLN:NE2	14:O:114:GLU:HB3	2.34	0.42
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.42
9:J:131:GLY:HA3	49:J:401:NDP:O3D	2.19	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.20	0.42
12:M:153:PHE:O	12:M:154:LEU:HD12	2.20	0.42
12:M:342:ALA:O	12:M:369:GLU:HG2	2.19	0.42
13:N:73:THR:HG22	13:N:74:PHE:N	2.34	0.42
20:V:133:TRP:CG	52:V:202:PEE:H7	2.54	0.42
21:W:72:LEU:HD23	21:W:72:LEU:HA	1.84	0.42
24:a:87:THR:CG2	47:b:201:PLX:C13	2.87	0.42
26:c:61:ASP:O	26:c:63:GLU:HG3	2.19	0.42
26:c:102:GLY:HA3	38:o:43:LEU:HD13	2.00	0.42
30:g:51:PRO:HB2	30:g:54:THR:OG1	2.19	0.42
30:g:61:LEU:O	30:g:65:THR:HG23	2.19	0.42
31:h:58:ILE:HD12	42:u:145:ARG:NH2	2.34	0.42
32:i:234:TRP:HH2	32:i:305:LEU:HB2	1.84	0.42
33:j:49:VAL:CG1	36:m:75:ILE:H	2.32	0.42
35:l:548:LEU:HD22	38:o:93:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:27:TYR:HA	36:m:30:LEU:HD12	2.01	0.42
40:r:179:LEU:O	40:r:248:LEU:HD13	2.19	0.42
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.42
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.00	0.42
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.42
2:B:117:CYS:HB2	45:B:301:SF4:S1	2.59	0.42
4:E:25:MET:O	4:E:29:LYS:N	2.44	0.42
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.42
12:M:254:MET:CB	12:M:290:THR:HG22	2.46	0.42
12:M:559:ASP:OD1	12:M:560:LEU:N	2.51	0.42
12:M:651:PRO:O	12:M:654:VAL:HG22	2.19	0.42
13:N:66:THR:HG23	13:N:74:PHE:H	1.85	0.42
14:O:163:THR:HG22	14:O:170:THR:HG22	2.01	0.42
15:P:109:LYS:O	15:P:110:SER:OG	2.31	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.42
17:S:53:ARG:HB2	31:h:105:ARG:CZ	2.49	0.42
18:T:79:GLU:OE1	18:T:122:HIS:HB3	2.19	0.42
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.52	0.42
24:a:78:THR:OG1	28:e:96:SER:O	2.24	0.42
30:g:87:ARG:HD2	42:u:156:GLY:O	2.19	0.42
36:m:43:ILE:HG22	36:m:48:GLY:HA3	2.00	0.42
36:m:86:VAL:O	36:m:90:VAL:HG23	2.19	0.42
39:p:90:SER:HB2	39:p:93:ARG:HE	1.84	0.42
41:s:169:GLN:NE2	41:s:241:ILE:O	2.42	0.42
42:u:67:ALA:O	42:u:70:PHE:HB3	2.19	0.42
43:v:5:LEU:HG	43:v:6:VAL:N	2.34	0.42
1:A:274:LYS:NZ	1:A:351:THR:O	2.51	0.42
2:B:158:GLU:O	16:Q:368:ARG:NH2	2.52	0.42
3:C:104:ASP:OD2	41:s:37:PRO:HD3	2.19	0.42
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	0.42
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.42
10:K:82:TYR:HB3	14:O:62:ARG:HH22	1.84	0.42
11:L:79:ILE:HD12	11:L:145:TYR:CD2	2.54	0.42
12:M:542:PRO:HB2	12:M:543:LYS:HD3	2.01	0.42
15:P:97:LEU:HD11	15:P:130:TYR:CE2	2.54	0.42
16:Q:39:PRO:HD2	32:i:304:LEU:O	2.19	0.42
16:Q:116:LEU:O	16:Q:118:ARG:HG3	2.19	0.42
16:Q:338:ARG:O	16:Q:341:LEU:HB2	2.19	0.42
18:T:52:ARG:O	18:T:55:ARG:HG2	2.20	0.42
18:T:102:ASN:HD21	18:T:104:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:40:LYS:O	19:U:44:MET:HG2	2.18	0.42
6:X:105:MET:HE2	6:X:139:MET:HE3	2.00	0.42
22:Y:40:ILE:HD11	35:l:446:ASN:ND2	2.34	0.42
24:a:54:LEU:CD2	25:b:26:GLN:C	2.87	0.42
25:b:51:LEU:HD22	25:b:59:LYS:HA	2.01	0.42
31:h:17:TRP:CZ3	31:h:18:LEU:HB2	2.55	0.42
35:l:149:ILE:HD12	40:r:369:LEU:HD11	2.01	0.42
37:n:51:PRO:O	37:n:53:GLU:HG3	2.20	0.42
51:n:101:CDL:H712	51:n:101:CDL:H512	2.01	0.42
40:r:10:MET:O	40:r:13:PRO:HD2	2.20	0.42
1:A:270:ASN:CG	1:A:338:ASP:HB2	2.44	0.42
1:A:314:LEU:O	1:A:315:LEU:HD12	2.19	0.42
2:B:176:GLU:OE1	3:C:200:LYS:HD2	2.20	0.42
8:I:40:LYS:HG2	21:W:8:GLN:HA	2.00	0.42
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	0.42
9:J:128:ASN:O	9:J:129:LEU:HD12	2.19	0.42
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	0.42
12:M:492:ALA:O	12:M:496:ILE:HG13	2.19	0.42
13:N:10:GLY:O	13:N:14:ILE:HG13	2.20	0.42
14:O:144:ASN:O	14:O:147:SER:OG	2.35	0.42
14:O:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
15:P:210:LEU:HA	15:P:221:ALA:HA	2.01	0.42
16:Q:116:LEU:HD11	16:Q:141:TYR:OH	2.20	0.42
16:Q:167:ALA:O	16:Q:171:ARG:HG3	2.18	0.42
17:S:55:SER:C	17:S:64:LYS:HZ1	2.28	0.42
24:a:101:ILE:HG13	27:d:58:TYR:CB	2.49	0.42
26:c:119:THR:HB	38:o:13:THR:HG23	2.02	0.42
28:e:87:MET:HE3	28:e:87:MET:HB3	1.77	0.42
30:g:37:GLY:O	30:g:40:SER:OG	2.28	0.42
32:i:109:ALA:CB	32:i:112:HIS:HD2	2.33	0.42
40:r:398:LEU:HA	40:r:398:LEU:HD23	1.82	0.42
47:r:502:PLX:H311	47:r:502:PLX:H282	1.75	0.42
41:s:18:ALA:O	41:s:21:MET:HG2	2.19	0.42
41:s:231:ILE:HG23	41:s:270:PHE:CD2	2.54	0.42
1:A:27:PRO:HB2	1:A:28:LYS:H	1.65	0.42
1:A:37:ASP:OD2	14:O:235:THR:N	2.49	0.42
1:A:159:ARG:HD3	1:A:162:PHE:CE2	2.55	0.42
1:A:282:VAL:HA	1:A:307:VAL:HA	2.00	0.42
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:46:GLU:C	14:O:49:PRO:HD3	2.44	0.42
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	0.42
26:c:101:TRP:CD1	38:o:62:ASN:HD22	2.38	0.42
32:i:26:TRP:HD1	32:i:84:TRP:O	2.02	0.42
35:l:14:SER:O	35:l:17:PRO:HD2	2.20	0.42
35:l:93:ALA:O	35:l:97:THR:OG1	2.38	0.42
35:l:404:THR:HB	35:l:405:ASN:H	1.66	0.42
37:n:40:ASN:HD22	37:n:56:THR:HG23	1.82	0.42
39:p:48:PHE:HE1	48:p:201:8Q1:C6	2.33	0.42
41:s:90:PRO:HB2	41:s:92:PRO:O	2.18	0.42
1:A:32:PHE:HB3	1:A:294:VAL:HA	2.02	0.42
4:E:78:VAL:O	4:E:82:LEU:HD13	2.20	0.42
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
11:L:154:LYS:HG2	12:M:279:GLU:HG3	2.02	0.42
12:M:49:VAL:HG23	12:M:94:MET:O	2.20	0.42
12:M:589:TYR:O	12:M:606:THR:HG21	2.19	0.42
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.42
16:Q:70:ASP:HB2	16:Q:71:PRO:HD3	2.02	0.42
16:Q:198:THR:HG21	41:s:275:THR:HB	2.02	0.42
18:T:110:GLY:N	18:T:119:PHE:O	2.28	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
25:b:117:ILE:CG2	25:b:118:PRO:HD2	2.50	0.42
25:b:117:ILE:HG23	25:b:118:PRO:HD2	2.01	0.42
47:b:201:PLX:C6	47:b:201:PLX:C11	2.85	0.42
26:c:94:GLN:OE1	26:c:99:LEU:HB2	2.20	0.42
26:c:125:SER:O	26:c:129:MET:HG3	2.20	0.42
26:c:183:HIS:CB	43:v:37:ARG:HA	2.50	0.42
27:d:24:ILE:HD11	35:l:56:CYS:HB3	2.02	0.42
31:h:74:ARG:HG2	36:m:116:VAL:HG13	2.02	0.42
31:h:94:PRO:O	31:h:97:HIS:N	2.52	0.42
35:l:336:LYS:HD3	35:l:336:LYS:HA	1.90	0.42
37:n:50:GLN:HG3	37:n:51:PRO:CD	2.50	0.42
43:v:79:ALA:C	43:v:81:LYS:H	2.26	0.42
44:w:143:TYR:OH	44:w:162:SER:HB2	2.20	0.42
2:B:133:ARG:NH2	18:T:69:ILE:HG13	2.34	0.42
3:C:104:ASP:HB2	41:s:34:ARG:NH1	2.35	0.42
3:C:150:MET:SD	3:C:190:LEU:HD13	2.60	0.42
4:E:102:HIS:HA	4:E:105:ARG:HG3	2.02	0.42
5:F:62:GLN:HE21	5:F:64:LYS:NZ	2.17	0.42
7:H:81:ILE:HG13	7:H:82:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:336:GLU:C	9:J:339:GLY:H	2.28	0.42
11:L:131:LYS:HD2	11:L:147:ILE:CG2	2.49	0.42
12:M:33:GLU:O	12:M:98:LYS:HA	2.20	0.42
12:M:433:GLY:HA3	12:M:684:LEU:HD23	2.01	0.42
15:P:240:GLU:OE1	15:P:246:ARG:NE	2.51	0.42
16:Q:233:HIS:CD2	16:Q:234:GLN:HB2	2.55	0.42
16:Q:275:ILE:HD13	16:Q:446:ASP:OD1	2.20	0.42
19:U:69:HIS:CE1	19:U:70:PRO:HA	2.54	0.42
52:W:201:PEE:H36	33:j:7:LEU:CD2	2.47	0.42
52:W:201:PEE:H60	36:m:56:PHE:HZ	1.84	0.42
24:a:57:ILE:HA	39:p:104:LEU:HD12	2.01	0.42
26:c:133:LEU:HD13	35:l:532:ILE:HD12	2.00	0.42
27:d:134:GLN:OE1	38:o:124:THR:HA	2.20	0.42
27:d:162:LYS:O	27:d:165:LYS:HB3	2.20	0.42
32:i:79:MET:HE3	34:k:5:TYR:CD2	2.55	0.42
32:i:217:LEU:HD23	32:i:217:LEU:HA	1.86	0.42
35:l:158:TRP:CH2	35:l:240:PRO:HB3	2.55	0.42
35:l:558:LEU:HB3	40:r:214:LEU:HD11	2.02	0.42
36:m:33:ILE:HD11	41:s:114:TYR:CE1	2.55	0.42
36:m:40:CYS:O	36:m:44:LEU:HG	2.19	0.42
39:p:31:CYS:HB3	39:p:36:LYS:HD2	2.02	0.42
39:p:174:PRO:O	39:p:175:ARG:HB3	2.19	0.42
40:r:344:LEU:O	40:r:420:THR:HG21	2.20	0.42
40:r:374:ASN:OD1	40:r:374:ASN:N	2.52	0.42
41:s:11:VAL:N	41:s:12:PRO:HD2	2.34	0.42
1:A:122:PRO:HB2	1:A:322:SER:HB2	2.01	0.42
1:A:453:PHE:O	1:A:456:GLN:HG2	2.20	0.42
3:C:106:PHE:CE1	41:s:39:VAL:HG21	2.54	0.42
6:G:103:HIS:N	6:G:107:ASP:HB2	2.35	0.42
9:J:171:ASN:O	9:J:181:LEU:HG	2.18	0.42
9:J:263:PHE:CE1	9:J:333:PRO:HG2	2.55	0.42
9:J:283:VAL:HG13	9:J:369:VAL:HG11	2.02	0.42
12:M:543:LYS:N	12:M:543:LYS:HD2	2.35	0.42
14:O:176:CYS:HA	50:O:301:FES:S1	2.60	0.42
16:Q:190:HIS:CE1	16:Q:268:TRP:CH2	3.08	0.42
16:Q:199:PRO:HB3	16:Q:258:LEU:HD21	2.00	0.42
17:S:53:ARG:CZ	31:h:105:ARG:NH2	2.83	0.42
18:T:80:VAL:O	18:T:121:GLN:HA	2.20	0.42
21:W:57:ARG:NH2	41:s:316:PRO:HG3	2.35	0.42
47:b:201:PLX:C10	47:b:201:PLX:C6	2.85	0.42
26:c:81:ARG:HD3	26:c:85:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:120:GLN:HA	32:i:176:ARG:HE	1.85	0.42
33:j:71:LEU:O	33:j:74:PRO:HD2	2.20	0.42
37:n:16:LEU:HD21	40:r:10:MET:HE3	2.02	0.42
43:v:59:CYS:O	43:v:87:TRP:HZ3	2.03	0.42
1:A:47:GLY:HA2	1:A:133:HIS:HB3	2.00	0.42
6:G:87:LEU:HA	6:G:90:TYR:HB3	2.00	0.42
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	0.42
9:J:179:ARG:HB3	9:J:179:ARG:HH11	1.84	0.42
11:L:130:THR:O	11:L:133:ASP:HB3	2.19	0.42
12:M:314:LEU:HD22	12:M:583:ILE:HD12	2.02	0.42
12:M:342:ALA:HA	12:M:547:LEU:HB2	2.00	0.42
12:M:560:LEU:HD12	12:M:561:PRO:HD2	2.02	0.42
16:Q:371:MET:HA	16:Q:377:SER:OG	2.20	0.42
20:V:23:TYR:O	20:V:24:SER:HB2	2.20	0.42
22:Y:95:GLU:CD	22:Y:95:GLU:N	2.77	0.42
24:a:98:LEU:HB2	27:d:57:TYR:CE1	2.39	0.42
24:a:180:ASP:HB3	31:h:24:GLU:HG3	2.02	0.42
26:c:100:ASN:HB2	26:c:103:GLU:HG3	2.02	0.42
30:g:44:ASP:OD1	32:i:327:PRO:HG2	2.20	0.42
32:i:2:ASN:ND2	32:i:4:LEU:HB2	2.35	0.42
32:i:294:LEU:HD23	32:i:294:LEU:HA	1.74	0.42
33:j:12:LEU:O	33:j:16:LEU:HB2	2.20	0.42
35:l:7:MET:O	35:l:11:THR:HG23	2.20	0.42
35:l:154:LEU:HD23	35:l:154:LEU:HA	1.85	0.42
35:l:305:SER:O	35:l:309:GLN:HG2	2.20	0.42
35:l:310:LEU:HD23	35:l:313:MET:HE3	2.01	0.42
35:l:414:ILE:O	35:l:417:SER:OG	2.29	0.42
35:l:536:THR:O	35:l:539:TYR:HB3	2.20	0.42
44:w:223:ASP:HA	44:w:224:PRO:HD3	1.85	0.42
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.41
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.41
2:B:96:ARG:HB3	2:B:167:GLU:HG2	2.01	0.41
2:B:166:VAL:HG11	2:B:199:ILE:CG2	2.49	0.41
47:B:303:PLX:H1A1	16:Q:269:ARG:HD2	2.02	0.41
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.84	0.41
9:J:240:VAL:HG22	9:J:266:VAL:C	2.45	0.41
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	0.41
12:M:128:CYS:CB	12:M:129:PRO:CD	2.86	0.41
12:M:357:LEU:O	12:M:361:VAL:HG22	2.20	0.41
12:M:711:VAL:O	12:M:715:THR:HG23	2.19	0.41
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.41
14:O:213:ILE:HG22	14:O:214:PRO:O	2.20	0.41
16:Q:83:ASN:CA	16:Q:98:VAL:HG22	2.44	0.41
16:Q:341:LEU:HA	16:Q:341:LEU:HD23	1.88	0.41
18:T:40:THR:OG1	18:T:44:GLN:HG2	2.20	0.41
18:T:83:ARG:HH12	18:T:103:LEU:H	1.68	0.41
19:U:19:LEU:O	19:U:22:SER:OG	2.29	0.41
24:a:149:LEU:HD23	24:a:149:LEU:HA	1.79	0.41
28:e:62:GLU:OE2	38:o:57:ARG:NH2	2.53	0.41
47:g:203:PLX:H22	47:g:203:PLX:H1B3	1.74	0.41
37:n:28:ASP:OD1	40:r:2:LEU:HB3	2.19	0.41
37:n:43:MET:HE3	37:n:43:MET:HB2	1.87	0.41
40:r:245:ARG:HA	40:r:245:ARG:HD3	1.86	0.41
44:w:93:TYR:CZ	44:w:142:GLN:OE1	2.73	0.41
44:w:240:ALA:O	44:w:244:THR:OG1	2.14	0.41
1:A:98:LYS:HD2	1:A:98:LYS:HA	1.92	0.41
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.56	0.41
12:M:381:LEU:C	12:M:383:SER:N	2.77	0.41
15:P:96:VAL:O	15:P:100:LEU:HG	2.20	0.41
15:P:202:PHE:HB2	15:P:207:TYR:CE2	2.55	0.41
16:Q:235:ASP:HA	16:Q:356:ILE:HD12	2.02	0.41
16:Q:368:ARG:HA	16:Q:371:MET:HG2	2.01	0.41
20:V:126:LYS:HE3	20:V:130:LEU:HD11	2.02	0.41
22:Y:81:LEU:HB3	35:l:480:THR:OG1	2.20	0.41
24:a:129:PRO:CG	27:d:60:ARG:HH22	2.33	0.41
25:b:118:PRO:HA	25:b:119:PRO:HD3	1.94	0.41
47:b:201:PLX:P1	47:b:201:PLX:O6	2.79	0.41
26:c:49:ALA:O	26:c:53:LYS:HG2	2.21	0.41
32:i:108:MET:SD	32:i:191:MET:HG3	2.60	0.41
33:j:70:ALA:HA	33:j:73:LEU:HD13	2.01	0.41
40:r:188:ASN:O	40:r:189:SER:OG	2.21	0.41
40:r:248:LEU:HD12	40:r:249:ILE:N	2.35	0.41
41:s:275:THR:OG1	41:s:276:ALA:N	2.53	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	0.41
2:B:133:ARG:C	2:B:136:GLY:H	2.29	0.41
3:C:118:ASP:CG	3:C:119:VAL:H	2.28	0.41
3:C:187:ALA:O	3:C:190:LEU:HB3	2.20	0.41
9:J:201:VAL:HG13	9:J:265:PHE:CD2	2.55	0.41
25:b:119:PRO:HB2	43:v:40:VAL:HG13	2.01	0.41
27:d:74:GLU:HB2	30:g:105:LYS:HD2	2.01	0.41
31:h:56:CYS:HA	42:u:145:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:307:MET:O	44:w:319:ILE:HD12	2.20	0.41
35:l:37:LYS:NZ	35:l:98:TRP:HE1	2.18	0.41
35:l:106:TRP:CZ2	35:l:348:HIS:HD2	2.38	0.41
35:l:188:TRP:O	35:l:192:HIS:HB2	2.20	0.41
47:r:501:PLX:H282	47:r:501:PLX:H251	1.77	0.41
42:u:104:GLN:HB3	42:u:108:ASP:OD2	2.20	0.41
44:w:77:ILE:HG23	44:w:81:LEU:HD13	2.03	0.41
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
1:A:382:CYS:HA	12:M:75:CYS:H	1.86	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
7:H:44:TYR:CD2	7:H:94:MET:HE2	2.54	0.41
12:M:83:GLU:HB2	12:M:101:ASN:HB3	2.02	0.41
12:M:598:ASN:N	12:M:602:ARG:O	2.48	0.41
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.36	0.41
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.41
16:Q:290:GLY:C	16:Q:294:ARG:HE	2.28	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
25:b:111:LEU:C	25:b:113:THR:N	2.78	0.41
30:g:46:LEU:CD1	32:i:239:TRP:HB3	2.49	0.41
30:g:51:PRO:HG2	30:g:55:ALA:CB	2.50	0.41
33:j:94:LEU:HD12	36:m:153:VAL:HG13	2.03	0.41
35:l:174:TYR:OH	35:l:534:HIS:HE1	2.03	0.41
35:l:562:LEU:O	35:l:566:ILE:HD12	2.21	0.41
51:l:703:CDL:HA61	51:l:703:CDL:H1	2.02	0.41
36:m:5:LEU:HD23	36:m:8:LEU:HD12	2.02	0.41
39:p:76:HIS:HA	39:p:77:PRO:HD3	1.86	0.41
39:p:135:ARG:HD3	39:p:162:ASP:OD1	2.21	0.41
41:s:173:TRP:HZ3	41:s:262:LYS:HE2	1.86	0.41
42:u:83:THR:O	42:u:87:THR:HG23	2.20	0.41
44:w:62:VAL:HG21	44:w:74:ALA:HB2	2.02	0.41
44:w:86:PHE:HE2	44:w:146:ALA:HB2	1.86	0.41
1:A:184:LYS:C	1:A:186:ALA:H	2.27	0.41
1:A:223:PRO:HB2	1:A:425:CYS:SG	2.60	0.41
2:B:184:ASN:ND2	13:N:126:PRO:HA	2.35	0.41
7:H:19:THR:N	7:H:20:PRO:HD3	2.35	0.41
7:H:50:GLN:HE22	8:I:93:LYS:HD2	1.85	0.41
9:J:152:ILE:HG22	9:J:164:PHE:CE1	2.55	0.41
11:L:131:LYS:HD2	11:L:147:ILE:HG23	2.03	0.41
12:M:598:ASN:HD22	12:M:602:ARG:NH1	2.19	0.41
13:N:117:VAL:HG11	13:N:122:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:156:LEU:HD13	14:O:158:ILE:HD12	2.03	0.41
18:T:32:VAL:HG22	18:T:38:LYS:HE3	2.03	0.41
6:X:131:PRO:HG3	26:c:89:TRP:CE3	2.55	0.41
26:c:151:PRO:O	26:c:153:TYR:HD1	2.03	0.41
32:i:69:ILE:HD12	32:i:104:MET:HE1	2.01	0.41
32:i:256:PRO:HB3	40:r:124:THR:HG22	2.01	0.41
34:k:10:LEU:O	34:k:14:ILE:HG13	2.20	0.41
35:l:197:ASP:O	35:l:201:MET:CG	2.68	0.41
35:l:452:ASN:CB	35:l:453:PRO:HD3	2.51	0.41
40:r:121:PHE:O	40:r:125:THR:HG23	2.20	0.41
40:r:355:MET:HA	40:r:358:TRP:CD1	2.54	0.41
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	0.41
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	0.41
12:M:557:ARG:HE	12:M:579:ILE:HG23	1.86	0.41
12:M:646:LEU:O	12:M:651:PRO:HA	2.20	0.41
16:Q:371:MET:HE1	16:Q:381:HIS:CE1	2.55	0.41
26:c:65:TYR:CE2	26:c:77:LYS:HG3	2.55	0.41
26:c:162:PRO:O	26:c:166:LEU:HD12	2.21	0.41
26:c:163:TYR:HB3	26:c:168:LEU:HD21	2.02	0.41
27:d:76:ILE:HG22	27:d:77:MET:HE2	2.02	0.41
30:g:27:ASP:O	30:g:31:LEU:HG	2.19	0.41
30:g:73:TYR:O	30:g:76:LYS:HB3	2.21	0.41
31:h:6:ILE:HD12	32:i:22:LEU:HD21	2.01	0.41
36:m:33:ILE:O	36:m:37:VAL:HG23	2.19	0.41
39:p:145:PRO:HA	39:p:146:PRO:HD3	1.84	0.41
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.41
2:B:75:LEU:HD12	41:s:31:MET:SD	2.60	0.41
3:C:213:ARG:O	3:C:213:ARG:HG2	2.19	0.41
5:F:23:LEU:HD21	5:F:34:ARG:HG2	2.03	0.41
9:J:50:SER:O	9:J:77:GLY:HA3	2.20	0.41
10:K:101:SER:OG	10:K:102:GLY:N	2.53	0.41
12:M:234:LYS:N	12:M:235:PRO:HD2	2.36	0.41
12:M:522:GLN:HE21	12:M:526:LEU:HG	1.85	0.41
12:M:528:LEU:HD23	12:M:528:LEU:HA	1.89	0.41
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.41
23:Z:53:TYR:HA	35:l:435:PRO:HG2	2.03	0.41
24:a:62:PHE:HB2	39:p:111:GLU:OE2	2.19	0.41
47:b:201:PLX:C6	47:b:201:PLX:P1	3.08	0.41
27:d:123:VAL:O	27:d:127:THR:HG23	2.21	0.41
32:i:167:TRP:HZ3	35:l:570:GLN:CA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:210:ILE:O	32:i:214:THR:HG23	2.20	0.41
33:j:36:PRO:HA	41:s:214:GLU:OE2	2.21	0.41
39:p:124:GLN:HA	39:p:127:LYS:NZ	2.36	0.41
40:r:153:THR:O	40:r:157:SER:N	2.54	0.41
41:s:150:LEU:HD23	41:s:150:LEU:HA	1.88	0.41
42:u:24:VAL:CG2	42:u:86:TRP:HE1	2.34	0.41
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	0.41
2:B:72:LEU:HD13	41:s:272:TRP:HH2	1.85	0.41
47:B:303:PLX:H12	16:Q:266:ARG:HG3	2.03	0.41
7:H:45:ARG:O	7:H:49:GLU:HG3	2.21	0.41
8:I:94:ALA:HB1	15:P:105:ASN:HD21	1.85	0.41
11:L:117:THR:OG1	15:P:229:GLU:OE1	2.39	0.41
15:P:77:GLN:HB2	15:P:85:GLU:HB2	2.03	0.41
16:Q:35:ARG:HH21	44:w:322:HIS:HB3	1.86	0.41
16:Q:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
19:U:56:PRO:HB3	42:u:129:THR:OG1	2.20	0.41
21:W:86:MET:HG2	21:W:128:ARG:HH22	1.86	0.41
24:a:106:VAL:HA	24:a:107:PRO:HD2	1.82	0.41
25:b:111:LEU:C	25:b:113:THR:H	2.27	0.41
26:c:73:GLY:C	26:c:75:TYR:H	2.28	0.41
26:c:159:LYS:HA	43:v:98:ARG:CZ	2.50	0.41
27:d:35:VAL:C	27:d:38:PRO:HD2	2.46	0.41
33:j:54:LYS:HB3	33:j:113:TRP:HE1	1.85	0.41
35:l:536:THR:OG1	35:l:537:ILE:N	2.53	0.41
39:p:134:GLU:O	39:p:138:LYS:HG3	2.21	0.41
40:r:229:MET:HE2	40:r:229:MET:HB3	1.90	0.41
41:s:86:TRP:HH2	41:s:232:ILE:HG22	1.85	0.41
41:s:164:THR:O	41:s:167:THR:OG1	2.38	0.41
44:w:42:HIS:O	44:w:46:GLY:N	2.54	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:244:ASN:ND2	46:A:502:FMN:HM82	2.35	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	0.41
1:A:339:PHE:HA	1:A:342:LEU:HD12	2.03	0.41
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	0.41
2:B:143:TYR:HB3	2:B:185:LYS:HB2	2.03	0.41
2:B:146:ASP:OD2	2:B:149:LYS:HE2	2.21	0.41
2:B:160:CYS:HA	2:B:161:PRO:HD2	1.83	0.41
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
5:F:89:ARG:HD2	5:F:92:GLU:OE2	2.21	0.41
9:J:130:ILE:HA	49:J:401:NDP:H8A	2.03	0.41
9:J:168:SER:CA	9:J:184:LYS:CE	2.99	0.41
9:J:202:LYS:N	9:J:263:PHE:O	2.54	0.41
9:J:271:TYR:HE1	9:J:374:THR:HB	1.85	0.41
12:M:209:TYR:H	14:O:110:MET:HE1	1.85	0.41
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
12:M:246:ARG:NH2	15:P:229:GLU:OE2	2.54	0.41
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.96	0.41
12:M:568:TYR:HB2	12:M:580:ALA:CB	2.51	0.41
15:P:157:VAL:HG21	15:P:181:HIS:CD2	2.46	0.41
16:Q:153:LEU:O	16:Q:157:LYS:HG3	2.21	0.41
17:S:47:LEU:O	17:S:50:ARG:HB3	2.20	0.41
18:T:33:SER:HB3	18:T:45:VAL:HG21	2.03	0.41
20:V:114:ALA:HB1	20:V:118:PHE:CE2	2.56	0.41
51:V:201:CDL:H722	51:V:201:CDL:H752	1.75	0.41
24:a:115:HIS:CG	24:a:116:PRO:HD2	2.56	0.41
24:a:130:GLU:HA	37:n:45:PHE:CD2	2.56	0.41
26:c:154:GLN:HE22	43:v:3:ALA:HB2	1.86	0.41
28:e:150:PRO:HD3	30:g:112:PHE:CD1	2.56	0.41
29:f:34:PRO:HG3	44:w:342:GLY:HA2	2.03	0.41
30:g:45:ASN:HD21	30:g:60:GLN:NE2	2.19	0.41
32:i:19:ILE:HD12	32:i:35:MET:HE1	2.02	0.41
32:i:112:HIS:HB2	32:i:184:ILE:HD13	2.03	0.41
34:k:3:LEU:O	34:k:3:LEU:HD13	2.20	0.41
34:k:10:LEU:CD1	36:m:102:LEU:HD12	2.49	0.41
34:k:14:ILE:HD13	36:m:17:VAL:HG22	2.02	0.41
35:l:311:GLY:O	35:l:315:VAL:HG23	2.21	0.41
35:l:396:ILE:HG22	35:l:400:ASN:HD21	1.85	0.41
35:l:452:ASN:N	35:l:453:PRO:HD2	2.35	0.41
36:m:106:VAL:HG11	36:m:117:ASN:ND2	2.34	0.41
36:m:114:VAL:O	36:m:115:VAL:HG22	2.20	0.41
38:o:112:LYS:NZ	40:r:389:SER:HA	2.36	0.41
38:o:124:THR:C	38:o:126:HIS:H	2.29	0.41
39:p:31:CYS:O	39:p:33:GLN:N	2.54	0.41
39:p:158:ARG:O	39:p:162:ASP:HB2	2.21	0.41
40:r:130:LEU:HD21	40:r:149:PHE:HD2	1.86	0.41
47:r:502:PLX:H392	47:r:502:PLX:H361	1.64	0.41
41:s:154:LEU:HA	41:s:154:LEU:HD23	1.73	0.41
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:B:303:PLX:H332	47:B:303:PLX:H301	1.80	0.41
7:H:75:GLY:CA	8:I:103:ARG:HH11	2.34	0.41
9:J:62:THR:HG21	49:J:401:NDP:O1X	2.21	0.41
9:J:329:LEU:HD13	9:J:332:LEU:HD12	2.03	0.41
11:L:123:ASN:HB3	15:P:232:LYS:HD2	2.02	0.41
12:M:401:LEU:HD13	12:M:462:PHE:CE2	2.56	0.41
14:O:148:ILE:O	14:O:152:ILE:HG13	2.21	0.41
16:Q:103:GLY:HA3	33:j:52:SER:CB	2.50	0.41
16:Q:169:TRP:C	16:Q:351:MET:HE2	2.47	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
24:a:96:ALA:CB	27:d:55:TYR:H	2.34	0.41
24:a:112:TYR:CD1	27:d:58:TYR:O	2.72	0.41
26:c:88:PRO:HB2	39:p:86:PRO:HG2	2.03	0.41
27:d:56:TYR:HD1	27:d:56:TYR:HA	1.78	0.41
30:g:37:GLY:HA2	30:g:67:PHE:CE2	2.56	0.41
32:i:189:TRP:HE1	32:i:286:THR:HG21	1.85	0.41
34:k:31:LEU:HD21	36:m:67:PHE:CE2	2.56	0.41
35:l:100:ILE:HD12	35:l:246:LEU:CD2	2.51	0.41
35:l:244:SER:HA	35:l:248:HIS:CD2	2.56	0.41
35:l:272:LEU:HD11	51:l:704:CDL:HB61	2.02	0.41
35:l:493:VAL:O	35:l:496:LEU:HB3	2.21	0.41
40:r:170:THR:OG1	40:r:171:LEU:N	2.53	0.41
41:s:195:ARG:HG3	41:s:196:ALA:N	2.36	0.41
41:s:311:ILE:O	41:s:312:SER:OG	2.28	0.41
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.40
2:B:96:ARG:HD2	2:B:154:GLY:HA3	2.03	0.40
2:B:120:ILE:O	2:B:121:CYS:C	2.64	0.40
2:B:155:PHE:HB2	45:B:302:SF4:S2	2.61	0.40
9:J:329:LEU:HD22	9:J:332:LEU:HD12	2.01	0.40
14:O:99:ASN:O	14:O:103:GLU:HG3	2.21	0.40
14:O:198:ALA:O	14:O:202:GLU:HG2	2.21	0.40
15:P:148:ASP:HB2	15:P:151:THR:HG23	2.02	0.40
16:Q:65:PRO:CG	16:Q:69:VAL:HG22	2.51	0.40
16:Q:71:PRO:HB2	16:Q:72:PRO:HD3	2.03	0.40
22:Y:62:SER:O	22:Y:65:MET:HB3	2.21	0.40
32:i:58:LYS:HZ1	34:k:92:ASN:CG	2.28	0.40
34:k:3:LEU:C	34:k:3:LEU:CD1	2.94	0.40
35:l:70:THR:HA	35:l:75:GLN:HB2	2.04	0.40
35:l:218:LEU:C	35:l:218:LEU:CD2	2.94	0.40
35:l:362:LEU:HA	35:l:365:THR:OG1	2.22	0.40
35:l:522:PHE:HA	35:l:528:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:6:TYR:HE2	38:o:14:LEU:HA	1.85	0.40
40:r:375:LEU:HD12	40:r:375:LEU:HA	1.85	0.40
41:s:193:THR:O	41:s:194:ASN:HB2	2.20	0.40
1:A:53:LEU:O	1:A:56:SER:OG	2.24	0.40
1:A:121:GLU:HA	1:A:122:PRO:HD3	1.87	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.40
2:B:84:TYR:CD1	2:B:85:PRO:HA	2.56	0.40
2:B:90:PRO:O	2:B:91:LEU:HD12	2.22	0.40
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	0.40
4:E:42:GLU:OE2	4:E:46:THR:OG1	2.40	0.40
14:O:197:THR:N	14:O:200:ASP:HB3	2.36	0.40
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
16:Q:52:MET:HE2	32:i:295:ARG:HH21	1.86	0.40
16:Q:316:PHE:HD1	16:Q:339:GLN:HE21	1.67	0.40
16:Q:331:LEU:O	16:Q:335:GLU:HG3	2.20	0.40
47:U:101:PLX:H22	47:U:101:PLX:H1B3	1.86	0.40
47:V:203:PLX:H371	47:V:203:PLX:H342	1.76	0.40
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.86	0.40
24:a:109:HIS:O	24:a:112:TYR:HD2	2.03	0.40
25:b:105:PHE:HD2	43:v:68:LYS:CB	2.34	0.40
27:d:72:LYS:HE3	30:g:105:LYS:O	2.20	0.40
28:e:67:TYR:CE2	40:r:428:PRO:HG2	2.56	0.40
32:i:61:LEU:O	32:i:65:THR:HG23	2.21	0.40
35:l:39:ILE:O	35:l:43:THR:HG23	2.21	0.40
39:p:30:TRP:NE1	39:p:76:HIS:HB2	2.36	0.40
40:r:196:TRP:NE1	40:r:250:LEU:HD13	2.36	0.40
41:s:2:PRO:O	41:s:5:ASN:HB2	2.20	0.40
41:s:273:ILE:HG23	41:s:277:TYR:HD2	1.86	0.40
43:v:75:PRO:O	43:v:77:PHE:N	2.43	0.40
44:w:72:LYS:HD2	44:w:75:LYS:HD2	2.03	0.40
5:F:22:HIS:ND1	5:F:64:LYS:HD2	2.36	0.40
6:G:154:VAL:O	6:G:156:GLU:HG3	2.22	0.40
11:L:163:ASN:O	11:L:171:ARG:N	2.55	0.40
12:M:128:CYS:HA	45:M:801:SF4:S4	2.61	0.40
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.40
12:M:483:ARG:O	12:M:483:ARG:HG3	2.21	0.40
12:M:634:LEU:HA	12:M:635:PRO:HD3	1.91	0.40
14:O:110:MET:HA	14:O:113:TYR:CD2	2.56	0.40
15:P:61:PHE:O	15:P:64:TYR:HB3	2.20	0.40
20:V:124:LEU:HA	20:V:127:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:93:GLU:OE1	31:h:93:THR:HG21	2.21	0.40
21:W:111:PHE:CE2	21:W:117:VAL:HG21	2.56	0.40
22:Y:45:ARG:O	22:Y:45:ARG:HG2	2.22	0.40
22:Y:68:TRP:CZ3	35:l:386:LEU:HA	2.56	0.40
22:Y:74:TRP:CZ3	22:Y:75:HIS:HA	2.53	0.40
24:a:54:LEU:HD23	24:a:54:LEU:HA	1.81	0.40
25:b:31:ARG:HH12	39:p:116:PRO:HG2	1.85	0.40
32:i:70:LEU:HD23	32:i:70:LEU:HA	1.76	0.40
32:i:342:PHE:CD2	32:i:343:MET:HE2	2.57	0.40
51:i:401:CDL:H311	51:i:401:CDL:H341	1.83	0.40
34:k:46:LEU:HD22	36:m:46:PHE:CE2	2.56	0.40
34:k:97:GLN:N	35:l:579:THR:OG1	2.41	0.40
35:l:84:TYR:HD1	35:l:88:MET:CE	2.01	0.40
35:l:417:SER:HB3	35:l:493:VAL:CG1	2.51	0.40
35:l:550:LEU:HD23	35:l:554:ASP:OD2	2.22	0.40
37:n:30:LYS:HZ2	51:n:101:CDL:HA31	1.86	0.40
39:p:158:ARG:O	39:p:159:LYS:HB2	2.21	0.40
40:r:89:LEU:O	40:r:93:LYS:HG3	2.20	0.40
40:r:235:LEU:O	40:r:238:LEU:HB3	2.22	0.40
47:r:501:PLX:H301	47:r:501:PLX:H271	1.66	0.40
44:w:68:THR:OG1	44:w:69:GLY:N	2.54	0.40
1:A:382:CYS:SG	1:A:424:ILE:HG22	2.62	0.40
2:B:52:THR:HA	19:U:13:TRP:HH2	1.87	0.40
3:C:81:PRO:HA	3:C:119:VAL:HG13	2.03	0.40
5:F:66:TRP:CZ2	12:M:648:GLU:HB2	2.57	0.40
49:J:401:NDP:P2B	49:J:401:NDP:O3B	2.79	0.40
12:M:436:VAL:HG21	12:M:686:PRO:HG2	2.02	0.40
12:M:645:ARG:O	12:M:649:VAL:HG12	2.21	0.40
13:N:39:VAL:HG12	13:N:40:GLY:O	2.21	0.40
15:P:227:ALA:O	15:P:229:GLU:N	2.47	0.40
16:Q:255:LEU:HA	16:Q:255:LEU:HD23	1.91	0.40
18:T:105:LYS:HB3	18:T:107:THR:HG22	2.04	0.40
47:b:201:PLX:C11	47:b:201:PLX:C7	3.00	0.40
27:d:138:GLN:HG2	27:d:139:ASP:OD1	2.22	0.40
30:g:11:ARG:O	30:g:13:LEU:N	2.54	0.40
32:i:124:LEU:HD13	32:i:219:LEU:HG	2.03	0.40
35:l:564:LYS:HG3	38:o:77:TYR:OH	2.21	0.40
40:r:80:SER:O	40:r:81:GLN:C	2.64	0.40
40:r:346:GLN:HA	40:r:413:THR:O	2.21	0.40
41:s:116:ILE:O	41:s:119:SER:OG	2.34	0.40
44:w:86:PHE:HA	44:w:87:PRO:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:C	1:A:95:THR:HG23	2.46	0.40
5:F:14:LEU:N	5:F:17:ARG:HH12	2.20	0.40
9:J:157:LYS:HB2	9:J:195:PHE:HD1	1.86	0.40
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40
15:P:52:ASP:O	15:P:56:LYS:HG3	2.22	0.40
15:P:114:LEU:HG	15:P:130:TYR:HE1	1.87	0.40
16:Q:120:THR:O	16:Q:124:ILE:HG13	2.22	0.40
16:Q:310:VAL:O	16:Q:314:VAL:HG23	2.20	0.40
16:Q:314:VAL:HG12	16:Q:316:PHE:HD2	1.87	0.40
19:U:8:PHE:O	19:U:11:ASN:HB3	2.21	0.40
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.03	0.40
23:Z:61:VAL:HB	35:l:432:THR:O	2.21	0.40
25:b:12:LEU:HD23	25:b:12:LEU:HA	1.90	0.40
25:b:33:PRO:HG2	39:p:116:PRO:HD3	2.03	0.40
25:b:88:TYR:HB2	47:b:201:PLX:C1B	2.51	0.40
26:c:168:LEU:HD12	26:c:169:GLU:N	2.36	0.40
28:e:74:HIS:HB3	28:e:87:MET:SD	2.61	0.40
29:f:63:ASN:O	29:f:67:LEU:HG	2.22	0.40
30:g:86:ASP:CG	42:u:166:ARG:HH22	2.27	0.40
32:i:73:ALA:HA	32:i:97:MET:HE3	2.03	0.40
32:i:86:MET:HE2	32:i:144:GLN:OE1	2.21	0.40
35:l:121:LEU:HD23	35:l:121:LEU:HA	1.92	0.40
40:r:233:ALA:HB2	40:r:324:SER:HB3	2.04	0.40
47:r:502:PLX:H1B2	47:r:502:PLX:H22	1.53	0.40
41:s:94:PRO:HB2	41:s:96:VAL:O	2.22	0.40
44:w:223:ASP:O	44:w:227:MET:HG3	2.20	0.40
44:w:319:ILE:HG21	44:w:324:THR:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	31
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	52
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	25
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	29
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	17
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	18
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	13
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	31
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	25
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	25
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	17
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	25
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	16
16	Q	428/430 (100%)	397 (93%)	24 (6%)	7 (2%)	7	35
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	26
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	19
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	40
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	31
21	W	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	3	26
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	5
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	31
25	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	2	20
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	18
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	52
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	25
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	31
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	17
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	34
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	27
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	25
35	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	6	32
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	15
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	22
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	25
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	32
41	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	4	27
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	26
43	v	107/137 (78%)	90 (84%)	14 (13%)	3 (3%)	4	27
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	27
All	All	8097/8236 (98%)	7338 (91%)	526 (6%)	233 (3%)	5	26

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE

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Mol	Chain	Res	Type
24	a	58	ARG
26	c	115	ASN
26	c	178	PRO
27	d	2	PRO
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU

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Mol	Chain	Res	Type
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE
31	h	24	GLU
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
35	l	512	LYS
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS
1	A	74	ASP
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU

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Mol	Chain	Res	Type
12	M	715	THR
13	N	113	HIS
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	511	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
1	A	50	ASP

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Mol	Chain	Res	Type
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN
8	I	108	SER
9	J	100	LEU
9	J	330	PRO
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU

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Mol	Chain	Res	Type
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
1	A	94	PRO
12	M	575	VAL
36	m	23	PRO
3	C	144	PRO
16	Q	307	PRO

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Mol	Chain	Res	Type
16	Q	69	VAL
10	K	102	GLY
32	i	338	PRO
28	e	135	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	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	77 (99%)	1 (1%)	61	71
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	74
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	70
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	83
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	76
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	22
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	76
25	b	118/122 (97%)	113 (96%)	5 (4%)	26	51
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	46
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	83
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	74
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	48
35	l	531/532 (100%)	512 (96%)	19 (4%)	31	54
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	71
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/121 (74%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
All	All	7093/7209 (98%)	7034 (99%)	59 (1%)	70	76

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	81	ILE
9	J	85	ARG
9	J	91	ILE

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Mol	Chain	Res	Type
9	J	206	ILE
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
16	Q	275	ILE
6	X	93	ILE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	87	PRO
22	Y	95	GLU
22	Y	97	LEU
24	a	53	ARG
25	b	21	ARG
25	b	38	GLN
25	b	82	ILE
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
32	i	149	LEU
33	j	86	LEU
34	k	1	MET
34	k	3	LEU
34	k	6	MET
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	94	LEU
35	l	97	THR
35	l	99	SER
35	l	191	LEU

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Mol	Chain	Res	Type
35	l	193	SER
35	l	195	SER
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	229	LEU
35	l	447	ASN
35	l	450	LEU
35	l	452	ASN
39	p	124	GLN
39	p	170	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	HIS
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	220	GLN
1	A	270	ASN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	72	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
4	E	108	HIS
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	101	ASN
6	G	142	GLN
7	H	50	GLN

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Mol	Chain	Res	Type
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	21	GLN
9	J	71	ASN
9	J	93	HIS
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	86	ASN
12	M	142	GLN
12	M	425	ASN
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	663	ASN
12	M	666	GLN
12	M	669	ASN
13	N	72	ASN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	69	ASN
14	O	187	GLN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
16	Q	38	GLN
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN

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Mol	Chain	Res	Type
17	S	44	HIS
18	T	64	ASN
20	V	44	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
6	X	142	GLN
22	Y	75	HIS
23	Z	33	GLN
24	a	90	ASN
24	a	109	HIS
24	a	115	HIS
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
26	c	56	ASN
26	c	84	HIS
26	c	127	HIS
26	c	154	GLN
26	c	165	ASN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	108	GLN
27	d	113	GLN
27	d	116	GLN
27	d	117	GLN
28	e	140	ASN
30	g	45	ASN
30	g	58	HIS
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS

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Mol	Chain	Res	Type
35	l	59	GLN
35	l	113	ASN
35	l	139	GLN
35	l	192	HIS
35	l	199	GLN
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	323	HIS
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	117	ASN
37	n	40	ASN
38	o	52	ASN
38	o	62	ASN
38	o	126	HIS
39	p	26	HIS
39	p	75	GLN
40	r	21	HIS
40	r	46	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	97	ASN
41	s	169	GLN
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS

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Mol	Chain	Res	Type
42	u	104	GLN
42	u	140	ASN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	92	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	GLN
44	w	323	GLN

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](#)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	A	501	1	0,12,12	-	-	-		
47	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
47	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
52	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
47	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
48	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
51	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
47	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
52	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
49	NDP	J	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.75	11 (16%)
46	FMN	A	502	-	33,33,33	1.40	6 (18%)	48,50,50	1.34	8 (16%)
47	PLX	g	202	-	51,51,51	0.75	1 (1%)	55,59,59	0.61	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
51	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
45	SF4	M	802	12	0,12,12	-	-	-		
50	FES	M	803	-	0,4,4	-	-	-		
47	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
47	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
51	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
51	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
52	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
52	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
47	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.59	1 (1%)
51	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
48	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
50	FES	O	301	14	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	B	303	-	-	21/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLX	b	201	-	-	27/55/55/55	-
47	PLX	U	101	-	-	22/55/55/55	-
52	PEE	W	201	-	-	32/54/54/54	-
47	PLX	r	502	-	-	36/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
48	8Q1	E	201	-	-	18/41/41/41	-
51	CDL	l	703	-	-	38/74/74/110	-
47	PLX	r	501	-	-	28/55/55/55	-
52	PEE	l	702	-	-	27/54/54/54	-
49	NDP	J	401	-	-	15/34/77/77	0/5/5/5
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
47	PLX	g	202	-	-	25/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
51	CDL	l	704	-	-	44/74/74/110	-
45	SF4	M	802	12	-	-	0/6/5/5
50	FES	M	803	-	-	-	0/1/1/1
47	PLX	g	201	-	-	25/55/55/55	-
47	PLX	g	203	-	-	24/55/55/55	-
51	CDL	n	101	-	-	33/74/74/110	-
51	CDL	i	401	-	-	39/74/74/110	-
52	PEE	V	202	-	-	27/54/54/54	-
52	PEE	l	701	-	-	32/52/52/54	-
47	PLX	V	203	-	-	26/55/55/55	-
51	CDL	V	201	-	-	42/69/69/110	-
45	SF4	B	302	2	-	-	0/6/5/5
48	8Q1	p	201	-	-	19/41/41/41	-
50	FES	O	301	14	-	-	0/1/1/1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	201	8Q1	C34-N36	5.30	1.45	1.33
48	E	201	8Q1	C34-N36	5.24	1.45	1.33
48	p	201	8Q1	C39-N41	5.24	1.45	1.33
48	E	201	8Q1	C39-N41	4.93	1.44	1.33
46	A	502	FMN	C9A-C5A	4.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	l	704	CDL	OB8-CB7	4.36	1.46	1.33
51	n	101	CDL	OA6-CA5	4.31	1.46	1.34
51	l	703	CDL	OA6-CA5	4.28	1.46	1.34
51	V	201	CDL	OA6-CA5	4.26	1.46	1.34
51	l	703	CDL	OB8-CB7	4.24	1.45	1.33
51	V	201	CDL	OB8-CB7	4.18	1.45	1.33
52	l	701	PEE	C39-C38	4.17	1.55	1.31
51	l	704	CDL	OA8-CA7	4.15	1.45	1.33
51	l	704	CDL	OA6-CA5	4.14	1.46	1.34
52	l	701	PEE	O3-C30	4.12	1.45	1.33
52	l	701	PEE	C18-C19	4.11	1.55	1.31
51	n	101	CDL	OB8-CB7	4.10	1.45	1.33
51	i	401	CDL	OB8-CB7	4.05	1.45	1.33
51	i	401	CDL	OA6-CA5	4.01	1.45	1.34
51	n	101	CDL	OA8-CA7	3.92	1.44	1.33
49	J	401	NDP	C5A-C4A	3.90	1.46	1.39
51	l	703	CDL	OA8-CA7	3.82	1.44	1.33
52	l	702	PEE	C18-C19	3.78	1.53	1.31
52	V	202	PEE	C18-C19	3.75	1.53	1.31
51	i	401	CDL	OA8-CA7	3.74	1.44	1.33
52	W	201	PEE	C18-C19	3.74	1.53	1.31
52	V	202	PEE	C39-C38	3.71	1.53	1.31
52	l	702	PEE	C39-C38	3.70	1.53	1.31
52	W	201	PEE	C39-C38	3.67	1.53	1.31
51	l	704	CDL	OB6-CB5	3.31	1.43	1.34
52	l	701	PEE	O2-C10	3.31	1.43	1.34
51	n	101	CDL	OB6-CB5	3.29	1.43	1.34
51	l	703	CDL	OB6-CB5	3.23	1.43	1.34
51	V	201	CDL	OB6-CB5	3.13	1.43	1.34
49	J	401	NDP	C6N-C5N	3.11	1.38	1.33
51	i	401	CDL	OB6-CB5	3.10	1.43	1.34
46	A	502	FMN	C8-C7	3.07	1.48	1.40
46	A	502	FMN	C4-N3	-3.04	1.33	1.38
51	V	201	CDL	OA8-CA7	3.00	1.44	1.33
47	B	303	PLX	O6-C4	-2.97	1.40	1.44
47	g	203	PLX	O6-C4	-2.92	1.40	1.44
49	J	401	NDP	C5A-N7A	-2.84	1.33	1.39
47	V	203	PLX	O6-C4	-2.82	1.40	1.44
47	g	201	PLX	O6-C4	-2.79	1.40	1.44
51	n	101	CDL	OB6-CB4	-2.75	1.39	1.46
51	V	201	CDL	OB6-CB4	-2.62	1.40	1.46
47	U	101	PLX	O6-C4	-2.54	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	i	401	CDL	OB6-CB4	-2.51	1.40	1.46
47	g	202	PLX	O6-C4	-2.48	1.41	1.44
48	E	201	8Q1	O35-C34	-2.48	1.18	1.23
48	p	201	8Q1	O35-C34	-2.46	1.18	1.23
52	V	202	PEE	O2-C10	2.41	1.41	1.34
52	l	702	PEE	O2-C10	2.39	1.41	1.34
47	r	501	PLX	O6-C4	-2.37	1.41	1.44
51	l	704	CDL	OB6-CB4	-2.36	1.40	1.46
51	l	703	CDL	OB6-CB4	-2.34	1.40	1.46
48	E	201	8Q1	C1-S44	2.34	1.81	1.76
48	E	201	8Q1	O40-C39	-2.34	1.18	1.23
48	p	201	8Q1	O40-C39	-2.34	1.18	1.23
52	l	702	PEE	O3-C30	2.33	1.40	1.33
46	A	502	FMN	C5A-N5	-2.26	1.35	1.39
52	l	702	PEE	O2-C2	-2.25	1.41	1.46
48	p	201	8Q1	C1-S44	2.25	1.81	1.76
52	V	202	PEE	O2-C2	-2.25	1.41	1.46
52	W	201	PEE	O3-C30	2.24	1.39	1.33
52	V	202	PEE	O3-C30	2.24	1.39	1.33
52	W	201	PEE	O2-C10	2.22	1.40	1.34
52	V	202	PEE	O3-C3	-2.22	1.40	1.45
48	E	201	8Q1	C6-C1	2.22	1.53	1.50
49	J	401	NDP	C5A-C6A	2.19	1.47	1.41
52	W	201	PEE	O2-C2	-2.19	1.41	1.46
52	l	702	PEE	O3-C3	-2.18	1.40	1.45
52	W	201	PEE	O3-C3	-2.15	1.40	1.45
46	A	502	FMN	C4A-N5	2.14	1.34	1.30
49	J	401	NDP	C8A-N7A	2.09	1.35	1.31
46	A	502	FMN	C2-N3	-2.03	1.34	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	J	401	NDP	C5A-C4A-N3A	-6.19	118.68	126.75
48	p	201	8Q1	C6-C1-S44	6.03	120.47	113.46
49	J	401	NDP	PN-O3-PA	-5.21	114.94	132.83
49	J	401	NDP	N3A-C4A-N9A	4.96	135.26	127.08
48	E	201	8Q1	C6-C1-S44	4.56	118.77	113.46
52	l	702	PEE	O2-C10-C11	4.38	120.95	111.50
51	l	703	CDL	OA6-CA5-C11	4.16	120.48	111.50
51	i	401	CDL	OA6-CA5-C11	4.13	120.39	111.50
51	l	704	CDL	OA6-CA5-C11	4.11	120.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	V	201	CDL	OB6-CB5-C51	4.09	120.32	111.50
51	n	101	CDL	OB6-CB5-C51	4.08	120.29	111.50
49	J	401	NDP	C2A-N3A-C4A	4.03	121.28	111.75
52	l	701	PEE	O2-C10-C11	4.01	120.14	111.50
51	l	703	CDL	OB6-CB5-C51	3.94	120.00	111.50
51	l	704	CDL	OB6-CB5-C51	3.92	119.96	111.50
51	n	101	CDL	OA6-CA5-C11	3.92	119.94	111.50
49	J	401	NDP	N3A-C2A-N1A	-3.71	122.81	128.60
52	W	201	PEE	O2-C10-C11	3.69	119.45	111.50
48	p	201	8Q1	O4-C1-C6	-3.63	119.70	123.99
52	V	202	PEE	O2-C10-C11	3.59	119.25	111.50
51	i	401	CDL	OB6-CB5-C51	3.51	119.06	111.50
51	V	201	CDL	OA6-CA5-C11	3.44	118.92	111.50
49	J	401	NDP	C4A-C5A-N7A	-3.08	106.87	110.62
51	l	703	CDL	OA8-CA7-C31	2.99	121.28	111.91
52	V	202	PEE	O3-C30-C31	2.85	120.86	111.91
52	l	702	PEE	O3-C30-C31	2.85	120.84	111.91
49	J	401	NDP	C5A-N7A-C8A	2.83	107.52	103.51
46	A	502	FMN	C4-C4A-N5	2.82	122.25	118.23
48	E	201	8Q1	C43-S44-C1	2.79	110.56	101.87
46	A	502	FMN	C4A-C10-N1	-2.76	118.33	124.73
51	i	401	CDL	OB8-CB7-C71	2.75	120.55	111.91
51	n	101	CDL	OA8-CA7-C31	2.74	120.49	111.91
48	E	201	8Q1	C32-C34-N36	2.73	122.01	116.58
51	l	704	CDL	OA8-CA7-C31	2.72	120.45	111.91
48	p	201	8Q1	C43-S44-C1	2.71	110.31	101.87
52	W	201	PEE	O3-C30-C31	2.70	120.38	111.91
51	n	101	CDL	OB8-CB7-C71	2.69	120.36	111.91
51	l	703	CDL	OB8-CB7-C71	2.68	120.32	111.91
49	J	401	NDP	C4A-N9A-C8A	2.68	108.63	105.73
51	l	704	CDL	OB8-CB7-C71	2.67	120.28	111.91
48	p	201	8Q1	C38-C39-N41	2.55	120.71	116.42
48	E	201	8Q1	O4-C1-C6	-2.53	121.00	123.99
51	V	201	CDL	OB8-CB7-C71	2.53	119.86	111.91
48	E	201	8Q1	C42-N41-C39	-2.43	118.33	122.84
46	A	502	FMN	C4A-C10-N10	2.42	120.02	116.48
51	i	401	CDL	OA8-CA7-C31	2.41	119.47	111.91
48	E	201	8Q1	C37-N36-C34	-2.39	118.33	122.59
47	B	303	PLX	C1C-N1-C1	2.36	119.59	109.92
47	V	203	PLX	C1C-N1-C1	2.32	119.40	109.92
46	A	502	FMN	O2-C2-N1	-2.31	118.00	121.83
47	U	101	PLX	C1C-N1-C1	2.29	119.30	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	l	701	PEE	O3-C30-C31	2.29	119.10	111.91
47	g	203	PLX	C1C-N1-C1	2.27	119.21	109.92
46	A	502	FMN	C4-N3-C2	-2.22	121.54	125.64
49	J	401	NDP	C3D-C2D-C1D	2.21	105.62	101.43
47	g	201	PLX	C1C-N1-C1	2.20	118.93	109.92
49	J	401	NDP	N9A-C8A-N7A	-2.20	110.91	113.91
47	g	202	PLX	C1C-N1-C1	2.19	118.90	109.92
46	A	502	FMN	C4A-C4-N3	2.15	118.66	113.19
48	p	201	8Q1	O4-C1-S44	-2.15	119.83	122.61
49	J	401	NDP	C6A-C5A-N7A	2.14	136.02	132.02
46	A	502	FMN	C10-N1-C2	2.14	121.18	116.90
48	E	201	8Q1	O35-C34-N36	-2.12	118.45	122.99
46	A	502	FMN	N3-C2-N1	2.10	123.51	119.38
47	r	502	PLX	C2-C1-N1	-2.09	108.79	115.78
47	U	101	PLX	C5-C4-C3	-2.08	106.87	111.79
47	r	501	PLX	C1C-N1-C1	2.06	118.35	109.92
51	i	401	CDL	OA6-CA5-OA7	-2.01	118.86	123.70

There are no chirality outliers.

All (607) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	B	303	PLX	C2-O1-P1-O2
47	B	303	PLX	N1-C1-C2-O1
47	U	101	PLX	O7-C6-C7-C8
47	U	101	PLX	O7-C6-O6-C4
47	U	101	PLX	C3-O4-P1-O2
47	U	101	PLX	N1-C1-C2-O1
47	U	101	PLX	O9-C24-C25-C26
47	V	203	PLX	O7-C6-C7-C8
47	V	203	PLX	N1-C1-C2-O1
47	V	203	PLX	O9-C24-C25-C26
47	b	201	PLX	O7-C6-O6-C4
47	b	201	PLX	N1-C1-C2-O1
47	b	201	PLX	O9-C24-O8-C5
47	g	201	PLX	O7-C6-C7-C8
47	g	201	PLX	O7-C6-O6-C4
47	g	201	PLX	C3-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
47	g	202	PLX	C2-O1-P1-O4
47	g	202	PLX	C2-O1-P1-O2
47	g	202	PLX	C2-O1-P1-O3
47	g	202	PLX	O9-C24-O8-C5
47	g	203	PLX	O7-C6-O6-C4
47	g	203	PLX	C2-O1-P1-O2
47	g	203	PLX	C25-C24-O8-C5
47	r	501	PLX	C3-O4-P1-O1
47	r	501	PLX	C3-O4-P1-O2
47	r	501	PLX	C3-O4-P1-O3
47	r	501	PLX	O8-C24-C25-C26
47	r	502	PLX	C7-C6-O6-C4
47	r	502	PLX	C3-O4-P1-O1
47	r	502	PLX	C3-O4-P1-O2
47	r	502	PLX	C3-O4-P1-O3
47	r	502	PLX	C2-O1-P1-O2
47	r	502	PLX	N1-C1-C2-O1
47	r	502	PLX	O9-C24-C25-C26
48	E	201	8Q1	C1-C6-C7-C8
48	E	201	8Q1	O4-C1-S44-C43
48	E	201	8Q1	C6-C1-S44-C43
48	E	201	8Q1	C29-C32-C34-N36
48	E	201	8Q1	C29-C32-C34-O35
48	E	201	8Q1	C42-C43-S44-C1
48	E	201	8Q1	C28-O27-P24-O3
48	E	201	8Q1	C28-O27-P24-O2
48	E	201	8Q1	C28-O27-P24-O1
48	p	201	8Q1	C1-C6-C7-C8
48	p	201	8Q1	O4-C1-S44-C43
48	p	201	8Q1	C6-C1-S44-C43
48	p	201	8Q1	C28-C29-C32-C34
48	p	201	8Q1	C28-C29-C32-O33
48	p	201	8Q1	C30-C29-C32-C34
48	p	201	8Q1	C31-C29-C32-C34
48	p	201	8Q1	C31-C29-C32-O33
48	p	201	8Q1	C28-O27-P24-O2
48	p	201	8Q1	C28-O27-P24-O1
49	J	401	NDP	C5B-O5B-PA-O1A
49	J	401	NDP	C5D-O5D-PN-O1N
51	V	201	CDL	CB2-C1-CA2-OA2
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	CA2-OA2-PA1-OA5
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CA3-OA5-PA1-OA4
51	V	201	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	C51-CB5-OB6-CB4
51	i	401	CDL	O1-C1-CA2-OA2
51	i	401	CDL	CB2-C1-CA2-OA2
51	i	401	CDL	CA2-OA2-PA1-OA3
51	i	401	CDL	CA2-OA2-PA1-OA4
51	i	401	CDL	CA2-OA2-PA1-OA5
51	i	401	CDL	CA3-OA5-PA1-OA3
51	i	401	CDL	CA3-OA5-PA1-OA4
51	i	401	CDL	OA6-CA4-CA6-OA8
51	i	401	CDL	CB2-OB2-PB2-OB4
51	i	401	CDL	CB3-OB5-PB2-OB3
51	i	401	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CA2-OA2-PA1-OA3
51	l	703	CDL	OB7-CB5-OB6-CB4
51	l	704	CDL	CA2-OA2-PA1-OA3
51	l	704	CDL	CA2-OA2-PA1-OA4
51	l	704	CDL	CA3-OA5-PA1-OA2
51	l	704	CDL	CA3-OA5-PA1-OA4
51	l	704	CDL	C11-CA5-OA6-CA4
51	l	704	CDL	CB2-OB2-PB2-OB3
51	n	101	CDL	CA2-OA2-PA1-OA3
51	n	101	CDL	CA2-OA2-PA1-OA4
51	n	101	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	OA7-CA5-OA6-CA4
51	n	101	CDL	C11-CA5-OA6-CA4
51	n	101	CDL	CB2-OB2-PB2-OB3
51	n	101	CDL	CB2-OB2-PB2-OB4
51	n	101	CDL	C51-CB5-OB6-CB4
52	V	202	PEE	C2-C1-O3P-P
52	V	202	PEE	O4P-C4-C5-N
52	W	201	PEE	C4-O4P-P-O3P
52	W	201	PEE	C4-O4P-P-O1P
52	l	701	PEE	C11-C10-O2-C2
52	l	701	PEE	C4-O4P-P-O2P
52	l	701	PEE	C4-O4P-P-O1P
51	l	704	CDL	OA9-CA7-OA8-CA6
51	l	704	CDL	OB9-CB7-OB8-CB6
51	n	101	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OB7-CB5-OB6-CB4
51	l	704	CDL	OA7-CA5-OA6-CA4
51	n	101	CDL	OB7-CB5-OB6-CB4
52	l	701	PEE	O4-C10-O2-C2
51	l	704	CDL	C31-CA7-OA8-CA6
51	l	704	CDL	C71-CB7-OB8-CB6
51	n	101	CDL	C31-CA7-OA8-CA6
51	n	101	CDL	C71-CB7-OB8-CB6
51	l	703	CDL	C51-CB5-OB6-CB4
48	E	201	8Q1	C38-C39-N41-C42
52	W	201	PEE	C17-C18-C19-C20
52	l	701	PEE	C37-C38-C39-C40
52	l	702	PEE	C37-C38-C39-C40
51	n	101	CDL	OB9-CB7-OB8-CB6
52	l	702	PEE	O5-C30-O3-C3
51	l	703	CDL	O1-C1-CA2-OA2
51	l	704	CDL	O1-C1-CA2-OA2
51	i	401	CDL	C11-CA5-OA6-CA4
52	W	201	PEE	C21-C22-C23-C24
52	V	202	PEE	C20-C21-C22-C23
47	r	502	PLX	C16-C17-C18-C19
52	l	701	PEE	C32-C33-C34-C35
49	J	401	NDP	O4B-C4B-C5B-O5B
49	J	401	NDP	C3B-C4B-C5B-O5B
52	l	702	PEE	C31-C30-O3-C3
47	g	203	PLX	C26-C27-C28-C29
47	r	501	PLX	C10-C11-C12-C13
47	b	201	PLX	C4-C3-O4-P1
47	b	201	PLX	C14-C15-C16-C17
47	g	203	PLX	C30-C31-C32-C33
47	r	502	PLX	C30-C31-C32-C33
52	W	201	PEE	C32-C33-C34-C35
49	J	401	NDP	C1B-C2B-O2B-P2B
47	g	202	PLX	C10-C11-C12-C13
48	E	201	8Q1	O40-C39-N41-C42
51	l	703	CDL	CB2-C1-CA2-OA2
47	r	502	PLX	C12-C13-C14-C15
51	i	401	CDL	C31-C32-C33-C34
52	W	201	PEE	C31-C30-O3-C3
51	l	703	CDL	C73-C74-C75-C76
51	l	703	CDL	OB5-CB3-CB4-OB6
52	W	201	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
52	l	701	PEE	C34-C35-C36-C37
51	V	201	CDL	O1-C1-CA2-OA2
51	l	703	CDL	O1-C1-CB2-OB2
47	r	501	PLX	C12-C13-C14-C15
52	W	201	PEE	O5-C30-O3-C3
51	V	201	CDL	C54-C55-C56-C57
51	i	401	CDL	OA7-CA5-OA6-CA4
47	V	203	PLX	C13-C14-C15-C16
51	l	704	CDL	CB5-C51-C52-C53
51	n	101	CDL	CA7-C31-C32-C33
52	l	702	PEE	C10-C11-C12-C13
52	l	702	PEE	C17-C18-C19-C20
52	W	201	PEE	C15-C16-C17-C18
51	i	401	CDL	CA5-C11-C12-C13
52	V	202	PEE	C10-C11-C12-C13
52	l	701	PEE	C30-C31-C32-C33
47	r	501	PLX	C27-C28-C29-C30
51	n	101	CDL	C31-C32-C33-C34
51	i	401	CDL	C31-CA7-OA8-CA6
49	J	401	NDP	C3B-C2B-O2B-P2B
52	l	701	PEE	C39-C40-C41-C42
52	V	202	PEE	C17-C18-C19-C20
52	l	701	PEE	C17-C18-C19-C20
47	B	303	PLX	C2-O1-P1-O4
47	U	101	PLX	C3-O4-P1-O1
47	b	201	PLX	C3-O4-P1-O1
47	g	201	PLX	C3-O4-P1-O1
47	g	202	PLX	C3-O4-P1-O1
47	g	203	PLX	C2-O1-P1-O4
47	r	502	PLX	C2-O1-P1-O4
51	V	201	CDL	CA3-OA5-PA1-OA2
51	V	201	CDL	CB3-OB5-PB2-OB2
51	i	401	CDL	CA3-OA5-PA1-OA2
51	i	401	CDL	CB2-OB2-PB2-OB5
51	i	401	CDL	CB3-OB5-PB2-OB2
51	l	703	CDL	CB3-OB5-PB2-OB2
51	l	704	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	CB2-OB2-PB2-OB5
52	V	202	PEE	C1-O3P-P-O4P
52	W	201	PEE	C1-O3P-P-O4P
52	l	701	PEE	C4-O4P-P-O3P
52	V	202	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	C71-CB7-OB8-CB6
47	B	303	PLX	O6-C6-C7-C8
47	U	101	PLX	O6-C6-C7-C8
47	g	203	PLX	O8-C24-C25-C26
47	g	201	PLX	C13-C14-C15-C16
51	l	704	CDL	C51-CB5-OB6-CB4
47	B	303	PLX	C27-C28-C29-C30
47	g	201	PLX	C7-C8-C9-C10
47	g	202	PLX	C7-C8-C9-C10
47	g	203	PLX	C29-C30-C31-C32
51	l	704	CDL	C31-C32-C33-C34
51	n	101	CDL	C12-C13-C14-C15
51	n	101	CDL	C13-C14-C15-C16
52	W	201	PEE	C14-C15-C16-C17
52	l	701	PEE	C22-C23-C24-C25
47	g	203	PLX	C34-C35-C36-C37
52	l	702	PEE	C20-C21-C22-C23
51	l	704	CDL	OB7-CB5-OB6-CB4
51	n	101	CDL	CB5-C51-C52-C53
48	p	201	8Q1	C11-C12-C13-C14
51	V	201	CDL	C71-C72-C73-C74
52	l	701	PEE	C21-C22-C23-C24
47	r	501	PLX	C13-C14-C15-C16
47	r	502	PLX	C14-C15-C16-C17
52	V	202	PEE	C12-C13-C14-C15
52	l	702	PEE	C33-C34-C35-C36
51	l	703	CDL	CB7-C71-C72-C73
51	l	704	CDL	CB7-C71-C72-C73
47	U	101	PLX	C33-C34-C35-C36
51	l	704	CDL	C51-C52-C53-C54
52	V	202	PEE	C40-C41-C42-C43
47	U	101	PLX	C10-C11-C12-C13
47	U	101	PLX	C35-C36-C37-C38
47	b	201	PLX	C16-C17-C18-C19
47	b	201	PLX	C29-C30-C31-C32
47	g	203	PLX	C15-C16-C17-C18
47	r	502	PLX	C11-C12-C13-C14
47	r	502	PLX	C10-C11-C12-C13
48	p	201	8Q1	C6-C7-C8-C9
47	U	101	PLX	C19-C20-C21-C22
47	U	101	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
47	U	101	PLX	C9-C10-C11-C12
47	V	203	PLX	C10-C11-C12-C13
47	b	201	PLX	C27-C28-C29-C30
47	g	202	PLX	C14-C15-C16-C17
48	E	201	8Q1	C12-C13-C14-C15
51	i	401	CDL	C13-C14-C15-C16
52	l	702	PEE	C40-C41-C42-C43
47	B	303	PLX	C9-C10-C11-C12
47	B	303	PLX	C28-C29-C30-C31
47	r	502	PLX	C9-C10-C11-C12
51	l	704	CDL	C32-C33-C34-C35
47	b	201	PLX	C18-C19-C20-C21
47	g	201	PLX	C16-C17-C18-C19
52	V	202	PEE	C14-C15-C16-C17
52	l	702	PEE	C34-C35-C36-C37
51	l	704	CDL	CA7-C31-C32-C33
47	U	101	PLX	C7-C8-C9-C10
47	V	203	PLX	C25-C26-C27-C28
47	g	201	PLX	C10-C11-C12-C13
51	l	703	CDL	C51-C52-C53-C54
52	l	702	PEE	C21-C22-C23-C24
47	b	201	PLX	C25-C26-C27-C28
51	l	703	CDL	C11-C12-C13-C14
47	V	203	PLX	C32-C33-C34-C35
47	g	202	PLX	C9-C10-C11-C12
51	n	101	CDL	C51-C52-C53-C54
51	n	101	CDL	CB7-C71-C72-C73
52	l	701	PEE	C20-C21-C22-C23
47	r	502	PLX	C32-C33-C34-C35
48	E	201	8Q1	N41-C42-C43-S44
47	g	203	PLX	C10-C11-C12-C13
52	V	202	PEE	C34-C35-C36-C37
52	V	202	PEE	O5-C30-O3-C3
47	B	303	PLX	C12-C13-C14-C15
47	g	203	PLX	C17-C18-C19-C20
47	r	502	PLX	C26-C27-C28-C29
52	W	201	PEE	C37-C38-C39-C40
47	g	203	PLX	C7-C8-C9-C10
47	r	502	PLX	C25-C26-C27-C28
51	i	401	CDL	C34-C35-C36-C37
51	i	401	CDL	OA9-CA7-OA8-CA6
47	g	202	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
48	p	201	8Q1	C7-C8-C9-C10
47	B	303	PLX	O7-C6-C7-C8
47	g	203	PLX	O9-C24-C25-C26
47	r	501	PLX	O9-C24-C25-C26
47	r	502	PLX	O7-C6-C7-C8
47	g	203	PLX	C14-C15-C16-C17
47	r	501	PLX	C7-C8-C9-C10
51	i	401	CDL	C11-C12-C13-C14
51	l	703	CDL	C33-C34-C35-C36
46	A	502	FMN	O2'-C2'-C3'-O3'
47	r	501	PLX	C35-C36-C37-C38
51	i	401	CDL	C32-C33-C34-C35
52	V	202	PEE	C43-C44-C45-C46
51	l	703	CDL	OB9-CB7-OB8-CB6
52	l	701	PEE	C13-C14-C15-C16
52	l	701	PEE	C41-C42-C43-C44
51	V	201	CDL	OA7-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-C4'
47	V	203	PLX	C11-C12-C13-C14
48	p	201	8Q1	C12-C13-C14-C15
52	W	201	PEE	C23-C24-C25-C26
51	l	703	CDL	C31-CA7-OA8-CA6
51	V	201	CDL	C11-CA5-OA6-CA4
47	g	201	PLX	C32-C33-C34-C35
47	r	501	PLX	C26-C27-C28-C29
51	V	201	CDL	CB5-C51-C52-C53
51	i	401	CDL	CB5-C51-C52-C53
51	n	101	CDL	C55-C56-C57-C58
52	W	201	PEE	C41-C42-C43-C44
52	l	701	PEE	C15-C16-C17-C18
52	l	702	PEE	C19-C20-C21-C22
47	r	502	PLX	C7-C8-C9-C10
47	r	502	PLX	C36-C37-C38-C39
51	i	401	CDL	C73-C74-C75-C76
52	V	202	PEE	C31-C32-C33-C34
47	r	502	PLX	C20-C21-C22-C23
51	n	101	CDL	C71-C72-C73-C74
52	l	702	PEE	C31-C32-C33-C34
51	i	401	CDL	C71-CB7-OB8-CB6
47	b	201	PLX	C30-C31-C32-C33
47	g	202	PLX	C26-C27-C28-C29
52	W	201	PEE	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
51	i	401	CDL	C51-CB5-OB6-CB4
47	r	502	PLX	C35-C36-C37-C38
51	V	201	CDL	C14-C15-C16-C17
47	B	303	PLX	C29-C30-C31-C32
47	b	201	PLX	C32-C33-C34-C35
47	r	501	PLX	C9-C10-C11-C12
52	V	202	PEE	C19-C20-C21-C22
52	W	201	PEE	C19-C20-C21-C22
47	g	203	PLX	C35-C36-C37-C38
47	b	201	PLX	C11-C12-C13-C14
47	g	202	PLX	C11-C10-C9-C8
51	l	704	CDL	C13-C14-C15-C16
51	l	703	CDL	OA9-CA7-OA8-CA6
47	r	502	PLX	C17-C18-C19-C20
52	l	701	PEE	C23-C24-C25-C26
52	l	701	PEE	C40-C41-C42-C43
52	l	701	PEE	C16-C17-C18-C19
47	g	201	PLX	C2-O1-P1-O4
51	l	703	CDL	CA2-OA2-PA1-OA5
47	B	303	PLX	C15-C16-C17-C18
51	n	101	CDL	C34-C35-C36-C37
51	l	704	CDL	OB5-CB3-CB4-CB6
52	l	701	PEE	O3P-C1-C2-C3
47	r	502	PLX	C15-C16-C17-C18
52	l	702	PEE	C42-C43-C44-C45
47	B	303	PLX	C11-C10-C9-C8
51	l	704	CDL	CB2-C1-CA2-OA2
51	i	401	CDL	OB7-CB5-OB6-CB4
51	V	201	CDL	C12-C13-C14-C15
51	n	101	CDL	C33-C34-C35-C36
52	W	201	PEE	C33-C34-C35-C36
47	r	501	PLX	C3-C4-C5-O8
51	l	703	CDL	CA3-CA4-CA6-OA8
52	V	202	PEE	C41-C42-C43-C44
47	r	501	PLX	C18-C19-C20-C21
52	W	201	PEE	C44-C45-C46-C47
47	g	201	PLX	C26-C27-C28-C29
47	U	101	PLX	O8-C24-C25-C26
52	l	702	PEE	C12-C13-C14-C15
51	i	401	CDL	OB9-CB7-OB8-CB6
48	p	201	8Q1	C13-C14-C15-C16
47	b	201	PLX	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
47	V	203	PLX	C7-C8-C9-C10
52	l	701	PEE	C42-C43-C44-C45
52	l	702	PEE	C44-C45-C46-C47
52	l	701	PEE	C2-C1-O3P-P
51	V	201	CDL	OA5-CA3-CA4-OA6
47	U	101	PLX	C26-C27-C28-C29
52	W	201	PEE	O2-C2-C3-O3
51	l	703	CDL	C75-C76-C77-C78
48	p	201	8Q1	C30-C29-C32-O33
51	i	401	CDL	C52-C51-CB5-OB6
47	V	203	PLX	C16-C17-C18-C19
51	i	401	CDL	C35-C36-C37-C38
51	V	201	CDL	C72-C73-C74-C75
52	W	201	PEE	C34-C35-C36-C37
47	U	101	PLX	C11-C10-C9-C8
47	V	203	PLX	C12-C13-C14-C15
47	g	201	PLX	C17-C18-C19-C20
47	g	201	PLX	C27-C28-C29-C30
51	l	703	CDL	OB5-CB3-CB4-CB6
52	W	201	PEE	O3P-C1-C2-C3
47	V	203	PLX	C31-C32-C33-C34
47	r	501	PLX	C25-C26-C27-C28
51	V	201	CDL	C52-C53-C54-C55
47	B	303	PLX	C30-C31-C32-C33
47	U	101	PLX	C28-C29-C30-C31
47	b	201	PLX	C13-C14-C15-C16
52	l	702	PEE	C11-C10-O2-C2
47	b	201	PLX	C11-C10-C9-C8
47	U	101	PLX	C27-C28-C29-C30
47	b	201	PLX	C36-C37-C38-C39
47	g	201	PLX	C3-C4-C5-O8
51	V	201	CDL	CB3-CB4-CB6-OB8
51	i	401	CDL	CA3-CA4-CA6-OA8
52	W	201	PEE	C1-C2-C3-O3
47	r	502	PLX	C27-C28-C29-C30
48	p	201	8Q1	C10-C11-C12-C13
48	E	201	8Q1	C7-C8-C9-C10
47	r	501	PLX	C28-C29-C30-C31
52	W	201	PEE	C13-C14-C15-C16
51	V	201	CDL	C53-C54-C55-C56
47	b	201	PLX	C5-C4-O6-C6
47	g	202	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
47	r	501	PLX	O7-C6-C7-C8
47	b	201	PLX	C35-C36-C37-C38
51	l	704	CDL	OA5-CA3-CA4-OA6
47	V	203	PLX	C26-C27-C28-C29
51	l	703	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	C12-C11-CA5-OA6
47	g	201	PLX	C20-C21-C22-C23
47	g	203	PLX	C4-C3-O4-P1
47	r	501	PLX	C4-C3-O4-P1
51	l	704	CDL	C73-C74-C75-C76
47	r	501	PLX	C19-C20-C21-C22
51	l	703	CDL	C15-C16-C17-C18
51	n	101	CDL	CA5-C11-C12-C13
52	W	201	PEE	O4-C10-O2-C2
52	W	201	PEE	C11-C10-O2-C2
47	B	303	PLX	C11-C12-C13-C14
52	l	702	PEE	O4-C10-O2-C2
47	B	303	PLX	C32-C33-C34-C35
52	l	701	PEE	C31-C32-C33-C34
51	V	201	CDL	C75-C76-C77-C78
47	r	501	PLX	C30-C31-C32-C33
47	g	202	PLX	C30-C31-C32-C33
47	g	202	PLX	O4-C3-C4-O6
51	V	201	CDL	OB5-CB3-CB4-OB6
51	l	703	CDL	OA5-CA3-CA4-OA6
52	V	202	PEE	C33-C34-C35-C36
52	V	202	PEE	C32-C33-C34-C35
47	b	201	PLX	O6-C4-C5-O8
47	r	501	PLX	O6-C4-C5-O8
51	V	201	CDL	OA6-CA4-CA6-OA8
51	V	201	CDL	OB6-CB4-CB6-OB8
48	E	201	8Q1	C6-C7-C8-C9
49	J	401	NDP	C5B-O5B-PA-O3
49	J	401	NDP	C5D-O5D-PN-O3
51	l	704	CDL	C12-C13-C14-C15
47	r	502	PLX	C24-C25-C26-C27
47	r	502	PLX	C34-C35-C36-C37
47	g	201	PLX	C35-C36-C37-C38
52	l	701	PEE	C24-C25-C26-C27
52	l	702	PEE	C11-C12-C13-C14
51	n	101	CDL	C35-C36-C37-C38
51	n	101	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
51	l	704	CDL	CB2-OB2-PB2-OB5
47	r	501	PLX	C31-C32-C33-C34
52	W	201	PEE	C31-C32-C33-C34
47	r	502	PLX	C4-C3-O4-P1
51	l	704	CDL	CA4-CA3-OA5-PA1
47	b	201	PLX	C3-O4-P1-O2
47	g	201	PLX	C3-O4-P1-O3
47	g	202	PLX	C3-O4-P1-O2
47	g	202	PLX	C3-O4-P1-O3
47	r	502	PLX	C2-O1-P1-O3
49	J	401	NDP	C5B-O5B-PA-O2A
49	J	401	NDP	C5D-O5D-PN-O2N
51	V	201	CDL	CB3-OB5-PB2-OB4
51	i	401	CDL	CB2-OB2-PB2-OB3
51	l	703	CDL	CA2-OA2-PA1-OA4
51	l	703	CDL	CB3-OB5-PB2-OB4
51	l	704	CDL	CA3-OA5-PA1-OA3
51	n	101	CDL	CA3-OA5-PA1-OA3
52	V	202	PEE	C1-O3P-P-O1P
47	g	202	PLX	O4-C3-C4-C5
51	V	201	CDL	OA5-CA3-CA4-CA6
51	V	201	CDL	OB5-CB3-CB4-CB6
51	l	703	CDL	OA5-CA3-CA4-CA6
51	l	704	CDL	OA5-CA3-CA4-CA6
47	r	501	PLX	C15-C16-C17-C18
47	U	101	PLX	C25-C24-O8-C5
47	b	201	PLX	C1-C2-O1-P1
47	g	203	PLX	C1-C2-O1-P1
47	r	501	PLX	C25-C24-O8-C5
52	W	201	PEE	C10-C11-C12-C13
47	V	203	PLX	C19-C20-C21-C22
47	g	203	PLX	C19-C20-C21-C22
51	V	201	CDL	C74-C75-C76-C77
51	l	704	CDL	OB5-CB3-CB4-OB6
52	l	701	PEE	O3P-C1-C2-O2
47	V	203	PLX	C14-C15-C16-C17
47	g	203	PLX	C3-C4-C5-O8
47	r	502	PLX	C3-C4-C5-O8
47	g	203	PLX	O6-C4-C5-O8
47	r	502	PLX	O6-C4-C5-O8
51	l	704	CDL	OA6-CA4-CA6-OA8
47	g	201	PLX	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
47	r	502	PLX	O8-C24-C25-C26
48	E	201	8Q1	O33-C32-C34-O35
47	g	202	PLX	O7-C6-C7-C8
51	l	704	CDL	C15-C16-C17-C18
47	B	303	PLX	C20-C21-C22-C23
47	U	101	PLX	C36-C37-C38-C39
49	J	401	NDP	O4D-C1D-N1N-C6N
47	r	502	PLX	C11-C10-C9-C8
51	n	101	CDL	C73-C74-C75-C76
47	g	201	PLX	C14-C15-C16-C17
51	V	201	CDL	CA3-CA4-OA6-CA5
51	l	703	CDL	CB6-CB4-OB6-CB5
51	l	704	CDL	CA6-CA4-OA6-CA5
52	l	701	PEE	C3-C2-O2-C10
52	l	702	PEE	C3-C2-O2-C10
51	V	201	CDL	CB7-C71-C72-C73
51	i	401	CDL	C32-C31-CA7-OA8
51	V	201	CDL	C55-C56-C57-C58
51	n	101	CDL	C53-C54-C55-C56
51	l	703	CDL	CA7-C31-C32-C33
52	V	202	PEE	C11-C10-O2-C2
51	n	101	CDL	C15-C16-C17-C18
47	U	101	PLX	C2-O1-P1-O4
47	V	203	PLX	C3-O4-P1-O1
47	g	203	PLX	C3-O4-P1-O1
51	V	201	CDL	CB2-OB2-PB2-OB5
51	l	703	CDL	CB2-OB2-PB2-OB5
52	V	202	PEE	C4-O4P-P-O3P
52	l	701	PEE	C1-O3P-P-O4P
52	l	702	PEE	C4-O4P-P-O3P
49	J	401	NDP	C2D-C1D-N1N-C6N
47	V	203	PLX	C29-C30-C31-C32
47	V	203	PLX	C3-C4-C5-O8
47	b	201	PLX	C28-C29-C30-C31
47	r	501	PLX	C11-C10-C9-C8
51	l	703	CDL	C34-C35-C36-C37
51	l	704	CDL	C1-CB2-OB2-PB2
52	V	202	PEE	C23-C24-C25-C26
52	V	202	PEE	O4-C10-O2-C2
52	V	202	PEE	C35-C36-C37-C38
52	l	702	PEE	C23-C24-C25-C26
52	l	701	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
47	g	202	PLX	C15-C16-C17-C18
47	g	201	PLX	C19-C20-C21-C22
47	V	203	PLX	O6-C6-C7-C8
47	g	201	PLX	O6-C6-C7-C8
51	i	401	CDL	C1-CB2-OB2-PB2
51	i	401	CDL	CB4-CB3-OB5-PB2
51	l	703	CDL	CA4-CA3-OA5-PA1
52	W	201	PEE	C11-C12-C13-C14
47	B	303	PLX	C6-C7-C8-C9
47	V	203	PLX	C6-C7-C8-C9
51	l	703	CDL	CB5-C51-C52-C53
47	g	201	PLX	C25-C26-C27-C28
48	E	201	8Q1	O27-C28-C29-C30
48	p	201	8Q1	O27-C28-C29-C31
51	V	201	CDL	C11-C12-C13-C14
47	g	203	PLX	C3-C4-O6-C6
47	r	501	PLX	C5-C4-O6-C6
52	V	202	PEE	C21-C22-C23-C24
47	V	203	PLX	C33-C34-C35-C36
51	i	401	CDL	C72-C71-CB7-OB8
48	p	201	8Q1	C42-C43-S44-C1
47	g	201	PLX	O6-C4-C5-O8
47	B	303	PLX	C7-C8-C9-C10
51	i	401	CDL	C52-C51-CB5-OB7
51	V	201	CDL	C73-C74-C75-C76
51	l	704	CDL	CA3-CA4-CA6-OA8
47	g	202	PLX	C16-C17-C18-C19
47	r	502	PLX	C28-C29-C30-C31
47	g	201	PLX	O4-C3-C4-O6
47	V	203	PLX	C24-C25-C26-C27
48	E	201	8Q1	O33-C32-C34-N36
51	l	704	CDL	C32-C31-CA7-OA8
52	W	201	PEE	C35-C36-C37-C38
51	l	703	CDL	C32-C31-CA7-OA8
52	W	201	PEE	C1-C2-O2-C10
47	g	202	PLX	C27-C28-C29-C30
47	B	303	PLX	C14-C15-C16-C17
47	V	203	PLX	C35-C36-C37-C38
52	V	202	PEE	C30-C31-C32-C33
47	b	201	PLX	C3-C4-C5-O8
51	V	201	CDL	CA3-CA4-CA6-OA8
49	J	401	NDP	O4D-C4D-C5D-O5D

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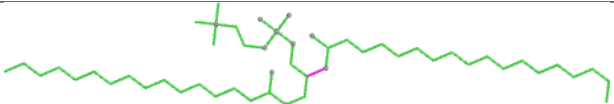
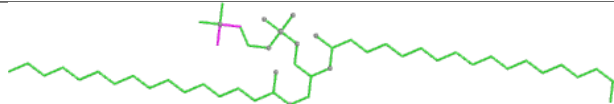
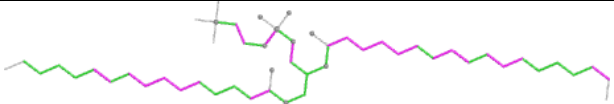
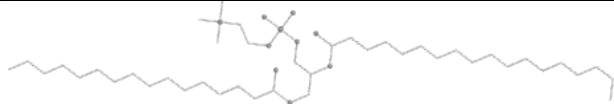
Mol	Chain	Res	Type	Atoms
47	r	502	PLX	C33-C34-C35-C36
49	J	401	NDP	O4D-C1D-N1N-C2N
51	l	704	CDL	C35-C36-C37-C38
47	B	303	PLX	O9-C24-C25-C26
52	l	701	PEE	C38-C39-C40-C41
52	l	702	PEE	C18-C19-C20-C21
51	l	703	CDL	C32-C31-CA7-OA9
51	l	703	CDL	C32-C33-C34-C35
52	l	702	PEE	C1-C2-C3-O3
47	b	201	PLX	C24-C25-C26-C27
52	l	702	PEE	C22-C23-C24-C25
47	B	303	PLX	C4-C3-O4-P1
47	V	203	PLX	C17-C18-C19-C20
47	V	203	PLX	C3-O4-P1-O2
47	g	201	PLX	C3-O4-P1-O2
51	l	703	CDL	CA3-OA5-PA1-OA3
51	l	704	CDL	CB3-OB5-PB2-OB3
51	n	101	CDL	CB3-OB5-PB2-OB3
52	l	702	PEE	C4-O4P-P-O1P
51	V	201	CDL	C12-C11-CA5-OA7
51	l	704	CDL	C32-C31-CA7-OA9
52	l	701	PEE	C33-C34-C35-C36
47	r	501	PLX	C14-C15-C16-C17
47	b	201	PLX	C25-C24-O8-C5
47	g	202	PLX	C25-C24-O8-C5
52	W	201	PEE	C5-C4-O4P-P
49	J	401	NDP	C2D-C1D-N1N-C2N
52	V	202	PEE	C39-C40-C41-C42
52	l	702	PEE	C41-C42-C43-C44
52	l	702	PEE	C32-C33-C34-C35
51	l	704	CDL	C52-C51-CB5-OB6
51	l	704	CDL	C74-C75-C76-C77
47	g	202	PLX	C6-C7-C8-C9
47	g	202	PLX	C24-C25-C26-C27
52	l	701	PEE	C11-C12-C13-C14
46	A	502	FMN	N10-C1'-C2'-O2'
47	V	203	PLX	C15-C16-C17-C18
47	g	203	PLX	C36-C37-C38-C39
52	W	201	PEE	C42-C43-C44-C45
51	l	704	CDL	C52-C51-CB5-OB7
51	V	201	CDL	C52-C51-CB5-OB6

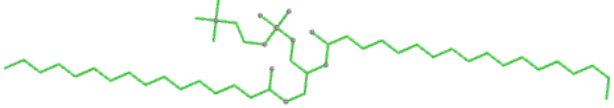
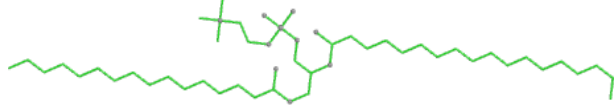
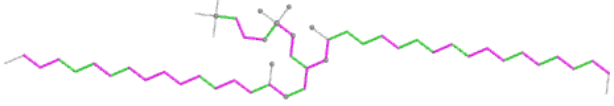
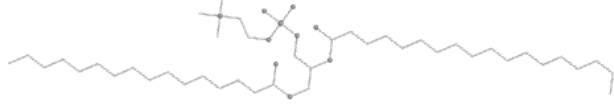
There are no ring outliers.

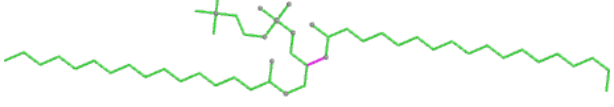
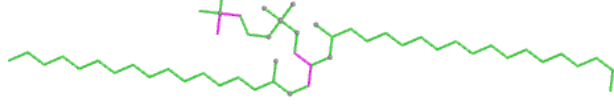
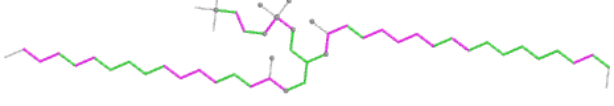
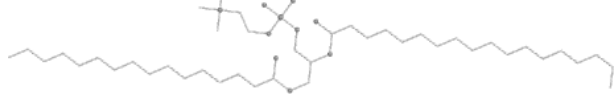
28 monomers are involved in 285 short contacts:

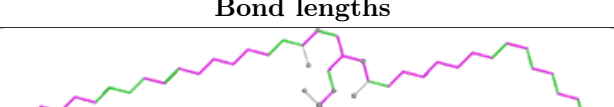
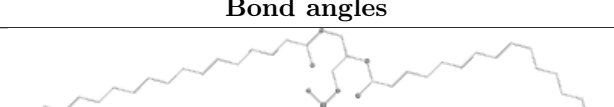
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	B	303	PLX	4	0
45	A	501	SF4	6	0
47	b	201	PLX	38	0
47	U	101	PLX	3	0
52	W	201	PEE	19	0
45	B	301	SF4	1	0
47	r	502	PLX	17	0
48	E	201	8Q1	4	0
51	l	703	CDL	2	0
47	r	501	PLX	6	0
52	l	702	PEE	18	0
49	J	401	NDP	26	0
46	A	502	FMN	16	0
47	g	202	PLX	3	0
45	M	801	SF4	3	0
51	l	704	CDL	2	0
50	M	803	FES	1	0
47	g	201	PLX	2	0
47	g	203	PLX	8	0
51	n	101	CDL	10	0
51	i	401	CDL	3	0
52	V	202	PEE	21	0
52	l	701	PEE	50	0
47	V	203	PLX	5	0
51	V	201	CDL	8	0
45	B	302	SF4	2	0
48	p	201	8Q1	12	0
50	O	301	FES	2	0

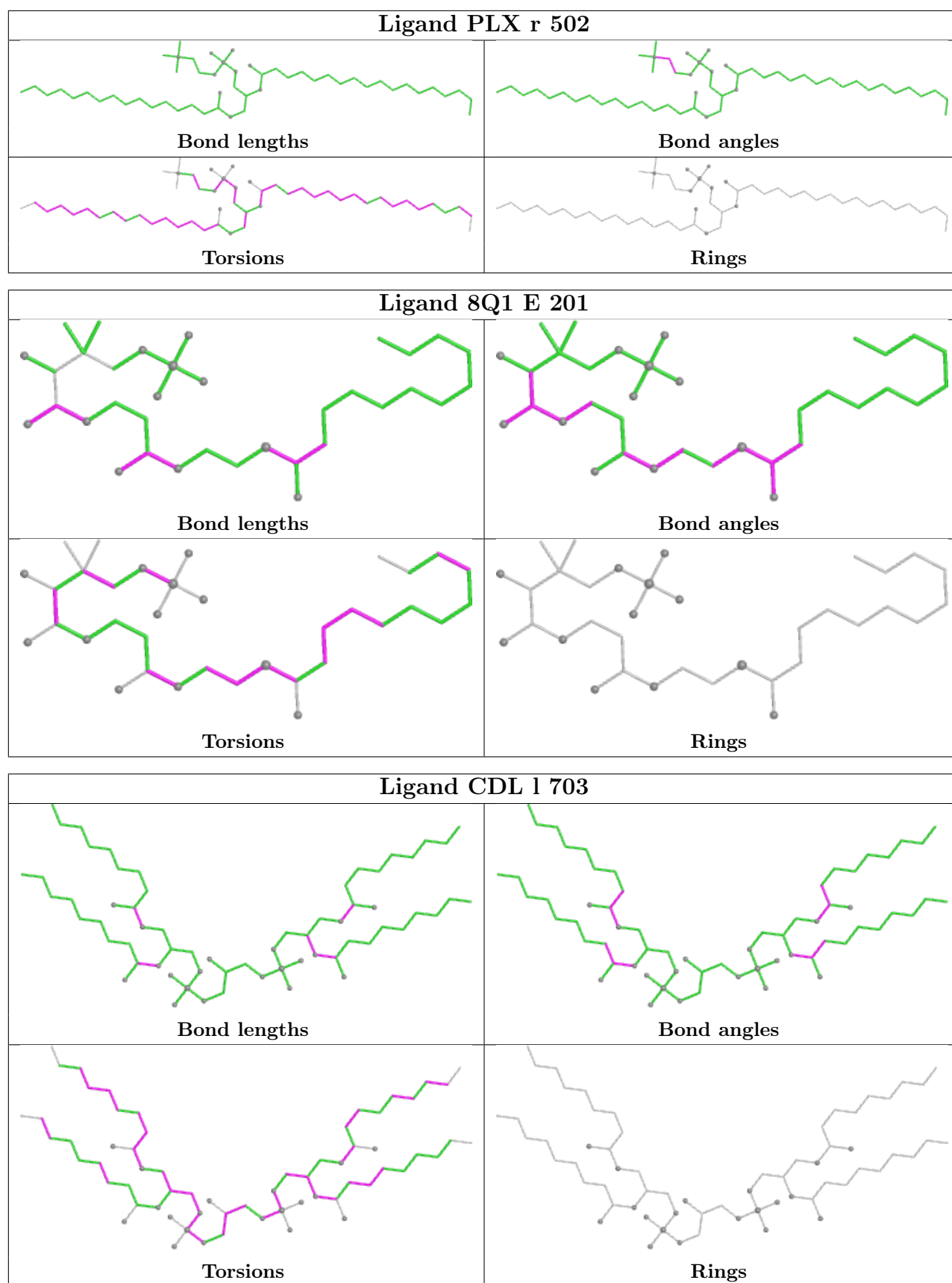
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

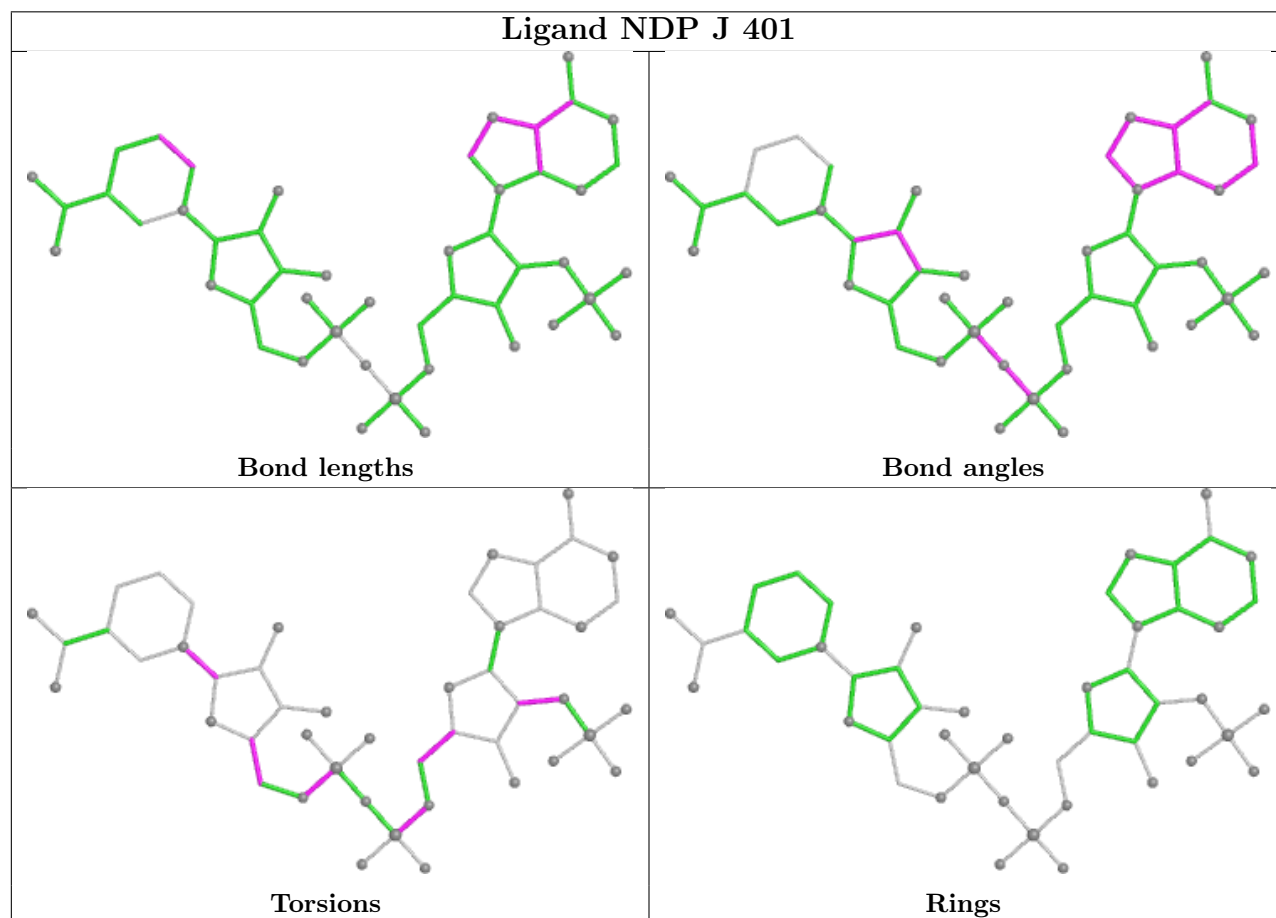
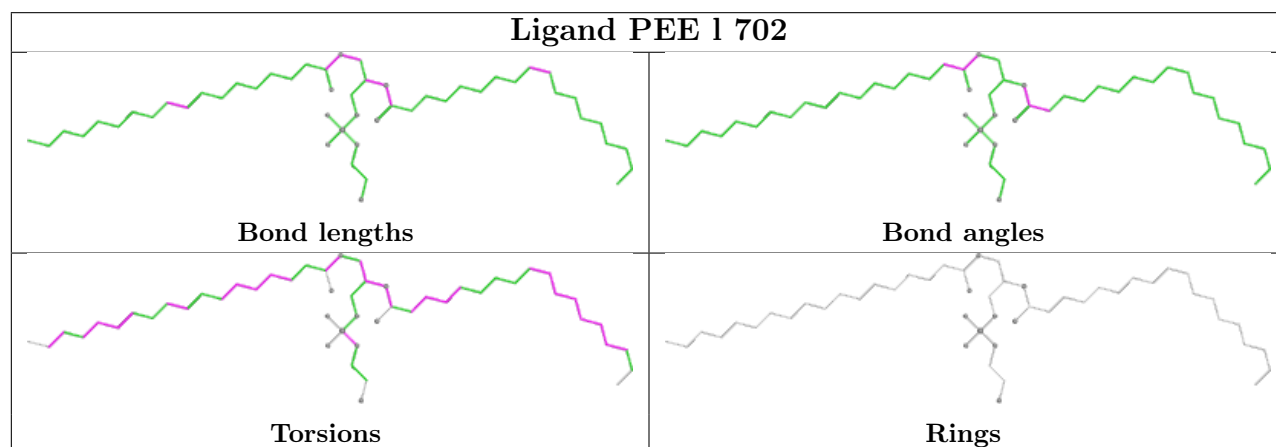
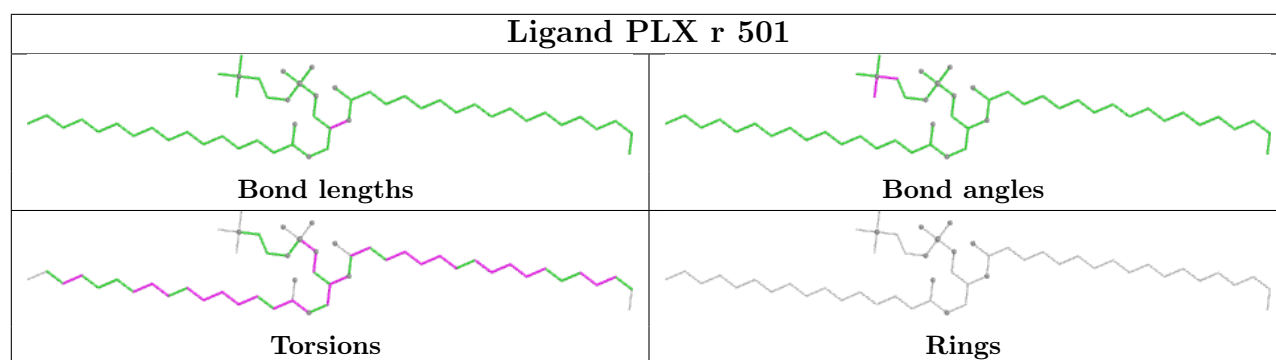
Ligand PLX B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

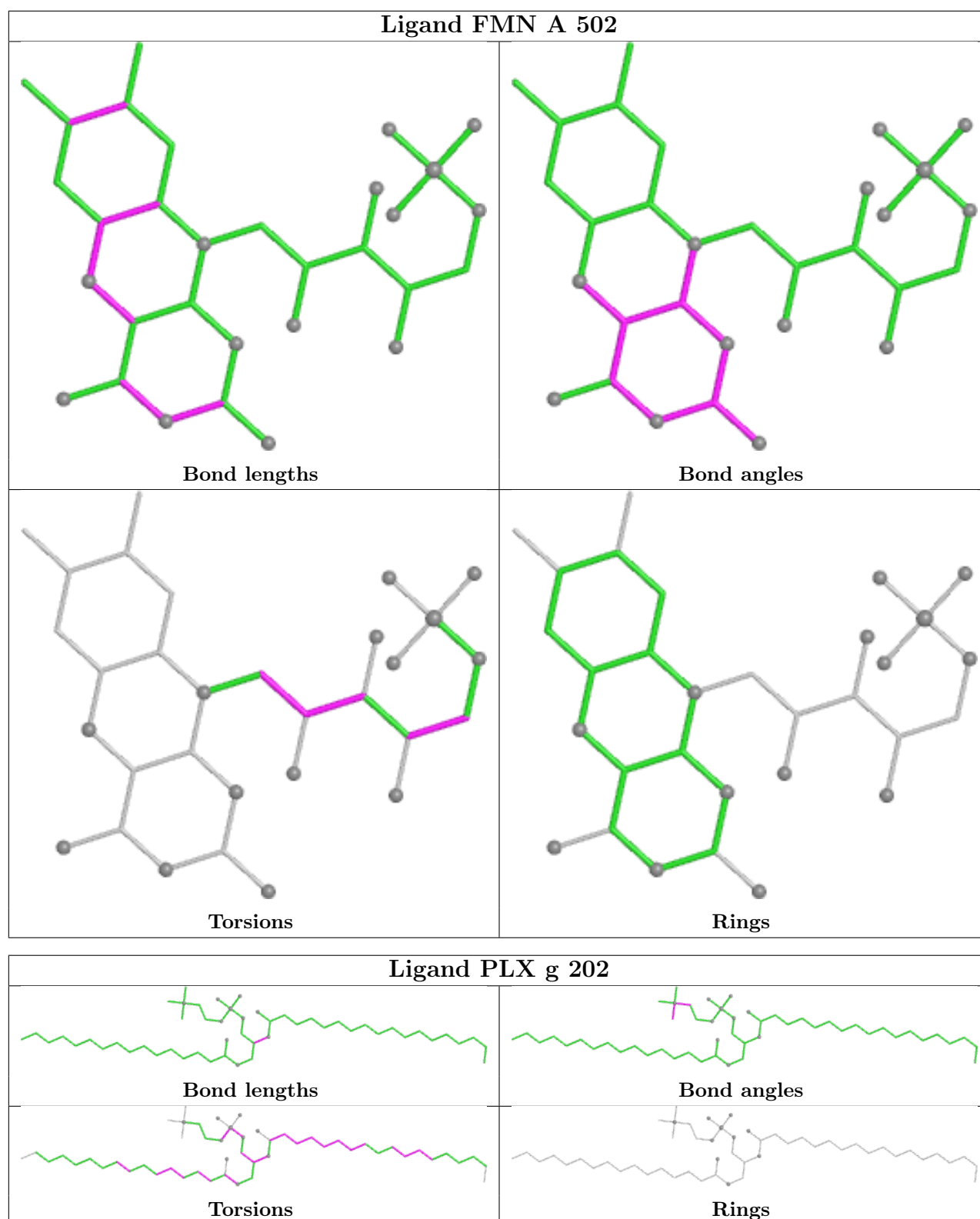
Ligand PLX b 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

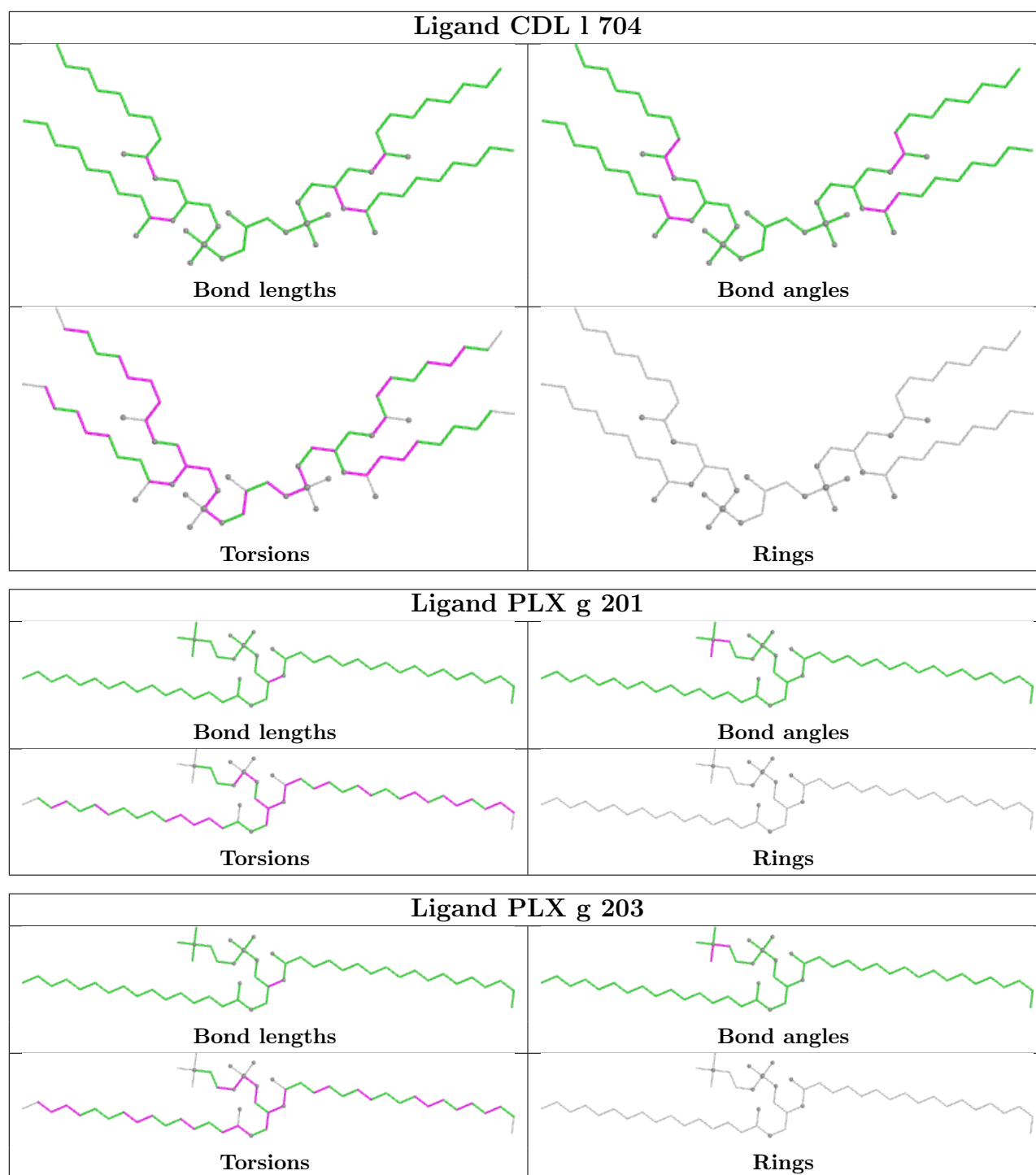
Ligand PLX U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

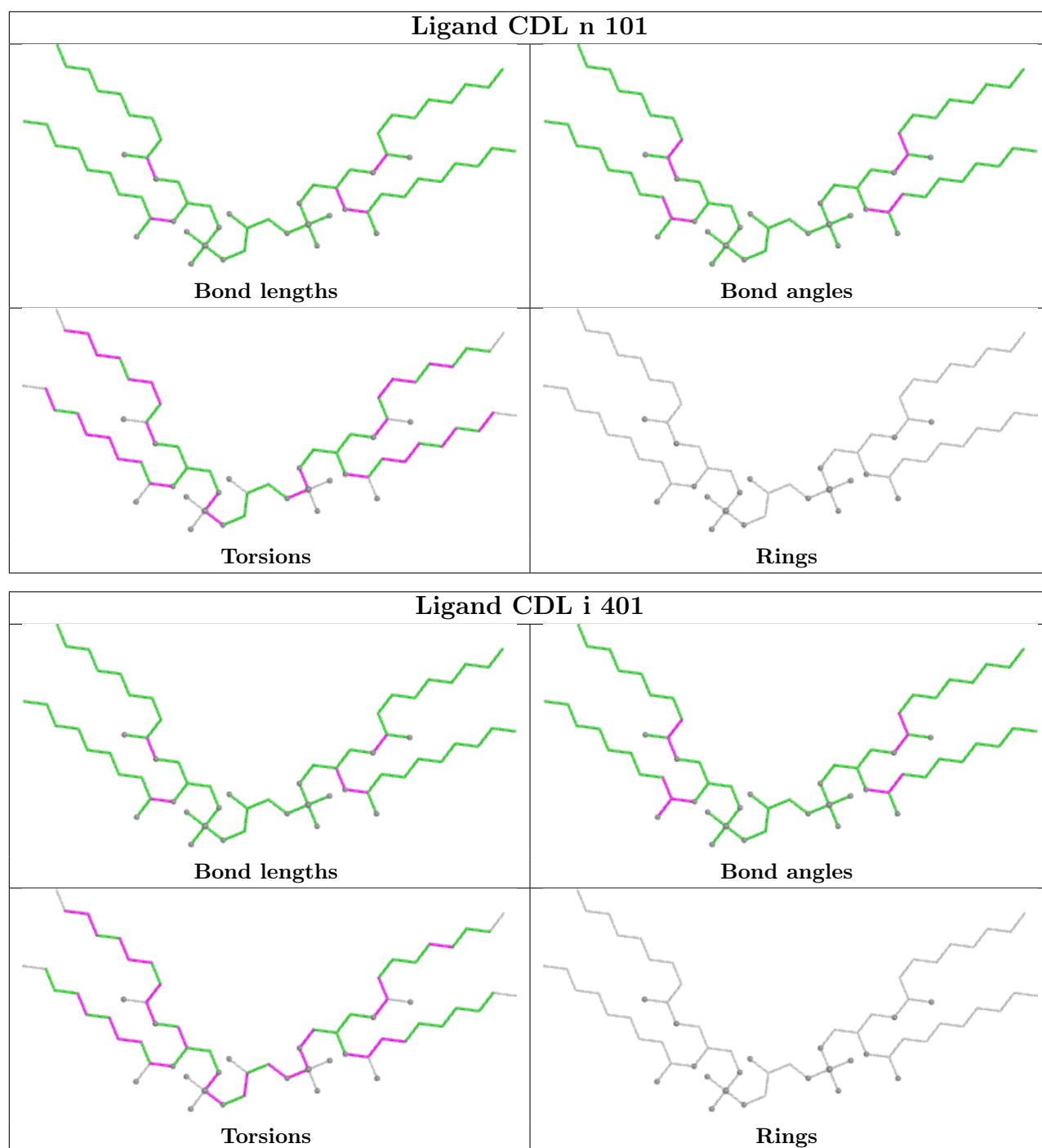
Ligand PEE W 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

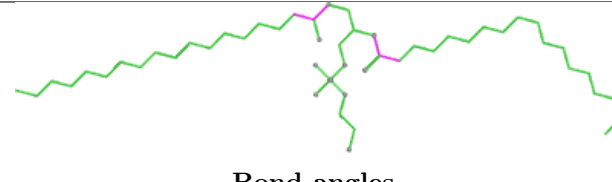
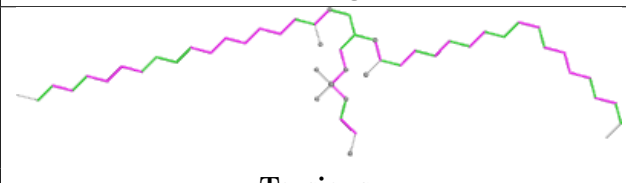
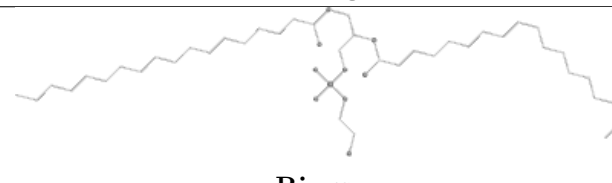


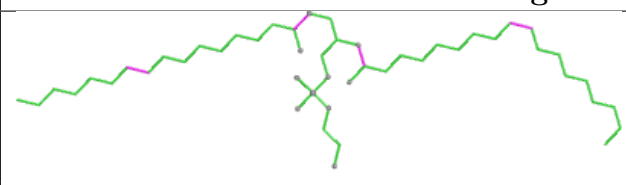
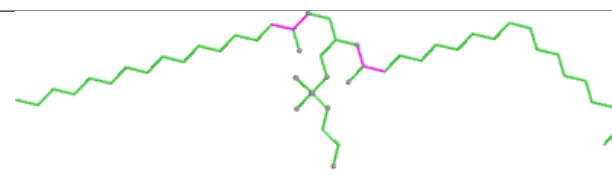
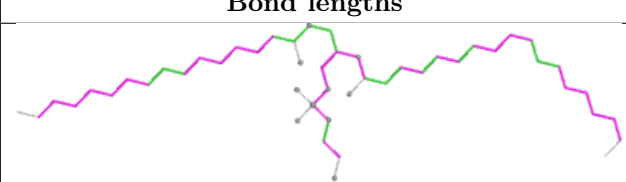
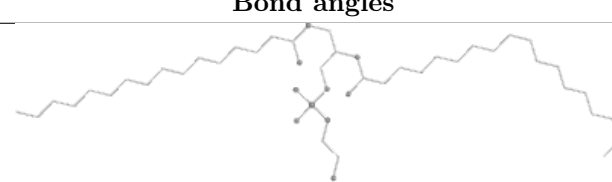


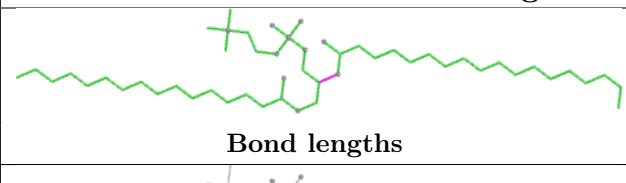
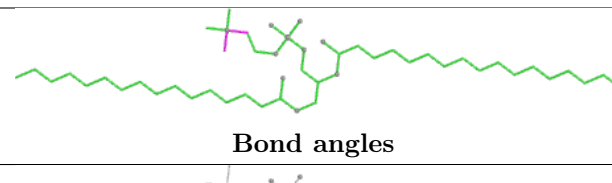
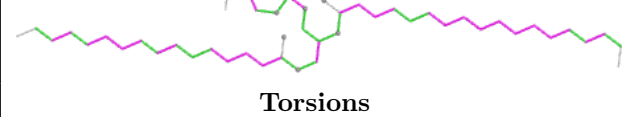


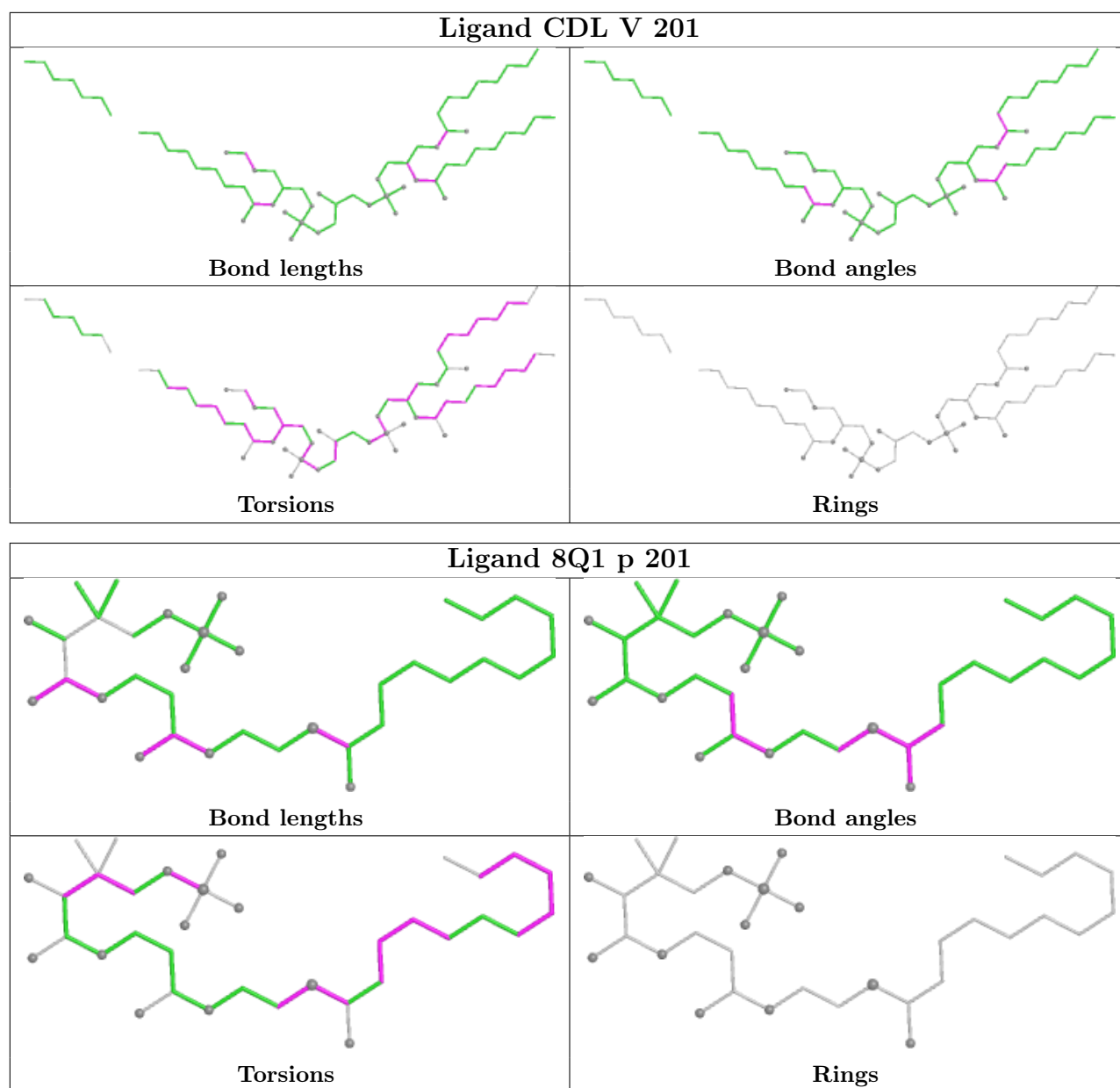




Ligand PEE V 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE I 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX V 203	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

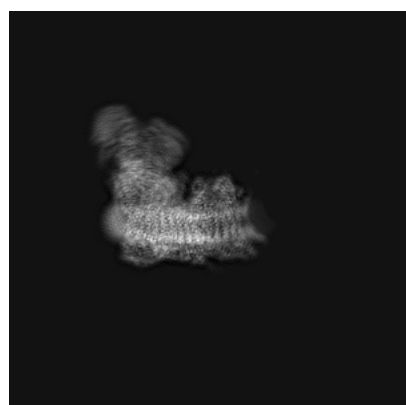
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6773. These allow visual inspection of the internal detail of the map and identification of artifacts.

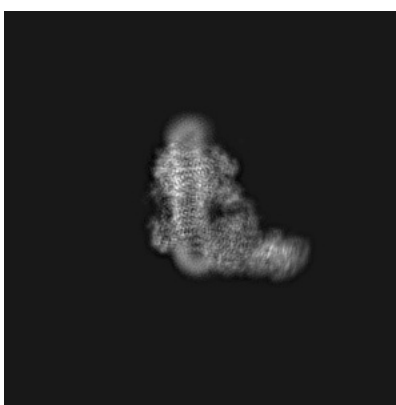
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

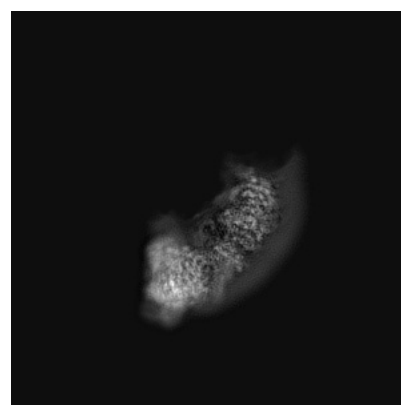
6.1.1 Primary map



X



Y



Z

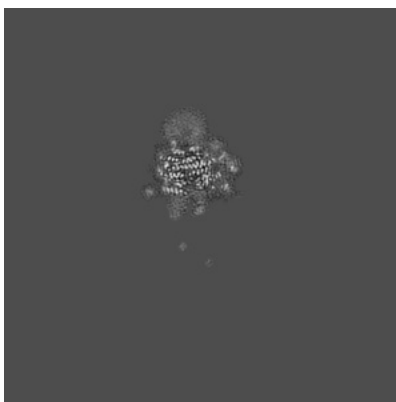
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

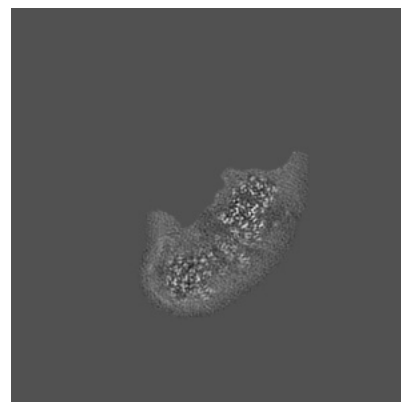
6.2.1 Primary map



X Index: 240



Y Index: 240

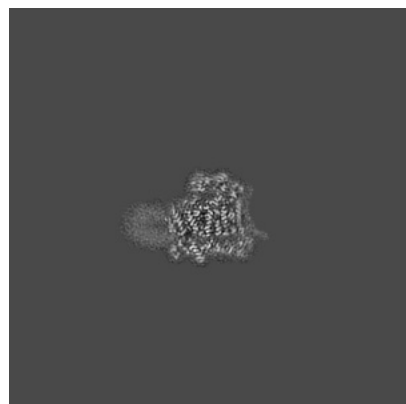


Z Index: 240

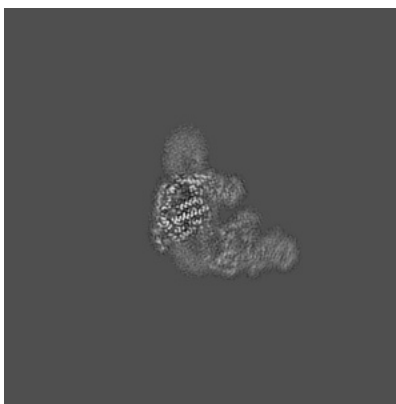
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

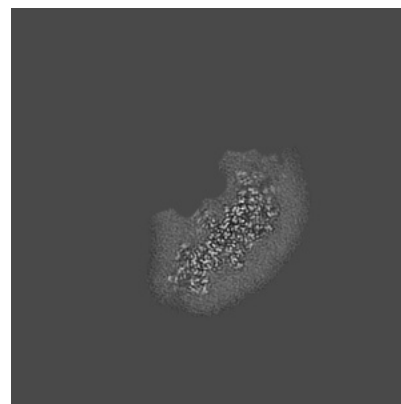
6.3.1 Primary map



X Index: 290



Y Index: 183

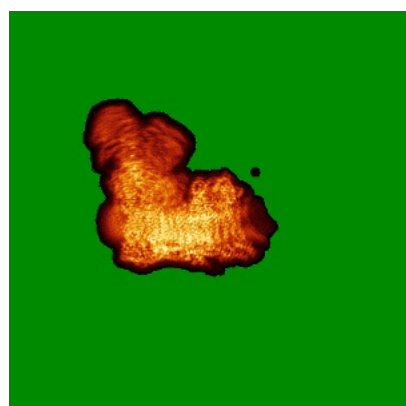


Z Index: 208

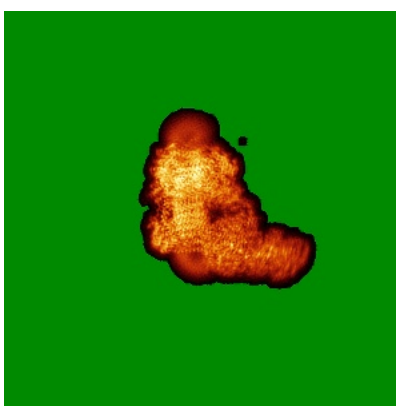
The images above show the largest variance slices of the map in three orthogonal directions.

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

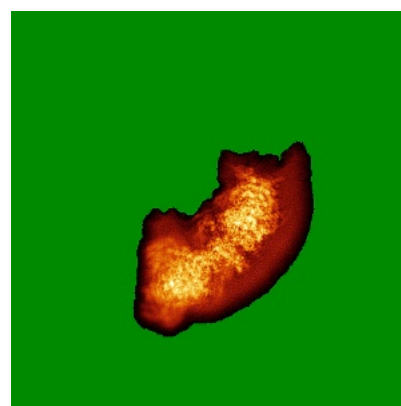
6.4.1 Primary map



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 0.0525. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

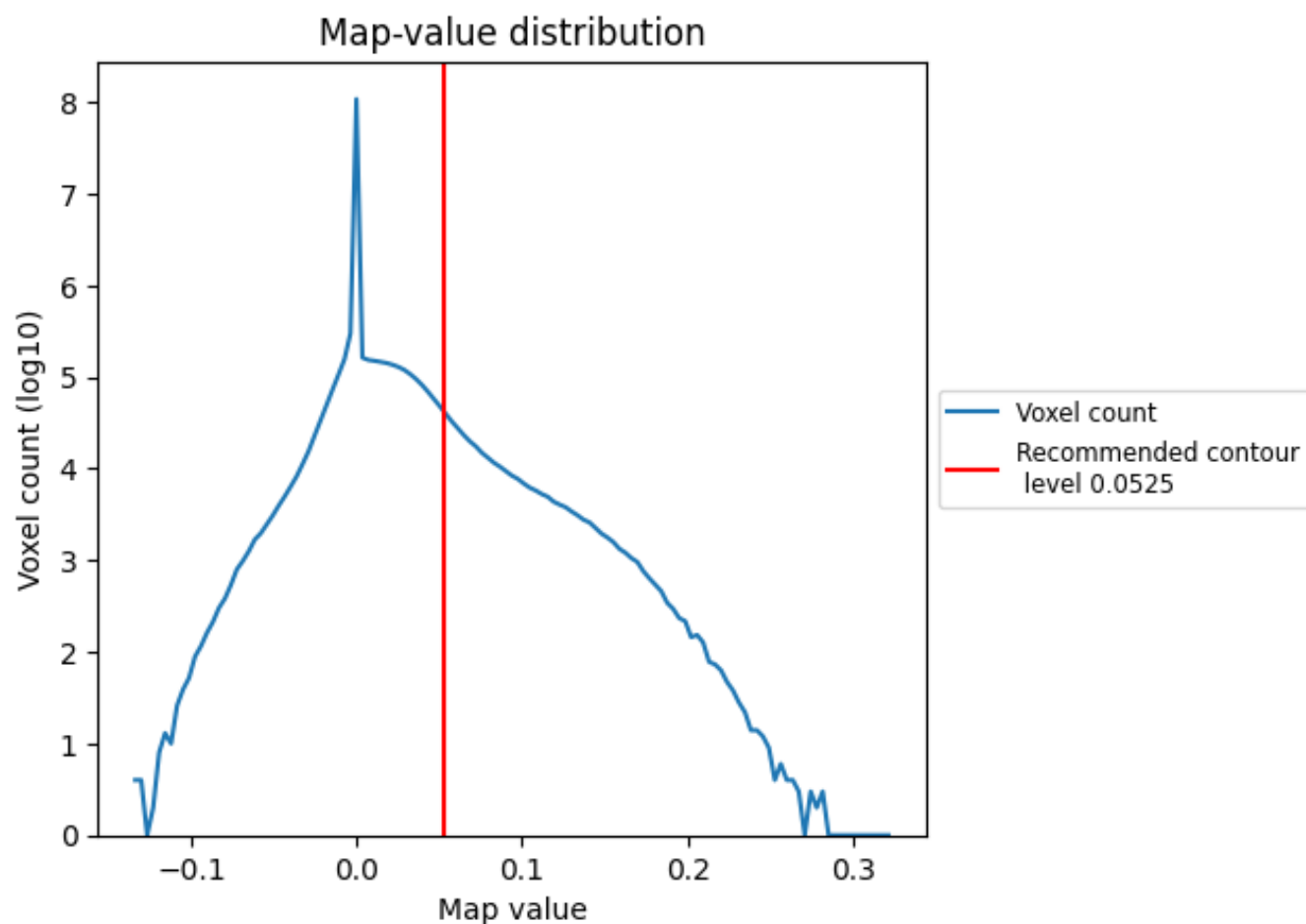
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

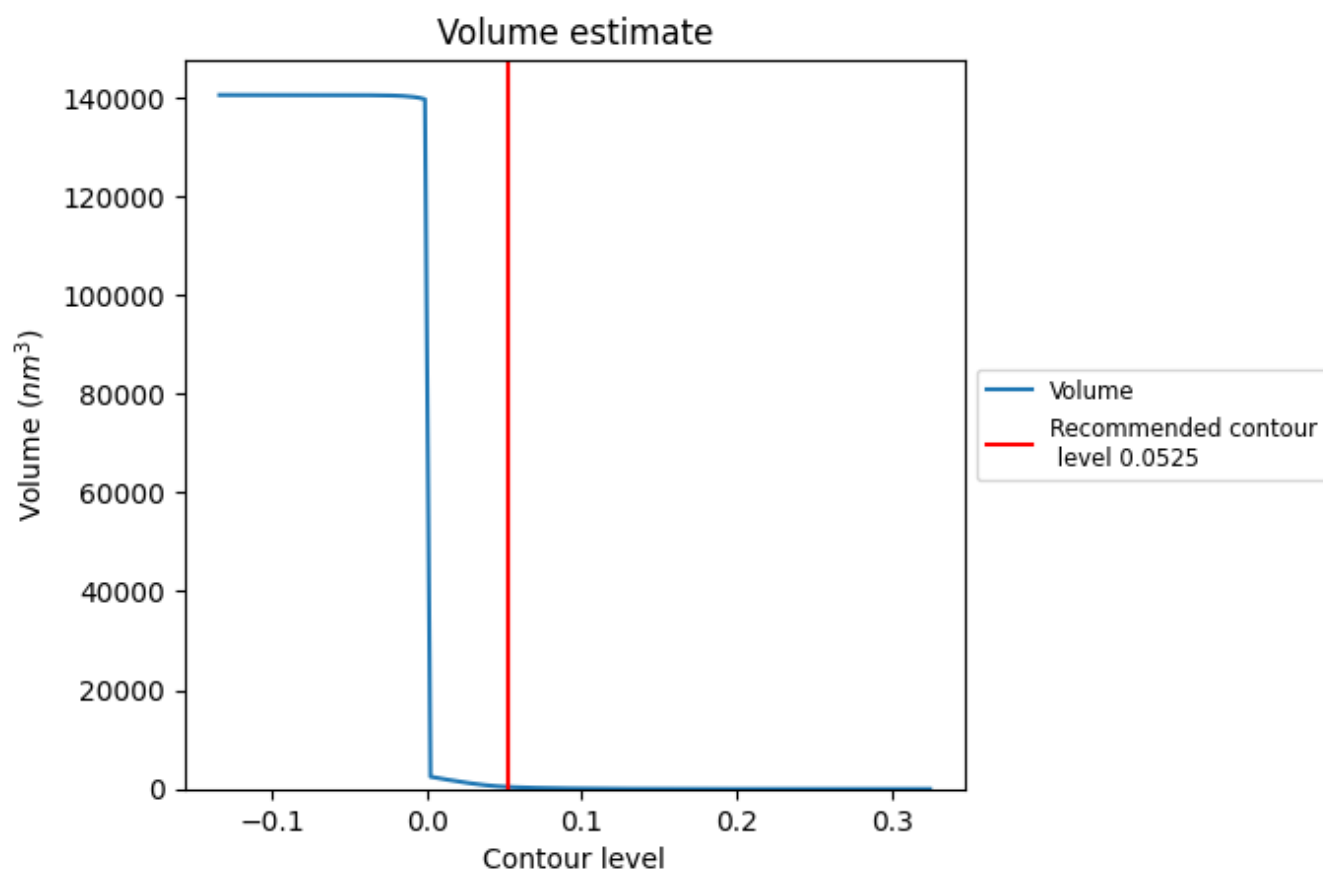
This section contains the results of statistical analysis of the map.

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.

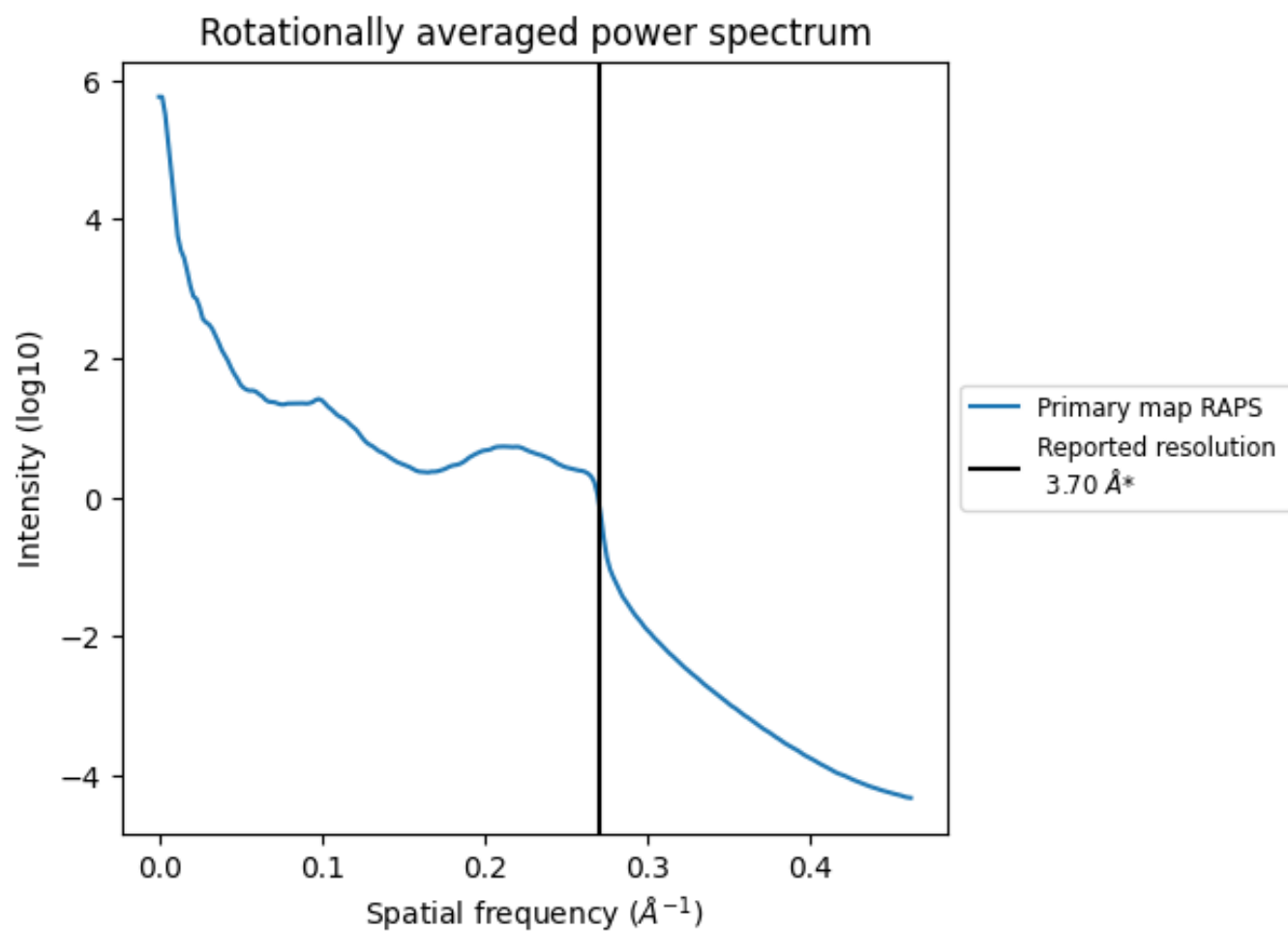
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm^3 ; this corresponds to an approximate mass of 372 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 0.270 Å⁻¹

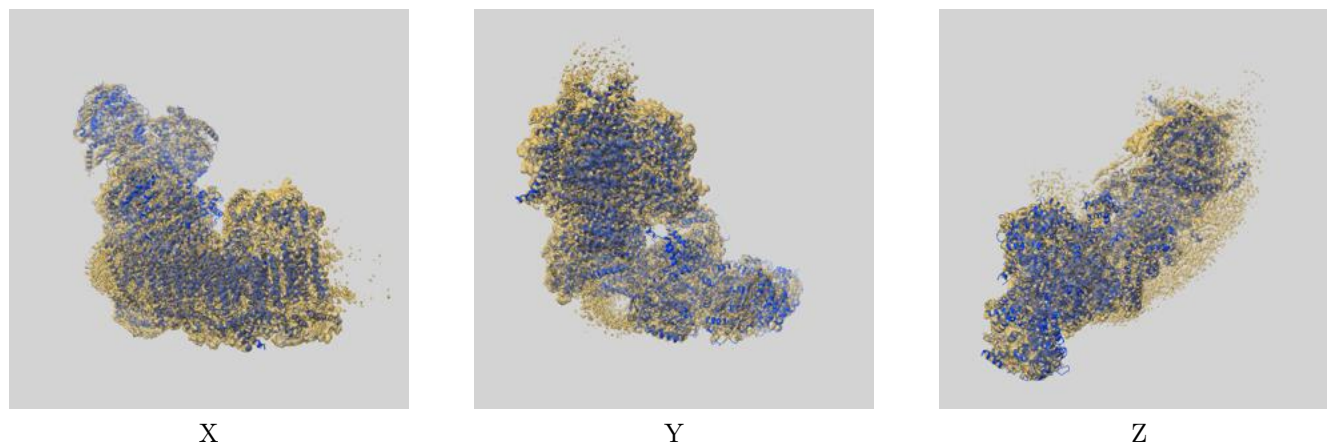
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

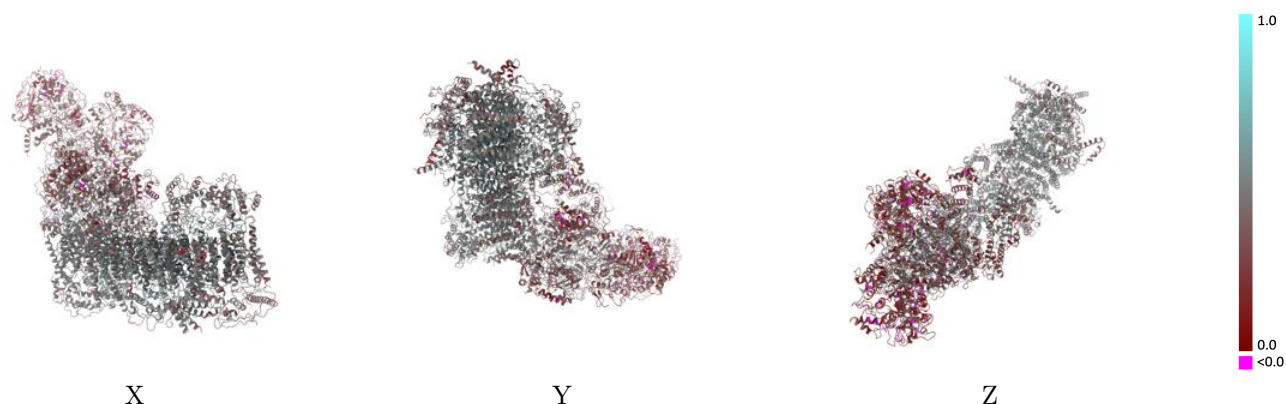
This section contains information regarding the fit between EMDB map EMD-6773 and PDB model 5XTD. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



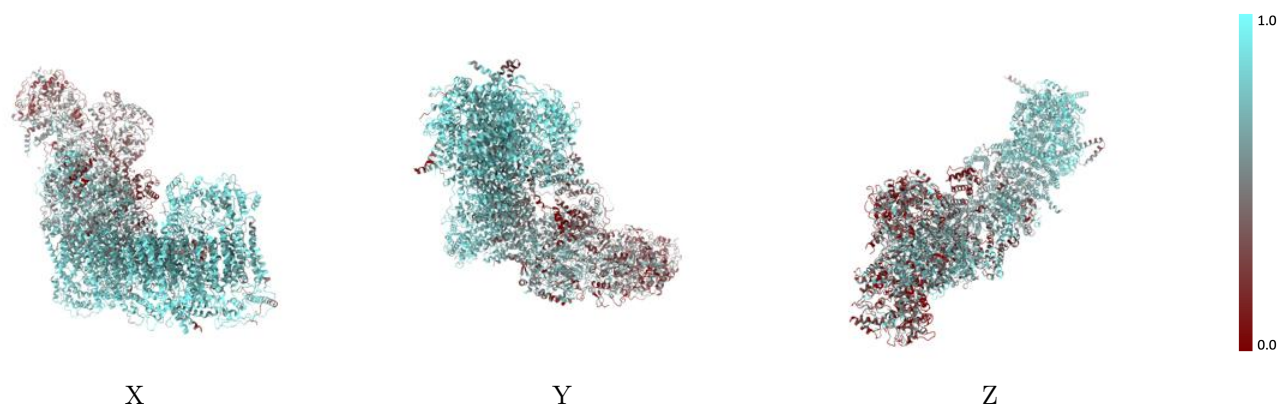
The images above show the 3D surface view of the map at the recommended contour level 0.0525 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



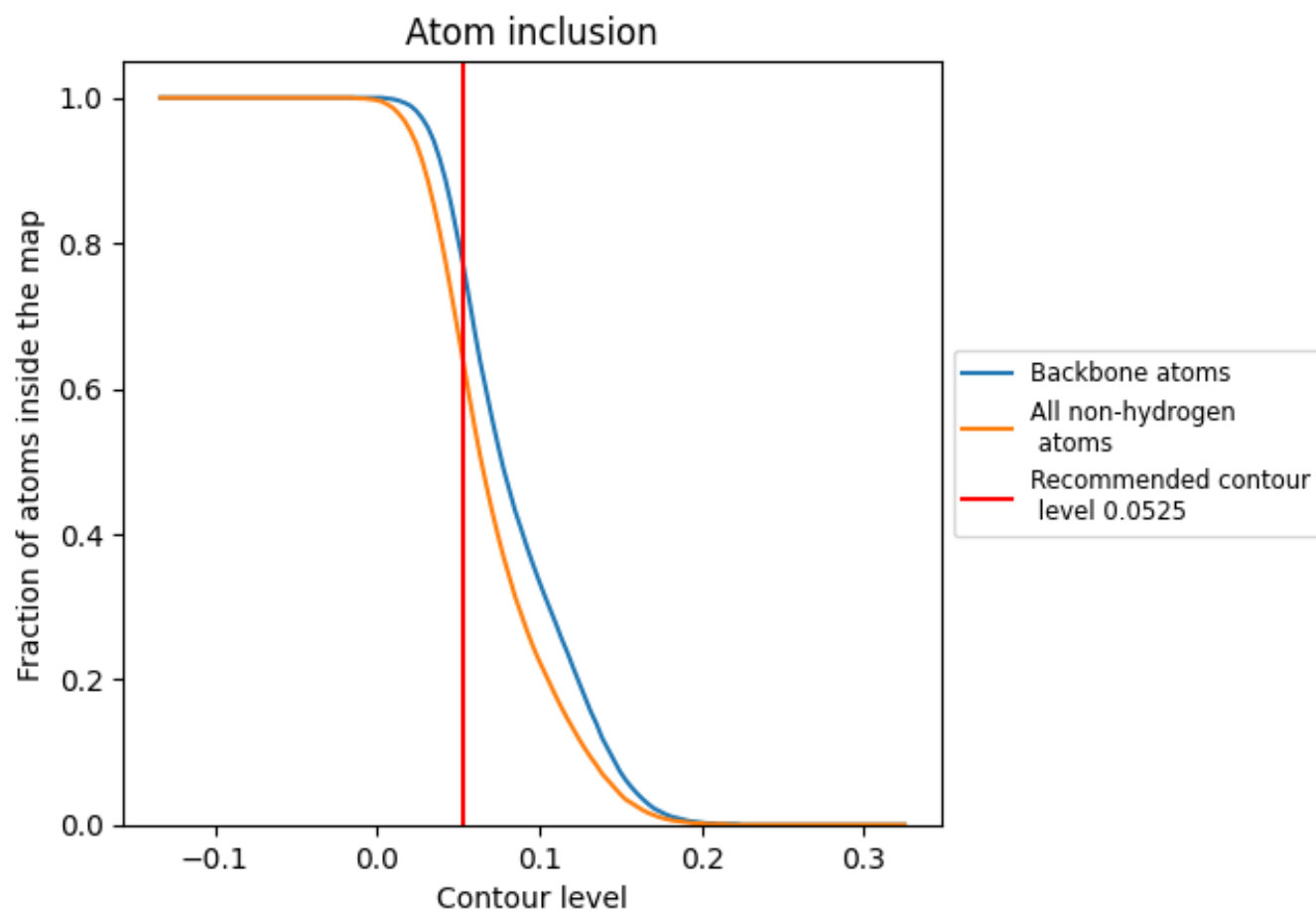
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0525).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.0525) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6410	 0.4010
A	 0.3440	 0.2340
B	 0.7530	 0.4320
C	 0.7910	 0.4590
E	 0.3910	 0.3140
F	 0.3690	 0.2200
G	 0.1290	 0.2310
H	 0.4360	 0.2870
I	 0.4070	 0.3250
J	 0.5260	 0.3290
K	 0.3020	 0.2340
L	 0.3510	 0.2970
M	 0.4030	 0.2840
N	 0.5340	 0.3760
O	 0.3390	 0.2460
P	 0.5330	 0.3350
Q	 0.6230	 0.3820
S	 0.8200	 0.4740
T	 0.4140	 0.3560
U	 0.7870	 0.4510
V	 0.6180	 0.4430
W	 0.8030	 0.4550
X	 0.7880	 0.4390
Y	 0.8360	 0.4350
Z	 0.7600	 0.4170
a	 0.8660	 0.5000
b	 0.7050	 0.3980
c	 0.8320	 0.4840
d	 0.8260	 0.4620
e	 0.7660	 0.4730
f	 0.6670	 0.3950
g	 0.7960	 0.4890
h	 0.8170	 0.4660
i	 0.7810	 0.5020
j	 0.6040	 0.4120



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Chain	Atom inclusion	Q-score
k	 0.7110	 0.4750
l	 0.7560	 0.4770
m	 0.7010	 0.4490
n	 0.7370	 0.4510
o	 0.7890	 0.4710
p	 0.8180	 0.4600
r	 0.8290	 0.5080
s	 0.7680	 0.4730
u	 0.8410	 0.4560
v	 0.7170	 0.3930
w	 0.6340	 0.3910