



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 11:25 AM UTC

PDB ID : 8IBB / pdb_00008ibb
EMDB ID : EMD-35338
Title : Respiratory complex Membrane domain of CI, focus-refined of type IB, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

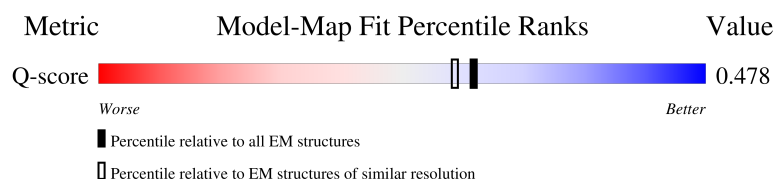
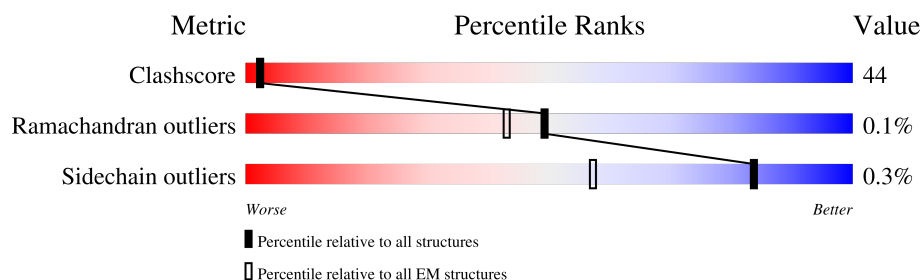
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.30 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	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	D	463	
2	J	172	
3	K	98	
4	L	607	

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Mol	Chain	Length	Quality of chain
5	M	459	
6	N	345	
7	O	355	
8	U	156	
9	X	172	
10	Y	143	
11	c	76	
12	d	120	
13	e	106	
14	f	57	
15	g	151	
16	h	189	
17	i	128	
18	j	105	
19	k	104	
20	l	186	
21	m	129	
22	n	179	
23	o	137	
24	p	176	

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
25	3PE	M	503	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	39	Total	C	N	O	S	0	0
			328	214	54	59	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	157	Total	C	N	O	S	0	0
			1193	806	169	203	15		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 8 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	27	Total	C	N	O	0	0
			221	146	39	36		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	52	Total	C	N	O	S	0	0
			447	290	80	75	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	100	Total	C	N	O	S	0	0
			842	545	135	158	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	92	Total	C	N	O	S	0	0
			773	506	132	132	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	70	Total	C	N	O	S	0	0
			587	383	98	105	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	72	Total	C	N	O	S	0	0
			578	381	101	94	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	125	Total	C	N	O	S	0	0
			1044	673	188	183			

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

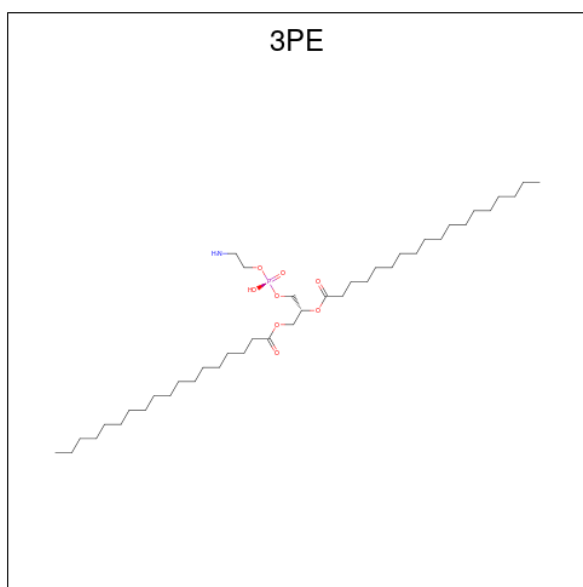
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	119	Total	C	N	O	S	0	0
			1019	642	191	178	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	170	Total	C	N	O	S	0	0
			1438	904	258	268	8		

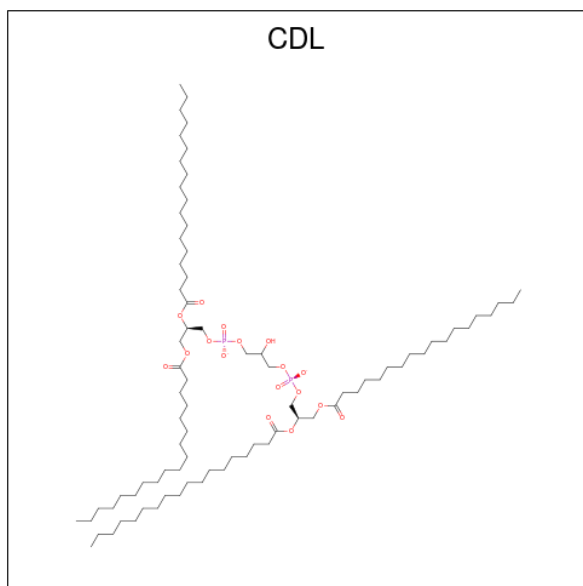
- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	O	1	Total	C	N	O	P	0
			44	34	1	8	1	
25	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	j	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

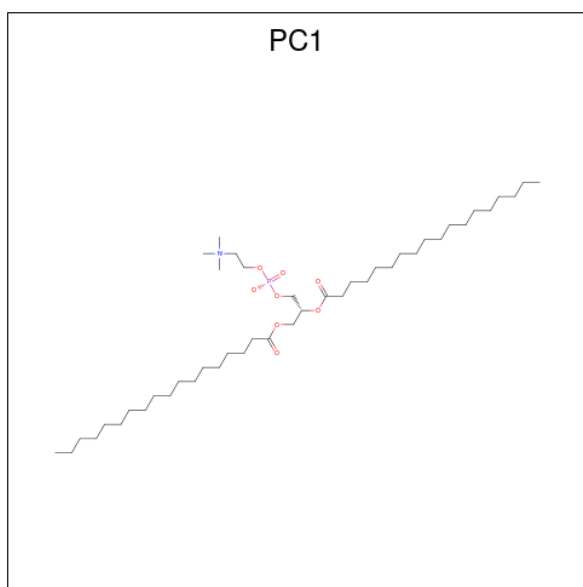
- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand

of Interest" by depositor).



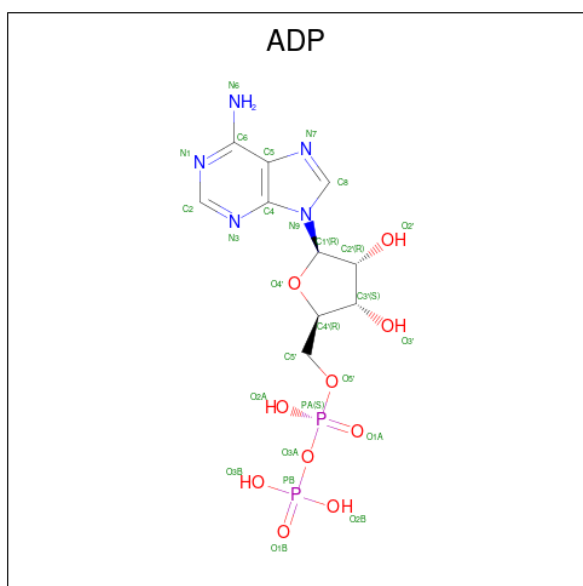
Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			77	58	17	2	
26	L	1	Total	C	O	P	0
			81	62	17	2	
26	d	1	Total	C	O	P	0
			67	48	17	2	
26	h	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

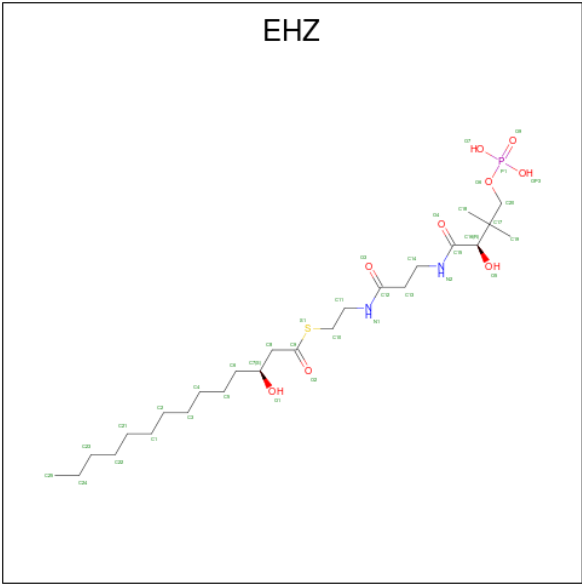
- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 29 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EH2) (formula:

C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

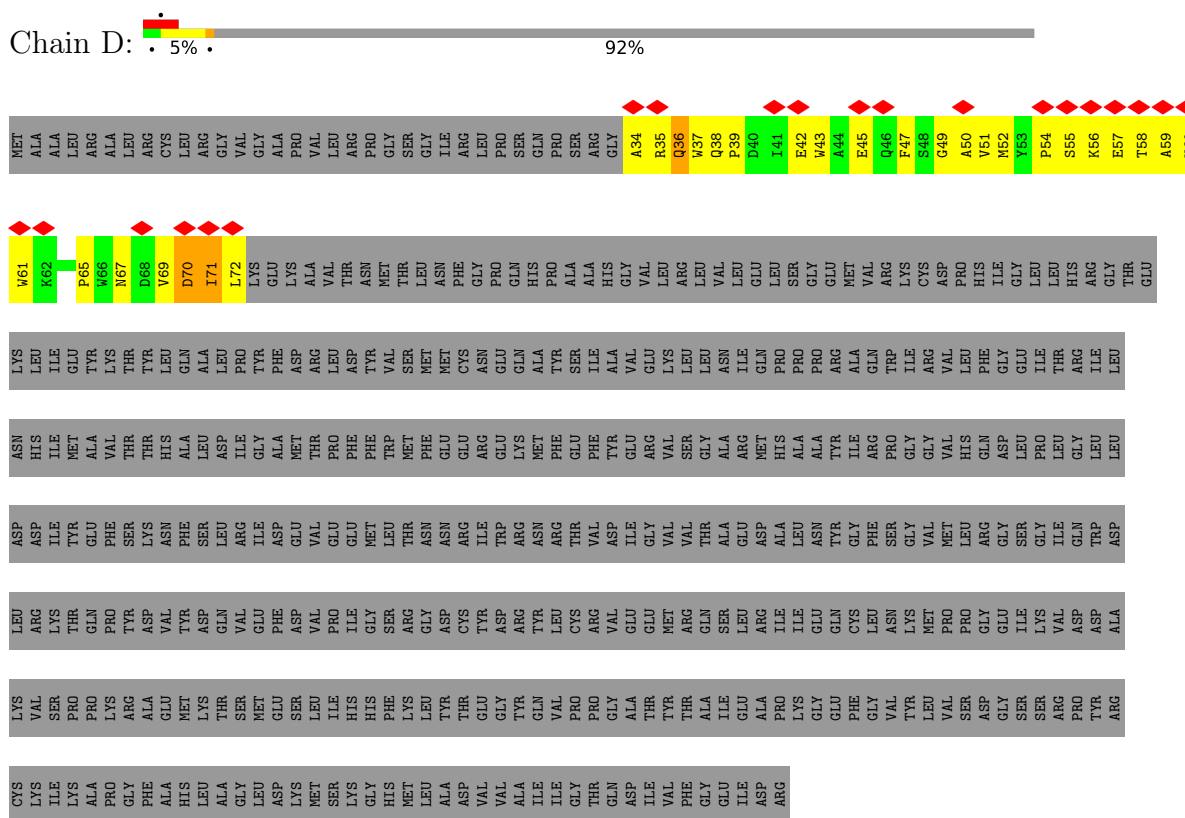


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
29	n	1	32	19	2	9	1	1	0

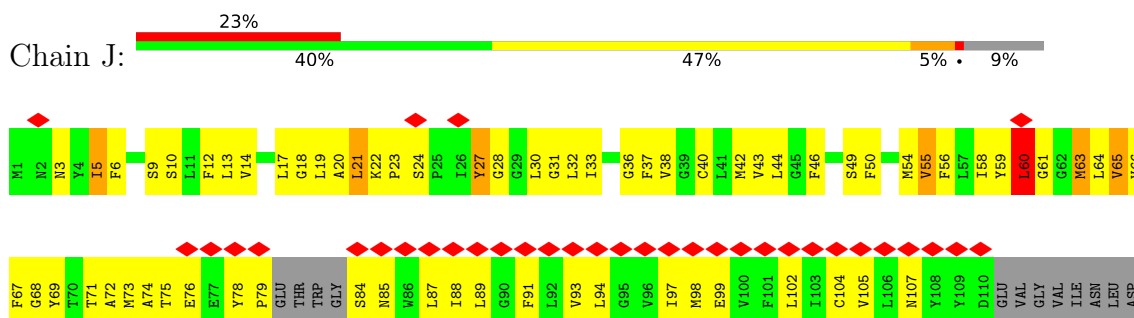
3 Residue-property plots [i](#)

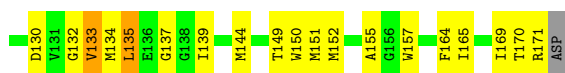
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

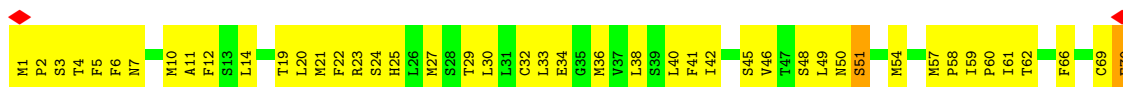


- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

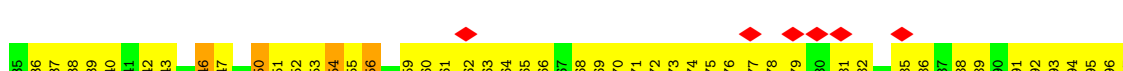
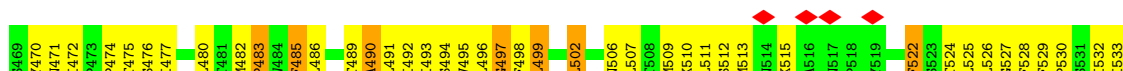
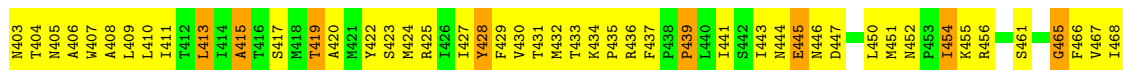
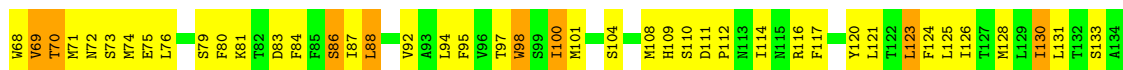


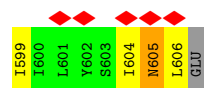


• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L



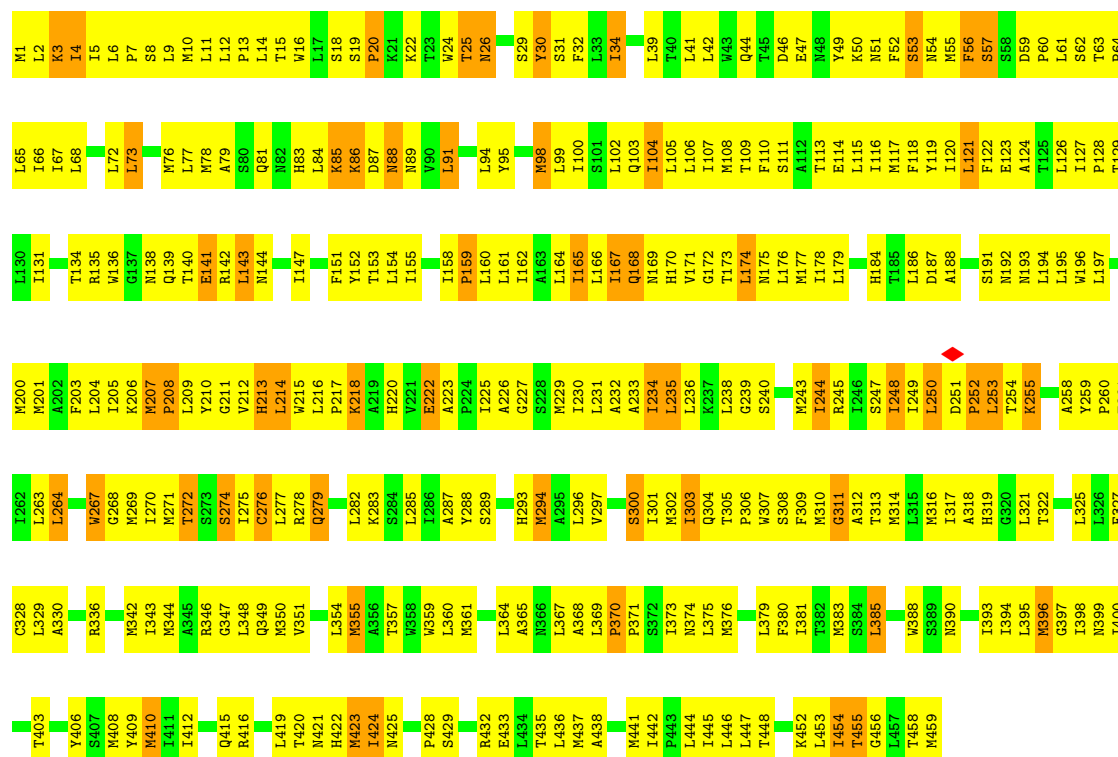
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5



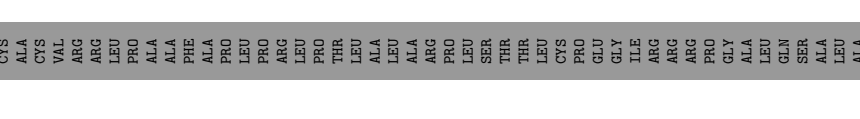


• Molecule 5: NADH-ubiquinone oxidoreductase chain 4

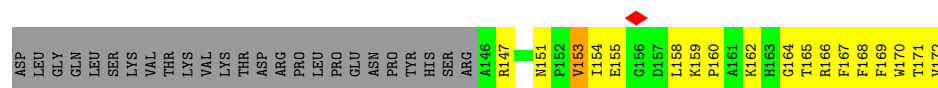
Chain M: 29% 59% 13%



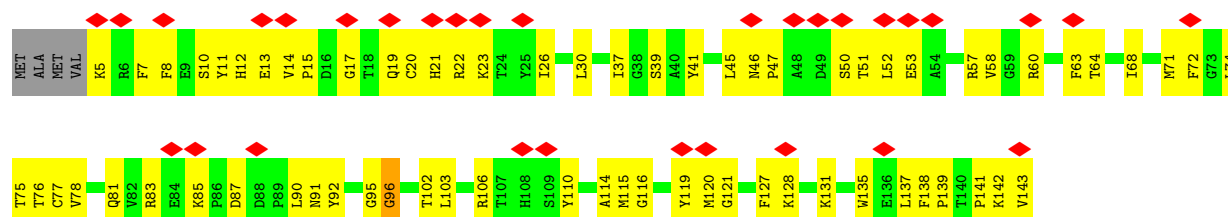
- [illegible]

- Chain U: 
- 
- VAL THR HIS LEU CYS ARG GLN TYR D70 A71 L72 T75 L76 I79 K80 D81 R82 V83 L84 Y85 V86 L87 K88 L89 Y90 D91 K92 I93 D94 P95 L98 S99 Y100 N101 S102 M105 L106 L107 D108 L109 D110 S111 L112 L113 D114 Q115 V116 E117 I118 I119 M120 A121 M122 E123 D124 Y125 F126
- MET ALA SER ARG VAL LEU CYS ARG VAL CYS ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO ARG LEU THR LEU ALA LEU ALA ARG PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG ARG PRO GLY ALA LEU GLN SER ALA LEU ALA LEU ALA GLN VAL PRO GLY THR

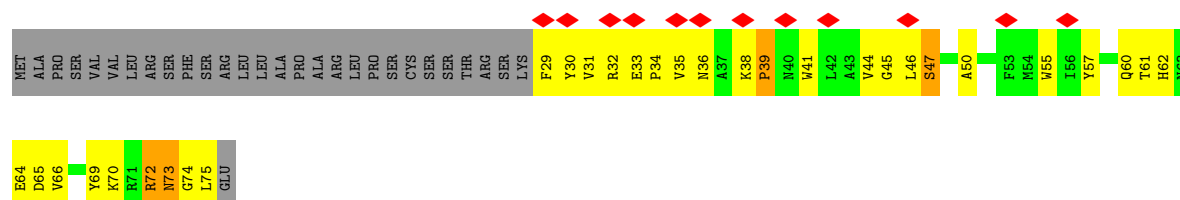
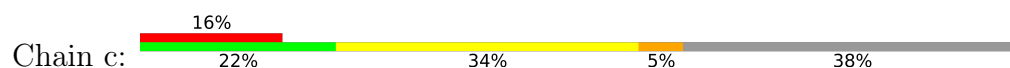
- Chain X:  84%
- | Chain X | Chain Y | Chain Z |
|---------|---------|---------|
| MET | LYS | GLY |
| PRO | LEU | VAL |
| GLY | VAL | ASN |
| ILE | ASN | GLY |
| VAL | GLY | CYS |
| GLU | CYS | ALA |
| LEU | ALA | LEU |
| PRO | LEU | ASN |
| THR | ASN | PHE |
| GLU | PHE | ARG |
| LEU | ARG | GLN |
| GLU | GLN | ILE |
| LEU | ILE | SER |
| VAL | SER | HIS |
| GLU | HIS | CYS |
| VAL | CYS | ALA |
| LYS | ALA | GLU |
| VAL | GLU | GLU |
| SER | GLU | THR |
| THR | THR | GLY |
| ALA | THR | TYR |
| VAL | GLY | TRP |
| LEU | TYR | THR |
| LEU | THR | CYS |
| ALA | CYS | ALA |
| HIS | ALA | LEU |
| HIS | LEU | ASP |
| TYR | ASP | TYR |
| SER | TYR | SER |
| ASN | SER | ASN |
| GLY | ASN | MET |
| ALA | MET | GLN |
| GLN | GLN | LEU |
| CYS | LEU | PHE |
| ASP | PHE | ARG |
| LYS | ARG | HIS |
| THR | HIS | CYS |
| ASN | CYS | ARG |
| LYS | ASN | ASP |
| GLU | ARG | GLN |
| GLU | GLN | GLN |
| PHE | GLN | ALA |
| LEU | ALA | LYS |
| CYS | LYS | PHE |
| ARG | PHE | ASP |
| TRP | ASP | GLN |
| GLU | GLN | CYS |
| GLY | CYS | VAL |
| LEU | VAL | LEU |
| ASP | LEU | ASP |
| PRO | ASP | LYS |
| ARG | LYS | LEU |
| ARG | LEU | GLY |
| CYS | GLY | TRP |
| LEU | TRP | VAL |
| LYS | VAL | ARG |
| GLY | ARG | PRO |



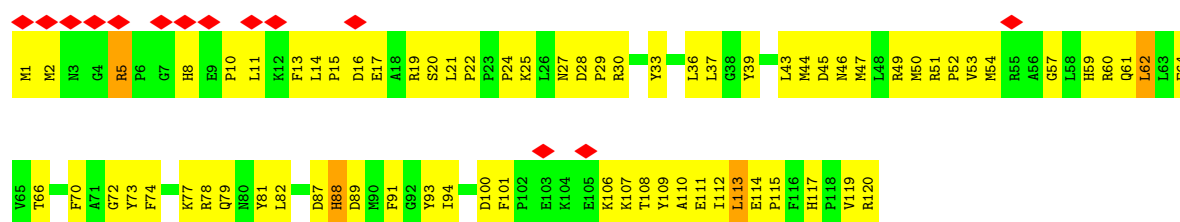
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



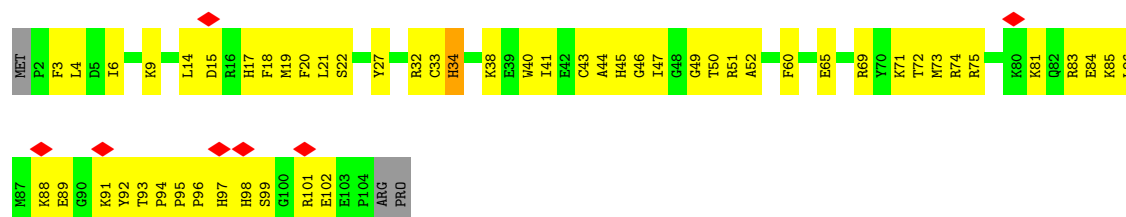
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



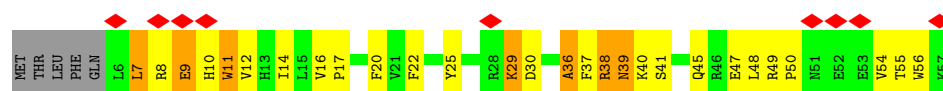
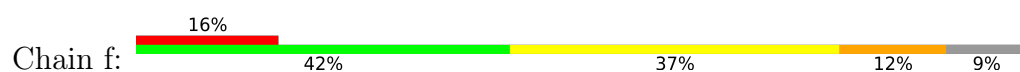
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 subunit C2



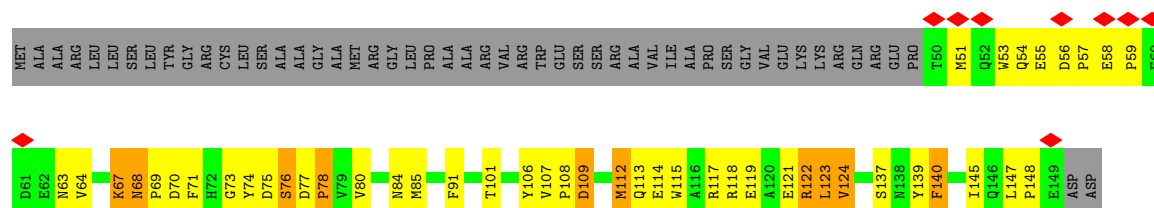
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



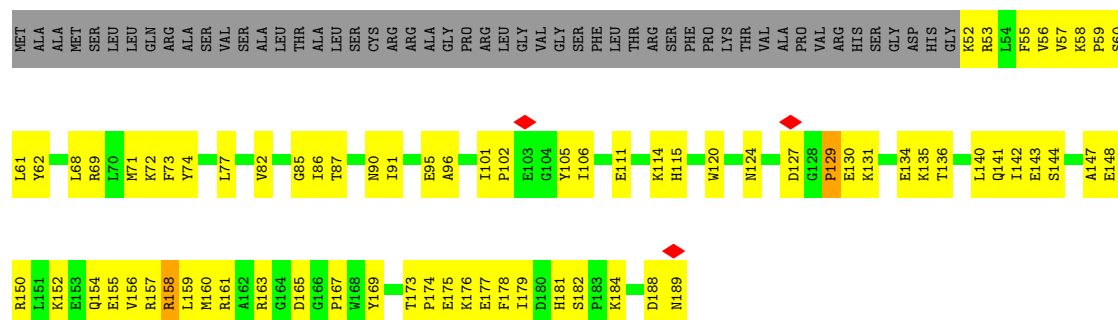
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



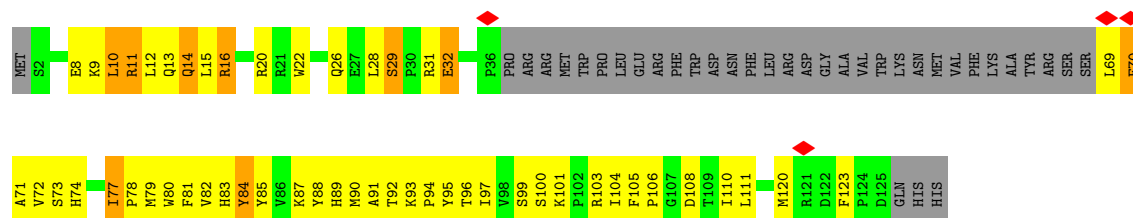
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



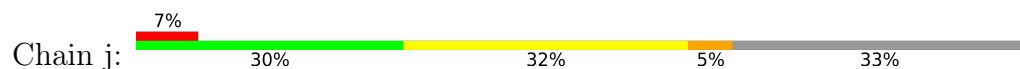
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

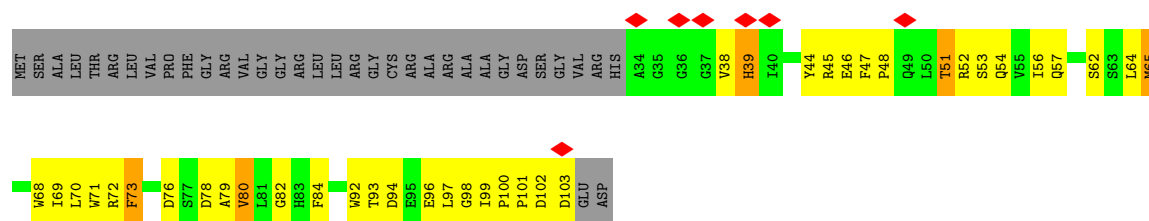


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

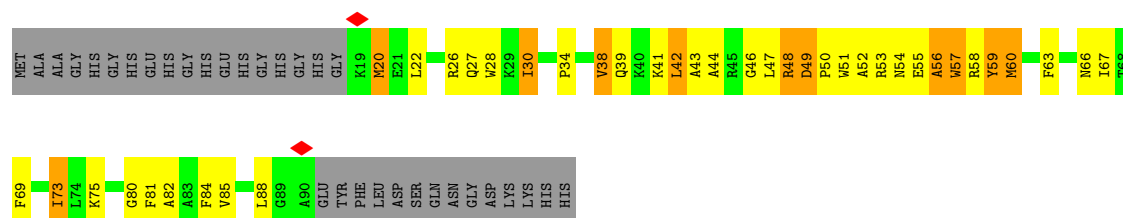
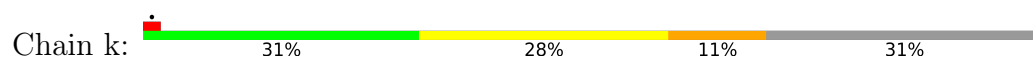


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

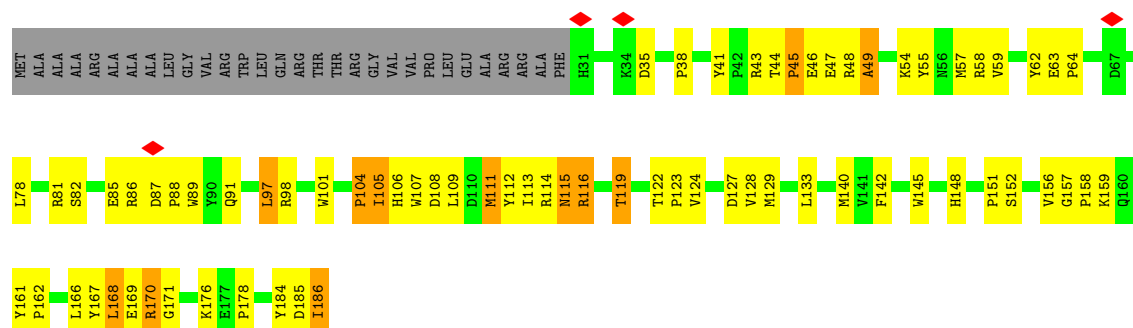




- Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

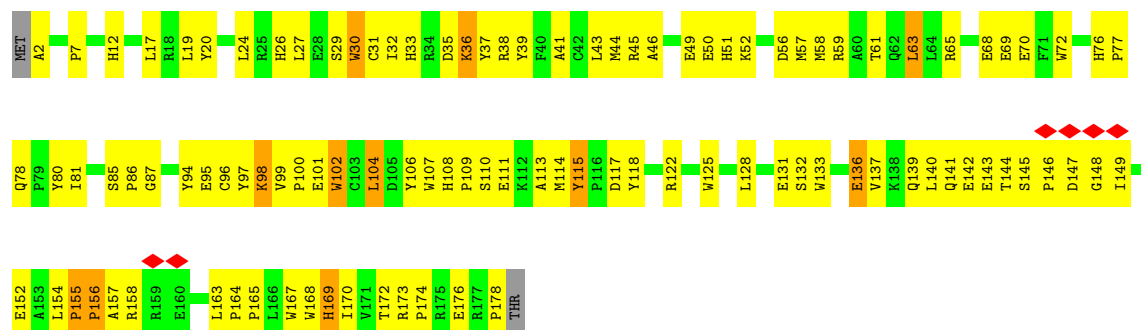


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

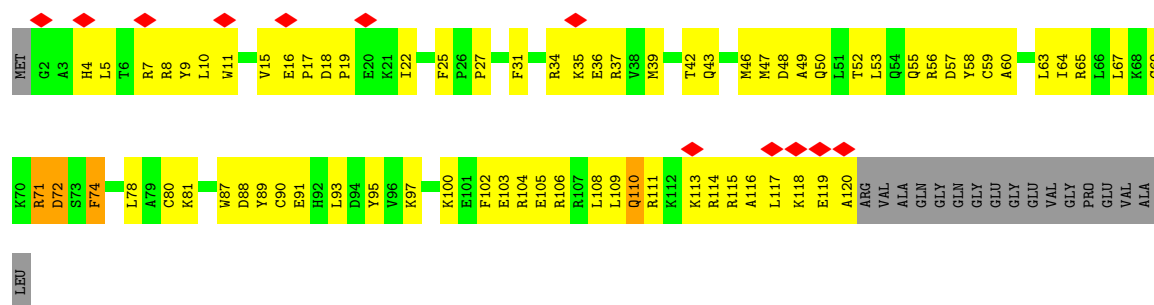


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

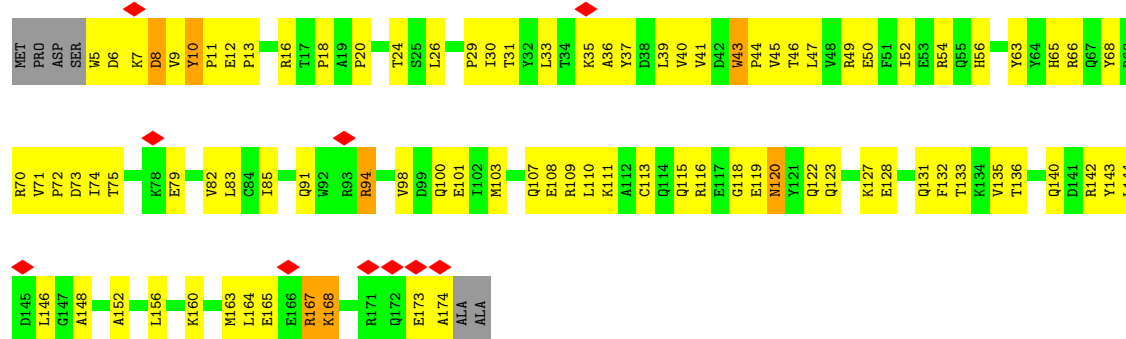




- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.253	Depositor
Minimum map value	-1.781	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 3PE, CDL, EHZ, PC1

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	D	0.65	0/343	1.10	3/472 (0.6%)
2	J	0.80	0/1221	1.34	16/1656 (1.0%)
3	K	0.91	0/740	1.50	14/1005 (1.4%)
4	L	0.98	5/4921 (0.1%)	1.57	109/6696 (1.6%)
5	M	1.01	7/3717 (0.2%)	1.57	87/5062 (1.7%)
6	N	1.00	4/2756 (0.1%)	1.43	50/3751 (1.3%)
7	O	0.87	6/2666 (0.2%)	1.22	27/3615 (0.7%)
8	U	1.02	1/712 (0.1%)	1.42	17/962 (1.8%)
9	X	0.81	0/230	1.16	1/313 (0.3%)
10	Y	0.87	0/1054	0.97	3/1429 (0.2%)
11	c	0.96	1/400 (0.2%)	1.34	11/544 (2.0%)
12	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
13	e	0.74	1/881 (0.1%)	1.00	2/1173 (0.2%)
14	f	0.90	1/459 (0.2%)	1.32	11/618 (1.8%)
15	g	0.88	3/870 (0.3%)	1.36	19/1185 (1.6%)
16	h	0.75	0/1197	1.22	6/1621 (0.4%)
17	i	0.85	0/798	1.38	17/1085 (1.6%)
18	j	0.87	2/612 (0.3%)	1.28	10/837 (1.2%)
19	k	1.12	2/596 (0.3%)	1.55	20/805 (2.5%)
20	l	1.02	4/1367 (0.3%)	1.27	10/1866 (0.5%)
21	m	0.85	1/1073 (0.1%)	1.20	15/1455 (1.0%)
22	n	0.95	1/1589 (0.1%)	1.26	17/2152 (0.8%)
23	o	0.82	0/1044	1.14	7/1401 (0.5%)
24	p	0.73	1/1471 (0.1%)	1.01	13/1988 (0.7%)
All	All	0.92	42/31745 (0.1%)	1.35	496/43078 (1.2%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	d	115	PRO	N-CD	-14.11	1.28	1.47
4	L	265	PRO	N-CD	13.82	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	50	PRO	N-CD	-13.63	1.28	1.47
6	N	255	PRO	N-CD	-13.58	1.28	1.47
11	c	39	PRO	N-CD	-13.26	1.29	1.47
7	O	315	PRO	N-CD	-12.07	1.30	1.47
7	O	210	PRO	N-CD	-11.39	1.31	1.47
4	L	234	PRO	N-CD	11.17	1.63	1.47
5	M	370	PRO	N-CD	-10.60	1.32	1.47
19	k	20	MET	C-N	9.61	1.47	1.33
15	g	78	PRO	N-CD	-9.51	1.34	1.47
12	d	15	PRO	N-CD	-9.38	1.34	1.47
5	M	20	PRO	N-CD	8.54	1.59	1.47
4	L	212	PRO	N-CD	-8.21	1.36	1.47
22	n	155	PRO	N-CD	8.07	1.59	1.47
20	l	115	ASN	C-N	-7.30	1.24	1.33
20	l	104	PRO	N-CD	-7.21	1.37	1.47
5	M	208	PRO	N-CD	7.15	1.57	1.47
6	N	238	PRO	N-CD	-7.00	1.38	1.47
18	j	38	VAL	C-N	6.98	1.43	1.33
7	O	206	TYR	C-N	6.83	1.42	1.33
15	g	113	GLN	CA-C	6.62	1.61	1.52
7	O	205	ILE	C-N	6.48	1.42	1.33
4	L	384	PRO	N-CD	6.28	1.56	1.47
24	p	10	TYR	CA-C	-6.23	1.46	1.52
15	g	137	SER	C-O	-6.04	1.16	1.24
4	L	112	PRO	N-CD	6.01	1.56	1.47
21	m	72	ARG	CA-C	5.89	1.60	1.52
13	e	34	HIS	C-O	-5.85	1.16	1.24
20	l	45	PRO	N-CD	-5.77	1.39	1.47
18	j	39	HIS	C-N	-5.73	1.28	1.33
7	O	87	PRO	N-CD	-5.72	1.39	1.47
5	M	454	ILE	CA-C	5.66	1.60	1.52
5	M	252	PRO	N-CD	-5.58	1.40	1.47
6	N	333	SER	C-O	-5.57	1.17	1.23
8	U	140	CYS	C-O	-5.41	1.17	1.24
7	O	103	PRO	N-CD	-5.24	1.40	1.47
14	f	38	ARG	CA-C	-5.16	1.46	1.52
20	l	111	MET	C-O	-5.12	1.17	1.24
5	M	424	ILE	CA-C	-5.11	1.45	1.52
5	M	159	PRO	N-CD	5.03	1.54	1.47
6	N	88	GLN	CA-C	5.00	1.59	1.52

All (496) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	370	PRO	N-CA-C	14.57	128.48	110.70
6	N	255	PRO	N-CA-C	14.49	128.38	110.70
7	O	118	TYR	N-CA-C	13.83	125.86	111.07
5	M	424	ILE	N-CA-C	-11.65	94.03	109.30
17	i	14	GLN	N-CA-C	11.58	123.90	111.28
5	M	104	ILE	N-CA-C	-11.56	99.09	110.30
4	L	194	ASN	N-CA-C	11.47	125.40	109.11
7	O	114	LEU	N-CA-C	-11.46	98.87	111.36
2	J	5	ILE	N-CA-C	11.42	121.90	110.82
5	M	311	GLY	N-CA-C	-11.38	99.30	112.50
20	l	116	ARG	N-CA-C	11.32	123.30	110.97
6	N	244	ILE	N-CA-C	-11.28	99.33	110.72
4	L	278	LEU	N-CA-C	-11.23	99.01	111.14
3	K	83	ASN	N-CA-C	-11.19	100.17	114.04
8	U	79	ILE	N-CA-C	-10.99	102.35	112.90
4	L	582	GLY	N-CA-C	-10.80	99.52	114.64
4	L	556	ILE	N-CA-C	10.70	121.36	110.23
4	L	231	PRO	N-CA-C	10.67	127.71	113.84
16	h	101	ILE	N-CA-C	-10.55	98.61	108.95
7	O	210	PRO	N-CA-CB	-10.36	94.62	103.32
5	M	276	CYS	N-CA-C	-10.35	99.99	111.28
7	O	96	THR	N-CA-C	-10.32	100.11	111.36
20	l	170	ARG	N-CA-C	-10.19	101.49	113.21
22	n	29	SER	N-CA-C	-10.05	101.52	113.88
5	M	117	MET	N-CA-C	-10.04	100.34	111.28
2	J	27	TYR	N-CA-C	-9.91	100.95	113.23
2	J	36	GLY	N-CA-C	-9.89	101.03	112.50
5	M	423	MET	N-CA-C	-9.71	96.95	110.35
6	N	255	PRO	CA-N-CD	9.70	125.58	112.00
19	k	50	PRO	CA-N-CD	9.69	125.56	112.00
6	N	286	ALA	N-CA-C	-9.68	100.73	111.28
5	M	83	HIS	N-CA-C	-9.64	97.24	110.35
12	d	115	PRO	N-CA-CB	-9.60	95.00	103.35
17	i	12	LEU	N-CA-C	-9.51	101.23	113.12
4	L	375	ILE	N-CA-C	-9.50	101.30	110.42
24	p	56	HIS	N-CA-C	9.43	121.56	111.28
6	N	228	ASN	N-CA-C	-9.41	101.00	111.07
12	d	115	PRO	CA-N-CD	9.37	125.12	112.00
14	f	12	VAL	N-CA-CB	9.37	124.01	110.52
5	M	104	ILE	N-CA-CB	9.36	120.82	110.62
19	k	60	MET	N-CA-C	9.33	121.14	110.97
19	k	56	ALA	N-CA-C	9.29	121.49	111.36
4	L	394	LEU	N-CA-C	-9.29	101.13	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	40	ILE	N-CA-C	-9.29	101.34	110.72
4	L	483	PRO	N-CA-C	-9.20	96.75	111.38
11	c	64	GLU	N-CA-C	-9.12	101.31	111.07
6	N	87	GLN	N-CA-C	9.11	123.26	109.41
4	L	467	VAL	N-CA-C	9.10	119.15	110.42
5	M	442	ILE	N-CA-CB	9.06	117.52	110.45
11	c	39	PRO	N-CA-CB	-9.01	95.32	103.25
14	f	12	VAL	N-CA-C	-9.00	102.09	110.82
24	p	115	GLN	N-CA-C	-8.97	102.85	113.88
3	K	70	GLU	N-CA-C	-8.96	100.35	111.11
7	O	183	CYS	N-CA-C	-8.86	100.47	111.11
4	L	344	GLY	N-CA-C	-8.86	102.22	112.50
6	N	233	LEU	N-CA-C	-8.82	101.66	111.28
4	L	406	ALA	N-CA-C	-8.80	101.76	111.36
23	o	72	ASP	N-CA-C	-8.77	98.96	110.53
22	n	70	GLU	N-CA-C	-8.74	101.71	111.07
6	N	255	PRO	N-CA-CB	-8.74	94.60	103.08
5	M	255	LYS	N-CA-C	-8.72	101.74	111.07
6	N	81	LEU	N-CA-C	-8.72	94.43	108.55
5	M	248	ILE	N-CA-C	-8.58	102.18	110.42
4	L	212	PRO	N-CA-C	8.57	125.73	113.47
4	L	265	PRO	N-CA-C	-8.50	101.32	113.47
7	O	315	PRO	CA-N-CD	8.50	123.90	112.00
4	L	287	PHE	N-CA-C	-8.46	102.02	111.07
6	N	109	ALA	CA-C-N	-8.45	110.74	120.12
6	N	109	ALA	C-N-CA	-8.45	110.74	120.12
6	N	221	LEU	N-CA-C	-8.43	101.13	111.33
4	L	281	GLY	N-CA-C	-8.41	102.75	112.50
6	N	272	LYS	N-CA-C	-8.40	102.12	111.28
22	n	19	LEU	N-CA-C	-8.31	103.27	113.41
19	k	50	PRO	N-CA-CB	-8.27	93.50	102.76
6	N	218	ALA	N-CA-C	-8.25	98.93	111.56
4	L	151	SER	N-CA-C	-8.24	102.38	111.36
5	M	274	SER	N-CA-C	8.20	120.22	111.28
2	J	133	VAL	N-CA-C	-8.18	96.73	108.42
4	L	169	LEU	N-CA-C	-8.16	102.46	111.36
1	D	36	GLN	N-CA-C	-8.15	98.53	110.42
4	L	88	LEU	N-CA-C	-8.15	102.34	111.14
5	M	26	ASN	N-CA-C	-8.14	102.35	111.14
19	k	38	VAL	N-CA-C	-8.10	102.54	110.72
6	N	32	GLY	N-CA-C	-8.08	103.12	112.50
12	d	15	PRO	N-CA-CB	-8.03	96.37	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	170	ILE	N-CA-C	-8.02	103.08	111.58
4	L	276	THR	N-CA-CB	8.00	121.62	110.01
2	J	60	LEU	N-CA-C	7.99	120.76	111.02
5	M	385	LEU	N-CA-C	-7.98	102.58	111.28
5	M	205	ILE	N-CA-C	7.98	118.08	110.42
5	M	141	GLU	N-CA-C	7.91	122.77	113.20
11	c	39	PRO	CA-N-CD	7.91	123.07	112.00
11	c	45	GLY	N-CA-C	7.91	123.60	113.24
4	L	265	PRO	N-CA-CB	7.88	111.66	103.23
2	J	3	ASN	N-CA-C	-7.82	101.18	111.74
4	L	111	ASP	N-CA-C	-7.82	100.24	109.93
14	f	30	ASP	N-CA-C	-7.80	103.37	113.12
2	J	137	GLY	N-CA-C	-7.79	103.76	112.33
5	M	330	ALA	N-CA-C	-7.77	102.75	111.14
5	M	85	LYS	N-CA-C	-7.77	101.45	113.02
3	K	51	SER	N-CA-C	-7.76	102.90	113.30
4	L	265	PRO	CA-N-CD	-7.76	101.13	112.00
6	N	336	THR	N-CA-C	-7.74	103.36	114.12
4	L	415	ALA	N-CA-C	-7.72	102.86	111.28
7	O	210	PRO	CA-N-CD	7.61	122.66	112.00
8	U	147	TYR	N-CA-C	-7.59	102.94	111.14
15	g	124	VAL	N-CA-C	-7.54	103.11	110.72
4	L	245	ALA	N-CA-C	7.52	119.11	111.07
23	o	81	LYS	N-CA-C	-7.49	104.66	113.88
3	K	14	LEU	N-CA-C	-7.49	103.20	111.36
13	e	46	GLY	N-CA-C	-7.49	104.94	114.37
4	L	138	PHE	N-CA-C	-7.42	103.19	111.28
4	L	605	ASN	N-CA-CB	7.42	121.23	110.47
18	j	82	GLY	N-CA-C	-7.42	103.51	112.48
5	M	250	LEU	N-CA-C	-7.39	103.56	112.58
12	d	113	LEU	N-CA-CB	-7.39	99.93	111.23
4	L	392	LYS	N-CA-C	7.38	118.97	111.07
4	L	123	LEU	N-CA-C	-7.38	103.31	111.36
4	L	21	ILE	N-CA-CB	7.33	121.57	110.58
5	M	455	THR	N-CA-C	-7.32	100.40	110.35
20	l	97	LEU	N-CA-C	-7.30	103.97	113.17
21	m	72	ARG	N-CA-C	7.30	122.48	113.50
5	M	289	SER	N-CA-C	-7.29	103.27	111.07
4	L	28	LYS	N-CA-C	-7.27	103.35	111.28
4	L	19	ILE	N-CA-C	7.24	117.37	110.42
3	K	24	SER	CB-CA-C	-7.22	107.40	117.23
19	k	73	ILE	N-CA-C	-7.21	103.27	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	81	VAL	N-CA-C	7.19	117.95	110.62
8	U	136	GLU	N-CA-C	-7.17	104.52	113.20
24	p	168	LYS	N-CA-C	-7.14	104.19	113.12
4	L	554	ASP	N-CA-CB	7.13	121.26	110.42
5	M	244	ILE	N-CA-C	7.13	117.90	110.62
8	U	74	LEU	N-CA-C	7.11	119.16	110.41
14	f	9	GLU	N-CA-C	7.11	121.70	113.38
3	K	48	SER	N-CA-C	-7.08	103.56	111.28
22	n	102	TRP	N-CA-C	-7.07	105.01	112.93
5	M	325	LEU	N-CA-C	-7.06	103.52	111.07
5	M	34	ILE	N-CA-C	-7.03	103.45	110.62
5	M	365	ALA	N-CA-C	-7.03	103.69	111.36
4	L	319	MET	N-CA-C	-7.03	104.70	112.72
18	j	65	MET	N-CA-C	-7.03	103.55	111.07
5	M	264	LEU	N-CA-C	-7.02	103.56	111.07
9	X	153	VAL	N-CA-C	7.02	117.97	107.80
5	M	213	HIS	CB-CA-C	-7.00	96.81	110.11
6	N	132	THR	N-CA-C	6.97	122.90	113.97
4	L	546	LEU	N-CA-C	6.94	119.49	111.02
4	L	471	ASN	N-CA-C	6.93	118.92	111.36
5	M	91	LEU	N-CA-C	-6.93	103.81	112.90
17	i	9	LYS	N-CA-C	-6.93	104.81	112.72
5	M	235	LEU	N-CA-C	6.93	119.42	111.11
4	L	100	ILE	N-CA-C	6.90	119.67	111.05
4	L	86	SER	N-CA-C	6.89	118.45	111.07
17	i	11	ARG	N-CA-C	-6.89	104.87	113.28
19	k	59	TYR	N-CA-CB	-6.89	98.83	110.41
4	L	26	LEU	N-CA-C	6.88	119.62	111.71
4	L	522	PHE	N-CA-C	-6.88	103.71	111.07
3	K	83	ASN	N-CA-CB	6.87	120.98	110.81
5	M	276	CYS	N-CA-CB	6.87	120.22	110.12
22	n	117	ASP	N-CA-C	-6.85	103.87	111.82
5	M	442	ILE	N-CA-C	-6.84	104.14	112.35
4	L	547	LYS	N-CA-C	6.83	118.73	111.28
21	m	49	LEU	N-CA-C	-6.81	104.95	112.72
3	K	70	GLU	N-CA-CB	6.79	120.06	109.94
15	g	78	PRO	CA-N-CD	6.79	121.51	112.00
5	M	165	ILE	N-CA-C	-6.78	102.61	111.09
7	O	93	TYR	N-CA-C	-6.77	103.98	111.36
21	m	127	ILE	N-CA-C	-6.76	106.21	112.43
2	J	58	ILE	N-CA-C	6.75	117.36	111.56
12	d	88	HIS	N-CA-C	-6.74	103.02	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	248	ILE	N-CA-CB	6.74	118.43	110.55
7	O	175	ASN	N-CA-C	-6.73	104.01	111.82
5	M	374	ASN	N-CA-C	-6.72	103.88	111.07
4	L	95	PHE	N-CA-C	-6.72	103.88	111.07
20	l	86	ARG	N-CA-C	-6.70	99.61	110.20
5	M	410	MET	N-CA-C	-6.69	103.91	111.07
8	U	150	ASP	CB-CA-C	6.69	121.90	110.79
6	N	228	ASN	N-CA-CB	6.69	119.71	110.01
18	j	53	SER	N-CA-C	6.68	119.42	111.33
21	m	51	TYR	N-CA-C	-6.68	105.70	114.31
8	U	140	CYS	CA-C-N	-6.66	114.04	120.83
8	U	140	CYS	C-N-CA	-6.66	114.04	120.83
15	g	76	SER	N-CA-C	6.66	118.19	111.07
5	M	143	LEU	N-CA-C	-6.65	103.96	111.07
7	O	315	PRO	N-CA-CB	-6.64	96.03	103.33
1	D	70	ASP	N-CA-C	6.63	120.69	110.42
17	i	8	GLU	N-CA-C	-6.62	104.79	114.39
17	i	70	PHE	N-CA-C	6.62	120.22	111.75
18	j	38	VAL	O-C-N	6.62	128.47	122.65
3	K	76	ALA	N-CA-C	-6.61	104.15	111.36
19	k	49	ASP	CA-C-N	-6.61	113.40	120.47
19	k	49	ASP	C-N-CA	-6.61	113.40	120.47
22	n	115	TYR	N-CA-CB	6.60	122.11	110.37
5	M	303	ILE	N-CA-C	-6.59	104.06	110.72
8	U	102	SER	N-CA-C	6.58	119.57	107.99
5	M	161	LEU	N-CA-C	-6.57	104.04	111.07
4	L	499	LEU	N-CA-C	-6.57	103.81	110.97
19	k	46	GLY	N-CA-C	-6.57	106.88	114.69
4	L	329	ILE	N-CA-C	-6.55	104.14	110.42
4	L	130	ILE	N-CA-C	-6.54	103.95	110.62
7	O	140	LEU	N-CA-C	-6.52	104.09	111.07
4	L	232	TRP	N-CA-C	6.52	120.49	112.54
7	O	118	TYR	N-CA-CB	-6.51	100.57	110.01
19	k	57	TRP	N-CA-C	-6.51	104.60	112.54
4	L	423	SER	N-CA-C	-6.50	104.11	111.07
2	J	21	LEU	N-CA-C	-6.49	105.67	112.93
24	p	54	ARG	N-CA-C	-6.47	103.74	111.69
10	Y	96	GLY	N-CA-C	-6.46	104.50	112.77
7	O	320	GLY	N-CA-C	-6.45	96.59	111.04
6	N	315	THR	N-CA-C	-6.44	104.18	111.07
2	J	139	ILE	N-CA-C	-6.44	102.81	111.44
19	k	42	LEU	N-CA-C	-6.42	103.53	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	325	ALA	N-CA-C	-6.42	104.28	111.28
5	M	32	PHE	N-CA-C	-6.40	104.22	111.07
3	K	11	ALA	N-CA-C	-6.40	104.23	111.07
11	c	72	ARG	N-CA-C	-6.40	104.23	111.07
20	l	119	THR	N-CA-C	-6.39	98.13	108.41
4	L	234	PRO	CA-N-CD	-6.35	103.11	112.00
5	M	317	ILE	N-CA-C	-6.35	104.56	110.53
12	d	15	PRO	CA-N-CD	6.35	120.89	112.00
15	g	112	MET	N-CA-C	6.35	120.81	113.38
4	L	439	PRO	N-CA-C	6.34	122.34	113.53
7	O	98	THR	N-CA-C	6.34	120.61	109.96
4	L	387	THR	N-CA-C	6.34	119.00	111.71
4	L	70	THR	N-CA-C	-6.33	103.91	111.69
4	L	337	ALA	N-CA-C	-6.30	104.41	111.28
5	M	26	ASN	N-CA-CB	6.29	119.19	110.07
17	i	32	GLU	CA-C-N	-6.29	111.98	119.84
17	i	32	GLU	C-N-CA	-6.29	111.98	119.84
4	L	490	ALA	N-CA-C	-6.27	104.36	111.07
7	O	113	SER	N-CA-C	6.27	118.63	108.41
4	L	502	LEU	N-CA-C	-6.26	104.46	111.28
6	N	337	LEU	CA-C-N	-6.25	113.70	119.82
6	N	337	LEU	C-N-CA	-6.25	113.70	119.82
20	l	105	ILE	CA-C-O	-6.24	115.16	121.59
18	j	78	ASP	N-CA-C	-6.24	102.82	110.61
6	N	91	ASN	N-CA-CB	6.23	119.13	109.97
11	c	47	SER	N-CA-CB	6.23	120.80	110.33
6	N	89	GLN	N-CA-C	6.22	120.43	112.34
22	n	63	LEU	N-CA-C	-6.21	104.05	111.69
6	N	276	LEU	N-CA-C	-6.20	105.36	113.17
6	N	46	ASN	N-CA-C	-6.19	105.75	113.55
19	k	59	TYR	N-CA-C	6.19	120.67	113.18
23	o	110	GLN	N-CA-C	-6.18	104.63	111.36
6	N	216	PHE	N-CA-C	6.17	118.08	111.36
15	g	123	LEU	N-CA-CB	6.16	119.01	110.07
4	L	361	ASN	CB-CA-C	-6.14	102.83	111.80
5	M	4	ILE	N-CA-C	-6.14	103.96	112.50
22	n	30	TRP	N-CA-C	-6.14	104.14	111.69
21	m	72	ARG	CA-C-O	6.14	125.89	119.14
5	M	121	LEU	N-CA-C	-6.13	104.68	111.36
6	N	47	LYS	N-CA-C	-6.13	104.71	111.82
4	L	287	PHE	N-CA-CB	6.11	118.87	110.01
14	f	39	ASN	N-CA-C	-6.10	104.00	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	k	30	ILE	N-CA-C	6.10	118.71	111.09
24	p	127	LYS	N-CA-C	-6.10	104.19	111.69
16	h	101	ILE	N-CA-CB	6.08	115.74	110.08
5	M	57	SER	N-CA-C	6.08	119.11	109.50
21	m	52	ASN	N-CA-C	-6.08	105.17	112.59
5	M	213	HIS	N-CA-C	6.07	120.54	113.20
6	N	91	ASN	N-CA-C	-6.07	101.30	110.28
4	L	98	TRP	N-CA-C	-6.05	104.76	111.36
5	M	168	GLN	N-CA-C	-6.05	104.76	111.36
15	g	109	ASP	CA-CB-CG	6.05	118.65	112.60
4	L	140	LEU	N-CA-C	-6.05	104.68	111.28
15	g	123	LEU	N-CA-C	-6.05	104.61	111.14
21	m	22	GLU	N-CA-C	-6.02	104.63	111.07
4	L	454	ILE	N-CA-C	-6.01	104.48	110.62
7	O	234	LEU	N-CA-C	-6.01	104.81	111.36
16	h	142	ILE	N-CA-C	-6.01	104.65	110.42
5	M	370	PRO	CA-N-CD	6.01	120.41	112.00
7	O	160	GLU	CB-CA-C	-6.00	109.64	116.54
5	M	396	MET	N-CA-C	-6.00	105.94	113.20
11	c	47	SER	N-CA-C	-6.00	104.70	112.68
7	O	181	LYS	N-CA-C	5.99	117.48	111.07
5	M	253	LEU	N-CA-C	5.98	117.80	111.28
2	J	135	LEU	N-CA-C	-5.98	106.52	113.88
5	M	3	LYS	N-CA-C	-5.98	106.11	113.41
7	O	183	CYS	N-CA-CB	5.98	118.85	109.94
4	L	234	PRO	N-CA-CB	5.98	109.62	103.23
15	g	78	PRO	N-CA-C	5.98	121.84	113.53
5	M	300	SER	N-CA-C	-5.97	106.98	114.56
5	M	222	GLU	N-CA-C	5.97	120.40	113.18
2	J	155	ALA	N-CA-C	-5.95	104.88	111.36
4	L	88	LEU	N-CA-CB	5.95	118.69	110.07
24	p	8	ASP	N-CA-C	5.94	120.59	113.23
4	L	112	PRO	CB-CA-C	-5.93	103.02	111.68
5	M	88	ASN	N-CA-C	5.93	120.14	113.02
4	L	248	HIS	CB-CA-C	5.92	120.91	110.85
6	N	295	ARG	N-CA-C	-5.91	104.84	111.28
4	L	278	LEU	N-CA-CB	5.91	118.63	110.07
5	M	272	THR	N-CA-C	-5.91	104.92	111.36
4	L	247	LEU	N-CA-CB	5.90	120.60	110.34
8	U	143	GLU	N-CA-C	-5.89	104.21	111.75
7	O	262	GLU	N-CA-C	-5.89	104.86	111.28
6	N	16	GLY	CA-C-N	-5.89	112.43	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	16	GLY	C-N-CA	-5.89	112.43	118.85
7	O	205	ILE	O-C-N	5.88	129.05	122.75
4	L	387	THR	CB-CA-C	-5.88	99.75	110.63
22	n	27	LEU	N-CA-C	-5.87	106.08	113.72
7	O	130	ARG	N-CA-C	-5.87	104.88	111.28
19	k	82	ALA	N-CA-C	-5.87	104.89	111.28
6	N	15	LEU	N-CA-C	-5.85	105.64	112.89
23	o	11	TRP	CB-CA-C	-5.84	109.85	116.63
4	L	428	TYR	N-CA-C	-5.83	104.84	111.14
17	i	105	PHE	CA-C-N	-5.83	113.69	119.99
17	i	105	PHE	C-N-CA	-5.83	113.69	119.99
17	i	10	LEU	N-CA-C	-5.82	107.17	114.56
19	k	80	GLY	N-CA-C	-5.82	105.75	112.50
5	M	424	ILE	O-C-N	5.81	128.42	122.79
12	d	62	LEU	N-CA-C	5.81	117.61	111.28
12	d	53	VAL	N-CA-C	5.80	116.45	110.36
6	N	66	ALA	N-CA-C	-5.79	105.05	111.36
6	N	321	LYS	N-CA-C	5.79	118.54	110.20
4	L	467	VAL	N-CA-CB	-5.79	103.78	110.55
20	l	186	ILE	N-CA-CB	-5.79	101.66	111.50
4	L	177	ILE	N-CA-C	-5.78	104.72	110.62
14	f	36	ALA	N-CA-C	-5.77	103.31	110.41
8	U	101	ASN	N-CA-C	-5.77	106.10	113.02
3	K	6	PHE	N-CA-C	-5.76	106.38	113.41
19	k	20	MET	CA-C-N	-5.76	111.13	122.02
19	k	20	MET	C-N-CA	-5.76	111.13	122.02
21	m	116	ILE	N-CA-C	-5.76	104.89	110.42
22	n	52	LYS	N-CA-C	-5.75	105.93	113.12
5	M	124	ALA	N-CA-C	-5.75	105.10	111.36
15	g	78	PRO	N-CA-CB	-5.74	97.02	103.33
4	L	495	VAL	N-CA-C	5.74	115.93	110.42
8	U	137	LYS	CA-C-N	-5.74	113.56	122.05
8	U	137	LYS	C-N-CA	-5.74	113.56	122.05
21	m	104	VAL	N-CA-C	-5.73	105.50	111.58
18	j	73	PHE	N-CA-C	-5.73	104.94	111.07
2	J	27	TYR	N-CA-CB	5.72	119.37	110.44
4	L	419	THR	N-CA-C	-5.72	105.04	111.28
5	M	279	GLN	N-CA-C	-5.72	98.57	108.69
15	g	67	LYS	N-CA-C	-5.70	102.02	110.46
4	L	342	CYS	N-CA-CB	5.69	118.26	110.01
13	e	34	HIS	N-CA-C	-5.68	106.19	113.01
23	o	71	ARG	N-CA-C	-5.67	104.48	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	220	LYS	N-CA-C	5.67	117.46	111.28
5	M	19	SER	N-CA-C	5.67	117.72	109.84
4	L	214	MET	N-CA-C	-5.65	105.20	111.36
4	L	20	LEU	N-CA-C	5.65	119.89	112.89
4	L	605	ASN	N-CA-C	-5.65	106.24	113.02
6	N	232	LEU	N-CA-C	-5.64	106.61	112.93
2	J	130	ASP	N-CA-C	5.64	117.43	111.28
5	M	214	LEU	N-CA-C	-5.64	105.66	112.54
14	f	7	LEU	CB-CA-C	-5.64	102.26	111.50
17	i	14	GLN	N-CA-CB	-5.63	101.84	110.12
20	l	49	ALA	N-CA-C	-5.63	106.57	113.50
4	L	371	SER	N-CA-C	-5.63	105.06	111.14
12	d	5	ARG	CA-C-N	-5.63	114.16	119.90
12	d	5	ARG	C-N-CA	-5.63	114.16	119.90
14	f	10	HIS	CB-CA-C	-5.62	100.67	110.17
21	m	31	ARG	N-CA-C	-5.62	106.55	113.41
2	J	132	GLY	N-CA-C	5.61	121.24	111.14
4	L	151	SER	N-CA-CB	5.60	118.45	110.16
17	i	84	TYR	N-CA-C	-5.59	105.18	111.28
4	L	445	GLU	CB-CA-C	-5.59	101.96	111.02
15	g	140	PHE	N-CA-CB	5.58	118.31	109.71
4	L	234	PRO	N-CA-C	-5.58	105.49	113.47
4	L	155	ILE	N-CA-C	-5.57	105.30	110.53
24	p	115	GLN	N-CA-CB	5.57	118.00	110.59
6	N	251	LEU	N-CA-C	-5.56	105.22	111.28
15	g	107	VAL	N-CA-C	-5.56	102.90	108.96
11	c	64	GLU	N-CA-CB	5.55	118.06	110.01
10	Y	13	GLU	N-CA-C	5.55	117.77	111.11
15	g	113	GLN	CA-C-O	5.55	126.21	119.11
6	N	36	SER	N-CA-C	-5.54	105.24	111.28
21	m	60	ILE	N-CA-C	-5.54	102.04	109.30
21	m	46	GLU	N-CA-C	-5.54	106.52	113.72
3	K	3	SER	N-CA-C	-5.53	106.43	114.12
15	g	122	ARG	N-CA-C	5.52	118.23	111.82
4	L	370	SER	N-CA-C	-5.51	105.35	111.36
24	p	120	ASN	N-CA-C	-5.51	105.19	113.89
4	L	465	GLY	N-CA-C	-5.50	105.72	112.77
22	n	136	GLU	CB-CA-C	5.50	121.37	110.42
14	f	29	LYS	N-CA-C	-5.50	106.16	112.92
5	M	73	LEU	N-CA-C	-5.50	105.28	112.75
18	j	64	LEU	N-CA-C	-5.50	105.45	111.82
4	L	194	ASN	CB-CA-C	-5.49	103.32	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	394	LEU	N-CA-CB	5.49	117.96	110.01
5	M	223	ALA	N-CA-CB	5.47	118.10	110.11
5	M	355	MET	N-CA-C	-5.47	104.71	111.33
18	j	80	VAL	CB-CA-C	-5.47	106.25	111.44
4	L	152	PHE	N-CA-C	-5.47	105.22	111.07
14	f	11	TRP	CA-C-O	5.46	125.68	119.18
5	M	370	PRO	N-CA-CB	-5.46	97.78	103.08
23	o	74	PHE	CA-C-N	-5.46	113.99	119.56
23	o	74	PHE	C-N-CA	-5.46	113.99	119.56
6	N	62	THR	N-CA-C	-5.43	105.26	111.07
7	O	154	GLY	N-CA-C	-5.43	107.53	114.37
6	N	108	LEU	N-CA-C	5.43	118.09	109.24
17	i	77	ILE	CB-CA-C	-5.43	108.60	114.35
6	N	89	GLN	N-CA-CB	-5.42	100.43	110.18
15	g	137	SER	N-CA-CB	-5.41	101.32	110.41
4	L	543	ASN	N-CA-C	-5.40	105.40	111.28
24	p	94	ARG	N-CA-C	5.38	116.83	111.07
5	M	174	LEU	N-CA-C	-5.38	106.49	112.57
4	L	386	LEU	N-CA-C	-5.37	100.96	108.96
5	M	117	MET	N-CA-CB	5.37	118.01	110.12
5	M	409	TYR	N-CA-C	-5.37	105.59	111.82
19	k	48	ARG	N-CA-C	-5.37	98.82	108.48
5	M	343	ILE	N-CA-C	5.37	116.09	110.62
5	M	234	ILE	N-CA-C	5.36	116.25	111.90
8	U	141	PRO	N-CA-C	-5.36	109.11	114.68
4	L	21	ILE	N-CA-C	-5.35	105.32	110.72
4	L	311	GLY	N-CA-C	-5.34	106.33	112.73
4	L	413	LEU	N-CA-C	5.34	117.10	111.28
5	M	53	SER	N-CA-C	5.34	115.58	108.38
5	M	169	ASN	N-CA-C	-5.33	105.55	111.36
4	L	550	LEU	CA-C-O	-5.33	115.29	120.89
16	h	173	THR	O-C-N	5.33	125.71	121.55
5	M	294	MET	N-CA-C	-5.32	106.80	113.72
6	N	218	ALA	N-CA-CB	5.31	118.43	110.14
15	g	80	VAL	N-CA-C	-5.31	105.32	110.42
22	n	104	LEU	N-CA-C	-5.30	106.84	113.15
7	O	264	GLU	N-CA-C	-5.30	107.18	113.38
4	L	415	ALA	N-CA-CB	5.30	117.91	110.12
4	L	183	ILE	N-CA-C	-5.30	105.22	110.62
5	M	25	THR	CB-CA-C	-5.30	100.50	110.67
4	L	231	PRO	CB-CA-C	-5.29	104.34	111.85
22	n	36	LYS	N-CA-C	-5.29	105.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	494	SER	N-CA-C	-5.27	105.44	111.14
2	J	65	VAL	N-CA-CB	5.27	116.15	110.62
5	M	212	VAL	CB-CA-C	-5.25	105.17	112.36
4	L	190	SER	N-CA-C	-5.24	106.73	113.23
15	g	68	ASN	N-CA-CB	5.24	119.01	111.51
16	h	129	PRO	N-CA-C	-5.24	106.70	113.57
5	M	167	ILE	N-CA-C	5.24	117.60	111.05
18	j	76	ASP	CB-CA-C	-5.24	104.60	112.09
5	M	98	MET	N-CA-C	-5.23	105.47	111.07
18	j	51	THR	O-C-N	-5.23	117.05	122.96
22	n	26	HIS	N-CA-C	-5.23	106.48	112.92
4	L	137	MET	N-CA-C	5.23	119.29	113.01
22	n	12	HIS	N-CA-C	-5.22	105.03	111.40
5	M	317	ILE	N-CA-CB	5.22	117.25	110.57
8	U	133	ILE	CB-CA-C	-5.22	104.08	112.16
5	M	20	PRO	N-CA-C	-5.21	106.29	113.53
8	U	133	ILE	N-CA-C	5.20	117.56	111.05
21	m	17	THR	N-CA-C	-5.20	103.66	110.53
4	L	485	PHE	N-CA-CB	5.19	117.54	110.01
4	L	386	LEU	CA-C-O	-5.19	115.89	121.45
4	L	375	ILE	N-CA-CB	5.18	116.62	110.55
6	N	335	MET	CB-CA-C	-5.18	104.44	111.95
24	p	167	ARG	CB-CA-C	5.17	117.20	109.13
7	O	206	TYR	CA-C-N	-5.17	115.01	122.45
7	O	206	TYR	C-N-CA	-5.17	115.01	122.45
6	N	222	ASN	N-CA-C	-5.17	106.22	112.88
4	L	332	HIS	N-CA-C	-5.17	105.65	111.28
24	p	43	TRP	CA-C-N	-5.16	113.60	118.97
24	p	43	TRP	C-N-CA	-5.16	113.60	118.97
4	L	284	THR	N-CA-C	-5.14	105.75	111.36
14	f	11	TRP	N-CA-C	-5.14	107.00	113.28
6	N	90	THR	N-CA-C	5.14	117.55	110.35
4	L	249	SER	N-CA-C	5.13	116.68	111.14
12	d	37	LEU	N-CA-C	-5.13	105.69	111.28
24	p	13	PRO	O-C-N	5.13	123.56	121.15
4	L	217	LEU	N-CA-C	-5.13	105.69	111.28
10	Y	72	PHE	N-CA-C	-5.13	105.58	111.07
6	N	225	MET	N-CA-C	-5.12	106.62	112.92
20	l	168	LEU	N-CA-C	-5.12	105.61	111.14
16	h	158	ARG	N-CA-C	-5.12	105.61	111.14
4	L	396	ILE	O-C-N	5.11	126.92	121.91
5	M	330	ALA	N-CA-CB	5.11	117.48	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	497	GLY	N-CA-C	-5.11	106.57	112.50
11	c	60	GLN	N-CA-C	-5.10	105.61	111.07
21	m	26	SER	N-CA-C	-5.10	102.75	109.84
21	m	61	GLU	N-CA-C	5.10	119.58	112.90
6	N	292	PHE	CA-CB-CG	5.10	118.90	113.80
5	M	86	LYS	N-CA-C	-5.09	106.31	112.88
1	D	71	ILE	N-CA-C	5.09	118.26	111.44
6	N	42	PRO	CB-CA-C	-5.09	104.97	113.06
19	k	44	ALA	N-CA-C	-5.09	105.73	111.28
11	c	39	PRO	N-CA-C	5.08	119.18	111.15
5	M	234	ILE	CB-CA-C	5.08	116.17	111.30
3	K	48	SER	N-CA-CB	5.07	117.57	110.12
6	N	282	MET	N-CA-C	-5.07	105.64	111.07
17	i	16	ARG	N-CA-C	-5.07	105.76	111.28
5	M	267	TRP	N-CA-C	-5.06	105.84	111.36
5	M	56	PHE	N-CA-C	5.06	116.77	108.52
15	g	137	SER	N-CA-C	5.06	119.30	113.18
5	M	229	MET	N-CA-C	-5.04	105.67	111.07
8	U	132	ASP	N-CA-C	5.04	117.17	111.02
8	U	81	ASP	N-CA-C	-5.04	106.30	112.90
20	l	45	PRO	N-CA-C	5.04	120.45	113.65
5	M	32	PHE	N-CA-CB	5.03	117.31	110.01
22	n	169	HIS	CB-CA-C	5.03	118.67	110.17
17	i	29	SER	CA-C-N	-5.03	114.61	119.78
17	i	29	SER	C-N-CA	-5.03	114.61	119.78
4	L	212	PRO	CA-N-CD	5.02	119.03	112.00
6	N	64	ALA	N-CA-C	5.02	116.44	111.07
5	M	30	TYR	N-CA-C	5.02	116.75	111.28
5	M	207	MET	N-CA-CB	5.02	119.31	110.37
6	N	217	MET	N-CA-C	-5.01	107.00	113.01
11	c	73	ASN	N-CA-C	-5.01	103.44	110.35
15	g	109	ASP	CB-CA-C	5.00	119.00	111.89
4	L	384	PRO	N-CA-CB	5.00	107.70	103.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	328	0	298	58	0
2	J	1193	0	1215	129	0
3	K	729	0	764	103	0
4	L	4798	0	4986	622	0
5	M	3630	0	3854	550	0
6	N	2694	0	2896	348	0
7	O	2599	0	2552	264	0
8	U	700	0	691	74	0
9	X	221	0	215	34	0
10	Y	1030	0	1015	90	0
11	c	389	0	385	38	0
12	d	996	0	1001	91	0
13	e	859	0	849	72	0
14	f	447	0	444	31	0
15	g	842	0	779	69	0
16	h	1162	0	1163	122	0
17	i	773	0	780	71	0
18	j	587	0	533	71	0
19	k	578	0	581	55	0
20	l	1312	0	1204	100	0
21	m	1044	0	1056	112	0
22	n	1534	0	1463	149	0
23	o	1019	0	1006	108	0
24	p	1438	0	1404	122	0
25	D	38	0	50	13	0
25	K	46	0	66	6	0
25	L	135	0	198	35	0
25	M	139	0	212	40	0
25	O	44	0	65	7	0
25	i	40	0	54	11	0
25	j	40	0	54	9	0
25	m	92	0	138	16	0
26	L	158	0	204	31	0
26	d	67	0	81	5	0
26	h	70	0	87	13	0
27	L	50	0	74	17	0
28	O	27	0	12	6	0
29	n	32	0	0	0	0
All	All	31880	0	32429	2851	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 44.

All (2851) 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)
4:L:302:ILE:HG22	4:L:340:PHE:CZ	1.64	1.31
26:L:705:CDL:H111	10:Y:115:MET:SD	1.75	1.27
25:M:503:3PE:HN3	7:O:338:LYS:CE	1.50	1.23
4:L:141:PHE:CE2	5:M:375:LEU:HD21	1.75	1.22
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.20
4:L:437:PHE:CE1	4:L:441:ILE:HG12	1.77	1.19
4:L:280:LEU:HD23	27:L:706:PC1:C3H	1.73	1.17
5:M:369:LEU:HD23	5:M:371:PRO:HD2	1.18	1.16
2:J:22:LYS:HD2	3:K:23:ARG:HG2	1.28	1.16
4:L:141:PHE:CE2	5:M:375:LEU:CD2	2.29	1.15
4:L:280:LEU:CD2	27:L:706:PC1:C3H	2.25	1.15
2:J:9:SER:CB	3:K:7:ASN:HD22	1.59	1.15
4:L:358:LYS:HG3	22:n:80:TYR:CZ	1.82	1.14
4:L:141:PHE:HE2	5:M:375:LEU:CD2	1.60	1.14
4:L:247:LEU:CD1	4:L:248:HIS:CD2	2.31	1.14
2:J:22:LYS:HD2	3:K:23:ARG:CG	1.77	1.13
25:M:503:3PE:N	7:O:338:LYS:CE	2.10	1.13
4:L:261:VAL:O	4:L:264:HIS:CD2	2.01	1.12
6:N:215:MET:CE	6:N:248:LEU:HD21	1.79	1.12
4:L:437:PHE:HE1	4:L:441:ILE:HG12	0.96	1.12
23:o:8:ARG:HB2	23:o:16:GLU:HG2	1.32	1.11
12:d:14:LEU:O	12:d:14:LEU:HD12	1.49	1.11
4:L:365:ILE:HD12	4:L:366:MET:HG3	1.32	1.11
25:M:503:3PE:HN3	7:O:338:LYS:NZ	1.48	1.11
8:U:90:TYR:OH	8:U:92:LYS:HD2	1.48	1.11
4:L:229:LEU:HD12	4:L:229:LEU:O	1.51	1.10
7:O:80:GLN:HG3	7:O:270:VAL:HG21	1.25	1.10
1:D:47:PHE:HB3	6:N:227:ILE:HD11	1.23	1.10
5:M:162:ILE:HG23	6:N:271:MET:HE3	1.33	1.09
4:L:550:LEU:HD12	5:M:275:ILE:HB	1.34	1.09
4:L:121:LEU:HD22	4:L:246:LEU:HD21	1.33	1.09
4:L:141:PHE:HE2	5:M:375:LEU:HD22	1.17	1.09
4:L:569:LEU:HB2	10:Y:115:MET:HE1	1.36	1.08
19:k:34:PRO:HG2	19:k:59:TYR:CE1	1.88	1.08
20:l:91:GLN:HE21	22:n:2:ALA:HB1	1.13	1.07
4:L:553:LEU:HD11	21:m:93:ALA:HB3	1.37	1.07
1:D:52:MET:HE3	25:D:501:3PE:N	1.68	1.07
4:L:16:LEU:HD23	4:L:126:ILE:HD13	1.30	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:141:PHE:HB2	4:L:182:PHE:CE2	1.92	1.05
18:j:97:LEU:HB3	23:o:104:ARG:HB2	1.36	1.04
6:N:233:LEU:HD23	6:N:241:LEU:HD12	1.36	1.04
4:L:141:PHE:CE2	5:M:370:PRO:HG3	1.91	1.03
5:M:249:ILE:O	5:M:250:LEU:HG	1.58	1.03
4:L:131:LEU:HD12	4:L:140:LEU:HD12	1.36	1.03
23:o:69:CYS:O	23:o:80:CYS:SG	2.17	1.02
5:M:179:LEU:HB3	5:M:249:ILE:HD11	1.42	1.02
4:L:228:GLY:O	4:L:229:LEU:HG	1.61	1.01
13:e:20:PHE:CZ	16:h:178:PHE:HB2	1.95	1.01
22:n:97:TYR:HB2	22:n:178:PRO:HG2	1.39	1.01
4:L:222:GLY:HA2	4:L:229:LEU:HD11	1.40	1.00
5:M:172:GLY:O	5:M:173:THR:HG23	1.61	1.00
2:J:60:LEU:HD13	2:J:60:LEU:C	1.86	1.00
16:h:163:ARG:HG2	16:h:165:ASP:HB2	1.44	1.00
4:L:358:LYS:CG	22:n:80:TYR:CZ	2.45	1.00
4:L:466:PHE:HB2	18:j:68:TRP:HZ2	1.27	0.99
25:L:703:3PE:H321	25:m:201:3PE:H342	1.44	0.99
5:M:196:TRP:CD1	5:M:250:LEU:HD13	1.96	0.99
2:J:87:LEU:HG	2:J:91:PHE:CZ	1.97	0.99
25:M:503:3PE:HN3	7:O:338:LYS:HE3	1.23	0.99
5:M:143:LEU:HD21	6:N:303:THR:HG21	1.44	0.99
6:N:232:LEU:HD23	6:N:307:THR:HG23	1.39	0.99
20:l:38:PRO:HB2	21:m:75:ASN:HD22	1.26	0.99
5:M:127:ILE:CD1	6:N:256:PRO:HG3	1.93	0.98
25:M:503:3PE:N	7:O:338:LYS:NZ	2.10	0.98
4:L:141:PHE:HB2	4:L:182:PHE:HE2	1.27	0.98
5:M:275:ILE:HD11	5:M:288:TYR:CG	1.98	0.98
3:K:22:PHE:HB2	4:L:585:LYS:HG2	1.40	0.98
7:O:254:GLU:HG2	7:O:276:LEU:HD22	1.45	0.98
4:L:383:MET:HB3	4:L:386:LEU:HD12	1.43	0.97
4:L:316:THR:HG23	4:L:325:ALA:HB2	1.45	0.97
10:Y:68:ILE:HD11	10:Y:103:LEU:HB2	1.46	0.97
4:L:216:LEU:HD22	4:L:259:LEU:HD21	1.44	0.97
2:J:9:SER:HB3	3:K:7:ASN:HD22	1.26	0.96
4:L:173:LEU:HD23	25:L:701:3PE:H321	1.46	0.96
4:L:174:TYR:HD2	4:L:232:TRP:CD1	1.82	0.96
4:L:174:TYR:CD2	4:L:232:TRP:HD1	1.83	0.96
5:M:250:LEU:HD12	5:M:250:LEU:O	1.65	0.96
4:L:363:THR:HG23	4:L:431:THR:HB	1.48	0.95
4:L:466:PHE:HB2	18:j:68:TRP:CZ2	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:90:TYR:HE2	8:U:92:LYS:HB2	1.25	0.95
4:L:174:TYR:HD2	4:L:232:TRP:HD1	1.03	0.95
4:L:319:MET:HE1	4:L:399:ILE:HA	1.47	0.95
5:M:143:LEU:HD21	6:N:303:THR:CG2	1.96	0.95
20:l:91:GLN:NE2	22:n:2:ALA:HB1	1.82	0.95
4:L:247:LEU:HD12	4:L:248:HIS:CD2	1.98	0.95
4:L:466:PHE:CZ	18:j:72:ARG:NH2	2.35	0.95
5:M:4:ILE:HG22	5:M:107:ILE:HD13	1.47	0.95
6:N:31:VAL:O	6:N:35:PHE:CD2	2.18	0.95
4:L:302:ILE:CG2	4:L:340:PHE:CZ	2.49	0.94
6:N:307:THR:HB	7:O:319:ILE:CD1	1.97	0.94
5:M:216:LEU:HG	5:M:220:HIS:CE1	2.01	0.94
5:M:369:LEU:CD2	5:M:371:PRO:HD2	1.97	0.94
4:L:246:LEU:HD12	4:L:247:LEU:N	1.81	0.94
5:M:173:THR:CG2	16:h:147:ALA:HB2	1.96	0.94
4:L:362:ILE:HD12	4:L:430:VAL:HG12	1.50	0.94
8:U:140:CYS:HB2	8:U:143:GLU:HG2	1.49	0.94
5:M:1:MET:HG3	5:M:4:ILE:HD13	1.50	0.93
4:L:247:LEU:HD11	4:L:248:HIS:NE2	1.83	0.93
4:L:274:LEU:HA	4:L:277:MET:HE3	1.49	0.93
13:e:20:PHE:HZ	16:h:178:PHE:HB2	1.28	0.93
5:M:142:ARG:HH21	6:N:303:THR:HG22	1.32	0.93
5:M:453:LEU:CD1	5:M:454:ILE:HG23	1.99	0.93
5:M:173:THR:HG21	16:h:147:ALA:HB2	1.48	0.93
4:L:41:LYS:HG3	4:L:98:TRP:CZ2	2.04	0.92
13:e:41:ILE:HG23	16:h:179:ILE:HD11	1.51	0.92
7:O:314:LEU:CD1	7:O:315:PRO:HD2	2.00	0.92
7:O:256:LEU:HD21	7:O:276:LEU:HD23	1.47	0.92
4:L:136:ASN:HD21	26:h:201:CDL:H273	1.34	0.92
2:J:12:PHE:CE2	3:K:42:ILE:HD13	2.05	0.92
2:J:12:PHE:CE2	3:K:42:ILE:CD1	2.53	0.91
20:l:158:PRO:HD3	23:o:22:ILE:HB	1.53	0.91
5:M:106:LEU:HD13	5:M:234:ILE:CG2	2.00	0.91
4:L:202:MET:HE3	4:L:265:PRO:HG3	1.53	0.91
4:L:560:LYS:HD2	21:m:80:PHE:HE2	1.35	0.91
25:M:503:3PE:HN3	7:O:338:LYS:HZ1	1.18	0.91
25:M:503:3PE:H261	25:O:401:3PE:H252	1.52	0.91
7:O:106:ILE:HG12	7:O:111:SER:HA	1.50	0.91
4:L:245:ALA:O	4:L:249:SER:HB3	1.70	0.91
20:l:156:VAL:HG11	23:o:95:TYR:CZ	2.05	0.91
5:M:231:LEU:HD12	5:M:235:LEU:CD1	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:347:VAL:O	7:O:347:VAL:HG12	1.71	0.90
3:K:40:LEU:HD13	6:N:71:LEU:HD23	1.54	0.90
25:M:503:3PE:N	7:O:338:LYS:HE3	1.78	0.90
4:L:280:LEU:HD21	27:L:706:PC1:C3H	2.00	0.90
5:M:2:LEU:HA	5:M:5:ILE:HG12	1.53	0.89
4:L:466:PHE:CB	18:j:68:TRP:HZ2	1.84	0.89
5:M:453:LEU:HD12	5:M:454:ILE:N	1.87	0.89
7:O:314:LEU:CG	7:O:315:PRO:HD2	2.02	0.89
4:L:123:LEU:HD22	4:L:150:MET:SD	2.12	0.89
5:M:380:PHE:HA	5:M:383:MET:HE2	1.55	0.89
17:i:94:PRO:HG3	24:p:10:TYR:CE2	2.07	0.89
4:L:466:PHE:CE1	18:j:72:ARG:NH2	2.41	0.89
5:M:168:GLN:OE1	9:X:168:PHE:CE1	2.24	0.89
4:L:261:VAL:O	4:L:264:HIS:HD2	1.50	0.89
4:L:364:LYS:HE2	19:k:67:ILE:CD1	2.03	0.89
2:J:24:SER:HB2	2:J:27:TYR:HD2	1.35	0.88
22:n:101:GLU:O	22:n:122:ARG:NH2	2.06	0.88
5:M:8:SER:HA	5:M:11:LEU:HD13	1.55	0.88
6:N:307:THR:HB	7:O:319:ILE:HD11	1.54	0.88
1:D:52:MET:HE3	25:D:501:3PE:HN3	1.37	0.88
5:M:310:MET:SD	5:M:455:THR:HB	2.13	0.88
4:L:428:TYR:HA	4:L:432:MET:HG2	1.56	0.87
5:M:447:LEU:HD11	5:M:454:ILE:HG21	1.55	0.87
4:L:362:ILE:HD12	4:L:430:VAL:CG1	2.03	0.87
4:L:496:LEU:HD12	4:L:497:GLY:N	1.90	0.87
2:J:9:SER:CB	3:K:7:ASN:ND2	2.37	0.87
27:L:706:PC1:H3C1	20:l:148:HIS:CE1	2.09	0.87
5:M:368:ALA:HB1	5:M:375:LEU:HD13	1.56	0.87
13:e:17:HIS:CD2	13:e:18:PHE:HD1	1.92	0.87
5:M:102:LEU:HD13	5:M:230:ILE:HG12	1.57	0.87
4:L:553:LEU:HD11	21:m:93:ALA:CB	2.04	0.87
26:L:705:CDL:C11	10:Y:115:MET:SD	2.63	0.87
4:L:79:SER:HB2	4:L:135:ASN:HB2	1.55	0.86
5:M:1:MET:HE1	5:M:111:SER:HB2	1.58	0.86
5:M:127:ILE:CD1	6:N:256:PRO:CG	2.54	0.86
5:M:127:ILE:HD12	6:N:256:PRO:HG3	1.56	0.86
1:D:52:MET:CE	25:D:501:3PE:H121	2.04	0.86
14:f:8:ARG:HG2	14:f:9:GLU:OE1	1.75	0.86
15:g:145:ILE:HG23	24:p:160:LYS:HE2	1.57	0.86
4:L:417:SER:HB3	4:L:493:ILE:HG13	1.58	0.85
20:l:167:TYR:HD2	20:l:168:LEU:HD12	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:MET:HE2	25:D:501:3PE:H121	1.58	0.85
4:L:54:PHE:O	4:L:58:ASN:N	2.10	0.85
5:M:175:ASN:HD22	16:h:143:GLU:HG2	1.42	0.85
4:L:247:LEU:HD11	4:L:248:HIS:CD2	2.11	0.85
4:L:437:PHE:HE1	4:L:441:ILE:CG1	1.85	0.85
5:M:115:LEU:HD21	5:M:176:LEU:HD21	1.59	0.84
5:M:208:PRO:HD3	5:M:236:LEU:HD22	1.59	0.84
4:L:128:MET:HG2	4:L:251:THR:HB	1.59	0.84
4:L:302:ILE:HG22	4:L:340:PHE:CE2	2.11	0.84
7:O:314:LEU:HD12	7:O:315:PRO:HD2	1.56	0.84
26:L:704:CDL:H782	5:M:371:PRO:HG3	1.57	0.84
5:M:447:LEU:HD11	5:M:454:ILE:CG2	2.07	0.84
13:e:14:LEU:HD12	13:e:15:ASP:HB2	1.57	0.84
4:L:445:GLU:HB2	4:L:450:LEU:HD23	1.59	0.84
6:N:215:MET:SD	6:N:248:LEU:HD21	2.18	0.84
20:l:167:TYR:CD2	20:l:168:LEU:HD12	2.13	0.84
5:M:196:TRP:NE1	5:M:250:LEU:HD13	1.92	0.84
4:L:20:LEU:HD12	4:L:21:ILE:N	1.92	0.84
4:L:466:PHE:CE1	18:j:72:ARG:CZ	2.60	0.84
21:m:125:PHE:HE1	24:p:133:THR:HG22	1.43	0.83
26:h:201:CDL:H171	25:i:201:3PE:H372	1.57	0.83
1:D:67:ASN:HB3	1:D:69:VAL:HG12	1.58	0.83
5:M:373:ILE:HG12	5:M:454:ILE:HD11	1.60	0.83
4:L:16:LEU:HD23	4:L:126:ILE:CD1	2.08	0.83
5:M:361:MET:HB3	5:M:441:MET:HE3	1.60	0.83
7:O:314:LEU:HG	7:O:315:PRO:HD2	1.58	0.83
4:L:9:LEU:HD21	25:i:201:3PE:H2A2	1.59	0.83
10:Y:143:VAL:HG23	16:h:157:ARG:HG2	1.59	0.83
7:O:347:VAL:HG11	11:c:29:PHE:HA	1.61	0.83
17:i:15:LEU:HD21	22:n:164:PRO:HB2	1.61	0.83
7:O:168:VAL:HG11	7:O:241:TYR:CD1	2.14	0.83
4:L:131:LEU:CD1	4:L:140:LEU:HD12	2.09	0.82
4:L:556:ILE:HG21	21:m:80:PHE:CE1	2.14	0.82
5:M:269:MET:HE1	5:M:396:MET:HA	1.61	0.82
4:L:432:MET:HG3	4:L:432:MET:O	1.78	0.82
4:L:222:GLY:HA2	4:L:229:LEU:CD1	2.08	0.82
5:M:151:PHE:CZ	6:N:291:PHE:HB2	2.14	0.82
6:N:335:MET:HG3	6:N:335:MET:O	1.79	0.82
5:M:162:ILE:HG23	6:N:271:MET:CE	2.08	0.82
7:O:339:TYR:OH	25:O:401:3PE:H122	1.79	0.82
4:L:493:ILE:HD12	4:L:496:LEU:HD21	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:29:SER:HB3	15:g:91:PHE:CD2	2.15	0.82
4:L:364:LYS:HE2	19:k:67:ILE:HD11	1.60	0.82
2:J:65:VAL:HG13	2:J:66:VAL:N	1.92	0.81
12:d:109:TYR:HA	12:d:112:ILE:HG22	1.61	0.81
19:k:34:PRO:HD2	19:k:59:TYR:CD1	2.15	0.81
4:L:358:LYS:HG3	22:n:80:TYR:OH	1.79	0.81
4:L:552:LEU:HD21	21:m:90:GLY:HA2	1.61	0.81
4:L:572:ASN:OD1	26:L:705:CDL:OA4	1.98	0.81
7:O:168:VAL:HG21	7:O:241:TYR:CE1	2.15	0.81
22:n:97:TYR:HB2	22:n:178:PRO:CG	2.10	0.81
26:L:705:CDL:H351	10:Y:114:ALA:HB1	1.61	0.81
21:m:125:PHE:CE1	24:p:133:THR:HG22	2.16	0.81
4:L:229:LEU:O	4:L:229:LEU:CD1	2.28	0.81
19:k:30:ILE:HD11	19:k:39:GLN:HB2	1.61	0.81
2:J:22:LYS:CD	3:K:23:ARG:HG2	2.10	0.81
4:L:424:MET:HE2	4:L:502:LEU:HB2	1.62	0.81
5:M:172:GLY:O	5:M:173:THR:CG2	2.28	0.81
6:N:277:ILE:CG2	6:N:278:MET:H	1.93	0.81
6:N:277:ILE:HG23	6:N:278:MET:N	1.96	0.81
6:N:307:THR:HG22	6:N:308:ASN:H	1.46	0.81
5:M:216:LEU:HD12	5:M:236:LEU:HD21	1.60	0.80
25:M:503:3PE:H3A2	6:N:246:LEU:HD11	1.63	0.80
6:N:200:LEU:HD21	6:N:265:ILE:HG12	1.62	0.80
24:p:6:ASP:HB3	24:p:9:VAL:HG22	1.61	0.80
5:M:453:LEU:HD12	5:M:454:ILE:HG23	1.63	0.80
5:M:458:THR:CG2	24:p:148:ALA:HB1	2.12	0.80
2:J:9:SER:HB2	3:K:7:ASN:ND2	1.96	0.80
5:M:168:GLN:OE1	9:X:168:PHE:HE1	1.62	0.80
7:O:117:PHE:CE1	7:O:173:MET:HE3	2.17	0.80
25:j:700:3PE:H3B2	23:o:78:LEU:HD13	1.63	0.80
2:J:22:LYS:CD	3:K:23:ARG:CG	2.60	0.79
7:O:199:LEU:HD11	7:O:294:LEU:HD22	1.64	0.79
1:D:52:MET:CE	25:D:501:3PE:N	2.44	0.79
1:D:47:PHE:CB	6:N:227:ILE:HD11	2.08	0.79
5:M:231:LEU:HA	5:M:235:LEU:HB2	1.62	0.79
4:L:16:LEU:CD2	4:L:126:ILE:HD13	2.10	0.79
4:L:130:ILE:HG23	4:L:139:GLN:HE21	1.46	0.79
2:J:61:GLY:O	2:J:65:VAL:CG1	2.31	0.79
8:U:76:LEU:HD12	8:U:156:GLU:HB2	1.62	0.79
4:L:73:SER:HB3	24:p:100:GLN:NE2	1.97	0.79
5:M:122:PHE:CZ	5:M:206:LYS:HD3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:367:LEU:HD21	5:M:408:MET:HE2	1.64	0.79
1:D:52:MET:CE	25:D:501:3PE:C12	2.61	0.79
13:e:41:ILE:CG2	16:h:179:ILE:HD11	2.13	0.79
4:L:131:LEU:HD12	4:L:140:LEU:CD1	2.12	0.79
5:M:29:SER:HB3	15:g:91:PHE:HD2	1.47	0.79
22:n:20:TYR:CE2	22:n:24:LEU:HD11	2.18	0.79
5:M:106:LEU:HD13	5:M:234:ILE:HG21	1.63	0.79
6:N:123:PRO:HG2	6:N:126:MET:HG2	1.63	0.79
4:L:565:SER:OG	26:L:705:CDL:H322	1.83	0.79
27:L:706:PC1:H3C1	20:l:148:HIS:HE1	1.47	0.78
6:N:319:LYS:HA	7:O:302:THR:HG21	1.64	0.78
5:M:370:PRO:HA	5:M:375:LEU:CD2	2.13	0.78
4:L:302:ILE:CG2	4:L:340:PHE:CE1	2.66	0.78
5:M:248:ILE:HG13	5:M:249:ILE:HD12	1.64	0.78
7:O:117:PHE:HE1	7:O:173:MET:CE	1.96	0.78
4:L:3:ILE:H	4:L:3:ILE:HD12	1.48	0.78
5:M:231:LEU:HD12	5:M:235:LEU:HD13	1.64	0.78
7:O:314:LEU:HD12	7:O:315:PRO:CD	2.13	0.78
13:e:89:GLU:HB2	13:e:91:LYS:HG2	1.65	0.78
4:L:475:THR:HA	23:o:55:GLN:NE2	1.97	0.78
7:O:250:SER:HA	7:O:255:VAL:HG23	1.66	0.78
4:L:534:HIS:O	4:L:538:PRO:HG3	1.83	0.78
17:i:69:LEU:HD12	17:i:71:ALA:H	1.48	0.78
3:K:42:ILE:O	3:K:46:VAL:HG23	1.84	0.78
4:L:136:ASN:HA	4:L:197:GLU:HA	1.66	0.78
5:M:9:LEU:HD23	5:M:104:ILE:HD13	1.65	0.78
9:X:168:PHE:O	9:X:170:TRP:CD1	2.37	0.78
20:l:44:THR:OG1	20:l:45:PRO:HD2	1.83	0.78
5:M:319:HIS:HA	5:M:322:THR:HG22	1.66	0.78
6:N:215:MET:CE	6:N:248:LEU:CD2	2.62	0.78
2:J:67:PHE:CE2	3:K:75:LEU:HD21	2.19	0.77
23:o:31:PHE:HE2	23:o:104:ARG:NH1	1.80	0.77
7:O:305:LEU:HD12	7:O:305:LEU:O	1.83	0.77
6:N:170:LEU:HD11	6:N:288:LEU:HG	1.65	0.77
5:M:204:LEU:HD22	5:M:209:LEU:HD12	1.65	0.77
5:M:274:SER:O	5:M:277:LEU:HB2	1.85	0.77
6:N:45:ILE:O	6:N:45:ILE:HG13	1.83	0.77
4:L:174:TYR:HE1	25:L:701:3PE:H362	1.49	0.77
21:m:18:LEU:HD21	22:n:69:GLU:HA	1.64	0.77
6:N:254:LEU:HD12	6:N:255:PRO:CD	2.14	0.77
13:e:17:HIS:CD2	13:e:18:PHE:CD1	2.72	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:503:3PE:H3I3	26:d:201:CDL:H651	1.67	0.77
5:M:173:THR:HG23	16:h:147:ALA:CB	2.15	0.77
5:M:208:PRO:HG2	5:M:216:LEU:HD13	1.67	0.77
6:N:31:VAL:O	6:N:35:PHE:HD2	1.68	0.77
2:J:40:CYS:SG	2:J:56:PHE:HB2	2.25	0.77
2:J:59:TYR:OH	3:K:34:GLU:HB3	1.84	0.77
4:L:594:ASN:ND2	6:N:110:PRO:HB2	1.99	0.77
5:M:98:MET:CE	5:M:128:PRO:HA	2.14	0.77
20:l:113:ILE:HG23	20:l:115:ASN:H	1.50	0.77
5:M:42:LEU:HG	5:M:67:ILE:HD11	1.67	0.76
5:M:453:LEU:HD11	5:M:454:ILE:HG23	1.66	0.76
6:N:232:LEU:CD2	6:N:307:THR:HG23	2.15	0.76
20:l:169:GLU:C	20:l:171:GLY:H	1.92	0.76
4:L:419:THR:HA	4:L:422:TYR:CE2	2.20	0.76
5:M:60:PRO:O	5:M:64:PRO:HD3	1.85	0.76
6:N:210:ILE:HG22	6:N:333:SER:HB3	1.65	0.76
7:O:339:TYR:OH	25:O:401:3PE:C12	2.34	0.76
8:U:86:VAL:HB	8:U:122:MET:HE1	1.67	0.76
8:U:123:GLU:HG2	8:U:130:ILE:HG12	1.67	0.76
4:L:302:ILE:HG22	4:L:340:PHE:CE1	2.20	0.76
4:L:496:LEU:HD12	4:L:496:LEU:C	2.09	0.76
5:M:171:VAL:HG11	5:M:179:LEU:HD21	1.65	0.76
5:M:231:LEU:HD12	5:M:235:LEU:HD12	1.67	0.76
4:L:232:TRP:CZ3	4:L:233:LEU:CD2	2.69	0.76
4:L:506:ASN:HA	4:L:509:MET:HE2	1.66	0.76
6:N:211:LEU:HD23	6:N:333:SER:HB2	1.68	0.76
4:L:605:ASN:OD1	4:L:605:ASN:O	2.04	0.76
6:N:215:MET:HE2	6:N:248:LEU:HD21	1.67	0.75
4:L:56:HIS:HA	23:o:74:PHE:CD1	2.21	0.75
7:O:121:PRO:O	7:O:122:LYS:HG2	1.85	0.75
17:i:110:ILE:HD13	24:p:16:ARG:HD2	1.68	0.75
22:n:20:TYR:CZ	22:n:24:LEU:HD11	2.21	0.75
2:J:60:LEU:C	2:J:60:LEU:CD1	2.59	0.75
2:J:61:GLY:O	2:J:65:VAL:HG12	1.86	0.75
4:L:387:THR:HG23	4:L:461:SER:O	1.85	0.75
16:h:57:VAL:HG22	22:n:104:LEU:HD11	1.69	0.75
17:i:22:TRP:CE2	22:n:172:THR:HG22	2.21	0.75
4:L:513:MET:HE3	4:L:515:LYS:HG3	1.68	0.75
2:J:63:MET:HA	2:J:63:MET:HE3	1.68	0.75
4:L:393:ASP:OD1	4:L:394:LEU:N	2.19	0.75
6:N:277:ILE:HG23	6:N:278:MET:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:71:MET:HG3	10:Y:102:THR:HG21	1.68	0.75
15:g:70:ASP:OD1	22:n:108:HIS:NE2	2.18	0.75
2:J:151:MET:HE2	6:N:28:LEU:HD13	1.69	0.74
5:M:314:MET:HA	5:M:454:ILE:HD12	1.69	0.74
6:N:227:ILE:HA	6:N:230:ILE:HG22	1.66	0.74
7:O:333:GLU:O	7:O:333:GLU:CD	2.30	0.74
4:L:9:LEU:HD11	25:i:201:3PE:H2A1	1.69	0.74
27:L:706:PC1:H321	27:L:706:PC1:H231	1.70	0.74
6:N:314:MET:HB2	7:O:305:LEU:HD11	1.69	0.74
4:L:362:ILE:HG23	4:L:366:MET:HE3	1.68	0.74
11:c:30:TYR:HB2	11:c:34:PRO:HD3	1.69	0.74
7:O:117:PHE:CE1	7:O:128:SER:HB2	2.22	0.74
1:D:67:ASN:HB2	7:O:193:LEU:HD23	1.69	0.74
4:L:285:THR:HG22	4:L:415:ALA:HB1	1.70	0.74
10:Y:76:THR:HG23	10:Y:95:GLY:HA3	1.70	0.74
20:l:38:PRO:HB2	21:m:75:ASN:ND2	2.00	0.74
5:M:173:THR:CG2	16:h:147:ALA:CB	2.65	0.74
5:M:310:MET:HG3	5:M:455:THR:HA	1.70	0.74
5:M:1:MET:HB2	5:M:52:PHE:CD2	2.23	0.74
5:M:200:MET:HE1	5:M:247:SER:HB2	1.69	0.74
6:N:202:LEU:O	6:N:206:MET:HG2	1.87	0.74
6:N:289:ASN:HA	6:N:292:PHE:CE2	2.23	0.74
7:O:217:ARG:O	7:O:220:LYS:HG2	1.88	0.73
4:L:174:TYR:CD2	4:L:232:TRP:CD1	2.68	0.73
5:M:260:PRO:O	5:M:264:LEU:HG	1.88	0.73
1:D:67:ASN:HB2	7:O:193:LEU:CD2	2.17	0.73
7:O:117:PHE:HE1	7:O:173:MET:HE3	1.53	0.73
4:L:20:LEU:HD12	4:L:20:LEU:C	2.13	0.73
5:M:73:LEU:HD22	5:M:103:GLN:CD	2.12	0.73
4:L:455:LYS:NZ	18:j:57:GLN:OE1	2.21	0.73
5:M:216:LEU:HG	5:M:220:HIS:HE1	1.48	0.73
6:N:275:CYS:SG	10:Y:139:PRO:HG2	2.28	0.73
4:L:232:TRP:CZ3	4:L:233:LEU:HD23	2.23	0.73
4:L:579:ASN:OD1	4:L:579:ASN:O	2.06	0.73
5:M:167:ILE:HD11	5:M:195:LEU:HD21	1.70	0.73
7:O:204:VAL:CG2	7:O:255:VAL:HG22	2.19	0.73
25:m:202:3PE:H261	25:m:202:3PE:H371	1.69	0.73
5:M:122:PHE:CD1	5:M:238:LEU:HG	2.23	0.73
20:l:89:TRP:CZ2	22:n:86:PRO:HD2	2.24	0.73
10:Y:68:ILE:CD1	10:Y:103:LEU:HB2	2.18	0.73
2:J:9:SER:HB2	3:K:7:ASN:HD22	1.45	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:141:PHE:CD2	5:M:370:PRO:HB3	2.24	0.72
4:L:153:LEU:HD11	5:M:360:LEU:HD11	1.70	0.72
4:L:358:LYS:HG3	22:n:80:TYR:CE2	2.23	0.72
5:M:441:MET:SD	5:M:444:LEU:HD23	2.29	0.72
5:M:458:THR:HG22	24:p:148:ALA:HB1	1.71	0.72
6:N:215:MET:SD	6:N:248:LEU:CD2	2.77	0.72
4:L:136:ASN:ND2	26:h:201:CDL:H273	2.03	0.72
24:p:7:LYS:O	24:p:11:PRO:HA	1.89	0.72
4:L:556:ILE:CG2	21:m:80:PHE:CZ	2.72	0.72
5:M:243:MET:HE1	5:M:302:MET:HE3	1.71	0.72
8:U:79:ILE:HD11	8:U:148:ILE:HG22	1.71	0.72
4:L:569:LEU:HB2	10:Y:115:MET:CE	2.17	0.72
7:O:168:VAL:HG21	7:O:241:TYR:CZ	2.24	0.72
19:k:34:PRO:HG2	19:k:59:TYR:HE1	1.54	0.72
4:L:316:THR:CG2	4:L:325:ALA:HB2	2.19	0.72
7:O:176:GLN:HB2	7:O:178:TYR:HD2	1.55	0.72
8:U:112:SER:HB2	22:n:17:LEU:HD11	1.72	0.72
4:L:553:LEU:HD21	21:m:93:ALA:C	2.15	0.72
7:O:80:GLN:HG3	7:O:270:VAL:CG2	2.11	0.72
2:J:165:ILE:HG23	6:N:42:PRO:HG3	1.69	0.72
4:L:576:LEU:HD12	4:L:577:THR:N	2.05	0.72
6:N:59:TYR:CE2	6:N:63:GLN:HG3	2.23	0.72
16:h:96:ALA:HB3	24:p:63:TYR:HD1	1.54	0.72
7:O:238:GLU:HA	7:O:241:TYR:HD2	1.54	0.72
16:h:163:ARG:HG2	16:h:165:ASP:CB	2.19	0.72
4:L:141:PHE:HD2	5:M:370:PRO:HB3	1.54	0.72
4:L:299:LYS:HB2	4:L:354:GLN:HE21	1.55	0.72
2:J:87:LEU:HG	2:J:91:PHE:CE2	2.25	0.71
4:L:9:LEU:HD22	17:i:82:VAL:HG13	1.72	0.71
4:L:247:LEU:HD12	4:L:248:HIS:N	2.04	0.71
5:M:106:LEU:HD13	5:M:234:ILE:HG22	1.71	0.71
5:M:373:ILE:CG1	5:M:454:ILE:HD11	2.19	0.71
7:O:336:GLY:H	7:O:344:ASN:ND2	1.88	0.71
1:D:35:ARG:HH22	15:g:56:ASP:C	1.99	0.71
6:N:146:TYR:CD1	6:N:147:PRO:HD3	2.26	0.71
23:o:39:MET:HE1	23:o:58:TYR:HA	1.71	0.71
4:L:358:LYS:HG2	22:n:80:TYR:CZ	2.26	0.71
5:M:263:LEU:HD11	21:m:102:TYR:HD1	1.54	0.71
6:N:273:ASN:ND2	10:Y:143:VAL:HA	2.04	0.71
20:l:38:PRO:HG2	21:m:71:ALA:HB2	1.73	0.71
20:l:106:HIS:CD2	20:l:107:TRP:H	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:9:ALA:HB1	21:m:10:PRO:HD2	1.71	0.71
1:D:52:MET:HE3	25:D:501:3PE:HN1	1.54	0.71
5:M:313:THR:HG21	5:M:456:GLY:HA3	1.71	0.71
5:M:370:PRO:HA	5:M:375:LEU:HD23	1.72	0.71
8:U:144:ILE:O	8:U:148:ILE:HG12	1.91	0.71
1:D:52:MET:HE2	25:D:501:3PE:C12	2.20	0.71
4:L:368:PHE:HB3	4:L:445:GLU:CD	2.15	0.71
5:M:220:HIS:CE1	5:M:231:LEU:HD23	2.26	0.71
8:U:102:SER:O	8:U:141:PRO:HD3	1.91	0.71
21:m:45:ARG:O	21:m:45:ARG:HG2	1.90	0.71
5:M:373:ILE:HG12	5:M:454:ILE:CD1	2.20	0.70
6:N:275:CYS:SG	10:Y:139:PRO:CG	2.78	0.70
4:L:141:PHE:CD2	5:M:375:LEU:HD21	2.26	0.70
4:L:556:ILE:HG23	21:m:80:PHE:CE2	2.26	0.70
5:M:388:TRP:CE2	21:m:109:ARG:HD2	2.26	0.70
6:N:237:THR:HG23	6:N:237:THR:O	1.88	0.70
21:m:127:ILE:CG2	24:p:136:THR:HG23	2.20	0.70
4:L:510:LYS:HE3	4:L:512:SER:HB3	1.72	0.70
6:N:313:MET:CG	7:O:305:LEU:HD22	2.22	0.70
6:N:342:GLN:HE21	12:d:30:ARG:HH11	1.38	0.70
7:O:135:LEU:HB3	7:O:139:ARG:HH12	1.57	0.70
4:L:428:TYR:HA	4:L:432:MET:CG	2.20	0.70
6:N:137:ALA:HB3	6:N:138:PRO:HD3	1.74	0.70
4:L:559:GLU:O	4:L:564:LYS:HB2	1.92	0.70
4:L:25:ASN:HB2	16:h:72:LYS:HZ1	1.55	0.70
5:M:123:GLU:HB3	6:N:255:PRO:HG2	1.74	0.70
5:M:142:ARG:NH2	6:N:303:THR:HG22	2.05	0.70
17:i:69:LEU:HD11	17:i:71:ALA:HB3	1.72	0.70
4:L:285:THR:HG22	4:L:415:ALA:CB	2.21	0.70
25:M:503:3PE:HN2	7:O:338:LYS:CE	2.04	0.70
5:M:134:THR:O	5:M:142:ARG:HD2	1.91	0.70
6:N:254:LEU:HD12	6:N:255:PRO:HD3	1.72	0.70
10:Y:143:VAL:CG2	16:h:157:ARG:HG2	2.22	0.70
17:i:22:TRP:CD2	22:n:172:THR:HG22	2.26	0.70
2:J:144:MET:O	2:J:149:THR:HA	1.92	0.69
4:L:142:ILE:HA	5:M:370:PRO:HB2	1.74	0.69
4:L:480:LEU:HD23	4:L:480:LEU:O	1.93	0.69
5:M:424:ILE:HG13	21:m:57:VAL:O	1.92	0.69
5:M:447:LEU:HD21	5:M:454:ILE:HD13	1.73	0.69
5:M:127:ILE:HD11	6:N:256:PRO:CG	2.22	0.69
20:l:122:THR:HG21	20:l:129:MET:HE1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:703:3PE:H291	25:L:703:3PE:H3D1	1.75	0.69
6:N:248:LEU:HD13	6:N:296:LEU:HD23	1.75	0.69
1:D:35:ARG:O	1:D:36:GLN:C	2.35	0.69
4:L:305:SER:HB2	4:L:422:TYR:HE1	1.57	0.69
4:L:306:THR:HA	4:L:336:LYS:HZ2	1.58	0.69
4:L:353:GLU:OE1	22:n:80:TYR:OH	2.10	0.69
21:m:25:VAL:HA	21:m:30:ARG:HD3	1.73	0.69
2:J:9:SER:OG	3:K:4:THR:HG23	1.93	0.69
4:L:149:ILE:HG13	5:M:369:LEU:HD12	1.75	0.69
5:M:216:LEU:HD11	5:M:236:LEU:HD11	1.72	0.69
5:M:369:LEU:HD23	5:M:371:PRO:CD	2.12	0.69
7:O:238:GLU:O	7:O:241:TYR:HB2	1.93	0.69
23:o:19:PRO:HA	23:o:22:ILE:HD11	1.74	0.69
4:L:332:HIS:NE2	4:L:336:LYS:HG3	2.07	0.69
12:d:106:LYS:HB3	24:p:79:GLU:HB3	1.74	0.69
4:L:18:PRO:O	4:L:21:ILE:HG22	1.92	0.69
4:L:436:ARG:HA	19:k:58:ARG:NH1	2.08	0.68
5:M:127:ILE:HB	5:M:128:PRO:HD3	1.75	0.68
19:k:34:PRO:CD	19:k:59:TYR:CD1	2.75	0.68
4:L:279:CYS:SG	27:L:706:PC1:H3D2	2.33	0.68
6:N:215:MET:HE2	6:N:248:LEU:CD2	2.23	0.68
10:Y:77:CYS:SG	10:Y:78:VAL:N	2.66	0.68
3:K:66:PHE:HE2	6:N:35:PHE:CZ	2.11	0.68
4:L:279:CYS:SG	27:L:706:PC1:C3D	2.82	0.68
4:L:312:LEU:HD21	4:L:395:ILE:HG21	1.75	0.68
7:O:60:ILE:HD12	7:O:203:ALA:HB3	1.74	0.68
20:l:78:LEU:HD11	20:l:104:PRO:HB2	1.74	0.68
4:L:385:PHE:CD1	18:j:72:ARG:HG3	2.29	0.68
25:M:503:3PE:H3D1	25:M:503:3PE:H2B2	1.76	0.68
2:J:65:VAL:CG1	2:J:66:VAL:N	2.57	0.68
4:L:73:SER:HB3	24:p:100:GLN:HE21	1.58	0.68
7:O:140:LEU:HG	7:O:304:VAL:HG12	1.74	0.68
10:Y:96:GLY:HA3	10:Y:121:GLY:HA2	1.75	0.68
4:L:211:ILE:N	4:L:212:PRO:HD2	2.08	0.68
6:N:243:MET:HG2	12:d:44:MET:HE2	1.75	0.68
20:l:158:PRO:HD3	23:o:22:ILE:CB	2.23	0.68
1:D:34:ALA:HB3	5:M:86:LYS:NZ	2.09	0.68
4:L:383:MET:SD	4:L:384:PRO:HD2	2.33	0.68
5:M:379:LEU:O	5:M:383:MET:HG3	1.93	0.68
6:N:215:MET:HE1	6:N:248:LEU:HD21	1.71	0.68
23:o:31:PHE:CD1	23:o:34:ARG:HB3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:L:704:CDL:HA62	16:h:68:LEU:HD13	1.76	0.68
8:U:100:VAL:O	8:U:141:PRO:HG2	1.94	0.68
1:D:49:GLY:O	6:N:173:THR:HG21	1.93	0.68
4:L:357:ARG:HG2	22:n:32:ILE:HG12	1.76	0.68
5:M:39:LEU:HD23	5:M:67:ILE:HD13	1.74	0.68
5:M:311:GLY:HA2	5:M:314:MET:HE3	1.76	0.68
20:l:157:GLY:HA2	23:o:22:ILE:HG13	1.76	0.68
4:L:228:GLY:C	4:L:229:LEU:HG	2.19	0.68
4:L:358:LYS:HG2	22:n:80:TYR:CE1	2.29	0.68
20:l:122:THR:HG23	20:l:123:PRO:HD2	1.75	0.68
5:M:446:LEU:HD13	15:g:101:THR:HG21	1.75	0.67
7:O:339:TYR:OH	25:O:401:3PE:N	2.27	0.67
12:d:5:ARG:HD2	12:d:89:ASP:OD2	1.93	0.67
15:g:140:PHE:CE2	24:p:74:ILE:CG2	2.77	0.67
20:l:152:SER:HA	23:o:5:LEU:HD21	1.76	0.67
4:L:80:PHE:C	4:L:135:ASN:ND2	2.52	0.67
5:M:127:ILE:CG1	6:N:254:LEU:HD21	2.24	0.67
5:M:275:ILE:HD11	5:M:288:TYR:CD1	2.29	0.67
5:M:395:LEU:HD21	21:m:101:TRP:CE2	2.29	0.67
6:N:149:LEU:HD13	6:N:154:ILE:HG21	1.75	0.67
7:O:347:VAL:O	7:O:347:VAL:CG1	2.42	0.67
4:L:141:PHE:CE2	5:M:375:LEU:HD22	2.08	0.67
5:M:30:TYR:O	5:M:34:ILE:HG12	1.95	0.67
6:N:26:LEU:HD23	6:N:29:MET:SD	2.35	0.67
7:O:114:LEU:HA	7:O:131:LEU:CD2	2.24	0.67
4:L:203:PHE:CZ	24:p:110:LEU:HD11	2.30	0.67
25:L:703:3PE:H252	25:L:703:3PE:H3A1	1.76	0.67
5:M:350:MET:HG2	22:n:99:VAL:HG12	1.77	0.67
15:g:109:ASP:CB	15:g:114:GLU:HB3	2.24	0.67
5:M:11:LEU:HB3	5:M:100:ILE:HD13	1.76	0.67
5:M:98:MET:HE2	5:M:131:ILE:HB	1.77	0.67
4:L:187:VAL:HG22	5:M:383:MET:HG2	1.77	0.67
5:M:44:GLN:HE22	5:M:49:TYR:HA	1.58	0.67
5:M:285:LEU:HD13	5:M:342:MET:HE1	1.75	0.67
6:N:313:MET:HG3	7:O:305:LEU:HD22	1.76	0.67
20:l:106:HIS:HD2	20:l:107:TRP:H	1.43	0.67
18:j:47:PHE:HA	19:k:63:PHE:CZ	2.30	0.67
1:D:36:GLN:HE21	1:D:38:GLN:NE2	1.93	0.67
4:L:81:LYS:N	4:L:135:ASN:ND2	2.43	0.67
4:L:552:LEU:CD2	4:L:553:LEU:HD12	2.25	0.67
5:M:282:LEU:HD21	5:M:359:TRP:HH2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:14:LEU:O	12:d:14:LEU:CD1	2.37	0.67
4:L:480:LEU:HD22	18:j:84:PHE:CD2	2.30	0.67
5:M:344:MET:HE1	21:m:59:HIS:NE2	2.10	0.67
10:Y:71:MET:HG3	10:Y:102:THR:CG2	2.26	0.67
4:L:180:ILE:HD11	5:M:400:ILE:HB	1.78	0.66
5:M:166:LEU:HD11	25:M:501:3PE:H11	1.77	0.66
5:M:270:ILE:HG22	5:M:271:MET:HE2	1.76	0.66
5:M:361:MET:CB	5:M:441:MET:HE3	2.25	0.66
10:Y:76:THR:HG22	10:Y:92:TYR:HA	1.77	0.66
13:e:14:LEU:CD1	13:e:15:ASP:HB2	2.25	0.66
3:K:22:PHE:CB	4:L:585:LYS:HG2	2.21	0.66
4:L:201:ILE:HG22	4:L:266:LEU:HD11	1.76	0.66
8:U:128:PHE:CZ	8:U:148:ILE:HD12	2.30	0.66
16:h:102:PRO:HD2	16:h:105:TYR:HB2	1.78	0.66
7:O:124:ASN:O	15:g:51:MET:HE3	1.95	0.66
23:o:89:TYR:CE2	23:o:93:LEU:HD11	2.30	0.66
4:L:522:PHE:O	4:L:527:GLY:N	2.25	0.66
4:L:562:ILE:HB	4:L:563:PRO:HD3	1.78	0.66
25:L:702:3PE:O32	26:L:705:CDL:H812	1.94	0.66
7:O:209:VAL:HG12	7:O:260:SER:HB2	1.76	0.66
4:L:407:TRP:CE3	4:L:410:LEU:HD11	2.29	0.66
5:M:318:ALA:HB2	5:M:373:ILE:HG23	1.75	0.66
7:O:343:TYR:HD1	7:O:352:ILE:HG23	1.59	0.66
5:M:446:LEU:HD13	15:g:101:THR:CG2	2.26	0.66
25:i:201:3PE:H2B2	25:i:201:3PE:H342	1.76	0.66
4:L:174:TYR:CE1	25:L:701:3PE:H331	2.30	0.66
7:O:62:VAL:HA	7:O:205:ILE:O	1.96	0.66
1:D:55:SER:HB2	4:L:575:THR:HG23	1.78	0.66
7:O:205:ILE:HD11	7:O:273:ILE:HG12	1.77	0.66
23:o:25:PHE:CE2	23:o:109:LEU:HD22	2.31	0.66
24:p:70:ARG:CZ	24:p:91:GLN:HE21	2.09	0.66
2:J:56:PHE:O	2:J:60:LEU:HB3	1.96	0.66
4:L:116:ARG:HG2	4:L:120:TYR:CE2	2.31	0.66
7:O:48:LYS:HD2	7:O:288:ASP:HB2	1.78	0.66
7:O:200:PRO:HG3	7:O:282:PRO:HD2	1.77	0.66
10:Y:141:PRO:HB2	16:h:161:ARG:NH1	2.11	0.66
4:L:66:TRP:HZ3	4:L:68:TRP:CD1	2.14	0.66
4:L:552:LEU:HD23	4:L:553:LEU:HD12	1.77	0.66
12:d:113:LEU:HD22	15:g:148:PRO:HG3	1.78	0.66
19:k:34:PRO:CG	19:k:59:TYR:CE1	2.72	0.66
4:L:25:ASN:OD1	4:L:25:ASN:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:373:ILE:CD1	5:M:454:ILE:HD11	2.25	0.65
6:N:25:ASN:ND2	13:e:18:PHE:CE2	2.65	0.65
7:O:38:TYR:HB3	7:O:299:GLN:NE2	2.11	0.65
2:J:12:PHE:HE2	3:K:42:ILE:CD1	2.05	0.65
8:U:134:ASP:OD2	22:n:2:ALA:N	2.29	0.65
11:c:72:ARG:HD2	12:d:20:SER:HA	1.78	0.65
21:m:15:PRO:CG	21:m:18:LEU:HD12	2.26	0.65
4:L:524:THR:HG22	22:n:78:GLN:HG2	1.78	0.65
6:N:220:MET:C	6:N:223:ASN:H	2.04	0.65
6:N:258:THR:HB	6:N:333:SER:O	1.96	0.65
4:L:190:SER:HB2	4:L:196:TRP:HE1	1.61	0.65
4:L:445:GLU:OE2	18:j:54:GLN:HG3	1.97	0.65
4:L:542:LEU:HB3	5:M:278:ARG:HD2	1.77	0.65
26:L:705:CDL:HA22	26:L:705:CDL:H512	1.79	0.65
26:L:705:CDL:H591	10:Y:68:ILE:HD12	1.77	0.65
1:D:47:PHE:HB3	6:N:227:ILE:CD1	2.13	0.65
5:M:367:LEU:CD2	5:M:408:MET:HE2	2.25	0.65
15:g:108:PRO:O	15:g:109:ASP:OD1	2.13	0.65
18:j:94:ASP:HB3	18:j:99:ILE:HB	1.78	0.65
20:l:82:SER:HA	20:l:112:TYR:HB3	1.79	0.65
4:L:88:LEU:HD23	4:L:326:PHE:CE2	2.32	0.65
22:n:30:TRP:CD2	22:n:76:HIS:HD2	2.15	0.65
4:L:70:THR:HG21	24:p:101:GLU:OE2	1.96	0.65
11:c:55:TRP:CZ2	12:d:66:THR:HG22	2.31	0.65
14:f:38:ARG:NH1	14:f:54:VAL:HB	2.11	0.65
20:l:162:PRO:HG3	23:o:39:MET:HE3	1.78	0.65
2:J:68:GLY:HA2	2:J:71:THR:HB	1.78	0.65
4:L:387:THR:HG22	4:L:465:GLY:H	1.61	0.65
6:N:23:SER:HB2	13:e:15:ASP:OD2	1.96	0.65
7:O:343:TYR:CE1	7:O:355:LYS:HB2	2.31	0.65
5:M:122:PHE:HD1	5:M:238:LEU:HG	1.62	0.65
5:M:127:ILE:HG12	6:N:254:LEU:HD21	1.77	0.65
7:O:117:PHE:CE1	7:O:173:MET:CE	2.77	0.65
9:X:162:LYS:HB3	9:X:166:ARG:HH21	1.61	0.65
24:p:24:THR:HG22	24:p:26:LEU:H	1.62	0.65
4:L:368:PHE:HB3	4:L:445:GLU:OE2	1.97	0.64
15:g:140:PHE:CE2	24:p:74:ILE:HG22	2.32	0.64
25:i:201:3PE:H292	25:i:201:3PE:H332	1.79	0.64
23:o:71:ARG:HB3	23:o:71:ARG:HH11	1.61	0.64
5:M:119:TYR:CD1	5:M:160:LEU:HD22	2.32	0.64
5:M:307:TRP:CD1	5:M:459:MET:SD	2.91	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:194:THR:HG23	7:O:307:TYR:HB2	1.79	0.64
16:h:127:ASP:OD1	16:h:127:ASP:O	2.15	0.64
24:p:74:ILE:HD13	24:p:85:ILE:HG13	1.80	0.64
5:M:167:ILE:O	5:M:171:VAL:HG12	1.98	0.64
5:M:300:SER:HB3	5:M:381:ILE:HG23	1.78	0.64
6:N:307:THR:HG22	6:N:308:ASN:N	2.12	0.64
9:X:167:PHE:HD2	9:X:170:TRP:NE1	1.94	0.64
10:Y:137:LEU:HD23	10:Y:138:PHE:CG	2.31	0.64
20:l:122:THR:CG2	20:l:123:PRO:HD2	2.27	0.64
25:M:503:3PE:C12	7:O:338:LYS:HE3	2.28	0.64
7:O:238:GLU:HA	7:O:241:TYR:CD2	2.32	0.64
3:K:22:PHE:O	4:L:585:LYS:HE3	1.97	0.64
4:L:40:ILE:HD13	4:L:97:THR:HG22	1.79	0.64
4:L:366:MET:CG	4:L:443:ILE:HG21	2.28	0.64
12:d:109:TYR:HA	12:d:112:ILE:CG2	2.28	0.64
19:k:38:VAL:HG13	22:n:39:TYR:HB2	1.78	0.64
23:o:105:GLU:O	23:o:106:ARG:C	2.39	0.64
4:L:41:LYS:HG3	4:L:98:TRP:CE2	2.33	0.64
4:L:81:LYS:N	4:L:135:ASN:HD21	1.96	0.64
6:N:254:LEU:HD12	6:N:255:PRO:HD2	1.78	0.64
7:O:347:VAL:CG1	11:c:29:PHE:HA	2.28	0.64
12:d:60:ARG:O	12:d:61:GLN:C	2.40	0.64
17:i:101:LYS:HG2	24:p:116:ARG:O	1.97	0.64
5:M:175:ASN:ND2	16:h:143:GLU:HG2	2.13	0.64
6:N:37:LEU:HD12	6:N:63:GLN:HB3	1.79	0.64
6:N:179:MET:HG3	6:N:216:PHE:HE1	1.63	0.64
24:p:5:TRP:HH2	24:p:12:GLU:OE1	1.81	0.64
4:L:246:LEU:HD12	4:L:246:LEU:C	2.23	0.64
7:O:323:GLN:HE22	15:g:54:GLN:HB3	1.63	0.64
22:n:31:CYS:SG	22:n:36:LYS:NZ	2.71	0.64
4:L:446:ASN:ND2	18:j:51:THR:HG21	2.12	0.64
5:M:160:LEU:HD11	5:M:203:PHE:CZ	2.33	0.64
19:k:47:LEU:HD12	22:n:43:LEU:HD23	1.79	0.64
4:L:446:ASN:HD21	18:j:51:THR:HG21	1.63	0.64
6:N:143:ILE:HA	6:N:194:LEU:HD11	1.79	0.64
17:i:29:SER:HB2	17:i:32:GLU:OE1	1.97	0.64
20:l:101:TRP:NE1	21:m:62:ASP:HA	2.13	0.64
20:l:106:HIS:CD2	20:l:107:TRP:N	2.67	0.64
5:M:267:TRP:CZ2	5:M:271:MET:HE3	2.32	0.63
6:N:220:MET:HA	6:N:223:ASN:HA	1.79	0.63
15:g:147:LEU:HD11	24:p:163:MET:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:31:PHE:CE2	23:o:104:ARG:NH1	2.63	0.63
4:L:433:THR:HG22	4:L:434:LYS:N	2.13	0.63
5:M:105:LEU:O	5:M:109:THR:HG23	1.98	0.63
5:M:196:TRP:HZ3	5:M:261:PHE:HE2	1.44	0.63
15:g:75:ASP:OD1	15:g:76:SER:N	2.32	0.63
4:L:100:ILE:HD13	4:L:341:MET:SD	2.38	0.63
4:L:145:GLU:HB3	5:M:370:PRO:CG	2.28	0.63
4:L:305:SER:HB2	4:L:422:TYR:CE1	2.34	0.63
5:M:1:MET:HB2	5:M:52:PHE:HD2	1.60	0.63
5:M:250:LEU:O	5:M:250:LEU:CD1	2.44	0.63
5:M:368:ALA:HB1	5:M:375:LEU:CD1	2.25	0.63
5:M:422:HIS:HB3	21:m:51:TYR:CE2	2.33	0.63
7:O:176:GLN:HB2	7:O:178:TYR:CD2	2.32	0.63
19:k:34:PRO:HG2	19:k:59:TYR:CD1	2.34	0.63
4:L:80:PHE:C	4:L:135:ASN:HD21	2.06	0.63
4:L:381:THR:HG21	4:L:498:PHE:CE2	2.33	0.63
4:L:410:LEU:HD12	4:L:411:ILE:N	2.13	0.63
5:M:118:PHE:O	5:M:122:PHE:N	2.25	0.63
5:M:220:HIS:NE2	5:M:231:LEU:HB3	2.13	0.63
13:e:69:ARG:HD2	13:e:72:THR:HG21	1.80	0.63
22:n:95:GLU:HA	22:n:98:LYS:HG3	1.81	0.63
4:L:202:MET:HE3	4:L:265:PRO:CG	2.25	0.63
5:M:231:LEU:HA	5:M:235:LEU:HD12	1.80	0.63
6:N:131:LEU:O	6:N:135:LYS:HG2	1.98	0.63
6:N:149:LEU:HD13	6:N:154:ILE:CG2	2.28	0.63
8:U:140:CYS:SG	8:U:143:GLU:OE2	2.53	0.63
18:j:52:ARG:HG3	18:j:56:ILE:HD12	1.78	0.63
4:L:361:ASN:OD1	4:L:361:ASN:O	2.17	0.63
25:L:702:3PE:H361	6:N:164:MET:HE1	1.81	0.63
25:M:502:3PE:H2A1	26:h:201:CDL:H202	1.80	0.63
7:O:305:LEU:HD12	7:O:305:LEU:C	2.24	0.63
7:O:326:ARG:HH21	15:g:56:ASP:CG	2.07	0.63
17:i:28:LEU:HD22	17:i:32:GLU:HG2	1.79	0.63
6:N:158:ALA:O	6:N:162:ILE:HG12	1.99	0.63
16:h:155:GLU:O	16:h:159:LEU:HD13	1.99	0.63
5:M:129:THR:HG21	5:M:235:LEU:HD13	1.80	0.62
8:U:74:LEU:N	8:U:74:LEU:HD12	2.15	0.62
22:n:141:GLN:O	22:n:144:THR:HG22	1.99	0.62
23:o:18:ASP:OD1	23:o:19:PRO:HD2	1.99	0.62
25:D:501:3PE:H272	6:N:288:LEU:HD13	1.81	0.62
4:L:445:GLU:HB2	4:L:450:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:73:LEU:CD2	5:M:103:GLN:NE2	2.61	0.62
5:M:395:LEU:HD21	21:m:101:TRP:CZ2	2.33	0.62
24:p:66:ARG:HD2	24:p:68:TYR:CZ	2.34	0.62
6:N:100:MET:HE3	6:N:111:PHE:CZ	2.34	0.62
7:O:113:SER:HB3	7:O:116:LYS:HB2	1.80	0.62
21:m:127:ILE:HG22	24:p:136:THR:HG23	1.81	0.62
4:L:365:ILE:HD11	4:L:366:MET:HE2	1.81	0.62
5:M:16:TRP:HZ2	25:M:503:3PE:H282	1.64	0.62
7:O:61:THR:HB	7:O:160:GLU:O	2.00	0.62
3:K:51:SER:HA	13:e:32:ARG:HD3	1.80	0.62
5:M:98:MET:SD	25:M:503:3PE:H3C1	2.40	0.62
5:M:307:TRP:CE3	5:M:383:MET:HE3	2.34	0.62
5:M:318:ALA:CB	5:M:373:ILE:HG23	2.29	0.62
23:o:17:PRO:HG3	23:o:106:ARG:HA	1.82	0.62
3:K:93:LEU:CD2	6:N:54:GLU:HG2	2.30	0.62
5:M:129:THR:HG21	5:M:235:LEU:CD1	2.30	0.62
5:M:307:TRP:HD1	5:M:459:MET:SD	2.23	0.62
6:N:324:LEU:HD11	12:d:64:PHE:HZ	1.64	0.62
21:m:129:TYR:CZ	24:p:144:LEU:O	2.53	0.62
22:n:168:TRP:O	22:n:172:THR:OG1	2.18	0.62
23:o:5:LEU:HB3	23:o:9:TYR:CE2	2.34	0.62
25:L:703:3PE:H3C1	25:L:703:3PE:H271	1.81	0.62
5:M:56:PHE:HE1	5:M:108:MET:HG2	1.64	0.62
7:O:117:PHE:HE1	7:O:128:SER:HB2	1.63	0.62
7:O:121:PRO:O	7:O:122:LYS:CG	2.46	0.62
10:Y:64:THR:OG1	10:Y:106:ARG:HG2	2.00	0.62
4:L:542:LEU:HD21	20:l:116:ARG:HD2	1.81	0.62
6:N:207:ILE:O	6:N:211:LEU:HG	2.00	0.62
6:N:335:MET:O	6:N:335:MET:CG	2.41	0.62
7:O:132:GLN:HE22	7:O:169:PHE:HB2	1.64	0.62
3:K:1:MET:N	3:K:2:PRO:HD2	2.15	0.62
4:L:437:PHE:CE1	4:L:441:ILE:CG1	2.69	0.62
5:M:98:MET:HE3	5:M:128:PRO:HA	1.81	0.62
17:i:69:LEU:HD12	17:i:71:ALA:N	2.14	0.62
21:m:17:THR:O	21:m:18:LEU:HB2	1.99	0.62
4:L:550:LEU:HB2	5:M:275:ILE:HG22	1.82	0.62
6:N:109:ALA:CB	6:N:110:PRO:HD3	2.30	0.62
6:N:218:ALA:HB1	6:N:240:MET:SD	2.40	0.61
7:O:140:LEU:HD11	7:O:198:TYR:CZ	2.35	0.61
9:X:164:GLY:O	9:X:165:THR:C	2.41	0.61
24:p:5:TRP:CH2	24:p:12:GLU:OE1	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:101:3PE:H3C1	4:L:593:ILE:HD11	1.82	0.61
4:L:10:LEU:HD23	4:L:46:ILE:HG21	1.82	0.61
4:L:141:PHE:CE2	5:M:370:PRO:CG	2.76	0.61
4:L:466:PHE:CB	18:j:68:TRP:CZ2	2.71	0.61
8:U:128:PHE:CZ	8:U:148:ILE:HG23	2.35	0.61
13:e:95:PRO:HD2	13:e:98:HIS:CE1	2.34	0.61
20:l:57:MET:HG2	20:l:104:PRO:HG2	1.82	0.61
4:L:149:ILE:HG21	5:M:364:LEU:HD21	1.83	0.61
4:L:556:ILE:HD11	21:m:76:ILE:HG22	1.82	0.61
4:L:559:GLU:HA	4:L:563:PRO:HG2	1.82	0.61
5:M:73:LEU:CB	5:M:103:GLN:OE1	2.48	0.61
5:M:81:GLN:O	5:M:85:LYS:HB2	2.01	0.61
5:M:151:PHE:CE2	6:N:291:PHE:HB2	2.34	0.61
6:N:175:MET:HE1	6:N:227:ILE:HA	1.80	0.61
7:O:117:PHE:HD1	7:O:128:SER:HA	1.64	0.61
21:m:100:PHE:O	21:m:104:VAL:HG23	2.00	0.61
26:L:705:CDL:H581	26:L:705:CDL:H762	1.81	0.61
5:M:158:ILE:HG12	6:N:287:LEU:HD11	1.82	0.61
5:M:373:ILE:H	5:M:448:THR:HG22	1.65	0.61
6:N:17:PRO:HG2	6:N:133:TRP:CE2	2.35	0.61
7:O:213:GLU:O	7:O:217:ARG:HG3	2.00	0.61
16:h:106:ILE:O	16:h:106:ILE:HG22	1.99	0.61
23:o:5:LEU:HB3	23:o:9:TYR:CD2	2.36	0.61
23:o:22:ILE:HA	23:o:105:GLU:OE2	2.00	0.61
23:o:111:ARG:NH1	23:o:115:ARG:HD3	2.14	0.61
4:L:468:ILE:O	4:L:472:ILE:HG23	2.00	0.61
26:L:704:CDL:H571	26:L:704:CDL:H792	1.82	0.61
5:M:139:GLN:HB3	5:M:222:GLU:HG3	1.83	0.61
5:M:422:HIS:NE2	5:M:425:ASN:OD1	2.33	0.61
5:M:433:GLU:O	5:M:437:MET:HG2	2.01	0.61
25:M:501:3PE:H112	6:N:276:LEU:HD21	1.81	0.61
4:L:100:ILE:HG21	4:L:246:LEU:HD23	1.82	0.61
5:M:98:MET:HE1	5:M:128:PRO:HA	1.83	0.61
5:M:143:LEU:HD21	6:N:303:THR:HG23	1.80	0.61
5:M:318:ALA:HB2	5:M:373:ILE:CG2	2.30	0.61
6:N:342:GLN:NE2	12:d:30:ARG:HH11	1.99	0.61
7:O:140:LEU:HD21	7:O:304:VAL:O	2.00	0.61
13:e:32:ARG:O	13:e:33:CYS:HB2	1.99	0.61
20:l:62:TYR:CZ	20:l:64:PRO:HG3	2.36	0.61
22:n:149:ILE:H	22:n:149:ILE:HD12	1.65	0.61
4:L:560:LYS:HD2	21:m:80:PHE:CE2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:138:LEU:HB3	8:U:144:ILE:HG12	1.83	0.61
23:o:69:CYS:C	23:o:80:CYS:SG	2.82	0.61
2:J:24:SER:O	2:J:27:TYR:N	2.32	0.61
4:L:424:MET:HE2	4:L:502:LEU:CB	2.31	0.61
5:M:11:MET:CE	5:M:111:SER:HB2	2.29	0.61
4:L:302:ILE:HB	4:L:340:PHE:CE1	2.36	0.61
9:X:160:PRO:HG3	12:d:22:PRO:HD3	1.83	0.61
10:Y:68:ILE:CG2	10:Y:120:MET:HE1	2.31	0.61
1:D:35:ARG:HE	15:g:59:PRO:CD	2.13	0.61
4:L:174:TYR:HE1	25:L:701:3PE:H331	1.64	0.61
4:L:182:PHE:CE2	4:L:186:MET:SD	2.94	0.61
4:L:594:ASN:CG	6:N:110:PRO:HB2	2.26	0.61
5:M:109:THR:HG22	5:M:121:LEU:HB3	1.82	0.61
14:f:38:ARG:NH1	14:f:56:TRP:O	2.34	0.61
15:g:109:ASP:HB3	15:g:114:GLU:HB3	1.82	0.61
23:o:50:GLN:OE1	24:p:120:ASN:ND2	2.34	0.61
2:J:71:THR:HA	3:K:27:MET:HE3	1.82	0.60
2:J:87:LEU:CG	2:J:91:PHE:CZ	2.81	0.60
3:K:12:PHE:CE1	6:N:72:LEU:HD22	2.35	0.60
3:K:66:PHE:CE2	6:N:35:PHE:CZ	2.89	0.60
5:M:209:LEU:HD23	5:M:210:TYR:N	2.16	0.60
6:N:59:TYR:CZ	6:N:63:GLN:HG3	2.36	0.60
5:M:423:MET:O	5:M:424:ILE:C	2.44	0.60
4:L:40:ILE:HD12	4:L:101:MET:HG3	1.82	0.60
4:L:180:ILE:HG21	25:L:703:3PE:H3G2	1.84	0.60
6:N:100:MET:HE3	6:N:111:PHE:HZ	1.66	0.60
4:L:42:PHE:O	4:L:46:ILE:HG12	2.01	0.60
4:L:556:ILE:HG21	21:m:80:PHE:CZ	2.34	0.60
9:X:159:LYS:O	9:X:160:PRO:C	2.43	0.60
12:d:16:ASP:O	12:d:19:ARG:HG3	2.01	0.60
15:g:63:ASN:OD1	22:n:106:TYR:HE1	1.85	0.60
4:L:222:GLY:CA	4:L:229:LEU:HD11	2.26	0.60
4:L:594:ASN:HD21	6:N:110:PRO:HB2	1.66	0.60
4:L:56:HIS:O	23:o:71:ARG:HG3	2.02	0.60
5:M:207:MET:HG3	5:M:239:GLY:HA3	1.83	0.60
5:M:269:MET:HE3	5:M:399:ASN:CB	2.32	0.60
6:N:112:HIS:HB2	6:N:184:ILE:HD13	1.84	0.60
6:N:224:SER:HB2	6:N:229:SER:CB	2.32	0.60
7:O:76:GLU:HG3	7:O:266:PRO:HG2	1.83	0.60
7:O:249:MET:HB3	7:O:253:CYS:SG	2.40	0.60
4:L:173:LEU:CD2	25:L:701:3PE:H321	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:L:705:CDL:H541	26:L:705:CDL:H142	1.82	0.60
5:M:178:ILE:HD12	16:h:143:GLU:HG3	1.84	0.60
5:M:370:PRO:HA	5:M:375:LEU:HD22	1.83	0.60
20:l:38:PRO:CB	21:m:75:ASN:HD22	2.09	0.60
20:l:184:TYR:CD1	23:o:36:GLU:HA	2.36	0.60
2:J:68:GLY:O	2:J:69:TYR:C	2.45	0.60
4:L:204:SER:HA	4:L:207:ASN:HD22	1.67	0.60
5:M:144:ASN:HA	5:M:147:ILE:HD12	1.82	0.60
16:h:73:PHE:HD2	16:h:74:TYR:CD1	2.20	0.60
22:n:143:GLU:OE1	22:n:155:PRO:HB3	2.02	0.60
5:M:77:LEU:HD23	5:M:99:LEU:HD12	1.83	0.60
25:M:503:3PE:H251	6:N:242:THR:HG21	1.84	0.60
7:O:256:LEU:HD11	7:O:276:LEU:CD2	2.32	0.60
10:Y:137:LEU:CD2	10:Y:138:PHE:CD2	2.84	0.60
16:h:102:PRO:HD2	16:h:105:TYR:CB	2.32	0.60
17:i:69:LEU:CD1	17:i:71:ALA:HB3	2.31	0.60
4:L:123:LEU:HD22	4:L:150:MET:CG	2.32	0.59
4:L:145:GLU:HG2	5:M:370:PRO:HD3	1.84	0.59
5:M:329:LEU:HD23	5:M:437:MET:HE3	1.84	0.59
6:N:258:THR:CG2	6:N:336:THR:HG22	2.32	0.59
6:N:276:LEU:C	6:N:276:LEU:HD12	2.27	0.59
16:h:73:PHE:CD2	16:h:74:TYR:CD1	2.90	0.59
22:n:176:GLU:O	22:n:178:PRO:HD3	2.02	0.59
2:J:9:SER:HB3	3:K:7:ASN:ND2	2.05	0.59
25:L:703:3PE:H232	25:m:201:3PE:H3B1	1.84	0.59
5:M:126:LEU:HD21	5:M:153:THR:HB	1.83	0.59
7:O:54:HIS:HB2	7:O:56:TYR:CE1	2.37	0.59
8:U:90:TYR:CZ	8:U:92:LYS:HD2	2.35	0.59
9:X:158:LEU:HB3	12:d:21:LEU:HD21	1.84	0.59
4:L:81:LYS:HB2	4:L:135:ASN:OD1	2.02	0.59
4:L:247:LEU:HD12	4:L:248:HIS:CG	2.36	0.59
5:M:115:LEU:O	5:M:118:PHE:HB3	2.02	0.59
17:i:104:ILE:HG13	23:o:48:ASP:HB3	1.84	0.59
2:J:134:MET:HE2	13:e:27:TYR:CZ	2.37	0.59
5:M:294:MET:HE3	5:M:319:HIS:CD2	2.37	0.59
7:O:126:GLY:HA3	15:g:51:MET:HE1	1.84	0.59
7:O:167:PHE:HE1	7:O:245:PHE:HB2	1.67	0.59
7:O:343:TYR:HE1	7:O:355:LYS:HB2	1.66	0.59
16:h:69:ARG:O	16:h:73:PHE:HB2	2.02	0.59
1:D:34:ALA:HB3	5:M:86:LYS:HZ3	1.67	0.59
4:L:302:ILE:CG2	4:L:340:PHE:CE2	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:313:MET:HE2	4:L:328:HIS:CE1	2.38	0.59
16:h:87:THR:HA	26:h:201:CDL:H512	1.83	0.59
20:l:38:PRO:C	21:m:75:ASN:ND2	2.60	0.59
1:D:65:PRO:HG3	1:D:70:ASP:OD1	2.02	0.59
2:J:19:LEU:HD21	2:J:31:GLY:HA3	1.83	0.59
4:L:227:PHE:CD2	4:L:283:LEU:CD2	2.86	0.59
5:M:14:LEU:HD21	5:M:26:ASN:HB2	1.84	0.59
5:M:209:LEU:HD23	5:M:211:GLY:H	1.67	0.59
6:N:200:LEU:HD22	6:N:269:GLU:HG3	1.84	0.59
2:J:12:PHE:CZ	3:K:42:ILE:CD1	2.86	0.59
4:L:312:LEU:CD2	4:L:395:ILE:HG21	2.33	0.59
4:L:605:ASN:O	4:L:606:LEU:C	2.46	0.59
5:M:255:LYS:NZ	12:d:117:HIS:HB3	2.18	0.59
5:M:388:TRP:NE1	21:m:109:ARG:HD2	2.18	0.59
26:L:704:CDL:H322	16:h:71:MET:HE1	1.83	0.59
6:N:324:LEU:HD11	12:d:64:PHE:CZ	2.37	0.59
15:g:139:TYR:HD2	15:g:140:PHE:CD1	2.20	0.59
4:L:570:HIS:O	4:L:571:THR:C	2.45	0.59
7:O:114:LEU:HA	7:O:131:LEU:HD21	1.84	0.59
8:U:105:MET:SD	8:U:139:MET:HE1	2.42	0.59
16:h:95:GLU:HB3	16:h:114:LYS:HG2	1.85	0.59
1:D:51:VAL:HG21	1:D:58:THR:HG22	1.83	0.59
25:D:501:3PE:H361	4:L:566:THR:HG21	1.85	0.59
2:J:21:LEU:HA	25:K:101:3PE:H252	1.85	0.59
4:L:466:PHE:CE1	4:L:470:TYR:HE2	2.21	0.59
5:M:263:LEU:CD1	21:m:102:TYR:HD1	2.16	0.59
5:M:275:ILE:HD11	5:M:288:TYR:CB	2.33	0.59
5:M:396:MET:HG3	5:M:396:MET:O	2.03	0.59
7:O:242:LYS:HA	7:O:246:LEU:HD12	1.84	0.59
18:j:71:TRP:CH2	25:j:700:3PE:H3B1	2.38	0.59
20:l:113:ILE:HG12	20:l:114:ARG:H	1.67	0.59
22:n:97:TYR:HB2	22:n:178:PRO:CB	2.32	0.59
22:n:111:GLU:O	22:n:114:MET:HG2	2.03	0.59
4:L:230:HIS:N	4:L:231:PRO:CD	2.66	0.58
5:M:210:TYR:O	5:M:213:HIS:CD2	2.56	0.58
6:N:77:ASN:OD1	6:N:81:LEU:HD12	2.03	0.58
6:N:179:MET:CG	6:N:216:PHE:HE1	2.16	0.58
6:N:300:THR:HG23	6:N:301:SER:N	2.17	0.58
13:e:101:ARG:CZ	13:e:102:GLU:H	2.16	0.58
3:K:19:THR:HG23	3:K:29:THR:HG23	1.85	0.58
4:L:417:SER:HB3	4:L:493:ILE:CG1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:109:ALA:CB	6:N:110:PRO:CD	2.81	0.58
9:X:151:ASN:ND2	13:e:51:ARG:HH11	2.01	0.58
24:p:37:TYR:CZ	24:p:41:VAL:HG11	2.38	0.58
6:N:307:THR:C	7:O:319:ILE:HG12	2.29	0.58
8:U:119:ILE:HD11	8:U:138:LEU:HB2	1.85	0.58
20:l:105:ILE:HG23	20:l:109:LEU:HD22	1.84	0.58
3:K:70:GLU:HA	6:N:38:LEU:HD21	1.84	0.58
5:M:131:ILE:CD1	6:N:302:LEU:HD21	2.34	0.58
6:N:308:ASN:C	7:O:319:ILE:HG23	2.29	0.58
1:D:37:TRP:CZ2	1:D:39:PRO:HA	2.38	0.58
4:L:407:TRP:CZ3	4:L:410:LEU:HD11	2.38	0.58
8:U:105:MET:CG	8:U:139:MET:HE1	2.33	0.58
12:d:14:LEU:HD12	12:d:14:LEU:C	2.27	0.58
16:h:96:ALA:HB3	24:p:63:TYR:CD1	2.37	0.58
21:m:75:ASN:O	21:m:75:ASN:OD1	2.20	0.58
24:p:128:GLU:O	24:p:131:GLN:N	2.37	0.58
2:J:33:ILE:HG23	2:J:60:LEU:HD21	1.85	0.58
4:L:15:LEU:O	4:L:18:PRO:HD2	2.03	0.58
4:L:261:VAL:C	4:L:264:HIS:HD2	2.12	0.58
4:L:404:THR:HG22	4:L:405:ASN:N	2.19	0.58
7:O:49:THR:O	7:O:53:LEU:HG	2.04	0.58
13:e:41:ILE:HG12	16:h:174:PRO:HB2	1.84	0.58
14:f:37:PHE:CE2	16:h:141:GLN:OE1	2.56	0.58
4:L:477:ILE:HG13	23:o:91:GLU:CD	2.29	0.58
5:M:154:LEU:HD13	6:N:287:LEU:CD2	2.33	0.58
5:M:196:TRP:HZ3	5:M:261:PHE:CE2	2.21	0.58
11:c:65:ASP:OD2	12:d:73:TYR:OH	2.18	0.58
12:d:113:LEU:O	12:d:113:LEU:HG	2.02	0.58
14:f:47:GLU:HG2	14:f:47:GLU:O	2.03	0.58
4:L:466:PHE:HE1	18:j:72:ARG:CZ	2.13	0.58
5:M:398:ILE:HD12	25:m:201:3PE:H2G1	1.86	0.58
6:N:26:LEU:O	6:N:27:MET:C	2.46	0.58
6:N:147:PRO:HB2	6:N:148:LEU:HD12	1.86	0.58
6:N:314:MET:CB	7:O:305:LEU:HD11	2.33	0.58
4:L:65:THR:HA	17:i:90:MET:HE2	1.86	0.58
4:L:542:LEU:HD11	25:L:701:3PE:H261	1.86	0.58
7:O:76:GLU:HG3	7:O:266:PRO:CG	2.34	0.58
17:i:95:TYR:OH	24:p:11:PRO:O	2.20	0.58
4:L:425:ARG:HG3	4:L:429:PHE:CE2	2.39	0.58
5:M:73:LEU:HB2	5:M:103:GLN:OE1	2.02	0.58
5:M:109:THR:HG22	5:M:121:LEU:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:149:LEU:HD11	6:N:195:PRO:HG3	1.84	0.58
7:O:117:PHE:CD1	7:O:128:SER:CB	2.87	0.58
8:U:155:TYR:OH	16:h:52:LYS:HD2	2.04	0.58
9:X:167:PHE:HB3	9:X:170:TRP:CD1	2.39	0.58
15:g:121:GLU:HA	15:g:124:VAL:HG22	1.86	0.58
4:L:232:TRP:CZ3	4:L:233:LEU:HD21	2.37	0.57
4:L:592:LEU:O	4:L:596:ILE:HG12	2.04	0.57
5:M:154:LEU:HD13	6:N:287:LEU:HD22	1.85	0.57
25:M:503:3PE:H382	6:N:246:LEU:CD1	2.34	0.57
8:U:100:VAL:C	8:U:141:PRO:HG2	2.28	0.57
4:L:456:ARG:HG2	25:j:700:3PE:H241	1.86	0.57
6:N:33:LEU:HD11	6:N:141:ILE:HD12	1.86	0.57
8:U:113:LEU:HD23	22:n:17:LEU:CD2	2.34	0.57
2:J:65:VAL:HG13	2:J:66:VAL:H	1.66	0.57
4:L:358:LYS:CG	22:n:80:TYR:CE2	2.83	0.57
4:L:441:ILE:HG21	18:j:48:PRO:HD3	1.86	0.57
5:M:172:GLY:C	5:M:173:THR:HG23	2.28	0.57
16:h:188:ASP:O	16:h:189:ASN:C	2.48	0.57
27:L:706:PC1:H2B2	27:L:706:PC1:H352	1.87	0.57
5:M:230:ILE:HG13	5:M:235:LEU:HG	1.87	0.57
5:M:296:LEU:HD22	5:M:396:MET:HE1	1.86	0.57
6:N:253:GLY:N	6:N:290:LEU:HD11	2.19	0.57
10:Y:63:PHE:HE2	10:Y:106:ARG:HE	1.53	0.57
13:e:14:LEU:HD12	13:e:15:ASP:CB	2.33	0.57
3:K:96:LEU:O	3:K:97:GLN:C	2.47	0.57
4:L:227:PHE:CD2	4:L:283:LEU:HD21	2.38	0.57
4:L:425:ARG:HG3	4:L:429:PHE:HE2	1.68	0.57
5:M:73:LEU:HD22	5:M:103:GLN:NE2	2.18	0.57
5:M:297:VAL:O	5:M:301:ILE:HG12	2.03	0.57
5:M:444:LEU:O	5:M:448:THR:HG23	2.04	0.57
6:N:154:ILE:HG12	6:N:195:PRO:HG2	1.87	0.57
6:N:179:MET:HG3	6:N:216:PHE:CE1	2.39	0.57
6:N:284:MET:O	6:N:287:LEU:HB2	2.04	0.57
15:g:123:LEU:HD12	24:p:98:VAL:CG1	2.35	0.57
3:K:20:LEU:HA	4:L:588:PHE:HD2	1.70	0.57
4:L:145:GLU:HB3	5:M:370:PRO:HG2	1.85	0.57
5:M:447:LEU:HD21	5:M:454:ILE:CD1	2.33	0.57
4:L:141:PHE:CD2	5:M:370:PRO:HG3	2.38	0.57
6:N:273:ASN:O	6:N:274:ASN:HB2	2.05	0.57
8:U:93:ILE:HD11	8:U:110:LEU:HD11	1.86	0.57
22:n:98:LYS:HG2	22:n:178:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:246:LEU:HD12	4:L:247:LEU:CA	2.34	0.57
4:L:407:TRP:HE1	20:l:140:MET:CE	2.18	0.57
5:M:4:ILE:CG2	5:M:107:ILE:HD13	2.29	0.57
5:M:14:LEU:HD11	5:M:26:ASN:HB3	1.87	0.57
7:O:38:TYR:HB3	7:O:299:GLN:HE22	1.70	0.57
8:U:130:ILE:HG23	8:U:147:TYR:CE2	2.40	0.57
14:f:8:ARG:C	14:f:9:GLU:OE1	2.48	0.57
17:i:87:LYS:HG2	17:i:87:LYS:O	2.05	0.57
20:l:166:LEU:HB2	20:l:170:ARG:NH2	2.19	0.57
23:o:39:MET:CE	23:o:58:TYR:HA	2.35	0.57
2:J:169:ILE:CD1	6:N:42:PRO:HA	2.35	0.57
5:M:12:LEU:HB2	5:M:13:PRO:HD3	1.85	0.57
5:M:282:LEU:HD13	5:M:342:MET:HE2	1.86	0.57
7:O:80:GLN:CG	7:O:270:VAL:HG21	2.18	0.57
7:O:167:PHE:CE1	7:O:245:PHE:HB2	2.40	0.57
7:O:258:TYR:HB3	7:O:262:GLU:HB2	1.86	0.57
4:L:25:ASN:HB2	16:h:72:LYS:NZ	2.20	0.57
4:L:88:LEU:HD23	4:L:326:PHE:HE2	1.69	0.57
4:L:253:VAL:CG2	4:L:310:LEU:HD11	2.35	0.57
5:M:42:LEU:HD11	5:M:67:ILE:CD1	2.34	0.57
5:M:264:LEU:HD23	21:m:98:LEU:HD11	1.87	0.57
5:M:278:ARG:HH22	20:l:108:ASP:CG	2.13	0.57
6:N:109:ALA:HB1	6:N:110:PRO:HD3	1.86	0.57
7:O:323:GLN:HB2	15:g:56:ASP:OD1	2.05	0.57
10:Y:57:ARG:HG2	10:Y:60:ARG:HH21	1.68	0.57
15:g:140:PHE:CZ	24:p:74:ILE:HG22	2.40	0.57
1:D:36:GLN:HE22	5:M:135:ARG:NH2	2.02	0.56
2:J:22:LYS:CD	3:K:23:ARG:HG3	2.35	0.56
4:L:60:GLU:CG	4:L:83:ASP:HA	2.35	0.56
5:M:269:MET:HE3	5:M:399:ASN:HB2	1.86	0.56
6:N:226:THR:HG22	6:N:228:ASN:H	1.70	0.56
16:h:175:GLU:HB3	16:h:177:GLU:HG2	1.86	0.56
5:M:310:MET:O	5:M:314:MET:HG3	2.04	0.56
25:M:501:3PE:H221	10:Y:135:TRP:CH2	2.40	0.56
7:O:125:ASP:OD1	7:O:126:GLY:N	2.38	0.56
7:O:209:VAL:HG23	7:O:209:VAL:O	2.05	0.56
14:f:49:ARG:HB2	14:f:50:PRO:HD2	1.87	0.56
4:L:229:LEU:HD12	4:L:229:LEU:C	2.28	0.56
4:L:247:LEU:CD1	4:L:248:HIS:NE2	2.52	0.56
4:L:279:CYS:SG	27:L:706:PC1:H3D1	2.45	0.56
4:L:367:PRO:HB3	19:k:75:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:703:3PE:N	25:L:703:3PE:H2	2.19	0.56
5:M:264:LEU:CD2	21:m:98:LEU:HD21	2.34	0.56
7:O:173:MET:HE2	7:O:179:ILE:HG23	1.87	0.56
9:X:168:PHE:O	9:X:169:PHE:CD1	2.58	0.56
10:Y:92:TYR:CE1	10:Y:128:LYS:HD3	2.40	0.56
17:i:108:ASP:OD2	24:p:18:PRO:CB	2.52	0.56
22:n:81:ILE:CD1	22:n:87:GLY:O	2.53	0.56
5:M:57:SER:HB3	5:M:113:THR:HG22	1.87	0.56
5:M:78:MET:O	5:M:432:ARG:HD2	2.05	0.56
5:M:118:PHE:O	5:M:122:PHE:CB	2.54	0.56
5:M:196:TRP:HE1	5:M:250:LEU:HD13	1.69	0.56
6:N:120:GLN:O	6:N:176:ARG:CZ	2.54	0.56
6:N:254:LEU:CD1	6:N:255:PRO:HD2	2.35	0.56
7:O:149:HIS:CE1	7:O:153:THR:HG21	2.40	0.56
8:U:91:ASP:OD2	19:k:48:ARG:NH2	2.38	0.56
17:i:93:LYS:HD3	25:i:201:3PE:H121	1.88	0.56
20:l:88:PRO:HB2	22:n:86:PRO:CB	2.35	0.56
21:m:15:PRO:HG3	21:m:18:LEU:HD12	1.86	0.56
24:p:39:LEU:O	24:p:44:PRO:HD3	2.06	0.56
7:O:114:LEU:O	7:O:117:PHE:HB3	2.06	0.56
13:e:14:LEU:HD12	13:e:14:LEU:C	2.31	0.56
22:n:50:GLU:HG2	22:n:51:HIS:N	2.20	0.56
2:J:169:ILE:HD13	6:N:42:PRO:HA	1.87	0.56
4:L:295:GLN:NE2	4:L:524:THR:O	2.38	0.56
6:N:196:TYR:HB3	6:N:273:ASN:OD1	2.05	0.56
6:N:314:MET:HB2	7:O:305:LEU:CD1	2.34	0.56
7:O:256:LEU:CD2	7:O:276:LEU:HD23	2.30	0.56
8:U:125:GLU:OE2	18:j:44:TYR:HE1	1.89	0.56
15:g:140:PHE:HB3	24:p:75:THR:HG21	1.87	0.56
2:J:38:VAL:O	2:J:42:MET:HG3	2.05	0.56
4:L:397:GLU:HB2	4:L:482:MET:SD	2.46	0.56
6:N:149:LEU:CD1	6:N:154:ILE:HG21	2.35	0.56
6:N:253:GLY:H	6:N:290:LEU:HD11	1.71	0.56
23:o:15:VAL:HG11	23:o:113:LYS:HD3	1.87	0.56
6:N:258:THR:OG1	6:N:336:THR:HG22	2.05	0.56
11:c:55:TRP:HE1	12:d:66:THR:HG21	1.71	0.56
17:i:69:LEU:HD11	17:i:71:ALA:CB	2.35	0.56
18:j:52:ARG:HG3	18:j:56:ILE:CD1	2.36	0.56
18:j:92:TRP:CZ3	23:o:100:LYS:HA	2.41	0.56
20:l:185:ASP:OD1	23:o:37:ARG:HA	2.05	0.56
23:o:4:HIS:HA	23:o:7:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:427:ILE:CD1	19:k:69:PHE:HE1	2.18	0.56
5:M:73:LEU:CD2	5:M:103:GLN:CD	2.79	0.56
5:M:370:PRO:CA	5:M:375:LEU:CD2	2.83	0.56
6:N:193:ILE:HD11	6:N:269:GLU:HB2	1.88	0.56
13:e:85:LYS:O	13:e:88:LYS:HB3	2.06	0.56
9:X:160:PRO:HG3	12:d:22:PRO:CD	2.35	0.56
10:Y:76:THR:CG2	10:Y:95:GLY:HA3	2.34	0.56
19:k:42:LEU:HG	22:n:39:TYR:HD1	1.71	0.56
20:l:111:MET:HE3	20:l:112:TYR:CZ	2.41	0.56
23:o:25:PHE:CZ	23:o:109:LEU:HD13	2.40	0.56
24:p:74:ILE:CD1	24:p:85:ILE:HG13	2.36	0.56
3:K:59:ILE:HD12	6:N:27:MET:HG2	1.88	0.55
4:L:94:LEU:HD23	4:L:125:LEU:HD21	1.88	0.55
4:L:597:LEU:HD21	10:Y:37:ILE:HD12	1.87	0.55
5:M:309:PHE:O	5:M:313:THR:HG23	2.06	0.55
9:X:158:LEU:HD13	12:d:17:GLU:HG3	1.88	0.55
16:h:129:PRO:HG3	24:p:66:ARG:CZ	2.37	0.55
4:L:94:LEU:CD2	4:L:125:LEU:HD21	2.35	0.55
4:L:385:PHE:CD1	18:j:72:ARG:CG	2.89	0.55
4:L:538:PRO:O	4:L:542:LEU:HD13	2.06	0.55
26:L:704:CDL:H171	5:M:361:MET:HE1	1.89	0.55
5:M:267:TRP:HZ3	25:m:201:3PE:H2F1	1.72	0.55
6:N:325:MET:HE3	6:N:329:LEU:HD11	1.88	0.55
7:O:316:GLU:HG3	15:g:51:MET:HE2	1.87	0.55
9:X:169:PHE:CD2	9:X:169:PHE:O	2.59	0.55
10:Y:71:MET:CG	10:Y:102:THR:HG21	2.37	0.55
2:J:65:VAL:CG1	2:J:66:VAL:H	2.19	0.55
10:Y:137:LEU:HD23	10:Y:138:PHE:CD2	2.41	0.55
22:n:57:MET:HE2	22:n:57:MET:HA	1.87	0.55
1:D:57:GLU:HA	1:D:60:HIS:CD2	2.41	0.55
4:L:336:LYS:O	4:L:340:PHE:HD2	1.89	0.55
4:L:578:THR:CG2	6:N:168:GLY:HA2	2.36	0.55
5:M:4:ILE:H	5:M:4:ILE:HD12	1.70	0.55
5:M:421:ASN:HB2	21:m:51:TYR:OH	2.06	0.55
23:o:69:CYS:O	23:o:69:CYS:SG	2.65	0.55
7:O:66:ILE:HD12	7:O:67:CYS:SG	2.46	0.55
2:J:55:VAL:HB	3:K:41:PHE:CE2	2.42	0.55
3:K:93:LEU:HD13	6:N:57:THR:HG21	1.88	0.55
4:L:54:PHE:O	4:L:58:ASN:CA	2.55	0.55
4:L:69:VAL:HG11	4:L:71:MET:HE2	1.89	0.55
4:L:162:THR:O	4:L:166:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:230:HIS:N	4:L:231:PRO:HD3	2.22	0.55
4:L:561:THR:O	4:L:565:SER:HB2	2.07	0.55
25:M:501:3PE:O22	6:N:276:LEU:HD13	2.07	0.55
6:N:224:SER:HB2	6:N:229:SER:HB3	1.89	0.55
6:N:237:THR:O	6:N:237:THR:CG2	2.55	0.55
7:O:135:LEU:HD13	28:O:402:ADP:C6	2.41	0.55
7:O:170:LEU:HG	7:O:179:ILE:HD13	1.87	0.55
8:U:89:LEU:HA	19:k:53:ARG:HH22	1.71	0.55
10:Y:68:ILE:HG21	10:Y:120:MET:HE1	1.87	0.55
6:N:230:ILE:O	6:N:233:LEU:HB2	2.07	0.55
13:e:14:LEU:HD12	13:e:15:ASP:N	2.21	0.55
18:j:97:LEU:O	23:o:104:ARG:NH1	2.39	0.55
2:J:75:THR:OG1	3:K:25:HIS:CD2	2.59	0.55
4:L:441:ILE:HD12	18:j:46:GLU:O	2.06	0.55
26:L:704:CDL:H341	16:h:71:MET:HE1	1.89	0.55
5:M:62:SER:C	5:M:64:PRO:HD2	2.32	0.55
7:O:319:ILE:HG13	7:O:320:GLY:H	1.72	0.55
8:U:120:MET:HE1	22:n:24:LEU:HD12	1.88	0.55
17:i:69:LEU:CD1	17:i:71:ALA:CB	2.85	0.55
4:L:197:GLU:HB2	24:p:111:LYS:HE3	1.88	0.55
5:M:231:LEU:CA	5:M:235:LEU:HD12	2.36	0.55
5:M:453:LEU:HD12	5:M:454:ILE:CG2	2.34	0.55
8:U:83:VAL:O	8:U:87:LEU:HG	2.07	0.55
17:i:83:HIS:HE1	17:i:87:LYS:HD2	1.71	0.55
19:k:30:ILE:CD1	19:k:39:GLN:HB2	2.33	0.55
3:K:45:SER:O	3:K:49:LEU:HG	2.07	0.55
4:L:258:PHE:HE1	4:L:262:ARG:HH21	1.55	0.55
4:L:586:LEU:HD21	10:Y:47:PRO:HD3	1.89	0.55
25:M:503:3PE:C3A	6:N:246:LEU:HD11	2.35	0.55
6:N:273:ASN:HD21	10:Y:143:VAL:HA	1.72	0.55
8:U:79:ILE:HD11	8:U:148:ILE:CG2	2.37	0.55
8:U:125:GLU:OE2	18:j:44:TYR:CE1	2.60	0.55
14:f:56:TRP:CD1	16:h:134:GLU:OE1	2.60	0.55
17:i:108:ASP:OD2	24:p:18:PRO:HB2	2.07	0.55
4:L:381:THR:HG21	4:L:498:PHE:CZ	2.43	0.54
4:L:477:ILE:HG13	23:o:91:GLU:OE1	2.07	0.54
14:f:38:ARG:HH12	14:f:54:VAL:HB	1.71	0.54
14:f:56:TRP:CE3	16:h:131:LYS:HG3	2.41	0.54
2:J:22:LYS:HD2	3:K:23:ARG:CD	2.35	0.54
4:L:54:PHE:O	4:L:58:ASN:HA	2.08	0.54
5:M:415:GLN:O	5:M:416:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:49:THR:HG21	7:O:151:LEU:HG	1.89	0.54
14:f:49:ARG:NH2	16:h:106:ILE:HG22	2.23	0.54
16:h:73:PHE:CD2	16:h:74:TYR:CE1	2.94	0.54
18:j:71:TRP:CZ3	25:j:700:3PE:H3B1	2.42	0.54
23:o:103:GLU:OE2	23:o:106:ARG:HD2	2.07	0.54
2:J:12:PHE:CZ	3:K:42:ILE:HD12	2.42	0.54
4:L:190:SER:HB2	4:L:196:TRP:NE1	2.22	0.54
7:O:63:ASP:OD2	7:O:241:TYR:CE1	2.60	0.54
9:X:158:LEU:HD13	12:d:17:GLU:CG	2.38	0.54
12:d:100:ASP:HB3	16:h:159:LEU:HD21	1.89	0.54
13:e:38:LYS:HG2	16:h:179:ILE:CG2	2.36	0.54
17:i:16:ARG:O	17:i:20:ARG:HG2	2.08	0.54
17:i:69:LEU:CD1	17:i:71:ALA:H	2.18	0.54
2:J:164:PHE:HE2	6:N:4:ILE:HG12	1.73	0.54
4:L:232:TRP:O	4:L:236:ALA:N	2.40	0.54
4:L:385:PHE:CE1	18:j:72:ARG:HG3	2.42	0.54
4:L:551:THR:HA	4:L:555:LEU:HD12	1.89	0.54
5:M:6:LEU:HB3	5:M:7:PRO:HD3	1.88	0.54
5:M:25:THR:HG22	15:g:84:ASN:CG	2.33	0.54
7:O:305:LEU:O	7:O:305:LEU:CD1	2.55	0.54
2:J:60:LEU:HD13	2:J:61:GLY:N	2.21	0.54
3:K:93:LEU:HA	6:N:54:GLU:OE2	2.06	0.54
4:L:131:LEU:CD1	4:L:140:LEU:CD1	2.78	0.54
4:L:362:ILE:HA	4:L:365:ILE:HG13	1.90	0.54
26:L:704:CDL:H211	26:L:704:CDL:H532	1.90	0.54
5:M:423:MET:SD	21:m:59:HIS:NE2	2.81	0.54
8:U:131:PRO:HG2	8:U:134:ASP:HB2	1.90	0.54
4:L:123:LEU:HD21	26:L:704:CDL:H741	1.90	0.54
4:L:232:TRP:CH2	4:L:233:LEU:HD21	2.42	0.54
4:L:539:MET:SD	21:m:11:LEU:HD21	2.48	0.54
5:M:231:LEU:O	5:M:236:LEU:HG	2.06	0.54
6:N:223:ASN:HB3	7:O:306:ASN:HD21	1.73	0.54
7:O:69:GLY:HA2	7:O:72:LYS:HZ3	1.72	0.54
7:O:170:LEU:HG	7:O:179:ILE:CD1	2.37	0.54
7:O:209:VAL:HG23	7:O:214:VAL:HG13	1.88	0.54
15:g:147:LEU:HD21	24:p:163:MET:HB2	1.90	0.54
25:m:201:3PE:H2D2	25:m:201:3PE:H2H1	1.89	0.54
25:L:702:3PE:C2F	6:N:100:MET:HE1	2.38	0.54
5:M:31:SER:HA	5:M:34:ILE:HG12	1.90	0.54
5:M:79:ALA:HB1	5:M:225:ILE:HD13	1.90	0.54
7:O:60:ILE:O	7:O:158:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:237:ILE:HG22	7:O:241:TYR:CE2	2.43	0.54
13:e:83:ARG:HD3	13:e:92:TYR:CD2	2.43	0.54
14:f:37:PHE:CZ	24:p:83:LEU:HD13	2.43	0.54
21:m:8:PRO:HB3	21:m:14:LEU:N	2.23	0.54
21:m:109:ARG:O	21:m:113:GLU:HG2	2.08	0.54
22:n:20:TYR:CE2	22:n:24:LEU:CD1	2.91	0.54
23:o:39:MET:HE1	23:o:57:ASP:O	2.07	0.54
23:o:93:LEU:O	23:o:97:LYS:HG2	2.07	0.54
1:D:58:THR:HG23	1:D:61:TRP:CZ3	2.41	0.54
3:K:1:MET:SD	3:K:50:ASN:ND2	2.77	0.54
4:L:264:HIS:HA	4:L:267:THR:HG23	1.89	0.54
5:M:160:LEU:HD23	5:M:164:LEU:HD13	1.89	0.54
5:M:373:ILE:HD11	5:M:454:ILE:HD11	1.89	0.54
8:U:85:TYR:CE2	18:j:44:TYR:HE2	2.25	0.54
16:h:57:VAL:HG12	22:n:99:VAL:HG21	1.89	0.54
17:i:103:ARG:O	24:p:18:PRO:HG3	2.08	0.54
4:L:247:LEU:HD11	4:L:248:HIS:CE1	2.43	0.54
4:L:427:ILE:HD11	19:k:69:PHE:CE1	2.43	0.54
4:L:507:LEU:O	4:L:510:LYS:HG2	2.07	0.54
5:M:158:ILE:HG21	6:N:283:ALA:HB1	1.90	0.54
5:M:276:CYS:HB3	5:M:285:LEU:HG	1.89	0.54
5:M:283:LYS:HG3	5:M:327:PHE:CE1	2.43	0.54
6:N:307:THR:CG2	6:N:308:ASN:H	2.19	0.54
16:h:57:VAL:HG12	22:n:99:VAL:CG2	2.38	0.54
5:M:1:MET:HE2	5:M:52:PHE:CE2	2.42	0.54
21:m:28:GLU:HG2	21:m:31:ARG:HH22	1.73	0.54
2:J:20:ALA:O	25:K:101:3PE:H242	2.08	0.53
4:L:193:MET:HE1	21:m:125:PHE:CD2	2.43	0.53
4:L:362:ILE:CD1	4:L:430:VAL:CG1	2.82	0.53
8:U:86:VAL:CB	8:U:122:MET:HE1	2.37	0.53
12:d:39:TYR:CE2	12:d:43:LEU:HD11	2.43	0.53
23:o:57:ASP:CG	23:o:59:CYS:H	2.16	0.53
24:p:31:THR:O	24:p:35:LYS:HG3	2.07	0.53
1:D:35:ARG:HH21	15:g:59:PRO:HD3	1.73	0.53
3:K:62:THR:HG23	3:K:66:PHE:CE1	2.43	0.53
4:L:149:ILE:HG21	5:M:364:LEU:CD2	2.38	0.53
5:M:173:THR:HB	16:h:143:GLU:OE2	2.08	0.53
25:M:501:3PE:H342	6:N:280:THR:HG21	1.90	0.53
6:N:179:MET:HE2	6:N:216:PHE:CE1	2.43	0.53
7:O:40:LEU:HG	7:O:292:HIS:CE1	2.44	0.53
17:i:22:TRP:CZ2	22:n:172:THR:HG22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:30:TRP:CD2	22:n:76:HIS:CD2	2.95	0.53
1:D:36:GLN:HE22	5:M:135:ARG:HH22	1.57	0.53
4:L:559:GLU:HG2	4:L:564:LYS:HD3	1.90	0.53
5:M:61:LEU:HD22	5:M:244:ILE:HG21	1.90	0.53
7:O:114:LEU:HA	7:O:131:LEU:HD22	1.91	0.53
7:O:164:TYR:CE1	7:O:195:LEU:HD21	2.43	0.53
7:O:332:ARG:NH1	12:d:50:MET:HE1	2.23	0.53
13:e:38:LYS:NZ	16:h:181:HIS:HD2	2.06	0.53
16:h:55:PHE:HB2	17:i:28:LEU:HD21	1.91	0.53
22:n:125:TRP:CE3	22:n:128:LEU:HD12	2.43	0.53
4:L:226:GLN:OE1	4:L:284:THR:HG21	2.07	0.53
4:L:362:ILE:HD12	4:L:430:VAL:HG13	1.88	0.53
4:L:387:THR:HG22	4:L:465:GLY:N	2.24	0.53
4:L:586:LEU:CD2	10:Y:47:PRO:HD3	2.37	0.53
5:M:263:LEU:HD11	21:m:102:TYR:CD1	2.39	0.53
7:O:140:LEU:HD11	7:O:198:TYR:OH	2.08	0.53
7:O:319:ILE:HG13	7:O:320:GLY:N	2.22	0.53
1:D:51:VAL:HG21	1:D:58:THR:CG2	2.38	0.53
4:L:79:SER:CB	4:L:135:ASN:HB2	2.35	0.53
4:L:400:ASN:HD21	4:L:413:LEU:HD11	1.74	0.53
25:L:701:3PE:H222	20:l:116:ARG:O	2.09	0.53
25:M:503:3PE:H382	6:N:246:LEU:HD11	1.91	0.53
8:U:74:LEU:N	8:U:74:LEU:CD1	2.72	0.53
15:g:106:TYR:CE2	16:h:86:ILE:HD12	2.44	0.53
24:p:103:MET:CE	24:p:135:VAL:HG12	2.38	0.53
2:J:22:LYS:HD2	3:K:23:ARG:HG3	1.80	0.53
4:L:97:THR:HG21	4:L:125:LEU:HD22	1.90	0.53
4:L:124:PHE:HZ	4:L:252:MET:HB2	1.74	0.53
5:M:269:MET:CE	5:M:396:MET:HA	2.36	0.53
12:d:109:TYR:O	12:d:110:ALA:C	2.50	0.53
13:e:40:TRP:CG	13:e:40:TRP:O	2.61	0.53
21:m:17:THR:HB	22:n:68:GLU:OE1	2.08	0.53
4:L:20:LEU:C	4:L:20:LEU:CD1	2.81	0.53
25:L:703:3PE:H382	25:L:703:3PE:H231	1.91	0.53
5:M:55:MET:HG3	5:M:56:PHE:CD2	2.44	0.53
5:M:57:SER:CB	5:M:113:THR:HG22	2.39	0.53
5:M:422:HIS:CE1	21:m:56:ARG:HH22	2.26	0.53
7:O:97:THR:HG22	11:c:32:ARG:HH12	1.73	0.53
10:Y:50:SER:HB3	10:Y:53:GLU:HG2	1.91	0.53
14:f:16:VAL:O	14:f:17:PRO:C	2.49	0.53
16:h:156:VAL:CG1	16:h:160:MET:HE3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:56:ASP:O	22:n:57:MET:C	2.50	0.53
23:o:15:VAL:CG1	23:o:113:LYS:HD3	2.39	0.53
4:L:361:ASN:HA	4:L:431:THR:O	2.09	0.53
5:M:15:THR:HG21	5:M:100:ILE:HD12	1.90	0.53
6:N:120:GLN:HE22	6:N:174:GLN:CB	2.21	0.53
9:X:171:THR:O	9:X:172:VAL:C	2.52	0.53
2:J:68:GLY:HA2	2:J:71:THR:CB	2.39	0.53
4:L:128:MET:CG	4:L:251:THR:HB	2.36	0.53
4:L:450:LEU:HG	4:L:454:ILE:HD12	1.91	0.53
5:M:73:LEU:HD23	5:M:103:GLN:NE2	2.23	0.53
5:M:310:MET:HG3	5:M:455:THR:CA	2.39	0.53
5:M:314:MET:HE1	5:M:380:PHE:CD2	2.44	0.53
5:M:348:LEU:HD12	5:M:415:GLN:NE2	2.24	0.53
5:M:453:LEU:HD12	5:M:453:LEU:C	2.33	0.53
7:O:170:LEU:HD13	7:O:187:TYR:CD2	2.44	0.53
15:g:139:TYR:CD2	15:g:140:PHE:CD1	2.96	0.53
20:l:55:TYR:O	20:l:104:PRO:HG3	2.09	0.53
21:m:18:LEU:HD11	22:n:72:TRP:CG	2.44	0.53
21:m:85:LYS:O	21:m:85:LYS:HG2	2.09	0.53
24:p:142:ARG:O	24:p:143:TYR:CD1	2.62	0.53
5:M:59:ASP:O	5:M:60:PRO:C	2.49	0.53
5:M:213:HIS:O	5:M:217:PRO:HD3	2.09	0.53
5:M:313:THR:HA	5:M:316:MET:HE3	1.89	0.53
5:M:354:LEU:O	5:M:357:THR:N	2.41	0.53
6:N:227:ILE:HA	6:N:230:ILE:CG2	2.38	0.53
15:g:106:TYR:OH	16:h:86:ILE:HD12	2.09	0.53
4:L:108:MET:HB2	4:L:114:ILE:HD13	1.90	0.52
4:L:247:LEU:O	4:L:252:MET:HB3	2.09	0.52
6:N:307:THR:HB	7:O:319:ILE:CG1	2.39	0.52
22:n:39:TYR:CZ	22:n:43:LEU:HD11	2.44	0.52
23:o:116:ALA:O	23:o:119:GLU:HB3	2.09	0.52
3:K:38:LEU:HG	3:K:42:ILE:CD1	2.39	0.52
3:K:89:TYR:HB3	3:K:91:GLN:OE1	2.09	0.52
4:L:400:ASN:HB3	4:L:486:LEU:HD22	1.90	0.52
4:L:480:LEU:HD22	18:j:84:PHE:HD2	1.72	0.52
4:L:536:ILE:HG23	4:L:537:THR:N	2.25	0.52
25:L:703:3PE:C32	25:m:201:3PE:H342	2.30	0.52
5:M:73:LEU:HD21	5:M:100:ILE:HG12	1.91	0.52
5:M:188:ALA:H	5:M:253:LEU:HD11	1.75	0.52
10:Y:141:PRO:HB2	16:h:161:ARG:CZ	2.39	0.52
21:m:103:TYR:HB3	25:m:201:3PE:H112	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:25:HIS:HD2	3:K:88:ASP:OD1	1.91	0.52
4:L:332:HIS:CD2	4:L:336:LYS:HG3	2.44	0.52
4:L:496:LEU:C	4:L:496:LEU:CD1	2.79	0.52
4:L:604:ILE:O	10:Y:5:LYS:HD2	2.09	0.52
27:L:706:PC1:H252	27:L:706:PC1:H341	1.90	0.52
5:M:160:LEU:CD2	5:M:164:LEU:HD13	2.40	0.52
5:M:447:LEU:HD11	5:M:454:ILE:HG23	1.90	0.52
6:N:81:LEU:HD23	13:e:60:PHE:HE1	1.74	0.52
7:O:121:PRO:C	7:O:122:LYS:HG2	2.33	0.52
7:O:310:ILE:HG13	7:O:311:PRO:HD2	1.91	0.52
7:O:336:GLY:N	7:O:344:ASN:ND2	2.56	0.52
10:Y:90:LEU:O	10:Y:91:ASN:C	2.51	0.52
20:l:169:GLU:C	20:l:171:GLY:N	2.55	0.52
3:K:20:LEU:O	4:L:588:PHE:HB3	2.08	0.52
5:M:196:TRP:HE1	5:M:254:THR:HB	1.75	0.52
5:M:403:THR:HA	5:M:406:TYR:CE2	2.44	0.52
6:N:313:MET:HG2	7:O:305:LEU:HD22	1.91	0.52
11:c:47:SER:HB2	12:d:59:HIS:HD2	1.74	0.52
13:e:38:LYS:HG2	16:h:179:ILE:HG23	1.90	0.52
22:n:173:ARG:O	22:n:174:PRO:C	2.52	0.52
3:K:57:MET:N	3:K:58:PRO:HD2	2.24	0.52
3:K:73:VAL:HG21	6:N:38:LEU:HD22	1.90	0.52
4:L:123:LEU:HD22	4:L:150:MET:HG3	1.91	0.52
4:L:427:ILE:HD11	19:k:69:PHE:HE1	1.75	0.52
4:L:446:ASN:HD21	18:j:51:THR:CG2	2.23	0.52
5:M:55:MET:HE1	26:d:201:CDL:H511	1.92	0.52
5:M:84:LEU:HD21	5:M:95:TYR:HB3	1.90	0.52
6:N:10:TYR:O	6:N:13:ILE:HG22	2.09	0.52
6:N:175:MET:HG2	6:N:219:LEU:CD2	2.40	0.52
12:d:1:MET:HG3	12:d:2:MET:N	2.24	0.52
3:K:93:LEU:HD23	6:N:54:GLU:HG2	1.91	0.52
4:L:123:LEU:HD21	26:L:704:CDL:C74	2.40	0.52
4:L:297:ASP:HB3	4:L:300:LYS:CG	2.40	0.52
4:L:441:ILE:HD13	18:j:48:PRO:HD3	1.91	0.52
5:M:68:LEU:HG	5:M:234:ILE:HD11	1.92	0.52
6:N:175:MET:HG2	6:N:219:LEU:HD22	1.91	0.52
7:O:170:LEU:HD13	7:O:187:TYR:CG	2.44	0.52
9:X:172:VAL:HG23	12:d:30:ARG:NH1	2.25	0.52
26:h:201:CDL:H721	17:i:84:TYR:CD2	2.45	0.52
4:L:228:GLY:O	4:L:229:LEU:CG	2.47	0.52
26:L:704:CDL:H111	26:L:704:CDL:H161	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:72:LEU:HD11	5:M:233:ALA:HB1	1.92	0.52
6:N:29:MET:HE2	6:N:141:ILE:HG12	1.92	0.52
13:e:81:LYS:O	13:e:84:GLU:HB3	2.10	0.52
17:i:31:ARG:O	17:i:32:GLU:C	2.51	0.52
17:i:88:TYR:CE2	24:p:49:ARG:HB2	2.44	0.52
4:L:108:MET:HB2	4:L:114:ILE:CD1	2.39	0.52
5:M:346:ARG:O	5:M:419:LEU:HA	2.09	0.52
7:O:172:ALA:HA	7:O:236:ASP:HB3	1.91	0.52
8:U:128:PHE:CE1	8:U:148:ILE:HG23	2.45	0.52
4:L:23:MET:HE3	26:L:704:CDL:H522	1.92	0.52
4:L:324:LEU:HB3	4:L:395:ILE:HD11	1.90	0.52
25:L:703:3PE:C23	25:m:201:3PE:H3B1	2.39	0.52
5:M:115:LEU:HD21	5:M:176:LEU:CD2	2.37	0.52
5:M:171:VAL:HG11	5:M:179:LEU:CD2	2.35	0.52
7:O:326:ARG:NH2	15:g:56:ASP:OD1	2.43	0.52
8:U:133:ILE:HG23	8:U:134:ASP:N	2.25	0.52
13:e:69:ARG:HG3	13:e:72:THR:OG1	2.10	0.52
22:n:37:TYR:C	22:n:39:TYR:N	2.67	0.52
22:n:168:TRP:HD1	22:n:169:HIS:CE1	2.27	0.52
4:L:533:ILE:HG23	4:L:534:HIS:HD2	1.74	0.52
5:M:103:GLN:O	5:M:107:ILE:HB	2.10	0.52
5:M:139:GLN:HB3	5:M:222:GLU:CG	2.40	0.52
5:M:168:GLN:O	5:M:172:GLY:N	2.43	0.52
7:O:121:PRO:HB3	7:O:178:TYR:CE1	2.45	0.52
10:Y:19:GLN:HE21	10:Y:22:ARG:HB2	1.75	0.52
20:l:156:VAL:HG11	23:o:95:TYR:CE1	2.43	0.52
2:J:60:LEU:CD1	2:J:61:GLY:N	2.72	0.51
3:K:1:MET:SD	6:N:79:LYS:HD2	2.50	0.51
4:L:52:LEU:HB2	24:p:30:ILE:HD11	1.91	0.51
4:L:286:LEU:HG	4:L:290:ILE:CD1	2.40	0.51
4:L:386:LEU:HD11	18:j:69:ILE:HD11	1.92	0.51
6:N:338:PRO:HG3	26:d:201:CDL:H611	1.92	0.51
10:Y:17:GLY:O	10:Y:81:GLN:HG2	2.09	0.51
12:d:87:ASP:O	12:d:88:HIS:C	2.50	0.51
13:e:44:ALA:HA	13:e:47:ILE:HG12	1.92	0.51
18:j:98:GLY:O	18:j:100:PRO:HD3	2.11	0.51
19:k:49:ASP:OD2	22:n:38:ARG:HG3	2.10	0.51
24:p:164:LEU:O	24:p:168:LYS:N	2.42	0.51
3:K:59:ILE:O	3:K:60:PRO:C	2.49	0.51
4:L:569:LEU:O	4:L:573:MET:HG2	2.11	0.51
6:N:168:GLY:O	6:N:172:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:LEU:HB3	4:L:50:PRO:HD3	1.91	0.51
4:L:202:MET:CE	4:L:265:PRO:HG3	2.32	0.51
5:M:173:THR:HG22	16:h:150:ARG:NH1	2.25	0.51
5:M:388:TRP:CD1	21:m:109:ARG:HD2	2.46	0.51
7:O:204:VAL:HG21	7:O:255:VAL:HG22	1.90	0.51
12:d:62:LEU:O	12:d:66:THR:OG1	2.22	0.51
17:i:77:ILE:HD13	17:i:80:TRP:CZ3	2.46	0.51
22:n:143:GLU:O	22:n:143:GLU:HG2	2.10	0.51
3:K:1:MET:H3	3:K:2:PRO:HD2	1.74	0.51
5:M:129:THR:CG2	5:M:235:LEU:HD11	2.40	0.51
5:M:154:LEU:HD22	6:N:287:LEU:HD21	1.93	0.51
5:M:251:ASP:N	5:M:252:PRO:HD2	2.26	0.51
6:N:240:MET:HE2	6:N:326:PHE:CZ	2.45	0.51
10:Y:143:VAL:HG21	16:h:169:TYR:CE2	2.45	0.51
14:f:37:PHE:HA	14:f:40:LYS:HB2	1.93	0.51
5:M:177:MET:CE	16:h:140:LEU:HD21	2.41	0.51
7:O:132:GLN:CD	28:O:402:ADP:HN62	2.19	0.51
9:X:168:PHE:C	9:X:169:PHE:CD1	2.88	0.51
16:h:52:LYS:O	16:h:53:ARG:C	2.53	0.51
20:l:151:PRO:HD2	23:o:9:TYR:OH	2.10	0.51
23:o:89:TYR:O	23:o:90:CYS:C	2.52	0.51
2:J:61:GLY:O	2:J:65:VAL:HG11	2.08	0.51
3:K:66:PHE:CE2	6:N:31:VAL:HB	2.46	0.51
4:L:161:ARG:NE	4:L:163:ASP:HB2	2.26	0.51
4:L:530:PRO:O	4:L:534:HIS:HB2	2.11	0.51
4:L:595:ILE:O	4:L:599:ILE:HG13	2.11	0.51
5:M:11:LEU:O	5:M:15:THR:HG23	2.10	0.51
5:M:31:SER:HA	5:M:34:ILE:CG1	2.41	0.51
5:M:201:MET:HG2	25:M:501:3PE:H3B1	1.91	0.51
8:U:79:ILE:HG13	8:U:126:PHE:CE2	2.45	0.51
17:i:10:LEU:HA	17:i:13:GLN:HB3	1.91	0.51
17:i:83:HIS:CE1	17:i:87:LYS:HD2	2.46	0.51
17:i:85:TYR:CE2	17:i:90:MET:HE3	2.46	0.51
4:L:60:GLU:HG3	4:L:83:ASP:HA	1.93	0.51
5:M:20:PRO:HB3	5:M:89:ASN:ND2	2.25	0.51
5:M:336:ARG:HH12	5:M:433:GLU:CD	2.19	0.51
17:i:70:PHE:O	17:i:73:SER:HB2	2.10	0.51
19:k:34:PRO:HD2	19:k:59:TYR:CG	2.46	0.51
3:K:93:LEU:HD22	6:N:54:GLU:HG2	1.93	0.51
4:L:66:TRP:CZ3	4:L:68:TRP:CD1	2.96	0.51
4:L:536:ILE:HD11	4:L:540:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:45:ILE:HA	6:N:52:SER:OG	2.11	0.51
7:O:289:TRP:HA	7:O:289:TRP:CE3	2.46	0.51
8:U:84:LEU:HD11	8:U:100:VAL:HG12	1.93	0.51
12:d:28:ASP:O	12:d:29:PRO:C	2.53	0.51
1:D:47:PHE:CE2	6:N:305:PHE:HZ	2.28	0.51
2:J:104:CYS:HA	2:J:107:ASN:CG	2.36	0.51
4:L:383:MET:CB	4:L:386:LEU:HD12	2.30	0.51
4:L:451:MET:O	4:L:452:ASN:C	2.53	0.51
4:L:563:PRO:HG3	5:M:152:TYR:OH	2.10	0.51
5:M:304:GLN:HA	5:M:309:PHE:CE1	2.45	0.51
6:N:321:LYS:HD2	12:d:49:ARG:NE	2.26	0.51
14:f:41:SER:O	14:f:45:GLN:HB2	2.11	0.51
16:h:73:PHE:CE2	16:h:74:TYR:CE1	2.98	0.51
16:h:159:LEU:HD23	16:h:163:ARG:HH12	1.75	0.51
4:L:141:PHE:CD2	5:M:370:PRO:CG	2.94	0.51
4:L:598:ILE:HG21	6:N:100:MET:HE2	1.93	0.51
25:L:703:3PE:H361	25:L:703:3PE:H222	1.93	0.51
26:L:705:CDL:H351	10:Y:114:ALA:CB	2.37	0.51
5:M:354:LEU:O	5:M:355:MET:C	2.52	0.51
8:U:89:LEU:HA	19:k:53:ARG:NH2	2.25	0.51
10:Y:14:VAL:HG13	10:Y:15:PRO:HD2	1.93	0.51
12:d:108:THR:HG23	12:d:110:ALA:HB3	1.93	0.51
18:j:97:LEU:HB3	23:o:104:ARG:CB	2.25	0.51
24:p:113:CYS:O	24:p:113:CYS:SG	2.69	0.51
4:L:362:ILE:CD1	4:L:430:VAL:HG13	2.41	0.50
4:L:404:THR:HG22	4:L:405:ASN:H	1.75	0.50
5:M:249:ILE:HG22	5:M:250:LEU:N	2.26	0.50
5:M:275:ILE:CD1	5:M:288:TYR:CG	2.84	0.50
8:U:86:VAL:HG13	19:k:54:ASN:ND2	2.26	0.50
10:Y:83:ARG:HH12	10:Y:90:LEU:HB3	1.76	0.50
11:c:72:ARG:HD2	12:d:20:SER:CA	2.40	0.50
15:g:115:TRP:HA	15:g:118:ARG:HH11	1.75	0.50
4:L:173:LEU:HD23	25:L:701:3PE:C32	2.30	0.50
4:L:349:SER:HB2	4:L:443:ILE:HG23	1.93	0.50
5:M:4:ILE:HD11	5:M:41:LEU:HD21	1.92	0.50
5:M:158:ILE:CG1	6:N:287:LEU:HD11	2.41	0.50
6:N:36:SER:HB2	6:N:134:GLN:HE22	1.76	0.50
7:O:182:GLN:O	7:O:183:CYS:C	2.54	0.50
8:U:74:LEU:CD1	8:U:74:LEU:H	2.24	0.50
8:U:122:MET:HA	8:U:122:MET:HE2	1.91	0.50
11:c:32:ARG:HB2	11:c:32:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:49:ARG:O	24:p:52:ILE:HB	2.11	0.50
1:D:54:PRO:HB2	1:D:59:ALA:HB2	1.94	0.50
4:L:21:ILE:HG12	4:L:27:ILE:HG23	1.93	0.50
4:L:145:GLU:CG	5:M:370:PRO:HD3	2.42	0.50
4:L:395:ILE:O	4:L:399:ILE:HG13	2.11	0.50
4:L:424:MET:HE2	4:L:502:LEU:HA	1.93	0.50
5:M:294:MET:HE3	5:M:319:HIS:HD2	1.76	0.50
5:M:370:PRO:CA	5:M:375:LEU:HD22	2.40	0.50
6:N:175:MET:O	6:N:179:MET:HG2	2.12	0.50
6:N:248:LEU:CD1	6:N:296:LEU:HD23	2.41	0.50
10:Y:57:ARG:HG2	10:Y:60:ARG:NH2	2.27	0.50
11:c:46:LEU:O	11:c:50:ALA:HB2	2.12	0.50
15:g:74:TYR:CE2	15:g:85:MET:HB3	2.47	0.50
20:l:87:ASP:OD1	20:l:88:PRO:HD2	2.11	0.50
2:J:164:PHE:HD2	6:N:5:THR:HA	1.77	0.50
4:L:117:PHE:HE1	4:L:243:VAL:CG2	2.24	0.50
4:L:365:ILE:CD1	4:L:366:MET:HE2	2.42	0.50
5:M:118:PHE:O	5:M:122:PHE:HB2	2.11	0.50
5:M:309:PHE:HB2	5:M:458:THR:HG21	1.93	0.50
23:o:71:ARG:HB3	23:o:71:ARG:NH1	2.27	0.50
24:p:5:TRP:HZ3	24:p:10:TYR:O	1.94	0.50
1:D:55:SER:HB3	1:D:58:THR:HB	1.94	0.50
4:L:109:HIS:O	4:L:110:SER:HB2	2.11	0.50
8:U:79:ILE:HG23	8:U:145:VAL:HG13	1.91	0.50
13:e:69:ARG:O	13:e:73:MET:HG3	2.11	0.50
19:k:34:PRO:CG	19:k:59:TYR:CD1	2.94	0.50
2:J:9:SER:HB3	3:K:7:ASN:HB2	1.93	0.50
2:J:98:MET:O	2:J:102:LEU:HG	2.11	0.50
4:L:336:LYS:O	4:L:340:PHE:CD2	2.65	0.50
5:M:328:CYS:SG	5:M:436:LEU:HD21	2.52	0.50
25:M:503:3PE:HN2	7:O:338:LYS:HE2	1.77	0.50
6:N:189:TRP:HB2	6:N:204:ASN:HD21	1.77	0.50
8:U:90:TYR:HD2	8:U:93:ILE:H	1.59	0.50
15:g:106:TYR:OH	16:h:86:ILE:HG23	2.12	0.50
17:i:10:LEU:HD12	17:i:13:GLN:HB3	1.94	0.50
19:k:55:GLU:OE1	22:n:38:ARG:HB2	2.12	0.50
20:l:49:ALA:HA	20:l:59:VAL:HG13	1.93	0.50
20:l:108:ASP:HB3	20:l:111:MET:HE2	1.92	0.50
20:l:119:THR:HG23	21:m:11:LEU:HA	1.92	0.50
3:K:1:MET:HA	3:K:4:THR:HB	1.94	0.50
4:L:141:PHE:CD2	5:M:370:PRO:CB	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:193:MET:CE	21:m:125:PHE:CD2	2.94	0.50
4:L:354:GLN:O	4:L:354:GLN:HG2	2.12	0.50
4:L:589:MET:O	4:L:592:LEU:N	2.45	0.50
7:O:352:ILE:HG21	12:d:52:PRO:HG2	1.94	0.50
8:U:142:GLN:O	8:U:145:VAL:N	2.43	0.50
26:h:201:CDL:H132	26:h:201:CDL:H172	1.92	0.50
22:n:114:MET:O	22:n:115:TYR:C	2.52	0.50
23:o:114:ARG:HG3	23:o:115:ARG:N	2.27	0.50
4:L:60:GLU:O	4:L:61:TYR:CD1	2.65	0.50
5:M:63:THR:N	5:M:64:PRO:HD2	2.27	0.50
5:M:432:ARG:HA	5:M:435:THR:HG22	1.94	0.50
6:N:258:THR:HG23	6:N:336:THR:HG22	1.93	0.50
7:O:136:TYR:OH	7:O:191:LYS:HA	2.11	0.50
10:Y:12:HIS:NE2	10:Y:127:PHE:HZ	2.09	0.50
18:j:84:PHE:HE2	23:o:88:ASP:HB3	1.77	0.50
21:m:91:ALA:HB2	25:m:202:3PE:H272	1.93	0.50
21:m:124:LYS:HE2	21:m:125:PHE:CE2	2.47	0.50
4:L:123:LEU:CD2	4:L:150:MET:HG3	2.42	0.50
4:L:302:ILE:CB	4:L:340:PHE:CE1	2.95	0.50
4:L:357:ARG:NH1	22:n:78:GLN:O	2.45	0.50
5:M:248:ILE:HG13	5:M:249:ILE:N	2.26	0.50
6:N:175:MET:HE1	6:N:227:ILE:HG22	1.94	0.50
6:N:190:MET:HB3	6:N:201:THR:HG23	1.94	0.50
10:Y:114:ALA:HB2	25:m:202:3PE:H231	1.94	0.50
2:J:55:VAL:HG13	2:J:56:PHE:H	1.77	0.49
3:K:38:LEU:HG	3:K:42:ILE:HD11	1.93	0.49
4:L:14:LEU:HD21	17:i:74:HIS:O	2.12	0.49
25:L:703:3PE:H222	25:L:703:3PE:H332	1.94	0.49
5:M:184:HIS:CD2	5:M:249:ILE:HG23	2.47	0.49
5:M:441:MET:HG3	5:M:445:ILE:HD12	1.94	0.49
6:N:133:TRP:CG	6:N:133:TRP:O	2.63	0.49
7:O:276:LEU:HD11	7:O:278:TYR:CE2	2.47	0.49
7:O:319:ILE:HD12	7:O:324:GLY:HA3	1.94	0.49
10:Y:141:PRO:HB2	16:h:161:ARG:HH11	1.77	0.49
4:L:142:ILE:HA	5:M:370:PRO:CB	2.42	0.49
4:L:393:ASP:OD1	4:L:393:ASP:C	2.56	0.49
5:M:122:PHE:CE1	5:M:238:LEU:HG	2.46	0.49
6:N:62:THR:HG21	6:N:114:TRP:CD1	2.47	0.49
13:e:45:HIS:CD2	16:h:176:LYS:HD3	2.47	0.49
16:h:96:ALA:O	24:p:63:TYR:HE1	1.94	0.49
4:L:578:THR:HG21	6:N:168:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:88:ASN:O	5:M:89:ASN:HB3	2.12	0.49
5:M:166:LEU:CD1	25:M:501:3PE:H11	2.41	0.49
5:M:207:MET:SD	5:M:240:SER:HA	2.52	0.49
6:N:313:MET:HG3	7:O:305:LEU:CD2	2.41	0.49
7:O:170:LEU:HD21	7:O:184:VAL:HG22	1.95	0.49
7:O:351:TRP:HB3	11:c:39:PRO:HG3	1.94	0.49
25:j:700:3PE:C3B	23:o:78:LEU:HD13	2.40	0.49
22:n:96:CYS:SG	22:n:97:TYR:CZ	3.05	0.49
22:n:163:LEU:O	22:n:164:PRO:C	2.54	0.49
24:p:74:ILE:O	24:p:75:THR:C	2.54	0.49
2:J:59:TYR:HH	3:K:34:GLU:C	2.19	0.49
4:L:217:LEU:HD13	4:L:273:ILE:HG23	1.94	0.49
4:L:399:ILE:HG22	4:L:409:LEU:HD13	1.93	0.49
4:L:542:LEU:CD2	20:l:116:ARG:HD2	2.43	0.49
5:M:285:LEU:HD22	5:M:410:MET:SD	2.53	0.49
5:M:348:LEU:HD12	5:M:415:GLN:HE22	1.77	0.49
25:M:502:3PE:O22	26:h:201:CDL:H141	2.13	0.49
6:N:230:ILE:HG21	6:N:296:LEU:HD11	1.94	0.49
12:d:11:LEU:HB2	13:e:9:LYS:HB2	1.94	0.49
17:i:90:MET:O	17:i:91:ALA:C	2.53	0.49
4:L:439:PRO:HA	19:k:57:TRP:CZ2	2.47	0.49
4:L:445:GLU:CB	4:L:450:LEU:HD23	2.37	0.49
5:M:139:GLN:HG3	5:M:140:THR:N	2.27	0.49
5:M:420:THR:HG21	5:M:423:MET:HG2	1.93	0.49
7:O:143:TYR:CZ	7:O:164:TYR:HE2	2.30	0.49
7:O:354:LEU:HD21	11:c:44:VAL:HG11	1.94	0.49
9:X:165:THR:OG1	9:X:172:VAL:HG11	2.12	0.49
12:d:109:TYR:HB3	24:p:156:LEU:HD21	1.94	0.49
4:L:316:THR:CG2	4:L:325:ALA:CB	2.89	0.49
5:M:131:ILE:HD12	6:N:302:LEU:HD21	1.93	0.49
6:N:231:SER:HA	6:N:300:THR:HA	1.93	0.49
15:g:53:TRP:H	15:g:53:TRP:HE3	1.58	0.49
26:h:201:CDL:C17	25:i:201:3PE:H372	2.36	0.49
20:l:81:ARG:HD3	20:l:85:GLU:OE2	2.13	0.49
4:L:67:HIS:HE2	4:L:69:VAL:C	2.20	0.49
4:L:183:ILE:HD13	5:M:400:ILE:HD13	1.94	0.49
4:L:296:ASN:OD1	4:L:357:ARG:NH1	2.45	0.49
4:L:405:ASN:OD1	20:l:148:HIS:CE1	2.66	0.49
4:L:477:ILE:HG13	23:o:91:GLU:OE2	2.13	0.49
5:M:193:ASN:HA	5:M:253:LEU:HD23	1.94	0.49
5:M:248:ILE:CG1	5:M:249:ILE:HD12	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:260:SER:O	7:O:263:ALA:HB3	2.13	0.49
15:g:121:GLU:OE2	24:p:10:TYR:CZ	2.66	0.49
16:h:111:GLU:O	24:p:63:TYR:HA	2.12	0.49
20:l:88:PRO:HB2	22:n:86:PRO:HB2	1.94	0.49
21:m:50:GLN:O	21:m:60:ILE:HD11	2.13	0.49
22:n:145:SER:HB2	22:n:146:PRO:HD2	1.94	0.49
2:J:68:GLY:O	2:J:71:THR:N	2.46	0.49
2:J:76:GLU:HG2	2:J:76:GLU:O	2.12	0.49
4:L:496:LEU:HA	4:L:499:LEU:HB2	1.94	0.49
5:M:114:GLU:HG3	9:X:169:PHE:HB3	1.95	0.49
5:M:227:GLY:HA2	5:M:230:ILE:HG22	1.95	0.49
8:U:133:ILE:CD1	22:n:7:PRO:HD3	2.42	0.49
11:c:62:HIS:O	11:c:66:VAL:HG23	2.12	0.49
21:m:129:TYR:HE2	24:p:146:LEU:O	1.95	0.49
22:n:20:TYR:OH	22:n:45:ARG:HB2	2.12	0.49
25:D:501:3PE:H3A2	5:M:155:ILE:HD13	1.94	0.49
2:J:99:GLU:HA	2:J:102:LEU:HD12	1.93	0.49
4:L:68:TRP:CE3	4:L:76:LEU:HD21	2.47	0.49
4:L:264:HIS:HA	4:L:267:THR:OG1	2.13	0.49
4:L:316:THR:HG23	4:L:325:ALA:CB	2.32	0.49
5:M:4:ILE:HG22	5:M:107:ILE:CD1	2.32	0.49
5:M:5:ILE:HG13	5:M:6:LEU:N	2.28	0.49
5:M:51:ASN:ND2	16:h:136:THR:HG23	2.27	0.49
5:M:178:ILE:HG12	24:p:82:VAL:HG11	1.94	0.49
15:g:140:PHE:HZ	24:p:152:ALA:HB1	1.78	0.49
22:n:114:MET:HG3	22:n:115:TYR:HD2	1.78	0.49
2:J:150:TRP:CD1	6:N:28:LEU:HD21	2.47	0.49
4:L:511:LEU:HD12	22:n:36:LYS:HA	1.94	0.49
25:L:703:3PE:H2	25:L:703:3PE:HN1	1.77	0.49
5:M:348:LEU:HB2	5:M:415:GLN:OE1	2.13	0.49
6:N:335:MET:CB	26:d:201:CDL:H642	2.43	0.49
7:O:78:ALA:HB2	7:O:85:HIS:HB2	1.95	0.49
8:U:118:ILE:O	8:U:119:ILE:C	2.55	0.49
9:X:168:PHE:O	9:X:170:TRP:NE1	2.45	0.49
20:l:101:TRP:HE1	21:m:62:ASP:HA	1.77	0.49
20:l:167:TYR:OH	20:l:176:LYS:O	2.14	0.49
21:m:75:ASN:OD1	21:m:79:ASN:ND2	2.46	0.49
22:n:81:ILE:HD12	22:n:87:GLY:O	2.12	0.49
1:D:35:ARG:HE	15:g:59:PRO:HD2	1.77	0.48
4:L:227:PHE:CD2	4:L:283:LEU:HD23	2.48	0.48
5:M:1:MET:HB2	5:M:52:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:216:LEU:HD12	5:M:236:LEU:CD2	2.38	0.48
7:O:135:LEU:HD13	28:O:402:ADP:C5	2.48	0.48
11:c:72:ARG:NH1	12:d:19:ARG:HD3	2.28	0.48
15:g:109:ASP:HB2	15:g:114:GLU:HB3	1.94	0.48
21:m:45:ARG:CZ	22:n:140:LEU:HD11	2.43	0.48
21:m:122:ASP:O	21:m:123:ARG:C	2.53	0.48
1:D:36:GLN:HG3	1:D:38:GLN:HE21	1.78	0.48
3:K:19:THR:HG23	3:K:29:THR:CG2	2.43	0.48
4:L:41:LYS:HG3	4:L:98:TRP:CH2	2.44	0.48
4:L:101:MET:HE1	4:L:121:LEU:CB	2.43	0.48
4:L:144:TRP:HH2	4:L:256:GLY:HA2	1.78	0.48
4:L:350:LEU:HD23	4:L:443:ILE:HD11	1.96	0.48
4:L:556:ILE:HG23	21:m:80:PHE:CZ	2.47	0.48
5:M:134:THR:O	5:M:142:ARG:CD	2.59	0.48
8:U:90:TYR:CD1	19:k:51:TRP:CE2	3.01	0.48
23:o:42:THR:O	23:o:43:GLN:C	2.56	0.48
4:L:361:ASN:O	4:L:361:ASN:CG	2.54	0.48
4:L:372:CYS:SG	4:L:454:ILE:HG22	2.54	0.48
4:L:390:TYR:CE2	18:j:68:TRP:HH2	2.32	0.48
5:M:59:ASP:OD1	5:M:245:ARG:NH2	2.47	0.48
5:M:311:GLY:HA2	5:M:314:MET:CE	2.42	0.48
6:N:31:VAL:HB	6:N:35:PHE:CE2	2.48	0.48
9:X:151:ASN:CG	13:e:51:ARG:HH11	2.21	0.48
10:Y:68:ILE:HG12	10:Y:102:THR:OG1	2.13	0.48
16:h:73:PHE:O	16:h:77:LEU:N	2.46	0.48
19:k:41:LYS:C	19:k:43:ALA:N	2.64	0.48
22:n:44:MET:O	22:n:45:ARG:C	2.53	0.48
22:n:51:HIS:HB3	22:n:63:LEU:HD13	1.95	0.48
23:o:8:ARG:HB2	23:o:16:GLU:CG	2.23	0.48
4:L:74:MET:HE3	5:M:307:TRP:HH2	1.78	0.48
4:L:141:PHE:HD1	4:L:182:PHE:CD2	2.31	0.48
4:L:316:THR:HG21	4:L:325:ALA:HA	1.94	0.48
4:L:402:CYS:SG	4:L:403:ASN:N	2.87	0.48
26:L:704:CDL:OB7	26:L:704:CDL:HB32	2.13	0.48
5:M:25:THR:HG22	15:g:84:ASN:OD1	2.13	0.48
5:M:166:LEU:HD21	5:M:170:HIS:CE1	2.48	0.48
5:M:313:THR:HA	5:M:316:MET:CE	2.43	0.48
11:c:70:LYS:O	11:c:75:LEU:HA	2.12	0.48
13:e:47:ILE:HG13	13:e:47:ILE:O	2.12	0.48
13:e:83:ARG:HD3	13:e:92:TYR:CE2	2.48	0.48
16:h:62:TYR:N	22:n:111:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:47:LEU:CD1	22:n:43:LEU:HD23	2.43	0.48
2:J:24:SER:O	2:J:28:GLY:N	2.44	0.48
4:L:296:ASN:ND2	4:L:425:ARG:HH21	2.12	0.48
4:L:424:MET:HE2	4:L:502:LEU:CA	2.43	0.48
5:M:127:ILE:CD1	6:N:256:PRO:HG2	2.42	0.48
6:N:146:TYR:CE1	6:N:198:PRO:HG2	2.48	0.48
6:N:227:ILE:CA	6:N:230:ILE:HG22	2.38	0.48
8:U:94:ASP:OD1	8:U:95:PRO:HD2	2.13	0.48
16:h:73:PHE:HE2	16:h:74:TYR:HE1	1.62	0.48
20:l:48:ARG:CZ	20:l:64:PRO:HD2	2.44	0.48
24:p:5:TRP:CZ3	24:p:10:TYR:O	2.66	0.48
3:K:21:MET:HB2	25:K:101:3PE:H231	1.94	0.48
4:L:319:MET:O	4:L:319:MET:HG2	2.13	0.48
4:L:433:THR:HG21	4:L:436:ARG:NH2	2.29	0.48
5:M:42:LEU:HG	5:M:67:ILE:CD1	2.42	0.48
5:M:123:GLU:CG	6:N:255:PRO:HG2	2.43	0.48
6:N:4:ILE:HG23	6:N:5:THR:N	2.29	0.48
11:c:57:TYR:HD2	12:d:70:PHE:CZ	2.30	0.48
17:i:14:GLN:HE22	22:n:157:ALA:HB3	1.79	0.48
22:n:144:THR:HG23	22:n:144:THR:O	2.13	0.48
22:n:155:PRO:HG2	22:n:165:PRO:HG2	1.95	0.48
4:L:149:ILE:CG2	5:M:364:LEU:HD21	2.43	0.48
4:L:197:GLU:HG3	24:p:111:LYS:HE2	1.94	0.48
4:L:274:LEU:O	4:L:277:MET:HG2	2.14	0.48
4:L:496:LEU:HD12	4:L:497:GLY:CA	2.44	0.48
5:M:6:LEU:HD21	14:f:22:PHE:HD2	1.79	0.48
5:M:307:TRP:CE3	5:M:383:MET:CE	2.97	0.48
17:i:22:TRP:CE3	22:n:172:THR:HG22	2.49	0.48
20:l:167:TYR:HD2	20:l:168:LEU:CD1	2.19	0.48
23:o:87:TRP:NE1	23:o:91:GLU:OE1	2.45	0.48
1:D:42:GLU:HA	1:D:45:GLU:HG2	1.96	0.48
2:J:5:ILE:CG2	3:K:4:THR:HG21	2.44	0.48
3:K:22:PHE:HZ	6:N:61:VAL:HG11	1.79	0.48
4:L:186:MET:HE1	5:M:379:LEU:HD21	1.96	0.48
4:L:389:PHE:CZ	18:j:79:ALA:HB1	2.48	0.48
5:M:269:MET:HE3	5:M:399:ASN:HB3	1.96	0.48
5:M:422:HIS:CE1	5:M:425:ASN:OD1	2.67	0.48
6:N:307:THR:CB	7:O:319:ILE:HD11	2.37	0.48
7:O:76:GLU:HB2	7:O:266:PRO:HB3	1.95	0.48
7:O:76:GLU:O	7:O:77:ILE:C	2.57	0.48
8:U:128:PHE:HZ	8:U:148:ILE:HD12	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:41:LYS:O	19:k:42:LEU:C	2.50	0.48
19:k:69:PHE:CE1	19:k:73:ILE:HD11	2.48	0.48
3:K:29:THR:O	3:K:30:LEU:C	2.54	0.48
5:M:177:MET:HE2	16:h:140:LEU:HD21	1.96	0.48
25:M:503:3PE:H231	12:d:47:MET:HE1	1.95	0.48
6:N:82:GLY:HA3	13:e:21:LEU:HG	1.96	0.48
6:N:308:ASN:HB3	7:O:317:ILE:HG22	1.96	0.48
12:d:119:VAL:O	12:d:120:ARG:C	2.55	0.48
17:i:90:MET:SD	17:i:97:ILE:HD11	2.54	0.48
20:l:48:ARG:HH21	20:l:63:GLU:HA	1.78	0.48
1:D:35:ARG:HE	15:g:59:PRO:HD3	1.77	0.48
2:J:18:GLY:O	2:J:23:PRO:HD3	2.14	0.48
4:L:152:PHE:HE1	5:M:412:ILE:HD11	1.79	0.48
5:M:94:LEU:O	5:M:98:MET:HG2	2.14	0.48
5:M:310:MET:CE	5:M:459:MET:SD	3.02	0.48
6:N:189:TRP:CZ3	6:N:282:MET:HE3	2.49	0.48
7:O:314:LEU:HD12	7:O:315:PRO:HD3	1.93	0.48
18:j:45:ARG:HD3	19:k:57:TRP:CD1	2.49	0.48
19:k:52:ALA:O	19:k:53:ARG:C	2.56	0.48
20:l:184:TYR:CD1	23:o:36:GLU:CA	2.97	0.48
21:m:124:LYS:C	21:m:126:ASN:N	2.70	0.48
22:n:37:TYR:O	22:n:39:TYR:N	2.47	0.48
2:J:65:VAL:O	2:J:66:VAL:C	2.54	0.47
4:L:554:ASP:OD2	5:M:213:HIS:HE1	1.97	0.47
26:L:705:CDL:H342	10:Y:115:MET:HG3	1.95	0.47
5:M:192:ASN:C	5:M:194:LEU:N	2.72	0.47
25:M:501:3PE:H321	25:M:501:3PE:C21	2.44	0.47
8:U:102:SER:C	8:U:141:PRO:HD3	2.39	0.47
18:j:44:TYR:CG	19:k:22:LEU:HD22	2.49	0.47
19:k:42:LEU:HG	22:n:39:TYR:CD1	2.49	0.47
21:m:45:ARG:NE	22:n:140:LEU:HD11	2.29	0.47
22:n:81:ILE:HD11	22:n:87:GLY:O	2.14	0.47
22:n:156:PRO:HD2	22:n:158:ARG:NH1	2.29	0.47
23:o:22:ILE:HD12	23:o:102:PHE:HD1	1.79	0.47
23:o:111:ARG:HG2	23:o:115:ARG:HG3	1.96	0.47
2:J:102:LEU:O	2:J:105:VAL:HB	2.14	0.47
3:K:12:PHE:CD1	6:N:72:LEU:HD22	2.49	0.47
4:L:31:ASN:HD22	4:L:34:LEU:HB2	1.79	0.47
4:L:54:PHE:CZ	4:L:84:PHE:HB2	2.49	0.47
26:L:705:CDL:H312	10:Y:115:MET:SD	2.54	0.47
12:d:8:HIS:O	12:d:10:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:84:PHE:CZ	19:k:88:LEU:HD22	2.49	0.47
2:J:66:VAL:O	2:J:69:TYR:HB3	2.14	0.47
2:J:104:CYS:HA	2:J:107:ASN:ND2	2.29	0.47
3:K:36:MET:HE3	6:N:68:MET:HG3	1.96	0.47
4:L:3:ILE:HG22	4:L:49:LEU:HD21	1.96	0.47
4:L:121:LEU:HD22	4:L:246:LEU:CD2	2.24	0.47
4:L:482:MET:HE2	4:L:486:LEU:HB3	1.96	0.47
4:L:483:PRO:HG2	4:L:486:LEU:HD12	1.96	0.47
27:L:706:PC1:H2D2	27:L:706:PC1:H371	1.96	0.47
5:M:176:LEU:HD13	5:M:245:ARG:HH11	1.79	0.47
25:M:503:3PE:H3I1	25:M:503:3PE:H2G1	1.96	0.47
7:O:242:LYS:O	7:O:247:PRO:HD3	2.14	0.47
7:O:341:PRO:HB2	11:c:34:PRO:HB3	1.95	0.47
17:i:79:MET:O	17:i:80:TRP:C	2.57	0.47
2:J:170:THR:O	2:J:171:ARG:C	2.57	0.47
4:L:277:MET:SD	4:L:318:GLY:HA2	2.54	0.47
4:L:433:THR:CG2	4:L:434:LYS:N	2.78	0.47
25:L:703:3PE:H231	25:L:703:3PE:H361	1.96	0.47
6:N:1:MET:HE1	6:N:43:MET:SD	2.54	0.47
6:N:89:GLN:H	6:N:89:GLN:CD	2.22	0.47
7:O:116:LYS:HA	7:O:119:ASP:OD1	2.13	0.47
7:O:343:TYR:CE1	7:O:355:LYS:CB	2.96	0.47
7:O:350:LYS:O	7:O:351:TRP:HB2	2.13	0.47
14:f:37:PHE:O	14:f:38:ARG:C	2.57	0.47
23:o:15:VAL:HB	23:o:110:GLN:HG2	1.96	0.47
24:p:6:ASP:C	24:p:8:ASP:N	2.69	0.47
1:D:36:GLN:HA	5:M:138:ASN:HA	1.97	0.47
2:J:24:SER:HB2	2:J:27:TYR:CD2	2.28	0.47
2:J:59:TYR:OH	3:K:34:GLU:O	2.29	0.47
3:K:69:CYS:O	3:K:70:GLU:C	2.57	0.47
4:L:390:TYR:HE2	18:j:68:TRP:CH2	2.33	0.47
4:L:474:PRO:HD2	23:o:67:LEU:HD21	1.96	0.47
4:L:513:MET:SD	22:n:36:LYS:NZ	2.86	0.47
4:L:576:LEU:HA	4:L:579:ASN:ND2	2.29	0.47
5:M:78:MET:HG2	5:M:432:ARG:HG3	1.97	0.47
6:N:1:MET:O	6:N:2:ASN:C	2.54	0.47
8:U:93:ILE:HD11	8:U:118:ILE:HD11	1.97	0.47
13:e:22:SER:HA	13:e:34:HIS:HD2	1.79	0.47
21:m:124:LYS:C	21:m:126:ASN:H	2.21	0.47
2:J:85:ASN:O	2:J:89:LEU:HG	2.15	0.47
3:K:75:LEU:O	3:K:79:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:93:LEU:HD22	6:N:54:GLU:HA	1.97	0.47
4:L:420:ALA:HB1	4:L:498:PHE:CD2	2.50	0.47
5:M:50:LYS:HE2	5:M:52:PHE:HE1	1.80	0.47
5:M:57:SER:OG	5:M:113:THR:HG22	2.15	0.47
5:M:122:PHE:HZ	5:M:206:LYS:HD3	1.75	0.47
5:M:264:LEU:HD23	21:m:98:LEU:HD21	1.96	0.47
6:N:26:LEU:O	6:N:29:MET:N	2.47	0.47
10:Y:142:LYS:O	10:Y:143:VAL:C	2.57	0.47
12:d:101:PHE:CZ	16:h:159:LEU:HD22	2.50	0.47
2:J:46:PHE:CE2	3:K:46:VAL:HG13	2.50	0.47
4:L:237:MET:HE1	4:L:248:HIS:HB2	1.96	0.47
4:L:353:GLU:CD	22:n:80:TYR:OH	2.57	0.47
4:L:386:LEU:HA	18:j:68:TRP:HZ3	1.79	0.47
4:L:428:TYR:OH	22:n:33:HIS:CE1	2.68	0.47
4:L:552:LEU:HD22	4:L:553:LEU:HD12	1.97	0.47
5:M:16:TRP:CZ2	25:M:503:3PE:H282	2.47	0.47
5:M:231:LEU:CD1	5:M:235:LEU:HD12	2.42	0.47
5:M:305:THR:O	5:M:306:PRO:C	2.58	0.47
5:M:370:PRO:CA	5:M:375:LEU:HD23	2.42	0.47
6:N:120:GLN:O	6:N:176:ARG:NH2	2.48	0.47
12:d:73:TYR:O	12:d:77:LYS:HB2	2.14	0.47
13:e:85:LYS:O	13:e:89:GLU:HG2	2.15	0.47
20:l:44:THR:CG2	20:l:47:GLU:HG3	2.45	0.47
21:m:14:LEU:HD12	21:m:15:PRO:HD2	1.96	0.47
22:n:96:CYS:SG	22:n:97:TYR:CE1	3.04	0.47
1:D:35:ARG:NH2	15:g:57:PRO:C	2.72	0.47
3:K:57:MET:C	3:K:60:PRO:HD2	2.39	0.47
5:M:196:TRP:HD1	5:M:250:LEU:HB2	1.80	0.47
5:M:428:PRO:HD3	22:n:106:TYR:CG	2.49	0.47
25:M:503:3PE:H122	7:O:338:LYS:HE3	1.96	0.47
6:N:25:ASN:HB3	13:e:15:ASP:CG	2.40	0.47
6:N:317:GLN:HG2	7:O:301:LYS:HB3	1.96	0.47
7:O:78:ALA:CB	7:O:85:HIS:HB2	2.45	0.47
7:O:135:LEU:HB3	7:O:139:ARG:NH1	2.26	0.47
8:U:130:ILE:HG21	8:U:138:LEU:HD11	1.97	0.47
12:d:51:ARG:O	12:d:52:PRO:C	2.55	0.47
24:p:65:HIS:O	24:p:66:ARG:C	2.57	0.47
4:L:63:ILE:HG23	17:i:97:ILE:CD1	2.45	0.47
25:L:703:3PE:H351	5:M:390:ASN:HB2	1.96	0.47
5:M:127:ILE:HG12	6:N:254:LEU:CD2	2.44	0.47
7:O:129:TYR:CE2	7:O:183:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:232:ALA:O	7:O:235:GLN:HB3	2.14	0.47
9:X:151:ASN:HD22	16:h:165:ASP:HA	1.80	0.47
9:X:154:ILE:HG12	16:h:167:PRO:HG2	1.97	0.47
11:c:46:LEU:O	11:c:50:ALA:CB	2.63	0.47
14:f:39:ASN:ND2	14:f:55:THR:HG21	2.30	0.47
22:n:57:MET:O	22:n:58:MET:C	2.58	0.47
2:J:37:PHE:HD1	2:J:56:PHE:CE1	2.33	0.47
12:d:93:TYR:OH	16:h:163:ARG:HD2	2.15	0.47
12:d:93:TYR:CD2	16:h:156:VAL:HG13	2.49	0.47
14:f:41:SER:OG	16:h:134:GLU:HG2	2.14	0.47
20:l:127:ASP:O	20:l:128:VAL:C	2.58	0.47
22:n:50:GLU:O	22:n:51:HIS:C	2.55	0.47
24:p:29:PRO:O	24:p:33:LEU:HD13	2.14	0.47
3:K:73:VAL:HG21	6:N:38:LEU:CD2	2.45	0.46
25:L:702:3PE:H231	25:L:702:3PE:H261	1.83	0.46
5:M:232:ALA:HA	5:M:236:LEU:HD12	1.97	0.46
5:M:348:LEU:O	5:M:351:VAL:N	2.38	0.46
7:O:50:THR:OG1	7:O:288:ASP:HB3	2.15	0.46
10:Y:116:GLY:O	10:Y:120:MET:HB2	2.15	0.46
20:l:119:THR:HG22	21:m:13:THR:HG23	1.96	0.46
22:n:133:TRP:O	22:n:137:VAL:HG22	2.15	0.46
2:J:75:THR:HG23	2:J:75:THR:O	2.14	0.46
4:L:86:SER:OG	4:L:133:SER:HB3	2.15	0.46
4:L:277:MET:CG	4:L:318:GLY:HA2	2.44	0.46
4:L:482:MET:HE2	4:L:486:LEU:CB	2.45	0.46
5:M:213:HIS:O	5:M:217:PRO:CD	2.63	0.46
6:N:17:PRO:HG2	6:N:133:TRP:NE1	2.30	0.46
12:d:59:HIS:CE1	12:d:60:ARG:HG3	2.50	0.46
12:d:78:ARG:O	12:d:81:TYR:N	2.48	0.46
15:g:147:LEU:HD11	24:p:163:MET:HE2	1.97	0.46
17:i:103:ARG:NH1	23:o:67:LEU:HD22	2.31	0.46
24:p:6:ASP:OD1	24:p:8:ASP:HB2	2.15	0.46
24:p:43:TRP:O	24:p:44:PRO:C	2.58	0.46
2:J:33:ILE:HG23	2:J:60:LEU:CD2	2.45	0.46
2:J:74:ALA:O	2:J:75:THR:C	2.56	0.46
2:J:135:LEU:O	3:K:54:MET:CE	2.64	0.46
4:L:172:ILE:O	4:L:176:ARG:HG2	2.16	0.46
4:L:367:PRO:HB3	19:k:75:LYS:HZ1	1.81	0.46
5:M:123:GLU:CB	6:N:255:PRO:HG2	2.42	0.46
7:O:62:VAL:HG13	7:O:62:VAL:O	2.15	0.46
7:O:258:TYR:HE2	7:O:272:ASP:OD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:34:HIS:CE1	16:h:184:LYS:NZ	2.83	0.46
17:i:89:HIS:ND1	25:i:201:3PE:H112	2.31	0.46
18:j:97:LEU:O	23:o:104:ARG:HG3	2.16	0.46
21:m:125:PHE:HE1	24:p:133:THR:CG2	2.21	0.46
1:D:58:THR:HA	1:D:61:TRP:CE2	2.50	0.46
2:J:135:LEU:O	3:K:54:MET:HE2	2.15	0.46
3:K:57:MET:N	3:K:58:PRO:CD	2.78	0.46
4:L:373:LEU:CD2	4:L:427:ILE:HG22	2.45	0.46
5:M:4:ILE:HD12	5:M:4:ILE:N	2.30	0.46
5:M:380:PHE:HD1	5:M:380:PHE:N	2.13	0.46
5:M:380:PHE:N	5:M:380:PHE:CD1	2.82	0.46
5:M:435:THR:O	5:M:436:LEU:C	2.59	0.46
6:N:275:CYS:SG	10:Y:139:PRO:HD2	2.56	0.46
16:h:73:PHE:HD2	16:h:74:TYR:CE1	2.33	0.46
20:l:38:PRO:CB	21:m:75:ASN:ND2	2.73	0.46
22:n:136:GLU:O	22:n:139:GLN:N	2.49	0.46
4:L:21:ILE:HG12	4:L:27:ILE:CG2	2.46	0.46
4:L:225:ALA:CB	4:L:233:LEU:HD12	2.45	0.46
4:L:264:HIS:HA	4:L:267:THR:CG2	2.45	0.46
4:L:581:LYS:HB2	4:L:586:LEU:HD22	1.97	0.46
25:L:703:3PE:H251	25:L:703:3PE:H221	1.48	0.46
5:M:10:MET:C	5:M:13:PRO:HD2	2.41	0.46
5:M:139:GLN:HG3	5:M:141:GLU:H	1.80	0.46
5:M:300:SER:HB2	5:M:308:SER:HB3	1.97	0.46
6:N:25:ASN:HB3	13:e:15:ASP:OD2	2.14	0.46
7:O:38:TYR:CE1	7:O:292:HIS:HD2	2.34	0.46
7:O:135:LEU:CD1	28:O:402:ADP:C6	2.99	0.46
23:o:111:ARG:HA	23:o:114:ARG:HG2	1.98	0.46
24:p:6:ASP:O	24:p:8:ASP:N	2.49	0.46
2:J:32:LEU:HG	2:J:64:LEU:HD21	1.97	0.46
4:L:261:VAL:CA	4:L:264:HIS:HD2	2.29	0.46
4:L:598:ILE:HD11	6:N:153:ILE:HG12	1.97	0.46
5:M:303:ILE:HG22	5:M:305:THR:HG23	1.98	0.46
6:N:154:ILE:HG12	6:N:195:PRO:CG	2.45	0.46
16:h:69:ARG:O	16:h:73:PHE:CB	2.63	0.46
23:o:31:PHE:CG	23:o:34:ARG:HB3	2.51	0.46
2:J:5:ILE:HG13	2:J:124:LEU:HD11	1.97	0.46
4:L:13:ILE:HD11	25:i:201:3PE:H2A2	1.98	0.46
4:L:306:THR:HA	4:L:336:LYS:NZ	2.27	0.46
4:L:466:PHE:CE2	25:j:700:3PE:H361	2.50	0.46
4:L:529:PHE:CZ	4:L:533:ILE:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:556:ILE:HD11	21:m:76:ILE:CG2	2.44	0.46
5:M:15:THR:HG21	5:M:100:ILE:CD1	2.46	0.46
6:N:123:PRO:HG2	6:N:126:MET:CG	2.40	0.46
6:N:239:ALA:HB1	12:d:47:MET:HG2	1.98	0.46
6:N:319:LYS:HA	7:O:302:THR:CG2	2.40	0.46
15:g:77:ASP:HA	15:g:78:PRO:HD3	1.70	0.46
16:h:95:GLU:OE1	16:h:114:LYS:HD3	2.15	0.46
20:l:184:TYR:HD1	23:o:36:GLU:HA	1.78	0.46
22:n:61:THR:O	22:n:65:ARG:HG3	2.15	0.46
4:L:31:ASN:ND2	4:L:34:LEU:HB2	2.31	0.46
4:L:101:MET:HE1	4:L:121:LEU:HB2	1.98	0.46
6:N:37:LEU:HD21	6:N:60:PHE:CD1	2.51	0.46
10:Y:74:LEU:HD23	10:Y:74:LEU:C	2.41	0.46
11:c:38:LYS:HA	11:c:39:PRO:HD3	1.58	0.46
12:d:108:THR:O	12:d:109:TYR:C	2.55	0.46
16:h:59:PRO:HD3	22:n:99:VAL:HG11	1.98	0.46
18:j:84:PHE:CE2	23:o:88:ASP:HB3	2.50	0.46
18:j:92:TRP:O	18:j:93:THR:C	2.59	0.46
21:m:15:PRO:HG2	21:m:18:LEU:HD12	1.97	0.46
2:J:94:LEU:HD23	2:J:94:LEU:C	2.40	0.46
4:L:324:LEU:HA	4:L:327:LEU:HD12	1.97	0.46
4:L:427:ILE:CD1	19:k:69:PHE:CE1	2.99	0.46
5:M:208:PRO:CD	5:M:236:LEU:HD22	2.38	0.46
5:M:319:HIS:CA	5:M:322:THR:HG22	2.41	0.46
7:O:231:SER:O	7:O:234:LEU:N	2.48	0.46
16:h:82:VAL:O	16:h:85:GLY:N	2.49	0.46
19:k:52:ALA:O	19:k:55:GLU:N	2.49	0.46
1:D:58:THR:HG23	1:D:61:TRP:CH2	2.51	0.46
3:K:57:MET:O	3:K:58:PRO:C	2.58	0.46
4:L:390:TYR:CE2	18:j:68:TRP:CH2	3.05	0.46
5:M:122:PHE:CZ	5:M:206:LYS:CD	2.95	0.46
7:O:140:LEU:HD11	7:O:198:TYR:CE2	2.51	0.46
9:X:168:PHE:O	9:X:169:PHE:CG	2.69	0.46
10:Y:143:VAL:HG21	16:h:169:TYR:CZ	2.51	0.46
11:c:55:TRP:HE1	12:d:66:THR:CG2	2.28	0.46
12:d:54:MET:HE2	12:d:54:MET:HB3	1.89	0.46
19:k:69:PHE:CZ	19:k:73:ILE:HG13	2.51	0.46
20:l:35:ASP:O	20:l:54:LYS:HD3	2.15	0.46
20:l:38:PRO:CG	21:m:71:ALA:HB2	2.43	0.46
21:m:9:ALA:O	21:m:10:PRO:C	2.56	0.46
1:D:55:SER:HB3	1:D:58:THR:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:74:ALA:O	2:J:75:THR:HG22	2.16	0.45
4:L:12:PHE:O	4:L:16:LEU:HG	2.15	0.45
4:L:74:MET:HE3	4:L:74:MET:HB2	1.76	0.45
4:L:339:LEU:HD11	4:L:376:GLY:HA3	1.99	0.45
4:L:550:LEU:O	4:L:554:ASP:HB3	2.16	0.45
5:M:56:PHE:CE1	5:M:108:MET:HG2	2.47	0.45
5:M:61:LEU:C	5:M:64:PRO:HD2	2.41	0.45
5:M:116:ILE:HD12	5:M:119:TYR:HB3	1.98	0.45
6:N:241:LEU:O	6:N:244:ILE:HG22	2.15	0.45
6:N:277:ILE:HG22	6:N:278:MET:H	1.79	0.45
7:O:40:LEU:O	7:O:44:ILE:HG13	2.16	0.45
7:O:126:GLY:CA	15:g:51:MET:HE1	2.45	0.45
7:O:344:ASN:OD1	7:O:346:GLU:HG2	2.15	0.45
11:c:35:VAL:HG23	11:c:36:ASN:OD1	2.16	0.45
11:c:57:TYR:CD2	12:d:70:PHE:HZ	2.34	0.45
2:J:12:PHE:HE2	3:K:42:ILE:HD11	1.77	0.45
3:K:51:SER:HA	13:e:32:ARG:CD	2.46	0.45
4:L:60:GLU:HG2	4:L:83:ASP:HA	1.98	0.45
4:L:277:MET:HG3	4:L:318:GLY:CA	2.46	0.45
4:L:475:THR:O	4:L:476:SER:HB2	2.16	0.45
4:L:550:LEU:HD11	5:M:279:GLN:NE2	2.31	0.45
5:M:186:LEU:HD22	5:M:250:LEU:HA	1.98	0.45
5:M:282:LEU:HD11	5:M:410:MET:HE3	1.96	0.45
5:M:309:PHE:O	5:M:312:ALA:HB3	2.16	0.45
5:M:393:ILE:O	5:M:397:GLY:N	2.49	0.45
6:N:300:THR:CG2	6:N:301:SER:N	2.79	0.45
7:O:204:VAL:O	7:O:205:ILE:C	2.59	0.45
10:Y:39:SER:HB2	10:Y:58:VAL:HA	1.98	0.45
13:e:89:GLU:HB3	13:e:91:LYS:HE2	1.98	0.45
19:k:38:VAL:CG1	22:n:39:TYR:HB2	2.46	0.45
20:l:166:LEU:HD12	20:l:170:ARG:HH22	1.81	0.45
25:m:201:3PE:H252	25:m:201:3PE:H3C1	1.97	0.45
23:o:5:LEU:H	23:o:5:LEU:HD12	1.81	0.45
24:p:24:THR:HG22	24:p:26:LEU:N	2.31	0.45
1:D:43:TRP:CZ2	5:M:143:LEU:CD1	2.98	0.45
2:J:44:LEU:CD2	2:J:49:SER:HA	2.47	0.45
2:J:84:SER:O	2:J:88:ILE:HG12	2.16	0.45
4:L:135:ASN:O	4:L:198:LEU:HD13	2.16	0.45
4:L:195:SER:O	4:L:201:ILE:HD11	2.16	0.45
4:L:204:SER:HA	4:L:207:ASN:ND2	2.31	0.45
4:L:366:MET:SD	4:L:443:ILE:HG21	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:22:LYS:HG2	5:M:22:LYS:O	2.17	0.45
5:M:458:THR:HG21	24:p:148:ALA:HB1	1.93	0.45
6:N:133:TRP:CE3	6:N:136:ILE:HD12	2.51	0.45
6:N:308:ASN:ND2	7:O:310:ILE:O	2.49	0.45
7:O:306:ASN:O	7:O:309:THR:HG22	2.16	0.45
9:X:147:ARG:HD2	13:e:43:CYS:HA	1.98	0.45
10:Y:75:THR:HB	10:Y:95:GLY:HA2	1.98	0.45
13:e:19:MET:HE2	13:e:19:MET:HB3	1.85	0.45
24:p:107:GLN:O	24:p:111:LYS:HG3	2.15	0.45
24:p:173:GLU:O	24:p:174:ALA:C	2.59	0.45
1:D:36:GLN:OE1	5:M:136:TRP:HA	2.17	0.45
3:K:29:THR:O	3:K:32:CYS:N	2.49	0.45
4:L:241:THR:N	4:L:242:PRO:HD2	2.31	0.45
4:L:444:ASN:ND2	18:j:39:HIS:HB2	2.32	0.45
25:L:703:3PE:H112	25:L:703:3PE:H11	1.99	0.45
5:M:42:LEU:HD21	5:M:67:ILE:HD12	1.97	0.45
5:M:65:LEU:O	5:M:66:ILE:C	2.59	0.45
5:M:131:ILE:HD12	25:M:503:3PE:H362	1.97	0.45
6:N:26:LEU:HG	6:N:85:MET:SD	2.56	0.45
7:O:265:ASP:O	7:O:266:PRO:C	2.58	0.45
7:O:342:GLY:O	7:O:355:LYS:NZ	2.50	0.45
26:h:201:CDL:H162	26:h:201:CDL:H191	1.75	0.45
17:i:123:PHE:CD1	23:o:65:ARG:NH2	2.85	0.45
19:k:26:ARG:O	19:k:27:GLN:C	2.57	0.45
2:J:33:ILE:HA	2:J:64:LEU:HD23	1.99	0.45
2:J:169:ILE:HG23	6:N:45:ILE:HD11	1.98	0.45
4:L:47:SER:O	4:L:50:PRO:HD2	2.16	0.45
4:L:532:ILE:HG23	4:L:533:ILE:N	2.31	0.45
5:M:42:LEU:HD11	5:M:67:ILE:HD12	1.99	0.45
5:M:207:MET:O	5:M:208:PRO:C	2.59	0.45
5:M:453:LEU:CD1	5:M:454:ILE:CG2	2.84	0.45
6:N:3:PRO:HG2	7:O:289:TRP:CH2	2.52	0.45
6:N:215:MET:SD	6:N:244:ILE:HD11	2.56	0.45
8:U:90:TYR:HD1	19:k:51:TRP:CE2	2.34	0.45
10:Y:83:ARG:NH1	10:Y:90:LEU:HD23	2.31	0.45
12:d:11:LEU:HD12	12:d:11:LEU:HA	1.69	0.45
23:o:63:LEU:O	23:o:64:ILE:C	2.59	0.45
4:L:210:LEU:HD23	4:L:210:LEU:C	2.41	0.45
4:L:247:LEU:HD12	4:L:247:LEU:C	2.41	0.45
4:L:310:LEU:HA	4:L:313:MET:HB2	1.99	0.45
4:L:385:PHE:HE2	18:j:73:PHE:HD1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:591:PHE:N	4:L:591:PHE:CD1	2.83	0.45
4:L:591:PHE:N	4:L:591:PHE:HD1	2.15	0.45
5:M:162:ILE:HD13	6:N:280:THR:HG23	1.97	0.45
7:O:351:TRP:HB2	7:O:355:LYS:HE3	1.98	0.45
8:U:113:LEU:HD23	22:n:17:LEU:HD23	1.97	0.45
10:Y:83:ARG:O	10:Y:85:LYS:HG2	2.17	0.45
11:c:57:TYR:CD2	12:d:70:PHE:CZ	3.04	0.45
13:e:18:PHE:O	13:e:18:PHE:CD2	2.69	0.45
13:e:41:ILE:CD1	16:h:174:PRO:HB2	2.46	0.45
15:g:67:LYS:O	15:g:68:ASN:C	2.60	0.45
16:h:144:SER:HB2	24:p:82:VAL:HG21	1.98	0.45
22:n:101:GLU:HG2	22:n:122:ARG:HH12	1.81	0.45
2:J:78:TYR:O	2:J:79:PRO:C	2.60	0.45
4:L:387:THR:HA	4:L:465:GLY:HA3	1.98	0.45
25:L:701:3PE:H362	25:L:701:3PE:H331	1.45	0.45
5:M:272:THR:O	5:M:275:ILE:HG13	2.17	0.45
5:M:283:LYS:HG3	5:M:327:PHE:HE1	1.78	0.45
6:N:155:LEU:O	6:N:159:ILE:HG22	2.16	0.45
7:O:112:CYS:HB3	7:O:131:LEU:HA	1.97	0.45
12:d:13:PHE:CE2	12:d:14:LEU:HD23	2.52	0.45
15:g:121:GLU:OE2	24:p:10:TYR:CE2	2.69	0.45
19:k:57:TRP:O	19:k:58:ARG:C	2.59	0.45
20:l:57:MET:HE2	20:l:57:MET:HB3	1.75	0.45
22:n:45:ARG:O	22:n:49:GLU:N	2.37	0.45
23:o:27:PRO:O	23:o:34:ARG:NH1	2.42	0.45
23:o:31:PHE:CD2	23:o:34:ARG:HD2	2.52	0.45
24:p:110:LEU:O	24:p:111:LYS:C	2.58	0.45
4:L:246:LEU:C	4:L:246:LEU:CD1	2.90	0.45
25:L:702:3PE:H122	10:Y:46:ASN:HD22	1.81	0.45
26:L:704:CDL:H161	26:L:704:CDL:C11	2.46	0.45
5:M:3:LYS:HA	5:M:7:PRO:HD2	1.99	0.45
5:M:87:ASP:HB3	5:M:91:LEU:HB2	1.99	0.45
5:M:452:LYS:NZ	25:M:502:3PE:O14	2.49	0.45
6:N:293:TYR:O	6:N:297:ILE:HG12	2.17	0.45
9:X:165:THR:N	9:X:172:VAL:HG11	2.32	0.45
11:c:32:ARG:O	11:c:33:GLU:C	2.58	0.45
18:j:71:TRP:CH2	25:j:700:3PE:H392	2.51	0.45
22:n:98:LYS:HD3	22:n:176:GLU:O	2.17	0.45
22:n:146:PRO:O	22:n:147:ASP:C	2.60	0.45
4:L:483:PRO:CG	4:L:486:LEU:HD12	2.47	0.45
4:L:527:GLY:O	4:L:528:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:L:704:CDL:H202	26:L:704:CDL:H511	1.99	0.45
5:M:42:LEU:CG	5:M:67:ILE:HD11	2.43	0.45
5:M:209:LEU:HD11	5:M:261:PHE:HD1	1.81	0.45
5:M:388:TRP:NE1	21:m:109:ARG:CD	2.79	0.45
6:N:153:ILE:O	6:N:154:ILE:C	2.58	0.45
9:X:166:ARG:HH22	12:d:87:ASP:CG	2.25	0.45
11:c:65:ASP:O	11:c:66:VAL:C	2.56	0.45
16:h:73:PHE:CE2	16:h:74:TYR:HE1	2.35	0.45
16:h:120:TRP:NE1	16:h:124:ASN:ND2	2.64	0.45
20:l:91:GLN:HG2	22:n:2:ALA:O	2.16	0.45
4:L:81:LYS:CA	4:L:135:ASN:HD21	2.29	0.45
4:L:226:GLN:HG3	4:L:314:MET:HE2	1.98	0.45
4:L:407:TRP:HE1	20:l:140:MET:HE3	1.82	0.45
4:L:437:PHE:CZ	4:L:441:ILE:HG12	2.43	0.45
5:M:42:LEU:CG	5:M:67:ILE:CD1	2.95	0.45
5:M:129:THR:CG2	5:M:235:LEU:CD1	2.95	0.45
5:M:187:ASP:H	5:M:192:ASN:ND2	2.15	0.45
5:M:249:ILE:O	5:M:250:LEU:CG	2.47	0.45
6:N:109:ALA:HB3	6:N:110:PRO:CD	2.46	0.45
6:N:154:ILE:CD1	6:N:195:PRO:HG2	2.47	0.45
6:N:217:MET:HA	6:N:220:MET:SD	2.57	0.45
6:N:220:MET:O	6:N:221:LEU:C	2.60	0.45
7:O:129:TYR:CD2	7:O:183:CYS:HB3	2.52	0.45
8:U:114:ASP:OD1	22:n:45:ARG:NH2	2.50	0.45
8:U:116:VAL:HG12	8:U:120:MET:HE2	1.98	0.45
11:c:72:ARG:HH11	12:d:19:ARG:HD3	1.82	0.45
15:g:64:VAL:HG11	15:g:71:PHE:CE1	2.52	0.45
17:i:106:PRO:HD2	23:o:64:ILE:CG2	2.46	0.45
22:n:145:SER:O	22:n:146:PRO:C	2.58	0.45
3:K:66:PHE:HE2	6:N:35:PHE:CE2	2.35	0.44
3:K:93:LEU:CD1	6:N:57:THR:HG21	2.47	0.44
4:L:100:ILE:O	4:L:104:SER:N	2.42	0.44
4:L:371:SER:HB2	18:j:62:SER:OG	2.17	0.44
4:L:375:ILE:HG12	18:j:65:MET:SD	2.57	0.44
5:M:73:LEU:HB3	5:M:103:GLN:OE1	2.16	0.44
6:N:163:PHE:CZ	6:N:285:MET:HG3	2.52	0.44
6:N:214:PRO:HB2	6:N:247:MET:SD	2.56	0.44
6:N:250:SER:O	6:N:259:GLY:HA3	2.17	0.44
7:O:250:SER:HA	7:O:255:VAL:CG2	2.41	0.44
10:Y:20:CYS:O	10:Y:21:HIS:C	2.60	0.44
11:c:73:ASN:OD1	11:c:75:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:38:ARG:HD3	14:f:56:TRP:NE1	2.32	0.44
16:h:55:PHE:C	16:h:55:PHE:CD1	2.94	0.44
16:h:56:VAL:O	16:h:58:LYS:HG3	2.16	0.44
26:h:201:CDL:HB61	17:i:84:TYR:CE2	2.51	0.44
23:o:110:GLN:O	23:o:111:ARG:C	2.59	0.44
24:p:6:ASP:HB3	24:p:9:VAL:CG2	2.39	0.44
3:K:61:ILE:O	3:K:62:THR:C	2.58	0.44
4:L:231:PRO:C	4:L:234:PRO:HD2	2.41	0.44
4:L:366:MET:SD	4:L:443:ILE:CG2	3.05	0.44
26:L:705:CDL:H591	10:Y:68:ILE:CD1	2.45	0.44
7:O:69:GLY:HA2	7:O:72:LYS:NZ	2.32	0.44
7:O:169:PHE:CD2	28:O:402:ADP:N6	2.85	0.44
7:O:351:TRP:O	7:O:355:LYS:HG2	2.16	0.44
12:d:78:ARG:O	12:d:79:GLN:C	2.59	0.44
13:e:92:TYR:OH	13:e:94:PRO:HA	2.16	0.44
21:m:49:LEU:HD12	21:m:49:LEU:HA	1.82	0.44
22:n:136:GLU:OE2	22:n:167:TRP:CD1	2.70	0.44
1:D:55:SER:OG	1:D:56:LYS:N	2.49	0.44
2:J:43:VAL:HG13	3:K:49:LEU:HD11	2.00	0.44
3:K:1:MET:N	3:K:2:PRO:CD	2.81	0.44
4:L:485:PHE:CE1	4:L:486:LEU:HG	2.52	0.44
25:L:702:3PE:H122	10:Y:46:ASN:ND2	2.32	0.44
5:M:24:TRP:CE3	5:M:81:GLN:HG2	2.52	0.44
5:M:415:GLN:O	5:M:416:ARG:CG	2.64	0.44
6:N:258:THR:CB	6:N:333:SER:O	2.64	0.44
7:O:336:GLY:HA2	7:O:344:ASN:HB3	1.99	0.44
9:X:154:ILE:CG1	16:h:167:PRO:HG2	2.47	0.44
10:Y:120:MET:HE2	10:Y:120:MET:HB3	1.90	0.44
18:j:39:HIS:ND1	18:j:39:HIS:N	2.65	0.44
21:m:125:PHE:HA	24:p:136:THR:HG21	1.99	0.44
22:n:35:ASP:OD1	22:n:35:ASP:N	2.51	0.44
22:n:97:TYR:HB2	22:n:178:PRO:HB2	1.99	0.44
23:o:49:ALA:O	23:o:50:GLN:C	2.60	0.44
2:J:68:GLY:O	2:J:71:THR:HB	2.18	0.44
4:L:2:ASN:O	4:L:3:ILE:C	2.59	0.44
4:L:54:PHE:CB	4:L:87:ILE:HD11	2.47	0.44
4:L:73:SER:CB	24:p:100:GLN:HE21	2.27	0.44
4:L:117:PHE:CE1	4:L:243:VAL:CG2	3.00	0.44
4:L:155:ILE:HG12	4:L:248:HIS:CE1	2.53	0.44
4:L:435:PRO:O	19:k:58:ARG:HD2	2.18	0.44
4:L:537:THR:N	4:L:538:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:200:MET:HE2	5:M:250:LEU:HD21	2.00	0.44
5:M:424:ILE:O	5:M:424:ILE:CG2	2.65	0.44
6:N:87:GLN:O	6:N:88:GLN:C	2.59	0.44
6:N:208:TYR:O	6:N:212:THR:HG22	2.18	0.44
7:O:223:ASP:O	7:O:224:PRO:C	2.60	0.44
17:i:94:PRO:HG3	24:p:10:TYR:CD2	2.50	0.44
22:n:149:ILE:HD12	22:n:149:ILE:N	2.32	0.44
2:J:133:VAL:O	2:J:134:MET:HB2	2.16	0.44
4:L:56:HIS:CA	23:o:74:PHE:CE1	3.01	0.44
27:L:706:PC1:H371	27:L:706:PC1:C2D	2.47	0.44
5:M:18:SER:OG	5:M:26:ASN:ND2	2.51	0.44
5:M:22:LYS:HG2	5:M:26:ASN:ND2	2.33	0.44
6:N:227:ILE:HG13	6:N:228:ASN:N	2.32	0.44
7:O:262:GLU:HB3	7:O:268:LYS:NZ	2.33	0.44
9:X:153:VAL:O	9:X:155:GLU:HG3	2.18	0.44
10:Y:7:PHE:CZ	10:Y:26:ILE:HG12	2.52	0.44
17:i:69:LEU:HD12	17:i:69:LEU:C	2.42	0.44
18:j:101:PRO:O	18:j:102:ASP:C	2.59	0.44
20:l:38:PRO:C	21:m:75:ASN:HD21	2.26	0.44
23:o:31:PHE:CG	23:o:34:ARG:HD2	2.53	0.44
3:K:33:LEU:HA	3:K:36:MET:HE2	2.00	0.44
4:L:66:TRP:CZ3	4:L:68:TRP:HD1	2.34	0.44
4:L:68:TRP:HE3	4:L:76:LEU:HD21	1.82	0.44
4:L:529:PHE:O	4:L:533:ILE:HG22	2.16	0.44
26:L:704:CDL:H561	26:L:704:CDL:H531	1.83	0.44
5:M:350:MET:HE2	22:n:96:CYS:HA	1.99	0.44
5:M:445:ILE:HG23	25:M:502:3PE:H292	1.99	0.44
6:N:45:ILE:O	6:N:45:ILE:CG1	2.58	0.44
6:N:338:PRO:HG2	12:d:33:TYR:CZ	2.52	0.44
25:O:401:3PE:H2A2	25:O:401:3PE:H272	1.83	0.44
13:e:74:ARG:O	13:e:75:ARG:C	2.59	0.44
14:f:25:TYR:O	14:f:29:LYS:HG2	2.17	0.44
14:f:39:ASN:CG	14:f:55:THR:HG21	2.41	0.44
2:J:74:ALA:C	2:J:75:THR:HG22	2.42	0.44
4:L:594:ASN:OD1	10:Y:41:TYR:OH	2.34	0.44
5:M:131:ILE:HD13	6:N:302:LEU:HD21	2.00	0.44
6:N:122:ILE:HD11	6:N:127:GLY:HA2	1.98	0.44
7:O:272:ASP:O	7:O:275:TYR:HB2	2.18	0.44
11:c:55:TRP:CE2	12:d:66:THR:HG22	2.53	0.44
11:c:61:THR:HG22	11:c:65:ASP:OD2	2.18	0.44
24:p:140:GLN:HG2	24:p:144:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:42:LEU:CD1	5:M:67:ILE:CD1	2.96	0.44
5:M:126:LEU:HD11	5:M:153:THR:HG21	2.00	0.44
5:M:186:LEU:HD13	5:M:250:LEU:HA	2.00	0.44
5:M:321:LEU:HD23	5:M:321:LEU:HA	1.81	0.44
6:N:146:TYR:CD1	6:N:198:PRO:HG2	2.53	0.44
6:N:146:TYR:O	6:N:147:PRO:C	2.53	0.44
7:O:206:TYR:CD1	7:O:246:LEU:HD21	2.53	0.44
8:U:88:LYS:HG3	8:U:98:LEU:HD23	1.98	0.44
17:i:92:THR:O	24:p:5:TRP:CD1	2.71	0.44
23:o:118:LYS:HA	23:o:118:LYS:HD2	1.81	0.44
4:L:152:PHE:HD2	4:L:153:LEU:HD12	1.83	0.44
4:L:588:PHE:O	4:L:589:MET:C	2.60	0.44
26:L:704:CDL:H1	5:M:357:THR:OG1	2.18	0.44
5:M:8:SER:O	5:M:11:LEU:HB2	2.18	0.44
5:M:158:ILE:CG2	6:N:283:ALA:HB1	2.47	0.44
5:M:277:LEU:O	20:l:116:ARG:NH2	2.44	0.44
5:M:344:MET:HE3	5:M:423:MET:CE	2.48	0.44
5:M:423:MET:C	5:M:424:ILE:O	2.56	0.44
6:N:202:LEU:HD11	13:e:3:PHE:CE1	2.53	0.44
7:O:323:GLN:HE21	15:g:55:GLU:HA	1.83	0.44
10:Y:12:HIS:CD2	10:Y:131:LYS:HE2	2.53	0.44
2:J:40:CYS:O	2:J:44:LEU:HG	2.17	0.43
2:J:44:LEU:HD23	2:J:49:SER:HA	2.00	0.43
2:J:157:TRP:HE1	6:N:11:PHE:HD2	1.65	0.43
2:J:164:PHE:HB3	6:N:5:THR:HG23	1.99	0.43
4:L:529:PHE:HB3	4:L:530:PRO:HD3	1.99	0.43
5:M:158:ILE:HG21	6:N:283:ALA:CB	2.48	0.43
25:M:503:3PE:H2I2	26:d:201:CDL:H602	2.00	0.43
6:N:31:VAL:C	6:N:35:PHE:CD2	2.91	0.43
6:N:120:GLN:HE22	6:N:174:GLN:HB3	1.83	0.43
10:Y:7:PHE:O	10:Y:8:PHE:C	2.61	0.43
12:d:57:GLY:O	12:d:60:ARG:N	2.51	0.43
12:d:72:GLY:O	12:d:73:TYR:C	2.60	0.43
13:e:92:TYR:CG	13:e:93:THR:N	2.86	0.43
24:p:165:GLU:C	24:p:167:ARG:H	2.26	0.43
3:K:21:MET:HB2	25:K:101:3PE:C23	2.48	0.43
3:K:57:MET:O	3:K:60:PRO:HD2	2.18	0.43
4:L:226:GLN:OE1	4:L:284:THR:CG2	2.66	0.43
4:L:305:SER:OG	4:L:336:LYS:HE2	2.18	0.43
5:M:151:PHE:HZ	6:N:291:PHE:HB2	1.78	0.43
6:N:12:THR:CG2	6:N:39:ALA:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:19:GLN:OE1	10:Y:19:GLN:HA	2.17	0.43
17:i:94:PRO:CB	24:p:10:TYR:CD2	3.02	0.43
25:i:201:3PE:H11	25:i:201:3PE:O22	2.18	0.43
18:j:70:LEU:HD13	19:k:81:PHE:HA	2.00	0.43
20:l:41:TYR:HD2	20:l:43:ARG:HD3	1.82	0.43
20:l:142:PHE:O	20:l:145:TRP:N	2.51	0.43
21:m:45:ARG:O	21:m:45:ARG:CG	2.61	0.43
22:n:131:GLU:O	22:n:131:GLU:HG2	2.17	0.43
2:J:55:VAL:HG13	2:J:56:PHE:N	2.33	0.43
4:L:564:LYS:HG2	21:m:77:TYR:OH	2.18	0.43
4:L:589:MET:O	4:L:592:LEU:HB3	2.18	0.43
5:M:278:ARG:HH22	20:l:108:ASP:CB	2.31	0.43
5:M:348:LEU:O	5:M:349:GLN:C	2.60	0.43
7:O:72:LYS:O	7:O:76:GLU:HG2	2.18	0.43
7:O:211:VAL:HB	7:O:212:PRO:HD3	2.00	0.43
10:Y:26:ILE:O	10:Y:30:LEU:HG	2.17	0.43
17:i:32:GLU:OE2	22:n:118:TYR:N	2.50	0.43
20:l:58:ARG:HD2	21:m:35:GLU:OE1	2.18	0.43
21:m:17:THR:O	21:m:18:LEU:CB	2.66	0.43
21:m:34:VAL:O	21:m:34:VAL:HG12	2.16	0.43
4:L:496:LEU:CD1	4:L:497:GLY:N	2.73	0.43
4:L:564:LYS:HG2	21:m:77:TYR:CZ	2.54	0.43
5:M:154:LEU:HA	5:M:154:LEU:HD23	1.84	0.43
6:N:254:LEU:HA	6:N:255:PRO:HD3	1.61	0.43
6:N:279:ALA:HA	6:N:282:MET:HE2	2.00	0.43
6:N:307:THR:HB	7:O:319:ILE:HG12	2.00	0.43
6:N:323:ASN:N	6:N:323:ASN:OD1	2.49	0.43
7:O:210:PRO:O	7:O:213:GLU:N	2.51	0.43
7:O:256:LEU:HD11	7:O:276:LEU:HD22	1.99	0.43
10:Y:19:GLN:O	10:Y:23:LYS:HG2	2.19	0.43
10:Y:143:VAL:O	16:h:158:ARG:NH2	2.52	0.43
12:d:78:ARG:HG2	12:d:82:LEU:HD23	2.00	0.43
15:g:58:GLU:CD	15:g:59:PRO:HD2	2.44	0.43
25:m:201:3PE:H2I3	25:m:201:3PE:H2F2	1.87	0.43
1:D:36:GLN:NE2	1:D:38:GLN:NE2	2.62	0.43
4:L:246:LEU:HD12	4:L:247:LEU:CB	2.49	0.43
4:L:407:TRP:HE1	20:l:140:MET:HE1	1.84	0.43
4:L:427:ILE:HG13	4:L:428:TYR:N	2.33	0.43
6:N:175:MET:HE2	6:N:175:MET:HB2	1.85	0.43
6:N:186:HIS:O	6:N:190:MET:HG3	2.18	0.43
6:N:240:MET:O	6:N:240:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:324:LEU:CD1	12:d:64:PHE:HZ	2.30	0.43
16:h:57:VAL:HG13	22:n:104:LEU:HG	2.01	0.43
20:l:97:LEU:O	20:l:98:ARG:C	2.60	0.43
24:p:75:THR:HG22	24:p:156:LEU:HD13	2.00	0.43
2:J:67:PHE:O	2:J:68:GLY:C	2.59	0.43
4:L:22:SER:HA	4:L:27:ILE:HG21	2.00	0.43
4:L:81:LYS:HD3	4:L:262:ARG:NH1	2.34	0.43
4:L:296:ASN:HD21	4:L:425:ARG:HH21	1.65	0.43
4:L:327:LEU:HD21	4:L:472:ILE:HD13	2.00	0.43
5:M:73:LEU:HD23	5:M:103:GLN:HE22	1.84	0.43
6:N:105:LYS:HE3	6:N:105:LYS:HB3	1.79	0.43
7:O:99:GLY:O	11:c:31:VAL:N	2.36	0.43
7:O:239:ASN:HB3	7:O:243:LYS:NZ	2.33	0.43
7:O:303:GLU:O	7:O:304:VAL:C	2.59	0.43
10:Y:115:MET:O	10:Y:119:TYR:HD2	2.02	0.43
10:Y:141:PRO:CB	16:h:161:ARG:NH1	2.81	0.43
13:e:41:ILE:HD11	16:h:174:PRO:O	2.18	0.43
21:m:28:GLU:HA	21:m:31:ARG:NH2	2.33	0.43
2:J:30:LEU:O	2:J:31:GLY:C	2.59	0.43
2:J:144:MET:HB3	2:J:152:MET:HB2	2.01	0.43
3:K:4:THR:O	3:K:4:THR:HG22	2.19	0.43
4:L:60:GLU:C	4:L:61:TYR:CD1	2.97	0.43
4:L:70:THR:O	4:L:75:GLU:HA	2.18	0.43
4:L:172:ILE:HD13	4:L:172:ILE:HA	1.89	0.43
4:L:446:ASN:O	4:L:447:ASP:C	2.57	0.43
5:M:95:TYR:OH	5:M:226:ALA:HB3	2.19	0.43
5:M:119:TYR:HD1	5:M:160:LEU:HD22	1.79	0.43
5:M:208:PRO:HG2	5:M:216:LEU:CD1	2.44	0.43
5:M:304:GLN:HA	5:M:309:PHE:HE1	1.83	0.43
6:N:219:LEU:CD2	6:N:230:ILE:HD12	2.49	0.43
6:N:275:CYS:SG	10:Y:139:PRO:CD	3.07	0.43
10:Y:22:ARG:O	10:Y:26:ILE:HG13	2.19	0.43
14:f:11:TRP:O	14:f:14:ILE:HG22	2.18	0.43
16:h:127:ASP:OD1	16:h:127:ASP:C	2.61	0.43
20:l:186:ILE:HG23	23:o:100:LYS:HZ1	1.84	0.43
22:n:37:TYR:O	22:n:38:ARG:C	2.61	0.43
24:p:103:MET:HE1	24:p:135:VAL:HG12	1.99	0.43
2:J:13:LEU:HD11	3:K:10:MET:SD	2.58	0.43
4:L:92:VAL:HG21	4:L:330:CYS:HB3	2.00	0.43
4:L:184:LEU:HD22	25:L:703:3PE:H3C2	2.01	0.43
4:L:187:VAL:HG13	5:M:383:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:196:TRP:HZ2	5:M:383:MET:SD	2.41	0.43
4:L:353:GLU:CD	22:n:80:TYR:HH	2.26	0.43
4:L:493:ILE:O	4:L:496:LEU:HG	2.19	0.43
5:M:63:THR:N	5:M:64:PRO:CD	2.81	0.43
5:M:207:MET:SD	5:M:240:SER:CA	3.06	0.43
6:N:11:PHE:O	6:N:15:LEU:N	2.49	0.43
6:N:154:ILE:HD12	6:N:155:LEU:N	2.33	0.43
7:O:76:GLU:CB	7:O:266:PRO:HB3	2.49	0.43
14:f:39:ASN:HA	16:h:134:GLU:OE2	2.18	0.43
21:m:129:TYR:CE2	24:p:146:LEU:O	2.72	0.43
22:n:81:ILE:HD12	22:n:87:GLY:C	2.44	0.43
24:p:49:ARG:O	24:p:50:GLU:C	2.59	0.43
24:p:118:GLY:O	24:p:119:GLU:HB2	2.19	0.43
1:D:47:PHE:CD1	6:N:227:ILE:CD1	3.01	0.43
1:D:52:MET:O	1:D:54:PRO:HD3	2.19	0.43
1:D:72:LEU:O	1:D:72:LEU:HD12	2.18	0.43
4:L:38:THR:O	4:L:41:LYS:HB3	2.19	0.43
4:L:53:MET:HE2	4:L:53:MET:HB3	1.78	0.43
4:L:145:GLU:HB3	5:M:370:PRO:CD	2.48	0.43
4:L:217:LEU:CD1	4:L:273:ILE:HG23	2.49	0.43
5:M:46:ASP:OD1	5:M:47:GLU:N	2.52	0.43
6:N:12:THR:HG22	6:N:39:ALA:HB2	2.00	0.43
6:N:39:ALA:O	6:N:42:PRO:HD2	2.19	0.43
6:N:193:ILE:HD12	6:N:266:ILE:HA	2.01	0.43
8:U:133:ILE:HD13	22:n:7:PRO:HD3	1.99	0.43
13:e:69:ARG:CD	13:e:72:THR:HG21	2.49	0.43
16:h:90:ASN:OD1	16:h:115:HIS:NE2	2.52	0.43
20:l:184:TYR:CE1	23:o:36:GLU:HB3	2.54	0.43
2:J:20:ALA:C	2:J:22:LYS:H	2.26	0.43
3:K:50:ASN:C	3:K:50:ASN:OD1	2.62	0.43
4:L:491:LEU:CD1	18:j:80:VAL:HG22	2.49	0.43
4:L:522:PHE:CD2	4:L:527:GLY:HA2	2.54	0.43
5:M:6:LEU:HD21	14:f:22:PHE:CD2	2.54	0.43
5:M:100:ILE:O	5:M:103:GLN:HG2	2.19	0.43
5:M:263:LEU:HD13	21:m:102:TYR:HB2	2.00	0.43
5:M:367:LEU:C	5:M:367:LEU:HD12	2.44	0.43
6:N:193:ILE:HD11	6:N:269:GLU:CB	2.49	0.43
6:N:272:LYS:HE3	16:h:154:GLN:HG2	2.00	0.43
10:Y:8:PHE:CD1	10:Y:30:LEU:HD21	2.53	0.43
13:e:96:PRO:O	13:e:97:HIS:C	2.62	0.43
14:f:37:PHE:HZ	24:p:83:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:59:PRO:O	16:h:61:LEU:HG	2.19	0.43
22:n:45:ARG:O	22:n:46:ALA:C	2.61	0.43
2:J:50:PHE:O	2:J:54:MET:HG2	2.20	0.42
4:L:466:PHE:HB2	18:j:68:TRP:CH2	2.50	0.42
4:L:553:LEU:HD21	21:m:94:GLY:N	2.33	0.42
4:L:569:LEU:CB	10:Y:115:MET:HE1	2.26	0.42
5:M:123:GLU:CD	6:N:255:PRO:HG2	2.44	0.42
5:M:214:LEU:C	5:M:217:PRO:HD2	2.44	0.42
6:N:170:LEU:HD12	6:N:292:PHE:CD2	2.54	0.42
7:O:117:PHE:HD1	7:O:128:SER:CA	2.31	0.42
7:O:209:VAL:HG23	7:O:214:VAL:CG1	2.49	0.42
8:U:100:VAL:HA	8:U:141:PRO:HG2	2.00	0.42
8:U:142:GLN:O	8:U:143:GLU:C	2.60	0.42
12:d:94:ILE:HD13	16:h:152:LYS:HE3	2.01	0.42
23:o:57:ASP:OD2	23:o:59:CYS:HB2	2.19	0.42
23:o:111:ARG:HA	23:o:114:ARG:NH1	2.34	0.42
4:L:5:THR:O	4:L:6:THR:C	2.62	0.42
4:L:60:GLU:N	4:L:60:GLU:OE2	2.52	0.42
4:L:197:GLU:HG3	24:p:111:LYS:CE	2.49	0.42
4:L:275:THR:HG23	4:L:276:THR:N	2.34	0.42
4:L:526:LEU:HD12	4:L:526:LEU:N	2.34	0.42
4:L:591:PHE:O	4:L:595:ILE:HG13	2.19	0.42
5:M:369:LEU:CD2	5:M:371:PRO:CD	2.84	0.42
6:N:80:GLN:O	6:N:81:LEU:HG	2.19	0.42
6:N:219:LEU:HD23	6:N:230:ILE:HD12	2.01	0.42
6:N:241:LEU:HG	6:N:301:SER:OG	2.19	0.42
7:O:86:TYR:HE1	7:O:157:VAL:HG12	1.82	0.42
7:O:323:GLN:HE21	15:g:55:GLU:CA	2.32	0.42
13:e:44:ALA:HA	13:e:47:ILE:CG1	2.50	0.42
13:e:49:GLY:O	13:e:50:THR:C	2.61	0.42
13:e:101:ARG:NE	13:e:101:ARG:HA	2.34	0.42
16:h:129:PRO:HD2	16:h:130:GLU:OE1	2.18	0.42
17:i:32:GLU:HG3	22:n:115:TYR:HA	2.00	0.42
19:k:28:TRP:CE3	19:k:60:MET:HG2	2.54	0.42
23:o:10:LEU:HD12	23:o:10:LEU:N	2.34	0.42
24:p:73:ASP:O	24:p:74:ILE:C	2.59	0.42
4:L:253:VAL:HG21	4:L:310:LEU:HD11	2.00	0.42
5:M:1:MET:HB3	5:M:1:MET:HE3	1.73	0.42
5:M:14:LEU:HD21	5:M:26:ASN:CB	2.50	0.42
5:M:68:LEU:HD23	5:M:234:ILE:CD1	2.50	0.42
5:M:72:LEU:HD12	5:M:234:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:210:TYR:O	5:M:213:HIS:HD2	2.01	0.42
7:O:121:PRO:HB3	7:O:178:TYR:HE1	1.83	0.42
7:O:170:LEU:HD21	7:O:184:VAL:HG13	2.00	0.42
7:O:256:LEU:N	7:O:256:LEU:HD12	2.34	0.42
7:O:297:LEU:C	7:O:297:LEU:HD23	2.43	0.42
7:O:310:ILE:HG23	7:O:312:VAL:HG23	2.01	0.42
25:O:401:3PE:H351	25:O:401:3PE:H391	2.01	0.42
12:d:27:ASN:O	12:d:28:ASP:C	2.60	0.42
12:d:114:GLU:O	12:d:114:GLU:HG2	2.18	0.42
13:e:22:SER:HB2	13:e:34:HIS:CD2	2.54	0.42
17:i:93:LYS:HE3	17:i:96:THR:HG21	2.01	0.42
23:o:46:MET:HE2	23:o:60:ALA:HB3	2.00	0.42
24:p:36:ALA:O	24:p:37:TYR:C	2.60	0.42
3:K:32:CYS:O	3:K:33:LEU:C	2.60	0.42
4:L:141:PHE:CB	4:L:182:PHE:CE2	2.81	0.42
4:L:220:ALA:HB2	4:L:260:LEU:CD1	2.49	0.42
4:L:335:PHE:O	4:L:339:LEU:HD13	2.19	0.42
4:L:489:THR:HG23	4:L:490:ALA:N	2.33	0.42
5:M:77:LEU:O	5:M:81:GLN:HG3	2.19	0.42
5:M:173:THR:HG23	16:h:147:ALA:HB2	1.78	0.42
5:M:200:MET:CE	5:M:247:SER:HB2	2.45	0.42
5:M:231:LEU:CD1	5:M:235:LEU:CD1	2.85	0.42
6:N:174:GLN:O	6:N:178:ILE:HG13	2.19	0.42
7:O:73:LEU:HD22	7:O:207:ILE:HD11	2.02	0.42
7:O:146:ALA:CB	7:O:159:LEU:HD21	2.49	0.42
8:U:119:ILE:HD13	8:U:119:ILE:HA	1.81	0.42
10:Y:87:ASP:HA	10:Y:128:LYS:NZ	2.34	0.42
11:c:69:TYR:O	11:c:73:ASN:ND2	2.53	0.42
17:i:11:ARG:HD2	22:n:154:LEU:O	2.20	0.42
17:i:22:TRP:O	17:i:26:GLN:HG2	2.19	0.42
20:l:57:MET:HG2	20:l:104:PRO:CG	2.49	0.42
24:p:6:ASP:C	24:p:8:ASP:H	2.27	0.42
24:p:43:TRP:NE1	24:p:47:LEU:HD11	2.33	0.42
4:L:272:PHE:O	4:L:275:THR:HG22	2.20	0.42
5:M:165:ILE:HD12	9:X:168:PHE:CZ	2.55	0.42
5:M:293:HIS:O	5:M:294:MET:HE2	2.20	0.42
5:M:347:GLY:O	5:M:348:LEU:C	2.63	0.42
5:M:422:HIS:CB	21:m:51:TYR:CE2	3.01	0.42
6:N:80:GLN:O	6:N:80:GLN:HG2	2.19	0.42
7:O:211:VAL:O	7:O:214:VAL:HG22	2.19	0.42
11:c:70:LYS:HB3	11:c:75:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:44:TYR:CE2	18:j:45:ARG:HG3	2.54	0.42
21:m:5:LYS:HB2	21:m:5:LYS:HE3	1.73	0.42
22:n:110:SER:O	22:n:113:ALA:HB3	2.20	0.42
23:o:35:LYS:HG3	23:o:36:GLU:O	2.19	0.42
2:J:13:LEU:C	2:J:13:LEU:HD23	2.45	0.42
2:J:55:VAL:O	2:J:56:PHE:C	2.62	0.42
3:K:19:THR:O	3:K:22:PHE:HE1	2.02	0.42
4:L:81:LYS:HD3	4:L:262:ARG:HH11	1.83	0.42
5:M:29:SER:CB	15:g:91:PHE:HD2	2.27	0.42
6:N:315:THR:O	6:N:316:HIS:C	2.61	0.42
6:N:331:ILE:HG23	6:N:335:MET:HE3	2.01	0.42
7:O:229:VAL:HG21	7:O:234:LEU:HD21	2.02	0.42
10:Y:83:ARG:NH1	10:Y:90:LEU:HB3	2.34	0.42
14:f:37:PHE:O	16:h:134:GLU:HB3	2.20	0.42
15:g:106:TYR:CZ	16:h:86:ILE:HD12	2.54	0.42
15:g:119:GLU:OE1	15:g:122:ARG:NH1	2.53	0.42
16:h:57:VAL:CG1	22:n:99:VAL:HG23	2.50	0.42
17:i:81:PHE:O	17:i:82:VAL:C	2.60	0.42
20:l:62:TYR:CE2	20:l:64:PRO:HG3	2.55	0.42
1:D:43:TRP:CZ2	5:M:143:LEU:HD12	2.54	0.42
2:J:21:LEU:O	2:J:22:LYS:C	2.62	0.42
2:J:55:VAL:HG23	2:J:59:TYR:HB3	2.02	0.42
2:J:74:ALA:O	2:J:75:THR:CG2	2.68	0.42
3:K:59:ILE:HB	3:K:60:PRO:HD3	2.01	0.42
4:L:189:PHE:CZ	4:L:212:PRO:HB2	2.55	0.42
4:L:226:GLN:OE1	4:L:281:GLY:HA2	2.20	0.42
4:L:277:MET:CG	4:L:318:GLY:CA	2.98	0.42
4:L:396:ILE:HD13	4:L:396:ILE:HA	1.89	0.42
4:L:405:ASN:HB2	4:L:408:ALA:HB3	2.01	0.42
4:L:525:LEU:O	4:L:526:LEU:C	2.61	0.42
4:L:534:HIS:O	4:L:538:PRO:CG	2.60	0.42
25:L:703:3PE:H271	25:L:703:3PE:C3C	2.48	0.42
5:M:118:PHE:HE2	5:M:203:PHE:CE1	2.37	0.42
5:M:123:GLU:OE2	5:M:154:LEU:HD21	2.20	0.42
5:M:206:LYS:HA	5:M:215:TRP:CZ2	2.54	0.42
5:M:207:MET:HE3	5:M:240:SER:HB2	2.02	0.42
5:M:216:LEU:HD23	5:M:287:ALA:HB1	2.02	0.42
6:N:154:ILE:HD11	6:N:155:LEU:HG	2.02	0.42
6:N:226:THR:HG22	6:N:228:ASN:N	2.34	0.42
6:N:340:ALA:N	6:N:341:PRO:CD	2.83	0.42
7:O:48:LYS:O	7:O:52:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:258:TYR:CZ	7:O:269:VAL:HG13	2.55	0.42
7:O:272:ASP:HA	7:O:275:TYR:HD2	1.85	0.42
25:O:401:3PE:H3A2	12:d:36:LEU:HD11	2.01	0.42
10:Y:45:LEU:O	10:Y:46:ASN:C	2.62	0.42
10:Y:76:THR:CG2	10:Y:92:TYR:HA	2.48	0.42
15:g:147:LEU:O	15:g:148:PRO:C	2.61	0.42
17:i:15:LEU:CD2	22:n:164:PRO:HB2	2.41	0.42
17:i:89:HIS:HB3	25:i:201:3PE:H122	2.02	0.42
18:j:52:ARG:HA	18:j:52:ARG:HD3	1.88	0.42
18:j:96:GLU:HG2	18:j:97:LEU:HD23	2.00	0.42
20:l:167:TYR:CG	20:l:178:PRO:HG3	2.55	0.42
22:n:85:SER:O	22:n:86:PRO:C	2.61	0.42
22:n:132:SER:O	22:n:133:TRP:C	2.62	0.42
22:n:139:GLN:HA	22:n:142:GLU:HG2	2.01	0.42
23:o:104:ARG:O	23:o:108:LEU:HG	2.20	0.42
24:p:6:ASP:O	24:p:7:LYS:C	2.63	0.42
1:D:35:ARG:NH2	15:g:57:PRO:O	2.53	0.42
2:J:23:PRO:O	2:J:24:SER:C	2.61	0.42
4:L:51:LEU:HA	4:L:87:ILE:HD12	2.02	0.42
4:L:246:LEU:CD1	4:L:247:LEU:N	2.68	0.42
4:L:346:ILE:HG21	4:L:362:ILE:HD11	2.02	0.42
5:M:51:ASN:ND2	16:h:136:THR:CG2	2.83	0.42
5:M:191:SER:O	5:M:194:LEU:HB2	2.20	0.42
5:M:230:ILE:HG23	5:M:235:LEU:HD11	2.01	0.42
5:M:301:ILE:HG22	5:M:301:ILE:O	2.19	0.42
6:N:109:ALA:HB3	6:N:110:PRO:HD3	2.01	0.42
6:N:338:PRO:O	9:X:170:TRP:HZ3	2.03	0.42
7:O:258:TYR:OH	7:O:272:ASP:HB2	2.20	0.42
7:O:343:TYR:HB3	12:d:52:PRO:HD3	2.02	0.42
15:g:117:ARG:NH2	24:p:10:TYR:OH	2.53	0.42
15:g:123:LEU:CD1	24:p:98:VAL:HG11	2.50	0.42
16:h:55:PHE:HE1	16:h:57:VAL:HA	1.84	0.42
16:h:163:ARG:CG	16:h:165:ASP:HB2	2.32	0.42
16:h:178:PHE:O	16:h:179:ILE:C	2.63	0.42
20:l:48:ARG:NE	20:l:64:PRO:HD2	2.35	0.42
20:l:109:LEU:HG	20:l:109:LEU:O	2.20	0.42
20:l:184:TYR:HD1	23:o:36:GLU:CA	2.32	0.42
21:m:15:PRO:HG2	21:m:18:LEU:HB2	2.01	0.42
21:m:125:PHE:CE1	24:p:133:THR:CG2	2.98	0.42
22:n:100:PRO:HB2	22:n:102:TRP:NE1	2.35	0.42
1:D:37:TRP:O	1:D:37:TRP:CE3	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:90:VAL:O	3:K:91:GLN:C	2.62	0.42
4:L:21:ILE:HG23	4:L:27:ILE:CG2	2.50	0.42
4:L:365:ILE:CD1	4:L:366:MET:HG3	2.24	0.42
4:L:466:PHE:HE2	25:j:700:3PE:H361	1.84	0.42
4:L:491:LEU:HD13	18:j:80:VAL:HG22	2.01	0.42
4:L:552:LEU:HD21	21:m:90:GLY:CA	2.41	0.42
4:L:568:THR:O	4:L:569:LEU:C	2.61	0.42
5:M:108:MET:HB3	5:M:121:LEU:HD13	2.01	0.42
6:N:108:LEU:HD22	6:N:191:LEU:HD22	2.02	0.42
6:N:239:ALA:HA	12:d:47:MET:HE2	2.02	0.42
6:N:243:MET:CG	12:d:44:MET:HE2	2.47	0.42
6:N:317:GLN:HG2	7:O:301:LYS:CB	2.49	0.42
12:d:24:PRO:HD2	12:d:73:TYR:CE2	2.55	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CE2	2.54	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CD2	2.55	0.42
15:g:145:ILE:CG2	24:p:160:LYS:HE2	2.39	0.42
20:l:59:VAL:O	20:l:59:VAL:HG12	2.19	0.42
3:K:1:MET:O	3:K:5:PHE:HB2	2.20	0.42
4:L:117:PHE:HZ	4:L:242:PRO:HG2	1.85	0.42
4:L:138:PHE:HZ	5:M:376:MET:HG2	1.85	0.42
4:L:390:TYR:HE2	18:j:68:TRP:HH2	1.67	0.42
27:L:706:PC1:H341	27:L:706:PC1:C25	2.50	0.42
6:N:180:ALA:O	6:N:184:ILE:HG13	2.20	0.42
7:O:195:LEU:N	7:O:196:PRO:HD2	2.35	0.42
8:U:120:MET:HE1	22:n:24:LEU:CD1	2.49	0.42
11:c:74:GLY:O	11:c:75:LEU:HB2	2.20	0.42
13:e:45:HIS:CD2	16:h:176:LYS:HZ2	2.36	0.42
18:j:71:TRP:HH2	25:j:700:3PE:C3A	2.33	0.42
21:m:8:PRO:HD3	21:m:14:LEU:HD13	2.02	0.42
23:o:59:CYS:SG	23:o:91:GLU:HG2	2.60	0.42
24:p:9:VAL:O	24:p:109:ARG:NH2	2.51	0.42
24:p:132:PHE:O	24:p:136:THR:OG1	2.17	0.42
2:J:37:PHE:HD1	2:J:56:PHE:HE1	1.66	0.41
2:J:43:VAL:HG13	3:K:49:LEU:CD1	2.50	0.41
4:L:52:LEU:CB	24:p:30:ILE:HD11	2.50	0.41
4:L:407:TRP:CE3	4:L:410:LEU:HD21	2.55	0.41
4:L:489:THR:O	4:L:492:ILE:HG13	2.20	0.41
4:L:524:THR:HG22	22:n:78:GLN:CG	2.49	0.41
4:L:525:LEU:HD21	22:n:77:PRO:HB3	2.02	0.41
6:N:108:LEU:CD2	6:N:191:LEU:HD22	2.50	0.41
6:N:215:MET:SD	6:N:244:ILE:CD1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:239:ALA:CB	12:d:47:MET:HG2	2.50	0.41
8:U:128:PHE:HZ	8:U:148:ILE:CD1	2.33	0.41
10:Y:10:SER:O	10:Y:11:TYR:C	2.62	0.41
21:m:41:ALA:HA	22:n:152:GLU:HG2	2.02	0.41
22:n:114:MET:HG3	22:n:115:TYR:CD2	2.55	0.41
2:J:10:SER:O	2:J:14:VAL:HG23	2.20	0.41
2:J:59:TYR:OH	3:K:34:GLU:C	2.63	0.41
6:N:218:ALA:CB	6:N:240:MET:SD	3.08	0.41
6:N:285:MET:HE1	6:N:288:LEU:HD22	2.03	0.41
7:O:179:ILE:HD12	7:O:184:VAL:HG22	2.02	0.41
8:U:93:ILE:CD1	8:U:110:LEU:HD11	2.49	0.41
11:c:61:THR:HG21	12:d:74:PHE:CE1	2.55	0.41
16:h:182:SER:O	16:h:184:LYS:HE3	2.20	0.41
18:j:100:PRO:O	18:j:101:PRO:C	2.63	0.41
18:j:102:ASP:O	18:j:103:ASP:HB2	2.20	0.41
20:l:159:LYS:HE3	20:l:161:TYR:HE1	1.86	0.41
23:o:47:MET:HE1	24:p:123:GLN:NE2	2.35	0.41
4:L:293:LEU:O	4:L:425:ARG:HD2	2.20	0.41
4:L:355:ASP:O	4:L:359:MET:HG3	2.20	0.41
5:M:165:ILE:HG21	6:N:268:THR:HA	2.01	0.41
5:M:258:ALA:O	5:M:259:TYR:C	2.62	0.41
7:O:179:ILE:CD1	7:O:184:VAL:HG22	2.50	0.41
7:O:267:THR:O	7:O:271:GLU:HG3	2.19	0.41
26:h:201:CDL:H732	17:i:84:TYR:HB2	2.01	0.41
17:i:20:ARG:HH11	17:i:20:ARG:HG3	1.84	0.41
17:i:111:LEU:HD11	24:p:20:PRO:HD3	2.02	0.41
22:n:56:ASP:O	22:n:59:ARG:N	2.54	0.41
1:D:67:ASN:HB3	1:D:69:VAL:CG1	2.41	0.41
25:D:501:3PE:H272	6:N:288:LEU:CD1	2.49	0.41
2:J:55:VAL:HB	3:K:41:PHE:HE2	1.86	0.41
25:K:101:3PE:H261	25:K:101:3PE:H232	1.92	0.41
4:L:159:TYR:CZ	22:n:96:CYS:HB2	2.55	0.41
4:L:218:ILE:HD11	25:L:703:3PE:H2A2	2.02	0.41
4:L:286:LEU:HG	4:L:290:ILE:HD11	2.01	0.41
5:M:7:PRO:HG3	14:f:20:PHE:HA	2.01	0.41
5:M:85:LYS:O	5:M:85:LYS:HG2	2.21	0.41
5:M:142:ARG:HG3	5:M:143:LEU:N	2.36	0.41
5:M:247:SER:OG	5:M:304:GLN:NE2	2.53	0.41
7:O:64:GLY:O	7:O:161:ARG:NH1	2.53	0.41
7:O:231:SER:O	7:O:232:ALA:C	2.62	0.41
7:O:239:ASN:HB3	7:O:243:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:141:PRO:HB2	16:h:161:ARG:NE	2.35	0.41
14:f:7:LEU:HG	14:f:11:TRP:HB3	2.02	0.41
15:g:69:PRO:HB2	22:n:109:PRO:CD	2.49	0.41
15:g:71:PHE:CE2	15:g:73:GLY:HA2	2.55	0.41
20:l:122:THR:HG22	20:l:124:VAL:H	1.85	0.41
21:m:42:ARG:O	21:m:43:LEU:C	2.62	0.41
1:D:47:PHE:CD1	6:N:227:ILE:HD11	2.55	0.41
1:D:71:ILE:O	1:D:72:LEU:C	2.62	0.41
2:J:17:LEU:O	2:J:21:LEU:HG	2.20	0.41
3:K:25:HIS:CD2	3:K:88:ASP:OD1	2.70	0.41
4:L:74:MET:CE	5:M:307:TRP:HH2	2.34	0.41
4:L:546:LEU:HD22	21:m:72:ARG:NH2	2.35	0.41
5:M:216:LEU:CG	5:M:220:HIS:CE1	2.88	0.41
5:M:270:ILE:HD11	5:M:395:LEU:HA	2.03	0.41
5:M:270:ILE:HD12	5:M:395:LEU:HD22	2.02	0.41
5:M:350:MET:HE3	5:M:350:MET:HB2	1.80	0.41
6:N:83:THR:HG22	6:N:84:TRP:N	2.35	0.41
6:N:159:ILE:HB	6:N:278:MET:HE1	2.01	0.41
6:N:191:LEU:HG	6:N:191:LEU:O	2.20	0.41
7:O:143:TYR:HD1	7:O:159:LEU:HD22	1.85	0.41
7:O:200:PRO:HG3	7:O:282:PRO:CD	2.47	0.41
7:O:261:TRP:H	7:O:261:TRP:HE3	1.68	0.41
7:O:263:ALA:C	7:O:265:ASP:N	2.77	0.41
16:h:144:SER:HB2	24:p:82:VAL:CG2	2.49	0.41
16:h:175:GLU:HB2	16:h:178:PHE:CE2	2.55	0.41
18:j:44:TYR:CD2	18:j:45:ARG:HG3	2.56	0.41
21:m:18:LEU:HD11	22:n:72:TRP:CB	2.50	0.41
21:m:124:LYS:O	21:m:126:ASN:N	2.54	0.41
23:o:53:LEU:HD23	23:o:56:ARG:NE	2.34	0.41
23:o:117:LEU:O	23:o:120:ALA:N	2.52	0.41
2:J:32:LEU:HD12	2:J:32:LEU:HA	1.86	0.41
4:L:202:MET:HE3	4:L:265:PRO:CB	2.50	0.41
4:L:231:PRO:O	4:L:234:PRO:HD2	2.20	0.41
5:M:263:LEU:CD1	21:m:102:TYR:CD1	3.00	0.41
7:O:262:GLU:O	7:O:265:ASP:HB3	2.21	0.41
7:O:355:LYS:O	12:d:59:HIS:HE1	2.04	0.41
8:U:89:LEU:HD12	18:j:45:ARG:HH12	1.86	0.41
13:e:41:ILE:HD11	16:h:174:PRO:N	2.36	0.41
13:e:49:GLY:O	13:e:52:ALA:N	2.54	0.41
18:j:99:ILE:HA	23:o:108:LEU:HD21	2.03	0.41
20:l:48:ARG:NH2	20:l:64:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:63:GLU:O	20:l:64:PRO:C	2.63	0.41
23:o:111:ARG:HG3	23:o:114:ARG:HH11	1.85	0.41
24:p:71:VAL:HB	24:p:72:PRO:CD	2.50	0.41
24:p:73:ASP:OD1	24:p:73:ASP:N	2.54	0.41
1:D:50:ALA:C	1:D:51:VAL:HG13	2.45	0.41
2:J:5:ILE:O	2:J:6:PHE:C	2.63	0.41
2:J:60:LEU:O	2:J:64:LEU:HB2	2.20	0.41
4:L:258:PHE:O	4:L:261:VAL:HG22	2.21	0.41
5:M:4:ILE:CD1	5:M:41:LEU:HD21	2.51	0.41
5:M:120:ILE:HD11	6:N:264:TRP:CH2	2.55	0.41
5:M:319:HIS:HA	5:M:322:THR:CG2	2.44	0.41
6:N:168:GLY:HA3	6:N:181:TYR:CE1	2.56	0.41
7:O:117:PHE:CZ	7:O:173:MET:HE3	2.54	0.41
7:O:229:VAL:HG13	7:O:229:VAL:O	2.21	0.41
24:p:91:GLN:O	24:p:91:GLN:HG2	2.21	0.41
2:J:72:ALA:O	2:J:76:GLU:HB2	2.21	0.41
4:L:253:VAL:HB	4:L:310:LEU:CD1	2.51	0.41
4:L:368:PHE:HB3	4:L:445:GLU:OE1	2.20	0.41
4:L:482:MET:CE	4:L:486:LEU:HB3	2.51	0.41
4:L:571:THR:O	4:L:574:THR:HG22	2.20	0.41
5:M:160:LEU:O	5:M:164:LEU:HD13	2.21	0.41
5:M:164:LEU:HB3	5:M:174:LEU:HD11	2.03	0.41
5:M:177:MET:HE3	5:M:177:MET:HB3	1.70	0.41
7:O:105:ASP:OD1	7:O:106:ILE:N	2.53	0.41
7:O:287:ASP:HB3	7:O:290:THR:HG23	2.02	0.41
7:O:332:ARG:O	7:O:338:LYS:HA	2.21	0.41
16:h:96:ALA:CB	24:p:63:TYR:HD1	2.29	0.41
19:k:20:MET:HE2	19:k:20:MET:HB3	1.98	0.41
19:k:81:PHE:O	19:k:85:VAL:HG23	2.21	0.41
20:l:129:MET:HE3	20:l:129:MET:HB2	1.89	0.41
2:J:72:ALA:O	2:J:73:MET:C	2.64	0.41
2:J:93:VAL:O	2:J:97:ILE:HG12	2.20	0.41
3:K:93:LEU:HD13	6:N:57:THR:CG2	2.50	0.41
4:L:58:ASN:HA	4:L:58:ASN:HD22	1.65	0.41
4:L:68:TRP:CE3	4:L:76:LEU:CD2	3.04	0.41
4:L:211:ILE:N	4:L:212:PRO:CD	2.82	0.41
4:L:321:GLN:NE2	4:L:324:LEU:HD13	2.36	0.41
4:L:511:LEU:CD1	22:n:36:LYS:HA	2.50	0.41
4:L:570:HIS:O	4:L:573:MET:N	2.54	0.41
26:L:705:CDL:H581	26:L:705:CDL:H741	2.02	0.41
5:M:22:LYS:HE3	5:M:26:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:51:ASN:O	16:h:135:LYS:HD2	2.21	0.41
5:M:53:SER:O	5:M:54:ASN:C	2.63	0.41
5:M:178:ILE:O	5:M:179:LEU:C	2.60	0.41
5:M:210:TYR:HB2	5:M:268:GLY:HA3	2.03	0.41
5:M:218:LYS:HE3	5:M:218:LYS:HB3	1.58	0.41
5:M:250:LEU:HD12	5:M:250:LEU:C	2.40	0.41
5:M:329:LEU:HD23	5:M:437:MET:CE	2.49	0.41
6:N:109:ALA:O	6:N:112:HIS:ND1	2.52	0.41
6:N:125:HIS:CE1	6:N:129:ILE:HD11	2.56	0.41
6:N:175:MET:O	6:N:176:ARG:C	2.63	0.41
6:N:215:MET:HE3	6:N:215:MET:HB3	1.96	0.41
6:N:233:LEU:CD2	6:N:241:LEU:HD12	2.26	0.41
6:N:307:THR:CG2	6:N:308:ASN:N	2.79	0.41
6:N:307:THR:O	7:O:319:ILE:N	2.50	0.41
6:N:331:ILE:HD12	6:N:335:MET:HE3	2.03	0.41
7:O:52:LYS:HD3	7:O:152:SER:O	2.20	0.41
7:O:90:GLY:H	7:O:93:TYR:HB2	1.85	0.41
7:O:104:LEU:HD23	7:O:104:LEU:HA	1.90	0.41
7:O:132:GLN:OE1	28:O:402:ADP:N6	2.45	0.41
7:O:254:GLU:OE2	7:O:276:LEU:HB2	2.21	0.41
7:O:354:LEU:HD12	7:O:354:LEU:HA	1.95	0.41
8:U:128:PHE:CZ	8:U:148:ILE:CD1	3.04	0.41
11:c:55:TRP:NE1	12:d:66:THR:CG2	2.84	0.41
12:d:25:LYS:HE3	12:d:27:ASN:OD1	2.21	0.41
13:e:65:GLU:CD	13:e:71:LYS:HB2	2.46	0.41
13:e:96:PRO:O	13:e:99:SER:N	2.53	0.41
13:e:101:ARG:HA	13:e:101:ARG:HE	1.86	0.41
14:f:47:GLU:O	14:f:48:LEU:C	2.60	0.41
15:g:117:ARG:NH2	24:p:108:GLU:OE1	2.54	0.41
17:i:29:SER:O	17:i:32:GLU:HB2	2.21	0.41
17:i:74:HIS:O	17:i:78:PRO:HG2	2.20	0.41
20:l:44:THR:HG23	20:l:46:GLU:HG2	2.03	0.41
20:l:156:VAL:CG1	23:o:95:TYR:CZ	2.91	0.41
22:n:94:TYR:HB3	22:n:178:PRO:HD2	2.03	0.41
23:o:5:LEU:HD12	23:o:5:LEU:N	2.35	0.41
23:o:17:PRO:HG3	23:o:106:ARG:CA	2.48	0.41
23:o:53:LEU:HD11	24:p:122:GLN:HG3	2.03	0.41
23:o:71:ARG:NH1	23:o:72:ASP:OD1	2.54	0.41
24:p:40:VAL:O	24:p:44:PRO:HG2	2.21	0.41
4:L:52:LEU:O	4:L:53:MET:C	2.62	0.41
4:L:56:HIS:N	23:o:74:PHE:CE1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:6:LEU:O	5:M:7:PRO:C	2.60	0.41
5:M:72:LEU:O	5:M:76:MET:N	2.45	0.41
25:M:503:3PE:O14	12:d:47:MET:HE3	2.20	0.41
7:O:117:PHE:CE1	7:O:128:SER:CB	2.96	0.41
7:O:268:LYS:HA	7:O:271:GLU:OE1	2.21	0.41
8:U:133:ILE:CG2	8:U:134:ASP:N	2.84	0.41
9:X:167:PHE:HD2	9:X:170:TRP:HE1	1.65	0.41
10:Y:5:LYS:C	10:Y:7:PHE:N	2.77	0.41
10:Y:51:THR:HG23	10:Y:52:LEU:N	2.35	0.41
12:d:45:ASP:O	12:d:46:ASN:C	2.62	0.41
14:f:36:ALA:O	14:f:37:PHE:C	2.61	0.41
16:h:60:SER:HB2	22:n:107:TRP:CD1	2.56	0.41
17:i:80:TRP:HE1	24:p:44:PRO:HG2	1.86	0.41
19:k:57:TRP:HA	19:k:60:MET:HB3	2.02	0.41
21:m:59:HIS:O	21:m:60:ILE:C	2.64	0.41
25:m:201:3PE:H362	25:m:201:3PE:H332	1.91	0.41
22:n:139:GLN:O	22:n:140:LEU:C	2.64	0.41
22:n:157:ALA:O	22:n:158:ARG:HB2	2.21	0.41
22:n:167:TRP:CD1	22:n:167:TRP:H	2.38	0.41
4:L:434:LYS:NZ	19:k:66:ASN:HA	2.36	0.40
27:L:706:PC1:H382	27:L:706:PC1:H351	1.93	0.40
5:M:151:PHE:HZ	6:N:291:PHE:CA	2.34	0.40
7:O:351:TRP:CZ3	11:c:41:TRP:HH2	2.39	0.40
8:U:91:ASP:OD2	19:k:48:ARG:NH1	2.53	0.40
16:h:87:THR:O	16:h:91:ILE:HG13	2.21	0.40
16:h:148:GLU:O	16:h:152:LYS:HG3	2.21	0.40
18:j:47:PHE:O	18:j:48:PRO:C	2.62	0.40
20:l:159:LYS:HE3	20:l:161:TYR:CE1	2.56	0.40
21:m:123:ARG:O	24:p:140:GLN:NE2	2.48	0.40
25:m:201:3PE:H2E2	25:m:201:3PE:H2B1	1.70	0.40
22:n:41:ALA:C	22:n:43:LEU:N	2.78	0.40
25:D:501:3PE:H322	25:D:501:3PE:H351	1.79	0.40
4:L:3:ILE:HG22	4:L:49:LEU:CD2	2.51	0.40
4:L:72:ASN:ND2	5:M:459:MET:HG2	2.36	0.40
4:L:138:PHE:CZ	5:M:376:MET:HG2	2.56	0.40
4:L:141:PHE:CD2	5:M:375:LEU:CD2	2.94	0.40
4:L:210:LEU:HD12	4:L:270:ASN:HD21	1.86	0.40
4:L:210:LEU:O	4:L:211:ILE:C	2.62	0.40
4:L:532:ILE:HG21	20:l:133:LEU:HD22	2.03	0.40
5:M:248:ILE:HG13	5:M:249:ILE:H	1.85	0.40
5:M:259:TYR:HB2	5:M:260:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:303:ILE:HG13	5:M:385:LEU:HD23	2.03	0.40
5:M:394:ILE:O	5:M:398:ILE:HG13	2.22	0.40
6:N:22:SER:HB2	13:e:6:ILE:HG22	2.03	0.40
6:N:146:TYR:CG	6:N:147:PRO:N	2.88	0.40
6:N:224:SER:HB2	6:N:229:SER:HB2	2.01	0.40
7:O:219:GLN:NE2	7:O:219:GLN:HA	2.36	0.40
7:O:263:ALA:C	7:O:265:ASP:H	2.30	0.40
13:e:49:GLY:HA2	13:e:52:ALA:HB3	2.02	0.40
15:g:112:MET:HE3	15:g:115:TRP:CE3	2.56	0.40
20:l:122:THR:CG2	20:l:129:MET:HE1	2.45	0.40
21:m:28:GLU:HG2	21:m:31:ARG:NH2	2.37	0.40
21:m:49:LEU:HD11	22:n:137:VAL:HG12	2.03	0.40
22:n:148:GLY:O	22:n:149:ILE:C	2.63	0.40
1:D:61:TRP:CD1	1:D:61:TRP:N	2.89	0.40
4:L:22:SER:HA	4:L:27:ILE:CG2	2.52	0.40
4:L:56:HIS:CA	23:o:74:PHE:CD1	2.98	0.40
4:L:138:PHE:CD1	26:h:201:CDL:H271	2.56	0.40
4:L:324:LEU:HB3	4:L:395:ILE:CD1	2.51	0.40
4:L:400:ASN:HD22	4:L:409:LEU:HD11	1.85	0.40
27:L:706:PC1:H331	27:L:706:PC1:H362	1.79	0.40
5:M:197:LEU:O	5:M:201:MET:HB2	2.21	0.40
6:N:106:LEU:HD21	6:N:138:PRO:HB2	2.03	0.40
7:O:248:LYS:HE2	7:O:248:LYS:HB3	1.82	0.40
8:U:93:ILE:CG1	8:U:110:LEU:HD11	2.51	0.40
12:d:107:LYS:HB3	12:d:111:GLU:HB3	2.04	0.40
15:g:140:PHE:HB3	24:p:75:THR:CG2	2.51	0.40
17:i:99:SER:O	17:i:100:SER:C	2.64	0.40
17:i:106:PRO:HD2	23:o:64:ILE:HG21	2.03	0.40
23:o:52:THR:O	23:o:53:LEU:C	2.62	0.40
24:p:43:TRP:HB3	24:p:44:PRO:HD3	2.03	0.40
4:L:399:ILE:HG22	4:L:409:LEU:CD1	2.51	0.40
5:M:264:LEU:HD23	21:m:98:LEU:CD1	2.51	0.40
5:M:313:THR:HG21	5:M:456:GLY:CA	2.47	0.40
5:M:435:THR:HG23	5:M:436:LEU:N	2.36	0.40
5:M:437:MET:O	5:M:438:ALA:C	2.62	0.40
6:N:59:TYR:O	6:N:63:GLN:HG2	2.21	0.40
6:N:202:LEU:HD21	13:e:3:PHE:CE1	2.56	0.40
6:N:211:LEU:CD2	6:N:333:SER:HB2	2.45	0.40
7:O:117:PHE:HE1	7:O:173:MET:HE1	1.80	0.40
7:O:170:LEU:CD2	7:O:184:VAL:HG13	2.51	0.40
7:O:276:LEU:C	7:O:276:LEU:HD12	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:110:TYR:HB2	25:m:202:3PE:H11	2.02	0.40
12:d:11:LEU:HD11	13:e:4:LEU:HD12	2.02	0.40
18:j:51:THR:O	18:j:52:ARG:C	2.61	0.40
18:j:71:TRP:HZ3	18:j:72:ARG:NH2	2.19	0.40
20:l:119:THR:CG2	21:m:13:THR:HG23	2.52	0.40
23:o:4:HIS:ND1	23:o:106:ARG:NH1	2.70	0.40
23:o:25:PHE:CD2	23:o:108:LEU:HB3	2.56	0.40
4:L:277:MET:HG3	4:L:318:GLY:HA3	2.04	0.40
4:L:371:SER:O	4:L:374:VAL:HG12	2.21	0.40
27:L:706:PC1:H3C2	27:L:706:PC1:H391	1.89	0.40
5:M:62:SER:HB2	5:M:110:PHE:O	2.22	0.40
5:M:151:PHE:CZ	6:N:291:PHE:CB	2.97	0.40
5:M:159:PRO:HG2	25:M:501:3PE:H391	2.03	0.40
5:M:186:LEU:CB	5:M:253:LEU:HD13	2.52	0.40
5:M:230:ILE:HG23	5:M:235:LEU:CD1	2.51	0.40
5:M:336:ARG:NH2	5:M:429:SER:HA	2.36	0.40
6:N:132:THR:HB	6:N:209:ILE:HG12	2.03	0.40
12:d:21:LEU:CD1	12:d:81:TYR:HA	2.51	0.40
13:e:86:LEU:HD23	13:e:86:LEU:HA	1.93	0.40
15:g:112:MET:HE1	24:p:94:ARG:HG3	2.04	0.40
17:i:70:PHE:O	17:i:71:ALA:C	2.65	0.40
17:i:120:MET:SD	17:i:123:PHE:CZ	3.15	0.40
19:k:56:ALA:O	19:k:60:MET:N	2.53	0.40
21:m:124:LYS:HG2	21:m:125:PHE:CD2	2.57	0.40
24:p:45:VAL:O	24:p:46:THR:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	37/463 (8%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	151/172 (88%)	140 (93%)	11 (7%)	0	100	100
3	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
4	L	604/607 (100%)	572 (95%)	32 (5%)	0	100	100
5	M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	65
7	O	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
8	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
9	X	25/172 (14%)	23 (92%)	2 (8%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	45 (100%)	0	0	100	100
12	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
13	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
14	f	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
15	g	98/151 (65%)	92 (94%)	6 (6%)	0	100	100
16	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
17	i	88/128 (69%)	79 (90%)	9 (10%)	0	100	100
18	j	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
19	k	70/104 (67%)	67 (96%)	3 (4%)	0	100	100
20	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
21	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
22	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	52
23	o	117/137 (85%)	113 (97%)	4 (3%)	0	100	100
24	p	168/176 (96%)	150 (89%)	18 (11%)	0	100	100
All	All	3761/4813 (78%)	3571 (95%)	188 (5%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	109	ALA
22	n	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	34/395 (9%)	34 (100%)	0	100	100
2	J	126/138 (91%)	123 (98%)	3 (2%)	43	65
3	K	87/88 (99%)	87 (100%)	0	100	100
4	L	549/550 (100%)	547 (100%)	2 (0%)	84	84
5	M	415/415 (100%)	414 (100%)	1 (0%)	87	88
6	N	307/308 (100%)	306 (100%)	1 (0%)	86	86
7	O	283/309 (92%)	283 (100%)	0	100	100
8	U	80/135 (59%)	79 (99%)	1 (1%)	61	74
9	X	23/154 (15%)	23 (100%)	0	100	100
10	Y	104/107 (97%)	104 (100%)	0	100	100
11	c	41/67 (61%)	41 (100%)	0	100	100
12	d	107/107 (100%)	107 (100%)	0	100	100
13	e	91/94 (97%)	91 (100%)	0	100	100
14	f	48/53 (91%)	48 (100%)	0	100	100
15	g	91/129 (70%)	91 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	87/120 (72%)	86 (99%)	1 (1%)	65	76
18	j	62/87 (71%)	62 (100%)	0	100	100
19	k	55/78 (70%)	55 (100%)	0	100	100
20	l	141/161 (88%)	141 (100%)	0	100	100
21	m	111/114 (97%)	111 (100%)	0	100	100
22	n	162/164 (99%)	161 (99%)	1 (1%)	78	81
23	o	109/121 (90%)	109 (100%)	0	100	100
24	p	154/158 (98%)	154 (100%)	0	100	100
All	All	3390/4214 (80%)	3380 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	55	VAL
2	J	60	LEU
2	J	63	MET
4	L	3	ILE
4	L	69	VAL
5	M	218	LYS
6	N	159	ILE
8	U	74	LEU
17	i	72	VAL
22	n	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	36	GLN
1	D	38	GLN
1	D	60	HIS
3	K	7	ASN
3	K	25	HIS
4	L	2	ASN
4	L	25	ASN
4	L	58	ASN
4	L	135	ASN
4	L	136	ASN
4	L	139	GLN
4	L	170	GLN
4	L	192	ASN
4	L	194	ASN
4	L	199	GLN
4	L	209	ASN
4	L	264	HIS
4	L	269	ASN
4	L	296	ASN
4	L	321	GLN
4	L	354	GLN
4	L	400	ASN
4	L	446	ASN
4	L	452	ASN
4	L	579	ASN
5	M	26	ASN
5	M	44	GLN
5	M	51	ASN
5	M	81	GLN

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Mol	Chain	Res	Type
5	M	92	GLN
5	M	170	HIS
5	M	175	ASN
5	M	213	HIS
5	M	279	GLN
5	M	293	HIS
5	M	304	GLN
5	M	374	ASN
5	M	415	GLN
6	N	120	GLN
6	N	134	GLN
6	N	174	GLN
6	N	273	ASN
6	N	289	ASN
6	N	310	ASN
6	N	342	GLN
7	O	80	GLN
7	O	175	ASN
7	O	219	GLN
7	O	286	GLN
7	O	292	HIS
7	O	306	ASN
7	O	323	GLN
10	Y	19	GLN
10	Y	91	ASN
11	c	62	HIS
12	d	59	HIS
12	d	79	GLN
16	h	109	HIS
16	h	170	GLN
16	h	181	HIS
17	i	83	HIS
18	j	41	GLN
19	k	39	GLN
19	k	66	ASN
20	l	83	GLN
20	l	91	GLN
20	l	106	HIS
21	m	75	ASN
21	m	79	ASN
22	n	12	HIS
22	n	13	GLN

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Mol	Chain	Res	Type
22	n	14	GLN
22	n	26	HIS
22	n	33	HIS
22	n	53	ASN
22	n	62	GLN
22	n	74	ASN
22	n	76	HIS
23	o	61	HIS
24	p	67	GLN
24	p	91	GLN
24	p	100	GLN
24	p	124	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.11	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	L	705	-	80,80,99	1.01	4 (5%)	86,92,111	1.14	7 (8%)
25	3PE	L	703	-	46,46,50	0.96	2 (4%)	49,51,55	1.04	3 (6%)
25	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.08	4 (7%)
25	3PE	D	501	-	37,37,50	1.05	2 (5%)	40,42,55	1.17	4 (10%)
26	CDL	L	704	-	76,76,99	1.03	4 (5%)	82,88,111	1.19	5 (6%)
26	CDL	d	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.31	7 (9%)
29	EHZ	n	201	-	29,31,37	1.76	7 (24%)	37,41,47	2.04	12 (32%)
28	ADP	O	402	-	28,29,29	1.37	5 (17%)	43,45,45	1.88	10 (23%)
26	CDL	h	201	-	69,69,99	1.09	4 (5%)	75,81,111	1.23	7 (9%)
25	3PE	M	503	-	50,50,50	0.91	2 (4%)	53,55,55	1.06	4 (7%)
25	3PE	m	201	-	50,50,50	0.90	2 (4%)	53,55,55	1.08	4 (7%)
25	3PE	m	202	-	40,40,50	1.01	2 (5%)	43,45,55	1.14	3 (6%)
25	3PE	L	701	-	48,48,50	0.92	2 (4%)	51,53,55	1.14	4 (7%)
25	3PE	i	201	-	39,39,50	1.05	2 (5%)	42,44,55	1.07	2 (4%)
25	3PE	O	401	-	43,43,50	0.99	2 (4%)	46,48,55	1.05	3 (6%)
25	3PE	M	501	-	36,36,50	1.08	2 (5%)	39,41,55	1.22	3 (7%)
25	3PE	L	702	-	38,38,50	1.06	2 (5%)	41,43,55	1.16	2 (4%)
27	PC1	L	706	-	49,49,53	0.98	2 (4%)	55,57,61	1.10	4 (7%)
25	3PE	j	700	-	39,39,50	1.03	2 (5%)	42,44,55	1.24	4 (9%)

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
25	3PE	K	101	-	-	14/49/49/54	-
26	CDL	L	705	-	-	19/91/91/110	-
25	3PE	L	703	-	-	8/50/50/54	-
25	3PE	M	502	-	-	16/54/54/54	-
25	3PE	D	501	-	-	8/41/41/54	-
26	CDL	L	704	-	-	24/87/87/110	-
26	CDL	d	201	-	-	24/77/77/110	-
29	EHZ	n	201	-	-	14/39/39/45	-
28	ADP	O	402	-	-	1/16/32/32	0/3/3/3
26	CDL	h	201	-	-	24/80/80/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	M	503	-	-	6/54/54/54	-
25	3PE	m	201	-	-	13/54/54/54	-
25	3PE	m	202	-	-	7/44/44/54	-
25	3PE	L	701	-	-	13/52/52/54	-
25	3PE	i	201	-	-	13/43/43/54	-
25	3PE	O	401	-	-	9/47/47/54	-
25	3PE	M	501	-	-	7/40/40/54	-
25	3PE	L	702	-	-	16/42/42/54	-
27	PC1	L	706	-	-	9/53/53/57	-
25	3PE	j	700	-	-	5/43/43/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C15-N2	4.88	1.45	1.33
29	n	201	EHZ	C12-N1	4.72	1.44	1.33
28	O	402	ADP	C5-C4	4.41	1.46	1.39
27	L	706	PC1	O31-C31	4.32	1.45	1.33
25	L	702	3PE	O31-C31	4.31	1.45	1.33
25	O	401	3PE	O31-C31	4.31	1.45	1.33
25	i	201	3PE	O31-C31	4.29	1.45	1.33
25	M	501	3PE	O31-C31	4.26	1.45	1.33
26	d	201	CDL	OB8-CB7	4.26	1.45	1.33
25	L	703	3PE	O31-C31	4.24	1.45	1.33
26	L	704	CDL	OB6-CB5	4.23	1.46	1.34
25	i	201	3PE	O21-C21	4.23	1.46	1.34
25	j	700	3PE	O31-C31	4.23	1.45	1.33
25	K	101	3PE	O31-C31	4.22	1.45	1.33
26	L	705	CDL	OA8-CA7	4.20	1.45	1.33
25	M	503	3PE	O31-C31	4.20	1.45	1.33
25	m	202	3PE	O31-C31	4.19	1.45	1.33
26	d	201	CDL	OA8-CA7	4.19	1.45	1.33
25	D	501	3PE	O31-C31	4.19	1.45	1.33
26	h	201	CDL	OA8-CA7	4.18	1.45	1.33
25	m	201	3PE	O31-C31	4.18	1.45	1.33
26	L	705	CDL	OB8-CB7	4.17	1.45	1.33
26	L	704	CDL	OB8-CB7	4.12	1.45	1.33
25	M	502	3PE	O31-C31	4.12	1.45	1.33
26	h	201	CDL	OB8-CB7	4.11	1.45	1.33
26	h	201	CDL	OB6-CB5	4.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	702	3PE	O21-C21	4.10	1.45	1.34
27	L	706	PC1	O21-C21	4.07	1.45	1.34
26	L	705	CDL	OA6-CA5	4.07	1.45	1.34
25	L	703	3PE	O21-C21	4.06	1.45	1.34
26	L	704	CDL	OA8-CA7	4.06	1.45	1.33
25	L	701	3PE	O31-C31	4.05	1.45	1.33
25	M	501	3PE	O21-C21	4.01	1.45	1.34
25	D	501	3PE	O21-C21	4.00	1.45	1.34
26	L	705	CDL	OB6-CB5	3.98	1.45	1.34
25	j	700	3PE	O21-C21	3.98	1.45	1.34
26	h	201	CDL	OA6-CA5	3.98	1.45	1.34
25	M	502	3PE	O21-C21	3.97	1.45	1.34
26	d	201	CDL	OA6-CA5	3.96	1.45	1.34
25	L	701	3PE	O21-C21	3.95	1.45	1.34
25	m	202	3PE	O21-C21	3.95	1.45	1.34
25	M	503	3PE	O21-C21	3.94	1.45	1.34
25	O	401	3PE	O21-C21	3.93	1.45	1.34
26	d	201	CDL	OB6-CB5	3.93	1.45	1.34
25	K	101	3PE	O21-C21	3.92	1.45	1.34
26	L	704	CDL	OA6-CA5	3.89	1.45	1.34
25	m	201	3PE	O21-C21	3.82	1.45	1.34
29	n	201	EHZ	P1-O7	2.70	1.64	1.54
29	n	201	EHZ	O4-C15	-2.58	1.18	1.23
28	O	402	ADP	C5-C6	2.55	1.48	1.41
29	n	201	EHZ	O3-C12	-2.44	1.18	1.23
29	n	201	EHZ	P1-OP3	-2.40	1.45	1.54
29	n	201	EHZ	C9-S1	2.31	1.81	1.76
28	O	402	ADP	C8-N7	2.31	1.36	1.31
28	O	402	ADP	C5-N7	-2.28	1.34	1.39
28	O	402	ADP	C4-N9	-2.04	1.33	1.37

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	402	ADP	C5-C4-N3	-5.58	119.04	126.72
29	n	201	EHZ	C8-C9-S1	5.57	120.59	113.56
29	n	201	EHZ	C14-C13-C12	-5.00	104.06	112.39
28	O	402	ADP	N3-C4-N9	4.61	135.01	127.17
25	j	700	3PE	O21-C21-C22	4.53	121.28	111.48
26	d	201	CDL	OA6-CA5-C11	4.49	121.20	111.48
26	h	201	CDL	OB6-CB5-C51	4.44	121.08	111.48
26	L	704	CDL	OB6-CB5-C51	4.42	121.05	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	706	PC1	O21-C21-C22	4.36	120.91	111.48
26	d	201	CDL	OB6-CB5-C51	4.32	120.82	111.48
25	M	501	3PE	O21-C21-C22	4.24	120.66	111.48
26	L	705	CDL	OB6-CB5-C51	4.05	120.24	111.48
25	i	201	3PE	O21-C21-C22	4.05	120.24	111.48
25	M	502	3PE	O21-C21-C22	4.02	120.19	111.48
25	L	702	3PE	O21-C21-C22	4.02	120.18	111.48
25	L	701	3PE	O21-C21-C22	3.99	120.11	111.48
26	h	201	CDL	OA6-CA5-C11	3.97	120.06	111.48
26	L	704	CDL	OA6-CA5-C11	3.96	120.05	111.48
25	D	501	3PE	O21-C21-C22	3.94	120.01	111.48
25	K	101	3PE	O21-C21-C22	3.86	119.83	111.48
25	O	401	3PE	O21-C21-C22	3.72	119.54	111.48
26	L	705	CDL	OA6-CA5-C11	3.72	119.54	111.48
25	m	201	3PE	O21-C21-C22	3.71	119.51	111.48
28	O	402	ADP	C2-N3-C4	3.68	120.82	111.83
25	m	202	3PE	O21-C21-C22	3.65	119.38	111.48
25	M	503	3PE	O21-C21-C22	3.59	119.25	111.48
25	L	703	3PE	O21-C21-C22	3.47	118.98	111.48
28	O	402	ADP	N3-C2-N1	-3.36	123.49	128.58
29	n	201	EHZ	C13-C12-N1	3.31	122.37	116.34
29	n	201	EHZ	C14-N2-C15	-3.29	116.63	122.55
25	M	501	3PE	C2-O21-C21	-3.25	110.02	117.80
25	K	101	3PE	C2-O21-C21	-3.22	110.08	117.80
28	O	402	ADP	C4-C5-N7	-3.21	106.92	110.58
26	d	201	CDL	CA4-OA6-CA5	-3.20	110.15	117.80
25	j	700	3PE	C2-O21-C21	-3.19	110.16	117.80
28	O	402	ADP	C4-N9-C8	3.19	109.09	105.74
25	L	702	3PE	O31-C31-C32	3.15	121.43	111.83
29	n	201	EHZ	C11-N1-C12	-3.13	117.00	122.82
25	m	202	3PE	C2-O21-C21	-3.11	110.36	117.80
25	M	502	3PE	C2-O21-C21	-3.04	110.52	117.80
26	h	201	CDL	OB8-CB7-C71	2.95	120.84	111.83
25	m	201	3PE	C2-O21-C21	-2.94	110.75	117.80
25	i	201	3PE	O31-C31-C32	2.94	120.80	111.83
26	L	705	CDL	OB8-CB7-C71	2.86	120.57	111.83
26	L	704	CDL	OB8-CB7-C71	2.83	120.46	111.83
25	j	700	3PE	O31-C31-C32	2.82	120.42	111.83
26	d	201	CDL	OB8-CB7-C71	2.80	120.38	111.83
25	K	101	3PE	O31-C31-C32	2.79	120.35	111.83
26	d	201	CDL	OA8-CA7-C31	2.78	120.32	111.83
25	M	502	3PE	O31-C31-C32	2.78	120.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	705	CDL	CA4-OA6-CA5	-2.77	111.17	117.80
25	m	202	3PE	O31-C31-C32	2.75	120.23	111.83
25	M	503	3PE	O31-C31-C32	2.75	120.21	111.83
25	m	201	3PE	O31-C31-C32	2.74	120.18	111.83
25	L	701	3PE	O31-C31-C32	2.73	120.17	111.83
25	O	401	3PE	C2-O21-C21	-2.73	111.27	117.80
28	O	402	ADP	O4'-C1'-N9	2.70	113.28	108.09
26	L	705	CDL	CB4-OB6-CB5	-2.70	111.34	117.80
29	n	201	EHZ	OP3-P1-O9	-2.69	100.37	110.83
25	M	503	3PE	C2-O21-C21	-2.68	111.37	117.80
26	L	705	CDL	OA8-CA7-C31	2.68	120.02	111.83
26	h	201	CDL	CA4-OA6-CA5	-2.67	111.39	117.80
27	L	706	PC1	O31-C31-C32	2.67	119.97	111.83
25	M	501	3PE	O31-C31-C32	2.66	119.94	111.83
25	O	401	3PE	O31-C31-C32	2.63	119.84	111.83
25	L	703	3PE	O31-C31-C32	2.62	119.81	111.83
26	L	704	CDL	OA8-CA7-C31	2.62	119.81	111.83
29	n	201	EHZ	C10-S1-C9	2.61	109.56	101.84
27	L	706	PC1	C2-O21-C21	-2.58	111.61	117.80
25	D	501	3PE	O31-C31-C32	2.58	119.71	111.83
25	D	501	3PE	C2-O21-C21	-2.58	111.63	117.80
26	L	704	CDL	CA4-OA6-CA5	-2.57	111.64	117.80
26	h	201	CDL	OA8-CA7-C31	2.57	119.67	111.83
25	L	703	3PE	C2-O21-C21	-2.56	111.67	117.80
25	L	701	3PE	C2-O21-C21	-2.54	111.72	117.80
26	h	201	CDL	CB4-OB6-CB5	-2.53	111.74	117.80
28	O	402	ADP	C5-N7-C8	2.47	107.33	103.45
29	n	201	EHZ	O2-C9-S1	-2.46	119.55	122.68
29	n	201	EHZ	O2-C9-C8	-2.46	119.86	123.74
28	O	402	ADP	N9-C8-N7	-2.27	110.71	113.94
25	m	201	3PE	O21-C21-O22	-2.21	118.54	123.70
26	d	201	CDL	OB6-CB5-OB7	-2.19	118.58	123.70
26	L	705	CDL	OA6-CA5-OA7	-2.18	118.60	123.70
29	n	201	EHZ	C16-C15-N2	2.18	120.62	116.48
25	L	701	3PE	O21-C21-O22	-2.15	118.68	123.70
29	n	201	EHZ	O3-C12-N1	-2.14	118.83	123.03
25	j	700	3PE	O21-C21-O22	-2.12	118.74	123.70
28	O	402	ADP	C6-C5-N7	2.11	136.16	132.09
29	n	201	EHZ	C5-C6-C7	-2.11	108.87	114.68
25	M	503	3PE	O21-C21-O22	-2.10	118.78	123.70
27	L	706	PC1	C11-C12-N	-2.09	109.12	115.82
26	d	201	CDL	OA6-CA5-OA7	-2.08	118.84	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	3PE	O21-C21-O22	-2.06	118.88	123.70
25	M	502	3PE	O21-C21-O22	-2.06	118.89	123.70
26	h	201	CDL	OA8-CA7-OA9	-2.03	118.56	123.63
25	D	501	3PE	O21-C21-O22	-2.01	119.01	123.70

There are no chirality outliers.

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O12
25	K	101	3PE	C11-O13-P-O11
25	K	101	3PE	C11-O13-P-O12
25	L	701	3PE	C1-O11-P-O12
25	L	701	3PE	C1-O11-P-O13
25	L	701	3PE	O22-C21-O21-C2
25	L	701	3PE	C22-C21-O21-C2
25	L	702	3PE	C1-O11-P-O14
25	L	702	3PE	C11-O13-P-O11
25	L	702	3PE	C11-O13-P-O12
25	L	702	3PE	C11-O13-P-O14
25	L	702	3PE	O32-C31-O31-C3
25	L	702	3PE	C32-C31-O31-C3
25	L	702	3PE	C22-C21-O21-C2
25	M	501	3PE	C1-O11-P-O13
25	M	502	3PE	C1-O11-P-O12
25	M	502	3PE	C1-O11-P-O13
25	M	502	3PE	C1-O11-P-O14
25	M	502	3PE	C11-O13-P-O11
25	M	502	3PE	C11-O13-P-O12
25	M	502	3PE	C11-O13-P-O14
25	i	201	3PE	C1-O11-P-O12
25	i	201	3PE	C1-O11-P-O13
25	m	201	3PE	C1-O11-P-O12
25	m	201	3PE	C11-O13-P-O11
25	m	201	3PE	C11-O13-P-O12
25	m	202	3PE	C1-O11-P-O12
25	m	202	3PE	C1-O11-P-O13
25	m	202	3PE	C1-O11-P-O14
25	m	202	3PE	C22-C21-O21-C2
26	L	704	CDL	CA2-OA2-PA1-OA3
26	L	704	CDL	CA2-OA2-PA1-OA4
26	L	704	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
26	L	704	CDL	CB2-OB2-PB2-OB3
26	L	704	CDL	C51-CB5-OB6-CB4
26	L	705	CDL	CA2-OA2-PA1-OA3
26	L	705	CDL	CA2-OA2-PA1-OA4
26	L	705	CDL	CA2-OA2-PA1-OA5
26	L	705	CDL	CB3-OB5-PB2-OB2
26	L	705	CDL	CB3-OB5-PB2-OB3
26	L	705	CDL	CB3-OB5-PB2-OB4
26	d	201	CDL	CA2-C1-CB2-OB2
26	d	201	CDL	CA3-OA5-PA1-OA2
26	d	201	CDL	CA3-OA5-PA1-OA3
26	d	201	CDL	CB2-OB2-PB2-OB3
26	d	201	CDL	CB2-OB2-PB2-OB5
26	d	201	CDL	C51-CB5-OB6-CB4
26	h	201	CDL	CA2-OA2-PA1-OA3
26	h	201	CDL	CA2-OA2-PA1-OA4
26	h	201	CDL	CA2-OA2-PA1-OA5
26	h	201	CDL	CA3-OA5-PA1-OA2
26	h	201	CDL	CA3-OA5-PA1-OA4
26	h	201	CDL	CB2-OB2-PB2-OB3
26	h	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	C51-CB5-OB6-CB4
27	L	706	PC1	C1-O11-P-O14
27	L	706	PC1	C22-C21-O21-C2
27	L	706	PC1	O32-C31-O31-C3
27	L	706	PC1	C32-C31-O31-C3
29	n	201	EHZ	C6-C7-C8-C9
29	n	201	EHZ	S1-C10-C11-N1
29	n	201	EHZ	C15-C16-C17-C18
29	n	201	EHZ	C15-C16-C17-C19
29	n	201	EHZ	C15-C16-C17-C20
29	n	201	EHZ	O5-C16-C17-C18
29	n	201	EHZ	O5-C16-C17-C19
29	n	201	EHZ	O5-C16-C17-C20
29	n	201	EHZ	O2-C9-S1-C10
29	n	201	EHZ	C8-C9-S1-C10
25	K	101	3PE	O32-C31-O31-C3
25	M	503	3PE	O32-C31-O31-C3
25	j	700	3PE	O32-C31-O31-C3
25	L	702	3PE	O22-C21-O21-C2
25	m	201	3PE	O22-C21-O21-C2
25	m	202	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
26	L	704	CDL	OB7-CB5-OB6-CB4
26	d	201	CDL	OB7-CB5-OB6-CB4
26	h	201	CDL	OB7-CB5-OB6-CB4
25	j	700	3PE	C32-C31-O31-C3
26	L	704	CDL	C31-CA7-OA8-CA6
26	L	705	CDL	C71-CB7-OB8-CB6
25	m	201	3PE	C22-C21-O21-C2
25	K	101	3PE	C32-C31-O31-C3
25	M	503	3PE	C32-C31-O31-C3
25	m	202	3PE	O32-C31-O31-C3
26	L	704	CDL	OA9-CA7-OA8-CA6
27	L	706	PC1	O22-C21-O21-C2
26	d	201	CDL	O1-C1-CB2-OB2
25	O	401	3PE	C32-C31-O31-C3
26	L	705	CDL	OB9-CB7-OB8-CB6
25	D	501	3PE	C22-C21-O21-C2
25	L	703	3PE	C22-C21-O21-C2
26	L	705	CDL	C11-CA5-OA6-CA4
25	m	202	3PE	C32-C31-O31-C3
26	h	201	CDL	CA4-CA3-OA5-PA1
25	O	401	3PE	O32-C31-O31-C3
25	L	703	3PE	C32-C31-O31-C3
25	L	703	3PE	O32-C31-O31-C3
26	d	201	CDL	C31-CA7-OA8-CA6
26	d	201	CDL	OA9-CA7-OA8-CA6
25	L	703	3PE	O22-C21-O21-C2
26	d	201	CDL	OA6-CA4-CA6-OA8
26	h	201	CDL	C71-CB7-OB8-CB6
25	m	201	3PE	C32-C31-O31-C3
25	M	501	3PE	C2-C3-O31-C31
25	D	501	3PE	O22-C21-O21-C2
26	L	705	CDL	OA7-CA5-OA6-CA4
25	M	501	3PE	C32-C31-O31-C3
25	m	201	3PE	O32-C31-O31-C3
25	M	501	3PE	C32-C33-C34-C35
25	M	502	3PE	C22-C21-O21-C2
26	h	201	CDL	OB9-CB7-OB8-CB6
25	M	502	3PE	O22-C21-O21-C2
26	L	704	CDL	C17-C18-C19-C20
26	h	201	CDL	C18-C19-C20-C21
26	L	704	CDL	C71-CB7-OB8-CB6
25	L	703	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	O	401	3PE	C22-C21-O21-C2
26	L	704	CDL	C11-CA5-OA6-CA4
25	M	501	3PE	C23-C24-C25-C26
25	M	501	3PE	O32-C31-O31-C3
26	L	704	CDL	C52-C53-C54-C55
26	L	705	CDL	C51-CB5-OB6-CB4
26	L	704	CDL	OB9-CB7-OB8-CB6
25	m	201	3PE	C24-C25-C26-C27
26	L	704	CDL	OA7-CA5-OA6-CA4
26	d	201	CDL	C71-CB7-OB8-CB6
25	K	101	3PE	C22-C21-O21-C2
26	d	201	CDL	C11-CA5-OA6-CA4
26	d	201	CDL	OA7-CA5-OA6-CA4
25	L	703	3PE	C22-C23-C24-C25
26	L	705	CDL	C72-C73-C74-C75
25	O	401	3PE	O22-C21-O21-C2
26	L	705	CDL	OB7-CB5-OB6-CB4
26	L	704	CDL	C12-C13-C14-C15
25	M	502	3PE	C3C-C3D-C3E-C3F
25	K	101	3PE	O22-C21-O21-C2
25	K	101	3PE	C22-C23-C24-C25
26	d	201	CDL	CA3-CA4-CA6-OA8
26	d	201	CDL	OB9-CB7-OB8-CB6
25	D	501	3PE	C24-C25-C26-C27
25	L	701	3PE	C32-C31-O31-C3
25	L	701	3PE	C24-C25-C26-C27
25	M	503	3PE	C24-C25-C26-C27
29	n	201	EHZ	C3-C4-C5-C6
26	L	705	CDL	C12-C13-C14-C15
25	i	201	3PE	C32-C33-C34-C35
25	L	702	3PE	C2-C1-O11-P
26	d	201	CDL	C1-CB2-OB2-PB2
25	i	201	3PE	C1-C2-C3-O31
25	m	201	3PE	C23-C24-C25-C26
25	K	101	3PE	C21-C22-C23-C24
25	M	503	3PE	C28-C29-C2A-C2B
25	L	702	3PE	C24-C25-C26-C27
25	M	502	3PE	C32-C31-O31-C3
25	L	702	3PE	C34-C35-C36-C37
29	n	201	EHZ	O1-C7-C8-C9
25	i	201	3PE	O21-C2-C3-O31
25	M	502	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	d	201	CDL	C52-C53-C54-C55
26	h	201	CDL	C14-C15-C16-C17
26	L	704	CDL	OB5-CB3-CB4-CB6
25	L	701	3PE	O32-C31-O31-C3
25	M	502	3PE	O32-C31-O31-C3
26	h	201	CDL	CB3-CB4-OB6-CB5
26	L	704	CDL	OB5-CB3-CB4-OB6
25	L	702	3PE	C25-C26-C27-C28
27	L	706	PC1	O13-C11-C12-N
25	L	701	3PE	C28-C29-C2A-C2B
25	L	702	3PE	C32-C33-C34-C35
26	L	705	CDL	C57-C58-C59-C60
25	O	401	3PE	C36-C37-C38-C39
26	L	704	CDL	C71-C72-C73-C74
25	i	201	3PE	C2-C1-O11-P
26	h	201	CDL	CB4-CB3-OB5-PB2
25	m	201	3PE	C2E-C2F-C2G-C2H
25	j	700	3PE	C22-C21-O21-C2
25	L	703	3PE	C29-C2A-C2B-C2C
25	L	701	3PE	C25-C26-C27-C28
25	K	101	3PE	C11-O13-P-O14
25	L	702	3PE	C1-O11-P-O13
25	O	401	3PE	C1-O11-P-O12
25	O	401	3PE	C1-O11-P-O13
25	O	401	3PE	C1-O11-P-O14
25	m	201	3PE	C1-O11-P-O13
25	m	201	3PE	C1-O11-P-O14
26	d	201	CDL	CA2-OA2-PA1-OA3
26	d	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	CA3-OA5-PA1-OA3
26	h	201	CDL	CB2-OB2-PB2-OB5
26	h	201	CDL	CB3-OB5-PB2-OB2
26	h	201	CDL	CB3-OB5-PB2-OB4
28	O	402	ADP	C5'-O5'-PA-O1A
25	m	201	3PE	C33-C34-C35-C36
26	L	704	CDL	CA4-CA3-OA5-PA1
26	L	705	CDL	CA4-CA3-OA5-PA1
26	L	704	CDL	CB6-CB4-OB6-CB5
25	M	503	3PE	C34-C35-C36-C37
26	L	705	CDL	C56-C57-C58-C59
27	L	706	PC1	C3B-C3C-C3D-C3E
25	D	501	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
25	O	401	3PE	C2-C1-O11-P
26	d	201	CDL	CB4-CB3-OB5-PB2
25	D	501	3PE	C32-C33-C34-C35
25	L	701	3PE	C33-C34-C35-C36
25	j	700	3PE	O22-C21-O21-C2
26	L	704	CDL	CB4-CB3-OB5-PB2
25	D	501	3PE	O32-C31-O31-C3
25	M	503	3PE	C23-C24-C25-C26
25	i	201	3PE	C3-C2-O21-C21
25	j	700	3PE	C2-C1-O11-P
25	M	502	3PE	C39-C3A-C3B-C3C
25	i	201	3PE	O22-C21-O21-C2
26	d	201	CDL	C59-C60-C61-C62
25	L	702	3PE	C23-C24-C25-C26
26	h	201	CDL	C31-CA7-OA8-CA6
26	L	704	CDL	OA5-CA3-CA4-OA6
26	L	704	CDL	C14-C15-C16-C17
26	h	201	CDL	OA9-CA7-OA8-CA6
29	n	201	EHZ	C2-C3-C4-C5
27	L	706	PC1	C2-C3-O31-C31
25	D	501	3PE	C34-C35-C36-C37
25	K	101	3PE	O11-C1-C2-O21
26	L	705	CDL	C52-C53-C54-C55
25	M	502	3PE	C26-C27-C28-C29
25	L	701	3PE	C39-C3A-C3B-C3C
25	i	201	3PE	O21-C21-C22-C23
25	K	101	3PE	C24-C25-C26-C27
25	M	501	3PE	C24-C25-C26-C27
25	M	502	3PE	C36-C37-C38-C39
26	L	704	CDL	C53-C54-C55-C56
25	K	101	3PE	C36-C37-C38-C39
25	K	101	3PE	C23-C24-C25-C26
25	L	701	3PE	C34-C35-C36-C37
25	L	701	3PE	C2B-C2C-C2D-C2E
25	M	502	3PE	C2B-C2C-C2D-C2E
26	d	201	CDL	C12-C11-CA5-OA6
26	L	705	CDL	CA7-C31-C32-C33
25	i	201	3PE	O22-C21-C22-C23
27	L	706	PC1	C27-C28-C29-C2A
25	L	703	3PE	C24-C25-C26-C27
26	d	201	CDL	C11-C12-C13-C14
25	i	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
25	K	101	3PE	C1-C2-C3-O31
29	n	201	EHZ	N2-C15-C16-O5
25	i	201	3PE	C32-C31-O31-C3
25	L	702	3PE	O21-C21-C22-C23
26	h	201	CDL	C72-C71-CB7-OB8
25	i	201	3PE	C22-C21-O21-C2
26	h	201	CDL	C11-C12-C13-C14

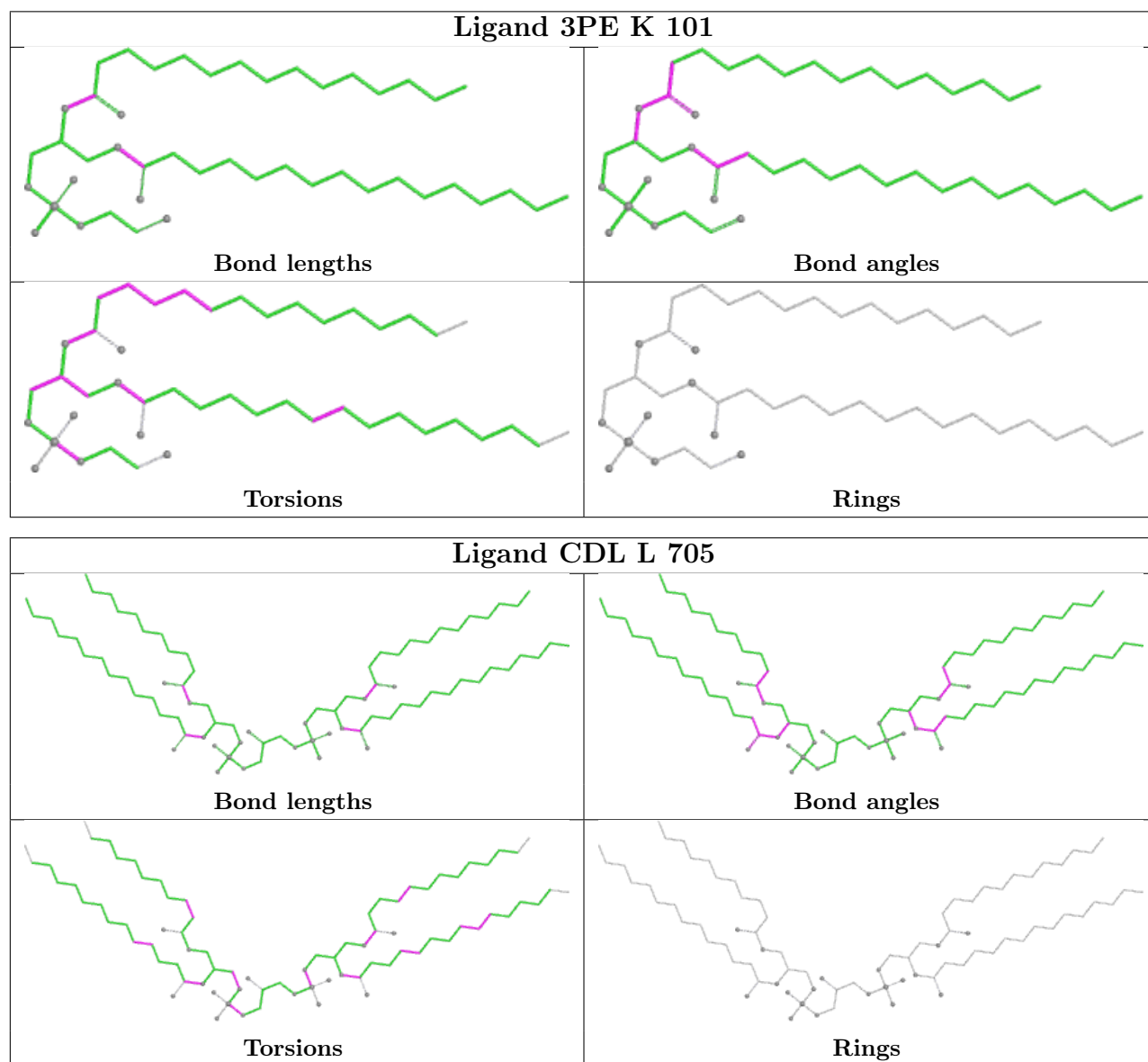
There are no ring outliers.

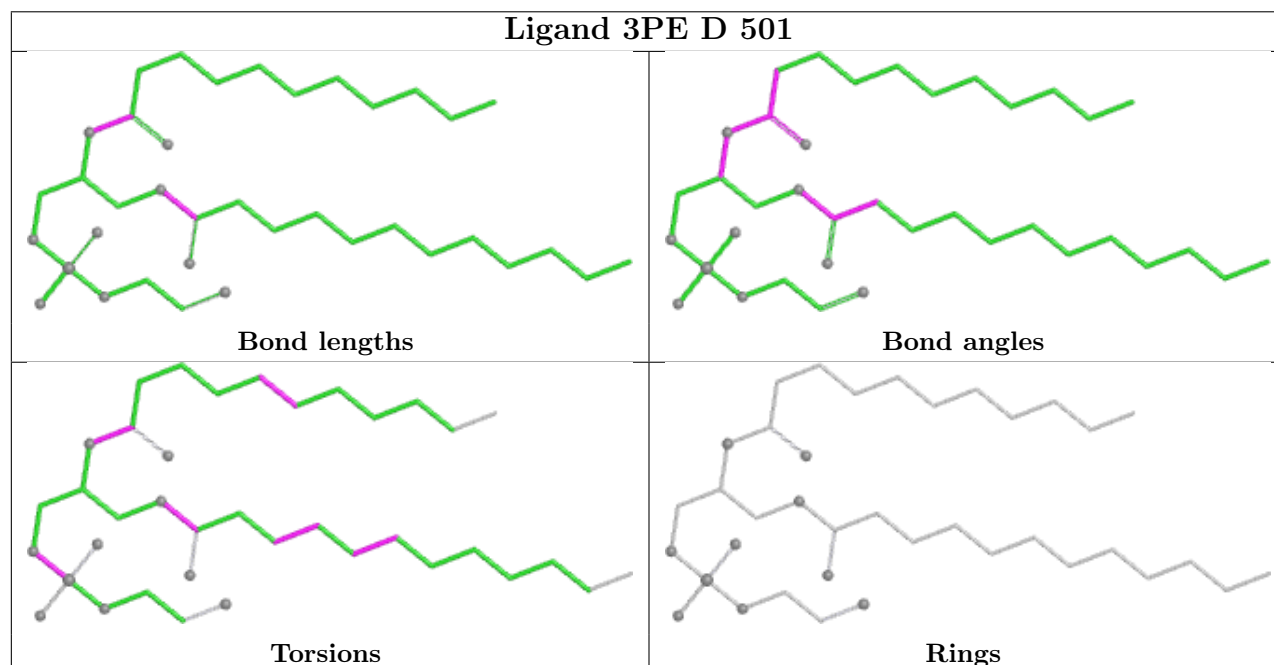
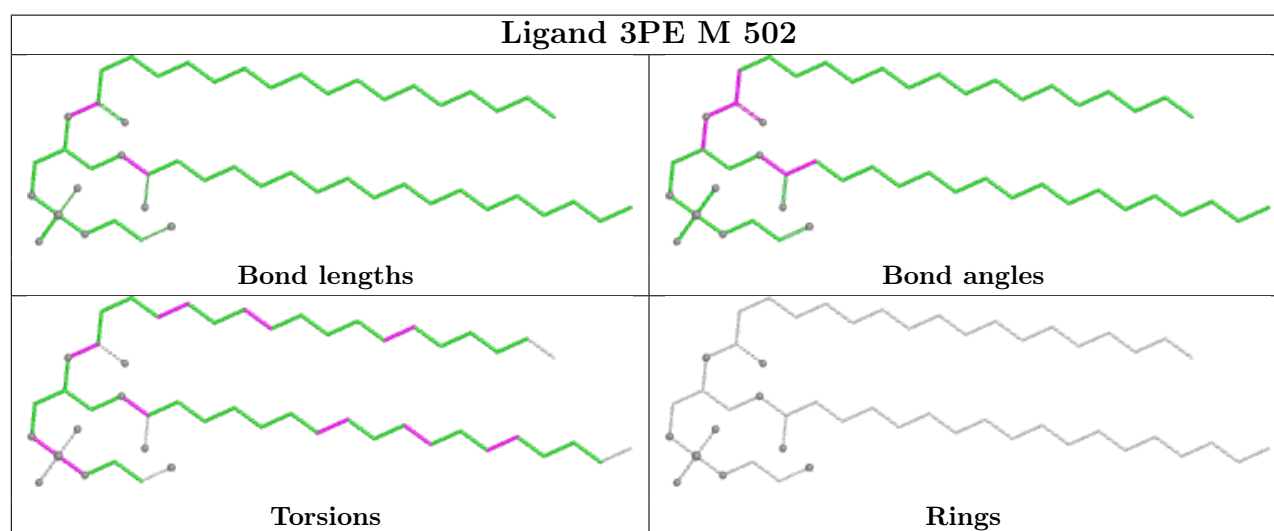
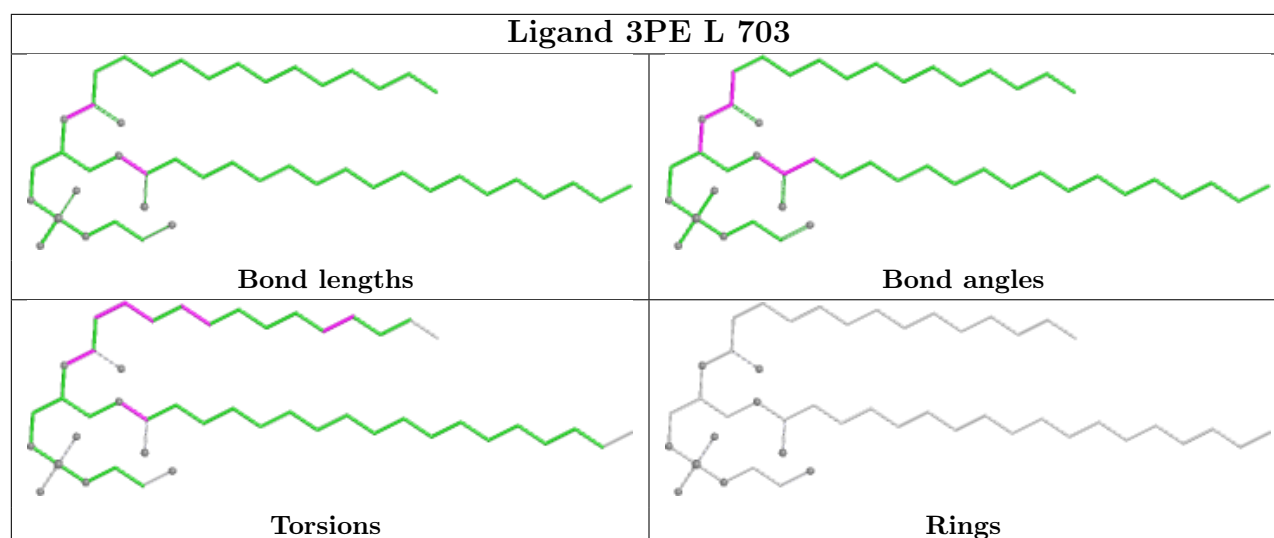
19 monomers are involved in 197 short contacts:

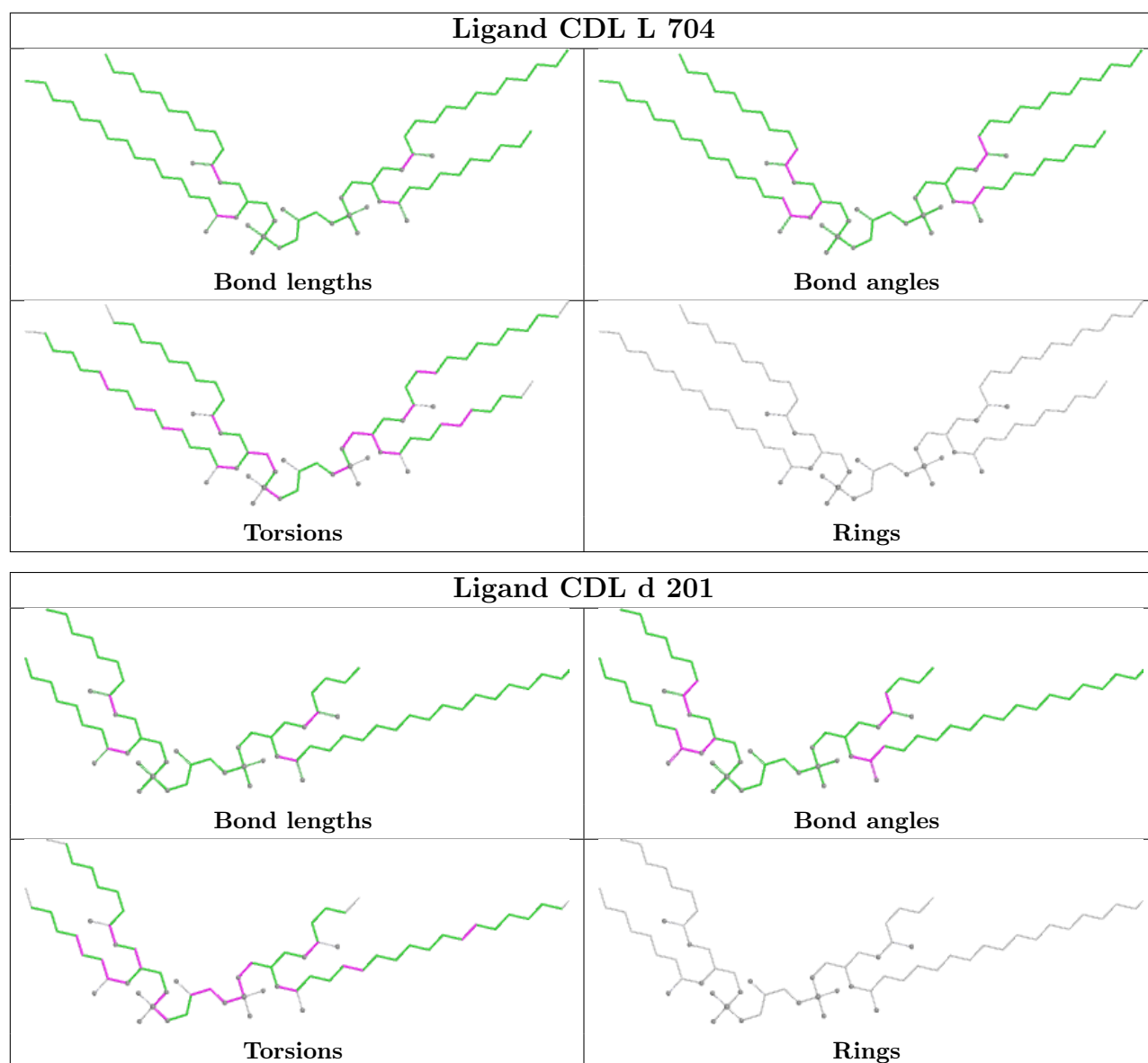
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	101	3PE	6	0
26	L	705	CDL	15	0
25	L	703	3PE	20	0
25	M	502	3PE	4	0
25	D	501	3PE	13	0
26	L	704	CDL	16	0
26	d	201	CDL	5	0
28	O	402	ADP	6	0
26	h	201	CDL	13	0
25	M	503	3PE	27	0
25	m	201	3PE	12	0
25	m	202	3PE	4	0
25	L	701	3PE	9	0
25	i	201	3PE	11	0
25	O	401	3PE	7	0
25	M	501	3PE	9	0
25	L	702	3PE	6	0
27	L	706	PC1	17	0
25	j	700	3PE	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

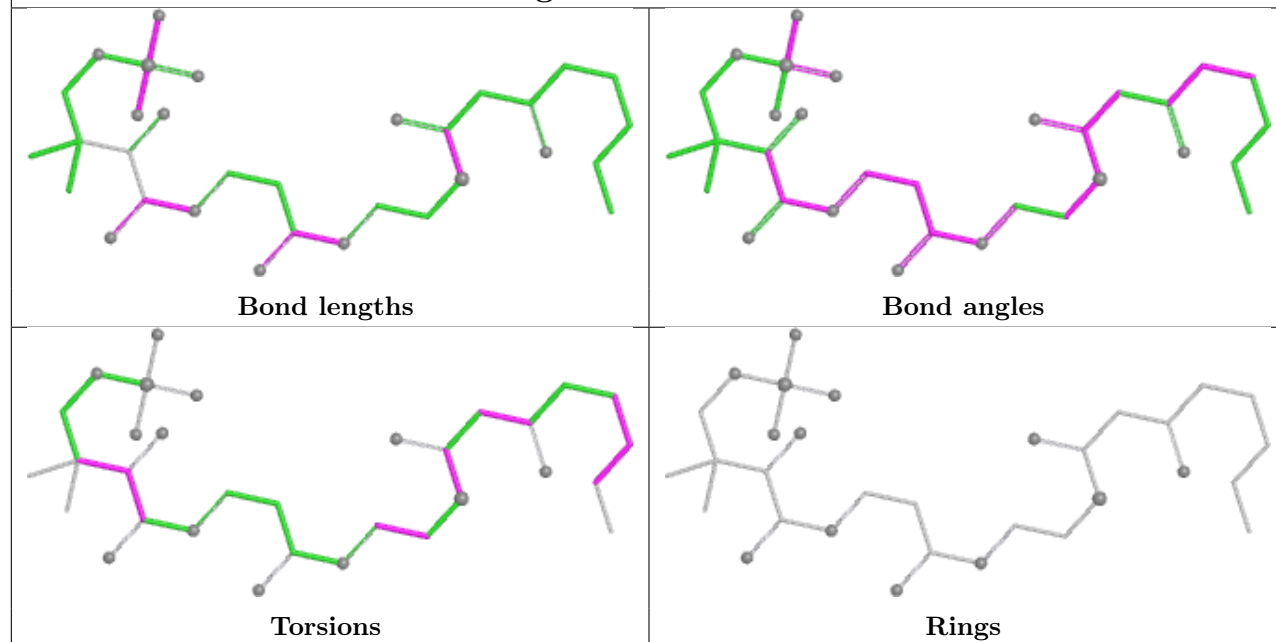
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



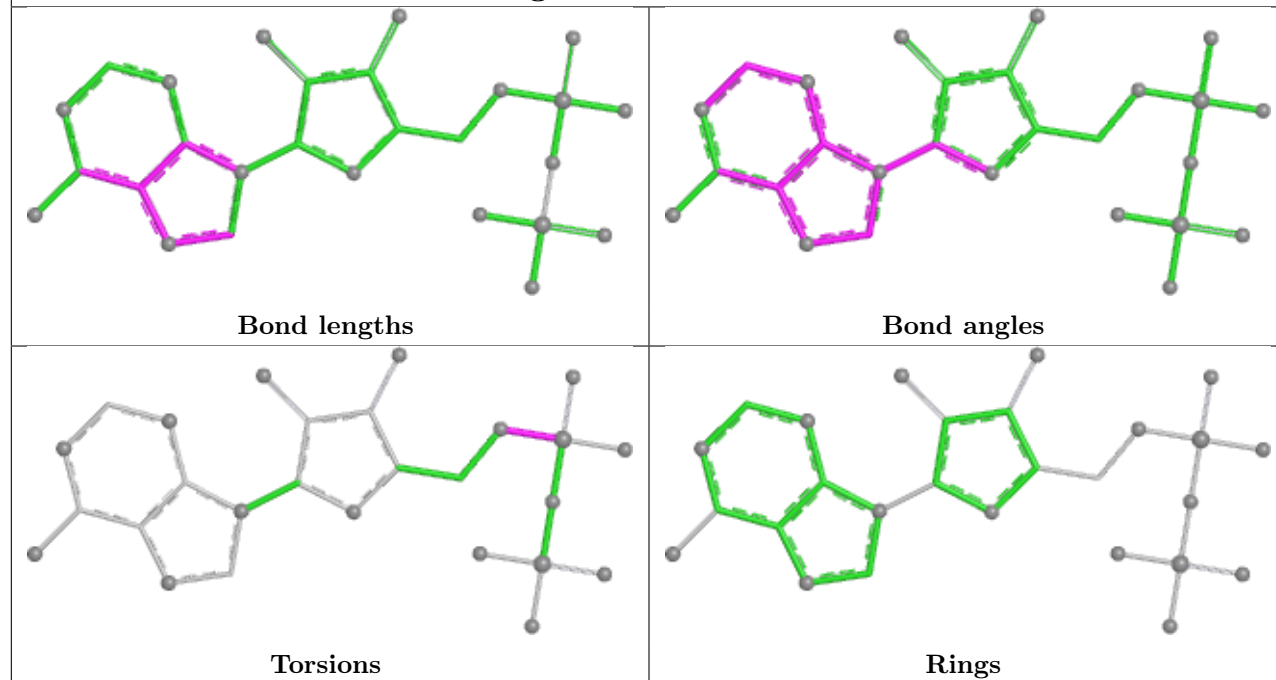


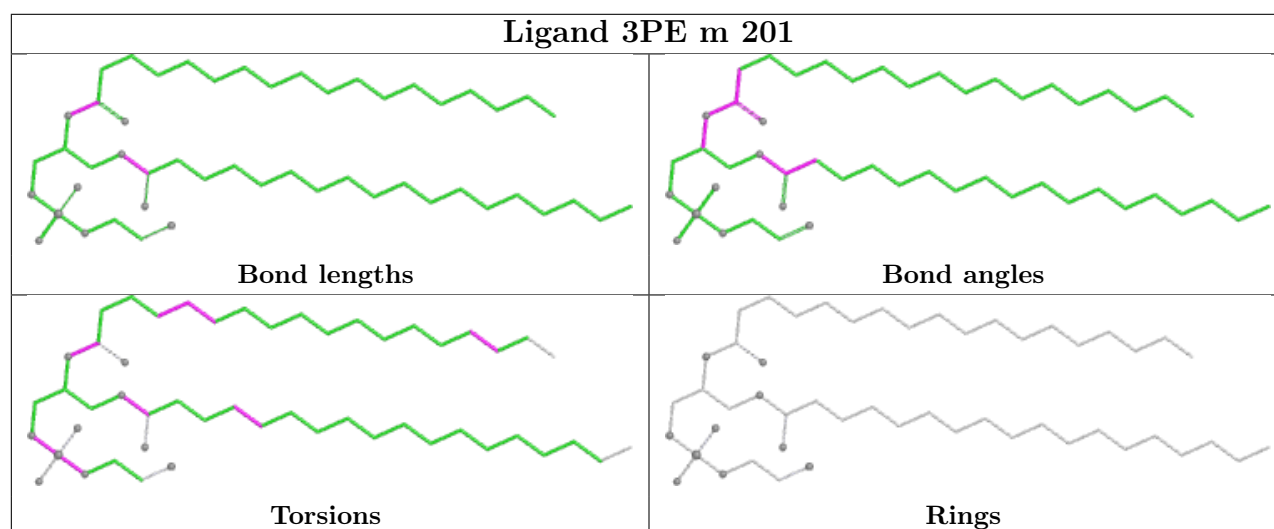
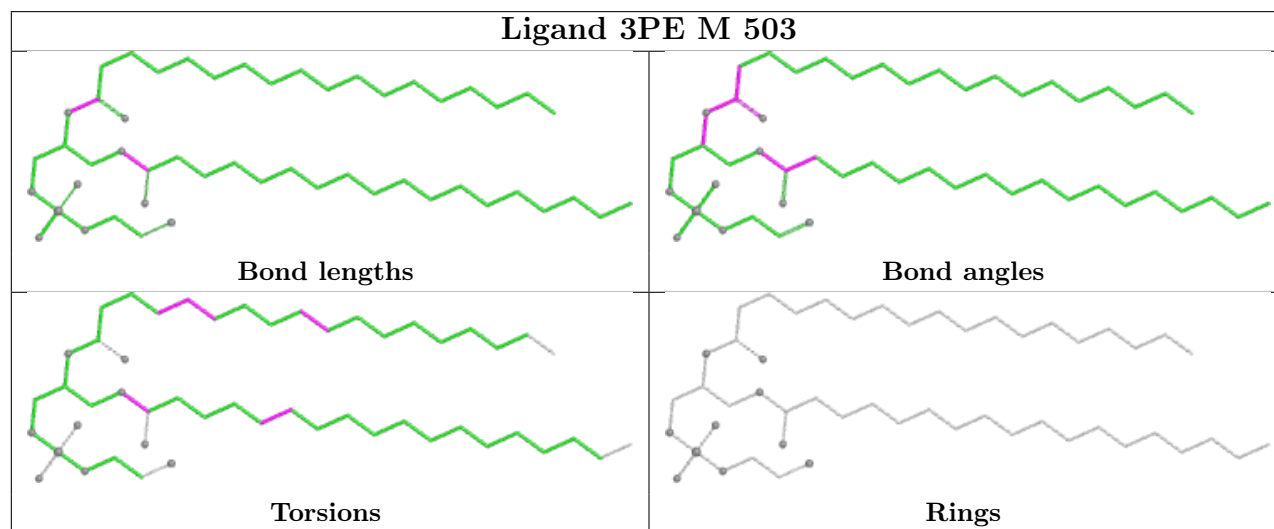
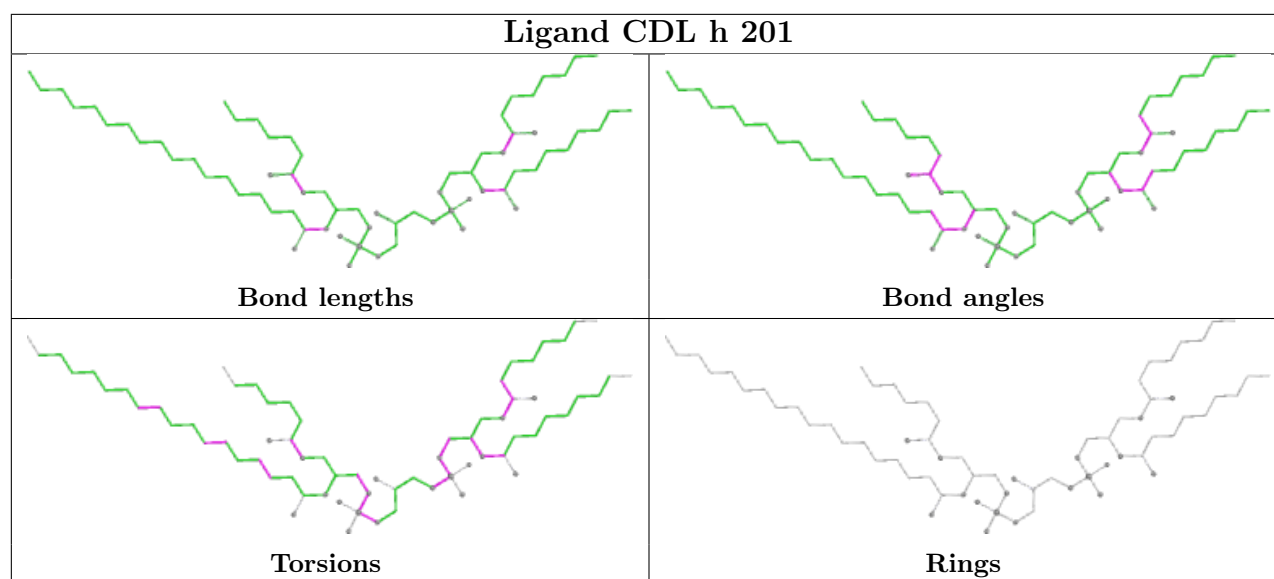


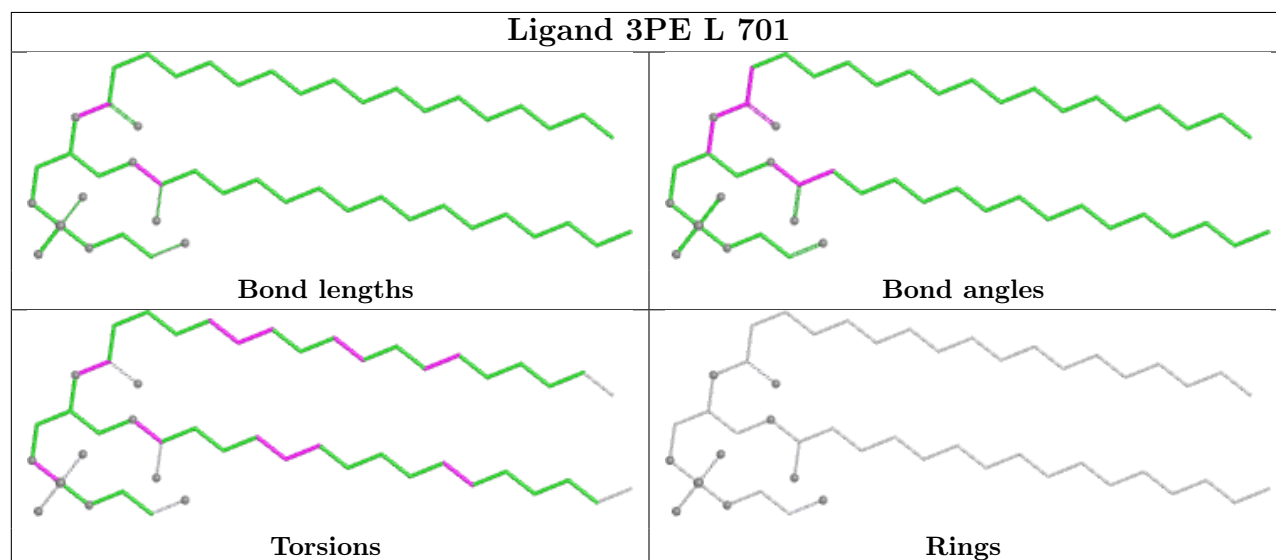
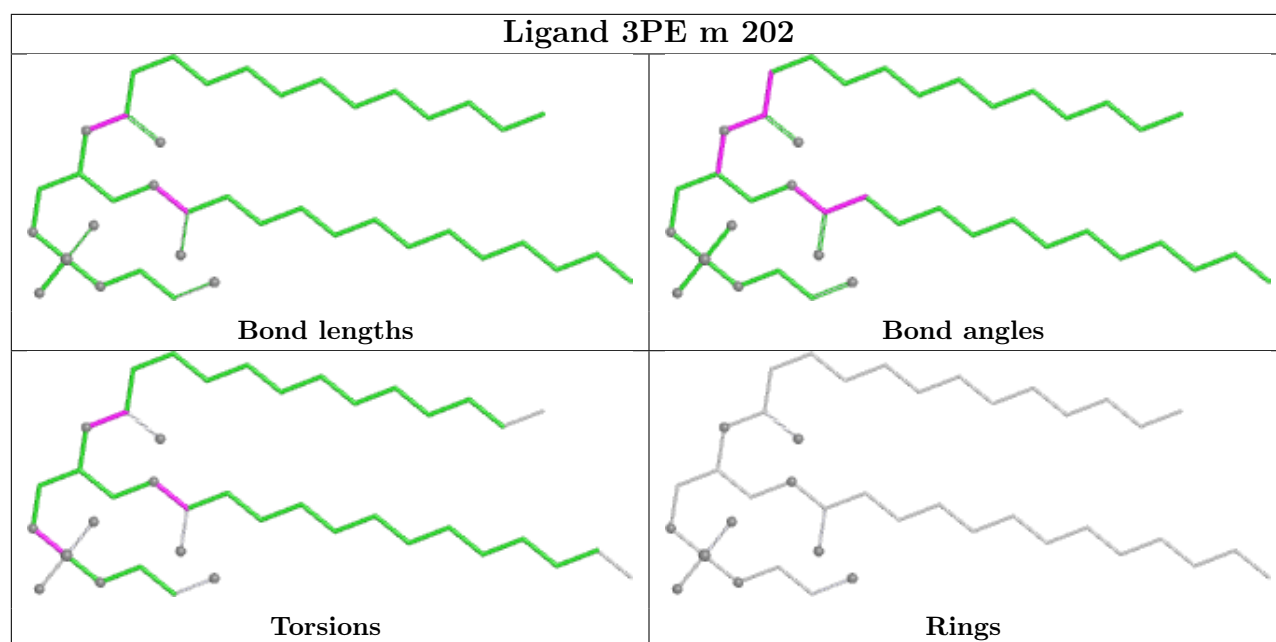
Ligand EHZ n 201

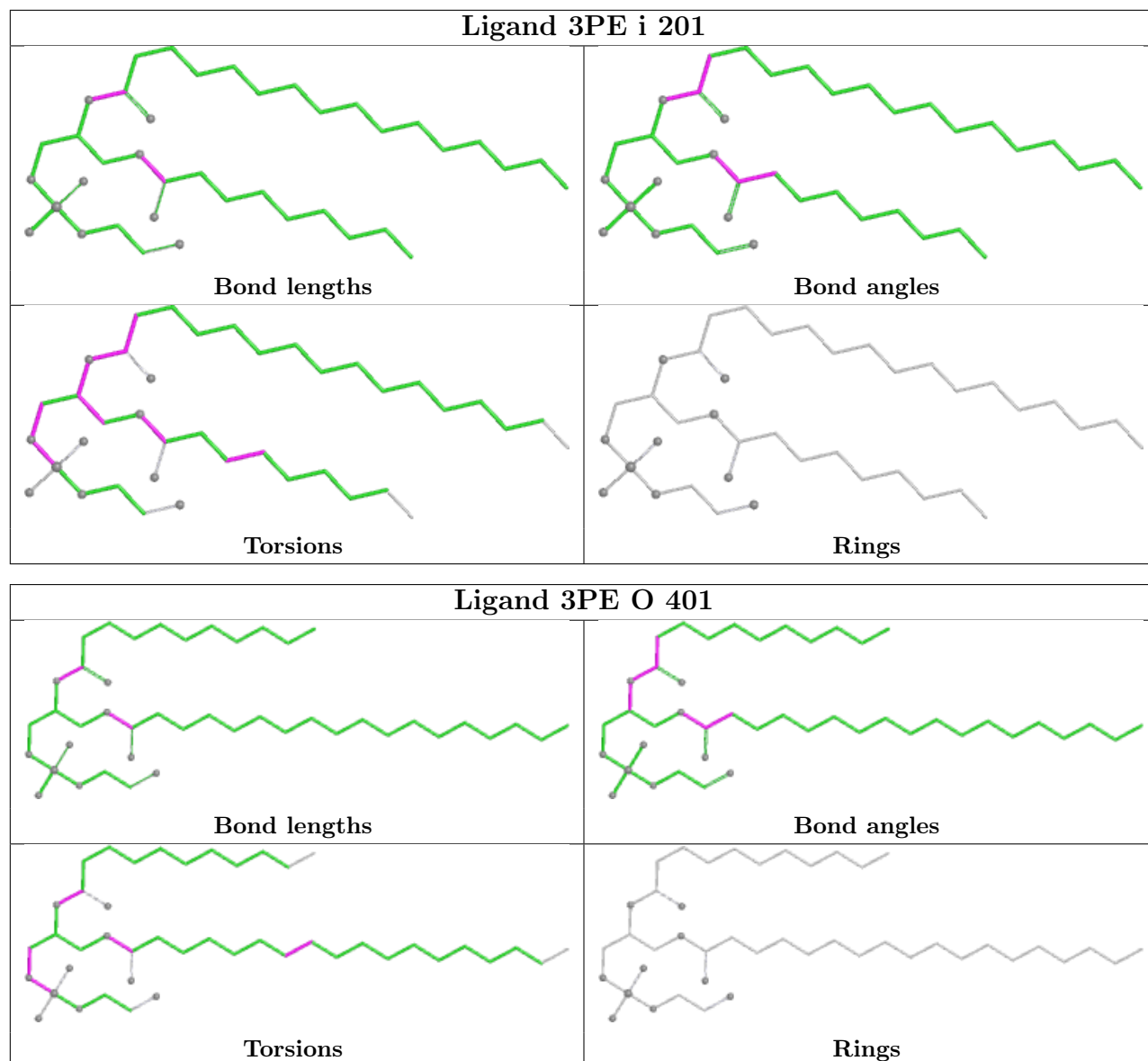


Ligand ADP O 402

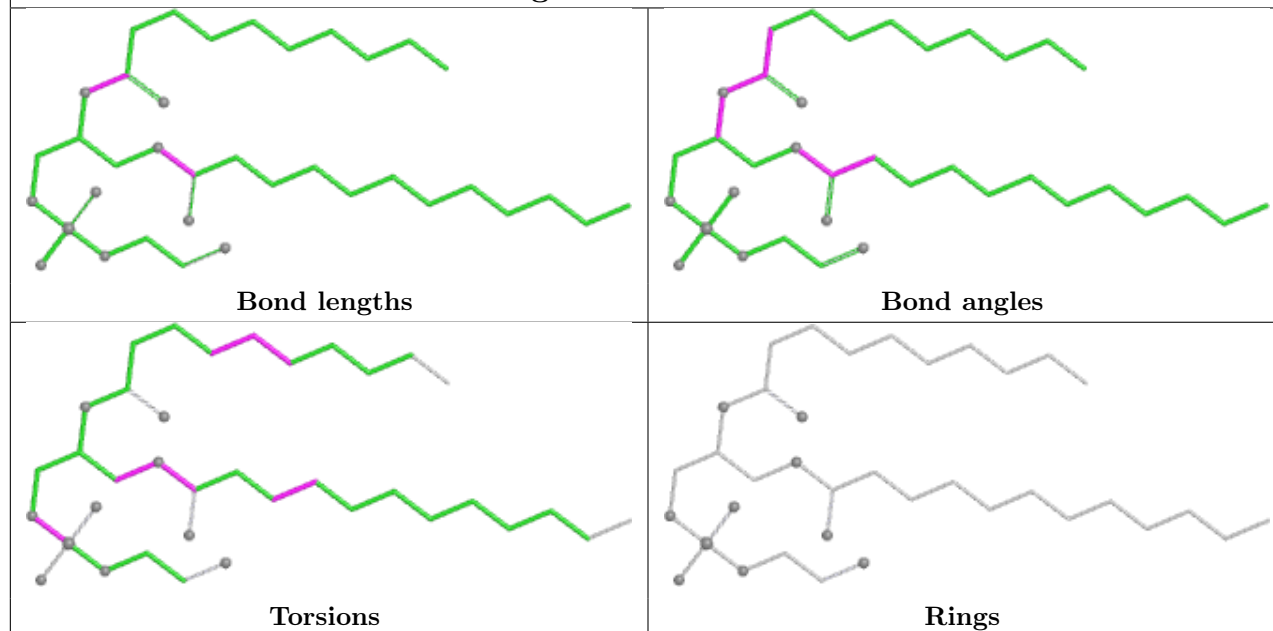




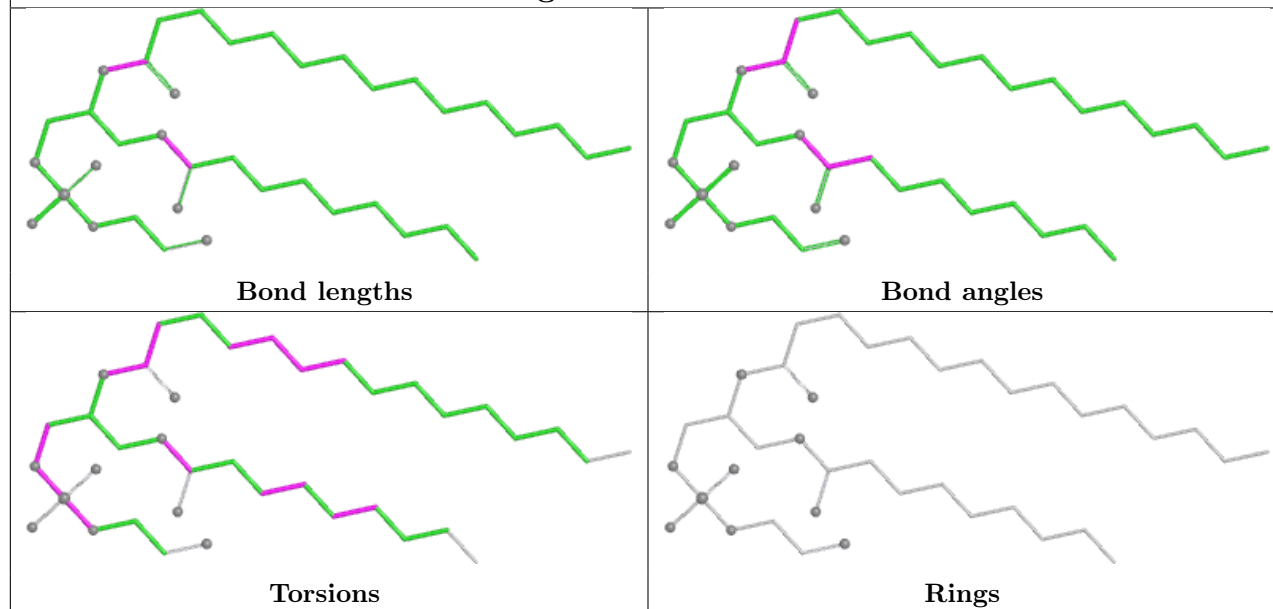


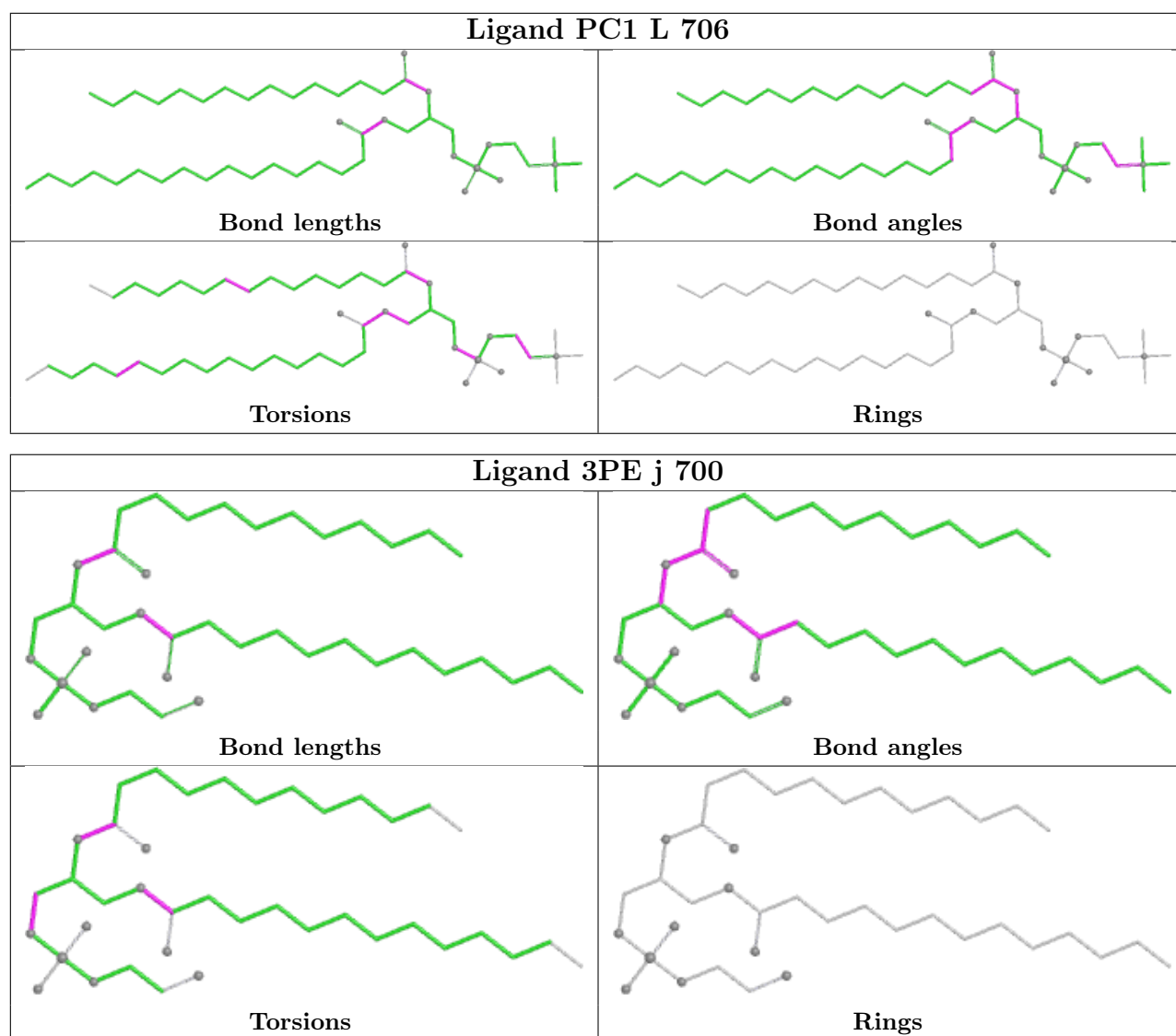


Ligand 3PE M 501



Ligand 3PE L 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

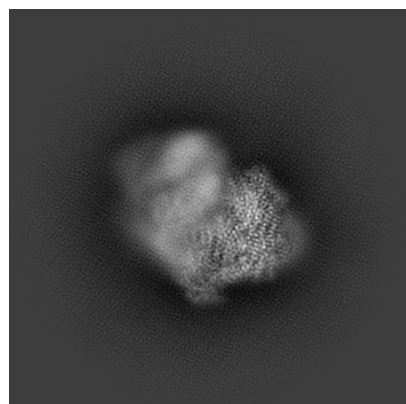
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35338. These allow visual inspection of the internal detail of the map and identification of artifacts.

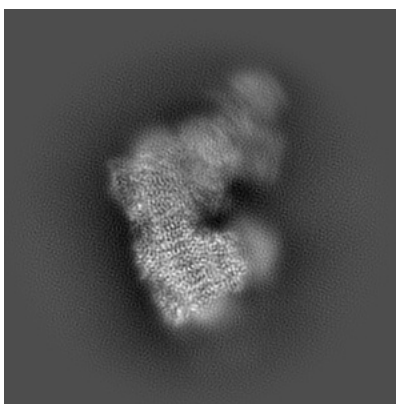
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

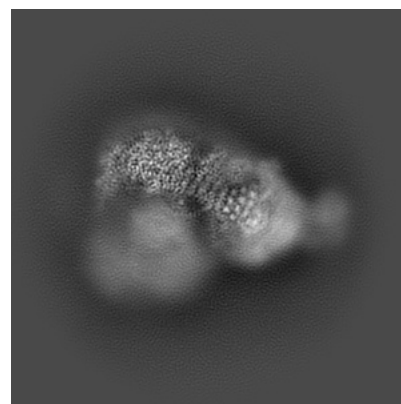
6.1.1 Primary map



X

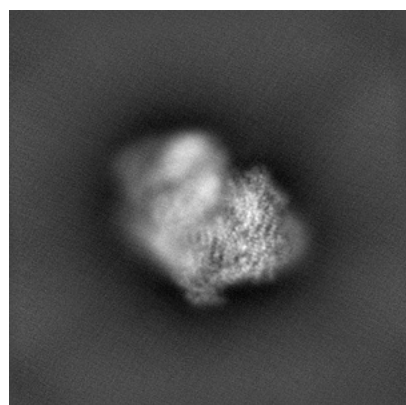


Y

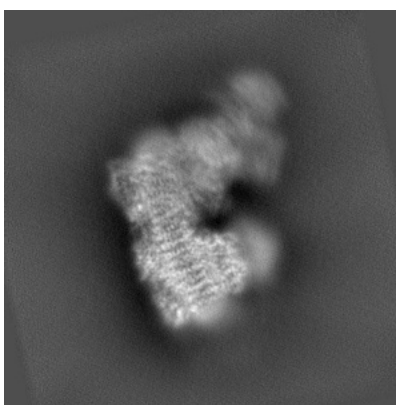


Z

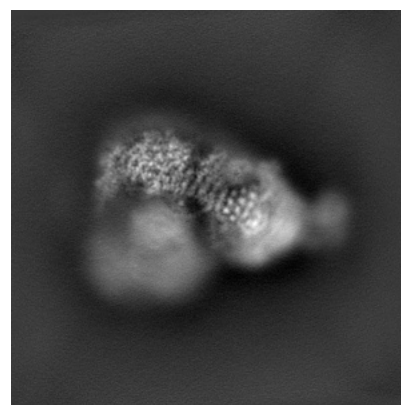
6.1.2 Raw map



X



Y

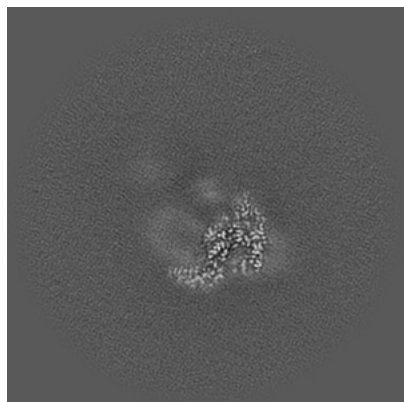


Z

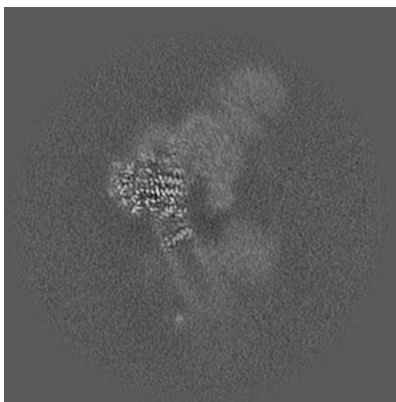
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

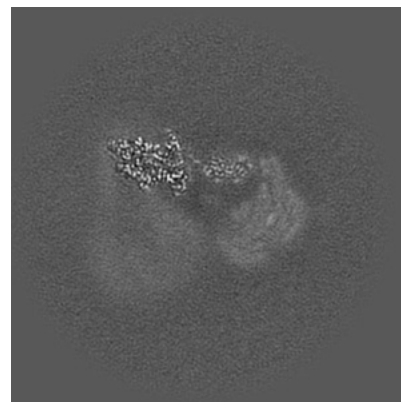
6.2.1 Primary map



X Index: 192

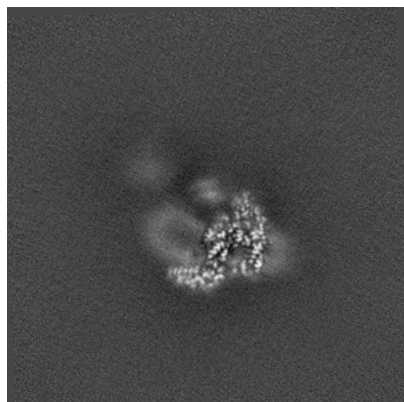


Y Index: 192

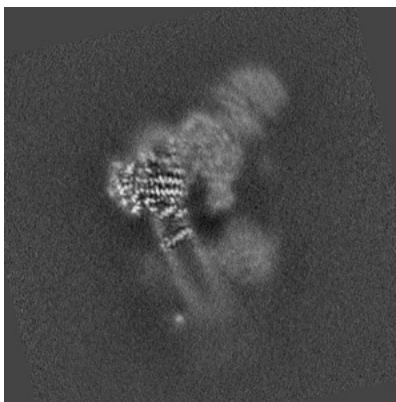


Z Index: 192

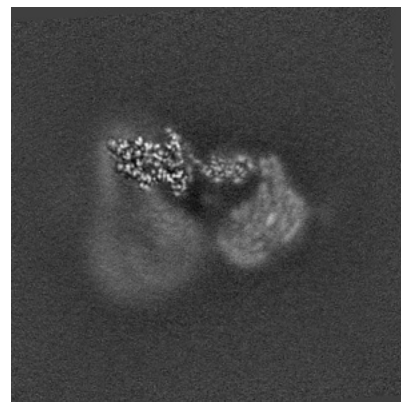
6.2.2 Raw map



X Index: 192



Y Index: 192

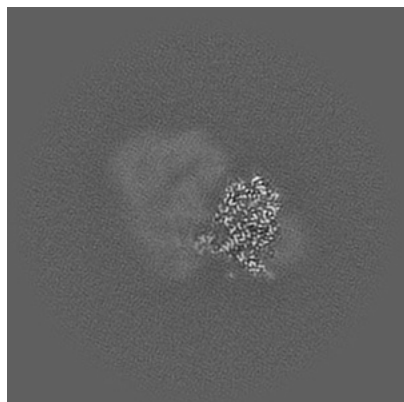


Z Index: 192

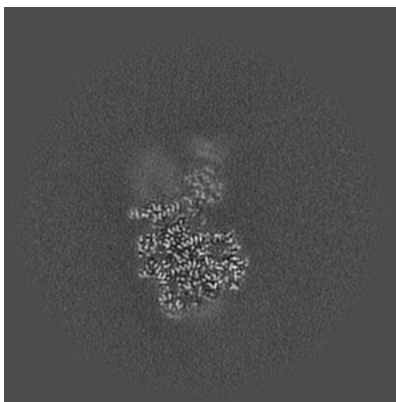
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

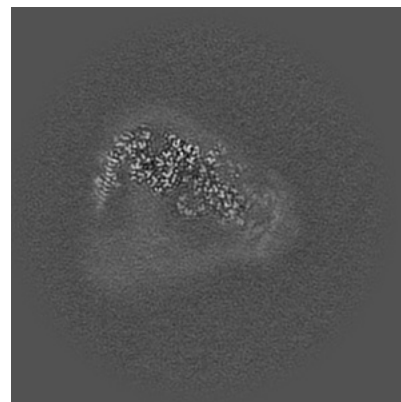
6.3.1 Primary map



X Index: 159

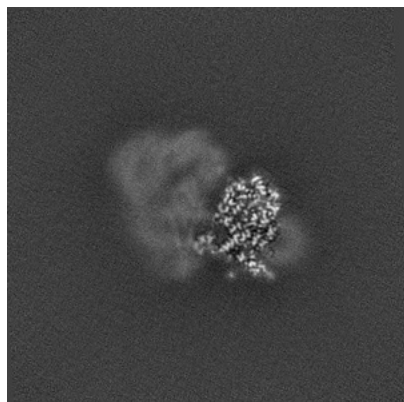


Y Index: 236

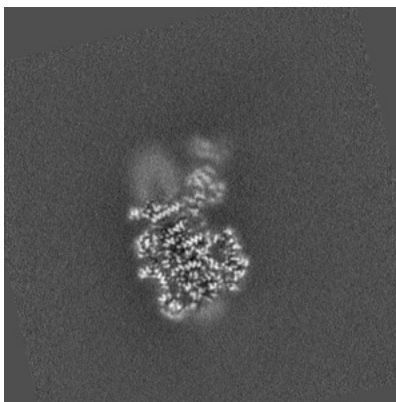


Z Index: 166

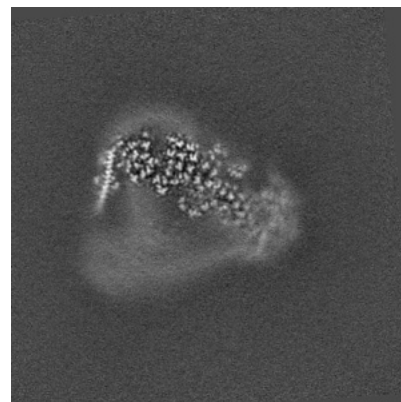
6.3.2 Raw map



X Index: 159



Y Index: 237

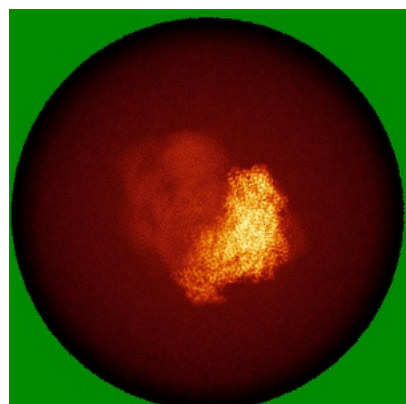


Z Index: 169

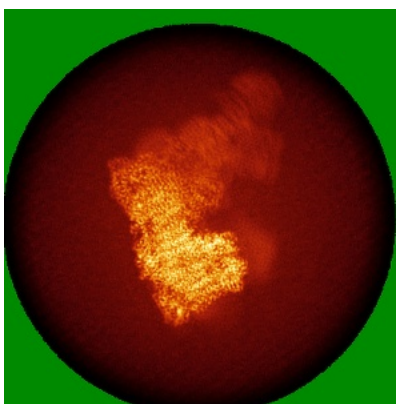
The images above show the largest variance slices of the map in three orthogonal directions.

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

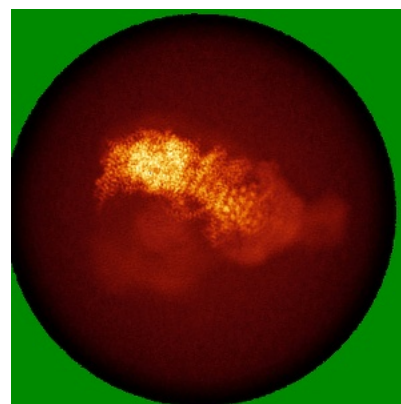
6.4.1 Primary map



X

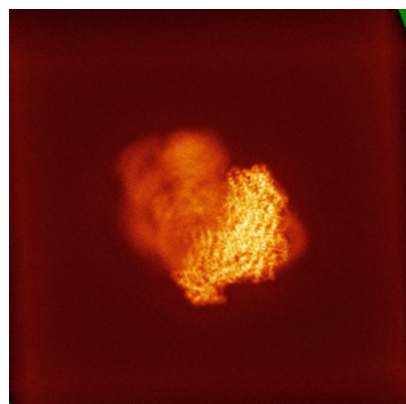


Y

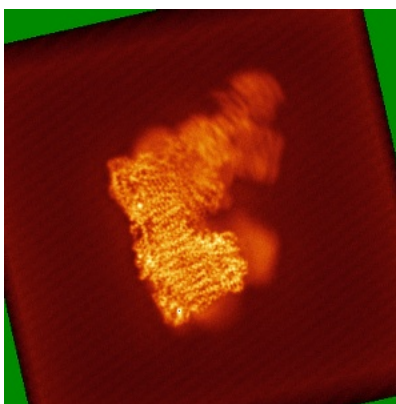


Z

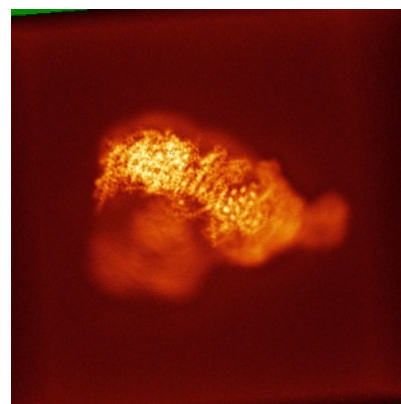
6.4.2 Raw map



X



Y



Z

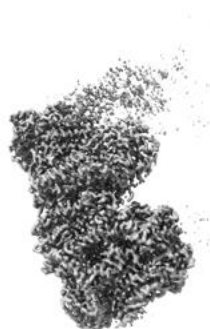
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



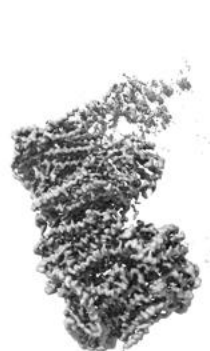
Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

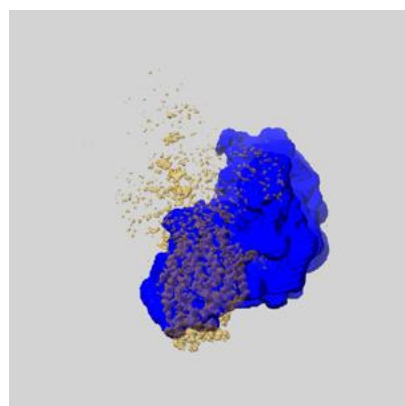
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

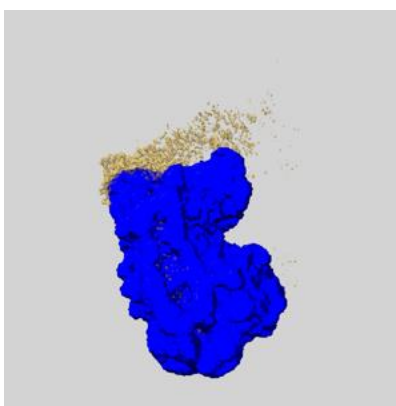
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

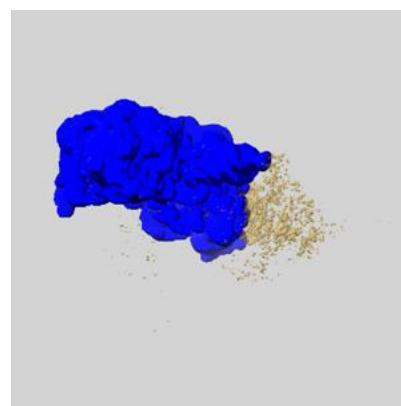
6.6.1 emd_35338_msk_1.map [i](#)



X



Y

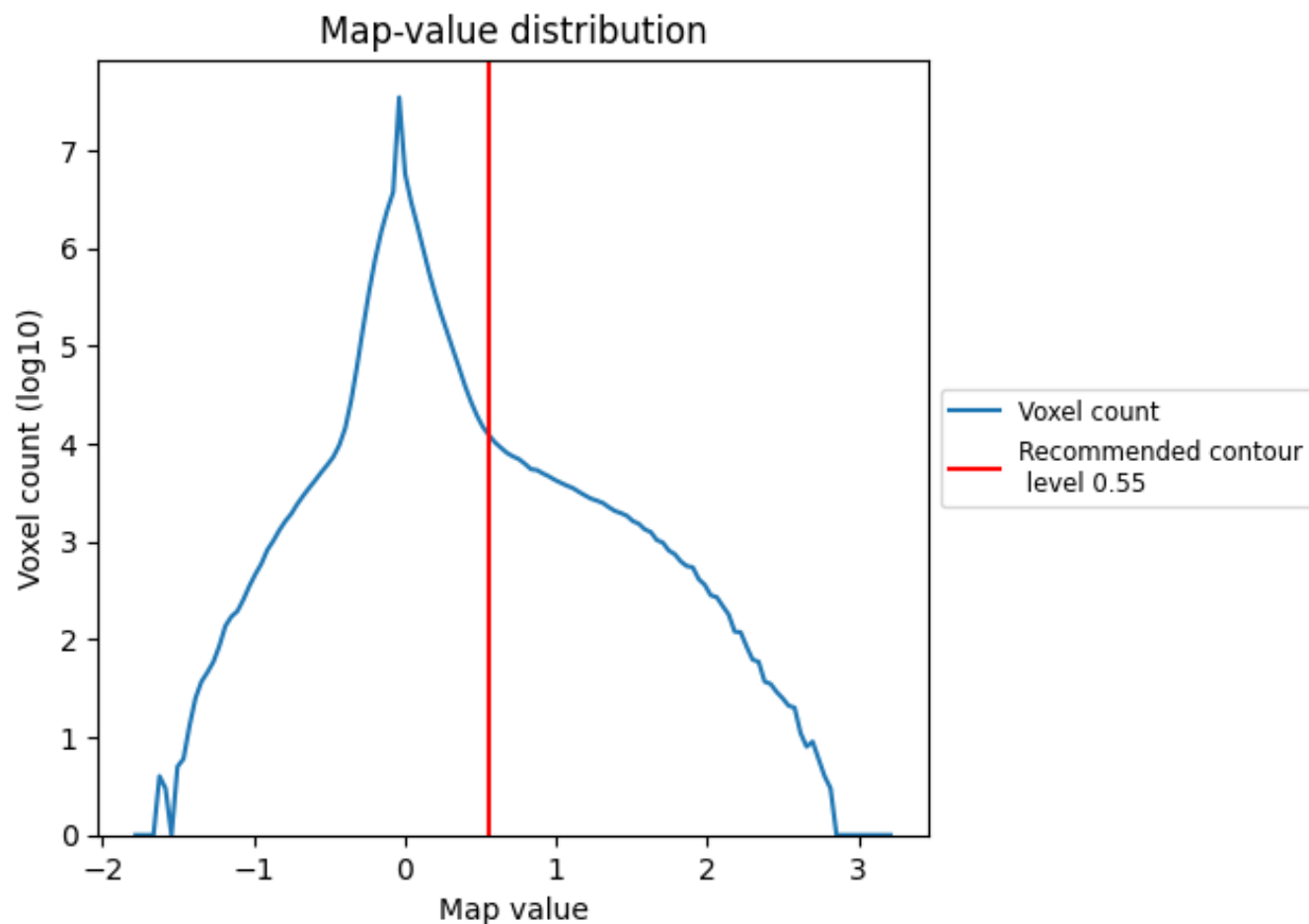


Z

7 Map analysis [i](#)

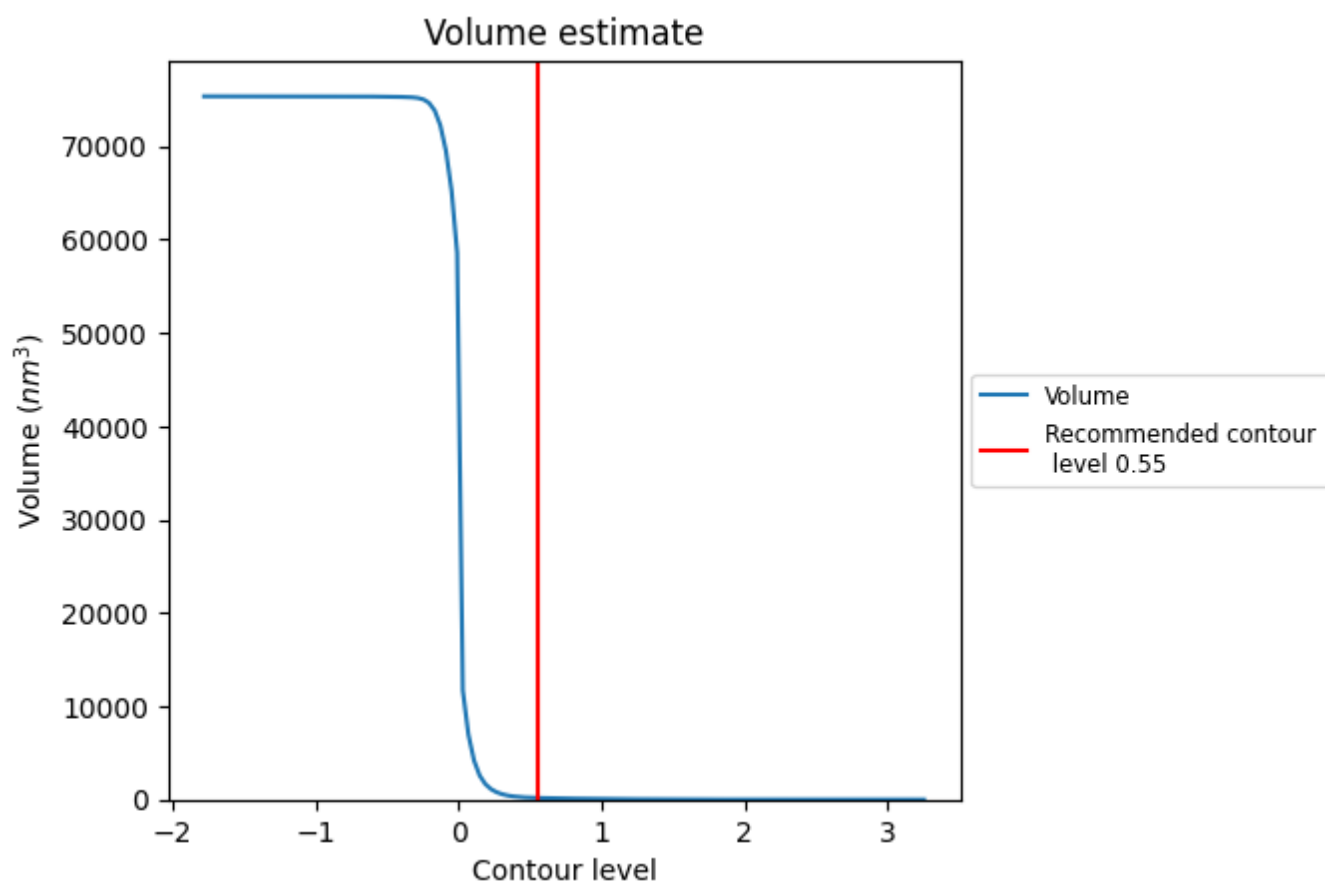
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

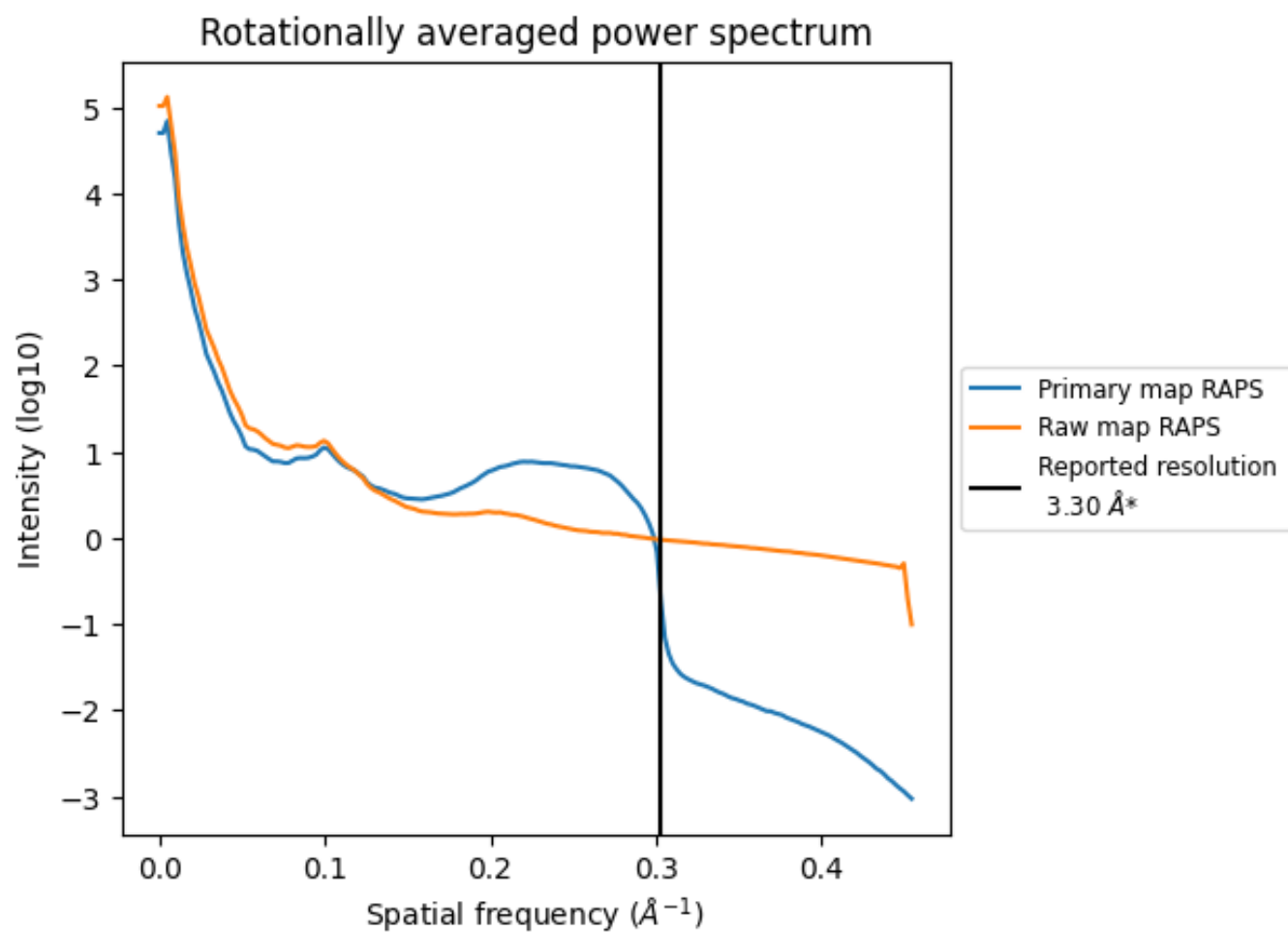
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

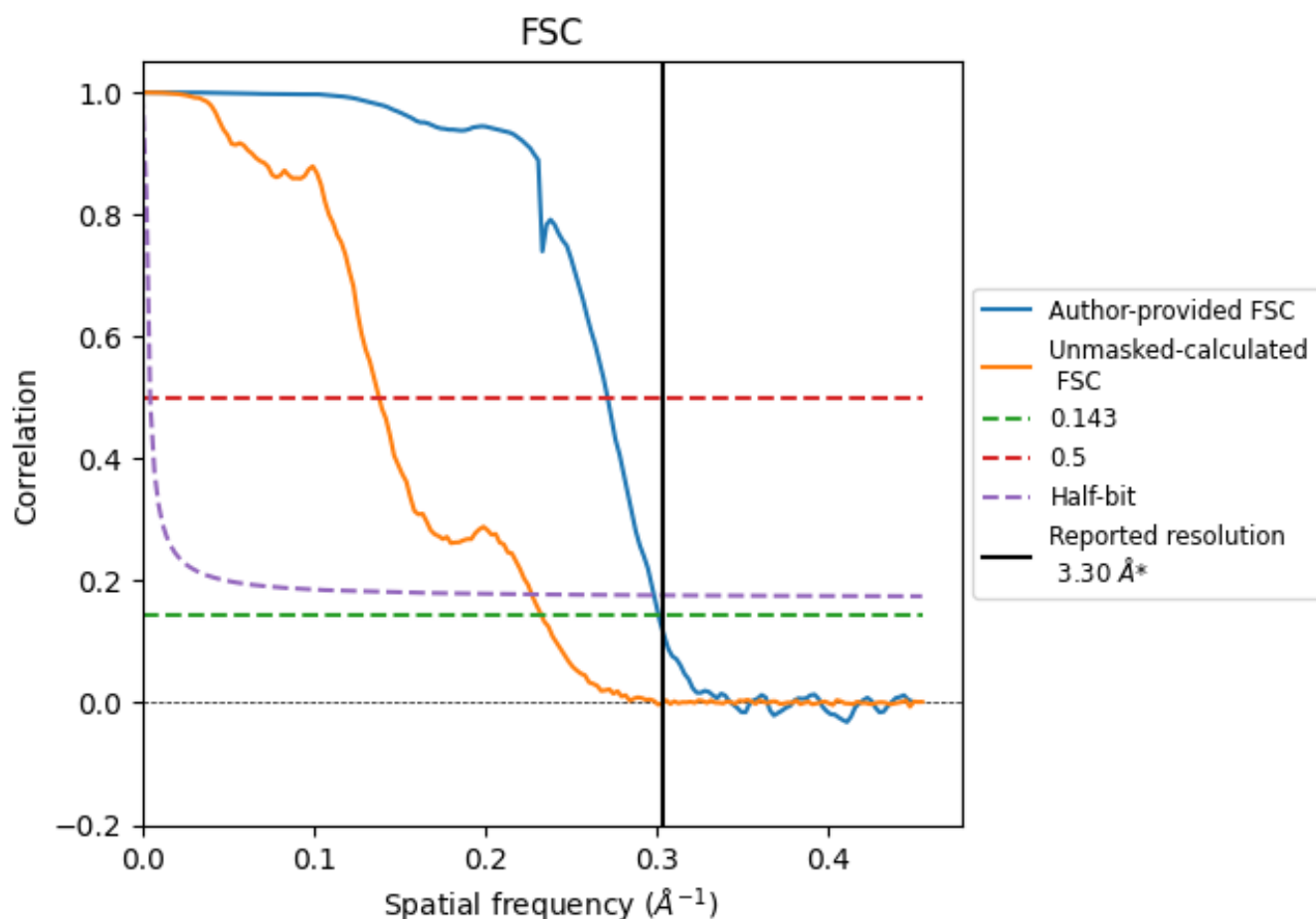


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates

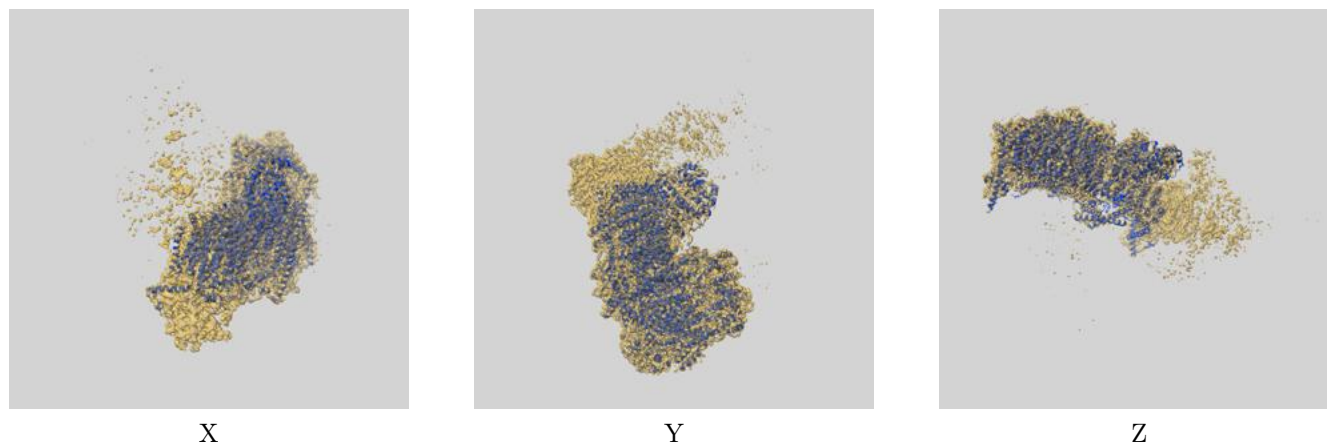
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.69	3.35
Unmasked-calculated*	4.30	7.24	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

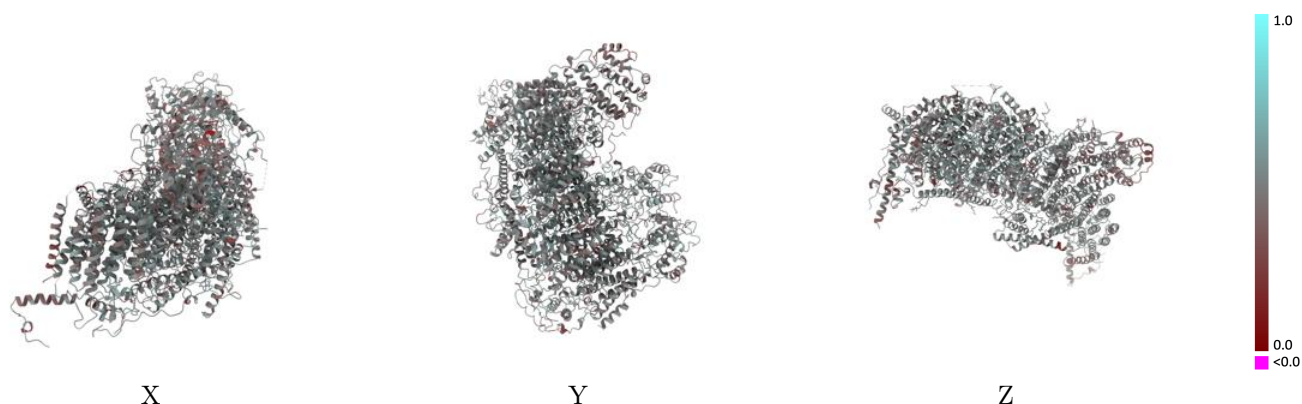
This section contains information regarding the fit between EMDB map EMD-35338 and PDB model 8IBB. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



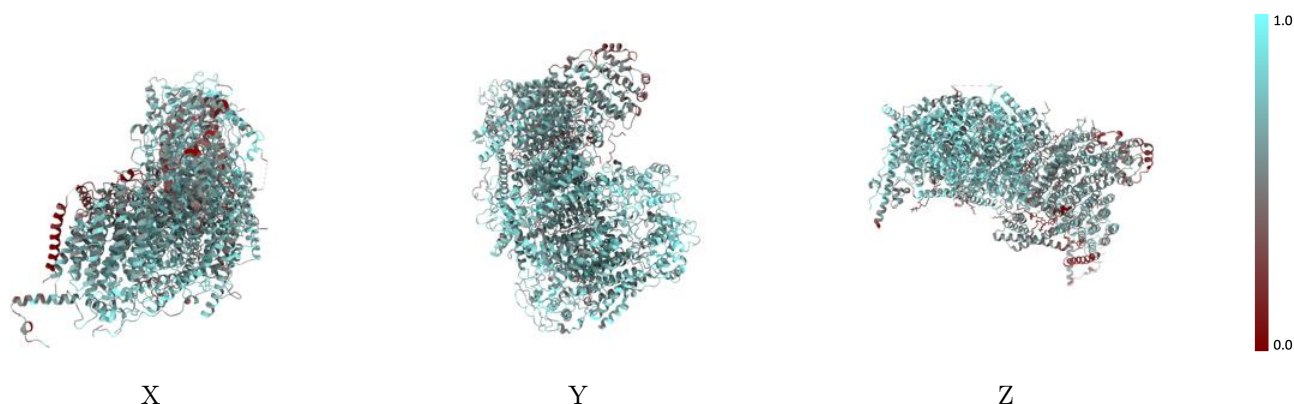
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



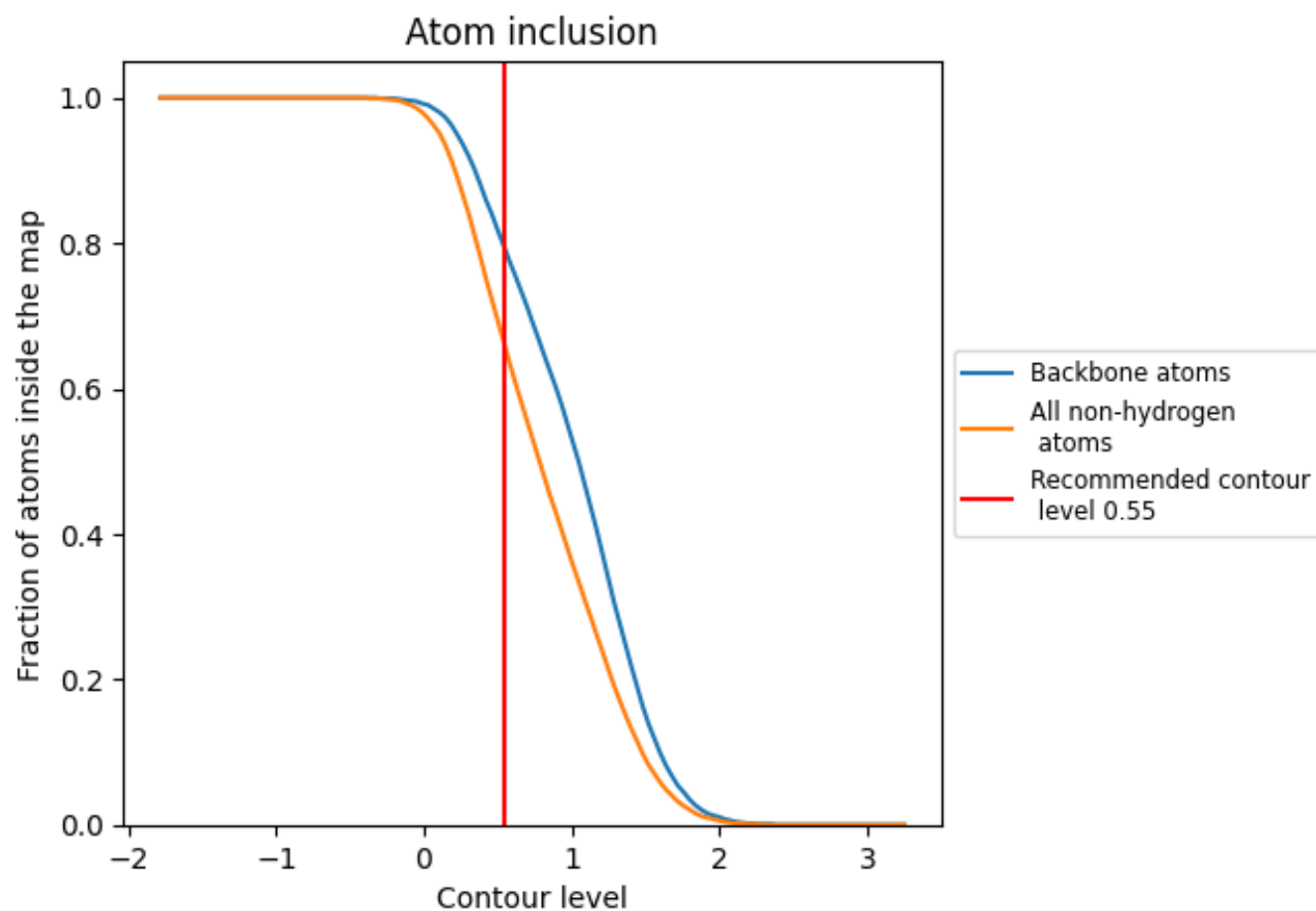
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4780
D	 0.3680	 0.4810
J	 0.4970	 0.4470
K	 0.5950	 0.4920
L	 0.6620	 0.4790
M	 0.6990	 0.5020
N	 0.6700	 0.4890
O	 0.5110	 0.4340
U	 0.7560	 0.5060
X	 0.7320	 0.5020
Y	 0.5270	 0.4580
c	 0.5640	 0.4600
d	 0.6580	 0.4910
e	 0.6270	 0.4580
f	 0.6360	 0.4860
g	 0.6960	 0.4750
h	 0.7100	 0.4840
i	 0.7340	 0.4900
j	 0.6880	 0.4580
k	 0.7460	 0.4760
l	 0.7440	 0.4950
m	 0.6680	 0.4880
n	 0.7740	 0.4980
o	 0.6910	 0.4560
p	 0.6940	 0.4670

