Full wwPDB EM Validation Report ⓘ

Aug 22, 2026 – 03:13 am BST

PDB ID	:	5LNK / pdb_00005lnk
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 initial model	:	4HEA

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

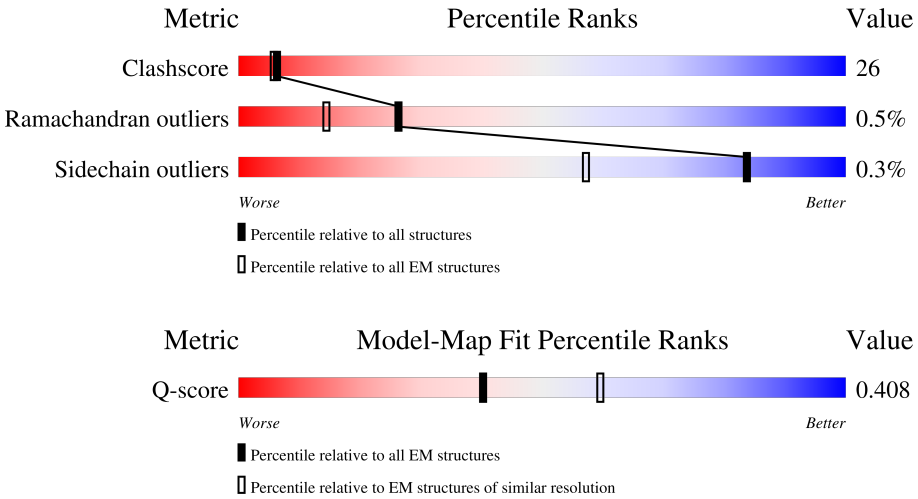
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



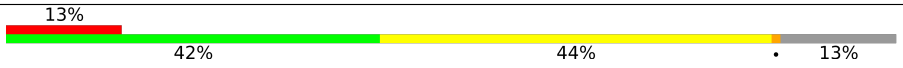
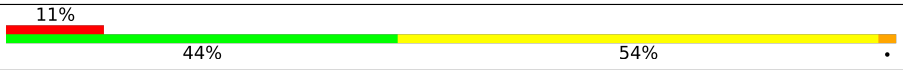
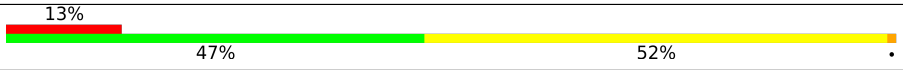
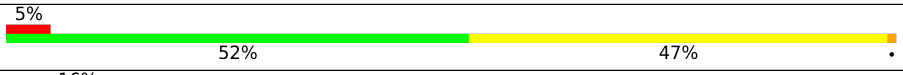
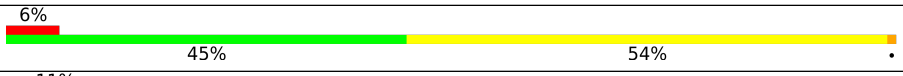
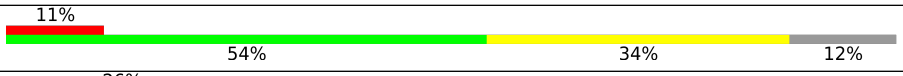
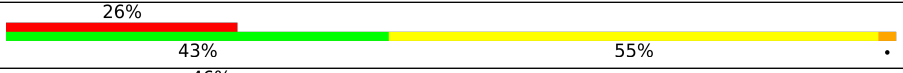
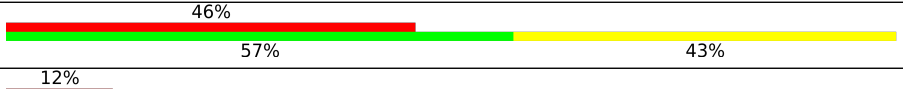
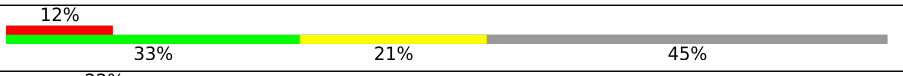
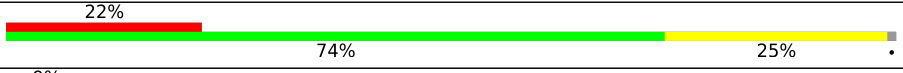
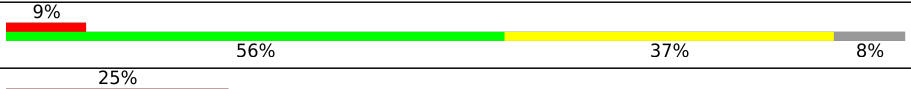
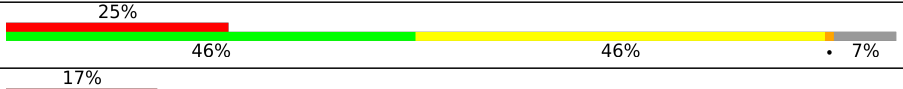
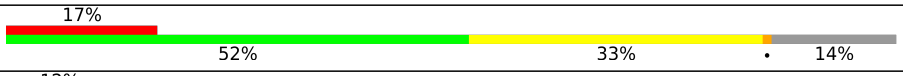
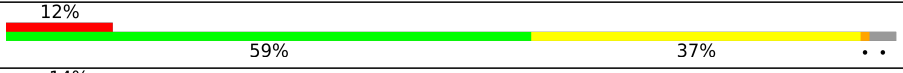
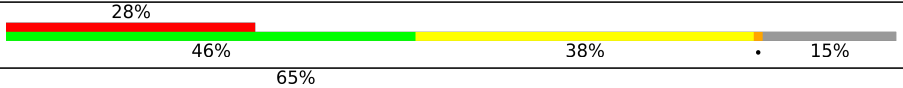
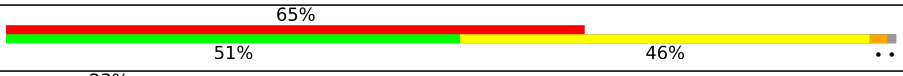
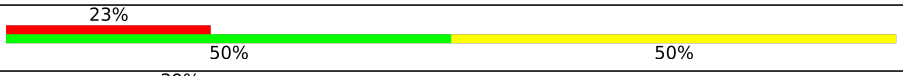
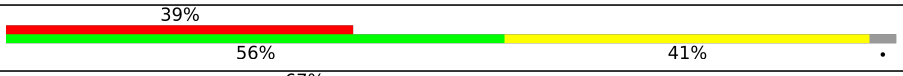
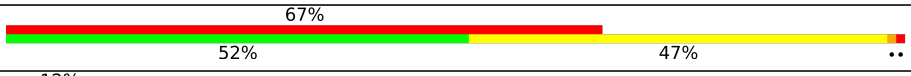
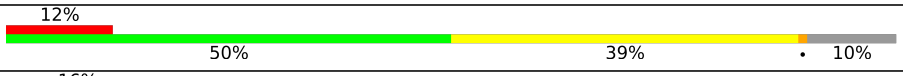
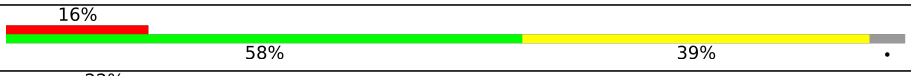
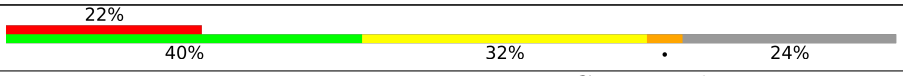
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	1	445	15% 51% 45% ·
2	2	217	19% 59% 38% ··
3	3	704	12% 58% 39% ·
4	4	412	14% 43% 50% · 6%

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Mol	Chain	Length	Quality of chain
5	5	228	
6	6	179	
7	9	176	
8	H	318	
9	N	347	
10	A	115	
11	M	459	
12	K	98	
13	L	599	
14	J	175	
15	a	75	
16	b	96	
17	c	133	
18	d	338	
19	e	98	
20	f	115	
21	g	127	
22	h	112	
23	i	145	
24	X	88	
24	j	88	
25	k	320	
26	l	105	
27	m	83	
28	n	97	

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Mol	Chain	Length	Quality of chain
29	o	120	18% 63% 37%
30	p	128	36% 52% 34% 12%
31	q	143	19% 56% 40%
32	r	127	20% 38% 33% 27%
33	s	136	30% 40% 45% 13%
34	t	178	16% 51% 40% 7%
35	u	72	29% 33% 58% 8%
36	v	158	37% 63% 24% 9%
37	w	125	5% 34% 34% 31%
38	x	49	16% 76% 22%
39	y	57	25% 65% 28% 7%
40	z	70	7% 54% 44%
41	Z	175	14% 54% 43%
42	Y	171	11% 37% 62%
43	W	143	6% 56% 41%
44	V	119	99% 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 (i)

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
			Total	C	N	O	S		
1	1	432	3328	2097	596	615	20	0	0

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

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

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

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

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

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

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

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

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

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

- 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	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		

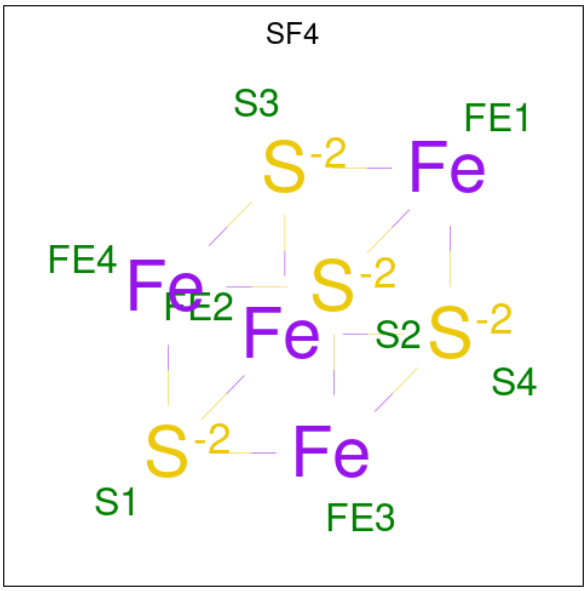
- Molecule 43 is a protein called Mitochondrial complex I, SGDH subunit.

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	0	0
			595	357	119	119		

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



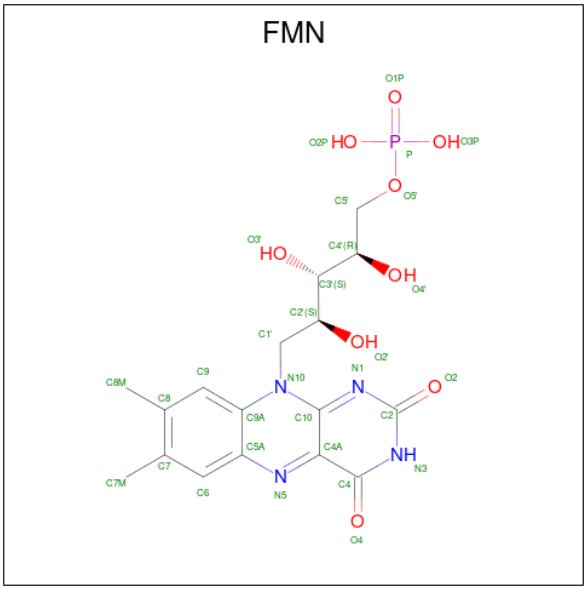
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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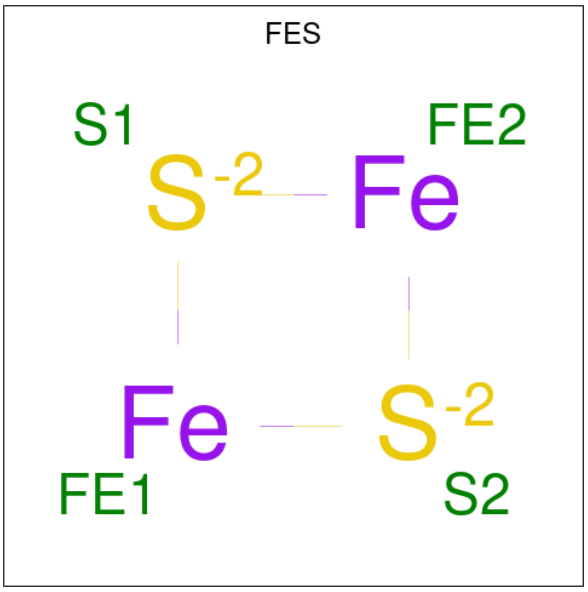
Mol	Chain	Residues	Atoms	AltConf
45	9	1	Total Fe S 8 4 4	0
45	9	1	Total Fe S 8 4 4	0

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



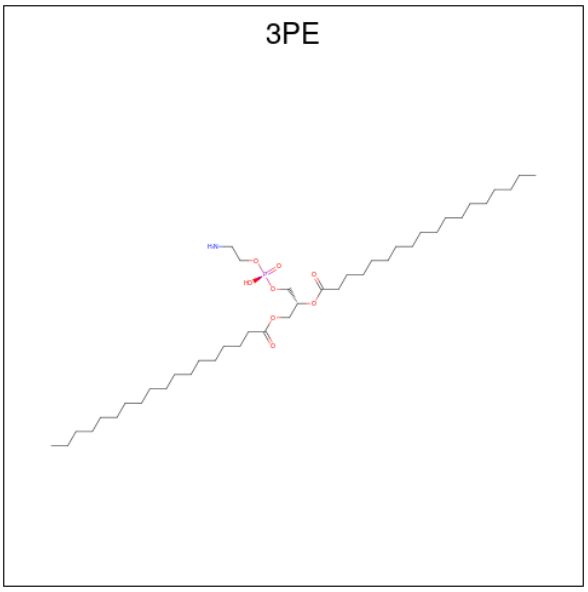
Mol	Chain	Residues	Atoms	AltConf
46	1	1	Total C N O P 31 17 4 9 1	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



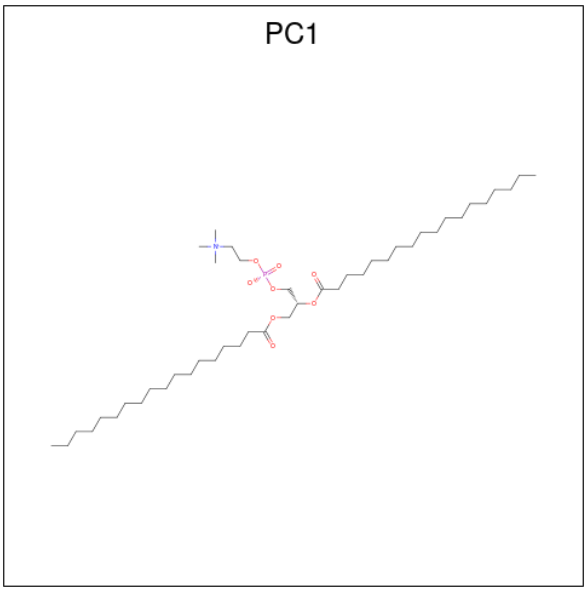
Mol	Chain	Residues	Atoms					AltConf
48	9	1	Total	C	N	O	P	0
			51	41	1	8	1	

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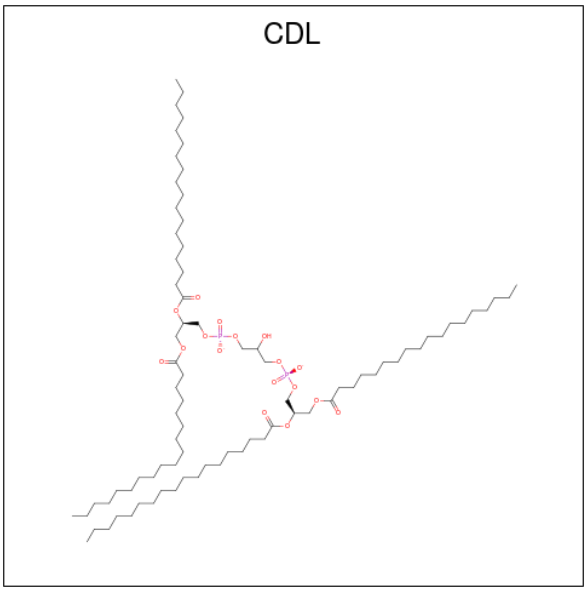
Mol	Chain	Residues	Atoms					AltConf
48	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	o	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	o	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: 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 (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

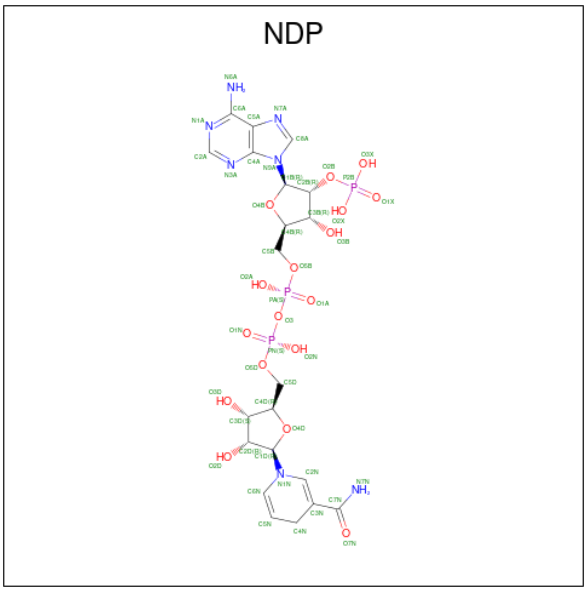


Mol	Chain	Residues	Atoms				AltConf
50	M	1	Total	C	O	P	0
			82	63	17	2	
50	L	1	Total	C	O	P	0
			84	65	17	2	
50	J	1	Total	C	O	P	0
			79	60	17	2	
50	i	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

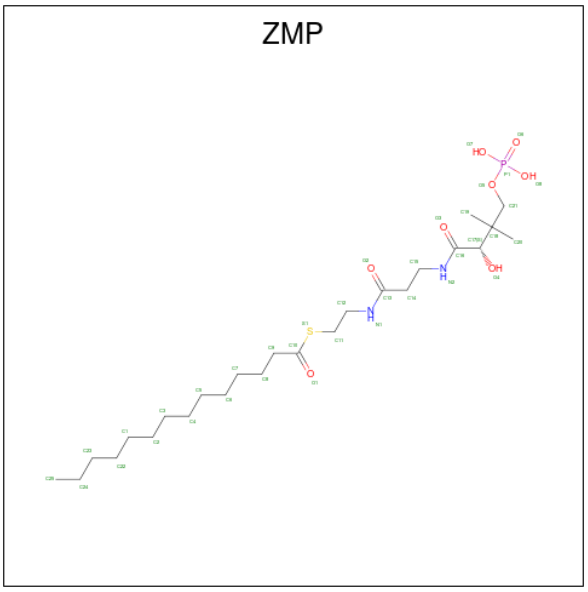
Mol	Chain	Residues	Atoms		AltConf
51	b	1	Total	Zn	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



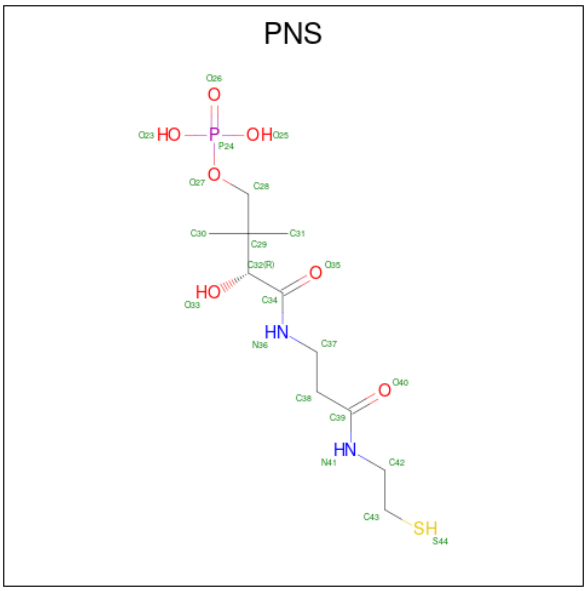
Mol	Chain	Residues	Atoms					AltConf
52	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



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 (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



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

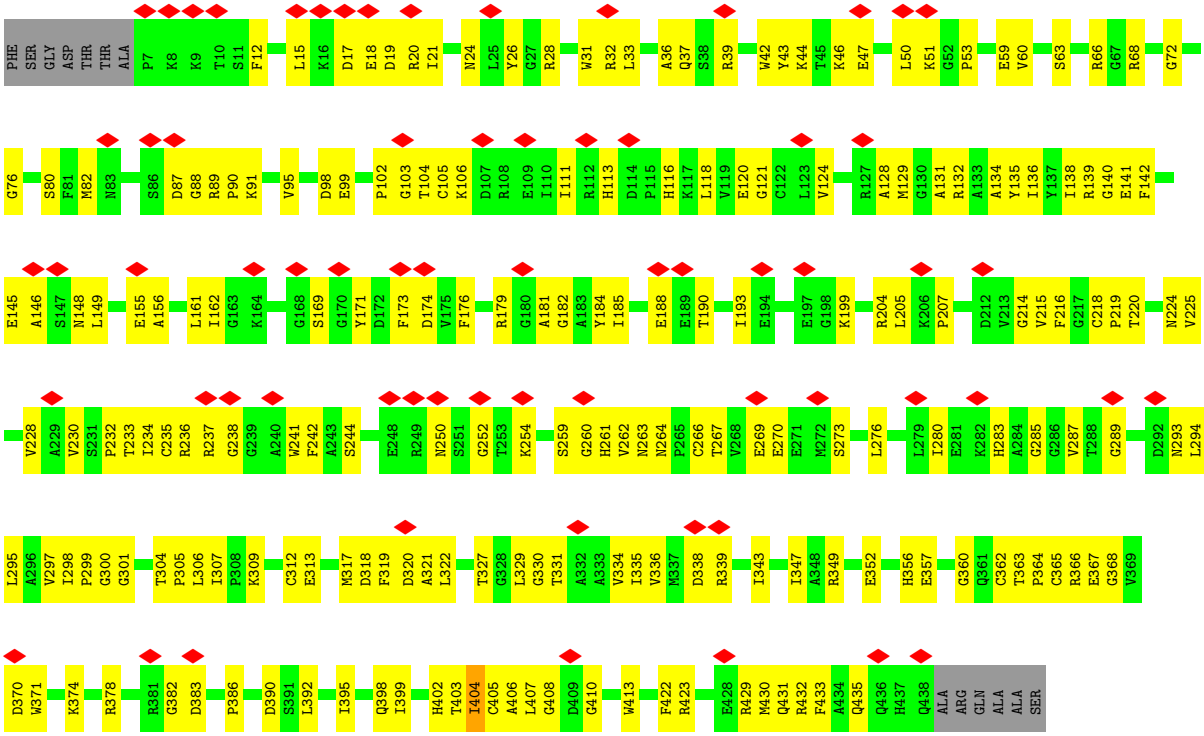
3 Residue-property plots (i)

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

• Molecule 1: Mitochondrial complex I, 51 kDa subunit

Chain 1:

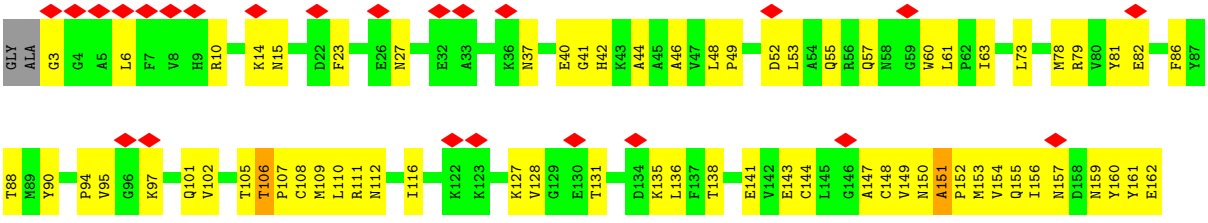


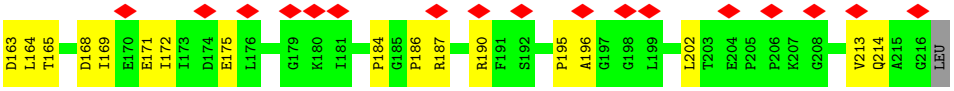


• Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:



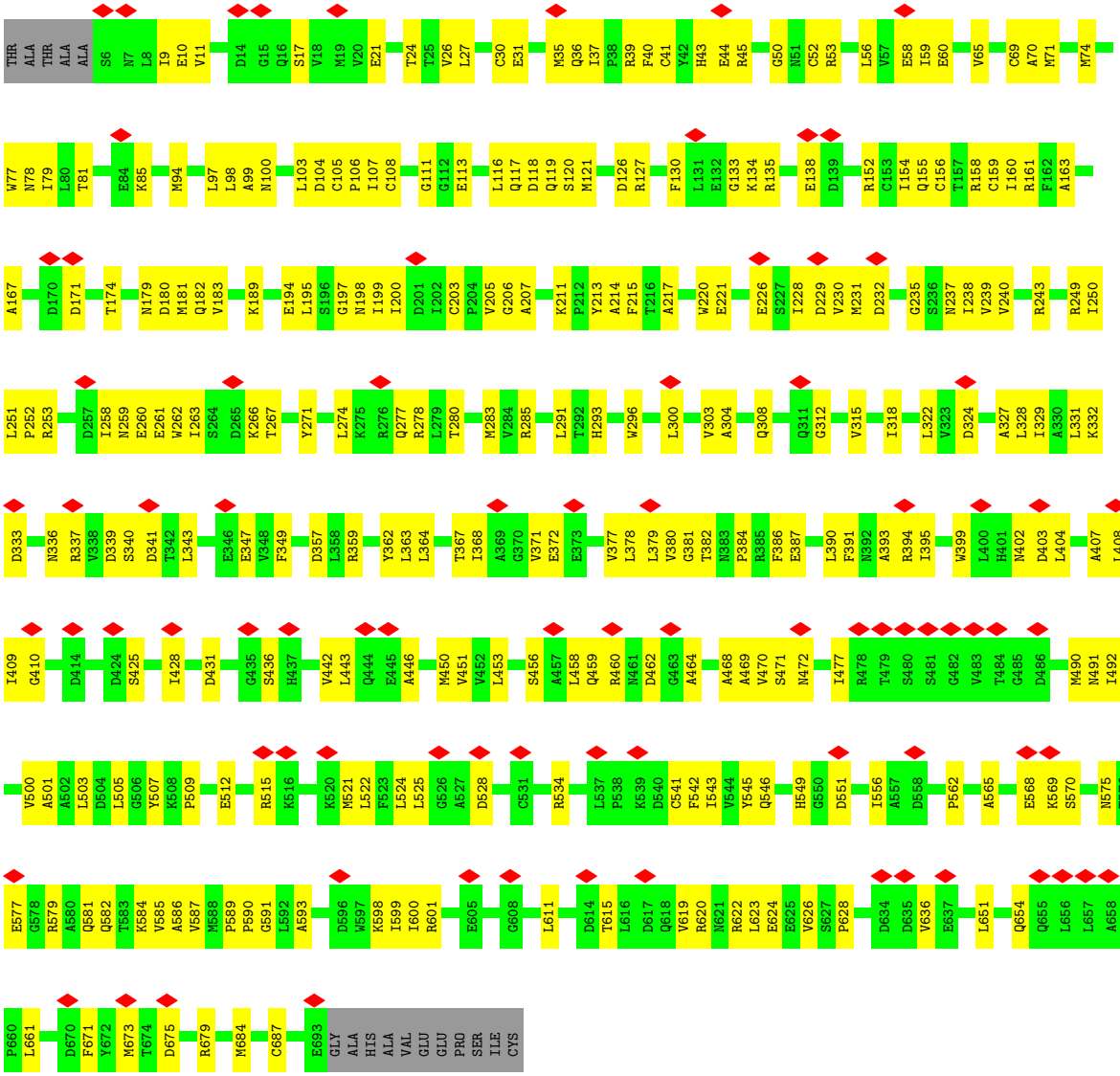




• Molecule 3: Mitochondrial complex I, 75 kDa subunit

Chain 3:

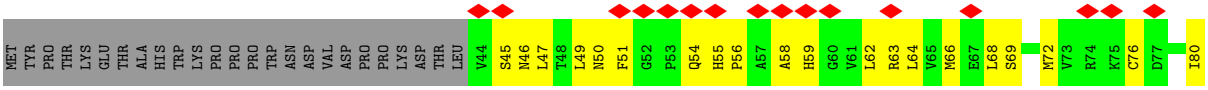


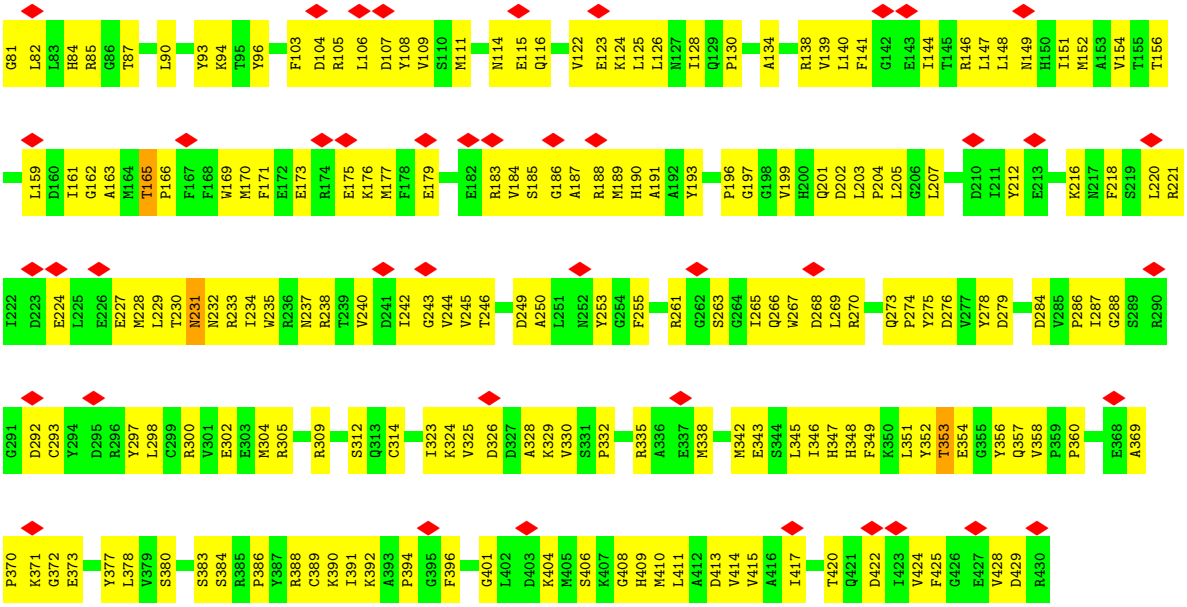


• Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:



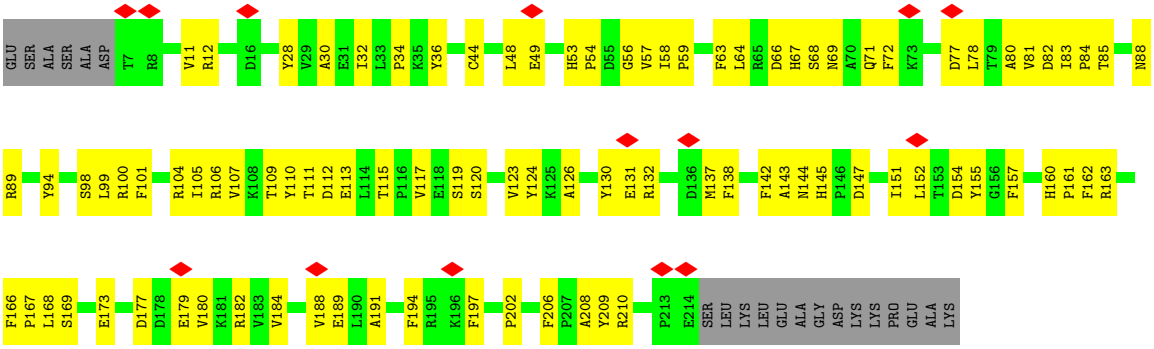




• Molecule 5: Mitochondrial complex I, 30 kDa subunit

Chain 5:

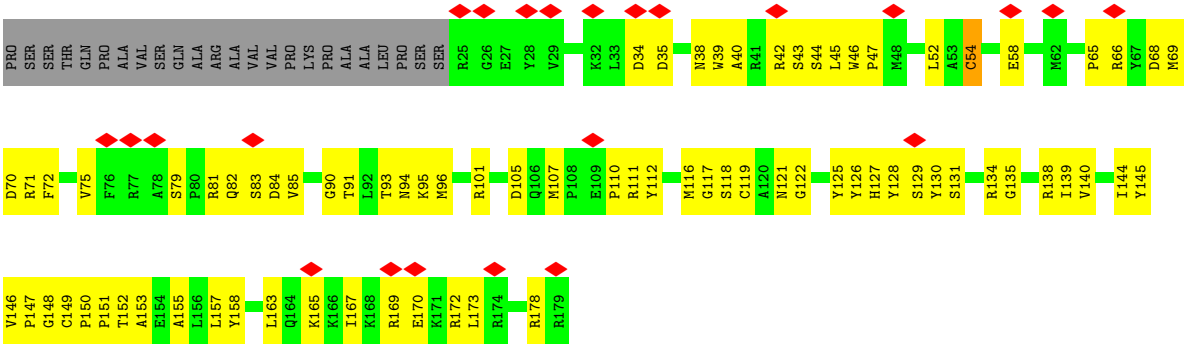




• Molecule 6: Mitochondrial complex I, PSST subunit

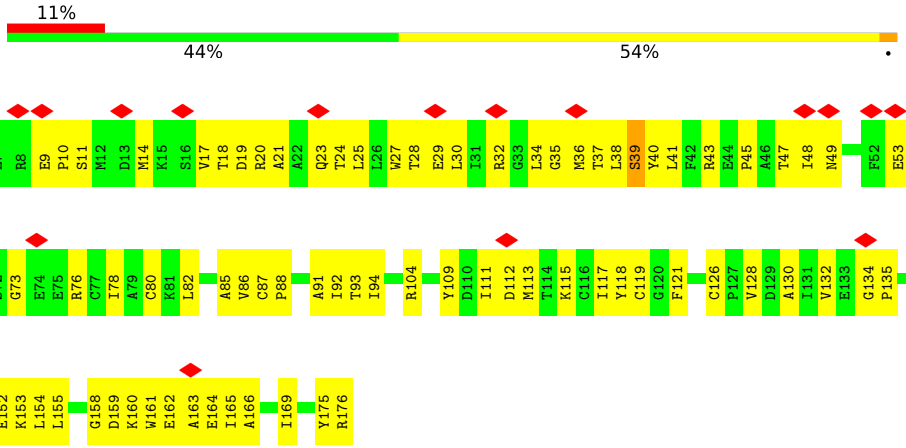
Chain 6:





• Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:



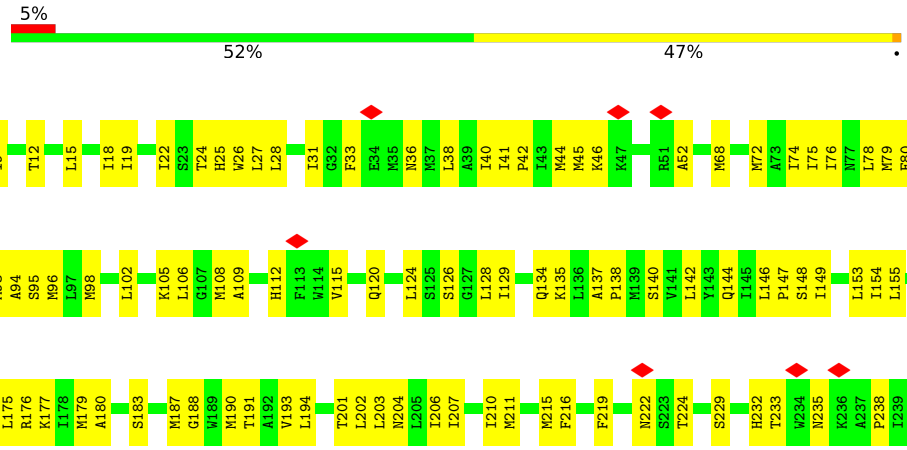
• Molecule 8: Mitochondrial complex I, ND1 subunit

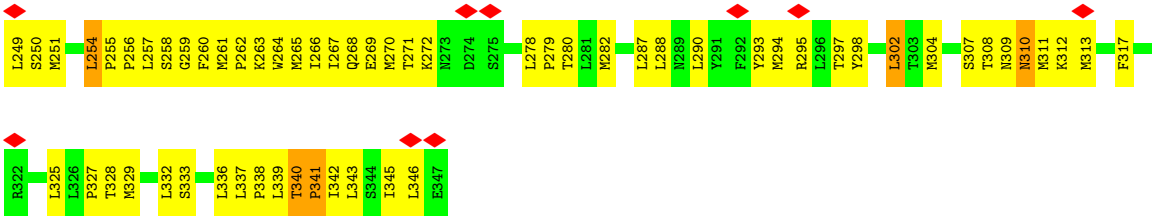
Chain H:



• Molecule 9: Mitochondrial complex I, ND2 subunit

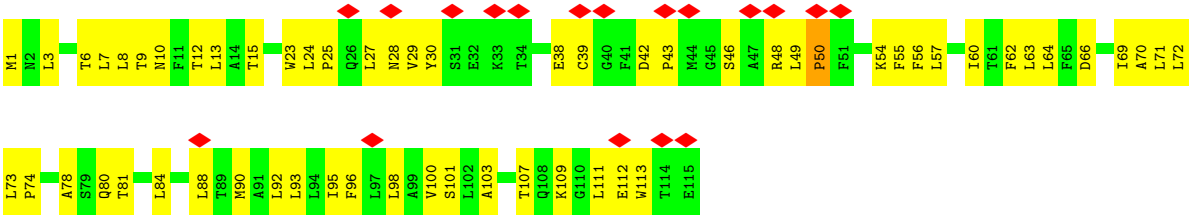
Chain N:





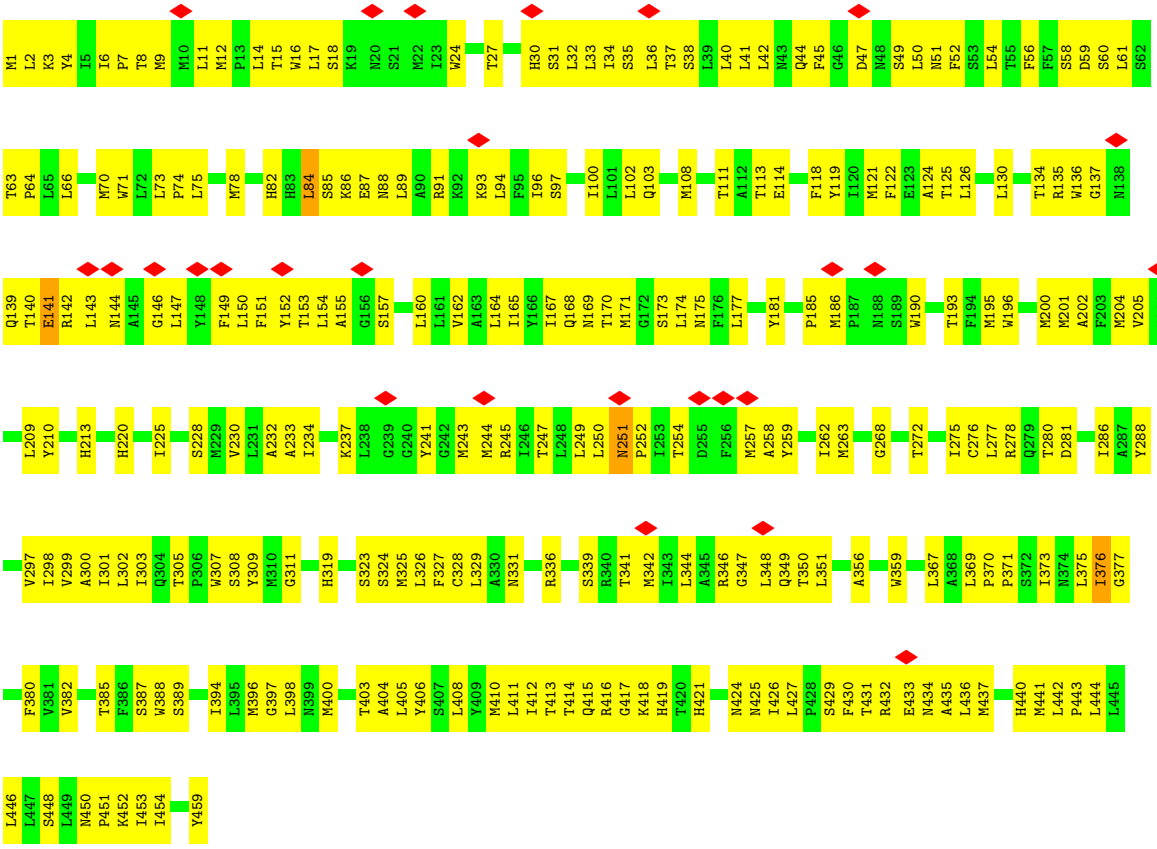
• Molecule 10: Mitochondrial complex I, ND3 subunit





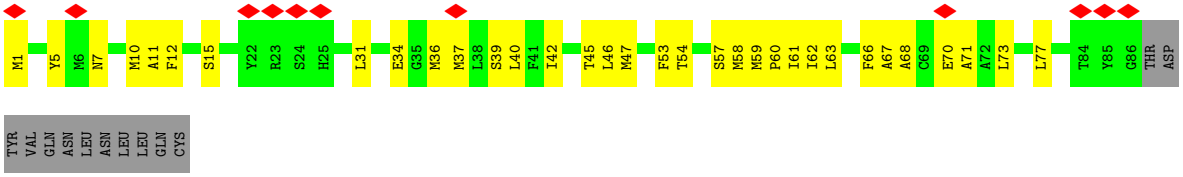
• Molecule 11: Mitochondrial complex I, ND4 subunit





• Molecule 12: Mitochondrial complex I, ND4L subunit

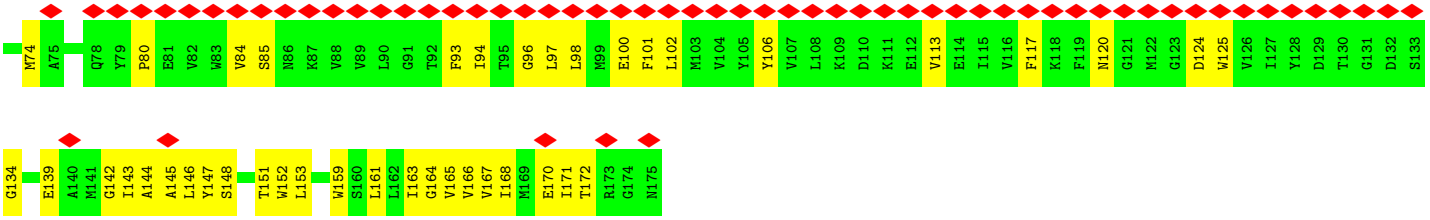




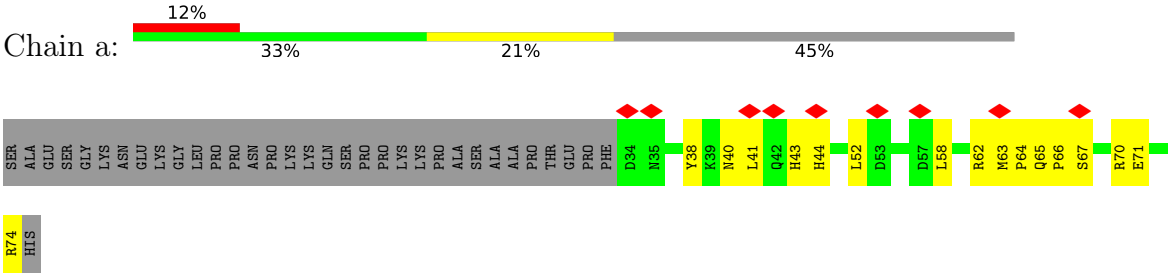
• Molecule 13: Mitochondrial complex I, ND5 subunit



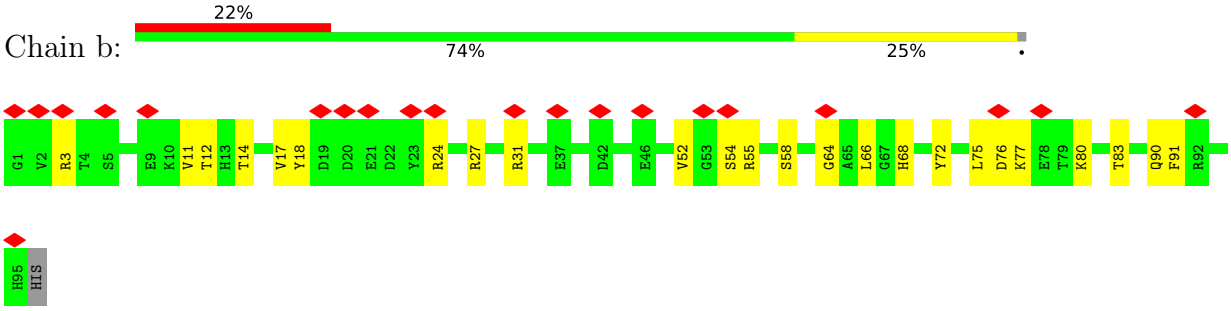
• Molecule 14: Mitochondrial complex I, ND6 subunit



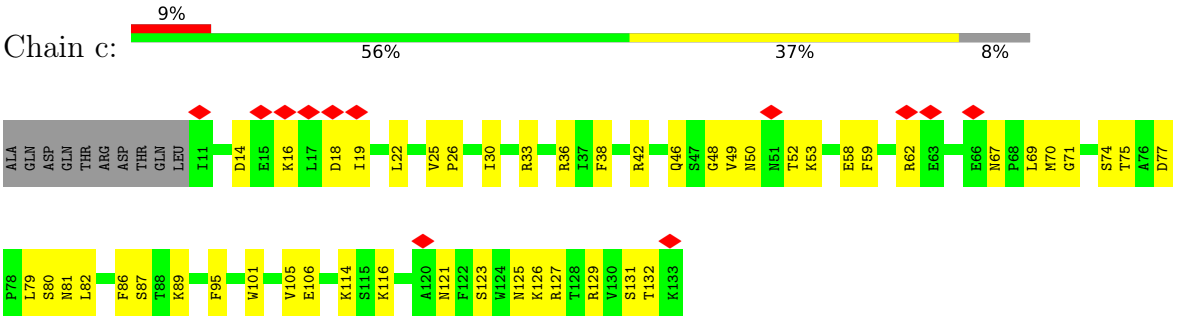
• Molecule 15: Mitochondrial complex I, 10 kDa subunit



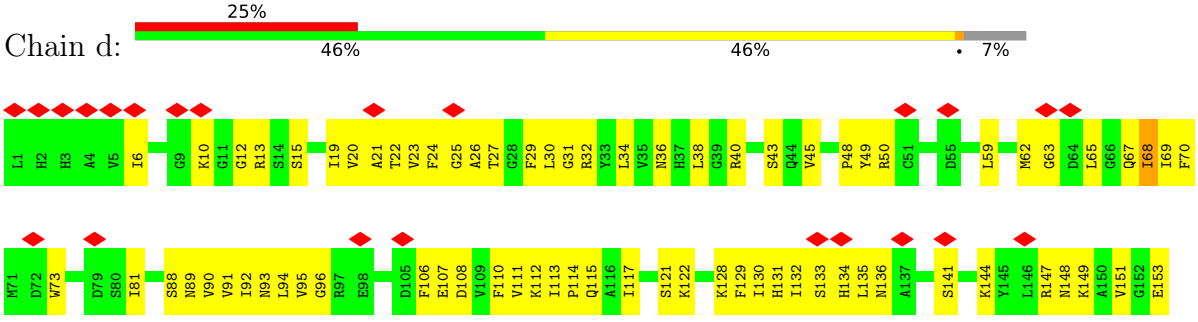
• Molecule 16: Mitochondrial complex I, 13 kDa subunit

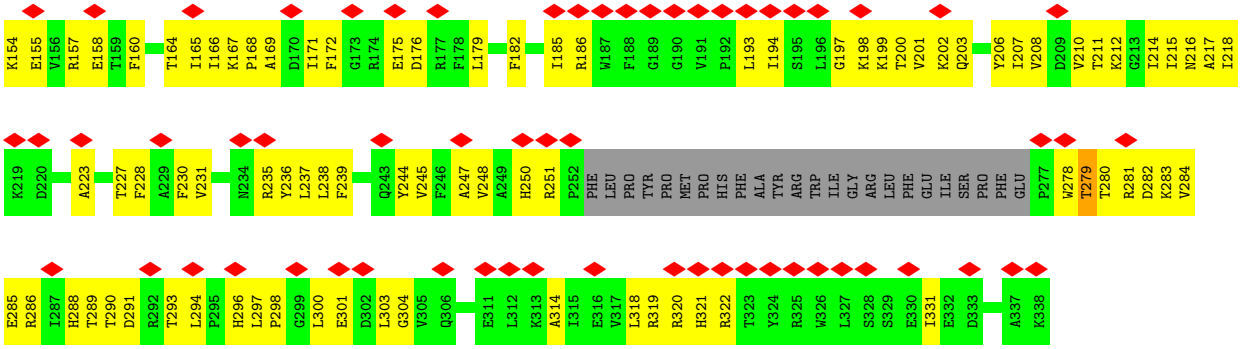


• Molecule 17: Mitochondrial complex I, 18 kDa subunit



• Molecule 18: Mitochondrial complex I, 39 kDa subunit

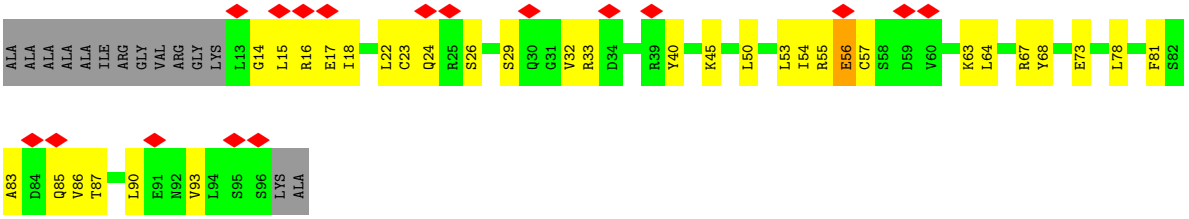




• Molecule 19: Mitochondrial complex I, B8 subunit

Chain e:

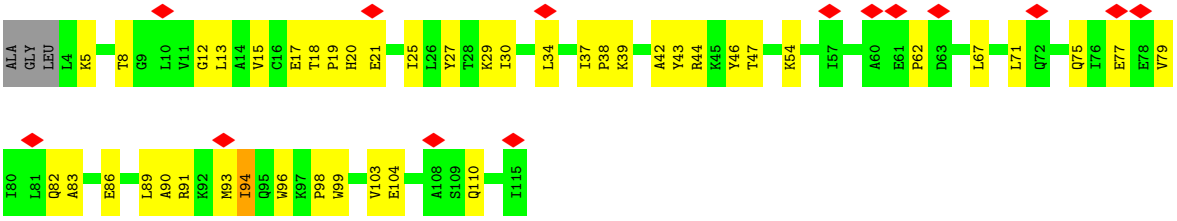




• Molecule 20: Mitochondrial complex I, B13 subunit

Chain f:

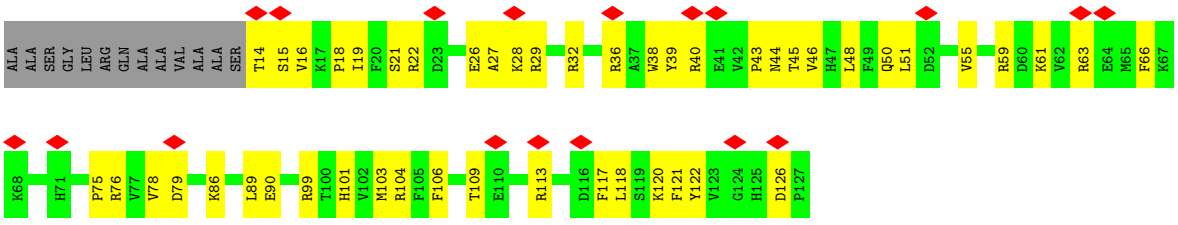




• Molecule 21: Mitochondrial complex I, B14 subunit

Chain g:

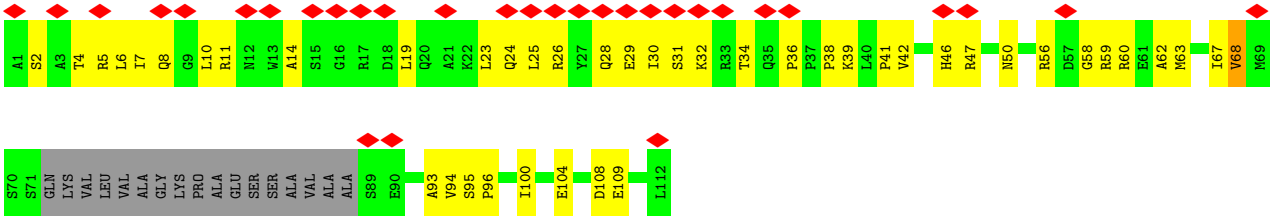




• Molecule 22: Mitochondrial complex I, B14.5a subunit

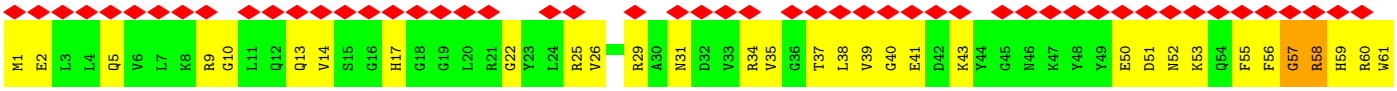
Chain h:

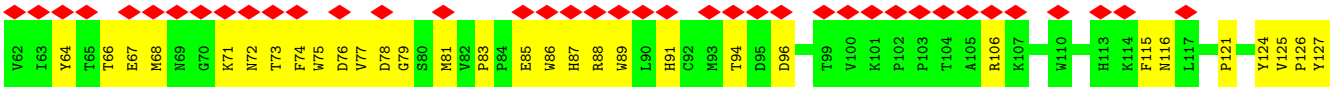


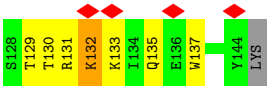


• Molecule 23: Mitochondrial complex I, B17.2 subunit



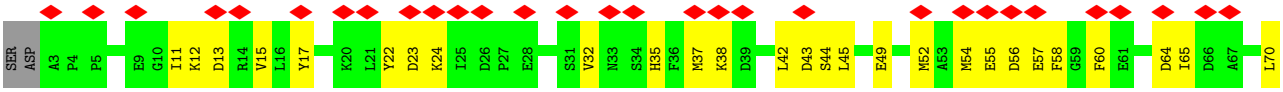


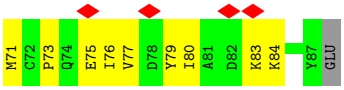




• Molecule 24: Acyl carrier protein

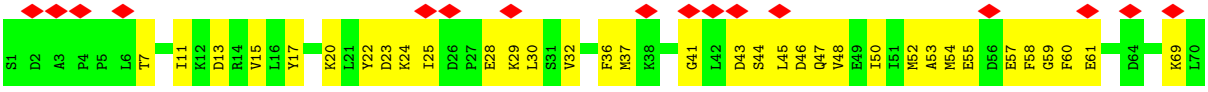


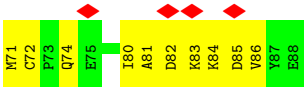




• Molecule 24: Acyl carrier protein

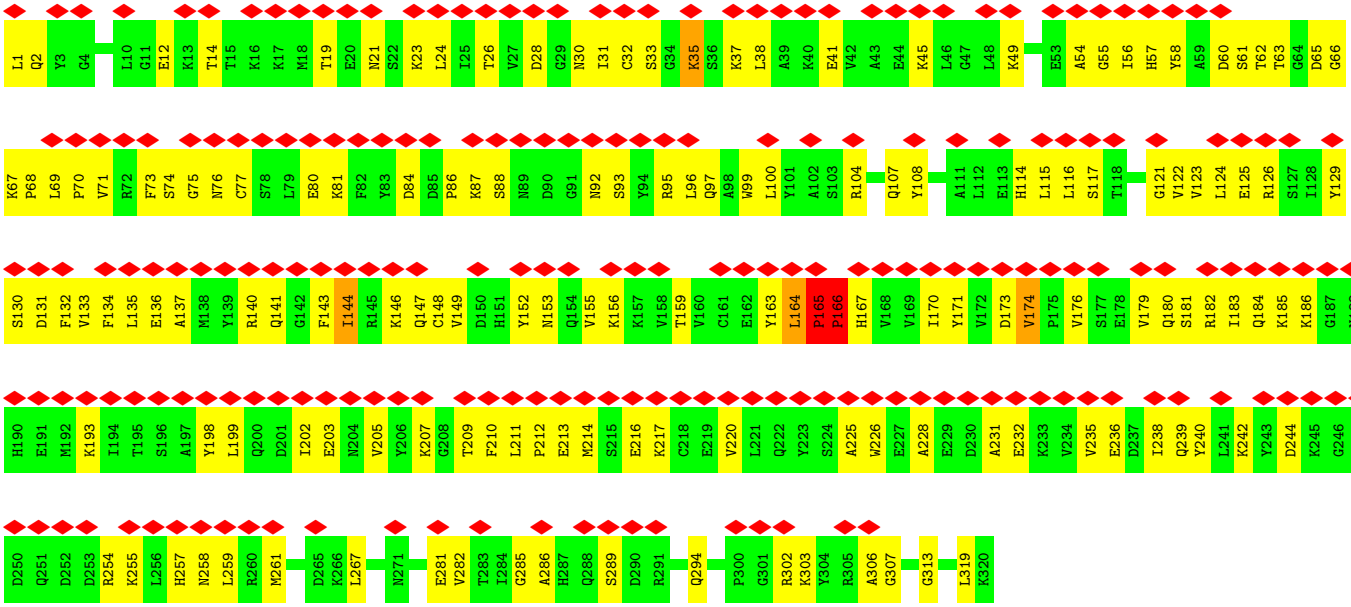






• Molecule 25: Mitochondrial complex I, 42 kDa subunit





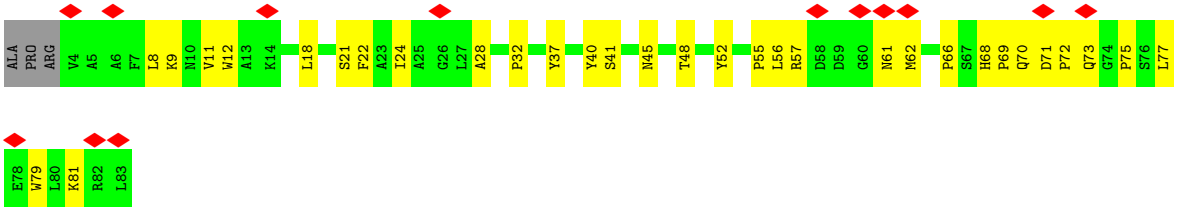
• Molecule 26: Mitochondrial complex I, 15 kDa subunit





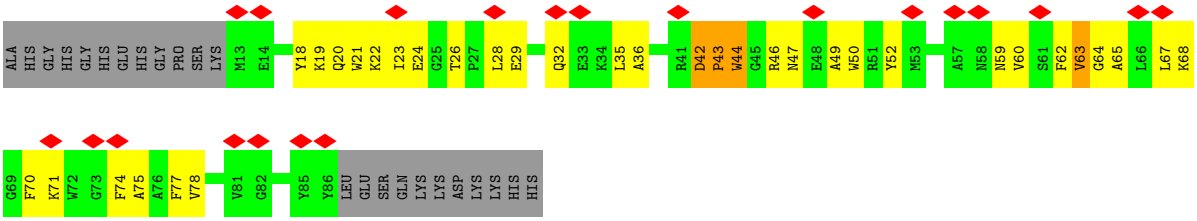
• Molecule 27: Mitochondrial complex I, B9 subunit





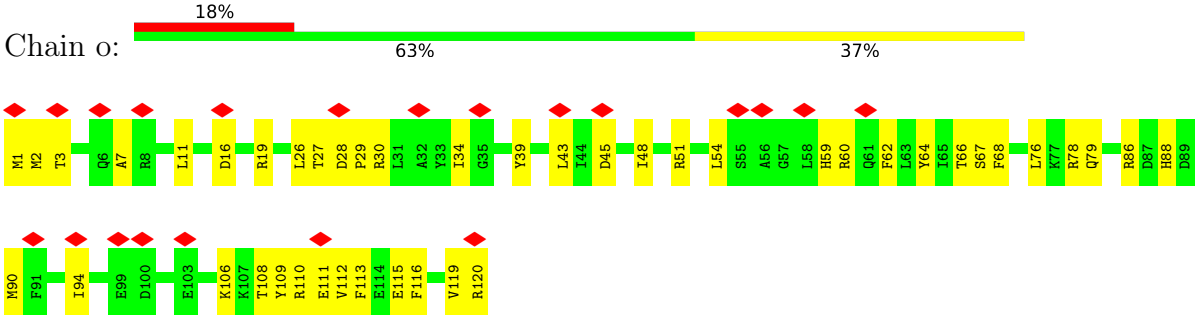
• Molecule 28: Mitochondrial complex I, B12 subunit





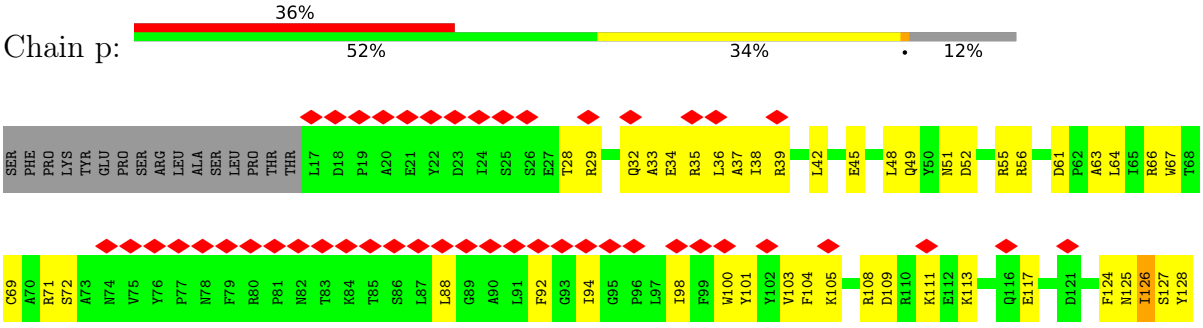
• Molecule 29: Mitochondrial complex I, B14.5b subunit

Chain o:



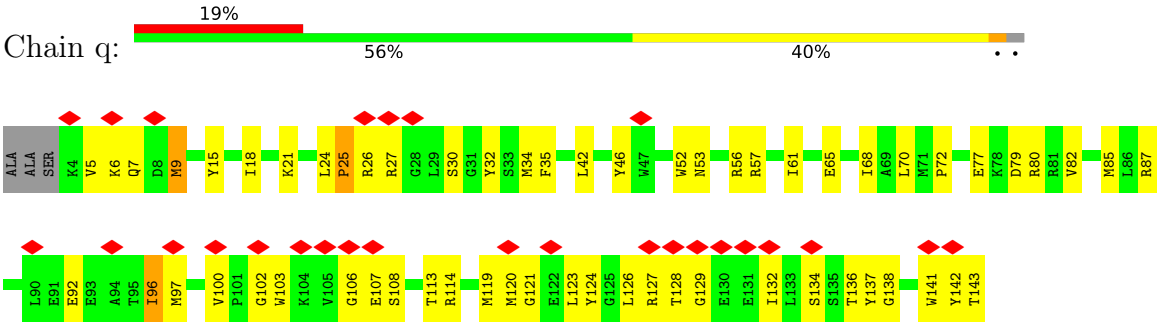
• Molecule 30: Mitochondrial complex I, B15 subunit

Chain p:



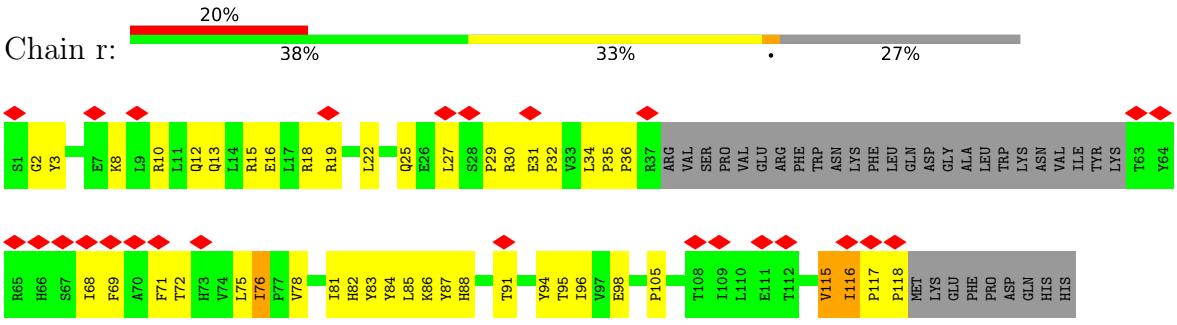
• Molecule 31: Mitochondrial complex I, B16.6 subunit

Chain q:



• Molecule 32: Mitochondrial complex I, B17 subunit

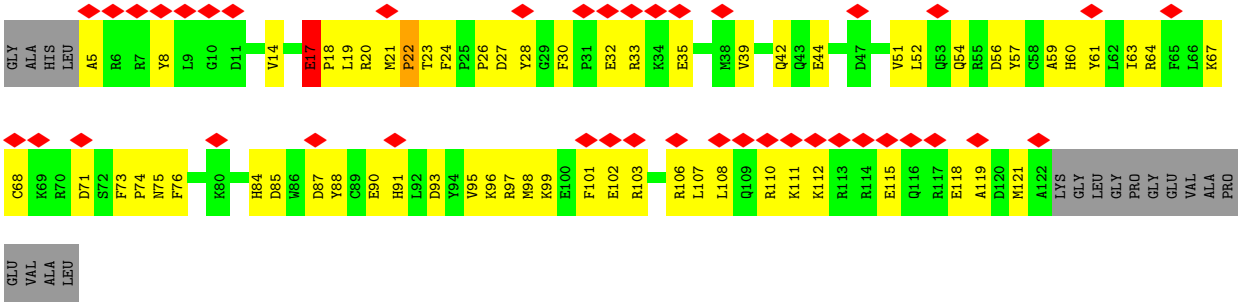
Chain r:



• Molecule 33: Mitochondrial complex I, B18 subunit

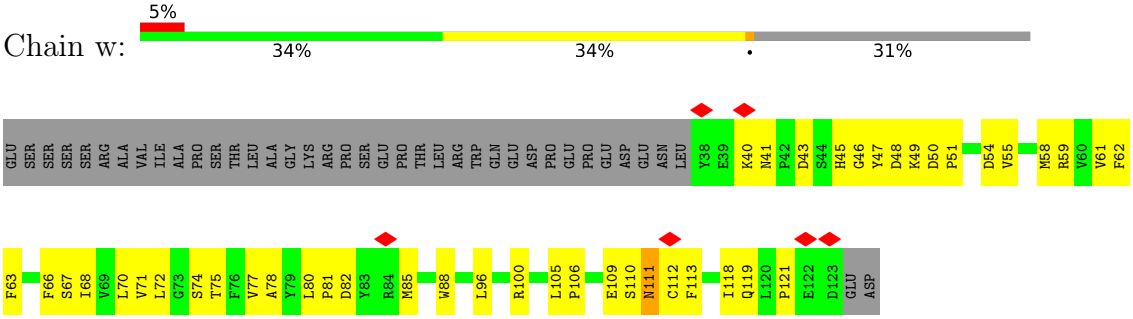
Chain s:





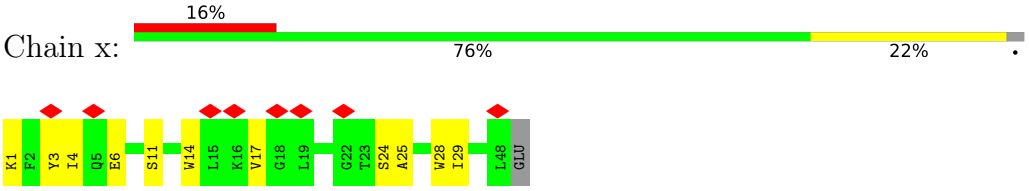
• Molecule 37: Mitochondrial complex I, ESSS subunit

Chain w:



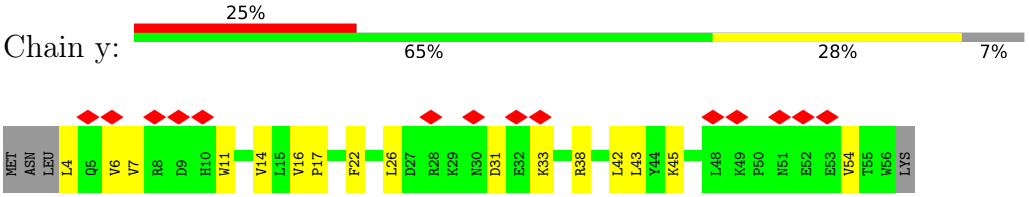
• Molecule 38: Mitochondrial complex I, KFYI subunit

Chain x:



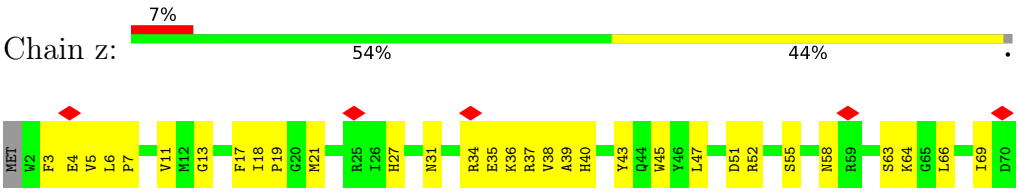
• Molecule 39: Mitochondrial complex I, MNLL subunit

Chain y:



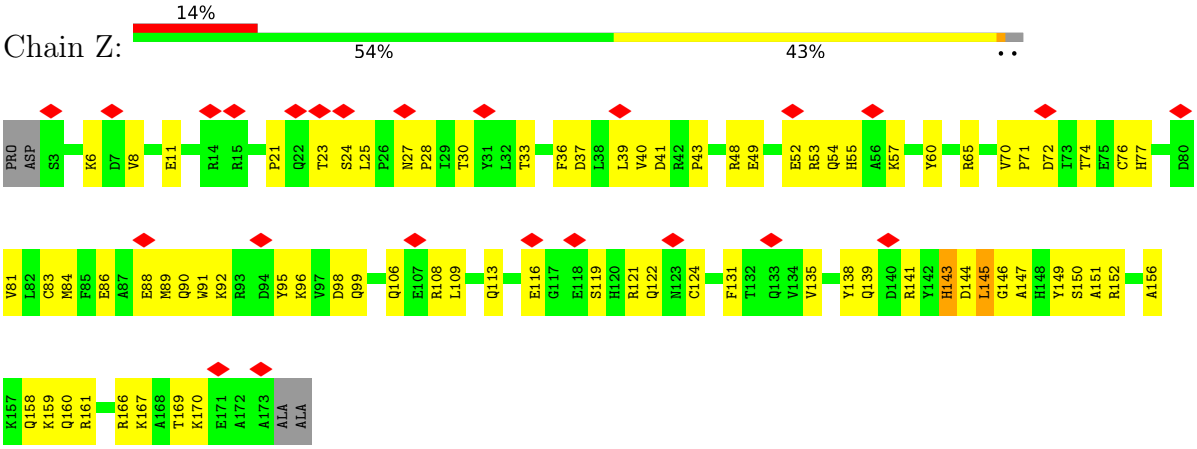
• Molecule 40: Mitochondrial complex I, MWFE subunit

Chain z:

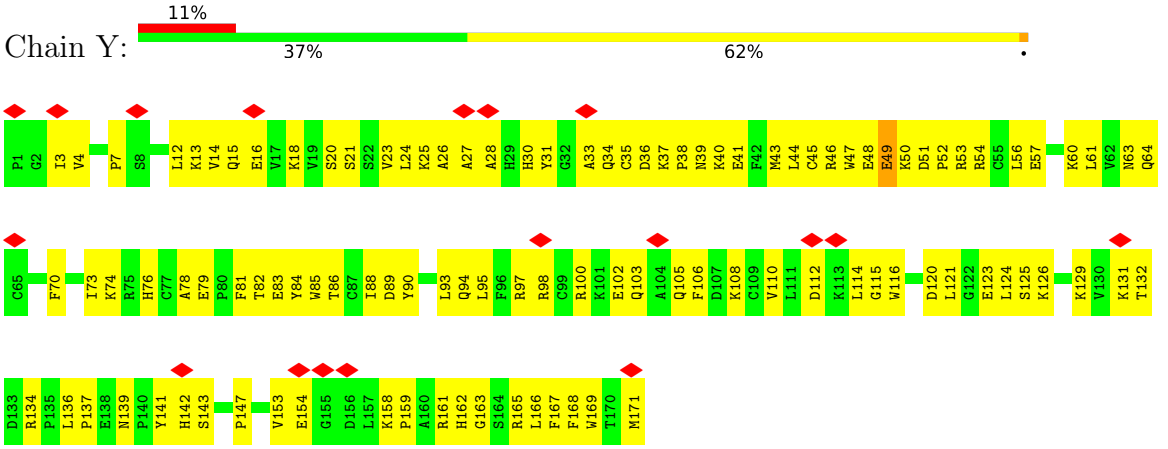


• Molecule 41: Mitochondrial complex I, PDSW subunit

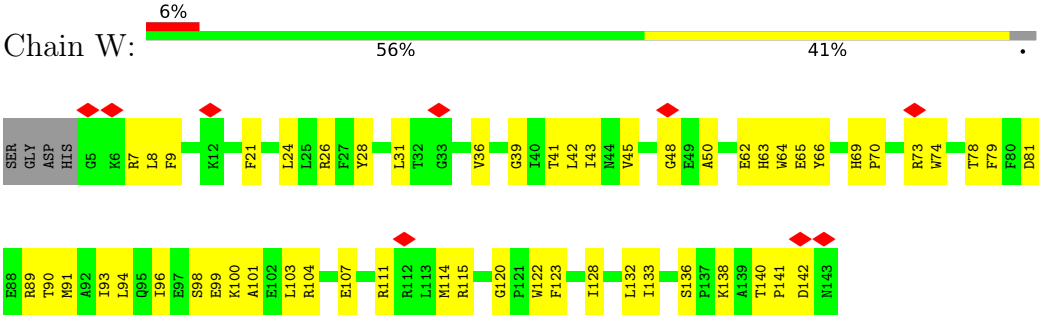
Chain Z:



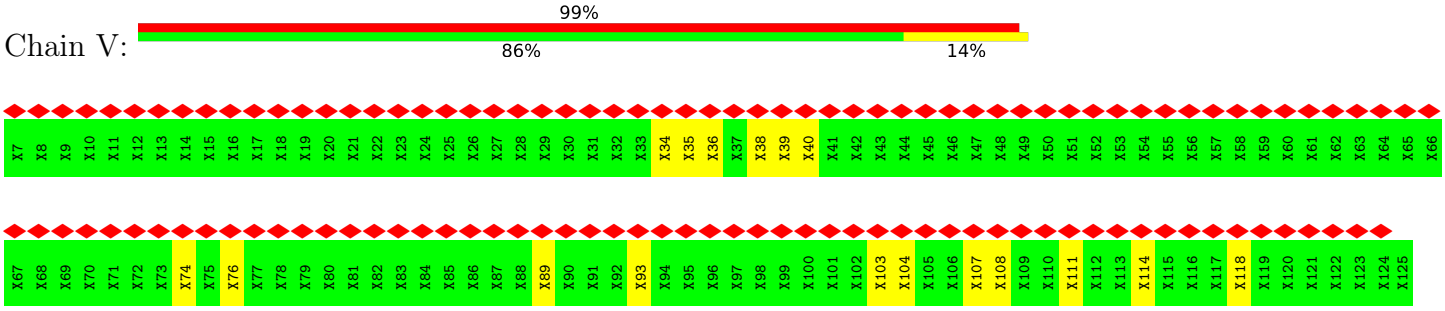
• Molecule 42: Mitochondrial complex I, PGIV subunit



• Molecule 43: Mitochondrial complex I, SGDH subunit



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	100720	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.314	Depositor
Minimum map value	-0.549	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	179.31, 195.99, 290.51	wwPDB
Map dimensions	209, 141, 129	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.3900001	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.24	0/3403	0.48	0/4597
2	2	0.25	0/1695	0.54	0/2305
3	3	0.26	0/5362	0.48	0/7266
4	4	0.32	0/3172	0.57	1/4288 (0.0%)
5	5	0.30	0/1776	0.50	0/2417
6	6	0.33	0/1272	0.56	0/1720
7	9	0.36	0/1445	0.69	3/1956 (0.2%)
8	H	0.36	0/2603	0.65	2/3561 (0.1%)
9	N	0.38	1/2787 (0.0%)	0.64	3/3795 (0.1%)
10	A	0.35	0/947	0.59	0/1296
11	M	0.34	0/3739	0.61	0/5095
12	K	0.34	0/658	0.54	0/888
13	L	0.32	0/4563	0.63	0/6227
14	J	0.31	0/1212	0.64	2/1652 (0.1%)
15	a	0.18	0/352	0.59	0/476
16	b	0.30	0/749	0.46	0/1009
17	c	0.29	0/1023	0.53	0/1382
18	d	0.25	0/2532	0.61	0/3430
19	e	0.36	1/688 (0.1%)	0.52	0/927
20	f	0.23	0/929	0.52	0/1260
21	g	0.26	0/993	0.49	0/1336
22	h	0.23	0/775	0.61	0/1048
23	i	0.21	0/1241	0.54	0/1687
24	X	0.24	0/719	0.58	1/971 (0.1%)
24	j	0.20	0/696	0.46	0/940
25	k	0.25	1/2309 (0.0%)	0.75	6/3141 (0.2%)
26	l	0.29	0/811	0.58	0/1085
27	m	0.25	0/647	0.45	0/890
28	n	0.25	0/595	0.72	0/805
29	o	0.27	0/1035	0.54	0/1398
30	p	0.23	0/855	0.59	0/1155
31	q	0.28	0/1180	0.69	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	r	0.31	0/774	0.68	0/1058
33	s	0.25	0/1011	0.66	0/1356
34	t	0.32	1/1483 (0.1%)	0.62	0/2006
35	u	0.27	0/590	0.61	0/809
36	v	0.25	0/877	0.82	1/1208 (0.1%)
37	w	0.29	0/737	0.60	0/999
38	x	0.19	0/416	0.40	0/564
39	y	0.25	0/470	0.50	0/636
40	z	0.28	0/583	0.55	0/785
41	Z	0.29	0/1475	0.58	0/1989
42	Y	0.31	0/1440	0.70	0/1942
43	W	0.30	0/1188	0.56	0/1607
All	All	0.29	4/63807 (0.0%)	0.59	19/86552 (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
2	2	0	1
4	4	0	1
7	9	0	1
8	H	0	3
9	N	0	3
10	A	0	2
13	L	0	6
17	c	0	1
19	e	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
42	Y	0	1
All	All	0	38

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	e	50	LEU	C-N	-7.86	1.15	1.33
34	t	163	PRO	C-N	7.55	1.51	1.33
25	k	174	VAL	C-N	-6.77	1.18	1.33
9	N	304	MET	C-N	-5.64	1.16	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	164	LEU	CA-C-N	17.32	138.22	120.38
25	k	164	LEU	C-N-CA	17.32	138.22	120.38
25	k	165	PRO	N-CA-C	7.07	119.33	110.70
25	k	165	PRO	CA-C-N	6.76	128.29	119.84
25	k	165	PRO	C-N-CA	6.76	128.29	119.84
9	N	310	ASN	N-CA-C	6.48	117.59	108.00
36	v	122	TYR	N-CA-C	6.40	115.67	108.25
8	H	272	TRP	CA-C-N	6.01	132.78	121.97
8	H	272	TRP	C-N-CA	6.01	132.78	121.97
9	N	341	PRO	N-CA-C	-5.99	105.86	114.18
7	9	65	HIS	N-CA-C	5.98	119.44	111.30
14	J	124	ASP	CA-C-N	5.91	132.82	121.54
14	J	124	ASP	C-N-CA	5.91	132.82	121.54
24	X	71	MET	CB-CA-C	-5.59	109.63	117.23
7	9	39	SER	CA-C-N	5.56	132.16	121.54
7	9	39	SER	C-N-CA	5.56	132.16	121.54
25	k	35	LYS	CB-CA-C	-5.42	110.31	116.54
9	N	310	ASN	CB-CA-C	-5.37	108.83	116.34
4	4	165	THR	N-CA-C	5.01	120.88	109.81

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

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Mol	Chain	Res	Type	Group
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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3328	0	3287	175	0
2	2	1655	0	1663	85	0
3	3	5275	0	5300	246	0
4	4	3098	0	3068	217	0
5	5	1726	0	1676	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	6	1241	0	1251	88	0
7	9	1414	0	1370	120	0
8	H	2528	0	2641	180	0
9	N	2723	0	2930	170	0
10	A	922	0	953	62	0
11	M	3645	0	3850	247	0
12	K	649	0	699	45	0
13	L	4456	0	4298	351	0
14	J	1188	0	1068	82	0
15	a	343	0	320	17	0
16	b	737	0	710	22	0
17	c	1000	0	997	61	0
18	d	2473	0	2461	156	0
19	e	677	0	686	30	0
20	f	909	0	947	41	0
21	g	969	0	980	45	0
22	h	757	0	771	54	0
23	i	1200	0	1169	70	0
24	X	707	0	700	35	0
24	j	684	0	682	26	0
25	k	2268	0	1995	125	0
26	l	792	0	798	55	0
27	m	626	0	635	31	0
28	n	578	0	558	40	0
29	o	1004	0	995	55	0
30	p	841	0	760	56	0
31	q	1151	0	1150	69	0
32	r	752	0	752	60	0
33	s	988	0	930	79	0
34	t	1434	0	1392	91	0
35	u	563	0	511	56	0
36	v	861	0	557	36	0
37	w	715	0	679	51	0
38	x	403	0	405	10	0
39	y	457	0	459	10	0
40	z	568	0	558	34	0
41	Z	1441	0	1416	82	0
42	Y	1403	0	1384	123	0
43	W	1155	0	1177	67	0
44	V	595	0	127	9	0
45	1	8	0	0	2	0
45	3	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10	0
48	J	51	0	82	6	0
48	o	87	0	128	8	0
49	A	47	0	71	5	0
49	M	46	0	66	2	0
49	N	46	0	66	3	0
49	o	39	0	55	3	0
50	J	79	0	108	1	0
50	L	84	0	118	13	0
50	M	82	0	114	3	0
50	i	58	0	60	1	0
51	b	1	0	0	0	0
52	d	48	0	26	8	0
53	j	34	0	40	3	0
54	X	21	0	21	8	0
All	All	63760	0	62771	3237	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 26.

All (3237) 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
37:w:68:ILE:O	37:w:72:LEU:HB2	1.51	1.10
13:L:374:ILE:O	13:L:378:LEU:HB3	1.62	0.98
31:q:134:SER:O	31:q:138:GLY:HA3	1.64	0.98
11:M:254:THR:O	11:M:258:ALA:HB2	1.64	0.97
33:s:5:ALA:N	33:s:23:THR:HG1	1.61	0.96
18:d:281:ARG:O	18:d:285:GLU:HB2	1.66	0.94
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
31:q:65:GLU:HA	42:Y:124:LEU:HD21	1.48	0.92
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
32:r:10:ARG:HD3	34:t:162:LEU:HD13	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:u:10:ARG:HD3	35:u:13:GLN:HB2	1.51	0.92
35:u:29:SER:HA	35:u:32:MET:HE3	1.50	0.91
2:2:79:ARG:HE	17:c:131:SER:HB3	1.33	0.90
25:k:149:VAL:O	25:k:153:ASN:HB2	1.71	0.90
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
37:w:40:LYS:HG2	37:w:41:ASN:H	1.34	0.89
4:4:82:LEU:HD21	6:6:96:MET:HE2	1.54	0.89
40:z:69:ILE:HD11	42:Y:18:LYS:H	1.37	0.89
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
25:k:212:PRO:O	25:k:216:GLU:HB2	1.74	0.88
37:w:74:SER:O	37:w:78:ALA:HB2	1.73	0.87
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
11:M:249:LEU:HD12	11:M:250:LEU:HG	1.57	0.86
13:L:375:ILE:O	13:L:379:ALA:HB2	1.75	0.86
32:r:13:GLN:HB2	34:t:162:LEU:HD11	1.56	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
13:L:17:MET:HE3	13:L:21:ALA:HB2	1.59	0.84
13:L:383:MET:HE3	13:L:388:GLY:H	1.42	0.84
22:h:67:ILE:HG22	22:h:68:VAL:HG23	1.59	0.84
11:M:254:THR:O	11:M:258:ALA:CB	2.26	0.84
18:d:235:ARG:HB3	18:d:237:LEU:HD13	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
35:u:66:ILE:HG13	35:u:67:PRO:HD3	1.61	0.83
13:L:366:MET:HE3	13:L:369:THR:HG21	1.59	0.83
28:n:44:TRP:HB3	34:t:37:ARG:HH22	1.43	0.82
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
3:3:36:GLN:HE22	17:c:48:GLY:HA2	1.44	0.82
14:J:16:GLY:O	14:J:20:PHE:HB2	1.79	0.81
5:5:71:GLN:HE21	20:f:82:GLN:HE22	1.26	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
9:N:79:MET:HA	12:K:47:MET:HE1	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
32:r:117:PRO:HG2	32:r:118:PRO:HD3	1.63	0.80
3:3:252:PRO:HB3	3:3:263:ILE:HB	1.64	0.80
28:n:74:PHE:HA	28:n:77:PHE:HB3	1.62	0.80
3:3:126:ASP:HA	4:4:347:HIS:HE1	1.46	0.80
29:o:86:ARG:HH22	42:Y:165:ARG:HD3	1.46	0.80
1:1:403:THR:OG1	45:1:500:SF4:S4	2.39	0.80
27:m:66:PRO:HD3	27:m:73:GLN:HB2	1.62	0.80
35:u:33:TRP:HA	35:u:36:ILE:HG22	1.64	0.79
40:z:66:LEU:O	42:Y:74:LYS:NZ	2.15	0.79
30:p:35:ARG:O	30:p:39:ARG:HB2	1.82	0.79
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
25:k:302:ARG:O	25:k:306:ALA:HB3	1.81	0.79
29:o:30:ARG:NH1	42:Y:171:MET:O	2.16	0.79
13:L:55:ILE:HG13	33:s:73:PHE:HE1	1.47	0.78
7:9:62:ARG:NH1	7:9:119:CYS:O	2.16	0.78
25:k:57:HIS:HA	25:k:60:ASP:HB2	1.65	0.78
33:s:106:ARG:HH12	35:u:59:TRP:HB3	1.48	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
30:p:66:ARG:NH1	36:v:23:ALA:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:u:34:PHE:O	35:u:38:TRP:HB2	1.83	0.78
11:M:220:HIS:HE2	11:M:228:SER:HG	1.31	0.78
25:k:37:LYS:O	25:k:41:GLU:HB2	1.83	0.78
4:4:64:LEU:HD22	4:4:66:MET:HE2	1.65	0.78
23:i:132:LYS:HG2	23:i:133:LYS:H	1.49	0.77
3:3:522:LEU:HB3	3:3:543:ILE:HG22	1.67	0.77
18:d:106:PHE:O	18:d:148:ASN:ND2	2.17	0.77
9:N:341:PRO:HB2	29:o:79:GLN:HE22	1.48	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
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
16:b:52:VAL:HG12	16:b:54:SER:H	1.49	0.77
13:L:441:ILE:HD13	35:u:15:PRO:HB3	1.68	0.76
16:b:31:ARG:HH22	18:d:69:ILE:HD11	1.50	0.76
25:k:31:ILE:HG22	25:k:126:ARG:HH22	1.50	0.76
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.51	0.76
23:i:129:THR:HG22	23:i:130:THR:H	1.49	0.76
29:o:34:ILE:HG22	29:o:68:PHE:HB3	1.66	0.76
33:s:19:LEU:HB2	41:Z:122:GLN:HE22	1.51	0.76
37:w:75:THR:HG21	43:W:36:VAL:HG11	1.66	0.76
1:1:301:GLY:H	1:1:330:GLY:HA3	1.50	0.76
25:k:240:TYR:O	25:k:244:ASP:CB	2.34	0.76
32:r:84:TYR:O	32:r:88:HIS:CB	2.34	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
32:r:115:VAL:HG13	32:r:116:ILE:HG23	1.68	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
25:k:255:LYS:O	25:k:259:LEU:CB	2.34	0.76
7:9:18:THR:HA	27:m:12:TRP:HH2	1.49	0.75
13:L:286:LEU:HD11	13:L:414:VAL:HG13	1.69	0.75
32:r:84:TYR:O	32:r:88:HIS:HB2	1.86	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
25:k:149:VAL:O	25:k:153:ASN:CB	2.35	0.75
21:g:40:ARG:NH1	24:j:52:MET:SD	2.60	0.75
14:J:161:LEU:O	14:J:164:GLY:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:37:LYS:HA	43:W:133:ILE:HD11	1.69	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
7:9:152:GLU:OE1	23:i:127:TYR:OH	2.04	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
5:5:69:ASN:OD1	22:h:95:SER:OG	2.05	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
16:b:11:VAL:HG12	16:b:17:VAL:HB	1.68	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:405:ASN:HD21	36:v:115:MET:HA	1.53	0.74
13:L:83:ASP:OD2	13:L:262:ARG:NH1	2.20	0.73
33:s:110:ARG:NH1	35:u:62:GLU:OE1	2.19	0.73
24:X:37:MET:O	24:X:41:GLY:N	2.21	0.73
1:1:132:ARG:NH2	15:a:64:PRO:O	2.21	0.73
2:2:151:ALA:HB3	2:2:163:ASP:HA	1.69	0.73
31:q:142:TYR:OH	40:z:37:ARG:O	2.04	0.73
3:3:43:HIS:O	17:c:116:LYS:NZ	2.20	0.73
3:3:45:ARG:HD3	17:c:114:LYS:HZ1	1.51	0.73
28:n:50:TRP:NE1	35:u:12:ARG:O	2.21	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
23:i:43:LYS:NZ	23:i:85:GLU:OE2	2.19	0.73
11:M:44:GLN:NE2	11:M:59:ASP:O	2.21	0.73
3:3:40:PHE:HB2	3:3:52:CYS:HB2	1.71	0.73
3:3:318:ILE:HG22	3:3:522:LEU:HD11	1.71	0.73
11:M:54:LEU:HA	43:W:93:ILE:HD12	1.69	0.73
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
34:t:172:ARG:HH21	43:W:8:LEU:HD13	1.52	0.72
41:Z:30:THR:HA	41:Z:33:THR:HG22	1.69	0.72
13:L:385:PHE:HB3	35:u:36:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:105:ARG:NH1	45:6:300:SF4:S3	2.62	0.72
5:5:68:SER:HA	20:f:82:GLN:HE21	1.52	0.72
5:5:202:PRO:HA	17:c:50:ASN:HB3	1.70	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
37:w:77:VAL:HA	37:w:80:LEU:HD23	1.69	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
25:k:302:ARG:O	25:k:306:ALA:CB	2.37	0.72
34:t:163:PRO:HG2	34:t:164:PRO:HD3	1.72	0.72
3:3:584:LYS:NZ	17:c:106:GLU:OE2	2.22	0.72
11:M:122:PHE:O	11:M:125:THR:OG1	2.08	0.72
30:p:29:ARG:O	30:p:33:ALA:HB3	1.90	0.72
13:L:22:ILE:O	43:W:26:ARG:NH2	2.22	0.72
13:L:177:ILE:O	13:L:180:ILE:HG22	1.89	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
34:t:44:ARG:O	34:t:48:ASP:HB2	1.90	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
9:N:254:LEU:HD23	9:N:256:PRO:HD2	1.70	0.71
11:M:114:GLU:HG2	11:M:175:ASN:HA	1.71	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:81:LYS:NZ	13:L:83:ASP:OD1	2.20	0.71
13:L:232:TRP:CD1	13:L:233:LEU:HD12	2.21	0.71
18:d:193:LEU:HG	18:d:194:ILE:H	1.56	0.71
11:M:387:SER:O	30:p:111:LYS:NZ	2.22	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
25:k:228:ALA:O	25:k:232:GLU:CB	2.39	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
8:H:93:TYR:OH	40:z:35:GLU:OE2	2.07	0.71
13:L:342:CYS:SG	13:L:369:THR:OG1	2.48	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:310:ASN:HA	25:k:294:GLN:HA	1.71	0.71
9:N:22:ILE:HD11	26:l:5:VAL:H	1.56	0.71
19:e:23:CYS:HA	19:e:57:CYS:HA	1.73	0.71
24:X:15:VAL:HG22	24:X:54:MET:HE2	1.73	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
18:d:30:LEU:HD22	18:d:94:LEU:HD21	1.71	0.70
25:k:88:SER:O	25:k:92:ASN:ND2	2.24	0.70
3:3:259:ASN:H	3:3:390:LEU:HD21	1.57	0.70
35:u:64:LEU:HB3	35:u:67:PRO:HD2	1.72	0.70
1:1:362:CYS:N	45:1:500:SF4:S2	2.63	0.70
11:M:388:TRP:O	30:p:108:ARG:NH2	2.24	0.70
11:M:459:TYR:O	41:Z:96:LYS:NZ	2.24	0.70
18:d:26:ALA:HA	18:d:31:GLY:HA3	1.74	0.70
18:d:179:LEU:HD21	18:d:318:LEU:HD11	1.73	0.70
33:s:21:MET:HB3	33:s:22:PRO:HD2	1.74	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
11:M:78:MET:HE3	11:M:432:ARG:HG3	1.73	0.70
25:k:26:THR:HG22	25:k:124:LEU:HB3	1.73	0.70
3:3:362:TYR:OH	3:3:500:VAL:O	2.10	0.70
14:J:125:TRP:HH2	26:l:79:LYS:HB3	1.55	0.70
3:3:333:ASP:O	3:3:337:ARG:HB2	1.92	0.69
40:z:34:ARG:HD2	42:Y:90:TYR:HA	1.73	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
23:i:87:HIS:O	23:i:91:HIS:ND1	2.23	0.69
34:t:138:GLN:HE22	34:t:156:ALA:HA	1.57	0.69
1:1:300:GLY:H	1:1:334:VAL:HG12	1.57	0.69
8:H:312:SER:OG	27:m:37:TYR:O	2.10	0.69
25:k:281:GLU:O	25:k:285:GLY:N	2.25	0.69
13:L:282:ALA:HB1	13:L:411:MET:HE3	1.73	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
19:e:56:GLU:HG2	19:e:57:CYS:H	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:140:THR:C	11:M:142:ARG:H	2.00	0.69
41:Z:27:ASN:HB3	41:Z:30:THR:OG1	1.92	0.69
24:X:81:ALA:HA	24:X:86:VAL:HG21	1.75	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
19:e:63:LYS:HA	19:e:78:LEU:H	1.57	0.69
13:L:272:PHE:O	13:L:275:SER:OG	2.08	0.69
25:k:236:GLU:O	25:k:240:TYR:CB	2.41	0.69
11:M:44:GLN:NE2	11:M:63:THR:OG1	2.25	0.69
13:L:494:THR:O	13:L:498:PHE:HB2	1.92	0.69
25:k:141:GLN:HB2	25:k:198:TYR:HE1	1.58	0.69
34:t:88:THR:O	34:t:92:ARG:NH1	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
4:4:246:THR:HG23	20:f:12:GLY:HA3	1.74	0.68
4:4:108:TYR:CG	6:6:54:CYS:HB3	2.27	0.68
13:L:56:HIS:HB3	33:s:73:PHE:CD1	2.28	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
18:d:133:SER:OG	18:d:153:GLU:OE2	2.12	0.68
32:r:27:LEU:HD12	32:r:29:PRO:HD2	1.75	0.68
8:H:209:SER:HA	8:H:212:ASN:HB3	1.75	0.68
15:a:70:ARG:NH1	17:c:125:ASN:O	2.26	0.68
23:i:60:ARG:NH2	23:i:89:TRP:O	2.25	0.68
30:p:100:TRP:HA	30:p:103:VAL:HG22	1.73	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
17:c:14:ASP:HB2	21:g:18:PRO:HG2	1.75	0.68
25:k:30:ASN:HD22	25:k:203:GLU:HB2	1.59	0.68
25:k:179:VAL:HA	25:k:182:ARG:HB3	1.76	0.68
34:t:103:LEU:HG	34:t:121:ARG:HH12	1.57	0.68
3:3:453:LEU:HB3	3:3:492:ILE:HG22	1.73	0.68
30:p:45:GLU:O	30:p:49:GLN:HB2	1.93	0.68
37:w:113:PHE:O	41:Z:158:GLN:NE2	2.25	0.68
5:5:209:TYR:OH	22:h:62:ALA:O	2.09	0.68
17:c:52:THR:HG22	17:c:53:LYS:H	1.58	0.68
5:5:154:ASP:HB3	5:5:157:PHE:HB2	1.74	0.68
18:d:201:VAL:H	18:d:290:THR:HG23	1.58	0.68
19:e:24:GLN:O	19:e:33:ARG:NH1	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:M:259:TYR:OH	30:p:101:TYR:O	2.11	0.68
13:L:365:ALA:HA	35:u:17:LEU:HD13	1.76	0.68
18:d:198:LYS:HG3	18:d:199:LYS:HG3	1.76	0.68
8:H:195:ARG:HD2	8:H:274:ARG:HB2	1.75	0.68
18:d:20:VAL:HB	18:d:89:ASN:H	1.58	0.68
3:3:315:VAL:HG23	3:3:521:MET:HB2	1.75	0.67
13:L:159:TYR:HB2	34:t:95:CYS:HB3	1.74	0.67
18:d:36:ASN:O	18:d:40:ARG:HB2	1.94	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
8:H:312:SER:HA	27:m:41:SER:HB3	1.75	0.67
11:M:24:TRP:HD1	37:w:49:LYS:HZ2	1.40	0.67
11:M:232:ALA:HB3	11:M:327:PHE:HE2	1.60	0.67
13:L:374:ILE:HA	13:L:377:SER:HG	1.59	0.67
31:q:77:GLU:OE2	31:q:80:ARG:NH2	2.27	0.67
4:4:273:GLN:OE1	5:5:104:ARG:NH1	2.25	0.67
13:L:1:MET:HB2	13:L:61:MET:HE1	1.76	0.67
25:k:56:ILE:HD11	25:k:77:CYS:HB2	1.76	0.67
3:3:159:CYS:HB2	3:3:199:ILE:HD11	1.77	0.67
13:L:466:PHE:O	13:L:469:SER:OG	2.12	0.67
18:d:34:LEU:HD11	18:d:214:ILE:HG21	1.77	0.67
34:t:51:LYS:NZ	54:X:401:PNS:O26	2.27	0.67
36:v:131:LYS:HG2	36:v:132:GLN:H	1.58	0.67
8:H:216:ALA:O	8:H:220:PHE:N	2.27	0.67
49:M:501:PC1:H152	49:M:501:PC1:H2	1.76	0.67
13:L:346:ILE:HD11	13:L:373:LEU:HD11	1.75	0.67
18:d:19:ILE:HA	18:d:89:ASN:HD22	1.60	0.67
36:v:124:THR:HG22	36:v:125:TYR:H	1.59	0.67
1:1:111:ILE:HD11	1:1:149:LEU:HD22	1.78	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
10:A:64:LEU:HD11	14:J:168:ILE:HD12	1.77	0.66
11:M:385:THR:HG21	11:M:396:MET:HE3	1.76	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
23:i:130:THR:HG22	23:i:131:ARG:H	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:313:GLY:HA2	29:o:51:ARG:HA	1.77	0.66
3:3:601:ARG:NH1	3:3:611:LEU:O	2.29	0.66
18:d:321:HIS:CG	18:d:322:ARG:H	2.13	0.66
32:r:69:PHE:O	32:r:72:THR:OG1	2.09	0.66
9:N:215:MET:HG3	9:N:219:PHE:HE2	1.60	0.66
13:L:482:MET:HE2	13:L:487:LYS:HB2	1.78	0.66
24:j:12:LYS:HE3	24:j:32:VAL:HG11	1.78	0.66
37:w:105:LEU:HD12	37:w:106:PRO:HD2	1.77	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
11:M:376:ILE:HG23	11:M:380:PHE:HE2	1.58	0.66
11:M:388:TRP:C	30:p:108:ARG:HH22	2.02	0.66
13:L:383:MET:HG3	13:L:389:PHE:N	2.10	0.66
3:3:106:PRO:O	7:9:104:ARG:NH2	2.29	0.66
49:N:401:PC1:H2E2	48:o:203:3PE:H2H1	1.78	0.66
11:M:339:SER:OG	11:M:341:THR:OG1	2.11	0.66
21:g:36:ARG:HH22	24:j:64:ASP:HA	1.61	0.66
29:o:54:LEU:HD11	48:o:202:3PE:H351	1.76	0.66
33:s:5:ALA:N	33:s:23:THR:OG1	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
13:L:237:MET:HE1	13:L:248:HIS:NE2	2.10	0.66
27:m:57:ARG:O	27:m:61:ASN:ND2	2.29	0.66
10:A:56:PHE:HB2	14:J:74:MET:HE1	1.78	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
8:H:316:PRO:HG3	31:q:56:ARG:HB3	1.78	0.66
9:N:19:ILE:HA	9:N:22:ILE:HG22	1.77	0.65
16:b:77:LYS:HD2	16:b:80:LYS:HE2	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
11:M:403:THR:HA	11:M:406:TYR:CE2	2.32	0.65
13:L:6:SER:O	13:L:9:LEU:HB2	1.97	0.65
34:t:50:HIS:NE2	54:X:401:PNS:S44	2.68	0.65
35:u:10:ARG:HH12	35:u:16:GLN:HE21	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:o:30:ARG:HE	29:o:76:LEU:HD22	1.61	0.65
32:r:2:GLY:O	24:X:69:LYS:HB2	1.95	0.65
34:t:104:ASP:OD1	34:t:121:ARG:NH2	2.30	0.65
13:L:568:LEU:O	13:L:572:LYS:N	2.28	0.65
18:d:319:ARG:HH12	21:g:50:GLN:HB3	1.62	0.65
30:p:66:ARG:HH12	36:v:24:ALA:HB2	1.61	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
16:b:83:THR:HG22	16:b:90:GLN:HG3	1.78	0.65
33:s:26:PRO:HG3	33:s:56:ASP:HA	1.78	0.65
40:z:47:LEU:HD23	42:Y:21:SER:HB2	1.78	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
3:3:226:GLU:HB2	17:c:36:ARG:HH22	1.61	0.65
5:5:179:GLU:HG3	18:d:36:ASN:ND2	2.11	0.65
9:N:18:ILE:HG12	49:o:201:PC1:H3E2	1.78	0.65
9:N:266:ILE:O	9:N:270:MET:HB2	1.96	0.65
11:M:12:MET:O	11:M:15:THR:OG1	2.10	0.65
2:2:131:THR:HG22	2:2:138:THR:HG22	1.79	0.65
4:4:227:GLU:OE2	31:q:27:ARG:NH2	2.30	0.65
18:d:19:ILE:O	18:d:43:SER:OG	2.13	0.65
25:k:41:GLU:OE2	25:k:45:LYS:NZ	2.29	0.65
28:n:28:LEU:HG	28:n:52:TYR:HE2	1.60	0.65
13:L:374:ILE:O	13:L:378:LEU:CB	2.40	0.65
21:g:118:LEU:O	21:g:122:TYR:HB2	1.97	0.65
33:s:106:ARG:HH22	35:u:59:TRP:CD1	2.15	0.64
33:s:115:GLU:O	33:s:119:ALA:CB	2.45	0.64
3:3:258:ILE:HD11	3:3:581:GLN:HE22	1.63	0.64
18:d:91:VAL:HG13	18:d:129:PHE:HD1	1.61	0.64
18:d:171:ILE:HG12	52:d:401:NDP:H42N	1.79	0.64
20:f:20:HIS:NE2	20:f:62:PRO:O	2.30	0.64
42:Y:166:LEU:O	43:W:104:ARG:NH2	2.30	0.64
6:6:165:LYS:NZ	23:i:76:ASP:O	2.29	0.64
31:q:70:LEU:HD21	42:Y:24:LEU:HG	1.79	0.64
37:w:68:ILE:HG23	37:w:72:LEU:HD22	1.80	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
14:J:145:ALA:HB2	26:l:25:PRO:HG3	1.79	0.64
33:s:17:GLU:OE1	41:Z:121:ARG:NH1	2.30	0.64
4:4:196:PRO:HG3	4:4:356:TYR:OH	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:30:ALA:HB1	22:h:68:VAL:HG11	1.79	0.64
13:L:361:GLY:O	13:L:364:LYS:NZ	2.30	0.64
13:L:386:LEU:HD12	35:u:36:ILE:HD13	1.80	0.64
18:d:108:ASP:HA	18:d:112:LYS:H	1.62	0.64
19:e:64:LEU:HD23	19:e:78:LEU:HD11	1.79	0.64
11:M:425:ASN:OD1	11:M:426:ILE:N	2.30	0.64
22:h:26:ARG:HA	23:i:56:PHE:HB3	1.79	0.64
37:w:80:LEU:HD12	37:w:81:PRO:O	1.97	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
17:c:25:VAL:HB	17:c:26:PRO:HD2	1.78	0.64
36:v:111:PHE:O	36:v:114:PHE:N	2.31	0.64
3:3:69:CYS:SG	3:3:70:ALA:N	2.71	0.64
7:9:65:HIS:HD2	7:9:113:MET:HE1	1.63	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
25:k:32:CYS:H	25:k:35:LYS:HE2	1.62	0.64
28:n:46:ARG:NH1	24:X:23:ASP:OD1	2.31	0.64
33:s:106:ARG:HH22	35:u:59:TRP:HD1	1.46	0.64
34:t:12:GLN:HG3	34:t:13:GLN:H	1.63	0.64
34:t:33:ARG:O	34:t:37:ARG:HG2	1.97	0.64
7:9:27:TRP:CZ2	48:9:501:3PE:H231	2.32	0.64
33:s:17:GLU:HB3	33:s:18:PRO:HD3	1.80	0.64
4:4:204:PRO:HD3	7:9:60:ARG:HH22	1.62	0.64
4:4:221:ARG:HH21	22:h:23:LEU:HA	1.63	0.64
34:t:102:CYS:O	34:t:103:LEU:HB3	1.97	0.64
1:1:20:ARG:NH1	1:1:269:GLU:O	2.31	0.63
1:1:135:TYR:HE1	1:1:176:PHE:HD2	1.47	0.63
30:p:39:ARG:HG3	34:t:148:PRO:HB3	1.80	0.63
39:y:38:ARG:HD3	39:y:54:VAL:HG23	1.80	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
17:c:42:ARG:HD2	17:c:48:GLY:H	1.63	0.63
25:k:136:GLU:O	25:k:140:ARG:HB2	1.99	0.63
9:N:287:LEU:HD23	9:N:290:LEU:HD12	1.80	0.63
25:k:129:TYR:OH	25:k:164:LEU:O	2.15	0.63
28:n:35:LEU:HD21	34:t:38:TYR:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:71:GLN:NE2	20:f:82:GLN:HE22	1.97	0.63
9:N:179:MET:HE1	9:N:251:MET:HE1	1.79	0.63
9:N:345:ILE:O	29:o:78:ARG:NH1	2.32	0.63
13:L:23:ASN:O	43:W:26:ARG:NH1	2.31	0.63
13:L:569:ALA:O	13:L:573:MET:N	2.31	0.63
18:d:281:ARG:HA	18:d:284:VAL:HG22	1.81	0.63
19:e:78:LEU:HD22	19:e:86:VAL:HG22	1.79	0.63
3:3:283:MET:HE2	3:3:291:LEU:HG	1.81	0.63
6:6:34:ASP:O	6:6:38:ASN:HB2	1.98	0.63
11:M:370:PRO:HA	11:M:375:LEU:HD22	1.80	0.63
13:L:81:LYS:HD3	13:L:135:ASN:HD22	1.62	0.63
13:L:460:GLY:O	13:L:464:ALA:N	2.30	0.63
20:f:30:ILE:O	20:f:34:LEU:HB3	1.98	0.63
34:t:34:ASP:OD1	34:t:35:LYS:N	2.32	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
26:l:92:THR:HB	26:l:94:PRO:HD2	1.81	0.63
1:1:429:ARG:HA	1:1:432:ARG:HG2	1.81	0.62
18:d:164:THR:OG1	18:d:223:ALA:O	2.17	0.62
24:j:56:ASP:OD1	24:j:57:GLU:N	2.32	0.62
29:o:108:THR:OG1	41:Z:74:THR:O	2.14	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
8:H:302:MET:HE3	10:A:92:LEU:HD22	1.80	0.62
25:k:129:TYR:HE2	25:k:166:PRO:HD2	1.64	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
2:2:40:GLU:HB3	15:a:67:SER:HA	1.81	0.62
31:q:5:VAL:HG12	31:q:6:LYS:H	1.64	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:30:HIS:HB3	39:y:16:VAL:HG21	1.80	0.62
11:M:342:MET:HG3	11:M:414:THR:HG22	1.81	0.62
17:c:33:ARG:HE	17:c:62:ARG:HE	1.47	0.62
18:d:115:GLN:NE2	18:d:155:GLU:OE1	2.22	0.62
18:d:212:LYS:HA	18:d:215:ILE:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:d:92:ILE:HG22	18:d:130:ILE:HB	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
3:3:357:ASP:OD2	19:e:40:TYR:OH	2.17	0.62
4:4:263:SER:O	4:4:265:ILE:HG22	2.00	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
2:2:53:LEU:HD12	15:a:52:LEU:HD13	1.82	0.62
4:4:202:ASP:HB3	4:4:323:ILE:HG12	1.81	0.62
17:c:33:ARG:NH1	17:c:77:ASP:OD1	2.33	0.62
29:o:116:PHE:CD2	41:Z:156:ALA:HB1	2.34	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:70:MET:HE1	14:J:27:ILE:HG13	1.82	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
9:N:144:GLN:HE21	26:l:2:PHE:HB2	1.65	0.62
10:A:54:LYS:NZ	10:A:111:LEU:O	2.27	0.62
11:M:4:TYR:HB3	11:M:70:MET:HE1	1.80	0.62
11:M:220:HIS:NE2	11:M:228:SER:OG	2.29	0.62
25:k:212:PRO:O	25:k:216:GLU:CB	2.47	0.62
34:t:132:TRP:HA	34:t:135:GLU:HB3	1.82	0.62
9:N:255:PRO:HA	9:N:260:PHE:CG	2.34	0.61
20:f:30:ILE:O	20:f:34:LEU:CB	2.47	0.61
31:q:143:THR:HA	40:z:45:TRP:HZ3	1.63	0.61
34:t:134:ARG:NH1	34:t:161:ASP:OD1	2.33	0.61
3:3:45:ARG:HD3	17:c:114:LYS:NZ	2.15	0.61
4:4:82:LEU:HA	6:6:95:LYS:HD3	1.81	0.61
4:4:228:MET:O	4:4:232:ASN:ND2	2.32	0.61
13:L:11:THR:HG22	13:L:129:LEU:HD21	1.82	0.61
32:r:10:ARG:NH2	34:t:154:PRO:O	2.30	0.61
34:t:135:GLU:HG3	34:t:163:PRO:HB2	1.81	0.61
44:V:35:UNK:O	44:V:39:UNK:CB	2.48	0.61
4:4:76:CYS:SG	4:4:406:SER:OG	2.58	0.61
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.13	0.61
25:k:37:LYS:O	25:k:41:GLU:CB	2.48	0.61
3:3:591:GLY:HA2	18:d:6:ILE:HG12	1.82	0.61
8:H:258:ASN:OD1	8:H:262:LYS:NZ	2.34	0.61
9:N:345:ILE:HD11	29:o:78:ARG:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:o:113:PHE:HB2	37:w:121:PRO:HG2	1.83	0.61
34:t:118:PHE:HA	34:t:121:ARG:HB3	1.82	0.61
8:H:195:ARG:HD2	8:H:274:ARG:HD2	1.81	0.61
11:M:86:LYS:O	11:M:87:GLU:HG3	2.00	0.61
13:L:595:ILE:O	13:L:598:SER:O	2.17	0.61
29:o:106:LYS:O	41:Z:77:HIS:ND1	2.33	0.61
4:4:80:ILE:HG13	4:4:81:GLY:H	1.66	0.61
15:a:38:TYR:CZ	15:a:40:ASN:HB2	2.35	0.61
28:n:18:TYR:CD2	28:n:19:LYS:HB2	2.35	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
21:g:44:ASN:O	21:g:48:LEU:HB2	2.00	0.61
32:r:85:LEU:HA	32:r:88:HIS:HB3	1.83	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
17:c:33:ARG:HH22	17:c:77:ASP:HA	1.64	0.61
37:w:85:MET:HG3	37:w:88:TRP:HB3	1.83	0.61
1:1:261:HIS:NE2	2:2:110:LEU:O	2.26	0.61
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:202:PHE:HB3	41:Z:113:GLN:HE22	1.66	0.61
13:L:518:ASN:O	13:L:522:PHE:N	2.34	0.61
18:d:228:PHE:HB3	18:d:298:PRO:HD2	1.82	0.61
25:k:28:ASP:N	25:k:170:ILE:O	2.34	0.61
42:Y:158:LYS:HB3	42:Y:159:PRO:HD2	1.82	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
14:J:134:GLY:HA2	40:z:43:TYR:HB2	1.84	0.60
42:Y:45:CYS:HA	42:Y:134:ARG:HH21	1.66	0.60
24:X:55:GLU:O	24:X:59:GLY:N	2.24	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
25:k:67:LYS:HB3	25:k:68:PRO:HD2	1.83	0.60
27:m:66:PRO:HG2	27:m:71:ASP:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:52:ASP:HB3	34:t:132:TRP:CZ2	2.36	0.60
13:L:12:LEU:HD12	32:r:81:ILE:HD11	1.82	0.60
25:k:148:CYS:O	25:k:152:TYR:HB3	2.02	0.60
33:s:108:LEU:HD22	33:s:112:LYS:HE3	1.83	0.60
36:v:126:GLN:HA	36:v:128:VAL:HG13	1.83	0.60
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.83	0.60
50:M:502:CDL:H572	50:M:502:CDL:H161	1.81	0.60
13:L:9:LEU:HD21	32:r:78:VAL:HG22	1.83	0.60
13:L:226:GLN:HE22	13:L:281:GLY:HA2	1.64	0.60
14:J:94:ILE:O	14:J:98:LEU:CB	2.49	0.60
25:k:61:SER:HB3	25:k:68:PRO:HD3	1.84	0.60
32:r:22:LEU:HD12	32:r:25:GLN:HB3	1.82	0.60
34:t:30:CYS:SG	34:t:31:VAL:N	2.68	0.60
37:w:70:LEU:O	37:w:74:SER:CB	2.49	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
18:d:194:ILE:HG23	18:d:197:GLY:HA2	1.82	0.60
21:g:46:VAL:HG23	21:g:51:LEU:HB2	1.83	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
11:M:59:ASP:CG	11:M:245:ARG:HH22	2.09	0.60
18:d:107:GLU:HA	18:d:148:ASN:HD21	1.65	0.60
18:d:135:LEU:HA	18:d:167:LYS:HB3	1.83	0.60
18:d:280:THR:O	18:d:283:LYS:N	2.35	0.60
3:3:362:TYR:OH	3:3:503:LEU:HB2	2.02	0.60
4:4:84:HIS:H	6:6:93:THR:HG21	1.66	0.60
6:6:107:MET:HB3	6:6:111:ARG:HE	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
26:l:48:SER:HA	26:l:51:ALA:HB3	1.82	0.60
33:s:98:MET:HE1	36:v:123:PRO:HG3	1.84	0.60
43:W:90:THR:HA	43:W:93:ILE:HG22	1.82	0.60
3:3:296:TRP:HE1	21:g:121:PHE:HE2	1.47	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
13:L:441:ILE:HD11	35:u:10:ARG:HB3	1.83	0.60
19:e:54:ILE:O	19:e:55:ARG:NH1	2.29	0.60
40:z:31:ASN:ND2	40:z:36:LYS:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:25:GLN:HE21	43:W:9:PHE:HB3	1.66	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
18:d:157:ARG:HH22	18:d:227:THR:HB	1.67	0.60
37:w:49:LYS:HG2	37:w:50:ASP:H	1.67	0.60
9:N:93:MET:HE3	14:J:117:PHE:HA	1.84	0.59
13:L:437:PHE:HB2	13:L:438:PRO:HD2	1.82	0.59
25:k:71:VAL:O	25:k:75:GLY:N	2.22	0.59
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
8:H:107:ALA:O	8:H:110:SER:OG	2.14	0.59
13:L:69:LEU:HD13	13:L:71:ILE:HG23	1.83	0.59
18:d:59:LEU:HD12	18:d:62:MET:HE3	1.84	0.59
22:h:26:ARG:HB3	23:i:55:PHE:HB2	1.84	0.59
25:k:181:SER:O	25:k:184:GLN:HB3	2.02	0.59
35:u:64:LEU:HD23	35:u:67:PRO:HG2	1.85	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
25:k:213:GLU:HA	25:k:216:GLU:HB3	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
9:N:180:ALA:O	9:N:183:SER:OG	2.11	0.59
11:M:60:SER:OG	11:M:61:LEU:N	2.35	0.59
11:M:119:TYR:O	11:M:122:PHE:HB3	2.02	0.59
16:b:55:ARG:NH2	16:b:76:ASP:OD1	2.35	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
22:h:26:ARG:HB3	23:i:56:PHE:H	1.68	0.59
41:Z:145:LEU:HD13	41:Z:149:TYR:HB3	1.85	0.59
9:N:72:MET:HE3	9:N:76:ILE:HD11	1.83	0.59
9:N:91:ASN:OD1	9:N:93:MET:N	2.35	0.59
14:J:166:VAL:O	14:J:170:GLU:HB2	2.02	0.59
18:d:95:VAL:O	52:d:401:NDP:O3D	2.21	0.59
19:e:15:LEU:HD21	19:e:93:VAL:HG12	1.84	0.59
33:s:24:PHE:HE1	33:s:42:GLN:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:z:18:ILE:HA	40:z:21:MET:HE3	1.85	0.59
6:6:46:TRP:N	6:6:84:ASP:OD2	2.35	0.59
11:M:75:LEU:HD21	11:M:440:HIS:CE1	2.38	0.59
13:L:43:ALA:O	13:L:47:SER:CB	2.51	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
24:j:58:PHE:CE2	24:j:80:ILE:HG21	2.38	0.59
28:n:21:TRP:CH2	28:n:50:TRP:HD1	2.21	0.59
1:1:233:THR:O	1:1:237:ARG:HG2	2.01	0.59
3:3:277:GLN:O	23:i:137:TRP:HB2	2.02	0.59
5:5:68:SER:HA	20:f:82:GLN:NE2	2.17	0.59
11:M:376:ILE:HG23	11:M:380:PHE:CE2	2.38	0.59
37:w:112:CYS:HB3	41:Z:141:ARG:HD2	1.85	0.59
9:N:298:TYR:HB3	11:M:147:LEU:HD22	1.84	0.58
11:M:397:GLY:HA3	13:L:180:ILE:HG13	1.85	0.58
20:f:8:THR:OG1	20:f:75:GLN:OE1	2.21	0.58
26:l:82:ARG:HH21	31:q:126:LEU:HD23	1.67	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
18:d:278:TRP:CG	18:d:279:THR:H	2.20	0.58
25:k:303:LYS:O	25:k:307:GLY:N	2.36	0.58
1:1:236:ARG:O	2:2:214:GLN:NE2	2.36	0.58
25:k:57:HIS:O	25:k:61:SER:OG	2.15	0.58
1:1:370:ASP:CG	3:3:179:ASN:HD21	2.11	0.58
7:9:160:LYS:HD2	7:9:161:TRP:HZ3	1.68	0.58
13:L:409:LEU:O	13:L:412:THR:OG1	2.20	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
9:N:249:LEU:HD11	9:N:297:THR:HG21	1.85	0.58
10:A:90:MET:HE1	14:J:151:THR:HB	1.85	0.58
11:M:2:LEU:HD22	49:M:501:PC1:H143	1.85	0.58
11:M:135:ARG:HD2	11:M:136:TRP:HZ3	1.68	0.58
13:L:40:ILE:HG13	13:L:101:MET:SD	2.44	0.58
18:d:48:PRO:HB2	18:d:73:TRP:CD1	2.38	0.58
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
18:d:134:HIS:ND1	18:d:135:LEU:O	2.35	0.58
12:K:1:MET:HE1	26:l:67:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:402:SER:HA	36:v:121:THR:HG22	1.84	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
35:u:51:PHE:CD1	35:u:52:PRO:HD2	2.39	0.58
37:w:80:LEU:HB2	37:w:81:PRO:HD2	1.86	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
9:N:1:MET:SD	9:N:46:LYS:NZ	2.71	0.58
9:N:325:LEU:HD13	48:o:203:3PE:H221	1.86	0.58
26:l:18:THR:HG22	26:l:19:ILE:HG23	1.86	0.58
32:r:78:VAL:HG12	41:Z:40:VAL:HG11	1.86	0.58
41:Z:8:VAL:O	41:Z:108:ARG:NH2	2.34	0.58
3:3:118:ASP:OD2	17:c:46:GLN:NE2	2.37	0.58
11:M:328:CYS:SG	11:M:436:LEU:HD23	2.43	0.58
25:k:69:LEU:HB2	25:k:70:PRO:HD2	1.86	0.58
25:k:77:CYS:HA	25:k:96:LEU:HG	1.86	0.58
31:q:42:LEU:HB3	31:q:46:TYR:HE2	1.67	0.58
31:q:114:ARG:HB2	42:Y:142:HIS:CE1	2.39	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
5:5:100:ARG:O	22:h:100:ILE:HD12	2.04	0.57
6:6:158:TYR:OH	23:i:116:ASN:ND2	2.34	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
26:l:46:ILE:HG22	26:l:47:GLY:H	1.69	0.57
35:u:37:LEU:HA	35:u:40:PHE:HB3	1.84	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
13:L:420:ALA:O	13:L:423:SER:OG	2.15	0.57
18:d:50:ARG:HH22	52:d:401:NDP:C6A	2.16	0.57
23:i:39:VAL:HG23	23:i:40:GLY:H	1.69	0.57
31:q:100:VAL:O	31:q:102:GLY:N	2.36	0.57
32:r:10:ARG:NH1	34:t:153:LEU:HD13	2.19	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
24:j:43:ASP:OD1	24:j:44:SER:N	2.36	0.57
35:u:11:TYR:OH	35:u:12:ARG:NH2	2.37	0.57
42:Y:165:ARG:NH2	43:W:103:LEU:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:325:MET:SD	11:M:441:MET:HG2	2.45	0.57
13:L:310:LEU:HA	13:L:313:MET:HE3	1.85	0.57
15:a:41:LEU:HG	15:a:44:HIS:HD2	1.69	0.57
25:k:210:PHE:O	25:k:214:MET:N	2.27	0.57
34:t:89:SER:HA	34:t:92:ARG:HG3	1.87	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
11:M:225:ILE:HD13	11:M:331:ASN:HB2	1.87	0.57
11:M:389:SER:OG	30:p:108:ARG:NH2	2.38	0.57
13:L:379:ALA:HA	13:L:383:MET:SD	2.45	0.57
20:f:93:MET:SD	20:f:98:PRO:HG3	2.45	0.57
26:l:82:ARG:O	26:l:86:ILE:HD12	2.04	0.57
28:n:47:ASN:O	28:n:50:TRP:HB3	2.04	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
11:M:35:SER:O	11:M:38:SER:OG	2.15	0.57
13:L:43:ALA:O	13:L:47:SER:HB2	2.05	0.57
13:L:55:ILE:HG13	33:s:73:PHE:CE1	2.35	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
27:m:55:PRO:HG2	42:Y:44:LEU:HB3	1.86	0.57
1:1:82:MET:HB2	1:1:129:MET:HB2	1.86	0.57
3:3:134:LYS:HB2	16:b:72:TYR:CE2	2.40	0.57
24:j:79:TYR:O	24:j:83:LYS:HB2	2.04	0.57
24:X:82:ASP:OD1	24:X:83:LYS:N	2.38	0.57
4:4:151:ILE:HD13	4:4:304:MET:HE1	1.87	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
9:N:329:MET:HE3	49:N:401:PC1:H282	1.86	0.57
13:L:22:ILE:HG21	50:L:601:CDL:H141	1.87	0.57
19:e:17:GLU:OE2	19:e:67:ARG:NE	2.26	0.57
21:g:38:TRP:CD2	21:g:89:LEU:HD12	2.39	0.57
30:p:125:ASN:H	41:Z:139:GLN:HE21	1.51	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
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.69	0.57
4:4:347:HIS:O	4:4:351:LEU:CB	2.53	0.57
8:H:218:GLY:O	8:H:221:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:273:ILE:O	8:H:276:SER:N	2.36	0.57
18:d:208:VAL:HA	18:d:211:THR:HG22	1.87	0.57
24:X:60:PHE:HD1	24:X:61:GLU:HB2	1.70	0.57
1:1:95:VAL:HB	1:1:136:ILE:HG12	1.87	0.56
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
5:5:101:PHE:CD2	22:h:96:PRO:HD2	2.40	0.56
8:H:316:PRO:HG3	31:q:56:ARG:CB	2.34	0.56
9:N:40:ILE:HG21	9:N:134:GLN:HE22	1.70	0.56
49:A:200:PC1:H3C1	27:m:22:PHE:CE1	2.40	0.56
11:M:309:TYR:CE2	41:Z:147:ALA:HB1	2.39	0.56
13:L:342:CYS:O	13:L:345:SER:OG	2.19	0.56
25:k:38:LEU:HD21	25:k:228:ALA:HB1	1.87	0.56
33:s:84:HIS:HA	33:s:87:ASP:HB2	1.87	0.56
37:w:66:PHE:HA	37:w:70:LEU:HD12	1.85	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
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
10:A:23:TRP:O	10:A:27:LEU:N	2.38	0.56
20:f:103:VAL:HG22	20:f:104:GLU:H	1.70	0.56
25:k:56:ILE:HG23	25:k:99:TRP:HE1	1.69	0.56
1:1:42:TRP:CD2	1:1:161:LEU:HD21	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:100:LEU:HD22	14:J:54:LEU:HD12	1.86	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
13:L:108:MET:HB2	13:L:114:ILE:HD13	1.87	0.56
34:t:91:GLU:HB3	34:t:94:GLU:HB2	1.87	0.56
41:Z:55:HIS:CD2	43:W:48:GLY:HA2	2.40	0.56
4:4:62:LEU:HD23	4:4:425:PHE:CZ	2.40	0.56
8:H:85:MET:SD	8:H:108:MET:HE3	2.46	0.56
9:N:88:LYS:HG3	9:N:148:SER:HB3	1.86	0.56
13:L:22:ILE:HG13	13:L:23:ASN:N	2.20	0.56
18:d:135:LEU:HD23	18:d:136:ASN:HB2	1.86	0.56
9:N:295:ARG:HA	9:N:298:TYR:CD2	2.40	0.56
14:J:96:GLY:O	14:J:100:GLU:CB	2.54	0.56
32:r:82:HIS:O	32:r:86:LYS:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:s:32:GLU:HG2	36:v:140:LEU:HD11	1.86	0.56
3:3:235:GLY:HA3	3:3:575:ASN:HB3	1.88	0.56
4:4:221:ARG:HE	22:h:23:LEU:HG	1.70	0.56
9:N:154:ILE:HG23	9:N:191:THR:HG22	1.88	0.56
11:M:1:MET:HE1	11:M:41:LEU:HD11	1.88	0.56
13:L:530:PRO:O	13:L:534:HIS:CB	2.54	0.56
33:s:106:ARG:NH1	35:u:59:TRP:HB3	2.18	0.56
35:u:27:PHE:O	35:u:31:THR:HG23	2.04	0.56
7:9:17:VAL:HG13	27:m:12:TRP:HZ3	1.69	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
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
3:3:74:MET:H	3:3:77:TRP:NE1	2.02	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
22:h:41:PRO:HB3	31:q:6:LYS:HD3	1.87	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
18:d:36:ASN:O	18:d:40:ARG:CB	2.54	0.56
18:d:291:ASP:CG	18:d:293:THR:H	2.13	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
11:M:32:LEU:O	11:M:35:SER:OG	2.19	0.56
11:M:210:TYR:HB2	11:M:268:GLY:HA3	1.88	0.56
11:M:432:ARG:HB2	37:w:48:ASP:OD1	2.05	0.56
13:L:227:PHE:HB2	13:L:284:THR:HG23	1.88	0.56
32:r:84:TYR:O	32:r:88:HIS:HB3	2.07	0.56
1:1:370:ASP:OD1	1:1:374:LYS:NZ	2.39	0.55
3:3:403:ASP:OD1	17:c:127:ARG:NH1	2.29	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
18:d:81:ILE:HG21	18:d:117:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:228:PHE:HA	18:d:297:LEU:HD23	1.87	0.55
34:t:58:LYS:HE3	34:t:62:LEU:HD11	1.88	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
9:N:339:LEU:HD21	29:o:34:ILE:HD11	1.88	0.55
11:M:89:LEU:HD11	11:M:93:LYS:HE3	1.87	0.55
11:M:281:ASP:HA	11:M:341:THR:HA	1.88	0.55
21:g:15:SER:O	21:g:16:VAL:HG23	2.06	0.55
25:k:183:ILE:HA	25:k:186:LYS:HG2	1.87	0.55
25:k:214:MET:HG2	25:k:220:VAL:HG11	1.88	0.55
29:o:68:PHE:HE1	48:o:203:3PE:H371	1.71	0.55
32:r:83:TYR:HE1	41:Z:48:ARG:HD3	1.70	0.55
33:s:106:ARG:NH1	35:u:58:GLN:O	2.39	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
4:4:298:LEU:HD12	7:9:6:ASN:HD21	1.71	0.55
4:4:338:MET:SD	4:4:348:HIS:ND1	2.79	0.55
7:9:47:THR:HG21	8:H:35:LYS:H	1.71	0.55
8:H:28:LEU:HD22	8:H:275:ALA:HB2	1.87	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
18:d:117:ILE:O	18:d:121:SER:OG	2.13	0.55
18:d:319:ARG:HG3	18:d:320:ARG:H	1.71	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
13:L:383:MET:HE3	13:L:388:GLY:N	2.17	0.55
8:H:115:SER:O	8:H:119:SER:HB3	2.06	0.55
8:H:167:ILE:HD12	42:Y:97:ARG:HH21	1.71	0.55
8:H:269:THR:O	8:H:272:TRP:O	2.24	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
49:A:200:PC1:H132	49:A:200:PC1:H12	1.88	0.55
12:K:1:MET:HG2	14:J:120:ASN:HA	1.89	0.55
15:a:58:LEU:O	15:a:62:ARG:NH1	2.40	0.55
17:c:33:ARG:NE	17:c:62:ARG:HE	2.05	0.55
18:d:22:THR:HB	18:d:91:VAL:HG23	1.88	0.55
42:Y:49:GLU:HA	42:Y:137:PRO:HG3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:280:THR:HG21	30:p:67:TRP:HE1	1.72	0.55
13:L:470:ASN:H	33:s:76:PHE:HZ	1.55	0.55
18:d:215:ILE:O	18:d:218:ILE:HG22	2.06	0.55
25:k:55:GLY:HA2	25:k:100:LEU:HD22	1.87	0.55
41:Z:143:HIS:HD1	41:Z:144:ASP:HB2	1.72	0.55
43:W:83:PRO:O	43:W:87:TYR:CB	2.55	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
20:f:13:LEU:HB3	20:f:77:GLU:HG2	1.88	0.55
23:i:56:PHE:HA	23:i:59:HIS:CE1	2.40	0.55
25:k:1:LEU:HB2	25:k:117:SER:HA	1.88	0.55
25:k:54:ALA:N	25:k:125:GLU:OE1	2.40	0.55
27:m:68:HIS:CD2	27:m:70:GLN:HB2	2.41	0.55
37:w:70:LEU:O	37:w:74:SER:HB2	2.05	0.55
4:4:342:MET:HE3	4:4:346:ILE:HD11	1.88	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
11:M:31:SER:OG	11:M:74:PRO:HG3	2.06	0.55
11:M:448:SER:O	13:L:68:TRP:HH2	1.89	0.55
13:L:283:MET:O	13:L:287:PHE:CB	2.55	0.55
18:d:285:GLU:O	18:d:289:THR:HG23	2.07	0.55
21:g:101:HIS:O	21:g:104:ARG:N	2.40	0.55
31:q:124:TYR:HB3	31:q:132:ILE:HG22	1.88	0.55
35:u:6:HIS:ND1	35:u:6:HIS:O	2.40	0.55
1:1:102:PRO:HA	2:2:144:CYS:SG	2.47	0.55
7:9:36:MET:HB3	22:h:14:ALA:HB1	1.89	0.55
9:N:36:ASN:O	9:N:40:ILE:HB	2.06	0.55
9:N:68:MET:HE3	12:K:40:LEU:HD12	1.88	0.55
21:g:38:TRP:CZ2	21:g:89:LEU:HB2	2.41	0.55
25:k:49:LYS:HB2	25:k:122:VAL:HG22	1.89	0.55
26:l:19:ILE:HG21	43:W:128:ILE:HG12	1.89	0.55
8:H:148:ILE:HG22	8:H:301:CYS:SG	2.46	0.55
9:N:120:GLN:OE1	9:N:177:LYS:HE2	2.07	0.55
13:L:76:LEU:HB2	13:L:136:ASN:HD21	1.71	0.55
13:L:260:LEU:HD13	13:L:277:MET:HE1	1.89	0.55
13:L:491:LEU:O	13:L:494:THR:OG1	2.20	0.55
52:d:401:NDP:O2X	52:d:401:NDP:O3B	2.24	0.55
22:h:4:THR:OG1	22:h:8:GLN:OE1	2.24	0.55
1:1:262:VAL:HG13	1:1:336:VAL:HG21	1.89	0.54
6:6:165:LYS:NZ	23:i:78:ASP:HB3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:N:22:ILE:CD1	26:l:5:VAL:H	2.19	0.54
19:e:16:ARG:H	19:e:68:TYR:HB3	1.72	0.54
23:i:13:GLN:HB3	23:i:35:VAL:HG22	1.89	0.54
1:1:174:ASP:OD2	15:a:63:MET:N	2.38	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
4:4:292:ASP:O	4:4:293:CYS:HB3	2.07	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
9:N:149:ILE:HG21	9:N:154:ILE:HD12	1.89	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
13:L:9:LEU:CD2	32:r:78:VAL:HG22	2.37	0.54
18:d:172:PHE:CE1	18:d:179:LEU:HD13	2.42	0.54
25:k:24:LEU:HD23	25:k:166:PRO:HB3	1.88	0.54
35:u:5:ALA:HB3	35:u:7:ILE:HG23	1.88	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
11:M:94:LEU:O	11:M:97:SER:OG	2.22	0.54
11:M:307:TRP:NE1	30:p:127:SER:HB2	2.22	0.54
13:L:63:ILE:HG22	32:r:96:ILE:HG22	1.89	0.54
18:d:157:ARG:HE	18:d:165:ILE:HD13	1.72	0.54
21:g:39:TYR:CE1	21:g:59:ARG:HD3	2.43	0.54
30:p:109:ASP:O	30:p:113:LYS:HG2	2.08	0.54
32:r:18:ARG:HH22	34:t:170:VAL:H	1.55	0.54
3:3:368:ILE:HG21	3:3:394:ARG:HD2	1.89	0.54
4:4:111:MET:HE1	4:4:189:MET:HG3	1.88	0.54
8:H:54:LYS:O	8:H:57:ILE:N	2.37	0.54
10:A:7:LEU:HD21	48:J:301:3PE:H362	1.89	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
13:L:479:GLN:C	13:L:481:THR:H	2.15	0.54
14:J:60:TYR:O	14:J:64:MET:HB2	2.07	0.54
24:j:54:MET:HE2	24:j:76:ILE:HG21	1.89	0.54
32:r:94:TYR:O	32:r:95:THR:HG23	2.07	0.54
33:s:74:PRO:HB2	41:Z:25:LEU:HD23	1.88	0.54
34:t:51:LYS:HA	54:X:401:PNS:H371	1.89	0.54
42:Y:110:VAL:HG12	42:Y:115:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:42:LEU:O	43:W:45:VAL:N	2.33	0.54
1:1:131:ALA:O	1:1:171:TYR:OH	2.26	0.54
1:1:338:ASP:OD1	1:1:339:ARG:N	2.40	0.54
4:4:176:LYS:HD3	22:h:25:LEU:HD13	1.87	0.54
9:N:106:LEU:HB2	9:N:187:MET:HE3	1.89	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
25:k:58:TYR:O	25:k:62:THR:OG1	2.22	0.54
35:u:19:ARG:O	35:u:23:ILE:HG12	2.08	0.54
37:w:70:LEU:O	37:w:74:SER:OG	2.21	0.54
42:Y:36:ASP:HA	42:Y:39:ASN:OD1	2.07	0.54
3:3:134:LYS:HB2	16:b:72:TYR:CD2	2.42	0.54
5:5:80:ALA:HB3	5:5:138:PHE:CE2	2.43	0.54
5:5:177:ASP:HB2	18:d:36:ASN:HD21	1.72	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
15:a:40:ASN:O	15:a:43:HIS:ND1	2.17	0.54
17:c:69:LEU:HD23	17:c:70:MET:HG2	1.90	0.54
18:d:90:VAL:HG21	18:d:218:ILE:HD11	1.90	0.54
25:k:33:SER:HB3	25:k:179:VAL:HG21	1.90	0.54
32:r:27:LEU:HG	32:r:32:PRO:HG2	1.90	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
6:6:165:LYS:HZ2	23:i:78:ASP:HB3	1.71	0.54
8:H:99:ASN:N	48:J:301:3PE:O14	2.35	0.54
11:M:326:LEU:HD21	11:M:410:MET:HE1	1.90	0.54
13:L:63:ILE:HD11	13:L:80:PHE:HD2	1.71	0.54
17:c:67:ASN:HB3	17:c:71:GLY:H	1.73	0.54
23:i:25:ARG:O	23:i:29:ARG:HG3	2.08	0.54
41:Z:116:GLU:OE2	41:Z:124:CYS: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
42:Y:120:ASP:OD1	42:Y:121:LEU: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
12:K:58:MET:HE2	12:K:58:MET:N	2.23	0.54
18:d:29:PHE:CZ	18:d:207:ILE:HD12	2.42	0.54
28:n:28:LEU:HG	28:n:52:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:o:90:MET:O	29:o:94:ILE:HG12	2.07	0.54
40:z:38:VAL:HG21	42:Y:93:LEU:HG	1.89	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
11:M:336:ARG:O	11:M:425:ASN:ND2	2.41	0.54
13:L:377:SER:O	13:L:381:THR:HG23	2.08	0.54
24:j:22:TYR:CE2	24:j:24:LYS:HB3	2.43	0.54
33:s:30:PHE:HB3	33:s:35:GLU:O	2.08	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
3:3:453:LEU:HD21	3:3:458:LEU:HD13	1.90	0.54
4:4:72:MET:HE1	4:4:408:GLY:C	2.33	0.54
4:4:233:ARG:NH2	7:9:24:THR:HG23	2.23	0.54
11:M:4:TYR:CE2	11:M:41:LEU:HD12	2.43	0.54
11:M:251:ASN:OD1	11:M:251:ASN:N	2.38	0.54
14:J:102:LEU:O	14:J:106:TYR:CB	2.56	0.54
18:d:90:VAL:HG12	18:d:128:LYS:HB2	1.90	0.54
18:d:107:GLU:HA	18:d:148:ASN:ND2	2.22	0.54
25:k:141:GLN:HB2	25:k:198:TYR:CE1	2.42	0.54
32:r:84:TYR:HA	32:r:87:TYR:CE2	2.43	0.54
35:u:8:GLU:OE2	35:u:10:ARG:NH2	2.38	0.54
37:w:62:PHE:HA	37:w:66:PHE:HD2	1.72	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:ND1	3:3:549:HIS:O	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:307:TRP:HE1	30:p:127:SER:HB2	1.71	0.53
11:M:408:LEU:HD23	13:L:172:ILE:HG21	1.89	0.53
13:L:98:TRP:HZ2	13:L:456:ARG:HH12	1.54	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
18:d:144:LYS:HA	18:d:147:ARG:NH1	2.22	0.53
33:s:28:TYR:CE1	33:s:30:PHE:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:165:ARG:NH2	43:W:100:LYS:O	2.42	0.53
9:N:250:SER:O	9:N:259:GLY:HA3	2.08	0.53
11:M:137:GLY:C	11:M:139:GLN:H	2.14	0.53
14:J:38:GLY:HA3	48:J:301:3PE:H2E2	1.89	0.53
18:d:29:PHE:HE2	18:d:171:ILE:HD12	1.73	0.53
18:d:32:ARG:HH22	18:d:175:GLU:CD	2.16	0.53
18:d:210:VAL:O	18:d:214:ILE:HD12	2.09	0.53
29:o:66:THR:HG23	38:x:28:TRP:HE3	1.73	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
25:k:115:LEU:HD13	25:k:121:GLY:HA2	1.90	0.53
25:k:235:VAL:O	25:k:239:GLN:CB	2.57	0.53
28:n:74:PHE:CA	28:n:77:PHE:HB3	2.35	0.53
30:p:35:ARG:O	30:p:39:ARG:CB	2.54	0.53
37:w:41:ASN:HB3	37:w:43:ASP:H	1.74	0.53
42:Y:76:HIS:CD2	42:Y:114:LEU:HB2	2.44	0.53
1:1:363:THR:HG21	3:3:97:LEU:HD21	1.90	0.53
3:3:382:THR:OG1	3:3:387:GLU:OE1	2.26	0.53
4:4:124:LYS:HG3	5:5:12:ARG:NH1	2.23	0.53
4:4:244:VAL:HG12	4:4:292:ASP:HA	1.88	0.53
9:N:108:MET:O	9:N:112:HIS:N	2.42	0.53
11:M:373:ILE:HD13	11:M:376:ILE:HD13	1.89	0.53
13:L:83:ASP:HB3	13:L:85:PHE:HD2	1.73	0.53
13:L:373:LEU:O	13:L:377:SER:OG	2.24	0.53
17:c:33:ARG:NH1	17:c:79:LEU:HB2	2.24	0.53
25:k:66:GLY:HA3	38:x:3:TYR:HD2	1.72	0.53
26:l:24:GLN:HB2	26:l:27:ARG:HA	1.91	0.53
32:r:18:ARG:HH22	34:t:170:VAL:HG22	1.74	0.53
34:t:77:GLN:N	34:t:77:GLN:OE1	2.41	0.53
37:w:72:LEU:O	37:w:75:THR:OG1	2.25	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:88:MET:HE2	13:L:468:ILE:HG12	1.90	0.53
13:L:362:LEU:HB3	13:L:431:LEU:HB3	1.91	0.53
17:c:121:ASN:O	17:c:129:ARG:HA	2.09	0.53
32:r:10:ARG:HB2	34:t:155:PRO:HG3	1.91	0.53
33:s:17:GLU:O	33:s:19:LEU:N	2.41	0.53
42:Y:30:HIS:O	42:Y:33:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:65:GLU:OE2	43:W:73:ARG:HD3	2.08	0.53
1:1:230:VAL:O	1:1:234:ILE:HG12	2.09	0.53
2:2:42:HIS:C	2:2:44:ALA:H	2.17	0.53
2:2:172:ILE:HD11	2:2:187:ARG:NH1	2.23	0.53
3:3:261:GLU:OE2	17:c:42:ARG:NH2	2.42	0.53
3:3:371:VAL:HG12	3:3:450:MET:HE1	1.91	0.53
4:4:309:ARG:O	4:4:312:SER:OG	2.21	0.53
5:5:113:GLU:OE1	17:c:22:LEU:HD21	2.09	0.53
11:M:114:GLU:OE1	42:Y:168:PHE:HB3	2.09	0.53
17:c:38:PHE:HE2	17:c:58:GLU:HG2	1.74	0.53
32:r:35:PRO:HB2	32:r:36:PRO:HD3	1.91	0.53
33:s:64:ARG:O	33:s:67:LYS:HB2	2.08	0.53
2:2:101:GLN:HB2	2:2:155:GLN:HB3	1.91	0.53
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
23:i:25:ARG:HE	23:i:29:ARG:HH21	1.56	0.53
29:o:45:ASP:OD2	29:o:64:TYR:OH	2.26	0.53
29:o:109:TYR:OH	41:Z:152:ARG:NH2	2.42	0.53
34:t:53:GLU:N	34:t:53:GLU:OE1	2.41	0.53
4:4:166:PRO:HD3	4:4:228:MET:HE2	1.90	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
9:N:31:ILE:HG12	12:K:66:PHE:CE2	2.43	0.53
9:N:106:LEU:HD22	9:N:187:MET:HE1	1.91	0.53
11:M:349:GLN:HG2	11:M:415:GLN:O	2.07	0.53
13:L:17:MET:HG2	13:L:36:VAL:HG22	1.91	0.53
24:j:80:ILE:HG22	24:j:84:LYS:HE2	1.90	0.53
31:q:30:SER:HA	31:q:34:MET:HG3	1.91	0.53
33:s:115:GLU:O	33:s:119:ALA:HB2	2.08	0.53
42:Y:165:ARG:HH22	43:W:103:LEU:HB3	1.71	0.53
5:5:191:ALA:O	17:c:74:SER:OG	2.26	0.53
11:M:329:LEU:HD23	11:M:359:TRP:CD2	2.44	0.53
12:K:53:PHE:CE1	26:l:20:GLN:HA	2.44	0.53
13:L:138:PHE:HB2	13:L:196:TRP:NE1	2.21	0.53
18:d:21:ALA:HA	18:d:90:VAL:O	2.09	0.53
22:h:30:ILE:HD12	22:h:32:LYS:H	1.74	0.53
23:i:83:PRO:HG2	23:i:86:TRP:HD1	1.74	0.53
33:s:28:TYR:HE1	33:s:30:PHE:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:9:175:TYR:CE2	22:h:38:PRO:HG3	2.43	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
18:d:63:GLY:HA3	18:d:68:ILE:HG12	1.91	0.53
28:n:65:ALA:HA	28:n:68:LYS:HG3	1.90	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
9:N:126:SER:HA	9:N:129:ILE:HG22	1.90	0.52
50:L:601:CDL:H531	50:L:601:CDL:H121	1.91	0.52
14:J:97:LEU:O	14:J:101:PHE:CB	2.57	0.52
18:d:40:ARG:HH21	21:g:109:THR:C	2.17	0.52
23:i:38:LEU:HD12	23:i:50:GLU:HG2	1.91	0.52
26:l:16:TRP:CZ3	26:l:17:MET:HB3	2.44	0.52
27:m:62:MET:O	42:Y:129:LYS:NZ	2.42	0.52
30:p:124:PHE:HB2	30:p:126:ILE:HD11	1.91	0.52
33:s:95:VAL:O	33:s:98:MET:HB2	2.09	0.52
33:s:107:LEU:HD21	35:u:62:GLU:OE2	2.08	0.52
33:s:115:GLU:O	33:s:119:ALA:HB3	2.09	0.52
42:Y:27:ALA:HB1	42:Y:70:PHE:HE1	1.74	0.52
1:1:299:PRO:O	1:1:304:THR:OG1	2.22	0.52
13:L:271:LYS:HA	13:L:274:GLN:OE1	2.09	0.52
13:L:358:LYS:HE2	34:t:33:ARG:HH22	1.74	0.52
18:d:216:ASN:HB2	18:d:303:LEU:HD21	1.91	0.52
19:e:15:LEU:HA	19:e:68:TYR:HB3	1.92	0.52
25:k:182:ARG:HG2	25:k:186:LYS:HE2	1.90	0.52
32:r:116:ILE:HB	32:r:117:PRO:HA	1.90	0.52
41:Z:49:GLU:OE2	41:Z:53:ARG:NH2	2.43	0.52
24:X:22:TYR:HD2	24:X:25:ILE:HG13	1.73	0.52
44:V:114:UNK:O	44:V:118:UNK:CB	2.57	0.52
3:3:378:LEU:HG	3:3:451:VAL:HG22	1.91	0.52
5:5:85:THR:OG1	17:c:86:PHE:HA	2.09	0.52
6:6:81:ARG:NH1	8:H:217:ALA:H	2.04	0.52
25:k:173:ASP:OD2	25:k:207:LYS:NZ	2.35	0.52
25:k:179:VAL:O	25:k:183:ILE:N	2.36	0.52
28:n:22:LYS:H	28:n:46:ARG:HD3	1.73	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
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:57:VAL:HG22	5:5:109:THR:HG21	1.91	0.52
9:N:146:LEU:HA	9:N:149:ILE:HD12	1.92	0.52
13:L:193:LEU:HD11	13:L:206:PRO:HG3	1.90	0.52
14:J:57:PHE:HA	14:J:61:LEU:HD12	1.90	0.52
18:d:157:ARG:HH21	18:d:165:ILE:HD13	1.74	0.52
18:d:281:ARG:O	18:d:285:GLU:CB	2.51	0.52
29:o:43:LEU:HD13	48:o:202:3PE:H231	1.91	0.52
30:p:42:LEU:HD22	34:t:151:GLU:HB3	1.92	0.52
33:s:33:ARG:NE	36:v:142:ARG:HG2	2.24	0.52
44:V:74:UNK:O	44:V:76:UNK:N	2.43	0.52
3:3:45:ARG:HH11	17:c:114:LYS:HZ1	1.58	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
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
20:f:71:LEU:HD21	20:f:79:VAL:HG11	1.92	0.52
34:t:128:ARG:HH11	34:t:166:TRP:HE3	1.58	0.52
41:Z:6:LYS:HE3	41:Z:11:GLU:HB2	1.90	0.52
43:W:85:LYS:HZ3	43:W:89:ARG:HH22	1.57	0.52
4:4:46:ASN:O	4:4:47:LEU:HD12	2.10	0.52
50:M:502:CDL:H841	50:M:502:CDL:H622	1.92	0.52
12:K:36:MET:O	12:K:39:SER:OG	2.18	0.52
13:L:441:ILE:HG13	35:u:10:ARG:O	2.10	0.52
14:J:45:LEU:HD23	14:J:50:SER:HA	1.91	0.52
18:d:129:PHE:HB3	18:d:160:PHE:CE2	2.45	0.52
18:d:278:TRP:O	18:d:279:THR:HG23	2.09	0.52
33:s:26:PRO:HD2	33:s:57:TYR:CE2	2.44	0.52
4:4:109:VAL:HG21	4:4:152:MET:HE1	1.92	0.52
6:6:38:ASN:O	6:6:42:ARG:HG2	2.09	0.52
9:N:25:HIS:HB2	26:l:14:ASP:HB2	1.91	0.52
13:L:595:ILE:O	13:L:598:SER:C	2.53	0.52
14:J:139:GLU:O	14:J:142:GLY:N	2.43	0.52
31:q:68:ILE:HB	42:Y:124:LEU:HD22	1.91	0.52
33:s:111:LYS:O	33:s:115:GLU:HB2	2.10	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
18:d:10:LYS:HD2	21:g:113:ARG:HH12	1.75	0.52
20:f:46:TYR:HB3	22:h:93:ALA:HB2	1.92	0.52
25:k:95:ARG:O	25:k:99:TRP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:18:TYR:CG	28:n:19:LYS:N	2.78	0.52
32:r:3:TYR:HB2	32:r:8:LYS:NZ	2.25	0.52
35:u:34:PHE:O	35:u:38:TRP:CB	2.58	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
7:9:18:THR:HA	27:m:12:TRP:CH2	2.38	0.52
7:9:155:LEU:O	7:9:158:GLY:N	2.43	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
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
29:o:116:PHE:HZ	41:Z:160:GLN:HB2	1.75	0.52
33:s:111:LYS:HG2	35:u:64:LEU:HD21	1.92	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
6:6:126:TYR:C	6:6:128:TYR:H	2.16	0.52
7:9:92:ILE:HD13	7:9:111:ILE:HG12	1.92	0.52
11:M:56:PHE:HA	11:M:113:THR:OG1	2.10	0.52
13:L:2:ASN:O	13:L:5:SER:HB2	2.10	0.52
13:L:265:PRO:HA	13:L:268:GLU:HG3	1.92	0.52
17:c:25:VAL:HB	17:c:26:PRO:CD	2.38	0.52
25:k:130:SER:HA	25:k:210:PHE:CZ	2.45	0.52
30:p:36:LEU:O	30:p:39:ARG:HB3	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
7:9:1:THR:HB	22:h:104:GLU:O	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
17:c:59:PHE:CD2	17:c:79:LEU:HB3	2.45	0.51
21:g:86:LYS:O	21:g:90:GLU:HB2	2.09	0.51
28:n:43:PRO:HB3	34:t:41:CYS:SG	2.50	0.51
33:s:19:LEU:HB2	41:Z:122:GLN:NE2	2.22	0.51
35:u:39:ARG:HA	35:u:42:HIS:HB2	1.92	0.51
36:v:132:GLN:HG3	36:v:133:TYR:N	2.25	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:61:MET:HB3	32:r:98:GLU:HB3	1.92	0.51
13:L:410:LEU:O	13:L:414:VAL:HG12	2.10	0.51
18:d:49:TYR:CE2	18:d:70:PHE:HB3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:211:LEU:HD23	25:k:214:MET:SD	2.50	0.51
32:r:31:GLU:HG2	43:W:7:ARG:HH22	1.75	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
8:H:314:ILE:HG13	31:q:57:ARG:NH2	2.26	0.51
11:M:168:GLN:OE1	43:W:104:ARG:NH1	2.44	0.51
11:M:196:TRP:CD1	11:M:250:LEU:HD13	2.46	0.51
13:L:119:LYS:NZ	50:L:601:CDL:OA5	2.37	0.51
13:L:585:LYS:O	13:L:589:LEU:CB	2.57	0.51
16:b:12:THR:OG1	16:b:14:THR:O	2.27	0.51
25:k:93:SER:OG	25:k:144:ILE:HD12	2.10	0.51
36:v:132:GLN:HG3	36:v:133:TYR:H	1.75	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
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
4:4:410:MET:HG2	8:H:281:ARG:NH2	2.24	0.51
8:H:127:TYR:HD1	10:A:46:SER:HB2	1.76	0.51
9:N:340:THR:HA	9:N:342:ILE:HG22	1.91	0.51
13:L:43:ALA:O	13:L:47:SER:OG	2.28	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
14:J:80:PRO:HA	18:d:322:ARG:HE	1.76	0.51
14:J:161:LEU:O	14:J:164:GLY:CA	2.58	0.51
20:f:17:GLU:HG2	20:f:18:THR:HG23	1.92	0.51
20:f:42:ALA:HB1	20:f:46:TYR:HE2	1.75	0.51
22:h:34:THR:OG1	22:h:36:PRO:O	2.28	0.51
31:q:25:PRO:HB2	31:q:26:ARG:HG2	1.93	0.51
34:t:51:LYS:HG3	54:X:401:PNS:C34	2.40	0.51
41:Z:96:LYS:O	41:Z:99:GLN:HB2	2.10	0.51
1:1:132:ARG:NH1	15:a:66:PRO:HD3	2.26	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
9:N:327:PRO:HG3	29:o:48:ILE:HD12	1.92	0.51
11:M:140:THR:C	11:M:142:ARG:N	2.63	0.51
23:i:71:LYS:HG3	23:i:72:ASN:ND2	2.25	0.51
29:o:62:PHE:HE2	38:x:24:SER:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:69:CYS:O	30:p:72:SER:OG	2.23	0.51
33:s:111:LYS:HZ3	36:v:139:TYR:HE2	1.57	0.51
41:Z:27:ASN:HB3	41:Z:30:THR:HG1	1.75	0.51
42:Y:28:ALA:HA	42:Y:31:TYR:CD2	2.45	0.51
42:Y:141:TYR:HD1	42:Y:142:HIS:H	1.56	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
8:H:100:LEU:HD21	14:J:51:PHE:HD1	1.76	0.51
10:A:57:LEU:HD21	14:J:172:THR:HG21	1.93	0.51
13:L:470:ASN:HB3	33:s:76:PHE:CZ	2.46	0.51
17:c:16:LYS:HZ2	21:g:76:ARG:HG3	1.76	0.51
25:k:74:SER:HB2	25:k:76:ASN:ND2	2.25	0.51
31:q:132:ILE:O	31:q:136:THR:OG1	2.16	0.51
34:t:147:GLY:N	34:t:148:PRO:HD3	2.26	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
10:A:1:MET:H3	31:q:141:TRP:CG	2.29	0.51
13:L:483:PRO:HG3	35:u:51:PHE:CE1	2.45	0.51
19:e:67:ARG:HA	19:e:73:GLU:HG2	1.92	0.51
35:u:53:TYR:CD1	35:u:54:PRO:HD2	2.45	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
4:4:90:LEU:HD23	5:5:168:LEU:HD11	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
7:9:30:LEU:HG	8:H:277:TYR:CE1	2.45	0.51
8:H:120:GLY:HA3	8:H:132:ALA:HB2	1.93	0.51
9:N:307:SER:HB2	9:N:309:ASN:ND2	2.25	0.51
11:M:412:ILE:O	11:M:413:THR:OG1	2.24	0.51
12:K:5:TYR:HE1	12:K:47:MET:HG2	1.76	0.51
18:d:301:GLU:C	18:d:304:GLY:H	2.17	0.51
22:h:5:ARG:HG3	23:i:2:GLU:HG3	1.93	0.51
28:n:23:ILE:HG13	28:n:46:ARG:HG3	1.93	0.51
28:n:26:THR:O	28:n:29:GLU:N	2.28	0.51
28:n:47:ASN:ND2	24:X:57:GLU:OE2	2.43	0.51
30:p:63:ALA:O	30:p:64:LEU:HG	2.09	0.51
30:p:125:ASN:C	30:p:126:ILE:HD12	2.36	0.51
32:r:18:ARG:NH2	34:t:170:VAL:HG22	2.26	0.51
1:1:134:ALA:HB2	1:1:173:PHE:HZ	1.75	0.51
1:1:406:ALA:HB3	46:1:501:FMN:HM83	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:63:ILE:HG13	2:2:81:TYR:HE1	1.75	0.51
2:2:168:ASP:CG	2:2:187:ARG:HD2	2.36	0.51
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
11:M:60:SER:O	11:M:64:PRO:HD2	2.10	0.51
11:M:154:LEU:HA	11:M:157:SER:HB2	1.92	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
18:d:215:ILE:HA	18:d:218:ILE:HG22	1.93	0.51
23:i:52:ASN:O	23:i:53:LYS:HB2	2.11	0.51
25:k:228:ALA:HA	25:k:231:ALA:HB3	1.93	0.51
25:k:244:ASP:O	25:k:248:TRP:N	2.44	0.51
28:n:59:ASN:OD1	28:n:60:VAL:N	2.40	0.51
29:o:108:THR:OG1	41:Z:76:CYS:O	2.29	0.51
32:r:117:PRO:CG	32:r:118:PRO:HD3	2.38	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
30:p:88:LEU:O	30:p:92:PHE:CB	2.59	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
7:9:43:ARG:HG2	22:h:11:ARG:HH11	1.76	0.50
8:H:168:THR:HG22	31:q:56:ARG:NH1	2.26	0.50
9:N:263:LYS:O	9:N:267:ILE:HG12	2.12	0.50
13:L:128:MET:HE2	13:L:251:THR:HA	1.93	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
4:4:352:TYR:CD1	7:9:86:VAL:HG11	2.39	0.50
4:4:396:PHE:HA	4:4:428:VAL:HG13	1.94	0.50
11:M:263:MET:HE2	30:p:101:TYR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:18:ASP:OD1	17:c:19:ILE:N	2.42	0.50
18:d:122:LYS:HB2	18:d:160:PHE:HD1	1.75	0.50
25:k:286:ALA:O	25:k:289:SER:N	2.44	0.50
31:q:42:LEU:HB3	31:q:46:TYR:CE2	2.46	0.50
34:t:51:LYS:HE2	54:X:401:PNS:O35	2.11	0.50
2:2:37:ASN:OD1	15:a:62:ARG:NH2	2.44	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
8:H:51:ASP:O	8:H:55:LEU:HB3	2.11	0.50
8:H:233:MET:O	8:H:236:ILE:N	2.45	0.50
9:N:162:ILE:HG13	9:N:188:GLY:HA3	1.94	0.50
10:A:72:LEU:HA	14:J:147:TYR:OH	2.12	0.50
11:M:45:PHE:HZ	43:W:86:ASN:HD22	1.60	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
13:L:195:THR:HB	41:Z:106:GLN:NE2	2.26	0.50
13:L:481:THR:HG22	33:s:91:HIS:CD2	2.47	0.50
13:L:506:ASN:OD1	13:L:507:THR:N	2.44	0.50
43:W:70:PRO:O	43:W:73:ARG:HB3	2.12	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
14:J:125:TRP:HB2	26:l:72:MET:HE1	1.93	0.50
25:k:19:THR:C	25:k:21:ASN:H	2.20	0.50
25:k:210:PHE:O	25:k:214:MET:HG3	2.11	0.50
33:s:24:PHE:CE1	33:s:42:GLN:HB2	2.45	0.50
39:y:4:LEU:HG	39:y:6:VAL:HG22	1.93	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
44:V:103:UNK:O	44:V:107:UNK:CB	2.60	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
7:9:14:MET:HE2	27:m:9:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:THR:O	8:H:66:SER:OG	2.21	0.50
8:H:185:TRP:HZ3	8:H:238:THR:HG1	1.56	0.50
9:N:294:MET:HE1	11:M:150:LEU:HD23	1.92	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
20:f:90:ALA:O	20:f:94:ILE:HD12	2.12	0.50
25:k:65:ASP:O	38:x:4:ILE:HD11	2.12	0.50
25:k:163:TYR:O	25:k:164:LEU:HG	2.11	0.50
28:n:74:PHE:O	28:n:78:VAL:HG23	2.12	0.50
30:p:38:ILE:O	30:p:42:LEU:HG	2.11	0.50
34:t:12:GLN:HG3	34:t:13:GLN:N	2.26	0.50
34:t:138:GLN:NE2	34:t:155:PRO:O	2.45	0.50
1:1:76:GLY:O	1:1:80:SER:HB3	2.12	0.50
1:1:237:ARG:C	2:2:214:GLN:HE22	2.20	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
5:5:69:ASN:ND2	22:h:93:ALA:O	2.44	0.50
8:H:97:ASN:OD1	40:z:40:HIS:NE2	2.34	0.50
8:H:222:LEU:O	8:H:225:MET:N	2.45	0.50
9:N:83:GLN:OE1	9:N:83:GLN:N	2.45	0.50
11:M:435:ALA:HB2	37:w:62:PHE:HE1	1.77	0.50
13:L:226:GLN:HE21	13:L:280:LEU:HG	1.77	0.50
18:d:296:HIS:O	18:d:297:LEU:HD12	2.12	0.50
28:n:70:PHE:HD1	28:n:74:PHE:CE2	2.30	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
21:g:36:ARG:O	21:g:40:ARG:HG2	2.12	0.50
29:o:39:TYR:CE2	29:o:43:LEU:HD11	2.47	0.50
29:o:68:PHE:CE1	48:o:203:3PE:H371	2.45	0.50
35:u:29:SER:O	35:u:32:MET:HG2	2.12	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
6:6:44:SER:OG	6:6:45:LEU:N	2.45	0.50
6:6:163:LEU:O	6:6:167:ILE:HG12	2.12	0.50
9:N:102:LEU:HD23	9:N:105:LYS:HG3	1.93	0.50
11:M:50:LEU:HD11	11:M:58:SER:HB3	1.94	0.50
29:o:112:VAL:O	41:Z:159:LYS:NZ	2.45	0.50
31:q:72:PRO:HA	42:Y:43:MET:HE2	1.93	0.50
4:4:141:PHE:CE1	4:4:184:VAL:HG21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:N:96:MET:HG3	9:N:153:LEU:HD11	1.93	0.50
13:L:53:MET:HA	13:L:56:HIS:NE2	2.26	0.50
20:f:42:ALA:HB1	20:f:46:TYR:CE2	2.47	0.50
22:h:26:ARG:HG2	23:i:56:PHE:HB3	1.93	0.50
34:t:16:LEU:HD22	24:X:48:VAL:HG21	1.94	0.50
1:1:87:ASP:OD1	1:1:88:GLY:N	2.43	0.49
1:1:392:LEU:HA	1:1:395:ILE:HD12	1.94	0.49
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.76	0.49
9:N:92:PRO:O	9:N:95:SER:OG	2.25	0.49
9:N:341:PRO:HB2	29:o:79:GLN:NE2	2.24	0.49
11:M:220:HIS:CE1	11:M:228:SER:HG	2.27	0.49
19:e:26:SER:O	19:e:29:SER:OG	2.17	0.49
33:s:61:TYR:CD1	33:s:85:ASP:HB3	2.46	0.49
41:Z:54:GLN:O	41:Z:57:LYS:HG2	2.11	0.49
43:W:81:ASP:HB3	43:W:85:LYS:HD3	1.94	0.49
1:1:33:LEU:O	1:1:37:GLN:CB	2.52	0.49
1:1:53:PRO:HB3	1:1:128:ALA:O	2.12	0.49
3:3:126:ASP:OD1	22:h:56:ARG:NH2	2.41	0.49
4:4:193:TYR:HE1	4:4:201:GLN:O	1.95	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
30:p:36:LEU:HA	30:p:39:ARG:HE	1.77	0.49
32:r:83:TYR:CE1	41:Z:48:ARG:HD3	2.47	0.49
34:t:30:CYS:SG	34:t:35:LYS:HB2	2.52	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
9:N:264:TRP:CZ2	42:Y:167:PHE:HD2	2.30	0.49
13:L:328:HIS:HB2	13:L:391:SER:HB2	1.94	0.49
19:e:15:LEU:HD23	19:e:18:ILE:HD11	1.93	0.49
24:j:35:HIS:CE1	24:j:38:LYS:HD3	2.48	0.49
27:m:8:LEU:HA	27:m:11:VAL:HG12	1.94	0.49
34:t:108:PRO:HA	34:t:111:LYS:HB3	1.94	0.49
37:w:45:HIS:CD2	37:w:46:GLY:H	2.30	0.49
41:Z:65:ARG:HG2	43:W:66:TYR:CD1	2.48	0.49
1:1:82:MET:HE1	1:1:219:PRO:HB2	1.94	0.49
3:3:349:PHE:H	3:3:509:PRO:HB2	1.78	0.49
3:3:431:ASP:O	3:3:436:SER:OG	2.21	0.49
8:H:9:LEU:HD22	8:H:95:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:3:LYS:HE2	11:M:4:TYR:CZ	2.46	0.49
11:M:450:ASN:OD1	11:M:452:LYS:HG2	2.13	0.49
27:m:57:ARG:HH22	42:Y:136:LEU:HA	1.77	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
9:N:91:ASN:HB3	9:N:94:ALA:HB3	1.93	0.49
11:M:12:MET:SD	11:M:16:TRP:NE1	2.85	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
18:d:238:LEU:HG	18:d:239:PHE:H	1.77	0.49
21:g:19:ILE:HB	21:g:79:ASP:OD2	2.12	0.49
25:k:14:THR:HG23	25:k:116:LEU:HD22	1.95	0.49
25:k:108:TYR:OH	25:k:166:PRO:HD3	2.12	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
9:N:26:TRP:HB3	9:N:74:ILE:HD13	1.94	0.49
9:N:207:ILE:O	9:N:211:MET:HG2	2.12	0.49
13:L:341:MET:HE3	13:L:454:ILE:HD13	1.95	0.49
13:L:455:LYS:O	13:L:459:ILE:HD12	2.12	0.49
14:J:4:TYR:O	14:J:7:PHE:N	2.45	0.49
18:d:91:VAL:HG13	18:d:129:PHE:CD1	2.45	0.49
27:m:52:TYR:OH	42:Y:43:MET:HG3	2.12	0.49
27:m:71:ASP:OD1	27:m:72:PRO:HD2	2.13	0.49
36:v:103:LYS:O	36:v:106:PHE:HB3	2.13	0.49
37:w:50:ASP:HB3	37:w:51:PRO:HD2	1.95	0.49
37:w:111:ASN:HA	41:Z:161:ARG:HH22	1.77	0.49
1:1:349:ARG:HE	2:2:105:THR:HA	1.76	0.49
1:1:363:THR:HA	1:1:366:ARG:HG2	1.94	0.49
8:H:115:SER:O	8:H:119:SER:HB2	2.11	0.49
9:N:240:MET:HE1	29:o:48:ILE:HG12	1.95	0.49
9:N:256:PRO:HB3	11:M:124:ALA:HB2	1.95	0.49
11:M:307:TRP:CZ2	30:p:127:SER:HB2	2.46	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
25:k:80:GLU:OE2	25:k:193:LYS:NZ	2.46	0.49
30:p:126:ILE:HG23	41:Z:138:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:143:THR:HA	40:z:45:TRP:CZ3	2.47	0.49
36:v:133:TYR:HB3	36:v:134:PRO:HD2	1.95	0.49
42:Y:15:GLN:NE2	42:Y:64:GLN:OE1	2.46	0.49
42:Y:139:ASN:HB3	42:Y:143:SER:OG	2.12	0.49
24:X:20:LYS:HG3	24:X:30:LEU:HD23	1.94	0.49
43:W:64:TRP:HD1	43:W:65:GLU:HG2	1.78	0.49
1:1:171:TYR:CE2	1:1:173:PHE:HB2	2.48	0.49
4:4:47:LEU:HD22	4:4:68:LEU:HD21	1.95	0.49
4:4:106:LEU:HD12	4:4:107:ASP:N	2.28	0.49
4:4:371:LYS:HZ1	4:4:424:VAL:HG23	1.77	0.49
9:N:78:LEU:HD12	9:N:84:TRP:CZ2	2.47	0.49
9:N:207:ILE:HD13	9:N:262:PRO:HD3	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
12:K:54:THR:HG22	26:l:24:GLN:HE21	1.78	0.49
18:d:279:THR:OG1	18:d:283:LYS:HB2	2.13	0.49
23:i:25:ARG:HH21	23:i:29:ARG:NH2	2.10	0.49
23:i:66:THR:OG1	23:i:74:PHE:HB2	2.12	0.49
33:s:103:ARG:HA	33:s:106:ARG:HE	1.78	0.49
33:s:112:LYS:HE2	36:v:130:PRO:HG2	1.94	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
3:3:113:GLU:O	17:c:46:GLN:NE2	2.22	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
5:5:11:VAL:HG22	22:h:58:GLY:HA3	1.95	0.49
5:5:206:PHE:HE1	22:h:59:ARG:HE	1.60	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
9:N:270:MET:HE3	9:N:282:MET:HE1	1.95	0.49
9:N:280:THR:HG22	11:M:162:VAL:HG21	1.95	0.49
13:L:135:ASN:HB2	13:L:198:LEU:HB3	1.95	0.49
18:d:134:HIS:H	18:d:149:LYS:HZ3	1.59	0.49
34:t:10:THR:HB	34:t:12:GLN:HG2	1.94	0.49
39:y:7:VAL:O	39:y:11:TRP:N	2.46	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
25:k:87:LYS:HG2	25:k:143:PHE:HD1	1.77	0.49
28:n:47:ASN:O	28:n:50:TRP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:51:ASN:HA	30:p:55:ARG:NH1	2.28	0.49
42:Y:165:ARG:NH1	43:W:103:LEU:HD23	2.28	0.49
44:V:107:UNK:O	44:V:111:UNK:CB	2.61	0.49
3:3:598:LYS:NZ	21:g:126:ASP:OD1	2.36	0.48
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
7:9:164:GLU:OE1	23:i:88:ARG:HB2	2.13	0.48
9:N:155:LEU:O	9:N:158:SER:OG	2.27	0.48
9:N:155:LEU:HD21	9:N:278:LEU:HD11	1.95	0.48
13:L:7:LEU:HD12	13:L:50:PRO:HG3	1.95	0.48
13:L:345:SER:O	13:L:349:SER:HB3	2.12	0.48
18:d:203:GLN:NE2	18:d:231:VAL:HG13	2.28	0.48
28:n:46:ARG:O	28:n:49:ALA:HB3	2.13	0.48
31:q:114:ARG:HG3	42:Y:141:TYR:C	2.38	0.48
33:s:101:PHE:HB2	36:v:122:TYR:HE1	1.78	0.48
41:Z:119:SER:O	41:Z:122:GLN:N	2.37	0.48
42:Y:15:GLN:HB2	42:Y:63:ASN:ND2	2.28	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
9:N:270:MET:HG2	9:N:279:PRO:HG3	1.95	0.48
9:N:311:MET:HE1	25:k:95:ARG:HG2	1.96	0.48
11:M:272:THR:HA	11:M:275:ILE:HG22	1.95	0.48
12:K:59:MET:O	12:K:63:LEU:HB3	2.13	0.48
14:J:30:GLY:O	14:J:34:ILE:HG12	2.14	0.48
23:i:41:GLU:HB2	23:i:86:TRP:CH2	2.48	0.48
25:k:30:ASN:ND2	25:k:203:GLU:HB2	2.28	0.48
34:t:23:LEU:O	34:t:27:GLU:HG3	2.13	0.48
42:Y:14:VAL:HG11	42:Y:60:LYS:HG3	1.95	0.48
24:X:7:THR:O	24:X:11:ILE:HG22	2.13	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
6:6:126:TYR:C	6:6:128:TYR:N	2.71	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
9:N:268:GLN:HB2	42:Y:167:PHE:HZ	1.77	0.48
9:N:328:THR:O	9:N:332:LEU:HB2	2.12	0.48
11:M:24:TRP:CD1	37:w:49:LYS:HZ2	2.27	0.48
11:M:394:ILE:O	11:M:398:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:12:LEU:O	13:L:16:THR:HG23	2.13	0.48
13:L:51:THR:HG21	13:L:91:PRO:HG2	1.95	0.48
13:L:137:LEU:HB3	13:L:196:TRP:CD1	2.48	0.48
13:L:154:LEU:HB3	13:L:243:VAL:HG11	1.95	0.48
13:L:592:LEU:O	13:L:596:LEU:CB	2.62	0.48
14:J:64:MET:HE2	14:J:64:MET:HA	1.94	0.48
24:j:79:TYR:O	24:j:83:LYS:CB	2.62	0.48
35:u:59:TRP:CD1	35:u:62:GLU:HB2	2.48	0.48
43:W:64:TRP:CD1	43:W:73:ARG:HG3	2.48	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
8:H:31:MET:HE3	8:H:272:TRP:CG	2.48	0.48
13:L:83:ASP:O	13:L:84:PHE:HB3	2.12	0.48
13:L:296:ASN:HB3	13:L:356:ILE:HG22	1.95	0.48
18:d:110:PHE:CD2	18:d:149:LYS:HB2	2.48	0.48
25:k:81:LYS:O	25:k:86:PRO:HG3	2.12	0.48
25:k:84:ASP:HB2	25:k:193:LYS:HD3	1.95	0.48
2:2:55:GLN:OE1	2:2:90:TYR:HA	2.13	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
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
9:N:83:GLN:HG2	9:N:85:THR:HG23	1.96	0.48
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
18:d:113:ILE:HB	18:d:114:PRO:HD3	1.95	0.48
18:d:294:LEU:HD21	18:d:296:HIS:CE1	2.48	0.48
32:r:115:VAL:O	32:r:116:ILE:HG12	2.14	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
4:4:305:ARG:HD3	31:q:21:LYS:HA	1.95	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
8:H:18:ALA:O	8:H:21:THR:OG1	2.24	0.48
9:N:146:LEU:HA	9:N:149:ILE:CD1	2.44	0.48
18:d:314:ALA:O	18:d:318:LEU:HD13	2.13	0.48
21:g:43:PRO:HG3	21:g:55:VAL:HG11	1.96	0.48
29:o:3:THR:O	29:o:7:ALA:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:117:PRO:HG3	33:s:88:TYR:CD2	2.48	0.48
1:1:46:LYS:HG2	1:1:50:LEU:HD23	1.96	0.48
3:3:45:ARG:NH1	17:c:114:LYS:HZ1	2.12	0.48
4:4:205:LEU:HA	31:q:9:MET:HE1	1.94	0.48
6:6:122:GLY:H	6:6:135:GLY:HA2	1.79	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
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
19:e:63:LYS:HA	19:e:78:LEU:N	2.27	0.48
25:k:155:VAL:O	25:k:159:THR:HB	2.14	0.48
30:p:48:LEU:HD22	30:p:61:ASP:OD2	2.13	0.48
30:p:125:ASN:HB3	41:Z:139:GLN:HE22	1.79	0.48
41:Z:60:TYR:HB2	43:W:50:ALA:HA	1.95	0.48
42:Y:41:GLU:HG2	42:Y:132:THR:HG22	1.94	0.48
24:X:84:LYS:HG3	24:X:85:ASP:H	1.79	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
11:M:30:HIS:O	11:M:34:ILE:HG12	2.13	0.48
13:L:81:LYS:HB2	13:L:135:ASN:HB3	1.96	0.48
18:d:10:LYS:O	18:d:15:SER:OG	2.21	0.48
18:d:12:GLY:H	18:d:15:SER:HB2	1.78	0.48
18:d:290:THR:O	18:d:291:ASP:HB2	2.14	0.48
25:k:146:LYS:O	25:k:147:GLN:HG2	2.14	0.48
25:k:152:TYR:O	25:k:156:LYS:HG3	2.13	0.48
26:l:82:ARG:HD3	26:l:85:LEU:HD11	1.96	0.48
32:r:115:VAL:HG22	32:r:116:ILE:H	1.78	0.48
39:y:14:VAL:C	39:y:17:PRO:HD2	2.38	0.48
42:Y:70:PHE:HA	42:Y:73:ILE:HG22	1.96	0.48
42:Y:165:ARG:HH21	43:W:104:ARG:N	2.12	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
5:5:66:ASP:HB2	20:f:89:LEU:HD22	1.96	0.48
7:9:87:CYS:HA	45:9:502:SF4:S2	2.53	0.48
9:N:109:ALA:HA	9:N:112:HIS:HD2	1.78	0.48
11:M:27:THR:HG21	11:M:96:ILE:HG21	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:226:GLN:HG3	13:L:227:PHE:H	1.78	0.48
18:d:21:ALA:O	18:d:22:THR:OG1	2.32	0.48
18:d:151:VAL:O	18:d:154:LYS:HB2	2.14	0.48
22:h:47:ARG:HH22	22:h:50:ASN:ND2	2.12	0.48
28:n:71:LYS:O	28:n:75:ALA:HB2	2.14	0.48
31:q:80:ARG:O	42:Y:12:LEU:HD11	2.12	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
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
17:c:123:SER:OG	17:c:126:LYS:HB2	2.14	0.48
19:e:26:SER:N	19:e:29:SER:OG	2.46	0.48
23:i:64:TYR:HD2	23:i:77:VAL:HB	1.79	0.48
25:k:30:ASN:OD1	25:k:31:ILE:N	2.46	0.48
26:l:49:ILE:HG23	26:l:50:ARG:H	1.78	0.48
29:o:59:HIS:CE1	29:o:60:ARG:HG2	2.49	0.48
32:r:13:GLN:O	32:r:16:GLU:HB2	2.13	0.48
34:t:59:ALA:HB1	54:X:401:PNS:H431	1.95	0.48
34:t:103:LEU:HG	34:t:121:ARG:NH1	2.26	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
2:2:82:GLU:OE2	17:c:132:THR:HG23	2.14	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
7:9:47:THR:O	23:i:58:ARG:NH2	2.46	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
9:N:4:ILE:O	9:N:7:ILE:N	2.46	0.47
11:M:49:SER:O	11:M:51:ASN:ND2	2.46	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
13:L:17:MET:HE2	13:L:32:TYR:CE1	2.48	0.47
31:q:57:ARG:O	31:q:61:ILE:HD12	2.13	0.47
31:q:137:TYR:HB3	31:q:141:TRP:CZ2	2.49	0.47
32:r:72:THR:O	32:r:76:ILE:HD12	2.14	0.47
33:s:24:PHE:HE2	33:s:39:VAL:HG23	1.78	0.47
33:s:75:ASN:CG	41:Z:25:LEU:HD21	2.39	0.47
34:t:19:TYR:CG	24:X:45:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:LEU:HD11	13:L:262:ARG:CG	2.44	0.47
13:L:233:LEU:HG	13:L:248:HIS:CE1	2.49	0.47
15:a:41:LEU:HG	15:a:44:HIS:CD2	2.49	0.47
32:r:75:LEU:HA	32:r:78:VAL:HG23	1.95	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
7:9:153:LYS:HB2	23:i:124:TYR:CE1	2.50	0.47
8:H:154:LEU:HD11	8:H:160:PHE:HA	1.95	0.47
11:M:371:PRO:HG3	50:L:601:CDL:H252	1.97	0.47
18:d:129:PHE:HB3	18:d:160:PHE:HE2	1.78	0.47
18:d:217:ALA:HB2	18:d:303:LEU:HD11	1.97	0.47
20:f:17:GLU:C	20:f:19:PRO:HD3	2.39	0.47
21:g:61:LYS:HE3	21:g:106:PHE:HA	1.96	0.47
26:l:35:PHE:HD2	26:l:65:CYS:HB2	1.79	0.47
33:s:108:LEU:HD13	36:v:131:LYS:HA	1.97	0.47
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.96	0.47
1:1:188:GLU:HG2	46:1:501:FMN:C7	2.44	0.47
1:1:264:ASN:OD1	2:2:196:ALA:HB3	2.14	0.47
2:2:213:VAL:HG23	2:2:214:GLN:H	1.78	0.47
5:5:44:CYS:HB3	22:h:62:ALA:HB1	1.95	0.47
5:5:85:THR:HG23	17:c:87:SER:H	1.79	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
13:L:4:PHE:HD2	13:L:61:MET:HE3	1.79	0.47
13:L:482:MET:O	13:L:487:LYS:HD3	2.15	0.47
18:d:135:LEU:HD13	18:d:169:ALA:HB2	1.97	0.47
19:e:14:GLY:O	19:e:68:TYR:HB2	2.14	0.47
24:j:70:LEU:HA	24:j:75:GLU:HG2	1.96	0.47
37:w:63:PHE:O	37:w:67:SER:HB3	2.14	0.47
41:Z:89:MET:SD	43:W:87:TYR:HE1	2.37	0.47
1:1:141:GLU:C	2:2:160:TYR:HH	2.22	0.47
3:3:624:GLU:HG3	3:3:628:PRO:HA	1.96	0.47
4:4:51:PHE:HD2	4:4:63:ARG:HG3	1.80	0.47
4:4:123:GLU:HG2	4:4:197:GLY:H	1.79	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
7:9:145:GLU:O	23:i:126:PRO:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:131:GLY:CA	8:H:208:VAL:HG22	2.45	0.47
8:H:302:MET:CB	10:A:95:ILE:HD11	2.38	0.47
9:N:45:MET:HA	9:N:52:ALA:HB1	1.97	0.47
11:M:232:ALA:HB3	11:M:327:PHE:CE2	2.46	0.47
18:d:321:HIS:CG	18:d:322:ARG:N	2.80	0.47
28:n:32:GLN:O	28:n:36:ALA:HB2	2.15	0.47
29:o:108:THR:HA	41:Z:77:HIS:HA	1.96	0.47
32:r:12:GLN:O	32:r:15:ARG:HB2	2.14	0.47
37:w:47:TYR:HB2	37:w:54:ASP:HB3	1.96	0.47
41:Z:24:SER:O	41:Z:25:LEU:HD12	2.15	0.47
42:Y:166:LEU:HG	42:Y:167:PHE:H	1.79	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
11:M:259:TYR:OH	30:p:105:LYS:N	2.47	0.47
11:M:431:THR:OG1	37:w:47:TYR:HD1	1.98	0.47
16:b:18:TYR:HE1	16:b:24:ARG:NH1	2.12	0.47
23:i:5:GLN:O	23:i:9:ARG:HG2	2.14	0.47
23:i:56:PHE:CD1	23:i:59:HIS:NE2	2.83	0.47
36:v:135:TYR:CE1	36:v:137:ASN:HB3	2.49	0.47
37:w:40:LYS:CG	37:w:41:ASN:H	2.17	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
4:4:84:HIS:CD2	5:5:152:LEU:HB3	2.50	0.47
4:4:255:PHE:HZ	4:4:401:GLY:HA3	1.80	0.47
4:4:270:ARG:HG2	4:4:278:TYR:HE2	1.79	0.47
5:5:209:TYR:HE1	22:h:63:MET:HA	1.78	0.47
8:H:284:GLN:O	8:H:288:LEU:CB	2.58	0.47
9:N:207:ILE:HD11	9:N:261:MET:HE3	1.95	0.47
10:A:8:LEU:O	10:A:12:THR:HG23	2.15	0.47
10:A:92:LEU:O	10:A:96:PHE:HB2	2.15	0.47
11:M:434:ASN:HB3	43:W:21:PHE:CE2	2.50	0.47
12:K:37:MET:SD	12:K:67:ALA:HA	2.55	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
14:J:143:ILE:O	14:J:146:LEU:HB3	2.15	0.47
16:b:58:SER:HB3	16:b:72:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:50:GLU:HB3	23:i:89:TRP:HH2	1.79	0.47
23:i:73:THR:HG22	23:i:74:PHE:N	2.30	0.47
25:k:49:LYS:HD2	25:k:114:HIS:CE1	2.49	0.47
28:n:52:TYR:OH	34:t:34:ASP:HB3	2.15	0.47
29:o:26:LEU:O	29:o:27:THR:HG22	2.14	0.47
30:p:33:ALA:O	30:p:37:ALA:CB	2.63	0.47
40:z:52:ARG:HG3	40:z:58:ASN:O	2.15	0.47
41:Z:167:LYS:HA	41:Z:170:LYS:HG2	1.96	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:79:GLU:O	42:Y:82:THR:OG1	2.20	0.47
42:Y:82:THR:HA	42:Y:85:TRP:NE1	2.30	0.47
43:W:114:MET:HE1	43:W:120:GLY:N	2.29	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
11:M:142:ARG:C	11:M:144:ASN:H	2.23	0.47
14:J:26:PRO:C	14:J:29:GLY:H	2.22	0.47
18:d:23:VAL:HG13	18:d:92:ILE:HD11	1.97	0.47
25:k:12:GLU:O	25:k:14:THR:N	2.48	0.47
33:s:39:VAL:O	33:s:60:HIS:HE1	1.97	0.47
1:1:386:PRO:HG3	1:1:430:MET:HG2	1.97	0.47
2:2:6:LEU:HD11	16:b:55:ARG:CZ	2.44	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
13:L:436:ARG:NH2	34:t:31:VAL:HG23	2.29	0.47
18:d:24:PHE:HE2	18:d:117:ILE:HB	1.80	0.47
22:h:108:ASP:OD1	22:h:109:GLU:N	2.46	0.47
24:j:13:ASP:O	24:j:17:TYR:HB2	2.15	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
24:X:11:ILE:HD11	24:X:80:ILE:HB	1.96	0.47
9:N:317:PHE:HB3	25:k:63:THR:HG21	1.96	0.47
11:M:7:PRO:HB2	11:M:34:ILE:CD1	2.45	0.47
11:M:451:PRO:O	11:M:454:ILE:HG13	2.15	0.47
13:L:463:PHE:CE2	13:L:467:ILE:HD11	2.50	0.47
25:k:165:PRO:HB3	25:k:217:LYS:HB3	1.95	0.47
25:k:180:GLN:HB2	25:k:199:LEU:HD23	1.97	0.47
29:o:3:THR:O	29:o:7:ALA:HB2	2.14	0.47
31:q:107:GLU:HB3	42:Y:3:ILE:HG22	1.97	0.47
33:s:97:ARG:HG2	36:v:122:TYR:OH	2.15	0.47
38:x:6:GLU:OE2	38:x:11:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:z:63:SER:O	42:Y:20:SER:HB3	2.14	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
5:5:179:GLU:HG3	18:d:36:ASN:HD22	1.77	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
9:N:210:ILE:HG22	9:N:333:SER:HB3	1.97	0.46
13:L:227:PHE:CG	13:L:228:GLY:N	2.83	0.46
25:k:209:THR:O	25:k:212:PRO:HD2	2.15	0.46
36:v:109:VAL:HA	36:v:112:MET:HE3	1.97	0.46
37:w:40:LYS:HG2	37:w:41:ASN:N	2.15	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
5:5:28:TYR:HE1	20:f:46:TYR:CG	2.33	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
8:H:313:SER:HB3	31:q:53:ASN:HB2	1.97	0.46
13:L:297:ASP:O	13:L:301:ILE:HD12	2.15	0.46
19:e:56:GLU:HG2	19:e:57:CYS:N	2.28	0.46
20:f:39:LYS:HB2	20:f:44:ARG:NH1	2.30	0.46
25:k:214:MET:SD	25:k:220:VAL:HG21	2.54	0.46
31:q:129:GLY:HA2	31:q:132:ILE:HG12	1.97	0.46
35:u:30:ALA:O	35:u:34:PHE:HB3	2.15	0.46
41:Z:81:VAL:O	41:Z:84:MET:N	2.49	0.46
4:4:47:LEU:HD22	4:4:68:LEU:HD11	1.97	0.46
4:4:233:ARG:O	4:4:237:ASN:HB2	2.16	0.46
5:5:110:TYR:CB	20:f:110:GLN:HE22	2.28	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
13:L:487:LYS:HZ2	13:L:488:MET:HG2	1.80	0.46
15:a:65:GLN:CD	15:a:65:GLN:H	2.23	0.46
17:c:89:LYS:HD2	17:c:105:VAL:HG11	1.95	0.46
25:k:49:LYS:O	25:k:123:VAL:HG12	2.16	0.46
25:k:86:PRO:HB2	25:k:92:ASN:CG	2.41	0.46
25:k:164:LEU:HA	25:k:165:PRO:HD3	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:127:ARG:O	31:q:128:THR:HG22	2.15	0.46
31:q:134:SER:O	31:q:138:GLY:CA	2.52	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
3:3:138:GLU:OE2	16:b:77:LYS:HE2	2.15	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
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
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
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
14:J:151:THR:OG1	14:J:152:TRP:N	2.48	0.46
18:d:90:VAL:CG1	18:d:128:LYS:HB2	2.45	0.46
18:d:133:SER:O	18:d:168:PRO:HD2	2.15	0.46
18:d:248:VAL:C	18:d:250:HIS:H	2.23	0.46
22:h:39:LYS:H	31:q:7:GLN:HB2	1.79	0.46
25:k:2:GLN:OE1	25:k:267:LEU:HA	2.15	0.46
34:t:103:LEU:HD13	34:t:106:TRP:CE2	2.50	0.46
40:z:69:ILE:HB	42:Y:74:LYS:HZ1	1.80	0.46
41:Z:167:LYS:O	41:Z:170:LYS:HG2	2.15	0.46
24:X:36:PHE:HE2	24:X:47:GLN:HB2	1.79	0.46
1:1:224:ASN:N	46:1:501:FMN:O3P	2.39	0.46
1:1:322:LEU:HB3	1:1:327:THR:O	2.16	0.46
2:2:202:LEU:O	2:2:202:LEU:HD12	2.16	0.46
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
7:9:9:GLU:HG2	7:9:9:GLU:O	2.15	0.46
7:9:37:THR:O	7:9:40:TYR:HB3	2.16	0.46
9:N:28:LEU:O	9:N:31:ILE:N	2.49	0.46
9:N:307:SER:O	9:N:308:THR:OG1	2.32	0.46
11:M:119:TYR:CD1	11:M:160:LEU:HD11	2.50	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
17:c:131:SER:O	17:c:132:THR:HB	2.15	0.46
18:d:45:VAL:HB	18:d:68:ILE:HG22	1.98	0.46
19:e:22:LEU:HD23	19:e:22:LEU:HA	1.75	0.46
34:t:45:ALA:HA	34:t:48:ASP:HB3	1.97	0.46
40:z:3:PHE:O	40:z:6:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:9:54:LYS:HD3	23:i:91:HIS:NE2	2.30	0.46
9:N:258:SER:OG	9:N:336:LEU:HB3	2.16	0.46
11:M:17:LEU:HD23	48:o:202:3PE:H372	1.98	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
13:L:22:ILE:HG22	50:L:601:CDL:HB4	1.98	0.46
13:L:41:SER:O	13:L:44:PHE:N	2.45	0.46
13:L:63:ILE:HD11	13:L:80:PHE:CD2	2.50	0.46
13:L:144:TRP:CE2	13:L:223:LYS:HE2	2.50	0.46
13:L:282:ALA:O	13:L:285:THR:OG1	2.23	0.46
13:L:484:HIS:CG	13:L:487:LYS:HE3	2.51	0.46
23:i:73:THR:HG22	23:i:74:PHE:H	1.81	0.46
25:k:153:ASN:O	25:k:156:LYS:HB2	2.16	0.46
26:l:14:ASP:O	26:l:18:THR:OG1	2.30	0.46
33:s:18:PRO:HD2	41:Z:121:ARG:HB2	1.98	0.46
34:t:153:LEU:HD22	34:t:164:PRO:HG2	1.97	0.46
3:3:213:TYR:CE1	3:3:249:ARG:HD3	2.51	0.46
4:4:94:LYS:HE2	7:9:88:PRO:O	2.15	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
6:6:138:ARG:NH1	18:d:13:ARG:HH21	2.13	0.46
8:H:247:HIS:O	8:H:249:PRO:HD3	2.15	0.46
10:A:71:LEU:O	14:J:147:TYR:OH	2.30	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
13:L:281:GLY:HA3	13:L:314:MET:HB3	1.96	0.46
13:L:310:LEU:HD23	13:L:313:MET:HE3	1.97	0.46
17:c:14:ASP:OD2	21:g:22:ARG:HG2	2.14	0.46
22:h:8:GLN:HA	22:h:11:ARG:HE	1.80	0.46
31:q:79:ASP:HA	31:q:82:VAL:HG22	1.98	0.46
34:t:15:VAL:HG22	34:t:63:LEU:HD12	1.96	0.46
34:t:76:PRO:C	34:t:78:PRO:HD3	2.39	0.46
35:u:54:PRO:O	35:u:57:SER:HB3	2.16	0.46
42:Y:100:ARG:NE	42:Y:103:GLN:OE1	2.49	0.46
43:W:114:MET:HE1	43:W:120:GLY:H	1.80	0.46
3:3:333:ASP:O	3:3:337:ARG:CB	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	6:6:127:HIS:ND1	2.48	0.46
7:9:27:TRP:NE1	48:9:501:3PE:O22	2.49	0.46
9:N:202:LEU:CB	9:N:346:LEU:HD21	2.46	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
11:M:425:ASN:HB3	30:p:56:ARG:O	2.16	0.46
13:L:57:THR:HG22	13:L:57:THR:O	2.16	0.46
13:L:213:LEU:HD12	13:L:266:LEU:HG	1.98	0.46
14:J:38:GLY:HA3	48:J:301:3PE:C2E	2.46	0.46
48:J:301:3PE:H3D2	48:J:301:3PE:H2G1	1.96	0.46
18:d:244:TYR:O	18:d:247:ALA:N	2.49	0.46
33:s:52:LEU:C	33:s:54:GLN:H	2.24	0.46
46:1:501:FMN:H9	46:1:501:FMN:H1'2	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
11:M:41:LEU:HD22	11:M:63:THR:HG23	1.98	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
32:r:16:GLU:O	32:r:19:ARG:HB2	2.15	0.46
33:s:67:LYS:O	33:s:71:ASP:N	2.47	0.46
39:y:31:ASP:CG	43:W:89:ARG:HH21	2.24	0.46
3:3:98:LEU:HD13	4:4:343:GLU:HG2	1.98	0.46
3:3:568:GLU:OE1	3:3:568:GLU:N	2.49	0.46
9:N:202:LEU:HB2	9:N:346:LEU:HD21	1.98	0.46
11:M:130:LEU:O	11:M:134:THR:HG22	2.16	0.46
13:L:83:ASP:C	13:L:85:PHE:H	2.24	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:O	13:L:350:LEU:HD23	2.16	0.46
13:L:418:PHE:O	13:L:421:ILE:HG12	2.16	0.46
17:c:30:ILE:HD12	17:c:101:TRP:HE3	1.81	0.46
18:d:134:HIS:N	18:d:149:LYS:HZ3	2.14	0.46
52:d:401:NDP:N3A	52:d:401:NDP:O3X	2.49	0.46
20:f:37:ILE:HD11	20:f:94:ILE:HD11	1.98	0.46
20:f:43:TYR:O	20:f:47:THR:OG1	2.27	0.46
22:h:8:GLN:NE2	22:h:19:LEU:HD22	2.31	0.46
23:i:74:PHE:CG	23:i:75:TRP:N	2.84	0.46
25:k:132:PHE:O	25:k:136:GLU:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:59:ASN:CG	28:n:60:VAL:H	2.23	0.46
35:u:54:PRO:O	35:u:57:SER:N	2.49	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
4:4:227:GLU:OE1	31:q:24:LEU:HD11	2.15	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
9:N:124:LEU:HD12	9:N:176:ARG:HH22	1.81	0.45
11:M:1:MET:HB3	11:M:56:PHE:HE1	1.81	0.45
11:M:417:GLY:HA2	13:L:160:GLY:HA2	1.97	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:472:ILE:O	13:L:473:PRO:C	2.58	0.45
13:L:484:HIS:HA	13:L:487:LYS:HG2	1.97	0.45
15:a:71:GLU:OE2	15:a:74:ARG:NH1	2.49	0.45
24:j:23:ASP:OD1	24:j:24:LYS:N	2.49	0.45
26:l:81:GLN:HG3	26:l:85:LEU:HD23	1.98	0.45
33:s:21:MET:HB2	33:s:23:THR:O	2.16	0.45
24:X:43:ASP:OD2	24:X:45:LEU:HB3	2.16	0.45
3:3:399:TRP:CH2	17:c:127:ARG:HD3	2.51	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
9:N:149:ILE:HD13	9:N:154:ILE:CD1	2.45	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
13:L:439:THR:OG1	13:L:440:LEU:N	2.50	0.45
13:L:477:ILE:HD12	33:s:90:GLU:OE1	2.16	0.45
25:k:199:LEU:O	25:k:202:ILE:HB	2.17	0.45
25:k:211:LEU:HB2	25:k:212:PRO:HD3	1.98	0.45
29:o:90:MET:SD	43:W:107:GLU:HB3	2.55	0.45
30:p:28:THR:O	30:p:32:GLN:N	2.43	0.45
30:p:125:ASN:H	41:Z:139:GLN:NE2	2.13	0.45
40:z:17:PHE:CE2	40:z:21:MET:HE2	2.51	0.45
41:Z:39:LEU:O	41:Z:43:PRO:HG2	2.17	0.45
41:Z:166:ARG:HA	41:Z:169:THR:HG22	1.97	0.45
43:W:115:ARG:HG3	43:W:123:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
49:A:200:PC1:H3C1	27:m:22:PHE:HE1	1.80	0.45
11:M:251:ASN:CG	11:M:252:PRO:HD3	2.41	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
18:d:108:ASP:HA	18:d:111:VAL:HB	1.98	0.45
18:d:319:ARG:HG3	18:d:320:ARG:N	2.31	0.45
22:h:24:GLN:HE21	22:h:26:ARG:CZ	2.29	0.45
34:t:128:ARG:CZ	34:t:165:LEU:HD13	2.46	0.45
35:u:10:ARG:HD3	35:u:13:GLN:CB	2.36	0.45
1:1:17:ASP:C	1:1:19:ASP:H	2.25	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
8:H:145:THR:O	8:H:149:ILE:HD12	2.17	0.45
8:H:303:TRP:HD1	27:m:28:ALA:HB2	1.81	0.45
9:N:25:HIS:CD2	26:l:17:MET:HG3	2.51	0.45
10:A:73:LEU:N	10:A:74:PRO:HD2	2.32	0.45
13:L:54:PHE:CD1	13:L:58:GLY:HA2	2.52	0.45
19:e:22:LEU:HD11	19:e:32:VAL:HG12	1.97	0.45
20:f:13:LEU:HD23	20:f:77:GLU:HG3	1.98	0.45
25:k:129:TYR:CE2	25:k:166:PRO:HD2	2.48	0.45
30:p:42:LEU:CD2	34:t:151:GLU:HB3	2.47	0.45
32:r:25:GLN:HE22	43:W:9:PHE:HD2	1.64	0.45
32:r:85:LEU:HA	32:r:85:LEU:HD23	1.75	0.45
33:s:68:CYS:HA	33:s:71:ASP:CG	2.42	0.45
33:s:112:LYS:HZ1	36:v:130:PRO:C	2.24	0.45
42:Y:27:ALA:HB2	42:Y:81:PHE:CZ	2.51	0.45
24:X:28:GLU:HG3	24:X:29:LYS:HD2	1.98	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
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
7:9:112:ASP:OD2	7:9:115:LYS:NZ	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:81:LYS:C	13:L:82:MET:HE2	2.41	0.45
14:J:166:VAL:O	14:J:170:GLU:CB	2.65	0.45
26:l:68:ARG:HH12	31:q:119:MET:HB2	1.82	0.45
31:q:5:VAL:HG12	31:q:6:LYS:N	2.31	0.45
32:r:68:ILE:O	32:r:72:THR:HG23	2.16	0.45
39:y:22:PHE:CE2	39:y:26:LEU:HD11	2.50	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
3:3:134:LYS:O	16:b:72:TYR:HD2	1.97	0.45
4:4:151:ILE:HD11	4:4:170:MET:HG3	1.98	0.45
4:4:161:ILE:HD11	4:4:238:ARG:NE	2.30	0.45
4:4:266:GLN:CD	7:9:2:TYR:HB3	2.40	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
11:M:14:LEU:HD22	11:M:30:HIS:ND1	2.32	0.45
13:L:67:HIS:ND1	13:L:69:LEU:O	2.49	0.45
18:d:96:GLY:HA3	18:d:110:PHE:HE1	1.82	0.45
25:k:132:PHE:CE1	25:k:133:VAL:HG23	2.51	0.45
27:m:48:THR:HG22	31:q:61:ILE:HG13	1.99	0.45
28:n:21:TRP:HB2	28:n:46:ARG:HD3	1.99	0.45
28:n:26:THR:O	28:n:28:LEU:N	2.49	0.45
30:p:64:LEU:HA	30:p:67:TRP:HB3	1.99	0.45
33:s:108:LEU:O	33:s:112:LYS:HB2	2.17	0.45
34:t:12:GLN:HA	54:X:401:PNS:H302	1.99	0.45
34:t:23:LEU:HB2	24:X:52:MET:HE3	1.98	0.45
35:u:58:GLN:HB3	35:u:60:THR:HG23	1.99	0.45
37:w:62:PHE:O	37:w:66:PHE:HB2	2.17	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
9:N:89:LEU:HD11	9:N:98:MET:SD	2.56	0.45
10:A:38:GLU:OE2	21:g:99:ARG:NH1	2.50	0.45
11:M:164:LEU:O	11:M:167:ILE:N	2.49	0.45
11:M:387:SER:O	29:o:120:ARG:NH2	2.31	0.45
50:M:502:CDL:H331	37:w:77:VAL:HG23	1.99	0.45
13:L:28:LYS:HB2	13:L:32:TYR:CD2	2.52	0.45
13:L:36:VAL:O	13:L:39:THR:OG1	2.23	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
14:J:17:PHE:HA	14:J:20:PHE:HB3	1.99	0.45
14:J:142:GLY:O	14:J:145:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:96:GLY:HA3	18:d:110:PHE:CE1	2.52	0.45
18:d:321:HIS:CD2	18:d:322:ARG:H	2.33	0.45
22:h:108:ASP:CG	22:h:109:GLU:H	2.24	0.45
26:l:8:LYS:HD2	29:o:11:LEU:HB2	1.99	0.45
40:z:13:GLY:O	40:z:17:PHE:HB3	2.17	0.45
43:W:140:THR:O	43:W:141:PRO:C	2.60	0.45
1:1:309:LYS:NZ	1:1:313:GLU:OE2	2.39	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
3:3:44:GLU:O	17:c:114:LYS:NZ	2.44	0.45
4:4:106:LEU:HD13	4:4:391:ILE:HD12	1.99	0.45
4:4:338:MET:SD	4:4:348:HIS:CE1	3.10	0.45
5:5:67:HIS:C	5:5:69:ASN:H	2.25	0.45
5:5:123:VAL:HG23	5:5:124:TYR:N	2.31	0.45
8:H:264:LEU:O	8:H:268:ILE:HG12	2.16	0.45
9:N:271:THR:HG22	9:N:279:PRO:HG2	1.98	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
18:d:245:VAL:HG23	18:d:318:LEU:HD21	1.98	0.45
27:m:18:LEU:O	27:m:21:SER:OG	2.28	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
3:3:303:VAL:HA	3:3:542:PHE:HZ	1.82	0.45
3:3:379:LEU:HD23	3:3:408:LEU:HD13	1.99	0.45
6:6:148:GLY:H	7:9:118:TYR:HE2	1.65	0.45
7:9:71:PRO:HG3	23:i:106:ARG:NH1	2.32	0.45
9:N:216:PHE:HA	9:N:219:PHE:HD2	1.82	0.45
11:M:17:LEU:O	11:M:18:SER:OG	2.34	0.45
11:M:146:GLY:C	11:M:149:PHE:HB3	2.41	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
13:L:282:ALA:HB1	13:L:411:MET:HG2	1.99	0.45
18:d:186:ARG:HH11	18:d:251:ARG:HH11	1.65	0.45
29:o:62:PHE:CE2	38:x:24:SER:HB2	2.52	0.45
31:q:87:ARG:HD2	42:Y:7:PRO:O	2.17	0.45
33:s:32:GLU:H	36:v:140:LEU:HD21	1.82	0.45
34:t:103:LEU:HD13	34:t:106:TRP:CD2	2.52	0.45
35:u:59:TRP:HD1	35:u:62:GLU:HB2	1.81	0.45
1:1:66:ARG:HD2	1:1:319:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:9:144:HIS:ND1	18:d:65:LEU:HD21	2.32	0.45
9:N:269:GLU:HG2	9:N:272:LYS:HE2	1.99	0.45
11:M:33:LEU:HA	11:M:36:LEU:HD13	1.97	0.45
11:M:350:THR:OG1	11:M:351:LEU:N	2.46	0.45
13:L:387:THR:HG21	13:L:461:SER:O	2.17	0.45
20:f:46:TYR:HD1	22:h:93:ALA:HB2	1.82	0.45
25:k:254:ARG:O	25:k:258:ASN:CB	2.65	0.45
33:s:98:MET:O	33:s:101:PHE:HB3	2.17	0.45
35:u:26:GLU:O	35:u:29:SER:OG	2.24	0.45
42:Y:78:ALA:O	42:Y:82:THR:HG23	2.17	0.45
44:V:104:UNK:O	44:V:108:UNK:CB	2.64	0.45
1:1:12:PHE:HB3	1:1:273:SER:O	2.17	0.44
1:1:91:LYS:HG2	1:1:219:PRO:HG2	1.98	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
5:5:194:PHE:HD2	17:c:81:ASN:HD22	1.63	0.44
9:N:158:SER:HB2	9:N:188:GLY:O	2.17	0.44
9:N:345:ILE:HD12	29:o:78:ARG:HH11	1.82	0.44
11:M:263:MET:SD	30:p:104:PHE:HD2	2.41	0.44
11:M:339:SER:HB2	11:M:344:LEU:HD23	1.99	0.44
11:M:369:LEU:HD22	50:L:601:CDL:H272	1.99	0.44
11:M:370:PRO:HB3	13:L:141:PHE:CD2	2.53	0.44
13:L:9:LEU:HA	32:r:81:ILE:HD13	1.99	0.44
13:L:274:GLN:HG2	13:L:319:ILE:O	2.17	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
14:J:125:TRP:CH2	26:l:79:LYS:HB3	2.43	0.44
17:c:77:ASP:CG	17:c:80:SER:HB3	2.42	0.44
23:i:22:GLY:O	23:i:26:VAL:HG12	2.17	0.44
25:k:319:LEU:O	38:x:1:LYS:HE2	2.17	0.44
29:o:116:PHE:CZ	41:Z:160:GLN:HB2	2.52	0.44
31:q:25:PRO:HG2	31:q:26:ARG:HG2	1.98	0.44
33:s:68:CYS:HA	33:s:71:ASP:OD2	2.17	0.44
39:y:43:LEU:HD12	43:W:87:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:56:GLY:C	5:5:59:PRO:HD2	2.42	0.44
5:5:173:GLU:CD	5:5:189:GLU:H	2.22	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
7:9:28:THR:HG21	31:q:34:MET:SD	2.56	0.44
9:N:26:TRP:HB2	9:N:84:TRP:CE3	2.52	0.44
11:M:220:HIS:CE1	11:M:327:PHE:CE1	3.05	0.44
13:L:68:TRP:HB3	13:L:76:LEU:O	2.17	0.44
13:L:217:ILE:O	13:L:221:THR:HG23	2.18	0.44
20:f:18:THR:HB	20:f:21:GLU:OE2	2.17	0.44
22:h:59:ARG:HG2	22:h:60:ARG:H	1.82	0.44
24:j:15:VAL:HG22	24:j:54:MET:HE1	1.99	0.44
25:k:143:PHE:O	25:k:144:ILE:HB	2.17	0.44
33:s:118:GLU:HA	33:s:121:MET:HG2	1.98	0.44
40:z:34:ARG:HD2	42:Y:90:TYR:CA	2.45	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
5:5:67:HIS:CE1	5:5:69:ASN:HB3	2.52	0.44
5:5:89:ARG:HH12	17:c:95:PHE:HE1	1.66	0.44
5:5:120:SER:HB3	5:5:131:GLU:OE2	2.16	0.44
8:H:309:ILE:HG21	10:A:88:LEU:HD21	1.99	0.44
9:N:91:ASN:CG	9:N:94:ALA:H	2.26	0.44
9:N:135:LYS:HD3	9:N:187:MET:HE2	1.99	0.44
9:N:258:SER:HB3	9:N:333:SER:O	2.16	0.44
11:M:347:GLY:N	11:M:418:LYS:O	2.50	0.44
13:L:4:PHE:CD2	13:L:61:MET:HE3	2.53	0.44
13:L:198:LEU:HD11	13:L:262:ARG:HG3	2.00	0.44
17:c:67:ASN:N	17:c:71:GLY:HA2	2.33	0.44
18:d:23:VAL:HG22	18:d:92:ILE:HD11	1.99	0.44
18:d:203:GLN:CD	18:d:231:VAL:HG13	2.42	0.44
20:f:25:ILE:O	20:f:29:LYS:HG2	2.17	0.44
20:f:46:TYR:CD1	22:h:93:ALA:HB2	2.52	0.44
23:i:1:MET:HG3	23:i:2:GLU:H	1.82	0.44
26:l:47:GLY:C	26:l:49:ILE:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:49:ILE:HG23	26:l:50:ARG:N	2.31	0.44
26:l:85:LEU:HD21	31:q:96:ILE:HG23	2.00	0.44
28:n:74:PHE:HA	28:n:77:PHE:CB	2.42	0.44
31:q:119:MET:HE3	31:q:121:GLY:HA3	1.97	0.44
33:s:99:LYS:O	33:s:103:ARG:HG3	2.18	0.44
33:s:108:LEU:HD11	36:v:132:GLN:HB3	2.00	0.44
35:u:36:ILE:HD12	35:u:36:ILE:HA	1.83	0.44
37:w:96:LEU:HD21	37:w:100:ARG:CZ	2.46	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
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
9:N:76:ILE:HG22	9:N:91:ASN:HD22	1.81	0.44
13:L:68:TRP:CD1	13:L:69:LEU:HG	2.52	0.44
13:L:253:VAL:HG22	13:L:310:LEU:HD13	1.99	0.44
18:d:29:PHE:O	18:d:32:ARG:N	2.51	0.44
18:d:282:ASP:O	18:d:286:ARG:HB2	2.17	0.44
23:i:35:VAL:O	23:i:37:THR:HG23	2.17	0.44
25:k:56:ILE:HG22	25:k:60:ASP:OD2	2.17	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
9:N:68:MET:SD	12:K:37:MET:HE2	2.57	0.44
9:N:85:THR:HG21	43:W:128:ILE:HD13	1.99	0.44
9:N:179:MET:SD	9:N:215:MET:HG2	2.58	0.44
11:M:196:TRP:CZ3	11:M:257:MET:HB3	2.52	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
18:d:93:ASN:O	18:d:94:LEU:HD12	2.17	0.44
25:k:257:HIS:O	25:k:261:MET:N	2.50	0.44
30:p:33:ALA:O	30:p:37:ALA:HB3	2.17	0.44
30:p:66:ARG:HH12	36:v:24:ALA:CB	2.30	0.44
37:w:55:VAL:HG12	37:w:59:ARG:HH12	1.82	0.44
37:w:74:SER:O	37:w:78:ALA:CB	2.57	0.44
40:z:18:ILE:HG23	40:z:19:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:9:152:GLU:OE2	16:b:12:THR:HG21	2.17	0.44
8:H:49:ILE:O	8:H:53:ILE:HG12	2.17	0.44
11:M:307:TRP:CE2	30:p:127:SER:HB2	2.53	0.44
11:M:319:HIS:CE1	11:M:323:SER:HB3	2.53	0.44
13:L:33:PRO:HB3	13:L:118:PHE:CE2	2.51	0.44
13:L:325:ALA:O	13:L:328:HIS:N	2.51	0.44
16:b:24:ARG:HB3	16:b:27:ARG:NH1	2.33	0.44
18:d:200:THR:O	18:d:238:LEU:HD12	2.17	0.44
21:g:117:PHE:O	21:g:120:LYS:N	2.51	0.44
23:i:60:ARG:HD2	23:i:89:TRP:CH2	2.53	0.44
34:t:19:TYR:HD1	34:t:47:PHE:HD2	1.66	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
3:3:60:GLU:OE2	3:3:78:ASN:ND2	2.51	0.44
3:3:343:LEU:HD23	3:3:507:TYR:CE1	2.43	0.44
9:N:167:TRP:CE3	9:N:288:LEU:HD13	2.53	0.44
9:N:224:THR:HG22	9:N:229:SER:HB3	2.00	0.44
9:N:278:LEU:HD23	9:N:282:MET:HE2	2.00	0.44
10:A:3:LEU:O	10:A:6:THR:OG1	2.24	0.44
11:M:258:ALA:HB1	11:M:302:LEU:HD23	1.98	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
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
14:J:57:PHE:CZ	48:J:301:3PE:H352	2.52	0.44
14:J:60:TYR:CZ	14:J:65:MET:HE3	2.52	0.44
14:J:145:ALA:HA	14:J:148:SER:OG	2.17	0.44
18:d:111:VAL:O	18:d:115:GLN:HG3	2.18	0.44
23:i:13:GLN:O	23:i:17:HIS:HB3	2.18	0.44
23:i:115:PHE:CG	23:i:116:ASN:N	2.85	0.44
25:k:198:TYR:O	25:k:202:ILE:HG13	2.18	0.44
33:s:8:TYR:O	33:s:20:ARG:NH2	2.36	0.44
35:u:10:ARG:NH1	35:u:14:PHE:O	2.50	0.44
38:x:4:ILE:H	38:x:4:ILE:HD12	1.83	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:6:72:PHE:HA	8:H:39:VAL:HB	2.00	0.44
7:9:56:PRO:HG3	23:i:56:PHE:HZ	1.83	0.44
8:H:102:VAL:HG13	8:H:162:LEU:HB2	1.98	0.44
8:H:114:TYR:OH	14:J:65:MET:HB2	2.16	0.44
8:H:220:PHE:O	8:H:224:PHE:HB2	2.18	0.44
9:N:85:THR:HG22	26:l:18:THR:CG2	2.48	0.44
10:A:24:LEU:HA	10:A:27:LEU:HB3	2.00	0.44
11:M:78:MET:HE2	37:w:61:VAL:HG21	2.00	0.44
11:M:442:LEU:O	11:M:446:LEU:HG	2.18	0.44
19:e:22:LEU:HD21	19:e:32:VAL:HB	1.99	0.44
21:g:45:THR:O	21:g:48:LEU:N	2.50	0.44
37:w:82:ASP:N	37:w:82:ASP:OD1	2.51	0.44
43:W:62:GLU:HG3	43:W:63:HIS:N	2.33	0.44
1:1:60:VAL:O	1:1:63:SER:OG	2.27	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
8:H:316:PRO:HA	31:q:57:ARG:HE	1.83	0.44
9:N:4:ILE:HG21	49:A:200:PC1:O12	2.18	0.44
9:N:80:PHE:O	9:N:81:SER:C	2.61	0.44
11:M:84:LEU:C	11:M:86:LYS:H	2.25	0.44
11:M:244:MET:O	11:M:247:THR:HG22	2.17	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
14:J:62:GLY:O	14:J:66:VAL:CB	2.63	0.44
18:d:141:SER:HA	18:d:147:ARG:HE	1.83	0.44
18:d:203:GLN:HB3	18:d:236:TYR:HA	2.00	0.44
25:k:28:ASP:O	25:k:171:TYR:HA	2.18	0.44
25:k:210:PHE:HA	25:k:213:GLU:HB3	1.99	0.44
31:q:142:TYR:OH	40:z:36:LYS:HE3	2.17	0.44
35:u:10:ARG:NH1	35:u:16:GLN:HE21	2.12	0.44
43:W:69:HIS:CG	43:W:70:PRO:HD2	2.53	0.44
1:1:176:PHE:HE1	15:a:62:ARG:HD2	1.82	0.43
2:2:42:HIS:O	2:2:44:ALA:N	2.51	0.43
3:3:127:ARG:HH22	4:4:326:ASP:CG	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:30:ALA:CB	22:h:68:VAL:HG11	2.45	0.43
7:9:63:GLY:N	7:9:134:GLY:O	2.50	0.43
7:9:113:MET:HE3	7:9:118:TYR:OH	2.18	0.43
8:H:104:PHE:CE2	8:H:108:MET:HE2	2.53	0.43
9:N:211:MET:HB3	9:N:211:MET:HE3	1.76	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
17:c:123:SER:O	17:c:129:ARG:NH2	2.51	0.43
18:d:202:LYS:O	18:d:237:LEU:N	2.51	0.43
20:f:5:LYS:HE2	20:f:15:VAL:HB	1.99	0.43
32:r:71:PHE:O	32:r:75:LEU:HB2	2.18	0.43
34:t:50:HIS:HE2	54:X:401:PNS:H41	1.65	0.43
34:t:103:LEU:HA	34:t:106:TRP:CD1	2.53	0.43
37:w:47:TYR:HB3	37:w:48:ASP:H	1.62	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
3:3:94:MET:HE3	3:3:120:SER:HA	2.00	0.43
6:6:72:PHE:CD1	8:H:39:VAL:HG21	2.53	0.43
6:6:75:VAL:HG22	8:H:25:ARG:CZ	2.49	0.43
11:M:200:MET:O	11:M:204:MET:HG2	2.18	0.43
12:K:46:LEU:HD21	14:J:43:ILE:HG22	1.98	0.43
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
20:f:34:LEU:HD23	20:f:44:ARG:HG3	1.99	0.43
25:k:238:ILE:O	25:k:242:LYS:CB	2.66	0.43
31:q:70:LEU:HA	31:q:70:LEU:HD23	1.77	0.43
37:w:45:HIS:CD2	37:w:47:TYR:CE2	3.07	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
4:4:87:THR:O	4:4:90:LEU:N	2.51	0.43
4:4:96:TYR:HE1	4:4:386:PRO:HB3	1.83	0.43
4:4:144:ILE:HG23	4:4:177:MET:HE3	1.99	0.43
4:4:233:ARG:O	4:4:237:ASN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:233:ARG:NH1	7:9:24:THR:HA	2.34	0.43
5:5:67:HIS:O	5:5:69:ASN:N	2.49	0.43
6:6:34:ASP:OD1	6:6:173:LEU:HB3	2.19	0.43
6:6:178:ARG:NH1	52:d:401:NDP:O1X	2.46	0.43
8:H:303:TRP:CZ3	8:H:307:LEU:HD22	2.54	0.43
9:N:26:TRP:CD1	9:N:85:THR:O	2.72	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
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
11:M:142:ARG:C	11:M:144:ASN:N	2.77	0.43
11:M:173:SER:HB2	43:W:101:ALA:HB2	2.00	0.43
11:M:186:MET:SD	11:M:195:MET:HE1	2.58	0.43
11:M:210:TYR:CB	11:M:268:GLY:HA3	2.48	0.43
13:L:28:LYS:HE3	13:L:29:PHE:CE1	2.53	0.43
13:L:165:ASN:OD1	13:L:166:THR:N	2.52	0.43
17:c:52:THR:HG22	17:c:53:LYS:N	2.29	0.43
18:d:235:ARG:HH11	18:d:237:LEU:HD21	1.82	0.43
19:e:23:CYS:SG	19:e:24:GLN:N	2.91	0.43
21:g:16:VAL:CG1	21:g:76:ARG:HD3	2.48	0.43
50:i:201:CDL:OB3	50:i:201:CDL:O1	2.31	0.43
25:k:182:ARG:HA	25:k:185:LYS:HD2	2.00	0.43
28:n:62:PHE:C	28:n:64:GLY:H	2.26	0.43
34:t:89:SER:HA	34:t:92:ARG:CG	2.47	0.43
36:v:60:PRO:O	36:v:61:TRP:C	2.61	0.43
42:Y:81:PHE:HD1	42:Y:106:PHE:CE1	2.37	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
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
3:3:324:ASP:CG	3:3:327:ALA:H	2.27	0.43
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.99	0.43
5:5:32:ILE:HD12	5:5:63:PHE:CZ	2.54	0.43
5:5:36:TYR:CD2	5:5:56:GLY:HA3	2.53	0.43
6:6:70:ASP:CG	8:H:34:ARG:HH12	2.21	0.43
6:6:107:MET:HB3	6:6:111:ARG:NE	2.33	0.43
9:N:9:ILE:O	9:N:12:THR:N	2.50	0.43
10:A:101:SER:HB2	14:J:165:VAL:HG21	2.00	0.43
11:M:346:ARG:HG2	11:M:413:THR:O	2.19	0.43
13:L:411:MET:O	13:L:415:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:133:SER:HB2	18:d:149:LYS:HZ3	1.83	0.43
21:g:63:ARG:HB2	24:j:45:LEU:HD21	2.00	0.43
29:o:116:PHE:CD1	29:o:116:PHE:O	2.71	0.43
36:v:27:TYR:O	36:v:31:VAL:N	2.28	0.43
40:z:3:PHE:HD1	40:z:6:LEU:HD21	1.83	0.43
7:9:34:LEU:HD23	8:H:276:SER:HB3	2.00	0.43
13:L:32:TYR:OH	13:L:115:ASN:O	2.32	0.43
13:L:479:GLN:O	13:L:481:THR:N	2.48	0.43
13:L:483:PRO:HG3	35:u:51:PHE:CD1	2.52	0.43
18:d:134:HIS:H	18:d:149:LYS:NZ	2.17	0.43
26:l:93:PRO:HG2	26:l:94:PRO:HD3	2.00	0.43
30:p:98:ILE:O	30:p:101:TYR:HB3	2.18	0.43
40:z:66:LEU:HD21	42:Y:73:ILE:HG23	2.00	0.43
43:W:87:TYR:O	43:W:90:THR:OG1	2.27	0.43
1:1:24:ASN:HB2	1:1:39:ARG:NH1	2.34	0.43
1:1:36:ALA:HA	1:1:39:ARG:HE	1.83	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:OE1	3:3:577:GLU:N	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
8:H:269:THR:O	8:H:272:TRP:C	2.62	0.43
9:N:75:ILE:HD12	12:K:40:LEU:HD22	2.00	0.43
11:M:8:THR:O	11:M:11:LEU:HB3	2.18	0.43
12:K:11:ALA:HB1	14:J:17:PHE:CD2	2.53	0.43
12:K:42:ILE:O	12:K:46:LEU:HG	2.19	0.43
18:d:228:PHE:HB2	18:d:298:PRO:O	2.18	0.43
19:e:29:SER:O	19:e:33:ARG:HG3	2.19	0.43
21:g:28:LYS:O	21:g:32:ARG:HG3	2.18	0.43
23:i:79:GLY:C	23:i:81:MET:H	2.27	0.43
25:k:95:ARG:O	25:k:99:TRP:CB	2.66	0.43
30:p:29:ARG:O	30:p:33:ALA:CB	2.63	0.43
36:v:104:HIS:O	36:v:107:GLY:N	2.52	0.43
37:w:96:LEU:O	37:w:100:ARG:HG2	2.18	0.43
41:Z:21:PRO:C	41:Z:23:THR:H	2.25	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
4:4:69:SER:N	4:4:72:MET:O	2.40	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
5:5:72:PHE:CE1	5:5:98:SER:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:132:ARG:HH21	5:5:147:ASP:HB3	1.84	0.43
7:9:53:GLU:HG2	23:i:61:TRP:HB3	1.99	0.43
7:9:126:CYS:HA	45:9:503:SF4:S3	2.58	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
10:A:81:THR:N	27:m:45:ASN:HD21	2.16	0.43
11:M:47:ASP:CB	41:Z:92:LYS:HD2	2.49	0.43
50:L:601:CDL:OA7	50:L:601:CDL:H592	2.19	0.43
17:c:16:LYS:O	21:g:14:THR:OG1	2.37	0.43
22:h:42:VAL:HG11	22:h:46:HIS:CG	2.54	0.43
23:i:29:ARG:HG2	23:i:74:PHE:CZ	2.54	0.43
23:i:94:THR:HG22	23:i:96:ASP:H	1.84	0.43
27:m:81:LYS:HB2	42:Y:121:LEU:HD21	2.00	0.43
31:q:142:TYR:HE1	40:z:39:ALA:H	1.67	0.43
33:s:102:GLU:O	33:s:106:ARG:HG2	2.19	0.43
40:z:51:ASP:OD1	42:Y:21:SER:N	2.48	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
4:4:284:ASP:OD1	4:4:284:ASP:N	2.50	0.43
7:9:150:ASN:ND2	23:i:127:TYR:O	2.51	0.43
8:H:165:LEU:O	8:H:169:GLN:HG2	2.17	0.43
11:M:419:HIS:HD1	11:M:421:HIS:HB3	1.83	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
18:d:68:ILE:O	18:d:68:ILE:HG13	2.19	0.43
18:d:281:ARG:HA	18:d:284:VAL:CG2	2.48	0.43
20:f:30:ILE:O	20:f:34:LEU:HB2	2.18	0.43
25:k:282:VAL:C	25:k:285:GLY:H	2.27	0.43
26:l:26:HIS:O	26:l:28:ILE:HG23	2.18	0.43
26:l:46:ILE:HD11	42:Y:147:PRO:HB2	2.00	0.43
3:3:121:MET:O	4:4:329:LYS:HE2	2.19	0.43
3:3:364:LEU:HB2	3:3:492:ILE:O	2.18	0.43
3:3:368:ILE:H	3:3:368:ILE:HD12	1.83	0.43
3:3:620:ARG:HA	3:3:623:LEU:HB3	2.01	0.43
5:5:78:LEU:HB3	5:5:130:TYR:HB3	2.00	0.43
5:5:117:VAL:HB	5:5:142:PHE:HE1	1.84	0.43
5:5:137:MET:HA	5:5:161:PRO:HD2	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
11:M:241:TYR:O	11:M:244:MET:HB2	2.18	0.43
13:L:98:TRP:HZ2	13:L:456:ARG:NH1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:226:GLN:NE2	13:L:280:LEU:HG	2.33	0.43
14:J:93:PHE:O	14:J:97:LEU:CB	2.66	0.43
18:d:110:PHE:HD2	18:d:149:LYS:HB2	1.84	0.43
23:i:51:ASP:C	23:i:53:LYS:H	2.25	0.43
30:p:66:ARG:HG2	36:v:6:LYS:O	2.18	0.43
31:q:113:THR:O	31:q:114:ARG:HG2	2.19	0.43
32:r:27:LEU:CG	32:r:32:PRO:HG2	2.48	0.43
32:r:78:VAL:HG11	41:Z:40:VAL:HG21	2.00	0.43
32:r:82:HIS:CE1	32:r:86:LYS:HD3	2.53	0.43
34:t:77:GLN:O	34:t:77:GLN:HG2	2.17	0.43
35:u:30:ALA:O	35:u:34:PHE:CB	2.67	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
8:H:62:ARG:O	8:H:215:TYR:HE1	2.01	0.43
8:H:138:GLN:HA	8:H:286:MET:HE1	2.00	0.43
8:H:269:THR:O	8:H:273:ILE:HG13	2.19	0.43
9:N:302:LEU:HD22	11:M:91:ARG:CZ	2.49	0.43
9:N:311:MET:C	9:N:313:MET:H	2.27	0.43
10:A:63:LEU:HA	10:A:63:LEU:HD23	1.79	0.43
11:M:7:PRO:HB2	11:M:34:ILE:HD12	2.00	0.43
11:M:102:LEU:HD21	11:M:230:VAL:HG11	2.01	0.43
11:M:141:GLU:C	11:M:143:LEU:H	2.27	0.43
13:L:67:HIS:HA	13:L:77:SER:HB3	2.01	0.43
13:L:396:ILE:O	13:L:400:ASN:CB	2.56	0.43
16:b:31:ARG:HE	23:i:125:VAL:CG1	2.31	0.43
21:g:51:LEU:HD22	21:g:103:MET:SD	2.58	0.43
23:i:56:PHE:CG	23:i:57:GLY:N	2.87	0.43
25:k:69:LEU:HD13	25:k:73:PHE:CD2	2.54	0.43
33:s:17:GLU:HB3	33:s:18:PRO:CD	2.48	0.43
34:t:26:LEU:HD22	34:t:43:LEU:HD12	2.01	0.43
35:u:53:TYR:CG	35:u:54:PRO:HD2	2.54	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
3:3:111:GLY:O	4:4:349:PHE:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:85:THR:CG2	17:c:87:SER:H	2.31	0.42
7:9:21:ALA:O	7:9:25:LEU:CB	2.67	0.42
11:M:151:PHE:O	11:M:155:ALA:HB2	2.19	0.42
11:M:325:MET:SD	11:M:441:MET:HE3	2.58	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:12:LEU:HD12	32:r:81:ILE:CD1	2.48	0.42
13:L:161:ARG:NH2	13:L:238:GLU:OE1	2.52	0.42
13:L:386:LEU:HD12	35:u:36:ILE:CD1	2.48	0.42
13:L:458:LEU:HD12	13:L:459:ILE:N	2.33	0.42
17:c:59:PHE:HD2	17:c:79:LEU:HB3	1.84	0.42
22:h:94:VAL:HG12	22:h:95:SER:O	2.18	0.42
26:l:15:HIS:HA	26:l:18:THR:OG1	2.19	0.42
34:t:25:HIS:O	34:t:29:ARG:HG2	2.18	0.42
34:t:29:ARG:NH1	34:t:75:HIS:HB3	2.34	0.42
39:y:42:LEU:HA	39:y:45:LYS:HE2	2.01	0.42
41:Z:86:GLU:HG3	43:W:91:MET:HE1	2.01	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
8:H:39:VAL:HA	23:i:31:ASN:ND2	2.34	0.42
8:H:179:TRP:HE1	31:q:42:LEU:HG	1.84	0.42
9:N:72:MET:O	9:N:76:ILE:HG12	2.19	0.42
11:M:237:LYS:NZ	11:M:319:HIS:HD2	2.16	0.42
12:K:12:PHE:O	12:K:15:SER:OG	2.27	0.42
13:L:99:SER:HB3	13:L:341:MET:HE1	2.01	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
18:d:19:ILE:HD11	18:d:38:LEU:HD22	2.00	0.42
18:d:132:ILE:HG22	18:d:166:ILE:HG23	2.01	0.42
18:d:206:TYR:CD2	18:d:208:VAL:HG22	2.54	0.42
21:g:27:ALA:HB1	21:g:78:VAL:HG11	2.00	0.42
24:j:55:GLU:HA	24:j:60:PHE:H	1.84	0.42
25:k:137:ALA:HA	25:k:140:ARG:HB2	2.01	0.42
25:k:155:VAL:O	25:k:159:THR:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:44:TRP:HB3	34:t:37:ARG:NH2	2.23	0.42
31:q:97:MET:HE2	31:q:103:TRP:HE1	1.84	0.42
40:z:63:SER:HB3	42:Y:20:SER:HB3	2.00	0.42
41:Z:88:GLU:HG2	41:Z:151:ALA:CB	2.49	0.42
42:Y:35:CYS:O	42:Y:36:ASP:HB2	2.19	0.42
8:H:146:LEU:HG	8:H:185:TRP:NE1	2.34	0.42
9:N:83:GLN:HG3	26:l:19:ILE:HG22	2.02	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
11:M:108:MET:HB3	11:M:121:MET:HG3	2.01	0.42
11:M:233:ALA:HB2	11:M:324:SER:HB2	2.01	0.42
11:M:234:ILE:O	11:M:237:LYS:N	2.53	0.42
11:M:278:ARG:NH1	30:p:71:ARG:HH22	2.16	0.42
13:L:14:LEU:HD23	13:L:14:LEU:HA	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
16:b:64:GLY:C	16:b:66:LEU:H	2.26	0.42
18:d:244:TYR:HE1	18:d:331:ILE:HA	1.83	0.42
35:u:8:GLU:OE1	35:u:16:GLN:HG3	2.19	0.42
42:Y:82:THR:HA	42:Y:85:TRP:CD1	2.54	0.42
24:X:58:PHE:HB3	24:X:60:PHE:HE2	1.82	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
2:2:106:THR:O	2:2:107:PRO:C	2.63	0.42
3:3:10:GLU:HG3	3:3:17:SER:OG	2.19	0.42
4:4:149:ASN:ND2	4:4:371:LYS:HG3	2.34	0.42
4:4:152:MET:HG3	4:4:171:PHE:HZ	1.84	0.42
7:9:117:ILE:HG22	45:9:502:SF4:S3	2.60	0.42
9:N:26:TRP:CH2	9:N:98:MET:HE1	2.54	0.42
10:A:66:ASP:O	10:A:69:ILE:N	2.53	0.42
11:M:84:LEU:CD1	11:M:85:SER:H	2.20	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
13:L:4:PHE:HE2	13:L:59:GLN:HG3	1.84	0.42
13:L:32:TYR:O	13:L:33:PRO:C	2.61	0.42
13:L:476:THR:N	33:s:54:GLN:OE1	2.52	0.42
17:c:70:MET:HE2	23:i:126:PRO:HB2	2.00	0.42
20:f:54:LYS:HG3	20:f:71:LEU:HD11	2.01	0.42
22:h:6:LEU:O	22:h:10:LEU:HG	2.19	0.42
23:i:10:GLY:O	23:i:14:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:37:MET:HA	24:j:42:LEU:H	1.84	0.42
26:l:13:LEU:O	26:l:16:TRP:NE1	2.52	0.42
38:x:14:TRP:HA	38:x:17:VAL:HG22	2.02	0.42
40:z:27:HIS:O	40:z:31:ASN:HB2	2.18	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
9:N:128:LEU:HA	9:N:216:PHE:HD2	1.85	0.42
12:K:7:ASN:HA	12:K:10:MET:HE3	2.02	0.42
13:L:2:ASN:O	13:L:5:SER:N	2.52	0.42
13:L:62:ILE:HG12	13:L:199:GLN:HE22	1.84	0.42
50:L:601:CDL:HA21	50:L:601:CDL:HB31	2.01	0.42
15:a:58:LEU:HB3	15:a:62:ARG:NH1	2.34	0.42
18:d:25:GLY:C	18:d:27:THR:H	2.28	0.42
18:d:27:THR:HB	52:d:401:NDP:O3B	2.20	0.42
21:g:118:LEU:O	21:g:122:TYR:CB	2.67	0.42
24:j:11:ILE:HD11	24:j:80:ILE:HB	2.00	0.42
28:n:18:TYR:CZ	24:X:20:LYS:HB3	2.55	0.42
37:w:58:MET:HE1	43:W:24:LEU:HD13	1.99	0.42
42:Y:25:LYS:NZ	42:Y:94:GLN:O	2.49	0.42
42:Y:108:LYS:O	42:Y:112:ASP:HB2	2.20	0.42
1:1:199:LYS:NZ	17:c:131:SER:HA	2.34	0.42
2:2:61:LEU:HD12	2:2:61:LEU:O	2.20	0.42
3:3:266:LYS:NZ	3:3:675:ASP:OD2	2.39	0.42
4:4:163:ALA:HB2	8:H:278:PRO:HG3	2.02	0.42
5:5:167:PRO:HA	17:c:82:LEU:HD21	2.01	0.42
8:H:226:ALA:O	8:H:230:ASN:HB2	2.20	0.42
9:N:337:LEU:N	9:N:338:PRO:HD2	2.35	0.42
11:M:50:LEU:HD13	11:M:52:PHE:CE1	2.54	0.42
11:M:196:TRP:HD1	11:M:250:LEU:HB3	1.85	0.42
12:K:54:THR:HG22	26:l:24:GLN:NE2	2.34	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
20:f:91:ARG:HA	20:f:94:ILE:HD13	2.01	0.42
29:o:109:TYR:HE2	41:Z:84:MET:HE2	1.84	0.42
36:v:67:PRO:O	36:v:69:LEU:N	2.53	0.42
36:v:112:MET:HA	36:v:115:MET:HB2	2.02	0.42
2:2:79:ARG:NE	17:c:131:SER:HB3	2.16	0.42
3:3:381:GLY:HA3	3:3:661:LEU:HD11	2.01	0.42
3:3:568:GLU:HG3	3:3:587:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:184:VAL:HG11	21:g:109:THR:HG21	2.00	0.42
9:N:24:THR:N	26:l:14:ASP:OD2	2.51	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
11:M:424:ASN:HA	34:t:101:TRP:CD2	2.54	0.42
12:K:47:MET:HE2	12:K:47:MET:HB3	1.69	0.42
13:L:145:GLU:OE2	13:L:176:ARG:NH1	2.53	0.42
14:J:23:LYS:HG2	14:J:85:SER:O	2.20	0.42
18:d:88:SER:HB3	18:d:90:VAL:O	2.20	0.42
18:d:182:PHE:O	18:d:185:ILE:HG22	2.19	0.42
18:d:281:ARG:HB3	18:d:285:GLU:CD	2.45	0.42
21:g:28:LYS:NZ	53:j:101:ZMP:H20B	2.33	0.42
24:j:49:GLU:O	24:j:52:MET:HB3	2.20	0.42
24:j:73:PRO:O	24:j:77:VAL:HG23	2.19	0.42
26:l:58:GLU:O	26:l:61:ASP:HB3	2.19	0.42
29:o:1:MET:HG2	29:o:2:MET:HG3	2.01	0.42
31:q:85:MET:HE2	31:q:123:LEU:C	2.45	0.42
33:s:107:LEU:HD23	33:s:107:LEU:HA	1.83	0.42
37:w:62:PHE:CD1	37:w:66:PHE:HE2	2.37	0.42
38:x:25:ALA:O	38:x:29:ILE:HG22	2.19	0.42
41:Z:152:ARG:O	41:Z:156:ALA:HB2	2.19	0.42
1:1:106:LYS:HD2	1:1:331:THR:HB	2.01	0.42
1:1:276:LEU:HD21	1:1:297:VAL:HG11	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
7:9:53:GLU:OE2	23:i:58:ARG:HG3	2.19	0.42
8:H:1:MET:HG3	8:H:2:PHE:N	2.34	0.42
8:H:26:LYS:HD3	40:z:4:GLU:HG2	2.02	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
18:d:129:PHE:CE2	18:d:131:HIS:HB2	2.55	0.42
23:i:34:ARG:NH2	23:i:51:ASP:OD2	2.53	0.42
26:l:12:ASP:OD1	26:l:15:HIS:HB2	2.20	0.42
31:q:108:SER:HB2	42:Y:4:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:v:108:PHE:O	36:v:111:PHE:HB3	2.20	0.42
40:z:38:VAL:HB	40:z:40:HIS:CE1	2.55	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
8:H:145:THR:HG22	8:H:149:ILE:CD1	2.49	0.42
9:N:240:MET:O	9:N:244:VAL:HG23	2.19	0.42
9:N:265:MET:HE1	42:Y:166:LEU:HD11	2.01	0.42
10:A:90:MET:SD	14:J:151:THR:HA	2.60	0.42
10:A:96:PHE:CE1	49:A:200:PC1:H3B2	2.55	0.42
11:M:78:MET:HG3	11:M:436:LEU:HD11	2.01	0.42
13:L:418:PHE:CA	13:L:421:ILE:HG12	2.48	0.42
13:L:484:HIS:C	13:L:486:LEU:H	2.27	0.42
18:d:200:THR:HA	18:d:290:THR:OG1	2.19	0.42
20:f:83:ALA:O	20:f:86:GLU:HB3	2.20	0.42
22:h:8:GLN:HE22	22:h:19:LEU:HD22	1.84	0.42
24:j:13:ASP:O	24:j:17:TYR:CB	2.67	0.42
26:l:12:ASP:CG	26:l:15:HIS:HB2	2.44	0.42
26:l:35:PHE:CD2	26:l:65:CYS:HB2	2.54	0.42
29:o:1:MET:HE1	43:W:111:ARG:NH2	2.34	0.42
29:o:110:ARG:HE	37:w:119:GLN:HG2	1.83	0.42
30:p:94:ILE:O	30:p:98:ILE:HG22	2.19	0.42
34:t:138:GLN:NE2	34:t:156:ALA:HA	2.32	0.42
40:z:7:PRO:O	40:z:11:VAL:HG23	2.20	0.42
41:Z:92:LYS:O	41:Z:95:TYR:HB3	2.19	0.42
42:Y:110:VAL:O	42:Y:114:LEU:N	2.51	0.42
43:W:78:THR:HG23	43:W:79:PHE:CD1	2.55	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
8:H:249:PRO:HG2	42:Y:98:ARG:NH2	2.35	0.42
9:N:293:TYR:O	9:N:297:THR:HG23	2.19	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
12:K:12:PHE:CD1	12:K:36:MET:HG3	2.55	0.42
12:K:57:SER:C	12:K:58:MET:HE2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:368:PHE:HE2	13:L:454:ILE:HB	1.83	0.42
13:L:385:PHE:O	13:L:385:PHE:CG	2.73	0.42
16:b:3:ARG:O	16:b:11:VAL:HG22	2.19	0.42
25:k:205:VAL:O	25:k:209:THR:CB	2.68	0.42
26:l:3:PHE:HD2	49:o:201:PC1:H3F1	1.85	0.42
27:m:69:PRO:O	42:Y:126:LYS:NZ	2.51	0.42
29:o:115:GLU:C	29:o:116:PHE:CD2	2.98	0.42
34:t:133:GLU:O	34:t:137:LYS:HG2	2.20	0.42
3:3:221:GLU:HG2	5:5:197:PHE:HE1	1.85	0.41
4:4:84:HIS:CD2	5:5:152:LEU:HD22	2.54	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
4:4:216:LYS:HA	31:q:18:ILE:CD1	2.50	0.41
9:N:340:THR:HG23	9:N:343:LEU:HB2	2.00	0.41
11:M:1:MET:HB3	11:M:56:PHE:CE1	2.55	0.41
11:M:453:ILE:HD11	37:w:77:VAL:HB	2.02	0.41
13:L:176:ARG:O	13:L:179:ASP:HB3	2.20	0.41
13:L:487:LYS:NZ	13:L:488:MET:HE3	2.35	0.41
28:n:28:LEU:HD12	28:n:49:ALA:HB2	2.02	0.41
29:o:28:ASP:OD1	29:o:29:PRO:HD2	2.20	0.41
29:o:111:GLU:O	29:o:112:VAL:HG23	2.20	0.41
33:s:88:TYR:O	33:s:91:HIS:HB3	2.20	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
3:3:468:ALA:O	3:3:471:SER:OG	2.34	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
5:5:208:ALA:HB1	22:h:63:MET:HG3	2.01	0.41
7:9:38:LEU:HD22	8:H:276:SER:OG	2.20	0.41
8:H:306:SER:HB2	27:m:32:PRO:CG	2.50	0.41
11:M:41:LEU:HD23	11:M:41:LEU:O	2.19	0.41
11:M:305:THR:O	11:M:308:SER:HB3	2.20	0.41
12:K:45:THR:HG21	14:J:44:VAL:HG13	2.00	0.41
13:L:88:MET:CE	13:L:468:ILE:HG12	2.50	0.41
13:L:120:TYR:CE1	13:L:153:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:28:TYR:HD1	14:J:31:LEU:HD12	1.86	0.41
18:d:122:LYS:HB2	18:d:160:PHE:CD1	2.54	0.41
18:d:278:TRP:CG	18:d:279:THR:N	2.88	0.41
18:d:283:LYS:O	18:d:286:ARG:HB3	2.19	0.41
20:f:34:LEU:HD11	20:f:47:THR:OG1	2.21	0.41
21:g:43:PRO:HA	21:g:46:VAL:HG12	2.00	0.41
21:g:66:PHE:HD1	53:j:101:ZMP:H12	1.84	0.41
22:h:7:ILE:HG13	22:h:8:GLN:N	2.34	0.41
22:h:26:ARG:HD3	23:i:55:PHE:HB2	2.02	0.41
26:l:16:TRP:CE3	26:l:17:MET:HB3	2.55	0.41
29:o:16:ASP:HA	29:o:19:ARG:NH1	2.34	0.41
32:r:105:PRO:HG3	33:s:44:GLU:HB3	2.01	0.41
42:Y:44:LEU:O	42:Y:48:GLU:HB2	2.20	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
3:3:116:LEU:HD23	3:3:116:LEU:HA	1.89	0.41
3:3:230:VAL:C	3:3:232:ASP:H	2.28	0.41
4:4:51:PHE:CD2	4:4:63:ARG:HA	2.56	0.41
7:9:38:LEU:C	7:9:40:TYR:N	2.78	0.41
8:H:200:LEU:H	8:H:200:LEU:HG	1.75	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:HE2	13:L:364:LYS:HB2	1.83	0.41
13:L:374:ILE:HD11	35:u:32:MET:HE1	2.02	0.41
14:J:9:LEU:HD13	14:J:42:GLY:HA3	2.02	0.41
22:h:68:VAL:O	22:h:68:VAL:HG12	2.20	0.41
23:i:68:MET:HE1	23:i:81:MET:O	2.20	0.41
25:k:56:ILE:HD11	25:k:77:CYS:CB	2.48	0.41
27:m:52:TYR:CZ	42:Y:43:MET:HG3	2.56	0.41
28:n:62:PHE:CG	28:n:63:VAL:N	2.88	0.41
34:t:29:ARG:HH21	34:t:73:GLY:C	2.28	0.41
34:t:89:SER:OG	34:t:90:TYR:N	2.52	0.41
42:Y:95:LEU:HB2	42:Y:98:ARG:HG2	2.02	0.41
43:W:83:PRO:O	43:W:87:TYR:HB2	2.20	0.41
1:1:181:ALA:HB2	2:2:48:LEU:HD11	2.02	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
7:9:43:ARG:HG2	22:h:11:ARG:NH1	2.35	0.41
48:9:501:3PE:H3C2	27:m:24:ILE:HD11	2.02	0.41
8:H:153:VAL:HG11	8:H:242:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:213:VAL:HG13	8:H:220:PHE:CE1	2.56	0.41
9:N:328:THR:HG23	29:o:68:PHE:HZ	1.85	0.41
10:A:9:THR:O	10:A:12:THR: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
12:K:70:GLU:O	12:K:73:LEU:HB3	2.20	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
14:J:34:ILE:HG22	14:J:65:MET:HG3	2.02	0.41
15:a:58:LEU:HB3	15:a:62:ARG:HH12	1.86	0.41
26:l:82:ARG:HA	26:l:85:LEU:HG	2.01	0.41
27:m:77:LEU:HA	27:m:79:TRP:NE1	2.35	0.41
28:n:70:PHE:HB2	28:n:74:PHE:CE2	2.55	0.41
34:t:135:GLU:HG3	34:t:163:PRO:CB	2.47	0.41
42:Y:26:ALA:HB1	42:Y:84:TYR:HE2	1.85	0.41
42:Y:131:LYS:HE3	42:Y:131:LYS:HB3	1.88	0.41
24:X:54:MET:O	24:X:57:GLU:HB2	2.20	0.41
44:V:89:UNK:O	44:V:93:UNK:CB	2.67	0.41
1:1:46:LYS:HE3	1:1:169:SER:HA	2.02	0.41
1:1:111:ILE:HD13	1:1:138:ILE:HD12	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
8:H:96:ILE:HG22	8:H:98:MET:HG3	2.01	0.41
8:H:314:ILE:HG13	31:q:57:ARG:HH22	1.85	0.41
9:N:40:ILE:HG21	9:N:134:GLN:NE2	2.34	0.41
10:A:103:ALA:O	10:A:107:THR:HG23	2.20	0.41
11:M:160:LEU:HD23	11:M:202:ALA:HB1	2.01	0.41
11:M:190:TRP:O	11:M:193:THR:HB	2.19	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
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
23:i:55:PHE:HE1	23:i:58:ARG:HD2	1.86	0.41
25:k:93:SER:O	25:k:96:LEU:HB2	2.20	0.41
26:l:90:LYS:HA	26:l:90:LYS:HD2	1.90	0.41
27:m:75:PRO:HD2	42:Y:126:LYS:HG2	2.02	0.41
28:n:20:GLN:HE21	28:n:22:LYS:NZ	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:24:GLU:C	28:n:26:THR:H	2.29	0.41
28:n:32:GLN:NE2	28:n:42:ASP:HB3	2.35	0.41
29:o:88:HIS:CE1	42:Y:153:VAL:HG13	2.56	0.41
31:q:85:MET:HE1	31:q:124:TYR:CD1	2.55	0.41
32:r:3:TYR:HB2	32:r:8:LYS:HZ1	1.86	0.41
34:t:34:ASP:O	34:t:37:ARG:HB2	2.20	0.41
35:u:29:SER:HA	35:u:32:MET:CE	2.37	0.41
36:v:137:ASN:OD1	36:v:138:LEU:N	2.54	0.41
1:1:26:TYR:HE1	2:2:195:PRO:HD3	1.86	0.41
1:1:241:TRP:O	1:1:244:SER:OG	2.37	0.41
1:1:299:PRO:HA	1:1:334:VAL:HG12	2.03	0.41
2:2:153:MET:HE1	2:2:160:TYR:CD1	2.55	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
3:3:521:MET:HE3	3:3:542:PHE:HE2	1.85	0.41
4:4:186:GLY:O	7:9:61:PHE:HA	2.21	0.41
6:6:144:ILE:HG13	6:6:163:LEU:HB2	2.02	0.41
7:9:39:SER:C	7:9:41:LEU:H	2.28	0.41
7:9:128:VAL:HG12	16:b:68:HIS:HA	2.03	0.41
8:H:27:VAL:HG23	40:z:5:VAL:HG21	2.03	0.41
8:H:60:PRO:CD	10:A:25:PRO:HB2	2.50	0.41
8:H:312:SER:OG	27:m:40:TYR:HB2	2.20	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
12:K:37:MET:HE3	12:K:37:MET:HB2	1.99	0.41
13:L:363:PHE:CE1	13:L:367:PRO:HG3	2.56	0.41
13:L:436:ARG:CZ	34:t:31:VAL:HG23	2.50	0.41
14:J:45:LEU:CD2	14:J:50:SER:HA	2.51	0.41
22:h:2:SER:O	22:h:4:THR:HG23	2.19	0.41
23:i:130:THR:HG22	23:i:131:ARG:N	2.30	0.41
25:k:97:GLN:HE22	25:k:134:PHE:HE2	1.69	0.41
30:p:34:GLU:O	30:p:38:ILE:HG22	2.19	0.41
31:q:32:TYR:O	31:q:35:PHE:N	2.53	0.41
37:w:62:PHE:HA	37:w:66:PHE:CD2	2.55	0.41
40:z:55:SER:O	40:z:64:LYS:HE2	2.20	0.41
41:Z:49:GLU:O	41:Z:52:GLU:HB2	2.19	0.41
24:X:43:ASP:HB3	24:X:46:ASP:CB	2.47	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
3:3:127:ARG:HH11	22:h:46:HIS:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:4:253:TYR:C	5:5:126:ALA:HB2	2.46	0.41
8:H:308:PRO:HB2	8:H:314:ILE:HG22	2.02	0.41
9:N:25:HIS:CE1	26:l:17:MET:HE2	2.55	0.41
9:N:144:GLN:NE2	26:l:2:PHE:HB2	2.31	0.41
11:M:50:LEU:HA	43:W:86:ASN:ND2	2.33	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
16:b:75:LEU:HD21	16:b:91:PHE:HB2	2.02	0.41
18:d:154:LYS:O	18:d:158:GLU:HG3	2.20	0.41
18:d:166:ILE:HD11	18:d:230:PHE:CE2	2.56	0.41
18:d:301:GLU:O	18:d:304:GLY:N	2.53	0.41
22:h:8:GLN:HB2	22:h:11:ARG:HH21	1.85	0.41
23:i:71:LYS:HD2	23:i:72:ASN:H	1.86	0.41
25:k:75:GLY:O	25:k:95:ARG:NH1	2.50	0.41
25:k:104:ARG:HG2	25:k:131:ASP:OD2	2.20	0.41
31:q:119:MET:O	31:q:120:MET:HB3	2.20	0.41
40:z:34:ARG:HH21	42:Y:89:ASP:CG	2.29	0.41
41:Z:70:VAL:HG22	41:Z:90:GLN:CD	2.45	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
4:4:108:TYR:CB	6:6:54:CYS:HB3	2.50	0.41
4:4:276:ASP:N	4:4:276:ASP:OD1	2.53	0.41
4:4:413:ASP:O	4:4:417:ILE:HG13	2.21	0.41
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
11:M:196:TRP:HD1	11:M:250:LEU:HD22	1.86	0.41
11:M:237:LYS:HZ1	11:M:319:HIS:HD2	1.68	0.41
13:L:74:LEU:O	13:L:74:LEU:HD12	2.21	0.41
13:L:362:LEU:N	13:L:431:LEU:O	2.54	0.41
13:L:494:THR:O	13:L:498:PHE:CB	2.63	0.41
50:L:601:CDL:H111	50:L:601:CDL:H632	2.01	0.41
14:J:41:CYS:SG	14:J:57:PHE:HB2	2.61	0.41
18:d:199:LYS:O	18:d:290:THR:HG21	2.20	0.41
21:g:46:VAL:HG11	21:g:55:VAL:HG22	2.02	0.41
27:m:56:LEU:HD11	42:Y:129:LYS:HG2	2.03	0.41
29:o:39:TYR:O	29:o:43:LEU:HG	2.21	0.41
30:p:42:LEU:HD13	34:t:150:THR:C	2.46	0.41
32:r:87:TYR:O	32:r:91:THR:HG23	2.21	0.41
32:r:88:HIS:O	32:r:91:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:s:74:PRO:HG3	41:Z:28:PRO:HG3	2.03	0.41
42:Y:34:GLN:HG3	42:Y:35:CYS:N	2.36	0.41
42:Y:125:SER:O	42:Y:126:LYS:C	2.64	0.41
24:X:84:LYS:HG3	24:X:85:ASP: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
3:3:26:VAL:HG23	3:3:71:MET:O	2.21	0.41
3:3:35:MET:HE2	3:3:81:THR:HG21	2.03	0.41
3:3:107:ILE:HA	7:9:104:ARG:HH21	1.84	0.41
3:3:239:VAL:HG12	3:3:251:LEU:O	2.21	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
3:3:347:GLU:OE2	3:3:496:ILE:HD12	2.21	0.41
3:3:410:GLY:HA3	3:3:661:LEU:HD11	2.03	0.41
3:3:469:ALA:O	3:3:472:ASN:HB2	2.21	0.41
4:4:125:LEU:HD23	4:4:125:LEU:O	2.21	0.41
4:4:378:LEU:HD23	4:4:389:CYS:HB3	2.01	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:79:LEU:HD11	8:H:222:LEU:HG	2.03	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
9:N:206:ILE:HD12	9:N:346:LEU:HD11	2.03	0.41
10:A:28:ASN:CG	10:A:29:VAL:H	2.29	0.41
11:M:9:MET:HG2	48:o:202:3PE:H2E2	2.03	0.41
11:M:181:TYR:O	41:Z:152:ARG:NH2	2.54	0.41
11:M:196:TRP:CD1	11:M:250:LEU:HD22	2.56	0.41
11:M:204:MET:HB3	11:M:209:LEU:HD23	2.03	0.41
11:M:424:ASN:HA	34:t:101:TRP:CE3	2.56	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:188:TRP:CD2	13:L:212:PRO: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
13:L:469:SER:OG	13:L:470:ASN:N	2.53	0.41
17:c:30:ILE:HG23	17:c:101:TRP:HB3	2.01	0.41
18:d:29:PHE:CZ	18:d:176:ASP:HB3	2.56	0.41
18:d:63:GLY:O	18:d:67:GLN:HB2	2.21	0.41
18:d:165:ILE:O	18:d:227:THR:OG1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:206:TYR:CE2	18:d:208:VAL:HG22	2.56	0.41
19:e:83:ALA:O	19:e:87:THR:OG1	2.35	0.41
20:f:27:TYR:OH	20:f:54:LYS:NZ	2.54	0.41
20:f:37:ILE:HG22	20:f:38:PRO:O	2.20	0.41
24:j:37:MET:HE3	24:j:71:MET:CE	2.51	0.41
25:k:97:GLN:HB3	25:k:135:LEU:HD12	2.02	0.41
25:k:174:VAL:HB	25:k:203:GLU:OE1	2.20	0.41
32:r:10:ARG:NH1	34:t:164:PRO:HD2	2.35	0.41
32:r:115:VAL:HG22	32:r:116:ILE:N	2.35	0.41
33:s:18:PRO:HG3	33:s:52:LEU:HD11	2.03	0.41
35:u:28:PHE:O	35:u:31:THR:OG1	2.25	0.41
42:Y:154:GLU:N	42:Y:154:GLU:OE1	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
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
9:N:240:MET:HE1	29:o:48:ILE:HG23	2.01	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
11:M:42:LEU:HD23	11:M:63:THR:HG21	2.03	0.41
11:M:204:MET:SD	11:M:298:ILE:HD12	2.60	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:379:ALA:HB1	13:L:383:MET:HE1	2.03	0.41
13:L:436:ARG:O	13:L:436:ARG:HG3	2.20	0.41
14:J:9:LEU:HD23	14:J:9:LEU:HA	1.95	0.41
18:d:294:LEU:HD21	18:d:296:HIS:CD2	2.56	0.41
21:g:28:LYS:NZ	53:j:101:ZMP:O7	2.45	0.41
22:h:28:GLN:HB3	22:h:29:GLU:H	1.66	0.41
26:l:12:ASP:OD1	26:l:13:LEU:N	2.54	0.41
29:o:116:PHE:CG	41:Z:156:ALA:HB1	2.55	0.41
31:q:52:TRP:NE1	31:q:56:ARG:HD2	2.36	0.41
31:q:142:TYR:CG	31:q:143:THR:N	2.83	0.41
41:Z:88:GLU:HG2	41:Z:151:ALA:HB2	2.03	0.41
41:Z:131:PHE:O	41:Z:135:VAL:HG12	2.21	0.41
1:1:68:ARG:O	46:1:501:FMN:O4'	2.39	0.40
1:1:398:GLN:O	1:1:402:HIS:ND1	2.53	0.40
2:2:42:HIS:C	2:2:44:ALA:N	2.79	0.40
3:3:36:GLN:OE1	17:c:49:VAL:HG22	2.21	0.40
3:3:194:GLU:OE1	3:3:194:GLU:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:M:174:LEU:HD23	11:M:174:LEU:HA	1.89	0.40
11:M:305:THR:HG21	30:p:128:TYR:OXT	2.21	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
14:J:54:LEU:HD23	14:J:54:LEU:HA	1.80	0.40
21:g:21:SER:HB2	21:g:26:GLU:HB2	2.03	0.40
23:i:132:LYS:HD2	23:i:135:GLN:OE1	2.22	0.40
33:s:59:ALA:O	33:s:63:ILE:HG22	2.21	0.40
34:t:161:ASP:HB2	34:t:165:LEU:HD23	2.03	0.40
34:t:162:LEU:HA	34:t:162:LEU:HD23	1.86	0.40
37:w:71:VAL:O	37:w:75:THR:HG23	2.21	0.40
41:Z:48:ARG:O	41:Z:52:GLU:HG3	2.21	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
1:1:124:VAL:HG21	1:1:232:PRO:HB3	2.03	0.40
3:3:357:ASP:HB2	19:e:53:LEU:HA	2.03	0.40
4:4:203:LEU:HD22	4:4:207:LEU:HD23	2.03	0.40
4:4:212:TYR:CE1	31:q:15:TYR:HB3	2.57	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:35:LYS:HE3	8:H:38:ASN:ND2	2.30	0.40
8:H:307:LEU:HB3	8:H:308:PRO:HD3	2.02	0.40
13:L:131:LEU:HD12	13:L:143:GLY:C	2.45	0.40
13:L:400:ASN:ND2	13:L:486:LEU:O	2.54	0.40
19:e:22:LEU:O	19:e:57:CYS:HA	2.20	0.40
20:f:67:LEU:O	20:f:71:LEU:HB2	2.21	0.40
25:k:58:TYR:OH	25:k:107:GLN:HA	2.22	0.40
26:l:64:GLU:O	26:l:68:ARG:HD3	2.20	0.40
28:n:67:LEU:O	28:n:70:PHE:CD2	2.74	0.40
33:s:27:ASP:OD2	33:s:28:TYR:HD2	2.04	0.40
33:s:93:ASP:O	33:s:96:LYS:HB2	2.21	0.40
36:v:30:ARG:C	36:v:33:ASP:H	2.30	0.40
36:v:126:GLN:HG3	36:v:126:GLN:O	2.21	0.40
42:Y:12:LEU:HD23	42:Y:13:LYS:N	2.30	0.40
3:3:53:ARG:HA	3:3:53:ARG:HD3	1.88	0.40
3:3:285:ARG:HG3	3:3:291:LEU:HD13	2.03	0.40
4:4:93:TYR:CE2	5:5:168:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:34:PRO:HD2	20:f:99:TRP:HA	2.02	0.40
6:6:70:ASP:O	6:6:71:ARG:C	2.64	0.40
7:9:10:PRO:CA	7:9:20:ARG:HH22	2.34	0.40
7:9:92:ILE:HG22	7:9:93:THR:N	2.36	0.40
8:H:54:LYS:O	8:H:57:ILE:HG22	2.22	0.40
8:H:142:TYR:CE1	8:H:289:LEU:HD13	2.56	0.40
9:N:9:ILE:O	9:N:12:THR:OG1	2.31	0.40
13:L:3:LEU:HD21	41:Z:36:PHE:CG	2.56	0.40
13:L:446:ASN:OD1	35:u:21:GLN:NE2	2.54	0.40
18:d:300:LEU:HD12	18:d:300:LEU:HA	1.89	0.40
21:g:16:VAL:HG13	21:g:76:ARG:HD3	2.03	0.40
21:g:29:ARG:HH12	24:j:65:ILE:HB	1.87	0.40
26:l:3:PHE:CD2	49:o:201:PC1:H3F1	2.56	0.40
26:l:93:PRO:HG2	31:q:92:GLU:OE2	2.21	0.40
29:o:64:TYR:O	29:o:67:SER:OG	2.32	0.40
30:p:52:ASP:HB3	34:t:132:TRP:CH2	2.56	0.40
31:q:103:TRP:HZ3	31:q:106:GLY:N	2.20	0.40
33:s:51:VAL:O	33:s:54:GLN:HB3	2.21	0.40
34:t:165:LEU:HD12	34:t:166:TRP:N	2.36	0.40
37:w:49:LYS:HG2	37:w:50:ASP:N	2.35	0.40
1:1:250:ASN:ND2	1:1:319:PHE:H	2.19	0.40
5:5:182:ARG:NE	21:g:103:MET:HG3	2.37	0.40
5:5:194:PHE:HD2	17:c:81:ASN:ND2	2.18	0.40
6:6:47:PRO:HB3	6:6:85:VAL:HG23	2.03	0.40
10:A:80:GLN:O	10:A:80:GLN:HG3	2.21	0.40
11:M:196:TRP:CE3	11:M:257:MET:HB3	2.56	0.40
11:M:200:MET:SD	11:M:243:MET:HE1	2.61	0.40
11:M:325:MET:O	11:M:328:CYS:N	2.54	0.40
13:L:331:THR:HB	13:L:335:PHE:CE2	2.56	0.40
14:J:163:ILE:HA	14:J:166:VAL:HG22	2.03	0.40
17:c:16:LYS:NZ	21:g:75:PRO:HG2	2.36	0.40
18:d:50:ARG:HH22	52:d:401:NDP:C5A	2.34	0.40
19:e:64:LEU:HD22	19:e:90:LEU:HD21	2.03	0.40
25:k:2:GLN:HE22	25:k:267:LEU:CB	2.35	0.40
30:p:113:LYS:O	30:p:117:GLU:HG2	2.21	0.40
30:p:125:ASN:N	30:p:126:ILE:HD12	2.36	0.40
31:q:137:TYR:HB3	31:q:141:TRP:CH2	2.56	0.40
32:r:30:ARG:O	32:r:30:ARG:HG2	2.21	0.40
37:w:109:GLU:O	37:w:110:SER:OG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:651:LEU:HD12	19:e:45:LYS:HE2	2.03	0.40
4:4:146:ARG:HA	4:4:370:PRO:CG	2.52	0.40
5:5:67:HIS:O	5:5:67:HIS:CG	2.75	0.40
5:5:131:GLU:OE1	5:5:145:HIS:HD2	2.04	0.40
6:6:42:ARG:HB3	6:6:167:ILE:HG21	2.03	0.40
9:N:33:PHE:HE1	9:N:137:ALA:HB1	1.87	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:345:ILE:HD12	9:N:345:ILE:HA	1.85	0.40
11:M:160:LEU:O	11:M:164:LEU:HG	2.22	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
16:b:31:ARG:HA	23:i:121:PRO:O	2.22	0.40
18:d:193:LEU:HD11	18:d:288:HIS:ND1	2.36	0.40
19:e:81:PHE:HD1	19:e:85:GLN:OE1	2.04	0.40
21:g:63:ARG:HH12	24:j:24:LYS:HZ3	1.68	0.40
22:h:30:ILE:O	22:h:31:SER:OG	2.31	0.40
23:i:66:THR:HG22	23:i:67:GLU:N	2.36	0.40
25:k:23:LYS:HB3	25:k:24:LEU:H	1.68	0.40
31:q:57:ARG:HA	31:q:57:ARG:HD3	1.90	0.40
34:t:70:PHE:O	34:t:73:GLY:N	2.42	0.40
39:y:33:LYS:NZ	42:Y:171:MET:HE1	2.36	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	430/445 (97%)	405 (94%)	24 (6%)	1 (0%)	43 74
2	2	212/217 (98%)	189 (89%)	22 (10%)	1 (0%)	24 59
3	3	686/704 (97%)	616 (90%)	70 (10%)	0	100 100
4	4	385/412 (93%)	337 (88%)	46 (12%)	2 (0%)	24 59
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%)	36 69
9	N	345/347 (99%)	315 (91%)	30 (9%)	0	100 100
10	A	113/115 (98%)	97 (86%)	15 (13%)	1 (1%)	14 47
11	M	457/459 (100%)	392 (86%)	64 (14%)	1 (0%)	43 74
12	K	84/98 (86%)	72 (86%)	12 (14%)	0	100 100
13	L	597/599 (100%)	518 (87%)	75 (13%)	4 (1%)	18 53
14	J	173/175 (99%)	142 (82%)	29 (17%)	2 (1%)	10 41
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%)	36 69
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%)	11 43
23	i	142/145 (98%)	116 (82%)	24 (17%)	2 (1%)	9 38
24	X	86/88 (98%)	77 (90%)	9 (10%)	0	100 100
24	j	83/88 (94%)	70 (84%)	13 (16%)	0	100 100
25	k	318/320 (99%)	263 (83%)	50 (16%)	5 (2%)	7 36
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%)	1 16
29	o	118/120 (98%)	105 (89%)	13 (11%)	0	100 100
30	p	110/128 (86%)	83 (76%)	26 (24%)	1 (1%)	14 47
31	q	138/143 (96%)	126 (91%)	12 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	r	89/127 (70%)	75 (84%)	12 (14%)	2 (2%)	5 31
33	s	116/136 (85%)	93 (80%)	21 (18%)	2 (2%)	7 35
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%)	3 23
37	w	84/125 (67%)	67 (80%)	15 (18%)	2 (2%)	4 29
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%)	21 55
42	Y	169/171 (99%)	137 (81%)	32 (19%)	0	100 100
43	W	137/143 (96%)	115 (84%)	21 (15%)	1 (1%)	18 53
All	All	7824/8344 (94%)	6800 (87%)	984 (13%)	40 (0%)	26 59

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
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

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Mol	Chain	Res	Type
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
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%)	73 77
7	9	151/151 (100%)	150 (99%)	1 (1%)	76 78
8	H	278/278 (100%)	278 (100%)	0	100 100
9	N	315/315 (100%)	315 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	A	103/103 (100%)	103 (100%)	0	100	100
11	M	412/412 (100%)	408 (99%)	4 (1%)	68	75
12	K	75/87 (86%)	75 (100%)	0	100	100
13	L	445/532 (84%)	439 (99%)	6 (1%)	61	71
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%)	256 (100%)	1 (0%)	84	83
19	e	75/81 (93%)	75 (100%)	0	100	100
20	f	100/101 (99%)	99 (99%)	1 (1%)	68	75
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%)	84 (99%)	1 (1%)	63	72
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%)	119 (99%)	1 (1%)	73	77
32	r	80/121 (66%)	78 (98%)	2 (2%)	42	62
33	s	100/119 (84%)	100 (100%)	0	100	100
34	t	151/160 (94%)	149 (99%)	2 (1%)	61	71
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	z	58/59 (98%)	58 (100%)	0	100 100
41	Z	155/157 (99%)	154 (99%)	1 (1%)	78 80
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%)	6548 (100%)	21 (0%)	84 85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE
11	M	6	ILE
11	M	84	LEU
11	M	251	ASN
11	M	376	ILE
13	L	126	ILE
13	L	155	ILE
13	L	396	ILE
13	L	427	ILE
13	L	459	ILE
13	L	495	ILE
18	d	279	THR
20	f	94	ILE
26	l	86	ILE
31	q	96	ILE
32	r	34	LEU
32	r	76	ILE
34	t	153	LEU
34	t	165	LEU
41	Z	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	150	GLN
1	1	200	GLN
1	1	263	ASN
1	1	293	ASN
1	1	435	GLN
2	2	99	HIS

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Mol	Chain	Res	Type
2	2	214	GLN
3	3	36	GLN
3	3	255	HIS
3	3	259	ASN
3	3	499	GLN
3	3	581	GLN
4	4	46	ASN
4	4	84	HIS
4	4	149	ASN
4	4	157	HIS
4	4	200	HIS
4	4	266	GLN
4	4	347	HIS
5	5	38	GLN
5	5	88	ASN
7	9	123	GLN
7	9	157	ASN
8	H	38	ASN
8	H	138	GLN
8	H	169	GLN
8	H	194	ASN
8	H	287	HIS
8	H	317	GLN
9	N	63	GLN
9	N	134	GLN
9	N	222	ASN
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
13	L	27	HIS
13	L	115	ASN
13	L	226	GLN
13	L	270	ASN
13	L	323	HIS
13	L	405	ASN
13	L	479	GLN
13	L	484	HIS
16	b	13	HIS

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Mol	Chain	Res	Type
18	d	8	HIS
18	d	37	HIS
18	d	89	ASN
18	d	119	GLN
18	d	131	HIS
18	d	148	ASN
18	d	203	GLN
18	d	250	HIS
19	e	24	GLN
19	e	75	ASN
20	f	72	GLN
20	f	82	GLN
21	g	94	ASN
22	h	46	HIS
22	h	50	ASN
23	i	31	ASN
23	i	72	ASN
25	k	50	HIS
25	k	141	GLN
25	k	180	GLN
25	k	184	GLN
25	k	200	GLN
26	l	15	HIS
26	l	24	GLN
26	l	26	HIS
26	l	69	GLN
26	l	81	GLN
27	m	45	ASN
27	m	70	GLN
28	n	20	GLN
29	o	59	HIS
29	o	79	GLN
31	q	84	GLN
32	r	25	GLN
32	r	82	HIS
32	r	88	HIS
33	s	42	GLN
33	s	43	GLN
33	s	60	HIS
34	t	13	GLN
34	t	25	HIS
34	t	168	HIS

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Mol	Chain	Res	Type
35	u	16	GLN
35	u	21	GLN
36	v	104	HIS
36	v	126	GLN
37	w	45	HIS
37	w	111	ASN
38	x	35	HIS
40	z	44	GLN
41	Z	99	GLN
41	Z	113	GLN
41	Z	130	GLN
41	Z	160	GLN
42	Y	150	ASN
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 oligosaccharides 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	$\#\|Z\|>2$
50	CDL	i	201	-	57,57,99	0.38	0	63,69,111	0.39	0
45	SF4	9	502	7	0,12,12	-	-	-		
50	CDL	J	300	-	78,78,99	0.34	0	84,90,111	0.38	0
50	CDL	M	502	-	81,81,99	0.33	0	87,93,111	0.37	0
45	SF4	3	802	3	0,12,12	-	-	-		
54	PNS	X	401	24	13,20,21	0.51	0	18,26,29	0.90	1 (5%)
49	PC1	A	200	-	46,46,53	0.32	0	52,54,61	0.34	0
50	CDL	L	601	-	83,83,99	0.32	0	89,95,111	0.41	0
45	SF4	3	801	3	0,12,12	-	-	-		
46	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.47	0
48	3PE	J	301	-	50,50,50	0.31	0	53,55,55	0.33	0
49	PC1	N	401	-	45,45,53	0.32	0	51,53,61	0.35	0
45	SF4	6	300	6	0,12,12	-	-	-		
49	PC1	o	201	-	38,38,53	0.34	0	44,46,61	0.34	0
48	3PE	o	203	-	45,45,50	0.34	0	48,50,55	0.39	0
48	3PE	o	202	-	40,40,50	0.36	0	43,45,55	0.36	0
47	FES	3	803	3	0,4,4	-	-	-		
47	FES	2	300	2	0,4,4	-	-	-		
52	NDP	d	401	-	49,52,52	0.43	0	66,80,80	0.47	0
53	ZMP	j	101	24	27,33,36	0.72	2 (7%)	32,40,45	1.11	1 (3%)
45	SF4	9	503	7	0,12,12	-	-	-		
48	3PE	9	501	-	50,50,50	0.31	0	53,55,55	0.41	0
49	PC1	M	501	-	45,45,53	0.31	0	51,53,61	0.35	0
45	SF4	1	500	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CDL	i	201	-	-	15/68/68/110	-
45	SF4	9	502	7	-	-	0/6/5/5
50	CDL	J	300	-	-	18/89/89/110	-
50	CDL	M	502	-	-	22/92/92/110	-
45	SF4	3	802	3	-	-	0/6/5/5
54	PNS	X	401	24	-	7/24/26/27	-
49	PC1	A	200	-	-	18/50/50/57	-
50	CDL	L	601	-	-	24/94/94/110	-
45	SF4	3	801	3	-	-	0/6/5/5
46	FMN	1	501	-	-	7/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	3PE	J	301	-	-	7/54/54/54	-
49	PC1	N	401	-	-	10/49/49/57	-
45	SF4	6	300	6	-	-	0/6/5/5
49	PC1	o	201	-	-	10/42/42/57	-
48	3PE	o	203	-	-	11/49/49/54	-
48	3PE	o	202	-	-	8/44/44/54	-
47	FES	3	803	3	-	-	0/1/1/1
53	ZMP	j	101	24	-	9/38/40/43	-
52	NDP	d	401	-	-	9/34/77/77	0/5/5/5
47	FES	2	300	2	-	-	0/1/1/1
45	SF4	9	503	7	-	-	0/6/5/5
48	3PE	9	501	-	-	14/54/54/54	-
49	PC1	M	501	-	-	13/49/49/57	-
45	SF4	1	500	1	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	j	101	ZMP	C10-S1	-2.23	1.70	1.76
53	j	101	ZMP	C9-C10	2.07	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	j	101	ZMP	O1-C10-C9	-2.78	120.71	123.99
54	X	401	PNS	C37-C38-C39	-2.22	108.66	112.36

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	501	FMN	C5'-O5'-P-O1P
46	1	501	FMN	C5'-O5'-P-O2P
48	9	501	3PE	C11-O13-P-O14
48	9	501	3PE	O13-C11-C12-N
48	J	301	3PE	C1-O11-P-O14
48	o	202	3PE	C11-O13-P-O12
48	o	202	3PE	C11-O13-P-O14
48	o	202	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
48	o	203	3PE	C1-O11-P-O12
48	o	203	3PE	O13-C11-C12-N
49	N	401	PC1	C1-O11-P-O12
49	A	200	PC1	C1-O11-P-O12
49	M	501	PC1	C12-C11-O13-P
49	o	201	PC1	C1-O11-P-O12
50	M	502	CDL	CA3-OA5-PA1-OA3
50	M	502	CDL	CB2-OB2-PB2-OB3
50	M	502	CDL	CB2-OB2-PB2-OB4
50	M	502	CDL	CB2-OB2-PB2-OB5
50	M	502	CDL	CB3-OB5-PB2-OB4
50	L	601	CDL	CB2-C1-CA2-OA2
50	L	601	CDL	CA3-OA5-PA1-OA3
50	J	300	CDL	CA2-OA2-PA1-OA3
50	J	300	CDL	CA2-OA2-PA1-OA4
50	J	300	CDL	CA2-OA2-PA1-OA5
50	J	300	CDL	CA3-OA5-PA1-OA4
50	J	300	CDL	CB3-OB5-PB2-OB3
50	J	300	CDL	CB3-OB5-PB2-OB4
50	i	201	CDL	CA3-OA5-PA1-OA3
50	i	201	CDL	CA3-OA5-PA1-OA4
50	i	201	CDL	OA6-CA4-CA6-OA8
52	d	401	NDP	C1B-C2B-O2B-P2B
52	d	401	NDP	C2B-O2B-P2B-O1X
52	d	401	NDP	C2B-O2B-P2B-O3X
53	j	101	ZMP	S1-C11-C12-N1
54	X	401	PNS	N36-C37-C38-C39
49	o	201	PC1	C11-C12-N-C13
50	L	601	CDL	O1-C1-CA2-OA2
46	1	501	FMN	O3'-C3'-C4'-C5'
46	1	501	FMN	C2'-C3'-C4'-C5'
49	M	501	PC1	C11-C12-N-C15
49	M	501	PC1	C11-C12-N-C14
48	9	501	3PE	C21-C22-C23-C24
50	M	502	CDL	CA5-C11-C12-C13
50	L	601	CDL	C15-C16-C17-C18
48	9	501	3PE	C11-O13-P-O11
48	o	202	3PE	C11-O13-P-O11
49	M	501	PC1	C11-O13-P-O11
50	M	502	CDL	CA3-OA5-PA1-OA2
50	M	502	CDL	CB3-OB5-PB2-OB2
50	L	601	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
50	L	601	CDL	CB2-OB2-PB2-OB5
50	J	300	CDL	CB3-OB5-PB2-OB2
50	i	201	CDL	CA3-OA5-PA1-OA2
50	L	601	CDL	C61-C62-C63-C64
49	o	201	PC1	C11-C12-N-C14
46	1	501	FMN	O3'-C3'-C4'-O4'
46	1	501	FMN	C2'-C3'-C4'-O4'
49	A	200	PC1	C3C-C3D-C3E-C3F
53	j	101	ZMP	C1-C2-C3-C4
49	o	201	PC1	C11-C12-N-C15
48	J	301	3PE	O13-C11-C12-N
48	o	203	3PE	C37-C38-C39-C3A
49	M	501	PC1	C11-C12-N-C13
48	o	202	3PE	C31-C32-C33-C34
48	J	301	3PE	C37-C38-C39-C3A
50	M	502	CDL	C79-C80-C81-C82
49	A	200	PC1	C34-C35-C36-C37
49	o	201	PC1	C3C-C3D-C3E-C3F
50	M	502	CDL	C72-C73-C74-C75
53	j	101	ZMP	C2-C3-C4-C5
48	J	301	3PE	C1-O11-P-O13
50	J	300	CDL	CA3-OA5-PA1-OA2
53	j	101	ZMP	C5-C6-C7-C8
49	A	200	PC1	O11-C1-C2-C3
48	o	202	3PE	C28-C29-C2A-C2B
50	i	201	CDL	CA3-CA4-CA6-OA8
49	N	401	PC1	O31-C31-C32-C33
50	M	502	CDL	C52-C53-C54-C55
53	j	101	ZMP	C2-C1-C22-C23
49	A	200	PC1	C37-C38-C39-C3A
50	i	201	CDL	CB5-C51-C52-C53
50	i	201	CDL	OB5-CB3-CB4-OB6
49	M	501	PC1	C21-C22-C23-C24
49	M	501	PC1	C22-C23-C24-C25
50	M	502	CDL	OB5-CB3-CB4-CB6
50	M	502	CDL	CB5-C51-C52-C53
49	N	401	PC1	C1-O11-P-O13
49	A	200	PC1	C11-O13-P-O11
48	9	501	3PE	O11-C1-C2-O21
50	L	601	CDL	OB5-CB3-CB4-OB6
48	J	301	3PE	C23-C24-C25-C26
46	1	501	FMN	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
50	J	300	CDL	C1-CA2-OA2-PA1
49	A	200	PC1	C11-C12-N-C15
50	L	601	CDL	C52-C51-CB5-OB6
53	j	101	ZMP	O1-C10-S1-C11
50	i	201	CDL	OB5-CB3-CB4-CB6
53	j	101	ZMP	C9-C10-S1-C11
50	i	201	CDL	CB3-CB4-CB6-OB8
48	o	203	3PE	O11-C1-C2-O21
49	A	200	PC1	O11-C1-C2-O21
50	M	502	CDL	OB5-CB3-CB4-OB6
50	J	300	CDL	OB5-CB3-CB4-OB6
50	L	601	CDL	C59-C60-C61-C62
50	L	601	CDL	C17-C18-C19-C20
48	9	501	3PE	C34-C35-C36-C37
52	d	401	NDP	PN-O3-PA-O2A
48	o	203	3PE	C1-O11-P-O13
49	o	201	PC1	C1-O11-P-O13
52	d	401	NDP	O4D-C1D-N1N-C6N
50	i	201	CDL	C1-CB2-OB2-PB2
48	9	501	3PE	C11-O13-P-O12
48	o	203	3PE	C1-O11-P-O14
49	N	401	PC1	C1-O11-P-O14
49	A	200	PC1	C11-C12-N-C14
49	M	501	PC1	C11-O13-P-O12
49	M	501	PC1	C11-O13-P-O14
49	o	201	PC1	C1-O11-P-O14
50	M	502	CDL	CA3-OA5-PA1-OA4
50	M	502	CDL	CB3-OB5-PB2-OB3
50	L	601	CDL	CA3-OA5-PA1-OA4
50	L	601	CDL	CB2-OB2-PB2-OB3
50	J	300	CDL	CA3-OA5-PA1-OA3
48	9	501	3PE	C38-C39-C3A-C3B
48	o	203	3PE	O11-C1-C2-C3
50	L	601	CDL	OB5-CB3-CB4-CB6
50	J	300	CDL	OB5-CB3-CB4-CB6
49	A	200	PC1	C12-C11-O13-P
48	9	501	3PE	C2F-C2G-C2H-C2I
48	o	202	3PE	C29-C2A-C2B-C2C
49	N	401	PC1	O13-C11-C12-N
49	A	200	PC1	O13-C11-C12-N
49	M	501	PC1	O13-C11-C12-N
49	o	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
50	L	601	CDL	C12-C13-C14-C15
49	N	401	PC1	C2-C1-O11-P
50	M	502	CDL	CA4-CA3-OA5-PA1
50	M	502	CDL	C51-C52-C53-C54
54	X	401	PNS	O33-C32-C34-O35
50	M	502	CDL	C64-C65-C66-C67
48	9	501	3PE	C37-C38-C39-C3A
49	N	401	PC1	C3-C2-O21-C21
48	o	202	3PE	O31-C31-C32-C33
50	J	300	CDL	C38-C39-C40-C41
50	M	502	CDL	C57-C58-C59-C60
50	i	201	CDL	CA2-OA2-PA1-OA5
50	L	601	CDL	C53-C54-C55-C56
50	L	601	CDL	C1-CA2-OA2-PA1
49	A	200	PC1	C3B-C3C-C3D-C3E
48	9	501	3PE	C2E-C2F-C2G-C2H
50	i	201	CDL	OB6-CB4-CB6-OB8
50	L	601	CDL	C51-C52-C53-C54
49	A	200	PC1	C11-C12-N-C13
49	N	401	PC1	O32-C31-C32-C33
54	X	401	PNS	C29-C32-C34-N36
48	9	501	3PE	C1-C2-O21-C21
50	J	300	CDL	CB6-CB4-OB6-CB5
49	o	201	PC1	C3B-C3C-C3D-C3E
53	j	101	ZMP	C12-C11-S1-C10
49	A	200	PC1	C38-C39-C3A-C3B
49	o	201	PC1	C3A-C3B-C3C-C3D
49	N	401	PC1	C36-C37-C38-C39
50	L	601	CDL	C54-C55-C56-C57
50	M	502	CDL	C58-C59-C60-C61
50	L	601	CDL	C72-C71-CB7-OB8
54	X	401	PNS	O33-C32-C34-N36
48	J	301	3PE	C24-C25-C26-C27
48	J	301	3PE	C2D-C2E-C2F-C2G
49	M	501	PC1	O21-C21-C22-C23
48	o	203	3PE	C24-C25-C26-C27
50	L	601	CDL	CB3-CB4-OB6-CB5
50	L	601	CDL	CB6-CB4-OB6-CB5
48	o	203	3PE	C21-C22-C23-C24
50	i	201	CDL	C32-C31-CA7-OA8
49	N	401	PC1	C34-C35-C36-C37
54	X	401	PNS	C37-C38-C39-O40

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Mol	Chain	Res	Type	Atoms
53	j	101	ZMP	C6-C7-C8-C9
50	J	300	CDL	OA6-CA4-CA6-OA8
49	A	200	PC1	O21-C21-C22-C23
50	J	300	CDL	C19-C20-C21-C22
50	M	502	CDL	C1-CA2-OA2-PA1
50	J	300	CDL	C12-C11-CA5-OA6
52	d	401	NDP	O4B-C4B-C5B-O5B
49	A	200	PC1	C3D-C3E-C3F-C3G
52	d	401	NDP	C2B-C1B-N9A-C8A
49	M	501	PC1	O22-C21-C22-C23
50	i	201	CDL	C32-C31-CA7-OA9
50	L	601	CDL	C72-C71-CB7-OB9
49	A	200	PC1	C1-O11-P-O14
52	d	401	NDP	C5D-O5D-PN-O1N
49	A	200	PC1	O22-C21-C22-C23
50	J	300	CDL	C12-C11-CA5-OA7
50	L	601	CDL	C52-C51-CB5-OB7
48	o	203	3PE	C12-C11-O13-P
54	X	401	PNS	C29-C32-C34-O35
48	9	501	3PE	O21-C21-C22-C23
49	M	501	PC1	O31-C31-C32-C33
52	d	401	NDP	C3B-C2B-O2B-P2B
48	9	501	3PE	O31-C31-C32-C33
50	i	201	CDL	C52-C51-CB5-OB6
48	o	203	3PE	C34-C35-C36-C37
54	X	401	PNS	C37-C38-C39-N41

There are no ring outliers.

22 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	i	201	CDL	1	0
45	9	502	SF4	3	0
50	J	300	CDL	1	0
50	M	502	CDL	3	0
45	3	802	SF4	1	0
54	X	401	PNS	8	0
49	A	200	PC1	5	0
50	L	601	CDL	13	0
45	3	801	SF4	1	0
46	1	501	FMN	8	0
48	J	301	3PE	6	0

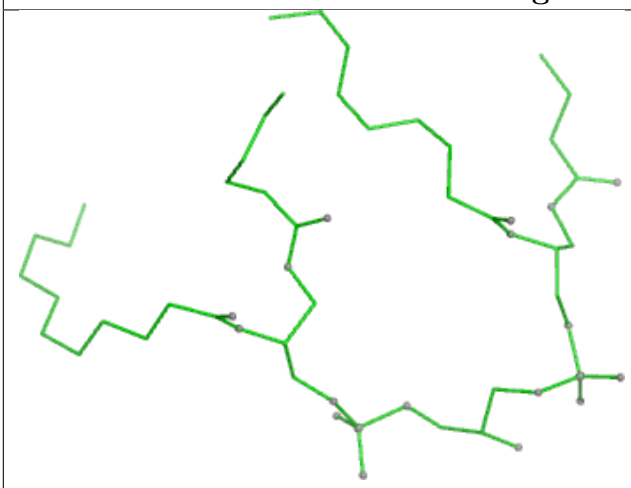
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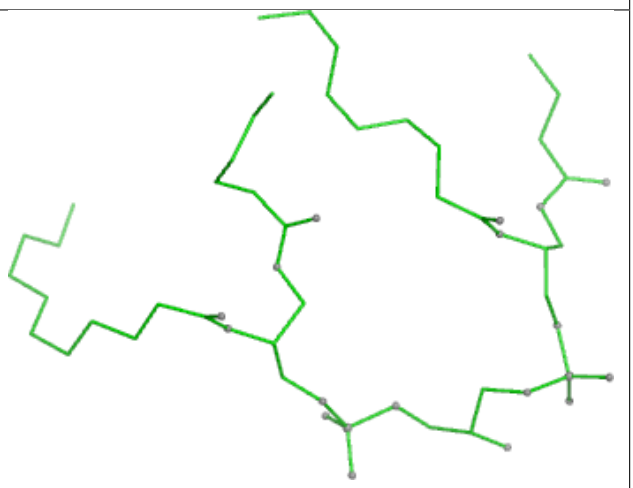
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	N	401	PC1	3	0
45	6	300	SF4	2	0
49	o	201	PC1	3	0
48	o	203	3PE	4	0
48	o	202	3PE	4	0
52	d	401	NDP	8	0
53	j	101	ZMP	3	0
45	9	503	SF4	1	0
48	9	501	3PE	10	0
49	M	501	PC1	2	0
45	1	500	SF4	2	0

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

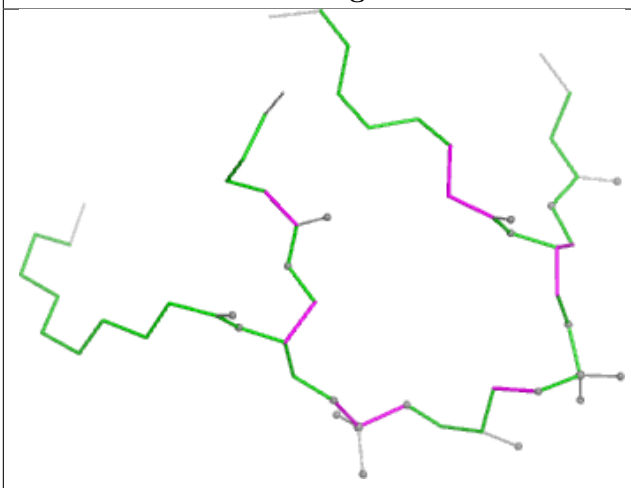
Ligand CDL i 201



Bond lengths



Bond angles

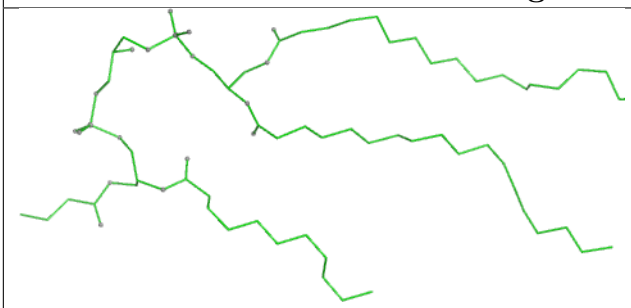


Torsions

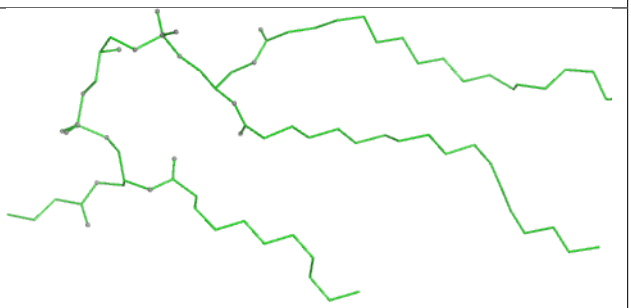


Rings

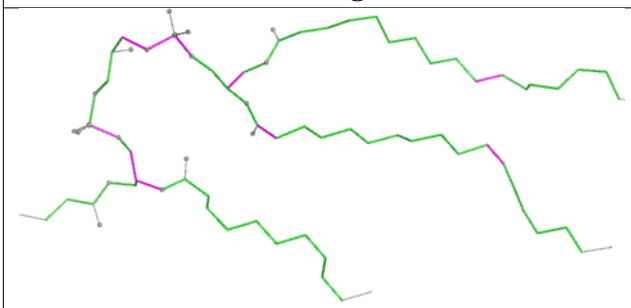
Ligand CDL J 300



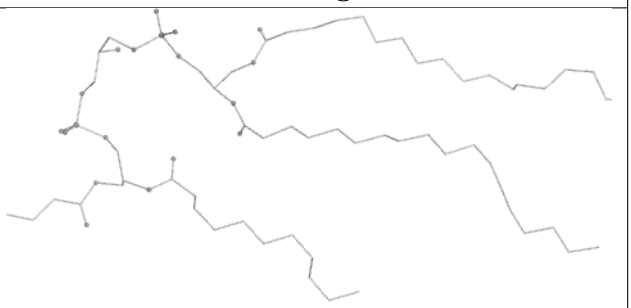
Bond lengths



Bond angles

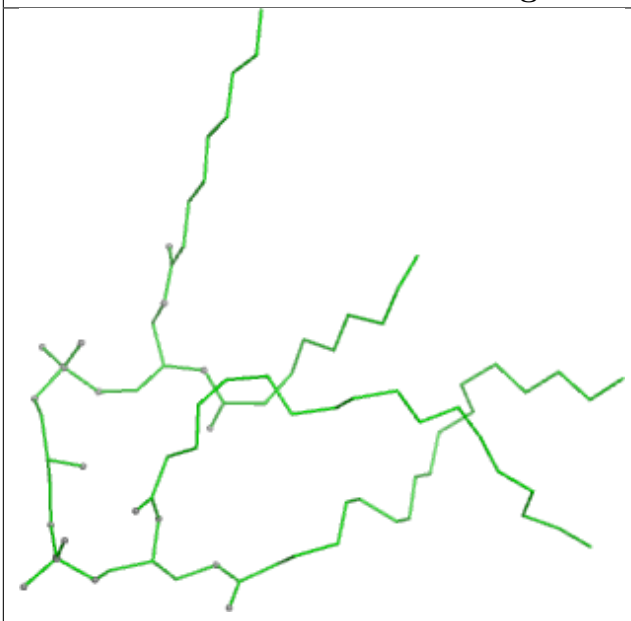


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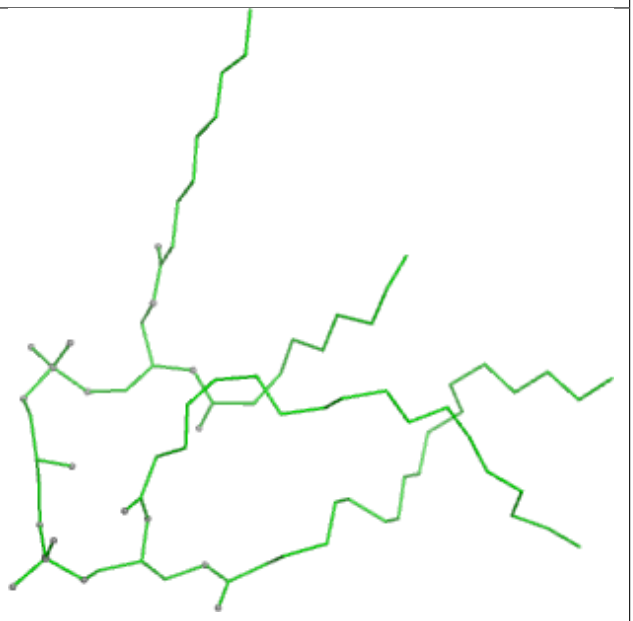


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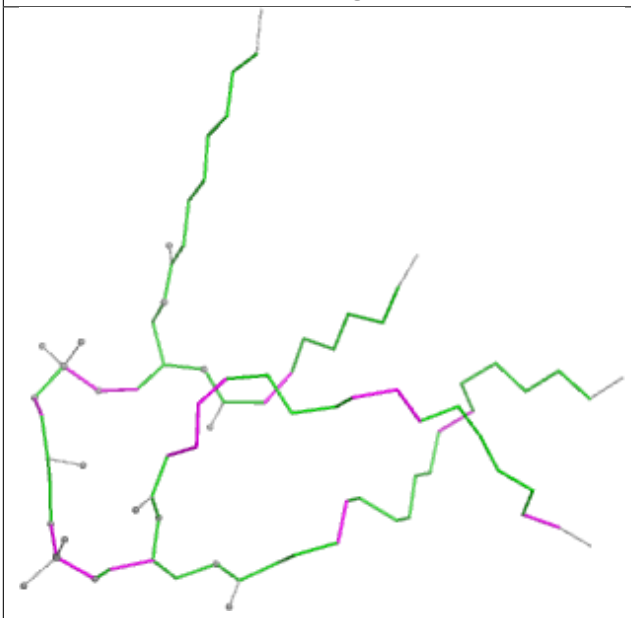
Ligand CDL M 502



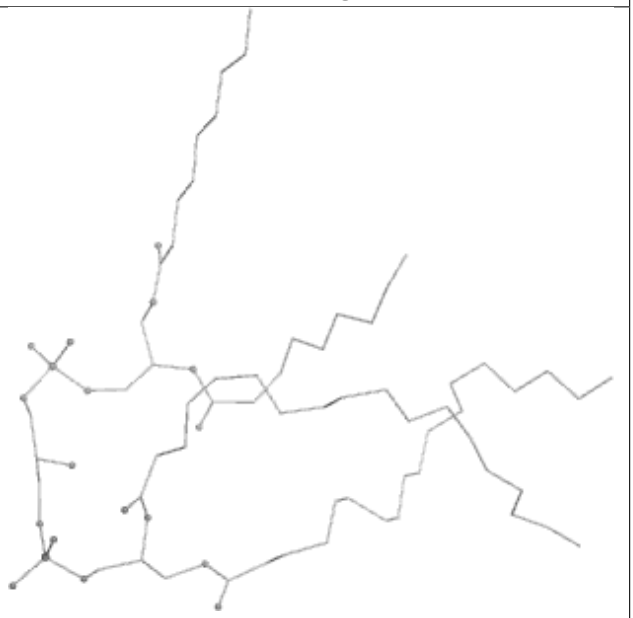
Bond lengths



Bond angles

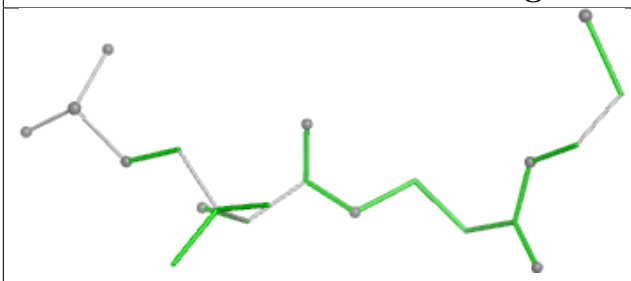


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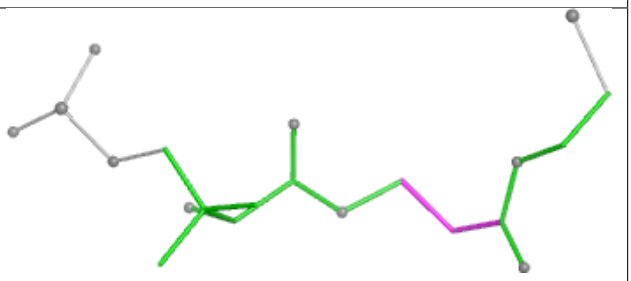


Rings

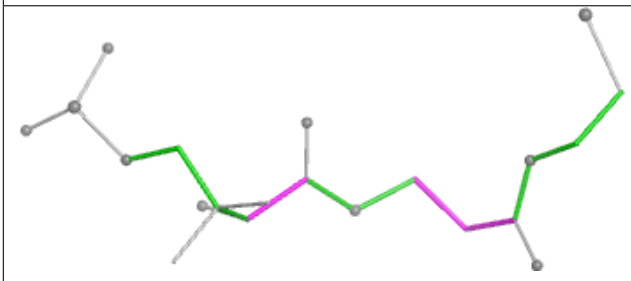
Ligand PNS X 401



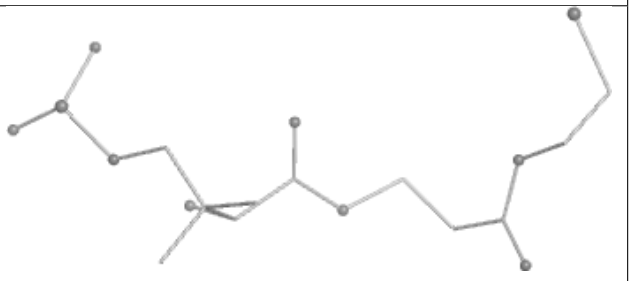
Bond lengths



Bond angles

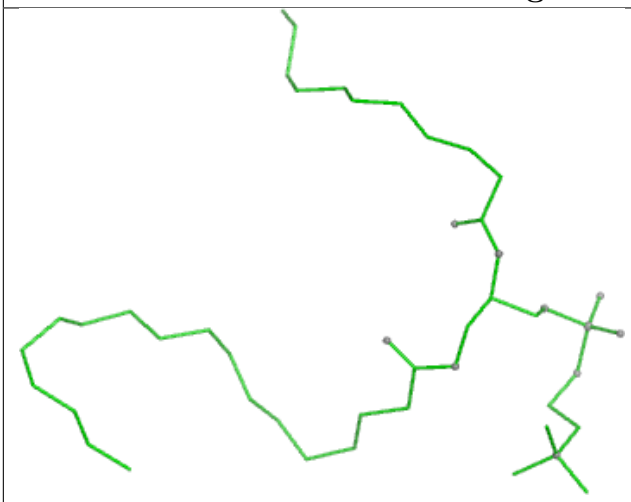


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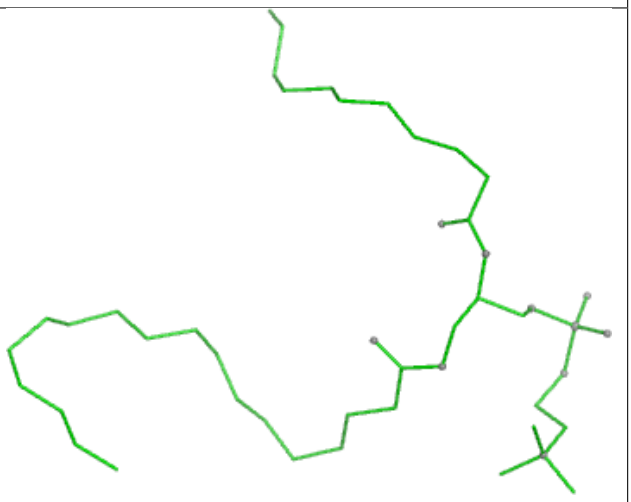


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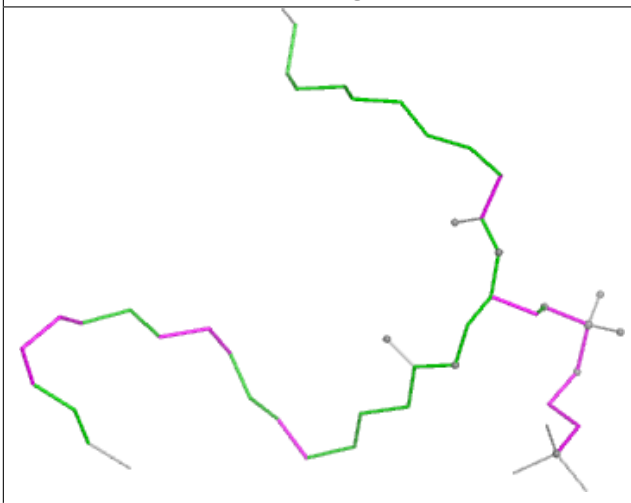
Ligand PC1 A 200



Bond lengths



Bond angles

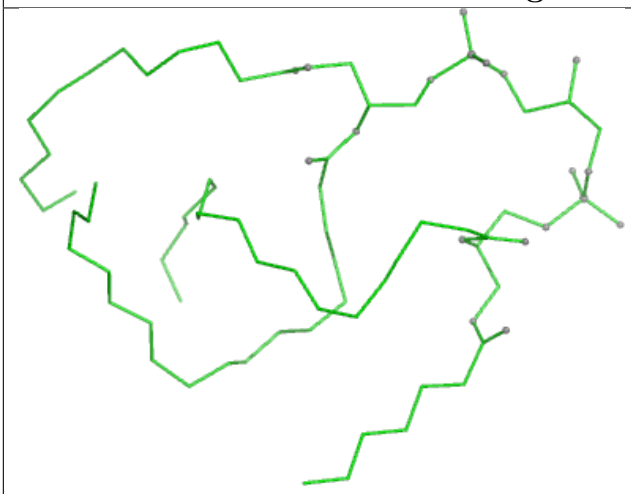


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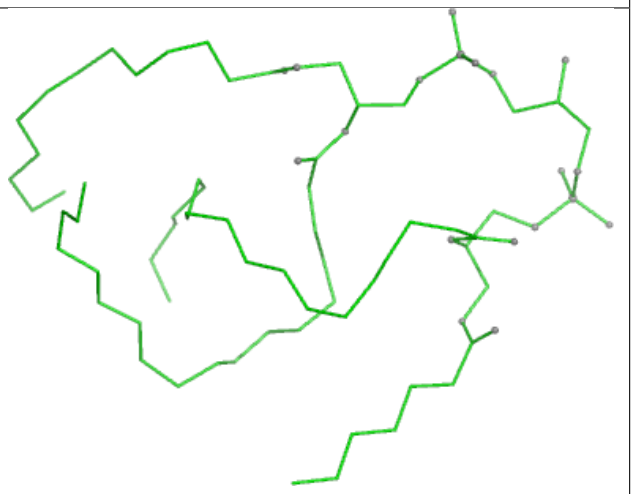


Rings

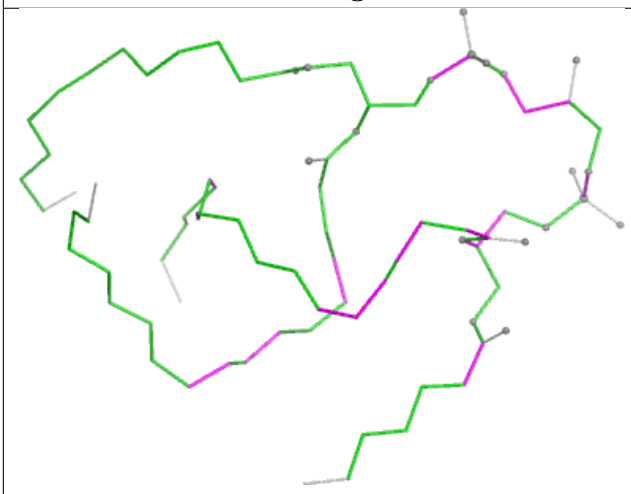
Ligand CDL L 601



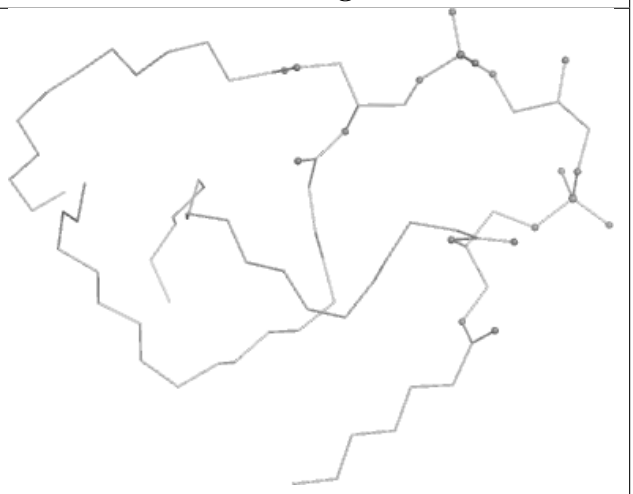
Bond lengths



Bond angles

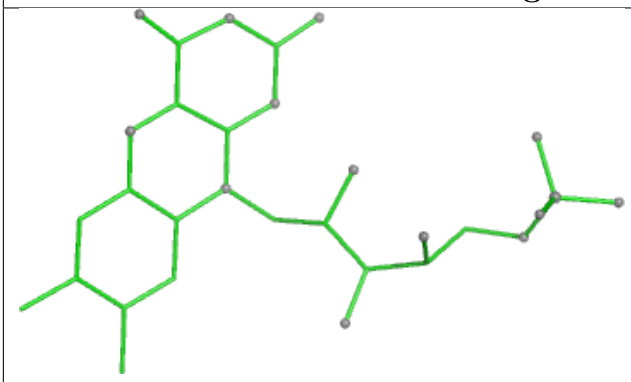


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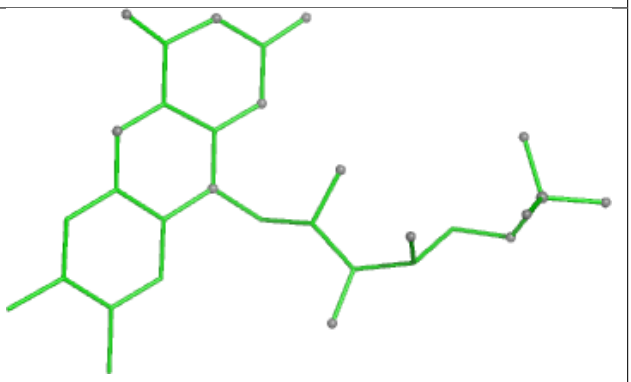


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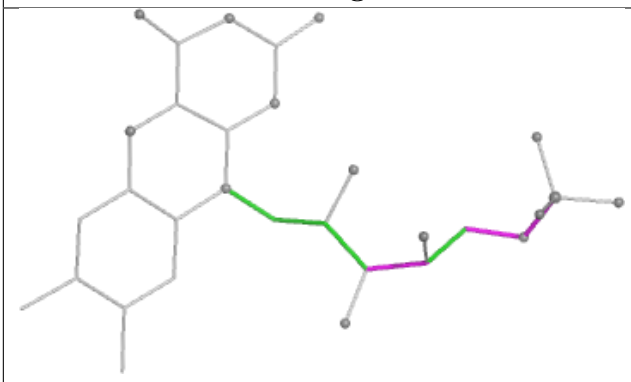
Ligand FMN 1 501



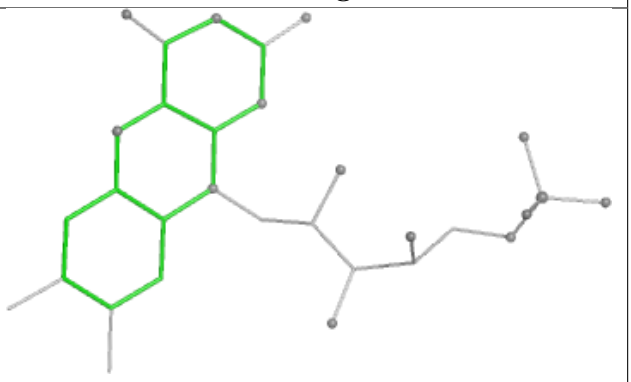
Bond lengths



Bond angles

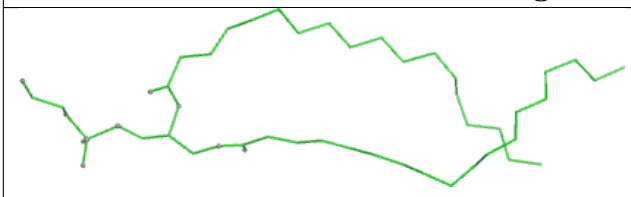


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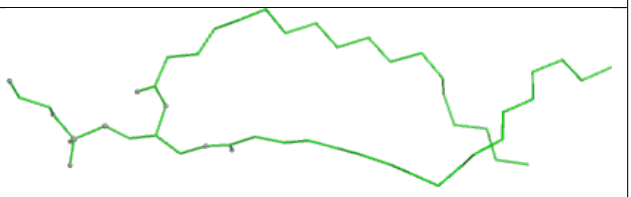


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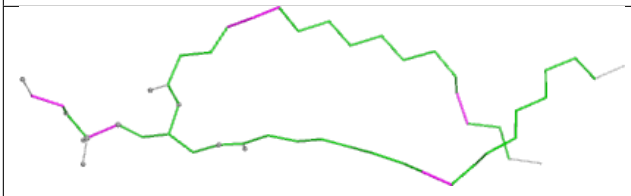
Ligand 3PE J 301



Bond lengths



Bond angles

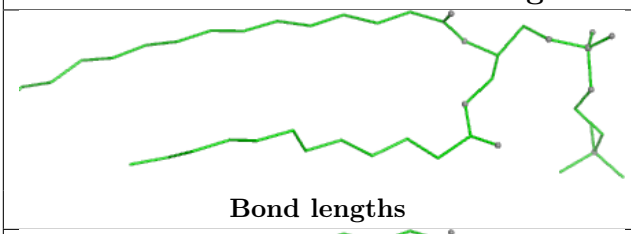


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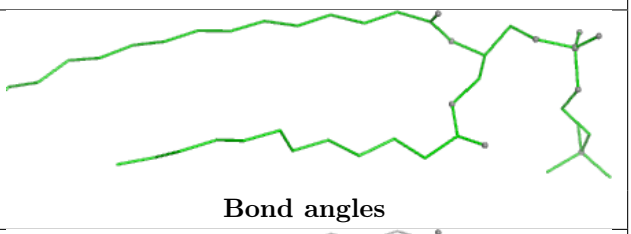


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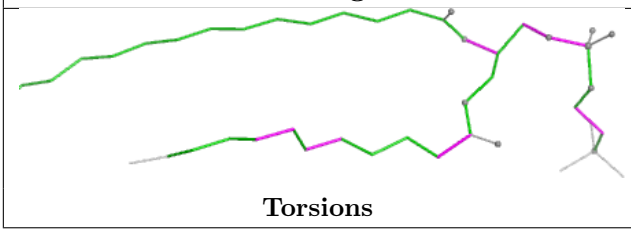
Ligand PC1 N 401



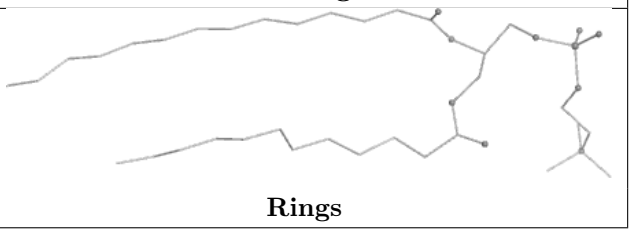
Bond lengths



Bond angles

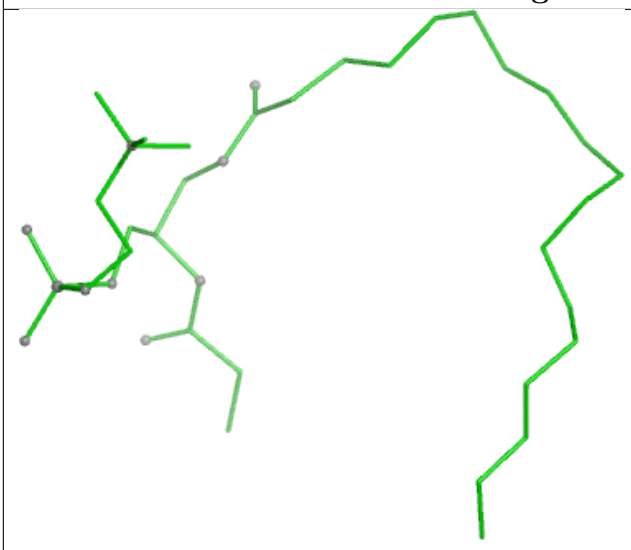


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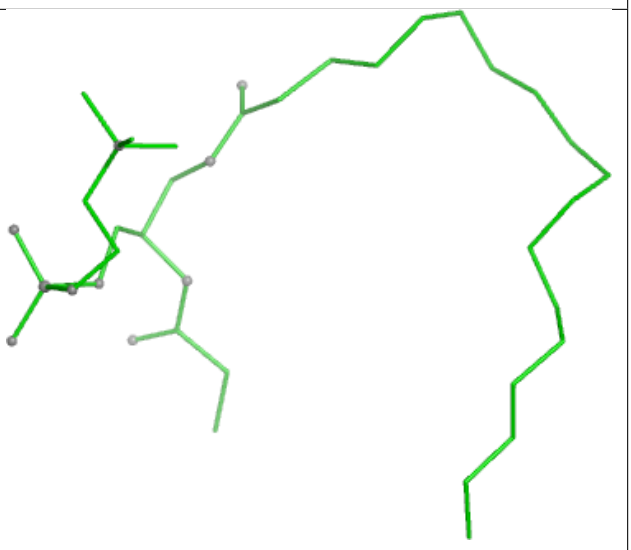


Rings

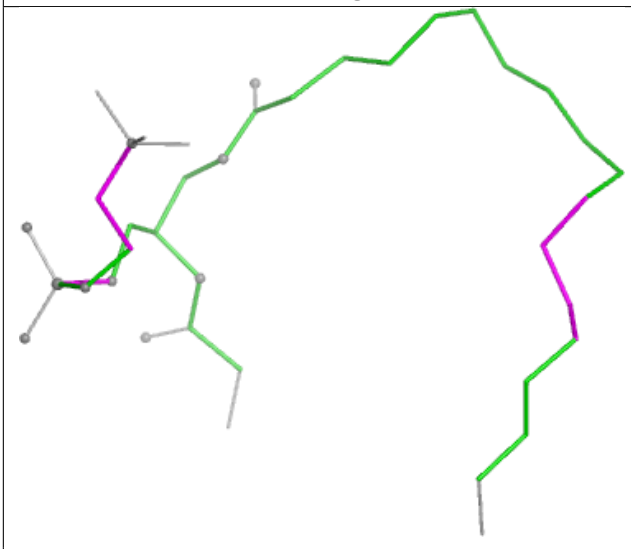
Ligand PC1 o 201



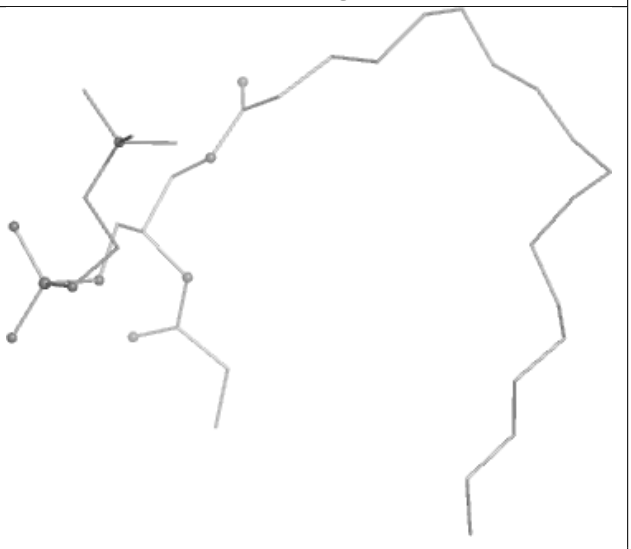
Bond lengths



Bond angles

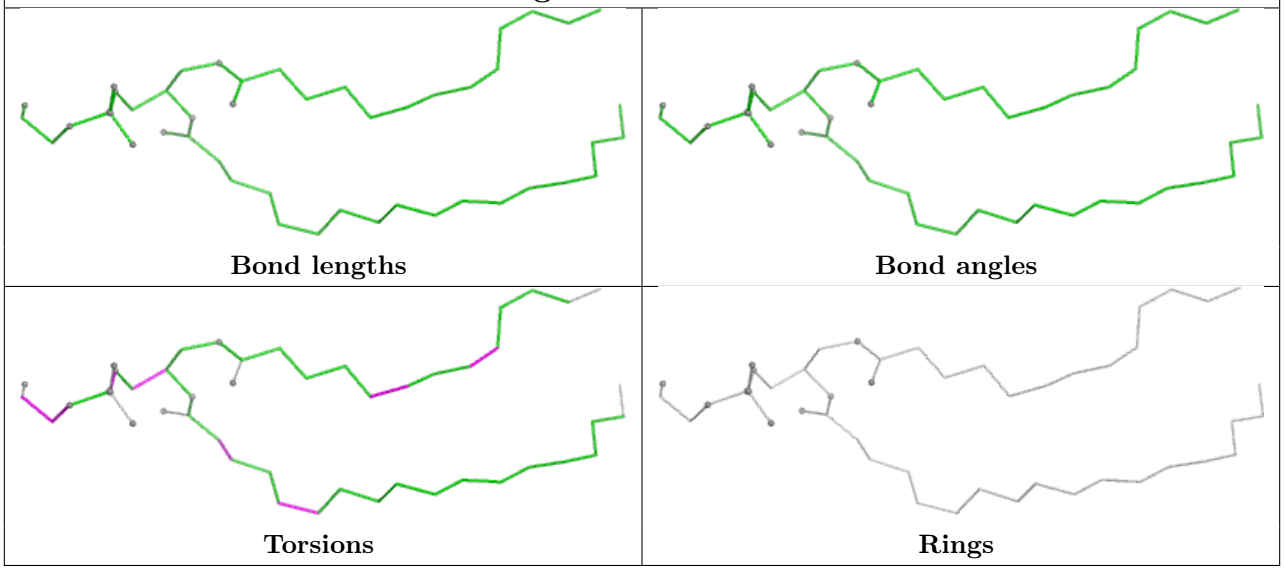


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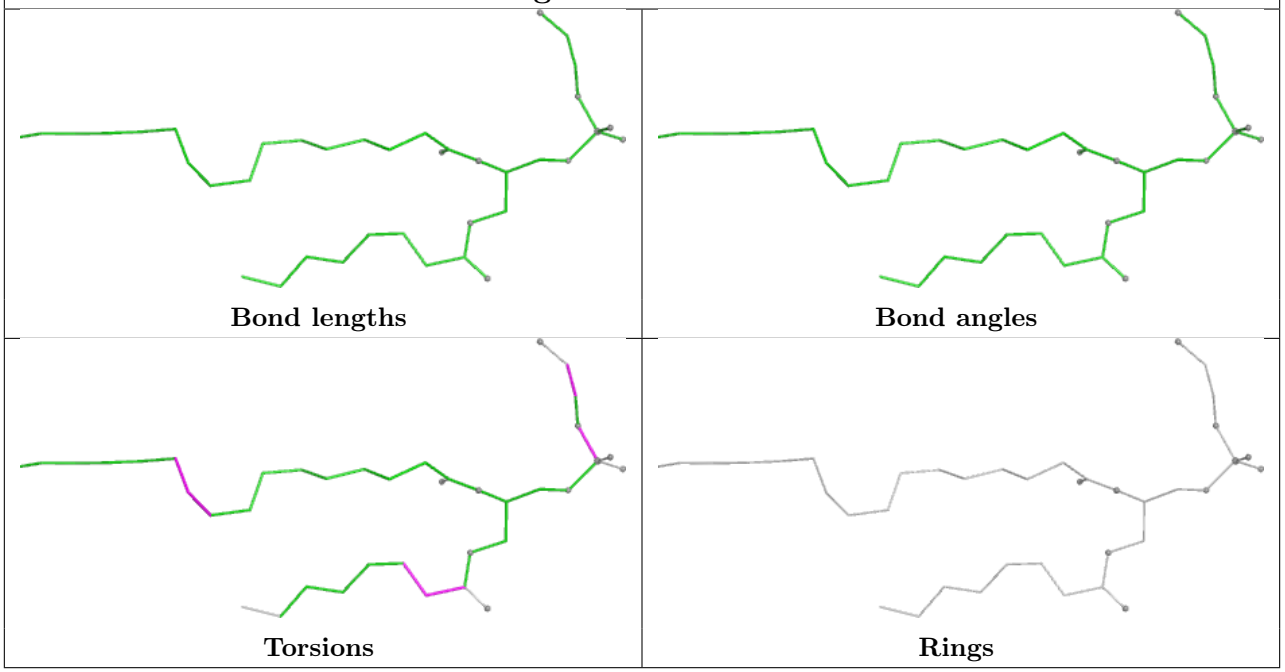


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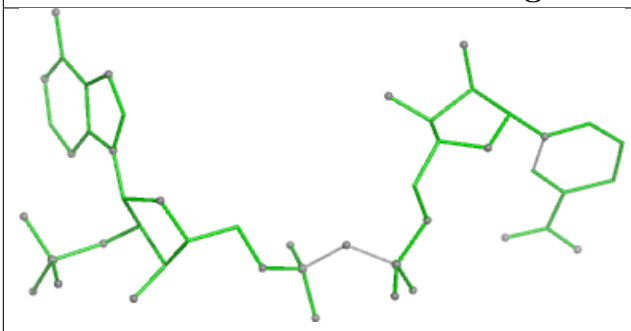
Ligand 3PE o 203



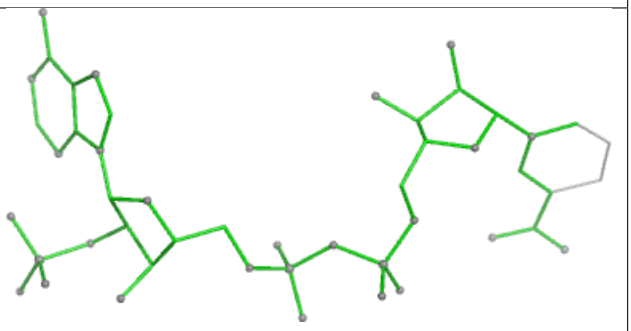
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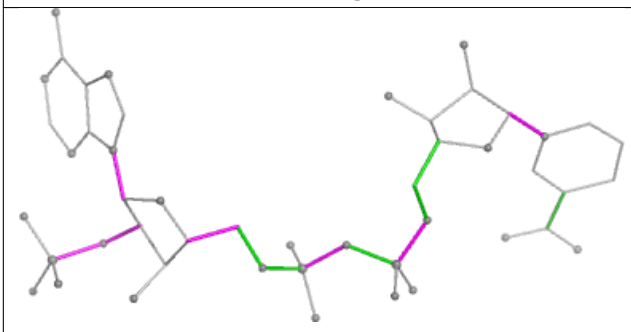
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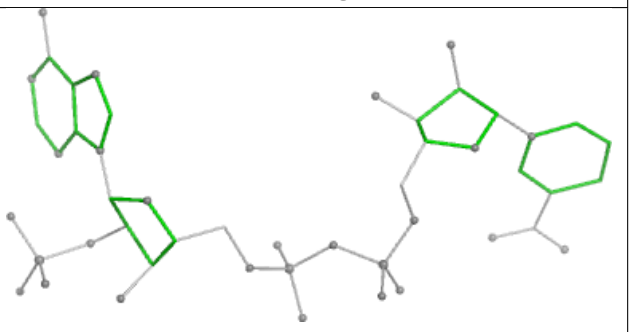
Bond lengths



Bond angles

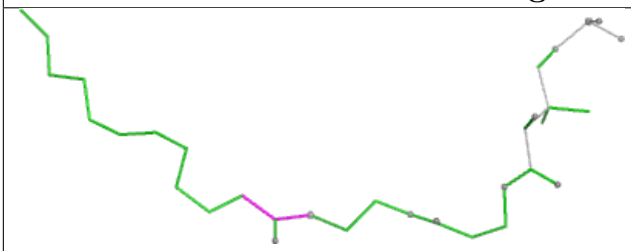


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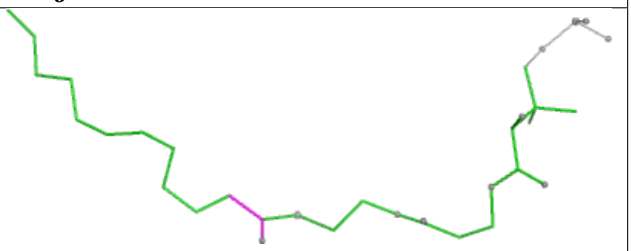


Rings

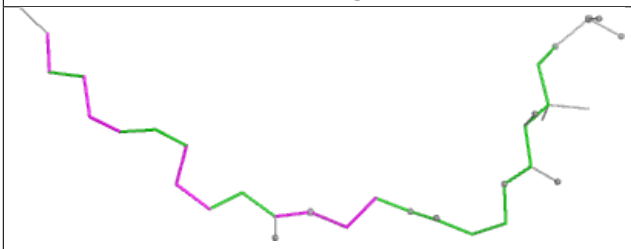
Ligand ZMP j 101



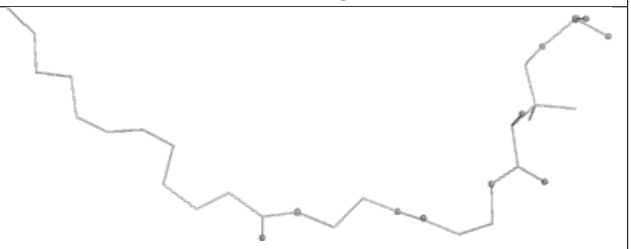
Bond lengths



Bond angles



Torsions



Rings

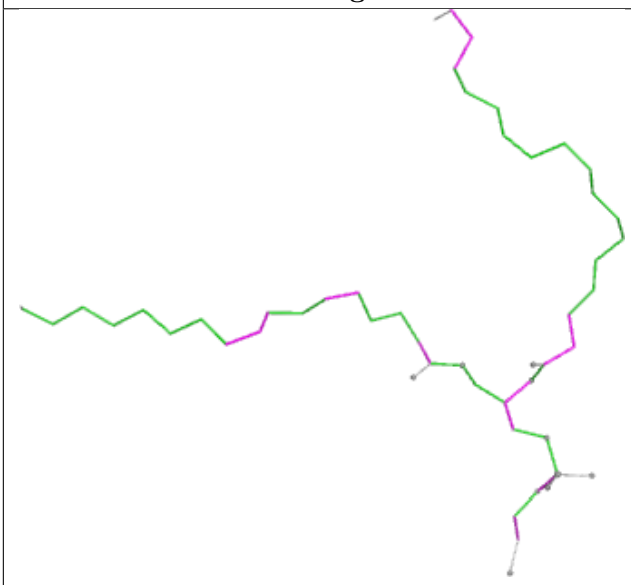
Ligand 3PE 9 501



Bond lengths



Bond angles

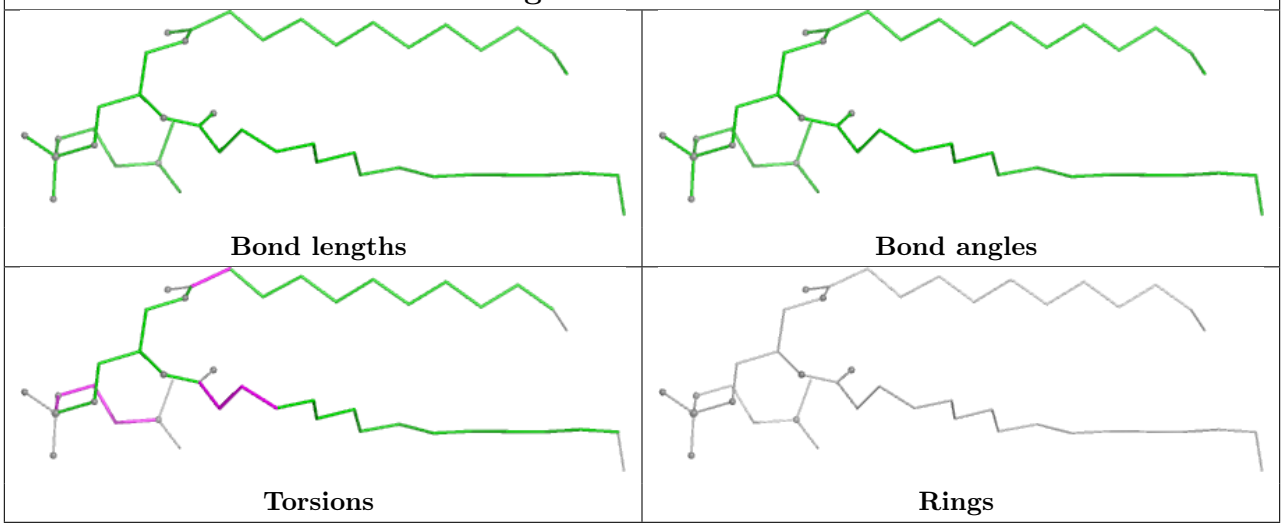


Torsions



Rings

Ligand PC1 M 501



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

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4093. These allow visual inspection of the internal detail of the map and identification of artifacts.

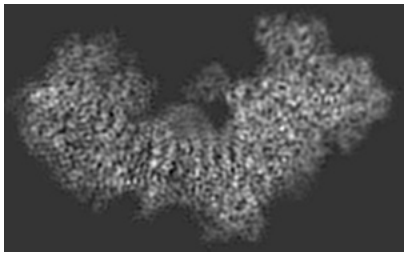
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

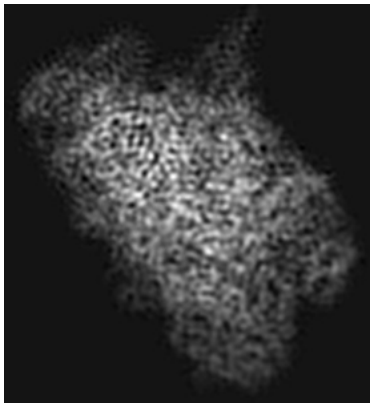
6.1.1 Primary map



X



Y

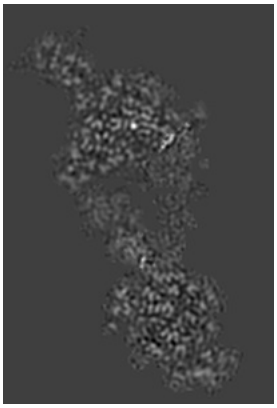


Z

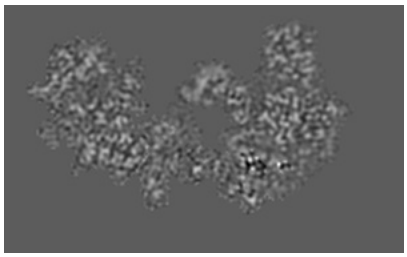
The images above show the map projected in three orthogonal directions.

6.2 Central slices

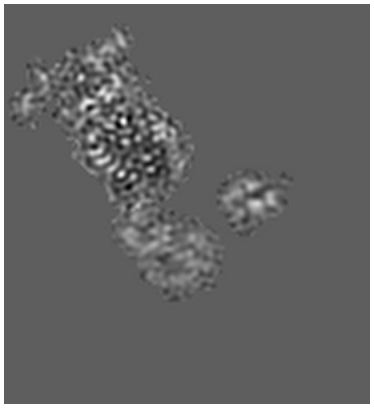
6.2.1 Primary map



X Index: 64



Y Index: 70

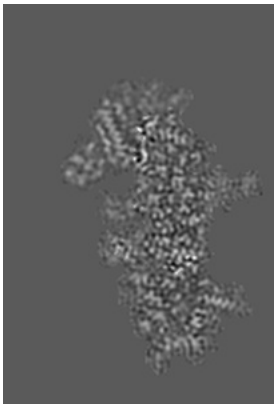


Z Index: 104

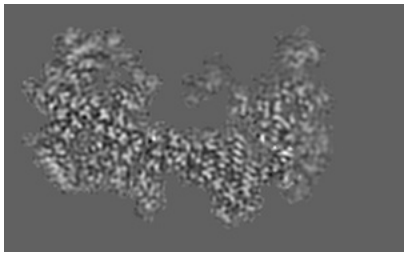
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

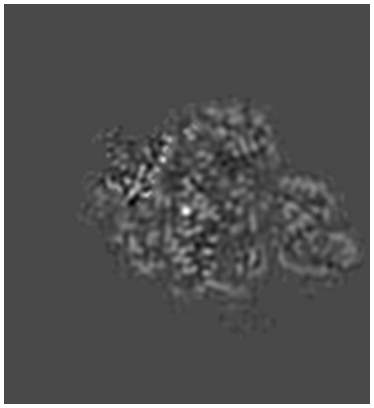
6.3.1 Primary map



X Index: 46



Y Index: 80

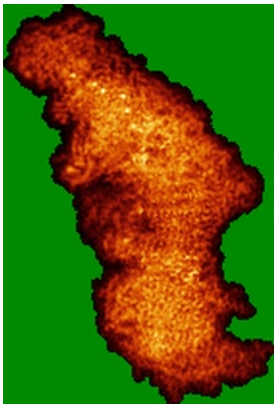


Z Index: 145

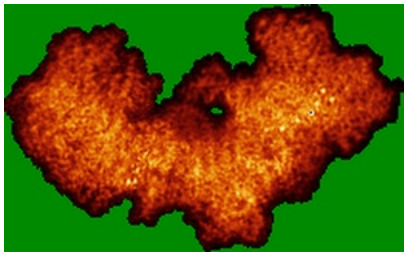
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

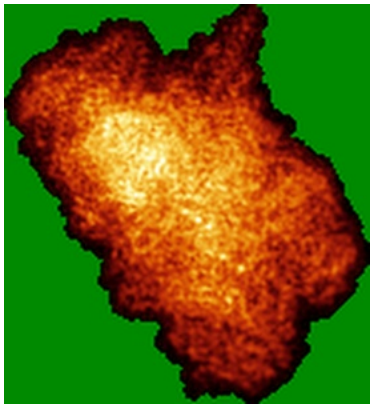
6.4.1 Primary map



X



Y

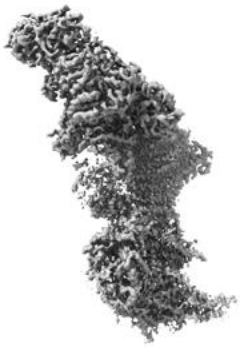


Z

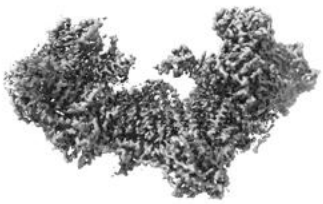
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

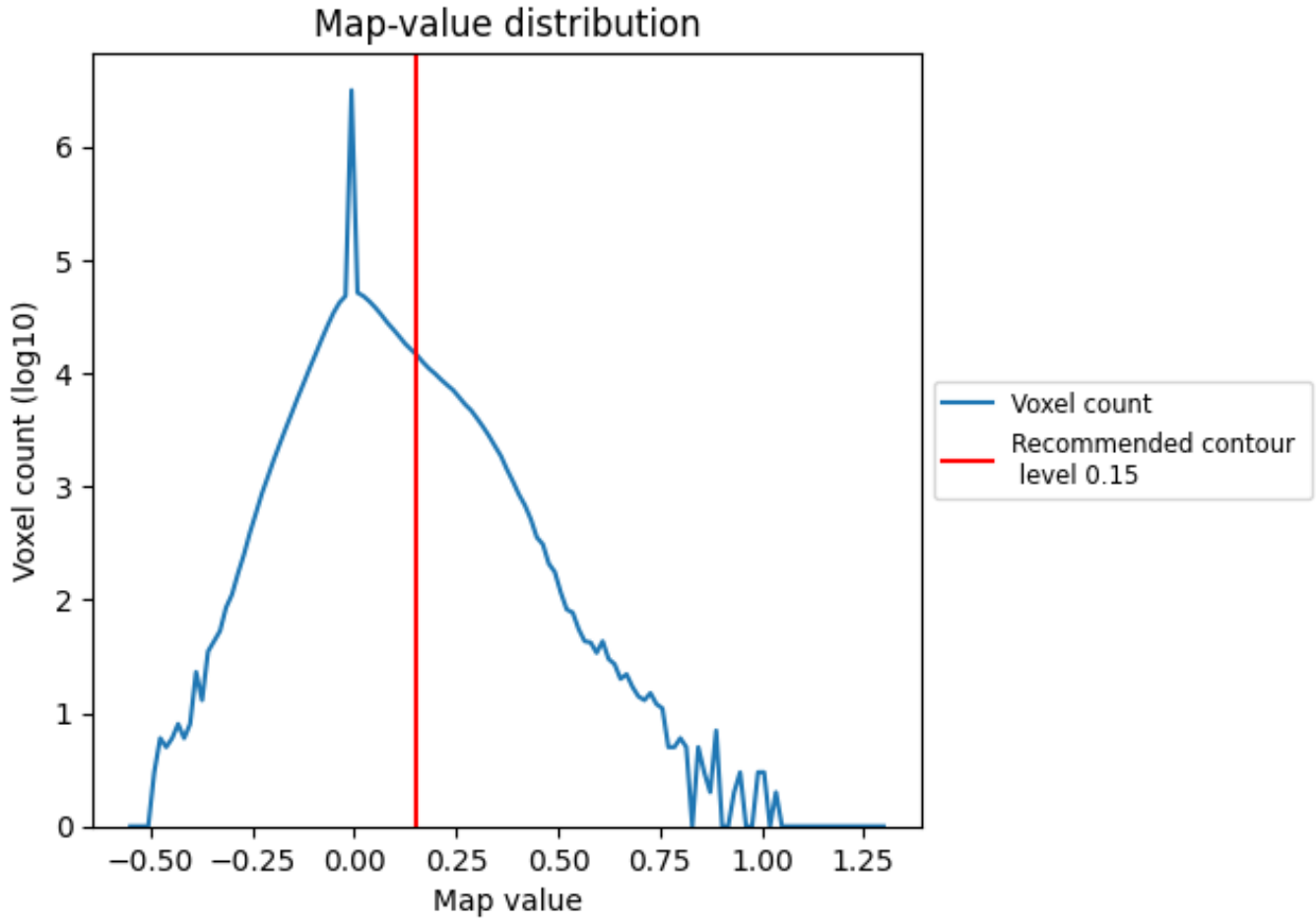
6.6 Mask visualisation (i)

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

7 Map analysis

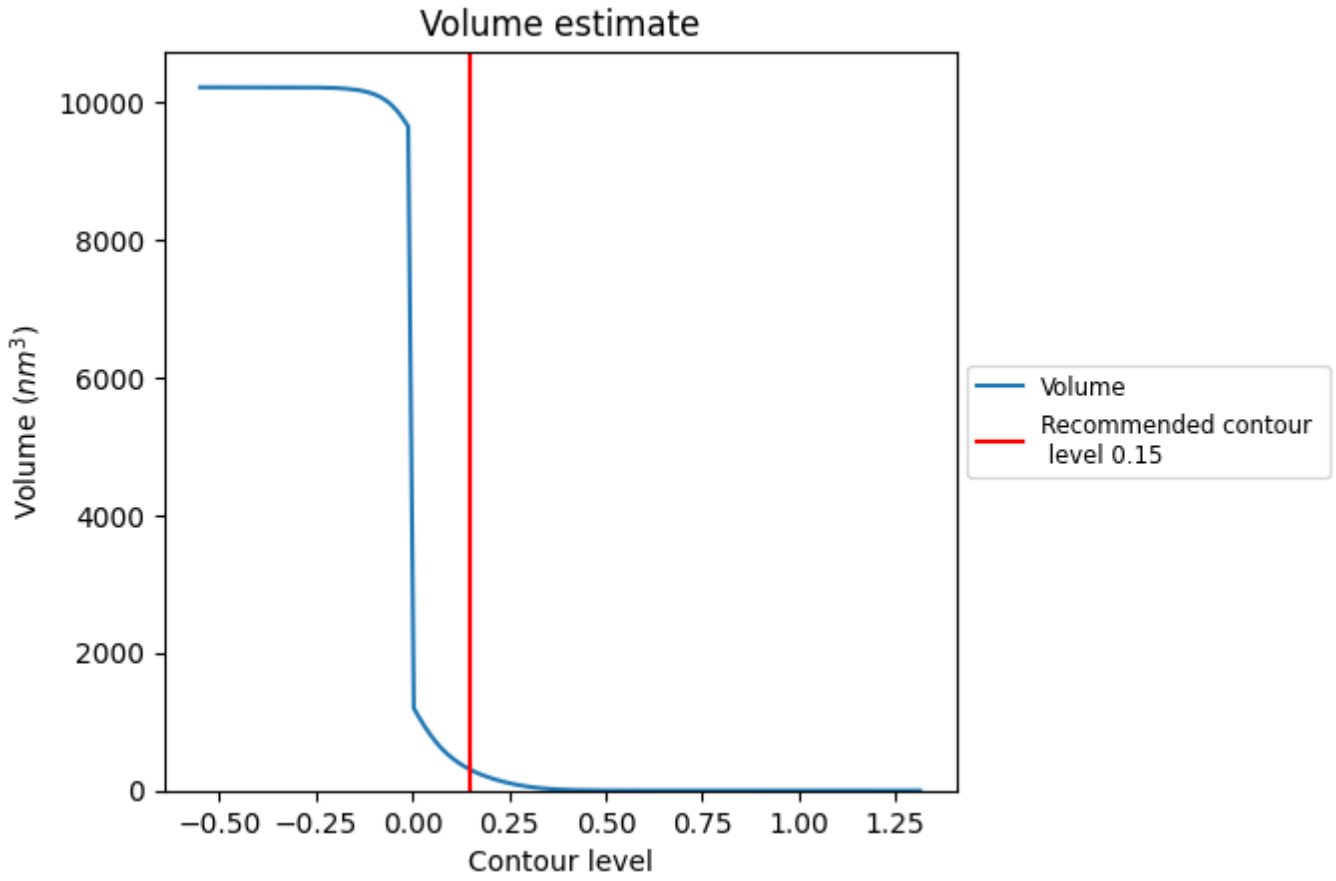
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate



The volume at the recommended contour level is 304 nm^3; this corresponds to an approximate mass of 275 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

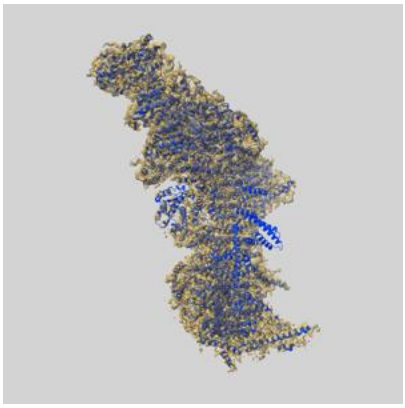
8 Fourier-Shell correlation

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

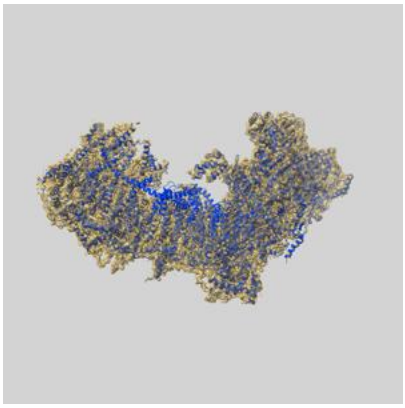
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4093 and PDB model 5LNK. Per-residue inclusion information can be found in section 3 on page 18.

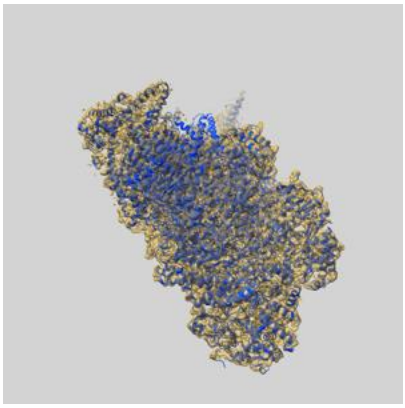
9.1 Map-model overlay



X



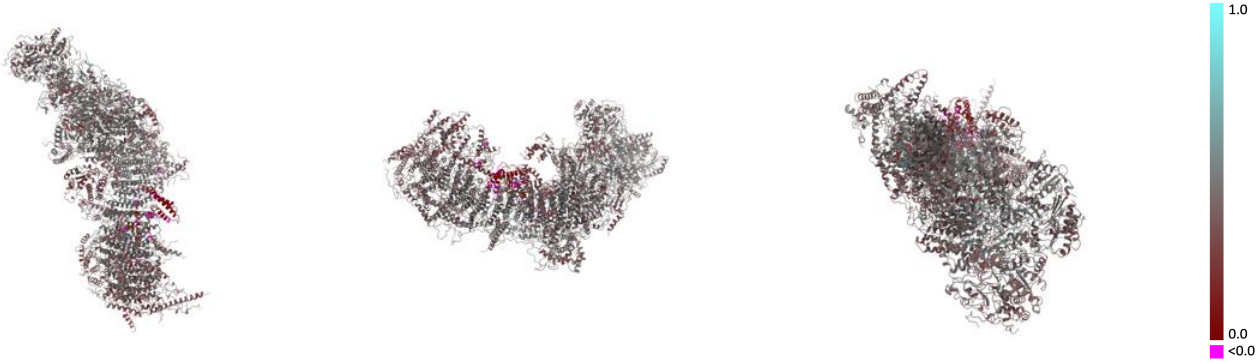
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

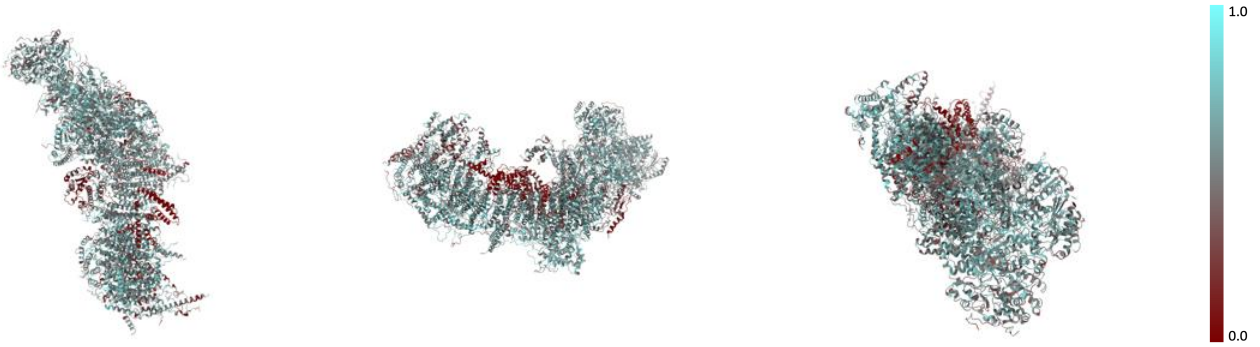
9.2 Q-score mapped to coordinate model



X Y Z

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

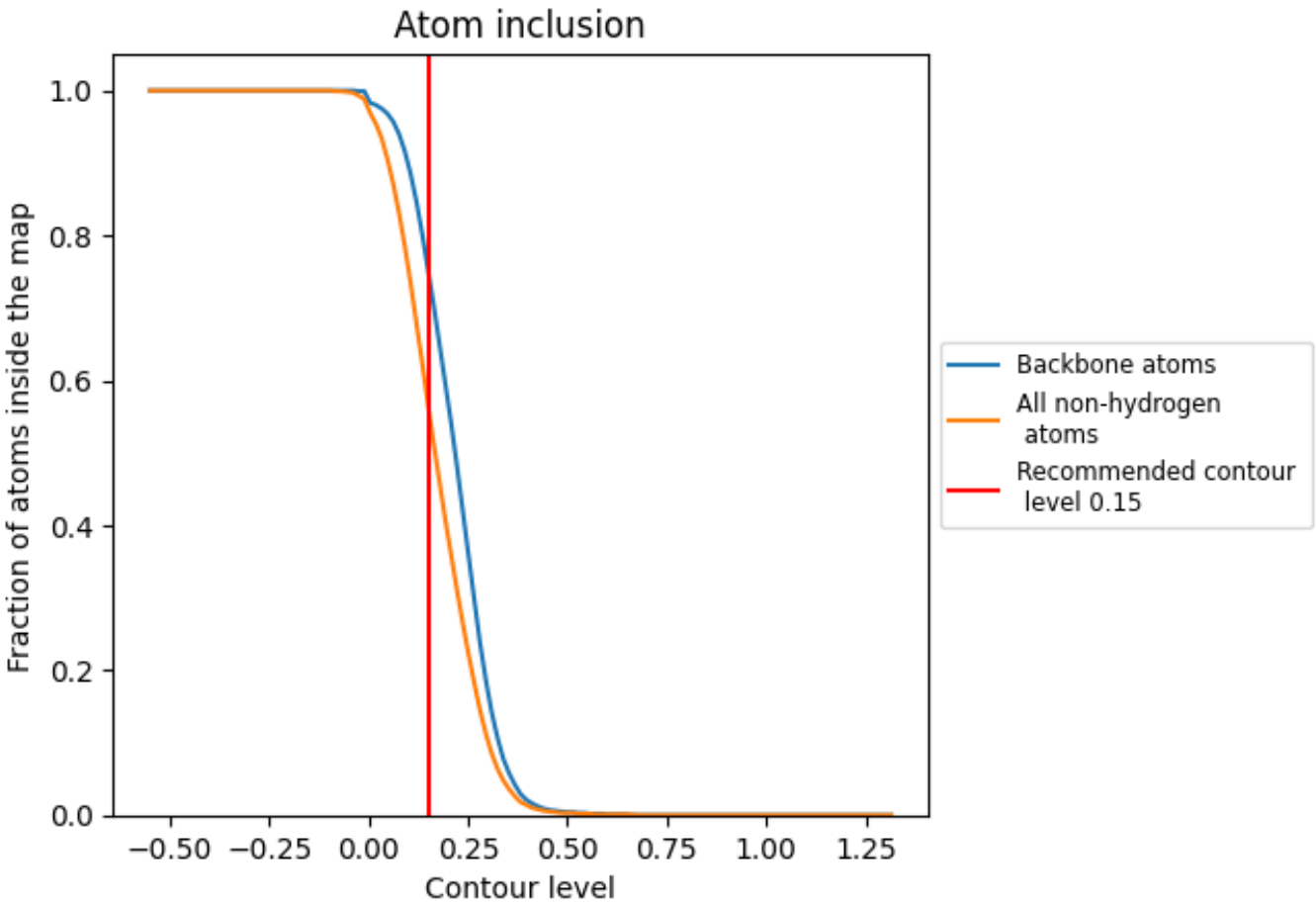
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.4080
1	0.5680	0.4170
2	0.5520	0.4100
3	0.5970	0.4350
4	0.5970	0.4320
5	0.6410	0.4560
6	0.6280	0.4200
9	0.6450	0.4310
A	0.5470	0.4270
H	0.6250	0.4320
J	0.4000	0.4110
K	0.5820	0.4330
L	0.5520	0.3890
M	0.6440	0.4460
N	0.6540	0.4480
V	0.0120	0.0190
W	0.6680	0.4390
X	0.5330	0.3640
Y	0.6240	0.4060
Z	0.6260	0.4120
a	0.5210	0.4050
b	0.5780	0.4570
c	0.5970	0.4570
d	0.5280	0.3940
e	0.5790	0.3900
f	0.5920	0.3920
g	0.5780	0.4250
h	0.4940	0.4070
i	0.3370	0.3900
j	0.4760	0.3610
k	0.3010	0.3100
l	0.6180	0.4400
m	0.6010	0.4360
n	0.5550	0.3680
o	0.5800	0.4420



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Chain	Atom inclusion	Q-score
p	0.4730	0.3660
q	0.5880	0.4050
r	0.5360	0.3660
s	0.5210	0.3630
t	0.6030	0.3700
u	0.5420	0.3750
v	0.4940	0.3360
w	0.6350	0.4340
x	0.5860	0.3870
y	0.5110	0.3860
z	0.6550	0.4260