



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:37 PM UTC

PDB ID : 8IBF / pdb_00008ibf
EMDB ID : EMD-35342
Title : Respiratory complex Membrane domain of CI, focus-refined of type II, 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

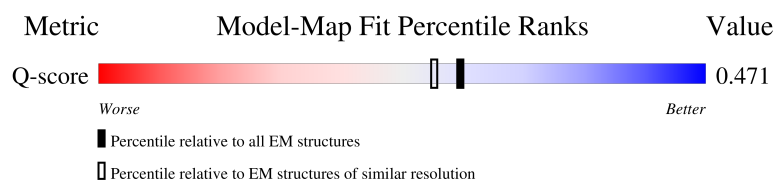
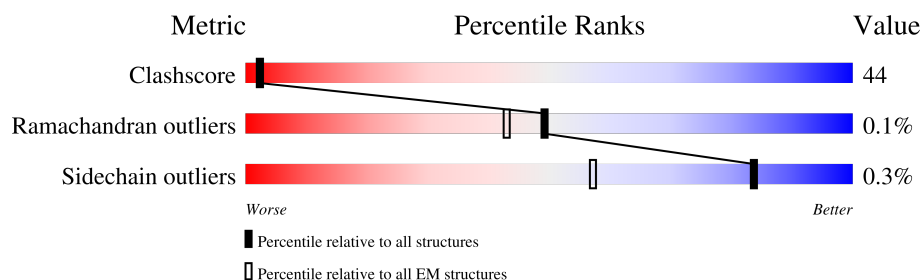
1 Overall quality at a glance

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
27	ADP	O	401	-	-	X	-

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 31948 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	42	Total	C	N	O	S	0	0
			350	227	58	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	163	Total	C	N	O	S	0	0
			1229	828	175	211	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	116	LEU	ASN	conflict	UNP P03925
J	117	GLY	LEU	conflict	UNP P03925

- 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	89	Total	C	N	O	S	0	0
			718	462	105	146	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	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	102	Total	C	N	O	S	0	0
			858	553	137	164	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	95	Total	C	N	O	S	0	0
			802	523	140	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	73	Total	C	N	O	S	0	0
			582	383	102	95	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	126	Total	C	N	O	S	0	0
			1050	676	189	185			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

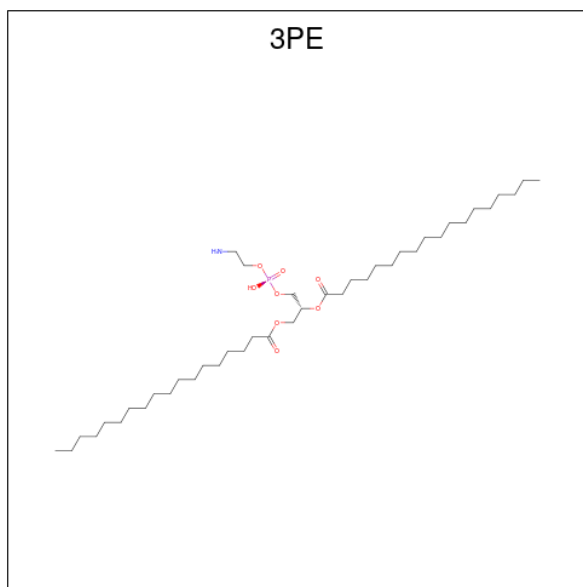
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

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

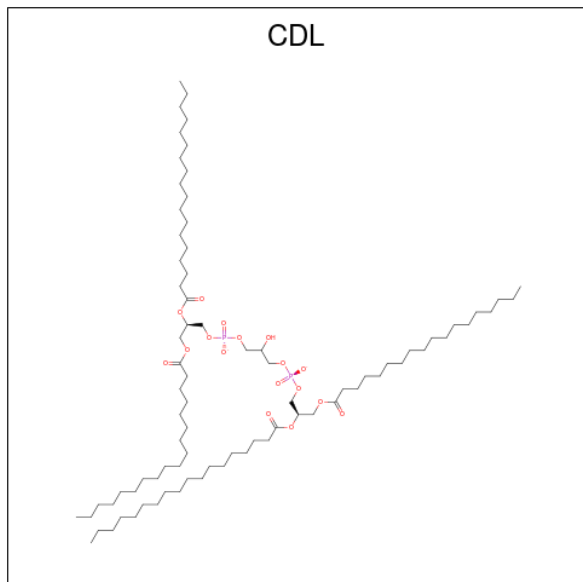
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

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



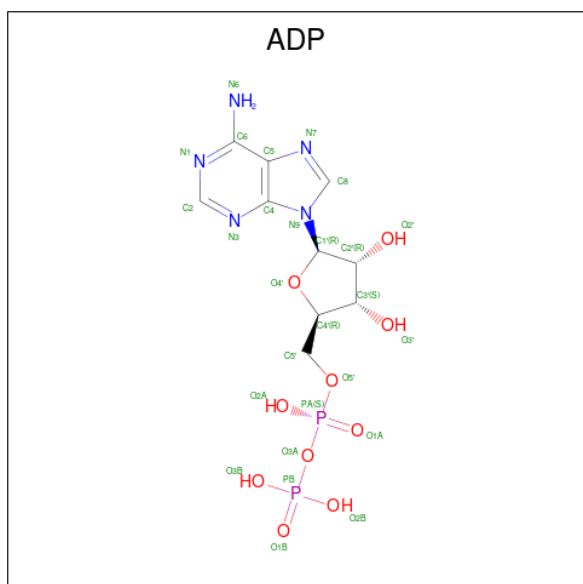
Mol	Chain	Residues	Atoms					AltConf
25	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
25	d	1	Total	C	N	O	P	0
			31	21	1	8	1	
25	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	m	1	Total	C	N	O	P	0
			47	37	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).



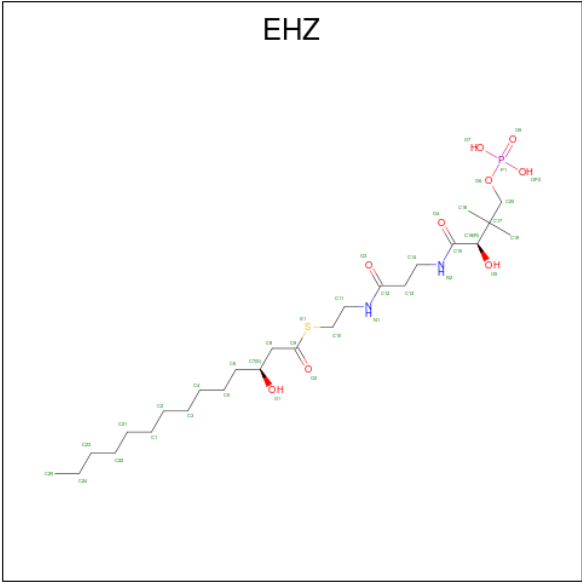
Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			78	59	17	2	
26	X	1	Total	C	O	P	0
			67	48	17	2	
26	h	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 27 is 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
27	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 28 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

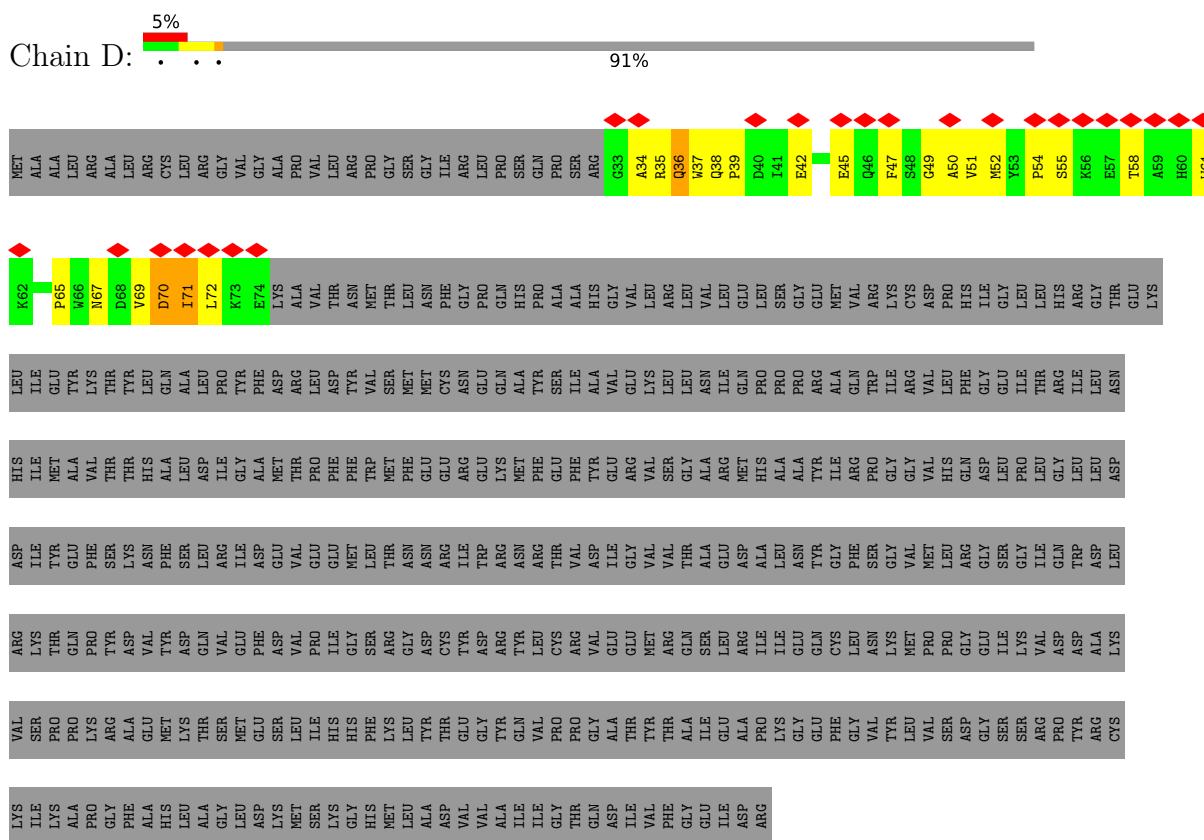


Mol	Chain	Residues	Atoms						AltConf
28	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

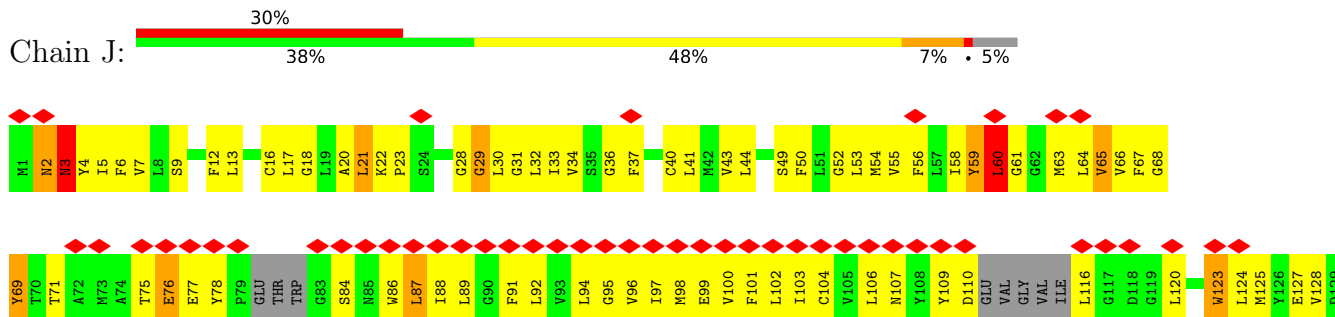
3 Residue-property plots

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

- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

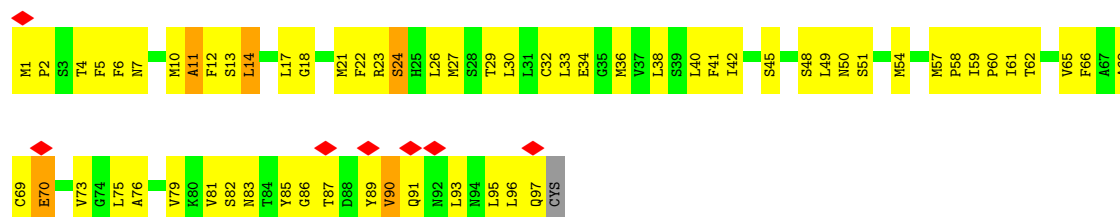


- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

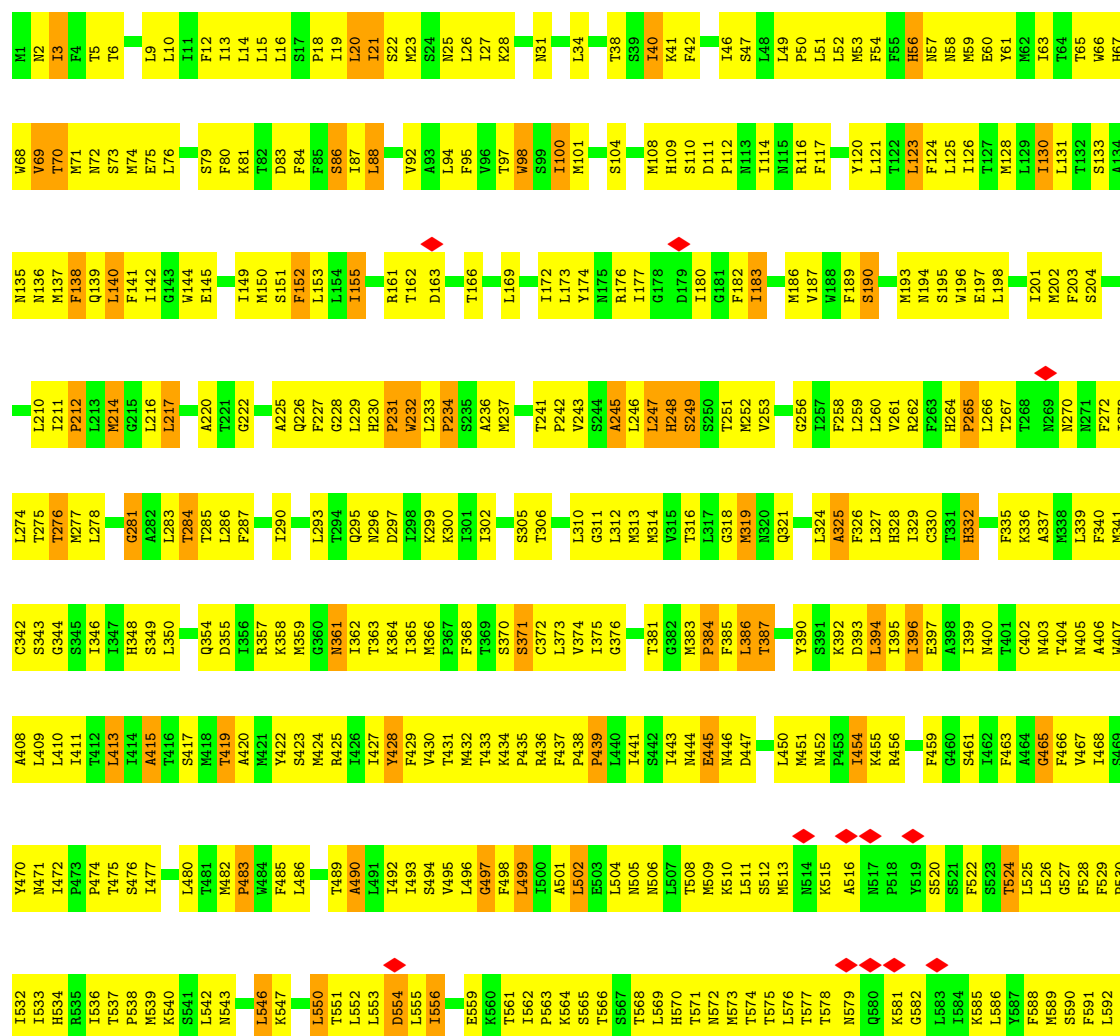


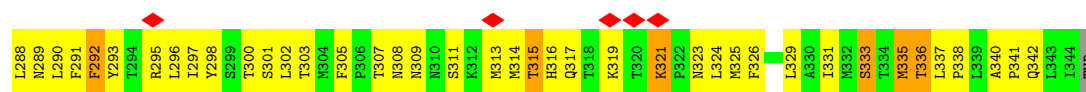


• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L

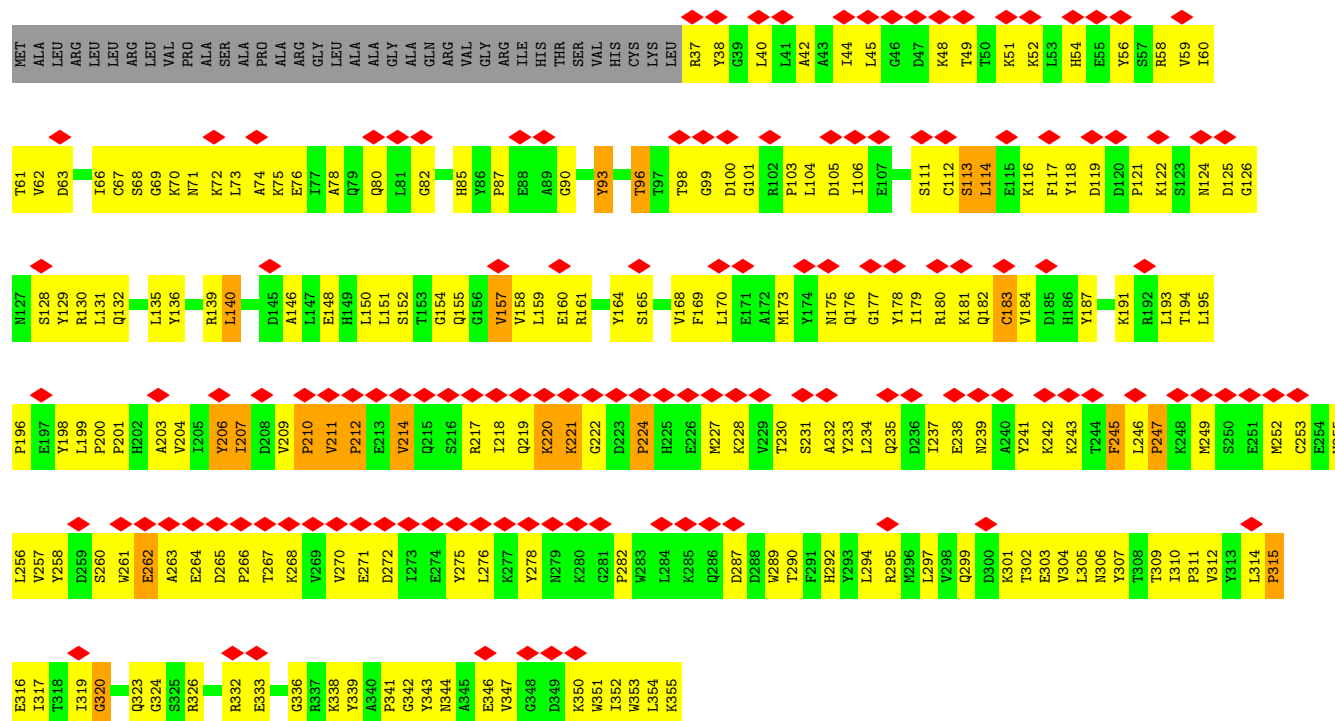


• Molecule 4: NADH-ubiquinone oxidoreductase chain 5

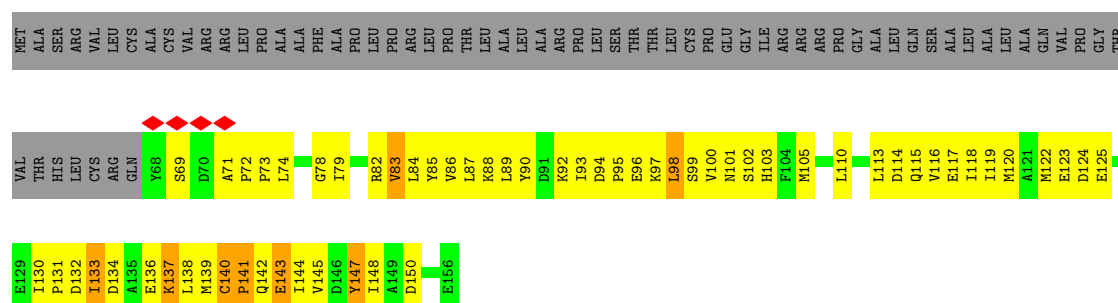




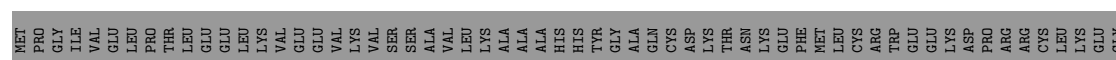
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 8: Acyl carrier protein, mitochondrial



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



LYS LEU VAL ASN GLY CYS ALA LEU ASN PHE LYS PHE ARG GLN TLE LYS SER PRO HIS CYS GLU ALA PRO PHE THR SER GLU TYR ARG TRP THR CYS LEU ASP TYR SER ASN MET GLN PHE ARG HIS ARG GLN GLN ALA LYS PHE ASP GLN VAL CYS LEU LYS ASP GLY TRP VAL ARG PRO

ASP LEU GLY VAL SER LYS VAL THR LYS VAL THR ASP ARG PRO LEU PRO GLU ASN ARG A146 R147 P148 N151 P152 V153 I154 E155 L158 K159 P160 A161 H163 G164 T165 R166 F167 F168 F169 W170 T171 V172

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

Chain Y: 32% 52% 44%

MET ALA VAL K5 R6 F7 F8 E9 A80 Y11 H12 E13 V14 P15 D16 G17 T18 Q19 C20 H21 R22 K23 I26 L30 G31 G35 I36 I37 G38 S39 V43 S44 L45 M46 P47 A48 D49 S50 T51 L52 E53 A56 R57 V58 G59 R60 F63 T64 A65 A66 A67 I68

M71 F72 G73 L74 T75 T76 C77 V78 S79 Q81 R82 R83 E84 D87 D88 P89 N91 Y92 F93 I94 G95 C97 A98 L101 T102 H103 S109 Y110 A114 M115 G116 Y119 M120 G121 A124 F127 K128 I129 G130 K131 L137 F138 P139 T140 P141 K142 V143

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

Chain c: 18% 25% 32% 5% 38%

MET ALA PRO VAL LEU ARG SER PHE SER ARG LEU ALA PRO ALA ARG LEU PRO SER CYS SER SER THR ARG SER LYS F29 Y30 V31 R32 E33 P34 V35 N36 A37 K38 P39 M40 W41 V44 G45 L46 S47 A50 F53 M54 W55 Y57 Q60 T61 H62 E64

D65 V66 L67 E68 Y69 K70 R71 R72 N73 G74 L75 GLU

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

Chain d: 11% 38% 59%

M1 M2 N3 G4 R5 P6 G7 H8 E9 P10 L11 K12 L13 L14 P15 D16 E17 A18 S19 S20 L21 P22 P23 P24 K25 N26 D27 D28 P29 R30 Y33 L37 G38 Y39 C40 L43 M44 D45 M46 M47 L48 R49 M50 R51 P52 V53 M54 R55 A56 G57 L58 H59 R60 D61 L62 L63 F64

V65 T66 F70 A71 G72 Y73 K77 R78 Q79 R80 Y81 L82 D87 H88 D89 M90 F91 G92 Y93 I94 E99 D100 F101 P102 E103 K104 E105 K106 T107 T108 Y109 A110 E111 I112 L113 E114 F115 H117 P118 V119 R120

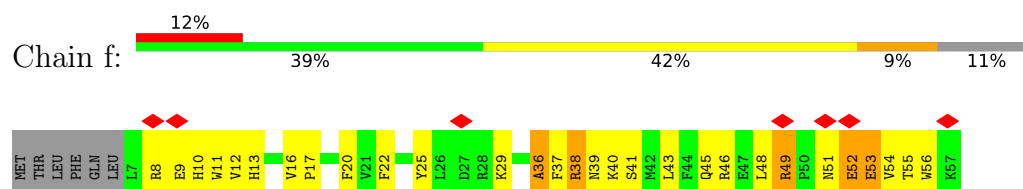
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 13% 47% 46% 6%

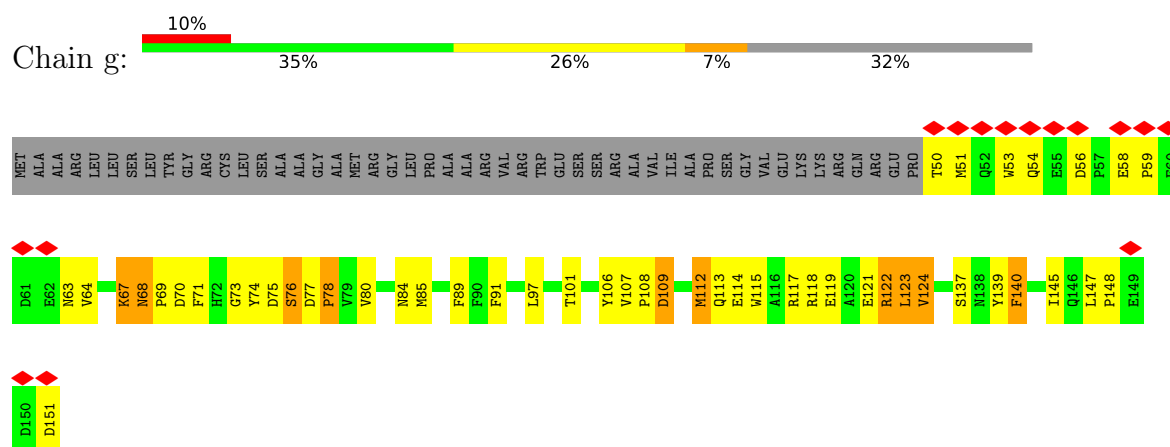
MET F2 F3 L4 D5 I6 L14 D15 R16 H17 F18 M19 F20 L21 R32 C33 D34 H35 F36 E37 K38 E39 V40 T41 E42 C43 A44 H45 G46 T47 G48 G49 T50 R51 A52 F60 D61 E65 R69 Y70 K71 T72 W73 R74 R75 I79 Q82 L86 M87 R88 E89 G90

K91 Y92 T93 F94 P95 P96 H97 H98 S99 G100 R101 E102 E103 P104 R105 P106

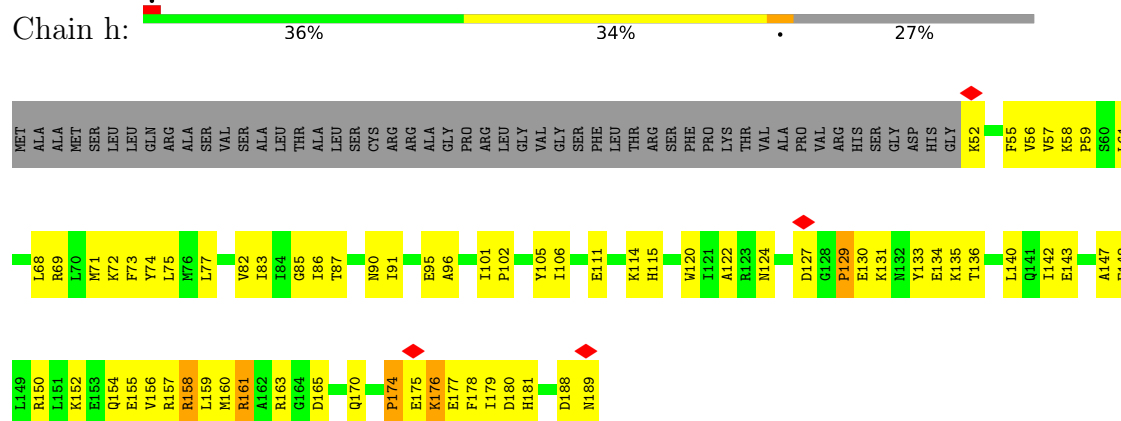
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



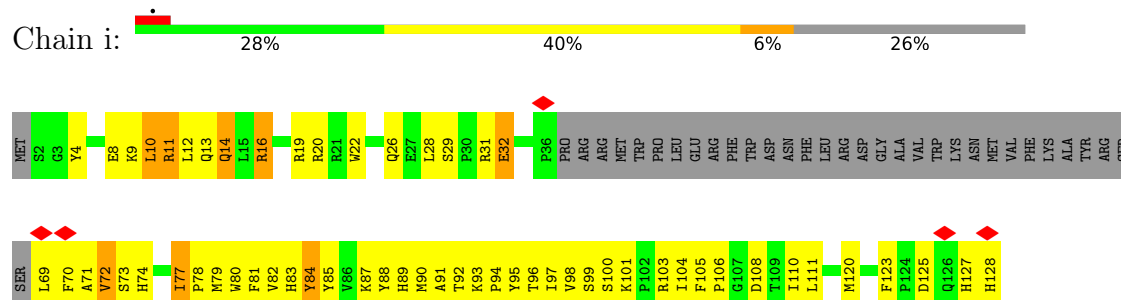
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

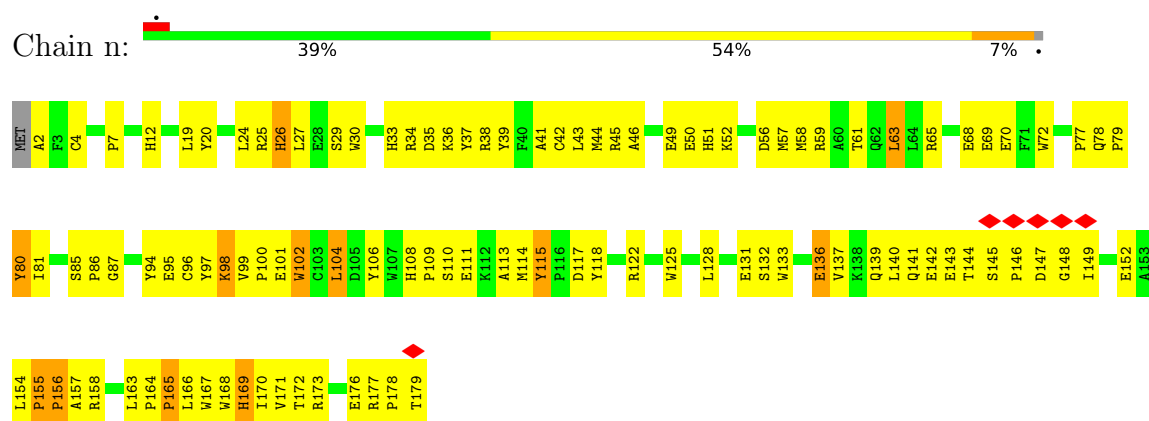


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

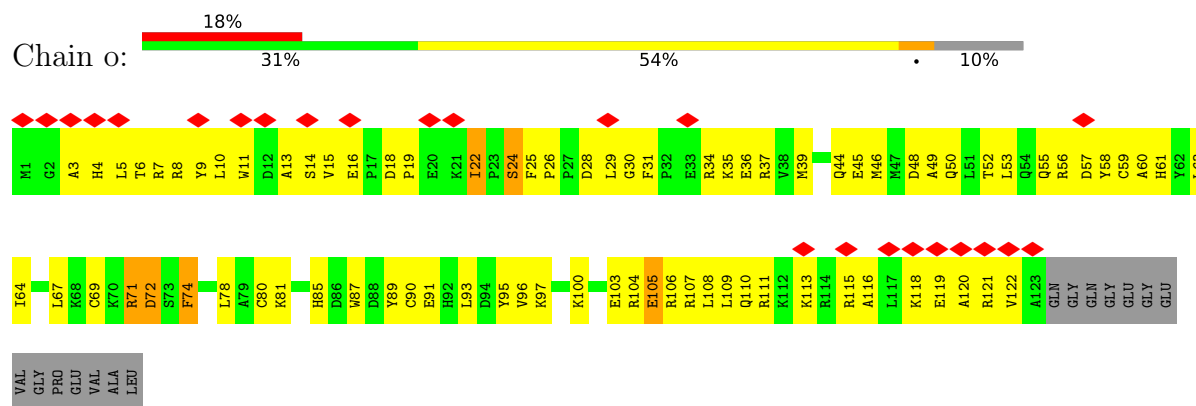


- | MET | SER | GLY |
|-----|-----|-----|
| S4 | K5 | Y6 |
| K7 | P8 | A9 |
| F10 | L11 | A12 |
| T13 | L14 | P15 |
| S16 | T17 | L18 |
| V25 | S26 | P27 |
| E28 | T29 | R30 |
| R31 | V34 | E35 |
| A41 | R42 | L43 |
| K44 | R45 | Y47 |
| L48 | L49 | Q50 |
| Y51 | N52 | V57 |
| S58 | H59 | I60 |
| E61 | D62 | Y70 |
| A71 | R72 | N75 |
| I76 | N79 | F80 |

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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177076	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	3.050	Depositor
Minimum map value	-1.895	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.085	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: CDL, 3PE, EH2, ADP

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	0.64	0/365	1.06	3/500 (0.6%)
2	J	0.84	1/1257 (0.1%)	1.26	20/1704 (1.2%)
3	K	0.90	0/740	1.54	13/1005 (1.3%)
4	L	0.99	7/4921 (0.1%)	1.57	107/6696 (1.6%)
5	M	1.01	7/3717 (0.2%)	1.57	86/5062 (1.7%)
6	N	1.01	3/2756 (0.1%)	1.44	51/3751 (1.4%)
7	O	1.00	8/2666 (0.3%)	1.40	41/3615 (1.1%)
8	U	0.98	1/731 (0.1%)	1.30	14/988 (1.4%)
9	X	0.72	0/230	0.98	0/313
10	Y	0.86	0/1054	0.98	2/1429 (0.1%)
11	c	0.93	1/400 (0.2%)	1.49	12/544 (2.2%)
12	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
13	e	0.69	1/900 (0.1%)	1.01	5/1199 (0.4%)
14	f	0.95	1/451 (0.2%)	1.38	12/607 (2.0%)
15	g	0.89	3/886 (0.3%)	1.35	19/1207 (1.6%)
16	h	0.77	1/1197 (0.1%)	1.26	8/1621 (0.5%)
17	i	0.84	0/829	1.35	14/1127 (1.2%)
18	j	0.80	0/588	1.32	8/805 (1.0%)
19	k	0.98	2/600 (0.3%)	1.44	14/810 (1.7%)
20	l	0.98	3/1367 (0.2%)	1.22	9/1866 (0.5%)
21	m	0.92	2/1079 (0.2%)	1.24	17/1463 (1.2%)
22	n	0.94	2/1596 (0.1%)	1.32	18/2162 (0.8%)
23	o	0.82	1/1075 (0.1%)	1.14	10/1442 (0.7%)
24	p	0.71	1/1485 (0.1%)	1.05	15/2007 (0.7%)
All	All	0.93	47/31918 (0.1%)	1.37	509/43310 (1.2%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	247	PRO	N-CD	16.66	1.71	1.47
12	d	115	PRO	N-CD	-14.15	1.27	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.84	1.67	1.47
6	N	255	PRO	N-CD	-13.65	1.28	1.47
11	c	39	PRO	N-CD	-13.22	1.29	1.47
21	m	27	PRO	N-CD	-12.93	1.29	1.47
7	O	315	PRO	N-CD	-12.04	1.30	1.47
4	L	234	PRO	N-CD	11.15	1.63	1.47
7	O	210	PRO	N-CD	-10.46	1.33	1.47
5	M	370	PRO	N-CD	-10.46	1.33	1.47
19	k	20	MET	C-N	10.35	1.47	1.33
7	O	224	PRO	N-CD	-10.21	1.33	1.47
4	L	57	ASN	C-O	-10.18	1.11	1.24
15	g	78	PRO	N-CD	-9.57	1.34	1.47
12	d	15	PRO	N-CD	-9.37	1.34	1.47
7	O	212	PRO	N-CD	-8.82	1.35	1.47
5	M	20	PRO	N-CD	8.61	1.59	1.47
4	L	212	PRO	N-CD	-8.26	1.36	1.47
22	n	155	PRO	N-CD	8.08	1.59	1.47
20	l	104	PRO	N-CD	-7.17	1.37	1.47
5	M	208	PRO	N-CD	7.16	1.57	1.47
6	N	238	PRO	N-CD	-7.02	1.38	1.47
7	O	211	VAL	CA-C	6.97	1.60	1.52
20	l	119	THR	CA-C	-6.86	1.45	1.53
13	e	106	PRO	N-CD	6.71	1.57	1.47
15	g	113	GLN	CA-C	6.68	1.61	1.52
4	L	384	PRO	N-CD	6.24	1.56	1.47
24	p	10	TYR	CA-C	-6.19	1.46	1.52
15	g	137	SER	C-O	-6.15	1.16	1.24
4	L	112	PRO	N-CD	5.95	1.56	1.47
2	J	69	TYR	CA-C	-5.91	1.45	1.52
21	m	72	ARG	CA-C	5.83	1.60	1.52
19	k	19	LYS	C-N	5.76	1.41	1.33
7	O	87	PRO	N-CD	-5.74	1.39	1.47
20	l	45	PRO	N-CD	-5.73	1.39	1.47
5	M	454	ILE	CA-C	5.69	1.60	1.52
6	N	333	SER	C-O	-5.58	1.17	1.23
5	M	252	PRO	N-CD	-5.54	1.40	1.47
8	U	140	CYS	C-O	-5.40	1.17	1.24
7	O	103	PRO	N-CD	-5.31	1.40	1.47
14	f	38	ARG	CA-C	-5.14	1.46	1.52
16	h	174	PRO	N-CD	-5.14	1.40	1.47
23	o	24	SER	C-N	-5.12	1.23	1.33
5	M	424	ILE	CA-C	-5.11	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	80	TYR	CA-C	-5.10	1.46	1.52
5	M	159	PRO	N-CD	5.09	1.54	1.47
4	L	56	HIS	CA-C	-5.03	1.46	1.52

All (509) 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	14.50	128.39	110.70
7	O	118	TYR	N-CA-C	13.84	125.88	111.07
22	n	165	PRO	N-CA-C	13.34	130.41	111.33
7	O	222	GLY	N-CA-C	13.25	129.73	112.77
24	p	128	GLU	N-CA-C	12.67	125.17	111.36
5	M	424	ILE	N-CA-C	-11.68	93.99	109.30
7	O	157	VAL	N-CA-C	11.67	124.45	108.11
17	i	14	GLN	N-CA-C	11.60	123.92	111.28
7	O	114	LEU	N-CA-C	-11.53	98.79	111.36
5	M	104	ILE	N-CA-C	-11.48	99.17	110.30
4	L	194	ASN	N-CA-C	11.43	125.34	109.11
6	N	244	ILE	N-CA-C	-11.37	99.24	110.72
5	M	311	GLY	N-CA-C	-11.35	99.33	112.50
4	L	278	LEU	N-CA-C	-11.25	98.99	111.14
3	K	83	ASN	N-CA-C	-11.16	100.21	114.04
2	J	4	TYR	N-CA-C	-10.94	99.44	113.12
2	J	76	GLU	N-CA-C	-10.81	97.09	110.61
4	L	582	GLY	N-CA-C	-10.80	99.52	114.64
18	j	82	GLY	N-CA-C	-10.74	91.04	111.02
4	L	556	ILE	N-CA-C	10.69	121.34	110.23
4	L	231	PRO	N-CA-C	10.67	127.72	113.84
16	h	101	ILE	N-CA-C	-10.57	98.59	108.95
7	O	96	THR	N-CA-C	-10.40	100.03	111.36
7	O	247	PRO	N-CA-CB	10.35	114.30	103.23
5	M	276	CYS	N-CA-C	-10.34	100.01	111.28
20	l	170	ARG	N-CA-C	-10.10	101.60	113.21
7	O	220	LYS	N-CA-C	10.07	124.92	112.23
5	M	117	MET	N-CA-C	-9.96	100.42	111.28
3	K	90	VAL	N-CA-C	-9.79	100.32	112.76
5	M	423	MET	N-CA-C	-9.76	96.89	110.35
6	N	255	PRO	CA-N-CD	9.72	125.61	112.00
6	N	286	ALA	N-CA-C	-9.70	100.71	111.28
5	M	83	HIS	N-CA-C	-9.63	97.25	110.35
12	d	115	PRO	N-CA-CB	-9.61	94.99	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	12	LEU	N-CA-C	-9.60	101.11	113.12
22	n	29	SER	N-CA-C	-9.56	101.50	113.55
4	L	375	ILE	N-CA-C	-9.53	101.27	110.42
2	J	36	GLY	N-CA-C	-9.46	101.04	112.49
6	N	228	ASN	N-CA-C	-9.46	100.95	111.07
24	p	56	HIS	N-CA-C	9.45	121.58	111.28
12	d	115	PRO	CA-N-CD	9.41	125.18	112.00
14	f	51	ASN	CB-CA-C	-9.38	97.33	112.06
4	L	40	ILE	N-CA-C	-9.33	101.30	110.72
19	k	60	MET	N-CA-C	9.32	121.12	110.97
19	k	56	ALA	N-CA-C	9.30	121.50	111.36
5	M	104	ILE	N-CA-CB	9.27	120.73	110.62
4	L	394	LEU	N-CA-C	-9.24	101.19	111.07
21	m	48	LEU	N-CA-C	9.22	124.07	113.01
4	L	483	PRO	N-CA-C	-9.16	96.81	111.38
4	L	524	THR	N-CA-C	9.13	122.20	111.71
7	O	247	PRO	CA-N-CD	-9.12	99.23	112.00
6	N	87	GLN	N-CA-C	9.11	123.25	109.41
11	c	64	GLU	N-CA-C	-9.08	101.35	111.07
5	M	442	ILE	N-CA-CB	9.08	117.53	110.45
4	L	467	VAL	N-CA-C	9.06	119.12	110.42
11	c	39	PRO	N-CA-CB	-9.00	95.33	103.25
24	p	115	GLN	N-CA-C	-8.94	102.88	113.88
3	K	70	GLU	N-CA-C	-8.93	100.39	111.11
4	L	344	GLY	N-CA-C	-8.87	102.22	112.50
4	L	406	ALA	N-CA-C	-8.87	101.70	111.36
7	O	206	TYR	N-CA-CB	-8.85	92.77	110.64
6	N	233	LEU	N-CA-C	-8.84	101.64	111.28
7	O	183	CYS	N-CA-C	-8.82	100.53	111.11
5	M	255	LYS	N-CA-C	-8.77	101.69	111.07
21	m	27	PRO	CA-N-CD	8.74	124.24	112.00
6	N	255	PRO	N-CA-CB	-8.74	94.61	103.08
6	N	81	LEU	N-CA-C	-8.72	94.42	108.55
22	n	70	GLU	N-CA-C	-8.69	101.77	111.07
23	o	72	ASP	N-CA-C	-8.69	99.06	110.53
5	M	248	ILE	N-CA-C	-8.60	102.17	110.42
4	L	212	PRO	N-CA-C	8.59	125.76	113.47
2	J	29	GLY	N-CA-C	-8.59	102.25	112.64
7	O	315	PRO	CA-N-CD	8.52	123.93	112.00
4	L	265	PRO	N-CA-C	-8.51	101.31	113.47
7	O	245	PHE	N-CA-C	8.48	120.15	111.07
6	N	221	LEU	N-CA-C	-8.45	101.11	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	272	LYS	N-CA-C	-8.42	102.10	111.28
4	L	281	GLY	N-CA-C	-8.41	102.75	112.50
4	L	287	PHE	N-CA-C	-8.40	102.08	111.07
7	O	212	PRO	N-CA-C	8.39	126.26	113.75
6	N	109	ALA	CA-C-N	-8.35	110.85	120.12
6	N	109	ALA	C-N-CA	-8.35	110.85	120.12
22	n	19	LEU	N-CA-C	-8.35	103.23	113.41
6	N	218	ALA	N-CA-C	-8.26	98.92	111.56
5	M	274	SER	N-CA-C	8.22	120.24	111.28
4	L	88	LEU	N-CA-C	-8.21	102.28	111.14
4	L	151	SER	N-CA-C	-8.17	102.46	111.36
6	N	32	GLY	N-CA-C	-8.16	103.03	112.50
1	D	36	GLN	N-CA-C	-8.16	98.50	110.42
4	L	169	LEU	N-CA-C	-8.15	102.48	111.36
5	M	26	ASN	N-CA-C	-8.12	102.37	111.14
19	k	38	VAL	N-CA-C	-8.11	102.53	110.72
5	M	385	LEU	N-CA-C	-8.06	102.50	111.28
7	O	217	ARG	N-CA-C	-8.05	102.46	111.07
22	n	170	ILE	N-CA-C	-8.03	103.06	111.58
4	L	276	THR	N-CA-CB	8.00	121.61	110.01
12	d	15	PRO	N-CA-CB	-7.99	96.40	103.35
2	J	60	LEU	N-CA-C	7.96	120.72	111.02
5	M	205	ILE	N-CA-C	7.92	118.02	110.42
11	c	39	PRO	CA-N-CD	7.92	123.08	112.00
5	M	141	GLU	N-CA-C	7.90	122.76	113.20
13	e	105	ARG	N-CA-C	7.86	122.45	110.50
24	p	128	GLU	N-CA-CB	-7.85	98.54	110.16
11	c	45	GLY	N-CA-C	7.85	123.53	113.24
4	L	111	ASP	N-CA-C	-7.84	100.20	109.93
4	L	265	PRO	N-CA-CB	7.84	111.62	103.23
5	M	85	LYS	N-CA-C	-7.82	101.37	113.02
21	m	50	GLN	N-CA-C	-7.81	102.77	114.64
5	M	330	ALA	N-CA-C	-7.77	102.75	111.14
3	K	51	SER	N-CA-C	-7.75	102.91	113.30
4	L	265	PRO	CA-N-CD	-7.75	101.14	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
14	f	51	ASN	N-CA-C	7.66	121.97	111.17
14	f	48	LEU	N-CA-C	7.60	121.69	110.30
15	g	124	VAL	N-CA-C	-7.59	103.06	110.72
8	U	147	TYR	N-CA-C	-7.55	102.98	111.14
23	o	81	LYS	N-CA-C	-7.55	104.59	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	m	27	PRO	N-CA-CB	-7.52	95.36	103.25
4	L	392	LYS	N-CA-C	7.50	119.09	111.07
4	L	245	ALA	N-CA-C	7.47	119.07	111.07
3	K	14	LEU	N-CA-C	-7.46	103.23	111.36
13	e	46	GLY	N-CA-C	-7.46	104.97	114.37
4	L	605	ASN	N-CA-CB	7.45	121.27	110.47
4	L	123	LEU	N-CA-C	-7.41	103.28	111.36
4	L	138	PHE	N-CA-C	-7.40	103.21	111.28
5	M	250	LEU	N-CA-C	-7.40	103.56	112.58
4	L	21	ILE	N-CA-CB	7.39	121.66	110.58
12	d	113	LEU	N-CA-CB	-7.38	99.93	111.23
4	L	28	LYS	N-CA-C	-7.35	103.27	111.28
21	m	72	ARG	N-CA-C	7.31	122.49	113.50
20	l	97	LEU	N-CA-C	-7.31	103.96	113.17
5	M	455	THR	N-CA-C	-7.28	100.44	110.35
3	K	81	VAL	N-CA-C	7.27	118.04	110.62
11	c	37	ALA	N-CA-C	7.27	119.83	111.11
4	L	19	ILE	N-CA-C	7.26	117.39	110.42
5	M	289	SER	N-CA-C	-7.25	103.31	111.07
2	J	21	LEU	N-CA-C	-7.24	104.53	113.15
16	h	174	PRO	N-CA-C	7.24	122.62	111.11
22	n	165	PRO	CB-CA-C	-7.24	100.25	111.40
7	O	224	PRO	N-CA-CB	-7.20	96.76	103.46
3	K	24	SER	CB-CA-C	-7.20	107.44	117.23
7	O	210	PRO	CA-N-CD	7.19	122.06	112.00
8	U	136	GLU	N-CA-C	-7.18	104.51	113.20
21	m	25	VAL	CB-CA-C	-7.18	102.89	111.65
19	k	73	ILE	N-CA-C	-7.15	103.33	110.62
4	L	554	ASP	N-CA-CB	7.14	121.28	110.42
5	M	244	ILE	N-CA-C	7.13	117.89	110.62
5	M	325	LEU	N-CA-C	-7.12	103.45	111.07
18	j	78	ASP	N-CA-C	-7.11	103.17	112.41
24	p	168	LYS	N-CA-C	-7.11	104.24	113.12
18	j	65	MET	N-CA-C	-7.10	103.48	111.07
7	O	210	PRO	N-CA-C	7.08	122.32	111.34
3	K	48	SER	N-CA-C	-7.07	103.58	111.28
5	M	34	ILE	N-CA-C	-7.05	103.43	110.62
5	M	365	ALA	N-CA-C	-7.04	103.69	111.36
22	n	102	TRP	N-CA-C	-7.03	105.06	112.93
23	o	11	TRP	CB-CA-C	-7.02	108.48	116.63
18	j	81	LEU	CA-C-O	7.02	126.02	119.00
4	L	319	MET	N-CA-C	-7.01	104.72	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	264	LEU	N-CA-C	-7.00	103.58	111.07
4	L	100	ILE	N-CA-C	6.99	119.79	111.05
5	M	213	HIS	CB-CA-C	-6.99	96.83	110.11
6	N	132	THR	N-CA-C	6.97	122.90	113.97
4	L	86	SER	N-CA-C	6.94	118.50	111.07
4	L	546	LEU	N-CA-C	6.94	119.49	111.02
7	O	220	LYS	CB-CA-C	-6.94	96.22	110.38
17	i	9	LYS	N-CA-C	-6.93	104.82	112.72
7	O	231	SER	N-CA-C	-6.92	103.81	111.36
5	M	91	LEU	N-CA-C	-6.92	103.84	112.90
17	i	11	ARG	N-CA-C	-6.92	104.84	113.28
5	M	235	LEU	N-CA-C	6.89	119.38	111.11
5	M	442	ILE	N-CA-C	-6.89	104.08	112.35
4	L	471	ASN	N-CA-C	6.88	118.86	111.36
4	L	26	LEU	N-CA-C	6.87	119.61	111.71
22	n	117	ASP	N-CA-C	-6.87	103.85	111.82
19	k	59	TYR	N-CA-CB	-6.87	98.87	110.41
5	M	276	CYS	N-CA-CB	6.87	120.21	110.12
4	L	547	LYS	N-CA-C	6.86	118.75	111.28
15	g	78	PRO	CA-N-CD	6.86	121.60	112.00
7	O	93	TYR	N-CA-C	-6.85	103.89	111.36
2	J	58	ILE	N-CA-C	6.84	117.44	111.56
5	M	165	ILE	N-CA-C	-6.84	102.54	111.09
3	K	83	ASN	N-CA-CB	6.83	120.92	110.81
18	j	79	ALA	N-CA-C	-6.80	103.95	111.36
3	K	70	GLU	N-CA-CB	6.77	120.03	109.94
12	d	88	HIS	N-CA-C	-6.72	103.04	111.11
21	m	127	ILE	N-CA-C	-6.72	106.25	112.43
7	O	207	ILE	N-CA-C	-6.71	97.27	107.73
5	M	248	ILE	N-CA-CB	6.71	118.39	110.55
5	M	374	ASN	N-CA-C	-6.70	103.90	111.07
8	U	140	CYS	CA-C-N	-6.70	114.00	120.83
8	U	140	CYS	C-N-CA	-6.70	114.00	120.83
6	N	228	ASN	N-CA-CB	6.69	119.71	110.01
15	g	76	SER	N-CA-C	6.69	118.22	111.07
4	L	95	PHE	N-CA-C	-6.68	103.93	111.07
7	O	315	PRO	N-CA-CB	-6.67	95.99	103.33
8	U	150	ASP	CB-CA-C	6.67	121.86	110.79
20	l	86	ARG	N-CA-C	-6.67	99.66	110.20
7	O	224	PRO	CA-N-CD	6.66	121.32	112.00
3	K	76	ALA	N-CA-C	-6.63	104.13	111.36
5	M	410	MET	N-CA-C	-6.63	103.98	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	143	LEU	N-CA-C	-6.62	103.98	111.07
5	M	303	ILE	N-CA-C	-6.62	104.03	110.72
1	D	70	ASP	N-CA-C	6.62	120.68	110.42
7	O	140	LEU	N-CA-C	-6.61	104.00	111.07
17	i	8	GLU	N-CA-C	-6.58	104.84	114.39
4	L	499	LEU	N-CA-C	-6.57	103.81	110.97
4	L	130	ILE	N-CA-C	-6.57	103.92	110.62
19	k	57	TRP	N-CA-C	-6.55	104.55	112.54
4	L	232	TRP	N-CA-C	6.54	120.52	112.54
22	n	115	TYR	N-CA-CB	6.54	122.00	110.37
5	M	161	LEU	N-CA-C	-6.53	104.08	111.07
4	L	423	SER	N-CA-C	-6.53	104.09	111.07
24	p	54	ARG	N-CA-C	-6.52	103.67	111.69
7	O	118	TYR	N-CA-CB	-6.52	100.56	110.01
4	L	329	ILE	N-CA-C	-6.49	104.19	110.42
21	m	51	TYR	N-CA-C	-6.49	105.67	113.97
10	Y	96	GLY	N-CA-C	-6.47	104.48	112.77
6	N	315	THR	N-CA-C	-6.47	104.15	111.07
20	l	119	THR	N-CA-C	-6.46	95.78	107.60
23	o	22	ILE	CA-C-N	-6.44	113.22	121.91
23	o	22	ILE	C-N-CA	-6.44	113.22	121.91
7	O	221	LYS	N-CA-C	-6.43	101.44	110.50
7	O	320	GLY	N-CA-C	-6.41	96.69	111.04
3	K	11	ALA	N-CA-C	-6.40	104.22	111.07
4	L	325	ALA	N-CA-C	-6.38	104.32	111.28
5	M	32	PHE	N-CA-C	-6.38	104.25	111.07
15	g	112	MET	N-CA-C	6.37	120.84	113.38
4	L	439	PRO	N-CA-C	6.36	122.37	113.53
4	L	234	PRO	CA-N-CD	-6.36	103.10	112.00
4	L	387	THR	N-CA-C	6.36	119.02	111.71
12	d	15	PRO	CA-N-CD	6.35	120.89	112.00
4	L	490	ALA	N-CA-C	-6.34	104.28	111.07
5	M	317	ILE	N-CA-C	-6.33	104.58	110.53
7	O	98	THR	N-CA-C	6.33	120.60	109.96
17	i	32	GLU	CA-C-N	-6.33	111.92	119.84
17	i	32	GLU	C-N-CA	-6.33	111.92	119.84
4	L	70	THR	N-CA-C	-6.32	103.91	111.69
2	J	136	GLU	CA-C-N	-6.32	113.56	120.44
2	J	136	GLU	C-N-CA	-6.32	113.56	120.44
14	f	52	GLU	N-CA-CB	6.29	121.16	110.71
6	N	89	GLN	N-CA-C	6.28	120.50	112.34
4	L	337	ALA	N-CA-C	-6.27	104.44	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	26	ASN	N-CA-CB	6.27	119.17	110.07
20	l	105	ILE	CA-C-O	-6.26	115.14	121.59
11	c	47	SER	N-CA-CB	6.26	120.84	110.33
4	L	502	LEU	N-CA-C	-6.24	104.48	111.28
6	N	46	ASN	N-CA-C	-6.24	105.69	113.55
7	O	210	PRO	N-CA-CB	-6.22	97.55	103.39
6	N	276	LEU	N-CA-C	-6.21	105.34	113.17
6	N	91	ASN	N-CA-CB	6.21	119.09	109.97
6	N	216	PHE	N-CA-C	6.21	118.12	111.36
7	O	113	SER	N-CA-C	6.20	118.52	108.41
21	m	72	ARG	CA-C-O	6.20	125.96	119.14
15	g	123	LEU	N-CA-CB	6.19	119.05	110.07
5	M	121	LEU	N-CA-C	-6.18	104.62	111.36
19	k	59	TYR	N-CA-C	6.18	120.66	113.18
4	L	361	ASN	CB-CA-C	-6.17	102.79	111.80
6	N	337	LEU	CA-C-N	-6.16	113.78	119.82
6	N	337	LEU	C-N-CA	-6.16	113.78	119.82
14	f	49	ARG	N-CA-CB	6.14	119.08	110.11
19	k	30	ILE	N-CA-C	6.13	118.75	111.09
22	n	63	LEU	N-CA-C	-6.13	104.15	111.69
6	N	47	LYS	N-CA-C	-6.13	104.71	111.82
2	J	123	TRP	N-CA-C	-6.12	102.55	111.30
23	o	105	GLU	N-CA-C	-6.12	104.69	111.36
5	M	4	ILE	N-CA-C	-6.11	104.00	112.50
4	L	98	TRP	N-CA-C	-6.11	104.70	111.36
4	L	454	ILE	N-CA-C	-6.11	104.39	110.62
11	c	33	GLU	CA-C-N	-6.10	113.99	120.03
11	c	33	GLU	C-N-CA	-6.10	113.99	120.03
5	M	57	SER	N-CA-C	6.10	119.14	109.50
14	f	39	ASN	N-CA-C	-6.09	104.02	112.30
15	g	109	ASP	CA-CB-CG	6.09	118.69	112.60
16	h	101	ILE	N-CA-CB	6.07	115.72	110.08
16	h	142	ILE	N-CA-C	-6.07	104.60	110.42
5	M	213	HIS	N-CA-C	6.06	120.53	113.20
4	L	287	PHE	N-CA-CB	6.05	118.79	110.01
6	N	91	ASN	N-CA-C	-6.05	101.33	110.28
4	L	140	LEU	N-CA-C	-6.04	104.70	111.28
15	g	123	LEU	N-CA-C	-6.03	104.63	111.14
5	M	3	LYS	N-CA-C	-6.03	106.06	113.41
5	M	396	MET	N-CA-C	-6.00	105.94	113.20
5	M	370	PRO	CA-N-CD	6.00	120.39	112.00
7	O	183	CYS	N-CA-CB	5.99	118.86	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	8	ASP	N-CA-C	5.97	120.64	113.23
5	M	168	GLN	N-CA-C	-5.97	104.86	111.36
4	L	234	PRO	N-CA-CB	5.97	109.61	103.23
6	N	295	ARG	N-CA-C	-5.96	104.78	111.28
11	c	47	SER	N-CA-C	-5.96	104.75	112.68
5	M	253	LEU	N-CA-C	5.95	117.77	111.28
15	g	78	PRO	N-CA-C	5.95	121.80	113.53
5	M	300	SER	N-CA-C	-5.95	107.01	114.56
4	L	112	PRO	CB-CA-C	-5.95	103.00	111.68
5	M	222	GLU	N-CA-C	5.95	120.37	113.18
7	O	234	LEU	N-CA-C	-5.95	104.88	111.36
2	J	155	ALA	N-CA-C	-5.94	104.89	111.36
4	L	278	LEU	N-CA-CB	5.92	118.66	110.07
14	f	53	GLU	N-CA-CB	-5.92	101.37	110.20
24	p	127	LYS	N-CA-C	-5.92	104.17	111.40
4	L	88	LEU	N-CA-CB	5.92	118.65	110.07
5	M	88	ASN	N-CA-C	5.91	120.12	113.02
7	O	181	LYS	N-CA-C	5.90	117.39	111.07
4	L	247	LEU	N-CA-CB	5.90	120.61	110.34
4	L	248	HIS	CB-CA-C	5.90	120.88	110.85
7	O	130	ARG	N-CA-C	-5.90	104.85	111.28
13	e	101	ARG	CB-CA-C	-5.87	109.82	116.63
4	L	387	THR	CB-CA-C	-5.87	99.77	110.63
19	k	80	GLY	N-CA-C	-5.86	105.70	112.50
5	M	272	THR	N-CA-C	-5.86	104.98	111.36
6	N	16	GLY	CA-C-N	-5.86	112.47	118.85
6	N	16	GLY	C-N-CA	-5.86	112.47	118.85
7	O	217	ARG	N-CA-CB	5.85	118.50	110.01
8	U	143	GLU	N-CA-C	-5.85	104.26	111.75
19	k	82	ALA	N-CA-C	-5.84	104.92	111.28
22	n	27	LEU	N-CA-C	-5.84	106.13	113.72
21	m	116	ILE	N-CA-C	-5.84	104.82	110.42
19	k	50	PRO	N-CA-C	5.83	121.64	113.53
6	N	66	ALA	N-CA-C	-5.82	105.02	111.36
7	O	262	GLU	N-CA-C	-5.81	104.95	111.28
6	N	15	LEU	N-CA-C	-5.80	105.69	112.89
12	d	62	LEU	N-CA-C	5.80	117.60	111.28
14	f	52	GLU	N-CA-C	-5.79	98.05	108.48
4	L	428	TYR	N-CA-C	-5.79	104.89	111.14
17	i	10	LEU	N-CA-C	-5.79	107.21	114.56
20	l	186	ILE	N-CA-CB	-5.78	101.67	111.50
18	j	73	PHE	N-CA-C	-5.78	104.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	105	PHE	CA-C-N	-5.77	113.75	119.99
17	i	105	PHE	C-N-CA	-5.77	113.75	119.99
15	g	78	PRO	N-CA-CB	-5.77	96.98	103.33
22	n	52	LYS	N-CA-C	-5.76	105.92	113.12
4	L	177	ILE	N-CA-C	-5.76	104.75	110.62
14	f	36	ALA	N-CA-C	-5.75	103.34	110.41
5	M	279	GLN	N-CA-C	-5.74	98.54	108.69
5	M	424	ILE	O-C-N	5.73	128.35	122.79
6	N	321	LYS	N-CA-C	5.73	118.45	110.20
14	f	10	HIS	N-CA-C	-5.73	104.51	112.30
2	J	134	MET	CA-C-N	-5.73	114.89	122.85
2	J	134	MET	C-N-CA	-5.73	114.89	122.85
4	L	467	VAL	N-CA-CB	-5.73	103.85	110.55
8	U	83	VAL	N-CA-C	-5.72	104.94	110.72
5	M	124	ALA	N-CA-C	-5.72	105.12	111.36
5	M	19	SER	N-CA-C	5.71	117.78	109.84
12	d	53	VAL	N-CA-C	5.71	116.36	110.36
4	L	605	ASN	N-CA-C	-5.71	106.17	113.02
4	L	495	VAL	N-CA-C	5.70	115.89	110.42
4	L	419	THR	N-CA-C	-5.69	105.07	111.28
15	g	67	LYS	N-CA-C	-5.69	102.04	110.46
23	o	71	ARG	N-CA-C	-5.69	104.46	111.40
8	U	137	LYS	CA-C-N	-5.67	113.66	122.05
8	U	137	LYS	C-N-CA	-5.67	113.66	122.05
17	i	84	TYR	N-CA-C	-5.67	105.10	111.28
21	m	104	VAL	N-CA-C	-5.67	105.57	111.58
7	O	214	VAL	N-CA-CB	5.66	119.07	110.58
4	L	371	SER	N-CA-C	-5.66	105.03	111.14
4	L	214	MET	N-CA-C	-5.65	105.20	111.36
17	i	14	GLN	N-CA-CB	-5.65	101.81	110.12
6	N	232	LEU	N-CA-C	-5.64	106.61	112.93
4	L	151	SER	N-CA-CB	5.63	118.50	110.16
4	L	342	CYS	N-CA-CB	5.62	118.16	110.01
5	M	214	LEU	N-CA-C	-5.62	105.68	112.54
20	l	49	ALA	N-CA-C	-5.61	106.59	113.50
4	L	20	LEU	N-CA-C	5.61	119.85	112.89
15	g	107	VAL	N-CA-C	-5.60	102.86	108.96
12	d	5	ARG	CA-C-N	-5.59	114.19	119.90
12	d	5	ARG	C-N-CA	-5.59	114.19	119.90
6	N	251	LEU	N-CA-C	-5.59	105.19	111.28
21	m	60	ILE	N-CA-C	-5.59	101.98	109.30
4	L	445	GLU	CB-CA-C	-5.59	101.97	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	115	GLN	N-CA-CB	5.58	118.02	110.59
5	M	370	PRO	N-CA-CB	-5.57	97.68	103.08
15	g	140	PHE	N-CA-CB	5.56	118.27	109.71
15	g	122	ARG	N-CA-C	5.56	118.27	111.82
4	L	234	PRO	N-CA-C	-5.56	105.53	113.47
4	L	370	SER	N-CA-C	-5.55	105.31	111.36
4	L	155	ILE	N-CA-C	-5.54	105.32	110.53
4	L	394	LEU	N-CA-CB	5.53	118.03	110.01
24	p	120	ASN	N-CA-C	-5.53	105.15	113.89
2	J	2	ASN	N-CA-C	-5.53	104.76	112.45
2	J	134	MET	N-CA-C	-5.53	105.31	113.72
15	g	113	GLN	CA-C-O	5.53	126.18	119.11
6	N	148	LEU	N-CA-C	5.52	120.02	113.28
5	M	355	MET	N-CA-C	-5.52	104.65	111.33
21	m	46	GLU	N-CA-C	-5.52	106.55	113.72
23	o	74	PHE	CA-C-N	-5.52	113.93	119.56
23	o	74	PHE	C-N-CA	-5.52	113.93	119.56
4	L	465	GLY	N-CA-C	-5.50	105.73	112.77
5	M	73	LEU	N-CA-C	-5.50	105.27	112.75
4	L	194	ASN	CB-CA-C	-5.48	103.33	111.72
11	c	64	GLU	N-CA-CB	5.48	117.96	110.01
22	n	136	GLU	CB-CA-C	5.47	121.31	110.42
5	M	223	ALA	N-CA-CB	5.46	118.09	110.11
4	L	152	PHE	N-CA-C	-5.46	105.23	111.07
24	p	94	ARG	N-CA-C	5.45	116.91	111.07
18	j	64	LEU	N-CA-C	-5.45	105.50	111.82
19	k	20	MET	CA-C-N	-5.45	111.20	121.66
19	k	20	MET	C-N-CA	-5.45	111.20	121.66
15	g	137	SER	N-CA-CB	-5.44	101.27	110.41
6	N	62	THR	N-CA-C	-5.44	105.25	111.07
8	U	98	LEU	N-CA-C	-5.43	102.16	110.30
6	N	89	GLN	N-CA-CB	-5.42	100.43	110.18
5	M	409	TYR	N-CA-C	-5.40	105.55	111.82
21	m	52	ASN	N-CA-C	-5.40	105.13	112.26
5	M	234	ILE	N-CA-C	5.40	116.27	111.90
6	N	108	LEU	N-CA-C	5.39	118.03	109.24
17	i	77	ILE	CB-CA-C	-5.39	108.63	114.35
5	M	174	LEU	N-CA-C	-5.39	106.48	112.57
4	L	543	ASN	N-CA-C	-5.39	105.41	111.28
4	L	550	LEU	CA-C-O	-5.38	115.24	120.89
4	L	21	ILE	N-CA-C	-5.38	105.29	110.72
7	O	175	ASN	N-CA-C	-5.37	105.42	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	311	GLY	N-CA-C	-5.37	106.28	112.73
4	L	183	ILE	N-CA-C	-5.37	105.14	110.62
4	L	413	LEU	N-CA-C	5.36	117.13	111.28
5	M	343	ILE	N-CA-C	5.35	116.08	110.62
4	L	415	ALA	N-CA-CB	5.35	117.98	110.12
5	M	169	ASN	N-CA-C	-5.35	105.53	111.36
5	M	53	SER	N-CA-C	5.35	115.60	108.38
4	L	386	LEU	N-CA-C	-5.33	101.01	108.96
23	o	24	SER	O-C-N	-5.33	115.98	122.22
5	M	117	MET	N-CA-CB	5.32	117.95	110.12
15	g	80	VAL	N-CA-C	-5.32	105.31	110.42
5	M	25	THR	CB-CA-C	-5.32	100.46	110.67
7	O	219	GLN	N-CA-C	5.32	117.49	111.11
4	L	494	SER	N-CA-C	-5.31	105.40	111.14
8	U	141	PRO	N-CA-C	-5.31	109.16	114.68
22	n	26	HIS	N-CA-C	-5.30	106.40	112.92
6	N	218	ALA	N-CA-CB	5.30	118.41	110.14
5	M	167	ILE	N-CA-C	5.29	117.67	111.05
7	O	206	TYR	N-CA-C	5.27	118.88	107.49
7	O	264	GLU	N-CA-C	-5.26	107.22	113.38
4	L	137	MET	N-CA-C	5.26	119.33	113.01
4	L	231	PRO	CB-CA-C	-5.26	104.38	111.85
22	n	104	LEU	N-CA-C	-5.26	106.89	113.15
16	h	129	PRO	N-CA-C	-5.25	106.69	113.57
4	L	375	ILE	N-CA-CB	5.25	116.69	110.55
4	L	190	SER	N-CA-C	-5.25	106.72	113.23
15	g	68	ASN	N-CA-CB	5.25	119.01	111.51
5	M	294	MET	N-CA-C	-5.25	106.90	113.72
22	n	12	HIS	N-CA-C	-5.25	105.00	111.40
24	p	13	PRO	O-C-N	5.24	123.61	121.15
5	M	212	VAL	CB-CA-C	-5.23	105.19	112.36
8	U	133	ILE	CB-CA-C	-5.23	104.05	112.16
4	L	497	GLY	N-CA-C	-5.23	106.44	112.50
2	J	3	ASN	N-CA-C	-5.22	99.43	108.52
18	j	76	ASP	CB-CA-C	-5.22	104.63	112.09
16	h	176	LYS	N-CA-C	-5.22	105.77	111.82
24	p	167	ARG	CB-CA-C	5.21	117.26	109.13
13	e	104	PRO	CB-CA-C	5.21	118.49	111.71
8	U	133	ILE	N-CA-C	5.21	117.56	111.05
5	M	317	ILE	N-CA-CB	5.20	117.23	110.57
6	N	90	THR	N-CA-C	5.20	117.63	110.35
5	M	20	PRO	N-CA-C	-5.19	106.31	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	284	THR	N-CA-C	-5.19	105.70	111.36
21	m	17	THR	N-CA-C	-5.19	103.68	110.53
4	L	332	HIS	N-CA-C	-5.18	105.63	111.28
4	L	217	LEU	N-CA-C	-5.18	105.64	111.28
4	L	396	ILE	O-C-N	5.17	126.98	121.91
5	M	98	MET	N-CA-C	-5.17	105.53	111.07
2	J	69	TYR	N-CA-C	-5.17	104.71	111.02
4	L	386	LEU	CA-C-O	-5.17	115.92	121.45
6	N	335	MET	CB-CA-C	-5.17	104.46	111.95
6	N	222	ASN	N-CA-C	-5.16	106.22	112.88
20	l	168	LEU	N-CA-C	-5.16	105.57	111.14
21	m	47	TYR	N-CA-C	-5.15	105.83	112.68
24	p	43	TRP	CA-C-N	-5.15	113.61	118.97
24	p	43	TRP	C-N-CA	-5.15	113.61	118.97
2	J	87	LEU	N-CA-C	-5.15	105.75	111.36
5	M	86	LYS	N-CA-C	-5.14	106.25	112.88
16	h	158	ARG	N-CA-C	-5.13	105.60	111.14
12	d	37	LEU	N-CA-C	-5.12	105.70	111.28
6	N	225	MET	N-CA-C	-5.12	106.62	112.92
14	f	12	VAL	N-CA-C	-5.12	107.99	112.90
21	m	61	GLU	N-CA-C	5.12	119.60	112.90
5	M	234	ILE	CB-CA-C	5.10	116.20	111.30
5	M	330	ALA	N-CA-CB	5.09	117.45	110.07
1	D	71	ILE	N-CA-C	5.09	118.26	111.44
3	K	48	SER	N-CA-CB	5.09	117.60	110.12
10	Y	72	PHE	N-CA-C	-5.09	105.63	111.07
11	c	60	GLN	N-CA-C	-5.08	105.63	111.07
4	L	249	SER	N-CA-C	5.07	116.62	111.14
6	N	292	PHE	CA-CB-CG	5.07	118.87	113.80
5	M	229	MET	N-CA-C	-5.06	105.66	111.07
5	M	32	PHE	N-CA-CB	5.06	117.34	110.01
14	f	55	THR	N-CA-C	5.06	116.48	110.97
5	M	56	PHE	N-CA-C	5.05	116.75	108.52
19	k	19	LYS	N-CA-C	-5.05	104.27	111.24
2	J	161	ALA	N-CA-C	-5.05	107.07	113.18
6	N	64	ALA	N-CA-C	5.05	116.47	111.07
5	M	30	TYR	N-CA-C	5.05	116.78	111.28
6	N	42	PRO	CB-CA-C	-5.05	105.04	113.06
8	U	132	ASP	N-CA-C	5.05	117.18	111.02
20	l	45	PRO	N-CA-C	5.05	120.46	113.65
6	N	217	MET	N-CA-C	-5.04	106.96	113.01
5	M	267	TRP	N-CA-C	-5.04	105.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	c	39	PRO	N-CA-C	5.03	119.10	111.15
15	g	137	SER	N-CA-C	5.03	119.27	113.18
6	N	36	SER	N-CA-C	-5.03	105.25	111.33
13	e	102	GLU	N-CA-C	-5.03	106.73	112.86
22	n	169	HIS	CB-CA-C	5.02	118.66	110.17
4	L	384	PRO	N-CA-CB	5.02	107.71	103.35
6	N	282	MET	N-CA-C	-5.01	105.71	111.07
17	i	16	ARG	N-CA-C	-5.01	105.82	111.28
22	n	42	CYS	N-CA-C	-5.01	107.00	113.01
15	g	109	ASP	CB-CA-C	5.00	119.00	111.89
16	h	161	ARG	N-CA-C	-5.00	105.51	110.97
2	J	59	TYR	N-CA-C	-5.00	105.30	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	350	0	320	40	0
2	J	1229	0	1250	130	0
3	K	729	0	764	96	0
4	L	4798	0	4986	608	0
5	M	3630	0	3854	544	0
6	N	2694	0	2896	336	0
7	O	2599	0	2552	306	0
8	U	718	0	705	89	0
9	X	221	0	215	34	0
10	Y	1030	0	1015	74	0
11	c	389	0	385	48	0
12	d	996	0	1001	93	0
13	e	877	0	869	92	0
14	f	439	0	433	37	0
15	g	858	0	787	75	0
16	h	1162	0	1163	134	0
17	i	802	0	802	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	j	563	0	510	72	0
19	k	582	0	584	46	0
20	l	1312	0	1204	103	0
21	m	1050	0	1061	109	0
22	n	1541	0	1470	151	0
23	o	1050	0	1045	103	0
24	p	1452	0	1413	140	0
25	K	46	0	66	9	0
25	L	167	0	233	28	0
25	M	88	0	130	8	0
25	N	51	0	82	11	0
25	Y	41	0	56	8	0
25	d	31	0	36	8	0
25	i	40	0	54	19	0
25	m	139	0	209	23	0
26	L	78	0	100	16	0
26	X	67	0	81	9	0
26	h	70	0	87	17	0
27	O	27	0	12	11	0
28	n	32	0	0	0	0
All	All	31948	0	32430	2862	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 (2862) 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)
7:O:247:PRO:CD	7:O:247:PRO:N	1.71	1.38
7:O:168:VAL:HG21	7:O:241:TYR:CZ	1.66	1.29
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.20
4:L:141:PHE:CE2	5:M:375:LEU:HD21	1.81	1.16
4:L:466:PHE:HB2	18:j:68:TRP:HZ2	1.11	1.15
4:L:247:LEU:CD1	4:L:248:HIS:CD2	2.30	1.14
4:L:261:VAL:O	4:L:264:HIS:CD2	2.02	1.12
6:N:215:MET:CE	6:N:248:LEU:HD21	1.79	1.12
7:O:80:GLN:HG3	7:O:270:VAL:HG21	1.25	1.11
12:d:14:LEU:O	12:d:14:LEU:HD12	1.49	1.11
1:D:47:PHE:HB3	6:N:227:ILE:HD11	1.25	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	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:365:ILE:HD12	4:L:366:MET:HG3	1.32	1.11
4:L:466:PHE:HB2	18:j:68:TRP:CZ2	1.85	1.10
5:M:127:ILE:CD1	6:N:256:PRO:HG3	1.82	1.10
4:L:141:PHE:CE2	5:M:375:LEU:CD2	2.35	1.10
4:L:121:LEU:HD22	4:L:246:LEU:HD21	1.32	1.09
7:O:66:ILE:HD12	7:O:67:CYS:SG	1.94	1.08
18:j:97:LEU:HB3	23:o:104:ARG:HB2	1.29	1.08
19:k:34:PRO:HG2	19:k:59:TYR:CE1	1.88	1.08
4:L:141:PHE:HE2	5:M:375:LEU:CD2	1.67	1.07
4:L:141:PHE:CE2	5:M:370:PRO:HG3	1.87	1.07
4:L:466:PHE:CZ	18:j:72:ARG:NH2	2.22	1.07
4:L:16:LEU:HD23	4:L:126:ILE:HD13	1.30	1.06
5:M:143:LEU:HD21	6:N:303:THR:CG2	1.85	1.06
4:L:550:LEU:HD12	5:M:275:ILE:HB	1.37	1.06
4:L:141:PHE:HB2	4:L:182:PHE:CE2	1.92	1.05
4:L:141:PHE:HE2	5:M:375:LEU:HD22	1.22	1.05
20:l:91:GLN:HE21	22:n:2:ALA:HB1	1.17	1.05
1:D:36:GLN:HE22	5:M:135:ARG:NH1	1.55	1.04
2:J:9:SER:CB	3:K:7:ASN:HD22	1.68	1.04
7:O:227:MET:O	7:O:228:LYS:HG2	1.57	1.04
5:M:162:ILE:HG23	6:N:271:MET:HE3	1.33	1.04
6:N:233:LEU:HD23	6:N:241:LEU:HD12	1.36	1.04
4:L:466:PHE:CE1	18:j:72:ARG:NH2	2.27	1.03
4:L:466:PHE:CB	18:j:68:TRP:HZ2	1.70	1.03
5:M:249:ILE:O	5:M:250:LEU:HG	1.58	1.03
7:O:168:VAL:HG21	7:O:241:TYR:CE1	1.92	1.03
4:L:131:LEU:HD12	4:L:140:LEU:HD12	1.36	1.02
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
22:n:97:TYR:HB2	22:n:178:PRO:HG2	1.39	1.02
4:L:123:LEU:HD21	26:L:704:CDL:H741	1.41	1.01
4:L:222:GLY:HA2	4:L:229:LEU:HD11	1.40	1.01
4:L:228:GLY:O	4:L:229:LEU:HG	1.61	1.01
2:J:60:LEU:HD13	2:J:60:LEU:C	1.86	1.00
5:M:172:GLY:O	5:M:173:THR:HG23	1.61	1.00
4:L:553:LEU:HD11	21:m:93:ALA:HB3	1.44	1.00
16:h:163:ARG:HG2	16:h:165:ASP:HB2	1.44	0.99
7:O:209:VAL:HG12	7:O:260:SER:HB2	1.43	0.99
5:M:143:LEU:HD21	6:N:303:THR:HG21	1.42	0.99
5:M:196:TRP:CD1	5:M:250:LEU:HD13	1.96	0.99
7:O:168:VAL:HG11	7:O:241:TYR:CD1	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:184:TYR:HA	23:o:36:GLU:HA	1.45	0.99
23:o:8:ARG:HB2	23:o:16:GLU:HG2	1.45	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
6:N:307:THR:HB	7:O:319:ILE:CD1	1.93	0.98
4:L:383:MET:HB3	4:L:386:LEU:HD12	1.43	0.98
5:M:173:THR:CG2	16:h:147:ALA:HB2	1.94	0.98
4:L:316:THR:HG23	4:L:325:ALA:HB2	1.45	0.97
4:L:216:LEU:HD22	4:L:259:LEU:HD21	1.44	0.96
4:L:174:TYR:HD2	4:L:232:TRP:CD1	1.82	0.96
5:M:250:LEU:HD12	5:M:250:LEU:O	1.65	0.96
4:L:174:TYR:CD2	4:L:232:TRP:HD1	1.83	0.96
2:J:9:SER:HB3	3:K:7:ASN:HD22	1.27	0.96
20:l:38:PRO:HB2	21:m:75:ASN:HD22	1.23	0.96
8:U:90:TYR:HE2	8:U:92:LYS:HB2	1.25	0.96
4:L:247:LEU:HD12	4:L:248:HIS:CD2	1.98	0.96
4:L:363:THR:HG23	4:L:431:THR:HB	1.48	0.96
4:L:466:PHE:CE1	18:j:72:ARG:CZ	2.49	0.95
4:L:319:MET:HE1	4:L:399:ILE:HA	1.47	0.95
4:L:174:TYR:HD2	4:L:232:TRP:HD1	1.02	0.95
5:M:4:ILE:HG22	5:M:107:ILE:HD13	1.47	0.94
5:M:216:LEU:HG	5:M:220:HIS:CE1	2.02	0.94
4:L:246:LEU:HD12	4:L:247:LEU:N	1.81	0.94
4:L:173:LEU:HD23	25:L:702:3PE:H321	1.47	0.94
4:L:274:LEU:HA	4:L:277:MET:HE3	1.49	0.94
4:L:362:ILE:HD12	4:L:430:VAL:HG12	1.50	0.94
5:M:1:MET:HG3	5:M:4:ILE:HD13	1.50	0.94
8:U:140:CYS:HB2	8:U:143:GLU:HG2	1.49	0.94
4:L:13:ILE:HD11	25:i:201:3PE:H2C2	1.49	0.93
4:L:247:LEU:HD11	4:L:248:HIS:NE2	1.83	0.93
3:K:40:LEU:HD13	6:N:71:LEU:HD23	1.50	0.93
5:M:453:LEU:CD1	5:M:454:ILE:HG23	1.99	0.93
7:O:314:LEU:CD1	7:O:315:PRO:HD2	2.00	0.92
5:M:127:ILE:CD1	6:N:256:PRO:CG	2.47	0.92
4:L:41:LYS:HG3	4:L:98:TRP:CZ2	2.04	0.92
5:M:127:ILE:HD12	6:N:256:PRO:HG3	1.50	0.92
10:Y:19:GLN:HE21	10:Y:22:ARG:HG2	1.32	0.91
4:L:136:ASN:HD21	26:h:201:CDL:H273	1.33	0.91
5:M:106:LEU:HD13	5:M:234:ILE:CG2	2.00	0.91
20:l:91:GLN:NE2	22:n:2:ALA:HB1	1.86	0.91
8:U:87:LEU:HB2	8:U:98:LEU:CD2	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:245:ALA:O	4:L:249:SER:HB3	1.70	0.91
4:L:202:MET:HE3	4:L:265:PRO:HG3	1.53	0.91
7:O:106:ILE:HG12	7:O:111:SER:HA	1.50	0.90
7:O:316:GLU:OE2	15:g:51:MET:HG3	1.72	0.90
4:L:364:LYS:HE2	19:k:67:ILE:CD1	2.02	0.90
5:M:231:LEU:HD12	5:M:235:LEU:CD1	2.00	0.90
7:O:347:VAL:O	7:O:347:VAL:HG12	1.71	0.90
7:O:314:LEU:CG	7:O:315:PRO:HD2	2.02	0.90
5:M:453:LEU:HD12	5:M:454:ILE:N	1.87	0.89
4:L:123:LEU:HD22	4:L:150:MET:SD	2.12	0.89
5:M:2:LEU:HA	5:M:5:ILE:HG12	1.53	0.89
4:L:455:LYS:NZ	18:j:57:GLN:OE1	2.04	0.89
5:M:380:PHE:HA	5:M:383:MET:HE2	1.55	0.89
2:J:12:PHE:CE2	3:K:42:ILE:HD13	2.07	0.89
5:M:50:LYS:HE2	5:M:52:PHE:HE1	1.36	0.89
5:M:8:SER:HA	5:M:11:LEU:HD13	1.54	0.88
7:O:59:VAL:HA	7:O:157:VAL:CG2	2.02	0.88
4:L:261:VAL:O	4:L:264:HIS:HD2	1.51	0.88
5:M:173:THR:HG21	16:h:147:ALA:HB2	1.55	0.88
22:n:101:GLU:O	22:n:122:ARG:NH2	2.06	0.88
4:L:428:TYR:HA	4:L:432:MET:HG2	1.56	0.88
5:M:310:MET:SD	5:M:455:THR:HB	2.13	0.88
4:L:594:ASN:ND2	6:N:110:PRO:HB2	1.88	0.87
5:M:368:ALA:HB1	5:M:375:LEU:HD13	1.56	0.87
4:L:362:ILE:HD12	4:L:430:VAL:CG1	2.04	0.87
5:M:447:LEU:HD11	5:M:454:ILE:HG21	1.55	0.87
4:L:496:LEU:HD12	4:L:497:GLY:N	1.90	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:79:SER:HB2	4:L:135:ASN:HB2	1.55	0.87
7:O:295:ARG:NH1	7:O:299:GLN:HB2	1.90	0.86
5:M:1:MET:HE1	5:M:111:SER:HB2	1.58	0.86
6:N:307:THR:HB	7:O:319:ILE:HD11	1.57	0.86
2:J:12:PHE:CE2	3:K:42:ILE:CD1	2.57	0.86
17:i:14:GLN:HB3	22:n:164:PRO:HG3	1.57	0.86
20:l:156:VAL:HG11	23:o:95:TYR:CZ	2.10	0.86
4:L:552:LEU:HD12	20:l:70:MET:HE1	1.56	0.86
2:J:37:PHE:CE2	2:J:41:LEU:HD11	2.10	0.85
20:l:167:TYR:HD2	20:l:168:LEU:HD12	1.41	0.85
4:L:417:SER:HB3	4:L:493:ILE:HG13	1.58	0.85
7:O:176:GLN:HG3	7:O:177:GLY:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:29:SER:HB3	15:g:91:PHE:CD2	2.12	0.85
4:L:54:PHE:O	4:L:58:ASN:N	2.10	0.85
5:M:115:LEU:HD21	5:M:176:LEU:HD21	1.59	0.84
4:L:128:MET:HG2	4:L:251:THR:HB	1.59	0.84
16:h:96:ALA:HB3	24:p:63:TYR:HD1	1.40	0.84
4:L:247:LEU:HD11	4:L:248:HIS:CD2	2.11	0.84
5:M:208:PRO:HD3	5:M:236:LEU:HD22	1.59	0.84
7:O:237:ILE:HG22	7:O:241:TYR:HE2	1.42	0.84
5:M:142:ARG:HH21	6:N:303:THR:HG22	1.40	0.84
7:O:314:LEU:HD12	7:O:315:PRO:HD2	1.56	0.84
5:M:447:LEU:HD11	5:M:454:ILE:CG2	2.07	0.84
5:M:391:PHE:CE2	25:m:202:3PE:H261	2.12	0.84
7:O:238:GLU:HA	7:O:241:TYR:HD2	1.43	0.84
8:U:110:LEU:CD1	8:U:118:ILE:HD11	2.06	0.84
13:e:14:LEU:HD12	13:e:15:ASP:HB2	1.57	0.84
5:M:196:TRP:NE1	5:M:250:LEU:HD13	1.92	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
8:U:100:VAL:HA	8:U:141:PRO:HG2	1.59	0.84
4:L:20:LEU:HD12	4:L:21:ILE:N	1.92	0.83
7:O:314:LEU:HG	7:O:315:PRO:HD2	1.58	0.83
4:L:16:LEU:HD23	4:L:126:ILE:CD1	2.08	0.83
17:i:94:PRO:HG3	24:p:10:TYR:CE2	2.13	0.83
5:M:361:MET:HB3	5:M:441:MET:HE3	1.60	0.83
1:D:67:ASN:HB3	1:D:69:VAL:HG12	1.58	0.83
4:L:364:LYS:HE2	19:k:67:ILE:HD11	1.58	0.83
5:M:373:ILE:HG12	5:M:454:ILE:HD11	1.60	0.83
7:O:99:GLY:HA2	11:c:30:TYR:HD1	1.42	0.83
2:J:33:ILE:HG23	2:J:60:LEU:CD2	2.09	0.83
2:J:135:LEU:HD12	3:K:54:MET:CE	2.09	0.83
15:g:53:TRP:CD1	15:g:53:TRP:H	1.95	0.83
5:M:269:MET:HE1	5:M:396:MET:HA	1.61	0.82
4:L:131:LEU:CD1	4:L:140:LEU:HD12	2.09	0.82
8:U:87:LEU:HB2	8:U:98:LEU:HD21	1.61	0.82
6:N:335:MET:HG3	6:N:335:MET:O	1.79	0.82
4:L:222:GLY:HA2	4:L:229:LEU:CD1	2.08	0.82
1:D:36:GLN:HE22	5:M:135:ARG:HH12	1.26	0.82
2:J:22:LYS:HD2	3:K:23:ARG:HG2	1.62	0.82
4:L:493:ILE:HD12	4:L:496:LEU:HD21	1.62	0.82
4:L:432:MET:HG3	4:L:432:MET:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:109:TYR:HA	12:d:112:ILE:HG22	1.60	0.82
22:n:97:TYR:HB2	22:n:178:PRO:CG	2.10	0.81
5:M:336:ARG:NH2	5:M:429:SER:HA	1.95	0.81
19:k:34:PRO:HD2	19:k:59:TYR:CD1	2.16	0.81
4:L:16:LEU:CD2	4:L:126:ILE:HD13	2.10	0.81
19:k:30:ILE:HD11	19:k:39:GLN:HB2	1.61	0.81
2:J:76:GLU:OE1	2:J:76:GLU:O	1.99	0.81
4:L:73:SER:HB3	24:p:100:GLN:NE2	1.96	0.81
4:L:428:TYR:OH	22:n:33:HIS:CE1	2.34	0.81
20:l:115:ASN:OD1	20:l:115:ASN:O	1.98	0.81
21:m:125:PHE:CE1	24:p:133:THR:HG22	2.16	0.81
24:p:6:ASP:HB3	24:p:9:VAL:HG22	1.61	0.81
2:J:33:ILE:HG23	2:J:60:LEU:HD21	1.61	0.81
4:L:229:LEU:O	4:L:229:LEU:CD1	2.28	0.81
4:L:506:ASN:HA	4:L:509:MET:HE2	1.63	0.81
6:N:277:ILE:HG23	6:N:278:MET:N	1.96	0.81
4:L:424:MET:HE2	4:L:502:LEU:HB2	1.62	0.80
5:M:172:GLY:O	5:M:173:THR:CG2	2.28	0.80
5:M:453:LEU:HD12	5:M:454:ILE:HG23	1.63	0.80
6:N:200:LEU:HD21	6:N:265:ILE:HG12	1.63	0.80
6:N:277:ILE:CG2	6:N:278:MET:H	1.93	0.80
7:O:227:MET:O	7:O:228:LYS:CG	2.30	0.80
25:i:201:3PE:H2E1	25:i:201:3PE:H342	1.63	0.80
21:m:18:LEU:HD21	22:n:69:GLU:HA	1.62	0.80
5:M:216:LEU:HD12	5:M:236:LEU:HD21	1.60	0.80
5:M:127:ILE:HD11	6:N:256:PRO:CG	2.09	0.80
5:M:29:SER:HB3	15:g:91:PHE:HD2	1.47	0.80
26:L:704:CDL:HA62	16:h:68:LEU:HD13	1.63	0.80
5:M:173:THR:HG23	16:h:147:ALA:CB	2.11	0.80
7:O:117:PHE:CE1	7:O:173:MET:HE3	2.17	0.80
4:L:553:LEU:HD11	21:m:93:ALA:CB	2.10	0.80
4:L:456:ARG:HG2	25:L:701:3PE:H241	1.62	0.79
7:O:199:LEU:HD11	7:O:294:LEU:HD22	1.64	0.79
13:e:38:LYS:HE3	16:h:181:HIS:HD2	1.45	0.79
5:M:231:LEU:HA	5:M:235:LEU:HB2	1.62	0.79
21:m:125:PHE:HE1	24:p:133:THR:HG22	1.47	0.79
4:L:552:LEU:HD21	21:m:90:GLY:HA2	1.62	0.79
7:O:59:VAL:HA	7:O:157:VAL:HG23	1.63	0.79
8:U:93:ILE:HD11	8:U:110:LEU:HD11	1.64	0.79
4:L:130:ILE:HG23	4:L:139:GLN:HE21	1.46	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	1.63	0.79
2:J:9:SER:CB	3:K:7:ASN:ND2	2.45	0.79
22:n:20:TYR:CE2	22:n:24:LEU:HD11	2.18	0.79
4:L:131:LEU:HD12	4:L:140:LEU:CD1	2.12	0.78
5:M:106:LEU:HD13	5:M:234:ILE:HG21	1.63	0.78
5:M:231:LEU:HD12	5:M:235:LEU:HD13	1.64	0.78
6:N:123:PRO:HG2	6:N:126:MET:HG2	1.63	0.78
8:U:90:TYR:HH	8:U:92:LYS:HD2	1.43	0.78
5:M:173:THR:HG23	16:h:147:ALA:HB2	1.65	0.78
5:M:370:PRO:HA	5:M:375:LEU:CD2	2.13	0.78
7:O:66:ILE:HD11	7:O:218:ILE:CG1	2.13	0.78
7:O:117:PHE:HE1	7:O:173:MET:CE	1.96	0.78
5:M:9:LEU:HD23	5:M:104:ILE:HD13	1.65	0.78
7:O:314:LEU:HD12	7:O:315:PRO:CD	2.13	0.78
4:L:3:ILE:H	4:L:3:ILE:HD12	1.48	0.78
4:L:136:ASN:HA	4:L:197:GLU:HA	1.66	0.78
4:L:534:HIS:O	4:L:538:PRO:HG3	1.83	0.78
5:M:143:LEU:HD21	6:N:303:THR:HG23	1.63	0.78
5:M:248:ILE:HG13	5:M:249:ILE:HD12	1.64	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
5:M:162:ILE:HG23	6:N:271:MET:CE	2.14	0.78
7:O:305:LEU:HD12	7:O:305:LEU:O	1.83	0.78
25:L:703:3PE:H361	6:N:164:MET:HE1	1.66	0.77
6:N:170:LEU:HD11	6:N:288:LEU:HG	1.65	0.77
7:O:206:TYR:CD2	7:O:257:VAL:HG13	2.19	0.77
7:O:256:LEU:HD11	7:O:276:LEU:HD23	1.64	0.77
20:l:89:TRP:CZ2	22:n:86:PRO:HD2	2.20	0.77
1:D:47:PHE:CB	6:N:227:ILE:HD11	2.12	0.77
5:M:274:SER:O	5:M:277:LEU:HB2	1.85	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
5:M:204:LEU:HD22	5:M:209:LEU:HD12	1.65	0.77
5:M:453:LEU:HD11	5:M:454:ILE:HG23	1.65	0.77
6:N:45:ILE:O	6:N:45:ILE:HG13	1.83	0.77
5:M:98:MET:CE	5:M:128:PRO:HA	2.14	0.77
20:l:169:GLU:C	20:l:171:GLY:H	1.92	0.77
4:L:419:THR:HA	4:L:422:TYR:CE2	2.20	0.77
7:O:168:VAL:HG21	7:O:241:TYR:OH	1.83	0.77
15:g:70:ASP:OD1	22:n:108:HIS:NE2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:56:HIS:HA	23:o:74:PHE:CD1	2.19	0.77
5:M:208:PRO:HG2	5:M:216:LEU:HD13	1.67	0.77
3:K:1:MET:HA	3:K:4:THR:HG22	1.67	0.76
7:O:99:GLY:HA2	11:c:30:TYR:CD1	2.20	0.76
5:M:42:LEU:HG	5:M:67:ILE:HD11	1.68	0.76
5:M:171:VAL:HG11	5:M:179:LEU:HD21	1.65	0.76
6:N:210:ILE:HG22	6:N:333:SER:HB3	1.65	0.76
7:O:66:ILE:CD1	7:O:218:ILE:HD11	2.14	0.76
8:U:123:GLU:HG2	8:U:130:ILE:HG12	1.67	0.76
17:i:22:TRP:CE2	22:n:172:THR:HG22	2.20	0.76
5:M:231:LEU:HD12	5:M:235:LEU:HD12	1.67	0.76
4:L:496:LEU:HD12	4:L:496:LEU:C	2.09	0.76
5:M:60:PRO:O	5:M:64:PRO:HD3	1.85	0.76
6:N:211:LEU:HD23	6:N:333:SER:HB2	1.68	0.76
15:g:145:ILE:HG23	24:p:160:LYS:HE2	1.66	0.76
16:h:175:GLU:HB3	16:h:177:GLU:HG2	1.65	0.76
5:M:344:MET:HE1	21:m:59:HIS:NE2	1.99	0.76
6:N:319:LYS:HA	7:O:302:THR:HG21	1.67	0.76
4:L:232:TRP:CZ3	4:L:233:LEU:CD2	2.69	0.76
4:L:605:ASN:OD1	4:L:605:ASN:O	2.03	0.76
7:O:168:VAL:HG11	7:O:241:TYR:CE1	2.19	0.76
20:l:38:PRO:HB2	21:m:75:ASN:ND2	2.00	0.76
2:J:40:CYS:SG	2:J:56:PHE:HB2	2.26	0.76
6:N:215:MET:HE2	6:N:248:LEU:HD21	1.67	0.76
4:L:16:LEU:HD21	26:L:704:CDL:H591	1.68	0.75
4:L:480:LEU:HD21	18:j:82:GLY:HA3	1.65	0.75
5:M:458:THR:CG2	24:p:148:ALA:HB1	2.16	0.75
6:N:314:MET:HB2	7:O:305:LEU:HD11	1.68	0.75
11:c:68:GLU:HG3	12:d:19:ARG:HH21	1.52	0.75
22:n:20:TYR:CZ	22:n:24:LEU:HD11	2.21	0.75
4:L:387:THR:HG23	4:L:461:SER:O	1.85	0.75
4:L:513:MET:HE3	4:L:515:LYS:HG3	1.68	0.75
2:J:60:LEU:C	2:J:60:LEU:CD1	2.59	0.75
7:O:121:PRO:O	7:O:122:LYS:HG2	1.86	0.75
4:L:446:ASN:ND2	18:j:51:THR:HG21	2.01	0.75
6:N:227:ILE:HA	6:N:230:ILE:HG22	1.66	0.75
1:D:34:ALA:HB3	5:M:86:LYS:NZ	2.01	0.75
10:Y:83:ARG:NH1	10:Y:90:LEU:HD22	2.00	0.75
1:D:36:GLN:NE2	5:M:135:ARG:NH1	2.34	0.75
4:L:393:ASP:OD1	4:L:394:LEU:N	2.19	0.75
4:L:482:MET:HE2	4:L:486:LEU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:277:ILE:HG23	6:N:278:MET:H	1.50	0.75
7:O:206:TYR:HD2	7:O:257:VAL:HG13	1.52	0.75
4:L:362:ILE:HG23	4:L:366:MET:HE3	1.68	0.74
4:L:475:THR:HA	23:o:55:GLN:NE2	2.01	0.74
17:i:127:HIS:HB3	23:o:89:TYR:HE2	1.52	0.74
3:K:95:LEU:HG	6:N:54:GLU:OE2	1.87	0.74
5:M:314:MET:HA	5:M:454:ILE:HD12	1.69	0.74
7:O:66:ILE:HD11	7:O:218:ILE:HD11	1.67	0.74
7:O:117:PHE:CE1	7:O:128:SER:HB2	2.22	0.74
7:O:333:GLU:O	7:O:333:GLU:CD	2.30	0.74
10:Y:71:MET:HG3	10:Y:102:THR:HG21	1.68	0.74
7:O:66:ILE:CD1	7:O:67:CYS:SG	2.76	0.74
2:J:52:GLY:O	2:J:55:VAL:HG12	1.87	0.74
4:L:136:ASN:ND2	26:h:201:CDL:H273	2.01	0.74
17:i:22:TRP:CD2	22:n:172:THR:HG22	2.21	0.74
4:L:285:THR:HG22	4:L:415:ALA:HB1	1.70	0.74
9:X:162:LYS:HB3	9:X:166:ARG:HH21	1.53	0.74
10:Y:76:THR:HG23	10:Y:95:GLY:HA3	1.70	0.74
5:M:310:MET:HG3	5:M:455:THR:HA	1.70	0.74
16:h:57:VAL:HG12	22:n:99:VAL:HG21	1.68	0.74
4:L:525:LEU:HD21	22:n:77:PRO:HB3	1.68	0.74
25:L:703:3PE:H272	6:N:164:MET:HE3	1.67	0.74
11:c:72:ARG:HH11	12:d:19:ARG:HD3	1.53	0.74
1:D:67:ASN:HB2	7:O:193:LEU:CD2	2.16	0.73
2:J:151:MET:HE2	6:N:28:LEU:HD13	1.70	0.73
25:L:705:3PE:H272	6:N:288:LEU:HD13	1.70	0.73
5:M:1:MET:HB2	5:M:52:PHE:CD2	2.23	0.73
5:M:260:PRO:O	5:M:264:LEU:HG	1.88	0.73
16:h:96:ALA:HB3	24:p:63:TYR:CD1	2.22	0.73
6:N:202:LEU:O	6:N:206:MET:HG2	1.87	0.73
6:N:289:ASN:HA	6:N:292:PHE:CE2	2.23	0.73
4:L:174:TYR:HE1	25:L:702:3PE:H362	1.53	0.73
5:M:200:MET:HE1	5:M:247:SER:HB2	1.69	0.73
5:M:263:LEU:HD11	21:m:102:TYR:HD1	1.53	0.73
7:O:117:PHE:HE1	7:O:173:MET:HE3	1.53	0.73
1:D:36:GLN:NE2	5:M:135:ARG:HH12	1.84	0.73
5:M:73:LEU:HD22	5:M:103:GLN:CD	2.12	0.73
16:h:175:GLU:HB2	16:h:178:PHE:HD2	1.53	0.73
25:m:201:3PE:H242	25:m:201:3PE:H362	1.69	0.73
5:M:167:ILE:HD11	5:M:195:LEU:HD21	1.70	0.73
8:U:110:LEU:HD11	8:U:118:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PRO:HG3	1:D:70:ASP:OD1	1.88	0.73
4:L:20:LEU:HD12	4:L:20:LEU:C	2.13	0.73
10:Y:143:VAL:HG23	16:h:157:ARG:HG2	1.69	0.73
2:J:75:THR:HG21	3:K:27:MET:CB	2.19	0.73
4:L:174:TYR:CD2	4:L:232:TRP:CD1	2.68	0.73
4:L:232:TRP:CZ3	4:L:233:LEU:HD23	2.23	0.73
4:L:428:TYR:OH	22:n:33:HIS:HE1	1.69	0.73
14:f:38:ARG:HH12	14:f:54:VAL:HG21	1.54	0.73
25:m:203:3PE:H261	25:m:203:3PE:H371	1.69	0.73
4:L:466:PHE:HE1	18:j:72:ARG:CZ	1.99	0.73
5:M:122:PHE:CD1	5:M:238:LEU:HG	2.23	0.73
2:J:67:PHE:CE2	3:K:75:LEU:HD21	2.24	0.73
4:L:445:GLU:OE2	18:j:54:GLN:HG3	1.89	0.73
4:L:579:ASN:OD1	4:L:579:ASN:O	2.06	0.73
5:M:441:MET:SD	5:M:444:LEU:HD23	2.29	0.73
4:L:9:LEU:HD22	17:i:82:VAL:HG13	1.71	0.72
15:g:106:TYR:CE2	16:h:86:ILE:HD12	2.24	0.72
2:J:71:THR:HG22	2:J:76:GLU:HB2	1.71	0.72
6:N:277:ILE:CG2	6:N:278:MET:N	2.52	0.72
7:O:80:GLN:HG3	7:O:270:VAL:CG2	2.11	0.72
19:k:34:PRO:HG2	19:k:59:TYR:HE1	1.54	0.72
24:p:7:LYS:O	24:p:11:PRO:HA	1.89	0.72
2:J:32:LEU:HG	2:J:64:LEU:HD21	1.71	0.72
5:M:216:LEU:HG	5:M:220:HIS:HE1	1.48	0.72
5:M:243:MET:HE1	5:M:302:MET:HE3	1.71	0.72
6:N:215:MET:SD	6:N:248:LEU:CD2	2.77	0.72
20:l:152:SER:HA	23:o:5:LEU:HD21	1.69	0.72
2:J:159:LEU:HD23	3:K:69:CYS:SG	2.29	0.72
4:L:141:PHE:HD2	5:M:370:PRO:HB3	1.54	0.72
6:N:59:TYR:CE2	6:N:63:GLN:HG3	2.23	0.72
16:h:163:ARG:HG2	16:h:165:ASP:CB	2.19	0.72
4:L:316:THR:CG2	4:L:325:ALA:HB2	2.18	0.72
1:D:67:ASN:HB2	7:O:193:LEU:HD23	1.70	0.72
11:c:72:ARG:HD2	12:d:20:SER:HA	1.70	0.72
4:L:576:LEU:HD12	4:L:577:THR:N	2.05	0.72
7:O:351:TRP:HB3	11:c:39:PRO:HG3	1.70	0.72
4:L:299:LYS:HB2	4:L:354:GLN:HE21	1.55	0.72
4:L:247:LEU:HD12	4:L:248:HIS:N	2.04	0.71
6:N:308:ASN:HB3	7:O:317:ILE:HG22	1.71	0.71
21:m:9:ALA:HB1	21:m:10:PRO:HD2	1.71	0.71
25:K:101:3PE:H2A2	25:K:101:3PE:H262	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:106:LEU:HD13	5:M:234:ILE:HG22	1.72	0.71
5:M:373:ILE:CG1	5:M:454:ILE:HD11	2.19	0.71
6:N:232:LEU:HD23	6:N:307:THR:HG23	1.70	0.71
7:O:100:ASP:OD1	7:O:101:GLY:N	2.24	0.71
5:M:173:THR:HB	16:h:143:GLU:OE2	1.90	0.71
6:N:146:TYR:CD1	6:N:147:PRO:HD3	2.26	0.71
5:M:370:PRO:HA	5:M:375:LEU:HD23	1.72	0.71
4:L:141:PHE:CD2	5:M:370:PRO:HB3	2.25	0.71
5:M:313:THR:HG21	5:M:456:GLY:HA3	1.71	0.71
20:l:106:HIS:CD2	20:l:107:TRP:H	2.08	0.71
7:O:336:GLY:H	7:O:344:ASN:ND2	1.89	0.71
7:O:354:LEU:HD21	11:c:44:VAL:HG11	1.72	0.71
4:L:466:PHE:CB	18:j:68:TRP:CZ2	2.57	0.71
5:M:220:HIS:CE1	5:M:231:LEU:HD23	2.26	0.71
7:O:237:ILE:HG22	7:O:241:TYR:CE2	2.24	0.71
8:U:144:ILE:O	8:U:148:ILE:HG12	1.91	0.71
21:m:45:ARG:O	21:m:45:ARG:HG2	1.90	0.71
4:L:73:SER:HB3	24:p:100:GLN:HE21	1.55	0.71
7:O:209:VAL:HG23	7:O:214:VAL:HG13	1.72	0.71
16:h:87:THR:HA	26:h:201:CDL:H512	1.73	0.71
4:L:556:ILE:HG21	21:m:80:PHE:CE1	2.25	0.71
4:L:368:PHE:HB3	4:L:445:GLU:CD	2.15	0.70
5:M:373:ILE:HG12	5:M:454:ILE:CD1	2.20	0.70
2:J:95:GLY:HA2	2:J:98:MET:HB3	1.73	0.70
6:N:237:THR:HG23	6:N:237:THR:O	1.88	0.70
9:X:167:PHE:HB3	9:X:170:TRP:CD1	2.25	0.70
4:L:436:ARG:HA	19:k:58:ARG:NH1	2.07	0.70
7:O:135:LEU:HB3	7:O:139:ARG:HH12	1.57	0.70
4:L:510:LYS:HE3	4:L:512:SER:HB3	1.72	0.70
4:L:306:THR:HA	4:L:336:LYS:HZ2	1.57	0.70
4:L:428:TYR:HA	4:L:432:MET:CG	2.20	0.70
4:L:559:GLU:O	4:L:564:LYS:HB2	1.92	0.70
5:M:446:LEU:HD13	15:g:101:THR:HG21	1.73	0.70
6:N:137:ALA:HB3	6:N:138:PRO:HD3	1.74	0.70
3:K:1:MET:HG3	3:K:50:ASN:HD22	1.57	0.70
7:O:161:ARG:HH22	27:O:401:ADP:H5'2	1.55	0.70
10:Y:19:GLN:HG3	10:Y:22:ARG:HB2	1.74	0.70
14:f:56:TRP:CE3	16:h:131:LYS:HG3	2.26	0.70
4:L:285:THR:HG22	4:L:415:ALA:CB	2.21	0.69
4:L:594:ASN:CG	6:N:110:PRO:HB2	2.17	0.69
5:M:134:THR:O	5:M:142:ARG:HD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:254:LEU:HD12	6:N:255:PRO:HD3	1.72	0.69
16:h:57:VAL:HG12	22:n:99:VAL:CG2	2.21	0.69
4:L:480:LEU:HD23	4:L:480:LEU:O	1.93	0.69
5:M:447:LEU:HD21	5:M:454:ILE:HD13	1.73	0.69
7:O:206:TYR:HB3	7:O:257:VAL:HA	1.72	0.69
11:c:34:PRO:HG2	11:c:37:ALA:HB2	1.74	0.69
15:g:106:TYR:OH	16:h:86:ILE:HG23	1.92	0.69
1:D:35:ARG:O	1:D:36:GLN:C	2.35	0.69
4:L:556:ILE:HD11	21:m:76:ILE:HG22	1.74	0.69
7:O:59:VAL:HA	7:O:157:VAL:HG22	1.71	0.69
6:N:248:LEU:HD13	6:N:296:LEU:HD23	1.75	0.69
4:L:305:SER:HB2	4:L:422:TYR:HE1	1.57	0.69
18:j:97:LEU:HB3	23:o:104:ARG:CB	2.16	0.69
20:l:122:THR:HG21	20:l:129:MET:HE1	1.73	0.69
20:l:158:PRO:HD3	23:o:22:ILE:HB	1.74	0.69
2:J:76:GLU:O	2:J:76:GLU:CD	2.36	0.69
4:L:153:LEU:HD11	5:M:360:LEU:HD11	1.73	0.69
5:M:216:LEU:HD11	5:M:236:LEU:HD11	1.72	0.69
8:U:87:LEU:HB2	8:U:98:LEU:HD22	1.72	0.69
5:M:50:LYS:HE2	5:M:52:PHE:CE1	2.25	0.69
5:M:151:PHE:CZ	6:N:291:PHE:HB2	2.27	0.69
19:k:34:PRO:CD	19:k:59:TYR:CD1	2.76	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
6:N:215:MET:HE2	6:N:248:LEU:CD2	2.23	0.69
17:i:104:ILE:HG13	23:o:48:ASP:HB3	1.75	0.69
4:L:312:LEU:HD21	4:L:395:ILE:HG21	1.75	0.68
4:L:18:PRO:O	4:L:21:ILE:HG22	1.92	0.68
5:M:127:ILE:HB	5:M:128:PRO:HD3	1.75	0.68
7:O:140:LEU:HG	7:O:304:VAL:HG12	1.74	0.68
10:Y:77:CYS:SG	10:Y:78:VAL:N	2.66	0.68
3:K:1:MET:HG3	3:K:50:ASN:ND2	2.08	0.68
5:M:369:LEU:HD12	5:M:370:PRO:HD3	1.74	0.68
6:N:215:MET:HE1	6:N:248:LEU:HD21	1.71	0.68
21:m:48:LEU:HB3	22:n:166:LEU:HD23	1.75	0.68
4:L:211:ILE:N	4:L:212:PRO:HD2	2.08	0.68
5:M:255:LYS:NZ	12:d:117:HIS:HB3	2.08	0.68
8:U:110:LEU:CD1	8:U:118:ILE:CD1	2.71	0.68
20:l:78:LEU:HD11	20:l:104:PRO:HB2	1.74	0.68
2:J:9:SER:HB2	3:K:7:ASN:ND2	2.09	0.68
5:M:446:LEU:HD13	15:g:101:THR:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:60:ILE:HD12	7:O:203:ALA:HB3	1.73	0.68
8:U:134:ASP:OD2	22:n:2:ALA:N	2.26	0.68
10:Y:96:GLY:HA3	10:Y:121:GLY:HA2	1.75	0.68
4:L:383:MET:SD	4:L:384:PRO:HD2	2.33	0.68
4:L:446:ASN:HD21	18:j:51:THR:HG21	1.56	0.68
25:M:501:3PE:H241	6:N:277:ILE:HD12	1.75	0.68
7:O:323:GLN:HE22	15:g:54:GLN:HB3	1.58	0.68
10:Y:143:VAL:CG2	16:h:157:ARG:HG2	2.23	0.68
5:M:379:LEU:O	5:M:383:MET:HG3	1.93	0.68
7:O:224:PRO:HA	7:O:227:MET:HE3	1.74	0.68
7:O:246:LEU:HG	7:O:255:VAL:HG11	1.76	0.68
5:M:311:GLY:HA2	5:M:314:MET:HE3	1.76	0.68
5:M:369:LEU:HD12	5:M:370:PRO:CD	2.24	0.68
4:L:9:LEU:HD21	25:i:201:3PE:H2A1	1.76	0.68
5:M:39:LEU:HD23	5:M:67:ILE:HD13	1.74	0.68
5:M:388:TRP:CE2	21:m:109:ARG:HD2	2.29	0.68
7:O:38:TYR:HB3	7:O:299:GLN:HE22	1.58	0.68
4:L:228:GLY:C	4:L:229:LEU:HG	2.19	0.67
12:d:5:ARG:HD2	12:d:89:ASP:OD2	1.93	0.67
4:L:203:PHE:CZ	24:p:110:LEU:HD11	2.30	0.67
8:U:119:ILE:HD11	8:U:138:LEU:HB2	1.76	0.67
15:g:140:PHE:CE2	24:p:74:ILE:HG22	2.28	0.67
16:h:96:ALA:O	24:p:63:TYR:HE1	1.77	0.67
4:L:80:PHE:C	4:L:135:ASN:ND2	2.52	0.67
5:M:275:ILE:HD11	5:M:288:TYR:CD1	2.29	0.67
6:N:26:LEU:HD23	6:N:29:MET:SD	2.35	0.67
15:g:109:ASP:CB	15:g:114:GLU:HB3	2.24	0.67
15:g:140:PHE:CE2	24:p:74:ILE:CG2	2.76	0.67
20:l:122:THR:HG23	20:l:123:PRO:HD2	1.75	0.67
6:N:25:ASN:ND2	13:e:18:PHE:CE2	2.63	0.67
6:N:149:LEU:HD13	6:N:154:ILE:HG21	1.75	0.67
7:O:114:LEU:HA	7:O:131:LEU:CD2	2.24	0.67
7:O:347:VAL:O	7:O:347:VAL:CG1	2.42	0.67
5:M:30:TYR:O	5:M:34:ILE:HG12	1.95	0.67
6:N:342:GLN:HE21	12:d:30:ARG:HH11	1.41	0.67
11:c:72:ARG:HD2	12:d:20:SER:CA	2.25	0.67
5:M:142:ARG:NH2	6:N:303:THR:HG22	2.08	0.67
19:k:55:GLU:CD	22:n:34:ARG:HD2	2.19	0.67
20:l:106:HIS:HD2	20:l:107:TRP:H	1.43	0.67
1:D:36:GLN:HE21	1:D:38:GLN:NE2	1.93	0.67
4:L:511:LEU:HD12	22:n:36:LYS:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:98:MET:HE2	5:M:131:ILE:HB	1.77	0.67
7:O:124:ASN:O	15:g:51:MET:SD	2.53	0.67
4:L:81:LYS:N	4:L:135:ASN:ND2	2.43	0.67
5:M:11:LEU:HB3	5:M:100:ILE:HD13	1.77	0.67
4:L:552:LEU:CD2	4:L:553:LEU:HD12	2.25	0.67
6:N:313:MET:CG	7:O:305:LEU:HD22	2.25	0.67
12:d:14:LEU:O	12:d:14:LEU:CD1	2.37	0.67
13:e:14:LEU:CD1	13:e:15:ASP:HB2	2.25	0.67
2:J:59:TYR:OH	3:K:34:GLU:HB3	1.94	0.67
3:K:66:PHE:HZ	6:N:35:PHE:CZ	2.12	0.67
5:M:282:LEU:HD21	5:M:359:TRP:HH2	1.60	0.67
7:O:66:ILE:HD12	7:O:67:CYS:HG	1.59	0.67
10:Y:76:THR:HG22	10:Y:92:TYR:HA	1.77	0.67
25:L:703:3PE:C36	6:N:164:MET:HE1	2.24	0.66
5:M:114:GLU:HG3	9:X:169:PHE:HB3	1.77	0.66
5:M:270:ILE:HG22	5:M:271:MET:HE2	1.76	0.66
5:M:285:LEU:HD13	5:M:342:MET:HE1	1.76	0.66
16:h:102:PRO:HD2	16:h:105:TYR:HB2	1.77	0.66
5:M:361:MET:CB	5:M:441:MET:HE3	2.25	0.66
7:O:66:ILE:HD11	7:O:218:ILE:CD1	2.24	0.66
25:i:201:3PE:H342	25:i:201:3PE:H2B1	1.77	0.66
25:m:201:3PE:H2	25:m:201:3PE:H241	1.78	0.66
23:o:89:TYR:CE2	23:o:93:LEU:HD11	2.30	0.66
4:L:201:ILE:HG22	4:L:266:LEU:HD11	1.76	0.66
5:M:173:THR:CG2	16:h:147:ALA:CB	2.69	0.66
6:N:307:THR:O	7:O:319:ILE:N	2.28	0.66
8:U:128:PHE:CZ	8:U:148:ILE:HD12	2.31	0.66
10:Y:71:MET:HG3	10:Y:102:THR:CG2	2.26	0.66
12:d:106:LYS:HB3	24:p:79:GLU:HB3	1.77	0.66
4:L:385:PHE:CD1	18:j:72:ARG:HG3	2.30	0.66
4:L:407:TRP:CE3	4:L:410:LEU:HD11	2.29	0.66
4:L:562:ILE:HB	4:L:563:PRO:HD3	1.78	0.66
13:e:38:LYS:HG2	16:h:179:ILE:HG21	1.78	0.66
7:O:343:TYR:HD1	7:O:352:ILE:HG23	1.59	0.66
17:i:101:LYS:HG2	24:p:116:ARG:O	1.95	0.66
2:J:165:ILE:HG23	6:N:42:PRO:HG3	1.78	0.66
14:f:41:SER:O	14:f:45:GLN:HB2	1.96	0.66
20:l:38:PRO:HG2	21:m:71:ALA:HB2	1.77	0.66
24:p:70:ARG:CZ	24:p:91:GLN:HE21	2.09	0.66
4:L:141:PHE:CD2	5:M:375:LEU:HD21	2.30	0.66
5:M:318:ALA:HB2	5:M:373:ILE:HG23	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:86:LEU:HB3	13:e:91:LYS:HB2	1.78	0.66
4:L:25:ASN:OD1	4:L:25:ASN:O	2.14	0.66
4:L:116:ARG:HG2	4:L:120:TYR:CE2	2.31	0.66
6:N:243:MET:HG2	12:d:44:MET:HE2	1.77	0.66
7:O:200:PRO:HG3	7:O:282:PRO:HD2	1.77	0.66
4:L:552:LEU:HD23	4:L:553:LEU:HD12	1.77	0.66
7:O:40:LEU:HG	7:O:292:HIS:CE1	2.31	0.66
13:e:38:LYS:CE	16:h:181:HIS:HD2	2.09	0.66
3:K:22:PHE:HB2	4:L:585:LYS:HG2	1.76	0.65
4:L:553:LEU:HD21	21:m:93:ALA:C	2.21	0.65
5:M:373:ILE:CD1	5:M:454:ILE:HD11	2.25	0.65
20:l:101:TRP:NE1	21:m:62:ASP:HA	2.11	0.65
4:L:66:TRP:HZ3	4:L:68:TRP:CD1	2.14	0.65
4:L:142:ILE:HA	5:M:370:PRO:HB2	1.78	0.65
5:M:175:ASN:HD22	16:h:143:GLU:HG2	1.61	0.65
5:M:350:MET:HG2	22:n:99:VAL:HG12	1.77	0.65
7:O:73:LEU:HD22	7:O:207:ILE:HD11	1.78	0.65
17:i:92:THR:O	24:p:4:SER:HB2	1.96	0.65
5:M:47:GLU:OE2	24:p:93:ARG:HB3	1.96	0.65
5:M:367:LEU:CD2	5:M:408:MET:HE2	2.25	0.65
4:L:190:SER:HB2	4:L:196:TRP:HE1	1.60	0.65
7:O:38:TYR:CE2	7:O:292:HIS:HD2	2.14	0.65
21:m:15:PRO:CG	21:m:18:LEU:HD12	2.27	0.65
23:o:25:PHE:HB3	23:o:26:PRO:HD2	1.78	0.65
4:L:141:PHE:CE2	5:M:370:PRO:CG	2.73	0.65
4:L:387:THR:HG22	4:L:465:GLY:H	1.61	0.65
25:M:502:3PE:H2A1	26:h:201:CDL:H202	1.78	0.65
6:N:258:THR:HB	6:N:333:SER:O	1.96	0.65
9:X:147:ARG:HH12	13:e:39:GLU:HG3	1.62	0.65
13:e:38:LYS:HE3	16:h:181:HIS:CD2	2.31	0.65
6:N:220:MET:C	6:N:223:ASN:H	2.04	0.65
15:g:108:PRO:O	15:g:109:ASP:OD1	2.13	0.65
2:J:33:ILE:CG2	2:J:60:LEU:HD21	2.26	0.65
14:f:38:ARG:NH1	14:f:54:VAL:HG21	2.11	0.65
20:l:38:PRO:CB	21:m:75:ASN:HD22	2.03	0.65
4:L:88:LEU:HD23	4:L:326:PHE:CE2	2.32	0.65
18:j:92:TRP:CZ3	23:o:100:LYS:HA	2.32	0.65
19:k:34:PRO:CG	19:k:59:TYR:CE1	2.72	0.65
23:o:71:ARG:HB3	23:o:71:ARG:HH11	1.61	0.65
4:L:13:ILE:HD11	25:i:201:3PE:C2C	2.26	0.65
4:L:368:PHE:HB3	4:L:445:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:594:ASN:HD21	6:N:110:PRO:HB2	1.57	0.65
7:O:38:TYR:HB3	7:O:299:GLN:NE2	2.12	0.65
7:O:343:TYR:CE1	7:O:355:LYS:HB2	2.32	0.65
19:k:38:VAL:HG13	22:n:39:TYR:HB2	1.76	0.65
5:M:122:PHE:HD1	5:M:238:LEU:HG	1.62	0.65
10:Y:137:LEU:HD23	10:Y:138:PHE:CG	2.31	0.65
15:g:106:TYR:OH	16:h:86:ILE:HD12	1.97	0.65
17:i:110:ILE:HD13	24:p:16:ARG:HD2	1.78	0.65
24:p:24:THR:HG22	24:p:26:LEU:H	1.62	0.65
1:D:47:PHE:HB3	6:N:227:ILE:CD1	2.16	0.64
5:M:300:SER:HB3	5:M:381:ILE:HG23	1.78	0.64
16:h:127:ASP:OD1	16:h:127:ASP:O	2.15	0.64
2:J:109:TYR:O	2:J:110:ASP:C	2.40	0.64
3:K:70:GLU:HA	6:N:38:LEU:HD21	1.78	0.64
3:K:96:LEU:O	3:K:97:GLN:C	2.40	0.64
4:L:141:PHE:CE2	5:M:375:LEU:HD22	2.12	0.64
5:M:167:ILE:O	5:M:171:VAL:HG12	1.98	0.64
5:M:307:TRP:CD1	5:M:459:MET:SD	2.91	0.64
6:N:254:LEU:HD12	6:N:255:PRO:HD2	1.78	0.64
4:L:81:LYS:N	4:L:135:ASN:HD21	1.96	0.64
5:M:119:TYR:CD1	5:M:160:LEU:HD22	2.32	0.64
7:O:117:PHE:CE1	7:O:173:MET:CE	2.77	0.64
7:O:194:THR:HG23	7:O:307:TYR:HB2	1.79	0.64
20:l:122:THR:CG2	20:l:123:PRO:HD2	2.27	0.64
24:p:74:ILE:HD13	24:p:85:ILE:HG13	1.80	0.64
4:L:247:LEU:CD1	4:L:248:HIS:NE2	2.52	0.64
4:L:366:MET:CG	4:L:443:ILE:HG21	2.28	0.64
16:h:175:GLU:HB2	16:h:178:PHE:CD2	2.31	0.64
18:j:97:LEU:O	23:o:104:ARG:NH1	2.29	0.64
4:L:174:TYR:CE1	25:L:702:3PE:H331	2.32	0.64
4:L:246:LEU:HD12	4:L:246:LEU:C	2.22	0.64
12:d:60:ARG:O	12:d:61:GLN:C	2.40	0.64
12:d:109:TYR:HA	12:d:112:ILE:CG2	2.28	0.64
16:h:57:VAL:HG22	22:n:104:LEU:HD11	1.78	0.64
5:M:458:THR:HG22	24:p:148:ALA:HB1	1.79	0.64
6:N:179:MET:HG3	6:N:216:PHE:HE1	1.63	0.64
18:j:47:PHE:HA	19:k:63:PHE:CZ	2.33	0.64
4:L:40:ILE:HD13	4:L:97:THR:HG22	1.79	0.64
6:N:37:LEU:HD12	6:N:63:GLN:HB3	1.79	0.64
15:g:139:TYR:HB2	24:p:142:ARG:CZ	2.28	0.64
24:p:5:TRP:HH2	24:p:12:GLU:OE1	1.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:104:CYS:HA	2:J:107:ASN:HB2	1.80	0.64
4:L:41:LYS:HG3	4:L:98:TRP:CE2	2.33	0.64
7:O:99:GLY:CA	11:c:30:TYR:HD1	2.11	0.64
17:i:89:HIS:HB3	25:i:201:3PE:H122	1.79	0.64
5:M:160:LEU:HD11	5:M:203:PHE:CZ	2.33	0.64
5:M:196:TRP:HZ3	5:M:261:PHE:HE2	1.44	0.64
7:O:168:VAL:CG2	7:O:241:TYR:CE1	2.77	0.64
7:O:168:VAL:CG2	7:O:241:TYR:CZ	2.62	0.64
10:Y:143:VAL:O	16:h:158:ARG:NH2	2.31	0.64
15:g:139:TYR:CD1	24:p:142:ARG:NH2	2.65	0.64
5:M:368:ALA:HB1	5:M:375:LEU:CD1	2.25	0.64
6:N:220:MET:HA	6:N:223:ASN:HA	1.79	0.64
6:N:313:MET:HG3	7:O:305:LEU:HD22	1.80	0.64
9:X:151:ASN:HD22	16:h:165:ASP:HA	1.62	0.64
17:i:29:SER:HB2	17:i:32:GLU:OE1	1.96	0.64
6:N:143:ILE:HA	6:N:194:LEU:HD11	1.79	0.63
7:O:342:GLY:HA3	11:c:36:ASN:OD1	1.98	0.63
14:f:41:SER:OG	16:h:134:GLU:HG2	1.99	0.63
20:l:106:HIS:CD2	20:l:107:TRP:N	2.67	0.63
20:l:119:THR:HG22	21:m:13:THR:HG23	1.79	0.63
25:m:201:3PE:H11	25:m:202:3PE:H331	1.81	0.63
4:L:305:SER:HB2	4:L:422:TYR:CE1	2.34	0.63
4:L:381:THR:HG21	4:L:498:PHE:CE2	2.33	0.63
5:M:220:HIS:NE2	5:M:231:LEU:HB3	2.13	0.63
5:M:250:LEU:O	5:M:250:LEU:CD1	2.44	0.63
8:U:72:PRO:HG3	18:j:42:PRO:HG2	1.79	0.63
13:e:38:LYS:HG2	16:h:179:ILE:CG2	2.28	0.63
4:L:100:ILE:HD13	4:L:341:MET:SD	2.38	0.63
4:L:202:MET:HE3	4:L:265:PRO:CG	2.25	0.63
26:L:704:CDL:H772	5:M:371:PRO:HG3	1.78	0.63
5:M:118:PHE:O	5:M:122:PHE:N	2.25	0.63
5:M:267:TRP:CZ2	5:M:271:MET:HE3	2.32	0.63
8:U:140:CYS:SG	8:U:143:GLU:OE2	2.53	0.63
13:e:75:ARG:O	13:e:79:ILE:HG13	1.98	0.63
15:g:63:ASN:OD1	22:n:106:TYR:HE1	1.82	0.63
4:L:80:PHE:C	4:L:135:ASN:HD21	2.06	0.63
4:L:410:LEU:HD12	4:L:411:ILE:N	2.13	0.63
4:L:433:THR:HG22	4:L:434:LYS:N	2.14	0.63
5:M:231:LEU:HA	5:M:235:LEU:HD12	1.80	0.63
8:U:86:VAL:HB	8:U:122:MET:HE1	1.79	0.63
14:f:38:ARG:NH1	14:f:54:VAL:CG2	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:75:ASP:OD1	15:g:76:SER:N	2.32	0.63
19:k:34:PRO:HG2	19:k:59:TYR:CD1	2.34	0.63
22:n:95:GLU:HA	22:n:98:LYS:HG3	1.81	0.63
2:J:116:LEU:HD23	2:J:123:TRP:CD2	2.34	0.63
4:L:56:HIS:O	23:o:71:ARG:HG3	1.99	0.63
5:M:1:MET:HB2	5:M:52:PHE:HD2	1.60	0.63
5:M:105:LEU:O	5:M:109:THR:HG23	1.98	0.63
6:N:149:LEU:HD13	6:N:154:ILE:CG2	2.28	0.63
6:N:308:ASN:CB	7:O:317:ILE:HG22	2.28	0.63
7:O:227:MET:C	7:O:228:LYS:HG2	2.23	0.63
7:O:305:LEU:HD12	7:O:305:LEU:C	2.24	0.63
5:M:129:THR:HG21	5:M:235:LEU:HD13	1.80	0.63
2:J:18:GLY:O	2:J:23:PRO:HD3	1.98	0.63
2:J:75:THR:HG21	3:K:27:MET:HB3	1.79	0.63
4:L:361:ASN:OD1	4:L:361:ASN:O	2.17	0.63
5:M:73:LEU:CD2	5:M:103:GLN:NE2	2.61	0.63
16:h:155:GLU:O	16:h:159:LEU:HD13	1.99	0.63
17:i:28:LEU:HD22	17:i:32:GLU:HG2	1.79	0.63
4:L:357:ARG:NH1	22:n:78:GLN:O	2.32	0.63
4:L:556:ILE:HG23	21:m:80:PHE:CE2	2.34	0.63
5:M:391:PHE:HE2	25:m:202:3PE:H261	1.61	0.63
6:N:100:MET:HE3	6:N:111:PHE:CZ	2.34	0.63
6:N:131:LEU:O	6:N:135:LYS:HG2	1.98	0.63
6:N:158:ALA:O	6:N:162:ILE:HG12	1.98	0.63
10:Y:19:GLN:NE2	10:Y:22:ARG:HG2	2.09	0.63
24:p:66:ARG:HD2	24:p:68:TYR:CZ	2.34	0.63
2:J:125:MET:HE2	2:J:128:VAL:HG21	1.80	0.62
2:J:77:GLU:OE1	3:K:87:THR:O	2.16	0.62
6:N:246:LEU:HD11	25:N:401:3PE:C3A	2.30	0.62
9:X:151:ASN:ND2	16:h:165:ASP:HA	2.14	0.62
20:l:38:PRO:C	21:m:75:ASN:ND2	2.58	0.62
21:m:49:LEU:HD12	21:m:49:LEU:O	1.99	0.62
22:n:141:GLN:O	22:n:144:THR:HG22	1.99	0.62
23:o:26:PRO:HB2	23:o:29:LEU:HB2	1.81	0.62
2:J:12:PHE:HE2	3:K:42:ILE:CD1	2.12	0.62
2:J:22:LYS:HB2	3:K:23:ARG:HD3	1.81	0.62
4:L:445:GLU:HB2	4:L:450:LEU:CD2	2.29	0.62
7:O:161:ARG:NH2	27:O:401:ADP:H5'2	2.15	0.62
13:e:101:ARG:NH2	13:e:104:PRO:HD2	2.14	0.62
4:L:9:LEU:HG	25:i:201:3PE:H2C1	1.80	0.62
5:M:123:GLU:HB3	6:N:255:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:307:TRP:CE3	5:M:383:MET:HE3	2.34	0.62
6:N:275:CYS:SG	10:Y:139:PRO:HG2	2.38	0.62
4:L:211:ILE:HG13	25:m:201:3PE:H272	1.81	0.62
4:L:365:ILE:HD11	4:L:366:MET:HE2	1.82	0.62
5:M:307:TRP:HD1	5:M:459:MET:SD	2.23	0.62
5:M:318:ALA:CB	5:M:373:ILE:HG23	2.29	0.62
7:O:113:SER:HB3	7:O:116:LYS:HB2	1.80	0.62
14:f:56:TRP:CZ3	16:h:131:LYS:HG3	2.35	0.62
23:o:18:ASP:OD1	23:o:19:PRO:HD2	1.99	0.62
5:M:129:THR:HG21	5:M:235:LEU:CD1	2.30	0.62
7:O:121:PRO:O	7:O:122:LYS:CG	2.46	0.62
7:O:132:GLN:HE22	7:O:169:PHE:HB2	1.64	0.62
8:U:71:ALA:HB1	8:U:72:PRO:HD2	1.81	0.62
17:i:93:LYS:HD3	25:i:201:3PE:H121	1.81	0.62
22:n:168:TRP:O	22:n:172:THR:OG1	2.18	0.62
3:K:4:THR:HG23	3:K:5:PHE:N	2.14	0.62
25:K:101:3PE:H3D2	4:L:593:ILE:HD13	1.81	0.62
6:N:109:ALA:CB	6:N:110:PRO:HD3	2.30	0.62
6:N:207:ILE:O	6:N:211:LEU:HG	2.00	0.62
6:N:307:THR:HB	7:O:319:ILE:CG1	2.30	0.62
2:J:9:SER:HB3	3:K:7:ASN:ND2	2.06	0.62
2:J:75:THR:HG21	3:K:27:MET:HB2	1.81	0.62
5:M:395:LEU:HD21	21:m:101:TRP:CE2	2.35	0.62
16:h:96:ALA:CB	24:p:63:TYR:HD1	2.12	0.62
21:m:127:ILE:CG2	24:p:136:THR:HG23	2.30	0.62
4:L:187:VAL:HG22	5:M:383:MET:HG2	1.82	0.62
5:M:56:PHE:HE1	5:M:108:MET:HG2	1.64	0.62
6:N:335:MET:O	6:N:335:MET:CG	2.41	0.62
7:O:117:PHE:HE1	7:O:128:SER:HB2	1.63	0.62
9:X:164:GLY:O	9:X:165:THR:C	2.41	0.62
21:m:17:THR:O	21:m:18:LEU:HB2	1.99	0.62
21:m:111:ARG:NE	25:m:202:3PE:H31	2.14	0.62
2:J:135:LEU:CD1	3:K:54:MET:CE	2.77	0.61
4:L:556:ILE:CG2	21:m:80:PHE:CZ	2.82	0.61
6:N:23:SER:HB2	13:e:15:ASP:OD2	1.99	0.61
24:p:5:TRP:CH2	24:p:12:GLU:OE1	2.53	0.61
4:L:10:LEU:HD23	4:L:46:ILE:HG21	1.82	0.61
5:M:98:MET:HE3	5:M:128:PRO:HA	1.81	0.61
7:O:117:PHE:HD1	7:O:128:SER:HA	1.64	0.61
7:O:249:MET:HE3	7:O:253:CYS:SG	2.40	0.61
8:U:128:PHE:CZ	8:U:148:ILE:HG23	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:19:ARG:HH11	22:n:173:ARG:HH21	1.48	0.61
23:o:69:CYS:C	23:o:80:CYS:SG	2.82	0.61
4:L:578:THR:CG2	6:N:168:GLY:HA2	2.30	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: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:76:GLU:HB3	7:O:266:PRO:HB3	1.82	0.61
7:O:99:GLY:O	11:c:30:TYR:HA	2.01	0.61
7:O:140:LEU:HD11	7:O:198:TYR:CZ	2.35	0.61
15:g:106:TYR:CZ	16:h:86:ILE:HD12	2.35	0.61
21:m:100:PHE:O	21:m:104:VAL:HG23	2.00	0.61
4:L:468:ILE:O	4:L:472:ILE:HG23	2.00	0.61
5:M:139:GLN:HB3	5:M:222:GLU:HG3	1.83	0.61
6:N:175:MET:HE1	6:N:227:ILE:HA	1.81	0.61
6:N:308:ASN:HB3	7:O:317:ILE:CG2	2.31	0.61
7:O:37:ARG:HB2	7:O:299:GLN:OE1	2.01	0.61
20:l:57:MET:HG2	20:l:104:PRO:HG2	1.82	0.61
5:M:422:HIS:NE2	5:M:425:ASN:OD1	2.33	0.61
7:O:140:LEU:HD21	7:O:304:VAL:O	2.00	0.61
18:j:102:ASP:OD1	23:o:111:ARG:HG3	1.99	0.61
4:L:542:LEU:HD11	25:L:702:3PE:H261	1.83	0.61
4:L:559:GLU:HA	4:L:563:PRO:HG2	1.82	0.61
5:M:98:MET:HE1	5:M:128:PRO:HA	1.82	0.61
5:M:318:ALA:HB2	5:M:373:ILE:CG2	2.30	0.61
5:M:433:GLU:O	5:M:437:MET:HG2	2.01	0.61
11:c:66:VAL:CG1	11:c:70:LYS:HE3	2.31	0.61
14:f:38:ARG:HH12	14:f:54:VAL:CG2	2.14	0.61
20:l:62:TYR:CZ	20:l:64:PRO:HG3	2.36	0.61
4:L:180:ILE:HD11	5:M:400:ILE:HB	1.83	0.61
5:M:1:MET:CE	5:M:111:SER:HB2	2.29	0.61
6:N:218:ALA:HB1	6:N:240:MET:SD	2.40	0.61
8:U:72:PRO:CD	18:j:42:PRO:HG2	2.31	0.61
8:U:138:LEU:HB3	8:U:144:ILE:HG12	1.82	0.61
4:L:70:THR:HG21	24:p:101:GLU:OE2	2.00	0.61
4:L:100:ILE:HG21	4:L:246:LEU:HD23	1.82	0.61
4:L:424:MET:HE2	4:L:502:LEU:CB	2.31	0.61
6:N:273:ASN:ND2	10:Y:143:VAL:HA	2.15	0.61
9:X:160:PRO:HG3	12:d:22:PRO:HD3	1.83	0.61
16:h:106:ILE:O	16:h:106:ILE:HG22	2.00	0.61
21:m:30:ARG:O	21:m:34:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:149:ILE:H	22:n:149:ILE:HD12	1.65	0.61
4:L:174:TYR:HE1	25:L:702:3PE:H331	1.64	0.61
5:M:109:THR:HG22	5:M:121:LEU:HB3	1.82	0.61
5:M:423:MET:O	5:M:424:ILE:C	2.43	0.61
6:N:275:CYS:SG	10:Y:139:PRO:CG	2.89	0.61
15:g:109:ASP:HB3	15:g:114:GLU:HB3	1.83	0.61
21:m:25:VAL:HA	21:m:30:ARG:HD3	1.83	0.61
25:m:201:3PE:H2A1	25:m:201:3PE:H3C2	1.82	0.61
23:o:15:VAL:HG11	23:o:113:LYS:HD3	1.83	0.61
4:L:538:PRO:HG2	20:l:117:VAL:HG22	1.83	0.61
5:M:209:LEU:HD23	5:M:210:TYR:N	2.16	0.61
11:c:55:TRP:CZ2	12:d:66:THR:HG22	2.36	0.61
5:M:178:ILE:HD12	16:h:143:GLU:HG3	1.83	0.60
11:c:66:VAL:HG12	11:c:70:LYS:HE3	1.83	0.60
20:l:108:ASP:HB3	20:l:111:MET:HE2	1.83	0.60
2:J:12:PHE:CZ	3:K:42:ILE:CD1	2.83	0.60
2:J:61:GLY:O	2:J:65:VAL:HB	2.02	0.60
4:L:40:ILE:HD12	4:L:101:MET:HG3	1.82	0.60
4:L:182:PHE:CE2	4:L:186:MET:SD	2.94	0.60
4:L:482:MET:CE	4:L:486:LEU:HB3	2.31	0.60
6:N:59:TYR:CZ	6:N:63:GLN:HG3	2.36	0.60
1:D:35:ARG:HH22	15:g:56:ASP:C	2.09	0.60
4:L:42:PHE:O	4:L:46:ILE:HG12	2.01	0.60
10:Y:83:ARG:HH11	10:Y:90:LEU:HD22	1.66	0.60
13:e:95:PRO:HD2	13:e:98:HIS:HB2	1.82	0.60
26:h:201:CDL:H171	25:i:201:3PE:H352	1.81	0.60
6:N:100:MET:HE3	6:N:111:PHE:HZ	1.66	0.60
9:X:159:LYS:O	9:X:160:PRO:C	2.43	0.60
2:J:133:VAL:O	2:J:134:MET:HB2	1.99	0.60
4:L:511:LEU:CD1	22:n:36:LYS:HA	2.31	0.60
20:l:162:PRO:HG3	23:o:39:MET:HE3	1.83	0.60
1:D:36:GLN:HA	5:M:138:ASN:HA	1.84	0.60
4:L:141:PHE:CD2	5:M:370:PRO:HG3	2.35	0.60
4:L:446:ASN:HD21	18:j:51:THR:CG2	2.14	0.60
4:L:204:SER:HA	4:L:207:ASN:HD22	1.67	0.60
5:M:207:MET:HG3	5:M:239:GLY:HA3	1.84	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
6:N:324:LEU:HD11	12:d:64:PHE:HZ	1.66	0.60
8:U:110:LEU:HD13	8:U:118:ILE:HD11	1.82	0.60
8:U:120:MET:HE1	22:n:24:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLN:HE22	5:M:135:ARG:HH11	1.45	0.60
2:J:68:GLY:O	2:J:69:TYR:C	2.41	0.60
4:L:65:THR:HA	17:i:90:MET:HE2	1.83	0.60
5:M:77:LEU:HD23	5:M:99:LEU:HD12	1.83	0.60
7:O:209:VAL:HG23	7:O:214:VAL:CG1	2.31	0.60
12:d:16:ASP:O	12:d:19:ARG:HG3	2.01	0.60
16:h:73:PHE:HD2	16:h:74:TYR:CD1	2.20	0.60
4:L:222:GLY:CA	4:L:229:LEU:HD11	2.26	0.60
5:M:126:LEU:HD21	5:M:153:THR:HB	1.83	0.60
5:M:269:MET:HE3	5:M:399:ASN:CB	2.32	0.60
10:Y:137:LEU:CD2	10:Y:138:PHE:CD2	2.84	0.60
5:M:370:PRO:HA	5:M:375:LEU:HD22	1.83	0.60
16:h:73:PHE:CD2	16:h:74:TYR:CD1	2.90	0.60
16:h:102:PRO:HD2	16:h:105:TYR:CB	2.32	0.60
22:n:176:GLU:O	22:n:178:PRO:HD3	2.02	0.60
2:J:120:LEU:CD2	2:J:124:LEU:HD22	2.32	0.59
4:L:173:LEU:CD2	25:L:702:3PE:H321	2.27	0.59
4:L:247:LEU:HD12	4:L:248:HIS:CG	2.36	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
7:O:54:HIS:HB2	7:O:56:TYR:CE1	2.37	0.59
11:c:65:ASP:OD2	12:d:73:TYR:OH	2.17	0.59
22:n:143:GLU:OE1	22:n:155:PRO:HB3	2.02	0.59
4:L:81:LYS:HB2	4:L:135:ASN:OD1	2.02	0.59
5:M:329:LEU:HD23	5:M:437:MET:HE3	1.85	0.59
8:U:90:TYR:CZ	8:U:92:LYS:HD2	2.35	0.59
12:d:113:LEU:HD22	15:g:148:PRO:HG3	1.84	0.59
4:L:123:LEU:HD22	4:L:150:MET:CG	2.32	0.59
4:L:313:MET:HE2	4:L:328:HIS:CE1	2.38	0.59
5:M:115:LEU:O	5:M:118:PHE:HB3	2.02	0.59
5:M:144:ASN:HA	5:M:147:ILE:HD12	1.82	0.59
7:O:164:TYR:CE2	7:O:195:LEU:HD21	2.36	0.59
9:X:158:LEU:HB3	12:d:21:LEU:HD21	1.84	0.59
11:c:34:PRO:CG	11:c:37:ALA:HB2	2.32	0.59
16:h:69:ARG:O	16:h:73:PHE:HB2	2.02	0.59
21:m:18:LEU:HD11	22:n:72:TRP:CG	2.37	0.59
23:o:39:MET:HE1	23:o:58:TYR:HA	1.84	0.59
2:J:55:VAL:HB	3:K:41:PHE:HE2	1.67	0.59
5:M:209:LEU:HD23	5:M:211:GLY:H	1.67	0.59
5:M:294:MET:HE3	5:M:319:HIS:CD2	2.37	0.59
18:j:94:ASP:HB3	18:j:99:ILE:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:4:HIS:HA	23:o:7:ARG:HH11	1.67	0.59
1:D:35:ARG:HH21	15:g:59:PRO:HD3	1.68	0.59
4:L:149:ILE:HG21	5:M:364:LEU:HD21	1.84	0.59
7:O:249:MET:HB3	7:O:253:CYS:SG	2.42	0.59
7:O:343:TYR:HE1	7:O:355:LYS:HB2	1.67	0.59
21:m:129:TYR:CZ	24:p:144:LEU:O	2.55	0.59
1:D:49:GLY:O	6:N:173:THR:HG21	2.03	0.59
4:L:227:PHE:CD2	4:L:283:LEU:CD2	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
6:N:223:ASN:HB3	7:O:306:ASN:HD21	1.67	0.59
7:O:114:LEU:HA	7:O:131:LEU:HD21	1.84	0.59
7:O:246:LEU:HD11	7:O:257:VAL:CG2	2.33	0.59
15:g:139:TYR:HD2	15:g:140:PHE:CD1	2.20	0.59
15:g:140:PHE:HB3	24:p:75:THR:HG21	1.84	0.59
20:l:109:LEU:O	20:l:113:ILE:HG23	2.03	0.59
3:K:12:PHE:CE1	6:N:72:LEU:HD22	2.38	0.59
4:L:358:LYS:HG3	22:n:80:TYR:CZ	2.38	0.59
4:L:390:TYR:CE2	18:j:68:TRP:HH2	2.21	0.59
5:M:275:ILE:HD11	5:M:288:TYR:CB	2.33	0.59
6:N:200:LEU:HD22	6:N:269:GLU:HG3	1.84	0.59
6:N:300:THR:HG23	6:N:301:SER:N	2.17	0.59
22:n:111:GLU:O	22:n:114:MET:HG2	2.03	0.59
4:L:466:PHE:CE1	4:L:470:TYR:HE2	2.21	0.59
4:L:570:HIS:O	4:L:571:THR:C	2.45	0.59
5:M:14:LEU:HD21	5:M:26:ASN:HB2	1.84	0.59
5:M:396:MET:HG3	5:M:396:MET:O	2.03	0.59
6:N:179:MET:CG	6:N:216:PHE:HE1	2.16	0.59
24:p:37:TYR:CZ	24:p:41:VAL:HG11	2.37	0.59
4:L:477:ILE:HG13	23:o:91:GLU:CD	2.28	0.58
6:N:342:GLN:NE2	12:d:30:ARG:HH11	2.01	0.58
7:O:351:TRP:CZ3	11:c:41:TRP:HH2	2.20	0.58
13:e:87:MET:HE3	13:e:94:PRO:HD3	1.85	0.58
16:h:95:GLU:HB3	16:h:114:LYS:HG2	1.85	0.58
22:n:97:TYR:HB2	22:n:178:PRO:CB	2.32	0.58
23:o:50:GLN:OE1	24:p:120:ASN:ND2	2.36	0.58
3:K:95:LEU:HG	6:N:54:GLU:CD	2.28	0.58
6:N:77:ASN:OD1	6:N:81:LEU:HD12	2.03	0.58
12:d:14:LEU:HD12	12:d:14:LEU:C	2.27	0.58
13:e:69:ARG:HD2	13:e:72:THR:HG21	1.85	0.58
21:m:49:LEU:HD22	22:n:140:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:ALA:CB	6:N:110:PRO:CD	2.81	0.58
21:m:75:ASN:O	21:m:75:ASN:OD1	2.20	0.58
4:L:407:TRP:CZ3	4:L:410:LEU:HD11	2.38	0.58
16:h:57:VAL:CG1	22:n:99:VAL:HG23	2.33	0.58
1:D:37:TRP:CZ2	1:D:39:PRO:HA	2.38	0.58
4:L:404:THR:HG22	4:L:405:ASN:N	2.19	0.58
4:L:417:SER:HB3	4:L:493:ILE:CG1	2.31	0.58
6:N:307:THR:CG2	6:N:311:SER:OG	2.52	0.58
25:N:401:3PE:H261	25:d:201:3PE:H222	1.84	0.58
17:i:95:TYR:OH	24:p:11:PRO:O	2.20	0.58
4:L:407:TRP:HE1	20:l:140:MET:CE	2.16	0.58
4:L:550:LEU:HB2	5:M:275:ILE:HG22	1.83	0.58
8:U:97:LYS:O	8:U:98:LEU:C	2.46	0.58
25:d:201:3PE:H111	25:d:201:3PE:H12	1.86	0.58
7:O:326:ARG:HH21	15:g:56:ASP:CG	2.12	0.58
21:m:129:TYR:HE2	24:p:146:LEU:O	1.85	0.58
4:L:261:VAL:C	4:L:264:HIS:HD2	2.12	0.58
4:L:390:TYR:CE2	18:j:68:TRP:CH2	2.92	0.58
5:M:123:GLU:CD	6:N:255:PRO:HG2	2.28	0.58
5:M:196:TRP:HZ3	5:M:261:PHE:CE2	2.21	0.58
6:N:314:MET:CB	7:O:305:LEU:HD11	2.33	0.58
12:d:113:LEU:O	12:d:113:LEU:HG	2.02	0.58
22:n:177:ARG:HG2	22:n:179:THR:OG1	2.04	0.58
3:K:59:ILE:HD12	6:N:27:MET:HG2	1.85	0.58
4:L:15:LEU:O	4:L:18:PRO:HD2	2.03	0.58
4:L:425:ARG:HG3	4:L:429:PHE:CE2	2.39	0.58
4:L:542:LEU:HB3	5:M:278:ARG:HD2	1.85	0.58
6:N:26:LEU:O	6:N:27:MET:C	2.46	0.58
6:N:149:LEU:HD11	6:N:195:PRO:HG3	1.84	0.58
7:O:351:TRP:CH2	11:c:41:TRP:HH2	2.22	0.58
15:g:121:GLU:HA	15:g:124:VAL:HG22	1.86	0.58
4:L:390:TYR:HE2	18:j:68:TRP:CH2	2.22	0.58
5:M:73:LEU:HB2	5:M:103:GLN:OE1	2.02	0.58
7:O:117:PHE:CD1	7:O:128:SER:CB	2.87	0.58
9:X:168:PHE:O	9:X:170:TRP:CD1	2.57	0.58
12:d:93:TYR:CD2	16:h:156:VAL:HG13	2.39	0.58
13:e:20:PHE:CZ	16:h:178:PHE:HB2	2.39	0.58
17:i:70:PHE:O	17:i:73:SER:HB3	2.04	0.58
23:o:116:ALA:O	23:o:120:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:232:TRP:CZ3	4:L:233:LEU:HD21	2.37	0.57
5:M:109:THR:HG22	5:M:121:LEU:CB	2.34	0.57
8:U:84:LEU:O	8:U:88:LYS:HG3	2.04	0.57
8:U:100:VAL:O	8:U:101:ASN:HB2	2.04	0.57
13:e:14:LEU:HD12	13:e:15:ASP:CB	2.33	0.57
1:D:36:GLN:OE1	5:M:136:TRP:HA	2.03	0.57
4:L:592:LEU:O	4:L:596:ILE:HG12	2.04	0.57
5:M:296:LEU:HD22	5:M:396:MET:HE1	1.85	0.57
5:M:423:MET:SD	21:m:59:HIS:NE2	2.78	0.57
6:N:33:LEU:HD11	6:N:141:ILE:HD12	1.86	0.57
22:n:26:HIS:CE1	22:n:79:PRO:HB3	2.39	0.57
23:o:5:LEU:HB3	23:o:9:TYR:CE2	2.38	0.57
7:O:66:ILE:CD1	7:O:218:ILE:CD1	2.82	0.57
18:j:101:PRO:O	18:j:102:ASP:C	2.46	0.57
5:M:73:LEU:HD22	5:M:103:GLN:NE2	2.18	0.57
5:M:172:GLY:C	5:M:173:THR:HG23	2.28	0.57
5:M:297:VAL:O	5:M:301:ILE:HG12	2.03	0.57
6:N:253:GLY:N	6:N:290:LEU:HD11	2.19	0.57
6:N:307:THR:O	7:O:319:ILE:HG12	2.05	0.57
9:X:171:THR:O	9:X:172:VAL:C	2.48	0.57
4:L:145:GLU:HB3	5:M:370:PRO:CG	2.34	0.57
4:L:227:PHE:CD2	4:L:283:LEU:HD21	2.38	0.57
5:M:230:ILE:HG13	5:M:235:LEU:HG	1.87	0.57
5:M:444:LEU:O	5:M:448:THR:HG23	2.04	0.57
5:M:447:LEU:HD21	5:M:454:ILE:CD1	2.33	0.57
6:N:179:MET:HG3	6:N:216:PHE:CE1	2.39	0.57
2:J:135:LEU:HA	3:K:54:MET:HE1	1.85	0.57
4:L:425:ARG:HG3	4:L:429:PHE:HE2	1.68	0.57
4:L:441:ILE:HG21	18:j:48:PRO:HD3	1.85	0.57
5:M:123:GLU:CG	6:N:255:PRO:HG2	2.35	0.57
5:M:255:LYS:HZ3	12:d:117:HIS:HB3	1.67	0.57
6:N:154:ILE:HG12	6:N:195:PRO:HG2	1.87	0.57
6:N:284:MET:O	6:N:287:LEU:HB2	2.04	0.57
15:g:147:LEU:HD11	24:p:163:MET:HB3	1.86	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
6:N:273:ASN:O	6:N:274:ASN:HB2	2.05	0.57
8:U:130:ILE:HG23	8:U:147:TYR:CE2	2.39	0.57
9:X:162:LYS:HB3	9:X:166:ARG:NH2	2.19	0.57
15:g:140:PHE:CZ	24:p:74:ILE:HG22	2.40	0.57
4:L:441:ILE:HD12	18:j:46:GLU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:14:LEU:HD11	5:M:26:ASN:HB3	1.87	0.57
5:M:421:ASN:HB2	21:m:51:TYR:OH	2.05	0.57
6:N:109:ALA:HB1	6:N:110:PRO:HD3	1.86	0.57
25:d:201:3PE:H232	25:d:201:3PE:H272	1.85	0.57
22:n:98:LYS:HG2	22:n:178:PRO:HG3	1.86	0.57
4:L:246:LEU:HD12	4:L:247:LEU:CA	2.34	0.57
5:M:12:LEU:HB2	5:M:13:PRO:HD3	1.86	0.57
5:M:424:ILE:HG13	21:m:57:VAL:O	2.05	0.57
7:O:135:LEU:HD13	27:O:401:ADP:C6	2.40	0.57
13:e:20:PHE:HZ	16:h:178:PHE:HB2	1.70	0.57
17:i:111:LEU:HD11	24:p:20:PRO:HD3	1.87	0.57
3:K:89:TYR:C	3:K:91:GLN:N	2.59	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:269:MET:HE3	5:M:399:ASN:HB2	1.86	0.57
5:M:310:MET:O	5:M:314:MET:HG3	2.04	0.57
7:O:80:GLN:CG	7:O:270:VAL:HG21	2.18	0.57
4:L:88:LEU:HD23	4:L:326:PHE:HE2	1.69	0.56
4:L:229:LEU:HD12	4:L:229:LEU:C	2.28	0.56
5:M:282:LEU:HD13	5:M:342:MET:HE2	1.87	0.56
10:Y:110:TYR:HB2	25:m:203:3PE:H11	1.87	0.56
16:h:57:VAL:CG1	22:n:99:VAL:CG2	2.83	0.56
2:J:33:ILE:HG23	2:J:60:LEU:HD22	1.85	0.56
2:J:136:GLU:HG3	2:J:139:ILE:HG12	1.87	0.56
2:J:150:TRP:CD1	6:N:28:LEU:HD21	2.40	0.56
4:L:60:GLU:CG	4:L:83:ASP:HA	2.35	0.56
4:L:456:ARG:CG	25:L:701:3PE:H241	2.34	0.56
5:M:4:ILE:CG2	5:M:107:ILE:HD13	2.30	0.56
5:M:263:LEU:CD1	21:m:102:TYR:HD1	2.16	0.56
6:N:226:THR:HG22	6:N:228:ASN:H	1.70	0.56
6:N:254:LEU:CD1	6:N:255:PRO:HD2	2.35	0.56
7:O:173:MET:HE2	7:O:179:ILE:HG23	1.87	0.56
7:O:176:GLN:HG3	7:O:177:GLY:N	2.16	0.56
7:O:201:PRO:O	7:O:253:CYS:HB3	2.05	0.56
10:Y:92:TYR:CE1	10:Y:128:LYS:HD3	2.40	0.56
22:n:81:ILE:CD1	22:n:87:GLY:O	2.53	0.56
1:D:58:THR:HG23	1:D:61:TRP:CD2	2.40	0.56
2:J:21:LEU:HA	25:K:101:3PE:H242	1.88	0.56
2:J:135:LEU:CD1	3:K:54:MET:HE3	2.35	0.56
3:K:89:TYR:C	3:K:91:GLN:H	2.13	0.56
4:L:9:LEU:CG	25:i:201:3PE:H2C1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:125:ASP:OD1	7:O:126:GLY:N	2.39	0.56
7:O:295:ARG:HH12	7:O:299:GLN:HB2	1.67	0.56
17:i:14:GLN:HE22	22:n:157:ALA:HB3	1.71	0.56
23:o:25:PHE:HZ	23:o:109:LEU:HA	1.70	0.56
24:p:132:PHE:O	24:p:136:THR:OG1	2.17	0.56
1:D:34:ALA:HB3	5:M:86:LYS:HZ3	1.71	0.56
3:K:1:MET:O	3:K:4:THR:HG22	2.04	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
6:N:196:TYR:HB3	6:N:273:ASN:OD1	2.05	0.56
14:f:38:ARG:NH1	14:f:56:TRP:O	2.39	0.56
14:f:43:LEU:HD21	24:p:68:TYR:HD1	1.69	0.56
3:K:45:SER:O	3:K:49:LEU:HG	2.06	0.56
6:N:120:GLN:O	6:N:176:ARG:CZ	2.54	0.56
7:O:66:ILE:CD1	7:O:218:ILE:CG1	2.84	0.56
13:e:14:LEU:HD12	13:e:14:LEU:C	2.31	0.56
20:l:105:ILE:HG23	20:l:109:LEU:HD22	1.86	0.56
21:m:15:PRO:HG3	21:m:18:LEU:HD12	1.87	0.56
23:o:115:ARG:O	23:o:119:GLU:HB3	2.06	0.56
24:p:39:LEU:O	24:p:44:PRO:HD3	2.06	0.56
25:M:501:3PE:H342	6:N:280:THR:HG21	1.87	0.56
6:N:149:LEU:CD1	6:N:154:ILE:HG21	2.35	0.56
6:N:324:LEU:HD11	12:d:64:PHE:CZ	2.40	0.56
7:O:114:LEU:O	7:O:117:PHE:HB3	2.06	0.56
8:U:87:LEU:HD21	8:U:118:ILE:HG23	1.86	0.56
18:j:97:LEU:O	23:o:104:ARG:HG3	2.05	0.56
4:L:385:PHE:CD1	18:j:72:ARG:CG	2.89	0.56
4:L:385:PHE:CE1	18:j:72:ARG:HG3	2.40	0.56
4:L:397:GLU:HB2	4:L:482:MET:SD	2.46	0.56
4:L:598:ILE:HD11	6:N:153:ILE:HG12	1.88	0.56
26:L:704:CDL:H1	5:M:357:THR:OG1	2.05	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
6:N:314:MET:HB2	7:O:305:LEU:CD1	2.34	0.56
13:e:42:GLU:HG2	16:h:176:LYS:HG3	1.88	0.56
4:L:14:LEU:HD21	17:i:74:HIS:O	2.06	0.56
25:L:701:3PE:H3B2	18:j:71:TRP:HH2	1.71	0.56
5:M:196:TRP:HE1	5:M:250:LEU:HD13	1.68	0.56
6:N:253:GLY:H	6:N:290:LEU:HD11	1.71	0.56
6:N:258:THR:OG1	6:N:336:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:50:GLU:HG2	22:n:51:HIS:N	2.20	0.56
4:L:589:MET:O	4:L:592:LEU:N	2.39	0.56
22:n:57:MET:HE2	22:n:57:MET:HA	1.86	0.56
23:o:121:ARG:NH1	23:o:122:VAL:HB	2.21	0.56
4:L:538:PRO:O	4:L:542:LEU:HD13	2.06	0.56
4:L:598:ILE:HG21	6:N:100:MET:HE2	1.87	0.56
5:M:73:LEU:CD2	5:M:103:GLN:CD	2.79	0.56
5:M:158:ILE:HG21	6:N:283:ALA:HB1	1.88	0.56
9:X:160:PRO:HG3	12:d:22:PRO:CD	2.35	0.56
24:p:74:ILE:CD1	24:p:85:ILE:HG13	2.36	0.56
5:M:309:PHE:O	5:M:313:THR:HG23	2.06	0.55
15:g:106:TYR:CE2	16:h:86:ILE:CD1	2.89	0.55
6:N:325:MET:HE3	6:N:329:LEU:HD11	1.88	0.55
10:Y:76:THR:CG2	10:Y:95:GLY:HA3	2.34	0.55
21:m:49:LEU:CD2	22:n:140:LEU:HD23	2.35	0.55
23:o:69:CYS:O	23:o:69:CYS:SG	2.64	0.55
2:J:6:PHE:O	2:J:7:VAL:C	2.50	0.55
4:L:94:LEU:HD23	4:L:125:LEU:HD21	1.89	0.55
4:L:466:PHE:HB2	18:j:68:TRP:CH2	2.39	0.55
4:L:556:ILE:HG21	21:m:80:PHE:CZ	2.39	0.55
4:L:586:LEU:CD2	10:Y:47:PRO:HD3	2.35	0.55
5:M:4:ILE:H	5:M:4:ILE:HD12	1.70	0.55
6:N:3:PRO:HG2	7:O:289:TRP:CH2	2.42	0.55
7:O:224:PRO:HA	7:O:227:MET:CE	2.36	0.55
8:U:87:LEU:CB	8:U:98:LEU:HD22	2.36	0.55
9:X:158:LEU:HD13	12:d:17:GLU:HG3	1.88	0.55
10:Y:137:LEU:HD23	10:Y:138:PHE:CD2	2.41	0.55
3:K:93:LEU:HA	6:N:54:GLU:OE2	2.06	0.55
4:L:54:PHE:O	4:L:58:ASN:CA	2.55	0.55
4:L:94:LEU:CD2	4:L:125:LEU:HD21	2.35	0.55
4:L:145:GLU:HG2	5:M:370:PRO:HD3	1.88	0.55
5:M:162:ILE:CG2	6:N:271:MET:HE3	2.23	0.55
10:Y:71:MET:CG	10:Y:102:THR:HG21	2.37	0.55
6:N:237:THR:O	6:N:237:THR:CG2	2.55	0.55
8:U:72:PRO:CG	18:j:42:PRO:HG2	2.35	0.55
19:k:30:ILE:CD1	19:k:39:GLN:HB2	2.33	0.55
4:L:230:HIS:N	4:L:231:PRO:HD3	2.22	0.55
5:M:453:LEU:HD12	5:M:454:ILE:CG2	2.34	0.55
6:N:224:SER:HB2	6:N:229:SER:HB3	1.89	0.55
7:O:230:THR:HG22	7:O:233:TYR:H	1.72	0.55
7:O:332:ARG:NH1	12:d:50:MET:HE1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:115:MET:HG3	25:Y:201:3PE:H322	1.89	0.55
14:f:43:LEU:HD21	24:p:68:TYR:CD1	2.41	0.55
14:f:49:ARG:HG3	14:f:52:GLU:HG2	1.89	0.55
18:j:99:ILE:HA	23:o:108:LEU:HD21	1.88	0.55
4:L:358:LYS:NZ	22:n:34:ARG:HH12	2.05	0.55
4:L:561:THR:O	4:L:565:SER:HB2	2.07	0.55
7:O:170:LEU:HG	7:O:179:ILE:HD13	1.87	0.55
7:O:256:LEU:HD11	7:O:276:LEU:CD2	2.35	0.55
13:e:14:LEU:HD12	13:e:15:ASP:N	2.21	0.55
20:l:109:LEU:O	20:l:109:LEU:HG	2.06	0.55
4:L:69:VAL:HG11	4:L:71:MET:HE2	1.89	0.55
4:L:258:PHE:HE1	4:L:262:ARG:HH21	1.55	0.55
5:M:17:LEU:HD13	14:f:11:TRP:CH2	2.42	0.55
5:M:62:SER:C	5:M:64:PRO:HD2	2.32	0.55
6:N:230:ILE:O	6:N:233:LEU:HB2	2.07	0.55
7:O:76:GLU:O	7:O:80:GLN:HG2	2.07	0.55
14:f:46:ARG:HD2	16:h:106:ILE:HD13	1.87	0.55
4:L:162:THR:O	4:L:166:THR:HG23	2.06	0.55
4:L:386:LEU:HD11	18:j:69:ILE:HD11	1.89	0.55
7:O:238:GLU:HA	7:O:241:TYR:CD2	2.32	0.55
7:O:354:LEU:HG	11:c:44:VAL:HG22	1.89	0.55
10:Y:115:MET:HE1	25:Y:201:3PE:H222	1.89	0.55
3:K:1:MET:HA	3:K:4:THR:CG2	2.37	0.55
4:L:459:PHE:HD2	25:L:701:3PE:H242	1.71	0.55
4:L:566:THR:HG21	25:L:705:3PE:H361	1.87	0.55
5:M:231:LEU:CA	5:M:235:LEU:HD12	2.36	0.55
7:O:319:ILE:HG13	7:O:320:GLY:H	1.72	0.55
23:o:25:PHE:CZ	23:o:109:LEU:HA	2.41	0.55
3:K:66:PHE:CZ	6:N:35:PHE:CZ	2.95	0.54
4:L:25:ASN:HB2	16:h:72:LYS:HZ1	1.71	0.54
4:L:54:PHE:O	4:L:58:ASN:HA	2.07	0.54
4:L:381:THR:HG21	4:L:498:PHE:CZ	2.43	0.54
5:M:6:LEU:HB3	5:M:7:PRO:HD3	1.88	0.54
13:e:101:ARG:O	13:e:104:PRO:HD3	2.06	0.54
17:i:83:HIS:HE1	17:i:87:LYS:HD2	1.71	0.54
21:m:129:TYR:CE2	24:p:146:LEU:O	2.60	0.54
23:o:103:GLU:OE2	23:o:106:ARG:HD2	2.07	0.54
4:L:190:SER:HB2	4:L:196:TRP:NE1	2.22	0.54
5:M:415:GLN:O	5:M:416:ARG:HG3	2.08	0.54
6:N:246:LEU:HD11	25:N:401:3PE:H3A1	1.89	0.54
7:O:305:LEU:O	7:O:305:LEU:CD1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:32:ARG:O	13:e:33:CYS:HB2	2.06	0.54
16:h:73:PHE:CD2	16:h:74:TYR:CE1	2.94	0.54
17:i:16:ARG:O	17:i:20:ARG:HG2	2.08	0.54
3:K:21:MET:O	25:K:101:3PE:H222	2.07	0.54
4:L:232:TRP:O	4:L:236:ALA:N	2.40	0.54
6:N:147:PRO:HB2	6:N:148:LEU:HD12	1.89	0.54
8:U:85:TYR:HA	8:U:88:LYS:HD3	1.89	0.54
9:X:158:LEU:HD13	12:d:17:GLU:CG	2.38	0.54
10:Y:17:GLY:O	10:Y:81:GLN:HG2	2.07	0.54
15:g:147:LEU:HD11	24:p:163:MET:HE2	1.89	0.54
23:o:24:SER:HB2	23:o:105:GLU:OE2	2.08	0.54
23:o:115:ARG:O	23:o:119:GLU:N	2.27	0.54
4:L:427:ILE:CD1	19:k:69:PHE:HE1	2.20	0.54
4:L:586:LEU:HD21	10:Y:47:PRO:HD3	1.89	0.54
6:N:307:THR:C	7:O:319:ILE:HG12	2.32	0.54
8:U:110:LEU:HD13	8:U:118:ILE:CD1	2.38	0.54
13:e:72:THR:O	13:e:73:MET:C	2.49	0.54
15:g:106:TYR:HE2	16:h:86:ILE:CD1	2.20	0.54
20:l:119:THR:HG23	21:m:11:LEU:HA	1.88	0.54
2:J:63:MET:HE3	3:K:68:ALA:HA	1.90	0.54
3:K:1:MET:CA	3:K:4:THR:HG22	2.36	0.54
4:L:551:THR:HA	4:L:555:LEU:HD12	1.89	0.54
5:M:127:ILE:CD1	6:N:256:PRO:HG2	2.37	0.54
5:M:336:ARG:HH22	5:M:429:SER:HA	1.73	0.54
25:N:401:3PE:H2I2	26:X:201:CDL:H602	1.88	0.54
7:O:60:ILE:O	7:O:158:VAL:HA	2.08	0.54
8:U:131:PRO:HG2	8:U:134:ASP:HB2	1.90	0.54
11:c:72:ARG:NE	12:d:19:ARG:HB2	2.23	0.54
11:c:72:ARG:NH1	12:d:19:ARG:HD3	2.22	0.54
25:d:201:3PE:H221	25:d:201:3PE:H362	1.89	0.54
2:J:60:LEU:HD13	2:J:61:GLY:N	2.21	0.54
2:J:120:LEU:HD21	2:J:124:LEU:HD22	1.89	0.54
4:L:362:ILE:HA	4:L:365:ILE:HG13	1.90	0.54
5:M:79:ALA:HB1	5:M:225:ILE:HD13	1.90	0.54
7:O:170:LEU:HG	7:O:179:ILE:CD1	2.37	0.54
16:h:179:ILE:HG22	16:h:180:ASP:H	1.73	0.54
18:j:98:GLY:O	18:j:100:PRO:HD3	2.06	0.54
21:m:109:ARG:O	21:m:113:GLU:HG2	2.08	0.54
2:J:168:GLU:OE2	6:N:1:MET:HE2	2.07	0.54
4:L:232:TRP:CH2	4:L:233:LEU:HD21	2.42	0.54
4:L:572:ASN:OD1	25:Y:201:3PE:H221	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:278:ARG:HG2	20:l:116:ARG:HH12	1.72	0.54
6:N:82:GLY:HA3	13:e:21:LEU:HG	1.89	0.54
3:K:4:THR:CG2	3:K:5:PHE:N	2.71	0.54
4:L:131:LEU:CD1	4:L:140:LEU:CD1	2.78	0.54
5:M:160:LEU:HD23	5:M:164:LEU:HD13	1.89	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
5:M:373:ILE:HD11	5:M:454:ILE:HD11	1.88	0.54
10:Y:114:ALA:HB2	25:m:203:3PE:H231	1.90	0.54
21:m:8:PRO:HB3	21:m:14:LEU:N	2.23	0.54
22:n:125:TRP:CE3	22:n:128:LEU:HD12	2.42	0.54
23:o:6:THR:HA	23:o:10:LEU:HD13	1.89	0.54
5:M:231:LEU:O	5:M:236:LEU:HG	2.06	0.54
6:N:307:THR:HB	7:O:319:ILE:HG12	1.89	0.54
4:L:141:PHE:CD2	5:M:370:PRO:CG	2.91	0.54
4:L:264:HIS:HA	4:L:267:THR:HG23	1.89	0.54
5:M:1:MET:HE2	5:M:52:PHE:CE2	2.42	0.54
5:M:17:LEU:HD22	14:f:11:TRP:HH2	1.73	0.54
5:M:31:SER:HA	5:M:34:ILE:HG12	1.90	0.54
8:U:95:PRO:HG2	8:U:96:GLU:HG3	1.88	0.54
8:U:99:SER:O	8:U:100:VAL:C	2.51	0.54
12:d:39:TYR:CE2	12:d:43:LEU:HD11	2.43	0.54
21:m:123:ARG:O	24:p:140:GLN:NE2	2.40	0.54
4:L:66:TRP:CZ3	4:L:68:TRP:CD1	2.96	0.53
4:L:226:GLN:OE1	4:L:284:THR:HG21	2.07	0.53
4:L:247:LEU:HD11	4:L:248:HIS:CE1	2.43	0.53
4:L:477:ILE:HG13	23:o:91:GLU:OE1	2.07	0.53
15:g:151:ASP:C	24:p:171:ARG:HH22	2.16	0.53
23:o:93:LEU:O	23:o:97:LYS:HG2	2.07	0.53
4:L:559:GLU:HG2	4:L:564:LYS:HD3	1.90	0.53
7:O:114:LEU:HA	7:O:131:LEU:HD22	1.91	0.53
13:e:41:ILE:HD13	16:h:174:PRO:HD2	1.89	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
2:J:59:TYR:HD1	2:J:63:MET:SD	2.31	0.53
4:L:400:ASN:HD21	4:L:413:LEU:HD11	1.73	0.53
5:M:269:MET:CE	5:M:396:MET:HA	2.36	0.53
5:M:395:LEU:HD21	21:m:101:TRP:CZ2	2.43	0.53
6:N:179:MET:HE2	6:N:216:PHE:CE1	2.43	0.53
23:o:25:PHE:HB3	23:o:26:PRO:CD	2.37	0.53
24:p:103:MET:CE	24:p:135:VAL:HG12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:387:THR:HG22	4:L:465:GLY:N	2.23	0.53
5:M:61:LEU:HD22	5:M:244:ILE:HG21	1.90	0.53
7:O:319:ILE:HG13	7:O:320:GLY:N	2.23	0.53
11:c:68:GLU:HG3	12:d:19:ARG:NH2	2.22	0.53
13:e:101:ARG:NE	13:e:104:PRO:HD2	2.24	0.53
4:L:362:ILE:HD12	4:L:430:VAL:HG13	1.87	0.53
4:L:362:ILE:CD1	4:L:430:VAL:CG1	2.82	0.53
7:O:140:LEU:HD11	7:O:198:TYR:OH	2.09	0.53
13:e:101:ARG:CZ	13:e:104:PRO:HD2	2.38	0.53
20:l:184:TYR:CA	23:o:36:GLU:HA	2.30	0.53
4:L:20:LEU:C	4:L:20:LEU:CD1	2.81	0.53
4:L:361:ASN:HA	4:L:431:THR:O	2.09	0.53
5:M:55:MET:HG3	5:M:56:PHE:CD2	2.44	0.53
5:M:453:LEU:HD12	5:M:453:LEU:C	2.33	0.53
10:Y:50:SER:HB3	10:Y:53:GLU:HG2	1.91	0.53
15:g:147:LEU:HD21	24:p:163:MET:HB2	1.90	0.53
21:m:17:THR:HB	22:n:68:GLU:OE1	2.09	0.53
4:L:124:PHE:HZ	4:L:252:MET:HB2	1.74	0.53
5:M:57:SER:CB	5:M:113:THR:HG22	2.39	0.53
5:M:73:LEU:HD23	5:M:103:GLN:NE2	2.23	0.53
6:N:120:GLN:HE22	6:N:174:GLN:CB	2.21	0.53
13:e:41:ILE:HG23	16:h:179:ILE:HD11	1.91	0.53
15:g:139:TYR:CD2	15:g:140:PHE:CD1	2.96	0.53
23:o:29:LEU:O	23:o:104:ARG:NH2	2.41	0.53
2:J:103:ILE:HG22	2:J:107:ASN:OD1	2.08	0.53
4:L:79:SER:CB	4:L:135:ASN:HB2	2.36	0.53
4:L:97:THR:HG21	4:L:125:LEU:HD22	1.90	0.53
4:L:128:MET:CG	4:L:251:THR:HB	2.36	0.53
5:M:15:THR:HG21	5:M:100:ILE:HD12	1.90	0.53
5:M:17:LEU:HD13	14:f:11:TRP:CZ3	2.43	0.53
7:O:170:LEU:HD13	7:O:187:TYR:CD2	2.44	0.53
8:U:78:GLY:O	8:U:79:ILE:C	2.51	0.53
12:d:109:TYR:O	12:d:110:ALA:C	2.51	0.53
13:e:40:TRP:CG	13:e:40:TRP:O	2.61	0.53
16:h:156:VAL:CG1	16:h:160:MET:HE3	2.39	0.53
20:l:55:TYR:O	20:l:104:PRO:HG3	2.09	0.53
4:L:501:ALA:HA	4:L:504:LEU:HD12	1.90	0.53
5:M:188:ALA:H	5:M:253:LEU:HD11	1.74	0.53
5:M:313:THR:HA	5:M:316:MET:HE3	1.89	0.53
5:M:314:MET:HE1	5:M:380:PHE:CD2	2.44	0.53
5:M:354:LEU:O	5:M:357:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:105:MET:CG	8:U:139:MET:HE1	2.39	0.53
17:i:108:ASP:OD2	24:p:18:PRO:CB	2.57	0.53
21:m:49:LEU:HD23	22:n:140:LEU:CD2	2.38	0.53
23:o:8:ARG:CB	23:o:16:GLU:HG2	2.30	0.53
2:J:2:ASN:HB3	2:J:120:LEU:O	2.09	0.53
5:M:73:LEU:HD21	5:M:100:ILE:HG12	1.90	0.53
5:M:213:HIS:O	5:M:217:PRO:HD3	2.09	0.53
5:M:348:LEU:HD12	5:M:415:GLN:NE2	2.24	0.53
13:e:41:ILE:CD1	16:h:174:PRO:HD2	2.39	0.53
17:i:106:PRO:HD2	23:o:64:ILE:CG2	2.38	0.53
21:m:85:LYS:O	21:m:85:LYS:HG2	2.09	0.53
22:n:39:TYR:CZ	22:n:43:LEU:HD11	2.44	0.53
22:n:136:GLU:OE2	22:n:167:TRP:NE1	2.42	0.53
1:D:52:MET:O	1:D:54:PRO:HD3	2.09	0.52
3:K:24:SER:O	3:K:90:VAL:HG13	2.10	0.52
4:L:108:MET:HB2	4:L:114:ILE:HD13	1.90	0.52
4:L:332:HIS:CD2	4:L:336:LYS:HG3	2.44	0.52
4:L:450:LEU:HG	4:L:454:ILE:HD12	1.91	0.52
5:M:310:MET:HG3	5:M:455:THR:CA	2.39	0.52
5:M:447:LEU:HD11	5:M:454:ILE:HG23	1.90	0.52
6:N:227:ILE:HA	6:N:230:ILE:CG2	2.39	0.52
7:O:66:ILE:O	27:O:401:ADP:H5'1	2.09	0.52
10:Y:65:ALA:O	10:Y:68:ILE:HG12	2.09	0.52
22:n:56:ASP:O	22:n:57:MET:C	2.50	0.52
4:L:228:GLY:O	4:L:229:LEU:CG	2.47	0.52
4:L:247:LEU:O	4:L:252:MET:HB3	2.09	0.52
4:L:385:PHE:HE2	18:j:73:PHE:HD1	1.56	0.52
4:L:536:ILE:HG23	4:L:537:THR:N	2.25	0.52
4:L:556:ILE:HD11	21:m:76:ILE:CG2	2.39	0.52
5:M:160:LEU:CD2	5:M:164:LEU:HD13	2.39	0.52
8:U:103:HIS:NE2	8:U:140:CYS:SG	2.82	0.52
13:e:101:ARG:HH21	13:e:104:PRO:HD2	1.74	0.52
14:f:49:ARG:CG	14:f:52:GLU:HG3	2.39	0.52
22:n:163:LEU:O	22:n:164:PRO:C	2.51	0.52
2:J:71:THR:O	2:J:76:GLU:HB2	2.08	0.52
4:L:586:LEU:HA	4:L:589:MET:CE	2.39	0.52
5:M:59:ASP:O	5:M:60:PRO:C	2.49	0.52
7:O:121:PRO:C	7:O:122:LYS:HG2	2.33	0.52
11:c:55:TRP:HE1	12:d:66:THR:HG21	1.75	0.52
2:J:162:GLY:O	2:J:166:ILE:HG12	2.10	0.52
3:K:14:LEU:HD22	25:K:101:3PE:H292	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:38:LEU:HG	3:K:42:ILE:CD1	2.39	0.52
4:L:123:LEU:HD22	4:L:150:MET:HG3	1.91	0.52
4:L:197:GLU:HB2	24:p:111:LYS:HE3	1.90	0.52
5:M:196:TRP:HE1	5:M:254:THR:HB	1.75	0.52
5:M:422:HIS:HB3	21:m:51:TYR:CE2	2.45	0.52
6:N:335:MET:CB	26:X:201:CDL:H642	2.40	0.52
7:O:168:VAL:CG2	7:O:241:TYR:OH	2.56	0.52
7:O:180:ARG:NH1	15:g:50:THR:HG21	2.25	0.52
7:O:220:LYS:HG3	7:O:221:LYS:N	2.24	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
8:U:114:ASP:O	8:U:115:GLN:C	2.53	0.52
12:d:1:MET:HG3	12:d:2:MET:N	2.24	0.52
13:e:34:HIS:O	13:e:38:LYS:HG3	2.08	0.52
17:i:31:ARG:O	17:i:32:GLU:C	2.51	0.52
20:l:169:GLU:C	20:l:171:GLY:N	2.55	0.52
4:L:522:PHE:HA	4:L:528:PHE:CZ	2.44	0.52
5:M:403:THR:HA	5:M:406:TYR:CE2	2.44	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:HD22	1.91	0.52
7:O:170:LEU:HD13	7:O:187:TYR:CG	2.44	0.52
8:U:133:ILE:CD1	22:n:7:PRO:HD3	2.39	0.52
26:h:201:CDL:H721	17:i:84:TYR:CD2	2.45	0.52
17:i:22:TRP:CE3	22:n:172:THR:HG22	2.45	0.52
21:m:125:PHE:HA	24:p:136:THR:HG21	1.91	0.52
2:J:92:LEU:O	2:J:96:VAL:HG23	2.10	0.52
2:J:99:GLU:O	2:J:103:ILE:HG13	2.10	0.52
3:K:36:MET:HE3	6:N:68:MET:HG3	1.92	0.52
3:K:57:MET:N	3:K:58:PRO:HD2	2.24	0.52
6:N:175:MET:HG2	6:N:219:LEU:CD2	2.40	0.52
12:d:94:ILE:HD13	16:h:152:LYS:HE3	1.92	0.52
18:j:99:ILE:HD12	23:o:107:ARG:HB2	1.91	0.52
23:o:31:PHE:HB3	23:o:34:ARG:HB3	1.90	0.52
4:L:108:MET:HB2	4:L:114:ILE:CD1	2.39	0.52
4:L:145:GLU:HB3	5:M:370:PRO:HG2	1.90	0.52
4:L:297:ASP:HB3	4:L:300:LYS:CG	2.39	0.52
4:L:483:PRO:HG2	4:L:486:LEU:HD13	1.91	0.52
4:L:496:LEU:C	4:L:496:LEU:CD1	2.79	0.52
5:M:84:LEU:HD21	5:M:95:TYR:HB3	1.90	0.52
6:N:335:MET:HB2	26:X:201:CDL:H642	1.90	0.52
16:h:87:THR:HG22	26:h:201:CDL:H512	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:128:HIS:O	23:o:85:HIS:NE2	2.41	0.52
2:J:168:GLU:OE2	6:N:1:MET:HG2	2.10	0.52
5:M:68:LEU:HG	5:M:234:ILE:HD11	1.92	0.52
5:M:72:LEU:HD11	5:M:233:ALA:HB1	1.91	0.52
5:M:115:LEU:HD21	5:M:176:LEU:CD2	2.37	0.52
5:M:346:ARG:O	5:M:419:LEU:HA	2.09	0.52
6:N:29:MET:HE2	6:N:141:ILE:HG12	1.92	0.52
8:U:128:PHE:CE1	8:U:148:ILE:HG23	2.45	0.52
8:U:133:ILE:HG23	8:U:134:ASP:N	2.25	0.52
15:g:123:LEU:HD12	24:p:98:VAL:CG1	2.40	0.52
4:L:202:MET:CE	4:L:265:PRO:HG3	2.33	0.52
4:L:324:LEU:HB3	4:L:395:ILE:HD11	1.90	0.52
4:L:513:MET:HE1	22:n:30:TRP:HB3	1.89	0.52
5:M:171:VAL:HG11	5:M:179:LEU:CD2	2.35	0.52
5:M:263:LEU:HD11	21:m:102:TYR:CD1	2.41	0.52
18:j:87:PRO:HG3	23:o:96:VAL:HG23	1.92	0.52
24:p:50:GLU:HG3	24:p:54:ARG:HH21	1.75	0.52
4:L:286:LEU:HG	4:L:290:ILE:CD1	2.40	0.52
4:L:533:ILE:HG23	4:L:534:HIS:HD2	1.74	0.52
5:M:139:GLN:HB3	5:M:222:GLU:CG	2.39	0.52
7:O:121:PRO:HB3	7:O:178:TYR:CE1	2.45	0.52
7:O:132:GLN:NE2	27:O:401:ADP:HN62	2.08	0.52
7:O:351:TRP:CZ3	11:c:41:TRP:CH2	2.97	0.52
17:i:108:ASP:OD2	24:p:18:PRO:HB2	2.10	0.52
22:n:143:GLU:O	22:n:143:GLU:HG2	2.10	0.52
5:M:103:GLN:O	5:M:107:ILE:HB	2.10	0.51
5:M:168:GLN:O	5:M:172:GLY:N	2.43	0.51
6:N:168:GLY:O	6:N:172:GLN:HG2	2.10	0.51
12:d:62:LEU:O	12:d:66:THR:OG1	2.22	0.51
12:d:87:ASP:O	12:d:88:HIS:C	2.51	0.51
13:e:44:ALA:HA	13:e:47:ILE:HG12	1.92	0.51
18:j:81:LEU:O	18:j:82:GLY:C	2.51	0.51
24:p:164:LEU:O	24:p:168:LYS:N	2.42	0.51
2:J:60:LEU:CD1	2:J:61:GLY:N	2.72	0.51
2:J:77:GLU:O	2:J:78:TYR:C	2.51	0.51
3:K:59:ILE:O	3:K:60:PRO:C	2.49	0.51
4:L:49:LEU:HB3	4:L:50:PRO:HD3	1.91	0.51
13:e:96:PRO:HB2	13:e:102:GLU:CD	2.36	0.51
17:i:77:ILE:HD13	17:i:80:TRP:CZ3	2.46	0.51
20:l:88:PRO:HB2	22:n:86:PRO:CB	2.40	0.51
4:L:569:LEU:O	4:L:573:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:151:PHE:CE2	6:N:291:PHE:HB2	2.44	0.51
7:O:66:ILE:CD1	7:O:218:ILE:HG12	2.40	0.51
25:Y:201:3PE:H122	25:Y:201:3PE:H231	1.91	0.51
17:i:106:PRO:HD2	23:o:64:ILE:HG21	1.93	0.51
3:K:22:PHE:HZ	6:N:61:VAL:HG11	1.75	0.51
4:L:295:GLN:OE1	22:n:78:GLN:NE2	2.41	0.51
4:L:427:ILE:HD11	19:k:69:PHE:CE1	2.46	0.51
4:L:578:THR:HG21	6:N:168:GLY:HA2	1.91	0.51
5:M:458:THR:HG21	24:p:148:ALA:HB1	1.92	0.51
14:f:37:PHE:HA	14:f:40:LYS:HB2	1.92	0.51
19:k:39:GLN:HE22	19:k:49:ASP:HB3	1.75	0.51
22:n:168:TRP:HD1	22:n:169:HIS:CE1	2.27	0.51
23:o:89:TYR:O	23:o:90:CYS:C	2.52	0.51
5:M:11:LEU:O	5:M:15:THR:HG23	2.09	0.51
5:M:20:PRO:HB3	5:M:89:ASN:ND2	2.25	0.51
5:M:129:THR:CG2	5:M:235:LEU:HD11	2.40	0.51
11:c:47:SER:HB2	12:d:59:HIS:HD2	1.76	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
25:m:201:3PE:H332	25:m:202:3PE:H341	1.93	0.51
23:o:39:MET:HE1	23:o:57:ASP:O	2.11	0.51
4:L:161:ARG:NE	4:L:163:ASP:HB2	2.26	0.51
4:L:249:SER:HB2	4:L:340:PHE:CE2	2.46	0.51
4:L:536:ILE:HD11	4:L:540:LYS:HD2	1.93	0.51
4:L:595:ILE:O	4:L:599:ILE:HG13	2.11	0.51
5:M:251:ASP:N	5:M:252:PRO:HD2	2.26	0.51
5:M:388:TRP:NE1	21:m:109:ARG:HD2	2.26	0.51
12:d:28:ASP:O	12:d:29:PRO:C	2.52	0.51
16:h:159:LEU:HD23	16:h:163:ARG:HH12	1.75	0.51
19:k:34:PRO:HD2	19:k:59:TYR:CG	2.46	0.51
2:J:22:LYS:HE2	3:K:18:GLY:O	2.10	0.51
4:L:13:ILE:CD1	25:i:201:3PE:H2C2	2.32	0.51
4:L:60:GLU:HG3	4:L:83:ASP:HA	1.93	0.51
4:L:530:PRO:O	4:L:534:HIS:HB2	2.11	0.51
4:L:590:SER:HB2	10:Y:45:LEU:HD11	1.91	0.51
5:M:31:SER:HA	5:M:34:ILE:CG1	2.41	0.51
5:M:304:GLN:HA	5:M:309:PHE:CE1	2.45	0.51
6:N:240:MET:HE2	6:N:326:PHE:CZ	2.45	0.51
9:X:151:ASN:ND2	13:e:51:ARG:HH11	2.08	0.51
17:i:10:LEU:HA	17:i:13:GLN:HB3	1.91	0.51
20:l:158:PRO:HD3	23:o:22:ILE:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:HG23	1:D:61:TRP:CE2	2.46	0.51
2:J:3:ASN:OD1	2:J:3:ASN:N	2.43	0.51
5:M:127:ILE:HG12	6:N:254:LEU:HD21	1.93	0.51
6:N:246:LEU:HD11	25:N:401:3PE:H3A2	1.91	0.51
6:N:313:MET:HG2	7:O:305:LEU:HD22	1.93	0.51
7:O:246:LEU:HD11	7:O:257:VAL:HG22	1.93	0.51
12:d:40:CYS:SG	25:d:201:3PE:H252	2.51	0.51
2:J:169:ILE:HD11	6:N:41:ILE:HG22	1.92	0.51
4:L:404:THR:HG22	4:L:405:ASN:H	1.75	0.51
5:M:178:ILE:HG12	24:p:82:VAL:HG11	1.93	0.51
5:M:354:LEU:O	5:M:355:MET:C	2.52	0.51
7:O:289:TRP:HA	7:O:289:TRP:CE3	2.46	0.51
12:d:108:THR:HG23	12:d:110:ALA:HB3	1.93	0.51
13:e:70:TYR:OH	13:e:74:ARG:HD3	2.11	0.51
14:f:49:ARG:CG	14:f:52:GLU:CG	2.88	0.51
15:g:115:TRP:HA	15:g:118:ARG:HH11	1.75	0.51
21:m:45:ARG:CZ	22:n:140:LEU:HD11	2.41	0.51
25:m:201:3PE:H261	25:m:201:3PE:H3B1	1.93	0.51
2:J:98:MET:O	2:J:101:PHE:HB3	2.11	0.51
4:L:477:ILE:HG13	23:o:91:GLU:OE2	2.11	0.51
6:N:45:ILE:HA	6:N:52:SER:OG	2.11	0.51
8:U:119:ILE:CD1	8:U:138:LEU:HB2	2.40	0.51
16:h:73:PHE:CE2	16:h:74:TYR:CE1	2.98	0.51
4:L:362:ILE:CD1	4:L:430:VAL:HG13	2.41	0.50
4:L:383:MET:CB	4:L:386:LEU:HD12	2.30	0.50
4:L:516:ALA:HB1	4:L:520:SER:CB	2.41	0.50
4:L:525:LEU:HD21	22:n:77:PRO:CB	2.39	0.50
7:O:62:VAL:HG21	7:O:73:LEU:HD23	1.93	0.50
7:O:182:GLN:O	7:O:183:CYS:C	2.54	0.50
8:U:86:VAL:HG13	19:k:54:ASN:ND2	2.26	0.50
10:Y:90:LEU:O	10:Y:94:ILE:HG12	2.11	0.50
13:e:101:ARG:NH2	13:e:103:GLU:HA	2.26	0.50
20:l:117:VAL:HG12	20:l:118:ASP:N	2.25	0.50
24:p:49:ARG:O	24:p:52:ILE:HB	2.11	0.50
2:J:77:GLU:OE1	3:K:87:THR:C	2.54	0.50
4:L:451:MET:O	4:L:452:ASN:C	2.53	0.50
4:L:483:PRO:HB2	4:L:485:PHE:CE1	2.46	0.50
5:M:4:ILE:HD11	5:M:41:LEU:HD21	1.92	0.50
5:M:249:ILE:HG22	5:M:250:LEU:N	2.26	0.50
17:i:22:TRP:CZ2	22:n:172:THR:HG22	2.46	0.50
17:i:103:ARG:NH1	23:o:67:LEU:HD22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:87:ASP:OD1	20:l:88:PRO:HD2	2.11	0.50
24:p:5:TRP:HZ3	24:p:10:TYR:O	1.93	0.50
24:p:113:CYS:O	24:p:113:CYS:SG	2.69	0.50
2:j:12:PHE:CZ	3:k:42:ILE:HD12	2.45	0.50
4:l:349:SER:HB2	4:l:443:ILE:HG23	1.93	0.50
5:m:118:PHE:O	5:m:122:PHE:HB2	2.11	0.50
6:n:36:SER:HB2	6:n:134:GLN:HE22	1.76	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
7:o:326:ARG:NH2	15:g:56:ASP:OD1	2.45	0.50
8:u:122:MET:HA	8:u:122:MET:HE2	1.91	0.50
8:u:124:ASP:OD1	22:n:25:ARG:NH2	2.41	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
26:h:201:CDL:H132	26:h:201:CDL:H172	1.92	0.50
21:m:45:ARG:NE	22:n:140:LEU:HD11	2.27	0.50
1:d:55:SER:HB2	4:l:575:THR:HG23	1.93	0.50
2:j:55:VAL:HB	3:k:41:PHE:CE2	2.47	0.50
4:l:21:ILE:HG12	4:l:27:ILE:HG23	1.93	0.50
5:m:127:ILE:CG1	6:n:254:LEU:HD21	2.41	0.50
5:m:275:ILE:CD1	5:m:288:TYR:CG	2.84	0.50
5:m:309:PHE:HB2	5:m:458:THR:HG21	1.93	0.50
5:m:370:PRO:CA	5:m:375:LEU:HD22	2.40	0.50
6:n:25:ASN:HB3	13:e:15:ASP:CG	2.37	0.50
6:n:189:TRP:HB2	6:n:204:ASN:HD21	1.77	0.50
7:o:135:LEU:HD13	27:o:401:ADP:C5	2.46	0.50
8:u:125:GLU:OE2	18:j:44:TYR:HE1	1.95	0.50
25:m:201:3PE:H3G2	25:m:201:3PE:H2D2	1.93	0.50
4:l:117:PHE:HE1	4:l:243:VAL:CG2	2.23	0.50
4:l:365:ILE:CD1	4:l:366:MET:HE2	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:248:ILE:HG13	5:m:249:ILE:N	2.25	0.50
5:m:294:MET:HE3	5:m:319:HIS:HD2	1.76	0.50
8:u:90:TYR:HD2	8:u:93:ILE:H	1.59	0.50
17:i:10:LEU:HD12	17:i:13:GLN:HB3	1.94	0.50
20:l:49:ALA:HA	20:l:59:VAL:HG13	1.93	0.50
23:o:39:MET:CE	23:o:58:TYR:HA	2.42	0.50
3:k:73:VAL:HG21	6:n:38:LEU:HD22	1.93	0.50
4:l:539:MET:SD	21:m:11:LEU:HD21	2.52	0.50
5:m:328:CYS:SG	5:m:436:LEU:HD21	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:371:PRO:HG2	25:M:502:3PE:H2F1	1.93	0.50
8:U:74:LEU:HB3	8:U:79:ILE:HG13	1.93	0.50
8:U:125:GLU:OE2	18:j:44:TYR:CE1	2.65	0.50
8:U:142:GLN:O	8:U:145:VAL:N	2.43	0.50
2:J:16:CYS:SG	3:K:11:ALA:HB1	2.52	0.50
4:L:60:GLU:O	4:L:61:TYR:CD1	2.65	0.50
4:L:109:HIS:O	4:L:110:SER:HB2	2.11	0.50
5:M:4:ILE:HG22	5:M:107:ILE:CD1	2.32	0.50
6:N:25:ASN:HB3	13:e:15:ASP:OD2	2.10	0.50
6:N:258:THR:HG23	6:N:336:THR:HG22	1.93	0.50
7:O:211:VAL:HB	7:O:212:PRO:HD3	1.92	0.50
8:U:93:ILE:HD11	8:U:118:ILE:HD11	1.92	0.50
9:X:166:ARG:HB3	16:h:150:ARG:HE	1.77	0.50
10:Y:12:HIS:NE2	10:Y:127:PHE:HZ	2.09	0.50
13:e:93:THR:O	13:e:94:PRO:C	2.55	0.50
15:g:53:TRP:H	15:g:53:TRP:HD1	1.56	0.50
19:k:34:PRO:CG	19:k:59:TYR:CD1	2.94	0.50
3:K:38:LEU:HG	3:K:42:ILE:HD11	1.93	0.50
4:L:149:ILE:HG21	5:M:364:LEU:CD2	2.42	0.50
5:M:63:THR:N	5:M:64:PRO:HD2	2.27	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
13:e:42:GLU:HG2	16:h:176:LYS:HE2	1.94	0.50
25:m:201:3PE:H241	25:m:201:3PE:C2	2.42	0.50
22:n:114:MET:O	22:n:115:TYR:C	2.52	0.50
4:L:141:PHE:CD2	5:M:370:PRO:CB	2.94	0.50
4:L:354:GLN:O	4:L:354:GLN:HG2	2.12	0.50
5:M:231:LEU:CD1	5:M:235:LEU:CD1	2.85	0.50
5:M:432:ARG:HA	5:M:435:THR:HG22	1.94	0.50
6:N:133:TRP:CG	6:N:133:TRP:O	2.63	0.50
8:U:105:MET:HG3	8:U:139:MET:HE1	1.94	0.50
9:X:151:ASN:CG	13:e:51:ARG:HH11	2.20	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	0.49
5:M:122:PHE:CE1	5:M:238:LEU:HG	2.46	0.49
5:M:207:MET:SD	5:M:240:SER:HA	2.52	0.49
5:M:441:MET:HG3	5:M:445:ILE:HD12	1.94	0.49
7:O:341:PRO:HB2	11:c:34:PRO:HB3	1.94	0.49
10:Y:115:MET:HE1	25:Y:201:3PE:C21	2.42	0.49
23:o:22:ILE:O	23:o:105:GLU:HG2	2.12	0.49
24:p:74:ILE:O	24:p:75:THR:C	2.54	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:184:HIS:CD2	5:M:249:ILE:HG23	2.47	0.49
7:O:48:LYS:H	7:O:51:LYS:HE3	1.75	0.49
7:O:136:TYR:OH	7:O:191:LYS:HA	2.11	0.49
7:O:319:ILE:HD12	7:O:324:GLY:HA3	1.94	0.49
22:n:20:TYR:CE2	22:n:24:LEU:CD1	2.91	0.49
22:n:96:CYS:SG	22:n:97:TYR:CZ	3.05	0.49
4:L:217:LEU:HD13	4:L:273:ILE:HG23	1.94	0.49
4:L:316:THR:CG2	4:L:325:ALA:CB	2.89	0.49
6:N:62:THR:HG21	6:N:114:TRP:CD1	2.47	0.49
7:O:170:LEU:HD21	7:O:184:VAL:HG22	1.95	0.49
7:O:276:LEU:HD11	7:O:278:TYR:CE2	2.47	0.49
4:L:9:LEU:HD21	25:i:201:3PE:C2A	2.41	0.49
4:L:173:LEU:HD23	25:L:702:3PE:C32	2.30	0.49
4:L:393:ASP:OD1	4:L:393:ASP:C	2.56	0.49
5:M:139:GLN:HG3	5:M:140:THR:N	2.27	0.49
5:M:348:LEU:HD12	5:M:415:GLN:HE22	1.77	0.49
6:N:230:ILE:HG21	6:N:296:LEU:HD11	1.94	0.49
7:O:132:GLN:CD	27:O:401:ADP:HN62	2.20	0.49
7:O:237:ILE:CG2	7:O:241:TYR:CE2	2.95	0.49
16:h:129:PRO:HG3	24:p:66:ARG:CZ	2.42	0.49
17:i:83:HIS:CD2	24:p:37:TYR:CE2	3.01	0.49
20:l:81:ARG:HD3	20:l:85:GLU:OE2	2.13	0.49
20:l:122:THR:O	21:m:6:TYR:CE1	2.65	0.49
1:D:35:ARG:HE	15:g:59:PRO:CD	2.24	0.49
4:L:264:HIS:HA	4:L:267:THR:OG1	2.12	0.49
4:L:399:ILE:HG22	4:L:409:LEU:HD13	1.93	0.49
5:M:278:ARG:HH22	20:l:108:ASP:CG	2.21	0.49
5:M:285:LEU:HD22	5:M:410:MET:SD	2.53	0.49
7:O:49:THR:HG21	7:O:151:LEU:HG	1.93	0.49
13:e:34:HIS:CE1	13:e:38:LYS:HD2	2.47	0.49
17:i:90:MET:O	17:i:91:ALA:C	2.53	0.49
19:k:47:LEU:CD1	22:n:43:LEU:HD23	2.42	0.49
20:l:101:TRP:HE1	21:m:62:ASP:HA	1.76	0.49
22:n:145:SER:HB2	22:n:146:PRO:HD2	1.94	0.49
4:L:23:MET:HE1	26:L:704:CDL:C19	2.43	0.49
4:L:445:GLU:CB	4:L:450:LEU:HD23	2.37	0.49
4:L:496:LEU:HA	4:L:499:LEU:HB2	1.94	0.49
7:O:352:ILE:HG21	12:d:52:PRO:HG2	1.94	0.49
21:m:127:ILE:HG22	24:p:136:THR:HG23	1.95	0.49
5:M:193:ASN:HA	5:M:253:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:420:THR:HG21	5:M:423:MET:HG2	1.93	0.49
6:N:231:SER:HA	6:N:300:THR:HA	1.93	0.49
7:O:72:LYS:O	7:O:73:LEU:C	2.56	0.49
7:O:146:ALA:HB2	7:O:159:LEU:HD21	1.95	0.49
7:O:260:SER:O	7:O:263:ALA:HB3	2.13	0.49
9:X:153:VAL:O	9:X:155:GLU:HG3	2.12	0.49
9:X:170:TRP:CZ3	26:X:201:CDL:H552	2.47	0.49
13:e:36:PHE:O	13:e:39:GLU:N	2.45	0.49
18:j:45:ARG:HD3	19:k:57:TRP:CD1	2.47	0.49
1:D:51:VAL:HG21	1:D:58:THR:HG22	1.95	0.49
4:L:67:HIS:HE2	4:L:69:VAL:C	2.21	0.49
4:L:590:SER:HB2	10:Y:45:LEU:CD1	2.42	0.49
5:M:5:ILE:HG13	5:M:6:LEU:N	2.28	0.49
5:M:248:ILE:CG1	5:M:249:ILE:HD12	2.39	0.49
8:U:94:ASP:OD1	8:U:95:PRO:HD2	2.12	0.49
11:c:62:HIS:O	11:c:66:VAL:HG23	2.12	0.49
14:f:25:TYR:OH	14:f:29:LYS:HE3	2.13	0.49
4:L:68:TRP:CE3	4:L:76:LEU:HD21	2.47	0.49
4:L:427:ILE:HD11	19:k:69:PHE:HE1	1.78	0.49
4:L:41:LYS:HG3	4:L:98:TRP:CH2	2.45	0.49
5:M:1:MET:HB2	5:M:52:PHE:CE2	2.47	0.49
5:M:227:GLY:HA2	5:M:230:ILE:HG22	1.95	0.49
7:O:256:LEU:HB3	7:O:258:TYR:CE1	2.48	0.49
10:Y:143:VAL:HG23	16:h:157:ARG:O	2.13	0.49
15:g:109:ASP:HB2	15:g:114:GLU:HB3	1.94	0.49
21:m:75:ASN:OD1	21:m:79:ASN:ND2	2.46	0.49
22:n:20:TYR:OH	22:n:45:ARG:HB2	2.12	0.49
22:n:81:ILE:HD12	22:n:87:GLY:O	2.12	0.49
22:n:114:MET:HG3	22:n:115:TYR:HD2	1.78	0.49
2:J:22:LYS:CD	3:K:23:ARG:HG2	2.40	0.48
4:L:101:MET:HE1	4:L:121:LEU:CB	2.43	0.48
4:L:227:PHE:CD2	4:L:283:LEU:HD23	2.48	0.48
4:L:361:ASN:O	4:L:361:ASN:CG	2.54	0.48
5:M:134:THR:O	5:M:142:ARG:CD	2.59	0.48
5:M:348:LEU:HB2	5:M:415:GLN:OE1	2.13	0.48
13:e:94:PRO:HB3	13:e:98:HIS:CD2	2.48	0.48
16:h:96:ALA:O	24:p:63:TYR:CE1	2.62	0.48
16:h:179:ILE:HG22	16:h:180:ASP:N	2.28	0.48
17:i:69:LEU:HG	17:i:71:ALA:HB3	1.94	0.48
19:k:38:VAL:CG1	22:n:39:TYR:HB2	2.43	0.48
1:D:36:GLN:HG3	1:D:38:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:56:HIS:CA	23:o:74:PHE:CD1	2.95	0.48
4:L:144:TRP:HH2	4:L:256:GLY:HA2	1.78	0.48
4:L:150:MET:HE3	26:L:704:CDL:H732	1.93	0.48
4:L:350:LEU:HD23	4:L:443:ILE:HD11	1.96	0.48
4:L:372:CYS:SG	4:L:454:ILE:HG22	2.54	0.48
4:L:424:MET:HE2	4:L:502:LEU:CA	2.43	0.48
5:M:351:VAL:HA	16:h:59:PRO:HB3	1.96	0.48
7:O:78:ALA:HB2	7:O:85:HIS:HB2	1.95	0.48
7:O:135:LEU:CD1	27:O:401:ADP:C6	2.96	0.48
7:O:355:LYS:O	12:d:59:HIS:HE1	1.96	0.48
17:i:19:ARG:HH11	22:n:173:ARG:NH2	2.11	0.48
22:n:51:HIS:HB3	22:n:63:LEU:HD13	1.95	0.48
5:M:166:LEU:HD21	5:M:170:HIS:CE1	2.48	0.48
5:M:190:TRP:CE2	10:Y:89:PRO:HG2	2.48	0.48
5:M:311:GLY:HA2	5:M:314:MET:CE	2.42	0.48
7:O:59:VAL:HG22	7:O:157:VAL:CG2	2.43	0.48
20:l:167:TYR:OH	20:l:176:LYS:O	2.14	0.48
4:L:152:PHE:HE1	5:M:412:ILE:HD11	1.79	0.48
4:L:296:ASN:ND2	4:L:425:ARG:HH21	2.12	0.48
4:L:316:THR:HG21	4:L:325:ALA:HA	1.95	0.48
4:L:402:CYS:SG	4:L:403:ASN:N	2.87	0.48
5:M:59:ASP:OD1	5:M:245:ARG:NH2	2.47	0.48
5:M:123:GLU:CB	6:N:255:PRO:HG2	2.44	0.48
6:N:321:LYS:HD2	12:d:49:ARG:NE	2.29	0.48
24:p:5:TRP:CZ3	24:p:10:TYR:O	2.66	0.48
2:J:5:ILE:HB	2:J:120:LEU:HD13	1.96	0.48
2:J:88:ILE:HD11	3:K:23:ARG:HH12	1.77	0.48
5:M:216:LEU:HD12	5:M:236:LEU:CD2	2.39	0.48
5:M:307:TRP:CE3	5:M:383:MET:CE	2.97	0.48
6:N:81:LEU:HD23	13:e:60:PHE:HE1	1.78	0.48
16:h:73:PHE:O	16:h:77:LEU:N	2.46	0.48
21:m:122:ASP:O	21:m:123:ARG:C	2.53	0.48
1:D:42:GLU:HA	1:D:45:GLU:HG2	1.96	0.48
2:J:91:PHE:O	2:J:94:LEU:HB3	2.13	0.48
2:J:169:ILE:CD1	6:N:42:PRO:HA	2.44	0.48
4:L:274:LEU:O	4:L:277:MET:HG2	2.14	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:313:THR:HA	5:M:316:MET:CE	2.43	0.48
6:N:4:ILE:HG23	6:N:5:THR:N	2.29	0.48
6:N:338:PRO:HG3	26:X:201:CDL:H611	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:170:TRP:CE3	26:X:201:CDL:H521	2.47	0.48
16:h:73:PHE:HE2	16:h:74:TYR:HE1	1.62	0.48
20:l:38:PRO:CB	21:m:75:ASN:ND2	2.70	0.48
2:J:106:LEU:HA	2:J:109:TYR:HB2	1.95	0.48
4:L:141:PHE:HD1	4:L:182:PHE:CD2	2.31	0.48
4:L:319:MET:O	4:L:319:MET:HG2	2.13	0.48
5:M:177:MET:HE1	24:p:86:TYR:CE1	2.49	0.48
5:M:422:HIS:CE1	5:M:425:ASN:OD1	2.66	0.48
6:N:227:ILE:CA	6:N:230:ILE:HG22	2.38	0.48
7:O:245:PHE:CE1	7:O:249:MET:HG3	2.48	0.48
8:U:128:PHE:HZ	8:U:148:ILE:HD12	1.76	0.48
13:e:47:ILE:HG13	13:e:47:ILE:O	2.12	0.48
13:e:105:ARG:O	13:e:106:PRO:C	2.56	0.48
17:i:69:LEU:O	17:i:72:VAL:HG22	2.13	0.48
17:i:69:LEU:HD23	17:i:72:VAL:HG13	1.95	0.48
23:o:87:TRP:NE1	23:o:91:GLU:OE1	2.46	0.48
2:J:20:ALA:C	2:J:22:LYS:H	2.21	0.48
2:J:28:GLY:O	2:J:31:GLY:N	2.46	0.48
3:K:12:PHE:CD1	6:N:72:LEU:HD22	2.49	0.48
4:L:435:PRO:O	19:k:58:ARG:HD2	2.14	0.48
4:L:496:LEU:HD12	4:L:497:GLY:CA	2.44	0.48
4:L:597:LEU:HD21	10:Y:37:ILE:HD12	1.96	0.48
5:M:344:MET:CE	21:m:59:HIS:NE2	2.74	0.48
6:N:146:TYR:CE1	6:N:198:PRO:HG2	2.49	0.48
17:i:83:HIS:CD2	24:p:37:TYR:HE2	2.31	0.48
19:k:69:PHE:CE1	19:k:73:ILE:HD11	2.48	0.48
20:l:167:TYR:HD2	20:l:168:LEU:CD1	2.19	0.48
22:n:144:THR:HG23	22:n:144:THR:O	2.13	0.48
5:M:269:MET:HE3	5:M:399:ASN:HB3	1.96	0.48
5:M:369:LEU:HD12	5:M:370:PRO:HD2	1.95	0.48
15:g:117:ARG:NH2	24:p:10:TYR:OH	2.47	0.48
19:k:18:GLY:O	19:k:19:LYS:C	2.55	0.48
21:m:49:LEU:HD23	22:n:140:LEU:HD21	1.95	0.48
6:N:189:TRP:CZ3	6:N:282:MET:HE3	2.49	0.48
7:O:76:GLU:HG3	7:O:266:PRO:CG	2.44	0.48
12:d:100:ASP:HB3	16:h:159:LEU:HD21	1.95	0.48
17:i:90:MET:SD	17:i:97:ILE:HD11	2.54	0.48
20:l:48:ARG:HH22	20:l:64:PRO:HD2	1.79	0.48
4:L:121:LEU:HD22	4:L:246:LEU:CD2	2.24	0.47
5:M:154:LEU:HD13	6:N:287:LEU:CD2	2.44	0.47
9:X:147:ARG:HH22	13:e:39:GLU:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:119:VAL:O	12:d:120:ARG:C	2.55	0.47
21:m:124:LYS:C	21:m:126:ASN:N	2.70	0.47
25:m:201:3PE:H361	25:m:202:3PE:H341	1.95	0.47
22:n:156:PRO:HD2	22:n:158:ARG:NH1	2.29	0.47
3:K:29:THR:O	3:K:32:CYS:N	2.47	0.47
4:L:3:ILE:HG22	4:L:49:LEU:HD21	1.96	0.47
4:L:54:PHE:CZ	4:L:84:PHE:HB2	2.49	0.47
5:M:94:LEU:O	5:M:98:MET:HG2	2.14	0.47
5:M:176:LEU:HD13	5:M:245:ARG:HH11	1.79	0.47
5:M:336:ARG:HH21	5:M:429:SER:HA	1.78	0.47
7:O:68:SER:C	7:O:70:LYS:N	2.70	0.47
7:O:71:ASN:O	7:O:75:LYS:HE3	2.14	0.47
17:i:79:MET:O	17:i:80:TRP:C	2.57	0.47
4:L:31:ASN:HD22	4:L:34:LEU:HB2	1.80	0.47
5:M:7:PRO:HG3	14:f:20:PHE:HA	1.94	0.47
5:M:147:ILE:HG13	6:N:298:TYR:OH	2.14	0.47
6:N:89:GLN:H	6:N:89:GLN:CD	2.22	0.47
7:O:314:LEU:HD12	7:O:315:PRO:HD3	1.93	0.47
13:e:94:PRO:HB3	13:e:98:HIS:CG	2.48	0.47
17:i:32:GLU:HG3	22:n:115:TYR:HA	1.96	0.47
22:n:81:ILE:HD11	22:n:87:GLY:O	2.14	0.47
22:n:96:CYS:SG	22:n:97:TYR:CE1	3.04	0.47
4:L:433:THR:CG2	4:L:434:LYS:N	2.78	0.47
4:L:576:LEU:HA	4:L:579:ASN:ND2	2.29	0.47
26:L:704:CDL:H161	5:M:361:MET:HE1	1.96	0.47
25:L:705:3PE:H322	25:L:705:3PE:H351	1.67	0.47
5:M:51:ASN:O	16:h:135:LYS:HD2	2.13	0.47
5:M:131:ILE:CD1	6:N:302:LEU:HD21	2.45	0.47
5:M:310:MET:CE	5:M:459:MET:SD	3.02	0.47
5:M:370:PRO:CA	5:M:375:LEU:HD23	2.42	0.47
12:d:8:HIS:O	12:d:10:PRO:HD3	2.14	0.47
16:h:91:ILE:O	24:p:56:HIS:NE2	2.48	0.47
19:k:84:PHE:CZ	19:k:88:LEU:HD22	2.49	0.47
3:K:69:CYS:O	3:K:70:GLU:C	2.57	0.47
4:L:277:MET:SD	4:L:318:GLY:HA2	2.54	0.47
4:L:437:PHE:HB2	4:L:438:PRO:HD2	1.96	0.47
5:M:78:MET:HG2	5:M:432:ARG:HG3	1.97	0.47
6:N:1:MET:HE1	6:N:43:MET:SD	2.54	0.47
7:O:52:LYS:HD3	7:O:152:SER:O	2.14	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	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:73:TYR:O	12:d:77:LYS:HB2	2.14	0.47
14:f:37:PHE:O	14:f:38:ARG:C	2.57	0.47
25:i:201:3PE:O22	25:i:201:3PE:H11	2.13	0.47
4:L:63:ILE:HG23	17:i:97:ILE:CD1	2.45	0.47
4:L:237:MET:HE1	4:L:248:HIS:HB2	1.96	0.47
4:L:420:ALA:HB1	4:L:498:PHE:CD2	2.50	0.47
6:N:120:GLN:O	6:N:176:ARG:NH2	2.48	0.47
7:O:116:LYS:HA	7:O:119:ASP:OD1	2.13	0.47
8:U:87:LEU:CB	8:U:98:LEU:CD2	2.83	0.47
8:U:133:ILE:HD13	22:n:7:PRO:HD3	1.95	0.47
10:Y:142:LYS:O	10:Y:143:VAL:C	2.57	0.47
17:i:19:ARG:NH1	22:n:173:ARG:HH21	2.11	0.47
17:i:123:PHE:CE2	23:o:61:HIS:HD2	2.32	0.47
20:l:38:PRO:CG	21:m:71:ALA:HB2	2.45	0.47
20:l:44:THR:CG2	20:l:47:GLU:HG3	2.45	0.47
20:l:48:ARG:NH2	20:l:64:PRO:HD2	2.29	0.47
21:m:28:GLU:O	21:m:31:ARG:HB3	2.14	0.47
21:m:124:LYS:C	21:m:126:ASN:H	2.21	0.47
24:p:6:ASP:C	24:p:8:ASP:N	2.69	0.47
1:D:37:TRP:CE3	5:M:140:THR:HA	2.50	0.47
2:J:59:TYR:CD1	2:J:63:MET:SD	3.07	0.47
3:K:75:LEU:O	3:K:79:VAL:HG23	2.15	0.47
4:L:183:ILE:HD13	5:M:400:ILE:HD13	1.96	0.47
4:L:390:TYR:HE2	18:j:68:TRP:HH2	1.61	0.47
4:L:441:ILE:HD13	18:j:48:PRO:HD3	1.97	0.47
4:L:552:LEU:HD22	4:L:553:LEU:HD12	1.97	0.47
26:L:704:CDL:H372	16:h:75:LEU:CD1	2.45	0.47
5:M:57:SER:OG	5:M:113:THR:HG22	2.15	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:430:HIS:HB3	15:g:73:GLY:HA3	1.97	0.47
5:M:445:ILE:HG23	25:M:502:3PE:H292	1.97	0.47
6:N:1:MET:O	6:N:2:ASN:C	2.54	0.47
6:N:26:LEU:O	6:N:29:MET:N	2.47	0.47
15:g:121:GLU:OE2	24:p:10:TYR:CZ	2.68	0.47
16:h:96:ALA:C	24:p:63:TYR:HE1	2.22	0.47
20:l:42:PRO:HB2	20:l:48:ARG:HG2	1.97	0.47
24:p:65:HIS:O	24:p:66:ARG:C	2.57	0.47
3:K:57:MET:C	3:K:60:PRO:HD2	2.39	0.47
4:L:23:MET:HE1	26:L:704:CDL:H191	1.96	0.47
4:L:348:HIS:HD2	8:U:69:SER:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:122:PHE:HZ	5:M:206:LYS:HD3	1.75	0.47
7:O:204:VAL:HG23	7:O:255:VAL:HG13	1.97	0.47
8:U:120:MET:HE1	22:n:24:LEU:CD1	2.44	0.47
8:U:130:ILE:HG21	8:U:138:LEU:HD11	1.97	0.47
9:X:172:VAL:HG23	12:d:30:ARG:NH1	2.30	0.47
11:c:46:LEU:O	11:c:50:ALA:CB	2.63	0.47
14:f:38:ARG:HD3	14:f:56:TRP:NE1	2.30	0.47
15:g:121:GLU:OE2	24:p:10:TYR:CE2	2.68	0.47
20:l:118:ASP:OD1	20:l:119:THR:N	2.47	0.47
21:m:14:LEU:HD12	21:m:15:PRO:HD2	1.96	0.47
21:m:18:LEU:HD11	22:n:72:TRP:CB	2.45	0.47
22:n:57:MET:O	22:n:58:MET:C	2.58	0.47
24:p:93:ARG:NH2	24:p:150:TYR:CE1	2.83	0.47
3:K:29:THR:O	3:K:30:LEU:C	2.56	0.47
4:L:357:ARG:NH2	22:n:78:GLN:O	2.48	0.47
4:L:546:LEU:HD22	21:m:72:ARG:NH2	2.29	0.47
5:M:16:TRP:CE3	25:d:201:3PE:H12	2.50	0.47
5:M:196:TRP:HD1	5:M:250:LEU:HB2	1.80	0.47
7:O:129:TYR:CE2	7:O:183:CYS:HB3	2.50	0.47
7:O:135:LEU:HB3	7:O:139:ARG:NH1	2.26	0.47
16:h:55:PHE:HB2	17:i:28:LEU:HD21	1.95	0.47
24:p:29:PRO:O	24:p:33:LEU:HD13	2.14	0.47
5:M:49:TYR:OH	5:M:457:LEU:HG	2.15	0.47
5:M:165:ILE:HD11	6:N:264:TRP:HE1	1.80	0.47
6:N:307:THR:HG22	6:N:308:ASN:N	2.30	0.47
7:O:78:ALA:CB	7:O:85:HIS:HB2	2.45	0.47
7:O:256:LEU:HD13	7:O:258:TYR:OH	2.15	0.47
10:Y:116:GLY:O	10:Y:120:MET:HB2	2.15	0.47
12:d:59:HIS:CE1	12:d:60:ARG:HG3	2.50	0.47
20:l:127:ASP:O	20:l:128:VAL:C	2.58	0.47
1:D:47:PHE:CE2	6:N:305:PHE:HZ	2.33	0.46
4:L:73:SER:CB	24:p:100:GLN:HE21	2.25	0.46
4:L:86:SER:OG	4:L:133:SER:HB3	2.15	0.46
5:M:232:ALA:HA	5:M:236:LEU:HD12	1.97	0.46
7:O:232:ALA:O	7:O:235:GLN:HB3	2.14	0.46
12:d:78:ARG:O	12:d:81:TYR:N	2.48	0.46
12:d:116:PHE:HB2	24:p:157:ALA:HB1	1.96	0.46
18:j:51:THR:O	18:j:52:ARG:C	2.53	0.46
22:n:35:ASP:OD1	22:n:36:LYS:N	2.47	0.46
22:n:50:GLU:O	22:n:51:HIS:C	2.55	0.46
24:p:43:TRP:O	24:p:44:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:13:SER:O	3:K:17:LEU:HG	2.15	0.46
4:L:172:ILE:O	4:L:176:ARG:HG2	2.16	0.46
4:L:277:MET:CG	4:L:318:GLY:HA2	2.45	0.46
4:L:302:ILE:HG22	4:L:340:PHE:CZ	2.49	0.46
4:L:405:ASN:OD1	20:l:148:HIS:CE1	2.69	0.46
4:L:474:PRO:HD2	23:o:67:LEU:HD21	1.96	0.46
4:L:589:MET:O	4:L:592:LEU:HB3	2.16	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
7:O:62:VAL:HG13	7:O:62:VAL:O	2.15	0.46
7:O:82:GLY:O	7:O:155:GLN:NE2	2.48	0.46
7:O:200:PRO:HB3	7:O:252:MET:SD	2.55	0.46
12:d:51:ARG:O	12:d:52:PRO:C	2.55	0.46
14:f:16:VAL:O	14:f:17:PRO:C	2.57	0.46
14:f:37:PHE:CZ	24:p:83:LEU:HD13	2.50	0.46
14:f:38:ARG:O	14:f:56:TRP:NE1	2.48	0.46
16:h:73:PHE:HD2	16:h:74:TYR:CE1	2.33	0.46
16:h:96:ALA:C	24:p:63:TYR:CE1	2.93	0.46
22:n:133:TRP:O	22:n:137:VAL:HG22	2.15	0.46
24:p:6:ASP:OD1	24:p:8:ASP:HB2	2.16	0.46
3:K:57:MET:N	3:K:58:PRO:CD	2.78	0.46
4:L:74:MET:HE3	5:M:307:TRP:HH2	1.80	0.46
4:L:581:LYS:HB2	4:L:586:LEU:HD22	1.97	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
7:O:38:TYR:CE2	7:O:292:HIS:CD2	3.01	0.46
13:e:16:ARG:HB3	16:h:178:PHE:CE2	2.50	0.46
14:f:37:PHE:O	16:h:134:GLU:HB3	2.15	0.46
4:L:407:TRP:HE1	20:l:140:MET:HE1	1.81	0.46
4:L:515:LYS:HA	22:n:30:TRP:CE3	2.51	0.46
5:M:255:LYS:CE	12:d:117:HIS:HB3	2.46	0.46
6:N:313:MET:HG3	7:O:305:LEU:CD2	2.44	0.46
17:i:98:VAL:HG13	24:p:115:GLN:HG2	1.98	0.46
2:J:21:LEU:HD23	25:K:101:3PE:H271	1.96	0.46
4:L:166:THR:HG22	20:l:115:ASN:HA	1.97	0.46
4:L:373:LEU:CD2	4:L:427:ILE:HG22	2.45	0.46
4:L:428:TYR:CD2	4:L:505:ASN:HB3	2.50	0.46
4:L:561:THR:O	25:Y:201:3PE:H381	2.16	0.46
4:L:588:PHE:O	4:L:589:MET:C	2.57	0.46
4:L:594:ASN:OD1	6:N:110:PRO:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:264:LEU:HD23	21:m:98:LEU:HD11	1.98	0.46
5:M:300:SER:HB2	5:M:308:SER:HB3	1.97	0.46
5:M:348:LEU:O	5:M:351:VAL:N	2.38	0.46
25:N:401:3PE:H3D1	25:N:401:3PE:H2B2	1.98	0.46
7:O:76:GLU:CB	7:O:266:PRO:HB3	2.45	0.46
12:d:13:PHE:O	12:d:78:ARG:NE	2.44	0.46
12:d:108:THR:O	12:d:109:TYR:C	2.55	0.46
13:e:20:PHE:HZ	16:h:178:PHE:CB	2.29	0.46
25:m:202:3PE:H392	25:m:202:3PE:H3C1	1.71	0.46
4:L:21:ILE:HG12	4:L:27:ILE:CG2	2.45	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
25:L:701:3PE:H3B2	18:j:71:TRP:CH2	2.50	0.46
5:M:10:MET:C	5:M:13:PRO:HD2	2.41	0.46
5:M:143:LEU:CD2	6:N:303:THR:HG21	2.30	0.46
5:M:158:ILE:HG12	6:N:287:LEU:HD11	1.96	0.46
5:M:173:THR:HG22	16:h:150:ARG:NH1	2.31	0.46
5:M:435:THR:O	5:M:436:LEU:C	2.59	0.46
6:N:154:ILE:HG12	6:N:195:PRO:CG	2.45	0.46
7:O:61:THR:HB	7:O:160:GLU:O	2.15	0.46
7:O:139:ARG:NH2	27:O:401:ADP:N7	2.61	0.46
7:O:339:TYR:CE1	12:d:52:PRO:HA	2.51	0.46
8:U:105:MET:SD	8:U:139:MET:HE1	2.55	0.46
8:U:114:ASP:O	8:U:117:GLU:N	2.48	0.46
11:c:67:LEU:O	11:c:68:GLU:C	2.59	0.46
19:k:55:GLU:OE1	22:n:38:ARG:HB2	2.15	0.46
24:p:6:ASP:O	24:p:8:ASP:N	2.49	0.46
1:D:34:ALA:HB3	5:M:86:LYS:HZ2	1.80	0.46
4:L:101:MET:HE1	4:L:121:LEU:HB2	1.98	0.46
4:L:193:MET:HE1	21:m:125:PHE:CD2	2.51	0.46
4:L:306:THR:HA	4:L:336:LYS:NZ	2.27	0.46
4:L:340:PHE:O	4:L:343:SER:OG	2.33	0.46
4:L:529:PHE:CZ	4:L:533:ILE:HG21	2.50	0.46
5:M:15:THR:HG21	5:M:100:ILE:CD1	2.46	0.46
5:M:105:LEU:CD2	25:N:401:3PE:H2H2	2.46	0.46
5:M:139:GLN:HG3	5:M:141:GLU:H	1.81	0.46
5:M:303:ILE:HG22	5:M:305:THR:HG23	1.98	0.46
7:O:354:LEU:HG	11:c:44:VAL:CG2	2.46	0.46
18:j:92:TRP:O	18:j:93:THR:C	2.59	0.46
20:l:57:MET:HE2	20:l:57:MET:HB3	1.75	0.46
20:l:156:VAL:HG11	23:o:95:TYR:CE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:9:ALA:O	21:m:10:PRO:C	2.56	0.46
22:n:136:GLU:O	22:n:139:GLN:N	2.49	0.46
2:J:29:GLY:O	2:J:30:LEU:C	2.58	0.46
2:J:75:THR:CG2	3:K:27:MET:HB3	2.46	0.46
2:J:127:GLU:CD	13:e:32:ARG:HG2	2.41	0.46
3:K:57:MET:O	3:K:58:PRO:C	2.58	0.46
4:L:31:ASN:ND2	4:L:34:LEU:HB2	2.31	0.46
4:L:261:VAL:CA	4:L:264:HIS:HD2	2.29	0.46
4:L:439:PRO:HA	19:k:57:TRP:CZ2	2.51	0.46
4:L:550:LEU:O	4:L:554:ASP:HB3	2.16	0.46
5:M:319:HIS:CA	5:M:322:THR:HG22	2.41	0.46
8:U:90:TYR:CD1	19:k:51:TRP:CE2	3.04	0.46
11:c:38:LYS:HA	11:c:39:PRO:HD3	1.58	0.46
17:i:123:PHE:CD2	23:o:61:HIS:HD2	2.32	0.46
20:l:35:ASP:O	20:l:54:LYS:HD3	2.15	0.46
20:l:117:VAL:CG1	20:l:118:ASP:N	2.79	0.46
21:m:15:PRO:HG2	21:m:18:LEU:HD12	1.97	0.46
22:n:61:THR:O	22:n:65:ARG:HG3	2.15	0.46
2:J:13:LEU:HD22	2:J:99:GLU:OE1	2.16	0.46
4:L:142:ILE:HA	5:M:370:PRO:CB	2.45	0.46
5:M:56:PHE:CE1	5:M:108:MET:HG2	2.47	0.46
6:N:123:PRO:HG2	6:N:126:MET:CG	2.40	0.46
6:N:241:LEU:O	6:N:244:ILE:HG22	2.15	0.46
6:N:277:ILE:HG22	6:N:278:MET:H	1.79	0.46
7:O:132:GLN:HE22	27:O:401:ADP:HN62	1.64	0.46
7:O:140:LEU:HD11	7:O:198:TYR:CE2	2.51	0.46
7:O:204:VAL:CG2	7:O:255:VAL:HG22	2.46	0.46
10:Y:74:LEU:HD23	10:Y:74:LEU:C	2.41	0.46
15:g:77:ASP:HA	15:g:78:PRO:HD3	1.70	0.46
16:h:69:ARG:O	16:h:73:PHE:CB	2.63	0.46
16:h:82:VAL:O	16:h:85:GLY:N	2.49	0.46
19:k:39:GLN:NE2	19:k:49:ASP:HB3	2.31	0.46
24:p:50:GLU:CG	24:p:54:ARG:HH21	2.28	0.46
4:L:135:ASN:O	4:L:198:LEU:HD13	2.16	0.46
4:L:324:LEU:HA	4:L:327:LEU:HD12	1.97	0.46
4:L:339:LEU:HD11	4:L:376:GLY:HA3	1.98	0.46
4:L:364:LYS:O	18:j:47:PHE:HZ	1.99	0.46
4:L:445:GLU:OE2	18:j:54:GLN:CG	2.62	0.46
4:L:598:ILE:HB	25:L:703:3PE:C2G	2.46	0.46
26:L:704:CDL:H141	26:L:704:CDL:H112	1.73	0.46
5:M:116:ILE:HD12	5:M:119:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:208:PRO:CD	5:M:236:LEU:HD22	2.38	0.46
6:N:37:LEU:HD21	6:N:60:PHE:CD1	2.51	0.46
7:O:68:SER:OG	7:O:70:LYS:HB3	2.16	0.46
12:d:94:ILE:HD13	16:h:152:LYS:CE	2.46	0.46
16:h:95:GLU:OE1	16:h:114:LYS:HD3	2.16	0.46
19:k:69:PHE:CZ	19:k:73:ILE:HG13	2.52	0.46
23:o:71:ARG:HB3	23:o:71:ARG:NH1	2.27	0.46
2:J:43:VAL:HG13	3:K:49:LEU:HD11	1.98	0.45
2:J:104:CYS:O	2:J:107:ASN:HB2	2.16	0.45
2:J:120:LEU:HA	2:J:123:TRP:CZ3	2.52	0.45
3:K:26:LEU:O	3:K:29:THR:N	2.48	0.45
4:L:12:PHE:O	4:L:16:LEU:HG	2.15	0.45
4:L:195:SER:O	4:L:201:ILE:HD11	2.16	0.45
5:M:61:LEU:C	5:M:64:PRO:HD2	2.41	0.45
5:M:393:ILE:O	5:M:397:GLY:N	2.49	0.45
7:O:72:LYS:O	7:O:75:LYS:HG2	2.16	0.45
7:O:76:GLU:HB3	7:O:266:PRO:CB	2.46	0.45
7:O:344:ASN:OD1	7:O:346:GLU:HG2	2.15	0.45
8:U:118:ILE:O	8:U:122:MET:HG2	2.16	0.45
8:U:124:ASP:CG	22:n:25:ARG:HH12	2.25	0.45
13:e:42:GLU:CG	16:h:176:LYS:HE2	2.46	0.45
14:f:49:ARG:HG2	14:f:52:GLU:HG3	1.98	0.45
20:l:166:LEU:HD12	20:l:170:ARG:HH22	1.81	0.45
21:m:49:LEU:CD2	22:n:140:LEU:CD2	2.94	0.45
22:n:37:TYR:O	22:n:38:ARG:C	2.58	0.45
22:n:44:MET:O	22:n:45:ARG:C	2.54	0.45
24:p:24:THR:HG22	24:p:26:LEU:N	2.30	0.45
4:L:204:SER:HA	4:L:207:ASN:ND2	2.31	0.45
4:L:475:THR:O	4:L:476:SER:HB2	2.16	0.45
4:L:508:THR:HG22	22:n:33:HIS:HD2	1.81	0.45
4:L:552:LEU:HD12	20:l:70:MET:CE	2.36	0.45
4:L:591:PHE:N	4:L:591:PHE:CD1	2.83	0.45
5:M:6:LEU:HD21	14:f:22:PHE:HD2	1.81	0.45
5:M:42:LEU:HD21	5:M:67:ILE:HD12	1.97	0.45
5:M:105:LEU:HD21	25:N:401:3PE:H2H2	1.98	0.45
6:N:133:TRP:CE3	6:N:136:ILE:HD12	2.51	0.45
6:N:300:THR:CG2	6:N:301:SER:N	2.79	0.45
2:J:99:GLU:HG3	2:J:100:VAL:N	2.32	0.45
25:K:101:3PE:H351	10:Y:43:VAL:HG12	1.99	0.45
4:L:47:SER:O	4:L:50:PRO:HD2	2.16	0.45
4:L:56:HIS:CA	23:o:74:PHE:CE1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:302:ILE:HG22	4:L:340:PHE:CE2	2.51	0.45
4:L:532:ILE:HG23	4:L:533:ILE:N	2.31	0.45
5:M:22:LYS:HG2	5:M:22:LYS:O	2.17	0.45
5:M:186:LEU:HD22	5:M:250:LEU:HA	1.98	0.45
5:M:249:ILE:O	5:M:250:LEU:CG	2.47	0.45
5:M:282:LEU:HD11	5:M:410:MET:HE3	1.96	0.45
6:N:26:LEU:HG	6:N:85:MET:SD	2.56	0.45
6:N:215:MET:SD	6:N:244:ILE:HD11	2.56	0.45
7:O:306:ASN:O	7:O:309:THR:HG22	2.16	0.45
7:O:342:GLY:O	7:O:355:LYS:NZ	2.50	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
17:i:103:ARG:O	24:p:18:PRO:HG3	2.17	0.45
25:i:201:3PE:H2E1	25:i:201:3PE:H362	1.98	0.45
23:o:63:LEU:O	23:o:64:ILE:C	2.59	0.45
24:p:107:GLN:O	24:p:111:LYS:HG3	2.16	0.45
24:p:173:GLU:O	24:p:174:ALA:C	2.59	0.45
2:J:28:GLY:O	2:J:29:GLY:C	2.59	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:358:LYS:HZ1	22:n:34:ARG:HH12	1.63	0.45
4:L:366:MET:SD	4:L:443:ILE:HG21	2.57	0.45
25:L:701:3PE:H3B2	25:L:701:3PE:H381	1.70	0.45
5:M:65:LEU:O	5:M:66:ILE:C	2.59	0.45
5:M:207:MET:O	5:M:208:PRO:C	2.59	0.45
5:M:283:LYS:HG3	5:M:327:PHE:HE1	1.78	0.45
5:M:309:PHE:O	5:M:312:ALA:HB3	2.16	0.45
8:U:102:SER:O	8:U:141:PRO:HD3	2.16	0.45
10:Y:19:GLN:HE21	10:Y:22:ARG:CG	2.15	0.45
10:Y:39:SER:HB2	10:Y:58:VAL:HA	1.98	0.45
13:e:18:PHE:O	13:e:18:PHE:CD2	2.69	0.45
19:k:57:TRP:O	19:k:58:ARG:C	2.59	0.45
20:l:110:ASP:O	20:l:116:ARG:NH1	2.50	0.45
4:L:210:LEU:HD23	4:L:210:LEU:C	2.41	0.45
4:L:310:LEU:HA	4:L:313:MET:HB2	1.99	0.45
4:L:407:TRP:HE1	20:l:140:MET:HE3	1.82	0.45
4:L:591:PHE:N	4:L:591:PHE:HD1	2.15	0.45
5:M:42:LEU:HD11	5:M:67:ILE:HD12	1.99	0.45
5:M:122:PHE:CZ	5:M:206:LYS:CD	2.95	0.45
5:M:453:LEU:CD1	5:M:454:ILE:CG2	2.84	0.45
6:N:155:LEU:O	6:N:159:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:351:TRP:HB3	11:c:39:PRO:CG	2.43	0.45
9:X:167:PHE:HB3	9:X:170:TRP:HD1	1.77	0.45
12:d:54:MET:HE2	12:d:54:MET:HB3	1.89	0.45
25:i:201:3PE:H2E1	25:i:201:3PE:C34	2.41	0.45
19:k:26:ARG:O	19:k:27:GLN:C	2.57	0.45
20:l:38:PRO:HD2	21:m:70:TYR:CD2	2.52	0.45
2:J:22:LYS:CE	3:K:18:GLY:O	2.65	0.45
4:L:515:LYS:HG2	22:n:30:TRP:CD2	2.51	0.45
6:N:293:TYR:O	6:N:297:ILE:HG12	2.16	0.45
7:O:112:CYS:HB3	7:O:131:LEU:HA	1.97	0.45
16:h:91:ILE:O	24:p:56:HIS:CD2	2.70	0.45
19:k:48:ARG:HG3	19:k:48:ARG:O	2.16	0.45
24:p:28:ASN:HA	24:p:29:PRO:HD3	1.86	0.45
24:p:49:ARG:O	24:p:50:GLU:C	2.57	0.45
2:J:17:LEU:O	2:J:21:LEU:HG	2.16	0.45
3:K:85:TYR:OH	3:K:95:LEU:HD11	2.17	0.45
4:L:74:MET:HE3	4:L:74:MET:HB2	1.76	0.45
4:L:81:LYS:CA	4:L:135:ASN:HD21	2.29	0.45
4:L:145:GLU:CG	5:M:370:PRO:HD3	2.47	0.45
4:L:241:THR:N	4:L:242:PRO:HD2	2.31	0.45
4:L:246:LEU:C	4:L:246:LEU:CD1	2.90	0.45
4:L:387:THR:HA	4:L:465:GLY:HA3	1.98	0.45
26:L:704:CDL:H322	16:h:71:MET:HE1	1.99	0.45
5:M:25:THR:HG22	15:g:84:ASN:CG	2.42	0.45
5:M:187:ASP:H	5:M:192:ASN:ND2	2.15	0.45
6:N:109:ALA:HB3	6:N:110:PRO:CD	2.46	0.45
6:N:153:ILE:O	6:N:154:ILE:C	2.58	0.45
25:N:401:3PE:H2I2	26:X:201:CDL:C60	2.46	0.45
7:O:265:ASP:O	7:O:266:PRO:C	2.58	0.45
7:O:351:TRP:HB2	7:O:355:LYS:HE3	1.98	0.45
9:X:168:PHE:O	9:X:169:PHE:CG	2.69	0.45
10:Y:88:ASP:H	10:Y:128:LYS:HZ3	1.63	0.45
15:g:67:LYS:O	15:g:68:ASN:C	2.60	0.45
21:m:25:VAL:O	21:m:26:SER:C	2.56	0.45
2:J:12:PHE:HE2	3:K:42:ILE:HD11	1.82	0.45
4:L:100:ILE:O	4:L:104:SER:N	2.42	0.45
4:L:226:GLN:HG3	4:L:314:MET:HE2	1.98	0.45
4:L:524:THR:HG22	22:n:78:GLN:HG3	1.99	0.45
4:L:565:SER:OG	25:Y:201:3PE:H331	2.16	0.45
5:M:3:LYS:HA	5:M:7:PRO:HD2	1.99	0.45
6:N:89:GLN:HB3	13:e:60:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:66:ILE:HD11	7:O:218:ILE:HG13	1.97	0.45
11:c:65:ASP:O	11:c:66:VAL:C	2.56	0.45
17:i:4:TYR:HE1	22:n:4:CYS:SG	2.40	0.45
17:i:88:TYR:CE2	24:p:49:ARG:HB2	2.52	0.45
22:n:146:PRO:O	22:n:147:ASP:C	2.60	0.45
23:o:44:GLN:O	23:o:45:GLU:C	2.58	0.45
3:K:73:VAL:HG21	6:N:38:LEU:CD2	2.47	0.45
4:L:295:GLN:NE2	4:L:524:THR:O	2.50	0.45
5:M:43:TRP:HZ2	16:h:122:ALA:HB2	1.82	0.45
5:M:87:ASP:HB3	5:M:91:LEU:HB2	1.99	0.45
5:M:272:THR:O	5:M:275:ILE:HG13	2.17	0.45
6:N:214:PRO:HB2	6:N:247:MET:SD	2.56	0.45
7:O:129:TYR:CD2	7:O:183:CYS:HB3	2.52	0.45
7:O:230:THR:HG22	7:O:232:ALA:N	2.32	0.45
12:d:11:LEU:HD11	13:e:4:LEU:HD12	1.98	0.45
12:d:13:PHE:CE2	12:d:14:LEU:HD23	2.52	0.45
12:d:78:ARG:O	12:d:79:GLN:C	2.59	0.45
16:h:73:PHE:CE2	16:h:74:TYR:HE1	2.35	0.45
22:n:101:GLU:HG2	22:n:122:ARG:HH12	1.81	0.45
22:n:145:SER:O	22:n:146:PRO:C	2.58	0.45
24:p:110:LEU:O	24:p:111:LYS:C	2.58	0.45
2:J:97:ILE:O	2:J:100:VAL:HB	2.17	0.45
4:L:527:GLY:O	4:L:528:PHE:HB2	2.17	0.45
5:M:73:LEU:HB3	5:M:103:GLN:OE1	2.16	0.45
5:M:129:THR:CG2	5:M:235:LEU:CD1	2.95	0.45
5:M:192:ASN:C	5:M:194:LEU:N	2.72	0.45
5:M:209:LEU:HD11	5:M:261:PHE:HD1	1.81	0.45
6:N:163:PHE:CZ	6:N:285:MET:HG3	2.52	0.45
6:N:217:MET:HA	6:N:220:MET:SD	2.57	0.45
6:N:258:THR:CB	6:N:333:SER:O	2.64	0.45
10:Y:83:ARG:HH12	10:Y:90:LEU:HD13	1.82	0.45
13:e:70:TYR:O	13:e:71:LYS:C	2.60	0.45
15:g:64:VAL:HG11	15:g:71:PHE:CE1	2.52	0.45
16:h:87:THR:HG22	26:h:201:CDL:C51	2.46	0.45
22:n:98:LYS:HD3	22:n:176:GLU:O	2.17	0.45
2:J:169:ILE:HG23	6:N:45:ILE:HD11	1.99	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:424:MET:HG3	4:L:505:ASN:HD21	1.82	0.44
5:M:42:LEU:CG	5:M:67:ILE:CD1	2.95	0.44
5:M:42:LEU:CG	5:M:67:ILE:HD11	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:154:ILE:CD1	6:N:195:PRO:HG2	2.47	0.44
10:Y:20:CYS:O	10:Y:21:HIS:C	2.60	0.44
26:h:201:CDL:H162	26:h:201:CDL:H191	1.75	0.44
19:k:47:LEU:HD12	22:n:43:LEU:HD23	1.99	0.44
25:K:101:3PE:H3F1	4:L:596:ILE:HG21	1.98	0.44
4:L:54:PHE:CB	4:L:87:ILE:HD11	2.47	0.44
4:L:117:PHE:CE1	4:L:243:VAL:CG2	3.00	0.44
4:L:149:ILE:CG2	5:M:364:LEU:HD21	2.47	0.44
4:L:366:MET:SD	4:L:443:ILE:CG2	3.06	0.44
4:L:598:ILE:HD11	6:N:153:ILE:CG1	2.47	0.44
6:N:220:MET:O	6:N:221:LEU:C	2.60	0.44
15:g:69:PRO:HB2	22:n:109:PRO:CD	2.47	0.44
16:h:55:PHE:C	16:h:55:PHE:CD1	2.94	0.44
16:h:120:TRP:NE1	16:h:124:ASN:ND2	2.64	0.44
22:n:97:TYR:HB2	22:n:178:PRO:HB2	1.99	0.44
2:J:94:LEU:HD23	2:J:94:LEU:C	2.42	0.44
4:L:155:ILE:HG12	4:L:248:HIS:CE1	2.53	0.44
6:N:87:GLN:O	6:N:88:GLN:C	2.59	0.44
6:N:250:SER:O	6:N:259:GLY:HA3	2.17	0.44
16:h:56:VAL:O	16:h:58:LYS:HG3	2.16	0.44
20:l:119:THR:CG2	21:m:13:THR:HG23	2.48	0.44
4:L:2:ASN:O	4:L:3:ILE:C	2.59	0.44
4:L:56:HIS:N	23:o:74:PHE:CE1	2.85	0.44
4:L:197:GLU:HG3	24:p:111:LYS:HE2	1.98	0.44
4:L:211:ILE:HA	25:m:201:3PE:H272	1.99	0.44
4:L:348:HIS:CD2	8:U:69:SER:CB	3.00	0.44
4:L:524:THR:CG2	22:n:78:GLN:HG3	2.48	0.44
25:L:702:3PE:H362	25:L:702:3PE:H331	1.45	0.44
5:M:24:TRP:CE3	5:M:81:GLN:HG2	2.52	0.44
5:M:26:ASN:OD1	14:f:13:HIS:HE1	2.00	0.44
5:M:29:SER:HB3	15:g:91:PHE:CE2	2.50	0.44
5:M:177:MET:HB3	16:h:140:LEU:HD21	2.00	0.44
5:M:200:MET:HE2	5:M:250:LEU:HD21	2.00	0.44
5:M:415:GLN:O	5:M:416:ARG:CG	2.64	0.44
25:M:501:3PE:H292	6:N:284:MET:HG3	1.99	0.44
6:N:275:CYS:SG	10:Y:139:PRO:HD2	2.58	0.44
7:O:262:GLU:HB3	7:O:268:LYS:NZ	2.33	0.44
7:O:336:GLY:HA2	7:O:344:ASN:HB3	1.99	0.44
7:O:351:TRP:O	7:O:355:LYS:HG2	2.16	0.44
10:Y:7:PHE:CZ	10:Y:26:ILE:HG12	2.52	0.44
10:Y:141:PRO:HB2	16:h:161:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:89:PRO:O	23:o:103:GLU:HG2	2.18	0.44
22:n:45:ARG:O	22:n:49:GLU:N	2.37	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
2:J:103:ILE:O	2:J:107:ASN:N	2.50	0.44
3:K:33:LEU:HA	3:K:36:MET:HE2	2.00	0.44
4:L:485:PHE:CD1	4:L:485:PHE:N	2.84	0.44
5:M:18:SER:OG	5:M:26:ASN:ND2	2.51	0.44
5:M:424:ILE:O	5:M:424:ILE:CG2	2.65	0.44
6:N:122:ILE:HD11	6:N:127:GLY:HA2	1.98	0.44
6:N:208:TYR:O	6:N:212:THR:HG22	2.18	0.44
7:O:169:PHE:CD2	27:O:401:ADP:N6	2.86	0.44
7:O:211:VAL:N	7:O:212:PRO:CD	2.80	0.44
13:e:38:LYS:NZ	16:h:181:HIS:HD2	2.15	0.44
13:e:91:LYS:NZ	13:e:91:LYS:HB3	2.32	0.44
20:l:88:PRO:HB2	22:n:86:PRO:HB2	1.98	0.44
23:o:49:ALA:O	23:o:50:GLN:C	2.60	0.44
2:J:136:GLU:HG3	2:J:136:GLU:O	2.18	0.44
4:L:66:TRP:CZ3	4:L:68:TRP:HD1	2.34	0.44
26:L:704:CDL:H132	5:M:361:MET:HE1	1.98	0.44
5:M:22:LYS:HG2	5:M:26:ASN:ND2	2.33	0.44
5:M:154:LEU:HD13	6:N:287:LEU:HD22	2.00	0.44
6:N:254:LEU:HA	6:N:255:PRO:HD3	1.60	0.44
12:d:109:TYR:HB3	24:p:156:LEU:HD21	1.99	0.44
4:L:529:PHE:O	4:L:533:ILE:HG22	2.16	0.44
4:L:537:THR:N	4:L:538:PRO:HD2	2.32	0.44
4:L:556:ILE:CG2	21:m:80:PHE:CE2	3.00	0.44
4:L:594:ASN:CG	6:N:110:PRO:CB	2.88	0.44
25:L:705:3PE:H11	25:L:705:3PE:H121	1.99	0.44
5:M:154:LEU:HA	5:M:154:LEU:HD23	1.84	0.44
5:M:186:LEU:HD13	5:M:250:LEU:HA	2.00	0.44
5:M:421:ASN:ND2	21:m:47:TYR:OH	2.51	0.44
7:O:148:GLU:HG3	7:O:295:ARG:NH1	2.32	0.44
7:O:272:ASP:O	7:O:275:TYR:HB2	2.18	0.44
11:c:61:THR:HG22	11:c:65:ASP:OD2	2.18	0.44
12:d:27:ASN:O	12:d:28:ASP:C	2.61	0.44
2:J:95:GLY:O	2:J:96:VAL:C	2.60	0.44
4:L:68:TRP:HE3	4:L:76:LEU:HD21	1.82	0.44
4:L:247:LEU:HD12	4:L:247:LEU:C	2.41	0.44
4:L:563:PRO:HG3	5:M:152:TYR:OH	2.18	0.44
5:M:42:LEU:CD1	5:M:67:ILE:CD1	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:126:LEU:HD11	5:M:153:THR:HG21	2.00	0.44
5:M:344:MET:HE3	5:M:423:MET:CE	2.48	0.44
5:M:446:LEU:CD1	15:g:97:LEU:HD12	2.47	0.44
6:N:35:PHE:O	6:N:36:SER:C	2.59	0.44
6:N:227:ILE:HG13	6:N:228:ASN:N	2.32	0.44
7:O:238:GLU:HG3	7:O:242:LYS:HD3	1.99	0.44
11:c:33:GLU:CD	11:c:33:GLU:H	2.26	0.44
12:d:57:GLY:O	12:d:60:ARG:N	2.51	0.44
13:e:20:PHE:CZ	16:h:178:PHE:CB	3.01	0.44
22:n:149:ILE:HD12	22:n:149:ILE:N	2.33	0.44
23:o:118:LYS:HD2	23:o:118:LYS:HA	1.85	0.44
1:D:36:GLN:NE2	1:D:38:GLN:NE2	2.62	0.44
2:J:165:ILE:HD13	6:N:38:LEU:HB3	1.99	0.44
3:K:57:MET:O	3:K:60:PRO:HD2	2.18	0.44
4:L:53:MET:HE2	4:L:53:MET:HB3	1.78	0.44
4:L:152:PHE:HD2	4:L:153:LEU:HD12	1.83	0.44
4:L:186:MET:HE1	5:M:379:LEU:HD21	2.00	0.44
4:L:305:SER:OG	4:L:336:LYS:HE2	2.18	0.44
4:L:586:LEU:HA	4:L:589:MET:HE3	1.99	0.44
4:L:598:ILE:HD11	6:N:153:ILE:CD1	2.48	0.44
5:M:8:SER:O	5:M:11:LEU:HB2	2.18	0.44
6:N:146:TYR:O	6:N:147:PRO:C	2.53	0.44
10:Y:120:MET:HE2	10:Y:120:MET:HB3	1.90	0.44
15:g:140:PHE:HZ	24:p:152:ALA:HB1	1.83	0.44
16:h:83:ILE:HG12	26:h:201:CDL:H561	2.00	0.44
20:l:58:ARG:HD2	21:m:35:GLU:OE1	2.18	0.44
23:o:5:LEU:HB3	23:o:9:TYR:CD2	2.53	0.44
24:p:140:GLN:HG2	24:p:144:LEU:CD1	2.47	0.44
24:p:165:GLU:C	24:p:167:ARG:H	2.26	0.44
2:J:13:LEU:HD11	3:K:10:MET:SD	2.58	0.43
3:K:26:LEU:HG	3:K:30:LEU:HD13	1.98	0.43
4:L:72:ASN:ND2	5:M:459:MET:HG2	2.33	0.43
4:L:172:ILE:HD13	4:L:172:ILE:HA	1.89	0.43
4:L:348:HIS:CD2	8:U:69:SER:HB3	2.53	0.43
4:L:529:PHE:HB3	4:L:530:PRO:HD3	1.99	0.43
5:M:98:MET:SD	25:N:401:3PE:H3C1	2.58	0.43
6:N:12:THR:CG2	6:N:39:ALA:HB2	2.48	0.43
6:N:120:GLN:HE22	6:N:174:GLN:HB3	1.83	0.43
6:N:146:TYR:CD1	6:N:198:PRO:HG2	2.53	0.43
6:N:175:MET:HE2	6:N:175:MET:HB2	1.85	0.43
6:N:323:ASN:N	6:N:323:ASN:OD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:LEU:O	7:O:44:ILE:HG13	2.18	0.43
7:O:72:LYS:O	7:O:76:GLU:HG2	2.16	0.43
9:X:169:PHE:HE1	26:X:201:CDL:H551	1.82	0.43
10:Y:7:PHE:O	10:Y:8:PHE:C	2.61	0.43
10:Y:12:HIS:CD2	10:Y:131:LYS:HE2	2.53	0.43
13:e:42:GLU:CD	16:h:176:LYS:HE2	2.42	0.43
17:i:19:ARG:HA	22:n:171:VAL:HG13	2.00	0.43
21:m:45:ARG:O	21:m:45:ARG:CG	2.61	0.43
25:L:703:3PE:P	10:Y:46:ASN:HD22	2.41	0.43
10:Y:89:PRO:HG3	10:Y:129:ILE:HG12	1.99	0.43
20:l:142:PHE:O	20:l:145:TRP:N	2.51	0.43
24:p:103:MET:HE1	24:p:135:VAL:HG12	1.98	0.43
2:J:30:LEU:O	2:J:34:VAL:HG23	2.17	0.43
2:J:55:VAL:HG13	2:J:56:PHE:N	2.33	0.43
2:J:77:GLU:OE1	3:K:87:THR:HA	2.18	0.43
4:L:141:PHE:CB	4:L:182:PHE:CE2	2.81	0.43
4:L:496:LEU:CD1	4:L:497:GLY:N	2.73	0.43
26:L:704:CDL:H792	26:L:704:CDL:H581	2.00	0.43
5:M:123:GLU:CD	6:N:255:PRO:CG	2.91	0.43
5:M:353:PRO:HG3	16:h:61:LEU:CD2	2.48	0.43
6:N:338:PRO:HG2	12:d:33:TYR:CZ	2.52	0.43
10:Y:19:GLN:OE1	10:Y:19:GLN:HA	2.17	0.43
11:c:55:TRP:HE1	12:d:66:THR:CG2	2.31	0.43
11:c:57:TYR:HD2	12:d:70:PHE:CZ	2.35	0.43
12:d:72:GLY:O	12:d:73:TYR:C	2.60	0.43
12:d:78:ARG:HG2	12:d:82:LEU:HD23	2.00	0.43
13:e:38:LYS:HB3	13:e:38:LYS:HE2	1.74	0.43
15:g:58:GLU:CD	15:g:59:PRO:HD2	2.44	0.43
20:l:41:TYR:HD2	20:l:43:ARG:HD3	1.82	0.43
2:J:155:ALA:HB1	3:K:65:VAL:HG11	2.00	0.43
4:L:92:VAL:HG21	4:L:330:CYS:HB3	2.00	0.43
4:L:226:GLN:OE1	4:L:284:THR:CG2	2.66	0.43
4:L:386:LEU:HA	18:j:68:TRP:HZ3	1.82	0.43
4:L:427:ILE:HG13	4:L:428:TYR:N	2.33	0.43
5:M:321:LEU:HD23	5:M:321:LEU:HA	1.81	0.43
7:O:214:VAL:O	7:O:218:ILE:HG13	2.18	0.43
8:U:137:LYS:HD3	17:i:4:TYR:CD1	2.53	0.43
9:X:165:THR:N	9:X:172:VAL:HG11	2.33	0.43
10:Y:26:ILE:O	10:Y:30:LEU:HG	2.17	0.43
12:d:116:PHE:HB2	24:p:157:ALA:CB	2.48	0.43
13:e:101:ARG:HH21	13:e:104:PRO:CD	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:139:TYR:HB2	24:p:142:ARG:NH2	2.34	0.43
16:h:127:ASP:OD1	16:h:127:ASP:C	2.61	0.43
18:j:44:TYR:CG	19:k:22:LEU:HD22	2.54	0.43
22:n:131:GLU:O	22:n:131:GLU:HG2	2.17	0.43
3:K:32:CYS:O	3:K:33:LEU:C	2.59	0.43
4:L:22:SER:HA	4:L:27:ILE:HG21	2.00	0.43
5:M:348:LEU:O	5:M:349:GLN:C	2.60	0.43
6:N:186:HIS:O	6:N:190:MET:HG3	2.18	0.43
6:N:319:LYS:HA	7:O:302:THR:CG2	2.43	0.43
7:O:315:PRO:O	15:g:53:TRP:HA	2.19	0.43
7:O:332:ARG:O	7:O:338:LYS:HA	2.19	0.43
10:Y:19:GLN:O	10:Y:23:LYS:HG2	2.19	0.43
15:g:89:PHE:HB3	16:h:74:TYR:HD2	1.84	0.43
20:l:38:PRO:HD2	21:m:70:TYR:HD2	1.82	0.43
24:p:75:THR:HG22	24:p:156:LEU:HD13	2.00	0.43
4:L:60:GLU:C	4:L:61:TYR:CD1	2.97	0.43
4:L:81:LYS:HD3	4:L:262:ARG:NH1	2.34	0.43
4:L:136:ASN:HD21	26:h:201:CDL:C27	2.18	0.43
4:L:246:LEU:HD12	4:L:247:LEU:CB	2.49	0.43
4:L:327:LEU:HD21	4:L:472:ILE:HD13	2.00	0.43
4:L:427:ILE:CD1	19:k:69:PHE:CE1	3.01	0.43
5:M:16:TRP:CD1	25:d:201:3PE:H361	2.53	0.43
5:M:207:MET:SD	5:M:240:SER:CA	3.06	0.43
5:M:304:GLN:HA	5:M:309:PHE:HE1	1.83	0.43
6:N:11:PHE:O	6:N:15:LEU:N	2.50	0.43
6:N:240:MET:O	6:N:240:MET:HG2	2.18	0.43
6:N:279:ALA:HA	6:N:282:MET:HE2	2.00	0.43
7:O:68:SER:O	7:O:69:GLY:C	2.59	0.43
7:O:239:ASN:HA	7:O:242:LYS:HE2	2.01	0.43
15:g:117:ARG:NE	24:p:10:TYR:OH	2.51	0.43
20:l:97:LEU:O	20:l:98:ARG:C	2.60	0.43
1:D:72:LEU:O	1:D:72:LEU:HD12	2.18	0.43
2:J:67:PHE:O	2:J:68:GLY:C	2.59	0.43
2:J:120:LEU:HA	2:J:123:TRP:CE3	2.53	0.43
4:L:70:THR:O	4:L:75:GLU:HA	2.18	0.43
4:L:217:LEU:CD1	4:L:273:ILE:HG23	2.49	0.43
5:M:73:LEU:HD23	5:M:103:GLN:HE22	1.84	0.43
5:M:95:TYR:OH	5:M:226:ALA:HB3	2.19	0.43
6:N:219:LEU:CD2	6:N:230:ILE:HD12	2.49	0.43
7:O:209:VAL:HA	7:O:210:PRO:HD3	1.80	0.43
8:U:73:PRO:HG3	16:h:52:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:11:ARG:HD2	22:m:154:LEU:O	2.19	0.43
20:l:152:SER:HA	23:o:5:LEU:CD2	2.43	0.43
21:m:5:LYS:HB2	21:m:5:LYS:HE3	1.73	0.43
21:m:34:VAL:O	21:m:34:VAL:HG12	2.16	0.43
25:m:202:3PE:H252	25:m:202:3PE:H381	1.99	0.43
24:p:118:GLY:O	24:p:119:GLU:HB2	2.19	0.43
4:L:296:ASN:HD21	4:L:425:ARG:HH21	1.65	0.43
5:M:1:MET:HB3	5:M:1:MET:HE3	1.73	0.43
5:M:119:TYR:HD1	5:M:160:LEU:HD22	1.80	0.43
6:N:39:ALA:O	6:N:42:PRO:HD2	2.19	0.43
6:N:309:ASN:N	7:O:317:ILE:O	2.49	0.43
8:U:115:GLN:O	8:U:116:VAL:C	2.61	0.43
10:Y:115:MET:O	10:Y:119:TYR:HD2	2.02	0.43
17:i:123:PHE:CE2	23:o:61:HIS:CD2	3.06	0.43
23:o:13:ALA:O	23:o:14:SER:C	2.60	0.43
4:L:138:PHE:CD1	26:h:201:CDL:H271	2.54	0.43
4:L:145:GLU:HG3	5:M:369:LEU:HD12	2.01	0.43
4:L:253:VAL:HG21	4:L:310:LEU:HD11	1.99	0.43
4:L:446:ASN:O	4:L:447:ASP:C	2.57	0.43
4:L:493:ILE:O	4:L:496:LEU:HG	2.19	0.43
4:L:526:LEU:HD12	4:L:526:LEU:N	2.34	0.43
5:M:51:ASN:ND2	16:h:136:THR:HG23	2.34	0.43
5:M:63:THR:N	5:M:64:PRO:CD	2.81	0.43
5:M:208:PRO:HG2	5:M:216:LEU:CD1	2.44	0.43
6:N:12:THR:HG22	6:N:39:ALA:HB2	2.00	0.43
6:N:193:ILE:HD11	6:N:269:GLU:CB	2.49	0.43
7:O:75:LYS:HE2	7:O:75:LYS:HB3	1.76	0.43
9:X:151:ASN:OD1	16:h:170:GLN:NE2	2.52	0.43
12:d:101:PHE:CZ	16:h:156:VAL:HG22	2.54	0.43
13:e:49:GLY:O	13:e:50:THR:C	2.61	0.43
16:h:90:ASN:OD1	16:h:115:HIS:NE2	2.52	0.43
17:i:111:LEU:CD2	24:p:19:ALA:HB2	2.48	0.43
17:i:123:PHE:CD2	23:o:61:HIS:CD2	3.07	0.43
22:n:81:ILE:HD12	22:n:87:GLY:C	2.44	0.43
23:o:57:ASP:OD2	23:o:59:CYS:HB2	2.19	0.43
24:p:73:ASP:O	24:p:74:ILE:C	2.59	0.43
2:J:50:PHE:O	2:J:54:MET:HG2	2.18	0.43
4:L:193:MET:CE	21:m:125:PHE:CD2	3.02	0.43
4:L:246:LEU:CD1	4:L:247:LEU:N	2.68	0.43
5:M:29:SER:CB	15:g:91:PHE:HD2	2.24	0.43
5:M:100:ILE:O	5:M:103:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:154:ILE:HD12	6:N:155:LEU:N	2.33	0.43
6:N:193:ILE:HD12	6:N:266:ILE:HA	2.01	0.43
6:N:239:ALA:HB1	12:d:47:MET:HG2	2.01	0.43
7:O:224:PRO:O	7:O:228:LYS:NZ	2.52	0.43
7:O:303:GLU:O	7:O:304:VAL:C	2.59	0.43
10:Y:8:PHE:CD1	10:Y:30:LEU:HD21	2.53	0.43
3:K:50:ASN:C	3:K:50:ASN:OD1	2.62	0.42
4:L:60:GLU:N	4:L:60:GLU:OE2	2.52	0.42
4:L:335:PHE:O	4:L:339:LEU:HD13	2.18	0.42
5:M:68:LEU:HD23	5:M:234:ILE:CD1	2.49	0.42
5:M:367:LEU:C	5:M:367:LEU:HD12	2.44	0.42
6:N:105:LYS:HE3	6:N:105:LYS:HB3	1.79	0.42
6:N:174:GLN:O	6:N:178:ILE:HG13	2.18	0.42
6:N:219:LEU:HD23	6:N:230:ILE:HD12	2.01	0.42
7:O:243:LYS:HB2	7:O:243:LYS:HE2	1.64	0.42
8:U:142:GLN:O	8:U:143:GLU:C	2.60	0.42
16:h:59:PRO:O	16:h:61:LEU:HG	2.19	0.42
16:h:129:PRO:HD2	16:h:130:GLU:OE1	2.18	0.42
16:h:163:ARG:CG	16:h:165:ASP:HB2	2.33	0.42
17:i:93:LYS:HD3	25:i:201:3PE:C12	2.46	0.42
17:i:93:LYS:HE3	17:i:96:THR:HG21	2.01	0.42
19:k:28:TRP:CE3	19:k:60:MET:HG2	2.54	0.42
4:L:5:THR:O	4:L:6:THR:C	2.62	0.42
4:L:38:THR:O	4:L:41:LYS:HB3	2.19	0.42
4:L:214:MET:HG2	25:m:201:3PE:H291	2.01	0.42
4:L:591:PHE:HE1	6:N:113:PHE:HD2	1.66	0.42
5:M:72:LEU:HD12	5:M:234:ILE:HG12	2.01	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:58:ARG:O	7:O:157:VAL:N	2.45	0.42
7:O:63:ASP:OD2	7:O:165:SER:HB2	2.20	0.42
7:O:117:PHE:HD1	7:O:128:SER:CA	2.31	0.42
7:O:310:ILE:HG23	7:O:312:VAL:HG23	2.01	0.42
7:O:323:GLN:HB2	15:g:56:ASP:OD1	2.18	0.42
8:U:74:LEU:HD11	8:U:82:ARG:NH1	2.33	0.42
17:i:22:TRP:O	17:i:26:GLN:HG2	2.19	0.42
17:i:81:PHE:O	17:i:82:VAL:C	2.60	0.42
23:o:46:MET:HE2	23:o:60:ALA:HB3	2.00	0.42
4:L:272:PHE:O	4:L:275:THR:HG22	2.19	0.42
4:L:275:THR:HG23	4:L:276:THR:N	2.34	0.42
4:L:444:ASN:HB2	18:j:40:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:489:THR:HG23	4:L:490:ALA:N	2.34	0.42
4:L:591:PHE:O	4:L:595:ILE:HG13	2.19	0.42
5:M:14:LEU:HD21	5:M:26:ASN:CB	2.50	0.42
6:N:80:GLN:O	6:N:81:LEU:HG	2.19	0.42
7:O:170:LEU:HD21	7:O:184:VAL:HG13	2.00	0.42
7:O:209:VAL:CG1	7:O:260:SER:HB2	2.31	0.42
7:O:351:TRP:CB	11:c:39:PRO:HG3	2.45	0.42
10:Y:68:ILE:HG22	10:Y:102:THR:OG1	2.19	0.42
13:e:89:GLU:HB2	13:e:91:LYS:HG2	2.00	0.42
20:l:57:MET:HG2	20:l:104:PRO:CG	2.49	0.42
22:n:45:ARG:O	22:n:46:ALA:C	2.61	0.42
22:n:85:SER:O	22:n:86:PRO:C	2.60	0.42
22:n:163:LEU:HA	22:n:164:PRO:HD2	1.75	0.42
24:p:43:TRP:NE1	24:p:47:LEU:HD11	2.33	0.42
2:J:44:LEU:HD13	2:J:49:SER:HA	2.01	0.42
4:L:81:LYS:HD3	4:L:262:ARG:HH11	1.83	0.42
5:M:200:MET:CE	5:M:247:SER:HB2	2.46	0.42
5:M:216:LEU:HD23	5:M:287:ALA:HB1	2.02	0.42
7:O:121:PRO:HB3	7:O:178:TYR:HE1	1.83	0.42
7:O:297:LEU:C	7:O:297:LEU:HD23	2.44	0.42
13:e:82:GLN:O	13:e:86:LEU:HG	2.20	0.42
13:e:101:ARG:HE	13:e:104:PRO:HD2	1.83	0.42
24:p:6:ASP:C	24:p:8:ASP:H	2.27	0.42
24:p:36:ALA:O	24:p:37:TYR:C	2.60	0.42
4:L:21:ILE:HG23	4:L:27:ILE:CG2	2.50	0.42
4:L:189:PHE:CZ	4:L:212:PRO:HB2	2.55	0.42
5:M:206:LYS:HA	5:M:215:TRP:CZ2	2.54	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
6:N:80:GLN:O	6:N:80:GLN:HG2	2.19	0.42
6:N:241:LEU:HG	6:N:301:SER:OG	2.19	0.42
7:O:180:ARG:HH22	15:g:51:MET:HE3	1.84	0.42
10:Y:141:PRO:HB2	16:h:161:ARG:NE	2.35	0.42
15:g:119:GLU:OE1	15:g:122:ARG:NH1	2.53	0.42
16:h:111:GLU:O	24:p:63:TYR:HA	2.18	0.42
21:m:15:PRO:HG2	21:m:18:LEU:HB2	2.01	0.42
21:m:41:ALA:HA	22:n:152:GLU:HG2	2.01	0.42
23:o:53:LEU:HD11	24:p:122:GLN:HG3	2.02	0.42
5:M:77:LEU:O	5:M:81:GLN:HG3	2.19	0.42
5:M:118:PHE:HE2	5:M:203:PHE:CE1	2.37	0.42
5:M:230:ILE:HG23	5:M:235:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:109:ALA:HB3	6:N:110:PRO:HD3	2.00	0.42
6:N:148:LEU:HD12	6:N:148:LEU:N	2.34	0.42
7:O:242:LYS:HE2	7:O:242:LYS:HB2	1.92	0.42
11:c:65:ASP:OD2	12:d:77:LYS:NZ	2.50	0.42
15:g:112:MET:HE1	24:p:94:ARG:HG3	2.02	0.42
15:g:147:LEU:O	15:g:148:PRO:C	2.62	0.42
17:i:32:GLU:OE2	22:n:118:TYR:N	2.52	0.42
17:i:94:PRO:HG3	24:p:10:TYR:CD2	2.52	0.42
18:j:96:GLU:HG2	18:j:97:LEU:HD23	2.00	0.42
20:l:38:PRO:C	21:m:75:ASN:HD21	2.25	0.42
20:l:62:TYR:CE2	20:l:64:PRO:HG3	2.55	0.42
20:l:120:SER:O	20:l:121:PRO:C	2.60	0.42
22:n:139:GLN:HA	22:n:142:GLU:HG2	2.01	0.42
23:o:3:ALA:O	23:o:4:HIS:C	2.61	0.42
2:J:84:SER:HB3	2:J:87:LEU:HG	2.02	0.42
4:L:52:LEU:HB2	24:p:30:ILE:HD11	2.01	0.42
4:L:220:ALA:HB2	4:L:260:LEU:CD1	2.49	0.42
4:L:405:ASN:HB2	4:L:408:ALA:HB3	2.01	0.42
4:L:534:HIS:O	4:L:538:PRO:CG	2.60	0.42
4:L:568:THR:O	4:L:569:LEU:C	2.61	0.42
5:M:207:MET:HE3	5:M:240:SER:HB2	2.02	0.42
5:M:210:TYR:O	5:M:213:HIS:HD2	2.02	0.42
6:N:226:THR:HG22	6:N:228:ASN:N	2.34	0.42
6:N:331:ILE:HG23	6:N:335:MET:HE3	2.01	0.42
8:U:72:PRO:CD	18:j:42:PRO:CG	2.96	0.42
10:Y:45:LEU:O	10:Y:46:ASN:C	2.62	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CD2	2.55	0.42
16:h:188:ASP:O	16:h:189:ASN:C	2.63	0.42
20:l:167:TYR:CG	20:l:178:PRO:HG3	2.55	0.42
22:n:110:SER:O	22:n:113:ALA:HB3	2.20	0.42
22:n:132:SER:O	22:n:133:TRP:C	2.62	0.42
24:p:6:ASP:O	24:p:7:LYS:C	2.63	0.42
3:K:59:ILE:HB	3:K:60:PRO:HD3	2.01	0.42
4:L:66:TRP:CZ3	26:h:201:CDL:H181	2.54	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:346:ILE:HG21	4:L:362:ILE:HD11	2.02	0.42
4:L:364:LYS:CE	19:k:67:ILE:HD11	2.41	0.42
4:L:396:ILE:HD13	4:L:396:ILE:HA	1.89	0.42
5:M:123:GLU:OE2	5:M:154:LEU:HD21	2.20	0.42
5:M:191:SER:O	5:M:194:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:428:PRO:HD3	22:n:106:TYR:CG	2.55	0.42
6:N:154:ILE:HD11	6:N:155:LEU:HG	2.02	0.42
6:N:340:ALA:N	6:N:341:PRO:CD	2.83	0.42
8:U:87:LEU:HD12	8:U:98:LEU:HD21	2.00	0.42
10:Y:76:THR:CG2	10:Y:92:TYR:HA	2.48	0.42
10:Y:91:ASN:HD22	10:Y:91:ASN:HA	1.71	0.42
12:d:114:GLU:O	12:d:114:GLU:HG2	2.18	0.42
13:e:36:PHE:O	13:e:37:GLU:C	2.62	0.42
18:j:44:TYR:CE2	18:j:45:ARG:HG3	2.54	0.42
18:j:99:ILE:CD1	23:o:107:ARG:HB2	2.50	0.42
21:m:91:ALA:HB2	25:m:203:3PE:H272	2.00	0.42
22:n:100:PRO:HB2	22:n:102:TRP:NE1	2.35	0.42
4:L:51:LEU:HA	4:L:87:ILE:HD12	2.02	0.42
4:L:463:PHE:CE2	18:j:64:LEU:HD21	2.54	0.42
5:M:216:LEU:CG	5:M:220:HIS:CE1	2.88	0.42
6:N:180:ALA:O	6:N:184:ILE:HG13	2.20	0.42
6:N:315:THR:O	6:N:316:HIS:C	2.61	0.42
6:N:338:PRO:HA	9:X:170:TRP:HZ3	1.84	0.42
7:O:195:LEU:N	7:O:196:PRO:HD2	2.35	0.42
7:O:272:ASP:HA	7:O:275:TYR:HD2	1.85	0.42
9:X:147:ARG:NH1	13:e:39:GLU:HG3	2.31	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CE2	2.54	0.42
25:d:201:3PE:O31	25:d:201:3PE:H342	2.19	0.42
23:o:104:ARG:O	23:o:108:LEU:HG	2.20	0.42
24:p:9:VAL:O	24:p:109:ARG:NH2	2.51	0.42
1:D:35:ARG:HE	15:g:59:PRO:HD3	1.85	0.42
1:D:37:TRP:CE3	1:D:37:TRP:O	2.73	0.42
2:J:165:ILE:O	2:J:169:ILE:HG12	2.20	0.42
3:K:4:THR:HA	3:K:7:ASN:ND2	2.35	0.42
4:L:117:PHE:HZ	4:L:242:PRO:HG2	1.85	0.42
4:L:286:LEU:HG	4:L:290:ILE:HD11	2.01	0.42
4:L:365:ILE:O	18:j:50:LEU:HD21	2.19	0.42
5:M:181:PHE:CZ	24:p:86:TYR:HD1	2.38	0.42
5:M:258:ALA:O	5:M:259:TYR:C	2.62	0.42
5:M:388:TRP:CD1	21:m:109:ARG:HD2	2.55	0.42
6:N:108:LEU:HD22	6:N:191:LEU:HD22	2.02	0.42
6:N:148:LEU:N	6:N:148:LEU:CD1	2.83	0.42
6:N:202:LEU:HD11	13:e:3:PHE:CE1	2.55	0.42
6:N:215:MET:SD	6:N:244:ILE:CD1	3.08	0.42
6:N:308:ASN:C	7:O:319:ILE:HG23	2.44	0.42
7:O:48:LYS:O	7:O:52:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:128:PHE:HZ	8:U:148:ILE:CD1	2.33	0.42
9:X:147:ARG:HH12	13:e:39:GLU:HA	1.85	0.42
12:d:24:PRO:HD2	12:d:73:TYR:CE2	2.55	0.42
16:h:55:PHE:HE1	16:h:57:VAL:HA	1.85	0.42
18:j:99:ILE:HA	23:o:108:LEU:CD2	2.50	0.42
20:l:159:LYS:HE3	20:l:161:TYR:HE1	1.85	0.42
20:l:184:TYR:HD1	23:o:35:LYS:C	2.27	0.42
21:m:8:PRO:HD3	21:m:14:LEU:HD13	2.02	0.42
25:K:101:3PE:H361	25:K:101:3PE:H392	1.68	0.41
4:L:293:LEU:O	4:L:425:ARG:HD2	2.20	0.41
4:L:489:THR:O	4:L:492:ILE:HG13	2.20	0.41
5:M:108:MET:HB3	5:M:121:LEU:HD13	2.01	0.41
5:M:158:ILE:CG1	6:N:287:LEU:HD11	2.50	0.41
6:N:108:LEU:CD2	6:N:191:LEU:HD22	2.50	0.41
13:e:33:CYS:O	13:e:34:HIS:C	2.62	0.41
13:e:44:ALA:HA	13:e:47:ILE:CG1	2.49	0.41
20:l:59:VAL:O	20:l:59:VAL:HG12	2.20	0.41
2:J:20:ALA:C	2:J:22:LYS:N	2.77	0.41
2:J:43:VAL:HG13	3:K:49:LEU:CD1	2.50	0.41
2:J:136:GLU:O	2:J:137:GLY:C	2.62	0.41
4:L:58:ASN:HA	4:L:58:ASN:HD22	1.65	0.41
4:L:355:ASP:O	4:L:359:MET:HG3	2.20	0.41
4:L:407:TRP:CE3	4:L:410:LEU:HD21	2.55	0.41
5:M:319:HIS:HA	5:M:322:THR:CG2	2.44	0.41
25:M:502:3PE:H371	25:M:502:3PE:H342	1.82	0.41
6:N:22:SER:HB2	13:e:6:ILE:HG22	2.02	0.41
6:N:285:MET:HE1	6:N:288:LEU:HD22	2.03	0.41
7:O:70:LYS:O	7:O:71:ASN:C	2.62	0.41
7:O:267:THR:O	7:O:271:GLU:HG3	2.19	0.41
8:U:118:ILE:HA	19:k:51:TRP:CH2	2.55	0.41
11:c:57:TYR:CD2	12:d:70:PHE:CZ	3.08	0.41
14:f:8:ARG:O	14:f:9:GLU:HB2	2.20	0.41
15:g:140:PHE:HB3	24:p:75:THR:CG2	2.50	0.41
17:i:20:ARG:HH11	17:i:20:ARG:HG3	1.84	0.41
25:m:202:3PE:H351	25:m:202:3PE:H321	1.75	0.41
22:n:56:ASP:O	22:n:59:ARG:N	2.53	0.41
22:n:114:MET:HG3	22:n:115:TYR:CD2	2.55	0.41
4:L:249:SER:HB2	4:L:340:PHE:CD2	2.55	0.41
4:L:434:LYS:HG3	19:k:59:TYR:CE1	2.55	0.41
4:L:437:PHE:HB2	4:L:438:PRO:CD	2.49	0.41
4:L:532:ILE:HG21	20:l:133:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:218:ALA:CB	6:N:240:MET:SD	3.08	0.41
7:O:76:GLU:HG3	7:O:266:PRO:HG2	2.00	0.41
7:O:146:ALA:CB	7:O:159:LEU:HD21	2.50	0.41
7:O:179:ILE:CD1	7:O:184:VAL:HG22	2.50	0.41
7:O:354:LEU:HD12	7:O:354:LEU:HA	1.95	0.41
10:Y:10:SER:O	10:Y:11:TYR:C	2.62	0.41
16:h:90:ASN:HD21	26:h:201:CDL:PA1	2.43	0.41
17:i:83:HIS:HD2	24:p:37:TYR:CE2	2.37	0.41
21:m:49:LEU:HA	22:n:133:TRP:HH2	1.84	0.41
23:o:59:CYS:SG	23:o:91:GLU:HG2	2.61	0.41
3:K:1:MET:O	3:K:2:PRO:C	2.62	0.41
3:K:73:VAL:CG2	6:N:38:LEU:HD22	2.50	0.41
26:L:704:CDL:HA62	16:h:68:LEU:CD1	2.42	0.41
5:M:85:LYS:O	5:M:85:LYS:HG2	2.21	0.41
5:M:127:ILE:HD11	6:N:256:PRO:HG2	1.96	0.41
5:M:270:ILE:HD12	5:M:395:LEU:HD22	2.02	0.41
5:M:394:ILE:HG21	25:m:202:3PE:H2C2	2.01	0.41
6:N:25:ASN:HB3	13:e:15:ASP:OD1	2.19	0.41
6:N:317:GLN:HG2	7:O:301:LYS:HB3	2.01	0.41
7:O:59:VAL:HG22	7:O:157:VAL:HG21	2.02	0.41
7:O:66:ILE:HD11	7:O:218:ILE:HG12	1.97	0.41
7:O:179:ILE:HD12	7:O:184:VAL:HG22	2.02	0.41
10:Y:83:ARG:O	10:Y:84:GLU:HB3	2.20	0.41
11:c:55:TRP:CE2	12:d:66:THR:HG22	2.55	0.41
14:f:36:ALA:O	14:f:37:PHE:C	2.61	0.41
15:g:71:PHE:CE2	15:g:73:GLY:HA2	2.55	0.41
18:j:44:TYR:CD2	18:j:45:ARG:HG3	2.56	0.41
21:m:42:ARG:O	21:m:43:LEU:C	2.62	0.41
2:J:29:GLY:O	2:J:33:ILE:HG13	2.21	0.41
3:K:1:MET:HB3	3:K:2:PRO:HD3	2.02	0.41
4:L:142:ILE:HG12	5:M:370:PRO:HB2	2.01	0.41
4:L:253:VAL:HB	4:L:310:LEU:CD1	2.50	0.41
4:L:365:ILE:CD1	4:L:366:MET:HG3	2.24	0.41
5:M:47:GLU:O	5:M:48:ASN:C	2.64	0.41
5:M:142:ARG:HG3	5:M:143:LEU:N	2.36	0.41
5:M:178:ILE:O	5:M:179:LEU:C	2.60	0.41
5:M:270:ILE:HD11	5:M:395:LEU:HA	2.03	0.41
6:N:159:ILE:HB	6:N:278:MET:HE1	2.01	0.41
6:N:168:GLY:HA3	6:N:181:TYR:CE1	2.56	0.41
6:N:324:LEU:CD1	12:d:64:PHE:HZ	2.32	0.41
6:N:338:PRO:HB3	26:X:201:CDL:H712	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:164:TYR:CE1	7:O:201:PRO:HD3	2.56	0.41
7:O:261:TRP:H	7:O:261:TRP:HE3	1.68	0.41
7:O:355:LYS:HE2	11:c:37:ALA:O	2.21	0.41
11:c:69:TYR:O	11:c:73:ASN:ND2	2.54	0.41
13:e:96:PRO:HB2	13:e:102:GLU:HG3	2.02	0.41
15:g:63:ASN:CG	22:n:106:TYR:HE1	2.29	0.41
16:h:133:TYR:OH	24:p:87:GLU:HA	2.21	0.41
17:i:22:TRP:CD2	22:n:172:THR:CG2	3.00	0.41
20:l:184:TYR:HD1	23:o:36:GLU:N	2.17	0.41
21:m:127:ILE:O	24:p:139:TYR:HE2	2.04	0.41
23:o:8:ARG:HH21	23:o:9:TYR:HE1	1.68	0.41
23:o:53:LEU:HD23	23:o:56:ARG:NE	2.34	0.41
24:p:71:VAL:HB	24:p:72:PRO:CD	2.50	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
25:L:703:3PE:H322	25:L:703:3PE:H351	1.84	0.41
5:M:247:SER:OG	5:M:304:GLN:NE2	2.53	0.41
5:M:250:LEU:HD12	5:M:250:LEU:C	2.39	0.41
5:M:301:ILE:HG22	5:M:301:ILE:O	2.19	0.41
6:N:233:LEU:CD2	6:N:241:LEU:HD12	2.27	0.41
7:O:117:PHE:CZ	7:O:173:MET:HE3	2.54	0.41
7:O:200:PRO:HG3	7:O:282:PRO:CD	2.47	0.41
7:O:263:ALA:C	7:O:265:ASP:N	2.77	0.41
7:O:295:ARG:HH12	7:O:299:GLN:CB	2.33	0.41
7:O:353:TRP:HB2	12:d:58:LEU:HD12	2.02	0.41
8:U:87:LEU:C	8:U:89:LEU:N	2.78	0.41
13:e:49:GLY:O	13:e:52:ALA:N	2.53	0.41
16:h:59:PRO:HD3	22:n:99:VAL:HG11	2.03	0.41
26:h:201:CDL:H171	25:i:201:3PE:H372	2.02	0.41
18:j:52:ARG:HG2	18:j:56:ILE:HD12	2.02	0.41
19:k:20:MET:HE2	19:k:20:MET:HB3	1.98	0.41
20:l:151:PRO:HD2	23:o:9:TYR:CZ	2.55	0.41
20:l:184:TYR:CD1	23:o:36:GLU:CA	3.03	0.41
21:m:124:LYS:O	21:m:126:ASN:N	2.53	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
1:D:67:ASN:HB2	7:O:193:LEU:HD22	2.00	0.41
1:D:71:ILE:O	1:D:72:LEU:C	2.62	0.41
2:J:60:LEU:O	2:J:64:LEU:HB2	2.20	0.41
2:J:124:LEU:O	2:J:125:MET:C	2.62	0.41
4:L:211:ILE:N	4:L:212:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:368:PHE:HB3	4:L:445:GLU:OE1	2.20	0.41
5:M:7:PRO:HG3	14:f:20:PHE:CA	2.50	0.41
5:M:22:LYS:HE3	5:M:26:ASN:HD21	1.86	0.41
6:N:272:LYS:HE3	16:h:154:GLN:HG2	2.02	0.41
7:O:42:ALA:O	7:O:45:LEU:O	2.39	0.41
7:O:150:LEU:O	7:O:154:GLY:HA2	2.20	0.41
7:O:287:ASP:HB3	7:O:290:THR:HG23	2.02	0.41
13:e:32:ARG:O	13:e:33:CYS:CB	2.69	0.41
13:e:101:ARG:C	13:e:104:PRO:HD3	2.46	0.41
17:i:74:HIS:O	17:i:78:PRO:HG2	2.20	0.41
20:l:122:THR:HG22	20:l:124:VAL:H	1.85	0.41
22:n:164:PRO:HA	22:n:165:PRO:HD3	1.94	0.41
24:p:91:GLN:O	24:p:91:GLN:HG2	2.21	0.41
2:J:33:ILE:HG12	2:J:64:LEU:HD23	2.02	0.41
2:J:101:PHE:HD2	2:J:102:LEU:HD22	1.86	0.41
2:J:116:LEU:HD11	13:e:73:MET:HG3	2.02	0.41
4:L:258:PHE:O	4:L:261:VAL:HG22	2.20	0.41
4:L:570:HIS:O	4:L:573:MET:N	2.54	0.41
4:L:571:THR:O	4:L:574:THR:HG22	2.20	0.41
5:M:4:ILE:CD1	5:M:41:LEU:HD21	2.51	0.41
5:M:218:LYS:HE3	5:M:218:LYS:HB3	1.58	0.41
6:N:83:THR:HG22	6:N:84:TRP:N	2.35	0.41
6:N:175:MET:O	6:N:176:ARG:C	2.63	0.41
7:O:262:GLU:O	7:O:265:ASP:HB3	2.21	0.41
7:O:343:TYR:HB3	12:d:52:PRO:HD3	2.03	0.41
12:d:101:PHE:CZ	16:h:159:LEU:HD22	2.55	0.41
20:l:63:GLU:O	20:l:64:PRO:C	2.63	0.41
21:m:50:GLN:O	21:m:50:GLN:HG2	2.20	0.41
24:p:40:VAL:O	24:p:44:PRO:HG2	2.21	0.41
2:J:5:ILE:O	2:J:6:PHE:C	2.63	0.41
2:J:86:TRP:CE3	2:J:89:LEU:HD12	2.56	0.41
3:K:6:PHE:O	3:K:7:ASN:C	2.63	0.41
4:L:61:TYR:HA	17:i:98:VAL:O	2.21	0.41
4:L:210:LEU:O	4:L:211:ILE:C	2.62	0.41
4:L:321:GLN:NE2	4:L:324:LEU:HD13	2.36	0.41
4:L:357:ARG:CZ	22:n:78:GLN:O	2.69	0.41
25:L:701:3PE:H382	23:o:78:LEU:CD1	2.51	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:175:ASN:ND2	16:h:143:GLU:HG2	2.31	0.41
5:M:210:TYR:HB2	5:M:268:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:303:ILE:HG13	5:M:385:LEU:HD23	2.02	0.41
5:M:412:ILE:HG21	20:l:115:ASN:ND2	2.35	0.41
6:N:125:HIS:CE1	6:N:129:ILE:HD11	2.56	0.41
6:N:191:LEU:HG	6:N:191:LEU:O	2.21	0.41
6:N:224:SER:HB2	6:N:229:SER:HB2	2.01	0.41
6:N:331:ILE:HD12	6:N:335:MET:HE3	2.03	0.41
7:O:71:ASN:OD1	7:O:71:ASN:N	2.54	0.41
7:O:90:GLY:H	7:O:93:TYR:HB2	1.86	0.41
7:O:96:THR:O	11:c:31:VAL:HG21	2.21	0.41
7:O:105:ASP:OD1	7:O:106:ILE:N	2.54	0.41
7:O:263:ALA:C	7:O:265:ASP:H	2.29	0.41
7:O:268:LYS:HA	7:O:271:GLU:OE1	2.21	0.41
8:U:83:VAL:HG13	8:U:122:MET:SD	2.61	0.41
10:Y:51:THR:HG23	10:Y:52:LEU:N	2.35	0.41
13:e:65:GLU:OE2	13:e:71:LYS:N	2.54	0.41
17:i:29:SER:O	17:i:32:GLU:HB2	2.21	0.41
17:i:92:THR:O	24:p:5:TRP:CD1	2.74	0.41
18:j:102:ASP:O	18:j:103:ASP:HB2	2.21	0.41
19:k:81:PHE:O	19:k:85:VAL:HG23	2.21	0.41
20:l:44:THR:HG23	20:l:46:GLU:HG2	2.03	0.41
20:l:80:ASN:HB3	20:l:112:TYR:OH	2.20	0.41
20:l:110:ASP:HB2	21:m:72:ARG:HH12	1.85	0.41
20:l:122:THR:CG2	20:l:129:MET:HE1	2.45	0.41
22:n:41:ALA:C	22:n:43:LEU:N	2.78	0.41
22:n:94:TYR:HB3	22:n:178:PRO:HD2	2.03	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:165:PRO:O	22:n:166:LEU:C	2.64	0.41
23:o:28:ASP:O	23:o:29:LEU:C	2.62	0.41
23:o:71:ARG:NH1	23:o:72:ASP:OD1	2.54	0.41
2:J:6:PHE:O	2:J:9:SER:N	2.54	0.41
4:L:3:ILE:HG22	4:L:49:LEU:CD2	2.51	0.41
5:M:120:ILE:HD11	6:N:264:TRP:CH2	2.56	0.41
5:M:248:ILE:HG13	5:M:249:ILE:H	1.85	0.41
5:M:329:LEU:HD23	5:M:437:MET:CE	2.49	0.41
5:M:422:HIS:HD2	22:n:102:TRP:CD1	2.39	0.41
7:O:117:PHE:CE1	7:O:128:SER:CB	2.96	0.41
7:O:246:LEU:HD23	7:O:246:LEU:C	2.46	0.41
8:U:133:ILE:CG2	8:U:134:ASP:N	2.84	0.41
10:Y:5:LYS:C	10:Y:7:PHE:N	2.77	0.41
12:d:25:LYS:HE3	12:d:27:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:49:GLY:HA2	13:e:52:ALA:HB3	2.02	0.41
17:i:111:LEU:HD21	24:p:19:ALA:CB	2.51	0.41
18:j:81:LEU:O	18:j:81:LEU:HD23	2.20	0.41
18:j:98:GLY:O	23:o:30:GLY:HA3	2.20	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
2:J:66:VAL:O	2:J:69:TYR:HB3	2.22	0.40
2:J:84:SER:C	2:J:86:TRP:N	2.78	0.40
4:L:22:SER:HA	4:L:27:ILE:CG2	2.52	0.40
4:L:68:TRP:CE3	4:L:76:LEU:CD2	3.04	0.40
4:L:324:LEU:HB3	4:L:395:ILE:CD1	2.51	0.40
4:L:554:ASP:OD2	5:M:213:HIS:HE1	2.04	0.40
5:M:6:LEU:O	5:M:7:PRO:C	2.60	0.40
5:M:177:MET:HB3	5:M:177:MET:HE3	1.70	0.40
5:M:350:MET:HE3	5:M:350:MET:HB2	1.80	0.40
6:N:139:LEU:HD23	6:N:139:LEU:HA	1.86	0.40
6:N:146:TYR:CG	6:N:147:PRO:N	2.88	0.40
6:N:211:LEU:CD2	6:N:333:SER:HB2	2.45	0.40
7:O:104:LEU:HD23	7:O:104:LEU:HA	1.90	0.40
8:U:113:LEU:HD11	22:n:20:TYR:CG	2.56	0.40
8:U:128:PHE:CZ	8:U:148:ILE:CD1	3.04	0.40
11:c:57:TYR:CD2	12:d:70:PHE:HZ	2.39	0.40
12:d:45:ASP:O	12:d:46:ASN:C	2.62	0.40
14:f:43:LEU:HD13	24:p:69:ARG:O	2.21	0.40
14:f:56:TRP:CD1	16:h:134:GLU:OE1	2.73	0.40
16:h:87:THR:O	16:h:91:ILE:HG13	2.21	0.40
17:i:69:LEU:HD23	17:i:69:LEU:N	2.36	0.40
20:l:159:LYS:HE3	20:l:161:TYR:CE1	2.56	0.40
22:n:148:GLY:O	22:n:149:ILE:C	2.63	0.40
24:p:43:TRP:HB3	24:p:44:PRO:HD3	2.03	0.40
2:J:32:LEU:O	2:J:33:ILE:C	2.64	0.40
4:L:14:LEU:CD2	17:i:74:HIS:O	2.69	0.40
4:L:52:LEU:O	4:L:53:MET:C	2.62	0.40
4:L:400:ASN:HD22	4:L:409:LEU:HD11	1.85	0.40
25:L:701:3PE:H381	18:j:71:TRP:CH2	2.56	0.40
5:M:53:SER:O	5:M:54:ASN:C	2.63	0.40
5:M:158:ILE:CG2	6:N:283:ALA:HB1	2.50	0.40
5:M:263:LEU:HD21	21:m:105:PHE:HD2	1.86	0.40
5:M:313:THR:HG21	5:M:456:GLY:CA	2.47	0.40
5:M:394:ILE:O	5:M:398:ILE:HG13	2.22	0.40
6:N:109:ALA:O	6:N:112:HIS:ND1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:215:MET:HE3	6:N:215:MET:HB3	1.96	0.40
15:g:115:TRP:CD1	24:p:65:HIS:CE1	3.10	0.40
26:h:201:CDL:H131	25:i:201:3PE:H321	2.03	0.40
18:j:47:PHE:O	18:j:48:PRO:C	2.62	0.40
23:o:52:THR:O	23:o:53:LEU:C	2.62	0.40
2:J:52:GLY:O	2:J:53:LEU:C	2.62	0.40
4:L:210:LEU:HD12	4:L:270:ASN:HD21	1.86	0.40
4:L:399:ILE:HG22	4:L:409:LEU:CD1	2.52	0.40
26:L:704:CDL:H372	16:h:75:LEU:HD13	2.04	0.40
5:M:197:LEU:O	5:M:201:MET:HB2	2.21	0.40
6:N:59:TYR:O	6:N:63:GLN:HG2	2.21	0.40
6:N:89:GLN:HG2	13:e:60:PHE:CD2	2.55	0.40
6:N:106:LEU:HD21	6:N:138:PRO:HB2	2.03	0.40
7:O:117:PHE:HE1	7:O:173:MET:HE1	1.80	0.40
7:O:168:VAL:CG1	7:O:241:TYR:CE1	2.97	0.40
7:O:170:LEU:CD2	7:O:184:VAL:HG13	2.51	0.40
7:O:176:GLN:CG	7:O:177:GLY:H	2.23	0.40
7:O:235:GLN:HE21	7:O:239:ASN:ND2	2.19	0.40
7:O:351:TRP:CH2	11:c:41:TRP:CH2	3.06	0.40
9:X:148:PRO:HG3	13:e:47:ILE:HD13	2.02	0.40
10:Y:115:MET:HE3	25:Y:201:3PE:H261	2.01	0.40
12:d:107:LYS:HB3	12:d:111:GLU:HB3	2.04	0.40
14:f:53:GLU:C	14:f:54:VAL:HG13	2.46	0.40
15:g:112:MET:HE3	15:g:115:TRP:CE3	2.56	0.40
18:j:71:TRP:HZ3	18:j:72:ARG:NH2	2.19	0.40
20:l:129:MET:HE3	20:l:129:MET:HB2	1.89	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
4:L:59:MET:HE2	4:L:59:MET:HB3	1.89	0.40
4:L:67:HIS:HD2	4:L:76:LEU:O	2.05	0.40
4:L:172:ILE:HG22	5:M:405:MET:HE1	2.04	0.40
4:L:348:HIS:HD2	8:U:69:SER:CB	2.34	0.40
25:L:702:3PE:H221	25:L:702:3PE:H2	1.84	0.40
5:M:131:ILE:HD12	25:N:401:3PE:H362	2.02	0.40
5:M:259:TYR:HB2	5:M:260:PRO:HD3	2.03	0.40
5:M:435:THR:HG23	5:M:436:LEU:N	2.36	0.40
6:N:132:THR:HB	6:N:209:ILE:HG12	2.03	0.40
7:O:74:ALA:HB1	7:O:85:HIS:CD2	2.56	0.40
13:e:69:ARG:CD	13:e:72:THR:HG21	2.50	0.40
14:f:37:PHE:HZ	24:p:83:LEU:HD13	1.86	0.40
16:h:148:GLU:O	16:h:152:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:89:HIS:NE2	25:i:201:3PE:H221	2.37	0.40
17:i:99:SER:O	17:i:100:SER:C	2.64	0.40
17:i:125:ASP:OD1	17:i:127:HIS:HB2	2.21	0.40
3:K:82:SER:HA	3:K:86:GLY:H	1.85	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
4:L:466:PHE:CD1	4:L:470:TYR:HE2	2.39	0.40
25:L:705:3PE:H3A2	5:M:155:ILE:HD13	2.03	0.40
5:M:5:ILE:CG1	5:M:6:LEU:N	2.85	0.40
5:M:186:LEU:CB	5:M:253:LEU:HD13	2.52	0.40
5:M:449:THR:OG1	25:M:502:3PE:H281	2.22	0.40
6:N:264:TRP:CZ2	9:X:168:PHE:CG	3.09	0.40
6:N:307:THR:CA	7:O:319:ILE:HG12	2.52	0.40
8:U:87:LEU:C	8:U:89:LEU:H	2.29	0.40
10:Y:64:THR:O	10:Y:68:ILE:HG23	2.20	0.40
12:d:99:GLU:HG2	12:d:100:ASP:OD1	2.22	0.40
13:e:87:MET:HG2	13:e:92:TYR:O	2.21	0.40
17:i:120:MET:SD	17:i:123:PHE:CZ	3.15	0.40
20:l:160:GLN:OE1	23:o:37:ARG:NH2	2.54	0.40
23:o:3:ALA:O	23:o:6:THR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	40/463 (9%)	38 (95%)	2 (5%)	0	100	100
2	J	157/172 (91%)	148 (94%)	9 (6%)	0	100	100
3	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
4	L	604/607 (100%)	573 (95%)	31 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	65
7	O	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
8	U	87/156 (56%)	81 (93%)	6 (7%)	0	100	100
9	X	25/172 (14%)	21 (84%)	4 (16%)	0	100	100
10	Y	137/143 (96%)	132 (96%)	5 (4%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
13	e	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
14	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
15	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
16	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
17	i	91/128 (71%)	81 (89%)	10 (11%)	0	100	100
18	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
19	k	71/104 (68%)	68 (96%)	3 (4%)	0	100	100
20	l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	176/179 (98%)	165 (94%)	10 (6%)	1 (1%)	21	52
23	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
24	p	170/176 (97%)	153 (90%)	17 (10%)	0	100	100
All	All	3782/4813 (79%)	3590 (95%)	190 (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	36/395 (9%)	36 (100%)	0	100	100
2	J	129/137 (94%)	126 (98%)	3 (2%)	44	66
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%)	305 (99%)	2 (1%)	76	80
7	O	283/309 (92%)	283 (100%)	0	100	100
8	U	82/135 (61%)	82 (100%)	0	100	100
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	93/94 (99%)	92 (99%)	1 (1%)	65	76
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	93/129 (72%)	93 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	90/120 (75%)	89 (99%)	1 (1%)	65	76
18	j	61/87 (70%)	61 (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	112/114 (98%)	112 (100%)	0	100	100
22	n	163/164 (99%)	162 (99%)	1 (1%)	78	81
23	o	112/121 (93%)	112 (100%)	0	100	100
24	p	156/158 (99%)	156 (100%)	0	100	100
All	All	3409/4213 (81%)	3398 (100%)	11 (0%)	84	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	3	ASN
2	J	60	LEU
2	J	65	VAL
4	L	3	ILE

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Mol	Chain	Res	Type
4	L	69	VAL
5	M	218	LYS
6	N	148	LEU
6	N	159	ILE
13	e	91	LYS
17	i	72	VAL
22	n	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	36	GLN
3	K	7	ASN
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	505	ASN
4	L	579	ASN
4	L	605	ASN
5	M	26	ASN
5	M	51	ASN
5	M	81	GLN
5	M	92	GLN
5	M	138	ASN
5	M	170	HIS
5	M	175	ASN

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Mol	Chain	Res	Type
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	273	ASN
6	N	289	ASN
6	N	310	ASN
7	O	80	GLN
7	O	155	GLN
7	O	175	ASN
7	O	225	HIS
7	O	239	ASN
7	O	286	GLN
7	O	292	HIS
7	O	306	ASN
7	O	323	GLN
8	U	101	ASN
10	Y	19	GLN
10	Y	46	ASN
10	Y	91	ASN
11	c	62	HIS
12	d	59	HIS
14	f	13	HIS
16	h	109	HIS
16	h	154	GLN
16	h	170	GLN
16	h	181	HIS
17	i	83	HIS
17	i	127	HIS
17	i	128	HIS
18	j	83	HIS
19	k	39	GLN
19	k	66	ASN
20	l	83	GLN
20	l	91	GLN
20	l	106	HIS
20	l	115	ASN
20	l	154	GLN

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Mol	Chain	Res	Type
21	m	75	ASN
21	m	79	ASN
22	n	12	HIS
22	n	13	GLN
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	139	GLN
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](#)

19 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	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.15	3 (7%)
25	3PE	L	703	-	39,39,50	1.02	2 (5%)	42,44,55	1.16	3 (7%)
25	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.14	4 (7%)
25	3PE	m	202	-	50,50,50	0.91	2 (4%)	53,55,55	1.15	4 (7%)
26	CDL	L	704	-	77,77,99	1.01	4 (5%)	83,89,111	1.14	6 (7%)
28	EHZ	n	201	-	29,31,37	1.78	7 (24%)	37,41,47	1.65	7 (18%)
25	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.06	2 (4%)
25	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.12	4 (8%)
25	3PE	m	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.14	3 (6%)
25	3PE	m	201	-	46,46,50	0.97	2 (4%)	49,51,55	1.12	3 (6%)
25	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.22	4 (10%)
25	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.16	5 (9%)
27	ADP	O	401	-	28,29,29	1.36	4 (14%)	43,45,45	1.87	10 (23%)
25	3PE	N	401	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	4 (7%)
26	CDL	h	201	-	69,69,99	1.09	4 (5%)	75,81,111	1.23	7 (9%)
26	CDL	X	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
25	3PE	Y	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.19	5 (11%)
25	3PE	L	705	-	37,37,50	1.04	2 (5%)	40,42,55	1.14	3 (7%)
25	3PE	d	201	-	30,30,50	1.15	2 (6%)	33,35,55	1.33	5 (15%)

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	L	701	-	-	5/43/43/54	-
25	3PE	L	703	-	-	6/43/43/54	-
25	3PE	L	702	-	-	13/52/52/54	-
25	3PE	m	202	-	-	9/54/54/54	-
26	CDL	L	704	-	-	27/88/88/110	-
28	EHZ	n	201	-	-	13/39/39/45	-
25	3PE	i	201	-	-	15/43/43/54	-
25	3PE	K	101	-	-	16/49/49/54	-
25	3PE	m	203	-	-	7/44/44/54	-
25	3PE	m	201	-	-	10/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	M	501	-	-	13/40/40/54	-
25	3PE	M	502	-	-	12/54/54/54	-
27	ADP	O	401	-	-	2/16/32/32	0/3/3/3
25	3PE	N	401	-	-	10/54/54/54	-
26	CDL	h	201	-	-	24/80/80/110	-
26	CDL	X	201	-	-	22/77/77/110	-
25	3PE	Y	201	-	-	10/44/44/54	-
25	3PE	L	705	-	-	14/41/41/54	-
25	3PE	d	201	-	-	7/34/34/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	201	EHZ	C12-N1	4.92	1.45	1.33
28	n	201	EHZ	C15-N2	4.87	1.45	1.33
27	O	401	ADP	C5-C4	4.35	1.46	1.39
26	X	201	CDL	OB8-CB7	4.28	1.45	1.33
25	K	101	3PE	O31-C31	4.25	1.45	1.33
25	m	202	3PE	O31-C31	4.24	1.45	1.33
25	N	401	3PE	O31-C31	4.24	1.45	1.33
25	m	201	3PE	O31-C31	4.23	1.45	1.33
25	i	201	3PE	O31-C31	4.22	1.45	1.33
25	m	201	3PE	O21-C21	4.21	1.46	1.34
26	X	201	CDL	OA8-CA7	4.21	1.45	1.33
25	M	501	3PE	O31-C31	4.20	1.45	1.33
25	M	501	3PE	O21-C21	4.20	1.46	1.34
25	L	703	3PE	O31-C31	4.20	1.45	1.33
26	L	704	CDL	OB8-CB7	4.19	1.45	1.33
25	L	701	3PE	O31-C31	4.18	1.45	1.33
25	m	203	3PE	O31-C31	4.18	1.45	1.33
25	Y	201	3PE	O21-C21	4.18	1.46	1.34
25	L	705	3PE	O31-C31	4.16	1.45	1.33
25	Y	201	3PE	O31-C31	4.14	1.45	1.33
25	M	502	3PE	O31-C31	4.14	1.45	1.33
26	h	201	CDL	OA8-CA7	4.14	1.45	1.33
25	L	701	3PE	O21-C21	4.13	1.45	1.34
26	h	201	CDL	OB8-CB7	4.12	1.45	1.33
26	L	704	CDL	OB6-CB5	4.11	1.45	1.34
25	i	201	3PE	O21-C21	4.11	1.45	1.34
26	h	201	CDL	OB6-CB5	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	201	3PE	O31-C31	4.05	1.45	1.33
25	L	702	3PE	O31-C31	4.03	1.45	1.33
26	h	201	CDL	OA6-CA5	4.03	1.45	1.34
26	L	704	CDL	OA8-CA7	4.00	1.45	1.33
25	m	202	3PE	O21-C21	3.99	1.45	1.34
26	X	201	CDL	OB6-CB5	3.97	1.45	1.34
25	L	703	3PE	O21-C21	3.97	1.45	1.34
25	K	101	3PE	O21-C21	3.97	1.45	1.34
25	d	201	3PE	O21-C21	3.96	1.45	1.34
25	L	702	3PE	O21-C21	3.95	1.45	1.34
26	X	201	CDL	OA6-CA5	3.94	1.45	1.34
25	N	401	3PE	O21-C21	3.94	1.45	1.34
25	m	203	3PE	O21-C21	3.92	1.45	1.34
25	M	502	3PE	O21-C21	3.91	1.45	1.34
25	L	705	3PE	O21-C21	3.88	1.45	1.34
26	L	704	CDL	OA6-CA5	3.81	1.45	1.34
28	n	201	EHZ	P1-O7	2.71	1.64	1.54
27	O	401	ADP	C5-C6	2.64	1.48	1.41
28	n	201	EHZ	O4-C15	-2.54	1.18	1.23
28	n	201	EHZ	C9-S1	2.47	1.82	1.76
28	n	201	EHZ	P1-OP3	-2.37	1.46	1.54
27	O	401	ADP	C5-N7	-2.34	1.34	1.39
28	n	201	EHZ	O3-C12	-2.33	1.18	1.23
27	O	401	ADP	C8-N7	2.24	1.36	1.31

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	401	ADP	C5-C4-N3	-5.69	118.88	126.72
28	n	201	EHZ	C8-C9-S1	4.96	119.83	113.56
25	m	201	3PE	O21-C21-C22	4.68	121.62	111.48
25	M	501	3PE	O21-C21-C22	4.64	121.52	111.48
27	O	401	ADP	N3-C4-N9	4.59	134.97	127.17
25	m	202	3PE	O21-C21-C22	4.43	121.07	111.48
26	h	201	CDL	OB6-CB5-C51	4.43	121.06	111.48
26	X	201	CDL	OB6-CB5-C51	4.34	120.88	111.48
25	M	502	3PE	O21-C21-C22	4.27	120.72	111.48
26	L	704	CDL	OA6-CA5-C11	4.26	120.69	111.48
26	X	201	CDL	OA6-CA5-C11	4.21	120.60	111.48
25	Y	201	3PE	O21-C21-C22	4.15	120.46	111.48
25	K	101	3PE	O21-C21-C22	4.11	120.38	111.48
25	L	703	3PE	O21-C21-C22	4.04	120.22	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	702	3PE	O21-C21-C22	4.00	120.13	111.48
26	h	201	CDL	OA6-CA5-C11	3.96	120.04	111.48
25	d	201	3PE	O21-C21-C22	3.91	119.94	111.48
25	L	701	3PE	O21-C21-C22	3.87	119.86	111.48
27	O	401	ADP	C2-N3-C4	3.79	121.08	111.83
25	N	401	3PE	O21-C21-C22	3.77	119.64	111.48
25	i	201	3PE	O21-C21-C22	3.76	119.62	111.48
26	L	704	CDL	OB6-CB5-C51	3.76	119.62	111.48
25	L	705	3PE	O21-C21-C22	3.71	119.50	111.48
25	m	203	3PE	O21-C21-C22	3.63	119.33	111.48
27	O	401	ADP	N3-C2-N1	-3.46	123.34	128.58
27	O	401	ADP	C4-C5-N7	-3.39	106.70	110.58
28	n	201	EHZ	C10-S1-C9	3.25	111.46	101.84
25	M	502	3PE	C2-O21-C21	-3.24	110.04	117.80
25	d	201	3PE	O31-C31-C32	3.20	121.60	111.83
25	m	202	3PE	C2-O21-C21	-3.17	110.22	117.80
25	d	201	3PE	C2-O21-C21	-3.16	110.24	117.80
26	X	201	CDL	CA4-OA6-CA5	-3.15	110.26	117.80
25	m	203	3PE	C2-O21-C21	-3.11	110.35	117.80
25	M	502	3PE	O31-C31-C32	3.11	121.32	111.83
27	O	401	ADP	C4-N9-C8	3.00	108.89	105.74
25	K	101	3PE	C2-O21-C21	-2.99	110.64	117.80
25	Y	201	3PE	O31-C31-C32	2.98	120.93	111.83
25	m	202	3PE	O31-C31-C32	2.94	120.81	111.83
25	i	201	3PE	O31-C31-C32	2.94	120.81	111.83
26	h	201	CDL	OB8-CB7-C71	2.91	120.70	111.83
25	m	201	3PE	O31-C31-C32	2.90	120.67	111.83
25	N	401	3PE	C2-O21-C21	-2.86	110.95	117.80
26	L	704	CDL	CA4-OA6-CA5	-2.83	111.03	117.80
26	X	201	CDL	OB8-CB7-C71	2.79	120.34	111.83
26	L	704	CDL	OB8-CB7-C71	2.77	120.30	111.83
25	m	203	3PE	O31-C31-C32	2.77	120.27	111.83
25	L	702	3PE	O31-C31-C32	2.75	120.23	111.83
25	K	101	3PE	O31-C31-C32	2.75	120.22	111.83
26	L	704	CDL	OA8-CA7-C31	2.75	120.22	111.83
25	L	703	3PE	O31-C31-C32	2.72	120.13	111.83
25	L	701	3PE	O31-C31-C32	2.72	120.12	111.83
25	N	401	3PE	O31-C31-C32	2.69	120.03	111.83
26	h	201	CDL	CA4-OA6-CA5	-2.68	111.38	117.80
26	X	201	CDL	OA8-CA7-C31	2.68	120.00	111.83
25	L	703	3PE	C2-O21-C21	-2.64	111.47	117.80
27	O	401	ADP	C5-N7-C8	2.60	107.54	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	201	CDL	OA8-CA7-C31	2.58	119.70	111.83
25	Y	201	3PE	C2-O21-C21	-2.56	111.67	117.80
26	h	201	CDL	CB4-OB6-CB5	-2.55	111.70	117.80
28	n	201	EHZ	OP3-P1-O9	-2.53	100.97	110.83
25	L	702	3PE	C2-O21-C21	-2.52	111.77	117.80
25	L	705	3PE	C2-O21-C21	-2.50	111.80	117.80
28	n	201	EHZ	O2-C9-C8	-2.48	119.83	123.74
25	M	501	3PE	C2-O21-C21	-2.48	111.86	117.80
25	L	705	3PE	O31-C31-C32	2.41	119.17	111.83
25	K	101	3PE	O21-C21-O22	-2.37	118.17	123.70
27	O	401	ADP	O4'-C1'-N9	2.35	112.60	108.09
28	n	201	EHZ	C10-C11-N1	-2.32	107.58	112.41
25	M	502	3PE	O21-C21-O22	-2.28	118.36	123.70
25	Y	201	3PE	O21-C21-O22	-2.28	118.37	123.70
25	m	202	3PE	O21-C21-O22	-2.28	118.37	123.70
25	d	201	3PE	O31-C31-O32	-2.28	117.92	123.63
27	O	401	ADP	N9-C8-N7	-2.27	110.72	113.94
25	N	401	3PE	O21-C21-O22	-2.25	118.44	123.70
25	M	501	3PE	O31-C31-C32	2.23	118.62	111.83
25	d	201	3PE	O21-C21-O22	-2.19	118.59	123.70
27	O	401	ADP	C6-C5-N7	2.17	136.28	132.09
28	n	201	EHZ	C5-C6-C7	-2.17	108.69	114.68
26	X	201	CDL	CB6-CB4-CB3	-2.15	106.78	111.78
25	L	702	3PE	O21-C21-O22	-2.13	118.71	123.70
26	X	201	CDL	OB6-CB5-OB7	-2.12	118.74	123.70
25	Y	201	3PE	O31-C31-O32	-2.09	118.41	123.63
26	L	704	CDL	OA6-CA5-OA7	-2.08	118.84	123.70
25	m	201	3PE	O21-C21-O22	-2.08	118.84	123.70
25	L	701	3PE	C2-O21-C21	-2.08	112.83	117.80
25	M	501	3PE	O21-C21-O22	-2.06	118.89	123.70
25	M	502	3PE	O31-C31-O32	-2.03	118.56	123.63
28	n	201	EHZ	C14-C13-C12	-2.03	109.02	112.39
26	h	201	CDL	OA8-CA7-OA9	-2.02	118.59	123.63

There are no chirality outliers.

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
25	L	702	3PE	C1-O11-P-O12
25	L	702	3PE	C1-O11-P-O13
25	L	702	3PE	O22-C21-O21-C2
25	L	702	3PE	C22-C21-O21-C2
25	L	703	3PE	C11-O13-P-O11
25	L	703	3PE	C11-O13-P-O12
25	L	703	3PE	C11-O13-P-O14
25	L	705	3PE	C1-O11-P-O12
25	L	705	3PE	C1-O11-P-O14
25	L	705	3PE	C11-O13-P-O11
25	L	705	3PE	C11-O13-P-O12
25	L	705	3PE	C11-O13-P-O14
25	M	501	3PE	C1-O11-P-O12
25	M	501	3PE	C1-O11-P-O13
25	M	501	3PE	C1-O11-P-O14
25	M	501	3PE	C11-O13-P-O11
25	M	501	3PE	C11-O13-P-O12
25	M	501	3PE	C11-O13-P-O14
25	M	502	3PE	C1-O11-P-O12
25	M	502	3PE	C11-O13-P-O11
25	M	502	3PE	C11-O13-P-O14
25	N	401	3PE	C11-O13-P-O11
25	N	401	3PE	C11-O13-P-O12
25	Y	201	3PE	C1-O11-P-O12
25	Y	201	3PE	C1-O11-P-O13
25	Y	201	3PE	C11-O13-P-O12
25	d	201	3PE	C11-O13-P-O11
25	d	201	3PE	O22-C21-O21-C2
25	i	201	3PE	C1-O11-P-O12
25	i	201	3PE	C1-O11-P-O13
25	i	201	3PE	C1-O11-P-O14
25	i	201	3PE	C11-O13-P-O11
25	i	201	3PE	C11-O13-P-O12
25	m	201	3PE	C1-O11-P-O14
25	m	201	3PE	C22-C21-O21-C2
25	m	202	3PE	C22-C21-O21-C2
25	m	203	3PE	C1-O11-P-O12
25	m	203	3PE	C1-O11-P-O13
25	m	203	3PE	C1-O11-P-O14
25	m	203	3PE	C22-C21-O21-C2
26	L	704	CDL	CA2-OA2-PA1-OA3
26	L	704	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
26	L	704	CDL	CB2-OB2-PB2-OB4
26	L	704	CDL	CB2-OB2-PB2-OB5
26	L	704	CDL	CB3-OB5-PB2-OB2
26	L	704	CDL	CB3-OB5-PB2-OB3
26	L	704	CDL	CB3-OB5-PB2-OB4
26	L	704	CDL	C51-CB5-OB6-CB4
26	X	201	CDL	CA3-OA5-PA1-OA2
26	X	201	CDL	CA3-OA5-PA1-OA3
26	X	201	CDL	CA3-OA5-PA1-OA4
26	X	201	CDL	CB2-OB2-PB2-OB3
26	X	201	CDL	CB3-OB5-PB2-OB3
26	X	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
28	n	201	EHZ	C12-C13-C14-N2
28	n	201	EHZ	N2-C15-C16-O5
28	n	201	EHZ	C15-C16-C17-C18
28	n	201	EHZ	C15-C16-C17-C19
28	n	201	EHZ	C15-C16-C17-C20
28	n	201	EHZ	O5-C16-C17-C18
28	n	201	EHZ	O5-C16-C17-C19
28	n	201	EHZ	O5-C16-C17-C20
26	L	704	CDL	OA9-CA7-OA8-CA6
25	m	202	3PE	O22-C21-O21-C2
25	m	203	3PE	O22-C21-O21-C2
26	L	704	CDL	OB7-CB5-OB6-CB4
26	X	201	CDL	OB7-CB5-OB6-CB4
26	h	201	CDL	OB7-CB5-OB6-CB4
25	K	101	3PE	C32-C31-O31-C3
25	d	201	3PE	C22-C21-O21-C2
25	N	401	3PE	C32-C31-O31-C3
26	L	704	CDL	C31-CA7-OA8-CA6
25	N	401	3PE	O32-C31-O31-C3
25	m	203	3PE	O32-C31-O31-C3
25	m	201	3PE	O22-C21-O21-C2
26	X	201	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
25	K	101	3PE	O32-C31-O31-C3
25	L	705	3PE	C22-C21-O21-C2
26	L	704	CDL	C11-CA5-OA6-CA4
25	m	203	3PE	C32-C31-O31-C3
26	h	201	CDL	CA4-CA3-OA5-PA1
25	L	705	3PE	O22-C21-O21-C2
25	i	201	3PE	C32-C31-O31-C3
26	X	201	CDL	C31-CA7-OA8-CA6
25	m	202	3PE	C32-C31-O31-C3
26	h	201	CDL	C71-CB7-OB8-CB6
26	X	201	CDL	OA9-CA7-OA8-CA6
25	M	501	3PE	C32-C33-C34-C35
25	i	201	3PE	O32-C31-O31-C3
26	L	704	CDL	OA7-CA5-OA6-CA4
25	m	202	3PE	O32-C31-O31-C3
26	X	201	CDL	CA2-C1-CB2-OB2
25	d	201	3PE	C32-C31-O31-C3
25	M	502	3PE	C22-C21-O21-C2
25	M	502	3PE	O22-C21-O21-C2
26	h	201	CDL	OB9-CB7-OB8-CB6
26	X	201	CDL	C1-CB2-OB2-PB2
26	X	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	C18-C19-C20-C21
25	M	501	3PE	C32-C31-O31-C3
25	L	703	3PE	C25-C26-C27-C28
25	m	201	3PE	C32-C31-O31-C3
25	K	101	3PE	C22-C23-C24-C25
25	d	201	3PE	O32-C31-O31-C3
25	m	201	3PE	C26-C27-C28-C29
25	m	201	3PE	O32-C31-O31-C3
26	X	201	CDL	OB9-CB7-OB8-CB6
25	M	501	3PE	O32-C31-O31-C3
25	M	502	3PE	C23-C24-C25-C26
25	Y	201	3PE	C2-C1-O11-P
28	n	201	EHZ	O4-C15-C16-O5
25	L	703	3PE	C32-C31-O31-C3
25	K	101	3PE	C33-C34-C35-C36
25	M	502	3PE	C3C-C3D-C3E-C3F
26	L	704	CDL	C55-C56-C57-C58
25	L	702	3PE	C32-C31-O31-C3
26	L	704	CDL	C71-CB7-OB8-CB6
26	L	704	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
26	L	704	CDL	OB5-CB3-CB4-OB6
25	L	705	3PE	C32-C31-O31-C3
25	L	702	3PE	C24-C25-C26-C27
25	N	401	3PE	C24-C25-C26-C27
25	L	703	3PE	O32-C31-O31-C3
25	i	201	3PE	C22-C21-O21-C2
25	m	201	3PE	C27-C28-C29-C2A
26	L	704	CDL	OB9-CB7-OB8-CB6
25	K	101	3PE	C36-C37-C38-C39
25	M	501	3PE	C2-C3-O31-C31
25	K	101	3PE	O11-C1-C2-O21
25	i	201	3PE	C2-C1-O11-P
28	n	201	EHZ	O2-C9-S1-C10
26	X	201	CDL	OA6-CA4-CA6-OA8
25	L	705	3PE	O32-C31-O31-C3
26	L	704	CDL	C32-C33-C34-C35
28	n	201	EHZ	C3-C4-C5-C6
28	n	201	EHZ	C8-C9-S1-C10
25	L	702	3PE	O32-C31-O31-C3
25	Y	201	3PE	C32-C31-O31-C3
26	h	201	CDL	C14-C15-C16-C17
25	Y	201	3PE	C22-C21-O21-C2
26	X	201	CDL	C11-CA5-OA6-CA4
25	i	201	3PE	O22-C21-O21-C2
25	i	201	3PE	C1-C2-O21-C21
26	h	201	CDL	CB3-CB4-OB6-CB5
27	O	401	ADP	PA-O3A-PB-O3B
26	L	704	CDL	C12-C13-C14-C15
25	M	501	3PE	O11-C1-C2-O21
26	X	201	CDL	CA3-CA4-CA6-OA8
25	d	201	3PE	C12-C11-O13-P
25	Y	201	3PE	O32-C31-O31-C3
25	L	702	3PE	C28-C29-C2A-C2B
25	Y	201	3PE	O22-C21-O21-C2
26	h	201	CDL	CB4-CB3-OB5-PB2
26	X	201	CDL	OA7-CA5-OA6-CA4
25	L	702	3PE	C25-C26-C27-C28
25	K	101	3PE	C1-O11-P-O12
25	K	101	3PE	C1-O11-P-O13
25	K	101	3PE	C1-O11-P-O14
25	K	101	3PE	C11-O13-P-O11
25	L	705	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	M	501	3PE	O13-C11-C12-N
25	M	502	3PE	C1-O11-P-O13
25	M	502	3PE	C11-O13-P-O12
25	N	401	3PE	C11-O13-P-O14
25	Y	201	3PE	C11-O13-P-O11
25	Y	201	3PE	C11-O13-P-O14
25	i	201	3PE	C11-O13-P-O14
25	m	201	3PE	C1-O11-P-O13
25	m	202	3PE	C1-O11-P-O14
26	L	704	CDL	CA2-OA2-PA1-OA4
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
25	K	101	3PE	C2-C1-O11-P
26	X	201	CDL	C1-CA2-OA2-PA1
25	m	201	3PE	C1-C2-O21-C21
26	X	201	CDL	CB6-CB4-OB6-CB5
25	M	501	3PE	O11-C1-C2-C3
26	L	704	CDL	OB5-CB3-CB4-CB6
26	X	201	CDL	C52-C53-C54-C55
25	L	701	3PE	C26-C27-C28-C29
28	n	201	EHZ	C2-C3-C4-C5
25	m	202	3PE	C32-C33-C34-C35
25	L	702	3PE	C33-C34-C35-C36
25	N	401	3PE	C34-C35-C36-C37
25	d	201	3PE	C24-C25-C26-C27
25	m	202	3PE	C23-C24-C25-C26
26	L	704	CDL	C34-C35-C36-C37
25	i	201	3PE	C24-C25-C26-C27
25	N	401	3PE	C28-C29-C2A-C2B
25	L	705	3PE	C24-C25-C26-C27
25	M	502	3PE	C2B-C2C-C2D-C2E
25	i	201	3PE	C2B-C2C-C2D-C2E
25	L	705	3PE	C2-C1-O11-P
26	L	704	CDL	CA4-CA3-OA5-PA1
26	L	704	CDL	C1-CB2-OB2-PB2
26	h	201	CDL	C31-CA7-OA8-CA6
26	h	201	CDL	OA9-CA7-OA8-CA6
25	K	101	3PE	O11-C1-C2-C3
25	M	502	3PE	C39-C3A-C3B-C3C
25	K	101	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	L	705	3PE	C34-C35-C36-C37
26	X	201	CDL	C59-C60-C61-C62
27	O	401	ADP	PA-O3A-PB-O2B
25	N	401	3PE	C23-C24-C25-C26
25	N	401	3PE	C12-C11-O13-P
25	L	702	3PE	C39-C3A-C3B-C3C
25	M	502	3PE	C3A-C3B-C3C-C3D
25	m	202	3PE	O11-C1-C2-O21
26	L	704	CDL	C11-C12-C13-C14
25	L	705	3PE	C33-C34-C35-C36
26	L	704	CDL	C77-C78-C79-C80
25	K	101	3PE	C2A-C2B-C2C-C2D
25	L	701	3PE	C38-C39-C3A-C3B
25	L	702	3PE	C34-C35-C36-C37
25	L	702	3PE	C2B-C2C-C2D-C2E
25	i	201	3PE	O21-C21-C22-C23
25	K	101	3PE	C27-C28-C29-C2A
25	m	202	3PE	C39-C3A-C3B-C3C
26	h	201	CDL	C11-C12-C13-C14
26	h	201	CDL	C72-C71-CB7-OB8
25	m	201	3PE	C29-C2A-C2B-C2C

There are no ring outliers.

18 monomers are involved in 160 short contacts:

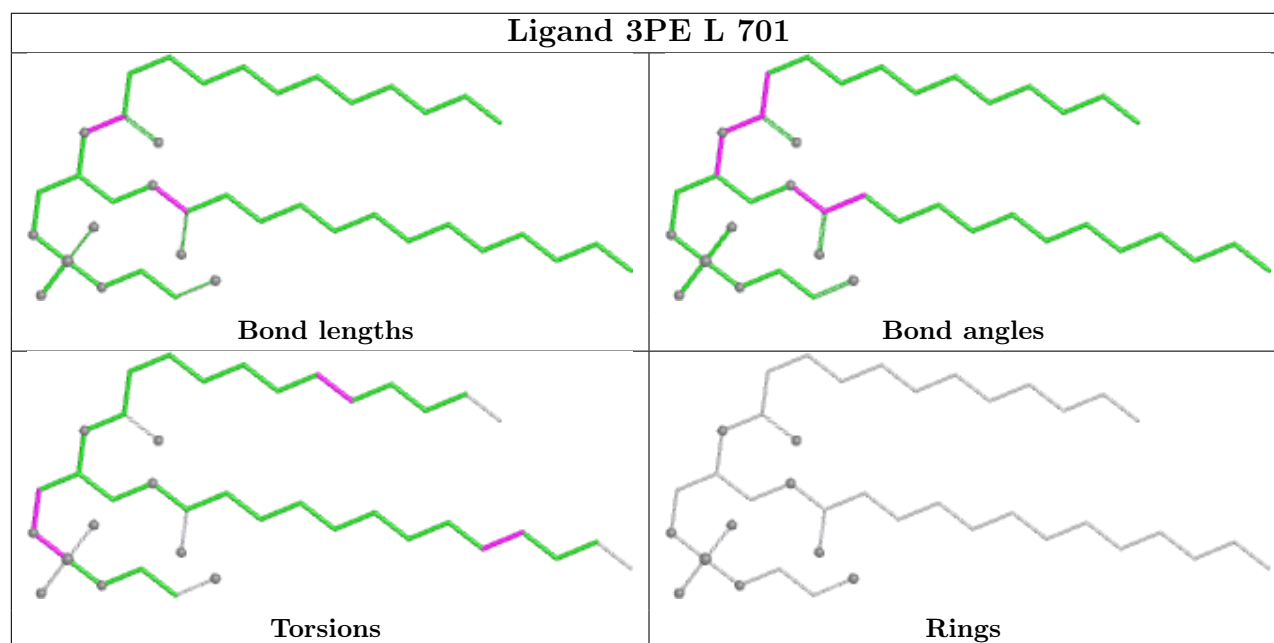
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	701	3PE	8	0
25	L	703	3PE	6	0
25	L	702	3PE	9	0
25	m	202	3PE	10	0
26	L	704	CDL	16	0
25	i	201	3PE	19	0
25	K	101	3PE	9	0
25	m	203	3PE	4	0
25	m	201	3PE	12	0
25	M	501	3PE	3	0
25	M	502	3PE	5	0
27	O	401	ADP	11	0
25	N	401	3PE	11	0
26	h	201	CDL	17	0
26	X	201	CDL	9	0
25	Y	201	3PE	8	0

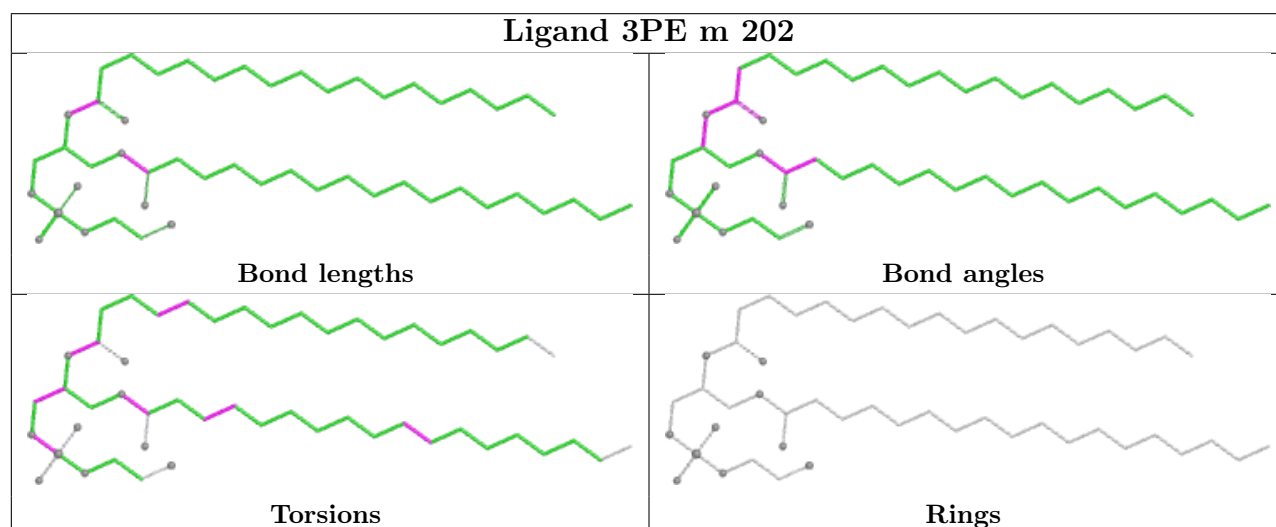
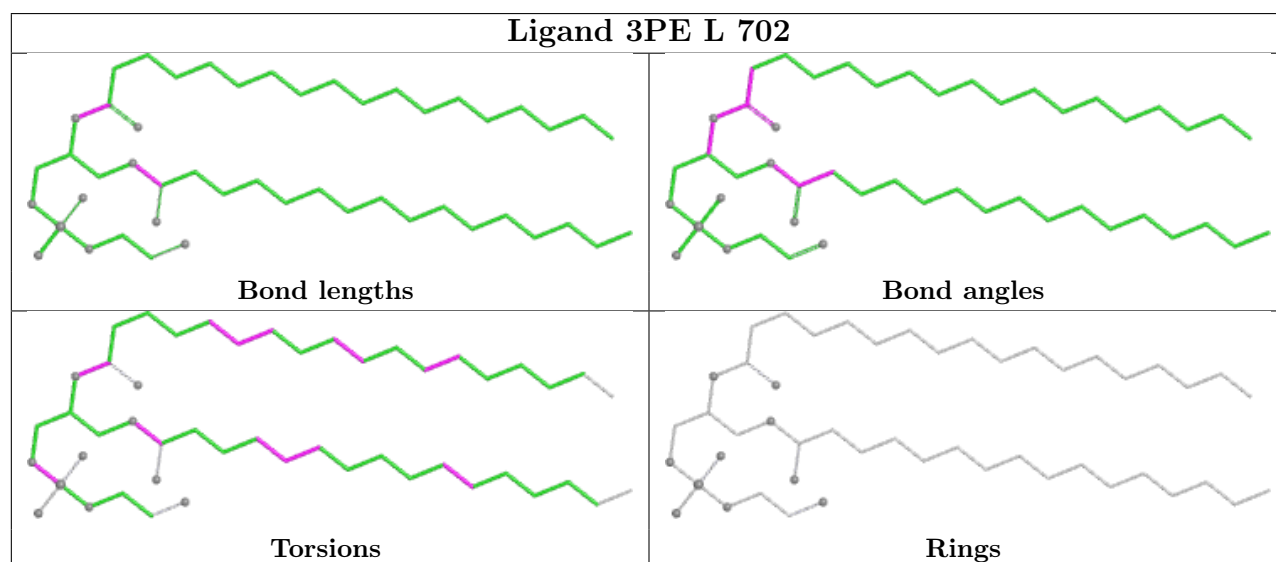
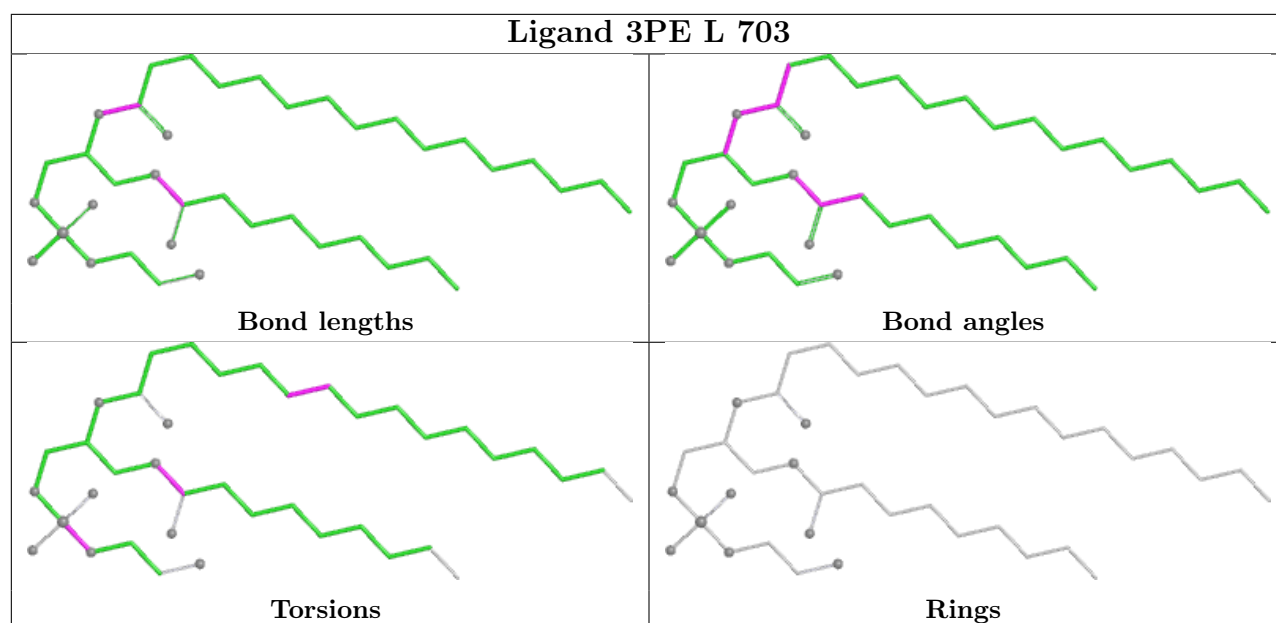
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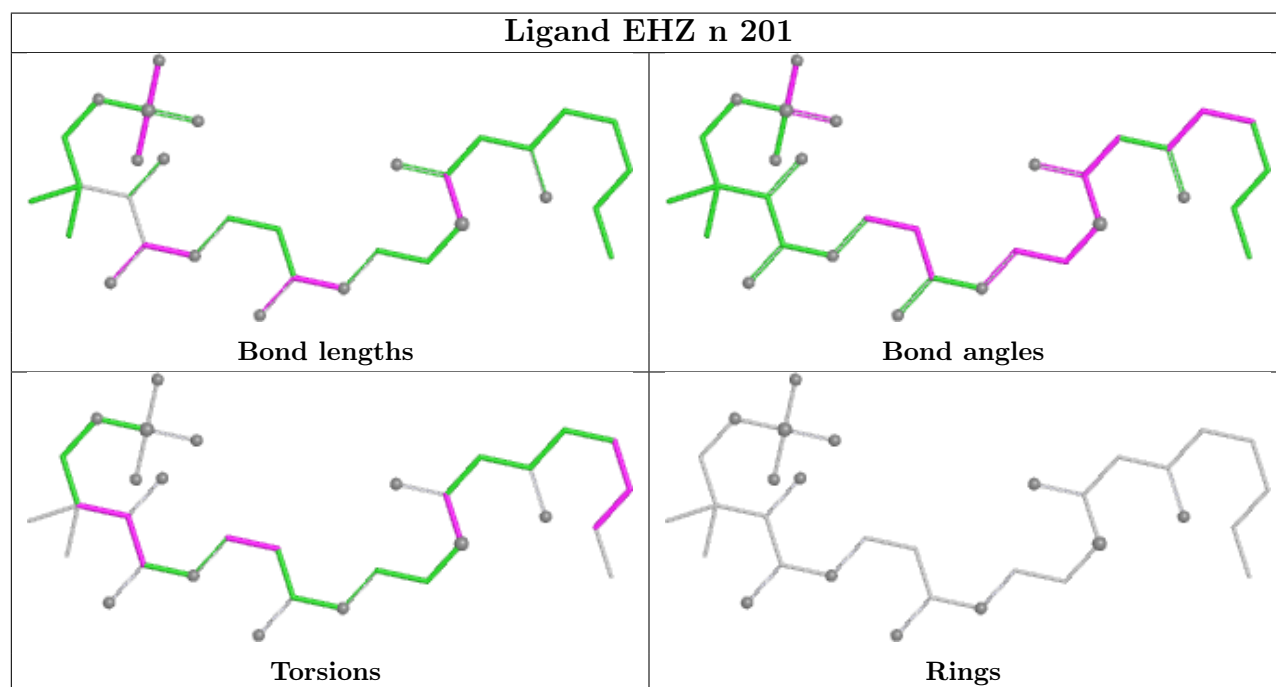
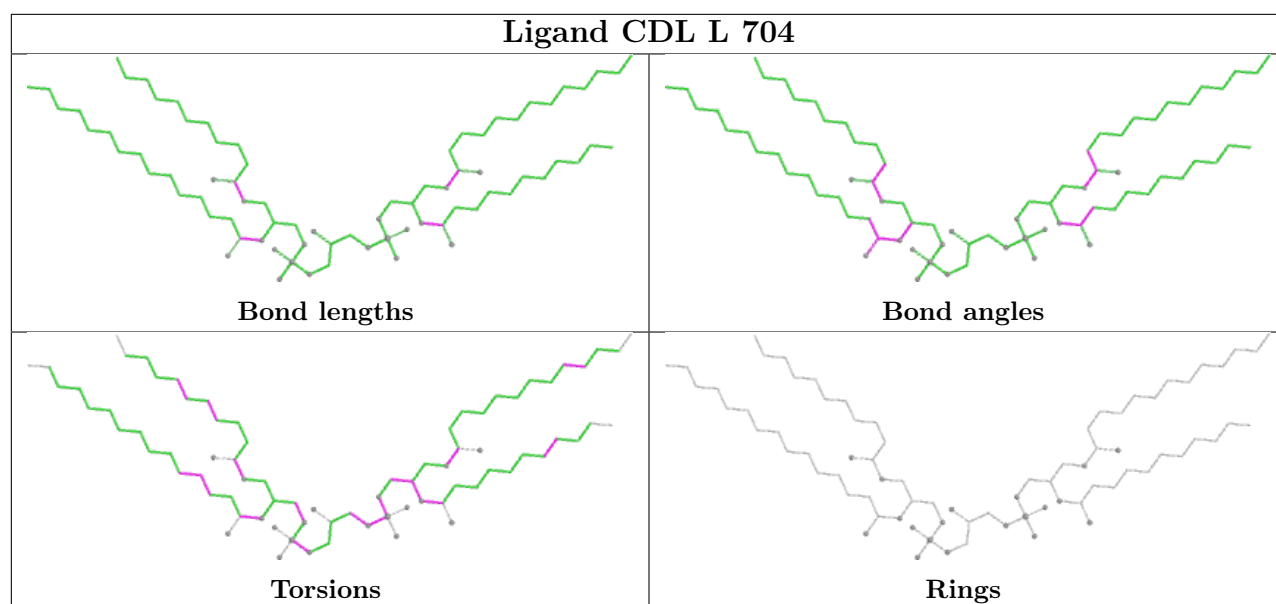
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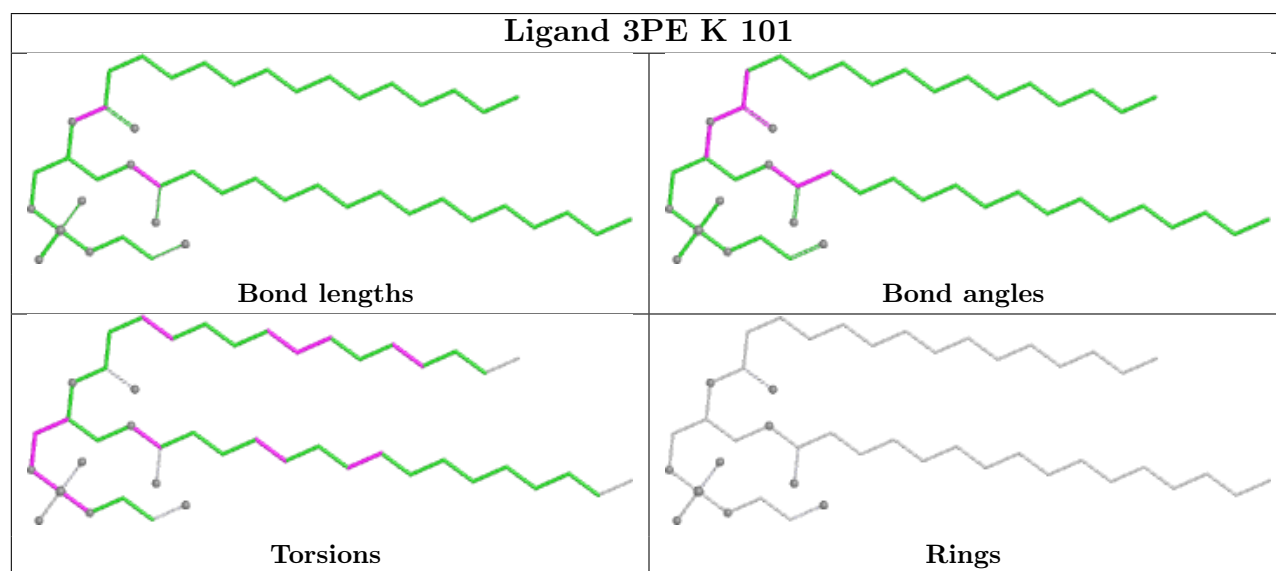
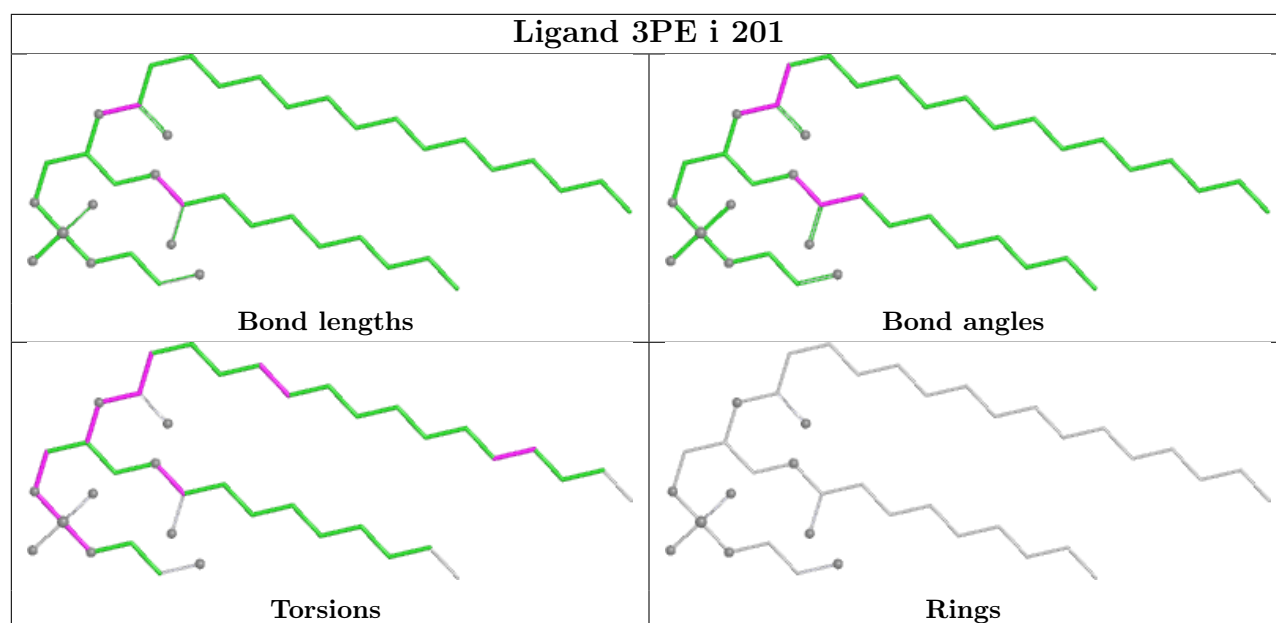
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	705	3PE	5	0
25	d	201	3PE	8	0

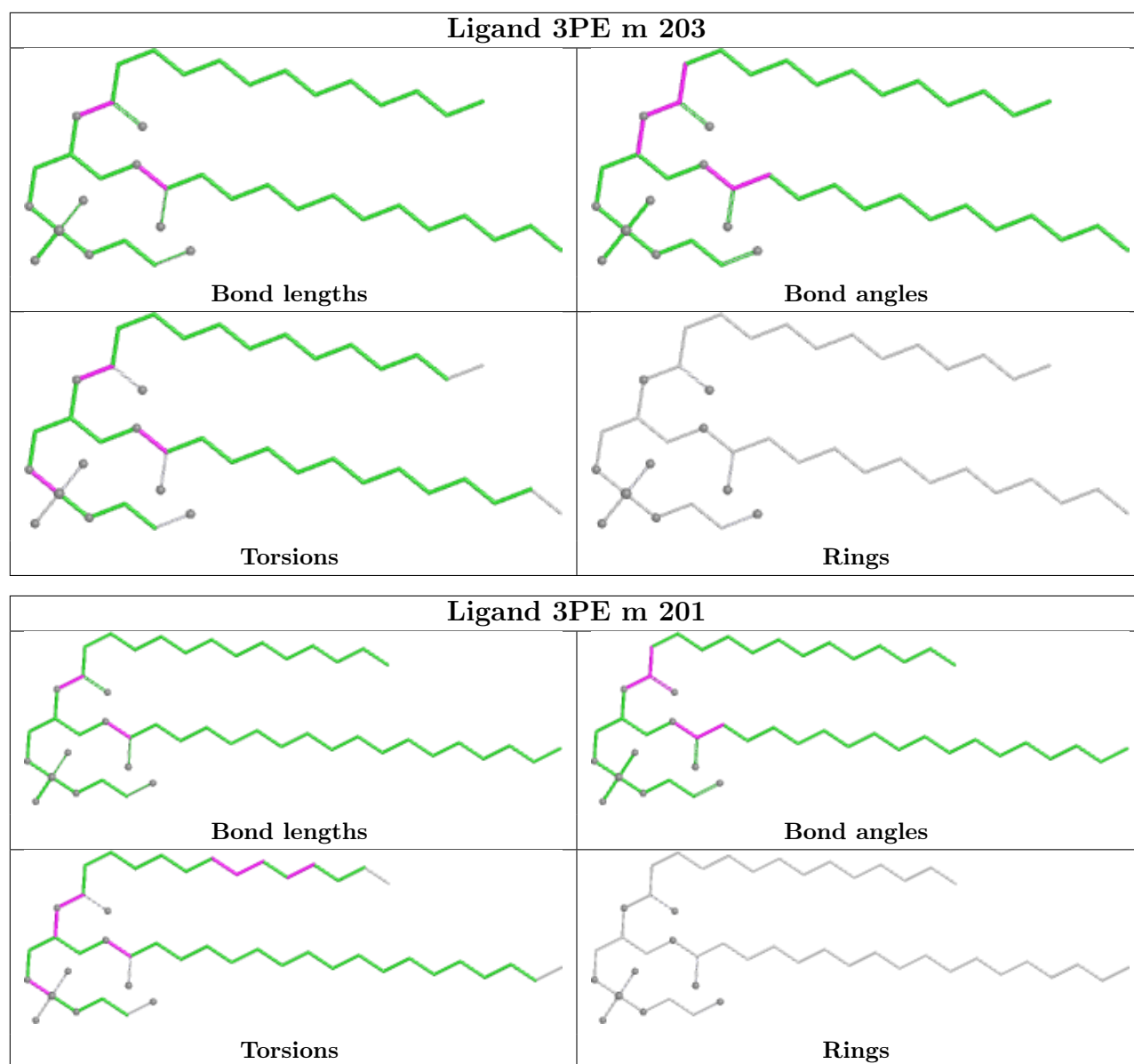
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



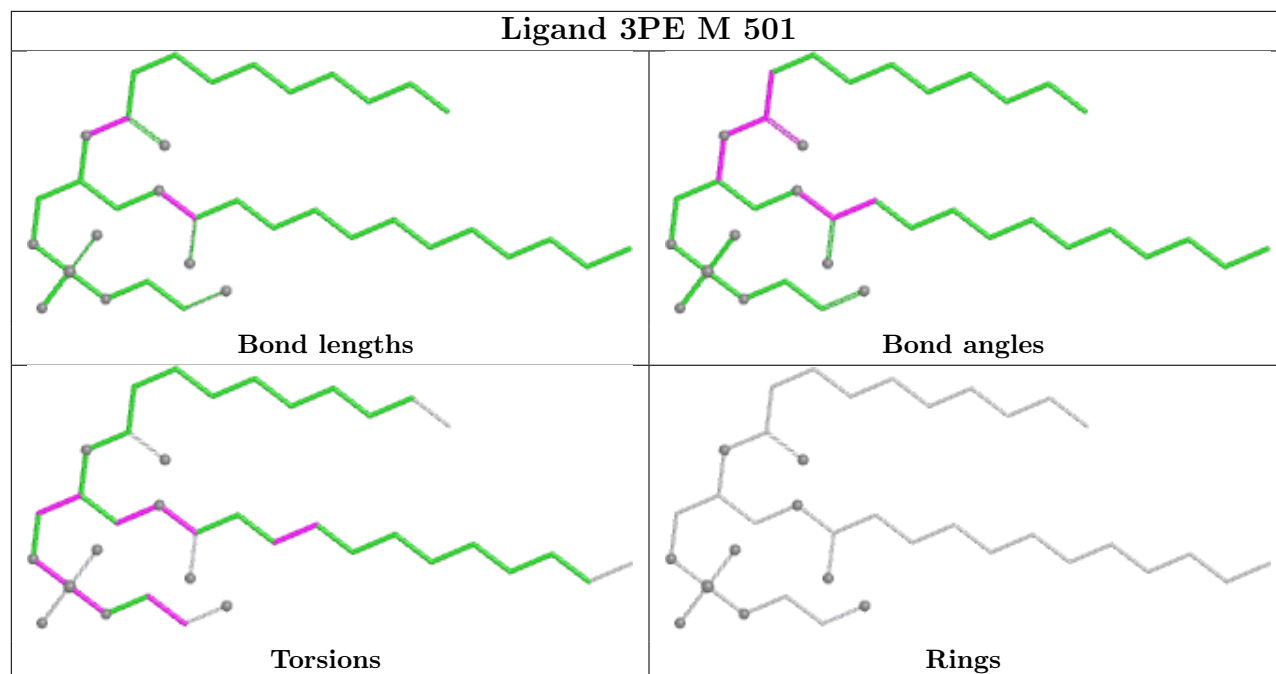




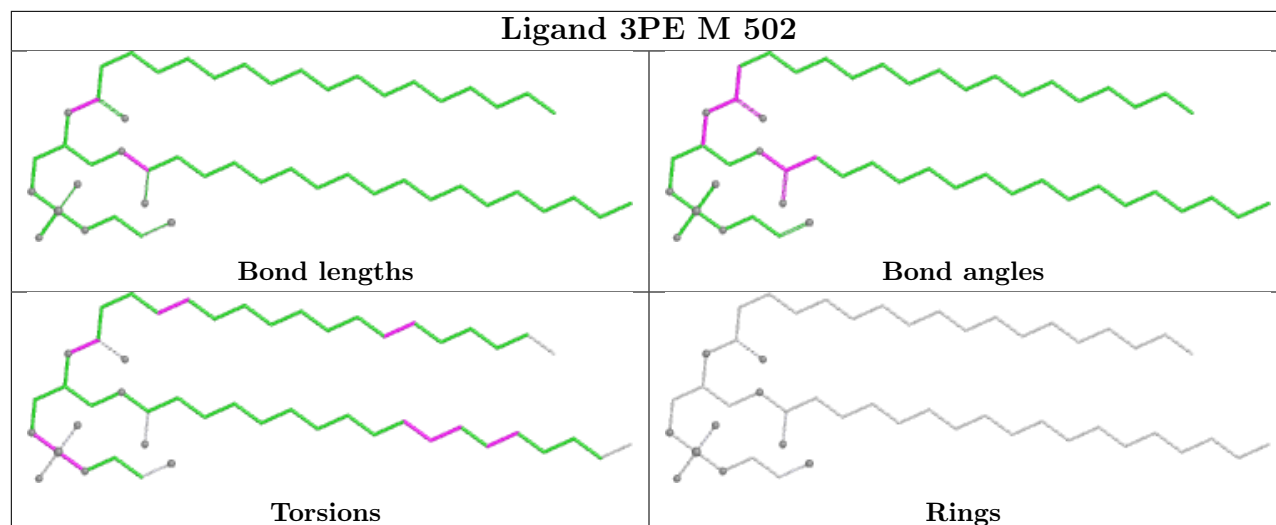


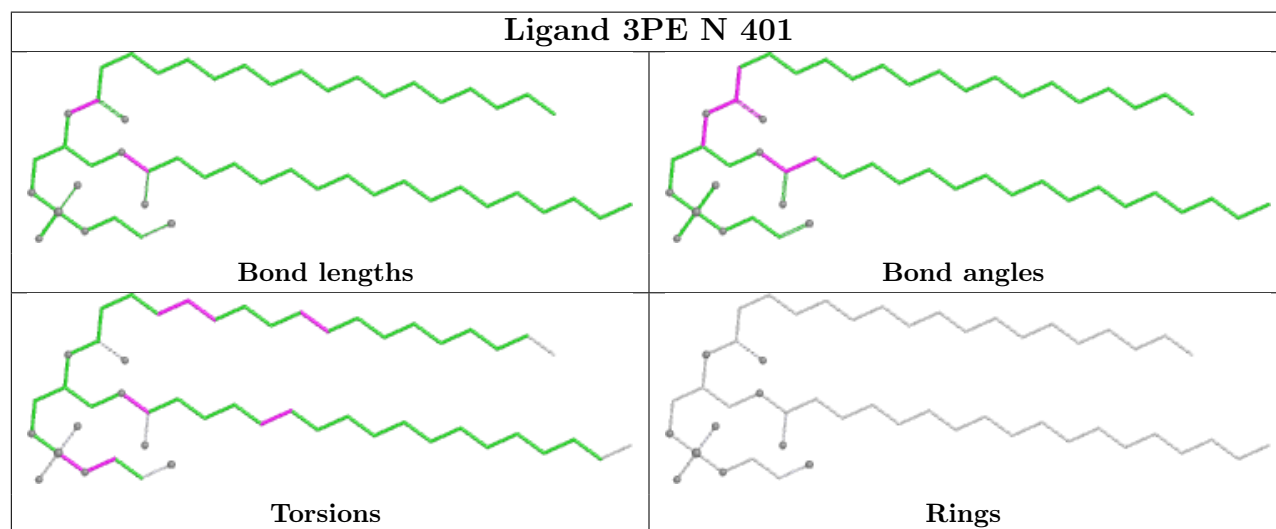
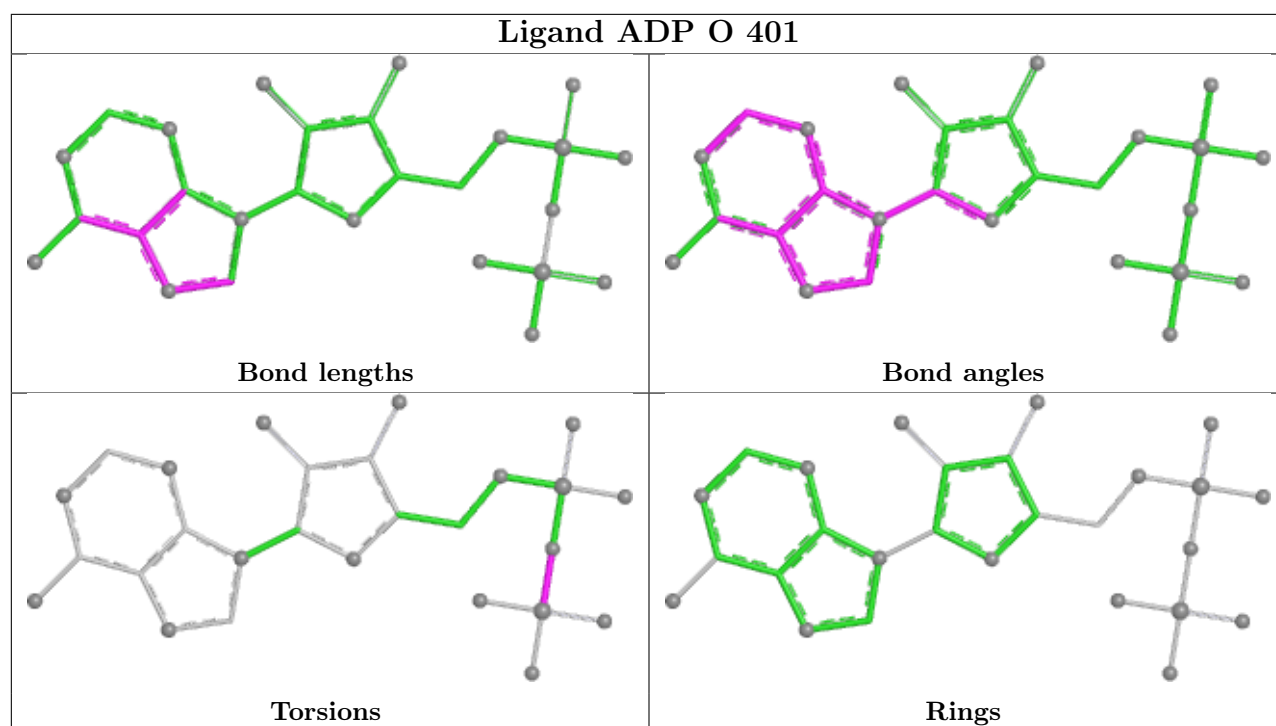


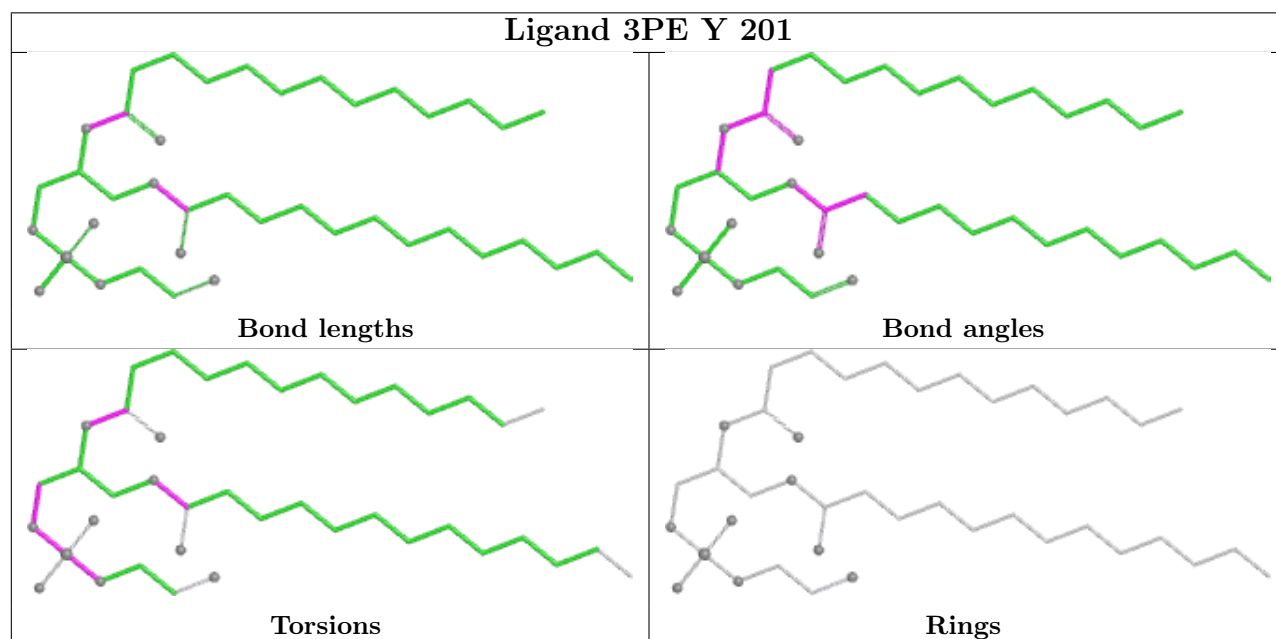
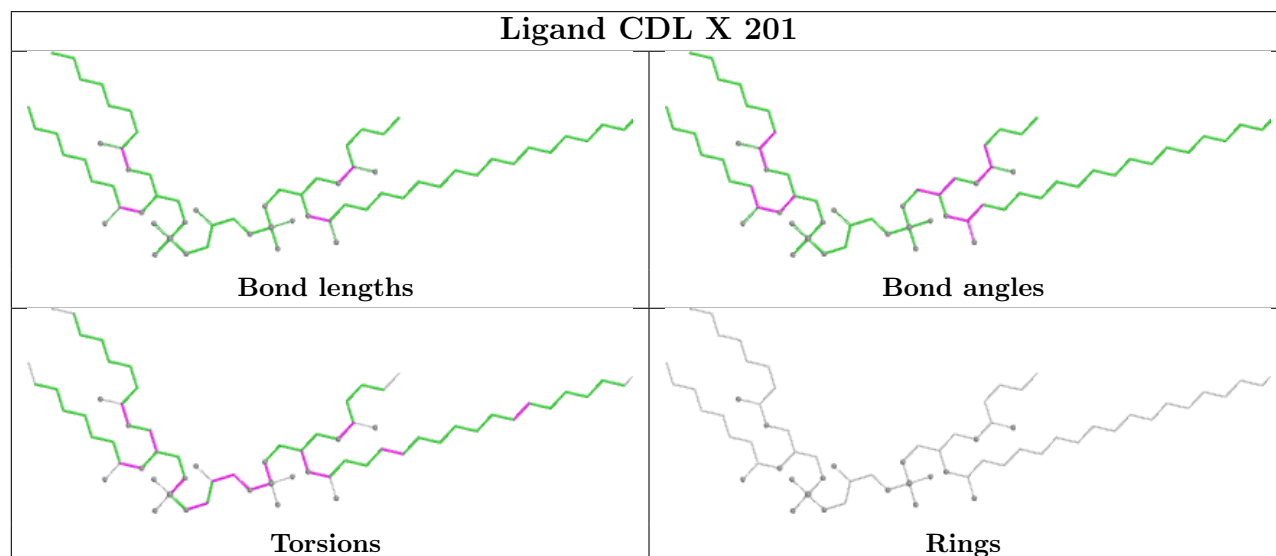
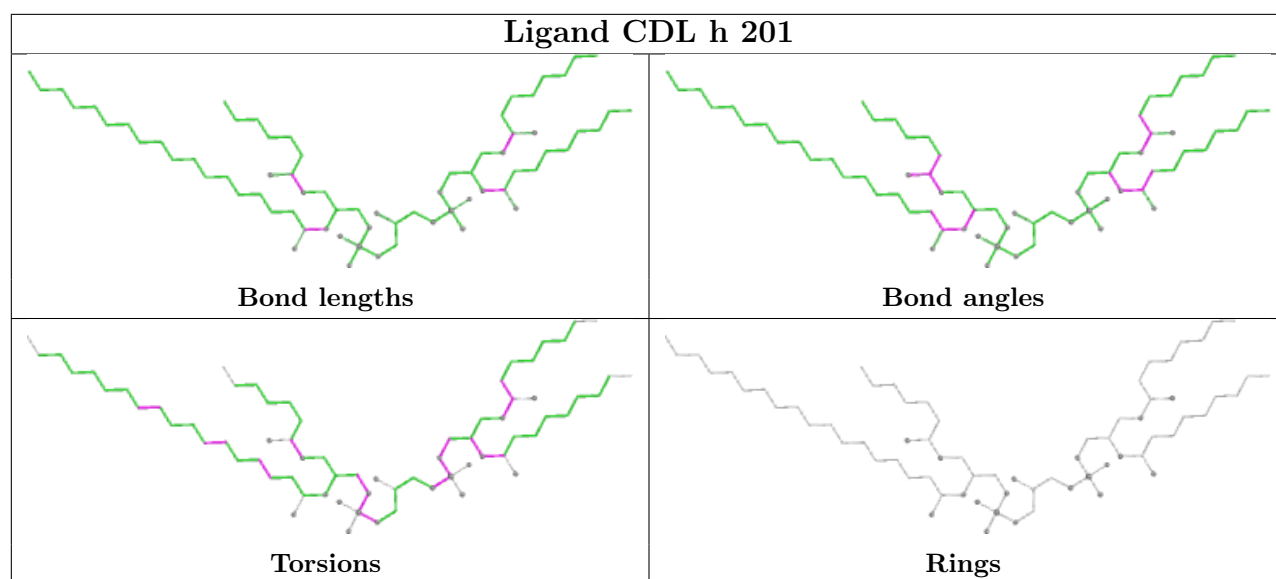
Ligand 3PE M 501

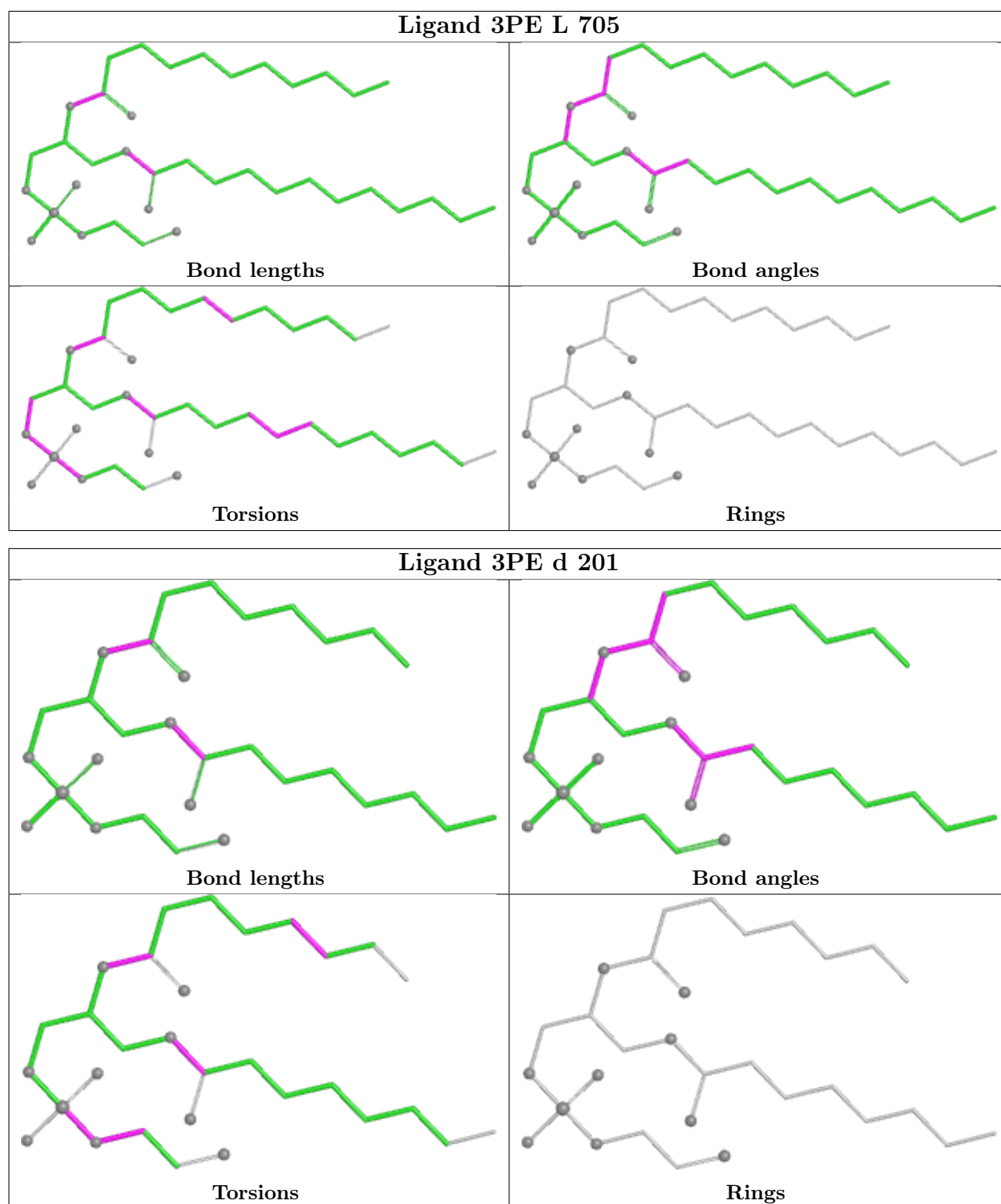


Ligand 3PE M 502









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

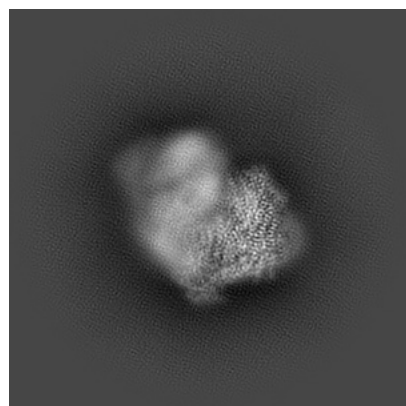
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35342. These allow visual inspection of the internal detail of the map and identification of artifacts.

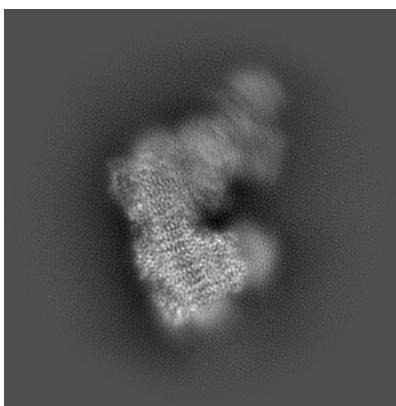
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

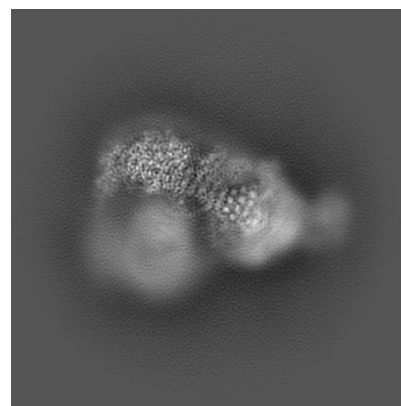
6.1.1 Primary map



X

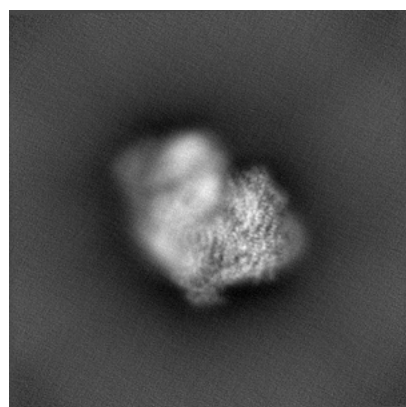


Y

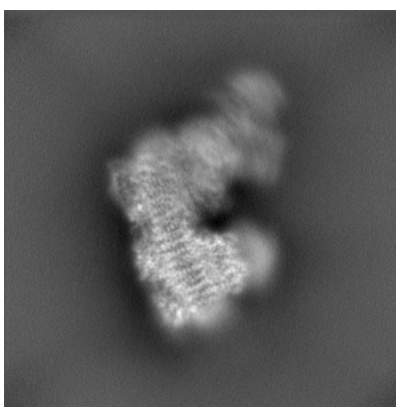


Z

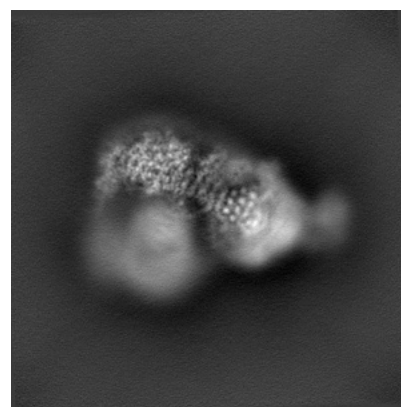
6.1.2 Raw map



X



Y

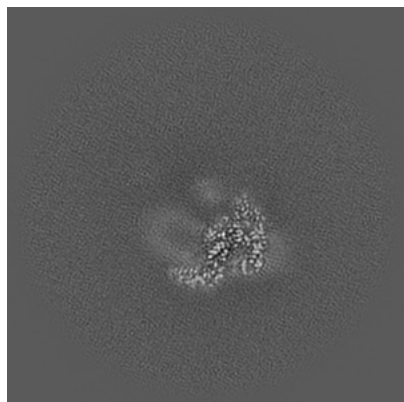


Z

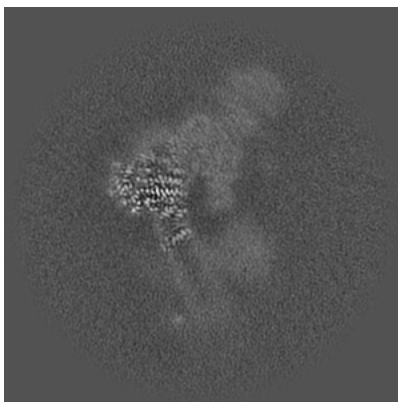
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

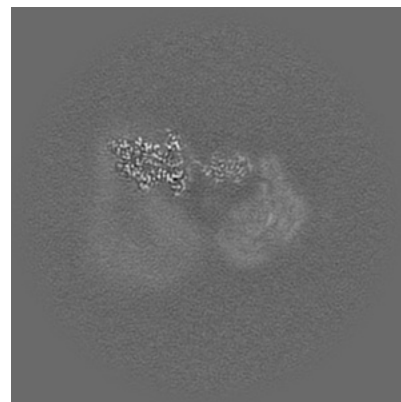
6.2.1 Primary map



X Index: 192

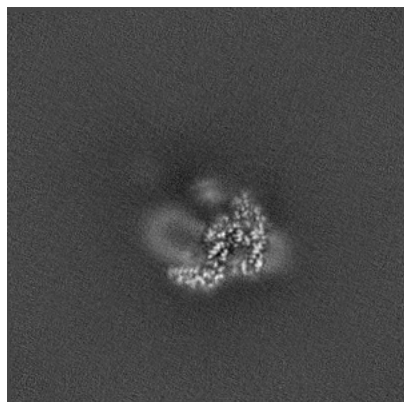


Y Index: 192

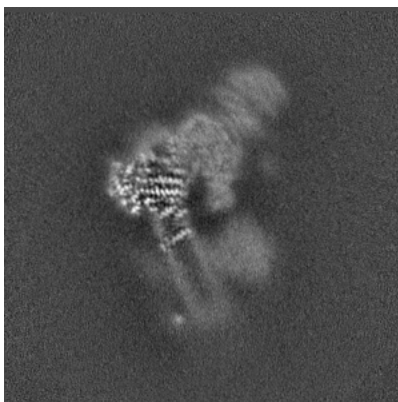


Z Index: 192

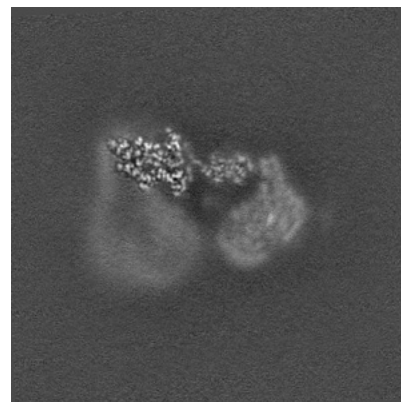
6.2.2 Raw map



X Index: 192



Y Index: 192

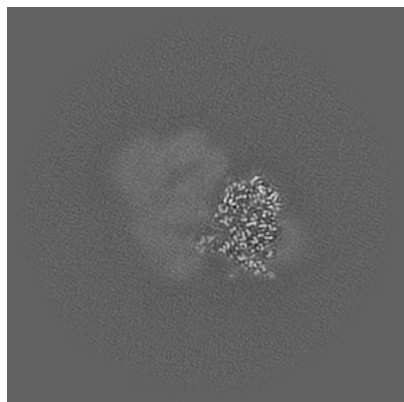


Z Index: 192

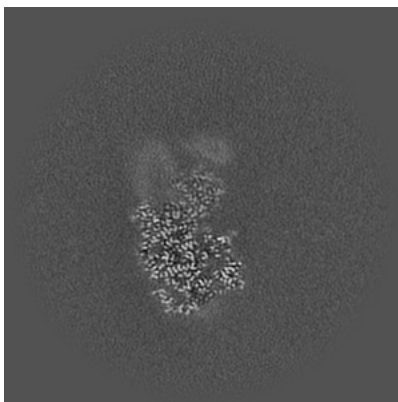
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

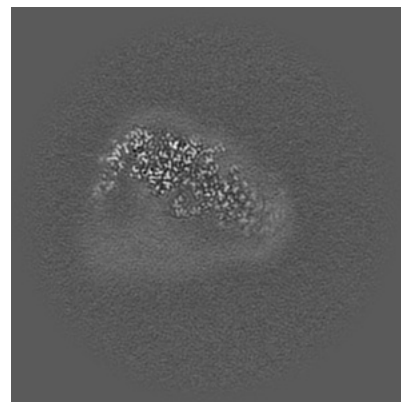
6.3.1 Primary map



X Index: 158

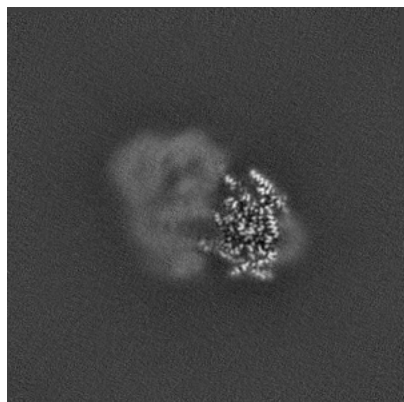


Y Index: 226

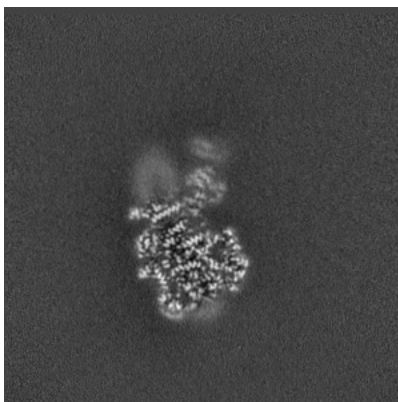


Z Index: 162

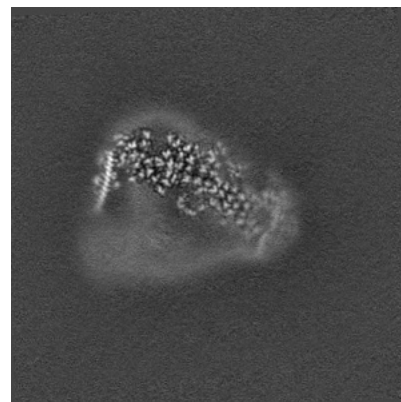
6.3.2 Raw map



X Index: 153



Y Index: 237

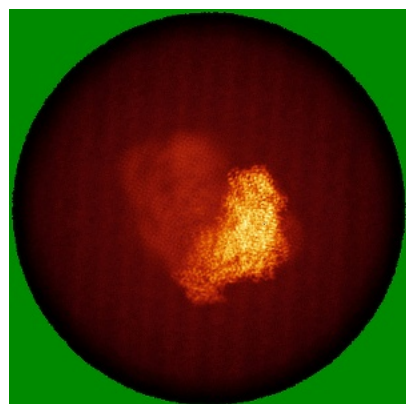


Z Index: 167

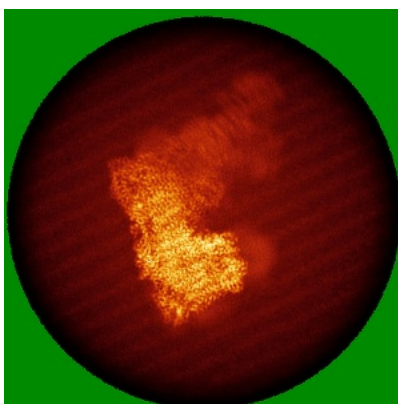
The images above show the largest variance slices of the map in three orthogonal directions.

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

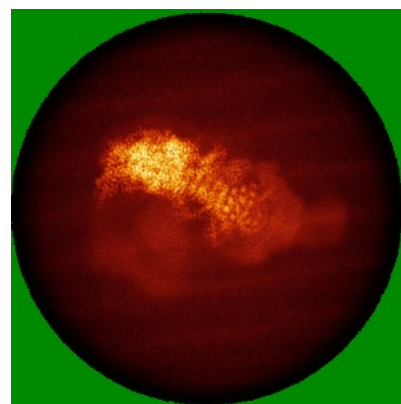
6.4.1 Primary map



X

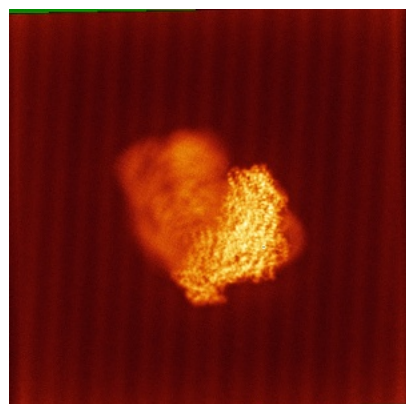


Y

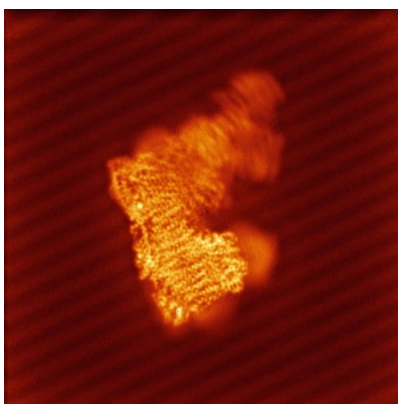


Z

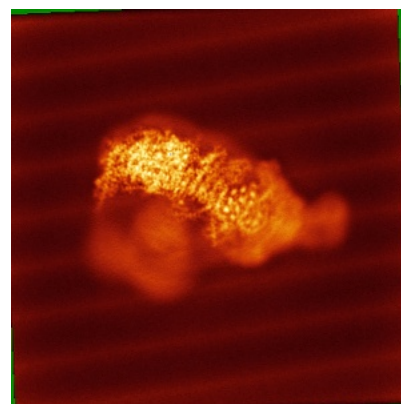
6.4.2 Raw map



X



Y



Z

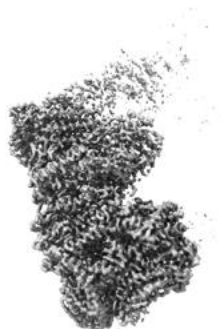
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



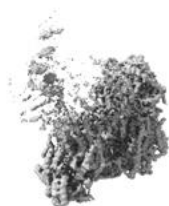
Y



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.

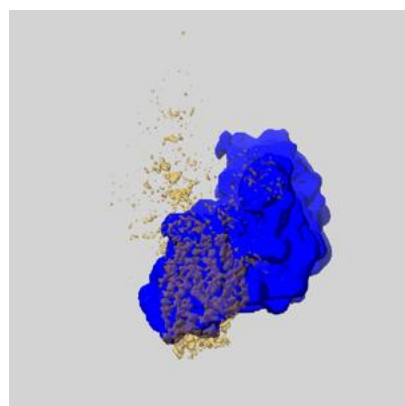
6.6 Mask visualisation [i](#)

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

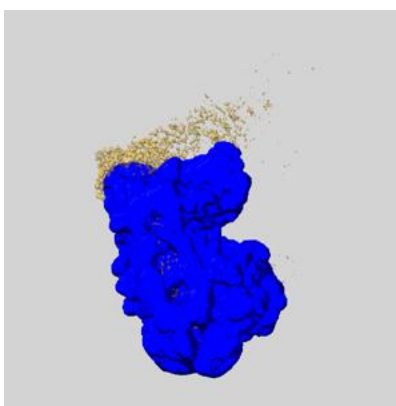
A mask typically either:

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

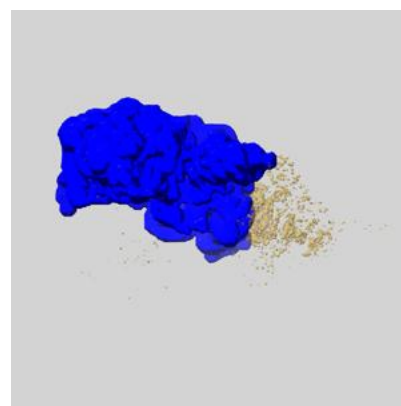
6.6.1 emd_35342_msk_1.map [i](#)



X



Y

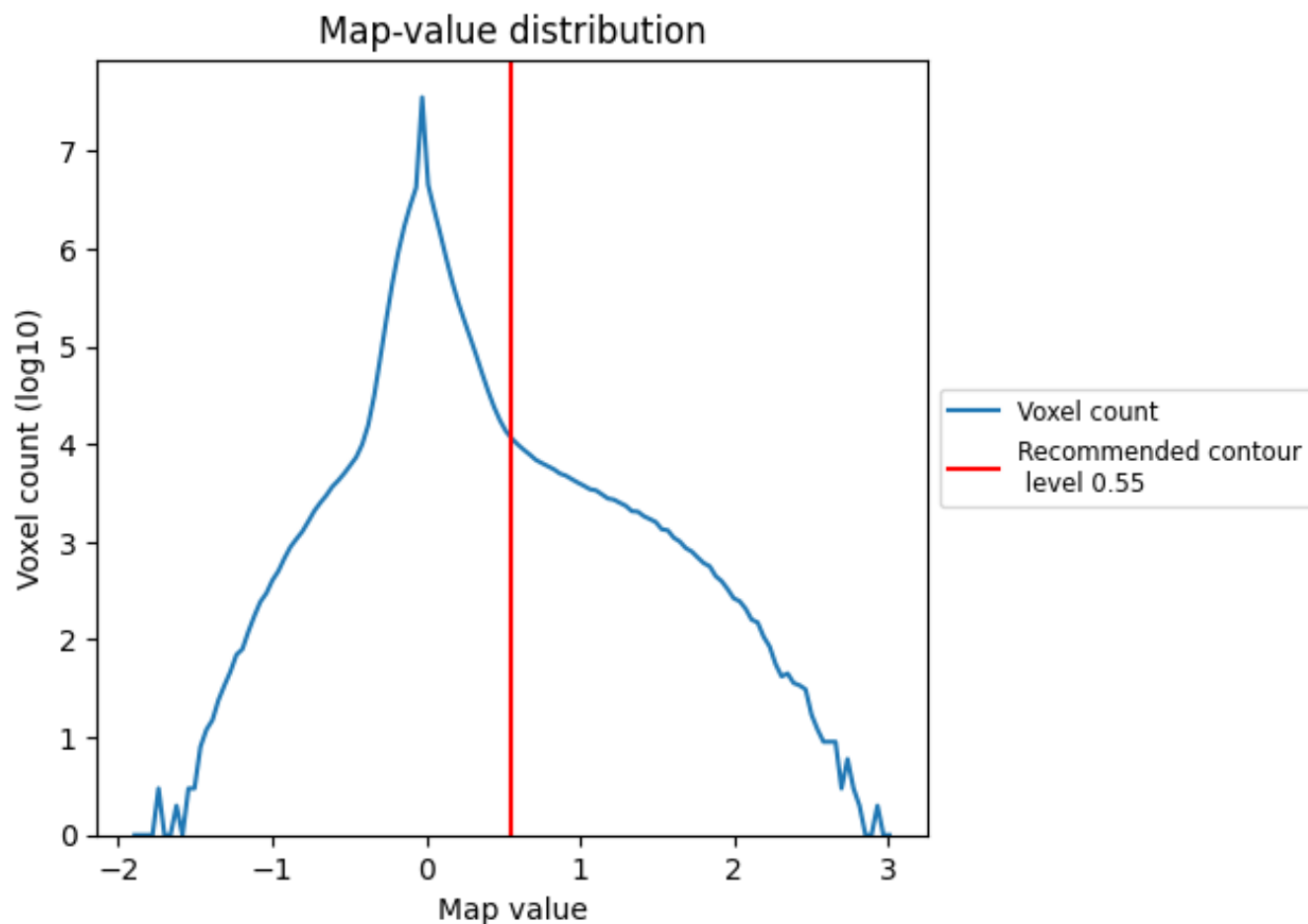


Z

7 Map analysis [i](#)

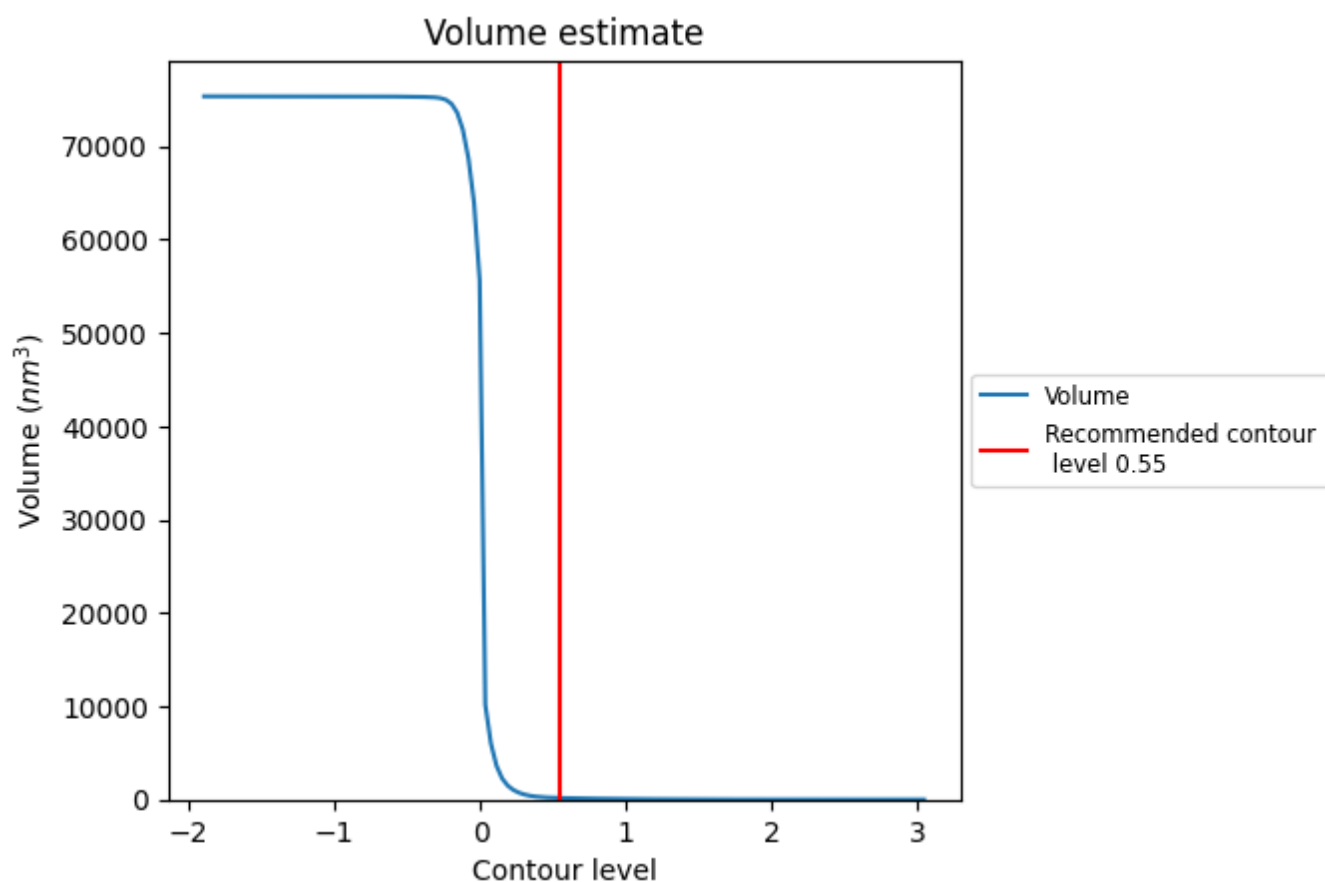
This section contains the results of statistical analysis of the map.

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.

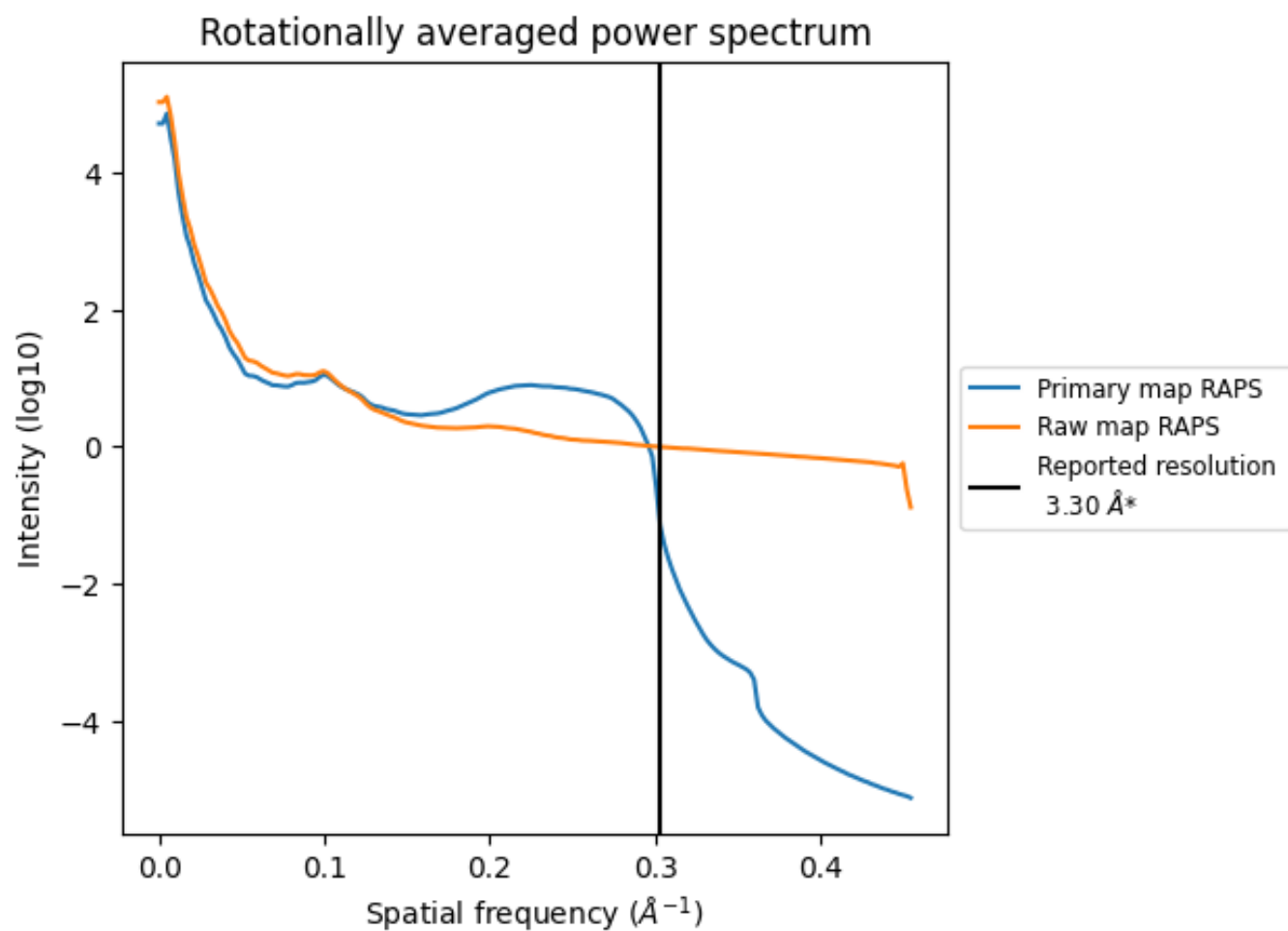
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 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 ⓘ

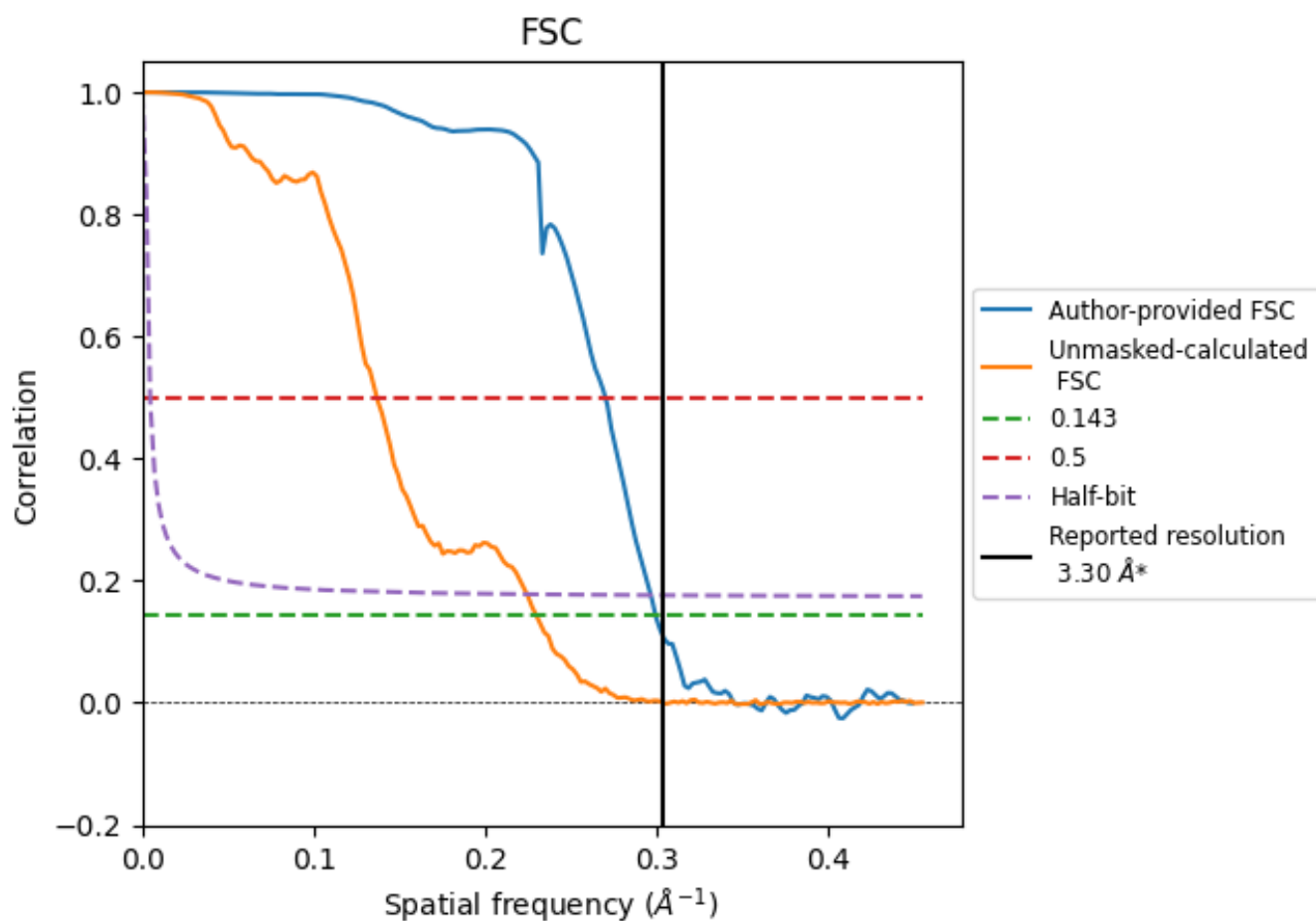


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 [i](#)

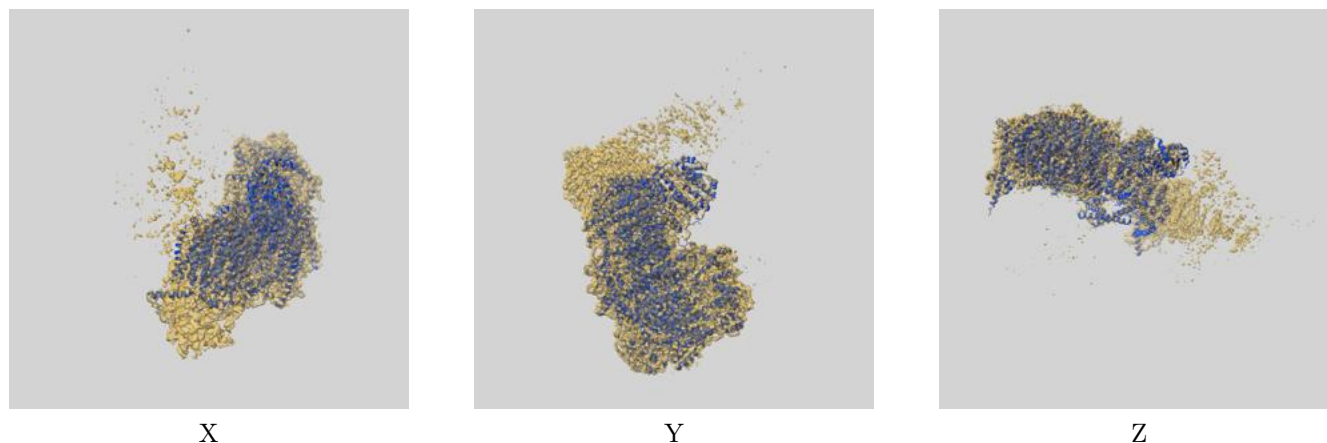
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.71	3.37
Unmasked-calculated*	4.35	7.31	4.46

*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 4.35 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

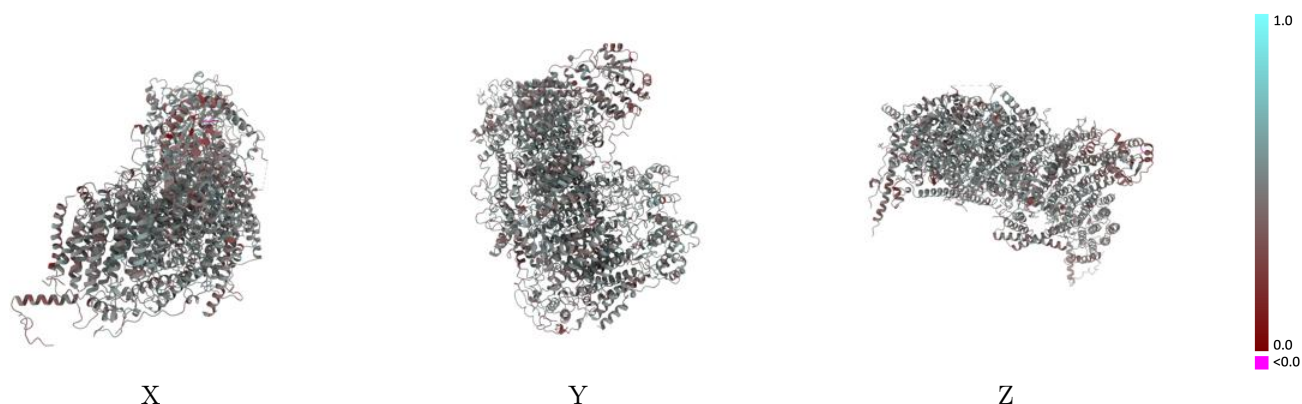
This section contains information regarding the fit between EMDB map EMD-35342 and PDB model 8IBF. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



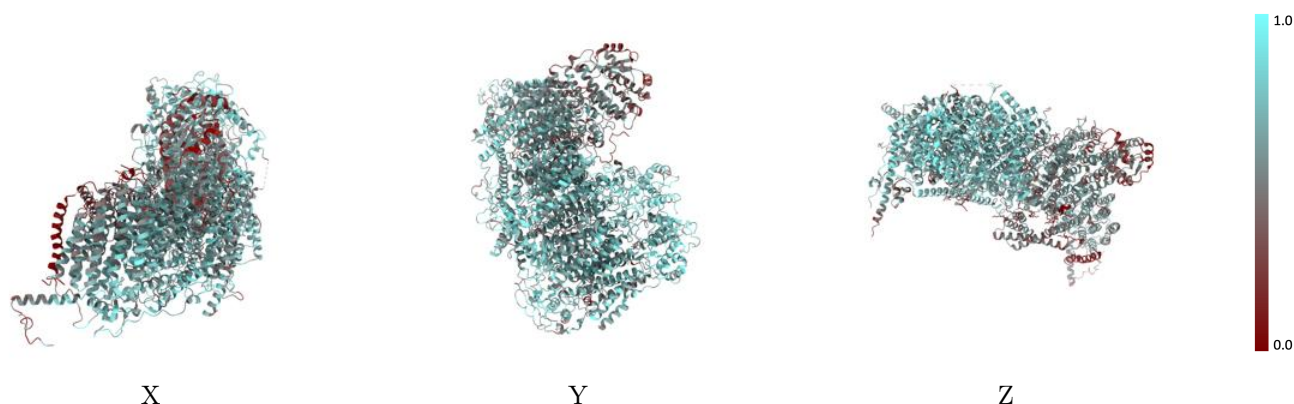
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



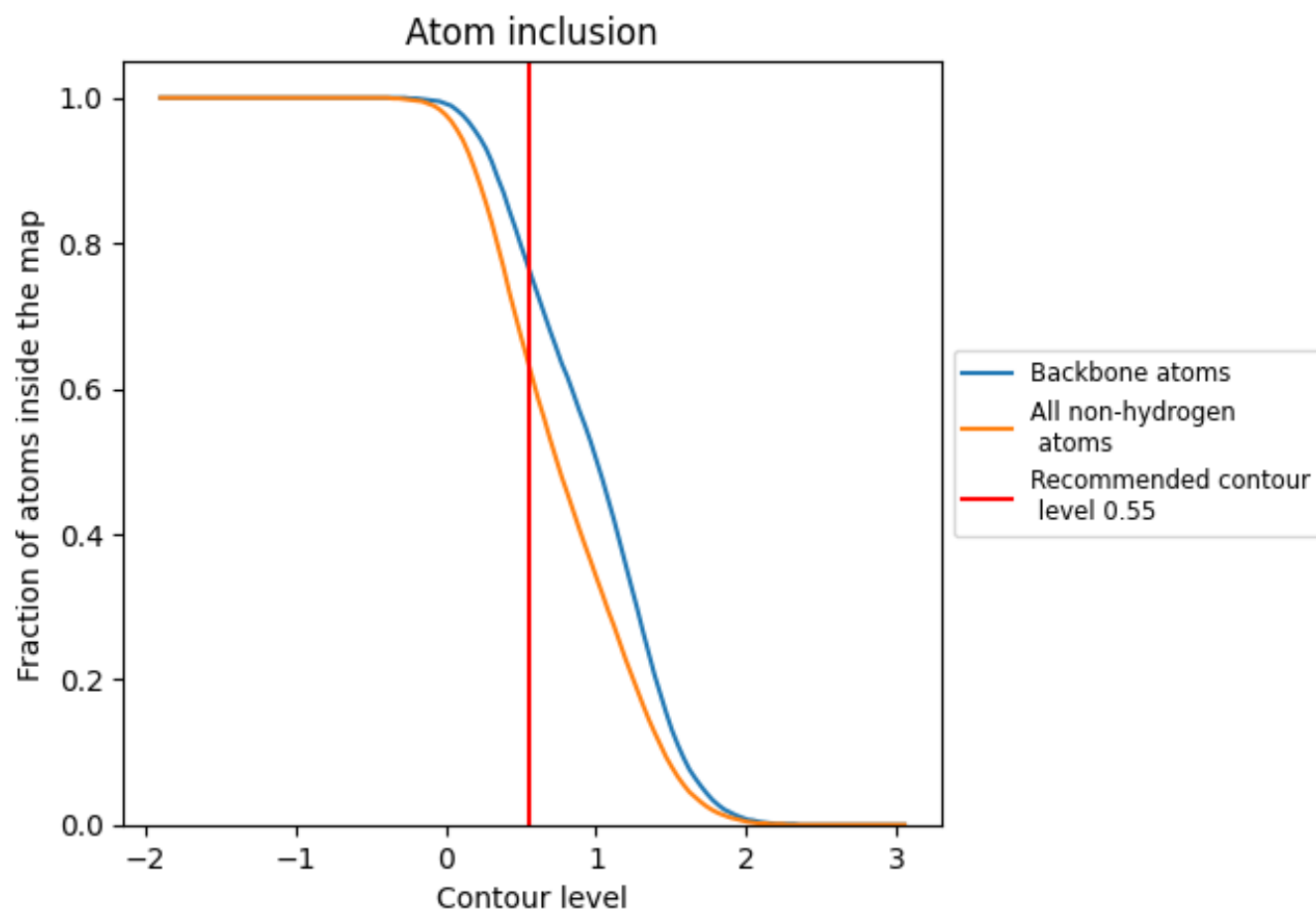
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.6350	 0.4710
D	 0.3180	 0.4700
J	 0.4500	 0.4350
K	 0.5620	 0.4800
L	 0.6700	 0.4800
M	 0.6990	 0.4960
N	 0.6570	 0.4930
O	 0.4340	 0.4140
U	 0.7270	 0.4810
X	 0.6470	 0.4890
Y	 0.4580	 0.4380
c	 0.5160	 0.4070
d	 0.6720	 0.4970
e	 0.5930	 0.4310
f	 0.6290	 0.4650
g	 0.6610	 0.4610
h	 0.6960	 0.4730
i	 0.7010	 0.4960
j	 0.6930	 0.4550
k	 0.7190	 0.4850
l	 0.7340	 0.4930
m	 0.6250	 0.4810
n	 0.7600	 0.5010
o	 0.6480	 0.4350
p	 0.6780	 0.4590

