



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 28, 2017 – 12:41 PM EST

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

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

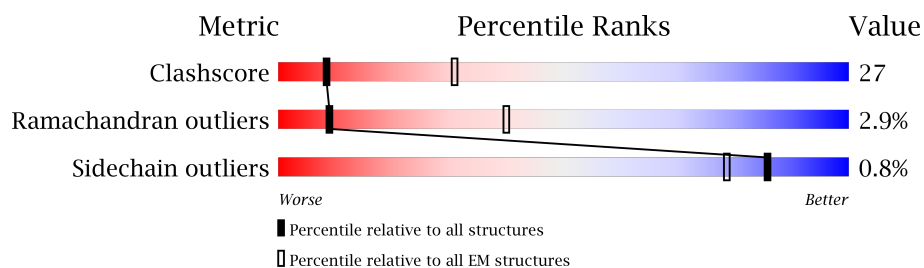
1 Overall quality at a glance

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.






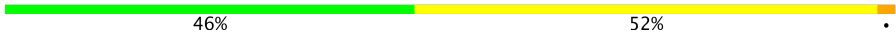

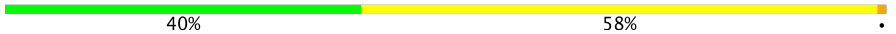
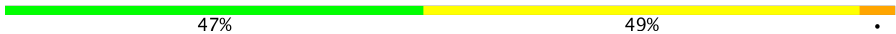






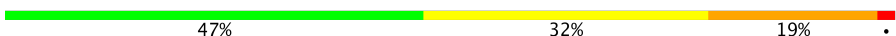

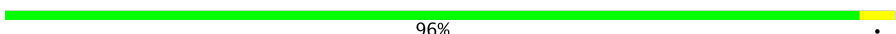

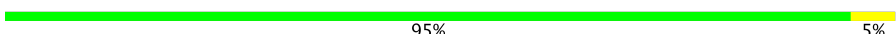
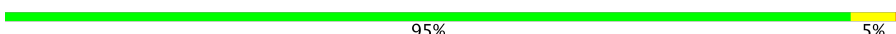
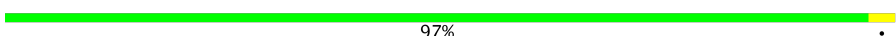
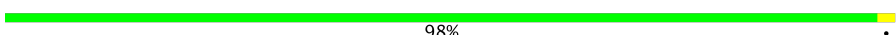
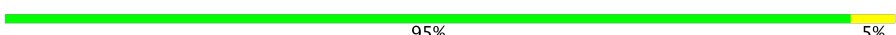
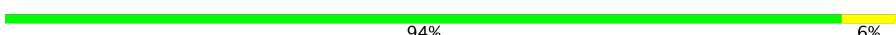
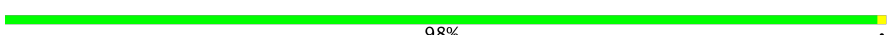

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	113	
5	F	83	
6	G	85	
6	X	85	
7	H	112	
8	I	110	


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Mol	Chain	Length	Quality of chain
9	J	337	 47% 51% .
10	K	33	 45% 45% 9% .
11	L	118	 44% 55% .
12	M	687	 46% 52% .
13	N	143	 59% 39% .
14	O	212	 40% 58% .
15	P	208	 47% 49% .
16	Q	430	 48% 51% .
17	S	70	 73% 26% .
18	T	95	 52% 45% .
19	U	83	 83% 17% .
20	V	140	 66% 33% .
21	W	138	 75% 23% .
22	Y	59	 47% 32% 19% .
23	Z	80	 79% 21% .
24	a	138	 96% .
25	b	128	 87% 9% . .
26	c	153	 95% 5% .
27	d	171	 95% 5% .
28	e	97	 97% .
29	f	47	 98% .
30	g	119	 95% 5% .
31	h	104	 94% 6% .
32	i	347	 98% .
33	j	115	 97% .

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Mol	Chain	Length	Quality of chain
34	k	97	 93% 6% .
35	l	603	 94% 5% .
36	m	174	 94% 6% .
37	n	56	 96% .
38	o	128	 97% .
39	p	172	 98% .
40	r	459	 98% .
41	s	318	 97% .
42	u	169	 97% .
43	v	137	 77% . 19%
44	w	320	 97% .

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	-
49	NDP	J	401	-	-	X	-
50	FES	O	301	-	-	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		

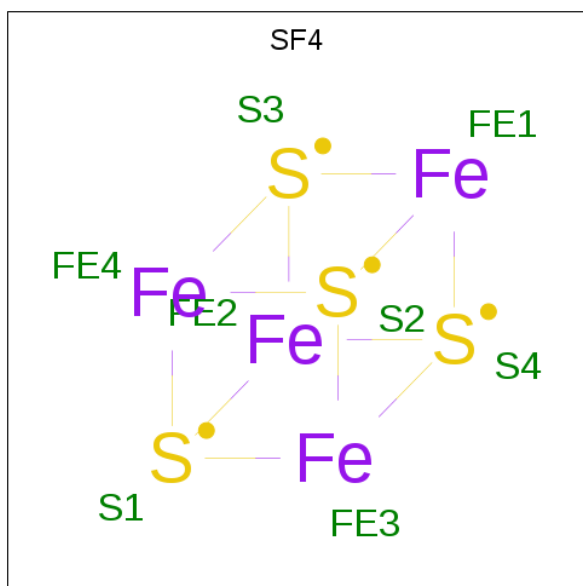
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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.

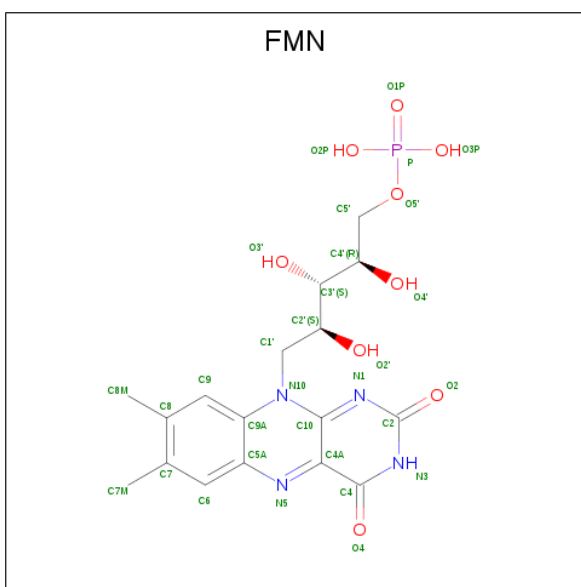
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



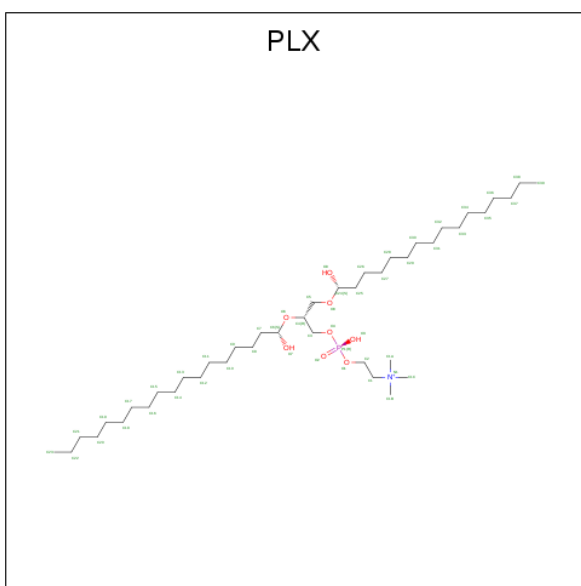
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			16	8	8	
45	B	1	Total	Fe	S	0
			16	8	8	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			16	8	8	
45	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



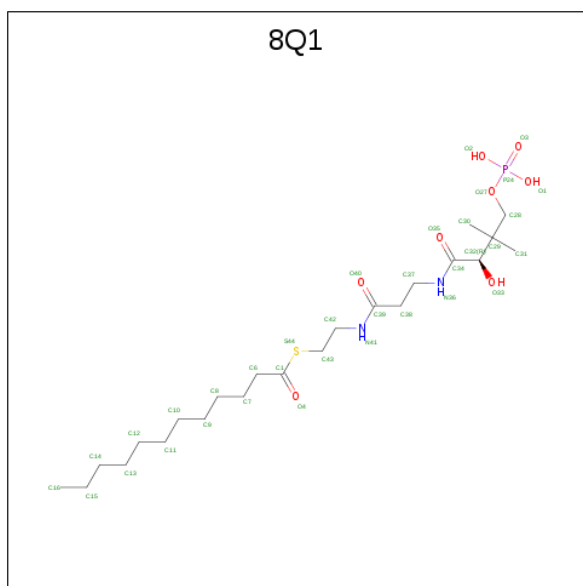
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total 52	C 42	N 1	O 8	P 1	0
47	U	1	Total 52	C 42	N 1	O 8	P 1	0

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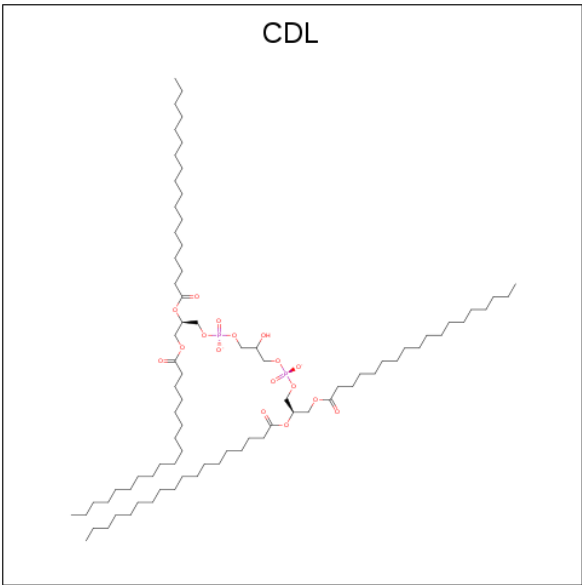
Mol	Chain	Residues	Atoms					AltConf
47	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
47	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
47	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



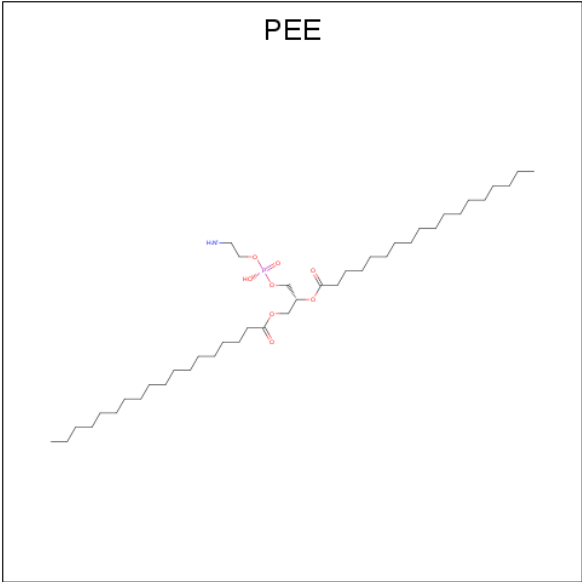
Mol	Chain	Residues	Atoms						AltConf
48	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
48	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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
			128	90	34	4	
51	l	1	Total	C	O	P	0
			128	90	34	4	
51	n	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 52 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).

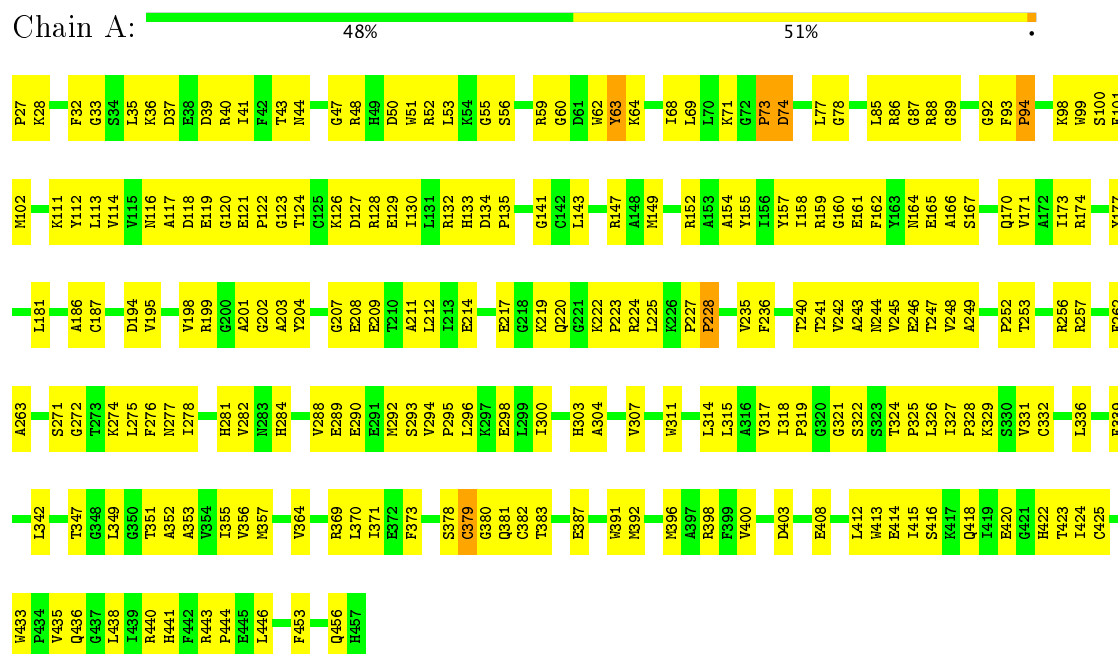


Mol	Chain	Residues	Atoms					AltConf
52	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1	1	Total	C	N	O	P	0
			100	80	2	16	2	
52	1	1	Total	C	N	O	P	0
			100	80	2	16	2	

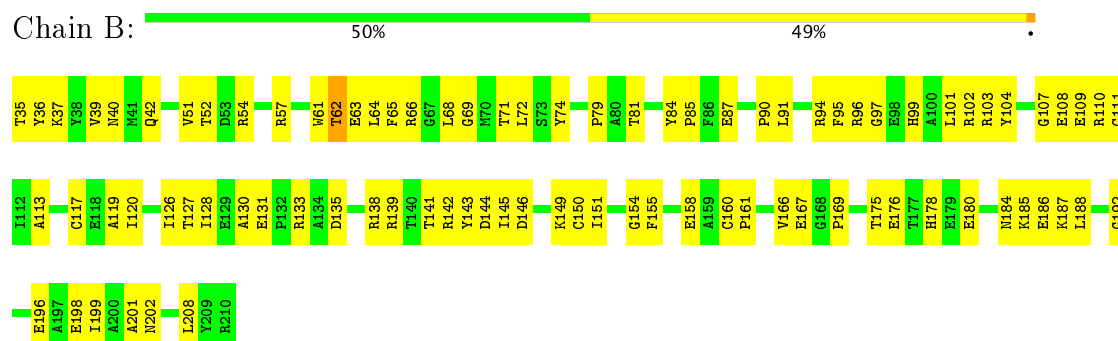
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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

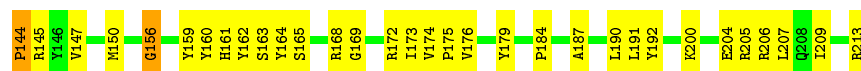


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

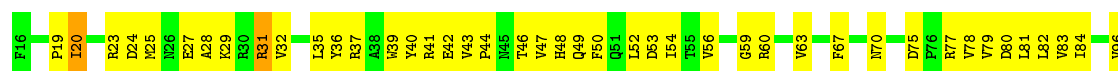


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

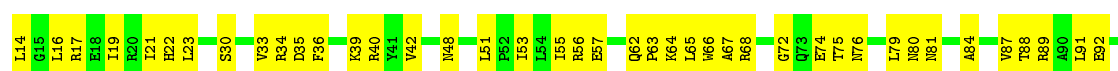




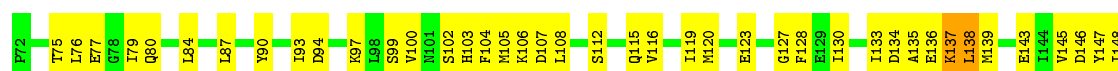
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



- Molecule 6: Acyl carrier protein, mitochondrial



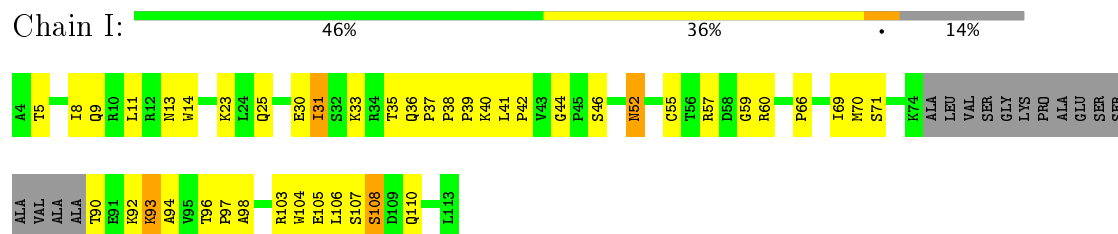
- Molecule 6: Acyl carrier protein, mitochondrial



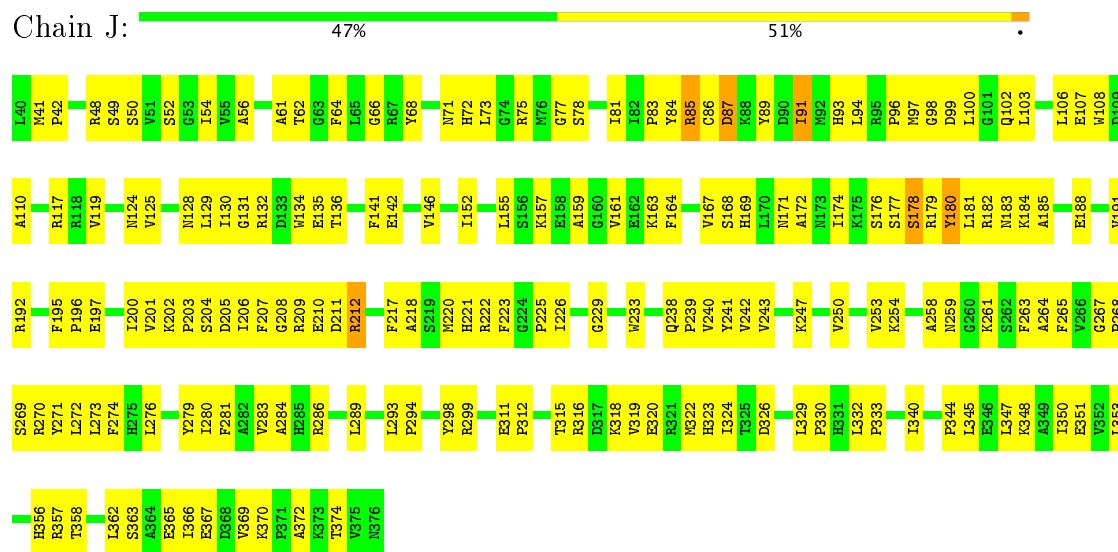
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



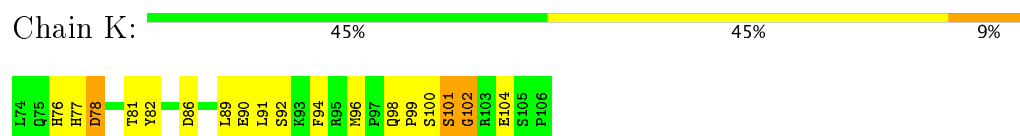
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



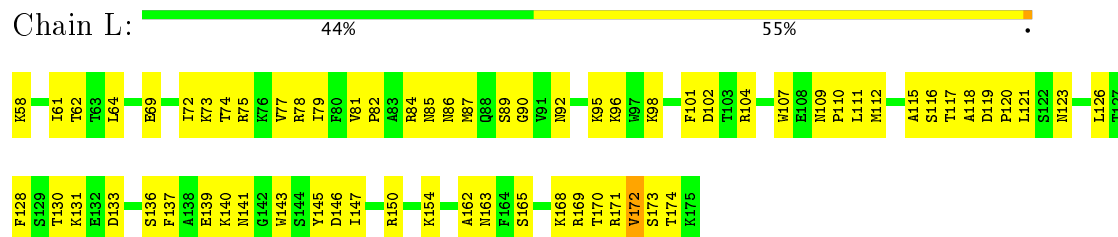
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



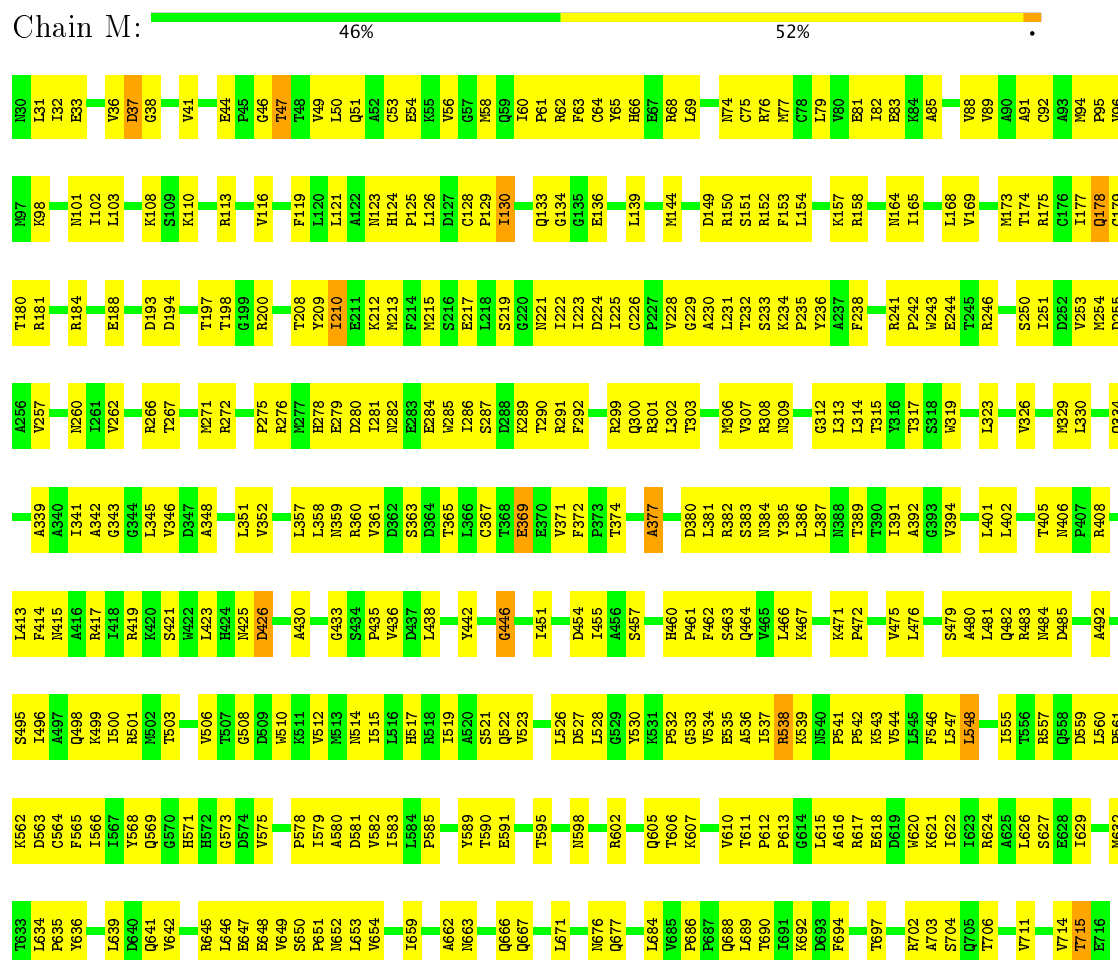
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



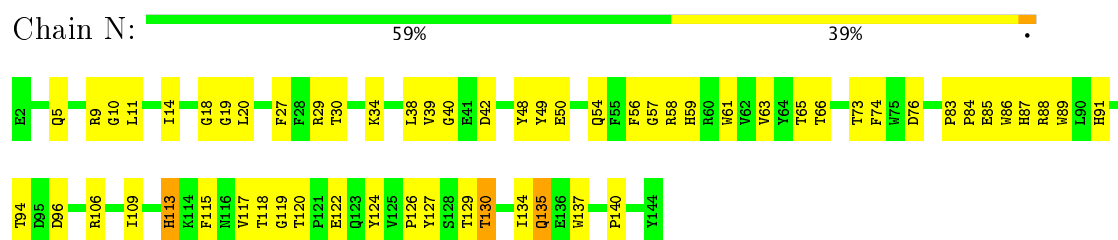
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



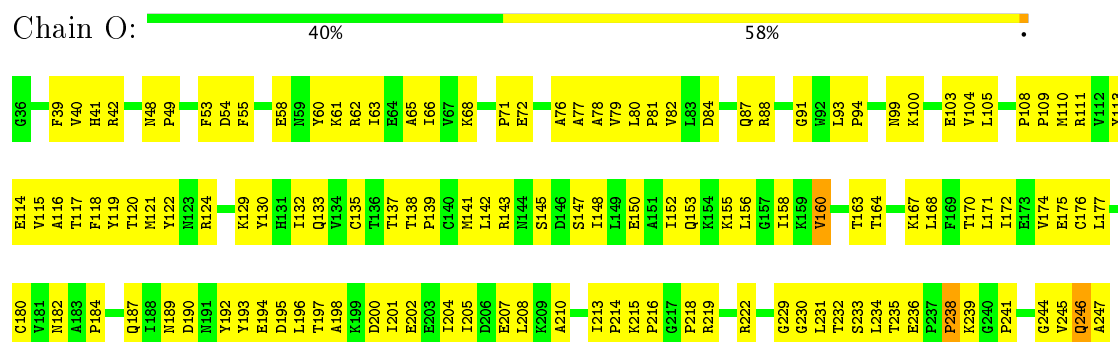
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



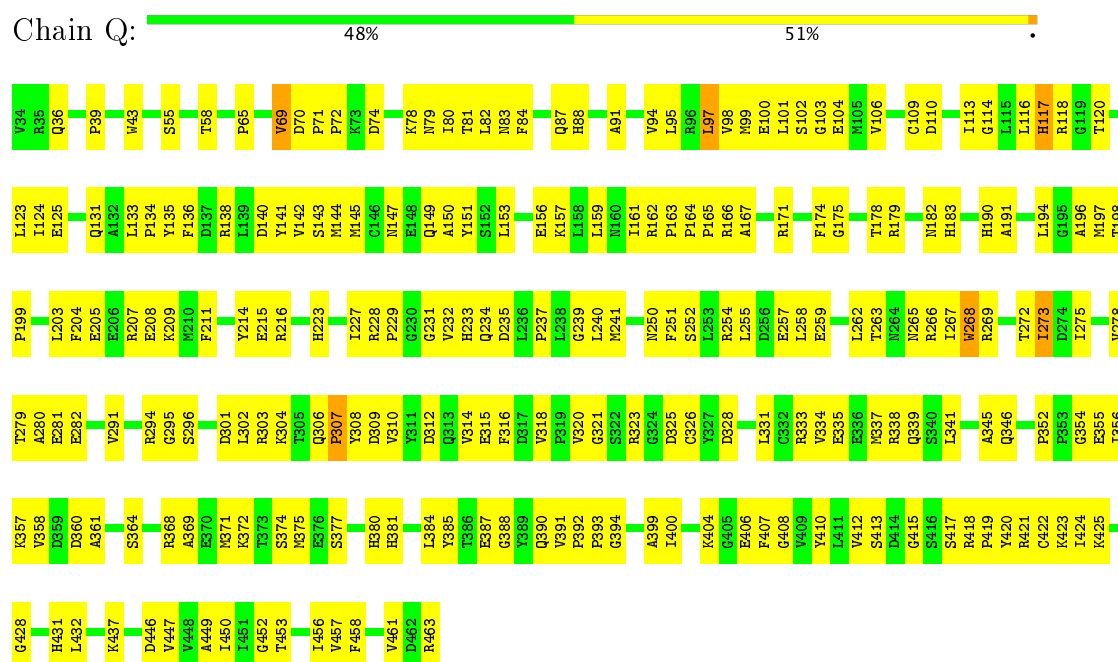
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



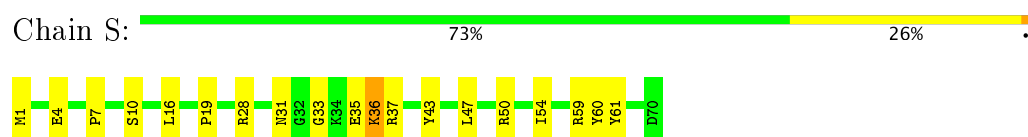
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



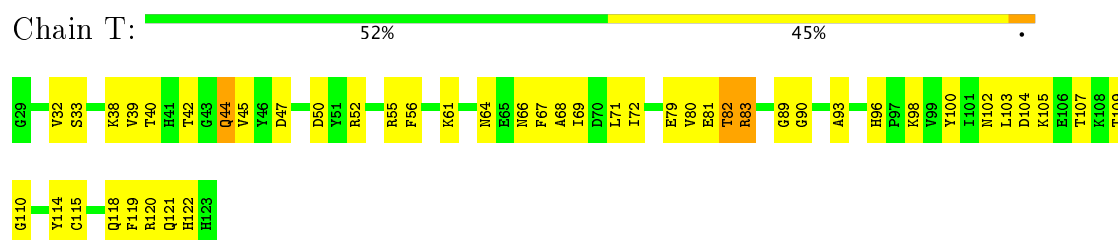
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



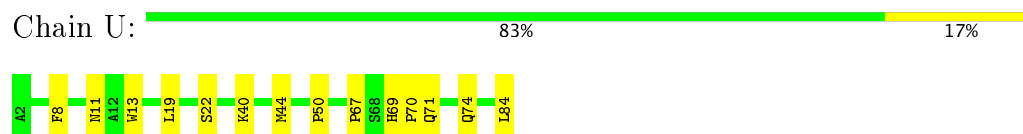
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



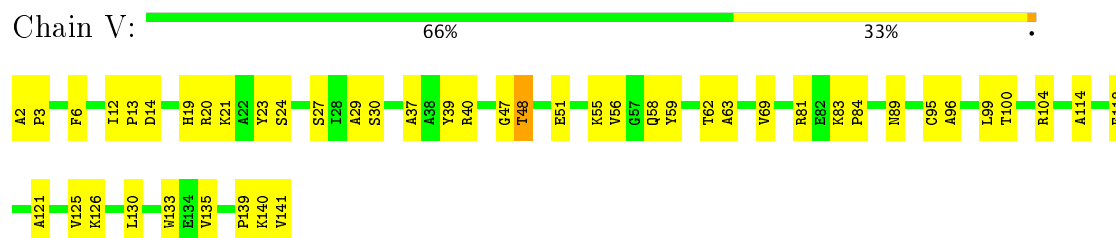
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



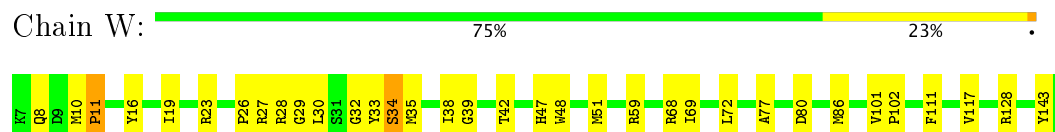
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



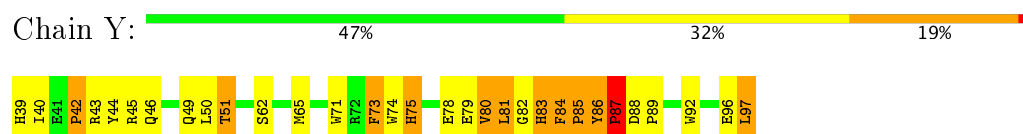
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



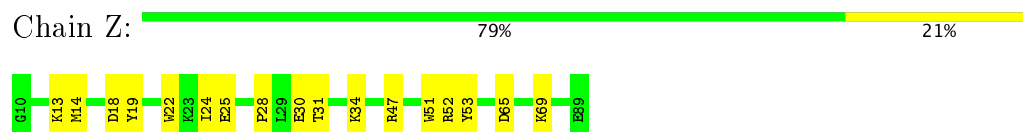
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



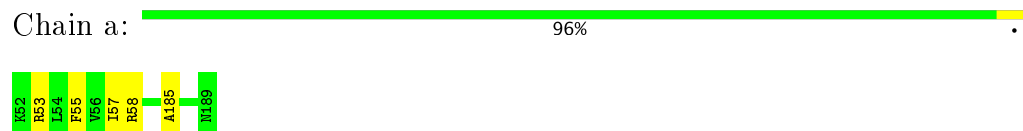
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



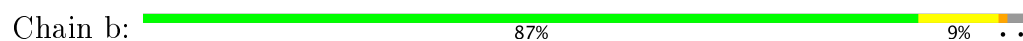
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- 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

Chain c: 95% 5%



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

Chain d: 95% 5%



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

Chain e: 97%



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

Chain f: 98%



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

Chain g: 95% 5%



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

Chain h: 94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 98%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 97% .



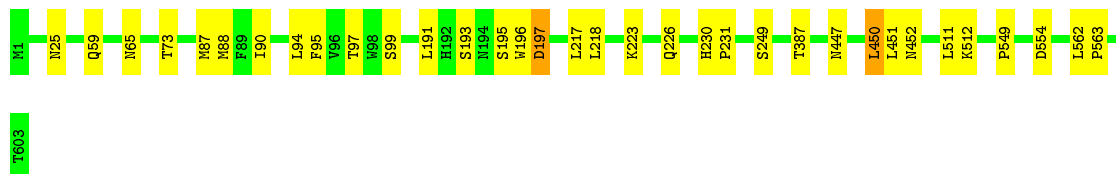
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 93% 6% .



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 94% 5% .



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m: 94% 6% .



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

Chain n: 96% .



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

Chain o: 97% .



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

Chain p: 98% .



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



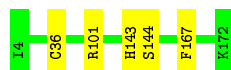
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97%



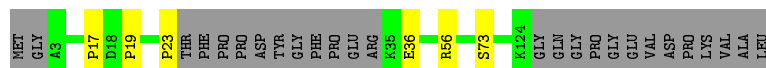
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97%



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

Chain v: 77% 19%



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

Chain w: 97%



4 Experimental information

Property	Value	Source
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.30	0/3398	0.49	0/4590
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.31	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
2	B	0.50	0/1452	0.57	0/1964
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.66	0/1579
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.58	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
3	C	0.58	0/1280	0.57	0/1732
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	1/4840 (0.0%)	0.69	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	p	0.59	0/1549	0.59	0/2098
4	E	0.34	0/993	0.54	0/1335
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.48	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
All	All	0.51	3/67276 (0.0%)	0.62	21/91300 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	118	PRO	N-CD	5.18	1.55	1.47
34	k	2	PRO	N-CD	5.14	1.55	1.47
35	l	231	PRO	N-CD	5.05	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.37	104.38	120.60
22	Y	92	TRP	N-CA-C	-7.00	92.10	111.00
27	d	2	PRO	N-CA-CB	6.79	111.44	103.30
22	Y	87	PRO	CA-N-CD	-6.57	102.30	111.50
25	b	36	PRO	C-N-CD	6.22	141.46	128.40
32	i	323	THR	C-N-CA	6.05	147.42	122.00
43	v	17	PRO	N-CA-CB	5.93	110.42	103.30
43	v	23	PRO	N-CA-CB	5.90	110.38	103.30
35	l	197	ASP	C-N-CD	5.88	140.74	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	105	PHE	C-N-CD	5.81	140.60	128.40
34	k	1	MET	C-N-CD	5.75	140.47	128.40
35	l	90	ILE	C-N-CD	5.72	140.41	128.40
43	v	19	PRO	N-CA-CB	5.69	110.13	103.30
35	l	230	HIS	C-N-CD	5.68	140.33	128.40
25	b	117	ILE	C-N-CD	5.67	140.31	128.40
16	Q	97	LEU	CA-CB-CG	5.65	128.29	115.30
25	b	37	PRO	CA-N-CD	-5.41	103.93	111.50
33	j	98	LEU	CB-CG-CD2	-5.40	101.82	111.00
22	Y	86	TYR	C-N-CD	5.12	139.15	128.40
40	r	408	LEU	CA-CB-CG	-5.10	103.58	115.30
40	r	238	LEU	CB-CG-CD2	-5.08	102.36	111.00

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 ⓘ

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	210	0
2	B	1420	0	1371	100	0
3	C	1249	0	1253	68	0
4	E	968	0	982	61	0
5	F	670	0	679	37	0
6	G	672	0	650	30	0
6	X	686	0	676	23	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	232	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	331	0
13	N	1195	0	1155	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	O	1643	0	1646	111	0
15	P	1730	0	1685	118	0
16	Q	3460	0	3419	252	0
17	S	568	0	567	15	0
18	T	742	0	723	40	0
19	U	647	0	653	10	0
20	V	1038	0	1027	34	0
21	W	1135	0	1129	33	0
22	Y	533	0	475	46	0
23	Z	648	0	627	13	0
24	a	1174	0	1177	0	0
25	b	1059	0	1079	0	0
26	c	1236	0	1092	0	0
27	d	1418	0	1375	0	0
28	e	810	0	772	0	0
29	f	405	0	407	0	0
30	g	1004	0	1008	0	0
31	h	863	0	861	0	0
32	i	2735	0	2893	0	0
33	j	919	0	968	0	0
34	k	740	0	792	0	0
35	l	4717	0	4893	0	0
36	m	1313	0	1330	0	0
37	n	473	0	480	0	0
38	o	1066	0	1086	0	0
39	p	1495	0	1440	0	0
40	r	3629	0	3825	0	0
41	s	2509	0	2617	0	0
42	u	1394	0	1367	0	0
43	v	921	0	892	0	0
44	w	2474	0	2304	0	0
45	A	8	0	0	6	0
45	B	16	0	0	3	0
45	C	8	0	0	0	0
45	M	16	0	0	3	0
46	A	31	0	19	17	0
47	B	52	0	88	3	0
47	U	52	0	88	1	0
47	V	52	0	88	2	0
47	b	52	0	88	0	0
47	g	156	0	264	0	0
47	r	104	0	176	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	E	35	0	0	4	0
48	p	35	0	0	0	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	0	0
51	l	128	0	144	0	0
51	n	64	0	72	0	0
52	V	51	0	82	12	0
52	W	51	0	82	5	0
52	l	100	0	157	0	0
All	All	66789	0	67204	1752	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 27.

All (1752) 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)
9:J:130:ILE:HG23	49:J:401:NDP:C8A	1.46	1.46
12:M:134:GLY:HA2	45:M:801:SF4:S3	1.57	1.42
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
9:J:206:ILE:HA	9:J:240:VAL:O	1.35	1.27
16:Q:82:LEU:O	16:Q:98:VAL:HG13	1.25	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.26
9:J:130:ILE:HG23	49:J:401:NDP:N7A	1.52	1.22
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
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
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
9:J:171:ASN:C	9:J:181:LEU:HD21	1.69	1.13
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
4:E:25:MET:HB3	4:E:29:LYS:HE3	1.32	1.07
12:M:134:GLY:CA	45:M:801:SF4:S3	2.42	1.06
22:Y:71:TRP:CH2	22:Y:75:HIS:HD2	1.76	1.04
9:J:221:HIS:CE1	9:J:222:ARG:HG3	1.91	1.04
16:Q:69:VAL:O	16:Q:72:PRO:HD2	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:82:LEU:O	16:Q:98:VAL:CG1	2.06	1.03
4:E:25:MET:CB	4:E:29:LYS:HE3	1.89	1.03
9:J:130:ILE:CG2	49:J:401:NDP:N7A	2.24	1.01
15:P:170:ILE:HD12	15:P:170:ILE:H	3.73	1.01
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:H60	52:V:202:PEE:C25	1.92	0.99
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
3:C:204:GLU:OE2	3:C:206:ARG:NH1	1.98	0.96
6:X:99:SER:HG	6:X:102:SER:HG	1.09	0.96
16:Q:262:LEU:HD22	16:Q:268:TRP:HD1	1.23	0.95
3:C:137:VAL:HG21	16:Q:87:GLN:HE21	1.29	0.94
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
14:O:177:LEU:N	50:O:301:FES:S1	2.39	0.94
1:A:116:ASN:HD22	46:A:502:FMN:C8	1.82	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
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
9:J:169:HIS:HD2	49:J:401:NDP:H5N	1.34	0.90
1:A:93:PHE:HE2	1:A:98:LYS:HD3	1.17	0.89
9:J:171:ASN:CB	9:J:181:LEU:HD11	2.02	0.89
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
3:C:137:VAL:CG2	16:Q:87:GLN:HE21	1.85	0.88
9:J:206:ILE:HB	9:J:242:VAL:CG2	2.04	0.88
22:Y:84:PHE:CG	22:Y:85:PRO:CD	2.57	0.87
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.38	0.87
9:J:212:ARG:HH11	9:J:212:ARG:HG2	1.37	0.86
16:Q:194:LEU:HD12	16:Q:268:TRP:CZ2	2.09	0.86
12:M:130:ILE:HD13	18:T:114:TYR:CE1	2.11	0.86
4:E:25:MET:HB3	4:E:29:LYS:HE2	1.55	0.86
22:Y:84:PHE:CD1	22:Y:85:PRO:CD	2.58	0.86
9:J:169:HIS:HD2	49:J:401:NDP:C5N	1.87	0.86
7:H:102:PRO:HA	15:P:70:PRO:HB2	1.57	0.86
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
2:B:81:THR:O	13:N:58:ARG:NH2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH21	16:Q:208:GLU:HB3	1.39	0.85
16:Q:273:ILE:CD1	16:Q:325:ASP:OD2	2.25	0.85
1:A:244:ASN:N	46:A:502:FMN:O2P	2.09	0.84
9:J:176:SER:CA	9:J:182:ARG:HH21	1.88	0.84
9:J:85:ARG:HH11	9:J:85:ARG:HG3	1.41	0.84
20:V:84:PRO:O	20:V:89:ASN:ND2	2.10	0.84
4:E:70:ASN:OD1	48:E:201:8Q1:O4	1.95	0.83
12:M:299:ARG:HG2	12:M:300:GLN:H	1.41	0.82
3:C:156:GLY:HA2	3:C:169:GLY:HA2	1.62	0.82
5:F:57:GLU:HB3	12:M:662:ALA:H	1.45	0.82
9:J:169:HIS:CD2	49:J:401:NDP:H5N	2.15	0.82
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.60	0.81
9:J:226:ILE:HD12	9:J:289:LEU:H	1.45	0.80
3:C:120:MET:HB3	3:C:147:VAL:HG12	1.64	0.80
22:Y:74:TRP:HZ3	22:Y:75:HIS:HD1	1.29	0.80
9:J:206:ILE:CA	9:J:240:VAL:O	2.24	0.80
16:Q:294:ARG:O	16:Q:321:GLY:N	2.11	0.80
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
16:Q:273:ILE:HD13	16:Q:325:ASP:OD2	1.81	0.79
9:J:217:PHE:HZ	9:J:322:MET:HE2	1.47	0.79
16:Q:70:ASP:O	16:Q:74:ASP:OD1	2.00	0.79
3:C:59:ARG:HH22	3:C:61:GLU:HB3	1.48	0.79
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.82	0.78
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
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
2:B:133:ARG:HG3	2:B:135:ASP:H	1.48	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
16:Q:83:ASN:HA	16:Q:98:VAL:HG22	1.65	0.78
9:J:176:SER:HA	9:J:182:ARG:NH2	1.98	0.78
9:J:270:ARG:NH2	9:J:326:ASP:O	2.16	0.78
16:Q:87:GLN:O	16:Q:88:HIS:C	2.22	0.77
22:Y:83:HIS:O	22:Y:84:PHE:CB	2.31	0.77
22:Y:84:PHE:CG	22:Y:85:PRO:HD2	2.19	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
16:Q:194:LEU:CD1	16:Q:268:TRP:CZ2	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:96:GLU:O	22:Y:97:LEU:HD23	1.84	0.77
3:C:59:ARG:NH2	3:C:61:GLU:HB3	1.98	0.77
1:A:64:LYS:NZ	14:O:244:GLY:O	2.18	0.77
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
4:E:79:VAL:HG22	48:E:201:8Q1:C38	2.16	0.76
3:C:143:GLU:OE1	9:J:89:TYR:OH	2.03	0.76
16:Q:125:GLU:HA	16:Q:419:PRO:HG2	1.67	0.76
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.19	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
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
9:J:221:HIS:ND1	9:J:222:ARG:N	2.35	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
16:Q:118:ARG:NH2	16:Q:138:ARG:O	2.20	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
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
16:Q:268:TRP:HZ3	16:Q:272:THR:HG21	1.52	0.74
16:Q:384:LEU:HA	16:Q:388:GLY:HA2	1.68	0.74
12:M:506:VAL:HG12	12:M:508:GLY:H	1.52	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
15:P:170:ILE:HD12	15:P:170:ILE:N	4.19	0.74
12:M:58:MET:SD	15:P:246:ARG:NH1	2.55	0.74
6:G:79:ILE:HG21	6:G:148:ILE:HG21	1.70	0.73
8:I:33:LYS:NZ	8:I:35:THR:O	2.18	0.73
3:C:67:LEU:HD22	3:C:207:LEU:HD21	1.70	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
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.71	0.73
12:M:128:CYS:HB2	12:M:129:PRO:CD	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.70	0.73
3:C:88:CYS:SG	16:Q:223:HIS:NE2	2.60	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
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
12:M:121:LEU:HD21	12:M:139:LEU:HD21	1.72	0.72
12:M:307:VAL:HG13	12:M:582:VAL:HG22	1.69	0.72
3:C:129:LYS:NZ	16:Q:113:ILE:O	2.23	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
14:O:116:ALA:O	14:O:124:ARG:NH1	2.22	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:391:TRP:HH2	12:M:153:PHE:HA	1.55	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
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
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
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
22:Y:86:TYR:HB3	22:Y:87:PRO:CA	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:55:HIS:NE2	15:P:78:VAL:O	2.24	0.71
15:P:134:SER:HG	15:P:139:SER:HG	1.25	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
9:J:176:SER:O	9:J:182:ARG:NH2	2.24	0.71
11:L:82:PRO:HG3	11:L:98:LYS:HE3	1.73	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
15:P:170:ILE:CD1	15:P:170:ILE:H	3.91	0.70
16:Q:281:GLU:N	16:Q:281:GLU:OE1	2.22	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
4:E:25:MET:O	4:E:29:LYS:CG	2.38	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
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
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
9:J:350:ILE:HD13	9:J:366:ILE:HG12	1.72	0.70
6:X:91:ASP:OD1	23:Z:47:ARG:NH1	2.24	0.70
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.71	0.70
9:J:85:ARG:HD2	9:J:85:ARG:O	1.92	0.70
9:J:210:GLU:HG2	9:J:210:GLU:O	1.92	0.69
7:H:12:VAL:HG13	16:Q:280:ALA:H	1.57	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
12:M:299:ARG:HD3	12:M:703:ALA:HB1	1.74	0.69
1:A:214:GLU:OE2	1:A:224:ARG:NH1	2.24	0.69
4:E:25:MET:C	4:E:29:LYS:HG3	2.13	0.69
12:M:613:PRO:HB2	13:N:134:ILE:HD13	1.73	0.69
1:A:60:GLY:HA3	14:O:241:PRO:HB3	1.74	0.69
12:M:595:THR:HA	12:M:605:GLN:HA	1.74	0.69
52:W:201:PEE:H24	52:W:201:PEE:H53	1.74	0.69
9:J:202:LYS:HB2	9:J:264:ALA:HA	1.75	0.69
12:M:466:LEU:HD23	12:M:500:ILE:HD11	1.75	0.69
4:E:25:MET:HB2	4:E:29:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:H9	46:A:502:FMN:O4'	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
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
1:A:318:ILE:HG22	1:A:326:LEU:HA	1.74	0.67
1:A:381:GLN:HG3	1:A:382:CYS:H	1.59	0.67
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
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
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:251:PHE:HB2	16:Q:254:ARG:HH21	1.59	0.67
16:Q:87:GLN:N	16:Q:87:GLN:OE1	2.26	0.67
1:A:63:TYR:HE2	1:A:64:LYS:HZ2	1.41	0.67
3:C:137:VAL:HG21	16:Q:87:GLN:NE2	2.05	0.67
3:C:136:LYS:O	3:C:140:GLN:HG3	1.94	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
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
1:A:118:ASP:O	1:A:159:ARG:HD2	1.95	0.67
1:A:43:THR:HG21	14:O:239:LYS:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:82:LEU:C	16:Q:98:VAL:HG13	2.10	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
1:A:379:CYS:SG	1:A:380:GLY:N	2.68	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
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
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
21:W:86:MET:SD	21:W:128:ARG:NH1	2.66	0.66
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.29	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
9:J:85:ARG:HH11	9:J:85:ARG:CG	2.09	0.66
11:L:81:VAL:HG11	11:L:150:ARG:HA	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
22:Y:81:LEU:HD23	22:Y:81:LEU:C	2.15	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
16:Q:450:ILE:O	16:Q:453:THR:OG1	2.07	0.65
4:E:23:ARG:N	4:E:27:GLU:OE1	2.24	0.65
9:J:206:ILE:CB	9:J:242:VAL:HG22	2.25	0.65
12:M:36:VAL:O	12:M:38:GLY:N	2.29	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
9:J:132:ARG:NH2	49:J:401:NDP:H2B	2.11	0.65
1:A:244:ASN:OD1	1:A:245:VAL:N	2.29	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:416:SER:HB3	1:A:436:GLN:HE21	1.63	0.64
11:L:89:SER:OG	15:P:239:TRP:NE1	2.26	0.64
18:T:39:VAL:HG12	18:T:45:VAL:HB	1.79	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:N	12:M:591:GLU:OE1	2.30	0.64
5:F:33:VAL:HG22	5:F:87:VAL:HG21	1.78	0.64
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.79	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
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
1:A:414:GLU:OE1	12:M:152:ARG:NH1	2.30	0.63
1:A:98:LYS:HD2	1:A:101:PHE:HE2	1.61	0.63
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.80	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
52:V:202:PEE:C24	52:V:202:PEE:H32	2.24	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
1:A:207:GLY:O	46:A:502:FMN:C5A	2.47	0.63
12:M:692:LYS:HD2	12:M:715:THR:HG22	1.79	0.63
16:Q:84:PHE:HE2	16:Q:91:ALA:HB2	1.63	0.63
1:A:391:TRP:CH2	12:M:153:PHE:HA	2.34	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:136:PHE:HB3	16:Q:147:ASN:HB3	1.79	0.63
2:B:99:HIS:NE2	45:B:302:SF4:S1	2.70	0.62
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:141:PHE:CZ	9:J:180:TYR:HD1	2.17	0.62
14:O:40:VAL:HG13	14:O:42:ARG:H	1.64	0.62
9:J:83:PRO:HB3	9:J:119:VAL:HG21	1.81	0.62
21:W:39:GLY:O	21:W:42:THR:OG1	2.15	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
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
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
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
10:K:98:GLN:HB3	14:O:71:PRO:HA	1.80	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
1:A:116:ASN:HD22	46:A:502:FMN:HM83	1.63	0.61
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
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
1:A:282:VAL:HG21	1:A:304:ALA:HB1	1.83	0.61
15:P:94:ILE:HG13	15:P:154:GLU:HB3	1.82	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:537:ILE:O	12:M:539:LYS:N	2.33	0.61
1:A:37:ASP:OD2	14:O:236:GLU:N	2.30	0.61
16:Q:428:GLY:HA2	16:Q:431:HIS:HD2	1.66	0.61
2:B:126:ILE:O	15:P:231:ARG:NH2	2.23	0.61
6:G:76:LEU:HD21	6:G:155:TYR:HA	1.82	0.61
2:B:187:LYS:HB2	13:N:124:TYR:CE1	2.36	0.61
13:N:130:THR:N	18:T:44:GLN:OE1	2.34	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
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
11:L:128:PHE:HA	15:P:121:THR:HG22	1.82	0.60
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.65	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
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
3:C:205:ARG:HG3	3:C:205:ARG:O	2.02	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
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
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.82	0.60
16:Q:179:ARG:CZ	16:Q:303:ARG:HH21	2.14	0.60
9:J:48:ARG:HH21	16:Q:78:LYS:HE2	43.62	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
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
4:E:37:ARG:HH21	4:E:41:ARG:NH2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:168:LEU:HD23	12:M:292:PHE:HD2	1.66	0.60
1:A:164:ASN:ND2	14:O:190:ASP:O	2.34	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
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
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
9:J:141:PHE:CZ	9:J:180:TYR:CA	2.84	0.59
11:L:89:SER:HG	15:P:239:TRP:HE1	1.39	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
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
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
7:H:40:LYS:HD3	7:H:45:ARG:NH1	2.18	0.59
12:M:334:GLN:HB2	12:M:361:VAL:HB	1.85	0.59
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.84	0.59
1:A:220:GLN:NE2	14:O:114:GLU:O	2.35	0.59
16:Q:142:VAL:HG11	16:Q:182:ASN:HA	1.84	0.59
9:J:315:THR:HG23	9:J:318:LYS:H	1.66	0.59
2:B:64:LEU:O	2:B:68:LEU:N	2.30	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
23:Z:25:GLU:HA	23:Z:30:GLU:HG3	1.84	0.59
9:J:358:THR:O	9:J:362:LEU:N	2.36	0.58
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.38	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
16:Q:273:ILE:HD13	16:Q:325:ASP:CG	2.23	0.58
2:B:186:GLU:OE2	18:T:64:ASN:N	2.36	0.58
9:J:181:LEU:HD23	9:J:181:LEU:O	2.03	0.58
4:E:126:HIS:NE2	12:M:612:PRO:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:39:VAL:HG22	16:Q:321:GLY:HA2	1.86	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
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:293:LEU:HD12	9:J:294:PRO:HD2	1.86	0.58
9:J:73:LEU:O	9:J:78:SER:OG	2.21	0.58
16:Q:182:ASN:HD21	16:Q:404:LYS:HE3	1.68	0.58
5:F:88:THR:HA	5:F:91:LEU:HD12	1.85	0.58
12:M:173:MET:C	12:M:175:ARG:H	2.05	0.58
12:M:385:TYR:HB2	12:M:517:HIS:HE2	1.69	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
1:A:243:ALA:HA	46:A:502:FMN:O2P	2.04	0.57
1:A:48:ARG:HH12	14:O:231:LEU:HD11	1.69	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
1:A:159:ARG:NH1	14:O:177:LEU:O	2.33	0.57
16:Q:412:VAL:HG12	16:Q:420:TYR:HB3	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
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.86	0.57
9:J:84:TYR:CB	9:J:91:ILE:HD11	2.34	0.57
12:M:222:ILE:O	12:M:225:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:226:CYS:HB2	12:M:231:LEU:HD12	1.85	0.57
12:M:257:VAL:HG11	12:M:413:LEU:HD22	1.85	0.57
12:M:251:ILE:HG22	12:M:260:ASN:HA	1.85	0.57
12:M:217:GLU:HB2	12:M:408:ARG:HH21	1.69	0.57
1:A:159:ARG:HH22	14:O:177:LEU:HA	1.70	0.57
16:Q:251:PHE:CD2	16:Q:341:LEU:HD21	2.40	0.57
16:Q:78:LYS:O	16:Q:79:ASN:HB3	2.04	0.57
20:V:40:ARG:HD3	20:V:59:TYR:HE2	1.68	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
12:M:177:ILE:O	12:M:177:ILE:HG13	2.04	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
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
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:283:VAL:HG12	9:J:369:VAL:HG21	1.86	0.57
9:J:75:ARG:NH1	15:P:215:GLU:OE2	2.34	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
8:I:39:PRO:HB2	8:I:41:LEU:HD12	1.87	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
1:A:126:LYS:HB2	1:A:275:LEU:HD22	1.85	0.56
12:M:591:GLU:HB3	12:M:612:PRO:HD3	1.87	0.56
2:B:87:GLU:HG2	13:N:61:TRP:HB3	1.87	0.56
16:Q:123:LEU:HB3	16:Q:135:TYR:OH	2.05	0.56
52:V:202:PEE:H40	52:V:202:PEE:H57	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:193:ASP:OD2	14:O:111:ARG:NH2	2.39	0.56
9:J:64:PHE:HD1	9:J:210:GLU:HB3	1.69	0.56
1:A:319:PRO:O	1:A:324:THR:OG1	2.23	0.56
9:J:221:HIS:HE1	9:J:222:ARG:HG3	1.61	0.56
9:J:84:TYR:O	9:J:107:GLU:HA	2.06	0.56
16:Q:390:GLN:OE1	16:Q:417:SER:N	2.39	0.56
16:Q:84:PHE:CE2	16:Q:91:ALA:HB2	2.40	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
1:A:222:LYS:HE2	1:A:379:CYS:HB2	1.88	0.56
1:A:86:ARG:HA	1:A:94:PRO:HA	1.88	0.56
6:G:97:LYS:HD3	6:G:108:LEU:HG	1.86	0.56
12:M:492:ALA:O	12:M:495:SER:OG	2.21	0.56
1:A:227:PRO:HB3	12:M:95:PRO:HD3	1.87	0.56
15:P:213:ASP:OD1	15:P:214:ASP:N	2.38	0.56
16:Q:326:CYS:SG	16:Q:453:THR:HG22	2.44	0.56
16:Q:94:VAL:HG11	16:Q:458:PHE:HB3	1.87	0.56
20:V:40:ARG:NH2	20:V:55:LYS:HD3	2.20	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
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
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
9:J:181:LEU:HD13	9:J:324:ILE:HD13	1.88	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
15:P:190:ASP:CG	15:P:191:TYR:H	2.08	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:PRO:HD3	13:N:113:HIS:CD2	2.41	0.55
13:N:48:TYR:HB3	13:N:89:TRP:CZ3	2.41	0.55
14:O:41:HIS:O	14:O:41:HIS:ND1	2.39	0.55
1:A:149:MET:HG3	1:A:241:THR:HG21	1.89	0.55
1:A:119:GLU:HB3	1:A:162:PHE:HE2	1.70	0.55
12:M:50:LEU:N	12:M:91:ALA:O	2.38	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
16:Q:273:ILE:HD11	16:Q:325:ASP:OD2	2.04	0.55
52:V:202:PEE:C24	52:V:202:PEE:H60	2.37	0.55
20:V:40:ARG:HD3	20:V:59:TYR:CE2	2.41	0.55
22:Y:74:TRP:HE3	22:Y:75:HIS:CA	2.19	0.55
9:J:141:PHE:CE1	9:J:180:TYR:HD1	2.25	0.55
9:J:49:SER:HB2	15:P:225:GLU:HB3	1.87	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
5:F:80:ASN:OD1	5:F:81:ASN:ND2	2.39	0.55
15:P:172:ASP:OD2	15:P:189:THR:OG1	2.24	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
9:J:134:TRP:CZ3	9:J:136:THR:HA	2.42	0.55
9:J:94:LEU:HG	9:J:97:MET:SD	2.46	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
1:A:278:ILE:HG12	1:A:304:ALA:HB2	1.89	0.55
1:A:116:ASN:ND2	46:A:502:FMN:HM83	2.20	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:94:ILE:N	15:P:154:GLU:OE1	2.28	0.55
15:P:51:ASN:HB2	15:P:82:ASN:HD21	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:620:TRP:HE1	12:M:639:LEU:HD13	1.71	0.54
9:J:164:PHE:HE2	9:J:191:VAL:HG13	1.71	0.54
9:J:141:PHE:HZ	9:J:180:TYR:CD1	2.26	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
7:H:12:VAL:HG11	16:Q:296:SER:HB2	1.90	0.54
7:H:31:ILE:HA	7:H:34:VAL:HG12	1.90	0.54
11:L:85:ASN:OD1	11:L:87:MET:N	2.36	0.54
11:L:61:ILE:HG21	15:P:149:GLU:OE1	2.07	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
1:A:328:PRO:HG2	1:A:441:HIS:CD2	2.43	0.54
1:A:207:GLY:O	46:A:502:FMN:C9A	2.56	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
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
22:Y:96:GLU:O	22:Y:97:LEU:CD2	2.54	0.54
22:Y:96:GLU:O	22:Y:97:LEU:CB	2.55	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:203:PRO:HG2	49:J:401:NDP:C5N	2.37	0.54
12:M:289:LYS:NZ	12:M:694:PHE:O	2.25	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
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.90	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:449:ALA:O	16:Q:453:THR:HG23	2.08	0.53
2:B:104:TYR:CE2	2:B:110:ARG:HA	2.43	0.53
2:B:68:LEU:O	2:B:71:THR:HG22	2.08	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:173:MET:C	12:M:175:ARG:N	2.60	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
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.91	0.53
14:O:204:ILE:O	14:O:208:LEU:HG	2.09	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
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
23:Z:24:ILE:HG22	23:Z:30:GLU:HB2	1.90	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:168:LEU:HB3	12:M:292:PHE:HE2	1.74	0.53
12:M:68:ARG:HD2	12:M:285:TRP:NE1	2.20	0.53
16:Q:136:PHE:HE2	16:Q:151:TYR:CD1	2.26	0.53
1:A:217:GLU:HB3	11:L:171:ARG:HH22	1.72	0.53
2:B:65:PHE:O	2:B:69:GLY:N	2.41	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
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.35	0.53
15:P:88:ILE:HG22	15:P:89:HIS:O	2.09	0.53
2:B:37:LYS:N	16:Q:318:VAL:O	2.37	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:196:ALA:O	16:Q:198:THR:N	2.41	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
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
1:A:77:LEU:HD21	1:A:100:SER:HA	1.90	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
12:M:46:GLY:O	12:M:96:VAL:HG22	2.09	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
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
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
1:A:116:ASN:HD22	46:A:502:FMN:C9	2.22	0.52
12:M:351:LEU:HD23	12:M:530:TYR:HE2	1.73	0.52
12:M:188:GLU:O	12:M:419:ARG:NE	2.40	0.52
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.43	0.52
9:J:141:PHE:HE2	9:J:183:ASN:HB2	1.74	0.52
9:J:141:PHE:CZ	9:J:180:TYR:CB	2.92	0.52
16:Q:159:LEU:HD21	16:Q:391:VAL:HA	1.90	0.52
7:H:32:LEU:O	7:H:36:GLU:HG3	2.10	0.52
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.92	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
1:A:281:HIS:NE2	14:O:142:LEU:O	2.38	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
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:338:ARG:NH2	21:W:23:ARG:HB3	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:385:TYR:HB2	12:M:517:HIS:NE2	2.25	0.52
8:I:41:LEU:C	21:W:8:GLN:HE22	2.13	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
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
9:J:176:SER:C	9:J:182:ARG:HH21	2.13	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
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
1:A:342:LEU:O	1:A:347:THR:N	2.42	0.52
48:E:201:8Q1:C30	48:E:201:8Q1:N36	2.73	0.52
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
2:B:66:ARG:HH12	21:W:28:ARG:HB3	1.74	0.52
10:K:77:HIS:CD2	14:O:215:LYS:HE2	2.44	0.51
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.74	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
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.91	0.51
19:U:84:LEU:O	21:W:59:ARG:NH1	2.41	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
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
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
12:M:573:GLY:HA3	13:N:137:TRP:NE1	2.25	0.51
8:I:25:GLN:OE1	16:Q:254:ARG:HD3	2.10	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

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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: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
12:M:50:LEU:HA	12:M:60:ILE:HD13	1.93	0.51
20:V:12:ILE:HG22	20:V:13:PRO:O	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
8:I:9:GLN:O	8:I:13:ASN:ND2	2.40	0.51
2:B:138:ARG:NH1	12:M:238:PHE:HA	2.26	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
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
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
7:H:111:GLN:NE2	15:P:122:ARG:HB3	2.26	0.51
4:E:19:PRO:HA	4:E:77:ARG:HD3	1.93	0.51
9:J:168:SER:C	9:J:184:LYS:HE2	2.31	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
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
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:308:ARG:HD3	12:M:314:LEU:HB3	1.92	0.51
12:M:460:HIS:O	12:M:463:SER:OG	2.13	0.51
6:X:85:TYR:HE2	22:Y:45:ARG:NH1	2.09	0.51
12:M:532:PRO:HB2	12:M:534:VAL:HG23	1.93	0.51
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.26	0.51
18:T:80:VAL:HG12	18:T:82:THR:H	1.76	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:113:ALA:HB1	2:B:130:ALA:HB2	1.94	0.50
2:B:37:LYS:HE2	8:I:110:GLN:O	2.11	0.50
7:H:107:PRO:HB2	7:H:111:GLN:HB2	1.93	0.50
7:H:83:GLN:HG2	15:P:107:GLN:NE2	2.26	0.50
9:J:178:SER:OG	9:J:181:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:54:ILE:HA	9:J:124:ASN:HD21	1.76	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
7:H:7:LYS:O	7:H:8:THR:OG1	2.29	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
22:Y:86:TYR:HB3	22:Y:87:PRO:HB3	1.93	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
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
5:F:36:PHE:HB2	5:F:84:ALA:HB1	1.92	0.50
9:J:161:VAL:HG12	9:J:163:LYS:H	1.76	0.50
9:J:141:PHE:CZ	9:J:180:TYR:HB2	2.47	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
7:H:90:LEU:HD11	15:P:99:PHE:HD1	1.76	0.50
2:B:108:GLU:OE1	18:T:68:ALA:HB1	2.12	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: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
12:M:77:MET:HA	12:M:116:VAL:HG21	1.92	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
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
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
12:M:464:GLN:NE2	12:M:467:LYS:HE2	2.27	0.50
12:M:92:CYS:SG	50:M:803:FES:S2	3.10	0.50
2:B:175:THR:HA	13:N:118:THR:HG21	1.94	0.50
15:P:74:GLN:HB2	15:P:87:CYS:SG	2.52	0.50
22:Y:74:TRP:CE3	22:Y:74:TRP:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:86:TYR:HB3	22:Y:87:PRO:CB	2.41	0.50
16:Q:145:MET:HB3	16:Q:227:ILE:HD12	1.92	0.50
16:Q:133:LEU:HD12	16:Q:229:PRO:HD3	1.93	0.50
16:Q:65:PRO:HG2	16:Q:69:VAL:HG22	1.94	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
12:M:88:VAL:HG13	12:M:108:LYS:HE2	1.94	0.50
11:L:92:ASN:HB2	15:P:239:TRP:H	1.77	0.50
20:V:14:ASP:O	20:V:21:LYS:NZ	2.45	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
5:F:21:ILE:HG12	5:F:55:ILE:HG12	1.93	0.49
9:J:221:HIS:HE1	9:J:222:ARG:CG	2.20	0.49
9:J:62:THR:HB	49:J:401:NDP:HO3A	1.76	0.49
1:A:152:ARG:HH12	10:K:99:PRO:HB3	1.76	0.49
7:H:115:PRO:O	15:P:247:GLN:NE2	2.45	0.49
16:Q:143:SER:HB2	16:Q:178:THR:HB	1.93	0.49
16:Q:428:GLY:HA2	16:Q:431:HIS:CD2	2.45	0.49
16:Q:87:GLN:O	16:Q:88:HIS:O	2.30	0.49
18:T:89:GLY:HA2	18:T:115:CYS:SG	2.52	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: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
7:H:107:PRO:HD3	15:P:74:GLN:HE22	1.76	0.49
52:V:202:PEE:C35	52:V:202:PEE:H40	2.42	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:168:LEU:HD23	12:M:292:PHE:CD2	2.47	0.49
7:H:111:GLN:HE22	15:P:122:ARG:HB3	1.77	0.49
12:M:126:LEU:HD23	16:Q:375:MET:SD	2.52	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:149:GLN:CD	16:Q:171:ARG:HB3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:334:VAL:O	16:Q:338:ARG:HG2	2.12	0.49
2:B:36:TYR:CD2	8:I:104:TRP:HB2	2.48	0.49
6:G:99:SER:OG	6:G:102:SER:OG	2.29	0.49
9:J:176:SER:C	9:J:182:ARG:NH2	2.65	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
16:Q:360:ASP:O	16:Q:364:SER:OG	2.29	0.49
7:H:114:TRP:NE1	16:Q:394:GLY:HA2	2.25	0.49
15:P:113:ASP:OD1	16:Q:425:LYS:HD2	2.13	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	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
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
1:A:102:MET:SD	1:A:149:MET:HB3	2.52	0.49
4:E:49:GLN:HE21	4:E:96:VAL:HG21	1.78	0.49
9:J:212:ARG:CG	9:J:212:ARG:NH1	2.73	0.49
9:J:85:ARG:NH1	9:J:85:ARG:CG	2.72	0.49
11:L:95:LYS:NZ	15:P:240:GLU:OE2	2.45	0.49
12:M:123:ASN:HA	12:M:157:LYS:HG2	1.94	0.49
12:M:66:HIS:HE1	12:M:68:ARG:HG2	1.78	0.49
9:J:209:ARG:HD2	15:P:217:LYS:HE2	1.93	0.49
16:Q:194:LEU:HD12	16:Q:268:TRP:CE2	2.45	0.49
16:Q:404:LYS:HZ3	16:Q:457:VAL:HB	1.75	0.49
20:V:39:TYR:HD2	51:V:201:CDL:H721	1.76	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:64:CYS:O	12:M:184:ARG:NH2	2.46	0.49
12:M:32:ILE:HG23	12:M:98:LYS:HB2	1.93	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
1:A:274:LYS:HZ2	1:A:352:ALA:HB3	1.77	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:197:THR:H	14:O:200:ASP:HB3	1.77	0.49
15:P:160:PHE:C	15:P:162:ALA:H	2.16	0.49
52:V:202:PEE:C37	52:V:202:PEE:H41	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	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
14:O:155:LYS:HZ3	14:O:205:ILE:HB	1.77	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:179:ARG:HG2	16:Q:183:HIS:CD2	2.48	0.48
20:V:62:THR:HG22	20:V:104:ARG:HD3	1.95	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
4:E:47:VAL:HG11	4:E:56:VAL:HG22	1.95	0.48
9:J:89:TYR:CD1	9:J:89:TYR:C	2.85	0.48
12:M:136:GLU:N	12:M:136:GLU:OE1	2.46	0.48
12:M:36:VAL:HG23	12:M:41:VAL:HG21	1.96	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
23:Z:28:PRO:O	23:Z:31:THR:OG1	2.22	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
20:V:29:ALA:O	20:V:63:ALA:HB1	2.13	0.48
1:A:158:ILE:N	1:A:198:VAL:O	2.47	0.48
9:J:197:GLU:N	9:J:197:GLU:OE1	2.45	0.48
12:M:302:LEU:N	12:M:571:HIS:O	2.33	0.48
2:B:94:ARG:CZ	16:Q:237:PRO:HG3	2.44	0.48
21:W:47:HIS:O	21:W:51:MET:HG3	2.13	0.48
9:J:217:PHE:CZ	9:J:322:MET:HE2	2.37	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: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:80:ILE:O	16:Q:100:GLU:C	2.52	0.48
16:Q:140:ASP:HB3	16:Q:147:ASN:ND2	2.28	0.48
1:A:130:ILE:HD11	1:A:275:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ARG:NH2	11:L:112:MET:O	2.47	0.48
9:J:141:PHE:HE2	9:J:183:ASN:HD22	1.62	0.48
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.48	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
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
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
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
14:O:207:GLU:HA	14:O:210:ALA:HB3	1.96	0.48
8:I:44:GLY:HA2	16:Q:355:GLU:HG3	1.95	0.48
22:Y:71:TRP:C	22:Y:71:TRP:CE3	2.87	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
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
20:V:47:GLY:O	20:V:48:THR:OG1	2.25	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
1:A:111:LYS:O	1:A:152:ARG:N	2.34	0.48
1:A:99:TRP:HH2	1:A:248:VAL:HA	1.78	0.48
2:B:198:GLU:OE2	2:B:202:ASN:ND2	2.46	0.48
7:H:18:ASN:O	7:H:19:THR:OG1	2.31	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
52:W:201:PEE:P	52:W:201:PEE:N	2.87	0.48
4:E:36:TYR:HD1	4:E:67:PHE:HE2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:HE1	10:K:76:HIS:HD1	1.62	0.47
20:V:40:ARG:HG3	51:V:201:CDL:HB22	1.96	0.47
20:V:37:ALA:HB1	20:V:56:VAL:HG22	1.95	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
2:B:133:ARG:NH1	2:B:139:ARG:HG3	2.29	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
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
1:A:123:GLY:N	14:O:180:CYS:SG	2.71	0.47
8:I:97:PRO:HG3	15:P:61:PHE:CG	2.49	0.47
3:C:95:HIS:HE1	16:Q:211:PHE:CE2	2.32	0.47
51:V:201:CDL:H522	51:V:201:CDL:H552	1.69	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	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
7:H:108:PRO:HG2	7:H:111:GLN:HG2	1.97	0.47
7:H:34:VAL:HG23	7:H:95:ARG:CZ	2.44	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
3:C:100:ARG:NH2	16:Q:208:GLU:HB3	2.18	0.47
16:Q:390:GLN:NE2	16:Q:417:SER:HB3	2.29	0.47
1:A:208:GLU:OE1	1:A:211:ALA:N	2.38	0.47
5:F:57:GLU:HB3	12:M:662:ALA:N	2.24	0.47
9:J:218:ALA:HB2	9:J:353:LEU:HD22	1.96	0.47
9:J:91:ILE:HA	9:J:93:HIS:CE1	2.49	0.47
12:M:266:ARG:NE	12:M:271:MET:HE3	2.29	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
4:E:98:LYS:HG2	15:P:191:TYR:HB3	1.96	0.47
16:Q:194:LEU:CD1	16:Q:268:TRP:CE2	2.97	0.47
20:V:96:ALA:HA	20:V:99:LEU:HD12	1.95	0.47
22:Y:73:PHE:CD1	22:Y:73:PHE:C	2.88	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
22:Y:50:LEU:O	22:Y:51:THR:OG1	2.27	0.47
1:A:126:LYS:HZ3	1:A:246:GLU:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:H:32:LEU:HG	7:H:52:THR:HG21	1.97	0.47
9:J:99:ASP:O	9:J:102:GLN:HG2	2.14	0.47
21:W:101:VAL:HG13	21:W:102:PRO:HD2	1.96	0.47
9:J:220:MET:SD	9:J:223:PHE:CD2	3.08	0.47
9:J:41:MET:HB3	9:J:42:PRO:HD2	1.97	0.47
15:P:186:ARG:NH2	15:P:193:PHE:HB3	2.29	0.47
52:W:201:PEE:H28	52:W:201:PEE:H22	1.50	0.47
3:C:96:MET:HG2	3:C:103:MET:HB3	1.96	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: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
12:M:198:THR:HG23	14:O:117:THR:HG21	1.97	0.47
15:P:201:ASP:OD1	15:P:202:PHE:N	2.48	0.47
9:J:52:SER:HB3	16:Q:103:GLY:HA3	59.47	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
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
14:O:135:CYS:O	14:O:145:SER:OG	2.25	0.47
16:Q:338:ARG:NH1	21:W:23:ARG:HB3	2.29	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:113:ILE:HG12	16:Q:114:GLY:H	1.80	0.47
16:Q:408:GLY:HA3	16:Q:425:LYS:HB3	1.97	0.47
16:Q:97:LEU:HA	16:Q:110:ASP:O	2.15	0.47
17:S:4:GLU:O	17:S:7:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HA	1:A:289:GLU:HA	1.97	0.46
9:J:365:GLU:OE1	9:J:365:GLU:N	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
22:Y:74:TRP:CE3	22:Y:75:HIS:CA	2.91	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
12:M:616:ALA:O	12:M:617:ARG:NH1	2.44	0.46
12:M:81:GLU:CD	12:M:108:LYS:HB3	2.36	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
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
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:200:ASP:O	14:O:204:ILE:HG12	2.16	0.46
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.79	0.46
14:O:84:ASP:O	14:O:88:ARG:N	2.47	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
1:A:311:TRP:CD1	1:A:314:LEU:HD12	2.50	0.46
7:H:36:GLU:HA	7:H:45:ARG:NH2	2.19	0.46
9:J:168:SER:HA	9:J:184:LYS:HE3	1.97	0.46
9:J:141:PHE:CE2	9:J:183:ASN:ND2	2.83	0.46
1:A:177:TYR:CE2	10:K:91:LEU:HD13	2.50	0.46
11:L:109:ASN:OD1	11:L:110:PRO:HD2	2.16	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
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
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
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
12:M:381:LEU:C	12:M:383:SER:H	2.16	0.46
15:P:124:ASN:HB3	15:P:146:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:64:TYR:CE2	15:P:68:ILE:HD11	2.50	0.46
1:A:113:LEU:HD23	1:A:113:LEU:C	2.35	0.46
1:A:119:GLU:O	1:A:159:ARG:NH1	2.45	0.46
1:A:116:ASN:HD21	46:A:502:FMN:C8	2.22	0.46
1:A:89:GLY:HA2	1:A:244:ASN:ND2	2.28	0.46
3:C:137:VAL:HA	3:C:140:GLN:CD	2.36	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
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
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
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
1:A:86:ARG:HB3	1:A:92:GLY:O	2.16	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:162:ALA:HA	11:L:168:LYS:HZ2	1.80	0.46
11:L:78:ARG:HA	11:L:146:ASP:OD1	2.16	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
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
23:Z:31:THR:O	23:Z:34:LYS:HB3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:59:GLY:O	4:E:63:VAL:HG23	2.16	0.45
6:G:77:GLU:N	6:G:77:GLU:OE1	2.38	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
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
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
18:T:68:ALA:O	18:T:72:ILE:HG13	2.16	0.45
21:W:111:PHE:CD2	21:W:117:VAL:HG21	2.51	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:168:ARG:HG3	3:C:172:ARG:NH1	2.31	0.45
3:C:163:SER:H	3:C:168:ARG:HH22	1.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:E:53:ASP:OD2	9:J:351:GLU:HB3	2.17	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
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
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
9:J:99:ASP:H	9:J:102:GLN:HB2	1.82	0.45
8:I:55:CYS:HB3	12:M:110:LYS:HE3	1.98	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
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:N	11:L:102:ASP:OD1	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
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: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
22:Y:74:TRP:HE3	22:Y:75:HIS:N	2.15	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
7:H:23:ARG:HH22	7:H:27:LEU:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:217:PHE:HZ	9:J:322:MET:HE1	1.80	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:546:PHE:HD2	12:M:568:TYR:HD1	1.63	0.44
12:M:501:ARG:HH12	12:M:666:GLN:HB2	1.82	0.44
14:O:145:SER:O	14:O:148:ILE:HB	2.18	0.44
15:P:97:LEU:HD23	15:P:100:LEU:HD12	1.97	0.44
8:I:97:PRO:HG3	15:P:61:PHE:CD1	2.52	0.44
15:P:97:LEU:HA	15:P:100:LEU:HD12	1.97	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
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
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
20:V:69:VAL:HG21	20:V:100:THR:HG21	1.98	0.44
20:V:40:ARG:HE	51:V:201:CDL:CA2	2.30	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
2:B:61:TRP:HB2	2:B:65:PHE:HE2	1.82	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
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:169:PRO:HG3	2:B:198:GLU:HG2	2.00	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
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.82	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
9:J:72:HIS:O	9:J:75:ARG:HG2	2.18	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
14:O:76:ALA:HA	14:O:79:VAL:HG23	1.98	0.44
15:P:63:GLU:O	15:P:67:GLU:HG3	2.17	0.44
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.66	0.44
7:H:13:GLY:HA2	16:Q:279:THR:HG22	2.00	0.44
1:A:157:TYR:HB2	1:A:212:LEU:HD21	1.99	0.44
2:B:127:THR:HA	15:P:231:ARG:HH12	1.81	0.44
2:B:79:PRO:HD2	17:S:1:MET:SD	2.57	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
15:P:188:LEU:HD22	16:Q:117:HIS:HB2	2.00	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:106:VAL:HG11	16:Q:109:CYS:HB2	2.00	0.44
8:I:60:ARG:HD3	16:Q:159:LEU:HD22	1.99	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
16:Q:82:LEU:HD23	16:Q:82:LEU:HA	1.78	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: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
52:W:201:PEE:H51	52:W:201:PEE:H56	1.33	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
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:147:SER:HA	14:O:150:GLU:OE1	2.18	0.43
14:O:143:ARG:CB	14:O:184:PRO:HD3	2.47	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
20:V:51:GLU:HB3	20:V:55:LYS:NZ	2.33	0.43
1:A:118:ASP:O	1:A:119:GLU:C	2.55	0.43
4:E:50:PHE:CD2	4:E:103:VAL:HG21	2.52	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
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
12:M:299:ARG:HG2	12:M:300:GLN:N	2.19	0.43
12:M:385:TYR:HE1	12:M:523:VAL:HG23	1.82	0.43
13:N:119:GLY:O	13:N:120:THR:OG1	2.27	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
16:Q:99:MET:HE2	16:Q:447:VAL:HG21	2.00	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
18:T:47:ASP:N	18:T:50:ASP:OD2	2.47	0.43
17:S:43:TYR:CE2	21:W:68:ARG:HD2	2.53	0.43
1:A:36:LYS:HB2	1:A:39:ASP:CG	2.38	0.43
2:B:35:THR:N	8:I:105:GLU:O	2.51	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
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
3:C:163:SER:HB3	16:Q:123:LEU:HD11	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:NH1	10:K:99:PRO:HB3	2.33	0.43
12:M:341:ILE:HD13	12:M:367:CYS:SG	2.59	0.43
12:M:66:HIS:CE1	12:M:68:ARG:HG2	2.53	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
1:A:40:ARG:NH1	1:A:289:GLU:O	2.40	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
4:E:126:HIS:HD2	12:M:612:PRO:HD2	1.84	0.43
4:E:80:ASP:OD1	4:E:81:LEU:N	2.52	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:H141	47:V:203:PLX:H332	2.01	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
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.54	0.43
1:A:134:ASP:N	1:A:135:PRO:HD3	2.34	0.43
1:A:73:PRO:HB2	1:A:74:ASP:H	1.58	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
4:E:118:PHE:HZ	12:M:621:LYS:HG3	1.83	0.43
4:E:43:VAL:O	4:E:47:VAL:HG23	2.19	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	17:S:43:TYR:CE1	60.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:E:28:ALA:HA	4:E:31:ARG:HG3	1.99	0.42
9:J:204:SER:OG	9:J:240:VAL:HG23	2.18	0.42
9:J:221:HIS:C	9:J:221:HIS:ND1	2.73	0.42
9:J:293:LEU:HD23	9:J:298:TYR:HD1	1.84	0.42
4:E:48:HIS:HE1	9:J:363:SER:O	2.02	0.42
3:C:175:PRO:HB3	9:J:96:PRO:HD3	2.01	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: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
1:A:257:ARG:HH12	14:O:239:LYS:NZ	2.17	0.42
9:J:180:TYR:O	9:J:184:LYS:HG3	2.20	0.42
9:J:131:GLY:HA3	49:J:401:NDP:O3D	2.19	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
1:A:220:GLN:NE2	14:O:114:GLU:HB3	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
1:A:227:PRO:HB2	1:A:228:PRO:HD3	2.00	0.42
1:A:52:ARG:O	1:A:55:GLY:N	2.51	0.42
2:B:117:CYS:HB2	45:B:301:SF4:S1	2.59	0.42
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	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
16:Q:164:PRO:HA	16:Q:165:PRO:HD3	1.83	0.42
15:P:200:LYS:HE2	16:Q:420:TYR:CE1	2.55	0.42
18:T:79:GLU:OE1	18:T:122:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:18:ASP:OD1	23:Z:19:TYR:N	2.52	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
6:G:116:VAL:HA	6:G:119:ILE:HG22	2.01	0.42
6:G:93:ILE:HG12	6:G:94:ASP:O	2.19	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:124:HIS:HD2	16:Q:375:MET:HE2	1.84	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: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:102:ASN:HD21	18:T:104:ASP:HB2	1.84	0.42
18:T:52:ARG:O	18:T:55:ARG:HG2	2.20	0.42
19:U:40:LYS:O	19:U:44:MET:HG2	2.18	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
9:J:128:ASN:O	9:J:129:LEU:HD12	2.19	0.42
9:J:98:GLY:HA3	9:J:103:LEU:HG	2.01	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:164:THR:HG23	14:O:167:LYS:N	2.34	0.42
12:M:198:THR:CG2	14:O:39:PHE:HB3	2.47	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:7:PRO:O	17:S:10:SER:OG	2.23	0.42
8:I:40:LYS:HG2	21:W:8:GLN:HA	2.00	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
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
7:H:21:HIS:NE2	7:H:63:PRO:O	2.52	0.42
12:M:319:TRP:HH2	12:M:617:ARG:NE	2.18	0.42
7:H:83:GLN:HG2	15:P:107:GLN:HE21	1.84	0.42
16:Q:358:VAL:O	16:Q:364:SER:OG	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:100:LYS:O	14:O:104:VAL:HG23	2.20	0.42
9:J:209:ARG:HD2	15:P:217:LYS:CE	2.50	0.42
8:I:60:ARG:HD2	16:Q:390:GLN:O	2.19	0.42
16:Q:70:ASP:HB2	16:Q:71:PRO:HD3	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
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
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
16:Q:281:GLU:N	16:Q:281:GLU:CD	2.73	0.42
2:B:133:ARG:NH2	18:T:69:ILE:HG13	2.34	0.42
19:U:69:HIS:CE1	19:U:70:PRO:HA	2.54	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
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:HD2	12:M:543:LYS:N	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
18:T:80:VAL:O	18:T:121:GLN:HA	2.20	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
8:I:23:LYS:NZ	16:Q:252:SER:HG	2.18	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
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TRP:HZ3	1:A:436:GLN:HB3	1.84	0.41
1:A:116:ASN:HB3	46:A:502:FMN:HM83	2.01	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
9:J:157:LYS:HA	9:J:195:PHE:HE1	1.84	0.41
12:M:128:CYS:CB	12:M:129:PRO:CD	2.86	0.41
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.53	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:213:ILE:HG22	14:O:214:PRO:O	2.20	0.41
14:O:53:PHE:HE2	14:O:55:PHE:CE1	2.38	0.41
14:O:93:LEU:HA	14:O:94:PRO:HD2	1.86	0.41
47:B:303:PLX:H1A1	16:Q:269:ARG:HD2	2.02	0.41
16:Q:341:LEU:HD23	16:Q:341:LEU:HA	1.88	0.41
16:Q:83:ASN:CA	16:Q:98:VAL:HG22	2.44	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
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.92	0.41
2:B:128:ILE:HG12	2:B:143:TYR:CD1	2.56	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
2:B:40:ASN:C	2:B:42:GLN:H	2.21	0.41
2:B:62:THR:OG1	2:B:63:GLU:N	2.53	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
1:A:222:LYS:NZ	12:M:197:THR:HG21	2.35	0.41
1:A:63:TYR:HE2	1:A:64:LYS:NZ	2.15	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
1:A:382:CYS:HA	12:M:75:CYS:H	1.86	0.41
13:N:34:LYS:NZ	13:N:54:GLN:HG2	2.36	0.41
4:E:84:ILE:HD13	15:P:177:PHE:CE1	2.56	0.41
16:Q:149:GLN:OE1	16:Q:171:ARG:HB3	2.20	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:296:LEU:HD22	1:A:332:CYS:SG	2.61	0.41
1:A:63:TYR:CD2	1:A:64:LYS:HG3	2.55	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
1:A:329:LYS:HA	1:A:332:CYS:HB3	2.02	0.41
3:C:213:ARG:HG2	3:C:213:ARG:O	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:236:GLU:C	14:O:238:PRO:HD2	2.41	0.41
14:O:87:GLN:OE1	14:O:122:TYR:HA	2.21	0.41
1:A:123:GLY:CA	1:A:355:ILE:HD11	2.48	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:204:PHE:CE1	16:Q:207:ARG:HD3	2.56	0.41
21:W:86:MET:HG2	21:W:128:ARG:HH22	1.86	0.41
1:A:113:LEU:HD23	1:A:114:VAL:N	2.35	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.21	0.41
1:A:387:GLU:HG2	12:M:119:PHE:O	2.20	0.41
2:B:160:CYS:HA	2:B:161:PRO:HD2	1.83	0.41
3:C:137:VAL:HA	3:C:140:GLN:OE1	2.20	0.41
3:C:98:ALA:HB1	3:C:99:PRO:HD2	2.03	0.41
4:E:41:ARG:HE	6:G:120:MET:HE3	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:394:GLY:O	16:Q:413:SER:OG	2.23	0.41
18:T:33:SER:HB3	18:T:45:VAL:HG21	2.03	0.41
51:V:201:CDL:H722	51:V:201:CDL:H752	1.75	0.41
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.41
1:A:339:PHE:HA	1:A:342:LEU:HD12	2.03	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:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.41
2:B:101:LEU:O	2:B:192:GLY:HA3	2.21	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
12:M:236:TYR:CE1	12:M:272:ARG:HB3	2.55	0.41
1:A:284:HIS:CE1	14:O:229:GLY:HA3	2.56	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
20:V:114:ALA:HB1	20:V:118:PHE:CE2	2.56	0.41
47:B:303:PLX:H332	47:B:303:PLX:H301	1.80	0.41
2:B:57:ARG:HG2	2:B:62:THR:OG1	2.21	0.41
7:H:75:GLY:CA	8:I:103:ARG:HH11	2.34	0.41
9:J:329:LEU:HD13	9:J:332:LEU:HD12	2.03	0.41
9:J:62:THR:HG21	49:J:401:NDP:O1X	2.21	0.41
9:J:52:SER:CB	16:Q:103:GLY:HA3	58.85	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
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
1:A:314:LEU:O	1:A:329:LYS:HD2	2.21	0.40
2:B:155:PHE:HB2	45:B:302:SF4:S2	2.61	0.40
2:B:96:ARG:HD2	2:B:154:GLY:HA3	2.03	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
1:A:121:GLU:HA	1:A:122:PRO:HD3	1.87	0.40
1:A:53:LEU:O	1:A:56:SER:OG	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ARG:HB2	2:B:196:GLU:OE2	2.21	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
4:E:42:GLU:OE2	4:E:46:THR:OG1	2.40	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.61	0.40
14:O:197:THR:N	14:O:200:ASP:HB3	2.36	0.40
15:P:100:LEU:O	15:P:108:PHE:HD2	2.05	0.40
15:P:81:PHE:HE1	16:Q:157:LYS:O	2.03	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:H1B3	47:U:101:PLX:H22	1.86	0.40
47:V:203:PLX:H342	47:V:203:PLX:H371	1.76	0.40
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.86	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:483:ARG:O	12:M:483:ARG:HG3	2.21	0.40
12:M:382:ARG:NE	12:M:527:ASP:OD1	2.54	0.40
12:M:634:LEU:HA	12:M:635:PRO:HD3	1.91	0.40
13:N:29:ARG:HH22	13:N:65:THR:C	2.17	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
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:74:TRP:CZ3	22:Y:75:HIS:HA	2.53	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
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
5:F:66:TRP:CZ2	12:M:648:GLU:HB2	2.57	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:HD23	16:Q:255:LEU:HA	1.91	0.40
18:T:105:LYS:HB3	18:T:107:THR:HG22	2.04	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:121:LEU:HA	11:L:121:LEU:HD23	4.49	0.40
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:114:LEU:HG	15:P:130:TYR:HE1	1.87	0.40
15:P:52:ASP:O	15:P:56:LYS:HG3	2.22	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
21:W:27:ARG:C	21:W:29:GLY:N	2.75	0.40
19:U:50:PRO:HB2	21:W:69:ILE:HD11	2.03	0.40
22:Y:73:PHE:C	22:Y:73:PHE:HD1	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	8	49
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	28	70
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	5	40
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	10	52
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	7	46
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	29
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	3	31
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	22
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	49
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	1	12
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	4	39
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	28
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	39
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	26
16	Q	428/430 (100%)	397 (93%)	24 (6%)	7 (2%)	11	54
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	5	42
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	3	32
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	15	59
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	8	48
21	W	136/138 (99%)	127 (93%)	5 (4%)	4 (3%)	5	42
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	10
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	8	48
25	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	3	33
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	3	30
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	28	70
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	5	40
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	8	48
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	28
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	2	24
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	11	53
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	6	43
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	5	40
35	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	9	50
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	2	24
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	4	36
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	5	40
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	10	52
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	9	50
41	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	6	43
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	5	41
43	v	107/137 (78%)	90 (84%)	14 (13%)	3 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	6	43
All	All	8097/8236 (98%)	7338 (91%)	526 (6%)	233 (3%)	9	42

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
16	Q	69	VAL
10	K	102	GLY
32	i	338	PRO
28	e	135	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	82	92
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%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	71	89
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%)	94	98
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%)	369 (100%)	2 (0%)	91	96
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
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%)	49 (86%)	8 (14%)	4	27
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	68	88
25	b	118/122 (97%)	114 (97%)	4 (3%)	42	75
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	25	64
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%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	41	75
35	l	531/532 (100%)	511 (96%)	20 (4%)	38	73
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%)	156 (99%)	1 (1%)	89	95
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%)	7038 (99%)	55 (1%)	86	93

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
22	Y	73	PHE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	83	HIS
22	Y	87	PRO
22	Y	97	LEU
24	a	53	ARG
24	a	55	PHE
25	b	21	ARG
25	b	38	GLN

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Mol	Chain	Res	Type
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	115	TYR
27	d	117	GLN
34	k	1	MET
34	k	3	LEU
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN
35	l	87	MET
35	l	88	MET
35	l	94	LEU
35	l	95	PHE
35	l	97	THR
35	l	99	SER
35	l	191	LEU
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	447	ASN
35	l	450	LEU
35	l	452	ASN
39	p	124	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
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	688	GLN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	59	ASN
14	O	69	ASN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN

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Mol	Chain	Res	Type
15	P	124	ASN
15	P	247	GLN
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
17	S	44	HIS
17	S	68	ASN
18	T	64	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
22	Y	75	HIS
24	a	90	ASN
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS
25	b	126	GLN
26	c	56	ASN
26	c	84	HIS
26	c	154	GLN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	113	GLN
27	d	117	GLN
27	d	138	GLN
30	g	60	GLN
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS

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Mol	Chain	Res	Type
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
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	320	ASN
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	45	ASN
36	m	117	ASN
37	n	40	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	48	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	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

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Mol	Chain	Res	Type
42	u	99	HIS
42	u	104	GLN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	85	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	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 carbohydrates 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	$\# Z > 2$
45	SF4	A	501	1	0,12,12	0.00	-	0,24,24	0.00	-
46	FMN	A	502	-	31,33,33	1.46	5 (16%)	38,50,50	1.95	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	B	301	2	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
47	PLX	B	303	-	51,51,51	0.75	1 (1%)	54,59,59	0.69	1 (1%)
45	SF4	C	301	3	0,12,12	0.00	-	0,24,24	0.00	-
48	8Q1	E	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.54	8 (20%)
49	NDP	J	401	-	43,52,52	0.98	2 (4%)	49,80,80	1.41	3 (6%)
45	SF4	M	801	12	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	M	802	12	0,12,12	0.00	-	0,24,24	0.00	-
50	FES	M	803	-	0,4,4	0.00	-	0,4,4	0.00	-
50	FES	O	301	14	0,4,4	0.00	-	0,4,4	0.00	-
47	PLX	U	101	-	51,51,51	0.73	1 (1%)	54,59,59	0.74	2 (3%)
51	CDL	V	201	-	61,61,99	1.24	5 (8%)	60,71,111	0.99	3 (5%)
52	PEE	V	202	-	50,50,50	0.87	4 (8%)	52,55,55	0.85	2 (3%)
47	PLX	V	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.61	1 (1%)
52	PEE	W	201	-	50,50,50	0.86	4 (8%)	52,55,55	0.92	2 (3%)
47	PLX	b	201	-	51,51,51	0.60	0	54,59,59	0.64	0
47	PLX	g	201	-	51,51,51	0.81	1 (1%)	54,59,59	0.69	1 (1%)
47	PLX	g	202	-	51,51,51	0.74	1 (1%)	54,59,59	0.62	1 (1%)
47	PLX	g	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.59	1 (1%)
51	CDL	i	401	-	63,63,99	1.19	5 (7%)	65,75,111	1.10	5 (7%)
52	PEE	l	701	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
52	PEE	l	702	-	50,50,50	0.88	4 (8%)	52,55,55	0.93	2 (3%)
51	CDL	l	703	-	63,63,99	1.19	5 (7%)	65,75,111	1.12	4 (6%)
51	CDL	l	704	-	63,63,99	1.24	5 (7%)	65,75,111	1.06	4 (6%)
51	CDL	n	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.12	4 (6%)
48	8Q1	p	201	-	32,34,34	1.67	5 (15%)	39,43,43	1.80	5 (12%)
47	PLX	r	501	-	51,51,51	0.74	1 (1%)	54,59,59	0.66	1 (1%)
47	PLX	r	502	-	51,51,51	0.67	0	54,59,59	0.67	1 (1%)

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
45	SF4	A	501	1	-	0/0/48/48	0/6/5/5
46	FMN	A	502	-	-	0/16/18/18	0/3/3/3
45	SF4	B	301	2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	B	302	2	-	0/0/48/48	0/6/5/5
47	PLX	B	303	-	-	0/54/55/55	0/0/0/0
45	SF4	C	301	3	-	0/0/48/48	0/6/5/5
48	8Q1	E	201	-	-	2/41/41/41	0/0/0/0
49	NDP	J	401	-	-	0/30/77/77	0/5/5/5
45	SF4	M	801	12	-	0/0/48/48	0/6/5/5
45	SF4	M	802	12	-	0/0/48/48	0/6/5/5
50	FES	M	803	-	-	0/0/4/4	0/1/1/1
50	FES	O	301	14	-	0/0/4/4	0/1/1/1
47	PLX	U	101	-	-	0/54/55/55	0/0/0/0
51	CDL	V	201	-	-	0/69/69/110	0/0/0/0
52	PEE	V	202	-	-	0/54/54/54	0/0/0/0
47	PLX	V	203	-	-	0/54/55/55	0/0/0/0
52	PEE	W	201	-	-	0/54/54/54	0/0/0/0
47	PLX	b	201	-	-	0/54/55/55	0/0/0/0
47	PLX	g	201	-	-	0/54/55/55	0/0/0/0
47	PLX	g	202	-	-	0/54/55/55	0/0/0/0
47	PLX	g	203	-	-	0/54/55/55	0/0/0/0
51	CDL	i	401	-	-	0/74/74/110	0/0/0/0
52	PEE	l	701	-	-	0/52/52/54	0/0/0/0
52	PEE	l	702	-	-	0/54/54/54	0/0/0/0
51	CDL	l	703	-	-	0/74/74/110	0/0/0/0
51	CDL	l	704	-	-	0/74/74/110	0/0/0/0
51	CDL	n	101	-	-	2/74/74/110	0/0/0/0
48	8Q1	p	201	-	-	2/41/41/41	0/0/0/0
47	PLX	r	501	-	-	0/54/55/55	0/0/0/0
47	PLX	r	502	-	-	0/54/55/55	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	B	303	PLX	O6-C4	-2.89	1.40	1.44
47	g	203	PLX	O6-C4	-2.85	1.40	1.44
47	V	203	PLX	O6-C4	-2.75	1.40	1.44
47	g	201	PLX	O6-C4	-2.72	1.40	1.44
51	n	101	CDL	OB6-CB4	-2.64	1.39	1.46
48	E	201	8Q1	O35-C34	-2.52	1.18	1.23
51	V	201	CDL	OB6-CB4	-2.51	1.40	1.46
48	p	201	8Q1	O35-C34	-2.50	1.18	1.23
47	U	101	PLX	O6-C4	-2.48	1.41	1.44
47	g	202	PLX	O6-C4	-2.42	1.41	1.44
51	i	401	CDL	OB6-CB4	-2.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	r	501	PLX	O6-C4	-2.31	1.41	1.44
48	E	201	8Q1	O40-C39	-2.27	1.18	1.23
52	V	202	PEE	O3-C3	-2.27	1.40	1.45
48	p	201	8Q1	O40-C39	-2.27	1.18	1.23
51	l	704	CDL	OB6-CB4	-2.26	1.40	1.46
51	l	703	CDL	OB6-CB4	-2.25	1.40	1.46
52	l	702	PEE	O3-C3	-2.23	1.40	1.45
52	W	201	PEE	O3-C3	-2.20	1.40	1.45
52	l	702	PEE	O2-C2	-2.15	1.41	1.46
52	V	202	PEE	O2-C2	-2.15	1.41	1.46
52	W	201	PEE	O2-C2	-2.09	1.41	1.46
46	A	502	FMN	C6-C5A	-2.02	1.38	1.41
48	E	201	8Q1	C6-C1	2.05	1.53	1.50
52	W	201	PEE	O2-C10	2.17	1.40	1.34
52	V	202	PEE	O3-C30	2.23	1.39	1.33
52	W	201	PEE	O3-C30	2.23	1.39	1.33
52	l	702	PEE	O3-C30	2.32	1.40	1.33
52	l	702	PEE	O2-C10	2.33	1.41	1.34
52	V	202	PEE	O2-C10	2.35	1.41	1.34
48	p	201	8Q1	C1-S44	2.49	1.81	1.76
49	J	401	NDP	C5A-C4A	2.57	1.46	1.40
48	E	201	8Q1	C1-S44	2.60	1.81	1.76
46	A	502	FMN	C9A-C5A	2.92	1.48	1.42
46	A	502	FMN	C8-C7	3.00	1.48	1.41
51	i	401	CDL	OB6-CB5	3.02	1.43	1.34
49	J	401	NDP	C6N-C5N	3.04	1.38	1.33
51	V	201	CDL	OB6-CB5	3.05	1.43	1.34
51	l	703	CDL	OB6-CB5	3.14	1.43	1.34
51	n	101	CDL	OB6-CB5	3.20	1.43	1.34
52	l	701	PEE	O2-C10	3.23	1.43	1.34
51	l	704	CDL	OB6-CB5	3.23	1.43	1.34
51	i	401	CDL	OA8-CA7	3.72	1.44	1.33
46	A	502	FMN	C4-C4A	3.76	1.48	1.41
46	A	502	FMN	C4A-C10	3.79	1.47	1.41
51	l	703	CDL	OA8-CA7	3.80	1.44	1.33
51	n	101	CDL	OA8-CA7	3.89	1.44	1.33
51	i	401	CDL	OA6-CA5	3.91	1.45	1.34
51	i	401	CDL	OB8-CB7	4.02	1.45	1.33
51	l	704	CDL	OA6-CA5	4.03	1.46	1.34
51	n	101	CDL	OB8-CB7	4.07	1.45	1.33
51	V	201	CDL	OA8-CA7	4.07	1.44	1.32
52	l	701	PEE	O3-C30	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	l	704	CDL	OA8-CA7	4.12	1.45	1.33
51	V	201	CDL	OA6-CA5	4.14	1.46	1.34
51	V	201	CDL	OB8-CB7	4.15	1.45	1.33
51	l	703	CDL	OA6-CA5	4.16	1.46	1.34
51	n	101	CDL	OA6-CA5	4.20	1.46	1.34
51	l	703	CDL	OB8-CB7	4.22	1.45	1.33
51	l	704	CDL	OB8-CB7	4.33	1.46	1.33
48	E	201	8Q1	C39-N41	4.75	1.44	1.33
48	p	201	8Q1	C39-N41	5.05	1.45	1.33
48	E	201	8Q1	C34-N36	5.62	1.45	1.33
48	p	201	8Q1	C34-N36	5.67	1.45	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	J	401	NDP	N3A-C2A-N1A	-6.95	122.81	128.86
48	p	201	8Q1	O4-C1-C6	-4.85	119.70	123.95
46	A	502	FMN	C4-C4A-C10	-3.94	116.78	119.96
46	A	502	FMN	C4A-C4-N3	-3.39	118.66	123.48
48	E	201	8Q1	O4-C1-C6	-3.37	121.00	123.95
48	p	201	8Q1	O4-C1-S44	-2.88	119.83	122.84
49	J	401	NDP	C4A-C5A-N7A	-2.63	106.87	109.41
48	E	201	8Q1	O4-C1-S44	-2.49	120.23	122.84
48	E	201	8Q1	O35-C34-N36	-2.40	118.45	123.07
48	E	201	8Q1	C42-N41-C39	-2.35	118.33	122.84
48	E	201	8Q1	C37-N36-C34	-2.29	118.33	122.59
47	U	101	PLX	C5-C4-C3	-2.21	106.87	111.86
47	r	502	PLX	C2-C1-N1	-2.09	108.79	115.86
51	i	401	CDL	CA4-OA6-CA5	-2.03	113.09	117.88
46	A	502	FMN	C1'-N10-C9A	2.01	120.19	118.35
49	J	401	NDP	C3D-C2D-C1D	2.18	105.62	101.43
47	r	501	PLX	C1C-N1-C1	2.20	118.35	109.93
47	g	202	PLX	C1C-N1-C1	2.34	118.90	109.93
47	g	201	PLX	C1C-N1-C1	2.35	118.93	109.93
47	g	203	PLX	C1C-N1-C1	2.42	119.21	109.93
47	U	101	PLX	C1C-N1-C1	2.44	119.30	109.93
48	p	201	8Q1	C38-C39-N41	2.45	120.71	116.49
47	V	203	PLX	C1C-N1-C1	2.47	119.40	109.93
52	l	701	PEE	O3-C30-C31	2.48	119.10	111.90
47	B	303	PLX	C1C-N1-C1	2.52	119.59	109.93
48	p	201	8Q1	C43-S44-C1	2.54	110.31	101.90
51	i	401	CDL	OA8-CA7-C31	2.60	119.47	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	E	201	8Q1	C32-C34-N36	2.61	122.01	116.58
48	E	201	8Q1	C43-S44-C1	2.62	110.56	101.90
51	V	201	CDL	OB8-CB7-C71	2.73	119.86	111.90
51	l	704	CDL	OB8-CB7-C71	2.88	120.28	111.90
51	l	703	CDL	OB8-CB7-C71	2.89	120.32	111.90
51	n	101	CDL	OB8-CB7-C71	2.91	120.36	111.90
52	W	201	PEE	O3-C30-C31	2.91	120.38	111.90
51	l	704	CDL	OA8-CA7-C31	2.94	120.45	111.90
46	A	502	FMN	C5A-C9A-N10	2.94	119.84	117.66
51	n	101	CDL	OA8-CA7-C31	2.95	120.49	111.90
51	i	401	CDL	OB8-CB7-C71	2.97	120.55	111.90
52	l	702	PEE	O3-C30-C31	3.07	120.84	111.90
52	V	202	PEE	O3-C30-C31	3.08	120.86	111.90
51	l	703	CDL	OA8-CA7-C31	3.22	121.28	111.90
46	A	502	FMN	C1'-N10-C10	3.25	121.83	118.50
46	A	502	FMN	C4-C4A-N5	3.25	122.25	118.68
46	A	502	FMN	C4A-N5-C5A	3.43	120.38	116.76
51	V	201	CDL	OA6-CA5-C11	3.55	118.92	111.55
51	i	401	CDL	OB6-CB5-C51	3.62	119.06	111.55
52	V	202	PEE	O2-C10-C11	3.71	119.25	111.55
52	W	201	PEE	O2-C10-C11	3.80	119.45	111.55
51	n	101	CDL	OA6-CA5-C11	4.04	119.94	111.55
51	l	704	CDL	OB6-CB5-C51	4.05	119.96	111.55
51	l	703	CDL	OB6-CB5-C51	4.07	120.00	111.55
52	l	701	PEE	O2-C10-C11	4.14	120.14	111.55
51	n	101	CDL	OB6-CB5-C51	4.21	120.29	111.55
51	V	201	CDL	OB6-CB5-C51	4.22	120.32	111.55
51	l	704	CDL	OA6-CA5-C11	4.24	120.36	111.55
51	i	401	CDL	OA6-CA5-C11	4.26	120.39	111.55
51	l	703	CDL	OA6-CA5-C11	4.30	120.48	111.55
52	l	702	PEE	O2-C10-C11	4.53	120.95	111.55
48	E	201	8Q1	C6-C1-S44	5.45	118.77	113.28
48	p	201	8Q1	C6-C1-S44	7.14	120.47	113.28
46	A	502	FMN	C4-N3-C2	7.29	121.54	115.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	E	201	8Q1	C29-C32-C34-N36
48	E	201	8Q1	O35-C34-C32-C29
51	n	101	CDL	CA4-OA6-CA5-OA7

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Mol	Chain	Res	Type	Atoms
51	n	101	CDL	CA4-OA6-CA5-C11
48	p	201	8Q1	C6-C1-S44-C43
48	p	201	8Q1	O4-C1-S44-C43

There are no ring outliers.

15 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	501	SF4	6	0
46	A	502	FMN	17	0
45	B	301	SF4	1	0
45	B	302	SF4	2	0
47	B	303	PLX	3	0
48	E	201	8Q1	4	0
49	J	401	NDP	26	0
45	M	801	SF4	3	0
50	M	803	FES	1	0
50	O	301	FES	2	0
47	U	101	PLX	1	0
51	V	201	CDL	8	0
52	V	202	PEE	12	0
47	V	203	PLX	2	0
52	W	201	PEE	5	0

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.