



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 29, 2016 – 11:02 AM EST

PDB ID : 5LNK
EMDB ID: : EMD-4093
Title : Entire ovine respiratory complex I
Authors : Fiedorczuk, K.; Letts, J.A.; Kaszuba, K.; Sazanov, L.A.
Deposited on : 2016-08-04
Resolution : 3.90 Å(reported)
Based on PDB ID : 4HEA

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 : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

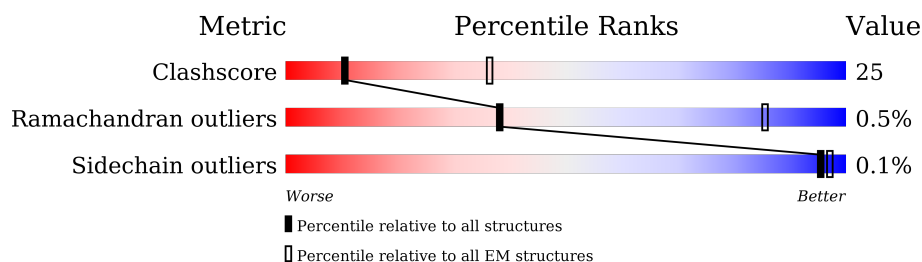
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.









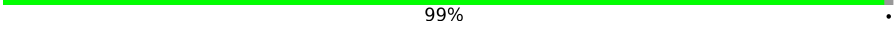

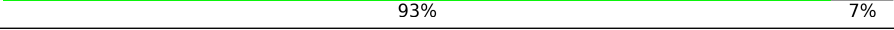

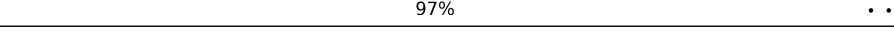
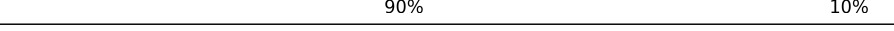

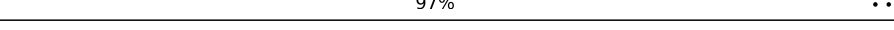

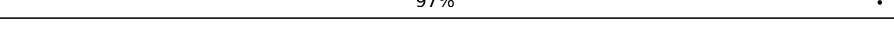
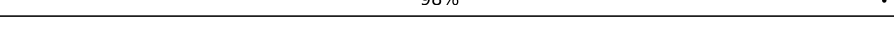

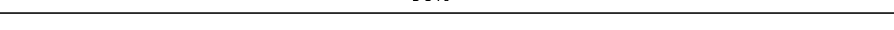
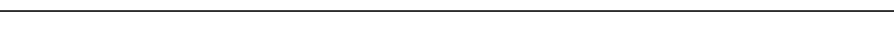

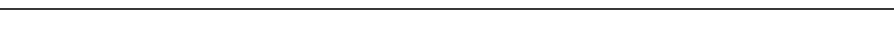
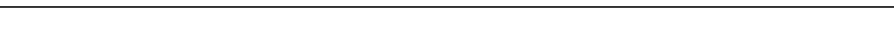


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	1	445	
2	2	217	
3	3	704	
4	4	412	
5	5	228	
6	6	179	
7	9	176	
8	H	318	
9	N	347	

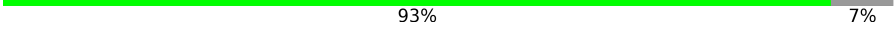
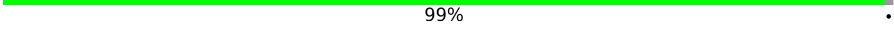


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Mol	Chain	Length	Quality of chain
10	A	115	 53% 45% .
11	M	459	 48% 52%
12	K	98	 58% 30% 12%
13	L	599	 45% 54% .
14	J	175	 61% 39%
15	a	75	 55% 45%
16	b	96	 99% .
17	c	133	 92% . 8%
18	d	338	 93% 7%
19	e	98	 84% . 14%
20	f	115	 97% . .
21	g	127	 90% 10%
22	h	112	 84% . 15%
23	i	145	 97% . .
24	X	88	 57% 43%
24	j	88	 97% .
25	k	320	 98% .
26	l	105	 90% 10%
27	m	83	 96% .
28	n	97	 72% . 24%
29	o	120	 99% .
30	p	128	 86% . 13%
31	q	143	 96% . .
32	r	127	 71% . 27%
33	s	136	 85% . . 13%

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Mol	Chain	Length	Quality of chain
34	t	178	 90% 7%
35	u	72	 92% 8%
36	v	158	 84% 5% 9%
37	w	125	 67% 31%
38	x	49	 98%
39	y	57	 93% 7%
40	z	70	 99%
41	Z	175	 61% 35%
42	Y	171	 47% 53%
43	W	143	 62% 35%
44	V	119	 86% 14%

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	1	500	-	-	X	-
45	SF4	6	300	-	-	X	-
45	SF4	9	502	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 63760 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 Mitochondrial complex I, 51 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	432	Total	C	N	O	S	0	0
			3328	2097	596	615	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	214	Total	C	N	O	S	0	0
			1655	1056	279	310	10		

- Molecule 3 is a protein called Mitochondrial complex I, 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	387	Total	C	N	O	S	0	0
			3098	1974	535	565	24		

- Molecule 5 is a protein called Mitochondrial complex I, 30 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called Mitochondrial complex I, ND1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

- Molecule 9 is a protein called Mitochondrial complex I, ND2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 10 is a protein called Mitochondrial complex I, ND3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

- Molecule 11 is a protein called Mitochondrial complex I, ND4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	459	Total	C	N	O	S	0	0
			3645	2428	571	606	40		

- Molecule 12 is a protein called Mitochondrial complex I, ND4L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	86	Total	C	N	O	S	0	0
			649	428	96	111	14		

- Molecule 13 is a protein called Mitochondrial complex I, ND5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	599	Total	C	N	O	S	0	0
			4456	2926	714	777	39		

- Molecule 14 is a protein called Mitochondrial complex I, ND6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	175	Total	C	N	O	S	0	0
			1188	780	184	214	10		

- Molecule 15 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	41	Total	C	N	O	S	0	0
			343	213	61	68	1		

- Molecule 16 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 17 is a protein called Mitochondrial complex I, 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	123	Total	C	N	O	S	0	0
			1000	631	178	188	3		

- Molecule 18 is a protein called Mitochondrial complex I, 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	314	Total	C	N	O	S	0	0
			2473	1585	448	435	5		

- Molecule 19 is a protein called Mitochondrial complex I, B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

- Molecule 20 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	112	Total	C	N	O	S	0	0
			909	589	152	166	2		

- Molecule 21 is a protein called Mitochondrial complex I, B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 22 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	95	Total	C	N	O	S	0	0
			757	473	144	137	3		

- Molecule 23 is a protein called Mitochondrial complex I, B17.2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	144	Total	C	N	O	S	0	0
			1200	772	214	209	5		

- Molecule 24 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	85	Total	C	N	O	S	0	0
			684	442	101	136	5		
24	X	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 25 is a protein called Mitochondrial complex I, 42 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	320	Total	C	N	O	S	0	0
			2268	1430	394	435	9		

- Molecule 26 is a protein called Mitochondrial complex I, 15 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	95	Total	C	N	O	S	0	0
			792	503	146	137	6		

- Molecule 27 is a protein called Mitochondrial complex I, B9 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 28 is a protein called Mitochondrial complex I, B12 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	74	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 29 is a protein called Mitochondrial complex I, B14.5b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 30 is a protein called Mitochondrial complex I, B15 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	112	Total	C	N	O	S	0	0
			841	526	162	152	1		

- Molecule 31 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	140	Total	C	N	O	S	0	0
			1151	739	202	201	9		

- Molecule 32 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	93	Total	C	N	O	S	0	0
			752	491	131	130			

- Molecule 33 is a protein called Mitochondrial complex I, B18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	s	118	Total	C	N	O	S	0	0
			988	616	187	176	9		

- Molecule 34 is a protein called Mitochondrial complex I, B22 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	166	Total	C	N	O	S	0	0
			1434	916	265	247	6		

- Molecule 35 is a protein called Mitochondrial complex I, AGGG subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	66	Total	C	N	O	S	0	0
			563	372	94	96	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	v	143	Total	C	N	O	S	0	0
			861	544	155	158	4		

- Molecule 37 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	w	86	Total	C	N	O	S	0	0
			715	462	119	130	4		

- Molecule 38 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	x	48	Total	C	N	O	0	0
			403	266	69	68		

- Molecule 39 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	y	53	Total	C	N	O	0	0
			457	301	80	76		

- Molecule 40 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	z	69	Total	C	N	O	S	0	0
			568	364	105	95	4		

- Molecule 41 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 42 is a protein called Mitochondrial complex I, PGIV subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

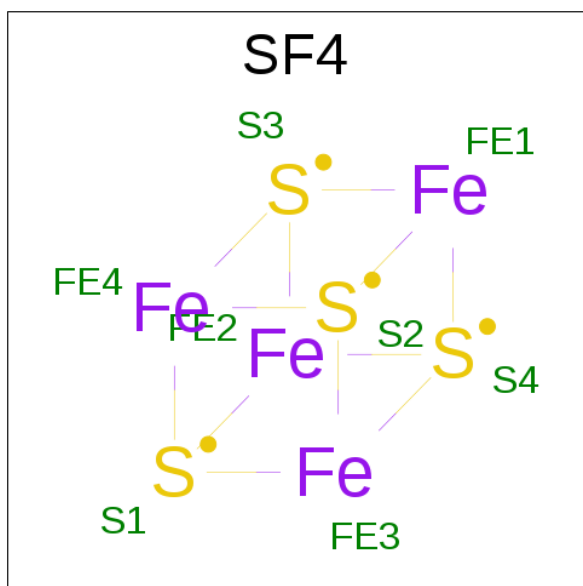
- Molecule 43 is a protein called Mitochondrial complex I, SGD1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 44 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	119	Total	C	N	O	S	0	0
			595	357	119	119			

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



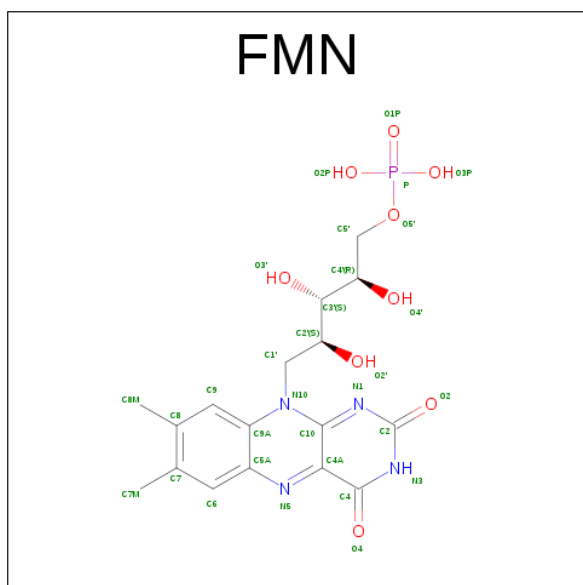
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			16	8	8	
45	3	1	Total	Fe	S	0
			16	8	8	
45	6	1	Total	Fe	S	0
			8	4	4	

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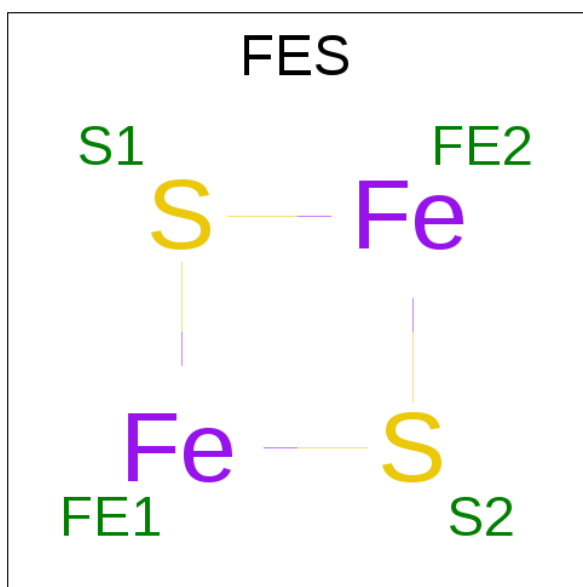
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			16	8	8	
45	9	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



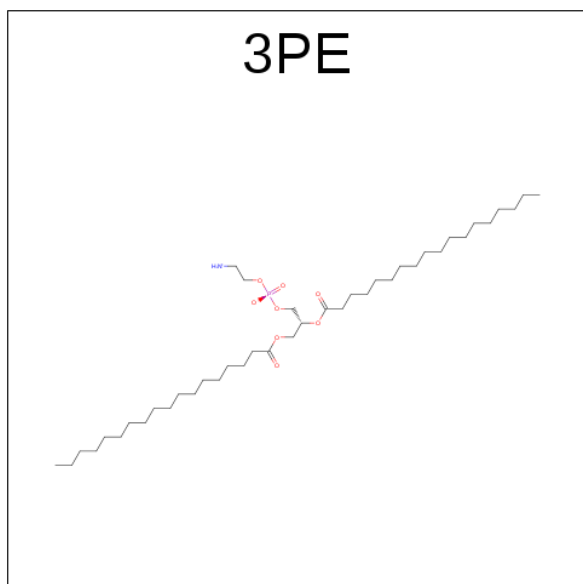
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	2	1	Total	Fe	S	0
			4	2	2	
47	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



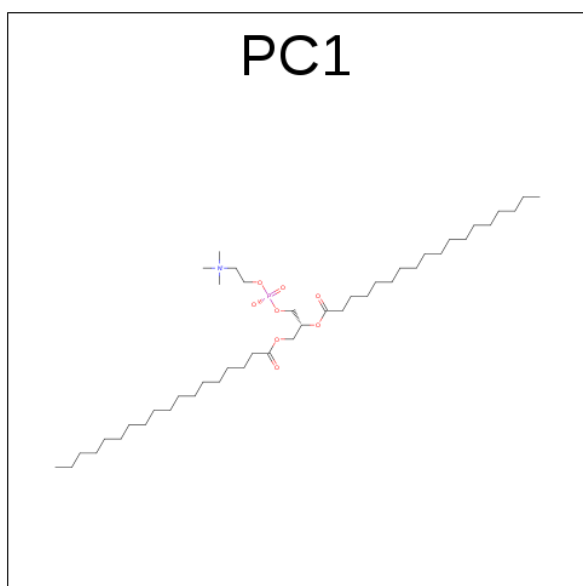
Mol	Chain	Residues	Atoms					AltConf
48	9	1	Total	C	N	O	P	0
			51	41	1	8	1	

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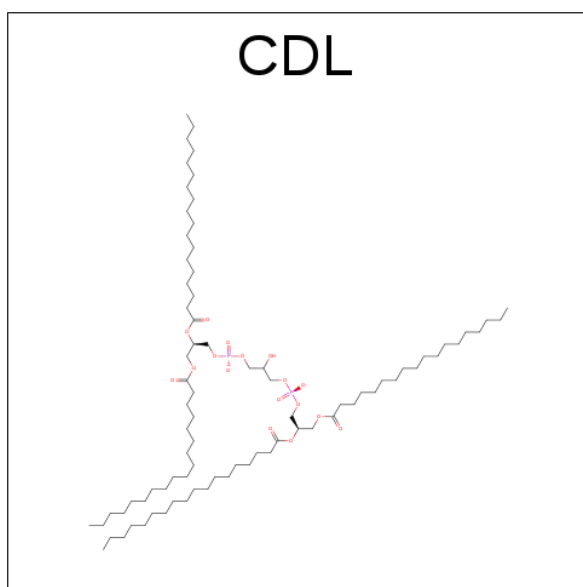
Mol	Chain	Residues	Atoms					AltConf
48	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	o	1	Total	C	N	O	P	0
			87	67	2	16	2	
48	o	1	Total	C	N	O	P	0
			87	67	2	16	2	

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
49	N	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	o	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

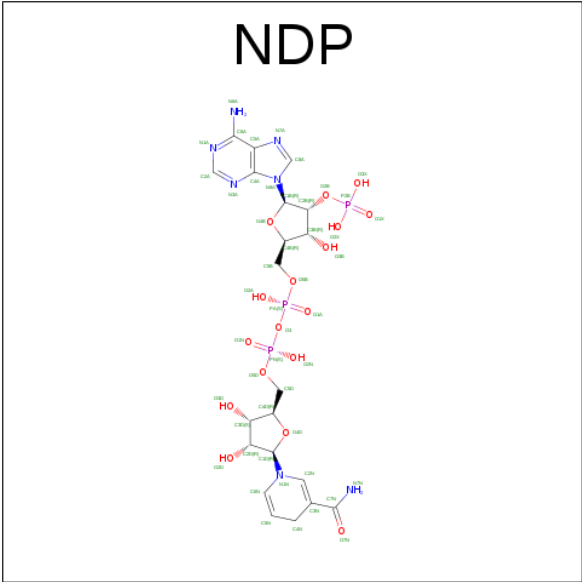


Mol	Chain	Residues	Atoms				AltConf
50	M	1	Total	C	O	P	0
			82	63	17	2	
50	L	1	Total	C	O	P	0
			84	65	17	2	
50	J	1	Total	C	O	P	0
			79	60	17	2	
50	i	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

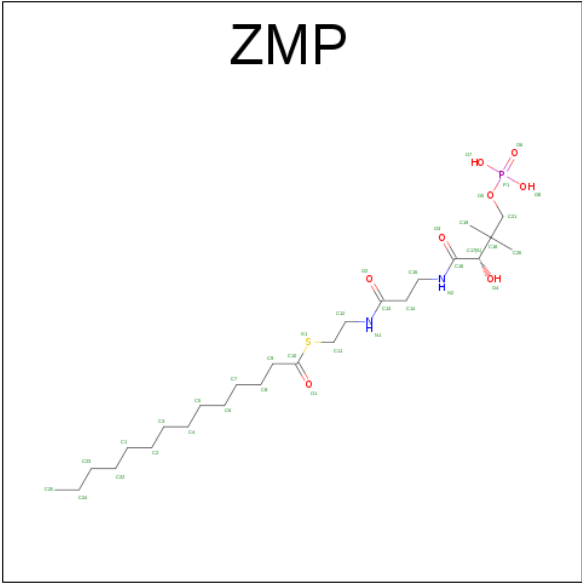
Mol	Chain	Residues	Atoms		AltConf
51	b	1	Total	Zn	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



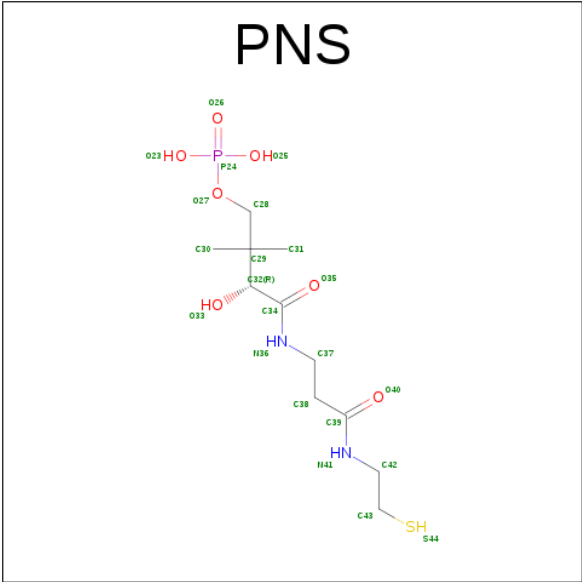
Mol	Chain	Residues	Atoms					AltConf
52	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
53	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 54 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).

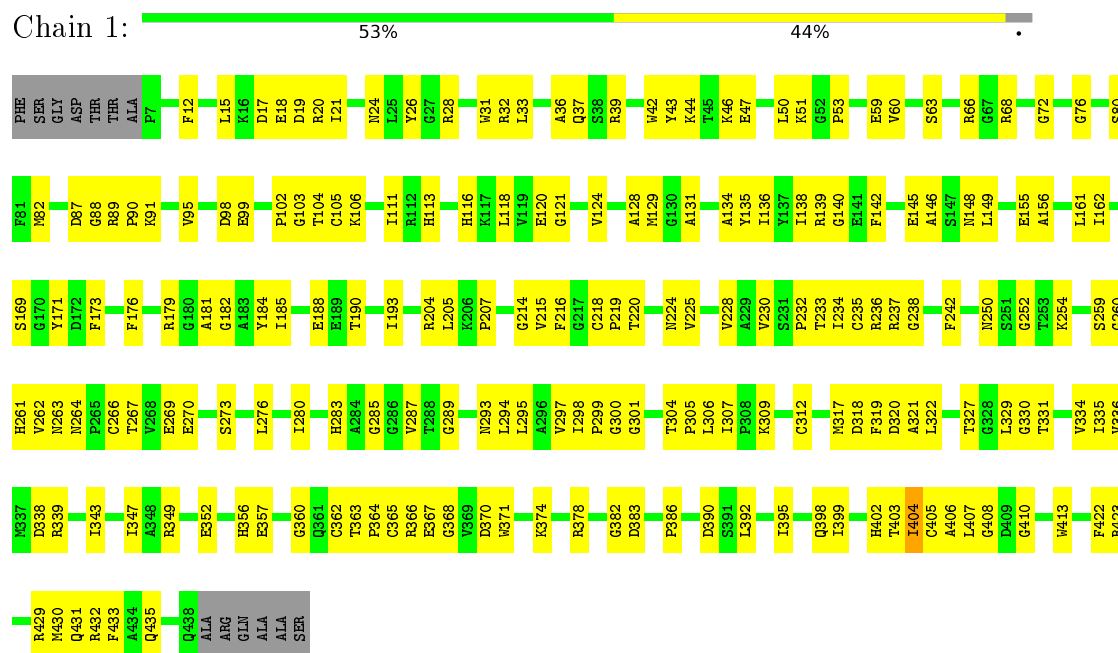


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
54	X	1	21	11	2	6	1	1	0

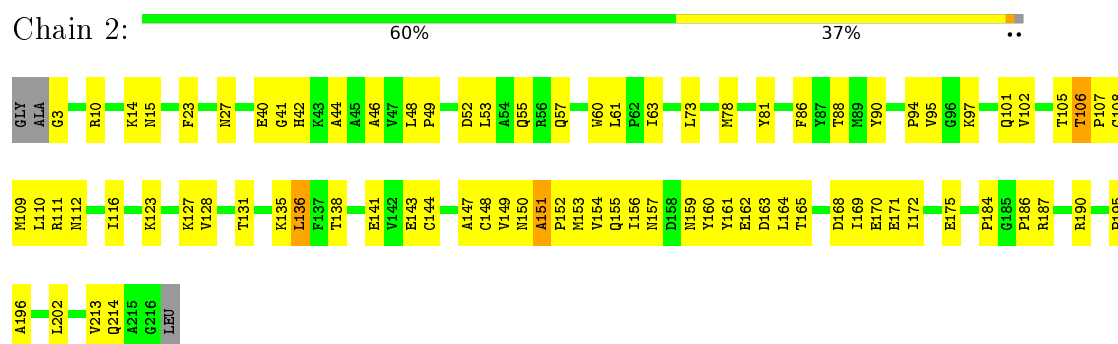
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Mitochondrial complex I, 51 kDa subunit

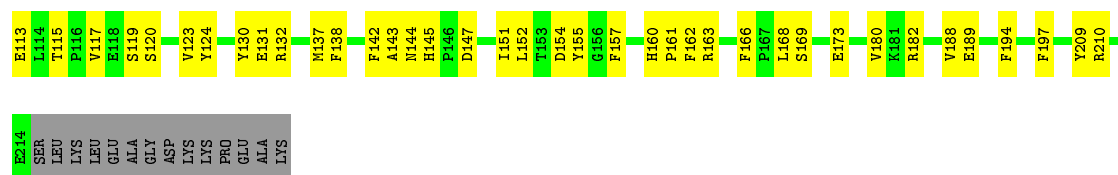


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

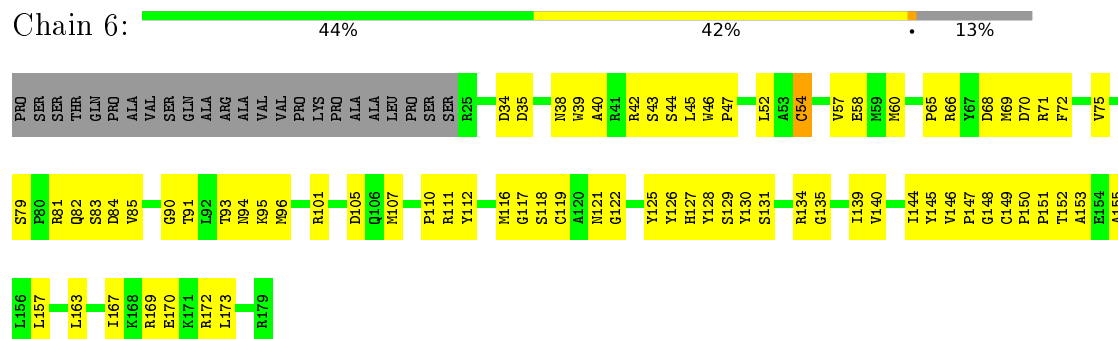


- Molecule 3: Mitochondrial complex I, 75 kDa subunit

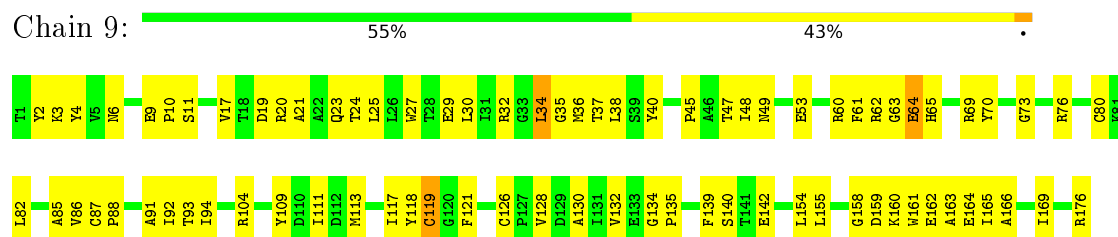




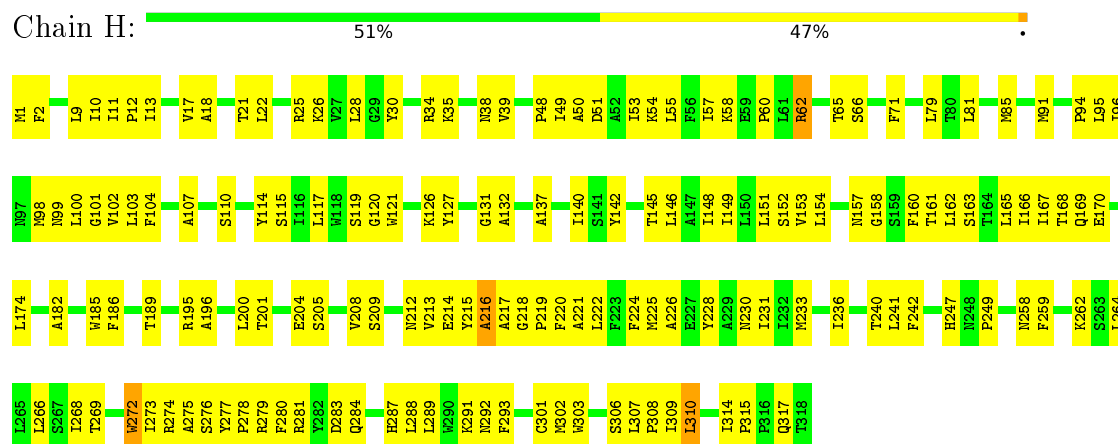
- Molecule 6: Mitochondrial complex I, PSST subunit



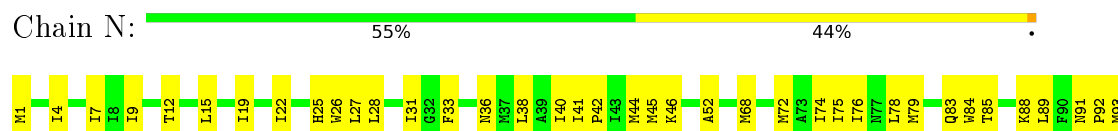
- Molecule 7: Mitochondrial complex I, TYKY subunit

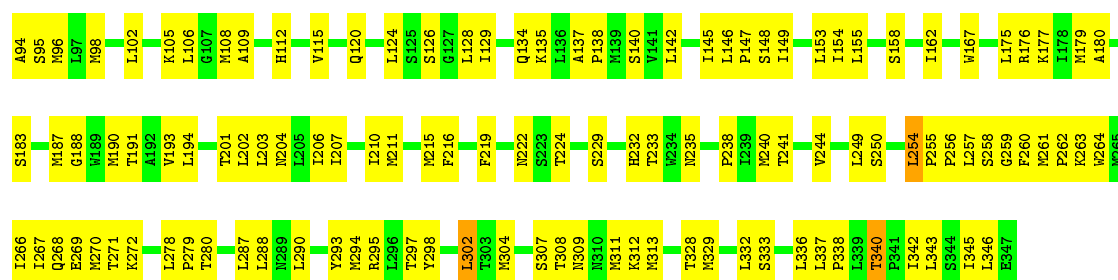


- Molecule 8: Mitochondrial complex I, ND1 subunit

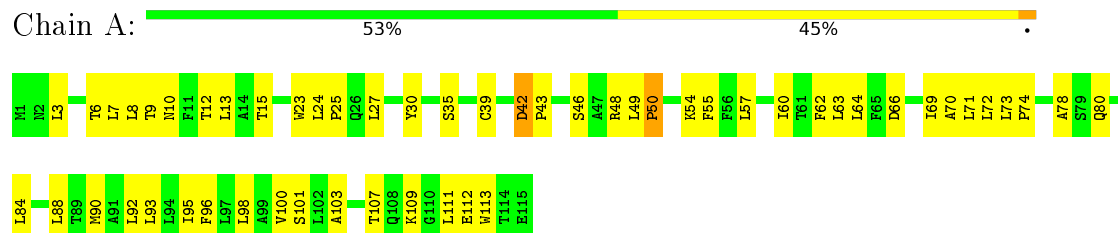


- Molecule 9: Mitochondrial complex I, ND2 subunit

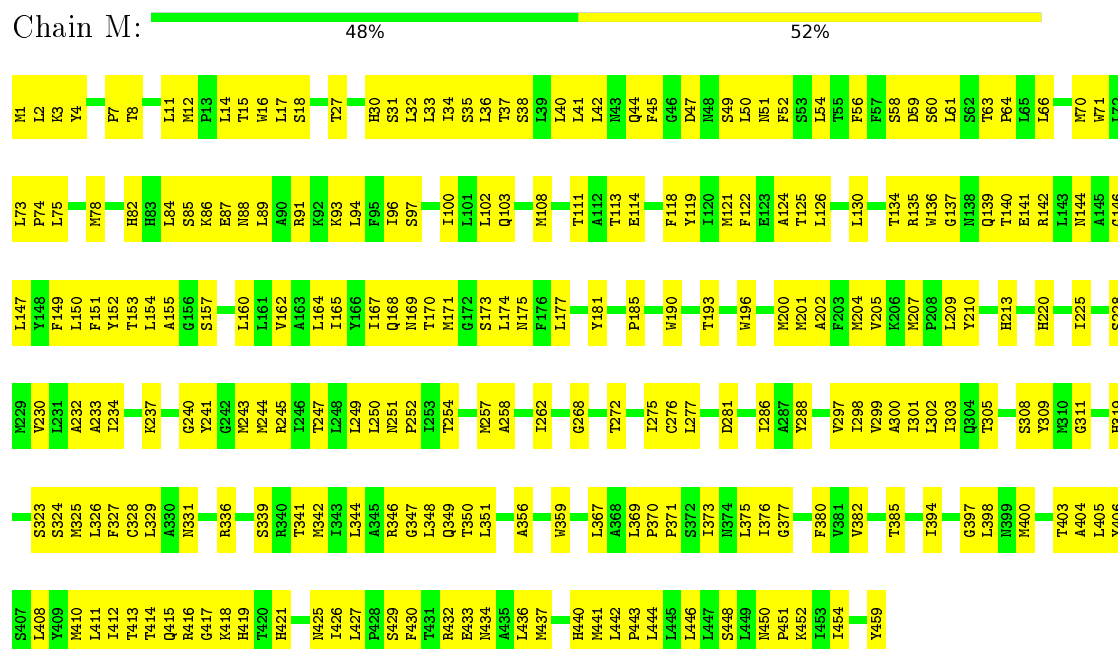




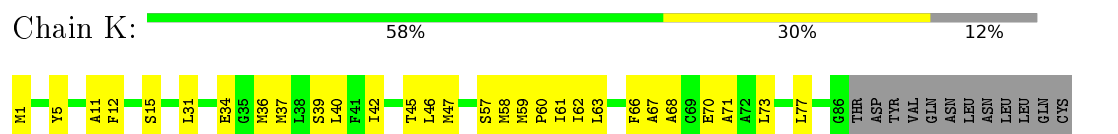
• Molecule 10: Mitochondrial complex I, ND3 subunit



• Molecule 11: Mitochondrial complex I, ND4 subunit

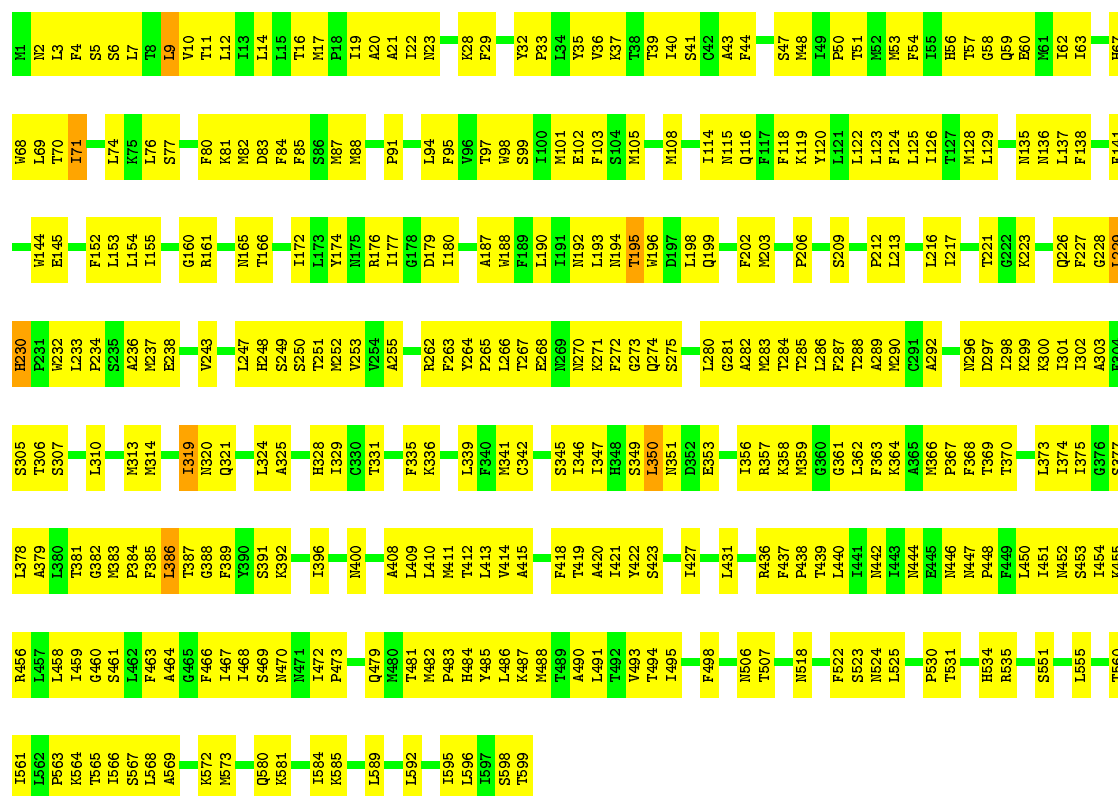


• Molecule 12: Mitochondrial complex I, ND4L subunit



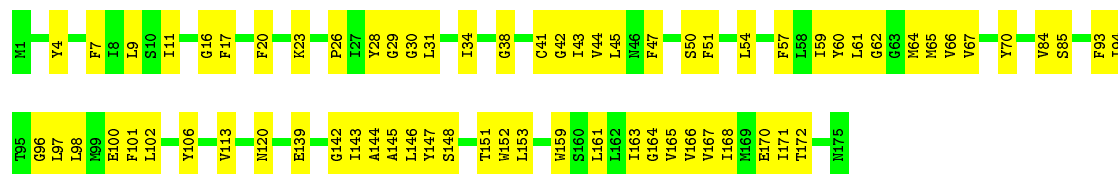
• Molecule 13: Mitochondrial complex I, ND5 subunit





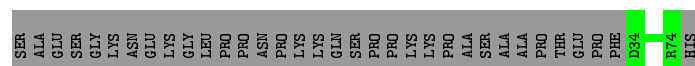
• Molecule 14: Mitochondrial complex I, ND6 subunit

Chain J: 61% 39%



• Molecule 15: Mitochondrial complex I, 10 kDa subunit

Chain a: 55% 45%



• Molecule 16: Mitochondrial complex I, 13 kDa subunit

Chain b: 99%



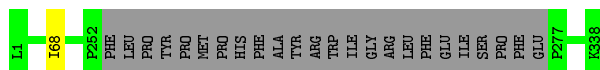
• Molecule 17: Mitochondrial complex I, 18 kDa subunit

Chain c: 92% 8%



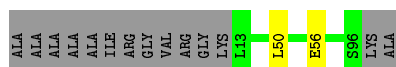
- Molecule 18: Mitochondrial complex I, 39 kDa subunit

Chain d: 93% 7%



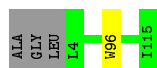
- Molecule 19: Mitochondrial complex I, B8 subunit

Chain e: 84% 14%



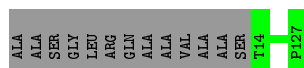
- Molecule 20: Mitochondrial complex I, B13 subunit

Chain f: 97% 2%



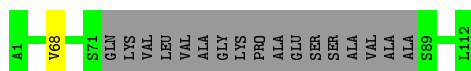
- Molecule 21: Mitochondrial complex I, B14 subunit

Chain g: 90% 10%



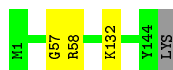
- Molecule 22: Mitochondrial complex I, B14.5a subunit

Chain h: 84% 15%



- Molecule 23: Mitochondrial complex I, B17.2 subunit

Chain i: 97% 2%

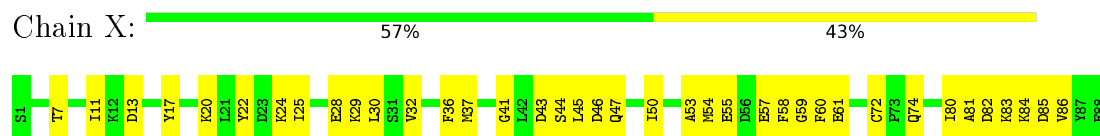


- Molecule 24: Acyl carrier protein

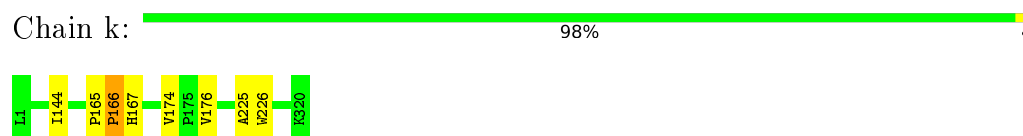
Chain j: 97% 2%



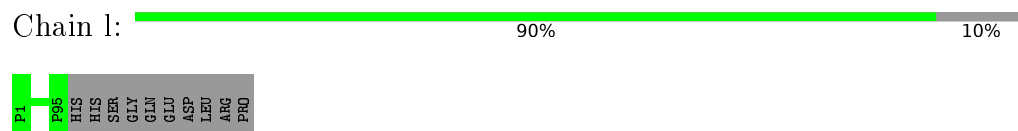
- Molecule 24: Acyl carrier protein



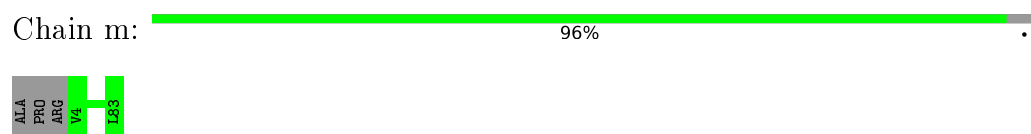
- Molecule 25: Mitochondrial complex I, 42 kDa subunit



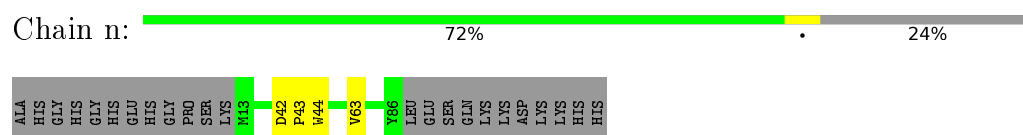
- Molecule 26: Mitochondrial complex I, 15 kDa subunit



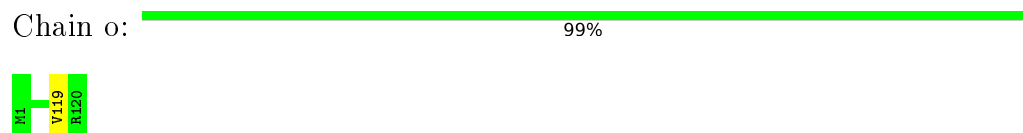
- Molecule 27: Mitochondrial complex I, B9 subunit



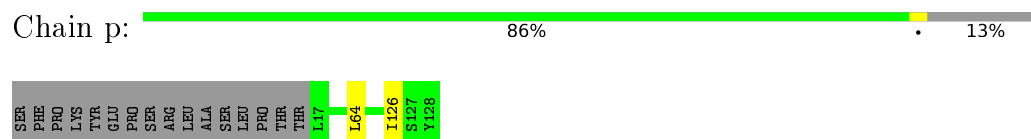
- Molecule 28: Mitochondrial complex I, B12 subunit



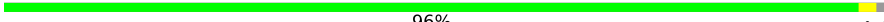
- Molecule 29: Mitochondrial complex I, B14.5b subunit



- Molecule 30: Mitochondrial complex I, B15 subunit



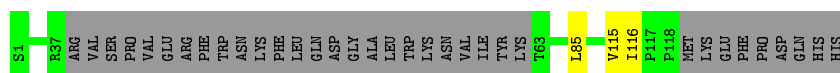
- Molecule 31: Mitochondrial complex I, B16.6 subunit

Chain q:  96% ..




- Molecule 32: Mitochondrial complex I, B17 subunit

Chain r:  71% . 27%



- Molecule 33: Mitochondrial complex I, B18 subunit

Chain s:  85% .. 13%



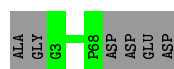
- Molecule 34: Mitochondrial complex I, B22 subunit

Chain t:  90% . 7%




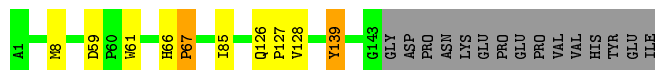
- Molecule 35: Mitochondrial complex I, AGGG subunit

Chain u:  92% 8%



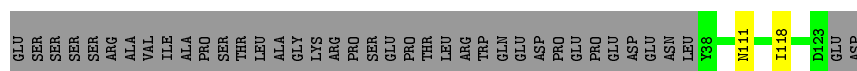
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:  84% 5% . 9%



- Molecule 37: Mitochondrial complex I, ESSS subunit

Chain w:  67% . 31%



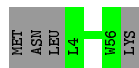
- Molecule 38: Mitochondrial complex I, KFYI subunit

Chain x:  98% .



- Molecule 39: Mitochondrial complex I, MNLL subunit

Chain y: 93% 7%



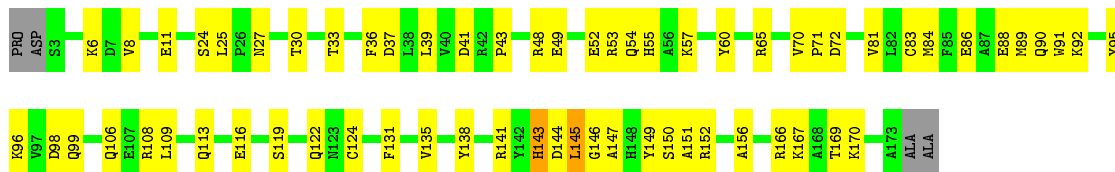
- Molecule 40: Mitochondrial complex I, MWFE subunit

Chain z: 99% .



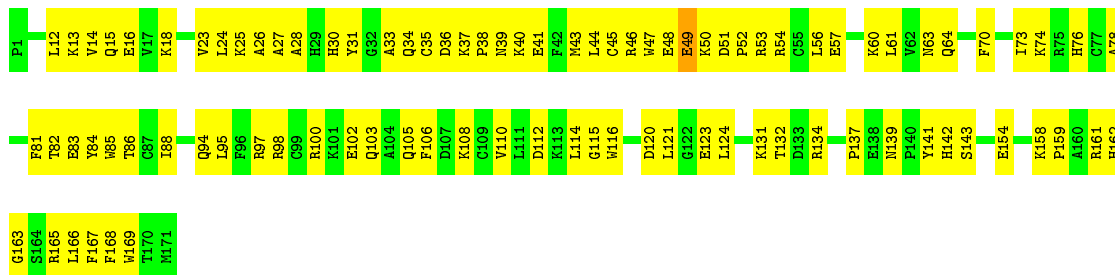
- Molecule 41: Mitochondrial complex I, PDSW subunit

Chain Z: 61% 35% ..



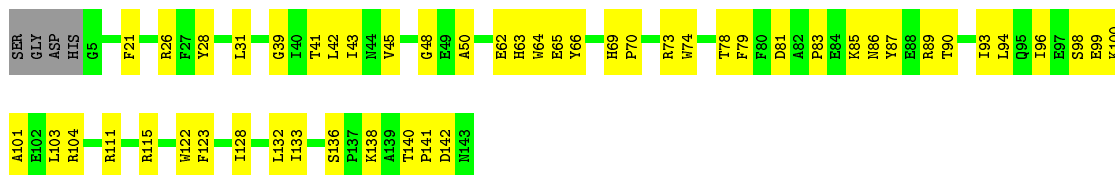
- Molecule 42: Mitochondrial complex I, PGIV subunit

Chain Y: 47% 53% .

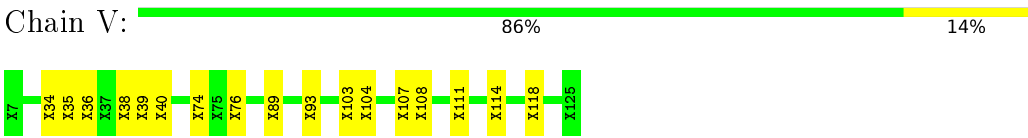


- Molecule 43: Mitochondrial complex I, SGDHI subunit

Chain W: 62% 35% .



- Molecule 44: Mitochondrial complex I, B14.7 subunit



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	82000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	100720	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CDL, PNS, PC1, FMN, FES, SF4, NDP, ZMP, 3PE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	1	0.34	0/3403	0.52	0/4597
10	A	0.42	1/947 (0.1%)	0.61	0/1296
11	M	0.38	0/3739	0.62	0/5095
12	K	0.36	0/658	0.62	0/888
13	L	0.37	0/4563	0.64	3/6227 (0.0%)
14	J	0.41	0/1212	0.57	0/1652
15	a	0.29	0/352	0.53	0/476
16	b	0.38	0/749	0.50	0/1009
17	c	0.36	0/1023	0.56	0/1382
18	d	0.33	0/2532	0.59	0/3430
19	e	0.47	1/688 (0.1%)	0.53	0/927
2	2	0.35	0/1695	0.59	1/2305 (0.0%)
20	f	0.32	0/929	0.51	0/1260
21	g	0.34	0/993	0.49	0/1336
22	h	0.33	0/775	0.61	0/1048
23	i	0.32	0/1241	0.54	0/1687
24	X	0.32	0/719	0.55	0/971
24	j	0.30	0/696	0.53	0/940
25	k	0.34	1/2309 (0.0%)	0.56	0/3141
26	l	0.36	0/811	0.57	0/1085
27	m	0.34	0/647	0.49	0/890
28	n	0.34	0/595	0.66	0/805
29	o	0.38	0/1035	0.55	0/1398
3	3	0.34	0/5362	0.53	0/7266
30	p	0.30	0/855	0.54	1/1155 (0.1%)
31	q	0.36	0/1180	0.63	1/1590 (0.1%)
32	r	0.37	0/774	0.62	1/1058 (0.1%)
33	s	0.32	0/1011	0.58	0/1356
34	t	0.41	1/1483 (0.1%)	0.56	1/2006 (0.0%)
35	u	0.35	0/590	0.59	0/809
36	v	0.30	0/877	0.65	0/1208
37	w	0.38	0/737	0.57	0/999

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	x	0.31	0/416	0.46	0/564
39	y	0.34	0/470	0.47	0/636
4	4	0.41	0/3172	0.57	1/4288 (0.0%)
40	z	0.38	0/583	0.55	0/785
41	Z	0.38	0/1475	0.55	0/1989
42	Y	0.39	0/1440	0.68	0/1942
43	W	0.39	0/1188	0.54	0/1607
5	5	0.40	0/1776	0.52	0/2417
6	6	0.42	0/1272	0.54	0/1720
7	9	0.45	1/1445 (0.1%)	0.64	1/1956 (0.1%)
8	H	0.43	0/2603	0.63	1/3561 (0.0%)
9	N	0.42	1/2787 (0.0%)	0.62	0/3795
All	All	0.37	6/63807 (0.0%)	0.58	11/86552 (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
10	A	0	2
13	L	0	6
17	c	0	1
19	e	0	1
2	2	0	1
20	f	0	1
23	i	0	1
25	k	0	3
29	o	0	1
31	q	0	2
33	s	0	2
34	t	0	1
36	v	0	7
4	4	0	1
42	Y	0	1
7	9	0	1
8	H	0	3
9	N	0	3
All	All	0	38

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	50	LEU	C-N	-9.90	1.15	1.34
34	t	163	PRO	C-N	9.08	1.51	1.34
25	k	174	VAL	C-N	-8.55	1.18	1.34
9	N	304	MET	C-N	-7.74	1.16	1.34
10	A	42	ASP	C-N	5.94	1.45	1.34
7	9	119	CYS	CB-SG	-5.03	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	74	GLN	C-N-CA	-6.59	105.21	121.70
4	4	47	LEU	CA-CB-CG	6.59	130.45	115.30
7	9	34	LEU	CA-CB-CG	-6.21	101.03	115.30
13	L	9	LEU	CA-CB-CG	6.18	129.52	115.30
30	p	64	LEU	CA-CB-CG	5.77	128.57	115.30
13	L	229	LEU	CA-CB-CG	5.60	128.18	115.30
8	H	310	LEU	CB-CG-CD2	-5.49	101.67	111.00
32	r	85	LEU	CA-CB-CG	-5.40	102.88	115.30
13	L	386	LEU	CA-CB-CG	5.36	127.64	115.30
2	2	136	LEU	CA-CB-CG	5.24	127.35	115.30
31	q	70	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	151	ALA	Peptide
4	4	54	GLN	Peptide
7	9	64	GLU	Peptide
10	A	112	GLU	Peptide
10	A	39	CYS	Peptide
8	H	216	ALA	Peptide
8	H	272	TRP	Peptide
8	H	62	ARG	Peptide
13	L	195	THR	Peptide
13	L	230	HIS	Peptide
13	L	350	LEU	Peptide
13	L	523	SER	Peptide
13	L	524	ASN	Peptide
13	L	525	LEU	Peptide
9	N	254	LEU	Peptide
9	N	302	LEU	Peptide

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Mol	Chain	Res	Type	Group
9	N	340	THR	Peptide
42	Y	49	GLU	Peptide
17	c	75	THR	Peptide
19	e	56	GLU	Peptide
20	f	96	TRP	Peptide
23	i	57	GLY	Peptide
25	k	165	PRO	Peptide
25	k	166	PRO	Peptide
25	k	225	ALA	Peptide
29	o	119	VAL	Peptide
31	q	25	PRO	Peptide
31	q	9	MET	Peptide
33	s	17	GLU	Peptide
33	s	22	PRO	Peptide
34	t	162	LEU	Peptide
36	v	126	GLN	Peptide
36	v	127	PRO	Peptide
36	v	128	VAL	Peptide
36	v	139	TYR	Peptide
36	v	61	TRP	Peptide
36	v	67	PRO	Peptide
36	v	8	MET	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	1	3328	0	3287	166	0
2	2	1655	0	1663	75	0
3	3	5275	0	5300	209	0
4	4	3098	0	3068	199	0
5	5	1726	0	1676	66	0
6	6	1241	0	1251	82	0
7	9	1414	0	1370	93	0
8	H	2528	0	2641	153	0
9	N	2723	0	2929	136	0
10	A	922	0	953	56	0
11	M	3645	0	3850	208	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	649	0	699	37	0
13	L	4456	0	4298	310	0
14	J	1188	0	1068	72	0
15	a	343	0	320	0	0
16	b	737	0	710	0	0
17	c	1000	0	997	0	0
18	d	2473	0	2461	0	0
19	e	677	0	686	0	0
20	f	909	0	947	0	0
21	g	969	0	980	0	0
22	h	757	0	771	0	0
23	i	1200	0	1169	0	0
24	X	707	0	700	27	0
24	j	684	0	682	0	0
25	k	2268	0	1995	0	0
26	l	792	0	798	0	0
27	m	626	0	635	0	0
28	n	578	0	558	0	0
29	o	1004	0	995	0	0
30	p	841	0	760	0	0
31	q	1151	0	1150	0	0
32	r	752	0	752	0	0
33	s	988	0	930	0	0
34	t	1434	0	1392	0	0
35	u	563	0	511	0	0
36	v	861	0	557	0	0
37	w	715	0	679	0	0
38	x	403	0	405	0	0
39	y	457	0	459	0	0
40	z	568	0	558	0	0
41	Z	1441	0	1416	49	0
42	Y	1403	0	1384	84	0
43	W	1155	0	1177	54	0
44	V	595	0	127	9	0
45	1	8	0	0	2	0
45	3	16	0	0	2	0
45	6	8	0	0	2	0
45	9	16	0	0	4	0
46	1	31	0	19	8	0
47	2	4	0	0	0	0
47	3	4	0	0	0	0
48	9	51	0	82	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	J	51	0	82	6	0
48	o	87	0	128	0	0
49	A	47	0	71	3	0
49	M	46	0	66	2	0
49	N	46	0	66	2	0
49	o	39	0	55	0	0
50	J	79	0	108	1	0
50	L	84	0	118	13	0
50	M	82	0	114	2	0
50	i	58	0	60	0	0
51	b	1	0	0	0	0
52	d	48	0	26	0	0
53	j	34	0	40	0	0
54	X	21	0	21	0	0
All	All	63760	0	62770	1861	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 25.

All (1861) 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)
13:L:451:ILE:O	13:L:455:LYS:HB2	1.43	1.15
13:L:374:ILE:O	13:L:378:LEU:HB3	1.62	0.98
11:M:254:THR:O	11:M:258:ALA:HB2	1.64	0.97
13:L:232:TRP:HD1	13:L:233:LEU:HD12	1.33	0.93
9:N:311:MET:HG2	9:N:312:LYS:H	1.32	0.93
1:1:33:LEU:O	1:1:37:GLN:HB2	1.70	0.92
3:3:237:ASN:H	3:3:259:ASN:HD21	1.09	0.92
14:J:20:PHE:HE1	14:J:29:GLY:HA2	1.35	0.90
13:L:396:ILE:O	13:L:400:ASN:HB2	1.71	0.90
41:Z:72:ASP:OD1	41:Z:90:GLN:NE2	2.06	0.88
42:Y:24:LEU:O	42:Y:28:ALA:HB2	1.73	0.88
1:1:33:LEU:HD23	1:1:155:GLU:HB3	1.54	0.88
2:2:162:GLU:HB2	2:2:186:PRO:HB3	1.53	0.88
42:Y:102:GLU:HA	42:Y:105:GLN:HB3	1.56	0.88
2:2:106:THR:O	2:2:109:MET:N	2.08	0.87
7:9:69:ARG:HD3	7:9:73:GLY:HA3	1.55	0.87
14:J:16:GLY:O	14:J:20:PHE:CB	2.22	0.87
3:3:116:LEU:O	3:3:120:SER:HB2	1.75	0.86
11:M:84:LEU:HD12	11:M:85:SER:H	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:375:ILE:O	13:L:379:ALA:HB2	1.75	0.86
11:M:249:LEU:HD12	11:M:250:LEU:HG	1.57	0.86
8:H:169:GLN:HE22	8:H:174:LEU:H	1.20	0.85
13:L:288:THR:O	13:L:292:ALA:HB2	1.76	0.85
3:3:237:ASN:OD1	3:3:253:ARG:NH2	2.09	0.85
9:N:261:MET:SD	9:N:340:THR:OG1	2.33	0.85
3:3:359:ARG:HA	3:3:362:TYR:HB3	1.56	0.85
11:M:126:LEU:HD22	11:M:150:LEU:HD13	1.57	0.85
8:H:302:MET:HB3	10:A:95:ILE:HD11	1.59	0.84
11:M:254:THR:O	11:M:258:ALA:CB	2.26	0.84
4:4:149:ASN:HD22	4:4:370:PRO:HB2	1.39	0.84
12:K:1:MET:N	14:J:120:ASN:O	2.11	0.83
13:L:32:TYR:O	13:L:35:TYR:N	2.10	0.83
13:L:451:ILE:O	13:L:455:LYS:CB	2.26	0.83
3:3:364:LEU:HA	3:3:491:ASN:HB2	1.60	0.83
11:M:336:ARG:HB3	11:M:426:ILE:HG22	1.60	0.83
11:M:400:MET:SD	13:L:176:ARG:NH2	2.52	0.83
4:4:105:ARG:NH1	6:6:149:CYS:SG	2.50	0.82
4:4:187:ALA:HB3	4:4:191:ALA:HB2	1.59	0.82
8:H:209:SER:O	8:H:213:VAL:HB	1.80	0.82
8:H:309:ILE:HD11	10:A:84:LEU:HD13	1.62	0.82
14:J:16:GLY:O	14:J:20:PHE:HB2	1.79	0.81
8:H:284:GLN:O	8:H:288:LEU:HB2	1.80	0.81
2:2:10:ARG:NH1	3:3:180:ASP:OD2	2.13	0.81
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.63	0.81
13:L:209:SER:OG	13:L:270:ASN:ND2	2.14	0.80
13:L:6:SER:HA	13:L:9:LEU:HD13	1.62	0.80
3:3:252:PRO:HB3	3:3:263:ILE:HB	1.64	0.80
3:3:126:ASP:HA	4:4:347:HIS:HE1	1.46	0.80
1:1:403:THR:OG1	45:1:500:SF4:S4	2.39	0.80
41:Z:145:LEU:HD12	41:Z:146:GLY:H	1.46	0.79
13:L:138:PHE:HB2	13:L:196:TRP:HE1	1.46	0.79
7:9:62:ARG:NH1	7:9:119:CYS:O	2.16	0.78
24:X:32:VAL:HB	24:X:74:GLN:HB2	1.66	0.78
11:M:369:LEU:HD23	11:M:371:PRO:HD2	1.63	0.78
3:3:237:ASN:H	3:3:259:ASN:ND2	1.82	0.78
11:M:56:PHE:HB2	11:M:111:THR:HG22	1.64	0.78
11:M:220:HIS:HE2	11:M:228:SER:HG	1.31	0.78
3:3:522:LEU:HB3	3:3:543:ILE:HG22	1.67	0.77
13:L:383:MET:HG3	13:L:389:PHE:H	1.49	0.77
14:J:62:GLY:O	14:J:66:VAL:HB	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:60:ILE:HG21	14:J:168:ILE:HG21	1.64	0.77
11:M:149:PHE:HA	11:M:152:TYR:HD2	1.49	0.77
13:L:135:ASN:OD1	13:L:136:ASN:N	2.18	0.77
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.51	0.76
1:1:301:GLY:H	1:1:330:GLY:HA3	1.50	0.76
3:3:278:ARG:HA	3:3:549:HIS:HB3	1.68	0.76
10:A:48:ARG:HG3	10:A:49:LEU:H	1.50	0.76
11:M:262:ILE:HD11	11:M:302:LEU:HB2	1.65	0.76
4:4:413:ASP:OD2	8:H:281:ARG:NH1	2.18	0.76
14:J:20:PHE:CE1	14:J:29:GLY:HA2	2.21	0.76
13:L:286:LEU:HD11	13:L:414:VAL:HG13	1.69	0.75
13:L:68:TRP:H	13:L:77:SER:HA	1.52	0.75
7:9:64:GLU:HB2	7:9:139:PHE:CZ	2.21	0.75
9:N:106:LEU:HD23	9:N:138:PRO:HB2	1.68	0.75
14:J:161:LEU:O	14:J:164:GLY:N	2.19	0.75
13:L:17:MET:HE3	13:L:21:ALA:HB2	1.67	0.75
13:L:37:LYS:HA	43:W:133:ILE:HD11	118.21	0.75
3:3:377:VAL:HG22	3:3:450:MET:HB3	1.68	0.74
13:L:288:THR:O	13:L:292:ALA:CB	2.35	0.74
1:1:214:GLY:HA3	1:1:220:THR:HG22	1.69	0.74
2:2:23:PHE:HA	2:2:57:GLN:HE22	1.52	0.74
11:M:300:ALA:O	11:M:308:SER:OG	2.05	0.74
3:3:35:MET:SD	5:5:210:ARG:NH1	2.58	0.74
5:5:137:MET:HB3	5:5:162:PHE:HD2	1.52	0.74
8:H:126:LYS:NZ	10:A:42:ASP:OD1	2.18	0.74
41:Z:99:GLN:NE2	41:Z:138:TYR:OH	2.20	0.74
4:4:352:TYR:HD1	7:9:86:VAL:HG11	1.50	0.74
11:M:243:MET:HG3	11:M:301:ILE:HG21	1.70	0.74
3:3:59:ILE:HG21	3:3:77:TRP:HE3	1.53	0.74
5:5:63:PHE:HD2	5:5:64:LEU:HD12	1.51	0.74
13:L:296:ASN:OD1	13:L:357:ARG:NH1	2.21	0.74
13:L:83:ASP:OD2	13:L:262:ARG:NH1	2.20	0.73
24:X:37:MET:O	24:X:41:GLY:N	2.21	0.73
2:2:151:ALA:HB3	2:2:163:ASP:HA	1.69	0.73
3:3:74:MET:H	3:3:77:TRP:HE1	1.35	0.73
8:H:165:LEU:HD21	8:H:241:LEU:HA	1.67	0.73
13:L:413:LEU:HD22	13:L:493:VAL:HG21	1.69	0.73
11:M:44:GLN:NE2	11:M:59:ASP:O	2.21	0.73
3:3:318:ILE:HG22	3:3:522:LEU:HD11	1.71	0.73
3:3:40:PHE:HB2	3:3:52:CYS:HB2	1.71	0.73
11:M:54:LEU:HA	43:W:93:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:172:ILE:HD11	2:2:187:ARG:HH12	1.53	0.72
6:6:81:ARG:HH12	8:H:217:ALA:H	1.35	0.72
41:Z:30:THR:HA	41:Z:33:THR:HG22	1.69	0.72
4:4:105:ARG:NH1	45:6:300:SF4:S3	2.62	0.72
8:H:65:THR:HG21	8:H:71:PHE:HB2	1.72	0.72
13:L:37:LYS:HG2	13:L:98:TRP:CZ3	2.25	0.72
7:9:64:GLU:HB2	7:9:139:PHE:HZ	1.52	0.72
41:Z:54:GLN:HA	41:Z:57:LYS:HE3	1.72	0.72
2:2:97:LYS:H	2:2:136:LEU:HA	1.53	0.72
3:3:116:LEU:O	3:3:120:SER:CB	2.37	0.72
13:L:84:PHE:HA	13:L:87:MET:HB2	1.71	0.72
13:L:177:ILE:O	13:L:180:ILE:HG22	1.89	0.72
13:L:22:ILE:O	43:W:26:ARG:NH2	2.22	0.72
3:3:45:ARG:HE	3:3:260:GLU:HB3	1.54	0.72
9:N:203:LEU:HD22	9:N:343:LEU:HD13	1.70	0.72
4:4:179:GLU:HG2	4:4:183:ARG:HH12	1.54	0.71
13:L:252:MET:O	13:L:255:ALA:N	2.23	0.71
4:4:126:LEU:HD13	4:4:358:VAL:HG22	1.69	0.71
11:M:114:GLU:HG2	11:M:175:ASN:HA	1.71	0.71
9:N:254:LEU:HD23	9:N:256:PRO:HD2	1.70	0.71
2:2:150:ASN:ND2	2:2:162:GLU:OE1	2.24	0.71
14:J:16:GLY:O	14:J:20:PHE:HB3	1.89	0.71
3:3:343:LEU:HD23	3:3:507:TYR:HE1	1.55	0.71
13:L:232:TRP:CD1	13:L:233:LEU:HD12	2.21	0.71
13:L:81:LYS:NZ	13:L:83:ASP:OD1	2.20	0.71
8:H:152:SER:OG	8:H:301:CYS:SG	2.47	0.71
9:N:194:LEU:HA	9:N:201:THR:HG21	1.72	0.71
9:N:307:SER:HB2	9:N:309:ASN:HD21	1.54	0.71
3:3:105:CYS:SG	3:3:117:GLN:NE2	2.63	0.71
7:9:135:PRO:HG2	7:9:164:GLU:HG3	1.71	0.71
13:L:342:CYS:SG	13:L:369:THR:OG1	2.48	0.71
4:4:175:GLU:OE1	4:4:188:ARG:NH2	2.24	0.71
6:6:35:ASP:O	6:6:39:TRP:HB2	1.91	0.71
5:5:113:GLU:OE2	5:5:163:ARG:NH2	2.24	0.70
9:N:193:VAL:HG21	9:N:266:ILE:HG12	1.72	0.70
3:3:259:ASN:H	3:3:390:LEU:HD21	1.57	0.70
1:1:362:CYS:N	45:1:500:SF4:S2	2.63	0.70
11:M:459:TYR:O	41:Z:96:LYS:NZ	2.24	0.70
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.57	0.70
12:K:58:MET:SD	14:J:146:LEU:HB2	2.32	0.70
3:3:362:TYR:OH	3:3:500:VAL:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:333:ASP:O	3:3:337:ARG:HB2	1.92	0.69
5:5:145:HIS:ND1	5:5:147:ASP:O	2.25	0.69
13:L:386:LEU:O	13:L:389:PHE:HB3	1.93	0.69
1:1:300:GLY:H	1:1:334:VAL:HG12	1.57	0.69
3:3:541:CYS:HB2	3:3:543:ILE:HG23	1.74	0.69
4:4:116:GLN:HG3	4:4:138:ARG:HD3	1.73	0.69
42:Y:14:VAL:HG12	42:Y:15:GLN:HG3	1.73	0.69
7:9:69:ARG:NH1	7:9:159:ASP:OD1	2.25	0.69
8:H:157:ASN:HD21	8:H:165:LEU:HD13	1.58	0.69
11:M:60:SER:O	11:M:63:THR:N	2.26	0.69
24:X:81:ALA:HA	24:X:86:VAL:HG21	1.75	0.69
41:Z:27:ASN:HB3	41:Z:30:THR:OG1	1.92	0.69
1:1:260:GLY:O	2:2:111:ARG:NH2	2.26	0.69
13:L:174:TYR:HB3	13:L:229:LEU:HD21	1.72	0.69
13:L:272:PHE:O	13:L:275:SER:OG	2.08	0.69
13:L:494:THR:O	13:L:498:PHE:HB2	1.92	0.69
11:M:44:GLN:NE2	11:M:63:THR:OG1	2.25	0.69
3:3:460:ARG:NH1	3:3:659:ASP:O	2.26	0.68
12:K:59:MET:O	12:K:63:LEU:HB2	1.93	0.68
13:L:3:LEU:O	13:L:6:SER:OG	2.08	0.68
1:1:17:ASP:O	1:1:18:GLU:HG2	1.93	0.68
4:4:108:TYR:CG	6:6:54:CYS:HB3	2.27	0.68
13:L:427:ILE:HG13	13:L:431:LEU:HD12	1.73	0.68
13:L:563:PRO:O	13:L:567:SER:CB	2.41	0.68
11:M:339:SER:OG	11:M:341:THR:OG1	2.11	0.68
8:H:209:SER:HA	8:H:212:ASN:HB3	1.75	0.68
42:Y:24:LEU:O	42:Y:28:ALA:CB	2.39	0.68
13:L:289:ALA:HB1	13:L:418:PHE:HD2	1.59	0.68
3:3:453:LEU:HB3	3:3:492:ILE:HG22	1.73	0.68
5:5:154:ASP:HB3	5:5:157:PHE:HB2	1.74	0.68
3:3:39:ARG:H	3:3:119:GLN:HE22	1.42	0.68
8:H:292:ASN:OD1	8:H:293:PHE:N	2.26	0.68
8:H:195:ARG:HD2	8:H:274:ARG:HB2	1.75	0.68
3:3:315:VAL:HG23	3:3:521:MET:HB2	1.75	0.67
1:1:305:PRO:HB2	1:1:327:THR:HG22	1.77	0.67
8:H:216:ALA:HB1	8:H:219:PRO:HB2	1.75	0.67
11:M:232:ALA:HB3	11:M:327:PHE:HE2	1.60	0.67
1:1:406:ALA:HB3	46:1:501:FMN:HM83	1.76	0.67
13:L:374:ILE:HA	13:L:377:SER:HG	1.59	0.67
4:4:273:GLN:OE1	5:5:104:ARG:NH1	2.25	0.67
3:3:159:CYS:HB2	3:3:199:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:122:PHE:O	11:M:125:THR:OG1	2.08	0.67
8:H:216:ALA:O	8:H:220:PHE:N	2.27	0.67
13:L:346:ILE:HD11	13:L:373:LEU:HD11	1.75	0.67
49:M:501:PC1:H2	49:M:501:PC1:H152	1.76	0.67
1:1:111:ILE:HD11	1:1:149:LEU:HD22	1.78	0.66
10:A:64:LEU:HD11	14:J:168:ILE:HD12	1.77	0.66
9:N:15:LEU:HD13	50:J:300:CDL:H171	1.76	0.66
9:N:232:HIS:NE2	9:N:313:MET:SD	2.69	0.66
3:3:174:THR:HG22	3:3:183:VAL:HG22	1.77	0.66
4:4:261:ARG:NH1	4:4:267:TRP:O	2.28	0.66
11:M:1:MET:HG2	11:M:111:THR:HG21	1.76	0.66
41:Z:70:VAL:HG23	41:Z:72:ASP:H	1.58	0.66
9:N:31:ILE:HG12	12:K:66:PHE:HE2	1.59	0.66
3:3:601:ARG:NH1	3:3:611:LEU:O	2.29	0.66
9:N:215:MET:HG3	9:N:219:PHE:HE2	1.60	0.66
5:5:119:SER:OG	5:5:143:ALA:O	2.12	0.66
5:5:154:ASP:OD1	5:5:155:TYR:N	2.29	0.66
8:H:101:GLY:O	8:H:104:PHE:N	2.26	0.66
13:L:383:MET:HG3	13:L:389:PHE:N	2.10	0.66
11:M:376:ILE:HG23	11:M:380:PHE:HE2	1.58	0.66
3:3:106:PRO:O	7:9:104:ARG:NH2	2.29	0.66
24:X:43:ASP:HB3	24:X:46:ASP:HB2	1.78	0.66
2:2:159:ASN:OD1	2:2:160:TYR:N	2.29	0.66
12:K:59:MET:O	12:K:63:LEU:CB	2.43	0.66
10:A:90:MET:HA	10:A:93:LEU:HB3	1.76	0.66
41:Z:98:ASP:OD2	41:Z:141:ARG:NH2	2.28	0.66
4:4:233:ARG:NH2	48:9:501:3PE:O14	2.28	0.66
9:N:19:ILE:HA	9:N:22:ILE:HG22	1.77	0.65
42:Y:12:LEU:HD23	42:Y:13:LYS:H	1.59	0.65
1:1:406:ALA:O	1:1:410:GLY:N	2.25	0.65
6:6:94:ASN:N	6:6:131:SER:O	2.21	0.65
13:L:6:SER:O	13:L:9:LEU:HB2	1.97	0.65
11:M:403:THR:HA	11:M:406:TYR:CE2	2.32	0.65
4:4:266:GLN:NE2	7:9:2:TYR:HB3	2.11	0.65
13:L:418:PHE:HA	13:L:421:ILE:HG12	1.77	0.65
13:L:568:LEU:O	13:L:572:LYS:N	2.28	0.65
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.79	0.65
14:J:26:PRO:O	14:J:29:GLY:N	2.29	0.65
3:3:534:ARG:NH1	3:3:541:CYS:SG	2.69	0.65
13:L:264:TYR:HA	13:L:267:THR:HG22	1.79	0.65
42:Y:45:CYS:HA	42:Y:134:ARG:NH2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:12:MET:O	11:M:15:THR:OG1	2.10	0.65
9:N:266:ILE:O	9:N:270:MET:HB2	1.96	0.65
2:2:131:THR:HG22	2:2:138:THR:HG22	1.79	0.65
13:L:374:ILE:O	13:L:378:LEU:CB	2.40	0.65
3:3:258:ILE:HD11	3:3:581:GLN:HE22	1.63	0.64
11:M:140:THR:C	11:M:142:ARG:H	2.00	0.64
42:Y:166:LEU:O	43:W:104:ARG:NH2	2.30	0.64
1:1:24:ASN:ND2	1:1:113:HIS:O	2.30	0.64
9:N:142:LEU:HB3	9:N:194:LEU:HD21	1.79	0.64
4:4:196:PRO:HG3	4:4:356:TYR:OH	1.98	0.64
13:L:361:GLY:O	13:L:364:LYS:NZ	2.30	0.64
11:M:425:ASN:OD1	11:M:426:ILE:N	2.30	0.64
42:Y:43:MET:O	42:Y:47:TRP:HB3	1.98	0.64
8:H:100:LEU:HD23	8:H:103:LEU:HD11	1.78	0.64
9:N:149:ILE:HD13	9:N:154:ILE:HD12	1.79	0.64
3:3:69:CYS:SG	3:3:70:ALA:N	2.71	0.64
10:A:74:PRO:HG2	14:J:147:TYR:HE2	1.62	0.64
13:L:375:ILE:O	13:L:379:ALA:CB	2.44	0.64
7:9:27:TRP:CZ2	48:9:501:3PE:H231	2.32	0.64
4:4:204:PRO:HD3	7:9:60:ARG:HH22	1.62	0.64
1:1:135:TYR:HE1	1:1:176:PHE:HD2	1.47	0.63
1:1:20:ARG:NH1	1:1:269:GLU:O	2.31	0.63
44:V:36:UNK:O	44:V:40:UNK:CB	2.46	0.63
1:1:95:VAL:HG22	1:1:228:VAL:HG21	1.79	0.63
7:9:132:VAL:HG21	7:9:169:ILE:HD11	1.80	0.63
9:N:287:LEU:HD23	9:N:290:LEU:HD12	1.80	0.63
1:1:105:CYS:SG	2:2:148:CYS:N	2.68	0.63
3:3:221:GLU:HB3	3:3:243:ARG:CZ	2.28	0.63
3:3:228:ILE:HG22	3:3:229:ASP:H	1.62	0.63
7:9:27:TRP:CH2	48:9:501:3PE:H332	2.33	0.63
1:1:185:ILE:HD11	2:2:86:PHE:HZ	1.63	0.63
3:3:367:THR:HG21	3:3:636:VAL:HG11	1.80	0.63
13:L:569:ALA:O	13:L:573:MET:N	2.31	0.63
13:L:23:ASN:O	43:W:26:ARG:NH1	2.31	0.63
6:6:34:ASP:O	6:6:38:ASN:HB2	1.98	0.63
13:L:460:GLY:O	13:L:464:ALA:N	2.30	0.63
13:L:81:LYS:HD3	13:L:135:ASN:HD22	1.62	0.63
11:M:370:PRO:HA	11:M:375:LEU:HD22	1.80	0.63
41:Z:86:GLU:HG2	43:W:87:TYR:OH	1.99	0.63
13:L:444:ASN:OD1	13:L:446:ASN:N	2.22	0.63
8:H:317:GLN:HB3	10:A:80:GLN:HE22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:429:ARG:HA	1:1:432:ARG:HG2	1.81	0.62
42:Y:43:MET:O	42:Y:47:TRP:CB	2.47	0.62
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.79	0.62
1:1:280:ILE:HG21	1:1:287:VAL:HG23	1.82	0.62
1:1:259:SER:HB3	1:1:335:ILE:HG22	1.80	0.62
1:1:15:LEU:HD21	1:1:270:GLU:HG2	1.82	0.62
2:2:27:ASN:ND2	2:2:57:GLN:OE1	2.29	0.62
11:M:342:MET:HG3	11:M:414:THR:HG22	1.81	0.62
3:3:104:ASP:OD2	3:3:152:ARG:NH1	2.26	0.62
3:3:230:VAL:HB	3:3:322:LEU:HD22	1.81	0.62
1:1:378:ARG:O	1:1:382:GLY:N	2.33	0.62
3:3:339:ASP:OD1	3:3:340:SER:N	2.30	0.62
4:4:263:SER:O	4:4:265:ILE:HG22	2.00	0.62
13:L:310:LEU:HA	13:L:313:MET:HE3	1.80	0.62
13:L:345:SER:HB3	13:L:450:LEU:HD11	1.80	0.62
1:1:205:LEU:HD11	3:3:50:GLY:HA3	1.81	0.62
4:4:202:ASP:HB3	4:4:323:ILE:HG12	1.81	0.62
3:3:312:GLY:N	3:3:339:ASP:OD2	2.33	0.62
6:6:35:ASP:O	6:6:39:TRP:CB	2.48	0.62
8:H:309:ILE:HG21	10:A:88:LEU:HD11	1.81	0.62
5:5:137:MET:HB3	5:5:162:PHE:CD2	2.35	0.62
10:A:54:LYS:NZ	10:A:111:LEU:O	2.27	0.62
11:M:220:HIS:NE2	11:M:228:SER:OG	2.29	0.62
9:N:255:PRO:HA	9:N:260:PHE:CG	2.34	0.61
4:4:228:MET:O	4:4:232:ASN:ND2	2.32	0.61
4:4:82:LEU:HA	6:6:95:LYS:HD3	1.81	0.61
13:L:11:THR:HG22	13:L:129:LEU:HD21	1.82	0.61
44:V:35:UNK:O	44:V:39:UNK:CB	2.48	0.61
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.13	0.61
4:4:76:CYS:SG	4:4:406:SER:OG	2.58	0.61
8:H:258:ASN:OD1	8:H:262:LYS:NZ	2.34	0.61
8:H:195:ARG:HD2	8:H:274:ARG:HD2	1.81	0.61
13:L:595:ILE:O	13:L:598:SER:O	2.17	0.61
11:M:86:LYS:O	11:M:87:GLU:HG3	2.00	0.61
4:4:80:ILE:HG13	4:4:81:GLY:H	1.66	0.61
8:H:115:SER:O	8:H:119:SER:CB	2.48	0.61
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.81	0.61
1:1:68:ARG:HD2	1:1:254:LYS:HE3	1.81	0.61
8:H:158:GLY:HA3	8:H:315:PRO:HB2	1.83	0.61
9:N:311:MET:HG2	9:N:312:LYS:N	2.11	0.61
1:1:261:HIS:NE2	2:2:110:LEU:O	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:460:ARG:HG2	3:3:462:ASP:H	1.66	0.61
4:4:190:HIS:HD2	6:6:150:PRO:HD3	1.66	0.61
5:5:151:ILE:HG22	5:5:152:LEU:HG	1.82	0.61
6:6:58:GLU:OE2	6:6:153:ALA:N	2.34	0.61
13:L:303:ALA:O	13:L:306:THR:HG22	2.00	0.61
4:4:124:LYS:HG3	5:5:12:ARG:HH12	1.66	0.61
13:L:518:ASN:O	13:L:522:PHE:N	2.34	0.61
42:Y:158:LYS:HB3	42:Y:159:PRO:HD2	1.82	0.61
13:L:202:PHE:HB3	41:Z:113:GLN:HE22	1.66	0.61
3:3:230:VAL:HG23	3:3:231:MET:HG3	1.82	0.60
7:9:160:LYS:HD2	7:9:161:TRP:CZ3	2.36	0.60
9:N:175:LEU:HD13	9:N:219:PHE:CE1	2.35	0.60
24:X:55:GLU:O	24:X:59:GLY:N	2.24	0.60
42:Y:45:CYS:HA	42:Y:134:ARG:HH21	1.66	0.60
8:H:151:LEU:HD21	10:A:72:LEU:HG	1.83	0.60
8:H:217:ALA:O	8:H:220:PHE:HB3	2.01	0.60
9:N:215:MET:HG3	9:N:219:PHE:CE2	2.35	0.60
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.83	0.60
14:J:94:ILE:O	14:J:98:LEU:CB	2.49	0.60
13:L:226:GLN:HE22	13:L:281:GLY:HA2	1.64	0.60
50:M:502:CDL:H161	50:M:502:CDL:H572	1.81	0.60
43:W:81:ASP:OD2	43:W:85:LYS:NZ	2.33	0.60
8:H:266:LEU:O	8:H:269:THR:OG1	2.13	0.60
3:3:575:ASN:OD1	3:3:579:ARG:N	2.33	0.60
10:A:12:THR:O	10:A:15:THR:N	2.34	0.60
3:3:362:TYR:OH	3:3:503:LEU:HB2	2.02	0.60
6:6:107:MET:HB3	6:6:111:ARG:HE	1.66	0.60
4:4:84:HIS:H	6:6:93:THR:HG21	1.66	0.60
13:L:230:HIS:O	13:L:232:TRP:N	2.35	0.60
13:L:561:ILE:O	13:L:565:THR:N	2.34	0.60
43:W:90:THR:HA	43:W:93:ILE:HG22	1.82	0.60
4:4:106:LEU:HD22	4:4:391:ILE:HD13	1.82	0.60
8:H:283:ASP:OD1	8:H:284:GLN:N	2.35	0.60
3:3:333:ASP:OD2	3:3:622:ARG:NE	2.28	0.60
10:A:78:ALA:HB2	14:J:144:ALA:HA	1.84	0.60
13:L:302:ILE:O	13:L:305:SER:OG	2.16	0.60
24:X:13:ASP:O	24:X:17:TYR:HB2	2.02	0.60
1:1:366:ARG:NH2	3:3:154:ILE:O	2.34	0.60
9:N:26:TRP:NE1	9:N:85:THR:O	2.34	0.60
4:4:151:ILE:HD13	4:4:304:MET:HE1	1.84	0.59
13:L:437:PHE:HB2	13:L:438:PRO:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:318:ASP:HB2	1:1:321:ALA:HB3	1.85	0.59
4:4:240:VAL:O	4:4:292:ASP:HB2	2.02	0.59
9:N:42:PRO:HG2	14:J:167:VAL:HG22	1.84	0.59
13:L:345:SER:O	13:L:349:SER:CB	2.50	0.59
13:L:419:THR:HA	13:L:422:TYR:CD2	2.38	0.59
1:1:242:PHE:CZ	1:1:252:GLY:HA3	2.38	0.59
13:L:69:LEU:HD13	13:L:71:ILE:HG23	1.83	0.59
4:4:85:ARG:HD2	6:6:126:TYR:CE2	2.37	0.59
13:L:97:THR:HG21	13:L:125:LEU:HD12	1.85	0.59
13:L:128:MET:HG3	13:L:251:THR:HG22	1.83	0.59
3:3:215:PHE:CD2	7:9:104:ARG:HB3	2.38	0.59
8:H:10:ILE:HD12	10:A:13:LEU:HD22	1.84	0.59
11:M:119:TYR:O	11:M:122:PHE:HB3	2.02	0.59
11:M:60:SER:OG	11:M:61:LEU:N	2.35	0.59
9:N:180:ALA:O	9:N:183:SER:OG	2.11	0.59
3:3:329:ILE:HD11	3:3:505:LEU:HD22	1.84	0.59
11:M:210:TYR:O	11:M:213:HIS:ND1	2.28	0.59
41:Z:145:LEU:HD13	41:Z:149:TYR:HB3	1.85	0.59
14:J:166:VAL:O	14:J:170:GLU:HB2	2.02	0.59
9:N:91:ASN:OD1	9:N:93:MET:N	2.35	0.59
6:6:46:TRP:N	6:6:84:ASP:OD2	2.35	0.59
13:L:319:ILE:HG22	13:L:320:ASN:H	1.68	0.59
13:L:383:MET:HB2	13:L:389:PHE:HB2	1.85	0.59
13:L:43:ALA:O	13:L:47:SER:CB	2.51	0.59
11:M:75:LEU:HD21	11:M:440:HIS:CE1	2.38	0.59
1:1:233:THR:O	1:1:237:ARG:HG2	2.01	0.59
11:M:376:ILE:HG23	11:M:380:PHE:CE2	2.38	0.59
11:M:397:GLY:HA3	13:L:180:ILE:HG13	1.85	0.58
9:N:298:TYR:HB3	11:M:147:LEU:HD22	1.84	0.58
1:1:99:GLU:OE2	1:1:104:THR:HG21	2.03	0.58
3:3:379:LEU:N	3:3:407:ALA:O	2.37	0.58
50:L:601:CDL:H601	50:L:601:CDL:H232	1.85	0.58
1:1:236:ARG:O	2:2:214:GLN:NE2	2.36	0.58
7:9:160:LYS:HD2	7:9:161:TRP:HZ3	1.68	0.58
3:3:332:LYS:NZ	3:3:505:LEU:O	2.27	0.58
4:4:62:LEU:HD23	4:4:425:PHE:CE1	2.38	0.58
8:H:60:PRO:HD3	10:A:25:PRO:HB2	1.85	0.58
13:L:40:ILE:HG13	13:L:101:MET:SD	2.44	0.58
11:M:135:ARG:HD2	11:M:136:TRP:HZ3	1.68	0.58
11:M:2:LEU:HD22	49:M:501:PC1:H143	1.85	0.58
9:N:249:LEU:HD11	9:N:297:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:283:MET:HA	3:3:293:HIS:HA	1.85	0.58
6:6:91:THR:OG1	6:6:119:CYS:SG	2.59	0.58
11:M:4:TYR:HE1	11:M:37:THR:HB	1.69	0.58
50:L:601:CDL:H122	50:L:601:CDL:H581	1.85	0.58
42:Y:76:HIS:NE2	42:Y:114:LEU:HB2	2.18	0.58
1:1:224:ASN:OD1	1:1:225:VAL:N	2.37	0.58
13:L:580:GLN:O	13:L:584:ILE:CB	2.52	0.58
1:1:17:ASP:OD1	1:1:18:GLU:N	2.36	0.58
8:H:170:GLU:OE2	42:Y:97:ARG:NH2	2.37	0.58
41:Z:8:VAL:O	41:Z:108:ARG:NH2	2.34	0.58
11:M:328:CYS:SG	11:M:436:LEU:HD23	2.43	0.58
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.30	0.57
4:4:56:PRO:HG2	4:4:159:LEU:HD21	1.86	0.57
7:9:94:ILE:HG12	7:9:109:TYR:HD1	1.69	0.57
8:H:200:LEU:HD11	8:H:209:SER:H	1.68	0.57
13:L:22:ILE:HD13	50:L:601:CDL:H141	1.85	0.57
8:H:85:MET:HB3	8:H:233:MET:SD	2.44	0.57
12:K:62:ILE:HD13	14:J:153:LEU:HG	1.86	0.57
9:N:68:MET:HE3	12:K:40:LEU:HD12	1.85	0.57
13:L:420:ALA:O	13:L:423:SER:OG	2.15	0.57
1:1:405:CYS:SG	1:1:407:LEU:HB3	2.44	0.57
3:3:40:PHE:HB2	3:3:52:CYS:CB	2.34	0.57
42:Y:165:ARG:NH2	43:W:103:LEU:HB3	2.19	0.57
11:M:325:MET:SD	11:M:441:MET:HG2	2.45	0.57
3:3:59:ILE:HG21	3:3:77:TRP:CE3	2.36	0.57
11:M:50:LEU:HA	43:W:86:ASN:HD21	1.69	0.57
1:1:215:VAL:HG12	1:1:216:PHE:CD2	2.40	0.57
1:1:295:LEU:HB2	1:1:339:ARG:HA	1.85	0.57
5:5:72:PHE:HA	5:5:98:SER:HA	1.86	0.57
13:L:379:ALA:HA	13:L:383:MET:SD	2.45	0.57
11:M:225:ILE:HD13	11:M:331:ASN:HB2	1.87	0.57
5:5:119:SER:OG	5:5:144:ASN:OD1	2.11	0.57
9:N:42:PRO:HG3	14:J:167:VAL:HG13	1.86	0.57
13:L:187:ALA:HA	13:L:190:LEU:HD13	1.85	0.57
13:L:364:LYS:O	13:L:366:MET:HG2	2.04	0.57
13:L:43:ALA:O	13:L:47:SER:HB2	2.05	0.57
11:M:35:SER:O	11:M:38:SER:OG	2.15	0.57
1:1:82:MET:HB2	1:1:129:MET:HB2	1.86	0.57
24:X:82:ASP:OD1	24:X:83:LYS:N	2.38	0.57
4:4:373:GLU:O	4:4:392:LYS:NZ	2.34	0.57
8:H:10:ILE:HG21	10:A:10:ASN:HD21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:22:ILE:HG21	50:L:601:CDL:H141	1.87	0.57
41:Z:70:VAL:HB	41:Z:71:PRO:HD2	1.86	0.57
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.85	0.57
4:4:347:HIS:O	4:4:351:LEU:CB	2.53	0.57
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.69	0.57
8:H:218:GLY:O	8:H:221:ALA:N	2.37	0.57
8:H:273:ILE:O	8:H:276:SER:N	2.36	0.57
24:X:60:PHE:HD1	24:X:61:GLU:HB2	1.70	0.57
1:1:182:GLY:O	2:2:88:THR:OG1	2.17	0.56
1:1:276:LEU:HD23	1:1:312:CYS:HB2	1.87	0.56
1:1:95:VAL:HB	1:1:136:ILE:HG12	1.87	0.56
9:N:40:ILE:HG21	9:N:134:GLN:HE22	1.70	0.56
11:M:309:TYR:CE2	41:Z:147:ALA:HB1	2.39	0.56
1:1:365:CYS:SG	1:1:366:ARG:N	2.78	0.56
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.86	0.56
3:3:126:ASP:HA	4:4:347:HIS:CE1	2.35	0.56
5:5:173:GLU:OE2	5:5:189:GLU:N	2.37	0.56
10:A:23:TRP:O	10:A:27:LEU:N	2.38	0.56
8:H:149:ILE:HG21	8:H:185:TRP:HB2	1.87	0.56
8:H:289:LEU:HD12	8:H:293:PHE:HB2	1.87	0.56
9:N:329:MET:HE3	49:N:401:PC1:H282	1.86	0.56
1:1:42:TRP:CD2	1:1:161:LEU:HD21	2.40	0.56
8:H:100:LEU:HD22	14:J:54:LEU:HD12	1.86	0.56
13:L:108:MET:HB2	13:L:114:ILE:HD13	1.87	0.56
41:Z:55:HIS:CD2	43:W:48:GLY:HA2	2.40	0.56
3:3:280:THR:HB	3:3:591:GLY:HA3	1.87	0.56
4:4:287:ILE:HB	7:9:4:TYR:HB3	1.87	0.56
8:H:195:ARG:HH21	8:H:274:ARG:HD2	1.69	0.56
13:L:60:GLU:HB3	13:L:82:MET:O	2.05	0.56
4:4:62:LEU:HD23	4:4:425:PHE:CZ	2.40	0.56
13:L:22:ILE:HG13	13:L:23:ASN:N	2.20	0.56
9:N:88:LYS:HG3	9:N:148:SER:HB3	1.86	0.56
14:J:96:GLY:O	14:J:100:GLU:CB	2.54	0.56
9:N:295:ARG:HA	9:N:298:TYR:CD2	2.40	0.56
3:3:235:GLY:HA3	3:3:575:ASN:HB3	1.88	0.56
13:L:530:PRO:O	13:L:534:HIS:CB	2.54	0.56
9:N:106:LEU:HB2	9:N:187:MET:HE3	1.87	0.56
9:N:154:ILE:HG23	9:N:191:THR:HG22	1.88	0.56
7:9:45:PRO:HG3	8:H:30:TYR:CE1	2.41	0.56
13:L:353:GLU:OE2	13:L:358:LYS:HG3	2.06	0.56
13:L:374:ILE:HA	13:L:377:SER:OG	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:34:GLN:OE1	42:Y:116:TRP:NE1	2.38	0.56
1:1:24:ASN:OD1	1:1:28:ARG:N	2.39	0.56
6:6:81:ARG:NH1	8:H:214:GLU:O	2.38	0.56
7:9:32:ARG:O	7:9:36:MET:HB2	2.06	0.56
4:4:146:ARG:NH1	4:4:270:ARG:HH11	2.04	0.56
4:4:265:ILE:HD11	5:5:99:LEU:HD21	1.87	0.56
8:H:151:LEU:HD13	10:A:73:LEU:HD12	1.88	0.56
13:L:116:GLN:NE2	50:L:601:CDL:OA4	2.39	0.56
42:Y:31:TYR:O	42:Y:35:CYS:N	2.37	0.56
3:3:21:GLU:HB3	3:3:24:THR:HG23	1.87	0.56
3:3:41:CYS:O	3:3:161:ARG:NH2	2.35	0.56
7:9:25:LEU:HD21	48:9:501:3PE:H392	1.87	0.56
8:H:94:PRO:O	8:H:95:LEU:HB3	2.06	0.56
13:L:227:PHE:HB2	13:L:284:THR:HG23	1.88	0.56
11:M:210:TYR:HB2	11:M:268:GLY:HA3	1.88	0.56
11:M:32:LEU:O	11:M:35:SER:OG	2.19	0.56
1:1:370:ASP:OD1	1:1:374:LYS:NZ	2.39	0.55
3:3:551:ASP:HB3	3:3:679:ARG:HH12	1.70	0.55
4:4:161:ILE:HD11	4:4:238:ARG:HE	1.71	0.55
4:4:349:PHE:CE1	7:9:82:LEU:HD21	2.41	0.55
13:L:56:HIS:CE1	13:L:57:THR:HG1	2.21	0.55
3:3:512:GLU:OE1	3:3:515:ARG:NH2	2.39	0.55
8:H:195:ARG:HH11	8:H:231:ILE:HD13	1.71	0.55
11:M:281:ASP:HA	11:M:341:THR:HA	1.88	0.55
11:M:59:ASP:CG	11:M:245:ARG:HH22	2.09	0.55
11:M:89:LEU:HD11	11:M:93:LYS:HE3	1.87	0.55
1:1:138:ILE:HD13	1:1:146:ALA:HB2	1.87	0.55
3:3:259:ASN:O	3:3:262:TRP:N	2.40	0.55
3:3:278:ARG:HH12	3:3:565:ALA:HB2	1.71	0.55
4:4:338:MET:SD	4:4:348:HIS:ND1	2.79	0.55
4:4:298:LEU:HD12	7:9:6:ASN:HD21	1.71	0.55
8:H:28:LEU:HD22	8:H:275:ALA:HB2	1.87	0.55
7:9:47:THR:HG21	8:H:35:LYS:H	1.71	0.55
11:M:41:LEU:HD13	11:M:66:LEU:HD22	1.87	0.55
13:L:203:MET:HG2	41:Z:109:LEU:HD11	1.87	0.55
2:2:97:LYS:N	2:2:136:LEU:HA	2.21	0.55
13:L:325:ALA:O	13:L:329:ILE:HD12	2.07	0.55
4:4:292:ASP:O	4:4:293:CYS:HB3	2.07	0.55
49:A:200:PC1:H132	49:A:200:PC1:H12	1.88	0.55
8:H:115:SER:O	8:H:119:SER:HB3	2.06	0.55
8:H:269:THR:O	8:H:272:TRP:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:1:MET:HG2	14:J:120:ASN:HA	1.89	0.55
9:N:222:ASN:HB3	9:N:233:THR:HG21	1.88	0.55
9:N:238:PRO:O	9:N:241:THR:OG1	2.18	0.55
42:Y:49:GLU:HA	42:Y:137:PRO:HG3	1.87	0.55
8:H:167:ILE:HD12	42:Y:97:ARG:HH21	1.71	0.55
6:6:70:ASP:OD2	8:H:34:ARG:NH1	2.33	0.55
8:H:22:LEU:HD11	8:H:26:LYS:HE3	1.88	0.55
11:M:44:GLN:OE1	11:M:60:SER:HA	2.07	0.55
43:W:83:PRO:O	43:W:87:TYR:CB	2.55	0.55
41:Z:143:HIS:HD1	41:Z:144:ASP:HB2	1.72	0.55
2:2:106:THR:HB	2:2:107:PRO:HD3	1.88	0.55
8:H:18:ALA:HB1	8:H:48:PRO:HB3	1.89	0.55
11:M:277:LEU:HD11	11:M:405:LEU:HD22	1.87	0.55
5:5:49:GLU:OE1	5:5:106:ARG:NH2	2.33	0.55
8:H:307:LEU:HA	8:H:310:LEU:HD12	1.89	0.55
13:L:283:MET:O	13:L:287:PHE:CB	2.55	0.55
11:M:448:SER:O	13:L:68:TRP:HH2	1.89	0.55
11:M:31:SER:OG	11:M:74:PRO:HG3	2.06	0.55
1:1:102:PRO:HA	2:2:144:CYS:SG	2.47	0.55
13:L:19:ILE:HG21	43:W:128:ILE:HG12	98.34	0.55
9:N:36:ASN:O	9:N:40:ILE:HB	2.06	0.55
8:H:148:ILE:HG22	8:H:301:CYS:SG	2.46	0.55
13:L:491:LEU:O	13:L:494:THR:OG1	2.20	0.55
13:L:76:LEU:HB2	13:L:136:ASN:HD21	1.71	0.55
9:N:120:GLN:OE1	9:N:177:LYS:HE2	2.07	0.55
1:1:262:VAL:HG13	1:1:336:VAL:HG21	1.89	0.54
7:9:76:ARG:HD2	7:9:130:ALA:HA	1.89	0.54
7:9:91:ALA:O	7:9:92:ILE:HG12	2.07	0.54
2:2:106:THR:O	2:2:108:CYS:N	2.40	0.54
3:3:220:TRP:HD1	5:5:197:PHE:CD1	2.25	0.54
5:5:160:HIS:O	5:5:163:ARG:HG2	2.07	0.54
6:6:75:VAL:HG13	8:H:25:ARG:HH12	1.72	0.54
13:L:466:PHE:O	13:L:469:SER:OG	2.12	0.54
11:M:146:GLY:O	11:M:149:PHE:HB3	2.07	0.54
11:M:347:GLY:O	11:M:348:LEU:HB2	2.07	0.54
9:N:149:ILE:HG21	9:N:154:ILE:HD12	1.89	0.54
42:Y:44:LEU:HD11	42:Y:132:THR:HG21	1.90	0.54
3:3:368:ILE:HD11	3:3:577:GLU:OE2	2.06	0.54
8:H:146:LEU:HG	8:H:185:TRP:HE1	1.71	0.54
3:3:368:ILE:HG21	3:3:394:ARG:HD2	1.89	0.54
10:A:7:LEU:HD21	48:J:301:3PE:H362	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:LYS:O	8:H:57:ILE:N	2.37	0.54
14:J:60:TYR:O	14:J:64:MET:HB2	2.07	0.54
10:A:63:LEU:HG	14:J:67:VAL:HG21	1.89	0.54
13:L:373:LEU:O	13:L:377:SER:CB	2.56	0.54
43:W:42:LEU:O	43:W:45:VAL:N	2.33	0.54
42:Y:110:VAL:HG12	42:Y:115:GLY:O	2.08	0.54
1:1:338:ASP:OD1	1:1:339:ARG:N	2.40	0.54
11:M:1:MET:HB2	11:M:52:PHE:HD2	1.72	0.54
11:M:82:HIS:HB2	11:M:432:ARG:HH12	1.72	0.54
42:Y:36:ASP:HA	42:Y:39:ASN:OD1	2.07	0.54
5:5:80:ALA:HB3	5:5:138:PHE:CE2	2.43	0.54
6:6:72:PHE:HE2	6:6:157:LEU:HD21	1.73	0.54
8:H:100:LEU:O	8:H:160:PHE:HB3	2.07	0.54
42:Y:57:GLU:O	42:Y:60:LYS:HB3	2.06	0.54
1:1:343:ILE:HD13	1:1:422:PHE:HE2	1.72	0.54
2:2:111:ARG:HG3	2:2:152:PRO:HD3	1.89	0.54
6:6:82:GLN:NE2	8:H:213:VAL:O	2.41	0.54
8:H:99:ASN:N	48:J:301:3PE:O14	2.35	0.54
13:L:63:ILE:HD11	13:L:80:PHE:HD2	1.71	0.54
42:Y:120:ASP:OD1	42:Y:121:LEU:N	2.41	0.54
42:Y:28:ALA:HA	42:Y:31:TYR:CE2	2.43	0.54
42:Y:85:TRP:HA	42:Y:88:ILE:HG22	1.89	0.54
41:Z:116:GLU:OE2	41:Z:124:CYS:N	2.41	0.54
4:4:347:HIS:O	4:4:351:LEU:HB3	2.08	0.54
5:5:169:SER:HA	6:6:129:SER:O	2.07	0.54
9:N:266:ILE:O	9:N:270:MET:CB	2.56	0.54
43:W:111:ARG:HB2	43:W:122:TRP:HZ3	1.71	0.54
1:1:305:PRO:HG3	1:1:413:TRP:HB3	1.90	0.54
3:3:460:ARG:NH2	3:3:661:LEU:HA	2.22	0.54
4:4:229:LEU:HA	4:4:232:ASN:ND2	2.23	0.54
5:5:49:GLU:HG3	5:5:106:ARG:HB2	1.89	0.54
6:6:58:GLU:HG2	6:6:151:PRO:O	2.08	0.54
6:6:68:ASP:OD1	6:6:69:MET:N	2.41	0.54
7:9:23:GLN:NE2	7:9:29:GLU:OE1	2.41	0.54
8:H:107:ALA:O	8:H:110:SER:OG	2.14	0.54
13:L:377:SER:O	13:L:381:THR:HG23	2.08	0.54
11:M:336:ARG:O	11:M:425:ASN:ND2	2.41	0.54
24:X:46:ASP:O	24:X:50:ILE:HG12	2.08	0.54
24:X:58:PHE:HB3	24:X:60:PHE:CE2	2.43	0.54
1:1:370:ASP:CG	3:3:179:ASN:HD21	2.11	0.54
3:3:453:LEU:HD21	3:3:458:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:233:ARG:NH2	7:9:24:THR:HG23	2.23	0.54
14:J:102:LEU:O	14:J:106:TYR:CB	2.56	0.54
11:M:251:ASN:N	11:M:251:ASN:OD1	2.38	0.54
11:M:4:TYR:CE2	11:M:41:LEU:HD12	2.43	0.54
1:1:135:TYR:CE1	1:1:176:PHE:HD2	2.25	0.53
3:3:258:ILE:HG22	3:3:368:ILE:HD13	1.90	0.53
3:3:368:ILE:O	3:3:371:VAL:HG22	2.08	0.53
3:3:549:HIS:O	3:3:549:HIS:ND1	2.40	0.53
4:4:199:VAL:O	4:4:323:ILE:HG22	2.07	0.53
8:H:200:LEU:CD1	8:H:209:SER:H	2.20	0.53
11:M:408:LEU:HD23	13:L:172:ILE:HG21	1.89	0.53
13:L:172:ILE:O	13:L:176:ARG:HG2	2.07	0.53
13:L:264:TYR:CD2	13:L:265:PRO:HD3	2.43	0.53
13:L:98:TRP:HZ2	13:L:456:ARG:HH12	1.54	0.53
42:Y:165:ARG:NH2	43:W:100:LYS:O	2.42	0.53
14:J:38:GLY:HA3	48:J:301:3PE:H2E2	1.89	0.53
9:N:250:SER:O	9:N:259:GLY:HA3	2.08	0.53
42:Y:70:PHE:O	42:Y:74:LYS:HG3	2.08	0.53
1:1:215:VAL:HG23	1:1:220:THR:HG21	1.90	0.53
11:M:121:MET:O	11:M:125:THR:HG23	2.07	0.53
42:Y:76:HIS:CD2	42:Y:114:LEU:HB2	2.44	0.53
3:3:382:THR:OG1	3:3:387:GLU:OE1	2.26	0.53
1:1:363:THR:HG21	3:3:97:LEU:HD21	1.90	0.53
4:4:244:VAL:HG12	4:4:292:ASP:HA	1.88	0.53
4:4:124:LYS:HG3	5:5:12:ARG:NH1	2.23	0.53
13:L:373:LEU:O	13:L:377:SER:OG	2.24	0.53
13:L:83:ASP:HB3	13:L:85:PHE:HD2	1.73	0.53
11:M:373:ILE:HD13	11:M:376:ILE:HD13	1.89	0.53
9:N:108:MET:O	9:N:112:HIS:N	2.42	0.53
3:3:278:ARG:HE	3:3:590:PRO:HG3	1.74	0.53
6:6:127:HIS:O	6:6:134:ARG:HD3	2.09	0.53
12:K:57:SER:O	12:K:60:PRO:HD2	2.08	0.53
13:L:28:LYS:HB2	13:L:32:TYR:HD2	1.74	0.53
13:L:362:LEU:HB3	13:L:431:LEU:HB3	1.91	0.53
43:W:65:GLU:OE2	43:W:73:ARG:HD3	2.08	0.53
42:Y:30:HIS:O	42:Y:33:ALA:HB3	2.08	0.53
1:1:230:VAL:O	1:1:234:ILE:HG12	2.09	0.53
2:2:172:ILE:HD11	2:2:187:ARG:NH1	2.23	0.53
4:4:309:ARG:O	4:4:312:SER:OG	2.21	0.53
11:M:114:GLU:OE1	42:Y:168:PHE:HB3	2.09	0.53
2:2:101:GLN:HB2	2:2:155:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:156:ILE:HG13	2:2:159:ASN:HB3	1.91	0.53
3:3:347:GLU:HB3	3:3:459:GLN:HE22	1.72	0.53
13:L:313:MET:SD	13:L:329:ILE:HG13	2.49	0.53
13:L:551:SER:O	13:L:555:LEU:CB	2.56	0.53
1:1:131:ALA:O	1:1:171:TYR:OH	2.26	0.53
4:4:268:ASP:OD1	4:4:269:LEU:N	2.42	0.53
5:5:48:LEU:HB3	5:5:105:ILE:HG22	1.89	0.53
8:H:137:ALA:O	8:H:140:ILE:HG22	2.09	0.53
13:L:17:MET:HG2	13:L:36:VAL:HG22	1.91	0.53
11:M:349:GLN:HG2	11:M:415:GLN:O	2.07	0.53
9:N:31:ILE:HG12	12:K:66:PHE:CE2	2.43	0.53
42:Y:165:ARG:HH22	43:W:103:LEU:HB3	1.71	0.53
13:L:138:PHE:HB2	13:L:196:TRP:NE1	2.21	0.53
11:M:329:LEU:HD23	11:M:359:TRP:CD2	2.44	0.53
43:W:132:LEU:HD12	43:W:132:LEU:O	2.08	0.53
4:4:128:ILE:HD13	4:4:330:VAL:HG11	1.92	0.53
4:4:388:ARG:HH22	4:4:390:LYS:HE2	1.74	0.53
11:M:140:THR:O	11:M:142:ARG:N	2.42	0.53
11:M:427:LEU:HD11	11:M:430:PHE:CZ	2.43	0.53
43:W:64:TRP:CD1	43:W:65:GLU:HG2	2.44	0.53
6:6:147:PRO:HD2	7:9:139:PHE:HB3	1.92	0.52
14:J:97:LEU:O	14:J:101:PHE:CB	2.57	0.52
50:L:601:CDL:H121	50:L:601:CDL:H531	1.91	0.52
9:N:126:SER:HA	9:N:129:ILE:HG22	1.90	0.52
42:Y:27:ALA:HB1	42:Y:70:PHE:HE1	1.74	0.52
13:L:271:LYS:HA	13:L:274:GLN:OE1	2.09	0.52
44:V:114:UNK:O	44:V:118:UNK:CB	2.57	0.52
24:X:22:TYR:HD2	24:X:25:ILE:HG13	1.73	0.52
41:Z:49:GLU:OE2	41:Z:53:ARG:NH2	2.43	0.52
3:3:378:LEU:HG	3:3:451:VAL:HG22	1.91	0.52
6:6:81:ARG:NH1	8:H:217:ALA:H	2.04	0.52
43:W:83:PRO:O	43:W:87:TYR:HB3	2.10	0.52
1:1:262:VAL:HG12	1:1:287:VAL:HA	1.90	0.52
5:5:57:VAL:HG22	5:5:109:THR:HG21	1.91	0.52
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.43	0.52
14:J:57:PHE:HA	14:J:61:LEU:HD12	1.90	0.52
13:L:193:LEU:HD11	13:L:206:PRO:HG3	1.90	0.52
9:N:146:LEU:HA	9:N:149:ILE:HD12	1.92	0.52
44:V:74:UNK:O	44:V:76:UNK:N	2.43	0.52
3:3:249:ARG:HH12	3:3:251:LEU:HD11	1.74	0.52
4:4:139:VAL:HG13	4:4:278:TYR:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:70:TYR:CE1	7:9:76:ARG:HG3	2.44	0.52
11:M:370:PRO:HA	11:M:375:LEU:HD13	1.91	0.52
43:W:85:LYS:HZ3	43:W:89:ARG:HH22	1.57	0.52
41:Z:6:LYS:HE3	41:Z:11:GLU:HB2	1.90	0.52
4:4:46:ASN:O	4:4:47:LEU:HD12	2.10	0.52
14:J:45:LEU:HD23	14:J:50:SER:HA	1.91	0.52
50:M:502:CDL:H622	50:M:502:CDL:H841	1.92	0.52
6:6:38:ASN:O	6:6:42:ARG:HG2	2.09	0.52
14:J:139:GLU:O	14:J:142:GLY:N	2.43	0.52
2:2:111:ARG:CG	2:2:152:PRO:HD3	2.39	0.52
3:3:171:ASP:OD2	3:3:189:LYS:NZ	2.31	0.52
3:3:229:ASP:OD1	3:3:230:VAL:N	2.42	0.52
7:9:76:ARG:HD3	7:9:128:VAL:O	2.10	0.52
43:W:94:LEU:O	43:W:98:SER:CB	2.58	0.52
1:1:68:ARG:NH1	1:1:254:LYS:HG3	2.24	0.52
1:1:98:ASP:O	46:1:501:FMN:N3	2.43	0.52
7:9:155:LEU:O	7:9:158:GLY:N	2.43	0.52
13:L:14:LEU:HD11	13:L:94:LEU:HD21	1.92	0.52
13:L:298:ILE:O	13:L:302:ILE:HG12	2.09	0.52
9:N:137:ALA:O	9:N:140:SER:OG	2.20	0.52
9:N:235:ASN:OD1	9:N:309:ASN:ND2	2.43	0.52
43:W:94:LEU:O	43:W:98:SER:HB2	2.09	0.52
1:1:139:ARG:NH2	2:2:144:CYS:O	2.42	0.52
7:9:92:ILE:HD13	7:9:111:ILE:HG12	1.92	0.52
13:L:265:PRO:HA	13:L:268:GLU:HG3	1.92	0.52
13:L:2:ASN:O	13:L:5:SER:HB2	2.10	0.52
11:M:56:PHE:HA	11:M:113:THR:OG1	2.10	0.52
24:X:36:PHE:HB2	24:X:72:CYS:HA	1.91	0.52
4:4:229:LEU:HD23	4:4:230:THR:N	2.25	0.51
6:6:145:TYR:O	7:9:140:SER:HA	2.10	0.51
10:A:60:ILE:O	10:A:63:LEU:N	2.42	0.51
13:L:345:SER:O	13:L:349:SER:HB2	2.10	0.51
3:3:103:LEU:HD23	4:4:342:MET:SD	2.50	0.51
4:4:45:SER:HA	10:A:50:PRO:HB3	1.91	0.51
13:L:410:LEU:O	13:L:414:VAL:HG12	2.10	0.51
42:Y:39:ASN:OD1	42:Y:40:LYS:N	2.43	0.51
3:3:103:LEU:HB3	4:4:345:LEU:HD22	1.91	0.51
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.43	0.51
7:9:162:GLU:O	7:9:165:ILE:N	2.44	0.51
8:H:182:ALA:HA	8:H:242:PHE:CE2	2.45	0.51
13:L:585:LYS:O	13:L:589:LEU:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:119:LYS:NZ	50:L:601:CDL:OA5	2.37	0.51
11:M:196:TRP:CD1	11:M:250:LEU:HD13	2.46	0.51
11:M:168:GLN:OE1	43:W:104:ARG:NH1	2.44	0.51
41:Z:83:CYS:SG	41:Z:84:MET:N	2.82	0.51
1:1:21:ILE:HG21	1:1:230:VAL:HG23	1.93	0.51
1:1:299:PRO:O	1:1:304:THR:OG1	2.22	0.51
2:2:40:GLU:HG3	2:2:41:GLY:H	1.75	0.51
3:3:347:GLU:HB3	3:3:459:GLN:NE2	2.25	0.51
8:H:127:TYR:HD1	10:A:46:SER:HB2	1.76	0.51
4:4:410:MET:HG2	8:H:281:ARG:NH2	2.24	0.51
14:J:161:LEU:O	14:J:164:GLY:CA	2.58	0.51
13:L:237:MET:SD	13:L:299:LYS:HG2	2.50	0.51
13:L:595:ILE:O	13:L:599:THR:CB	2.59	0.51
9:N:340:THR:HA	9:N:342:ILE:HG22	1.91	0.51
41:Z:96:LYS:O	41:Z:99:GLN:HB2	2.10	0.51
3:3:568:GLU:HG2	3:3:589:PRO:HA	1.91	0.51
4:4:55:HIS:HB2	4:4:56:PRO:HD2	1.92	0.51
5:5:56:GLY:HA2	5:5:59:PRO:HD2	1.91	0.51
42:Y:141:TYR:HD1	42:Y:142:HIS:H	1.56	0.51
42:Y:28:ALA:HA	42:Y:31:TYR:CD2	2.45	0.51
3:3:372:GLU:O	3:3:402:ASN:ND2	2.42	0.51
6:6:107:MET:O	6:6:111:ARG:NH2	2.41	0.51
6:6:139:ILE:HG22	6:6:140:VAL:HG13	1.92	0.51
10:A:57:LEU:HD21	14:J:172:THR:HG21	1.93	0.51
8:H:100:LEU:HD21	14:J:51:PHE:HD1	1.76	0.51
24:X:44:SER:O	24:X:47:GLN:HG2	2.10	0.51
4:4:371:LYS:NZ	4:4:422:ASP:OD1	2.43	0.51
13:L:383:MET:HE3	13:L:388:GLY:H	1.75	0.51
11:M:94:LEU:O	11:M:97:SER:OG	2.22	0.51
1:1:104:THR:HG22	1:1:106:LYS:H	1.76	0.51
3:3:329:ILE:HD12	3:3:626:VAL:HG21	1.93	0.51
4:4:166:PRO:HA	4:4:169:TRP:HE3	1.76	0.51
4:4:268:ASP:OD2	4:4:270:ARG:NE	2.44	0.51
4:4:90:LEU:HD23	5:5:168:LEU:HD11	1.93	0.51
8:H:120:GLY:HA3	8:H:132:ALA:HB2	1.93	0.51
7:9:30:LEU:HG	8:H:277:TYR:CE1	2.45	0.51
12:K:5:TYR:HE1	12:K:47:MET:HG2	1.76	0.51
11:M:412:ILE:O	11:M:413:THR:OG1	2.24	0.51
9:N:307:SER:HB2	9:N:309:ASN:ND2	2.25	0.51
1:1:134:ALA:HB2	1:1:173:PHE:HZ	1.75	0.51
2:2:63:ILE:HG13	2:2:81:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:195:LEU:HD11	3:3:393:ALA:HB2	1.91	0.51
4:4:80:ILE:HG13	4:4:429:ASP:OD1	2.11	0.51
6:6:84:ASP:OD2	8:H:54:LYS:NZ	2.42	0.51
8:H:287:HIS:HB3	10:A:113:TRP:CD1	2.46	0.51
8:H:317:GLN:HB3	10:A:80:GLN:NE2	2.25	0.51
9:N:12:THR:HG22	14:J:159:TRP:HE1	1.76	0.51
13:L:116:GLN:HG2	13:L:120:TYR:HE2	1.76	0.51
13:L:286:LEU:HB2	13:L:411:MET:SD	2.51	0.51
11:M:154:LEU:HA	11:M:157:SER:HB2	1.92	0.51
11:M:60:SER:O	11:M:64:PRO:HD2	2.10	0.51
42:Y:16:GLU:HB3	42:Y:18:LYS:HD3	1.93	0.51
1:1:66:ARG:NH1	1:1:72:GLY:O	2.41	0.51
4:4:360:PRO:HD2	5:5:209:TYR:CD2	2.46	0.51
13:L:53:MET:HA	13:L:56:HIS:CD2	2.46	0.51
1:1:188:GLU:HG2	46:1:501:FMN:C8	2.41	0.50
2:2:107:PRO:HA	2:2:110:LEU:HB2	1.92	0.50
3:3:180:ASP:OD1	3:3:182:GLN:NE2	2.44	0.50
3:3:570:SER:HB2	3:3:585:VAL:HG23	1.94	0.50
4:4:146:ARG:HA	4:4:370:PRO:HG3	1.92	0.50
9:N:263:LYS:O	9:N:267:ILE:HG12	2.12	0.50
42:Y:123:GLU:OE1	42:Y:124:LEU:HD23	2.11	0.50
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.93	0.50
1:1:266:CYS:SG	2:2:195:PRO:HG3	2.51	0.50
3:3:220:TRP:HD1	5:5:197:PHE:HD1	1.58	0.50
3:3:362:TYR:CE1	3:3:503:LEU:HB2	2.46	0.50
4:4:396:PHE:HA	4:4:428:VAL:HG13	1.94	0.50
4:4:352:TYR:CD1	7:9:86:VAL:HG11	2.39	0.50
11:M:140:THR:C	11:M:142:ARG:N	2.63	0.50
2:2:48:LEU:HB3	2:2:49:PRO:HD3	1.92	0.50
3:3:160:ILE:HD11	3:3:174:THR:HG23	1.92	0.50
3:3:367:THR:HB	3:3:579:ARG:HH22	1.76	0.50
6:6:125:TYR:CG	7:9:117:ILE:HD12	2.46	0.50
10:A:72:LEU:HA	14:J:147:TYR:OH	2.12	0.50
8:H:233:MET:O	8:H:236:ILE:N	2.45	0.50
8:H:51:ASP:O	8:H:55:LEU:HB3	2.11	0.50
13:L:195:THR:HB	41:Z:106:GLN:NE2	2.26	0.50
13:L:506:ASN:OD1	13:L:507:THR:N	2.44	0.50
11:M:153:THR:O	11:M:157:SER:OG	2.24	0.50
11:M:367:LEU:HD12	11:M:404:ALA:HA	1.93	0.50
9:N:162:ILE:HG13	9:N:188:GLY:HA3	1.94	0.50
9:N:98:MET:HE1	9:N:145:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:70:PRO:O	43:W:73:ARG:HB3	2.12	0.50
11:M:45:PHE:HZ	43:W:86:ASN:HD22	1.60	0.50
2:2:102:VAL:HG22	2:2:154:VAL:HG22	1.93	0.50
3:3:237:ASN:N	3:3:259:ASN:HD21	1.93	0.50
3:3:296:TRP:HZ2	3:3:599:ILE:HG12	1.76	0.50
4:4:130:PRO:HA	4:4:325:VAL:HG12	1.93	0.50
8:H:169:GLN:OE1	8:H:174:LEU:HB2	2.11	0.50
8:H:201:THR:O	8:H:205:SER:OG	2.29	0.50
44:V:103:UNK:O	44:V:107:UNK:CB	2.60	0.50
42:Y:162:HIS:NE2	43:W:99:GLU:OE2	2.41	0.50
42:Y:163:GLY:O	42:Y:165:ARG:HG3	2.11	0.50
1:1:297:VAL:HG22	1:1:336:VAL:HG12	1.94	0.50
3:3:442:VAL:O	3:3:446:ALA:N	2.45	0.50
5:5:111:THR:OG1	5:5:115:THR:O	2.28	0.50
5:5:173:GLU:HG3	5:5:188:VAL:HA	1.94	0.50
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.93	0.50
10:A:42:ASP:HB3	10:A:43:PRO:HD3	1.92	0.50
13:L:95:PHE:O	13:L:98:TRP:HB3	2.11	0.50
9:N:106:LEU:HD22	9:N:187:MET:HE1	1.93	0.50
1:1:263:ASN:O	1:1:285:GLY:HA3	2.11	0.50
1:1:267:THR:HG23	2:2:149:VAL:HG21	1.92	0.50
1:1:76:GLY:O	1:1:80:SER:HB3	2.12	0.50
8:H:222:LEU:O	8:H:225:MET:N	2.45	0.50
13:L:226:GLN:HE21	13:L:280:LEU:HG	1.77	0.50
9:N:83:GLN:N	9:N:83:GLN:OE1	2.45	0.50
4:4:147:LEU:HD11	4:4:218:PHE:CZ	2.46	0.50
6:6:40:ALA:HB1	8:H:50:ALA:HA	1.92	0.50
13:L:234:PRO:O	13:L:300:LYS:NZ	2.45	0.50
13:L:560:THR:O	13:L:564:LYS:N	2.45	0.50
1:1:59:GLU:HG2	1:1:235:CYS:HA	1.93	0.50
3:3:525:LEU:HD23	3:3:546:GLN:HB3	1.93	0.50
6:6:163:LEU:O	6:6:167:ILE:HG12	2.12	0.50
6:6:44:SER:OG	6:6:45:LEU:N	2.45	0.50
13:L:36:VAL:O	13:L:39:THR:OG1	2.23	0.50
11:M:50:LEU:HD11	11:M:58:SER:HB3	1.94	0.50
9:N:102:LEU:HD23	9:N:105:LYS:HG3	1.93	0.50
4:4:141:PHE:CE1	4:4:184:VAL:HG21	2.47	0.50
4:4:373:GLU:O	4:4:394:PRO:HG3	2.12	0.50
7:9:119:CYS:N	45:9:502:SF4:S4	2.84	0.50
8:H:65:THR:O	8:H:66:SER:OG	2.21	0.50
13:L:53:MET:HA	13:L:56:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:96:MET:HG3	9:N:153:LEU:HD11	1.93	0.50
1:1:392:LEU:HA	1:1:395:ILE:HD12	1.94	0.49
1:1:87:ASP:OD1	1:1:88:GLY:N	2.43	0.49
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.76	0.49
11:M:220:HIS:CE1	11:M:228:SER:HG	2.27	0.49
9:N:92:PRO:O	9:N:95:SER:OG	2.25	0.49
43:W:81:ASP:HB3	43:W:85:LYS:HD3	1.94	0.49
41:Z:54:GLN:O	41:Z:57:LYS:HG2	2.11	0.49
1:1:53:PRO:HB3	1:1:128:ALA:O	2.12	0.49
1:1:33:LEU:O	1:1:37:GLN:CB	2.52	0.49
4:4:193:TYR:HE1	4:4:201:GLN:O	1.95	0.49
13:L:479:GLN:C	13:L:481:THR:H	2.15	0.49
11:M:153:THR:O	11:M:157:SER:CB	2.60	0.49
11:M:286:ILE:HG12	11:M:326:LEU:HG	1.94	0.49
1:1:15:LEU:HD21	1:1:270:GLU:HA	1.93	0.49
4:4:228:MET:SD	7:9:34:LEU:HD11	2.52	0.49
7:9:119:CYS:HB3	7:9:121:PHE:CD2	2.47	0.49
13:L:328:HIS:HB2	13:L:391:SER:HB2	1.94	0.49
41:Z:65:ARG:HG2	43:W:66:TYR:CD1	2.48	0.49
9:N:264:TRP:CZ2	42:Y:167:PHE:HD2	2.30	0.49
3:3:431:ASP:O	3:3:436:SER:OG	2.21	0.49
3:3:349:PHE:H	3:3:509:PRO:HB2	1.78	0.49
8:H:9:LEU:HD22	8:H:95:LEU:HD23	1.94	0.49
11:M:450:ASN:OD1	11:M:452:LYS:HG2	2.13	0.49
11:M:3:LYS:HE2	11:M:4:TYR:CZ	2.46	0.49
1:1:42:TRP:HE1	1:1:116:HIS:HB3	1.77	0.49
1:1:47:GLU:O	1:1:51:LYS:HB2	2.11	0.49
4:4:85:ARG:HD2	6:6:126:TYR:HE2	1.76	0.49
5:5:58:ILE:HB	5:5:59:PRO:HD3	1.93	0.49
13:L:286:LEU:HD13	13:L:411:MET:SD	2.53	0.49
13:L:495:ILE:HA	13:L:498:PHE:HB3	1.94	0.49
11:M:12:MET:SD	11:M:16:TRP:NE1	2.85	0.49
9:N:1:MET:SD	9:N:46:LYS:NZ	2.71	0.49
9:N:91:ASN:HB3	9:N:94:ALA:HB3	1.93	0.49
42:Y:161:ARG:HG2	42:Y:162:HIS:CD2	2.47	0.49
4:4:193:TYR:O	4:4:199:VAL:HG13	2.12	0.49
4:4:249:ASP:OD2	4:4:404:LYS:NZ	2.45	0.49
7:9:80:CYS:HA	7:9:104:ARG:HH22	1.77	0.49
8:H:140:ILE:HG13	10:A:62:PHE:CE1	2.47	0.49
8:H:18:ALA:O	8:H:21:THR:OG1	2.24	0.49
14:J:4:TYR:O	14:J:7:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:455:LYS:O	13:L:459:ILE:HD12	2.12	0.49
9:N:207:ILE:O	9:N:211:MET:HG2	2.12	0.49
9:N:26:TRP:HB3	9:N:74:ILE:HD13	1.94	0.49
1:1:363:THR:HA	1:1:366:ARG:HG2	1.94	0.49
1:1:349:ARG:HE	2:2:105:THR:HA	1.76	0.49
8:H:115:SER:O	8:H:119:SER:HB2	2.11	0.49
13:L:7:LEU:O	13:L:10:VAL:HG22	2.12	0.49
13:L:396:ILE:HD11	13:L:490:ALA:HB2	1.94	0.49
13:L:83:ASP:O	13:L:84:PHE:HB3	2.12	0.49
9:N:256:PRO:HB3	11:M:124:ALA:HB2	1.95	0.49
43:W:64:TRP:HD1	43:W:65:GLU:HG2	1.78	0.49
24:X:20:LYS:HG3	24:X:30:LEU:HD23	1.94	0.49
42:Y:139:ASN:HB3	42:Y:143:SER:OG	2.12	0.49
42:Y:15:GLN:NE2	42:Y:64:GLN:OE1	2.46	0.49
1:1:171:TYR:CE2	1:1:173:PHE:HB2	2.48	0.49
4:4:106:LEU:HD12	4:4:107:ASP:N	2.28	0.49
4:4:47:LEU:HD22	4:4:68:LEU:HD21	1.95	0.49
10:A:48:ARG:CG	10:A:49:LEU:H	2.24	0.49
12:K:31:LEU:O	12:K:34:GLU:N	2.46	0.49
11:M:137:GLY:C	11:M:139:GLN:H	2.14	0.49
9:N:207:ILE:HD13	9:N:262:PRO:HD3	1.95	0.49
9:N:78:LEU:HD12	9:N:84:TRP:CZ2	2.47	0.49
24:X:22:TYR:CE2	24:X:24:LYS:HB3	2.48	0.49
2:2:46:ALA:HB3	2:2:73:LEU:HD21	1.95	0.49
4:4:287:ILE:HG22	4:4:288:GLY:N	2.28	0.49
4:4:383:SER:OG	4:4:384:SER:N	2.46	0.49
8:H:13:ILE:O	8:H:17:VAL:HG23	2.12	0.49
8:H:224:PHE:CE1	8:H:228:TYR:HE2	2.31	0.49
8:H:288:LEU:HG	8:H:292:ASN:HD21	1.77	0.49
13:L:135:ASN:HB2	13:L:198:LEU:HB3	1.95	0.49
9:N:280:THR:HG22	11:M:162:VAL:HG21	1.95	0.49
41:Z:88:GLU:HB3	41:Z:150:SER:OG	2.13	0.49
1:1:368:GLY:HA3	1:1:399:ILE:HD11	1.95	0.49
8:H:186:PHE:O	8:H:189:THR:OG1	2.21	0.49
44:V:107:UNK:O	44:V:111:UNK:CB	2.61	0.49
42:Y:165:ARG:NH1	43:W:103:LEU:HD23	2.28	0.49
4:4:154:VAL:HG13	4:4:297:TYR:HE1	1.78	0.48
6:6:110:PRO:HG2	8:H:58:LYS:NZ	2.28	0.48
6:6:117:GLY:O	6:6:121:ASN:ND2	2.46	0.48
13:L:345:SER:O	13:L:349:SER:HB3	2.12	0.48
13:L:7:LEU:HD12	13:L:50:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:155:LEU:HD21	9:N:278:LEU:HD11	1.95	0.48
42:Y:15:GLN:HB2	42:Y:63:ASN:ND2	2.28	0.48
41:Z:119:SER:O	41:Z:122:GLN:N	2.37	0.48
1:1:306:LEU:HD21	1:1:347:ILE:HD11	1.94	0.48
8:H:11:ILE:HB	8:H:12:PRO:HD3	1.95	0.48
8:H:165:LEU:HD23	8:H:240:THR:HG22	1.95	0.48
14:J:30:GLY:O	14:J:34:ILE:HG12	2.14	0.48
12:K:59:MET:O	12:K:63:LEU:HB3	2.13	0.48
11:M:272:THR:HA	11:M:275:ILE:HG22	1.95	0.48
9:N:270:MET:HG2	9:N:279:PRO:HG3	1.95	0.48
24:X:7:THR:O	24:X:11:ILE:HG22	2.13	0.48
42:Y:14:VAL:HG11	42:Y:60:LYS:HG3	1.95	0.48
1:1:138:ILE:HG21	1:1:146:ALA:HB2	1.95	0.48
2:2:116:ILE:HG23	2:2:169:ILE:HG13	1.95	0.48
5:5:83:ILE:HG22	5:5:84:PRO:O	2.13	0.48
6:6:152:THR:O	6:6:155:ALA:N	2.46	0.48
8:H:81:LEU:O	8:H:85:MET:HG2	2.14	0.48
13:L:154:LEU:HB3	13:L:243:VAL:HG11	1.95	0.48
13:L:12:LEU:O	13:L:16:THR:HG23	2.13	0.48
13:L:137:LEU:HB3	13:L:196:TRP:CD1	2.48	0.48
13:L:51:THR:HG21	13:L:91:PRO:HG2	1.95	0.48
13:L:592:LEU:O	13:L:596:LEU:CB	2.62	0.48
11:M:394:ILE:O	11:M:398:LEU:HB2	2.13	0.48
9:N:193:VAL:HG22	9:N:270:MET:HE1	1.95	0.48
9:N:328:THR:O	9:N:332:LEU:HB2	2.12	0.48
43:W:64:TRP:CD1	43:W:73:ARG:HG3	2.48	0.48
9:N:268:GLN:HB2	42:Y:167:PHE:HZ	1.77	0.48
2:2:42:HIS:C	2:2:44:ALA:H	2.17	0.48
1:1:366:ARG:NH2	3:3:155:GLN:HB2	2.28	0.48
3:3:304:ALA:O	3:3:308:GLN:HG2	2.13	0.48
3:3:386:PHE:CD1	3:3:671:PHE:HB2	2.49	0.48
4:4:106:LEU:HD22	4:4:391:ILE:HG21	1.95	0.48
5:5:53:HIS:CG	5:5:54:PRO:HD2	2.47	0.48
7:9:113:MET:HE3	7:9:118:TYR:HE1	1.78	0.48
10:A:3:LEU:O	10:A:6:THR:OG1	2.24	0.48
13:L:296:ASN:HB3	13:L:356:ILE:HG22	1.95	0.48
2:2:135:LYS:O	2:2:136:LEU:HG	2.13	0.48
2:2:168:ASP:OD2	2:2:187:ARG:NH1	2.46	0.48
2:2:55:GLN:OE1	2:2:90:TYR:HA	2.13	0.48
4:4:103:PHE:HA	4:4:106:LEU:HD23	1.96	0.48
4:4:353:THR:OG1	4:4:354:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:14:LEU:O	11:M:18:SER:OG	2.31	0.48
11:M:88:ASN:OD1	11:M:89:LEU:N	2.46	0.48
9:N:83:GLN:HG2	9:N:85:THR:HG23	1.96	0.48
1:1:403:THR:HG21	1:1:408:GLY:HA3	1.95	0.48
3:3:456:SER:HB3	3:3:495:ARG:HD3	1.96	0.48
7:9:126:CYS:SG	7:9:130:ALA:N	2.77	0.48
7:9:163:ALA:HA	7:9:166:ALA:HB3	1.96	0.48
9:N:146:LEU:HA	9:N:149:ILE:CD1	2.44	0.48
1:1:46:LYS:HG2	1:1:50:LEU:HD23	1.96	0.48
6:6:122:GLY:H	6:6:135:GLY:HA2	1.79	0.48
13:L:264:TYR:CG	13:L:265:PRO:HD3	2.49	0.48
13:L:283:MET:O	13:L:287:PHE:HB3	2.14	0.48
13:L:289:ALA:HA	13:L:422:TYR:OH	2.13	0.48
11:M:196:TRP:CE2	11:M:200:MET:HG3	2.49	0.48
11:M:408:LEU:HD11	13:L:152:PHE:CE2	2.49	0.48
41:Z:60:TYR:HB2	43:W:50:ALA:HA	1.95	0.48
24:X:84:LYS:HG3	24:X:85:ASP:H	1.79	0.48
42:Y:41:GLU:HG2	42:Y:132:THR:HG22	1.94	0.48
1:1:294:LEU:HD11	1:1:309:LYS:HG3	1.94	0.48
2:2:49:PRO:O	2:2:52:ASP:HB2	2.13	0.48
3:3:156:CYS:N	45:3:802:SF4:S4	2.87	0.48
10:A:55:PHE:HB3	14:J:70:TYR:OH	2.14	0.48
13:L:81:LYS:HB2	13:L:135:ASN:HB3	1.96	0.48
11:M:30:HIS:O	11:M:34:ILE:HG12	2.13	0.48
9:N:155:LEU:O	9:N:158:SER:OG	2.27	0.48
42:Y:165:ARG:HH21	43:W:104:ARG:N	2.12	0.48
42:Y:70:PHE:HA	42:Y:73:ILE:HG22	1.96	0.48
1:1:171:TYR:HE2	1:1:173:PHE:HB2	1.79	0.48
4:4:176:LYS:O	4:4:179:GLU:HB3	2.14	0.48
7:9:87:CYS:HA	45:9:502:SF4:S2	2.53	0.48
12:K:46:LEU:HD22	14:J:47:PHE:CD2	2.49	0.48
13:L:114:ILE:HD11	13:L:118:PHE:CE2	2.48	0.48
13:L:226:GLN:HG3	13:L:227:PHE:H	1.78	0.48
13:L:409:LEU:O	13:L:412:THR:OG1	2.20	0.48
11:M:27:THR:HG21	11:M:96:ILE:HG21	1.95	0.48
11:M:350:THR:OG1	11:M:351:LEU:N	2.46	0.48
9:N:109:ALA:HA	9:N:112:HIS:HD2	1.78	0.48
43:W:74:TRP:O	43:W:78:THR:HG22	2.14	0.48
1:1:349:ARG:NH1	1:1:352:GLU:OE1	2.41	0.48
1:1:363:THR:N	1:1:364:PRO:HD2	2.28	0.48
4:4:51:PHE:CD2	4:4:63:ARG:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:135:PRO:HG2	7:9:164:GLU:CG	2.42	0.48
14:J:7:PHE:O	14:J:11:ILE:HG12	2.14	0.48
42:Y:83:GLU:HA	42:Y:86:THR:HG22	1.95	0.48
1:1:238:GLY:N	2:2:214:GLN:HE22	2.11	0.47
3:3:240:VAL:HG21	3:3:586:ALA:HB2	1.95	0.47
3:3:425:SER:HB3	3:3:428:ILE:HG13	1.96	0.47
4:4:229:LEU:HD11	4:4:235:TRP:CE2	2.49	0.47
7:9:82:LEU:O	7:9:85:ALA:N	2.46	0.47
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.48	0.47
11:M:165:ILE:O	11:M:168:GLN:HB3	2.14	0.47
11:M:276:CYS:HB3	11:M:288:TYR:HB2	1.95	0.47
11:M:49:SER:O	11:M:51:ASN:ND2	2.46	0.47
9:N:211:MET:HE1	9:N:250:SER:HB2	1.95	0.47
9:N:4:ILE:O	9:N:7:ILE:N	2.46	0.47
42:Y:100:ARG:HD3	42:Y:103:GLN:HB3	1.96	0.47
1:1:431:GLN:HE21	1:1:435:GLN:HE21	1.62	0.47
2:2:164:LEU:HB3	2:2:169:ILE:HD11	1.96	0.47
13:L:233:LEU:HG	13:L:248:HIS:CE1	2.49	0.47
13:L:198:LEU:HD11	13:L:262:ARG:CG	2.44	0.47
41:Z:88:GLU:O	41:Z:91:TRP:HB3	2.14	0.47
6:6:71:ARG:NH2	7:9:48:ILE:O	2.47	0.47
7:9:69:ARG:HA	7:9:76:ARG:HB2	1.95	0.47
8:H:154:LEU:HD11	8:H:160:PHE:HA	1.95	0.47
13:L:32:TYR:OH	13:L:115:ASN:O	2.32	0.47
11:M:371:PRO:HG3	50:L:601:CDL:H252	1.97	0.47
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.96	0.47
1:1:264:ASN:OD1	2:2:196:ALA:HB3	2.14	0.47
1:1:188:GLU:HG2	46:1:501:FMN:C7	2.44	0.47
2:2:213:VAL:HG23	2:2:214:GLN:H	1.78	0.47
13:L:233:LEU:O	13:L:237:MET:HE2	2.14	0.47
13:L:482:MET:O	13:L:487:LYS:HD3	2.15	0.47
11:M:96:ILE:O	11:M:100:ILE:HG12	2.13	0.47
11:M:196:TRP:CZ2	11:M:200:MET:HG3	2.49	0.47
41:Z:89:MET:SD	43:W:87:TYR:HE1	2.37	0.47
3:3:624:GLU:HG3	3:3:628:PRO:HA	1.96	0.47
4:4:123:GLU:HG2	4:4:197:GLY:H	1.79	0.47
4:4:371:LYS:HZ1	4:4:424:VAL:HG23	1.79	0.47
4:4:51:PHE:HD2	4:4:63:ARG:HG3	1.80	0.47
6:6:126:TYR:C	6:6:128:TYR:H	2.16	0.47
6:6:65:PRO:O	7:9:47:THR:HG22	2.15	0.47
6:6:72:PHE:CD2	6:6:157:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:302:MET:CB	10:A:95:ILE:HD11	2.38	0.47
8:H:131:GLY:CA	8:H:208:VAL:HG22	2.45	0.47
13:L:595:ILE:O	13:L:598:SER:C	2.53	0.47
11:M:232:ALA:HB3	11:M:327:PHE:CE2	2.46	0.47
9:N:45:MET:HA	9:N:52:ALA:HB1	1.97	0.47
42:Y:166:LEU:HG	42:Y:167:PHE:H	1.79	0.47
41:Z:24:SER:O	41:Z:25:LEU:HD12	2.15	0.47
3:3:501:ALA:O	3:3:505:LEU:HG	2.13	0.47
4:4:388:ARG:HH12	4:4:390:LYS:HB2	1.79	0.47
4:4:411:LEU:O	4:4:414:VAL:N	2.48	0.47
6:6:118:SER:HA	6:6:121:ASN:HD21	1.79	0.47
11:M:201:MET:O	11:M:205:VAL:HG23	2.15	0.47
2:2:151:ALA:HB2	2:2:190:ARG:HH12	1.80	0.47
3:3:238:ILE:O	3:3:253:ARG:NH1	2.39	0.47
4:4:270:ARG:HG2	4:4:278:TYR:HE2	1.79	0.47
10:A:92:LEU:O	10:A:96:PHE:HB2	2.15	0.47
8:H:284:GLN:O	8:H:288:LEU:CB	2.58	0.47
12:K:37:MET:SD	12:K:67:ALA:HA	2.55	0.47
41:Z:167:LYS:HA	41:Z:170:LYS:HG2	1.96	0.47
4:4:255:PHE:HZ	4:4:401:GLY:HA3	1.80	0.47
4:4:84:HIS:CD2	5:5:152:LEU:HB3	2.50	0.47
10:A:8:LEU:O	10:A:12:THR:HG23	2.15	0.47
14:J:143:ILE:O	14:J:146:LEU:HB3	2.15	0.47
13:L:116:GLN:HG2	13:L:120:TYR:CE2	2.50	0.47
13:L:128:MET:HG3	13:L:251:THR:CG2	2.45	0.47
13:L:270:ASN:O	13:L:273:GLY:N	2.37	0.47
13:L:531:THR:O	13:L:535:ARG:CB	2.63	0.47
11:M:434:ASN:HB3	43:W:21:PHE:CE2	2.50	0.47
42:Y:23:VAL:HG23	42:Y:81:PHE:CZ	2.49	0.47
42:Y:46:ARG:O	42:Y:50:LYS:HG2	2.15	0.47
42:Y:82:THR:HA	42:Y:85:TRP:NE1	2.30	0.47
4:4:351:LEU:HD11	4:4:356:TYR:HD2	1.80	0.47
9:N:311:MET:CG	9:N:312:LYS:H	2.17	0.47
1:1:386:PRO:HG3	1:1:430:MET:HG2	1.97	0.47
2:2:27:ASN:OD1	2:2:53:LEU:HD21	2.14	0.47
3:3:524:LEU:HB2	3:3:545:TYR:HA	1.95	0.47
24:X:11:ILE:HD11	24:X:80:ILE:HB	1.96	0.47
42:Y:51:ASP:O	42:Y:54:ARG:N	2.35	0.47
42:Y:53:ARG:HA	42:Y:56:LEU:HD23	1.97	0.47
13:L:463:PHE:CE2	13:L:467:ILE:HD11	2.50	0.47
11:M:7:PRO:HB2	11:M:34:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:451:PRO:O	11:M:454:ILE:HG13	2.15	0.47
1:1:31:TRP:O	1:1:32:ARG:HG2	2.14	0.46
1:1:343:ILE:HD13	1:1:422:PHE:CE2	2.49	0.46
1:1:367:GLU:O	1:1:370:ASP:HB3	2.16	0.46
3:3:130:PHE:CZ	3:3:133:GLY:HA3	2.51	0.46
4:4:229:LEU:HD21	4:4:235:TRP:CZ3	2.49	0.46
6:6:112:TYR:OH	6:6:170:GLU:OE2	2.18	0.46
7:9:19:ASP:O	7:9:23:GLN:HB2	2.15	0.46
8:H:158:GLY:CA	8:H:315:PRO:HB2	2.44	0.46
13:L:227:PHE:CG	13:L:228:GLY:N	2.83	0.46
9:N:210:ILE:HG22	9:N:333:SER:HB3	1.97	0.46
1:1:431:GLN:NE2	1:1:435:GLN:HE21	2.13	0.46
3:3:528:ASP:OD2	3:3:679:ARG:NH2	2.48	0.46
5:5:94:TYR:HB2	5:5:107:VAL:HB	1.97	0.46
5:5:123:VAL:HG23	5:5:124:TYR:H	1.81	0.46
8:H:161:THR:O	8:H:162:LEU:HB3	2.15	0.46
13:L:297:ASP:O	13:L:301:ILE:HD12	2.15	0.46
41:Z:81:VAL:O	41:Z:84:MET:N	2.49	0.46
4:4:233:ARG:O	4:4:237:ASN:HB2	2.16	0.46
4:4:47:LEU:HD22	4:4:68:LEU:HD11	1.97	0.46
5:5:180:VAL:HB	5:5:182:ARG:NH1	2.30	0.46
7:9:27:TRP:HE1	48:9:501:3PE:C21	2.28	0.46
10:A:98:LEU:O	10:A:101:SER:OG	2.25	0.46
1:1:360:GLY:O	1:1:366:ARG:NH1	2.49	0.46
2:2:95:VAL:HB	2:2:138:THR:HG21	1.96	0.46
4:4:162:GLY:HA2	8:H:279:ARG:NH1	2.31	0.46
4:4:243:GLY:H	4:4:409:HIS:CD2	2.33	0.46
4:4:46:ASN:HA	4:4:68:LEU:O	2.15	0.46
4:4:96:TYR:CE1	4:4:386:PRO:HB3	2.51	0.46
5:5:82:ASP:OD2	5:5:163:ARG:HA	2.15	0.46
6:6:79:SER:O	6:6:83:SER:OG	2.27	0.46
8:H:163:SER:O	8:H:166:ILE:HG22	2.14	0.46
14:J:151:THR:OG1	14:J:152:TRP:N	2.48	0.46
13:L:487:LYS:HZ2	13:L:488:MET:HG2	1.80	0.46
11:M:297:VAL:O	11:M:301:ILE:HG12	2.15	0.46
11:M:441:MET:O	11:M:444:LEU:N	2.48	0.46
24:X:36:PHE:HE2	24:X:47:GLN:HB2	1.79	0.46
41:Z:167:LYS:O	41:Z:170:LYS:HG2	2.15	0.46
1:1:322:LEU:HB3	1:1:327:THR:O	2.16	0.46
1:1:224:ASN:N	46:1:501:FMN:O3P	2.39	0.46
2:2:202:LEU:O	2:2:202:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:107:ILE:HA	7:9:104:ARG:HE	1.80	0.46
4:4:134:ALA:HB2	4:4:323:ILE:O	2.15	0.46
7:9:37:THR:O	7:9:40:TYR:HB3	2.16	0.46
7:9:9:GLU:HG2	7:9:9:GLU:O	2.15	0.46
13:L:32:TYR:O	13:L:35:TYR:HB3	2.15	0.46
13:L:368:PHE:CE2	13:L:454:ILE:HB	2.51	0.46
11:M:119:TYR:CD1	11:M:160:LEU:HD11	2.50	0.46
9:N:28:LEU:O	9:N:31:ILE:N	2.49	0.46
42:Y:36:ASP:HB3	42:Y:40:LYS:HG2	1.98	0.46
1:1:135:TYR:CD1	1:1:176:PHE:HB2	2.51	0.46
2:2:168:ASP:CG	2:2:187:ARG:HD2	2.36	0.46
3:3:379:LEU:HD21	3:3:384:PRO:HG2	1.98	0.46
3:3:673:MET:O	3:3:679:ARG:HG3	2.15	0.46
4:4:165:THR:HG23	4:4:166:PRO:HD3	1.97	0.46
13:L:144:TRP:CE2	13:L:223:LYS:HE2	2.50	0.46
13:L:22:ILE:HG22	50:L:601:CDL:HB4	1.98	0.46
13:L:282:ALA:O	13:L:285:THR:OG1	2.23	0.46
13:L:342:CYS:O	13:L:345:SER:OG	2.19	0.46
13:L:41:SER:O	13:L:44:PHE:N	2.45	0.46
13:L:484:HIS:CG	13:L:487:LYS:HE3	2.51	0.46
13:L:63:ILE:HD11	13:L:80:PHE:CD2	2.50	0.46
11:M:73:LEU:HD22	11:M:103:GLN:OE1	2.16	0.46
11:M:429:SER:OG	11:M:430:PHE:N	2.36	0.46
9:N:258:SER:OG	9:N:336:LEU:HB3	2.16	0.46
3:3:213:TYR:CE1	3:3:249:ARG:HD3	2.51	0.46
4:4:369:ALA:O	4:4:372:GLY:N	2.40	0.46
6:6:42:ARG:HA	6:6:45:LEU:HG	1.98	0.46
4:4:94:LYS:HE2	7:9:88:PRO:O	2.15	0.46
10:A:71:LEU:O	14:J:147:TYR:OH	2.30	0.46
8:H:247:HIS:O	8:H:249:PRO:HD3	2.15	0.46
13:L:281:GLY:HA3	13:L:314:MET:HB3	1.96	0.46
11:M:356:ALA:HA	11:M:415:GLN:NE2	2.31	0.46
11:M:397:GLY:O	11:M:400:MET:HB3	2.16	0.46
42:Y:100:ARG:NE	42:Y:103:GLN:OE1	2.49	0.46
3:3:333:ASP:O	3:3:337:ARG:CB	2.61	0.46
3:3:464:ALA:HB3	3:3:654:GLN:OE1	2.16	0.46
4:4:47:LEU:HD13	4:4:68:LEU:HD11	1.97	0.46
6:6:127:HIS:ND1	6:6:127:HIS:O	2.48	0.46
7:9:27:TRP:NE1	48:9:501:3PE:O22	2.49	0.46
48:J:301:3PE:H3D2	48:J:301:3PE:H2G1	1.96	0.46
14:J:38:GLY:HA3	48:J:301:3PE:C2E	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:213:LEU:HD12	13:L:266:LEU:HG	1.98	0.46
13:L:57:THR:HG22	13:L:57:THR:O	2.16	0.46
11:M:311:GLY:HA2	11:M:377:GLY:HA2	1.97	0.46
11:M:408:LEU:CD2	13:L:172:ILE:HG21	2.46	0.46
9:N:202:LEU:CB	9:N:346:LEU:HD21	2.46	0.46
46:1:501:FMN:H1'2	46:1:501:FMN:H9	1.74	0.46
2:2:161:TYR:HE1	2:2:184:PRO:HA	1.81	0.46
4:4:144:ILE:HG23	4:4:177:MET:CE	2.46	0.46
7:9:69:ARG:NH2	7:9:155:LEU:HD22	2.31	0.46
13:L:190:LEU:O	13:L:194:ASN:N	2.44	0.46
13:L:382:GLY:HA2	13:L:392:LYS:HD2	1.98	0.46
11:M:41:LEU:HD22	11:M:63:THR:HG23	1.98	0.46
3:3:568:GLU:N	3:3:568:GLU:OE1	2.49	0.46
3:3:98:LEU:HD13	4:4:343:GLU:HG2	1.98	0.46
13:L:233:LEU:O	13:L:236:ALA:N	2.48	0.46
13:L:237:MET:HG3	13:L:300:LYS:HG2	1.97	0.46
13:L:350:LEU:HD23	13:L:350:LEU:O	2.16	0.46
13:L:418:PHE:O	13:L:421:ILE:HG12	2.16	0.46
11:M:130:LEU:O	11:M:134:THR:HG22	2.16	0.46
11:M:441:MET:HE1	11:M:444:LEU:HD23	1.97	0.46
9:N:202:LEU:HB2	9:N:346:LEU:HD21	1.98	0.46
24:X:53:ALA:O	24:X:57:GLU:HG2	2.16	0.46
3:3:58:GLU:OE1	3:3:85:LYS:HB3	2.15	0.45
4:4:104:ASP:HB2	4:4:115:GLU:OE2	2.16	0.45
4:4:105:ARG:NH2	7:9:117:ILE:HD11	2.30	0.45
4:4:242:ILE:HA	4:4:409:HIS:NE2	2.31	0.45
5:5:131:GLU:HB3	5:5:142:PHE:CD2	2.51	0.45
13:L:120:TYR:O	13:L:123:LEU:N	2.49	0.45
13:L:188:TRP:CE2	13:L:192:ASN:OD1	2.69	0.45
13:L:484:HIS:HA	13:L:487:LYS:HG2	1.97	0.45
11:M:417:GLY:HA2	13:L:160:GLY:HA2	1.97	0.45
11:M:1:MET:HB3	11:M:56:PHE:HE1	1.81	0.45
9:N:124:LEU:HD12	9:N:176:ARG:HH22	1.81	0.45
24:X:43:ASP:OD2	24:X:45:LEU:HB3	2.16	0.45
1:1:237:ARG:C	2:2:214:GLN:HE22	2.20	0.45
6:6:149:CYS:SG	7:9:117:ILE:HG13	2.56	0.45
7:9:49:ASN:O	7:9:53:GLU:N	2.50	0.45
8:H:287:HIS:ND1	8:H:291:LYS:HE3	2.32	0.45
13:L:439:THR:OG1	13:L:440:LEU:N	2.50	0.45
11:M:412:ILE:HG13	11:M:416:ARG:HB3	1.97	0.45
11:M:417:GLY:O	11:M:418:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:149:ILE:HD13	9:N:154:ILE:CD1	2.45	0.45
43:W:115:ARG:HG3	43:W:123:PHE:CE2	2.51	0.45
41:Z:166:ARG:HA	41:Z:169:THR:HG22	1.97	0.45
41:Z:39:LEU:O	41:Z:43:PRO:HG2	2.17	0.45
1:1:390:ASP:OD1	1:1:423:ARG:NH1	2.50	0.45
2:2:78:MET:HA	2:2:81:TYR:HD2	1.80	0.45
3:3:211:LYS:O	3:3:214:ALA:HB2	2.15	0.45
4:4:286:PRO:HA	7:9:3:LYS:O	2.16	0.45
10:A:109:LYS:O	10:A:109:LYS:HG2	2.15	0.45
13:L:99:SER:HB3	13:L:341:MET:HE1	1.98	0.45
13:L:491:LEU:O	13:L:495:ILE:HD12	2.16	0.45
13:L:581:LYS:O	13:L:585:LYS:CB	2.65	0.45
3:3:155:GLN:NE2	3:3:181:MET:O	2.50	0.45
3:3:379:LEU:O	3:3:409:ILE:N	2.49	0.45
7:9:34:LEU:HD12	7:9:34:LEU:HA	1.57	0.45
10:A:73:LEU:N	10:A:74:PRO:HD2	2.32	0.45
8:H:145:THR:O	8:H:149:ILE:HD12	2.17	0.45
13:L:54:PHE:CD1	13:L:58:GLY:HA2	2.52	0.45
9:N:25:HIS:CD2	13:L:17:MET:HG3	103.38	0.45
24:X:28:GLU:HG3	24:X:29:LYS:HD2	1.98	0.45
42:Y:27:ALA:HB2	42:Y:81:PHE:CZ	2.51	0.45
3:3:9:ILE:HG22	3:3:11:VAL:HG13	1.98	0.45
3:3:163:ALA:HA	3:3:167:ALA:HB3	1.98	0.45
3:3:101:HIS:HD2	4:4:342:MET:HE1	1.81	0.45
4:4:300:ARG:NH2	4:4:420:THR:O	2.50	0.45
5:5:77:ASP:OD1	5:5:78:LEU:N	2.49	0.45
5:5:80:ALA:HB3	5:5:138:PHE:HE2	1.81	0.45
14:J:166:VAL:O	14:J:170:GLU:CB	2.65	0.45
12:K:11:ALA:HB1	14:J:17:PHE:HD2	1.81	0.45
13:L:62:ILE:HG12	13:L:199:GLN:NE2	2.32	0.45
11:M:411:LEU:HD12	11:M:415:GLN:OE1	2.17	0.45
11:M:433:GLU:O	11:M:437:MET:HG2	2.17	0.45
1:1:362:CYS:SG	1:1:404:ILE:HG12	2.57	0.45
3:3:41:CYS:H	3:3:52:CYS:HB3	1.81	0.45
4:4:161:ILE:HD11	4:4:238:ARG:NE	2.30	0.45
4:4:151:ILE:HD11	4:4:170:MET:HG3	1.98	0.45
4:4:284:ASP:OD1	4:4:284:ASP:N	2.50	0.45
5:5:54:PRO:HB3	5:5:110:TYR:O	2.17	0.45
7:9:65:HIS:O	7:9:154:LEU:HD22	2.17	0.45
10:A:92:LEU:O	10:A:96:PHE:CB	2.65	0.45
13:L:67:HIS:ND1	13:L:69:LEU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:14:LEU:HD22	11:M:30:HIS:ND1	2.32	0.45
3:3:331:LEU:HB2	3:3:600:ILE:HD13	1.99	0.45
4:4:229:LEU:HD21	4:4:235:TRP:CE3	2.51	0.45
14:J:142:GLY:O	14:J:145:ALA:HB3	2.17	0.45
14:J:17:PHE:HA	14:J:20:PHE:HB3	1.99	0.45
13:L:28:LYS:HB2	13:L:32:TYR:CD2	2.52	0.45
13:L:98:TRP:HE1	13:L:456:ARG:HH11	1.63	0.45
13:L:487:LYS:HG3	13:L:488:MET:HG2	1.99	0.45
11:M:164:LEU:O	11:M:167:ILE:N	2.49	0.45
9:N:89:LEU:HD11	9:N:98:MET:SD	2.56	0.45
2:2:97:LYS:O	2:2:157:ASN:ND2	2.49	0.45
3:3:27:LEU:HD13	3:3:37:ILE:HB	1.99	0.45
4:4:338:MET:SD	4:4:348:HIS:CE1	3.10	0.45
4:4:106:LEU:HD13	4:4:391:ILE:HD12	1.99	0.45
5:5:123:VAL:HG23	5:5:124:TYR:N	2.31	0.45
7:9:113:MET:HE3	7:9:118:TYR:CE1	2.51	0.45
8:H:264:LEU:O	8:H:268:ILE:HG12	2.16	0.45
10:A:70:ALA:HB2	14:J:59:ILE:HD11	1.99	0.45
11:M:185:PRO:HA	11:M:251:ASN:HD21	1.82	0.45
11:M:419:HIS:CE1	11:M:421:HIS:HB3	2.52	0.45
9:N:271:THR:HG22	9:N:279:PRO:HG2	1.98	0.45
2:2:161:TYR:CE1	2:2:184:PRO:HA	2.52	0.45
3:3:221:GLU:O	3:3:243:ARG:NH1	2.50	0.45
3:3:240:VAL:HG12	3:3:250:ILE:HG22	1.99	0.45
3:3:379:LEU:HD23	3:3:408:LEU:HD13	1.99	0.45
3:3:303:VAL:HA	3:3:542:PHE:HZ	1.82	0.45
6:6:148:GLY:H	7:9:118:TYR:HE2	1.65	0.45
13:L:282:ALA:HB1	13:L:411:MET:HG2	1.99	0.45
11:M:17:LEU:O	11:M:18:SER:OG	2.34	0.45
11:M:351:LEU:HD13	11:M:426:ILE:HD11	1.98	0.45
11:M:442:LEU:HB2	11:M:443:PRO:HD3	1.98	0.45
9:N:135:LYS:HD3	9:N:187:MET:HE2	1.99	0.45
9:N:216:PHE:HA	9:N:219:PHE:HD2	1.82	0.45
1:1:66:ARG:HD2	1:1:319:PHE:CE2	2.52	0.45
3:3:197:GLY:O	3:3:200:ILE:HG12	2.16	0.45
3:3:198:ASN:ND2	3:3:263:ILE:O	2.39	0.45
4:4:49:LEU:HD23	4:4:50:ASN:O	2.16	0.45
5:5:88:ASN:HD22	5:5:112:ASP:HB3	1.82	0.45
6:6:81:ARG:HD3	8:H:214:GLU:HB3	1.98	0.45
13:L:387:THR:HG21	13:L:461:SER:O	2.17	0.45
11:M:33:LEU:HA	11:M:36:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:269:GLU:HG2	9:N:272:LYS:HE2	1.99	0.45
44:V:104:UNK:O	44:V:108:UNK:CB	2.64	0.45
42:Y:78:ALA:O	42:Y:82:THR:HG23	2.17	0.45
1:1:91:LYS:HG2	1:1:219:PRO:HG2	1.98	0.44
1:1:12:PHE:HB3	1:1:273:SER:O	2.17	0.44
1:1:322:LEU:HD12	1:1:329:LEU:HB2	2.00	0.44
3:3:391:PHE:O	3:3:395:ILE:HG12	2.17	0.44
4:4:59:HIS:NE2	4:4:152:MET:SD	2.90	0.44
4:4:197:GLY:O	4:4:325:VAL:HG13	2.17	0.44
11:M:370:PRO:HB3	13:L:141:PHE:CD2	2.53	0.44
13:L:274:GLN:HG2	13:L:319:ILE:O	2.17	0.44
13:L:284:THR:O	13:L:288:THR:OG1	2.25	0.44
13:L:313:MET:CG	13:L:328:HIS:HD2	2.30	0.44
13:L:362:LEU:HD12	13:L:363:PHE:N	2.32	0.44
11:M:369:LEU:HD22	50:L:601:CDL:H272	1.99	0.44
11:M:339:SER:HB2	11:M:344:LEU:HD23	1.99	0.44
9:N:158:SER:HB2	9:N:188:GLY:O	2.17	0.44
1:1:250:ASN:HD22	1:1:319:PHE:HD2	1.64	0.44
1:1:298:ILE:HD12	1:1:335:ILE:HD11	1.98	0.44
2:2:171:GLU:O	2:2:175:GLU:HG2	2.16	0.44
3:3:359:ARG:HD3	3:3:363:LEU:HD21	1.98	0.44
7:9:11:SER:N	7:9:20:ARG:HH22	2.15	0.44
7:9:25:LEU:HD12	48:9:501:3PE:O32	2.18	0.44
13:L:217:ILE:O	13:L:221:THR:HG23	2.18	0.44
13:L:68:TRP:HB3	13:L:76:LEU:O	2.17	0.44
11:M:220:HIS:CE1	11:M:327:PHE:CE1	3.05	0.44
9:N:26:TRP:HB2	9:N:84:TRP:CE3	2.52	0.44
42:Y:37:LYS:CG	42:Y:38:PRO:HD3	2.47	0.44
3:3:30:CYS:HB3	3:3:35:MET:HB2	2.00	0.44
3:3:104:ASP:HB2	45:3:801:SF4:S1	2.56	0.44
4:4:234:ILE:HD12	8:H:280:PHE:CZ	2.52	0.44
4:4:286:PRO:HG3	4:4:302:GLU:HB3	1.98	0.44
5:5:120:SER:HB3	5:5:131:GLU:OE2	2.16	0.44
5:5:67:HIS:CE1	5:5:69:ASN:HB3	2.52	0.44
8:H:309:ILE:HG21	10:A:88:LEU:HD21	1.99	0.44
13:L:198:LEU:HD11	13:L:262:ARG:HG3	2.00	0.44
11:M:347:GLY:N	11:M:418:LYS:O	2.50	0.44
9:N:258:SER:HB3	9:N:333:SER:O	2.16	0.44
24:X:58:PHE:CD2	24:X:80:ILE:HD13	2.52	0.44
4:4:107:ASP:HB3	4:4:114:ASN:OD1	2.17	0.44
4:4:116:GLN:NE2	4:4:275:TYR:HE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:172:ARG:HH21	10:A:30:TYR:HB2	1.82	0.44
8:H:306:SER:O	8:H:309:ILE:HG22	2.16	0.44
9:N:38:LEU:HD21	12:K:70:GLU:HA	1.99	0.44
13:L:253:VAL:HG22	13:L:310:LEU:HD13	1.99	0.44
13:L:68:TRP:CD1	13:L:69:LEU:HG	2.52	0.44
9:N:219:PHE:HD1	9:N:224:THR:HG1	1.65	0.44
9:N:76:ILE:HG22	9:N:91:ASN:HD22	1.81	0.44
42:Y:44:LEU:O	42:Y:48:GLU:CB	2.66	0.44
1:1:363:THR:HG22	1:1:366:ARG:HH21	1.82	0.44
3:3:568:GLU:HB3	3:3:589:PRO:HG3	1.99	0.44
3:3:684:MET:HA	3:3:687:CYS:SG	2.58	0.44
4:4:185:SER:HB3	4:4:193:TYR:HB2	1.99	0.44
4:4:233:ARG:HH21	48:9:501:3PE:P	2.40	0.44
8:H:157:ASN:HA	8:H:168:THR:HG21	2.00	0.44
13:L:154:LEU:HD23	13:L:154:LEU:HA	1.85	0.44
13:L:373:LEU:O	13:L:377:SER:HB3	2.17	0.44
11:M:196:TRP:CZ3	11:M:257:MET:HB3	2.52	0.44
9:N:179:MET:SD	9:N:215:MET:HG2	2.58	0.44
9:N:85:THR:HG21	43:W:128:ILE:HD13	1.99	0.44
41:Z:145:LEU:HD13	41:Z:149:TYR:CB	2.47	0.44
3:3:205:VAL:HG23	3:3:207:ALA:H	1.83	0.44
3:3:285:ARG:HG2	3:3:291:LEU:HB2	2.00	0.44
4:4:377:TYR:O	4:4:389:CYS:HA	2.17	0.44
6:6:122:GLY:N	6:6:135:GLY:HA2	2.33	0.44
8:H:49:ILE:O	8:H:53:ILE:HG12	2.17	0.44
13:L:325:ALA:O	13:L:328:HIS:N	2.51	0.44
13:L:33:PRO:HB3	13:L:118:PHE:CE2	2.51	0.44
11:M:319:HIS:CE1	11:M:323:SER:HB3	2.53	0.44
42:Y:52:PRO:O	42:Y:53:ARG:HG2	2.18	0.44
2:2:127:LYS:HG2	2:2:128:VAL:H	1.82	0.44
3:3:343:LEU:HD23	3:3:507:TYR:CE1	2.43	0.44
3:3:60:GLU:OE2	3:3:78:ASN:ND2	2.51	0.44
14:J:145:ALA:HA	14:J:148:SER:OG	2.17	0.44
14:J:57:PHE:CZ	48:J:301:3PE:H352	2.52	0.44
13:L:122:LEU:O	13:L:126:ILE:HD12	2.18	0.44
13:L:288:THR:HG21	13:L:307:SER:OG	2.18	0.44
13:L:3:LEU:HB2	13:L:53:MET:SD	2.58	0.44
13:L:70:THR:HG23	13:L:71:ILE:N	2.32	0.44
11:M:258:ALA:HB1	11:M:302:LEU:HD23	1.98	0.44
9:N:224:THR:HG22	9:N:229:SER:HB3	2.00	0.44
9:N:167:TRP:CE3	9:N:288:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:PRO:O	1:1:218:CYS:HB3	2.18	0.44
2:2:60:TRP:NE1	2:2:94:PRO:HB3	2.33	0.44
3:3:221:GLU:HB3	3:3:243:ARG:NH1	2.31	0.44
3:3:250:ILE:HD11	3:3:267:THR:O	2.18	0.44
3:3:328:LEU:HD22	3:3:507:TYR:CE2	2.53	0.44
5:5:84:PRO:O	5:5:85:THR:HB	2.18	0.44
6:6:126:TYR:C	6:6:128:TYR:N	2.71	0.44
10:A:24:LEU:HA	10:A:27:LEU:HB3	2.00	0.44
8:H:102:VAL:HG13	8:H:162:LEU:HB2	1.98	0.44
8:H:220:PHE:O	8:H:224:PHE:HB2	2.18	0.44
6:6:72:PHE:HA	8:H:39:VAL:HB	2.00	0.44
8:H:114:TYR:OH	14:J:65:MET:HB2	2.16	0.44
11:M:442:LEU:O	11:M:446:LEU:HG	2.18	0.44
43:W:62:GLU:HG3	43:W:63:HIS:N	2.33	0.44
1:1:190:THR:CG2	1:1:204:ARG:H	2.31	0.44
4:4:324:LYS:NZ	4:4:332:PRO:O	2.40	0.44
5:5:161:PRO:O	5:5:166:PHE:HB3	2.18	0.44
7:9:30:LEU:HD21	48:9:501:3PE:H292	1.99	0.44
8:H:117:LEU:O	8:H:121:TRP:HB2	2.18	0.44
14:J:62:GLY:O	14:J:66:VAL:CB	2.63	0.44
12:K:58:MET:HB3	12:K:62:ILE:HD12	2.00	0.44
13:L:302:ILE:HD12	13:L:339:LEU:HD21	1.98	0.44
11:M:244:MET:O	11:M:247:THR:HG22	2.17	0.44
9:N:4:ILE:HG21	49:A:200:PC1:O12	2.18	0.44
43:W:69:HIS:CG	43:W:70:PRO:HD2	2.53	0.44
2:2:42:HIS:O	2:2:44:ALA:N	2.51	0.43
3:3:135:ARG:HD3	3:3:179:ASN:HB3	2.00	0.43
3:3:403:ASP:OD1	3:3:404:LEU:N	2.51	0.43
3:3:615:THR:O	3:3:619:VAL:HG23	2.18	0.43
4:4:173:GLU:OE1	4:4:176:LYS:HD2	2.17	0.43
7:9:63:GLY:N	7:9:134:GLY:O	2.50	0.43
10:A:96:PHE:O	10:A:100:VAL:HG23	2.18	0.43
12:K:34:GLU:O	12:K:37:MET:HB3	2.18	0.43
13:L:124:PHE:CE2	13:L:251:THR:HG21	2.53	0.43
43:W:39:GLY:O	43:W:43:ILE:HD12	2.18	0.43
1:1:89:ARG:HH12	1:1:219:PRO:HD3	1.83	0.43
1:1:121:GLY:HA2	1:1:232:PRO:HD3	2.00	0.43
1:1:60:VAL:O	1:1:63:SER:OG	2.27	0.43
6:6:75:VAL:HG22	8:H:25:ARG:CZ	2.49	0.43
6:6:72:PHE:CD1	8:H:39:VAL:HG21	2.53	0.43
12:K:46:LEU:HD21	14:J:43:ILE:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:108:MET:CB	13:L:114:ILE:HD13	2.48	0.43
13:L:287:PHE:O	13:L:290:MET:N	2.50	0.43
13:L:453:SER:OG	13:L:454:ILE:N	2.51	0.43
11:M:200:MET:O	11:M:204:MET:HG2	2.18	0.43
1:1:156:ALA:HB1	1:1:162:ILE:HG12	2.01	0.43
2:2:165:THR:O	2:2:169:ILE:HG12	2.18	0.43
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.52	0.43
4:4:233:ARG:NH1	7:9:24:THR:HA	2.34	0.43
4:4:233:ARG:O	4:4:237:ASN:CB	2.66	0.43
4:4:96:TYR:HE1	4:4:386:PRO:HB3	1.83	0.43
4:4:87:THR:O	4:4:90:LEU:N	2.51	0.43
5:5:67:HIS:O	5:5:69:ASN:N	2.49	0.43
6:6:105:ASP:OD1	10:A:35:SER:OG	2.29	0.43
6:6:34:ASP:OD1	6:6:173:LEU:HB3	2.19	0.43
8:H:303:TRP:CZ3	8:H:307:LEU:HD22	2.54	0.43
13:L:165:ASN:OD1	13:L:166:THR:N	2.52	0.43
13:L:28:LYS:HE3	13:L:29:PHE:CE1	2.53	0.43
11:M:210:TYR:CB	11:M:268:GLY:HA3	2.48	0.43
11:M:37:THR:O	11:M:40:LEU:HB3	2.18	0.43
11:M:71:TRP:O	11:M:74:PRO:HD2	2.18	0.43
9:N:109:ALA:O	9:N:112:HIS:CD2	2.72	0.43
9:N:146:LEU:HG	9:N:147:PRO:HD3	2.00	0.43
9:N:340:THR:O	9:N:340:THR:HG22	2.18	0.43
9:N:26:TRP:CD1	9:N:85:THR:O	2.72	0.43
11:M:173:SER:HB2	43:W:101:ALA:HB2	2.00	0.43
43:W:41:THR:O	43:W:45:VAL:HG23	2.18	0.43
43:W:85:LYS:NZ	43:W:89:ARG:HH22	2.15	0.43
42:Y:81:PHE:HD1	42:Y:106:PHE:CE1	2.37	0.43
1:1:47:GLU:HA	1:1:50:LEU:HG	2.00	0.43
3:3:26:VAL:HG13	3:3:79:ILE:HD13	2.01	0.43
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.99	0.43
5:5:36:TYR:CD2	5:5:56:GLY:HA3	2.53	0.43
5:5:32:ILE:HD12	5:5:63:PHE:CZ	2.54	0.43
6:6:107:MET:HB3	6:6:111:ARG:NE	2.33	0.43
10:A:101:SER:HB2	14:J:165:VAL:HG21	2.00	0.43
13:L:411:MET:O	13:L:415:ALA:HB2	2.19	0.43
13:L:43:ALA:O	13:L:47:SER:OG	2.28	0.43
11:M:346:ARG:HG2	11:M:413:THR:O	2.19	0.43
9:N:9:ILE:O	9:N:12:THR:N	2.50	0.43
7:9:34:LEU:HD23	8:H:276:SER:HB3	2.00	0.43
13:L:479:GLN:O	13:L:481:THR:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:87:TYR:O	43:W:90:THR:OG1	2.27	0.43
1:1:36:ALA:HA	1:1:39:ARG:HE	1.83	0.43
1:1:24:ASN:HB2	1:1:39:ARG:NH1	2.34	0.43
1:1:188:GLU:HA	46:1:501:FMN:C9	2.49	0.43
1:1:366:ARG:HH22	3:3:155:GLN:HB2	1.84	0.43
3:3:577:GLU:N	3:3:577:GLU:OE1	2.52	0.43
4:4:229:LEU:HD22	4:4:297:TYR:CZ	2.54	0.43
4:4:357:GLN:OE1	4:4:357:GLN:N	2.52	0.43
12:K:11:ALA:HB1	14:J:17:PHE:CD2	2.53	0.43
9:N:75:ILE:HD12	12:K:40:LEU:HD22	2.00	0.43
12:K:42:ILE:O	12:K:46:LEU:HG	2.19	0.43
11:M:8:THR:O	11:M:11:LEU:HB3	2.18	0.43
43:W:28:TYR:O	43:W:31:LEU:N	2.52	0.43
3:3:534:ARG:NH2	3:3:556:ILE:O	2.51	0.43
4:4:265:ILE:HG23	4:4:265:ILE:O	2.19	0.43
4:4:347:HIS:O	4:4:351:LEU:HB2	2.19	0.43
4:4:69:SER:N	4:4:72:MET:O	2.40	0.43
5:5:132:ARG:HH21	5:5:147:ASP:HB3	1.84	0.43
5:5:72:PHE:CE1	5:5:98:SER:HB2	2.54	0.43
7:9:126:CYS:HA	45:9:503:SF4:S3	2.58	0.43
50:L:601:CDL:OA7	50:L:601:CDL:H592	2.19	0.43
9:N:115:VAL:HG12	9:N:180:ALA:HB1	2.00	0.43
9:N:190:MET:HG2	9:N:204:ASN:HB3	2.00	0.43
11:M:47:ASP:CB	41:Z:92:LYS:HD2	2.49	0.43
1:1:356:HIS:ND1	2:2:143:GLU:OE2	2.51	0.43
2:2:3:GLY:HA2	3:3:135:ARG:HB2	2.01	0.43
8:H:165:LEU:O	8:H:169:GLN:HG2	2.17	0.43
13:L:448:PRO:O	13:L:452:ASN:HB2	2.19	0.43
13:L:566:ILE:O	13:L:569:ALA:HB3	2.19	0.43
3:3:368:ILE:H	3:3:368:ILE:HD12	1.83	0.43
3:3:364:LEU:HB2	3:3:492:ILE:O	2.18	0.43
3:3:620:ARG:HA	3:3:623:LEU:HB3	2.01	0.43
3:3:121:MET:O	4:4:329:LYS:HE2	2.19	0.43
5:5:137:MET:HA	5:5:161:PRO:HD2	2.00	0.43
5:5:117:VAL:HB	5:5:142:PHE:HE1	1.84	0.43
5:5:78:LEU:HB3	5:5:130:TYR:HB3	2.00	0.43
6:6:126:TYR:O	6:6:128:TYR:N	2.52	0.43
7:9:93:THR:O	7:9:109:TYR:HA	2.19	0.43
14:J:93:PHE:O	14:J:97:LEU:CB	2.66	0.43
12:K:36:MET:O	12:K:39:SER:OG	2.18	0.43
13:L:226:GLN:NE2	13:L:280:LEU:HG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:98:TRP:HZ2	13:L:456:ARG:NH1	2.16	0.43
11:M:241:TYR:O	11:M:244:MET:HB2	2.18	0.43
44:V:34:UNK:O	44:V:38:UNK:CB	2.67	0.43
1:1:42:TRP:CE2	1:1:120:GLU:HB2	2.54	0.43
3:3:503:LEU:HD22	3:3:509:PRO:HD3	2.00	0.43
4:4:148:LEU:O	4:4:151:ILE:HG22	2.18	0.43
4:4:406:SER:HA	4:4:417:ILE:HD13	2.00	0.43
5:5:194:PHE:HB2	6:6:128:TYR:CE1	2.54	0.43
7:9:119:CYS:HB2	7:9:121:PHE:H	1.84	0.43
10:A:63:LEU:HA	10:A:63:LEU:HD23	1.79	0.43
8:H:62:ARG:O	8:H:215:TYR:HE1	2.01	0.43
8:H:269:THR:O	8:H:273:ILE:HG13	2.19	0.43
13:L:396:ILE:O	13:L:400:ASN:CB	2.56	0.43
13:L:67:HIS:HA	13:L:77:SER:HB3	2.01	0.43
11:M:102:LEU:HD21	11:M:230:VAL:HG11	2.01	0.43
11:M:7:PRO:HB2	11:M:34:ILE:HD12	2.00	0.43
9:N:302:LEU:HD22	11:M:91:ARG:CZ	2.49	0.43
42:Y:50:LYS:HD2	43:W:142:ASP:HA	2.01	0.43
1:1:205:LEU:HB3	1:1:207:PRO:HD2	2.00	0.42
1:1:273:SER:HA	1:1:317:MET:O	2.19	0.42
3:3:27:LEU:O	3:3:31:GLU:HG3	2.18	0.42
3:3:565:ALA:O	3:3:569:LYS:HG2	2.19	0.42
3:3:579:ARG:HG2	3:3:636:VAL:HB	2.01	0.42
4:4:229:LEU:HD23	4:4:230:THR:H	1.84	0.42
4:4:298:LEU:HD12	7:9:6:ASN:ND2	2.33	0.42
3:3:111:GLY:O	4:4:349:PHE:HE2	2.02	0.42
7:9:21:ALA:O	7:9:25:LEU:CB	2.67	0.42
12:K:40:LEU:HD23	12:K:40:LEU:HA	1.83	0.42
12:K:58:MET:O	12:K:61:ILE:N	2.52	0.42
13:L:161:ARG:NH2	13:L:238:GLU:OE1	2.52	0.42
13:L:458:LEU:HD12	13:L:459:ILE:N	2.33	0.42
11:M:151:PHE:O	11:M:155:ALA:HB2	2.19	0.42
1:1:15:LEU:HD22	1:1:283:HIS:NE2	2.34	0.42
1:1:43:TYR:HB3	1:1:236:ARG:NH2	2.34	0.42
1:1:371:TRP:HE1	3:3:99:ALA:HB1	1.83	0.42
4:4:139:VAL:HG22	4:4:278:TYR:HB2	2.00	0.42
6:6:130:TYR:CD1	6:6:131:SER:N	2.87	0.42
12:K:12:PHE:O	12:K:15:SER:OG	2.27	0.42
13:L:221:THR:HG22	13:L:226:GLN:HG2	2.00	0.42
13:L:388:GLY:O	13:L:391:SER:OG	2.28	0.42
11:M:237:LYS:NZ	11:M:319:HIS:HD2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:72:MET:O	9:N:76:ILE:HG12	2.19	0.42
42:Y:35:CYS:O	42:Y:36:ASP:HB2	2.19	0.42
41:Z:88:GLU:HG2	41:Z:151:ALA:CB	2.49	0.42
8:H:146:LEU:HG	8:H:185:TRP:NE1	2.34	0.42
13:L:14:LEU:HA	13:L:14:LEU:HD23	1.80	0.42
13:L:155:ILE:HD11	13:L:247:LEU:HD22	2.00	0.42
13:L:484:HIS:O	13:L:485:TYR:CG	2.73	0.42
11:M:108:MET:HB3	11:M:121:MET:HG3	2.01	0.42
11:M:234:ILE:O	11:M:237:LYS:N	2.53	0.42
11:M:233:ALA:HB2	11:M:324:SER:HB2	2.01	0.42
9:N:206:ILE:HD13	49:N:401:PC1:H2F1	2.01	0.42
9:N:342:ILE:O	9:N:345:ILE:HG22	2.18	0.42
9:N:83:GLN:HG3	13:L:19:ILE:HG22	99.43	0.42
24:X:58:PHE:HB3	24:X:60:PHE:HE2	1.82	0.42
42:Y:82:THR:HA	42:Y:85:TRP:CD1	2.54	0.42
1:1:134:ALA:HB2	1:1:173:PHE:CZ	2.53	0.42
1:1:140:GLY:O	1:1:179:ARG:NH2	2.51	0.42
1:1:362:CYS:SG	1:1:403:THR:OG1	2.78	0.42
3:3:10:GLU:HG3	3:3:17:SER:OG	2.19	0.42
4:4:152:MET:HG3	4:4:171:PHE:HZ	1.84	0.42
4:4:149:ASN:ND2	4:4:371:LYS:HG3	2.34	0.42
7:9:117:ILE:HG22	45:9:502:SF4:S3	2.60	0.42
10:A:66:ASP:O	10:A:69:ILE:N	2.53	0.42
12:K:58:MET:HE3	14:J:142:GLY:O	2.18	0.42
13:L:4:PHE:HE2	13:L:59:GLN:HG3	1.84	0.42
11:M:243:MET:CG	11:M:301:ILE:HG21	2.46	0.42
11:M:299:VAL:O	11:M:303:ILE:HG12	2.19	0.42
11:M:84:LEU:CD1	11:M:85:SER:H	2.20	0.42
1:1:43:TYR:CD2	1:1:44:LYS:HG2	2.55	0.42
2:2:106:THR:CB	2:2:107:PRO:HD3	2.50	0.42
2:2:111:ARG:O	2:2:112:ASN:HB2	2.20	0.42
6:6:101:ARG:O	6:6:105:ASP:HB2	2.19	0.42
13:L:2:ASN:O	13:L:5:SER:N	2.52	0.42
50:L:601:CDL:HB31	50:L:601:CDL:HA21	2.01	0.42
13:L:62:ILE:HG12	13:L:199:GLN:HE22	1.84	0.42
9:N:128:LEU:HA	9:N:216:PHE:HD2	1.85	0.42
42:Y:108:LYS:O	42:Y:112:ASP:HB2	2.20	0.42
42:Y:25:LYS:NZ	42:Y:94:GLN:O	2.49	0.42
2:2:61:LEU:O	2:2:61:LEU:HD12	2.20	0.42
8:H:226:ALA:O	8:H:230:ASN:HB2	2.20	0.42
4:4:163:ALA:HB2	8:H:278:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:26:PRO:C	14:J:29:GLY:H	2.22	0.42
13:L:17:MET:O	13:L:20:ALA:N	2.52	0.42
13:L:249:SER:OG	13:L:250:SER:N	2.52	0.42
11:M:142:ARG:C	11:M:144:ASN:H	2.23	0.42
11:M:196:TRP:HD1	11:M:250:LEU:HB3	1.85	0.42
11:M:50:LEU:HD13	11:M:52:PHE:CE1	2.54	0.42
9:N:337:LEU:N	9:N:338:PRO:HD2	2.35	0.42
3:3:568:GLU:HG3	3:3:587:VAL:O	2.19	0.42
3:3:381:GLY:HA3	3:3:661:LEU:HD11	2.01	0.42
4:4:55:HIS:CE1	4:4:58:ALA:HA	2.54	0.42
4:4:68:LEU:HB2	4:4:72:MET:O	2.19	0.42
14:J:23:LYS:HG2	14:J:85:SER:O	2.20	0.42
13:L:145:GLU:OE2	13:L:176:ARG:NH1	2.53	0.42
11:M:16:TRP:O	11:M:93:LYS:NZ	2.39	0.42
11:M:382:VAL:HA	11:M:385:THR:HG22	2.02	0.42
11:M:419:HIS:ND1	11:M:421:HIS:HB3	2.34	0.42
41:Z:152:ARG:O	41:Z:156:ALA:HB2	2.19	0.42
1:1:276:LEU:HD21	1:1:297:VAL:HG11	2.01	0.42
1:1:106:LYS:HD2	1:1:331:THR:HB	2.01	0.42
3:3:237:ASN:N	3:3:259:ASN:ND2	2.61	0.42
4:4:163:ALA:O	4:4:166:PRO:HD2	2.20	0.42
4:4:274:PRO:HB3	4:4:279:ASP:HB2	2.02	0.42
6:6:40:ALA:O	6:6:43:SER:N	2.53	0.42
6:6:66:ARG:HG3	7:9:48:ILE:HD13	2.01	0.42
6:6:81:ARG:CZ	8:H:215:TYR:HA	2.49	0.42
8:H:1:MET:HG3	8:H:2:PHE:N	2.34	0.42
13:L:216:LEU:HD13	13:L:263:PHE:HD2	1.83	0.42
13:L:336:LYS:HB2	13:L:336:LYS:HE2	1.87	0.42
13:L:362:LEU:O	13:L:370:THR:HG21	2.19	0.42
1:1:82:MET:CB	1:1:129:MET:HB2	2.50	0.42
1:1:320:ASP:OD1	1:1:320:ASP:N	2.53	0.42
3:3:104:ASP:HB2	3:3:152:ARG:HD3	2.00	0.42
4:4:84:HIS:N	6:6:93:THR:HG21	2.34	0.42
10:A:96:PHE:CE1	49:A:200:PC1:H3B2	2.55	0.42
8:H:145:THR:HG22	8:H:149:ILE:CD1	2.49	0.42
10:A:90:MET:SD	14:J:151:THR:HA	2.60	0.42
13:L:418:PHE:CA	13:L:421:ILE:HG12	2.48	0.42
11:M:78:MET:HG3	11:M:436:LEU:HD11	2.01	0.42
9:N:240:MET:O	9:N:244:VAL:HG23	2.19	0.42
43:W:78:THR:HG23	43:W:79:PHE:CD1	2.55	0.42
42:Y:110:VAL:O	42:Y:114:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Z:92:LYS:O	41:Z:95:TYR:HB3	2.19	0.42
1:1:193:ILE:HG23	1:1:215:VAL:HA	2.01	0.42
2:2:14:LYS:HG2	2:2:15:ASN:N	2.35	0.42
3:3:378:LEU:HD13	3:3:409:ILE:HD12	2.01	0.42
4:4:171:PHE:HD1	4:4:171:PHE:HA	1.72	0.42
6:6:116:MET:HA	6:6:146:VAL:HG23	2.01	0.42
6:6:57:VAL:HA	6:6:60:MET:HE3	2.01	0.42
12:K:12:PHE:CD1	12:K:36:MET:HG3	2.55	0.42
13:L:120:TYR:HE1	13:L:153:LEU:HD13	1.85	0.42
13:L:226:GLN:HA	13:L:284:THR:HG21	2.01	0.42
13:L:385:PHE:CG	13:L:385:PHE:O	2.73	0.42
13:L:368:PHE:HE2	13:L:454:ILE:HB	1.83	0.42
11:M:11:LEU:O	11:M:15:THR:HG23	2.20	0.42
11:M:241:TYR:OH	11:M:245:ARG:NE	2.47	0.42
9:N:293:TYR:O	9:N:297:THR:HG23	2.19	0.42
9:N:79:MET:HA	12:K:47:MET:CE	2.50	0.42
8:H:249:PRO:HG2	42:Y:98:ARG:NH2	2.35	0.42
3:3:221:GLU:HG2	5:5:197:PHE:HE1	1.85	0.41
4:4:122:VAL:O	4:4:126:LEU:CB	2.68	0.41
4:4:140:LEU:HB2	4:4:314:CYS:SG	2.60	0.41
4:4:202:ASP:H	4:4:323:ILE:HD13	1.85	0.41
4:4:84:HIS:CD2	5:5:152:LEU:HD22	2.54	0.41
13:L:176:ARG:O	13:L:179:ASP:HB3	2.20	0.41
11:M:1:MET:HB3	11:M:56:PHE:CE1	2.55	0.41
9:N:340:THR:HG23	9:N:343:LEU:HB2	2.00	0.41
42:Y:168:PHE:O	42:Y:169:TRP:HB2	2.20	0.41
1:1:103:GLY:HA2	2:2:148:CYS:HB3	2.01	0.41
3:3:203:CYS:SG	3:3:207:ALA:HB3	2.60	0.41
3:3:213:TYR:OH	3:3:217:ALA:HB3	2.20	0.41
3:3:336:ASN:OD1	3:3:341:ASP:HB3	2.19	0.41
4:4:105:ARG:CZ	7:9:117:ILE:HD11	2.50	0.41
4:4:201:GLN:HE21	7:9:176:ARG:HD3	1.85	0.41
4:4:229:LEU:HD22	4:4:297:TYR:OH	2.19	0.41
4:4:414:VAL:HA	4:4:417:ILE:HD12	2.02	0.41
7:9:38:LEU:HD22	8:H:276:SER:OG	2.20	0.41
14:J:28:TYR:HD1	14:J:31:LEU:HD12	1.86	0.41
12:K:45:THR:HG21	14:J:44:VAL:HG13	2.00	0.41
13:L:120:TYR:CE1	13:L:153:LEU:HD13	2.55	0.41
13:L:88:MET:CE	13:L:468:ILE:HG12	2.50	0.41
11:M:207:MET:HE1	11:M:240:GLY:HA3	2.02	0.41
11:M:305:THR:O	11:M:308:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:41:LEU:HD23	11:M:41:LEU:O	2.19	0.41
42:Y:44:LEU:O	42:Y:48:GLU:HB2	2.20	0.41
3:3:116:LEU:HA	3:3:116:LEU:HD23	1.89	0.41
1:1:404:ILE:HG12	3:3:53:ARG:NH2	2.35	0.41
3:3:56:LEU:HB3	3:3:65:VAL:HG11	2.03	0.41
4:4:51:PHE:CD2	4:4:63:ARG:HA	2.56	0.41
8:H:200:LEU:H	8:H:200:LEU:HG	1.75	0.41
14:J:9:LEU:HD13	14:J:42:GLY:HA3	2.02	0.41
12:K:68:ALA:O	12:K:71:ALA:N	2.54	0.41
13:L:138:PHE:CB	13:L:196:TRP:HE1	2.27	0.41
13:L:286:LEU:HD22	13:L:411:MET:SD	2.60	0.41
13:L:364:LYS:HB2	13:L:364:LYS:HE2	1.83	0.41
43:W:83:PRO:O	43:W:87:TYR:HB2	2.20	0.41
42:Y:95:LEU:HB2	42:Y:98:ARG:HG2	2.02	0.41
1:1:181:ALA:HB2	2:2:48:LEU:HD11	2.02	0.41
3:3:266:LYS:NZ	3:3:675:ASP:OD2	2.39	0.41
4:4:300:ARG:HH21	4:4:422:ASP:H	1.67	0.41
6:6:47:PRO:HB3	6:6:85:VAL:CG2	2.50	0.41
10:A:9:THR:O	10:A:12:THR:N	2.53	0.41
8:H:153:VAL:HG11	8:H:242:PHE:CE1	2.56	0.41
8:H:213:VAL:HG13	8:H:220:PHE:CE1	2.56	0.41
14:J:34:ILE:HG22	14:J:65:MET:HG3	2.02	0.41
12:K:70:GLU:O	12:K:73:LEU:HB3	2.20	0.41
13:L:366:MET:CE	13:L:369:THR:HG21	2.50	0.41
13:L:383:MET:CB	13:L:389:PHE:HB2	2.50	0.41
13:L:483:PRO:O	13:L:487:LYS:N	2.53	0.41
11:M:118:PHE:O	11:M:122:PHE:HB2	2.19	0.41
11:M:170:THR:HG23	11:M:171:MET:N	2.35	0.41
44:V:89:UNK:O	44:V:93:UNK:CB	2.67	0.41
24:X:54:MET:O	24:X:57:GLU:HB2	2.20	0.41
42:Y:131:LYS:HE3	42:Y:131:LYS:HB3	1.88	0.41
42:Y:26:ALA:HB1	42:Y:84:TYR:HE2	1.85	0.41
1:1:111:ILE:HD13	1:1:138:ILE:HD12	2.02	0.41
1:1:46:LYS:HE3	1:1:169:SER:HA	2.02	0.41
3:3:158:ARG:HA	3:3:161:ARG:HH21	1.85	0.41
3:3:362:TYR:CZ	3:3:503:LEU:HB2	2.55	0.41
4:4:152:MET:O	4:4:156:THR:HG22	2.20	0.41
4:4:193:TYR:O	4:4:193:TYR:CG	2.73	0.41
4:4:335:ARG:HA	4:4:338:MET:HB3	2.02	0.41
7:9:35:GLY:O	8:H:272:TRP:HZ2	2.03	0.41
10:A:103:ALA:O	10:A:107:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:96:ILE:HG22	8:H:98:MET:HG3	2.01	0.41
13:L:363:PHE:HE1	13:L:367:PRO:HG3	1.85	0.41
13:L:408:ALA:O	13:L:412:THR:HG23	2.21	0.41
13:L:48:MET:O	13:L:51:THR:OG1	2.32	0.41
13:L:88:MET:O	13:L:91:PRO:HD2	2.21	0.41
11:M:190:TRP:O	11:M:193:THR:HB	2.19	0.41
11:M:160:LEU:HD23	11:M:202:ALA:HB1	2.01	0.41
9:N:307:SER:O	9:N:308:THR:OG1	2.32	0.41
9:N:40:ILE:HG21	9:N:134:GLN:NE2	2.34	0.41
1:1:299:PRO:HA	1:1:334:VAL:HG12	2.03	0.41
1:1:26:TYR:HE1	2:2:195:PRO:HD3	1.86	0.41
3:3:45:ARG:NE	3:3:260:GLU:HB3	2.29	0.41
3:3:271:TYR:O	3:3:274:LEU:HB3	2.21	0.41
6:6:144:ILE:HG13	6:6:163:LEU:HB2	2.02	0.41
4:4:186:GLY:O	7:9:61:PHE:HA	2.21	0.41
8:H:60:PRO:CD	10:A:25:PRO:HB2	2.50	0.41
14:J:45:LEU:CD2	14:J:50:SER:HA	2.51	0.41
13:L:363:PHE:CE1	13:L:367:PRO:HG3	2.56	0.41
13:L:379:ALA:HB1	13:L:383:MET:HE2	2.02	0.41
11:M:369:LEU:HG	11:M:370:PRO:HD2	2.02	0.41
11:M:440:HIS:O	11:M:443:PRO:HD2	2.21	0.41
24:X:43:ASP:HB3	24:X:46:ASP:CB	2.47	0.41
41:Z:49:GLU:O	41:Z:52:GLU:HB2	2.19	0.41
1:1:31:TRP:CZ2	1:1:148:ASN:HB3	2.56	0.41
2:2:147:ALA:HB3	2:2:153:MET:SD	2.61	0.41
3:3:108:CYS:SG	3:3:206:GLY:HA3	2.60	0.41
3:3:470:VAL:HG12	3:3:490:MET:SD	2.61	0.41
4:4:220:LEU:O	4:4:224:GLU:HG3	2.21	0.41
8:H:308:PRO:HB2	8:H:314:ILE:HG22	2.02	0.41
13:L:213:LEU:HA	13:L:216:LEU:HD12	2.01	0.41
13:L:351:ASN:N	13:L:442:ASN:HD21	2.19	0.41
13:L:359:MET:HB3	13:L:359:MET:HE2	1.88	0.41
11:M:193:THR:HA	11:M:257:MET:HE3	2.03	0.41
11:M:50:LEU:HA	43:W:86:ASN:ND2	2.33	0.41
43:W:136:SER:O	43:W:138:LYS:HG3	2.20	0.41
1:1:135:TYR:HD1	1:1:176:PHE:HB2	1.85	0.41
2:2:123:LYS:HZ2	2:2:170:GLU:HB3	1.86	0.41
4:4:108:TYR:CB	6:6:54:CYS:HB3	2.50	0.41
4:4:276:ASP:OD1	4:4:276:ASP:N	2.53	0.41
4:4:413:ASP:O	4:4:417:ILE:HG13	2.21	0.41
4:4:82:LEU:HD21	6:6:96:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:415:VAL:HG22	8:H:204:GLU:HB3	2.01	0.41
8:H:307:LEU:O	8:H:310:LEU:HB2	2.20	0.41
14:J:41:CYS:SG	14:J:57:PHE:HB2	2.61	0.41
13:L:362:LEU:N	13:L:431:LEU:O	2.54	0.41
13:L:341:MET:HE3	13:L:454:ILE:HD13	2.03	0.41
13:L:494:THR:O	13:L:498:PHE:CB	2.63	0.41
50:L:601:CDL:H632	50:L:601:CDL:H111	2.01	0.41
13:L:74:LEU:HD12	13:L:74:LEU:O	2.21	0.41
13:L:83:ASP:C	13:L:85:PHE:H	2.24	0.41
11:M:196:TRP:HD1	11:M:250:LEU:HD22	1.86	0.41
11:M:251:ASN:CG	11:M:252:PRO:HD3	2.41	0.41
24:X:84:LYS:HG3	24:X:85:ASP:N	2.36	0.41
42:Y:34:GLN:HG3	42:Y:35:CYS:N	2.36	0.41
1:1:307:ILE:HD11	1:1:327:THR:OG1	2.21	0.41
1:1:370:ASP:OD1	3:3:179:ASN:ND2	2.43	0.41
3:3:107:ILE:HA	7:9:104:ARG:HH21	1.84	0.41
3:3:258:ILE:O	3:3:259:ASN:HB2	2.21	0.41
3:3:296:TRP:NE1	3:3:300:LEU:HD11	2.36	0.41
3:3:469:ALA:O	3:3:472:ASN:HB2	2.21	0.41
3:3:410:GLY:HA3	3:3:661:LEU:HD11	2.03	0.41
3:3:26:VAL:HG23	3:3:71:MET:O	2.21	0.41
4:4:378:LEU:HD23	4:4:389:CYS:HB3	2.01	0.41
8:H:79:LEU:HD11	8:H:222:LEU:HG	2.03	0.41
13:L:188:TRP:CD2	13:L:212:PRO:HG3	2.56	0.41
13:L:469:SER:OG	13:L:470:ASN:N	2.53	0.41
13:L:472:ILE:O	13:L:473:PRO:C	2.58	0.41
11:M:204:MET:HB3	11:M:209:LEU:HD23	2.03	0.41
3:3:239:VAL:HG12	3:3:251:LEU:O	2.21	0.41
3:3:347:GLU:OE2	3:3:496:ILE:HD12	2.21	0.41
4:4:125:LEU:HD23	4:4:125:LEU:O	2.21	0.41
5:5:117:VAL:HB	5:5:142:PHE:CE1	2.56	0.41
6:6:75:VAL:HG22	8:H:25:ARG:NH2	2.36	0.41
7:9:17:VAL:HA	7:9:20:ARG:HB2	2.02	0.41
7:9:21:ALA:O	7:9:25:LEU:HB3	2.20	0.41
8:H:215:TYR:CG	8:H:216:ALA:N	2.89	0.41
9:N:27:LEU:HD22	12:K:59:MET:HG2	2.03	0.41
12:K:77:LEU:HD11	14:J:171:ILE:HD13	2.03	0.41
13:L:103:PHE:CG	13:L:341:MET:HG3	2.56	0.41
13:L:283:MET:O	13:L:287:PHE:HB2	2.19	0.41
13:L:447:ASN:OD1	13:L:448:PRO:HD2	2.20	0.41
11:M:196:TRP:CD1	11:M:250:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:206:ILE:HD12	9:N:346:LEU:HD11	2.03	0.41
42:Y:154:GLU:OE1	42:Y:154:GLU:N	2.54	0.41
11:M:181:TYR:O	41:Z:152:ARG:NH2	2.54	0.41
1:1:383:ASP:HA	1:1:433:PHE:CE2	2.55	0.41
2:2:40:GLU:HG3	2:2:41:GLY:N	2.35	0.41
6:6:90:GLY:HA2	45:6:300:SF4:S2	2.61	0.41
14:J:9:LEU:HD23	14:J:9:LEU:HA	1.95	0.41
13:L:102:GLU:HA	13:L:105:MET:HE2	2.03	0.41
13:L:362:LEU:HD12	13:L:363:PHE:HB2	2.02	0.41
13:L:378:LEU:O	13:L:381:THR:OG1	2.33	0.41
13:L:436:ARG:HG3	13:L:436:ARG:O	2.20	0.41
11:M:204:MET:SD	11:M:298:ILE:HD12	2.60	0.41
11:M:42:LEU:HD23	11:M:63:THR:HG21	2.03	0.41
9:N:241:THR:O	9:N:244:VAL:N	2.53	0.41
9:N:294:MET:HA	9:N:297:THR:HG23	2.03	0.41
9:N:41:ILE:HG13	12:K:73:LEU:HD21	2.03	0.41
9:N:44:MET:O	9:N:45:MET:HB2	2.21	0.41
41:Z:131:PHE:O	41:Z:135:VAL:HG12	2.21	0.41
41:Z:88:GLU:HG2	41:Z:151:ALA:HB2	2.03	0.41
1:1:17:ASP:C	1:1:19:ASP:H	2.25	0.40
1:1:398:GLN:O	1:1:402:HIS:ND1	2.53	0.40
1:1:68:ARG:O	46:1:501:FMN:O4'	2.39	0.40
3:3:194:GLU:OE1	3:3:194:GLU:N	2.47	0.40
3:3:562:PRO:O	3:3:593:ALA:HA	2.21	0.40
7:9:117:ILE:HG23	7:9:119:CYS:SG	2.61	0.40
14:J:54:LEU:HD23	14:J:54:LEU:HA	1.80	0.40
13:L:213:LEU:O	13:L:217:ILE:HG12	2.21	0.40
13:L:321:GLN:HB3	13:L:324:LEU:HD12	2.03	0.40
11:M:174:LEU:HD23	11:M:174:LEU:HA	1.89	0.40
11:M:51:ASN:OD1	11:M:177:LEU:HD11	2.21	0.40
11:M:70:MET:HG2	11:M:103:GLN:HE21	1.86	0.40
42:Y:37:LYS:HG2	42:Y:38:PRO:HD3	2.03	0.40
42:Y:45:CYS:O	42:Y:49:GLU:HG2	2.21	0.40
41:Z:48:ARG:O	41:Z:52:GLU:HG3	2.21	0.40
1:1:124:VAL:HG21	1:1:232:PRO:HB3	2.03	0.40
4:4:203:LEU:HD22	4:4:207:LEU:HD23	2.03	0.40
4:4:245:VAL:HG11	4:4:250:ALA:HB2	2.03	0.40
4:4:417:ILE:O	4:4:420:THR:HG22	2.21	0.40
8:H:307:LEU:HB3	8:H:308:PRO:HD3	2.02	0.40
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.30	0.40
13:L:400:ASN:ND2	13:L:486:LEU:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:12:LEU:HD23	42:Y:13:LYS:N	2.30	0.40
3:3:285:ARG:HG3	3:3:291:LEU:HD13	2.03	0.40
3:3:53:ARG:HA	3:3:53:ARG:HD3	1.88	0.40
4:4:230:THR:O	4:4:231:ASN:ND2	2.54	0.40
4:4:360:PRO:HA	4:4:380:SER:O	2.21	0.40
4:4:93:TYR:CE2	5:5:168:LEU:HB2	2.56	0.40
7:9:10:PRO:CA	7:9:20:ARG:HH22	2.34	0.40
4:4:266:GLN:CD	7:9:2:TYR:HB3	2.40	0.40
7:9:92:ILE:HG22	7:9:93:THR:N	2.36	0.40
8:H:142:TYR:CE1	8:H:289:LEU:HD13	2.56	0.40
8:H:54:LYS:O	8:H:57:ILE:HG22	2.22	0.40
13:L:3:LEU:HD21	41:Z:36:PHE:CG	2.56	0.40
1:1:250:ASN:ND2	1:1:319:PHE:H	2.19	0.40
6:6:47:PRO:HB3	6:6:85:VAL:HG23	2.03	0.40
10:A:80:GLN:HG3	10:A:80:GLN:O	2.21	0.40
14:J:163:ILE:HA	14:J:166:VAL:HG22	2.03	0.40
13:L:331:THR:HB	13:L:335:PHE:CE2	2.56	0.40
11:M:196:TRP:CE3	11:M:257:MET:HB3	2.56	0.40
11:M:325:MET:O	11:M:328:CYS:N	2.54	0.40
43:W:140:THR:O	43:W:141:PRO:C	2.60	0.40
42:Y:61:LEU:O	42:Y:64:GLN:HB3	2.21	0.40
2:2:141:GLU:OE1	2:2:141:GLU:N	2.52	0.40
3:3:380:VAL:CG2	3:3:453:LEU:HA	2.52	0.40
4:4:146:ARG:HA	4:4:370:PRO:CG	2.52	0.40
5:5:131:GLU:OE1	5:5:145:HIS:HD2	2.04	0.40
5:5:67:HIS:O	5:5:67:HIS:CG	2.75	0.40
5:5:67:HIS:C	5:5:69:ASN:H	2.25	0.40
6:6:42:ARG:HB3	6:6:167:ILE:HG21	2.03	0.40
12:K:58:MET:HE3	14:J:142:GLY:C	2.42	0.40
13:L:366:MET:N	13:L:367:PRO:HD3	2.36	0.40
13:L:450:LEU:O	13:L:453:SER:N	2.55	0.40
11:M:160:LEU:O	11:M:164:LEU:HG	2.22	0.40
11:M:326:LEU:HD21	11:M:410:MET:HE3	2.03	0.40
9:N:250:SER:OG	9:N:257:LEU:HD23	2.21	0.40
9:N:272:LYS:HA	11:M:169:ASN:ND2	2.36	0.40
9:N:33:PHE:HE1	9:N:137:ALA:HB1	1.87	0.40
9:N:345:ILE:HA	9:N:345:ILE:HD12	1.85	0.40
41:Z:37:ASP:O	41:Z:41:ASP:HB3	2.22	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	1	430/445 (97%)	405 (94%)	24 (6%)	1 (0%)	52	86
2	2	212/217 (98%)	189 (89%)	22 (10%)	1 (0%)	34	76
3	3	686/704 (97%)	616 (90%)	70 (10%)	0	100	100
4	4	385/412 (93%)	337 (88%)	46 (12%)	2 (0%)	34	76
5	5	206/228 (90%)	183 (89%)	23 (11%)	0	100	100
6	6	153/179 (86%)	138 (90%)	15 (10%)	0	100	100
7	9	174/176 (99%)	150 (86%)	24 (14%)	0	100	100
8	H	316/318 (99%)	278 (88%)	37 (12%)	1 (0%)	46	82
9	N	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
10	A	113/115 (98%)	97 (86%)	15 (13%)	1 (1%)	21	65
11	M	457/459 (100%)	392 (86%)	64 (14%)	1 (0%)	52	86
12	K	84/98 (86%)	72 (86%)	12 (14%)	0	100	100
13	L	597/599 (100%)	518 (87%)	75 (13%)	4 (1%)	26	70
14	J	173/175 (99%)	142 (82%)	29 (17%)	2 (1%)	16	61
15	a	39/75 (52%)	33 (85%)	6 (15%)	0	100	100
16	b	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
17	c	121/133 (91%)	109 (90%)	12 (10%)	0	100	100
18	d	310/338 (92%)	253 (82%)	56 (18%)	1 (0%)	46	82
19	e	82/98 (84%)	74 (90%)	8 (10%)	0	100	100
20	f	110/115 (96%)	95 (86%)	15 (14%)	0	100	100
21	g	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
22	h	91/112 (81%)	73 (80%)	17 (19%)	1 (1%)	17	63
23	i	142/145 (98%)	116 (82%)	24 (17%)	2 (1%)	14	58
24	X	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
24	j	83/88 (94%)	70 (84%)	13 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	k	318/320 (99%)	263 (83%)	50 (16%)	5 (2%)	12	56
26	l	93/105 (89%)	83 (89%)	10 (11%)	0	100	100
27	m	78/83 (94%)	72 (92%)	6 (8%)	0	100	100
28	n	72/97 (74%)	50 (69%)	18 (25%)	4 (6%)	2	29
29	o	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
30	p	110/128 (86%)	83 (76%)	26 (24%)	1 (1%)	21	65
31	q	138/143 (96%)	126 (91%)	12 (9%)	0	100	100
32	r	89/127 (70%)	75 (84%)	12 (14%)	2 (2%)	8	50
33	s	116/136 (85%)	93 (80%)	21 (18%)	2 (2%)	11	55
34	t	164/178 (92%)	142 (87%)	22 (13%)	0	100	100
35	u	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
36	v	141/158 (89%)	103 (73%)	33 (23%)	5 (4%)	4	41
37	w	84/125 (67%)	67 (80%)	15 (18%)	2 (2%)	7	49
38	x	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
39	y	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
40	z	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
41	Z	169/175 (97%)	147 (87%)	21 (12%)	1 (1%)	30	73
42	Y	169/171 (99%)	137 (81%)	32 (19%)	0	100	100
43	W	137/143 (96%)	115 (84%)	21 (15%)	1 (1%)	26	70
All	All	7824/8344 (94%)	6800 (87%)	984 (13%)	40 (0%)	38	76

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	106	THR
28	n	63	VAL
33	s	14	VAL
13	L	71	ILE
13	L	319	ILE
22	h	68	VAL
23	i	58	ARG
37	w	111	ASN
11	M	141	GLU
13	L	384	PRO
14	J	84	VAL

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Mol	Chain	Res	Type
28	n	43	PRO
28	n	44	TRP
30	p	126	ILE
36	v	59	ASP
36	v	85	ILE
14	J	113	VAL
36	v	139	TYR
4	4	231	ASN
8	H	91	MET
25	k	144	ILE
25	k	167	HIS
25	k	226	TRP
32	r	115	VAL
36	v	66	HIS
36	v	67	PRO
37	w	118	ILE
41	Z	143	HIS
4	4	353	THR
23	i	132	LYS
33	s	17	GLU
10	A	50	PRO
25	k	166	PRO
1	1	404	ILE
13	L	347	ILE
28	n	42	ASP
43	W	96	ILE
18	d	68	ILE
25	k	176	VAL
32	r	116	ILE

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	1	346/354 (98%)	346 (100%)	0	100	100
2	2	182/183 (100%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	578/588 (98%)	578 (100%)	0	100	100
4	4	334/358 (93%)	334 (100%)	0	100	100
5	5	189/204 (93%)	189 (100%)	0	100	100
6	6	131/150 (87%)	130 (99%)	1 (1%)	86	93
7	9	151/151 (100%)	151 (100%)	0	100	100
8	H	278/278 (100%)	278 (100%)	0	100	100
9	N	315/315 (100%)	315 (100%)	0	100	100
10	A	103/103 (100%)	103 (100%)	0	100	100
11	M	412/412 (100%)	412 (100%)	0	100	100
12	K	75/87 (86%)	75 (100%)	0	100	100
13	L	445/532 (84%)	445 (100%)	0	100	100
14	J	101/144 (70%)	101 (100%)	0	100	100
15	a	40/68 (59%)	40 (100%)	0	100	100
16	b	79/80 (99%)	79 (100%)	0	100	100
17	c	110/119 (92%)	110 (100%)	0	100	100
18	d	257/292 (88%)	257 (100%)	0	100	100
19	e	75/81 (93%)	75 (100%)	0	100	100
20	f	100/101 (99%)	100 (100%)	0	100	100
21	g	107/113 (95%)	107 (100%)	0	100	100
22	h	83/94 (88%)	83 (100%)	0	100	100
23	i	130/131 (99%)	130 (100%)	0	100	100
24	X	81/81 (100%)	81 (100%)	0	100	100
24	j	78/81 (96%)	78 (100%)	0	100	100
25	k	199/284 (70%)	199 (100%)	0	100	100
26	l	85/94 (90%)	85 (100%)	0	100	100
27	m	69/71 (97%)	69 (100%)	0	100	100
28	n	53/75 (71%)	53 (100%)	0	100	100
29	o	107/107 (100%)	107 (100%)	0	100	100
30	p	71/114 (62%)	71 (100%)	0	100	100
31	q	120/121 (99%)	120 (100%)	0	100	100
32	r	80/121 (66%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	s	100/119 (84%)	100 (100%)	0	100	100
34	t	151/160 (94%)	149 (99%)	2 (1%)	76	89
35	u	58/62 (94%)	58 (100%)	0	100	100
36	v	38/142 (27%)	38 (100%)	0	100	100
37	w	77/112 (69%)	77 (100%)	0	100	100
38	x	43/44 (98%)	43 (100%)	0	100	100
39	y	49/53 (92%)	49 (100%)	0	100	100
40	z	58/59 (98%)	58 (100%)	0	100	100
41	Z	155/157 (99%)	154 (99%)	1 (1%)	90	95
42	Y	154/154 (100%)	154 (100%)	0	100	100
43	W	122/125 (98%)	122 (100%)	0	100	100
All	All	6569/7274 (90%)	6565 (100%)	4 (0%)	95	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
34	t	153	LEU
34	t	165	LEU
41	Z	145	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	150	GLN
1	1	293	ASN
1	1	361	GLN
1	1	431	GLN
2	2	99	HIS
2	2	214	GLN
3	3	36	GLN
3	3	255	HIS
3	3	259	ASN
3	3	581	GLN
4	4	149	ASN
4	4	157	HIS
4	4	200	HIS

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Mol	Chain	Res	Type
4	4	266	GLN
4	4	347	HIS
5	5	88	ASN
7	9	157	ASN
8	H	169	GLN
8	H	194	ASN
8	H	317	GLN
9	N	63	GLN
9	N	134	GLN
9	N	309	ASN
9	N	310	ASN
10	A	10	ASN
10	A	80	GLN
10	A	108	GLN
11	M	44	GLN
11	M	319	HIS
11	M	366	ASN
13	L	27	HIS
13	L	115	ASN
13	L	226	GLN
13	L	270	ASN
13	L	405	ASN
13	L	479	GLN
16	b	13	HIS
17	c	44	ASN
18	d	8	HIS
18	d	36	ASN
18	d	37	HIS
18	d	89	ASN
18	d	148	ASN
18	d	203	GLN
18	d	250	HIS
19	e	24	GLN
20	f	82	GLN
22	h	50	ASN
23	i	31	ASN
23	i	72	ASN
25	k	50	HIS
25	k	184	GLN
25	k	200	GLN
26	l	15	HIS
26	l	24	GLN

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Mol	Chain	Res	Type
26	l	26	HIS
27	m	45	ASN
27	m	70	GLN
28	n	20	GLN
29	o	59	HIS
29	o	79	GLN
30	p	125	ASN
32	r	25	GLN
32	r	82	HIS
32	r	88	HIS
33	s	42	GLN
33	s	60	HIS
34	t	17	GLN
34	t	25	HIS
34	t	168	HIS
35	u	16	GLN
35	u	21	GLN
36	v	104	HIS
37	w	45	HIS
37	w	111	ASN
37	w	119	GLN
39	y	30	ASN
41	Z	99	GLN
41	Z	139	GLN
43	W	135	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
45	SF4	1	500	1	0,12,12	0.00	-	0,24,24	0.00	-
46	FMN	1	501	-	32,33,33	1.10	2 (6%)	34,50,50	2.94	5 (14%)
47	FES	2	300	2	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	3	801	3	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	3	802	3	0,12,12	0.00	-	0,24,24	0.00	-
47	FES	3	803	3	0,4,4	0.00	-	0,4,4	0.00	-
45	SF4	6	300	6	0,12,12	0.00	-	0,24,24	0.00	-
48	3PE	9	501	-	50,50,50	0.32	0	52,55,55	0.41	0
45	SF4	9	502	7	0,12,12	0.00	-	0,24,24	0.00	-
45	SF4	9	503	7	0,12,12	0.00	-	0,24,24	0.00	-
49	PC1	A	200	-	46,46,53	0.34	0	50,54,61	0.32	0
50	CDL	J	300	-	78,78,99	0.36	0	80,90,111	0.37	0
48	3PE	J	301	-	50,50,50	0.33	0	52,55,55	0.31	0
50	CDL	L	601	-	83,83,99	0.34	0	85,95,111	0.40	0
49	PC1	M	501	-	45,45,53	0.33	0	49,53,61	0.31	0
50	CDL	M	502	-	81,81,99	0.35	0	83,93,111	0.36	0
49	PC1	N	401	-	45,45,53	0.34	0	49,53,61	0.35	0
54	PNS	X	401	24	13,20,21	0.51	0	16,26,29	0.91	1 (6%)
52	NDP	d	401	-	44,52,52	0.48	0	55,80,80	0.65	1 (1%)
50	CDL	i	201	-	57,57,99	0.41	0	59,69,111	0.36	0
53	ZMP	j	101	24	26,33,36	1.07	2 (7%)	31,40,45	1.41	3 (9%)
49	PC1	o	201	-	38,38,53	0.36	0	42,46,61	0.31	0
48	3PE	o	202	-	40,40,50	0.38	0	42,45,55	0.34	0
48	3PE	o	203	-	45,45,50	0.35	0	47,50,55	0.38	0

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	1	500	1	-	0/0/48/48	0/6/5/5
46	FMN	1	501	-	-	0/18/18/18	0/3/3/3
47	FES	2	300	2	-	0/0/4/4	0/1/1/1
45	SF4	3	801	3	-	0/0/48/48	0/6/5/5
45	SF4	3	802	3	-	0/0/48/48	0/6/5/5
47	FES	3	803	3	-	0/0/4/4	0/1/1/1
45	SF4	6	300	6	-	0/0/48/48	0/6/5/5
48	3PE	9	501	-	-	0/54/54/54	0/0/0/0
45	SF4	9	502	7	-	0/0/48/48	0/6/5/5
45	SF4	9	503	7	-	0/0/48/48	0/6/5/5
49	PC1	A	200	-	-	0/50/50/57	0/0/0/0
50	CDL	J	300	-	-	0/89/89/110	0/0/0/0
48	3PE	J	301	-	-	0/54/54/54	0/0/0/0
50	CDL	L	601	-	-	0/94/94/110	0/0/0/0
49	PC1	M	501	-	-	0/49/49/57	0/0/0/0
50	CDL	M	502	-	-	0/92/92/110	0/0/0/0
49	PC1	N	401	-	-	0/49/49/57	0/0/0/0
54	PNS	X	401	24	-	0/24/26/27	0/0/0/0
52	NDP	d	401	-	-	0/30/77/77	0/5/5/5
50	CDL	i	201	-	-	0/68/68/110	0/0/0/0
53	ZMP	j	101	24	-	0/38/40/43	0/0/0/0
49	PC1	o	201	-	-	0/42/42/57	0/0/0/0
48	3PE	o	202	-	-	0/44/44/54	0/0/0/0
48	3PE	o	203	-	-	0/49/49/54	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	j	101	ZMP	C10-S1	-4.27	1.70	1.76
46	1	501	FMN	C5A-N5	2.26	1.38	1.35
53	j	101	ZMP	C9-C10	2.60	1.53	1.50
46	1	501	FMN	C4-N3	3.07	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	501	FMN	C4A-C4-N3	-7.33	113.93	123.52
46	1	501	FMN	C4A-C10-N10	-5.37	116.62	120.52
46	1	501	FMN	N3-C2-N1	-4.72	119.75	127.69
53	j	101	ZMP	O1-C10-C9	-4.69	120.71	123.94
46	1	501	FMN	C4-C4A-C10	-3.97	117.40	119.94
53	j	101	ZMP	C8-C9-C10	-3.30	108.24	113.12
54	X	401	PNS	C37-C38-C39	-2.07	108.66	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	j	101	ZMP	C9-C10-S1	2.46	115.57	113.36
52	d	401	NDP	P2B-O2B-C2B	2.65	128.34	121.56
46	1	501	FMN	C4-N3-C2	12.97	125.98	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1	500	SF4	2	0
46	1	501	FMN	8	0
45	3	801	SF4	1	0
45	3	802	SF4	1	0
45	6	300	SF4	2	0
48	9	501	3PE	9	0
45	9	502	SF4	3	0
45	9	503	SF4	1	0
49	A	200	PC1	3	0
50	J	300	CDL	1	0
48	J	301	3PE	6	0
50	L	601	CDL	13	0
49	M	501	PC1	2	0
50	M	502	CDL	2	0
49	N	401	PC1	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	k	1
9	N	1
19	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	174:VAL	C	175:PRO	N	1.18
1	N	304:MET	C	305:PHE	N	1.16
1	e	50:LEU	C	51:PRO	N	1.15