



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 8IC4 / pdb_00008ic4
EMDB ID : EMD-35354
Title : Respiratory complex Membrane domain of CI, focus-refined of type I, PERK
-/- mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.20 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:

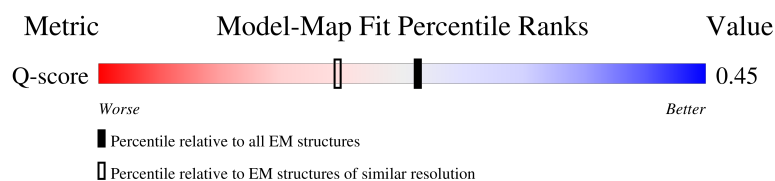
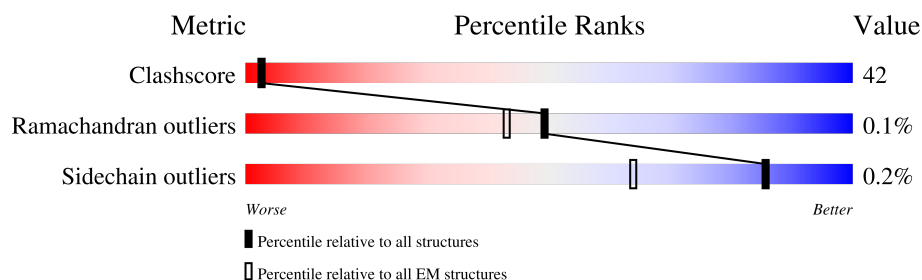
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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.



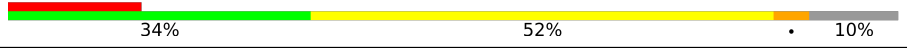
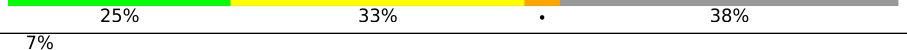
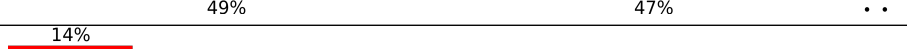
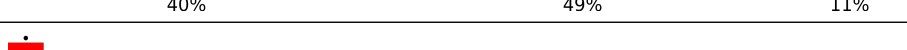
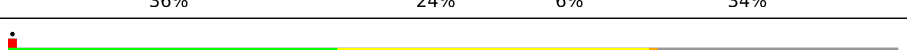
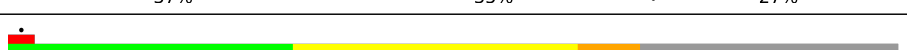
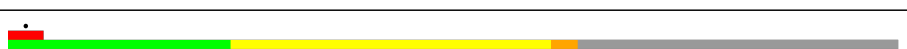
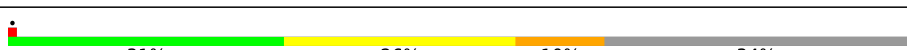
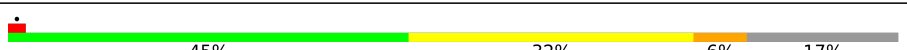
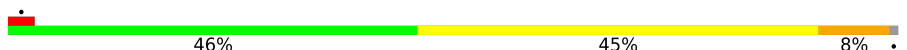
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31638 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
			355	231	59	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- 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	318	Total	C	N	O	S	0	0
			2588	1662	426	490	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	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	99	Total	C	N	O	S	0	0
			835	541	134	156	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	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	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	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

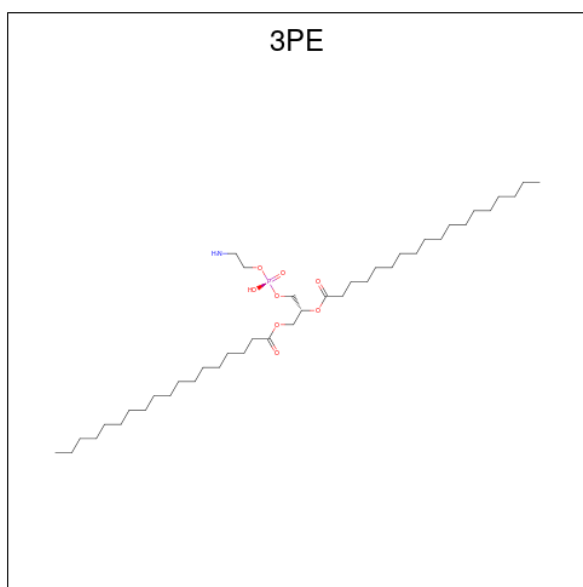
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

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

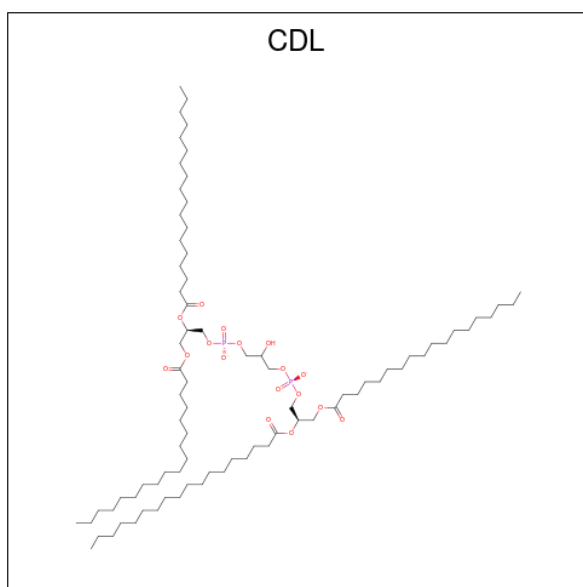
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

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



Mol	Chain	Residues	Atoms					AltConf
25	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	J	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
			44	34	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
			49	39	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
			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
			73	54	17	2	
26	M	1	Total	C	O	P	0
			82	63	17	2	
26	Y	1	Total	C	O	P	0
			71	52	17	2	
26	d	1	Total	C	O	P	0
			65	46	17	2	
26	h	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

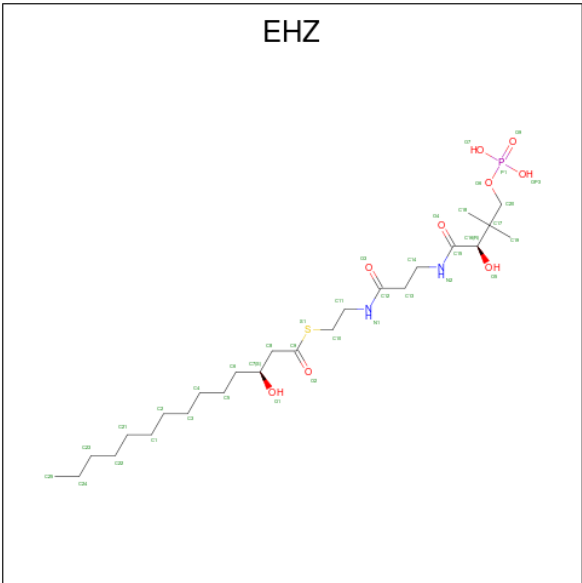
Mol	Chain	Residues	Atoms		AltConf
27	L	1	Total	Zn	0
			1	1	

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

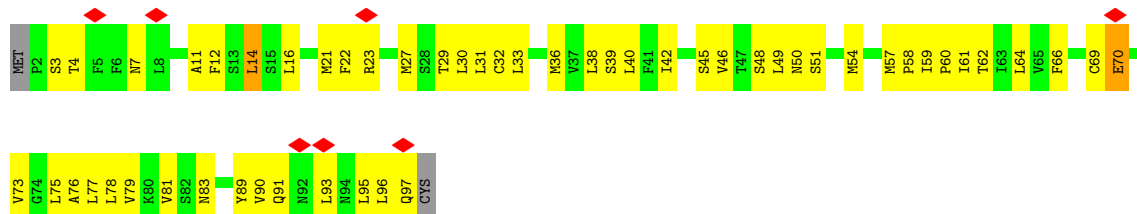
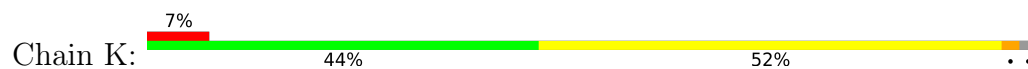
- Molecule 29 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



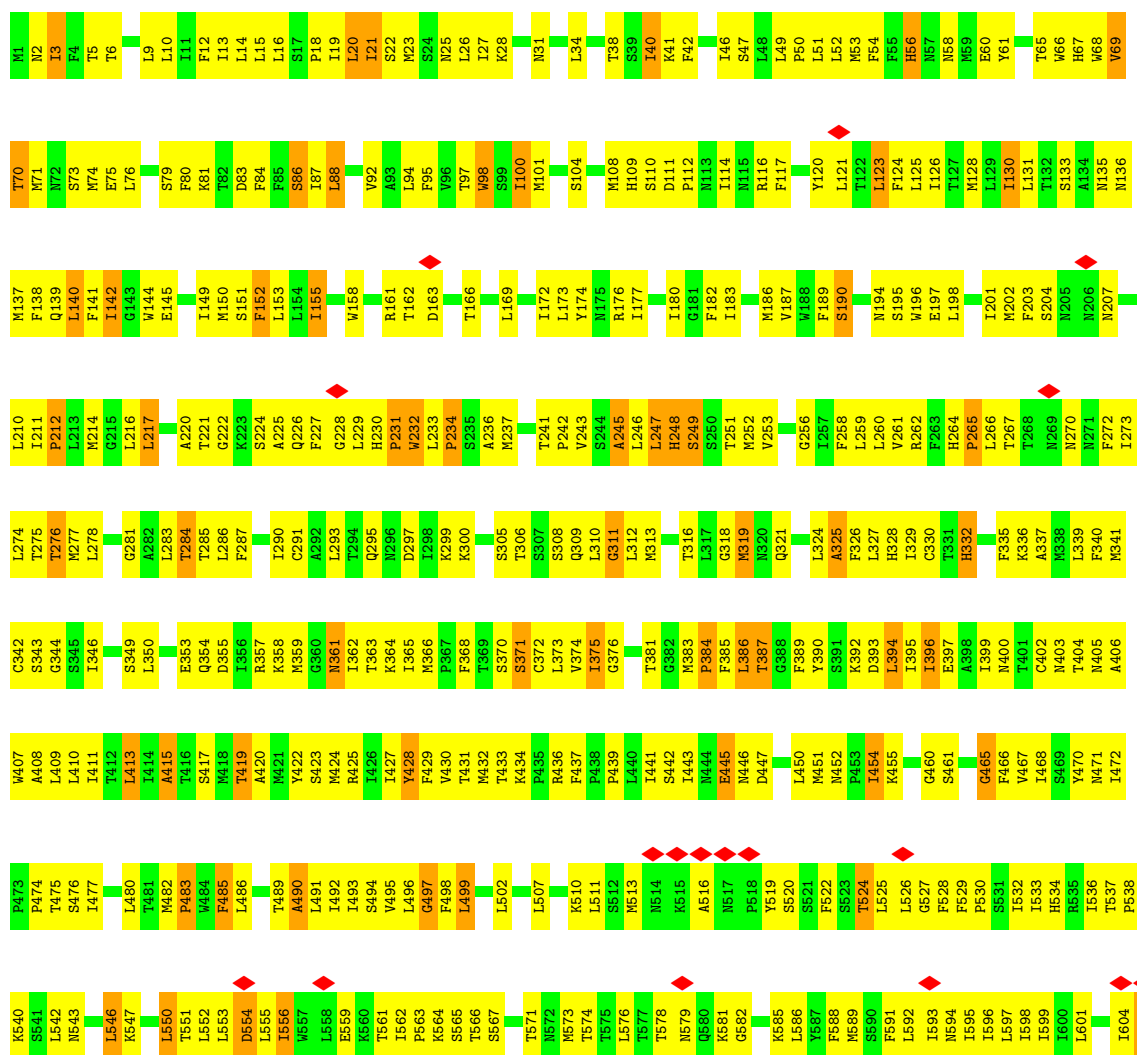
Mol	Chain	Residues	Atoms						AltConf
29	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	



• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L

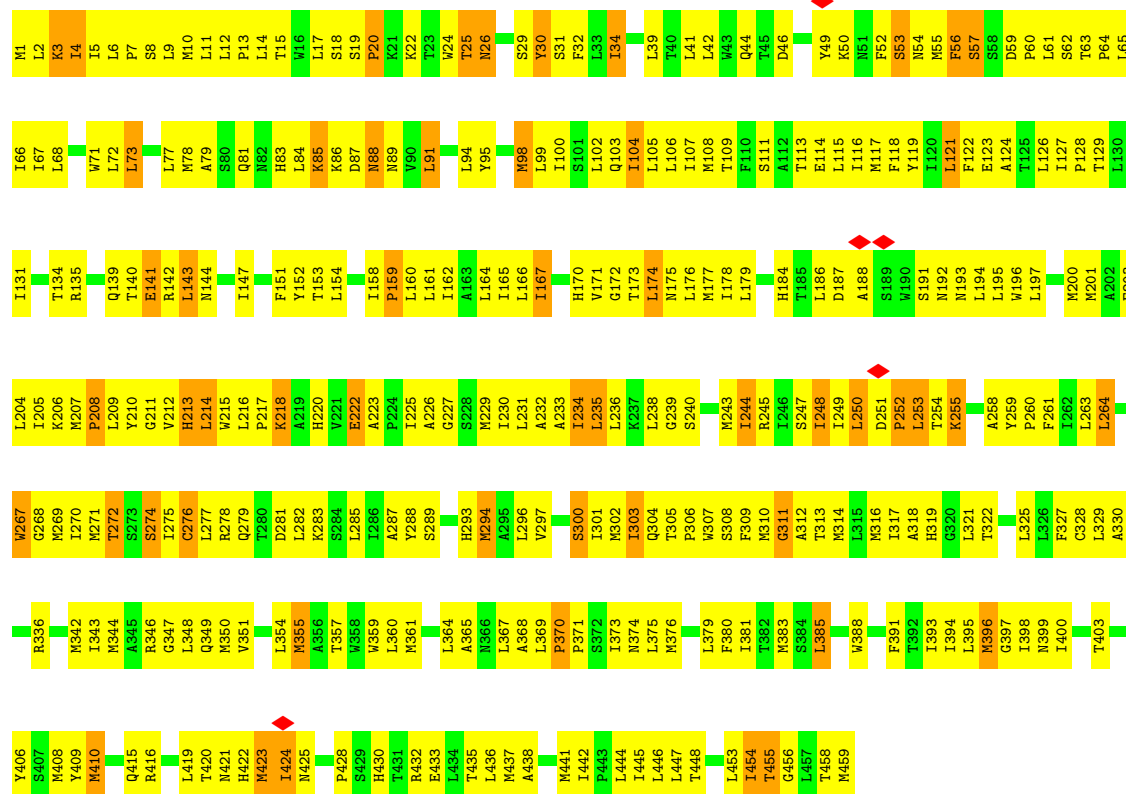
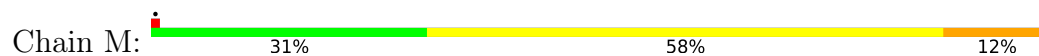


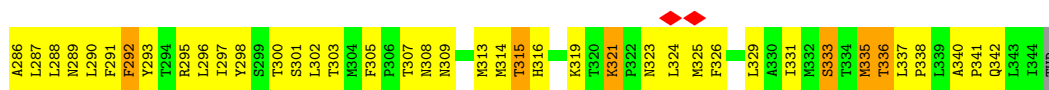
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5



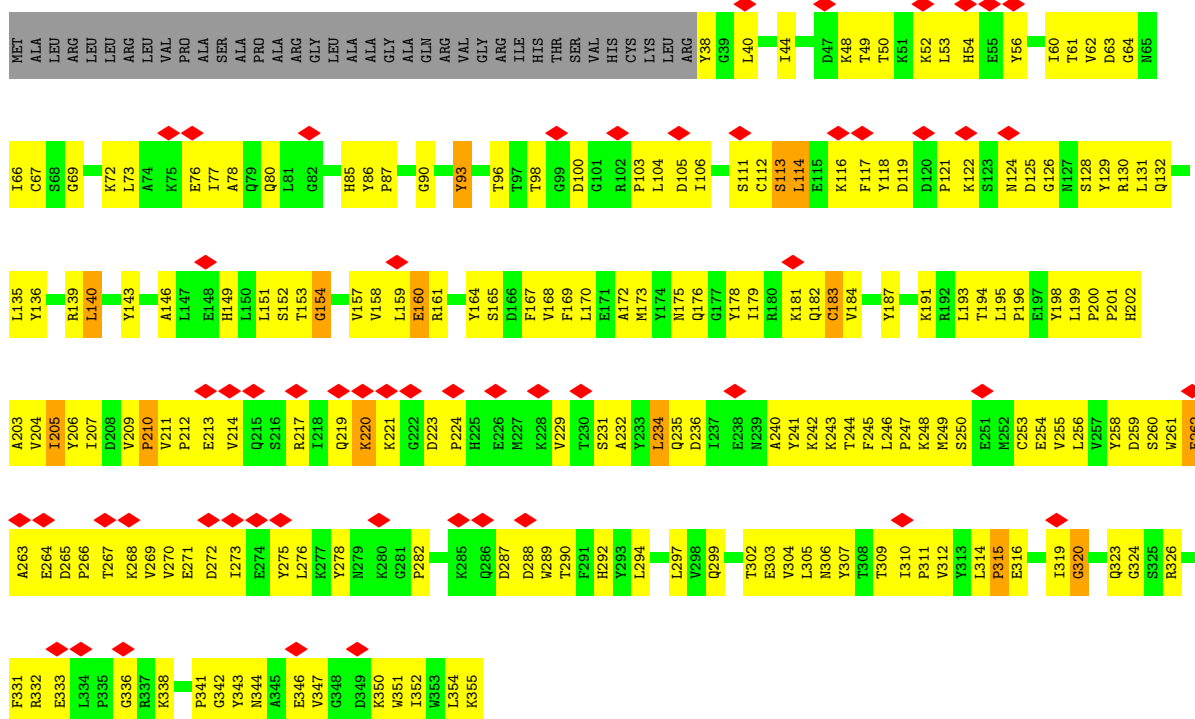


• Molecule 5: NADH-ubiquinone oxidoreductase chain 4

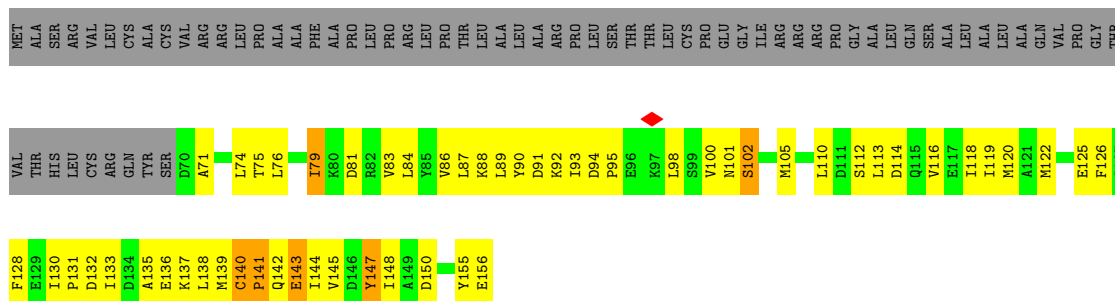
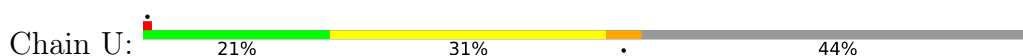




- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 8: Acyl carrier protein, mitochondrial



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



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

ASP LEU GLN VAL SER LYS VAL THR VAL LYS THR ASP ARG PRO LEU PRO GLU ASN PRO THR HIS SER ARG A146 A147 P148 V153 I154 E155 L158 K159 P160 A161 K162 H163 G164 T165 R166 F167 F168 F169 W170 T171 V172

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

Chain Y: 25% 50% 47% ..

MET ALA MET VAL K5 R6 F7 F8 E9 S10 Y11 H12 H13 E13 L14 P15 D16 G17 T18 Q19 C20 H21 R22 K23 T24 Y25 I26 A29 L30 I37 G38 S39 A40 Y41 L45 M46 P47 A48 D49 S50 T51 L52 E53 A54 R57 V58 G59 R60 F63 T64 A65 I68 M71 F72

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

Chain c: 12% 25% 33% 38%

MET ALA PRO SER VAL VAL LEU ARG SER PHE ARG ARG LEU LEU ALA PRO ARG ALA LEU PRO PRO CYS SER SER THR ARG LYS F29 Y30 V31 R32 E33 P34 V35 N36 A37 K38 P39 N40 M41 L42 A43 V44 G45 L46 S47 A50 W55 Q60 T61 H62 R63 E64 V66 Y69 K70 R71 N73 G74 L75 G11J

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

Chain d: 7% 48% 49%

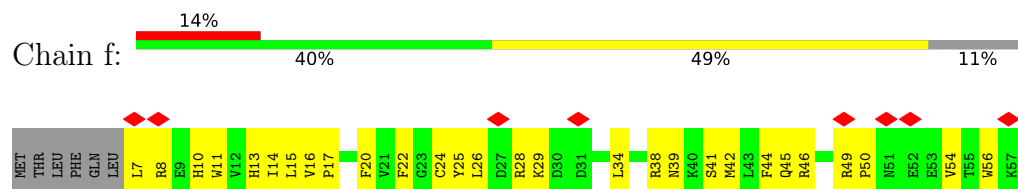
M1 M2 N3 G4 R5 P6 G7 H8 E9 P10 L11 K12 F13 L14 P15 D16 E17 A18 R19 S20 L21 P22 P23 P24 K25 L26 N27 D28 P29 R30 L37 Y39 L43 M44 D45 N46 M47 L48 R49 M50 R51 P52 V53 M54 G57 L58 H59 R60 Q61 L62 L63 F64 T65 T66 G72 Y73 F74 K77 R78 Q79 R80 Y81 L82 D87 H88 H89 R90 F91 G92 Y93 D100 F101 P102 E103 A104 E105 Y109 I112 L113 E114 H117 P118 V119 M120

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

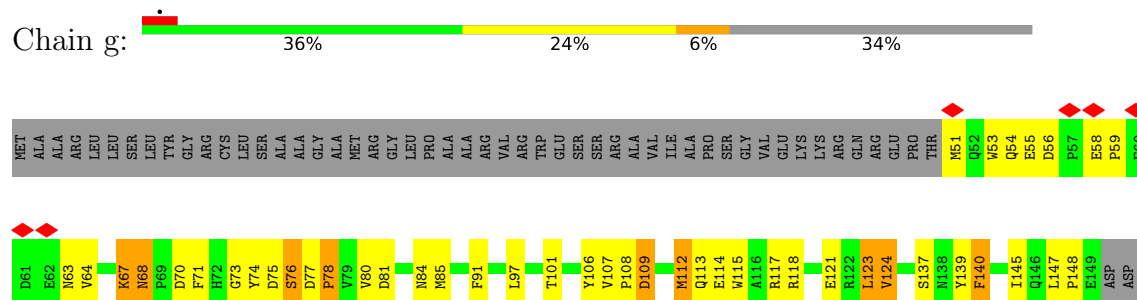
Chain e: 11% 49% 47%

MET F2 F3 I6 K9 L14 D15 R16 H17 F18 M19 F20 S22 A30 A31 R32 C33 H34 K38 E39 W40 L41 E42 C43 A44 H45 C46 G47 C48 C49 T50 R51 A52 E64 E65 C66 L67 L68 R69 Y70 K71 T72 M73 R74 R75 M76 K81 Q82 R83 E84 K85 L86 M87 K88 E89 G90 K91 Y92 T93 F94 P95 H97 H98 S99 G100 R101 E102 E103 P104 ARG PRO

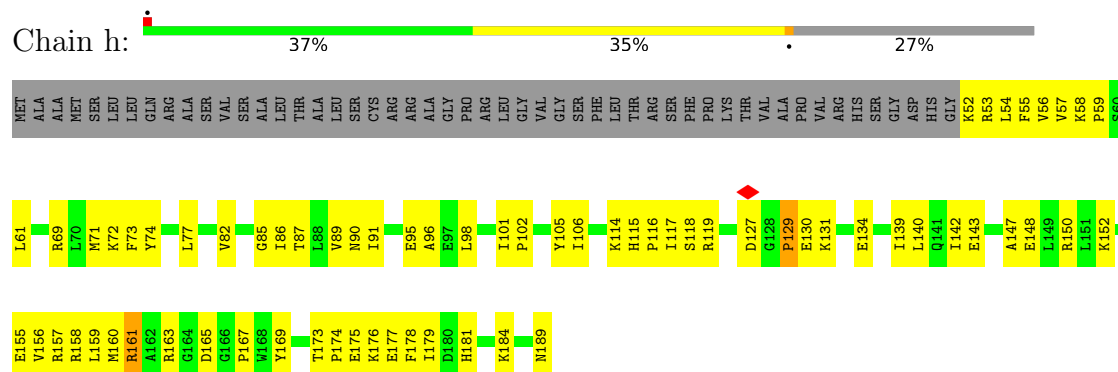
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



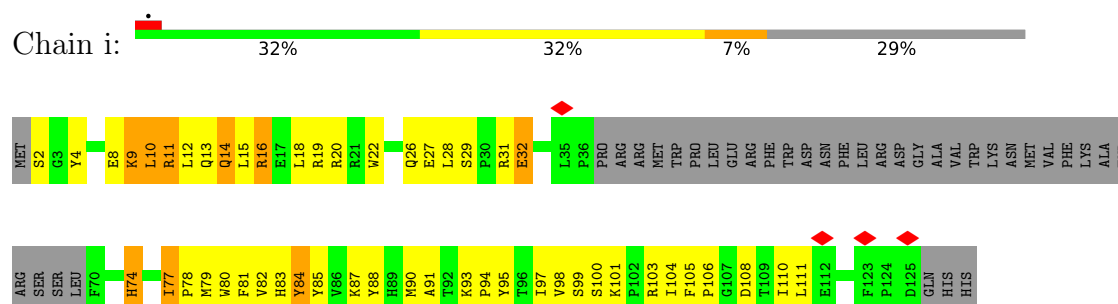
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



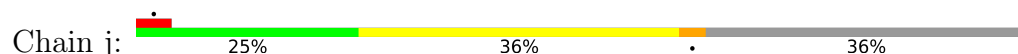
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

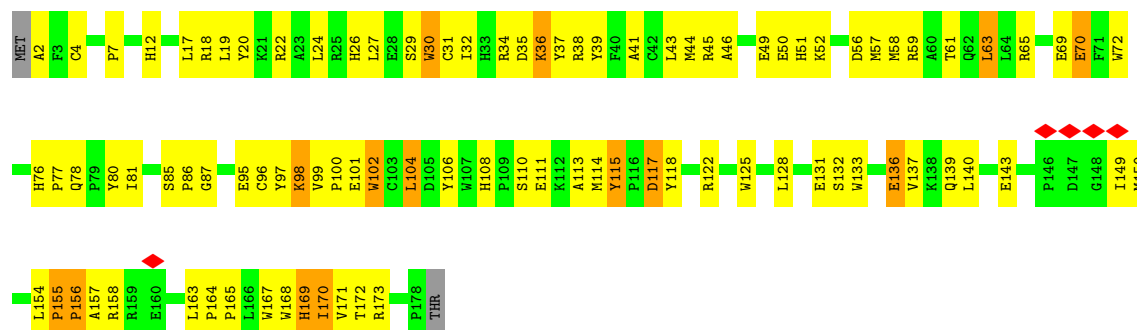


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

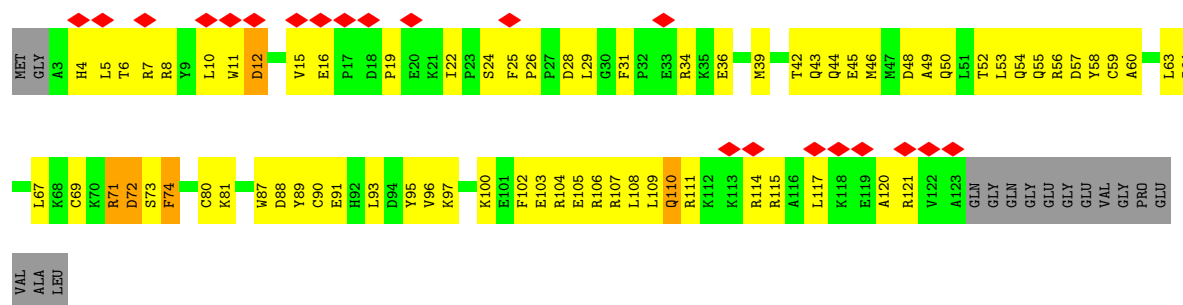


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

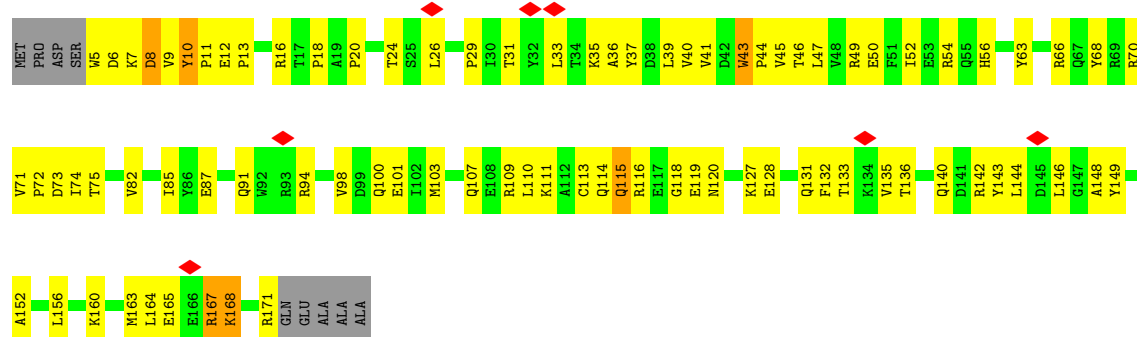




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.164	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.62	0/370	1.06	3/506 (0.6%)
2	J	0.55	1/1205 (0.1%)	0.92	6/1633 (0.4%)
3	K	0.85	0/732	1.44	11/994 (1.1%)
4	L	0.97	6/4921 (0.1%)	1.56	108/6696 (1.6%)
5	M	1.01	7/3717 (0.2%)	1.56	85/5062 (1.7%)
6	N	1.00	3/2756 (0.1%)	1.43	50/3751 (1.3%)
7	O	0.86	6/2655 (0.2%)	1.21	27/3601 (0.7%)
8	U	0.96	1/712 (0.1%)	1.35	12/962 (1.2%)
9	X	0.81	0/230	1.16	1/313 (0.3%)
10	Y	0.85	0/1054	0.96	3/1429 (0.2%)
11	c	0.69	0/400	1.24	8/544 (1.5%)
12	d	0.88	1/1028 (0.1%)	1.01	8/1387 (0.6%)
13	e	0.77	1/881 (0.1%)	1.01	4/1173 (0.3%)
14	f	0.59	0/451	0.75	0/607
15	g	0.87	3/863 (0.3%)	1.36	18/1175 (1.5%)
16	h	0.76	0/1197	1.22	7/1621 (0.4%)
17	i	0.85	0/790	1.38	16/1074 (1.5%)
18	j	0.75	0/599	1.23	8/820 (1.0%)
19	k	1.05	1/578 (0.2%)	1.56	18/782 (2.3%)
20	l	1.02	4/1359 (0.3%)	1.25	9/1855 (0.5%)
21	m	0.82	1/1079 (0.1%)	1.21	17/1463 (1.2%)
22	n	0.93	1/1589 (0.1%)	1.22	17/2152 (0.8%)
23	o	0.78	0/1063	1.14	7/1427 (0.5%)
24	p	0.72	1/1448 (0.1%)	1.01	13/1957 (0.7%)
All	All	0.89	37/31677 (0.1%)	1.32	456/42984 (1.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.82	1.67	1.47
19	k	50	PRO	N-CD	-13.63	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	255	PRO	N-CD	-13.45	1.28	1.47
13	e	91	LYS	C-N	12.91	1.51	1.33
7	O	315	PRO	N-CD	-12.15	1.30	1.47
7	O	210	PRO	N-CD	-11.31	1.31	1.47
4	L	234	PRO	N-CD	11.18	1.63	1.47
5	M	370	PRO	N-CD	-10.63	1.32	1.47
15	g	78	PRO	N-CD	-9.61	1.34	1.47
12	d	15	PRO	N-CD	-9.37	1.34	1.47
5	M	20	PRO	N-CD	8.52	1.59	1.47
4	L	212	PRO	N-CD	-8.26	1.36	1.47
22	n	155	PRO	N-CD	8.19	1.59	1.47
20	l	115	ASN	C-N	-7.42	1.24	1.33
5	M	208	PRO	N-CD	7.23	1.57	1.47
20	l	104	PRO	N-CD	-7.16	1.37	1.47
6	N	238	PRO	N-CD	-6.91	1.38	1.47
7	O	206	TYR	C-N	6.82	1.42	1.33
15	g	113	GLN	CA-C	6.64	1.61	1.52
2	J	136	GLU	CA-C	-6.55	1.44	1.52
7	O	205	ILE	C-N	6.40	1.42	1.33
4	L	384	PRO	N-CD	6.31	1.56	1.47
24	p	10	TYR	CA-C	-6.14	1.46	1.52
21	m	72	ARG	CA-C	6.06	1.60	1.52
15	g	137	SER	C-O	-6.04	1.16	1.24
4	L	112	PRO	N-CD	6.02	1.56	1.47
20	l	45	PRO	N-CD	-5.74	1.39	1.47
6	N	333	SER	C-O	-5.72	1.17	1.23
7	O	87	PRO	N-CD	-5.70	1.39	1.47
5	M	454	ILE	CA-C	5.69	1.60	1.52
5	M	252	PRO	N-CD	-5.53	1.40	1.47
8	U	140	CYS	C-O	-5.41	1.17	1.24
7	O	103	PRO	N-CD	-5.36	1.40	1.47
5	M	424	ILE	CA-C	-5.14	1.45	1.52
20	l	111	MET	C-O	-5.10	1.17	1.24
4	L	56	HIS	CA-C	-5.06	1.46	1.52
5	M	159	PRO	N-CD	5.04	1.54	1.47

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	370	PRO	N-CA-C	14.56	128.46	110.70
6	N	255	PRO	N-CA-C	14.41	128.28	110.70
7	O	118	TYR	N-CA-C	13.89	125.94	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	424	ILE	N-CA-C	-11.65	94.03	109.30
5	M	104	ILE	N-CA-C	-11.57	99.08	110.30
17	i	14	GLN	N-CA-C	11.54	123.86	111.28
4	L	194	ASN	N-CA-C	11.51	125.45	109.11
5	M	311	GLY	N-CA-C	-11.38	99.31	112.50
20	l	116	ARG	N-CA-C	11.33	123.32	110.97
4	L	278	LEU	N-CA-C	-11.26	98.98	111.14
3	K	83	ASN	N-CA-C	-11.21	100.14	114.04
6	N	244	ILE	N-CA-C	-11.20	99.41	110.72
8	U	79	ILE	N-CA-C	-11.04	102.30	112.90
4	L	582	GLY	N-CA-C	-10.82	99.49	114.64
4	L	231	PRO	N-CA-C	10.75	127.82	113.84
16	h	101	ILE	N-CA-C	-10.64	98.52	108.95
4	L	556	ILE	N-CA-C	10.63	121.29	110.23
5	M	276	CYS	N-CA-C	-10.38	99.97	111.28
7	O	210	PRO	N-CA-CB	-10.35	94.62	103.32
7	O	96	THR	N-CA-C	-10.31	100.13	111.36
20	l	170	ARG	N-CA-C	-10.18	101.51	113.21
5	M	117	MET	N-CA-C	-10.03	100.35	111.28
5	M	423	MET	N-CA-C	-9.72	96.94	110.35
19	k	50	PRO	CA-N-CD	9.72	125.61	112.00
6	N	286	ALA	N-CA-C	-9.66	100.75	111.28
6	N	255	PRO	CA-N-CD	9.65	125.50	112.00
5	M	83	HIS	N-CA-C	-9.64	97.24	110.35
2	J	136	GLU	CA-C-N	-9.58	110.00	120.44
2	J	136	GLU	C-N-CA	-9.58	110.00	120.44
17	i	12	LEU	N-CA-C	-9.54	101.20	113.12
4	L	375	ILE	N-CA-C	-9.49	101.31	110.42
5	M	104	ILE	N-CA-CB	9.45	120.92	110.62
24	p	56	HIS	N-CA-C	9.42	121.55	111.28
6	N	228	ASN	N-CA-C	-9.35	101.07	111.07
19	k	60	MET	N-CA-C	9.34	121.15	110.97
4	L	40	ILE	N-CA-C	-9.29	101.33	110.72
19	k	56	ALA	N-CA-C	9.29	121.49	111.36
4	L	394	LEU	N-CA-C	-9.23	101.19	111.07
4	L	483	PRO	N-CA-C	-9.16	96.81	111.38
21	m	48	LEU	N-CA-C	9.15	123.99	113.01
6	N	87	GLN	N-CA-C	9.14	123.30	109.41
5	M	442	ILE	N-CA-CB	9.12	117.57	110.45
11	c	64	GLU	N-CA-C	-9.11	101.32	111.07
4	L	467	VAL	N-CA-C	9.07	119.13	110.42
4	L	524	THR	N-CA-C	9.00	122.26	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	115	GLN	N-CA-C	-8.98	102.83	113.88
3	K	70	GLU	N-CA-C	-8.97	100.34	111.11
4	L	344	GLY	N-CA-C	-8.92	102.16	112.50
4	L	406	ALA	N-CA-C	-8.87	101.70	111.36
7	O	183	CYS	N-CA-C	-8.80	100.55	111.11
6	N	233	LEU	N-CA-C	-8.78	101.72	111.28
5	M	255	LYS	N-CA-C	-8.75	101.71	111.07
6	N	81	LEU	N-CA-C	-8.73	94.40	108.55
23	o	72	ASP	N-CA-C	-8.71	99.03	110.53
22	n	70	GLU	N-CA-C	-8.71	101.76	111.07
5	M	248	ILE	N-CA-C	-8.62	102.15	110.42
6	N	255	PRO	N-CA-CB	-8.61	94.73	103.08
15	g	80	VAL	N-CA-C	-8.60	102.03	110.72
7	O	315	PRO	CA-N-CD	8.56	123.98	112.00
6	N	109	ALA	CA-C-N	-8.50	110.68	120.12
6	N	109	ALA	C-N-CA	-8.50	110.68	120.12
4	L	212	PRO	N-CA-C	8.47	125.59	113.47
8	U	74	LEU	N-CA-C	8.43	120.78	110.41
6	N	272	LYS	N-CA-C	-8.43	102.10	111.28
4	L	281	GLY	N-CA-C	-8.42	102.73	112.50
6	N	221	LEU	N-CA-C	-8.40	101.16	111.33
4	L	287	PHE	N-CA-C	-8.36	102.13	111.07
22	n	19	LEU	N-CA-C	-8.32	103.26	113.41
6	N	218	ALA	N-CA-C	-8.26	98.92	111.56
4	L	151	SER	N-CA-C	-8.24	102.38	111.36
19	k	50	PRO	N-CA-CB	-8.23	93.54	102.76
5	M	274	SER	N-CA-C	8.21	120.23	111.28
5	M	26	ASN	N-CA-C	-8.18	102.31	111.14
4	L	88	LEU	N-CA-C	-8.16	102.33	111.14
4	L	169	LEU	N-CA-C	-8.15	102.48	111.36
6	N	32	GLY	N-CA-C	-8.09	103.12	112.50
12	d	15	PRO	N-CA-CB	-8.08	96.32	103.35
22	n	170	ILE	N-CA-C	-8.05	103.04	111.58
19	k	38	VAL	N-CA-C	-8.05	102.59	110.72
13	e	91	LYS	CA-C-N	-8.03	109.04	122.29
13	e	91	LYS	C-N-CA	-8.03	109.04	122.29
5	M	385	LEU	N-CA-C	-8.00	102.56	111.28
4	L	276	THR	N-CA-CB	8.00	121.61	110.01
5	M	141	GLU	N-CA-C	7.99	122.87	113.20
11	c	45	GLY	N-CA-C	7.95	123.66	113.24
5	M	205	ILE	N-CA-C	7.88	117.98	110.42
4	L	265	PRO	N-CA-CB	7.84	111.70	103.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	330	ALA	N-CA-C	-7.83	102.69	111.14
21	m	50	GLN	N-CA-C	-7.83	102.74	114.64
4	L	415	ALA	N-CA-C	-7.82	102.76	111.28
4	L	111	ASP	N-CA-C	-7.79	100.27	109.93
3	K	51	SER	N-CA-C	-7.79	102.86	113.30
4	L	265	PRO	CA-N-CD	-7.79	101.09	112.00
6	N	336	THR	N-CA-C	-7.76	103.33	114.12
5	M	85	LYS	N-CA-C	-7.71	101.53	113.02
4	L	265	PRO	N-CA-C	-7.68	101.33	113.78
7	O	210	PRO	CA-N-CD	7.57	122.60	112.00
15	g	124	VAL	N-CA-C	-7.56	103.09	110.72
8	U	147	TYR	N-CA-C	-7.52	103.02	111.14
23	o	81	LYS	N-CA-C	-7.50	104.66	113.88
4	L	245	ALA	N-CA-C	7.49	119.09	111.07
13	e	46	GLY	N-CA-C	-7.48	104.94	114.37
4	L	138	PHE	N-CA-C	-7.47	103.13	111.28
3	K	14	LEU	N-CA-C	-7.45	103.23	111.36
18	j	82	GLY	N-CA-C	-7.45	103.47	112.48
4	L	392	LYS	N-CA-C	7.41	119.00	111.07
4	L	605	ASN	N-CA-CB	7.40	121.20	110.47
4	L	123	LEU	N-CA-C	-7.38	103.31	111.36
5	M	250	LEU	N-CA-C	-7.37	103.58	112.58
4	L	21	ILE	N-CA-CB	7.37	121.64	110.58
20	l	97	LEU	N-CA-C	-7.36	103.90	113.17
22	n	29	SER	N-CA-C	-7.33	104.85	114.31
5	M	455	THR	N-CA-C	-7.31	100.40	110.35
4	L	28	LYS	N-CA-C	-7.29	103.34	111.28
23	o	12	ASP	N-CA-C	7.27	121.33	109.85
21	m	72	ARG	N-CA-C	7.26	122.43	113.50
4	L	19	ILE	N-CA-C	7.23	117.36	110.42
5	M	289	SER	N-CA-C	-7.23	103.33	111.07
22	n	30	TRP	N-CA-C	-7.21	104.11	113.12
3	K	81	VAL	N-CA-C	7.19	117.95	110.62
19	k	73	ILE	N-CA-C	-7.19	103.28	110.62
24	p	168	LYS	N-CA-C	-7.16	104.17	113.12
5	M	244	ILE	N-CA-C	7.13	117.89	110.62
4	L	554	ASP	N-CA-CB	7.13	121.25	110.42
5	M	34	ILE	N-CA-C	-7.13	103.35	110.62
18	j	65	MET	N-CA-C	-7.06	103.51	111.07
9	X	153	VAL	N-CA-C	7.06	118.03	107.80
22	n	102	TRP	N-CA-C	-7.03	105.05	112.93
3	K	48	SER	N-CA-C	-7.03	103.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	325	LEU	N-CA-C	-7.03	103.55	111.07
4	L	319	MET	N-CA-C	-7.02	104.71	112.72
5	M	365	ALA	N-CA-C	-7.01	103.72	111.36
5	M	213	HIS	CB-CA-C	-6.98	96.84	110.11
4	L	471	ASN	N-CA-C	6.98	118.97	111.36
6	N	132	THR	N-CA-C	6.96	122.89	113.97
4	L	100	ILE	N-CA-C	6.96	119.75	111.05
2	J	125	MET	N-CA-C	-6.95	101.80	111.39
5	M	264	LEU	N-CA-C	-6.95	103.64	111.07
17	i	9	LYS	N-CA-C	-6.94	104.80	112.72
4	L	546	LEU	N-CA-C	6.94	119.49	111.02
5	M	91	LEU	N-CA-C	-6.92	103.84	112.90
4	L	86	SER	N-CA-C	6.90	118.46	111.07
5	M	235	LEU	N-CA-C	6.90	119.39	111.11
17	i	11	ARG	N-CA-C	-6.88	104.89	113.28
19	k	59	TYR	N-CA-CB	-6.87	98.86	110.41
4	L	26	LEU	N-CA-C	6.87	119.61	111.71
5	M	276	CYS	N-CA-CB	6.85	120.19	110.12
22	n	117	ASP	N-CA-C	-6.84	103.88	111.82
5	M	442	ILE	N-CA-C	-6.84	104.14	112.35
3	K	83	ASN	N-CA-CB	6.84	120.93	110.81
21	m	127	ILE	N-CA-C	-6.83	106.14	112.43
4	L	547	LYS	N-CA-C	6.82	118.72	111.28
15	g	78	PRO	CA-N-CD	6.80	121.52	112.00
5	M	165	ILE	N-CA-C	-6.77	102.62	111.09
3	K	70	GLU	N-CA-CB	6.77	120.02	109.94
5	M	248	ILE	N-CA-CB	6.75	118.45	110.55
5	M	374	ASN	N-CA-C	-6.75	103.85	111.07
7	O	93	TYR	N-CA-C	-6.74	104.01	111.36
20	l	86	ARG	N-CA-C	-6.71	99.59	110.20
4	L	95	PHE	N-CA-C	-6.70	103.90	111.07
8	U	140	CYS	CA-C-N	-6.69	114.01	120.83
8	U	140	CYS	C-N-CA	-6.69	114.01	120.83
3	K	76	ALA	N-CA-C	-6.67	104.09	111.36
4	L	499	LEU	N-CA-C	-6.67	103.70	110.97
5	M	410	MET	N-CA-C	-6.67	103.93	111.07
7	O	315	PRO	N-CA-CB	-6.67	95.99	103.33
18	j	53	SER	N-CA-C	6.67	119.40	111.33
2	J	132	GLY	N-CA-C	-6.66	100.98	110.91
7	O	175	ASN	N-CA-C	-6.65	104.10	111.82
8	U	150	ASP	CB-CA-C	6.65	121.83	110.79
17	i	8	GLU	N-CA-C	-6.64	104.76	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	143	LEU	N-CA-C	-6.63	103.97	111.07
15	g	76	SER	N-CA-C	6.63	118.16	111.07
19	k	49	ASP	CA-C-N	-6.63	113.38	120.47
19	k	49	ASP	C-N-CA	-6.63	113.38	120.47
6	N	228	ASN	N-CA-CB	6.62	119.61	110.01
22	n	115	TYR	N-CA-CB	6.62	122.15	110.37
5	M	161	LEU	N-CA-C	-6.61	103.99	111.07
8	U	102	SER	N-CA-C	6.61	119.62	107.99
5	M	303	ILE	N-CA-C	-6.60	104.06	110.72
7	O	140	LEU	N-CA-C	-6.59	104.02	111.07
21	m	51	TYR	N-CA-C	-6.54	105.60	113.97
4	L	130	ILE	N-CA-C	-6.53	103.96	110.62
4	L	329	ILE	N-CA-C	-6.52	104.16	110.42
7	O	114	LEU	N-CA-C	-6.51	104.26	111.36
7	O	118	TYR	N-CA-CB	-6.51	100.58	110.01
4	L	232	TRP	N-CA-C	6.50	120.47	112.54
4	L	423	SER	N-CA-C	-6.50	104.12	111.07
19	k	57	TRP	N-CA-C	-6.48	104.63	112.54
19	k	46	GLY	N-CA-C	-6.48	106.98	114.69
24	p	54	ARG	N-CA-C	-6.47	103.73	111.69
6	N	315	THR	N-CA-C	-6.46	104.16	111.07
7	O	320	GLY	N-CA-C	-6.46	96.57	111.04
10	Y	96	GLY	N-CA-C	-6.45	104.51	112.77
3	K	11	ALA	N-CA-C	-6.45	104.17	111.07
11	c	72	ARG	N-CA-C	-6.42	104.20	111.07
5	M	32	PHE	N-CA-C	-6.41	104.21	111.07
19	k	42	LEU	N-CA-C	-6.41	103.55	111.75
4	L	325	ALA	N-CA-C	-6.40	104.30	111.28
4	L	439	PRO	N-CA-C	6.39	122.41	113.53
15	g	112	MET	N-CA-C	6.38	120.85	113.38
4	L	70	THR	N-CA-C	-6.38	103.85	111.69
12	d	15	PRO	CA-N-CD	6.37	120.92	112.00
5	M	317	ILE	N-CA-C	-6.37	104.55	110.53
20	l	119	THR	N-CA-C	-6.36	98.17	108.41
7	O	98	THR	N-CA-C	6.32	120.58	109.96
4	L	234	PRO	CA-N-CD	-6.31	103.17	112.00
15	g	123	LEU	N-CA-CB	6.31	119.15	110.01
4	L	387	THR	N-CA-C	6.30	118.96	111.71
17	i	32	GLU	CA-C-N	-6.30	111.97	119.84
17	i	32	GLU	C-N-CA	-6.30	111.97	119.84
4	L	337	ALA	N-CA-C	-6.29	104.42	111.28
1	D	73	LYS	N-CA-C	6.28	118.50	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	490	ALA	N-CA-C	-6.28	104.36	111.07
6	N	89	GLN	N-CA-C	6.27	120.49	112.34
20	l	105	ILE	CA-C-O	-6.26	115.14	121.59
7	O	113	SER	N-CA-C	6.25	118.60	108.41
5	M	26	ASN	N-CA-CB	6.24	119.11	110.07
11	c	47	SER	N-CA-CB	6.24	120.80	110.33
18	j	78	ASP	N-CA-C	-6.23	102.82	110.61
6	N	91	ASN	N-CA-CB	6.23	119.12	109.97
6	N	337	LEU	CA-C-N	-6.22	113.72	119.82
6	N	337	LEU	C-N-CA	-6.22	113.72	119.82
19	k	59	TYR	N-CA-C	6.22	120.70	113.18
6	N	276	LEU	N-CA-C	-6.19	105.38	113.17
22	n	63	LEU	N-CA-C	-6.18	104.09	111.69
23	o	110	GLN	N-CA-C	-6.18	104.62	111.36
5	M	121	LEU	N-CA-C	-6.16	104.65	111.36
24	p	127	LYS	N-CA-C	-6.15	104.12	111.69
4	L	98	TRP	N-CA-C	-6.14	104.67	111.36
6	N	47	LYS	N-CA-C	-6.14	104.70	111.82
4	L	361	ASN	CB-CA-C	-6.13	102.84	111.80
15	g	109	ASP	CA-CB-CG	6.13	118.73	112.60
6	N	216	PHE	N-CA-C	6.12	118.04	111.36
6	N	46	ASN	N-CA-C	-6.12	105.84	113.55
19	k	30	ILE	N-CA-C	6.10	118.72	111.09
16	h	142	ILE	N-CA-C	-6.10	104.56	110.42
5	M	4	ILE	N-CA-C	-6.09	104.04	112.50
5	M	3	LYS	N-CA-C	-6.09	105.98	113.41
4	L	287	PHE	N-CA-CB	6.08	118.82	110.01
11	c	47	SER	N-CA-C	-6.07	104.60	112.68
4	L	140	LEU	N-CA-C	-6.07	104.67	111.28
5	M	57	SER	N-CA-C	6.06	119.08	109.50
6	N	91	ASN	N-CA-C	-6.06	101.31	110.28
16	h	101	ILE	N-CA-CB	6.06	115.72	110.08
2	J	135	LEU	N-CA-C	6.05	118.39	108.52
15	g	123	LEU	N-CA-C	-6.05	104.60	111.07
21	m	72	ARG	CA-C-O	6.05	125.79	119.14
7	O	160	GLU	CB-CA-C	-6.04	109.59	116.54
21	m	52	ASN	N-CA-C	-6.04	105.22	112.59
7	O	234	LEU	N-CA-C	-6.03	104.79	111.36
5	M	213	HIS	N-CA-C	6.02	120.48	113.20
5	M	370	PRO	CA-N-CD	6.01	120.42	112.00
4	L	454	ILE	N-CA-C	-6.01	104.49	110.62
21	m	22	GLU	N-CA-C	-6.00	104.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	8	ASP	N-CA-C	6.00	120.67	113.23
5	M	396	MET	N-CA-C	-5.98	105.96	113.20
6	N	295	ARG	N-CA-C	-5.97	104.78	111.28
1	D	72	LEU	N-CA-C	5.96	117.38	108.31
15	g	78	PRO	N-CA-C	5.96	121.82	113.53
5	M	88	ASN	N-CA-C	5.96	120.17	113.02
7	O	183	CYS	N-CA-CB	5.96	118.81	109.94
4	L	247	LEU	N-CA-CB	5.95	120.69	110.34
4	L	112	PRO	CB-CA-C	-5.94	103.01	111.68
22	n	27	LEU	N-CA-C	-5.94	106.00	113.72
4	L	88	LEU	N-CA-CB	5.93	118.67	110.07
5	M	300	SER	N-CA-C	-5.92	107.04	114.56
19	k	82	ALA	N-CA-C	-5.92	104.83	111.28
4	L	278	LEU	N-CA-CB	5.91	118.64	110.07
5	M	222	GLU	N-CA-C	5.91	120.33	113.18
6	N	16	GLY	CA-C-N	-5.89	112.43	118.85
6	N	16	GLY	C-N-CA	-5.89	112.43	118.85
5	M	253	LEU	N-CA-C	5.89	117.70	111.28
7	O	181	LYS	N-CA-C	5.88	117.36	111.07
4	L	387	THR	CB-CA-C	-5.88	99.76	110.63
7	O	205	ILE	O-C-N	5.87	129.04	122.75
8	U	75	THR	N-CA-CB	5.87	121.77	111.55
7	O	130	ARG	N-CA-C	-5.87	104.88	111.28
7	O	262	GLU	N-CA-C	-5.87	104.89	111.28
8	U	143	GLU	N-CA-C	-5.86	104.25	111.75
19	k	80	GLY	N-CA-C	-5.86	105.70	112.50
4	L	248	HIS	CB-CA-C	5.86	120.81	110.85
4	L	234	PRO	N-CA-CB	5.85	109.49	103.23
6	N	15	LEU	N-CA-C	-5.85	105.64	112.89
17	i	10	LEU	N-CA-C	-5.84	107.15	114.56
17	i	105	PHE	CA-C-N	-5.83	113.69	119.99
17	i	105	PHE	C-N-CA	-5.83	113.69	119.99
13	e	91	LYS	O-C-N	5.83	129.44	122.27
12	d	53	VAL	N-CA-C	5.82	116.47	110.36
5	M	272	THR	N-CA-C	-5.80	105.03	111.36
21	m	116	ILE	N-CA-C	-5.80	104.85	110.42
5	M	424	ILE	O-C-N	5.80	128.41	122.79
8	U	101	ASN	N-CA-C	-5.79	106.07	113.02
18	j	73	PHE	N-CA-C	-5.79	104.88	111.07
4	L	428	TYR	N-CA-C	-5.78	104.89	111.14
6	N	321	LYS	N-CA-C	5.78	118.53	110.20
22	n	52	LYS	N-CA-C	-5.78	105.90	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	d	62	LEU	N-CA-C	5.76	117.56	111.28
15	g	78	PRO	N-CA-CB	-5.75	97.00	103.33
4	L	419	THR	N-CA-C	-5.73	105.03	111.28
4	L	467	VAL	N-CA-CB	-5.72	103.85	110.55
5	M	124	ALA	N-CA-C	-5.72	105.13	111.36
5	M	279	GLN	N-CA-C	-5.71	98.58	108.69
4	L	342	CYS	N-CA-CB	5.71	118.29	110.01
6	N	66	ALA	N-CA-C	-5.71	105.14	111.36
4	L	495	VAL	N-CA-C	5.71	115.90	110.42
4	L	177	ILE	N-CA-C	-5.70	104.81	110.62
4	L	605	ASN	N-CA-C	-5.69	106.19	113.02
23	o	71	ARG	N-CA-C	-5.69	104.46	111.40
4	L	214	MET	N-CA-C	-5.69	105.16	111.36
15	g	67	LYS	N-CA-C	-5.68	102.05	110.46
4	L	371	SER	N-CA-C	-5.67	105.01	111.14
5	M	214	LEU	N-CA-C	-5.66	105.64	112.54
6	N	232	LEU	N-CA-C	-5.66	106.60	112.93
4	L	20	LEU	N-CA-C	5.65	119.89	112.89
17	i	14	GLN	N-CA-CB	-5.65	101.82	110.12
20	l	49	ALA	N-CA-C	-5.65	106.55	113.50
21	m	104	VAL	N-CA-C	-5.64	105.60	111.58
21	m	31	ARG	N-CA-C	-5.64	106.53	113.41
5	M	19	SER	N-CA-C	5.62	117.65	109.84
24	p	115	GLN	N-CA-CB	5.62	118.06	110.59
4	L	151	SER	N-CA-CB	5.61	118.46	110.16
7	O	220	LYS	N-CA-C	5.60	117.39	111.28
1	D	72	LEU	CB-CA-C	-5.60	110.10	116.54
15	g	140	PHE	N-CA-CB	5.59	118.32	109.71
4	L	445	GLU	CB-CA-C	-5.59	101.96	111.02
4	L	155	ILE	N-CA-C	-5.59	105.28	110.53
15	g	107	VAL	N-CA-C	-5.59	102.87	108.96
17	i	74	HIS	CA-C-N	-5.58	115.76	122.35
17	i	74	HIS	C-N-CA	-5.58	115.76	122.35
21	m	60	ILE	N-CA-C	-5.58	101.99	109.30
18	j	80	VAL	CB-CA-C	-5.57	106.15	111.44
12	d	5	ARG	CA-C-N	-5.57	114.22	119.90
12	d	5	ARG	C-N-CA	-5.57	114.22	119.90
17	i	84	TYR	N-CA-C	-5.56	105.22	111.28
6	N	251	LEU	N-CA-C	-5.54	105.24	111.28
10	Y	13	GLU	N-CA-C	5.54	117.76	111.11
4	L	152	PHE	N-CA-C	-5.54	105.14	111.07
21	m	46	GLU	N-CA-C	-5.54	106.52	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	120	ASN	N-CA-C	-5.53	105.15	113.89
4	L	234	PRO	N-CA-C	-5.53	105.56	113.47
11	c	64	GLU	N-CA-CB	5.52	118.02	110.01
15	g	113	GLN	CA-C-O	5.51	126.17	119.11
4	L	370	SER	N-CA-C	-5.51	105.36	111.36
23	o	74	PHE	CA-C-N	-5.51	113.94	119.56
23	o	74	PHE	C-N-CA	-5.51	113.94	119.56
5	M	370	PRO	N-CA-CB	-5.50	97.75	103.08
4	L	394	LEU	N-CA-CB	5.49	117.97	110.01
6	N	36	SER	N-CA-C	-5.49	105.29	111.28
5	M	223	ALA	N-CA-CB	5.48	118.11	110.11
5	M	355	MET	N-CA-C	-5.48	104.70	111.33
4	L	465	GLY	N-CA-C	-5.47	105.77	112.77
5	M	73	LEU	N-CA-C	-5.47	105.31	112.75
22	n	136	GLU	CB-CA-C	5.47	121.30	110.42
4	L	194	ASN	CB-CA-C	-5.46	103.36	111.72
5	M	174	LEU	N-CA-C	-5.46	106.40	112.57
11	c	31	VAL	N-CA-C	-5.46	105.01	110.30
17	i	77	ILE	CB-CA-C	-5.44	108.58	114.35
7	O	154	GLY	N-CA-C	-5.44	107.52	114.37
15	g	137	SER	N-CA-CB	-5.44	101.28	110.41
4	L	413	LEU	N-CA-C	5.43	117.20	111.28
18	j	64	LEU	N-CA-C	-5.43	105.44	111.36
24	p	94	ARG	N-CA-C	5.41	116.86	111.07
16	h	173	THR	O-C-N	5.41	125.77	121.55
6	N	108	LEU	N-CA-C	5.41	118.05	109.24
5	M	234	ILE	N-CA-C	5.40	116.28	111.90
6	N	89	GLN	N-CA-CB	-5.40	100.46	110.18
4	L	21	ILE	N-CA-C	-5.40	105.27	110.72
6	N	62	THR	N-CA-C	-5.39	105.30	111.07
4	L	386	LEU	N-CA-C	-5.36	100.97	108.96
4	L	494	SER	N-CA-C	-5.36	105.35	111.14
4	L	543	ASN	N-CA-C	-5.36	105.44	111.28
5	M	53	SER	N-CA-C	5.35	115.60	108.38
19	k	48	ARG	N-CA-C	-5.35	98.85	108.48
5	M	117	MET	N-CA-CB	5.35	117.98	110.12
4	L	550	LEU	CA-C-O	-5.34	115.28	120.89
8	U	141	PRO	N-CA-C	-5.34	109.13	114.68
4	L	311	GLY	N-CA-C	-5.33	106.33	112.73
6	N	218	ALA	N-CA-CB	5.33	118.45	110.14
5	M	343	ILE	N-CA-C	5.30	116.03	110.62
5	M	409	TYR	N-CA-C	-5.30	105.67	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	104	LEU	N-CA-C	-5.30	106.84	113.15
4	L	231	PRO	CB-CA-C	-5.30	104.33	111.85
5	M	25	THR	CB-CA-C	-5.30	100.50	110.67
5	M	167	ILE	N-CA-C	5.29	117.67	111.05
4	L	415	ALA	N-CA-CB	5.28	117.89	110.12
15	g	68	ASN	N-CA-CB	5.28	119.05	111.51
4	L	183	ILE	N-CA-C	-5.26	105.25	110.62
22	n	36	LYS	N-CA-C	-5.26	105.55	111.28
5	M	212	VAL	CB-CA-C	-5.26	105.16	112.36
5	M	294	MET	N-CA-C	-5.25	106.89	113.72
16	h	129	PRO	N-CA-C	-5.25	106.69	113.57
22	n	12	HIS	N-CA-C	-5.25	105.00	111.40
6	N	335	MET	CB-CA-C	-5.23	104.37	111.95
4	L	190	SER	N-CA-C	-5.23	106.75	113.23
24	p	13	PRO	O-C-N	5.23	123.61	121.15
4	L	375	ILE	N-CA-CB	5.23	116.66	110.55
5	M	20	PRO	N-CA-C	-5.22	106.27	113.53
7	O	264	GLU	N-CA-C	-5.22	107.27	113.38
5	M	98	MET	N-CA-C	-5.22	105.49	111.07
18	j	76	ASP	CB-CA-C	-5.21	104.64	112.09
4	L	386	LEU	CA-C-O	-5.21	115.88	121.45
4	L	217	LEU	N-CA-C	-5.20	105.61	111.28
2	J	124	LEU	N-CA-C	-5.20	101.39	109.14
4	L	485	PHE	N-CA-CB	5.20	117.54	110.01
21	m	17	THR	N-CA-C	-5.19	103.67	110.53
22	n	26	HIS	N-CA-C	-5.19	106.54	112.92
4	L	137	MET	N-CA-C	5.19	119.23	113.01
5	M	317	ILE	N-CA-CB	5.17	117.19	110.57
12	d	37	LEU	N-CA-C	-5.17	105.64	111.28
24	p	167	ARG	CB-CA-C	5.17	117.19	109.13
7	O	206	TYR	CA-C-N	-5.17	115.01	122.45
7	O	206	TYR	C-N-CA	-5.17	115.01	122.45
6	N	90	THR	N-CA-C	5.15	117.56	110.35
4	L	332	HIS	N-CA-C	-5.15	105.66	111.28
6	N	222	ASN	N-CA-C	-5.15	106.24	112.88
4	L	497	GLY	N-CA-C	-5.14	106.53	112.50
6	N	225	MET	N-CA-C	-5.14	106.59	112.92
11	c	60	GLN	N-CA-C	-5.13	105.58	111.07
24	p	43	TRP	CA-C-N	-5.13	113.63	118.97
24	p	43	TRP	C-N-CA	-5.13	113.63	118.97
5	M	86	LYS	N-CA-C	-5.13	106.26	112.88
21	m	61	GLU	N-CA-C	5.13	119.62	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	284	THR	N-CA-C	-5.12	105.78	111.36
20	l	168	LEU	N-CA-C	-5.12	105.61	111.14
4	L	396	ILE	O-C-N	5.11	126.91	121.91
5	M	32	PHE	N-CA-CB	5.11	117.41	110.01
19	k	44	ALA	N-CA-C	-5.10	105.72	111.28
5	M	30	TYR	N-CA-C	5.10	116.84	111.28
6	N	292	PHE	CA-CB-CG	5.10	118.90	113.80
16	h	158	ARG	N-CA-C	-5.10	105.63	111.14
21	m	47	TYR	N-CA-C	-5.10	105.90	112.68
4	L	249	SER	N-CA-C	5.09	116.64	111.14
5	M	234	ILE	CB-CA-C	5.08	116.18	111.30
17	i	16	ARG	N-CA-C	-5.08	105.74	111.28
5	M	330	ALA	N-CA-CB	5.08	117.44	110.07
21	m	26	SER	N-CA-C	-5.07	102.79	109.84
15	g	137	SER	N-CA-C	5.07	119.32	113.18
22	n	169	HIS	CB-CA-C	5.06	118.73	110.17
6	N	42	PRO	CB-CA-C	-5.06	105.02	113.06
20	l	45	PRO	N-CA-C	5.05	120.47	113.65
10	Y	72	PHE	N-CA-C	-5.05	105.67	111.07
6	N	217	MET	N-CA-C	-5.05	106.95	113.01
16	h	161	ARG	N-CA-C	-5.04	105.47	110.97
15	g	124	VAL	N-CA-CB	5.04	118.13	110.58
5	M	56	PHE	N-CA-C	5.03	116.72	108.52
3	K	48	SER	N-CA-CB	5.03	117.51	110.12
5	M	267	TRP	N-CA-C	-5.03	105.88	111.36
8	U	81	ASP	N-CA-C	-5.02	106.32	112.90
4	L	384	PRO	N-CA-CB	5.01	107.71	103.35
6	N	64	ALA	N-CA-C	5.01	116.44	111.07
5	M	229	MET	N-CA-C	-5.01	105.71	111.07
4	L	142	ILE	N-CA-C	-5.01	105.51	110.62
6	N	282	MET	N-CA-C	-5.01	105.71	111.07
5	M	281	ASP	N-CA-CB	5.00	118.57	110.17
12	d	60	ARG	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	355	0	330	43	0
2	J	1178	0	1204	158	0
3	K	721	0	753	83	0
4	L	4798	0	4986	584	0
5	M	3630	0	3854	500	0
6	N	2694	0	2896	345	0
7	O	2588	0	2539	246	0
8	U	700	0	691	70	0
9	X	221	0	215	29	0
10	Y	1030	0	1015	80	0
11	c	389	0	385	34	0
12	d	996	0	1001	71	0
13	e	859	0	849	87	0
14	f	439	0	433	35	0
15	g	835	0	772	67	0
16	h	1162	0	1163	119	0
17	i	765	0	769	60	0
18	j	574	0	522	91	0
19	k	560	0	560	47	0
20	l	1304	0	1193	95	0
21	m	1050	0	1061	114	0
22	n	1534	0	1463	135	0
23	o	1038	0	1030	105	0
24	p	1415	0	1385	106	0
25	D	38	0	50	6	0
25	J	46	0	66	1	0
25	L	133	0	194	18	0
25	M	86	0	123	15	0
25	i	40	0	54	11	0
25	m	41	0	56	9	0
26	L	73	0	90	12	0
26	M	82	0	114	12	0
26	Y	71	0	86	5	0
26	d	65	0	74	8	0
26	h	68	0	83	13	0
27	L	1	0	0	0	0
28	O	27	0	12	3	0
29	n	32	0	0	1	0
All	All	31638	0	32071	2683	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 42.

All (2683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:141:PHE:CE2	5:M:370:PRO:HG3	1.75	1.21
3:K:66:PHE:HZ	6:N:35:PHE:CZ	1.56	1.21
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.20
4:L:437:PHE:CE1	4:L:441:ILE:HG12	1.77	1.19
4:L:358:LYS:HG3	22:n:80:TYR:CZ	1.79	1.17
4:L:466:PHE:CZ	18:j:72:ARG:NH2	2.14	1.16
5:M:369:LEU:HD23	5:M:371:PRO:HD2	1.18	1.16
17:i:74:HIS:O	17:i:78:PRO:HG2	1.46	1.14
4:L:247:LEU:CD1	4:L:248:HIS:CD2	2.31	1.14
3:K:66:PHE:CZ	6:N:35:PHE:CZ	2.35	1.13
1:D:72:LEU:HD11	6:N:50:PRO:CG	1.79	1.12
4:L:437:PHE:HE1	4:L:441:ILE:HG12	0.97	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
4:L:229:LEU:HD12	4:L:229:LEU:O	1.51	1.10
4:L:365:ILE:HD12	4:L:366:MET:HG3	1.32	1.10
8:U:90:TYR:OH	8:U:92:LYS:HD2	1.48	1.10
4:L:121:LEU:HD22	4:L:246:LEU:HD21	1.32	1.09
4:L:594:ASN:ND2	6:N:110:PRO:HB2	1.66	1.09
4:L:553:LEU:HD11	21:m:93:ALA:HB3	1.34	1.09
5:M:127:ILE:CD1	6:N:256:PRO:HG3	1.82	1.09
13:e:41:ILE:HG23	16:h:179:ILE:HD11	1.36	1.08
20:l:184:TYR:HB3	23:o:34:ARG:HD2	1.34	1.08
2:J:123:TRP:CE3	13:e:73:MET:HG2	1.88	1.08
4:L:466:PHE:HB2	18:j:68:TRP:CZ2	1.89	1.08
19:k:34:PRO:HG2	19:k:59:TYR:CE1	1.88	1.08
6:N:307:THR:HB	7:O:319:ILE:HD11	1.36	1.07
4:L:466:PHE:CB	18:j:68:TRP:HZ2	1.68	1.06
4:L:16:LEU:HD23	4:L:126:ILE:HD13	1.30	1.06
1:D:47:PHE:HB3	6:N:227:ILE:HD11	1.32	1.06
4:L:141:PHE:HB2	4:L:182:PHE:CE2	1.92	1.05
2:J:22:LYS:NZ	3:K:22:PHE:HA	1.72	1.04
4:L:364:LYS:HE2	19:k:67:ILE:CD1	1.86	1.04
4:L:466:PHE:HB2	18:j:68:TRP:HZ2	1.17	1.04
4:L:466:PHE:CE1	18:j:72:ARG:CZ	2.40	1.04
6:N:307:THR:HB	7:O:319:ILE:CD1	1.87	1.04
20:l:38:PRO:HB2	21:m:75:ASN:HD22	1.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:466:PHE:CE1	18:j:72:ARG:NH2	2.25	1.04
5:M:249:ILE:O	5:M:250:LEU:HG	1.58	1.03
6:N:233:LEU:HD23	6:N:241:LEU:HD12	1.36	1.03
18:j:97:LEU:HB3	23:o:104:ARG:HB2	1.05	1.03
4:L:131:LEU:HD12	4:L:140:LEU:HD12	1.36	1.03
23:o:69:CYS:O	23:o:80:CYS:SG	2.17	1.02
2:J:169:ILE:HD11	3:K:77:LEU:HD23	1.40	1.02
5:M:179:LEU:HB3	5:M:249:ILE:HD11	1.42	1.01
2:J:135:LEU:HG	3:K:54:MET:HE1	1.40	1.01
4:L:141:PHE:CE2	5:M:375:LEU:HD21	1.96	1.01
7:O:323:GLN:HE22	15:g:54:GLN:HB3	1.21	1.01
2:J:154:VAL:HG22	6:N:35:PHE:HZ	1.21	1.01
4:L:228:GLY:O	4:L:229:LEU:HG	1.61	1.01
2:J:154:VAL:HG22	6:N:35:PHE:CZ	1.95	1.00
4:L:222:GLY:HA2	4:L:229:LEU:HD11	1.40	1.00
5:M:172:GLY:O	5:M:173:THR:HG23	1.61	1.00
18:j:97:LEU:HB3	23:o:104:ARG:CB	1.91	1.00
20:l:91:GLN:HE21	22:n:2:ALA:HB1	1.26	1.00
4:L:358:LYS:CG	22:n:80:TYR:CZ	2.44	0.99
5:M:196:TRP:CD1	5:M:250:LEU:HD13	1.96	0.99
6:N:232:LEU:HD23	6:N:307:THR:HG23	1.39	0.99
2:J:9:SER:CB	3:K:7:ASN:HD22	1.76	0.98
5:M:143:LEU:HD21	6:N:303:THR:CG2	1.94	0.98
20:l:158:PRO:HD3	23:o:22:ILE:HB	1.45	0.98
12:d:109:TYR:HA	12:d:112:ILE:HG22	1.44	0.98
4:L:141:PHE:HB2	4:L:182:PHE:HE2	1.27	0.98
4:L:553:LEU:HD11	21:m:93:ALA:CB	1.94	0.98
5:M:275:ILE:HD11	5:M:288:TYR:CG	1.98	0.98
5:M:458:THR:CG2	24:p:148:ALA:HB1	1.93	0.98
4:L:383:MET:HB3	4:L:386:LEU:HD12	1.43	0.97
4:L:316:THR:HG23	4:L:325:ALA:HB2	1.45	0.97
4:L:216:LEU:HD22	4:L:259:LEU:HD21	1.44	0.96
4:L:141:PHE:CE2	5:M:375:LEU:CD2	2.48	0.96
4:L:174:TYR:HD2	4:L:232:TRP:CD1	1.82	0.96
1:D:72:LEU:HD11	6:N:50:PRO:HG2	1.44	0.96
2:J:169:ILE:HG13	6:N:45:ILE:HD11	1.47	0.96
7:O:347:VAL:HG11	11:c:29:PHE:HA	1.47	0.96
4:L:174:TYR:CD2	4:L:232:TRP:HD1	1.83	0.96
5:M:250:LEU:HD12	5:M:250:LEU:O	1.65	0.96
4:L:363:THR:HG23	4:L:431:THR:HB	1.48	0.96
4:L:174:TYR:HD2	4:L:232:TRP:HD1	1.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:550:LEU:HD12	5:M:275:ILE:HB	1.43	0.95
2:J:123:TRP:CZ3	13:e:73:MET:HG2	2.01	0.95
5:M:173:THR:HG21	16:h:147:ALA:HB2	1.48	0.95
8:U:90:TYR:HE2	8:U:92:LYS:HB2	1.24	0.95
2:J:164:PHE:CE2	6:N:8:ILE:HG13	2.01	0.95
4:L:319:MET:HE1	4:L:399:ILE:HA	1.47	0.95
4:L:364:LYS:HE2	19:k:67:ILE:HD11	1.47	0.95
6:N:31:VAL:O	6:N:35:PHE:CD2	2.18	0.95
4:L:247:LEU:HD12	4:L:248:HIS:CD2	1.98	0.95
2:J:123:TRP:CH2	13:e:73:MET:HA	2.02	0.94
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
16:h:57:VAL:HG22	22:n:104:LEU:HD11	1.49	0.94
4:L:362:ILE:HD12	4:L:430:VAL:HG12	1.50	0.94
5:M:369:LEU:CD2	5:M:371:PRO:HD2	1.97	0.94
2:J:151:MET:HE1	6:N:28:LEU:HD13	1.47	0.94
4:L:246:LEU:HD12	4:L:247:LEU:N	1.81	0.94
1:D:67:ASN:HB2	7:O:193:LEU:CD2	1.97	0.94
5:M:1:MET:HG3	5:M:4:ILE:HD13	1.50	0.94
5:M:458:THR:HG22	24:p:148:ALA:HB1	1.50	0.93
8:U:140:CYS:HB2	8:U:143:GLU:HG2	1.49	0.93
4:L:247:LEU:HD11	4:L:248:HIS:NE2	1.83	0.93
4:L:274:LEU:HA	4:L:277:MET:HE3	1.49	0.93
4:L:141:PHE:HE2	5:M:375:LEU:CD2	1.81	0.93
5:M:453:LEU:CD1	5:M:454:ILE:HG23	1.99	0.93
4:L:41:LYS:HG3	4:L:98:TRP:CZ2	2.04	0.93
7:O:314:LEU:CD1	7:O:315:PRO:HD2	2.00	0.92
5:M:143:LEU:HD21	6:N:303:THR:HG21	1.48	0.92
2:J:169:ILE:HD11	3:K:77:LEU:CD2	1.99	0.91
4:L:245:ALA:O	4:L:249:SER:HB3	1.70	0.91
2:J:59:TYR:HA	2:J:63:MET:HB3	1.51	0.91
2:J:135:LEU:HG	3:K:54:MET:CE	2.00	0.91
4:L:202:MET:HE3	4:L:265:PRO:HG3	1.53	0.91
5:M:106:LEU:HD13	5:M:234:ILE:CG2	2.00	0.91
3:K:40:LEU:HD13	6:N:71:LEU:HD23	1.52	0.91
1:D:72:LEU:CD1	6:N:50:PRO:CG	2.49	0.91
5:M:162:ILE:HG23	6:N:271:MET:HE3	1.52	0.90
18:j:97:LEU:CB	23:o:104:ARG:HB2	1.99	0.90
2:J:62:GLY:HA2	2:J:65:VAL:HB	1.53	0.90
2:J:71:THR:HG22	3:K:27:MET:HG2	1.53	0.90
7:O:106:ILE:HG12	7:O:111:SER:HA	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:165:ILE:HG23	6:N:42:PRO:HG3	1.53	0.90
1:D:72:LEU:CD1	6:N:50:PRO:HG2	2.00	0.90
5:M:127:ILE:CD1	6:N:256:PRO:CG	2.49	0.90
1:D:67:ASN:HB2	7:O:193:LEU:HD23	1.54	0.90
4:L:358:LYS:HG3	22:n:80:TYR:OH	1.72	0.90
5:M:231:LEU:HD12	5:M:235:LEU:CD1	2.00	0.90
7:O:314:LEU:CG	7:O:315:PRO:HD2	2.02	0.90
7:O:347:VAL:O	7:O:347:VAL:HG12	1.71	0.90
4:L:141:PHE:HE2	5:M:375:LEU:HD22	1.35	0.90
2:J:164:PHE:HE2	6:N:8:ILE:HG13	1.34	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
2:J:124:LEU:HD23	2:J:125:MET:N	1.87	0.89
5:M:453:LEU:HD12	5:M:454:ILE:N	1.88	0.89
5:M:142:ARG:HH21	6:N:303:THR:HG22	1.37	0.89
5:M:380:PHE:HA	5:M:383:MET:HE2	1.55	0.89
2:J:59:TYR:CE1	3:K:64:LEU:HD22	2.07	0.89
25:L:701:3PE:H321	25:L:701:3PE:H361	1.55	0.88
5:M:50:LYS:HE2	5:M:52:PHE:HE1	1.36	0.88
2:J:22:LYS:HZ3	3:K:22:PHE:HA	1.39	0.88
5:M:8:SER:HA	5:M:11:LEU:HD13	1.54	0.88
22:n:101:GLU:O	22:n:122:ARG:NH2	2.06	0.88
2:J:123:TRP:CZ3	13:e:73:MET:CG	2.57	0.88
5:M:173:THR:CG2	16:h:147:ALA:HB2	2.03	0.88
5:M:310:MET:SD	5:M:455:THR:HB	2.13	0.88
4:L:362:ILE:HD12	4:L:430:VAL:CG1	2.03	0.88
13:e:17:HIS:CD2	13:e:18:PHE:HD1	1.92	0.88
5:M:447:LEU:HD11	5:M:454:ILE:HG21	1.55	0.87
4:L:428:TYR:HA	4:L:432:MET:HG2	1.56	0.87
5:M:368:ALA:HB1	5:M:375:LEU:HD13	1.56	0.87
4:L:496:LEU:HD12	4:L:497:GLY:N	1.90	0.87
2:J:9:SER:OG	3:K:7:ASN:ND2	2.08	0.87
5:M:102:LEU:HD13	5:M:230:ILE:HG12	1.57	0.87
4:L:594:ASN:CG	6:N:110:PRO:HB2	2.00	0.86
4:L:79:SER:HB2	4:L:135:ASN:HB2	1.55	0.86
5:M:1:MET:HE1	5:M:111:SER:HB2	1.58	0.86
20:l:157:GLY:HA2	23:o:22:ILE:HG13	1.57	0.86
5:M:127:ILE:HD12	6:N:256:PRO:HG3	1.56	0.86
23:o:15:VAL:HG23	23:o:16:GLU:OE2	1.76	0.86
7:O:314:LEU:HG	7:O:315:PRO:HD2	1.58	0.86
7:O:347:VAL:CG1	11:c:29:PHE:HA	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:145:ILE:HG23	24:p:160:LYS:HE2	1.57	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
4:L:455:LYS:NZ	18:j:57:GLN:OE1	2.10	0.85
4:L:54:PHE:O	4:L:58:ASN:N	2.10	0.85
20:l:89:TRP:CZ2	22:n:86:PRO:HD2	2.11	0.85
4:L:437:PHE:HE1	4:L:441:ILE:CG1	1.85	0.85
5:M:115:LEU:HD21	5:M:176:LEU:HD21	1.59	0.85
5:M:208:PRO:HD3	5:M:236:LEU:HD22	1.59	0.85
4:L:247:LEU:HD11	4:L:248:HIS:CD2	2.11	0.84
3:K:66:PHE:HZ	6:N:35:PHE:HZ	1.25	0.84
4:L:128:MET:HG2	4:L:251:THR:HB	1.59	0.84
4:L:594:ASN:HD21	6:N:110:PRO:HB2	1.43	0.84
4:L:445:GLU:HB2	4:L:450:LEU:HD23	1.59	0.84
7:O:314:LEU:HD12	7:O:315:PRO:HD2	1.56	0.84
13:e:14:LEU:HD12	13:e:15:ASP:HB2	1.57	0.84
5:M:447:LEU:HD11	5:M:454:ILE:CG2	2.06	0.84
20:l:167:TYR:CD2	20:l:168:LEU:HD12	2.13	0.84
6:N:215:MET:SD	6:N:248:LEU:HD21	2.18	0.84
4:L:20:LEU:HD12	4:L:21:ILE:N	1.92	0.84
5:M:196:TRP:NE1	5:M:250:LEU:HD13	1.92	0.84
6:N:273:ASN:ND2	10:Y:143:VAL:HA	1.92	0.84
2:J:9:SER:HB2	3:K:7:ASN:HD22	1.42	0.83
2:J:22:LYS:HD2	3:K:23:ARG:HG3	1.61	0.83
5:M:373:ILE:HG12	5:M:454:ILE:HD11	1.60	0.83
13:e:87:MET:HE3	13:e:93:THR:HA	1.60	0.83
2:J:122:ASP:O	2:J:123:TRP:HD1	1.61	0.83
4:L:16:LEU:HD23	4:L:126:ILE:CD1	2.08	0.83
5:M:361:MET:HB3	5:M:441:MET:HE3	1.60	0.83
7:O:63:ASP:OD1	7:O:161:ARG:HA	1.79	0.83
10:Y:38:GLY:HA2	26:Y:201:CDL:H532	1.58	0.83
7:O:124:ASN:O	15:g:51:MET:HE3	1.79	0.83
4:L:131:LEU:CD1	4:L:140:LEU:HD12	2.09	0.82
20:l:91:GLN:NE2	22:n:2:ALA:HB1	1.94	0.82
4:L:432:MET:HG3	4:L:432:MET:O	1.78	0.82
5:M:269:MET:HE1	5:M:396:MET:HA	1.61	0.82
6:N:335:MET:HG3	6:N:335:MET:O	1.79	0.82
4:L:493:ILE:HD12	4:L:496:LEU:HD21	1.61	0.82
4:L:222:GLY:HA2	4:L:229:LEU:CD1	2.08	0.82
4:L:141:PHE:CE2	5:M:370:PRO:CG	2.61	0.82
13:e:41:ILE:CG2	16:h:179:ILE:HD11	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:16:LEU:CD2	4:L:126:ILE:HD13	2.10	0.81
19:k:34:PRO:HD2	19:k:59:TYR:CD1	2.16	0.81
13:e:45:HIS:CD2	16:h:176:LYS:HD3	2.15	0.81
4:L:229:LEU:O	4:L:229:LEU:CD1	2.28	0.81
6:N:277:ILE:HG23	6:N:278:MET:N	1.95	0.81
5:M:172:GLY:O	5:M:173:THR:CG2	2.28	0.81
19:k:30:ILE:HD11	19:k:39:GLN:HB2	1.61	0.81
1:D:72:LEU:HD11	6:N:50:PRO:CB	2.09	0.80
6:N:307:THR:HG22	6:N:308:ASN:H	1.47	0.80
16:h:163:ARG:HG2	16:h:165:ASP:HB2	1.63	0.80
5:M:263:LEU:HD11	21:m:102:TYR:HD1	1.45	0.80
6:N:200:LEU:HD21	6:N:265:ILE:HG12	1.62	0.80
5:M:216:LEU:HD12	5:M:236:LEU:HD21	1.60	0.80
6:N:277:ILE:CG2	6:N:278:MET:H	1.93	0.80
5:M:453:LEU:HD12	5:M:454:ILE:HG23	1.63	0.80
6:N:275:CYS:SG	10:Y:139:PRO:HG2	2.22	0.80
18:j:99:ILE:HA	23:o:108:LEU:HD21	1.63	0.80
24:p:6:ASP:HB3	24:p:9:VAL:HG22	1.61	0.80
20:l:38:PRO:HB2	21:m:75:ASN:ND2	1.94	0.80
7:O:117:PHE:CE1	7:O:173:MET:HE3	2.17	0.80
7:O:199:LEU:HD11	7:O:294:LEU:HD22	1.64	0.79
4:L:507:LEU:HD12	4:L:510:LYS:HD3	1.63	0.79
5:M:231:LEU:HA	5:M:235:LEU:HB2	1.62	0.79
18:j:97:LEU:O	23:o:104:ARG:NH1	2.15	0.79
8:U:76:LEU:HD12	8:U:156:GLU:HB2	1.62	0.79
4:L:516:ALA:HB2	22:n:30:TRP:CH2	2.18	0.79
5:M:122:PHE:CZ	5:M:206:LYS:HD3	2.18	0.79
4:L:130:ILE:HG23	4:L:139:GLN:HE21	1.46	0.79
4:L:552:LEU:HD21	21:m:90:GLY:HA2	1.65	0.79
5:M:367:LEU:HD21	5:M:408:MET:HE2	1.64	0.79
13:e:30:ALA:HB2	16:h:184:LYS:HG3	1.65	0.79
4:L:446:ASN:ND2	18:j:51:THR:HG21	1.98	0.79
6:N:338:PRO:HG3	26:d:201:CDL:H592	1.65	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	0.79
4:L:475:THR:HA	23:o:55:GLN:NE2	1.97	0.79
5:M:106:LEU:HD13	5:M:234:ILE:HG21	1.63	0.78
6:N:123:PRO:HG2	6:N:126:MET:HG2	1.64	0.78
7:O:117:PHE:HE1	7:O:173:MET:CE	1.96	0.78
5:M:248:ILE:HG13	5:M:249:ILE:HD12	1.64	0.78
26:M:503:CDL:H122	12:d:47:MET:HE1	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:159:LEU:HB3	16:h:163:ARG:HH12	1.47	0.78
4:L:3:ILE:H	4:L:3:ILE:HD12	1.48	0.78
4:L:466:PHE:CB	18:j:68:TRP:CZ2	2.56	0.78
5:M:231:LEU:HD12	5:M:235:LEU:HD13	1.64	0.78
5:M:370:PRO:HA	5:M:375:LEU:CD2	2.13	0.78
9:X:168:PHE:O	9:X:170:TRP:CD1	2.37	0.78
17:i:81:PHE:HB3	25:i:201:3PE:H242	1.64	0.78
4:L:534:HIS:O	4:L:538:PRO:HG3	1.83	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
13:e:89:GLU:HB2	13:e:91:LYS:HG2	1.65	0.78
20:l:44:THR:OG1	20:l:45:PRO:HD2	1.83	0.78
3:K:42:ILE:O	3:K:46:VAL:HG23	1.84	0.78
5:M:319:HIS:HA	5:M:322:THR:HG22	1.66	0.78
23:o:7:ARG:HA	23:o:11:TRP:CD1	2.19	0.78
4:L:136:ASN:HA	4:L:197:GLU:HA	1.66	0.78
6:N:215:MET:CE	6:N:248:LEU:CD2	2.62	0.78
5:M:127:ILE:HD11	6:N:256:PRO:CG	2.13	0.78
4:L:466:PHE:HE1	18:j:72:ARG:CZ	1.94	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
5:M:204:LEU:HD22	5:M:209:LEU:HD12	1.65	0.77
7:O:305:LEU:HD12	7:O:305:LEU:O	1.83	0.77
13:e:17:HIS:CD2	13:e:18:PHE:CD1	2.72	0.77
6:N:170:LEU:HD11	6:N:288:LEU:HG	1.65	0.77
25:i:201:3PE:H362	25:i:201:3PE:H2A1	1.66	0.77
20:l:169:GLU:C	20:l:171:GLY:H	1.92	0.77
5:M:208:PRO:HG2	5:M:216:LEU:HD13	1.67	0.77
6:N:31:VAL:O	6:N:35:PHE:HD2	1.68	0.77
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
5:M:453:LEU:HD11	5:M:454:ILE:HG23	1.66	0.77
6:N:232:LEU:CD2	6:N:307:THR:HG23	2.15	0.77
20:l:113:ILE:HG23	20:l:115:ASN:H	1.50	0.77
4:L:598:ILE:HD11	6:N:153:ILE:HG12	1.66	0.76
5:M:171:VAL:HG11	5:M:179:LEU:HD21	1.65	0.76
4:L:419:THR:HA	4:L:422:TYR:CE2	2.20	0.76
5:M:175:ASN:HD22	16:h:143:GLU:HG2	1.50	0.76
6:N:210:ILE:HG22	6:N:333:SER:HB3	1.65	0.76
18:j:97:LEU:O	23:o:104:ARG:HG3	1.85	0.76
8:U:86:VAL:HB	8:U:122:MET:HE1	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:42:LEU:HG	5:M:67:ILE:HD11	1.68	0.76
5:M:60:PRO:O	5:M:64:PRO:HD3	1.85	0.76
26:M:503:CDL:H742	26:M:503:CDL:H151	1.68	0.76
5:M:231:LEU:HD12	5:M:235:LEU:HD12	1.67	0.76
2:J:29:GLY:N	3:K:31:LEU:HD21	2.00	0.76
2:J:124:LEU:HD23	2:J:125:MET:H	1.50	0.76
4:L:496:LEU:HD12	4:L:496:LEU:C	2.09	0.76
20:l:158:PRO:HD3	23:o:22:ILE:CB	2.16	0.76
4:L:516:ALA:HB2	22:n:30:TRP:HH2	1.49	0.76
4:L:556:ILE:HG21	21:m:80:PHE:CE1	2.21	0.76
6:N:211:LEU:HD23	6:N:333:SER:HB2	1.68	0.76
2:J:59:TYR:HE1	3:K:64:LEU:HD22	1.49	0.76
17:i:94:PRO:HG3	24:p:10:TYR:CE2	2.20	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	0.75
6:N:215:MET:HE2	6:N:248:LEU:HD21	1.67	0.75
7:O:121:PRO:O	7:O:122:LYS:HG2	1.86	0.75
21:m:125:PHE:HE1	24:p:133:THR:HG22	1.51	0.75
22:n:20:TYR:CZ	22:n:24:LEU:HD11	2.21	0.75
4:L:23:MET:HE1	26:L:703:CDL:H192	1.67	0.75
4:L:387:THR:HG23	4:L:461:SER:O	1.85	0.75
6:N:275:CYS:SG	10:Y:139:PRO:CG	2.75	0.75
6:N:227:ILE:HA	6:N:230:ILE:HG22	1.66	0.75
26:L:703:CDL:H731	26:L:703:CDL:H542	1.68	0.75
6:N:307:THR:C	7:O:319:ILE:HG12	2.12	0.75
2:J:88:ILE:HD11	3:K:23:ARG:HH12	1.51	0.75
4:L:393:ASP:OD1	4:L:394:LEU:N	2.19	0.75
4:L:553:LEU:HD21	21:m:93:ALA:C	2.11	0.75
6:N:277:ILE:HG23	6:N:278:MET:H	1.50	0.75
23:o:117:LEU:HA	23:o:120:ALA:HB3	1.69	0.75
5:M:388:TRP:CE2	21:m:109:ARG:HD2	2.22	0.74
7:O:117:PHE:CE1	7:O:128:SER:HB2	2.22	0.74
2:J:169:ILE:HG13	6:N:45:ILE:CD1	2.17	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
5:M:314:MET:HA	5:M:454:ILE:HD12	1.70	0.74
18:j:92:TRP:CZ3	23:o:100:LYS:HA	2.22	0.74
4:L:362:ILE:HG23	4:L:366:MET:HE3	1.68	0.74
5:M:29:SER:HB3	15:g:91:PHE:CD2	2.22	0.74
5:M:29:SER:HB3	15:g:91:PHE:HD2	1.52	0.74
21:m:45:ARG:HD2	22:n:150:MET:CE	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:310:MET:HG3	5:M:455:THR:HA	1.70	0.74
7:O:254:GLU:HG3	7:O:276:LEU:HD13	1.68	0.74
2:J:154:VAL:CG2	6:N:35:PHE:CZ	2.70	0.74
4:L:285:THR:HG22	4:L:415:ALA:HB1	1.70	0.74
10:Y:76:THR:HG23	10:Y:95:GLY:HA3	1.70	0.74
4:L:14:LEU:HD21	17:i:74:HIS:O	1.87	0.74
6:N:289:ASN:HA	6:N:292:PHE:CE2	2.23	0.74
2:J:123:TRP:CE3	13:e:73:MET:CG	2.68	0.74
5:M:200:MET:HE1	5:M:247:SER:HB2	1.69	0.74
2:J:24:SER:HB2	2:J:27:TYR:HD1	1.53	0.73
5:M:1:MET:HB2	5:M:52:PHE:CD2	2.23	0.73
7:O:217:ARG:O	7:O:220:LYS:HG2	1.89	0.73
2:J:2:ASN:HB3	2:J:121:GLY:HA3	1.70	0.73
6:N:202:LEU:O	6:N:206:MET:HG2	1.87	0.73
5:M:260:PRO:O	5:M:264:LEU:HG	1.88	0.73
7:O:117:PHE:HE1	7:O:173:MET:HE3	1.53	0.73
7:O:323:GLN:NE2	15:g:54:GLN:HB3	2.00	0.73
4:L:20:LEU:HD12	4:L:20:LEU:C	2.13	0.73
26:L:703:CDL:H312	26:L:703:CDL:H351	1.69	0.73
5:M:167:ILE:HD11	5:M:195:LEU:HD21	1.70	0.73
4:L:232:TRP:CZ3	4:L:233:LEU:HD23	2.23	0.73
2:J:57:LEU:HD12	2:J:58:ILE:HG12	1.69	0.73
4:L:579:ASN:OD1	4:L:579:ASN:O	2.06	0.73
5:M:216:LEU:HG	5:M:220:HIS:HE1	1.49	0.73
6:N:308:ASN:C	7:O:319:ILE:HG23	2.13	0.73
4:L:150:MET:HE1	26:L:703:CDL:H511	1.69	0.73
5:M:73:LEU:HD22	5:M:103:GLN:CD	2.13	0.73
5:M:122:PHE:CD1	5:M:238:LEU:HG	2.23	0.73
25:D:501:3PE:H232	4:L:567:SER:HA	1.71	0.72
2:J:123:TRP:CZ3	13:e:73:MET:HA	2.24	0.72
4:L:358:LYS:HG2	22:n:80:TYR:CE1	2.24	0.72
6:N:277:ILE:CG2	6:N:278:MET:N	2.52	0.72
2:J:9:SER:CB	3:K:7:ASN:ND2	2.52	0.72
7:O:80:GLN:HG3	7:O:270:VAL:CG2	2.11	0.72
8:U:79:ILE:HD11	8:U:148:ILE:HG22	1.71	0.72
24:p:7:LYS:O	24:p:11:PRO:HA	1.89	0.72
4:L:136:ASN:HD21	26:h:201:CDL:H273	1.54	0.72
5:M:243:MET:HE1	5:M:302:MET:HE3	1.71	0.72
5:M:441:MET:SD	5:M:444:LEU:HD23	2.30	0.72
6:N:215:MET:SD	6:N:248:LEU:CD2	2.77	0.72
4:L:141:PHE:CD2	5:M:370:PRO:HB3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:34:PRO:HG2	19:k:59:TYR:HE1	1.54	0.72
4:L:316:THR:CG2	4:L:325:ALA:HB2	2.19	0.72
7:O:176:GLN:HB2	7:O:178:TYR:HD2	1.55	0.72
7:O:126:GLY:HA3	15:g:51:MET:HE1	1.71	0.72
4:L:141:PHE:HD2	5:M:370:PRO:HB3	1.53	0.72
26:M:503:CDL:H671	26:d:201:CDL:H151	1.69	0.72
17:i:74:HIS:O	17:i:78:PRO:CG	2.33	0.72
6:N:59:TYR:CE2	6:N:63:GLN:HG3	2.23	0.72
4:L:247:LEU:HD12	4:L:248:HIS:N	2.03	0.72
4:L:299:LYS:HB2	4:L:354:GLN:HE21	1.55	0.72
5:M:373:ILE:CG1	5:M:454:ILE:HD11	2.19	0.72
5:M:395:LEU:HD21	21:m:101:TRP:CE2	2.25	0.71
1:D:67:ASN:HB3	1:D:69:VAL:HG12	1.71	0.71
2:J:151:MET:HE1	6:N:28:LEU:CD1	2.19	0.71
4:L:441:ILE:HG21	18:j:48:PRO:HD3	1.71	0.71
5:M:106:LEU:HD13	5:M:234:ILE:HG22	1.72	0.71
6:N:146:TYR:CD1	6:N:147:PRO:HD3	2.26	0.71
7:O:336:GLY:H	7:O:344:ASN:ND2	1.89	0.71
5:M:313:THR:HG21	5:M:456:GLY:HA3	1.71	0.71
21:m:9:ALA:HB1	21:m:10:PRO:HD2	1.71	0.71
4:L:368:PHE:HB3	4:L:445:GLU:CD	2.15	0.71
8:U:144:ILE:O	8:U:148:ILE:HG12	1.91	0.71
20:l:106:HIS:CD2	20:l:107:TRP:H	2.08	0.71
5:M:220:HIS:CE1	5:M:231:LEU:HD23	2.26	0.71
5:M:370:PRO:HA	5:M:375:LEU:HD23	1.72	0.71
1:D:47:PHE:CB	6:N:227:ILE:HD11	2.16	0.71
8:U:102:SER:O	8:U:141:PRO:HD3	1.91	0.71
21:m:45:ARG:O	21:m:45:ARG:HG2	1.90	0.71
5:M:373:ILE:HG12	5:M:454:ILE:CD1	2.20	0.70
6:N:237:THR:HG23	6:N:237:THR:O	1.88	0.70
7:O:241:TYR:HA	7:O:245:PHE:HB3	1.73	0.70
7:O:135:LEU:HB3	7:O:139:ARG:HH12	1.56	0.70
13:e:83:ARG:HH11	13:e:92:TYR:HE2	1.38	0.70
20:l:184:TYR:HA	23:o:36:GLU:HA	1.72	0.70
21:m:45:ARG:NH2	22:n:150:MET:HE3	2.06	0.70
2:J:13:LEU:HD21	3:K:14:LEU:HD12	1.74	0.70
2:J:123:TRP:CH2	13:e:73:MET:CA	2.74	0.70
4:L:559:GLU:O	4:L:564:LYS:HB2	1.92	0.70
4:L:604:ILE:O	10:Y:5:LYS:HD2	1.91	0.70
6:N:156:MET:HE2	10:Y:138:PHE:CE2	2.27	0.70
6:N:254:LEU:HD12	6:N:255:PRO:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:55:TRP:CZ2	12:d:66:THR:HG22	2.25	0.70
20:l:38:PRO:HG2	21:m:71:ALA:HB2	1.73	0.70
25:D:501:3PE:H361	4:L:566:THR:HG21	1.73	0.70
4:L:445:GLU:OE2	18:j:54:GLN:HG3	1.91	0.70
4:L:446:ASN:HD21	18:j:51:THR:HG21	1.55	0.70
4:L:593:ILE:HG21	10:Y:41:TYR:CE2	2.25	0.70
6:N:137:ALA:HB3	6:N:138:PRO:HD3	1.74	0.70
4:L:428:TYR:HA	4:L:432:MET:CG	2.21	0.70
5:M:447:LEU:HD21	5:M:454:ILE:HD13	1.73	0.70
5:M:134:THR:O	5:M:142:ARG:HD2	1.91	0.70
4:L:480:LEU:HD23	4:L:480:LEU:O	1.92	0.70
23:o:22:ILE:HA	23:o:105:GLU:OE2	1.91	0.70
23:o:25:PHE:HE2	23:o:109:LEU:HD22	1.57	0.70
4:L:285:THR:HG22	4:L:415:ALA:CB	2.22	0.69
5:M:17:LEU:HD21	26:M:503:CDL:H522	1.74	0.69
17:i:104:ILE:HG13	23:o:48:ASP:HB3	1.74	0.69
2:J:123:TRP:CZ3	13:e:73:MET:CA	2.75	0.69
6:N:248:LEU:HD13	6:N:296:LEU:HD23	1.75	0.69
5:M:216:LEU:HD11	5:M:236:LEU:HD11	1.72	0.69
10:Y:143:VAL:HG22	16:h:161:ARG:HD2	1.73	0.69
2:J:22:LYS:HZ2	3:K:22:PHE:HA	1.56	0.69
5:M:50:LYS:HE2	5:M:52:PHE:CE1	2.25	0.69
5:M:142:ARG:NH2	6:N:303:THR:HG22	2.07	0.69
5:M:369:LEU:HD23	5:M:371:PRO:CD	2.12	0.69
20:l:122:THR:HG21	20:l:129:MET:HE1	1.73	0.69
21:m:25:VAL:HA	21:m:30:ARG:HD3	1.73	0.69
4:L:305:SER:HB2	4:L:422:TYR:HE1	1.58	0.69
16:h:96:ALA:HB3	24:p:63:TYR:HD1	1.57	0.69
21:m:127:ILE:CG2	24:p:136:THR:HG23	2.23	0.69
4:L:542:LEU:HD21	20:l:116:ARG:HD2	1.73	0.69
5:M:173:THR:CG2	16:h:147:ALA:CB	2.71	0.69
6:N:215:MET:HE2	6:N:248:LEU:CD2	2.23	0.69
23:o:19:PRO:HA	23:o:22:ILE:HD11	1.74	0.69
4:L:18:PRO:O	4:L:21:ILE:HG22	1.92	0.68
4:L:312:LEU:HD21	4:L:395:ILE:HG21	1.75	0.68
4:L:332:HIS:NE2	4:L:336:LYS:HG3	2.07	0.68
5:M:127:ILE:HB	5:M:128:PRO:HD3	1.75	0.68
5:M:263:LEU:CD1	21:m:102:TYR:HD1	2.05	0.68
19:k:34:PRO:CD	19:k:59:TYR:CD1	2.75	0.68
7:O:140:LEU:HG	7:O:304:VAL:HG12	1.74	0.68
13:e:95:PRO:HG2	13:e:97:HIS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:78:LEU:HD11	20:l:104:PRO:HB2	1.74	0.68
7:O:60:ILE:HD12	7:O:203:ALA:HB3	1.73	0.68
10:Y:77:CYS:SG	10:Y:78:VAL:N	2.66	0.68
4:L:516:ALA:HB1	4:L:520:SER:HB2	1.74	0.68
7:O:256:LEU:HB3	7:O:258:TYR:CE1	2.29	0.68
4:L:578:THR:CG2	6:N:168:GLY:HA2	2.23	0.68
5:M:143:LEU:HD21	6:N:303:THR:HG23	1.72	0.68
5:M:379:LEU:O	5:M:383:MET:HG3	1.93	0.68
4:L:9:LEU:HD11	25:i:201:3PE:H2A2	1.74	0.68
4:L:211:ILE:N	4:L:212:PRO:HD2	2.08	0.68
4:L:383:MET:SD	4:L:384:PRO:HD2	2.33	0.68
6:N:215:MET:HE1	6:N:248:LEU:HD21	1.71	0.68
13:e:95:PRO:HD2	13:e:98:HIS:ND1	2.08	0.68
20:l:156:VAL:HG11	23:o:95:TYR:CZ	2.29	0.68
23:o:7:ARG:HA	23:o:11:TRP:HD1	1.58	0.68
5:M:39:LEU:HD23	5:M:67:ILE:HD13	1.74	0.68
8:U:100:VAL:O	8:U:141:PRO:HG2	1.94	0.68
15:g:140:PHE:CE2	24:p:74:ILE:CG2	2.77	0.68
2:J:100:VAL:O	2:J:103:ILE:HG12	1.94	0.68
5:M:173:THR:HG23	16:h:147:ALA:CB	2.24	0.68
7:O:323:GLN:HE22	15:g:54:GLN:CB	2.03	0.68
7:O:352:ILE:HG21	12:d:52:PRO:HG2	1.75	0.68
10:Y:96:GLY:HA3	10:Y:121:GLY:HA2	1.75	0.68
20:l:101:TRP:NE1	21:m:62:ASP:HA	2.09	0.68
2:J:59:TYR:HA	2:J:63:MET:CB	2.24	0.68
2:J:25:PRO:HB3	3:K:27:MET:HG3	1.75	0.68
20:l:122:THR:HG23	20:l:123:PRO:HD2	1.75	0.68
4:L:228:GLY:C	4:L:229:LEU:HG	2.19	0.67
4:L:358:LYS:HG2	22:n:80:TYR:CZ	2.29	0.67
5:M:311:GLY:HA2	5:M:314:MET:HE3	1.76	0.67
5:M:423:MET:SD	21:m:59:HIS:NE2	2.67	0.67
6:N:313:MET:CG	7:O:305:LEU:HD22	2.23	0.67
7:O:347:VAL:O	7:O:347:VAL:CG1	2.42	0.67
12:d:5:ARG:HD2	12:d:89:ASP:OD2	1.93	0.67
20:l:152:SER:HA	23:o:5:LEU:HD21	1.75	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	2.30	0.67
9:X:158:LEU:HB3	12:d:21:LEU:HD21	1.75	0.67
5:M:11:LEU:HB3	5:M:100:ILE:HD13	1.76	0.67
6:N:26:LEU:HD23	6:N:29:MET:SD	2.35	0.67
6:N:149:LEU:HD13	6:N:154:ILE:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:125:PHE:CE1	24:p:133:THR:HG22	2.29	0.67
5:M:30:TYR:O	5:M:34:ILE:HG12	1.95	0.67
15:g:109:ASP:CB	15:g:114:GLU:HB3	2.24	0.67
5:M:98:MET:HE2	5:M:131:ILE:HB	1.77	0.67
9:X:158:LEU:HD13	12:d:17:GLU:HG3	1.77	0.67
21:m:45:ARG:HD2	22:n:150:MET:HE1	1.76	0.67
21:m:49:LEU:HD23	22:n:140:LEU:HD23	1.76	0.67
5:M:282:LEU:HD21	5:M:359:TRP:HH2	1.60	0.67
5:M:424:ILE:HG13	21:m:57:VAL:O	1.95	0.67
10:Y:76:THR:HG22	10:Y:92:TYR:HA	1.77	0.67
12:d:14:LEU:O	12:d:14:LEU:CD1	2.37	0.67
4:L:81:LYS:N	4:L:135:ASN:ND2	2.43	0.67
7:O:249:MET:HB3	7:O:253:CYS:SG	2.34	0.67
18:j:99:ILE:HA	23:o:108:LEU:CD2	2.25	0.67
20:l:106:HIS:HD2	20:l:107:TRP:H	1.43	0.67
4:L:552:LEU:CD2	4:L:553:LEU:HD12	2.25	0.67
5:M:285:LEU:HD13	5:M:342:MET:HE1	1.76	0.67
13:e:14:LEU:CD1	13:e:15:ASP:HB2	2.25	0.67
4:L:389:PHE:CZ	18:j:79:ALA:HB1	2.30	0.66
5:M:270:ILE:HG22	5:M:271:MET:HE2	1.76	0.66
7:O:209:VAL:HG12	7:O:260:SER:HB2	1.76	0.66
7:O:326:ARG:NH2	15:g:56:ASP:OD1	2.27	0.66
4:L:201:ILE:HG22	4:L:266:LEU:HD11	1.76	0.66
8:U:128:PHE:CZ	8:U:148:ILE:HD12	2.30	0.66
20:l:38:PRO:CB	21:m:75:ASN:HD22	2.02	0.66
23:o:89:TYR:CE2	23:o:93:LEU:HD11	2.30	0.66
4:L:446:ASN:HD21	18:j:51:THR:CG2	2.08	0.66
5:M:361:MET:CB	5:M:441:MET:HE3	2.25	0.66
10:Y:71:MET:HG3	10:Y:102:THR:CG2	2.26	0.66
18:j:38:VAL:HG12	18:j:39:HIS:N	2.10	0.66
23:o:42:THR:HG22	23:o:44:GLN:H	1.59	0.66
4:L:562:ILE:HB	4:L:563:PRO:HD3	1.78	0.66
7:O:343:TYR:HD1	7:O:352:ILE:HG23	1.59	0.66
4:L:364:LYS:CE	19:k:67:ILE:HD11	2.25	0.66
4:L:407:TRP:CE3	4:L:410:LEU:HD11	2.30	0.66
5:M:151:PHE:CZ	6:N:291:PHE:HB2	2.31	0.66
7:O:205:ILE:HD11	7:O:273:ILE:HG12	1.77	0.66
16:h:102:PRO:HD2	16:h:105:TYR:HB2	1.78	0.66
22:n:149:ILE:H	22:n:149:ILE:HD12	1.59	0.66
5:M:318:ALA:HB2	5:M:373:ILE:HG23	1.75	0.66
14:f:38:ARG:HD3	14:f:56:TRP:NE1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:TYR:CD2	2:J:63:MET:HG2	2.31	0.66
4:L:116:ARG:HG2	4:L:120:TYR:CE2	2.31	0.66
4:L:174:TYR:CD2	4:L:232:TRP:CD1	2.68	0.66
7:O:132:GLN:NE2	28:O:401:ADP:HN62	1.93	0.66
7:O:200:PRO:HG3	7:O:282:PRO:HD2	1.78	0.66
21:m:129:TYR:CZ	24:p:144:LEU:O	2.49	0.66
4:L:25:ASN:OD1	4:L:25:ASN:O	2.14	0.66
7:O:48:LYS:HD2	7:O:288:ASP:HB2	1.78	0.66
7:O:62:VAL:HA	7:O:205:ILE:O	1.96	0.66
19:k:34:PRO:CG	19:k:59:TYR:CE1	2.72	0.66
4:L:66:TRP:HZ3	4:L:68:TRP:CD1	2.14	0.66
4:L:552:LEU:HD23	4:L:553:LEU:HD12	1.77	0.66
2:J:44:LEU:CD2	2:J:52:GLY:HA3	2.26	0.65
17:i:15:LEU:HD21	22:n:164:PRO:HB2	1.78	0.65
24:p:70:ARG:CZ	24:p:91:GLN:HE21	2.09	0.65
5:M:373:ILE:CD1	5:M:454:ILE:HD11	2.25	0.65
7:O:38:TYR:HB3	7:O:299:GLN:NE2	2.11	0.65
9:X:160:PRO:HG3	12:d:22:PRO:HD3	1.78	0.65
6:N:307:THR:CB	7:O:319:ILE:HD11	2.22	0.65
21:m:15:PRO:CG	21:m:18:LEU:HD12	2.27	0.65
6:N:220:MET:C	6:N:223:ASN:H	2.04	0.65
26:h:201:CDL:H112	25:i:201:3PE:H331	1.77	0.65
5:M:367:LEU:CD2	5:M:408:MET:HE2	2.25	0.65
20:l:82:SER:HA	20:l:112:TYR:HB3	1.79	0.65
4:L:190:SER:HB2	4:L:196:TRP:HE1	1.60	0.65
4:L:386:LEU:HD11	18:j:69:ILE:HD11	1.79	0.65
6:N:258:THR:HB	6:N:333:SER:O	1.96	0.65
4:L:88:LEU:HD23	4:L:326:PHE:CE2	2.32	0.65
15:g:108:PRO:O	15:g:109:ASP:OD1	2.13	0.65
20:l:185:ASP:O	23:o:34:ARG:HD3	1.96	0.65
22:n:30:TRP:CD2	22:n:76:HIS:HD2	2.15	0.65
25:L:705:3PE:H2A1	25:L:705:3PE:H261	1.79	0.65
5:M:263:LEU:HD11	21:m:102:TYR:CD1	2.31	0.65
7:O:343:TYR:CE1	7:O:355:LYS:HB2	2.31	0.65
18:j:47:PHE:HA	19:k:63:PHE:CZ	2.32	0.65
4:L:141:PHE:CD2	5:M:370:PRO:HG3	2.31	0.65
4:L:591:PHE:HE1	6:N:113:PHE:HD2	1.42	0.65
5:M:122:PHE:HD1	5:M:238:LEU:HG	1.62	0.65
25:M:501:3PE:H12	6:N:276:LEU:HD22	1.79	0.65
16:h:127:ASP:OD1	16:h:127:ASP:O	2.15	0.65
24:p:24:THR:HG22	24:p:26:LEU:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:66:PHE:CZ	6:N:35:PHE:CE1	2.84	0.65
4:L:387:THR:HG22	4:L:465:GLY:H	1.61	0.65
4:L:594:ASN:CG	6:N:110:PRO:CB	2.69	0.65
9:X:162:LYS:HB3	9:X:166:ARG:HH21	1.62	0.65
4:L:368:PHE:HB3	4:L:445:GLU:OE2	1.97	0.64
6:N:254:LEU:HD12	6:N:255:PRO:HD2	1.77	0.64
7:O:194:THR:HG23	7:O:307:TYR:HB2	1.79	0.64
23:o:71:ARG:HB3	23:o:71:ARG:HH11	1.61	0.64
24:p:74:ILE:HD13	24:p:85:ILE:HG13	1.80	0.64
5:M:119:TYR:CD1	5:M:160:LEU:HD22	2.32	0.64
5:M:166:LEU:HD11	25:M:501:3PE:H11	1.77	0.64
5:M:167:ILE:O	5:M:171:VAL:HG12	1.98	0.64
9:X:167:PHE:HD2	9:X:170:TRP:NE1	1.94	0.64
2:J:22:LYS:NZ	3:K:22:PHE:CA	2.56	0.64
5:M:307:TRP:CD1	5:M:459:MET:SD	2.91	0.64
14:f:8:ARG:HE	14:f:8:ARG:HA	1.63	0.64
20:l:38:PRO:C	21:m:75:ASN:ND2	2.55	0.64
20:l:122:THR:CG2	20:l:123:PRO:HD2	2.27	0.64
4:L:556:ILE:CG2	21:m:80:PHE:CZ	2.81	0.64
6:N:307:THR:HG22	6:N:308:ASN:N	2.12	0.64
10:Y:137:LEU:HD23	10:Y:138:PHE:CG	2.31	0.64
2:J:25:PRO:HB3	3:K:27:MET:CG	2.28	0.64
4:L:81:LYS:N	4:L:135:ASN:HD21	1.96	0.64
12:d:60:ARG:O	12:d:61:GLN:C	2.40	0.64
15:g:140:PHE:CE2	24:p:74:ILE:HG22	2.33	0.64
26:h:201:CDL:HA62	26:h:201:CDL:H551	1.78	0.64
4:L:385:PHE:HE2	18:j:73:PHE:HD1	1.45	0.64
5:M:300:SER:HB3	5:M:381:ILE:HG23	1.78	0.64
6:N:37:LEU:HD12	6:N:63:GLN:HB3	1.79	0.64
7:O:117:PHE:CE1	7:O:173:MET:CE	2.77	0.64
7:O:132:GLN:HE22	28:O:401:ADP:HN62	1.45	0.64
18:j:84:PHE:HE2	23:o:88:ASP:HB3	1.63	0.64
23:o:105:GLU:O	23:o:106:ARG:C	2.39	0.64
4:L:40:ILE:HD13	4:L:97:THR:HG22	1.79	0.64
4:L:56:HIS:HA	23:o:74:PHE:CD1	2.33	0.64
4:L:366:MET:CG	4:L:443:ILE:HG21	2.28	0.64
5:M:160:LEU:HD11	5:M:203:PHE:CZ	2.33	0.64
5:M:344:MET:HE1	21:m:59:HIS:NE2	2.13	0.64
24:p:5:TRP:HH2	24:p:12:GLU:OE1	1.81	0.64
4:L:41:LYS:HG3	4:L:98:TRP:CE2	2.33	0.64
4:L:385:PHE:CD1	18:j:72:ARG:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:441:ILE:HD12	18:j:46:GLU:O	1.98	0.64
4:L:480:LEU:HD22	18:j:84:PHE:CD2	2.33	0.64
6:N:179:MET:HG3	6:N:216:PHE:HE1	1.63	0.64
12:d:100:ASP:HB3	16:h:159:LEU:HD21	1.80	0.64
4:L:246:LEU:HD12	4:L:246:LEU:C	2.23	0.64
5:M:196:TRP:HZ3	5:M:261:PHE:HE2	1.44	0.64
4:L:586:LEU:HD21	10:Y:47:PRO:HD3	1.80	0.63
25:L:701:3PE:H262	25:L:701:3PE:H342	1.78	0.63
5:M:267:TRP:CZ2	5:M:271:MET:HE3	2.32	0.63
26:M:503:CDL:H132	6:N:242:THR:HG21	1.80	0.63
6:N:220:MET:HA	6:N:223:ASN:HA	1.79	0.63
26:d:201:CDL:H531	26:d:201:CDL:H711	1.79	0.63
14:f:56:TRP:CD1	16:h:134:GLU:OE1	2.51	0.63
17:i:29:SER:HB2	17:i:32:GLU:OE1	1.97	0.63
2:J:51:LEU:H	2:J:51:LEU:HD12	1.63	0.63
6:N:143:ILE:HA	6:N:194:LEU:HD11	1.79	0.63
18:j:84:PHE:CE2	23:o:88:ASP:HB3	2.34	0.63
20:l:106:HIS:CD2	20:l:107:TRP:N	2.67	0.63
22:n:95:GLU:HA	22:n:98:LYS:HG3	1.80	0.63
23:o:6:THR:HA	23:o:10:LEU:HD13	1.80	0.63
4:L:381:THR:HG21	4:L:498:PHE:CE2	2.33	0.63
7:O:167:PHE:HZ	7:O:244:THR:HB	1.61	0.63
7:O:176:GLN:HB2	7:O:178:TYR:CD2	2.32	0.63
23:o:15:VAL:HG23	23:o:16:GLU:N	2.13	0.63
2:J:151:MET:CE	6:N:28:LEU:HD13	2.24	0.63
5:M:250:LEU:O	5:M:250:LEU:CD1	2.44	0.63
5:M:368:ALA:HB1	5:M:375:LEU:CD1	2.25	0.63
13:e:87:MET:HG2	13:e:92:TYR:O	1.99	0.63
15:g:75:ASP:OD1	15:g:76:SER:N	2.32	0.63
2:J:46:PHE:CZ	3:K:46:VAL:HG13	2.34	0.63
4:L:100:ILE:HD13	4:L:341:MET:SD	2.39	0.63
4:L:305:SER:HB2	4:L:422:TYR:CE1	2.34	0.63
5:M:1:MET:HB2	5:M:52:PHE:HD2	1.60	0.63
5:M:105:LEU:O	5:M:109:THR:HG23	1.98	0.63
5:M:118:PHE:O	5:M:122:PHE:N	2.25	0.63
5:M:231:LEU:HA	5:M:235:LEU:HD12	1.80	0.63
7:O:63:ASP:OD2	7:O:165:SER:HB3	1.99	0.63
19:k:34:PRO:HG2	19:k:59:TYR:CD1	2.34	0.63
4:L:80:PHE:C	4:L:135:ASN:HD21	2.06	0.63
4:L:202:MET:HE3	4:L:265:PRO:CG	2.25	0.63
4:L:410:LEU:HD12	4:L:411:ILE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:433:THR:HG22	4:L:434:LYS:N	2.14	0.63
5:M:220:HIS:NE2	5:M:231:LEU:HB3	2.13	0.63
22:n:133:TRP:HA	22:n:136:GLU:OE2	1.98	0.63
4:L:358:LYS:HG3	22:n:80:TYR:CE2	2.32	0.63
6:N:149:LEU:HD13	6:N:154:ILE:CG2	2.28	0.63
8:U:140:CYS:SG	8:U:143:GLU:OE2	2.53	0.63
9:X:160:PRO:HG3	12:d:22:PRO:CD	2.28	0.63
17:i:28:LEU:HD22	17:i:32:GLU:HG2	1.79	0.63
4:L:361:ASN:OD1	4:L:361:ASN:O	2.17	0.63
6:N:131:LEU:O	6:N:135:LYS:HG2	1.98	0.63
7:O:305:LEU:HD12	7:O:305:LEU:C	2.24	0.63
13:e:69:ARG:HD2	13:e:72:THR:HG21	1.80	0.63
16:h:155:GLU:O	16:h:159:LEU:HD13	1.99	0.63
18:j:89:PRO:O	23:o:103:GLU:HG2	1.98	0.63
5:M:129:THR:HG21	5:M:235:LEU:HD13	1.80	0.63
19:k:42:LEU:HG	22:n:39:TYR:HD1	1.64	0.63
4:L:598:ILE:HG21	6:N:100:MET:HE2	1.81	0.62
4:L:445:GLU:HB2	4:L:450:LEU:CD2	2.29	0.62
6:N:100:MET:HE3	6:N:111:PHE:CZ	2.34	0.62
6:N:158:ALA:O	6:N:162:ILE:HG12	1.99	0.62
22:n:31:CYS:SG	22:n:36:LYS:NZ	2.71	0.62
4:L:437:PHE:CE1	4:L:441:ILE:CG1	2.69	0.62
7:O:61:THR:HB	7:O:160:GLU:O	2.00	0.62
15:g:106:TYR:CE2	16:h:86:ILE:HD12	2.35	0.62
4:L:539:MET:SD	21:m:11:LEU:HD21	2.38	0.62
5:M:73:LEU:CD2	5:M:103:GLN:NE2	2.61	0.62
5:M:318:ALA:CB	5:M:373:ILE:HG23	2.29	0.62
7:O:121:PRO:O	7:O:122:LYS:CG	2.46	0.62
14:f:13:HIS:O	14:f:17:PRO:HD2	2.00	0.62
5:M:307:TRP:CE3	5:M:383:MET:HE3	2.34	0.62
7:O:132:GLN:HE22	7:O:169:PHE:HB2	1.64	0.62
10:Y:64:THR:OG1	10:Y:106:ARG:HG2	2.00	0.62
14:f:41:SER:OG	16:h:134:GLU:HG2	2.00	0.62
4:L:365:ILE:HD11	4:L:366:MET:HE2	1.82	0.62
5:M:129:THR:HG21	5:M:235:LEU:CD1	2.30	0.62
5:M:307:TRP:HD1	5:M:459:MET:SD	2.23	0.62
7:O:113:SER:HB3	7:O:116:LYS:HB2	1.80	0.62
21:m:17:THR:O	21:m:18:LEU:HB2	1.99	0.62
4:L:153:LEU:HD11	5:M:360:LEU:HD11	1.81	0.62
6:N:207:ILE:O	6:N:211:LEU:HG	2.00	0.62
4:L:9:LEU:HD22	17:i:82:VAL:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:56:PHE:HE1	5:M:108:MET:HG2	1.64	0.62
8:U:112:SER:HB2	22:n:17:LEU:HD11	1.82	0.62
20:l:57:MET:HG2	20:l:104:PRO:HG2	1.82	0.62
23:o:25:PHE:HB3	23:o:29:LEU:HD22	1.82	0.62
2:J:129:ASP:OD2	2:J:135:LEU:HD13	2.00	0.62
5:M:395:LEU:HD21	21:m:101:TRP:CZ2	2.34	0.62
6:N:109:ALA:CB	6:N:110:PRO:HD3	2.30	0.62
23:o:39:MET:HE1	23:o:58:TYR:HA	1.81	0.62
3:K:12:PHE:CE1	6:N:72:LEU:HD22	2.34	0.62
5:M:98:MET:HE3	5:M:128:PRO:HA	1.81	0.62
6:N:335:MET:O	6:N:335:MET:CG	2.41	0.62
7:O:117:PHE:HD1	7:O:128:SER:HA	1.64	0.62
9:X:164:GLY:O	9:X:165:THR:C	2.41	0.62
12:d:109:TYR:HB3	24:p:156:LEU:HD21	1.80	0.62
4:L:559:GLU:HA	4:L:563:PRO:HG2	1.82	0.61
6:N:338:PRO:HB3	26:d:201:CDL:H712	1.80	0.61
8:U:128:PHE:CZ	8:U:148:ILE:HG23	2.35	0.61
4:L:173:LEU:HD23	25:L:702:3PE:C32	2.30	0.61
23:o:69:CYS:C	23:o:80:CYS:SG	2.82	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:73:LEU:CB	5:M:103:GLN:OE1	2.48	0.61
5:M:422:HIS:NE2	5:M:425:ASN:OD1	2.33	0.61
6:N:218:ALA:HB1	6:N:240:MET:SD	2.40	0.61
7:O:117:PHE:HE1	7:O:128:SER:HB2	1.63	0.61
7:O:326:ARG:HH21	15:g:56:ASP:CG	2.06	0.61
9:X:158:LEU:HD13	12:d:17:GLU:CG	2.30	0.61
5:M:81:GLN:O	5:M:85:LYS:HB2	2.01	0.61
5:M:458:THR:HG21	24:p:148:ALA:HB1	1.81	0.61
6:N:17:PRO:HG2	6:N:133:TRP:CE2	2.35	0.61
17:i:95:TYR:OH	24:p:11:PRO:O	2.18	0.61
21:m:100:PHE:O	21:m:104:VAL:HG23	2.00	0.61
5:M:98:MET:HE1	5:M:128:PRO:HA	1.83	0.61
5:M:139:GLN:HB3	5:M:222:GLU:HG3	1.83	0.61
5:M:318:ALA:HB2	5:M:373:ILE:CG2	2.30	0.61
5:M:373:ILE:H	5:M:448:THR:HG22	1.65	0.61
5:M:433:GLU:O	5:M:437:MET:HG2	2.01	0.61
6:N:175:MET:HE1	6:N:227:ILE:HA	1.80	0.61
7:O:140:LEU:HD21	7:O:304:VAL:O	2.00	0.61
8:U:138:LEU:HB3	8:U:144:ILE:HG12	1.82	0.61
23:o:25:PHE:CE2	23:o:109:LEU:HD22	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:468:ILE:O	4:L:472:ILE:HG23	2.00	0.61
5:M:162:ILE:HG23	6:N:271:MET:CE	2.29	0.61
6:N:273:ASN:HD21	10:Y:143:VAL:HA	1.63	0.61
7:O:213:GLU:O	7:O:217:ARG:HG3	2.00	0.61
15:g:123:LEU:HD12	24:p:98:VAL:CG1	2.31	0.61
20:l:62:TYR:CZ	20:l:64:PRO:HG3	2.36	0.61
7:O:114:LEU:HA	7:O:131:LEU:CD2	2.30	0.61
7:O:140:LEU:HD11	7:O:198:TYR:CZ	2.35	0.61
16:h:106:ILE:O	16:h:106:ILE:HG22	1.99	0.61
4:L:100:ILE:HG21	4:L:246:LEU:HD23	1.82	0.61
5:M:109:THR:HG22	5:M:121:LEU:HB3	1.82	0.61
11:c:55:TRP:HE1	12:d:66:THR:HG21	1.66	0.61
19:k:47:LEU:HD12	22:n:43:LEU:HD23	1.83	0.61
2:J:56:PHE:HA	2:J:60:LEU:HD13	1.82	0.61
4:L:182:PHE:CE2	4:L:186:MET:SD	2.94	0.61
5:M:1:MET:CE	5:M:111:SER:HB2	2.29	0.61
2:J:166:ILE:HA	2:J:169:ILE:HG22	1.83	0.60
5:M:423:MET:O	5:M:424:ILE:C	2.44	0.60
10:Y:18:THR:HG22	10:Y:19:GLN:HG3	1.83	0.60
15:g:109:ASP:HB3	15:g:114:GLU:HB3	1.83	0.60
5:M:209:LEU:HD23	5:M:210:TYR:N	2.16	0.60
9:X:159:LYS:O	9:X:160:PRO:C	2.43	0.60
4:L:466:PHE:HB3	18:j:68:TRP:HZ2	1.65	0.60
6:N:59:TYR:CZ	6:N:63:GLN:HG3	2.36	0.60
16:h:89:VAL:HG21	16:h:117:ILE:HD11	1.83	0.60
4:L:40:ILE:HD12	4:L:101:MET:HG3	1.83	0.60
14:f:49:ARG:NH2	16:h:106:ILE:HG22	2.15	0.60
4:L:9:LEU:HD21	25:i:201:3PE:H2B1	1.83	0.60
6:N:100:MET:HE3	6:N:111:PHE:HZ	1.66	0.60
4:L:42:PHE:O	4:L:46:ILE:HG12	2.01	0.60
4:L:222:GLY:CA	4:L:229:LEU:HD11	2.26	0.60
12:d:16:ASP:O	12:d:19:ARG:HG3	2.01	0.60
16:h:87:THR:HA	26:h:201:CDL:H512	1.83	0.60
2:J:150:TRP:CD1	6:N:28:LEU:HD21	2.36	0.60
5:M:207:MET:HG3	5:M:239:GLY:HA3	1.83	0.60
5:M:269:MET:HE3	5:M:399:ASN:CB	2.32	0.60
6:N:112:HIS:HB2	6:N:184:ILE:HD13	1.84	0.60
6:N:224:SER:HB2	6:N:229:SER:CB	2.32	0.60
26:Y:201:CDL:H361	26:Y:201:CDL:H151	1.83	0.60
15:g:106:TYR:OH	16:h:86:ILE:HG23	2.02	0.60
2:J:37:PHE:O	2:J:41:LEU:HG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:73:PHE:HD2	16:h:74:TYR:CD1	2.20	0.60
4:L:141:PHE:CD2	5:M:370:PRO:CG	2.85	0.60
4:L:204:SER:HA	4:L:207:ASN:HD22	1.67	0.60
5:M:144:ASN:HA	5:M:147:ILE:HD12	1.82	0.60
5:M:370:PRO:HA	5:M:375:LEU:HD22	1.83	0.60
6:N:276:LEU:C	6:N:276:LEU:HD12	2.26	0.60
17:i:74:HIS:C	17:i:78:PRO:HG2	2.24	0.60
22:n:143:GLU:OE1	22:n:155:PRO:HB3	2.02	0.60
4:L:56:HIS:O	23:o:71:ARG:HG3	2.01	0.60
26:L:703:CDL:H341	16:h:71:MET:SD	2.42	0.60
5:M:77:LEU:HD23	5:M:99:LEU:HD12	1.83	0.60
5:M:329:LEU:HD23	5:M:437:MET:HE3	1.84	0.60
7:O:76:GLU:HG3	7:O:266:PRO:HG2	1.83	0.60
4:L:556:ILE:HG23	21:m:80:PHE:CE2	2.37	0.59
5:M:126:LEU:HD21	5:M:153:THR:HB	1.83	0.59
6:N:258:THR:CG2	6:N:336:THR:HG22	2.32	0.59
7:O:54:HIS:HB2	7:O:56:TYR:CE1	2.37	0.59
10:Y:137:LEU:CD2	10:Y:138:PHE:CD2	2.84	0.59
16:h:102:PRO:HD2	16:h:105:TYR:CB	2.32	0.59
2:J:123:TRP:HH2	13:e:72:THR:C	2.09	0.59
2:J:168:GLU:CD	6:N:5:THR:HG21	2.27	0.59
8:U:90:TYR:CZ	8:U:92:LYS:HD2	2.35	0.59
16:h:73:PHE:CD2	16:h:74:TYR:CD1	2.90	0.59
4:L:123:LEU:HD22	4:L:150:MET:CG	2.33	0.59
4:L:247:LEU:HD12	4:L:248:HIS:CG	2.36	0.59
5:M:115:LEU:O	5:M:118:PHE:HB3	2.02	0.59
4:L:313:MET:HE2	4:L:328:HIS:CE1	2.38	0.59
4:L:598:ILE:HD11	6:N:153:ILE:CG1	2.32	0.59
5:M:127:ILE:HG12	6:N:254:LEU:HD21	1.84	0.59
5:M:294:MET:HE3	5:M:319:HIS:CD2	2.37	0.59
7:O:126:GLY:CA	15:g:51:MET:HE1	2.32	0.59
18:j:94:ASP:HB3	18:j:99:ILE:HB	1.83	0.59
2:J:2:ASN:HB3	2:J:121:GLY:CA	2.31	0.59
4:L:81:LYS:HB2	4:L:135:ASN:OD1	2.03	0.59
16:h:69:ARG:O	16:h:73:PHE:HB2	2.02	0.59
4:L:312:LEU:CD2	4:L:395:ILE:HG21	2.33	0.59
8:U:120:MET:HE1	22:n:24:LEU:HD12	1.83	0.59
14:f:38:ARG:HD3	14:f:56:TRP:CD1	2.38	0.59
18:j:52:ARG:NE	18:j:52:ARG:HA	2.17	0.59
21:m:37:LEU:HA	21:m:40:ARG:HG2	1.83	0.59
4:L:227:PHE:CD2	4:L:283:LEU:CD2	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:424:MET:HE2	4:L:502:LEU:HB2	1.85	0.59
4:L:460:GLY:HA2	25:L:701:3PE:O12	2.02	0.59
5:M:209:LEU:HD23	5:M:211:GLY:H	1.67	0.59
5:M:350:MET:HG2	22:n:99:VAL:HG12	1.83	0.59
7:O:343:TYR:HE1	7:O:355:LYS:HB2	1.66	0.59
10:Y:141:PRO:HB2	16:h:161:ARG:NH1	2.17	0.59
15:g:139:TYR:HD2	15:g:140:PHE:CD1	2.20	0.59
26:h:201:CDL:H531	26:h:201:CDL:HA31	1.85	0.59
4:L:605:ASN:O	4:L:606:LEU:C	2.46	0.59
5:M:275:ILE:HD11	5:M:288:TYR:CB	2.33	0.59
6:N:300:THR:HG23	6:N:301:SER:N	2.17	0.59
10:Y:110:TYR:CD2	25:m:201:3PE:H112	2.37	0.59
13:e:41:ILE:CD1	16:h:174:PRO:HB2	2.33	0.59
16:h:96:ALA:O	24:p:63:TYR:HE1	1.85	0.59
1:D:67:ASN:HB2	7:O:193:LEU:HD22	1.84	0.59
4:L:173:LEU:HD23	25:L:702:3PE:H322	1.85	0.59
4:L:542:LEU:CD2	20:l:116:ARG:HD2	2.32	0.59
5:M:14:LEU:HD21	5:M:26:ASN:HB2	1.84	0.59
6:N:200:LEU:HD22	6:N:269:GLU:HG3	1.84	0.59
7:O:167:PHE:CZ	7:O:244:THR:HB	2.38	0.59
8:U:105:MET:SD	8:U:139:MET:HE1	2.42	0.59
19:k:58:ARG:HD2	22:n:34:ARG:HG3	1.83	0.59
22:n:111:GLU:O	22:n:114:MET:HG2	2.03	0.59
6:N:243:MET:HG2	12:d:44:MET:HE2	1.85	0.59
2:J:19:LEU:HD21	3:K:31:LEU:O	2.03	0.58
2:J:56:PHE:CE1	2:J:60:LEU:HD22	2.38	0.58
2:J:164:PHE:CD2	6:N:8:ILE:HG13	2.36	0.58
4:L:230:HIS:N	4:L:231:PRO:CD	2.66	0.58
4:L:417:SER:HB3	4:L:493:ILE:CG1	2.31	0.58
4:L:532:ILE:HG21	20:l:133:LEU:HD22	1.85	0.58
5:M:210:TYR:O	5:M:213:HIS:CD2	2.56	0.58
5:M:396:MET:HG3	5:M:396:MET:O	2.03	0.58
6:N:319:LYS:HA	7:O:302:THR:HG21	1.84	0.58
7:O:323:GLN:NE2	15:g:54:GLN:C	2.61	0.58
13:e:45:HIS:CD2	16:h:176:LYS:HZ2	2.21	0.58
16:h:95:GLU:HB3	16:h:114:LYS:HG2	1.85	0.58
20:l:155:PRO:HG3	23:o:4:HIS:CG	2.38	0.58
23:o:26:PRO:HB2	23:o:28:ASP:OD1	2.02	0.58
4:L:466:PHE:CE1	4:L:470:TYR:HE2	2.21	0.58
6:N:77:ASN:OD1	6:N:81:LEU:HD12	2.04	0.58
6:N:109:ALA:CB	6:N:110:PRO:CD	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:119:ILE:HD11	8:U:138:LEU:HB2	1.85	0.58
11:c:30:TYR:HB2	11:c:34:PRO:HD3	1.85	0.58
17:i:111:LEU:HD11	24:p:20:PRO:HD3	1.84	0.58
23:o:12:ASP:HB3	23:o:15:VAL:HG22	1.84	0.58
1:D:51:VAL:HG21	1:D:58:THR:HG22	1.83	0.58
4:L:556:ILE:HD11	21:m:76:ILE:HG22	1.83	0.58
6:N:179:MET:CG	6:N:216:PHE:HE1	2.16	0.58
7:O:124:ASN:O	15:g:51:MET:HG2	2.03	0.58
14:f:11:TRP:O	14:f:14:ILE:HG22	2.02	0.58
20:l:113:ILE:HG12	20:l:114:ARG:H	1.67	0.58
24:p:37:TYR:CZ	24:p:41:VAL:HG11	2.38	0.58
1:D:37:TRP:CZ2	1:D:39:PRO:HA	2.38	0.58
4:L:407:TRP:CZ3	4:L:410:LEU:HD11	2.38	0.58
4:L:525:LEU:HD21	22:n:77:PRO:HB3	1.86	0.58
8:U:105:MET:CG	8:U:139:MET:HE1	2.33	0.58
20:l:105:ILE:HG23	20:l:109:LEU:HD22	1.84	0.58
4:L:404:THR:HG22	4:L:405:ASN:N	2.19	0.58
24:p:128:GLU:O	24:p:131:GLN:N	2.37	0.58
5:M:196:TRP:HZ3	5:M:261:PHE:CE2	2.21	0.58
7:O:49:THR:O	7:O:53:LEU:HG	2.04	0.58
15:g:147:LEU:HD11	24:p:163:MET:HB3	1.86	0.58
21:m:75:ASN:O	21:m:75:ASN:OD1	2.20	0.58
6:N:147:PRO:HB2	6:N:148:LEU:HD12	1.86	0.58
16:h:96:ALA:HB3	24:p:63:TYR:CD1	2.38	0.58
4:L:15:LEU:O	4:L:18:PRO:HD2	2.03	0.58
5:M:73:LEU:HB2	5:M:103:GLN:OE1	2.02	0.58
25:M:501:3PE:O22	6:N:276:LEU:HD13	2.03	0.58
6:N:26:LEU:O	6:N:27:MET:C	2.46	0.58
9:X:167:PHE:HB3	9:X:170:TRP:CD1	2.39	0.58
12:d:14:LEU:HD12	12:d:14:LEU:C	2.27	0.58
21:m:127:ILE:HG22	24:p:136:THR:HG23	1.84	0.58
4:L:550:LEU:HB2	5:M:275:ILE:HG22	1.86	0.58
6:N:149:LEU:HD11	6:N:195:PRO:HG3	1.84	0.58
8:U:100:VAL:C	8:U:141:PRO:HG2	2.28	0.58
9:X:154:ILE:HG22	12:d:88:HIS:CE1	2.38	0.58
14:f:39:ASN:O	14:f:45:GLN:HG3	2.04	0.58
4:L:232:TRP:CZ3	4:L:233:LEU:HD21	2.37	0.58
5:M:109:THR:HG22	5:M:121:LEU:CB	2.34	0.58
6:N:33:LEU:HD11	6:N:141:ILE:HD12	1.86	0.58
13:e:14:LEU:HD12	13:e:15:ASP:CB	2.33	0.58
15:g:121:GLU:HA	15:g:124:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:425:ARG:HG3	4:L:429:PHE:CE2	2.39	0.57
7:O:63:ASP:OD2	7:O:165:SER:CB	2.52	0.57
7:O:76:GLU:HG3	7:O:266:PRO:CG	2.34	0.57
7:O:117:PHE:CD1	7:O:128:SER:CB	2.87	0.57
15:g:140:PHE:CZ	24:p:74:ILE:HG22	2.39	0.57
4:L:593:ILE:CG2	10:Y:41:TYR:CE2	2.87	0.57
8:U:125:GLU:OE2	18:j:44:TYR:OH	2.21	0.57
10:Y:63:PHE:HE2	10:Y:106:ARG:HE	1.53	0.57
3:K:96:LEU:O	3:K:97:GLN:C	2.47	0.57
4:L:592:LEU:O	4:L:596:ILE:HG12	2.04	0.57
23:o:15:VAL:HG23	23:o:16:GLU:H	1.69	0.57
2:J:151:MET:HE2	2:J:151:MET:HA	1.86	0.57
5:M:230:ILE:HG13	5:M:235:LEU:HG	1.87	0.57
5:M:296:LEU:HD22	5:M:396:MET:HE1	1.85	0.57
5:M:297:VAL:O	5:M:301:ILE:HG12	2.03	0.57
6:N:154:ILE:HG12	6:N:195:PRO:HG2	1.86	0.57
6:N:253:GLY:N	6:N:290:LEU:HD11	2.19	0.57
5:M:172:GLY:C	5:M:173:THR:HG23	2.28	0.57
5:M:447:LEU:HD21	5:M:454:ILE:CD1	2.33	0.57
7:O:80:GLN:CG	7:O:270:VAL:HG21	2.18	0.57
13:e:101:ARG:NE	13:e:101:ARG:HA	2.20	0.57
2:J:122:ASP:O	2:J:123:TRP:CD1	2.50	0.57
5:M:444:LEU:O	5:M:448:THR:HG23	2.04	0.57
6:N:284:MET:O	6:N:287:LEU:HB2	2.04	0.57
7:O:354:LEU:HG	11:c:44:VAL:HG22	1.86	0.57
20:l:166:LEU:HB2	20:l:170:ARG:NH2	2.19	0.57
2:J:85:ASN:O	2:J:89:LEU:HG	2.04	0.57
4:L:227:PHE:CD2	4:L:283:LEU:HD21	2.38	0.57
4:L:425:ARG:HG3	4:L:429:PHE:HE2	1.68	0.57
5:M:4:ILE:CG2	5:M:107:ILE:HD13	2.29	0.57
5:M:14:LEU:HD11	5:M:26:ASN:HB3	1.87	0.57
5:M:73:LEU:HD22	5:M:103:GLN:NE2	2.19	0.57
7:O:100:ASP:O	11:c:31:VAL:HG23	2.04	0.57
8:U:93:ILE:HD11	8:U:110:LEU:HD11	1.86	0.57
8:U:155:TYR:OH	16:h:52:LYS:HD2	2.04	0.57
5:M:388:TRP:NE1	21:m:109:ARG:HD2	2.20	0.57
7:O:354:LEU:HD21	11:c:44:VAL:HG11	1.87	0.57
17:i:103:ARG:O	24:p:18:PRO:HG3	2.04	0.57
4:L:306:THR:HA	4:L:336:LYS:HZ2	1.67	0.57
5:M:42:LEU:HD11	5:M:67:ILE:CD1	2.34	0.57
6:N:179:MET:HG3	6:N:216:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:273:ASN:O	6:N:274:ASN:HB2	2.05	0.57
4:L:246:LEU:HD12	4:L:247:LEU:CA	2.34	0.57
4:L:253:VAL:CG2	4:L:310:LEU:HD11	2.35	0.57
5:M:269:MET:HE3	5:M:399:ASN:HB2	1.86	0.57
6:N:109:ALA:HB1	6:N:110:PRO:HD3	1.86	0.57
6:N:314:MET:HB2	7:O:305:LEU:HD11	1.86	0.57
16:h:175:GLU:HB3	16:h:177:GLU:HG2	1.86	0.57
17:i:87:LYS:HG2	17:i:87:LYS:O	2.05	0.57
23:o:6:THR:O	23:o:10:LEU:HB2	2.05	0.57
2:J:138:GLY:HA2	2:J:141:VAL:HG12	1.86	0.56
4:L:60:GLU:CG	4:L:83:ASP:HA	2.35	0.56
4:L:247:LEU:CD1	4:L:248:HIS:NE2	2.53	0.56
4:L:553:LEU:HD11	21:m:93:ALA:HB1	1.86	0.56
5:M:12:LEU:HB2	5:M:13:PRO:HD3	1.86	0.56
5:M:282:LEU:HD13	5:M:342:MET:HE2	1.87	0.56
5:M:310:MET:O	5:M:314:MET:HG3	2.04	0.56
7:O:38:TYR:HB3	7:O:299:GLN:HE22	1.70	0.56
7:O:125:ASP:OD1	7:O:126:GLY:N	2.38	0.56
14:f:49:ARG:HB2	14:f:50:PRO:HD2	1.87	0.56
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
4:L:594:ASN:OD1	6:N:110:PRO:CB	2.53	0.56
5:M:264:LEU:HD23	21:m:98:LEU:HD11	1.87	0.56
10:Y:57:ARG:HG2	10:Y:60:ARG:HH21	1.69	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
2:J:19:LEU:HD22	2:J:32:LEU:HD13	1.87	0.56
5:M:196:TRP:HE1	5:M:250:LEU:HD13	1.68	0.56
25:M:501:3PE:H12	6:N:276:LEU:CD2	2.35	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
6:N:313:MET:HG2	7:O:305:LEU:HD22	1.85	0.56
7:O:173:MET:HE2	7:O:179:ILE:HG23	1.87	0.56
7:O:209:VAL:HG23	7:O:209:VAL:O	2.05	0.56
7:O:242:LYS:HA	7:O:246:LEU:HD12	1.88	0.56
9:X:168:PHE:O	9:X:169:PHE:CD1	2.58	0.56
15:g:140:PHE:HB3	24:p:75:THR:HG21	1.86	0.56
3:K:16:LEU:HA	3:K:36:MET:HE2	1.85	0.56
5:M:57:SER:HB3	5:M:113:THR:HG22	1.87	0.56
5:M:118:PHE:O	5:M:122:PHE:CB	2.54	0.56
7:O:149:HIS:CE1	7:O:153:THR:HG21	2.40	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
23:o:7:ARG:NH1	23:o:106:ARG:HH12	2.03	0.56
24:p:39:LEU:O	24:p:44:PRO:HD3	2.06	0.56
2:J:123:TRP:CZ3	13:e:73:MET:N	2.74	0.56
5:M:78:MET:O	5:M:432:ARG:HD2	2.06	0.56
6:N:120:GLN:O	6:N:176:ARG:CZ	2.54	0.56
17:i:101:LYS:HG2	24:p:116:ARG:O	2.05	0.56
1:D:72:LEU:CD1	6:N:50:PRO:HG3	2.34	0.56
6:N:149:LEU:CD1	6:N:154:ILE:HG21	2.35	0.56
6:N:196:TYR:HB3	6:N:273:ASN:OD1	2.05	0.56
6:N:253:GLY:H	6:N:290:LEU:HD11	1.71	0.56
16:h:55:PHE:HB2	17:i:28:LEU:HD21	1.87	0.56
17:i:110:ILE:HD13	24:p:16:ARG:HD2	1.88	0.56
5:M:25:THR:HG22	15:g:84:ASN:CG	2.31	0.56
7:O:316:GLU:HG3	15:g:51:MET:HE2	1.87	0.56
13:e:14:LEU:HD12	13:e:14:LEU:C	2.31	0.56
21:m:15:PRO:HG3	21:m:18:LEU:HD12	1.86	0.56
22:n:133:TRP:HA	22:n:136:GLU:HG2	1.87	0.56
5:M:370:PRO:CA	5:M:375:LEU:CD2	2.83	0.56
6:N:258:THR:OG1	6:N:336:THR:HG22	2.05	0.56
18:j:99:ILE:HD12	23:o:107:ARG:HB2	1.86	0.56
21:m:6:TYR:CE2	21:m:15:PRO:HD3	2.40	0.56
24:p:74:ILE:CD1	24:p:85:ILE:HG13	2.36	0.56
2:J:71:THR:O	2:J:72:ALA:C	2.49	0.56
4:L:397:GLU:HB2	4:L:482:MET:SD	2.46	0.56
8:U:90:TYR:CD1	19:k:51:TRP:CE2	2.94	0.56
8:U:90:TYR:HD1	19:k:51:TRP:CE2	2.23	0.56
13:e:85:LYS:O	13:e:88:LYS:HB3	2.06	0.56
4:L:597:LEU:HD21	10:Y:37:ILE:HD12	1.87	0.56
5:M:309:PHE:O	5:M:313:THR:HG23	2.06	0.56
6:N:25:ASN:HB3	13:e:15:ASP:OD2	2.06	0.56
6:N:313:MET:HG3	7:O:305:LEU:HD22	1.87	0.56
9:X:169:PHE:CD2	9:X:169:PHE:O	2.59	0.56
10:Y:76:THR:CG2	10:Y:95:GLY:HA3	2.34	0.56
20:l:111:MET:HE3	20:l:112:TYR:CZ	2.41	0.56
2:J:22:LYS:HZ2	3:K:22:PHE:CA	2.16	0.55
2:J:161:ALA:O	2:J:165:ILE:HD12	2.06	0.55
4:L:94:LEU:HD23	4:L:125:LEU:HD21	1.88	0.55
4:L:375:ILE:HG12	18:j:65:MET:SD	2.46	0.55
5:M:4:ILE:H	5:M:4:ILE:HD12	1.70	0.55
5:M:73:LEU:CD2	5:M:103:GLN:CD	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:193:ILE:HD11	6:N:269:GLU:HB2	1.89	0.55
7:O:114:LEU:HA	7:O:131:LEU:HD22	1.88	0.55
13:e:101:ARG:CZ	13:e:102:GLU:H	2.19	0.55
23:o:8:ARG:HD2	23:o:16:GLU:HB3	1.88	0.55
1:D:57:GLU:HA	1:D:60:HIS:CD2	2.41	0.55
4:L:538:PRO:O	4:L:542:LEU:HD13	2.06	0.55
7:O:256:LEU:HD23	7:O:258:TYR:OH	2.05	0.55
8:U:130:ILE:HD11	8:U:148:ILE:CD1	2.36	0.55
10:Y:137:LEU:HD23	10:Y:138:PHE:CD2	2.41	0.55
17:i:19:ARG:HA	22:n:171:VAL:HG13	1.89	0.55
19:k:47:LEU:CD1	22:n:43:LEU:HD23	2.36	0.55
22:n:57:MET:HE2	22:n:57:MET:HA	1.87	0.55
4:L:94:LEU:CD2	4:L:125:LEU:HD21	2.35	0.55
6:N:325:MET:HE3	6:N:329:LEU:HD11	1.88	0.55
13:e:45:HIS:CD2	16:h:176:LYS:CD	2.89	0.55
16:h:116:PRO:O	16:h:119:ARG:HG2	2.06	0.55
23:o:73:SER:HA	24:p:24:THR:OG1	2.05	0.55
4:L:54:PHE:O	4:L:58:ASN:CA	2.55	0.55
4:L:150:MET:HE3	26:L:703:CDL:H552	1.88	0.55
4:L:466:PHE:HB2	18:j:68:TRP:CH2	2.40	0.55
7:O:170:LEU:HG	7:O:179:ILE:HD13	1.87	0.55
10:Y:71:MET:CG	10:Y:102:THR:HG21	2.37	0.55
16:h:90:ASN:HD21	26:h:201:CDL:PA1	2.29	0.55
2:J:46:PHE:CE2	3:K:46:VAL:HG13	2.41	0.55
4:L:69:VAL:HG11	4:L:71:MET:HE2	1.88	0.55
4:L:149:ILE:HG13	5:M:369:LEU:HD12	1.89	0.55
4:L:513:MET:HE1	22:n:30:TRP:HB3	1.89	0.55
3:K:66:PHE:CE1	6:N:35:PHE:CE1	2.95	0.55
4:L:230:HIS:N	4:L:231:PRO:HD3	2.22	0.55
4:L:561:THR:O	4:L:565:SER:HB2	2.07	0.55
5:M:244:ILE:O	24:p:149:TYR:OH	2.19	0.55
6:N:224:SER:HB2	6:N:229:SER:HB3	1.89	0.55
6:N:237:THR:O	6:N:237:THR:CG2	2.55	0.55
21:m:18:LEU:HD21	22:n:69:GLU:HA	1.89	0.55
23:o:69:CYS:O	23:o:69:CYS:SG	2.65	0.55
4:L:162:THR:O	4:L:166:THR:HG23	2.06	0.55
6:N:230:ILE:O	6:N:233:LEU:HB2	2.07	0.55
7:O:319:ILE:HG13	7:O:320:GLY:H	1.72	0.55
13:e:14:LEU:HD12	13:e:15:ASP:N	2.21	0.55
14:f:8:ARG:HA	14:f:8:ARG:NE	2.21	0.55
24:p:66:ARG:HD3	24:p:68:TYR:CZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:231:LEU:CA	5:M:235:LEU:HD12	2.36	0.55
5:M:453:LEU:HD12	5:M:454:ILE:CG2	2.34	0.55
7:O:66:ILE:HD12	7:O:67:CYS:SG	2.47	0.55
7:O:258:TYR:CZ	7:O:269:VAL:HG13	2.42	0.55
17:i:83:HIS:HE1	17:i:87:LYS:HD2	1.71	0.55
19:k:30:ILE:CD1	19:k:39:GLN:HB2	2.33	0.55
3:K:45:SER:O	3:K:49:LEU:HG	2.07	0.55
5:M:62:SER:C	5:M:64:PRO:HD2	2.32	0.55
8:U:83:VAL:O	8:U:87:LEU:HG	2.07	0.55
15:g:78:PRO:O	15:g:81:ASP:HB3	2.07	0.55
2:J:19:LEU:HD11	3:K:31:LEU:HG	1.88	0.55
4:L:73:SER:HB3	24:p:100:GLN:NE2	2.22	0.55
4:L:261:VAL:O	4:L:264:HIS:HD2	1.89	0.55
4:L:357:ARG:HG2	22:n:32:ILE:HG12	1.89	0.55
4:L:381:THR:HG21	4:L:498:PHE:CZ	2.42	0.55
16:h:73:PHE:CD2	16:h:74:TYR:CE1	2.94	0.55
17:i:83:HIS:CD2	24:p:37:TYR:CE2	2.95	0.55
2:J:8:LEU:HD12	2:J:38:VAL:HG13	1.89	0.54
5:M:6:LEU:HB3	5:M:7:PRO:HD3	1.88	0.54
5:M:55:MET:HE1	26:d:201:CDL:H511	1.89	0.54
7:O:209:VAL:HG23	7:O:214:VAL:HG13	1.88	0.54
8:U:79:ILE:HD11	8:U:148:ILE:CG2	2.36	0.54
4:L:54:PHE:O	4:L:58:ASN:HA	2.08	0.54
4:L:258:PHE:HE1	4:L:262:ARG:HH21	1.56	0.54
4:L:371:SER:HB2	18:j:62:SER:OG	2.06	0.54
15:g:106:TYR:OH	16:h:86:ILE:HD12	2.07	0.54
21:m:18:LEU:HD11	22:n:72:TRP:CG	2.42	0.54
4:L:353:GLU:OE1	22:n:80:TYR:OH	2.24	0.54
4:L:362:ILE:HA	4:L:365:ILE:HG13	1.90	0.54
5:M:415:GLN:O	5:M:416:ARG:HG3	2.08	0.54
7:O:49:THR:HG21	7:O:151:LEU:HG	1.89	0.54
7:O:305:LEU:O	7:O:305:LEU:CD1	2.55	0.54
14:f:56:TRP:CE3	16:h:131:LYS:HG3	2.42	0.54
17:i:16:ARG:O	17:i:20:ARG:HG2	2.08	0.54
1:D:35:ARG:O	1:D:36:GLN:C	2.47	0.54
2:J:122:ASP:C	2:J:123:TRP:CD1	2.86	0.54
4:L:190:SER:HB2	4:L:196:TRP:NE1	2.22	0.54
4:L:232:TRP:O	4:L:236:ALA:N	2.40	0.54
5:M:127:ILE:CG1	6:N:254:LEU:HD21	2.37	0.54
5:M:446:LEU:HD13	15:g:101:THR:CG2	2.37	0.54
23:o:103:GLU:OE2	23:o:106:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:GLY:CA	3:K:31:LEU:HD21	2.37	0.54
2:J:77:GLU:O	2:J:78:TYR:C	2.51	0.54
4:L:131:LEU:CD1	4:L:140:LEU:CD1	2.78	0.54
4:L:389:PHE:CZ	18:j:79:ALA:CB	2.90	0.54
5:M:373:ILE:HD11	5:M:454:ILE:HD11	1.88	0.54
16:h:90:ASN:OD1	16:h:115:HIS:NE2	2.40	0.54
1:D:58:THR:HG23	1:D:61:TRP:CZ3	2.41	0.54
4:L:65:THR:HA	17:i:90:MET:HE2	1.90	0.54
4:L:141:PHE:CD2	5:M:370:PRO:CB	2.91	0.54
7:O:170:LEU:HG	7:O:179:ILE:CD1	2.37	0.54
18:j:98:GLY:O	18:j:100:PRO:HD3	2.07	0.54
2:J:123:TRP:CZ3	13:e:73:MET:HG3	2.41	0.54
2:J:124:LEU:O	2:J:125:MET:C	2.49	0.54
2:J:164:PHE:HB3	6:N:5:THR:HG23	1.90	0.54
4:L:551:THR:HA	4:L:555:LEU:HD12	1.90	0.54
5:M:79:ALA:HB1	5:M:225:ILE:HD13	1.90	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
10:Y:141:PRO:HB2	16:h:161:ARG:HH11	1.72	0.54
4:L:232:TRP:CH2	4:L:233:LEU:HD21	2.42	0.54
6:N:24:THR:HB	13:e:2:PRO:HG3	1.90	0.54
7:O:60:ILE:O	7:O:158:VAL:HA	2.07	0.54
7:O:69:GLY:HA2	7:O:72:LYS:HZ3	1.72	0.54
14:f:44:PHE:HE1	24:p:66:ARG:HH11	1.54	0.54
21:m:8:PRO:HB3	21:m:14:LEU:N	2.23	0.54
21:m:109:ARG:O	21:m:113:GLU:HG2	2.08	0.54
4:L:221:THR:HA	4:L:226:GLN:HG2	1.90	0.54
4:L:247:LEU:HD11	4:L:248:HIS:CE1	2.43	0.54
5:M:31:SER:HA	5:M:34:ILE:HG12	1.90	0.54
5:M:231:LEU:O	5:M:236:LEU:HG	2.06	0.54
5:M:283:LYS:HG3	5:M:327:PHE:CE1	2.43	0.54
8:U:86:VAL:CB	8:U:122:MET:HE1	2.37	0.54
18:j:101:PRO:O	18:j:102:ASP:C	2.49	0.54
20:l:119:THR:HG23	21:m:11:LEU:HA	1.89	0.54
22:n:20:TYR:CE2	22:n:24:LEU:CD1	2.91	0.54
4:L:66:TRP:CZ3	4:L:68:TRP:CD1	2.96	0.54
4:L:586:LEU:CD2	10:Y:47:PRO:HD3	2.38	0.54
6:N:307:THR:CG2	6:N:308:ASN:H	2.19	0.54
18:j:97:LEU:O	23:o:104:ARG:CG	2.55	0.54
22:n:133:TRP:CA	22:n:136:GLU:HG2	2.38	0.54
23:o:93:LEU:O	23:o:97:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:31:THR:O	24:p:35:LYS:HG3	2.07	0.54
2:J:123:TRP:CH2	13:e:73:MET:N	2.76	0.53
4:L:158:TRP:CD1	22:n:97:TYR:HH	2.26	0.53
5:M:1:MET:HE2	5:M:52:PHE:CE2	2.43	0.53
5:M:175:ASN:ND2	16:h:143:GLU:HG2	2.21	0.53
6:N:179:MET:HE2	6:N:216:PHE:CE1	2.43	0.53
7:O:319:ILE:HG13	7:O:320:GLY:N	2.22	0.53
7:O:355:LYS:HE2	11:c:38:LYS:HA	1.90	0.53
12:d:39:TYR:CE2	12:d:43:LEU:HD11	2.43	0.53
23:o:57:ASP:CG	23:o:59:CYS:H	2.16	0.53
4:L:491:LEU:CD1	18:j:80:VAL:HG22	2.38	0.53
7:O:40:LEU:HG	7:O:292:HIS:CE1	2.44	0.53
7:O:250:SER:HA	7:O:255:VAL:CG2	2.38	0.53
11:c:72:ARG:NH1	12:d:19:ARG:HD3	2.24	0.53
22:n:30:TRP:CD2	22:n:76:HIS:CD2	2.95	0.53
4:L:79:SER:CB	4:L:135:ASN:HB2	2.36	0.53
4:L:109:HIS:O	4:L:110:SER:HB2	2.08	0.53
4:L:362:ILE:CD1	4:L:430:VAL:CG1	2.82	0.53
4:L:400:ASN:HD21	4:L:413:LEU:HD11	1.73	0.53
4:L:559:GLU:HG2	4:L:564:LYS:HD3	1.90	0.53
5:M:61:LEU:HD22	5:M:244:ILE:HG21	1.90	0.53
5:M:154:LEU:HD13	6:N:287:LEU:CD2	2.39	0.53
18:j:38:VAL:CG1	18:j:39:HIS:N	2.72	0.53
21:m:28:GLU:HG2	21:m:31:ARG:HH22	1.73	0.53
22:n:56:ASP:O	22:n:57:MET:C	2.50	0.53
22:n:133:TRP:HA	22:n:136:GLU:CG	2.38	0.53
24:p:142:ARG:O	24:p:143:TYR:CD1	2.61	0.53
4:L:362:ILE:HD12	4:L:430:VAL:HG13	1.88	0.53
5:M:105:LEU:HD11	26:M:503:CDL:H472	1.91	0.53
20:l:101:TRP:HE1	21:m:62:ASP:HA	1.72	0.53
22:n:125:TRP:CE3	22:n:128:LEU:HD12	2.43	0.53
24:p:103:MET:CE	24:p:135:VAL:HG12	2.38	0.53
2:J:59:TYR:CZ	3:K:64:LEU:HD22	2.43	0.53
4:L:141:PHE:CE2	5:M:375:LEU:HD22	2.23	0.53
4:L:387:THR:HG22	4:L:465:GLY:N	2.24	0.53
6:N:120:GLN:HE22	6:N:174:GLN:CB	2.21	0.53
7:O:140:LEU:HD11	7:O:198:TYR:OH	2.09	0.53
10:Y:50:SER:HB3	10:Y:53:GLU:HG2	1.91	0.53
16:h:57:VAL:HG12	22:n:99:VAL:HG21	1.89	0.53
20:l:38:PRO:CB	21:m:75:ASN:ND2	2.67	0.53
21:m:94:GLY:HA3	25:m:201:3PE:H2C1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG21	1:D:58:THR:CG2	2.38	0.53
2:J:14:VAL:O	2:J:17:LEU:HB3	2.07	0.53
2:J:94:LEU:O	2:J:97:ILE:HG12	2.08	0.53
4:L:124:PHE:HZ	4:L:252:MET:HB2	1.74	0.53
5:M:55:MET:HG3	5:M:56:PHE:CD2	2.44	0.53
7:O:164:TYR:CE1	7:O:195:LEU:HD21	2.43	0.53
17:i:98:VAL:HG13	24:p:115:GLN:HG2	1.91	0.53
2:J:25:PRO:HG2	2:J:75:THR:OG1	2.08	0.53
2:J:104:CYS:O	2:J:107:ASN:HB3	2.08	0.53
4:L:97:THR:HG21	4:L:125:LEU:HD22	1.90	0.53
4:L:450:LEU:HG	4:L:454:ILE:HD12	1.91	0.53
4:L:466:PHE:CE2	25:L:701:3PE:H331	2.44	0.53
4:L:542:LEU:HB3	5:M:278:ARG:HD2	1.91	0.53
5:M:57:SER:CB	5:M:113:THR:HG22	2.39	0.53
5:M:446:LEU:HD13	15:g:101:THR:HG21	1.89	0.53
2:J:136:GLU:N	2:J:139:ILE:HD12	2.24	0.53
4:L:20:LEU:C	4:L:20:LEU:CD1	2.81	0.53
4:L:187:VAL:HG22	5:M:383:MET:HG2	1.90	0.53
4:L:361:ASN:HA	4:L:431:THR:O	2.09	0.53
4:L:511:LEU:HD11	19:k:38:VAL:HG22	1.91	0.53
5:M:269:MET:CE	5:M:396:MET:HA	2.36	0.53
5:M:310:MET:HG3	5:M:455:THR:CA	2.38	0.53
5:M:314:MET:HE1	5:M:380:PHE:CD2	2.44	0.53
6:N:307:THR:HB	7:O:319:ILE:CG1	2.39	0.53
15:g:139:TYR:CD2	15:g:140:PHE:CD1	2.96	0.53
16:h:156:VAL:CG1	16:h:160:MET:HE3	2.39	0.53
18:j:52:ARG:HA	18:j:52:ARG:HE	1.74	0.53
21:m:49:LEU:HD23	22:n:140:LEU:CD2	2.39	0.53
5:M:59:ASP:O	5:M:60:PRO:C	2.49	0.53
5:M:73:LEU:HD23	5:M:103:GLN:NE2	2.23	0.53
5:M:154:LEU:HD13	6:N:287:LEU:HD22	1.91	0.53
5:M:348:LEU:HD12	5:M:415:GLN:NE2	2.24	0.53
5:M:453:LEU:HD12	5:M:453:LEU:C	2.33	0.53
9:X:171:THR:O	9:X:172:VAL:C	2.52	0.53
13:e:32:ARG:O	13:e:33:CYS:HB2	2.08	0.53
20:l:55:TYR:O	20:l:104:PRO:HG3	2.09	0.53
4:L:247:LEU:O	4:L:252:MET:HB3	2.09	0.53
5:M:188:ALA:H	5:M:253:LEU:HD11	1.74	0.53
5:M:264:LEU:CD2	21:m:98:LEU:HD21	2.38	0.53
6:N:227:ILE:HA	6:N:230:ILE:CG2	2.38	0.53
11:c:55:TRP:HE1	12:d:66:THR:CG2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:40:TRP:CG	13:e:40:TRP:O	2.61	0.53
21:m:85:LYS:O	21:m:85:LYS:HG2	2.09	0.53
22:n:132:SER:O	22:n:136:GLU:HG2	2.09	0.53
4:L:128:MET:CG	4:L:251:THR:HB	2.36	0.52
4:L:400:ASN:HB3	4:L:486:LEU:HD22	1.91	0.52
5:M:15:THR:HG21	5:M:100:ILE:HD12	1.90	0.52
5:M:213:HIS:O	5:M:217:PRO:HD3	2.09	0.52
5:M:313:THR:HA	5:M:316:MET:HE3	1.89	0.52
5:M:447:LEU:HD11	5:M:454:ILE:HG23	1.90	0.52
7:O:170:LEU:HD13	7:O:187:TYR:CD2	2.44	0.52
7:O:347:VAL:HG11	11:c:29:PHE:CA	2.31	0.52
10:Y:65:ALA:O	10:Y:68:ILE:HG12	2.09	0.52
22:n:39:TYR:CZ	22:n:43:LEU:HD11	2.44	0.52
3:K:89:TYR:HB3	3:K:91:GLN:OE1	2.09	0.52
4:L:108:MET:HB2	4:L:114:ILE:HD13	1.90	0.52
4:L:145:GLU:HG2	5:M:370:PRO:HD3	1.90	0.52
4:L:536:ILE:HG23	4:L:537:THR:N	2.25	0.52
5:M:73:LEU:HD21	5:M:100:ILE:HG12	1.91	0.52
5:M:160:LEU:CD2	5:M:164:LEU:HD13	2.39	0.52
5:M:354:LEU:O	5:M:357:THR:N	2.41	0.52
5:M:393:ILE:CG2	25:M:502:3PE:H381	2.39	0.52
7:O:121:PRO:C	7:O:122:LYS:HG2	2.33	0.52
17:i:83:HIS:CD2	24:p:37:TYR:HE2	2.27	0.52
2:J:141:VAL:HG23	3:K:58:PRO:HA	1.91	0.52
4:L:228:GLY:O	4:L:229:LEU:CG	2.47	0.52
5:M:403:THR:HA	5:M:406:TYR:CE2	2.44	0.52
7:O:310:ILE:HG13	7:O:311:PRO:HD2	1.91	0.52
23:o:22:ILE:O	23:o:105:GLU:CD	2.52	0.52
2:J:123:TRP:HZ2	13:e:76:MET:SD	2.32	0.52
3:K:38:LEU:HG	3:K:42:ILE:CD1	2.39	0.52
4:L:332:HIS:CD2	4:L:336:LYS:HG3	2.44	0.52
10:Y:90:LEU:O	10:Y:91:ASN:C	2.51	0.52
13:e:69:ARG:HG3	13:e:72:THR:OG1	2.09	0.52
20:l:119:THR:HG22	21:m:13:THR:HG23	1.90	0.52
3:K:57:MET:N	3:K:58:PRO:HD2	2.24	0.52
4:L:297:ASP:HB3	4:L:300:LYS:CG	2.39	0.52
5:M:68:LEU:HG	5:M:234:ILE:HD11	1.92	0.52
7:O:336:GLY:N	7:O:344:ASN:ND2	2.56	0.52
12:d:101:PHE:CZ	16:h:159:LEU:HD22	2.45	0.52
17:i:31:ARG:O	17:i:32:GLU:C	2.50	0.52
20:l:162:PRO:HG3	23:o:39:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:324:LEU:HB3	4:L:395:ILE:HD11	1.90	0.52
4:L:496:LEU:C	4:L:496:LEU:CD1	2.79	0.52
4:L:578:THR:HG21	6:N:168:GLY:HA2	1.92	0.52
5:M:17:LEU:HD13	14:f:11:TRP:CH2	2.45	0.52
5:M:196:TRP:HE1	5:M:254:THR:HB	1.75	0.52
6:N:10:TYR:O	6:N:13:ILE:HG22	2.09	0.52
15:g:70:ASP:OD1	22:n:108:HIS:NE2	2.42	0.52
4:L:123:LEU:HD22	4:L:150:MET:HG3	1.91	0.52
4:L:264:HIS:O	4:L:265:PRO:C	2.53	0.52
26:L:703:CDL:H741	26:L:703:CDL:H781	1.92	0.52
5:M:84:LEU:HD21	5:M:95:TYR:HB3	1.90	0.52
5:M:171:VAL:HG11	5:M:179:LEU:CD2	2.35	0.52
5:M:346:ARG:O	5:M:419:LEU:HA	2.09	0.52
6:N:175:MET:HG2	6:N:219:LEU:CD2	2.40	0.52
7:O:170:LEU:HD13	7:O:187:TYR:CG	2.44	0.52
11:c:47:SER:HB2	12:d:59:HIS:HD2	1.74	0.52
4:L:108:MET:HB2	4:L:114:ILE:CD1	2.39	0.52
4:L:533:ILE:HG23	4:L:534:HIS:HD2	1.74	0.52
6:N:175:MET:HG2	6:N:219:LEU:HD22	1.91	0.52
7:O:172:ALA:HA	7:O:236:ASP:HB3	1.91	0.52
13:e:81:LYS:O	13:e:84:GLU:HB3	2.10	0.52
16:h:57:VAL:HG13	22:n:104:LEU:HG	1.92	0.52
1:D:35:ARG:HH12	15:g:56:ASP:HB2	1.74	0.52
5:M:72:LEU:HD11	5:M:233:ALA:HB1	1.92	0.52
5:M:103:GLN:O	5:M:107:ILE:HB	2.10	0.52
6:N:29:MET:HE2	6:N:141:ILE:HG12	1.92	0.52
7:O:121:PRO:HB3	7:O:178:TYR:CE1	2.45	0.52
7:O:245:PHE:HA	7:O:248:LYS:HE2	1.91	0.52
12:d:1:MET:HG3	12:d:2:MET:N	2.25	0.52
13:e:44:ALA:HA	13:e:47:ILE:HG12	1.92	0.52
20:l:169:GLU:C	20:l:171:GLY:N	2.55	0.52
22:n:37:TYR:C	22:n:39:TYR:N	2.67	0.52
2:J:106:LEU:HD12	2:J:109:TYR:HB3	1.92	0.52
8:U:128:PHE:CE1	8:U:148:ILE:HG23	2.45	0.52
12:d:62:LEU:O	12:d:66:THR:OG1	2.22	0.52
22:n:168:TRP:HD1	22:n:169:HIS:CE1	2.27	0.52
5:M:115:LEU:HD21	5:M:176:LEU:CD2	2.37	0.51
5:M:139:GLN:HB3	5:M:222:GLU:CG	2.40	0.51
8:U:120:MET:HE1	22:n:24:LEU:CD1	2.40	0.51
10:Y:17:GLY:O	10:Y:81:GLN:HG2	2.09	0.51
22:n:143:GLU:O	22:n:143:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:164:LEU:O	24:p:168:LYS:N	2.42	0.51
4:L:180:ILE:HD11	5:M:400:ILE:HB	1.92	0.51
4:L:286:LEU:HG	4:L:290:ILE:CD1	2.40	0.51
5:M:422:HIS:HB3	21:m:51:TYR:CE2	2.44	0.51
4:L:202:MET:CE	4:L:265:PRO:HG3	2.32	0.51
4:L:556:ILE:HD11	21:m:76:ILE:CG2	2.40	0.51
6:N:168:GLY:O	6:N:172:GLN:HG2	2.10	0.51
8:U:125:GLU:OE2	18:j:44:TYR:CE1	2.63	0.51
17:i:10:LEU:HA	17:i:13:GLN:HB3	1.91	0.51
18:j:87:PRO:HG3	23:o:96:VAL:HG23	1.92	0.51
3:K:59:ILE:O	3:K:60:PRO:C	2.49	0.51
6:N:25:ASN:ND2	13:e:18:PHE:CE2	2.78	0.51
14:f:34:LEU:HD22	16:h:139:ILE:HG13	1.91	0.51
16:h:52:LYS:O	16:h:53:ARG:C	2.53	0.51
17:i:77:ILE:HD13	17:i:80:TRP:CZ3	2.46	0.51
4:L:49:LEU:HB3	4:L:50:PRO:HD3	1.91	0.51
4:L:595:ILE:O	4:L:599:ILE:HG13	2.11	0.51
5:M:129:THR:CG2	5:M:235:LEU:HD11	2.40	0.51
6:N:240:MET:HE2	6:N:326:PHE:CZ	2.45	0.51
6:N:342:GLN:HE21	12:d:30:ARG:HH11	1.59	0.51
7:O:354:LEU:HG	11:c:44:VAL:CG2	2.41	0.51
9:X:168:PHE:C	9:X:169:PHE:CD1	2.89	0.51
10:Y:143:VAL:HG23	16:h:157:ARG:HG2	1.92	0.51
17:i:83:HIS:CE1	17:i:87:LYS:HD2	2.46	0.51
17:i:85:TYR:CE2	17:i:90:MET:HE3	2.46	0.51
4:L:530:PRO:O	4:L:534:HIS:HB2	2.11	0.51
5:M:31:SER:HA	5:M:34:ILE:CG1	2.41	0.51
5:M:251:ASP:N	5:M:252:PRO:HD2	2.26	0.51
19:k:34:PRO:HD2	19:k:59:TYR:CG	2.46	0.51
2:J:159:LEU:HD23	3:K:69:CYS:SG	2.51	0.51
4:L:161:ARG:NE	4:L:163:ASP:HB2	2.26	0.51
4:L:536:ILE:HD11	4:L:540:LYS:HD2	1.93	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	2.26	0.51
5:M:263:LEU:CD1	21:m:102:TYR:CD1	2.90	0.51
5:M:275:ILE:CD1	5:M:288:TYR:CG	2.84	0.51
5:M:336:ARG:HH12	5:M:433:GLU:CD	2.19	0.51
7:O:240:ALA:O	7:O:244:THR:N	2.44	0.51
12:d:28:ASP:O	12:d:29:PRO:C	2.53	0.51
16:h:57:VAL:HG13	22:n:104:LEU:HD21	1.92	0.51
19:k:42:LEU:HG	22:n:39:TYR:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:89:TYR:O	23:o:90:CYS:C	2.52	0.51
4:L:9:LEU:HD11	25:i:201:3PE:C2A	2.41	0.51
4:L:60:GLU:HG3	4:L:83:ASP:HA	1.93	0.51
5:M:304:GLN:HA	5:M:309:PHE:CE1	2.45	0.51
6:N:45:ILE:HA	6:N:52:SER:OG	2.11	0.51
7:O:289:TRP:HA	7:O:289:TRP:CE3	2.46	0.51
4:L:451:MET:O	4:L:452:ASN:C	2.53	0.51
7:O:182:GLN:O	7:O:183:CYS:C	2.54	0.51
8:U:79:ILE:HG13	8:U:126:PHE:CE2	2.45	0.51
15:g:140:PHE:HZ	24:p:152:ALA:HB1	1.76	0.51
23:o:4:HIS:HA	23:o:7:ARG:NH1	2.25	0.51
2:J:25:PRO:HD2	2:J:75:THR:HG21	1.93	0.51
3:K:73:VAL:HG21	6:N:38:LEU:HD22	1.93	0.51
4:L:404:THR:HG22	4:L:405:ASN:H	1.75	0.51
5:M:4:ILE:HD11	5:M:41:LEU:HD21	1.92	0.51
8:U:84:LEU:HD11	8:U:100:VAL:HG12	1.93	0.51
10:Y:14:VAL:HG13	10:Y:15:PRO:HD2	1.93	0.51
15:g:115:TRP:HA	15:g:118:ARG:HH11	1.74	0.51
16:h:73:PHE:CE2	16:h:74:TYR:CE1	2.98	0.51
23:o:7:ARG:HH11	23:o:106:ARG:HH12	1.59	0.51
1:D:49:GLY:O	6:N:173:THR:HG21	2.10	0.50
3:K:93:LEU:HD13	6:N:57:THR:HG21	1.92	0.50
4:L:362:ILE:CD1	4:L:430:VAL:HG13	2.41	0.50
5:M:249:ILE:HG22	5:M:250:LEU:N	2.26	0.50
10:Y:83:ARG:HH12	10:Y:90:LEU:HB3	1.76	0.50
24:p:113:CYS:O	24:p:113:CYS:SG	2.69	0.50
2:J:7:VAL:O	2:J:11:LEU:HD13	2.12	0.50
4:L:395:ILE:O	4:L:399:ILE:HG13	2.11	0.50
6:N:175:MET:O	6:N:179:MET:HG2	2.12	0.50
8:U:79:ILE:HG23	8:U:145:VAL:HG13	1.91	0.50
24:p:49:ARG:O	24:p:52:ILE:HB	2.10	0.50
4:L:349:SER:HB2	4:L:443:ILE:HG23	1.93	0.50
4:L:383:MET:CB	4:L:386:LEU:HD12	2.30	0.50
5:M:294:MET:HE3	5:M:319:HIS:HD2	1.76	0.50
5:M:354:LEU:O	5:M:355:MET:C	2.52	0.50
6:N:36:SER:HB2	6:N:134:GLN:HE22	1.76	0.50
6:N:248:LEU:CD1	6:N:296:LEU:HD23	2.41	0.50
8:U:122:MET:HA	8:U:122:MET:HE2	1.91	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
17:i:32:GLU:HG3	22:n:115:TYR:HA	1.93	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
4:L:21:ILE:HG12	4:L:27:ILE:HG23	1.93	0.50
4:L:117:PHE:HE1	4:L:243:VAL:CG2	2.23	0.50
4:L:385:PHE:CD1	18:j:72:ARG:CG	2.95	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
10:Y:57:ARG:HG2	10:Y:60:ARG:NH2	2.27	0.50
24:p:5:TRP:HZ3	24:p:10:TYR:O	1.93	0.50
1:D:54:PRO:HB2	1:D:59:ALA:HB2	1.94	0.50
1:D:55:SER:HB3	1:D:58:THR:HB	1.94	0.50
2:J:13:LEU:CD2	3:K:14:LEU:HD12	2.41	0.50
4:L:365:ILE:CD1	4:L:366:MET:HE2	2.42	0.50
4:L:441:ILE:HD13	18:j:48:PRO:HD3	1.94	0.50
5:M:118:PHE:O	5:M:122:PHE:HB2	2.11	0.50
5:M:123:GLU:HB3	6:N:255:PRO:HG2	1.93	0.50
17:i:10:LEU:HD12	17:i:13:GLN:HB3	1.94	0.50
19:k:34:PRO:CG	19:k:59:TYR:CD1	2.94	0.50
22:n:114:MET:O	22:n:115:TYR:C	2.52	0.50
3:K:38:LEU:HG	3:K:42:ILE:HD11	1.93	0.50
4:L:403:ASN:OD1	20:l:153:TYR:HB3	2.11	0.50
6:N:189:TRP:HB2	6:N:204:ASN:HD21	1.77	0.50
10:Y:115:MET:SD	10:Y:119:TYR:HE2	2.34	0.50
20:l:108:ASP:HB3	20:l:111:MET:HE2	1.93	0.50
21:m:124:LYS:HE2	21:m:125:PHE:CE2	2.47	0.50
4:L:60:GLU:O	4:L:61:TYR:CD1	2.65	0.50
5:M:4:ILE:HG22	5:M:107:ILE:CD1	2.32	0.50
5:M:63:THR:N	5:M:64:PRO:HD2	2.27	0.50
5:M:248:ILE:HG13	5:M:249:ILE:N	2.26	0.50
5:M:278:ARG:HH22	20:l:108:ASP:CG	2.20	0.50
5:M:328:CYS:SG	5:M:436:LEU:HD21	2.52	0.50
5:M:432:ARG:HA	5:M:435:THR:HG22	1.94	0.50
6:N:258:THR:HG23	6:N:336:THR:HG22	1.93	0.50
8:U:90:TYR:HD2	8:U:93:ILE:H	1.60	0.50
20:l:38:PRO:C	21:m:75:ASN:HD21	2.20	0.50
2:J:37:PHE:CE2	2:J:41:LEU:HD11	2.46	0.50
4:L:589:MET:O	4:L:592:LEU:N	2.45	0.50
7:O:319:ILE:HD12	7:O:324:GLY:HA3	1.94	0.50
8:U:142:GLN:O	8:U:145:VAL:N	2.43	0.50
10:Y:12:HIS:NE2	10:Y:127:PHE:HZ	2.09	0.50
15:g:106:TYR:CZ	16:h:86:ILE:HD12	2.47	0.50
20:l:49:ALA:HA	20:l:59:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:LEU:CD2	3:K:32:CYS:HA	2.42	0.50
4:L:354:GLN:O	4:L:354:GLN:HG2	2.12	0.50
9:X:170:TRP:CZ3	26:d:201:CDL:H522	2.47	0.50
16:h:57:VAL:HG13	22:n:104:LEU:CD2	2.41	0.50
4:L:123:LEU:CD2	4:L:150:MET:HG3	2.43	0.49
4:L:217:LEU:HD13	4:L:273:ILE:HG23	1.93	0.49
4:L:306:THR:HA	4:L:336:LYS:NZ	2.27	0.49
5:M:25:THR:HG22	15:g:84:ASN:OD1	2.11	0.49
5:M:158:ILE:HG12	6:N:287:LEU:HD11	1.94	0.49
6:N:175:MET:HE1	6:N:227:ILE:HG22	1.94	0.49
6:N:190:MET:HB3	6:N:201:THR:HG23	1.94	0.49
6:N:307:THR:O	7:O:319:ILE:HG12	2.11	0.49
11:c:55:TRP:CE2	12:d:66:THR:HG22	2.47	0.49
18:j:92:TRP:O	23:o:107:ARG:NH2	2.45	0.49
1:D:70:ASP:HB2	1:D:72:LEU:HG	1.94	0.49
2:J:22:LYS:HZ2	3:K:21:MET:C	2.20	0.49
2:J:68:GLY:O	2:J:69:TYR:C	2.55	0.49
3:K:66:PHE:CE1	6:N:35:PHE:CZ	2.97	0.49
4:L:445:GLU:CB	4:L:450:LEU:HD23	2.37	0.49
5:M:122:PHE:CE1	5:M:238:LEU:HG	2.46	0.49
5:M:184:HIS:CD2	5:M:249:ILE:HG23	2.47	0.49
5:M:441:MET:HG3	5:M:445:ILE:HD12	1.94	0.49
6:N:62:THR:HG21	6:N:114:TRP:CD1	2.47	0.49
6:N:133:TRP:CG	6:N:133:TRP:O	2.63	0.49
7:O:170:LEU:HD21	7:O:184:VAL:HG22	1.95	0.49
8:U:132:ASP:HA	8:U:135:ALA:HB3	1.93	0.49
10:Y:143:VAL:CG2	16:h:161:ARG:HD2	2.41	0.49
11:c:40:ASN:O	11:c:43:ALA:N	2.45	0.49
4:L:393:ASP:OD1	4:L:393:ASP:C	2.56	0.49
5:M:88:ASN:O	5:M:89:ASN:HB3	2.12	0.49
5:M:207:MET:SD	5:M:240:SER:HA	2.52	0.49
5:M:388:TRP:CD1	21:m:109:ARG:HD2	2.47	0.49
5:M:422:HIS:CE1	21:m:56:ARG:HH22	2.29	0.49
6:N:342:GLN:NE2	12:d:30:ARG:HH11	2.09	0.49
7:O:136:TYR:OH	7:O:191:LYS:HA	2.11	0.49
7:O:259:ASP:O	7:O:260:SER:C	2.54	0.49
9:X:165:THR:OG1	9:X:172:VAL:HG11	2.12	0.49
13:e:41:ILE:HG12	16:h:174:PRO:HB2	1.93	0.49
22:n:96:CYS:SG	22:n:97:TYR:CZ	3.05	0.49
22:n:163:LEU:O	22:n:164:PRO:C	2.54	0.49
24:p:74:ILE:O	24:p:75:THR:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:66:VAL:O	2:J:67:PHE:C	2.55	0.49
2:J:124:LEU:HD23	2:J:125:MET:HG2	1.95	0.49
4:L:399:ILE:HG22	4:L:409:LEU:HD13	1.93	0.49
4:L:564:LYS:HG2	21:m:77:TYR:CZ	2.47	0.49
7:O:276:LEU:HD11	7:O:278:TYR:CE2	2.47	0.49
13:e:20:PHE:CZ	16:h:178:PHE:HB2	2.47	0.49
21:m:45:ARG:CZ	22:n:140:LEU:HD11	2.43	0.49
4:L:553:LEU:HD21	21:m:93:ALA:O	2.12	0.49
5:M:348:LEU:HD12	5:M:415:GLN:HE22	1.77	0.49
5:M:420:THR:HG21	5:M:423:MET:HG2	1.93	0.49
7:O:143:TYR:CZ	7:O:164:TYR:HE2	2.30	0.49
17:i:90:MET:O	17:i:91:ALA:C	2.53	0.49
20:l:81:ARG:HD3	20:l:85:GLU:OE2	2.13	0.49
4:L:316:THR:CG2	4:L:325:ALA:CB	2.89	0.49
5:M:178:ILE:HD12	16:h:143:GLU:HG3	1.94	0.49
5:M:285:LEU:HD22	5:M:410:MET:SD	2.53	0.49
6:N:230:ILE:HG21	6:N:296:LEU:HD11	1.94	0.49
6:N:231:SER:HA	6:N:300:THR:HA	1.93	0.49
1:D:47:PHE:CD1	6:N:227:ILE:HD11	2.48	0.49
2:J:123:TRP:CZ2	13:e:76:MET:SD	3.05	0.49
4:L:68:TRP:CE3	4:L:76:LEU:HD21	2.47	0.49
4:L:491:LEU:HD13	18:j:80:VAL:HG22	1.94	0.49
4:L:496:LEU:HA	4:L:499:LEU:HB2	1.94	0.49
5:M:193:ASN:HA	5:M:253:LEU:HD23	1.94	0.49
7:O:260:SER:O	7:O:263:ALA:HB3	2.13	0.49
9:X:168:PHE:O	9:X:170:TRP:NE1	2.45	0.49
14:f:38:ARG:O	16:h:134:GLU:OE2	2.30	0.49
20:l:158:PRO:CD	23:o:22:ILE:HB	2.31	0.49
23:o:22:ILE:HD12	23:o:102:PHE:HD1	1.77	0.49
4:L:67:HIS:HE2	4:L:69:VAL:C	2.21	0.49
5:M:5:ILE:HG13	5:M:6:LEU:N	2.28	0.49
5:M:139:GLN:HG3	5:M:140:THR:N	2.27	0.49
5:M:248:ILE:CG1	5:M:249:ILE:HD12	2.39	0.49
9:X:166:ARG:HH22	12:d:87:ASP:CG	2.20	0.49
11:c:70:LYS:O	11:c:75:LEU:HA	2.13	0.49
14:f:24:CYS:SG	14:f:28:ARG:NH1	2.86	0.49
15:g:53:TRP:H	15:g:53:TRP:HE3	1.58	0.49
21:m:75:ASN:OD1	21:m:79:ASN:ND2	2.46	0.49
5:M:348:LEU:HB2	5:M:415:GLN:OE1	2.13	0.49
6:N:309:ASN:HA	7:O:319:ILE:CG2	2.42	0.49
7:O:256:LEU:CD2	7:O:276:LEU:HD23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:h:201:CDL:H181	26:h:201:CDL:H221	1.95	0.49
17:i:4:TYR:HE1	22:n:4:CYS:SG	2.35	0.49
19:k:55:GLU:OE1	22:n:38:ARG:HB2	2.13	0.49
3:K:59:ILE:HD12	6:N:27:MET:HG2	1.95	0.49
4:L:141:PHE:HE2	5:M:370:PRO:HG3	1.60	0.49
4:L:227:PHE:CD2	4:L:283:LEU:HD23	2.48	0.49
4:L:316:THR:HG23	4:L:325:ALA:CB	2.32	0.49
5:M:134:THR:O	5:M:142:ARG:CD	2.59	0.49
5:M:216:LEU:HD12	5:M:236:LEU:CD2	2.38	0.49
5:M:227:GLY:HA2	5:M:230:ILE:HG22	1.95	0.49
7:O:78:ALA:HB2	7:O:85:HIS:HB2	1.95	0.49
8:U:118:ILE:O	8:U:119:ILE:C	2.55	0.49
12:d:103:GLU:HG3	12:d:105:GLU:OE2	2.13	0.49
20:l:167:TYR:OH	20:l:176:LYS:O	2.14	0.49
22:n:20:TYR:OH	22:n:45:ARG:HB2	2.12	0.49
22:n:114:MET:HG3	22:n:115:TYR:HD2	1.78	0.49
2:J:125:MET:HE3	2:J:128:VAL:HG21	1.94	0.48
15:g:109:ASP:HB2	15:g:114:GLU:HB3	1.94	0.48
22:n:81:ILE:HD12	22:n:87:GLY:O	2.12	0.48
1:D:72:LEU:HD11	6:N:50:PRO:HB3	1.93	0.48
5:M:1:MET:HB2	5:M:52:PHE:CE2	2.48	0.48
5:M:313:THR:HA	5:M:316:MET:CE	2.43	0.48
11:c:62:HIS:O	11:c:66:VAL:HG23	2.12	0.48
15:g:108:PRO:HB3	16:h:118:SER:OG	2.12	0.48
18:j:97:LEU:HD13	23:o:104:ARG:N	2.28	0.48
18:j:99:ILE:CD1	23:o:107:ARG:HB2	2.42	0.48
21:m:122:ASP:O	21:m:123:ARG:C	2.54	0.48
24:p:5:TRP:CZ3	24:p:10:TYR:O	2.66	0.48
2:J:52:GLY:O	2:J:55:VAL:HG12	2.13	0.48
3:K:70:GLU:HA	6:N:38:LEU:HD21	1.94	0.48
4:L:101:MET:HE1	4:L:121:LEU:CB	2.43	0.48
4:L:144:TRP:HH2	4:L:256:GLY:HA2	1.78	0.48
4:L:350:LEU:HD23	4:L:443:ILE:HD11	1.96	0.48
4:L:372:CYS:SG	4:L:454:ILE:HG22	2.54	0.48
5:M:59:ASP:OD1	5:M:245:ARG:NH2	2.47	0.48
6:N:31:VAL:HB	6:N:35:PHE:CE2	2.48	0.48
7:O:256:LEU:HB3	7:O:258:TYR:HE1	1.73	0.48
16:h:73:PHE:O	16:h:77:LEU:N	2.46	0.48
1:D:42:GLU:HA	1:D:45:GLU:HG2	1.96	0.48
2:J:151:MET:O	2:J:154:VAL:HG12	2.13	0.48
4:L:41:LYS:HG3	4:L:98:TRP:CH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:402:CYS:SG	4:L:403:ASN:N	2.87	0.48
4:L:550:LEU:HD12	5:M:275:ILE:CB	2.30	0.48
5:M:114:GLU:HG3	9:X:169:PHE:HB3	1.94	0.48
5:M:166:LEU:HD21	5:M:170:HIS:CE1	2.48	0.48
6:N:321:LYS:HD2	12:d:49:ARG:NE	2.29	0.48
22:n:44:MET:O	22:n:45:ARG:C	2.54	0.48
22:n:51:HIS:HB3	22:n:63:LEU:HD13	1.95	0.48
2:J:39:GLY:HA2	2:J:42:MET:HE2	1.94	0.48
4:L:316:THR:HG21	4:L:325:ALA:HA	1.95	0.48
4:L:361:ASN:O	4:L:361:ASN:CG	2.54	0.48
4:L:433:THR:HG21	4:L:436:ARG:NH2	2.29	0.48
5:M:178:ILE:HG12	24:p:82:VAL:HG11	1.95	0.48
7:O:323:GLN:HE22	15:g:54:GLN:C	2.20	0.48
8:U:94:ASP:OD1	8:U:95:PRO:HD2	2.13	0.48
13:e:101:ARG:NH1	13:e:102:GLU:O	2.47	0.48
16:h:73:PHE:HE2	16:h:74:TYR:HE1	1.62	0.48
16:h:86:ILE:HG21	26:h:201:CDL:HA61	1.95	0.48
19:k:41:LYS:C	19:k:43:ALA:N	2.64	0.48
22:n:155:PRO:HG2	22:n:165:PRO:HG2	1.95	0.48
2:J:92:LEU:O	2:J:96:VAL:HG23	2.14	0.48
4:L:141:PHE:HD1	4:L:182:PHE:CD2	2.31	0.48
4:L:264:HIS:HA	4:L:267:THR:OG1	2.13	0.48
4:L:274:LEU:O	4:L:277:MET:HG2	2.14	0.48
4:L:358:LYS:CG	22:n:80:TYR:CE2	2.92	0.48
4:L:542:LEU:HD11	25:L:702:3PE:H261	1.94	0.48
5:M:311:GLY:HA2	5:M:314:MET:CE	2.42	0.48
6:N:4:ILE:HG23	6:N:5:THR:N	2.29	0.48
13:e:47:ILE:HG13	13:e:47:ILE:O	2.12	0.48
16:h:96:ALA:O	24:p:63:TYR:CE1	2.66	0.48
16:h:159:LEU:HB3	16:h:163:ARG:NH1	2.22	0.48
19:k:38:VAL:HG13	22:n:39:TYR:HB2	1.96	0.48
20:l:48:ARG:CZ	20:l:64:PRO:HD2	2.44	0.48
4:L:496:LEU:HD12	4:L:497:GLY:CA	2.44	0.48
5:M:173:THR:HG22	16:h:150:ARG:NH1	2.29	0.48
5:M:307:TRP:CE3	5:M:383:MET:CE	2.97	0.48
6:N:227:ILE:CA	6:N:230:ILE:HG22	2.38	0.48
7:O:314:LEU:HD12	7:O:315:PRO:HD3	1.93	0.48
8:U:132:ASP:O	8:U:136:GLU:HG3	2.14	0.48
14:f:25:TYR:CE1	14:f:29:LYS:HD3	2.48	0.48
17:i:108:ASP:OD2	24:p:18:PRO:HB2	2.13	0.48
20:l:48:ARG:HH21	20:l:63:GLU:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:201:3PE:H242	25:m:201:3PE:H3B1	1.95	0.48
23:o:87:TRP:NE1	23:o:91:GLU:OE1	2.45	0.48
2:J:104:CYS:HA	2:J:107:ASN:HB2	1.96	0.48
2:J:123:TRP:CH2	13:e:72:THR:C	2.91	0.48
4:L:308:SER:O	4:L:311:GLY:N	2.47	0.48
4:L:319:MET:O	4:L:319:MET:HG2	2.13	0.48
5:M:269:MET:HE3	5:M:399:ASN:HB3	1.96	0.48
5:M:422:HIS:CE1	5:M:425:ASN:OD1	2.66	0.48
6:N:146:TYR:CE1	6:N:198:PRO:HG2	2.49	0.48
7:O:76:GLU:HB2	7:O:266:PRO:HB3	1.95	0.48
10:Y:143:VAL:HG22	16:h:161:ARG:CD	2.40	0.48
19:k:69:PHE:CE1	19:k:73:ILE:HD11	2.48	0.48
23:o:111:ARG:O	23:o:115:ARG:HG3	2.14	0.48
1:D:72:LEU:HD12	6:N:50:PRO:HG2	1.90	0.48
11:c:65:ASP:O	11:c:66:VAL:C	2.56	0.48
13:e:38:LYS:HG2	16:h:179:ILE:HG23	1.95	0.48
13:e:102:GLU:HG2	13:e:103:GLU:H	1.79	0.48
14:f:39:ASN:ND2	14:f:46:ARG:O	2.47	0.48
17:i:90:MET:SD	17:i:97:ILE:HD11	2.53	0.48
19:k:41:LYS:O	19:k:42:LEU:C	2.50	0.48
20:l:167:TYR:HD2	20:l:168:LEU:CD1	2.19	0.48
7:O:76:GLU:O	7:O:77:ILE:C	2.57	0.48
8:U:86:VAL:HG13	19:k:54:ASN:ND2	2.29	0.48
8:U:102:SER:C	8:U:141:PRO:HD3	2.39	0.48
8:U:128:PHE:HZ	8:U:148:ILE:HD12	1.76	0.48
16:h:96:ALA:CB	24:p:63:TYR:HD1	2.26	0.48
4:L:31:ASN:HD22	4:L:34:LEU:HB2	1.79	0.47
4:L:145:GLU:HB3	5:M:370:PRO:HG2	1.96	0.47
4:L:513:MET:HE1	22:n:30:TRP:CB	2.44	0.47
5:M:42:LEU:HG	5:M:67:ILE:CD1	2.42	0.47
5:M:176:LEU:HD13	5:M:245:ARG:HH11	1.79	0.47
5:M:310:MET:CE	5:M:459:MET:SD	3.02	0.47
6:N:189:TRP:CZ3	6:N:282:MET:HE3	2.49	0.47
7:O:250:SER:HA	7:O:255:VAL:HG23	1.96	0.47
7:O:343:TYR:CE1	7:O:355:LYS:CB	2.96	0.47
22:n:37:TYR:O	22:n:39:TYR:N	2.47	0.47
22:n:81:ILE:HD11	22:n:87:GLY:O	2.14	0.47
22:n:156:PRO:HD2	22:n:158:ARG:NH1	2.29	0.47
4:L:3:ILE:HG22	4:L:49:LEU:HD21	1.96	0.47
4:L:483:PRO:HG2	4:L:486:LEU:HD12	1.96	0.47
5:M:49:TYR:CD1	5:M:59:ASP:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:192:ASN:C	5:M:194:LEU:N	2.72	0.47
13:e:83:ARG:HD3	13:e:92:TYR:CD2	2.48	0.47
19:k:52:ALA:O	19:k:53:ARG:C	2.56	0.47
19:k:84:PHE:CZ	19:k:88:LEU:HD22	2.49	0.47
24:p:6:ASP:C	24:p:8:ASP:N	2.69	0.47
3:K:95:LEU:HG	6:N:54:GLU:OE2	2.15	0.47
4:L:54:PHE:CZ	4:L:84:PHE:HB2	2.49	0.47
4:L:466:PHE:HE2	25:L:701:3PE:H331	1.79	0.47
4:L:482:MET:HE2	4:L:486:LEU:HB3	1.96	0.47
4:L:598:ILE:HD13	6:N:153:ILE:HG23	1.97	0.47
5:M:94:LEU:O	5:M:98:MET:HG2	2.14	0.47
5:M:391:PHE:HE1	25:M:502:3PE:H12	1.79	0.47
6:N:26:LEU:O	6:N:29:MET:N	2.47	0.47
8:U:93:ILE:HD11	8:U:118:ILE:HD11	1.97	0.47
8:U:130:ILE:HD12	8:U:147:TYR:CE2	2.50	0.47
12:d:8:HIS:O	12:d:10:PRO:HD3	2.14	0.47
16:h:98:LEU:HA	24:p:63:TYR:O	2.15	0.47
17:i:79:MET:O	17:i:80:TRP:C	2.57	0.47
21:m:124:LYS:C	21:m:126:ASN:H	2.21	0.47
4:L:277:MET:SD	4:L:318:GLY:HA2	2.54	0.47
5:M:421:ASN:HB2	21:m:51:TYR:OH	2.15	0.47
5:M:421:ASN:ND2	21:m:47:TYR:OH	2.47	0.47
6:N:89:GLN:H	6:N:89:GLN:CD	2.22	0.47
6:N:309:ASN:N	7:O:319:ILE:HG23	2.30	0.47
3:K:69:CYS:O	3:K:70:GLU:C	2.57	0.47
4:L:433:THR:CG2	4:L:434:LYS:N	2.78	0.47
5:M:122:PHE:HZ	5:M:206:LYS:HD3	1.75	0.47
5:M:159:PRO:CG	25:M:501:3PE:H391	2.44	0.47
17:i:83:HIS:HD2	24:p:37:TYR:CE2	2.31	0.47
18:j:45:ARG:HD3	19:k:57:TRP:CD1	2.50	0.47
4:L:340:PHE:O	4:L:343:SER:OG	2.32	0.47
4:L:420:ALA:HB1	4:L:498:PHE:CD2	2.50	0.47
5:M:9:LEU:HD13	26:M:503:CDL:H631	1.96	0.47
5:M:78:MET:HG2	5:M:432:ARG:HG3	1.97	0.47
5:M:370:PRO:CA	5:M:375:LEU:HD23	2.42	0.47
6:N:1:MET:HE1	6:N:43:MET:SD	2.54	0.47
6:N:1:MET:O	6:N:2:ASN:C	2.54	0.47
9:X:154:ILE:CG1	16:h:167:PRO:HG2	2.44	0.47
23:o:24:SER:OG	23:o:109:LEU:HD21	2.14	0.47
2:J:24:SER:HB2	2:J:27:TYR:CD1	2.43	0.47
3:K:75:LEU:O	3:K:79:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:121:LEU:HD22	4:L:246:LEU:CD2	2.24	0.47
4:L:174:TYR:HE1	25:L:702:3PE:H362	1.78	0.47
4:L:237:MET:HE1	4:L:248:HIS:HB2	1.96	0.47
4:L:386:LEU:HA	18:j:68:TRP:HZ3	1.80	0.47
4:L:390:TYR:HE2	18:j:68:TRP:CH2	2.33	0.47
4:L:424:MET:HE2	4:L:502:LEU:CB	2.45	0.47
4:L:524:THR:HG21	22:n:77:PRO:HG2	1.96	0.47
4:L:552:LEU:HD22	4:L:553:LEU:HD12	1.97	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
6:N:120:GLN:O	6:N:176:ARG:NH2	2.48	0.47
7:O:116:LYS:HA	7:O:119:ASP:OD1	2.14	0.47
7:O:232:ALA:O	7:O:235:GLN:HB3	2.14	0.47
7:O:350:LYS:O	7:O:351:TRP:HB2	2.13	0.47
10:Y:142:LYS:O	10:Y:143:VAL:C	2.57	0.47
12:d:73:TYR:O	12:d:77:LYS:HB2	2.14	0.47
12:d:100:ASP:HB3	16:h:159:LEU:CD2	2.45	0.47
13:e:41:ILE:HD11	16:h:174:PRO:HB2	1.96	0.47
13:e:102:GLU:HG2	13:e:103:GLU:HG2	1.95	0.47
14:f:41:SER:O	14:f:42:MET:C	2.58	0.47
20:l:44:THR:CG2	20:l:47:GLU:HG3	2.45	0.47
21:m:84:PRO:HG3	25:m:201:3PE:H331	1.97	0.47
4:L:142:ILE:HA	5:M:370:PRO:HB2	1.96	0.47
4:L:474:PRO:HD2	23:o:67:LEU:HD21	1.97	0.47
4:L:556:ILE:HG21	21:m:80:PHE:CZ	2.45	0.47
5:M:305:THR:O	5:M:306:PRO:C	2.58	0.47
7:O:205:ILE:HD13	7:O:256:LEU:HB2	1.96	0.47
7:O:243:LYS:O	7:O:247:PRO:CG	2.63	0.47
11:c:46:LEU:O	11:c:50:ALA:CB	2.63	0.47
12:d:51:ARG:O	12:d:52:PRO:C	2.55	0.47
22:n:50:GLU:O	22:n:51:HIS:C	2.56	0.47
22:n:96:CYS:SG	22:n:97:TYR:CE1	3.04	0.47
1:D:47:PHE:CD1	6:N:227:ILE:CD1	2.98	0.47
2:J:9:SER:HB2	3:K:7:ASN:ND2	2.20	0.47
5:M:196:TRP:HD1	5:M:250:LEU:HB2	1.80	0.47
5:M:232:ALA:HA	5:M:236:LEU:HD12	1.97	0.47
7:O:129:TYR:CE2	7:O:183:CYS:HB3	2.50	0.47
13:e:85:LYS:O	13:e:89:GLU:HG2	2.15	0.47
3:K:57:MET:C	3:K:60:PRO:HD2	2.39	0.47
7:O:78:ALA:CB	7:O:85:HIS:HB2	2.45	0.47
7:O:125:ASP:C	15:g:51:MET:HE3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:135:LEU:HB3	7:O:139:ARG:NH1	2.25	0.47
10:Y:116:GLY:O	10:Y:120:MET:HB2	2.15	0.47
12:d:78:ARG:O	12:d:81:TYR:N	2.48	0.47
12:d:93:TYR:CD2	16:h:156:VAL:HG13	2.50	0.47
15:g:123:LEU:CD1	24:p:98:VAL:HG11	2.45	0.47
21:m:14:LEU:HD12	21:m:15:PRO:HD2	1.96	0.47
22:n:57:MET:O	22:n:58:MET:C	2.58	0.47
24:p:29:PRO:O	24:p:33:LEU:HD13	2.14	0.47
2:J:5:ILE:HG13	2:J:124:LEU:HD13	1.97	0.46
4:L:277:MET:CG	4:L:318:GLY:HA2	2.44	0.46
4:L:482:MET:HE2	4:L:486:LEU:CB	2.45	0.46
26:L:703:CDL:H322	26:L:703:CDL:H161	1.97	0.46
7:O:62:VAL:HG13	7:O:62:VAL:O	2.15	0.46
20:l:127:ASP:O	20:l:128:VAL:C	2.58	0.46
3:K:30:LEU:HD22	3:K:78:LEU:CD1	2.44	0.46
3:K:57:MET:N	3:K:58:PRO:CD	2.78	0.46
4:L:42:PHE:CD2	17:i:74:HIS:HE1	2.33	0.46
4:L:203:PHE:CE1	24:p:114:GLN:HG3	2.50	0.46
4:L:305:SER:C	4:L:336:LYS:HZ3	2.24	0.46
4:L:373:LEU:CD2	4:L:427:ILE:HG22	2.45	0.46
4:L:385:PHE:CE1	18:j:72:ARG:HG3	2.50	0.46
4:L:390:TYR:CE2	18:j:68:TRP:CH2	3.03	0.46
4:L:556:ILE:HG23	21:m:80:PHE:CZ	2.50	0.46
5:M:263:LEU:HD13	21:m:102:TYR:HB2	1.97	0.46
5:M:388:TRP:NE1	21:m:109:ARG:CD	2.78	0.46
26:M:503:CDL:H382	6:N:242:THR:HG23	1.97	0.46
6:N:17:PRO:HG2	6:N:133:TRP:NE1	2.30	0.46
12:d:11:LEU:HB2	13:e:9:LYS:HB2	1.96	0.46
12:d:59:HIS:CE1	12:d:60:ARG:HG3	2.50	0.46
4:L:86:SER:OG	4:L:133:SER:HB3	2.15	0.46
4:L:172:ILE:O	4:L:176:ARG:HG2	2.16	0.46
4:L:225:ALA:CB	4:L:233:LEU:HD12	2.45	0.46
4:L:390:TYR:OH	18:j:72:ARG:HG2	2.15	0.46
4:L:480:LEU:HD22	18:j:84:PHE:HD2	1.78	0.46
4:L:581:LYS:HB2	4:L:586:LEU:HD22	1.97	0.46
5:M:213:HIS:O	5:M:217:PRO:CD	2.63	0.46
7:O:258:TYR:OH	7:O:272:ASP:HB2	2.15	0.46
19:k:57:TRP:O	19:k:58:ARG:C	2.58	0.46
21:m:91:ALA:HB2	25:m:201:3PE:H261	1.98	0.46
24:p:6:ASP:OD1	24:p:8:ASP:HB2	2.16	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)
2:J:32:LEU:HD23	2:J:64:LEU:HD11	1.96	0.46
3:K:12:PHE:CD1	6:N:72:LEU:HD22	2.50	0.46
4:L:21:ILE:HG12	4:L:27:ILE:CG2	2.45	0.46
4:L:226:GLN:OE1	4:L:284:THR:HG21	2.14	0.46
4:L:605:ASN:HA	10:Y:5:LYS:HZ2	1.80	0.46
5:M:4:ILE:HD12	5:M:4:ILE:N	2.30	0.46
5:M:139:GLN:HG3	5:M:141:GLU:H	1.80	0.46
5:M:300:SER:HB2	5:M:308:SER:HB3	1.97	0.46
5:M:348:LEU:O	5:M:351:VAL:N	2.38	0.46
5:M:380:PHE:HD1	5:M:380:PHE:N	2.13	0.46
5:M:380:PHE:N	5:M:380:PHE:CD1	2.82	0.46
5:M:435:THR:O	5:M:436:LEU:C	2.58	0.46
7:O:38:TYR:CE1	7:O:292:HIS:HD2	2.34	0.46
7:O:50:THR:OG1	7:O:288:ASP:HB3	2.15	0.46
8:U:133:ILE:HD11	22:n:7:PRO:HD3	1.98	0.46
22:n:133:TRP:O	22:n:137:VAL:HG22	2.15	0.46
22:n:136:GLU:O	22:n:139:GLN:N	2.49	0.46
4:L:573:MET:O	4:L:576:LEU:HG	2.15	0.46
5:M:151:PHE:CE2	6:N:291:PHE:HB2	2.49	0.46
6:N:154:ILE:HG12	6:N:195:PRO:CG	2.45	0.46
10:Y:110:TYR:HD2	25:m:201:3PE:H112	1.79	0.46
1:D:58:THR:HA	1:D:61:TRP:CE2	2.50	0.46
25:D:501:3PE:H272	6:N:288:LEU:CD1	2.46	0.46
4:L:31:ASN:ND2	4:L:34:LEU:HB2	2.31	0.46
5:M:10:MET:C	5:M:13:PRO:HD2	2.41	0.46
5:M:388:TRP:CD2	21:m:109:ARG:HD2	2.51	0.46
11:c:55:TRP:NE1	12:d:66:THR:CG2	2.79	0.46
12:d:13:PHE:O	12:d:78:ARG:NE	2.43	0.46
23:o:71:ARG:HB3	23:o:71:ARG:NH1	2.27	0.46
24:p:6:ASP:O	24:p:8:ASP:N	2.49	0.46
1:D:36:GLN:HE22	5:M:135:ARG:HH22	1.64	0.46
1:D:47:PHE:CE2	6:N:305:PHE:HZ	2.32	0.46
5:M:44:GLN:HG2	5:M:46:ASP:O	2.15	0.46
5:M:303:ILE:HG22	5:M:305:THR:HG23	1.98	0.46
25:M:501:3PE:H321	25:M:501:3PE:C21	2.46	0.46
6:N:37:LEU:HD21	6:N:60:PHE:CD1	2.51	0.46
7:O:40:LEU:O	7:O:44:ILE:HG13	2.16	0.46
7:O:231:SER:O	7:O:234:LEU:N	2.48	0.46
7:O:243:LYS:O	7:O:247:PRO:HG3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:155:PRO:HG3	23:o:4:HIS:CD2	2.51	0.46
20:l:158:PRO:HD3	23:o:22:ILE:CG1	2.45	0.46
21:m:9:ALA:O	21:m:10:PRO:C	2.56	0.46
2:J:49:SER:O	2:J:50:PHE:C	2.57	0.46
4:L:475:THR:O	4:L:476:SER:HB2	2.15	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:116:ILE:HD12	5:M:119:TYR:HB3	1.97	0.46
5:M:319:HIS:CA	5:M:322:THR:HG22	2.41	0.46
16:h:95:GLU:OE1	16:h:114:LYS:HD3	2.15	0.46
2:J:3:ASN:OD1	2:J:6:PHE:HB3	2.16	0.46
2:J:17:LEU:O	2:J:21:LEU:HG	2.16	0.46
2:J:136:GLU:HG2	2:J:139:ILE:HG13	1.98	0.46
3:K:57:MET:O	3:K:58:PRO:C	2.58	0.46
4:L:101:MET:HE1	4:L:121:LEU:HB2	1.98	0.46
4:L:324:LEU:HA	4:L:327:LEU:HD12	1.97	0.46
5:M:453:LEU:CD1	5:M:454:ILE:CG2	2.84	0.46
26:M:503:CDL:H342	6:N:242:THR:HA	1.98	0.46
6:N:123:PRO:HG2	6:N:126:MET:CG	2.40	0.46
7:O:247:PRO:O	7:O:248:LYS:C	2.59	0.46
10:Y:74:LEU:HD23	10:Y:74:LEU:C	2.41	0.46
16:h:82:VAL:O	16:h:85:GLY:N	2.49	0.46
18:j:92:TRP:O	18:j:93:THR:C	2.59	0.46
19:k:69:PHE:CZ	19:k:73:ILE:HG13	2.51	0.46
25:m:201:3PE:O31	25:m:201:3PE:H342	2.16	0.46
22:n:61:THR:O	22:n:65:ARG:HG3	2.15	0.46
4:L:277:MET:HG3	4:L:318:GLY:CA	2.46	0.46
4:L:550:LEU:O	4:L:554:ASP:HB3	2.16	0.46
5:M:122:PHE:CZ	5:M:206:LYS:CD	2.94	0.46
6:N:277:ILE:HG22	6:N:278:MET:H	1.79	0.46
7:O:344:ASN:OD1	7:O:346:GLU:HG2	2.15	0.46
12:d:54:MET:HE2	12:d:54:MET:HB3	1.89	0.46
12:d:114:GLU:CD	12:d:114:GLU:H	2.23	0.46
17:i:85:TYR:CD2	25:i:201:3PE:H291	2.51	0.46
19:k:52:ALA:O	19:k:55:GLU:N	2.49	0.46
22:n:45:ARG:O	22:n:49:GLU:N	2.37	0.46
23:o:15:VAL:CG2	23:o:16:GLU:N	2.79	0.46
4:L:12:PHE:O	4:L:16:LEU:HG	2.15	0.45
4:L:145:GLU:HB3	5:M:370:PRO:CG	2.46	0.45
4:L:339:LEU:HD11	4:L:376:GLY:HA3	1.99	0.45
6:N:241:LEU:O	6:N:244:ILE:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:140:LEU:HD11	7:O:198:TYR:CE2	2.51	0.45
9:X:168:PHE:O	9:X:169:PHE:CG	2.69	0.45
20:l:166:LEU:HD12	20:l:170:ARG:HH22	1.81	0.45
21:m:124:LYS:C	21:m:126:ASN:N	2.70	0.45
22:n:168:TRP:O	22:n:172:THR:OG1	2.33	0.45
1:D:55:SER:HB3	1:D:58:THR:CB	2.46	0.45
2:J:91:PHE:O	2:J:94:LEU:HB3	2.16	0.45
4:L:60:GLU:HG2	4:L:83:ASP:HA	1.98	0.45
4:L:74:MET:HE3	4:L:74:MET:HB2	1.76	0.45
4:L:204:SER:HA	4:L:207:ASN:ND2	2.31	0.45
4:L:424:MET:HE2	4:L:502:LEU:HA	1.97	0.45
4:L:532:ILE:CG2	20:l:133:LEU:HD22	2.46	0.45
5:M:186:LEU:HD22	5:M:250:LEU:HA	1.98	0.45
5:M:208:PRO:CD	5:M:236:LEU:HD22	2.38	0.45
5:M:309:PHE:O	5:M:312:ALA:HB3	2.16	0.45
5:M:393:ILE:O	5:M:397:GLY:N	2.49	0.45
6:N:215:MET:SD	6:N:244:ILE:HD11	2.56	0.45
7:O:204:VAL:O	7:O:205:ILE:C	2.60	0.45
7:O:306:ASN:O	7:O:309:THR:HG22	2.16	0.45
7:O:323:GLN:NE2	15:g:55:GLU:N	2.64	0.45
13:e:89:GLU:HB3	13:e:91:LYS:HE2	1.98	0.45
14:f:16:VAL:HB	14:f:17:PRO:HD3	1.97	0.45
20:l:35:ASP:O	20:l:54:LYS:HD3	2.15	0.45
21:m:15:PRO:HG2	21:m:18:LEU:HD12	1.97	0.45
23:o:63:LEU:O	23:o:64:ILE:C	2.59	0.45
1:D:58:THR:HG23	1:D:61:TRP:CH2	2.51	0.45
4:L:135:ASN:O	4:L:198:LEU:HD13	2.16	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:56:PHE:CE1	5:M:108:MET:HG2	2.47	0.45
5:M:61:LEU:C	5:M:64:PRO:HD2	2.42	0.45
5:M:207:MET:O	5:M:208:PRO:C	2.59	0.45
5:M:282:LEU:HD11	5:M:410:MET:HE3	1.96	0.45
6:N:300:THR:CG2	6:N:301:SER:N	2.79	0.45
7:O:342:GLY:O	7:O:355:LYS:NZ	2.50	0.45
17:i:11:ARG:HD2	22:n:154:LEU:O	2.15	0.45
25:D:501:3PE:O31	25:D:501:3PE:H231	2.16	0.45
4:L:247:LEU:HD12	4:L:247:LEU:C	2.41	0.45
5:M:42:LEU:HD11	5:M:67:ILE:HD12	1.99	0.45
5:M:264:LEU:HD23	21:m:98:LEU:HD21	1.98	0.45
6:N:133:TRP:CE3	6:N:136:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:155:LEU:O	6:N:159:ILE:HG22	2.16	0.45
6:N:313:MET:HG3	7:O:305:LEU:CD2	2.46	0.45
7:O:265:ASP:O	7:O:266:PRO:C	2.58	0.45
8:U:113:LEU:HD23	22:n:17:LEU:CD2	2.47	0.45
10:Y:39:SER:HB2	10:Y:58:VAL:HA	1.98	0.45
10:Y:75:THR:HB	10:Y:95:GLY:HA2	1.98	0.45
16:h:73:PHE:HD2	16:h:74:TYR:CE1	2.33	0.45
19:k:26:ARG:O	19:k:27:GLN:C	2.57	0.45
24:p:24:THR:HG22	24:p:26:LEU:N	2.31	0.45
4:L:47:SER:O	4:L:50:PRO:HD2	2.16	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:366:MET:SD	4:L:443:ILE:HG21	2.57	0.45
4:L:445:GLU:OE2	18:j:54:GLN:CG	2.62	0.45
5:M:65:LEU:O	5:M:66:ILE:C	2.59	0.45
6:N:26:LEU:HG	6:N:85:MET:SD	2.56	0.45
6:N:144:GLN:OE1	13:e:3:PHE:N	2.50	0.45
7:O:351:TRP:HB2	7:O:355:LYS:HE3	1.98	0.45
8:U:125:GLU:OE2	18:j:44:TYR:HE1	2.00	0.45
12:d:11:LEU:HD12	12:d:11:LEU:HA	1.69	0.45
13:e:18:PHE:O	13:e:18:PHE:CD2	2.69	0.45
18:j:97:LEU:HB3	23:o:104:ARG:CA	2.45	0.45
24:p:107:GLN:O	24:p:111:LYS:HG3	2.16	0.45
4:L:195:SER:O	4:L:201:ILE:HD11	2.16	0.45
4:L:390:TYR:CE2	18:j:68:TRP:HH2	2.34	0.45
4:L:591:PHE:N	4:L:591:PHE:CD1	2.83	0.45
4:L:591:PHE:N	4:L:591:PHE:HD1	2.15	0.45
5:M:42:LEU:HD21	5:M:67:ILE:HD12	1.97	0.45
5:M:272:THR:O	5:M:275:ILE:HG13	2.17	0.45
7:O:112:CYS:HB3	7:O:131:LEU:HA	1.97	0.45
7:O:114:LEU:HA	7:O:131:LEU:HD21	1.98	0.45
7:O:341:PRO:HB2	11:c:34:PRO:HB3	1.99	0.45
10:Y:83:ARG:O	10:Y:85:LYS:HG2	2.17	0.45
10:Y:83:ARG:NH1	10:Y:90:LEU:HD23	2.31	0.45
15:g:67:LYS:O	15:g:68:ASN:C	2.60	0.45
15:g:121:GLU:OE2	24:p:10:TYR:CZ	2.70	0.45
20:l:57:MET:HE2	20:l:57:MET:HB3	1.75	0.45
22:n:101:GLU:HG2	22:n:122:ARG:HH12	1.81	0.45
23:o:8:ARG:HB2	23:o:16:GLU:HG2	1.99	0.45
23:o:111:ARG:HA	23:o:114:ARG:HH11	1.82	0.45
24:p:110:LEU:O	24:p:111:LYS:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:LYS:NZ	3:K:21:MET:O	2.43	0.45
2:J:62:GLY:O	2:J:63:MET:C	2.58	0.45
2:J:150:TRP:HA	2:J:153:VAL:HG12	1.98	0.45
4:L:241:THR:N	4:L:242:PRO:HD2	2.31	0.45
4:L:407:TRP:HE1	20:l:140:MET:CE	2.29	0.45
4:L:483:PRO:CG	4:L:486:LEU:HD12	2.47	0.45
5:M:283:LYS:HG3	5:M:327:PHE:HE1	1.78	0.45
25:M:501:3PE:H221	10:Y:135:TRP:CZ2	2.52	0.45
6:N:25:ASN:HB3	13:e:15:ASP:CG	2.41	0.45
6:N:307:THR:O	7:O:319:ILE:N	2.49	0.45
7:O:168:VAL:HG21	7:O:241:TYR:CE2	2.51	0.45
9:X:165:THR:N	9:X:172:VAL:HG11	2.32	0.45
10:Y:19:GLN:HA	10:Y:21:HIS:CE1	2.52	0.45
17:i:108:ASP:OD2	24:p:18:PRO:CB	2.65	0.45
20:l:38:PRO:CG	21:m:71:ALA:HB2	2.43	0.45
4:L:81:LYS:CA	4:L:135:ASN:HD21	2.29	0.45
4:L:246:LEU:C	4:L:246:LEU:CD1	2.90	0.45
4:L:527:GLY:O	4:L:528:PHE:HB2	2.17	0.45
5:M:42:LEU:CG	5:M:67:ILE:HD11	2.43	0.45
5:M:129:THR:CG2	5:M:235:LEU:CD1	2.95	0.45
5:M:158:ILE:CG1	6:N:287:LEU:HD11	2.46	0.45
6:N:153:ILE:O	6:N:154:ILE:C	2.58	0.45
6:N:214:PRO:HB2	6:N:247:MET:SD	2.56	0.45
6:N:293:TYR:O	6:N:297:ILE:HG12	2.17	0.45
8:U:130:ILE:HG22	8:U:135:ALA:HB2	1.99	0.45
8:U:133:ILE:O	8:U:137:LYS:HE2	2.17	0.45
26:Y:201:CDL:H552	26:Y:201:CDL:H592	1.97	0.45
12:d:13:PHE:CE2	12:d:14:LEU:HD23	2.52	0.45
20:l:38:PRO:HD2	21:m:70:TYR:HD2	1.81	0.45
23:o:42:THR:O	23:o:45:GLU:N	2.49	0.45
24:p:6:ASP:HB3	24:p:9:VAL:CG2	2.39	0.45
2:J:102:LEU:O	2:J:105:VAL:HB	2.16	0.45
4:L:387:THR:HA	4:L:465:GLY:HA3	1.99	0.45
4:L:522:PHE:O	4:L:527:GLY:HA2	2.17	0.45
4:L:605:ASN:HA	10:Y:5:LYS:NZ	2.32	0.45
5:M:3:LYS:HA	5:M:7:PRO:HD2	1.99	0.45
5:M:209:LEU:HD11	5:M:261:PHE:HD1	1.81	0.45
25:M:501:3PE:H221	10:Y:135:TRP:CH2	2.52	0.45
6:N:109:ALA:HB3	6:N:110:PRO:CD	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:129:TYR:CD2	7:O:183:CYS:HB3	2.52	0.45
12:d:78:ARG:O	12:d:79:GLN:C	2.59	0.45
13:e:87:MET:HE3	13:e:92:TYR:O	2.16	0.45
14:f:38:ARG:HA	14:f:56:TRP:HE1	1.82	0.45
2:J:153:VAL:HG23	25:J:201:3PE:H3D2	1.99	0.45
4:L:485:PHE:CE1	4:L:486:LEU:HG	2.52	0.45
5:M:55:MET:HE1	26:d:201:CDL:C51	2.47	0.45
5:M:87:ASP:HB3	5:M:91:LEU:HB2	1.99	0.45
12:d:93:TYR:CG	16:h:160:MET:HE2	2.52	0.45
16:h:57:VAL:HG13	22:n:104:LEU:CG	2.46	0.45
16:h:73:PHE:CE2	16:h:74:TYR:HE1	2.35	0.45
23:o:22:ILE:O	23:o:105:GLU:OE2	2.35	0.45
25:D:501:3PE:H272	6:N:288:LEU:HD13	1.98	0.44
4:L:71:MET:CE	5:M:376:MET:HE1	2.47	0.44
4:L:100:ILE:O	4:L:104:SER:N	2.42	0.44
4:L:264:HIS:O	4:L:267:THR:N	2.49	0.44
4:L:532:ILE:HG21	20:l:133:LEU:CD2	2.47	0.44
5:M:42:LEU:CG	5:M:67:ILE:CD1	2.95	0.44
5:M:187:ASP:H	5:M:192:ASN:ND2	2.15	0.44
5:M:249:ILE:O	5:M:250:LEU:CG	2.47	0.44
6:N:154:ILE:CD1	6:N:195:PRO:HG2	2.47	0.44
7:O:241:TYR:HD1	7:O:245:PHE:CD2	2.35	0.44
7:O:351:TRP:O	7:O:355:LYS:HG2	2.16	0.44
8:U:116:VAL:HG12	8:U:120:MET:HE2	1.98	0.44
10:Y:110:TYR:HB3	25:m:201:3PE:H31	1.97	0.44
15:g:64:VAL:HG11	15:g:71:PHE:CE1	2.52	0.44
16:h:56:VAL:O	16:h:58:LYS:HG3	2.16	0.44
26:h:201:CDL:HA21	25:i:201:3PE:H112	1.99	0.44
22:n:35:ASP:OD1	22:n:35:ASP:N	2.51	0.44
22:n:170:ILE:O	22:n:173:ARG:NH1	2.50	0.44
3:K:93:LEU:CD2	6:N:54:GLU:HG2	2.47	0.44
4:L:117:PHE:CE1	4:L:243:VAL:CG2	3.00	0.44
4:L:437:PHE:CZ	4:L:441:ILE:HG12	2.43	0.44
4:L:604:ILE:O	10:Y:5:LYS:CD	2.63	0.44
5:M:131:ILE:CD1	6:N:302:LEU:HD21	2.48	0.44
5:M:415:GLN:O	5:M:416:ARG:CG	2.64	0.44
6:N:220:MET:O	6:N:221:LEU:C	2.60	0.44
6:N:250:SER:O	6:N:259:GLY:HA3	2.17	0.44
6:N:258:THR:CB	6:N:333:SER:O	2.64	0.44
6:N:324:LEU:HD11	12:d:64:PHE:HZ	1.82	0.44
7:O:69:GLY:HA2	7:O:72:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:114:ASP:OD1	22:n:45:ARG:NH2	2.50	0.44
9:X:154:ILE:HG12	16:h:167:PRO:HG2	1.98	0.44
16:h:54:LEU:HD23	17:i:27:GLU:HA	2.00	0.44
23:o:110:GLN:O	23:o:111:ARG:C	2.59	0.44
4:L:231:PRO:C	4:L:234:PRO:HD2	2.41	0.44
4:L:389:PHE:HZ	18:j:79:ALA:CB	2.28	0.44
4:L:477:ILE:HG13	23:o:91:GLU:CD	2.42	0.44
5:M:73:LEU:HB3	5:M:103:GLN:OE1	2.16	0.44
5:M:200:MET:HE2	5:M:250:LEU:HD21	2.00	0.44
7:O:201:PRO:HG2	7:O:249:MET:HE2	1.98	0.44
7:O:202:HIS:O	7:O:253:CYS:HB2	2.17	0.44
7:O:223:ASP:O	7:O:224:PRO:C	2.60	0.44
7:O:262:GLU:HB3	7:O:268:LYS:NZ	2.33	0.44
10:Y:115:MET:O	10:Y:119:TYR:HD2	2.01	0.44
11:c:61:THR:HG21	12:d:74:PHE:CE1	2.52	0.44
16:h:55:PHE:C	16:h:55:PHE:CD1	2.94	0.44
3:K:61:ILE:O	3:K:62:THR:C	2.58	0.44
4:L:2:ASN:O	4:L:3:ILE:C	2.59	0.44
4:L:155:ILE:HG12	4:L:248:HIS:CE1	2.53	0.44
4:L:366:MET:SD	4:L:443:ILE:CG2	3.06	0.44
5:M:22:LYS:HG2	5:M:26:ASN:ND2	2.33	0.44
5:M:24:TRP:CE3	5:M:81:GLN:HG2	2.52	0.44
5:M:321:LEU:HD23	5:M:321:LEU:HA	1.81	0.44
5:M:424:ILE:O	5:M:424:ILE:CG2	2.65	0.44
10:Y:120:MET:HE2	10:Y:120:MET:HB3	1.90	0.44
23:o:4:HIS:CD2	23:o:7:ARG:HH12	2.35	0.44
4:L:249:SER:HB2	4:L:340:PHE:CD2	2.53	0.44
4:L:537:THR:N	4:L:538:PRO:HD2	2.32	0.44
5:M:123:GLU:CD	6:N:255:PRO:HG2	2.43	0.44
6:N:23:SER:HB2	13:e:15:ASP:OD2	2.17	0.44
6:N:87:GLN:O	6:N:88:GLN:C	2.59	0.44
6:N:208:TYR:O	6:N:212:THR:HG22	2.18	0.44
7:O:336:GLY:HA2	7:O:344:ASN:HB3	1.99	0.44
8:U:136:GLU:O	17:i:2:SER:OG	2.36	0.44
13:e:42:GLU:OE2	16:h:181:HIS:NE2	2.46	0.44
17:i:11:ARG:NH1	22:n:154:LEU:HD12	2.32	0.44
23:o:49:ALA:O	23:o:50:GLN:C	2.60	0.44
2:J:3:ASN:O	2:J:4:TYR:C	2.60	0.44
2:J:33:ILE:CD1	2:J:60:LEU:HA	2.48	0.44
2:J:59:TYR:C	2:J:61:GLY:N	2.71	0.44
2:J:61:GLY:O	2:J:65:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:129:ASP:O	2:J:130:ASP:C	2.61	0.44
4:L:54:PHE:CB	4:L:87:ILE:HD11	2.48	0.44
4:L:556:ILE:CG2	21:m:80:PHE:CE1	2.96	0.44
5:M:186:LEU:HD13	5:M:250:LEU:HA	2.00	0.44
6:N:31:VAL:C	6:N:35:PHE:CD2	2.91	0.44
6:N:122:ILE:HD11	6:N:127:GLY:HA2	1.98	0.44
7:O:272:ASP:O	7:O:275:TYR:HB2	2.18	0.44
9:X:153:VAL:O	9:X:155:GLU:HG3	2.18	0.44
10:Y:7:PHE:CZ	10:Y:26:ILE:HG12	2.52	0.44
11:c:61:THR:HG22	11:c:65:ASP:OD2	2.18	0.44
11:c:73:ASN:OD1	11:c:75:LEU:N	2.50	0.44
12:d:27:ASN:O	12:d:28:ASP:C	2.61	0.44
14:f:14:ILE:O	14:f:15:LEU:C	2.61	0.44
18:j:102:ASP:O	18:j:103:ASP:HB2	2.17	0.44
2:J:5:ILE:HG13	2:J:124:LEU:CD1	2.48	0.44
3:K:29:THR:C	3:K:31:LEU:N	2.76	0.44
4:L:68:TRP:HE3	4:L:76:LEU:HD21	1.82	0.44
4:L:524:THR:HG23	4:L:525:LEU:HG	1.98	0.44
4:L:550:LEU:CD1	5:M:275:ILE:HB	2.31	0.44
5:M:18:SER:OG	5:M:26:ASN:ND2	2.51	0.44
5:M:42:LEU:CD1	5:M:67:ILE:CD1	2.96	0.44
5:M:126:LEU:HD11	5:M:153:THR:HG21	2.00	0.44
6:N:120:GLN:HE22	6:N:174:GLN:HB3	1.83	0.44
6:N:146:TYR:CD1	6:N:198:PRO:HG2	2.53	0.44
7:O:200:PRO:HG3	7:O:282:PRO:CD	2.47	0.44
9:X:172:VAL:HG23	12:d:30:ARG:NH1	2.33	0.44
11:c:40:ASN:O	11:c:41:TRP:C	2.60	0.44
13:e:19:MET:HE2	13:e:19:MET:HB3	1.85	0.44
14:f:7:LEU:HD13	14:f:11:TRP:HA	1.99	0.44
17:i:88:TYR:CE2	24:p:49:ARG:HB2	2.52	0.44
21:m:45:ARG:NE	22:n:140:LEU:HD11	2.33	0.44
1:D:55:SER:OG	1:D:56:LYS:N	2.50	0.44
4:L:66:TRP:CZ3	4:L:68:TRP:HD1	2.34	0.44
4:L:529:PHE:HB3	4:L:530:PRO:HD3	1.99	0.44
4:L:529:PHE:O	4:L:533:ILE:HG22	2.16	0.44
6:N:227:ILE:HG13	6:N:228:ASN:N	2.32	0.44
7:O:132:GLN:HE22	28:O:401:ADP:N6	2.14	0.44
8:U:88:LYS:HG3	8:U:98:LEU:HD23	1.98	0.44
13:e:74:ARG:O	13:e:75:ARG:C	2.59	0.44
18:j:43:ARG:HG3	18:j:48:PRO:HA	2.00	0.44
18:j:96:GLU:O	23:o:31:PHE:HZ	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:152:PHE:HD2	4:L:153:LEU:HD12	1.83	0.44
5:M:344:MET:HE3	5:M:423:MET:CE	2.48	0.44
6:N:146:TYR:O	6:N:147:PRO:C	2.53	0.44
11:c:55:TRP:HZ2	12:d:66:THR:HG22	1.76	0.44
12:d:57:GLY:O	12:d:60:ARG:N	2.51	0.44
16:h:55:PHE:CD2	22:n:115:TYR:CD1	3.06	0.44
18:j:38:VAL:HG12	18:j:39:HIS:H	1.80	0.44
21:m:37:LEU:HA	21:m:40:ARG:CG	2.46	0.44
24:p:140:GLN:HG2	24:p:144:LEU:CD1	2.47	0.44
1:D:72:LEU:HD12	6:N:50:PRO:CG	2.42	0.43
3:K:57:MET:O	3:K:60:PRO:HD2	2.18	0.43
4:L:73:SER:HB3	24:p:100:GLN:HE21	1.82	0.43
4:L:305:SER:OG	4:L:336:LYS:HE2	2.18	0.43
4:L:588:PHE:O	4:L:589:MET:C	2.60	0.43
4:L:589:MET:O	4:L:592:LEU:HB3	2.18	0.43
5:M:123:GLU:CG	6:N:255:PRO:HG2	2.48	0.43
6:N:12:THR:CG2	6:N:39:ALA:HB2	2.48	0.43
6:N:175:MET:HE2	6:N:175:MET:HB2	1.85	0.43
6:N:309:ASN:HA	7:O:319:ILE:HG22	1.99	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:72:THR:O	13:e:73:MET:C	2.58	0.43
20:l:38:PRO:HD2	21:m:70:TYR:CD2	2.53	0.43
20:l:119:THR:CG2	21:m:13:THR:HG23	2.48	0.43
22:n:131:GLU:O	22:n:131:GLU:HG2	2.17	0.43
24:p:165:GLU:C	24:p:167:ARG:H	2.26	0.43
4:L:446:ASN:HD21	18:j:40:ILE:HD11	1.82	0.43
5:M:8:SER:O	5:M:11:LEU:HB2	2.18	0.43
5:M:423:MET:C	5:M:424:ILE:O	2.56	0.43
25:M:502:3PE:H2A1	25:M:502:3PE:H3A2	2.00	0.43
7:O:211:VAL:HB	7:O:212:PRO:HD3	2.00	0.43
7:O:316:GLU:HG3	15:g:51:MET:CE	2.48	0.43
12:d:72:GLY:O	12:d:73:TYR:C	2.60	0.43
13:e:102:GLU:HG2	13:e:103:GLU:N	2.33	0.43
20:l:142:PHE:O	20:l:145:TRP:N	2.51	0.43
1:D:67:ASN:HB3	1:D:69:VAL:CG1	2.44	0.43
2:J:162:GLY:O	2:J:166:ILE:HD12	2.19	0.43
4:L:226:GLN:O	4:L:230:HIS:HB3	2.17	0.43
4:L:291:CYS:O	4:L:295:GLN:HG2	2.18	0.43
4:L:309:GLN:HB2	4:L:336:LYS:HZ1	1.83	0.43
4:L:598:ILE:CD1	6:N:153:ILE:HG12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:L:703:CDL:H321	16:h:71:MET:HE1	1.99	0.43
6:N:324:LEU:HD13	12:d:45:ASP:OD2	2.19	0.43
5:M:348:LEU:O	5:M:349:GLN:C	2.60	0.43
6:N:202:LEU:HD11	13:e:3:PHE:CE1	2.53	0.43
6:N:240:MET:O	6:N:240:MET:HG2	2.18	0.43
6:N:323:ASN:N	6:N:323:ASN:OD1	2.49	0.43
7:O:210:PRO:O	7:O:213:GLU:N	2.51	0.43
12:d:78:ARG:HG2	12:d:82:LEU:HD23	2.00	0.43
13:e:38:LYS:HG2	16:h:179:ILE:CG2	2.48	0.43
15:g:58:GLU:CD	15:g:59:PRO:HD2	2.44	0.43
18:j:38:VAL:CG1	18:j:39:HIS:H	2.31	0.43
20:l:41:TYR:HD2	20:l:43:ARG:HD3	1.82	0.43
20:l:97:LEU:O	20:l:98:ARG:C	2.60	0.43
21:m:17:THR:O	21:m:18:LEU:CB	2.66	0.43
21:m:28:GLU:HA	21:m:31:ARG:NH2	2.33	0.43
21:m:34:VAL:O	21:m:34:VAL:HG12	2.17	0.43
23:o:39:MET:HE1	23:o:57:ASP:O	2.18	0.43
24:p:75:THR:HG22	24:p:156:LEU:HD13	2.00	0.43
4:L:203:PHE:CZ	24:p:110:LEU:HD11	2.54	0.43
4:L:553:LEU:CD1	21:m:93:ALA:CB	2.83	0.43
4:L:564:LYS:HG2	21:m:77:TYR:OH	2.19	0.43
5:M:304:GLN:HA	5:M:309:PHE:HE1	1.83	0.43
6:N:186:HIS:O	6:N:190:MET:HG3	2.18	0.43
10:Y:26:ILE:O	10:Y:30:LEU:HG	2.17	0.43
13:e:22:SER:HA	13:e:34:HIS:HD2	1.84	0.43
13:e:38:LYS:HB3	13:e:38:LYS:HE2	1.74	0.43
21:m:45:ARG:O	21:m:45:ARG:CG	2.61	0.43
24:p:103:MET:HE1	24:p:135:VAL:HG12	1.98	0.43
2:J:54:MET:HE2	2:J:54:MET:N	2.34	0.43
2:J:97:ILE:HB	2:J:101:PHE:CZ	2.54	0.43
2:J:101:PHE:O	2:J:105:VAL:HG23	2.18	0.43
4:L:22:SER:HA	4:L:27:ILE:HG21	2.00	0.43
4:L:92:VAL:HG21	4:L:330:CYS:HB3	2.00	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:HG13	4:L:428:TYR:N	2.33	0.43
4:L:563:PRO:HG3	5:M:152:TYR:OH	2.18	0.43
5:M:95:TYR:OH	5:M:226:ALA:HB3	2.19	0.43
5:M:119:TYR:HD1	5:M:160:LEU:HD22	1.80	0.43
5:M:159:PRO:HG2	25:M:501:3PE:H391	1.99	0.43
6:N:223:ASN:HB3	7:O:306:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:254:LEU:HA	6:N:255:PRO:HD3	1.61	0.43
6:N:279:ALA:HA	6:N:282:MET:HE2	2.00	0.43
7:O:72:LYS:O	7:O:76:GLU:HG2	2.18	0.43
16:h:127:ASP:OD1	16:h:127:ASP:C	2.60	0.43
22:n:37:TYR:O	22:n:38:ARG:C	2.61	0.43
2:J:39:GLY:HA2	2:J:42:MET:CE	2.49	0.43
4:L:53:MET:HE2	4:L:53:MET:HB3	1.78	0.43
4:L:70:THR:O	4:L:75:GLU:HA	2.18	0.43
4:L:81:LYS:HD3	4:L:262:ARG:NH1	2.34	0.43
4:L:172:ILE:HD13	4:L:172:ILE:HA	1.88	0.43
4:L:442:SER:OG	8:U:71:ALA:HB2	2.18	0.43
4:L:574:THR:O	4:L:578:THR:N	2.46	0.43
5:M:1:MET:HB3	5:M:1:MET:HE3	1.73	0.43
5:M:63:THR:N	5:M:64:PRO:CD	2.81	0.43
5:M:207:MET:SD	5:M:240:SER:CA	3.06	0.43
6:N:11:PHE:O	6:N:15:LEU:N	2.49	0.43
6:N:154:ILE:HD12	6:N:155:LEU:N	2.33	0.43
7:O:86:TYR:HE1	7:O:157:VAL:HG12	1.82	0.43
12:d:87:ASP:O	12:d:88:HIS:C	2.59	0.43
16:h:57:VAL:HG12	22:n:99:VAL:CG2	2.49	0.43
23:o:22:ILE:CA	23:o:105:GLU:OE2	2.65	0.43
2:J:67:PHE:CE1	3:K:75:LEU:HD21	2.53	0.43
2:J:169:ILE:CD1	3:K:77:LEU:CD2	2.86	0.43
4:L:38:THR:O	4:L:41:LYS:HB3	2.19	0.43
4:L:60:GLU:C	4:L:61:TYR:CD1	2.97	0.43
4:L:68:TRP:CD2	26:h:201:CDL:H242	2.54	0.43
4:L:217:LEU:CD1	4:L:273:ILE:HG23	2.49	0.43
4:L:446:ASN:O	4:L:447:ASP:C	2.58	0.43
4:L:496:LEU:CD1	4:L:497:GLY:N	2.73	0.43
26:L:703:CDL:H142	26:L:703:CDL:OA9	2.18	0.43
25:L:705:3PE:H2A1	25:L:705:3PE:H232	2.01	0.43
25:L:705:3PE:H3B2	5:M:71:TRP:CD2	2.54	0.43
5:M:73:LEU:HD23	5:M:103:GLN:HE22	1.84	0.43
5:M:127:ILE:HD11	6:N:256:PRO:CD	2.49	0.43
5:M:154:LEU:HA	5:M:154:LEU:HD23	1.84	0.43
5:M:231:LEU:CD1	5:M:235:LEU:CD1	2.85	0.43
6:N:12:THR:HG22	6:N:39:ALA:HB2	2.00	0.43
6:N:219:LEU:CD2	6:N:230:ILE:HD12	2.49	0.43
7:O:76:GLU:CB	7:O:266:PRO:HB3	2.49	0.43
8:U:100:VAL:HA	8:U:141:PRO:HG2	2.00	0.43
10:Y:22:ARG:O	10:Y:26:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:45:ARG:O	22:n:46:ALA:C	2.61	0.43
24:p:118:GLY:O	24:p:119:GLU:HB2	2.19	0.43
1:D:52:MET:O	1:D:54:PRO:HD3	2.19	0.43
4:L:441:ILE:HG21	18:j:48:PRO:CD	2.42	0.43
4:L:493:ILE:O	4:L:496:LEU:HG	2.19	0.43
5:M:208:PRO:HG2	5:M:216:LEU:CD1	2.44	0.43
6:N:39:ALA:O	6:N:42:PRO:HD2	2.19	0.43
8:U:137:LYS:O	8:U:139:MET:N	2.50	0.43
21:m:49:LEU:HA	22:n:133:TRP:HH2	1.83	0.43
23:o:120:ALA:O	23:o:121:ARG:C	2.61	0.43
2:J:125:MET:HE3	2:J:128:VAL:CG2	2.49	0.43
7:O:121:PRO:HB3	7:O:178:TYR:HE1	1.83	0.43
7:O:303:GLU:O	7:O:304:VAL:C	2.59	0.43
8:U:91:ASP:OD2	19:k:48:ARG:NH2	2.51	0.43
11:c:72:ARG:HH11	12:d:19:ARG:HD3	1.83	0.43
14:f:25:TYR:CZ	14:f:29:LYS:HD3	2.54	0.43
16:h:129:PRO:HD2	16:h:130:GLU:OE1	2.18	0.43
2:J:134:MET:O	2:J:139:ILE:HD13	2.19	0.42
3:K:22:PHE:HB2	4:L:585:LYS:HG2	2.00	0.42
3:K:50:ASN:C	3:K:50:ASN:OD1	2.62	0.42
4:L:601:LEU:HD13	6:N:156:MET:SD	2.59	0.42
5:M:100:ILE:O	5:M:103:GLN:HG2	2.19	0.42
5:M:214:LEU:C	5:M:217:PRO:HD2	2.44	0.42
5:M:367:LEU:C	5:M:367:LEU:HD12	2.44	0.42
6:N:193:ILE:HD11	6:N:269:GLU:CB	2.49	0.42
6:N:193:ILE:HD12	6:N:266:ILE:HA	2.01	0.42
6:N:219:LEU:HD23	6:N:230:ILE:HD12	2.01	0.42
6:N:316:HIS:HA	7:O:331:PHE:HZ	1.83	0.42
8:U:142:GLN:O	8:U:143:GLU:C	2.60	0.42
26:Y:201:CDL:H151	26:Y:201:CDL:H381	2.00	0.42
14:f:38:ARG:HD3	14:f:56:TRP:CE2	2.54	0.42
16:h:59:PRO:O	16:h:61:LEU:HG	2.19	0.42
19:k:28:TRP:CE3	19:k:60:MET:HG2	2.54	0.42
22:n:81:ILE:HD12	22:n:87:GLY:C	2.44	0.42
23:o:46:MET:HE2	23:o:60:ALA:HB3	2.00	0.42
24:p:49:ARG:O	24:p:50:GLU:C	2.59	0.42
2:J:66:VAL:O	2:J:70:THR:N	2.42	0.42
4:L:5:THR:O	4:L:6:THR:C	2.62	0.42
4:L:141:PHE:CB	4:L:182:PHE:CE2	2.81	0.42
4:L:253:VAL:HG21	4:L:310:LEU:HD11	2.00	0.42
5:M:369:LEU:CD2	5:M:371:PRO:CD	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:73:LEU:HD22	7:O:207:ILE:HD11	2.02	0.42
7:O:114:LEU:O	7:O:117:PHE:HB3	2.19	0.42
7:O:117:PHE:HD1	7:O:128:SER:CA	2.31	0.42
7:O:146:ALA:CB	7:O:159:LEU:HD21	2.49	0.42
7:O:209:VAL:HG23	7:O:214:VAL:CG1	2.49	0.42
7:O:297:LEU:C	7:O:297:LEU:HD23	2.43	0.42
10:Y:68:ILE:HG22	10:Y:102:THR:OG1	2.19	0.42
11:c:40:ASN:HB3	11:c:43:ALA:HB3	2.00	0.42
13:e:49:GLY:O	13:e:50:THR:C	2.61	0.42
15:g:117:ARG:NH2	24:p:10:TYR:OH	2.52	0.42
15:g:148:PRO:O	24:p:167:ARG:NH2	2.52	0.42
16:h:89:VAL:HG11	16:h:117:ILE:HG12	2.01	0.42
18:j:98:GLY:HA3	23:o:104:ARG:NH1	2.33	0.42
23:o:57:ASP:OD2	23:o:59:CYS:HB2	2.19	0.42
24:p:43:TRP:NE1	24:p:47:LEU:HD11	2.33	0.42
3:K:3:SER:O	3:K:4:THR:C	2.61	0.42
4:L:13:ILE:HD11	25:i:201:3PE:C2B	2.49	0.42
4:L:60:GLU:N	4:L:60:GLU:OE2	2.53	0.42
4:L:246:LEU:CD1	4:L:247:LEU:N	2.68	0.42
4:L:264:HIS:HA	4:L:267:THR:HG23	2.02	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	2.35	0.42
4:L:526:LEU:HD12	4:L:526:LEU:N	2.34	0.42
4:L:591:PHE:O	4:L:595:ILE:HG13	2.19	0.42
5:M:68:LEU:HD23	5:M:234:ILE:CD1	2.49	0.42
6:N:80:GLN:O	6:N:81:LEU:HG	2.19	0.42
6:N:170:LEU:HD12	6:N:292:PHE:CD2	2.54	0.42
7:O:211:VAL:O	7:O:214:VAL:HG22	2.19	0.42
10:Y:8:PHE:CD1	10:Y:30:LEU:HD21	2.53	0.42
10:Y:87:ASP:HA	10:Y:128:LYS:NZ	2.34	0.42
13:e:44:ALA:HA	13:e:47:ILE:CG1	2.49	0.42
13:e:69:ARG:O	13:e:73:MET:HG3	2.19	0.42
17:i:22:TRP:O	17:i:26:GLN:HG2	2.19	0.42
3:K:32:CYS:O	3:K:33:LEU:C	2.60	0.42
4:L:220:ALA:HB2	4:L:260:LEU:CD1	2.49	0.42
4:L:357:ARG:NH2	22:n:78:GLN:O	2.53	0.42
4:L:489:THR:HG23	4:L:490:ALA:N	2.34	0.42
5:M:14:LEU:HD21	5:M:26:ASN:CB	2.50	0.42
5:M:72:LEU:HD12	5:M:234:ILE:HG12	2.01	0.42
5:M:200:MET:CE	5:M:247:SER:HB2	2.46	0.42
5:M:207:MET:HE3	5:M:240:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:210:TYR:O	5:M:213:HIS:HD2	2.01	0.42
6:N:80:GLN:O	6:N:80:GLN:HG2	2.19	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	2.19	0.42
6:N:342:GLN:H	6:N:342:GLN:CD	2.27	0.42
7:O:170:LEU:HD21	7:O:184:VAL:HG13	2.00	0.42
10:Y:143:VAL:HG21	16:h:169:TYR:CZ	2.54	0.42
16:h:87:THR:HG22	26:h:201:CDL:C51	2.49	0.42
17:i:81:PHE:O	17:i:82:VAL:C	2.60	0.42
25:i:201:3PE:H2B2	25:i:201:3PE:H281	1.88	0.42
20:l:57:MET:HG2	20:l:104:PRO:CG	2.49	0.42
24:p:6:ASP:C	24:p:8:ASP:H	2.27	0.42
24:p:73:ASP:O	24:p:74:ILE:C	2.59	0.42
1:D:36:GLN:HG3	1:D:38:GLN:HE21	1.83	0.42
3:K:36:MET:O	3:K:39:SER:N	2.52	0.42
4:L:224:SER:HB3	4:L:226:GLN:HE21	1.84	0.42
4:L:277:MET:CG	4:L:318:GLY:CA	2.97	0.42
4:L:519:TYR:O	4:L:520:SER:C	2.60	0.42
5:M:77:LEU:O	5:M:81:GLN:HG3	2.19	0.42
5:M:293:HIS:O	5:M:294:MET:HE2	2.20	0.42
5:M:446:LEU:CD1	15:g:97:LEU:HD12	2.50	0.42
6:N:241:LEU:HG	6:N:301:SER:OG	2.19	0.42
7:O:310:ILE:HG23	7:O:312:VAL:HG23	2.02	0.42
10:Y:83:ARG:NH1	10:Y:90:LEU:HB3	2.34	0.42
18:j:44:TYR:CE2	18:j:45:ARG:HG3	2.54	0.42
20:l:62:TYR:CE2	20:l:64:PRO:HG3	2.55	0.42
4:L:70:THR:HG21	24:p:101:GLU:OE2	2.20	0.42
4:L:309:GLN:CG	4:L:336:LYS:HZ1	2.32	0.42
4:L:335:PHE:O	4:L:339:LEU:HD13	2.19	0.42
4:L:365:ILE:CD1	4:L:366:MET:HG3	2.24	0.42
4:L:405:ASN:HB2	4:L:408:ALA:HB3	2.01	0.42
4:L:594:ASN:CG	6:N:110:PRO:CG	2.92	0.42
5:M:206:LYS:HA	5:M:215:TRP:CZ2	2.54	0.42
5:M:347:GLY:O	5:M:348:LEU:C	2.63	0.42
7:O:229:VAL:HG21	7:O:234:LEU:HD21	2.02	0.42
10:Y:45:LEU:O	10:Y:46:ASN:C	2.62	0.42
10:Y:76:THR:CG2	10:Y:92:TYR:HA	2.48	0.42
11:c:69:TYR:O	11:c:73:ASN:ND2	2.52	0.42
14:f:10:HIS:HB3	14:f:13:HIS:CD2	2.54	0.42
22:n:18:ARG:O	22:n:22:ARG:HD3	2.19	0.42
24:p:36:ALA:O	24:p:37:TYR:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:18:GLY:O	2:J:23:PRO:HD3	2.19	0.42
2:J:168:GLU:OE1	6:N:5:THR:HG21	2.20	0.42
3:K:59:ILE:HB	3:K:60:PRO:HD3	2.01	0.42
4:L:81:LYS:HD3	4:L:262:ARG:HH11	1.83	0.42
4:L:136:ASN:ND2	26:h:201:CDL:H273	2.29	0.42
4:L:396:ILE:HD13	4:L:396:ILE:HA	1.89	0.42
4:L:466:PHE:HZ	18:j:72:ARG:HH22	1.62	0.42
5:M:17:LEU:CD2	26:M:503:CDL:H522	2.46	0.42
5:M:118:PHE:HE2	5:M:203:PHE:CE1	2.37	0.42
5:M:216:LEU:HD23	5:M:287:ALA:HB1	2.02	0.42
5:M:344:MET:CE	21:m:59:HIS:NE2	2.83	0.42
5:M:430:HIS:HB3	15:g:73:GLY:HA3	2.02	0.42
6:N:154:ILE:HD11	6:N:155:LEU:HG	2.02	0.42
6:N:226:THR:HG22	6:N:228:ASN:N	2.34	0.42
6:N:331:ILE:HG23	6:N:335:MET:HE3	2.01	0.42
7:O:323:GLN:HE21	15:g:55:GLU:CA	2.33	0.42
8:U:91:ASP:OD2	19:k:48:ARG:NH1	2.53	0.42
16:h:178:PHE:O	16:h:179:ILE:C	2.63	0.42
20:l:167:TYR:CG	20:l:178:PRO:HG3	2.55	0.42
24:p:6:ASP:O	24:p:7:LYS:C	2.63	0.42
2:J:124:LEU:CD2	2:J:125:MET:H	2.26	0.42
4:L:21:ILE:HG23	4:L:27:ILE:CG2	2.50	0.42
4:L:49:LEU:HD12	24:p:33:LEU:HD23	2.02	0.42
4:L:51:LEU:HA	4:L:87:ILE:HD12	2.02	0.42
4:L:189:PHE:CZ	4:L:212:PRO:HB2	2.55	0.42
4:L:346:ILE:HG21	4:L:362:ILE:HD11	2.02	0.42
25:L:702:3PE:H3A1	25:L:702:3PE:H372	1.87	0.42
5:M:123:GLU:OE2	5:M:154:LEU:HD21	2.20	0.42
5:M:230:ILE:HG23	5:M:235:LEU:HD11	2.01	0.42
6:N:109:ALA:HB3	6:N:110:PRO:HD3	2.00	0.42
6:N:315:THR:O	6:N:316:HIS:C	2.61	0.42
6:N:340:ALA:N	6:N:341:PRO:CD	2.83	0.42
7:O:48:LYS:O	7:O:52:LYS:HE3	2.20	0.42
7:O:272:ASP:HA	7:O:275:TYR:HD2	1.85	0.42
11:c:70:LYS:HB3	11:c:75:LEU:HD12	2.01	0.42
14:f:22:PHE:CE2	14:f:26:LEU:HD11	2.55	0.42
14:f:25:TYR:HA	14:f:28:ARG:HH11	1.84	0.42
16:h:159:LEU:CB	16:h:163:ARG:HH12	2.25	0.42
20:l:109:LEU:HG	20:l:109:LEU:O	2.20	0.42
22:n:85:SER:O	22:n:86:PRO:C	2.61	0.42
22:n:110:SER:O	22:n:113:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:132:SER:O	22:n:133:TRP:C	2.62	0.42
1:D:37:TRP:O	1:D:37:TRP:CE3	2.73	0.42
4:L:141:PHE:CD2	5:M:375:LEU:HD21	2.48	0.42
4:L:385:PHE:HE2	18:j:73:PHE:CD1	2.32	0.42
4:L:477:ILE:HG22	23:o:54:GLN:NE2	2.34	0.42
4:L:571:THR:O	4:L:574:THR:HG22	2.19	0.42
5:M:191:SER:O	5:M:194:LEU:HB2	2.20	0.42
6:N:108:LEU:HD22	6:N:191:LEU:HD22	2.02	0.42
10:Y:41:TYR:CZ	26:Y:201:CDL:H772	2.55	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CE2	2.54	0.42
14:f:42:MET:HB2	24:p:87:GLU:OE1	2.19	0.42
18:j:51:THR:O	18:j:52:ARG:C	2.61	0.42
18:j:96:GLU:HG2	18:j:97:LEU:HD23	2.01	0.42
20:l:48:ARG:NE	20:l:64:PRO:HD2	2.35	0.42
20:l:59:VAL:O	20:l:59:VAL:HG12	2.19	0.42
22:n:100:PRO:HB2	22:n:102:TRP:NE1	2.35	0.42
23:o:5:LEU:H	23:o:5:LEU:HD12	1.84	0.42
2:J:3:ASN:O	2:J:7:VAL:HG23	2.19	0.42
2:J:28:GLY:C	3:K:31:LEU:HD21	2.44	0.42
2:J:51:LEU:HD12	2:J:51:LEU:N	2.31	0.42
4:L:117:PHE:HZ	4:L:242:PRO:HG2	1.85	0.42
25:L:702:3PE:H222	25:L:702:3PE:H2	1.94	0.42
5:M:127:ILE:CD1	6:N:256:PRO:HG2	2.44	0.42
8:U:89:LEU:HA	19:k:53:ARG:HH22	1.85	0.42
8:U:93:ILE:CD1	8:U:110:LEU:HD11	2.49	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CD2	2.55	0.42
14:f:38:ARG:NH1	14:f:54:VAL:HB	2.35	0.42
23:o:59:CYS:SG	23:o:91:GLU:HG2	2.60	0.42
3:K:90:VAL:O	3:K:91:GLN:C	2.62	0.41
3:K:93:LEU:HA	6:N:54:GLU:OE2	2.20	0.41
4:L:224:SER:CB	4:L:226:GLN:HE21	2.33	0.41
4:L:293:LEU:O	4:L:425:ARG:HD2	2.20	0.41
4:L:407:TRP:CE3	4:L:410:LEU:HD21	2.54	0.41
5:M:108:MET:HB3	5:M:121:LEU:HD13	2.02	0.41
5:M:177:MET:HE2	16:h:140:LEU:HD21	2.02	0.41
6:N:108:LEU:CD2	6:N:191:LEU:HD22	2.50	0.41
6:N:180:ALA:O	6:N:184:ILE:HG13	2.20	0.41
6:N:285:MET:HE1	6:N:288:LEU:HD22	2.02	0.41
7:O:261:TRP:H	7:O:261:TRP:HE3	1.68	0.41
8:U:131:PRO:O	8:U:135:ALA:N	2.52	0.41
15:g:106:TYR:CE2	16:h:86:ILE:CD1	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:55:PHE:HE1	16:h:57:VAL:HA	1.85	0.41
20:l:101:TRP:HE1	21:m:62:ASP:CA	2.32	0.41
21:m:8:PRO:HD3	21:m:14:LEU:HD13	2.02	0.41
21:m:15:PRO:HG2	21:m:18:LEU:HB2	2.01	0.41
23:o:42:THR:O	23:o:43:GLN:C	2.61	0.41
23:o:104:ARG:O	23:o:108:LEU:HG	2.20	0.41
2:J:19:LEU:HD21	3:K:32:CYS:HA	2.03	0.41
4:L:534:HIS:O	4:L:538:PRO:CG	2.60	0.41
4:L:546:LEU:HD23	20:l:108:ASP:OD1	2.19	0.41
6:N:215:MET:SD	6:N:244:ILE:CD1	3.08	0.41
6:N:218:ALA:CB	6:N:240:MET:SD	3.08	0.41
7:O:143:TYR:HD1	7:O:159:LEU:HD22	1.84	0.41
7:O:179:ILE:CD1	7:O:184:VAL:HG22	2.50	0.41
7:O:195:LEU:N	7:O:196:PRO:HD2	2.35	0.41
7:O:231:SER:O	7:O:232:ALA:C	2.62	0.41
7:O:267:THR:O	7:O:271:GLU:HG3	2.19	0.41
9:X:148:PRO:HG3	13:e:47:ILE:HD13	2.02	0.41
10:Y:10:SER:O	10:Y:11:TYR:C	2.62	0.41
12:d:24:PRO:HD2	12:d:73:TYR:CE2	2.55	0.41
12:d:119:VAL:O	12:d:120:ARG:C	2.62	0.41
18:j:100:PRO:HD3	23:o:108:LEU:CD2	2.50	0.41
22:n:114:MET:HG3	22:n:115:TYR:CD2	2.55	0.41
22:n:133:TRP:C	22:n:136:GLU:HG2	2.45	0.41
23:o:28:ASP:OD1	23:o:28:ASP:N	2.53	0.41
23:o:53:LEU:HD23	23:o:56:ARG:NE	2.34	0.41
2:J:36:GLY:C	2:J:60:LEU:HD11	2.45	0.41
2:J:136:GLU:H	2:J:139:ILE:HD12	1.85	0.41
4:L:25:ASN:HB2	16:h:72:LYS:HZ1	1.85	0.41
4:L:355:ASP:O	4:L:359:MET:HG3	2.21	0.41
4:L:489:THR:O	4:L:492:ILE:HG13	2.20	0.41
25:L:702:3PE:H362	25:L:702:3PE:H331	1.74	0.41
5:M:85:LYS:O	5:M:85:LYS:HG2	2.21	0.41
5:M:255:LYS:NZ	12:d:117:HIS:HB3	2.35	0.41
5:M:258:ALA:O	5:M:259:TYR:C	2.62	0.41
6:N:233:LEU:CD2	6:N:241:LEU:HD12	2.26	0.41
7:O:117:PHE:CE1	7:O:128:SER:CB	2.96	0.41
8:U:119:ILE:HD13	8:U:119:ILE:HA	1.81	0.41
8:U:128:PHE:HZ	8:U:148:ILE:CD1	2.33	0.41
11:c:74:GLY:O	11:c:75:LEU:HB2	2.20	0.41
13:e:22:SER:HB2	13:e:34:HIS:CD2	2.55	0.41
15:g:106:TYR:HE2	16:h:86:ILE:CD1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:14:GLN:HE22	22:n:157:ALA:HB3	1.85	0.41
17:i:20:ARG:HH11	17:i:20:ARG:HG3	1.84	0.41
18:j:40:ILE:HD11	18:j:51:THR:HG23	2.02	0.41
18:j:44:TYR:CD2	19:k:22:LEU:HD22	2.56	0.41
20:l:159:LYS:HE3	20:l:161:TYR:HE1	1.86	0.41
21:m:129:TYR:HE2	24:p:146:LEU:O	2.03	0.41
22:n:56:ASP:O	22:n:59:ARG:N	2.54	0.41
24:p:9:VAL:O	24:p:109:ARG:NH2	2.51	0.41
1:D:50:ALA:C	1:D:51:VAL:HG13	2.45	0.41
4:L:202:MET:HE3	4:L:265:PRO:CB	2.50	0.41
5:M:142:ARG:HG3	5:M:143:LEU:N	2.36	0.41
6:N:83:THR:HG22	6:N:84:TRP:N	2.35	0.41
7:O:64:GLY:O	7:O:161:ARG:NH1	2.53	0.41
7:O:117:PHE:CZ	7:O:173:MET:HE3	2.54	0.41
7:O:179:ILE:HD12	7:O:184:VAL:HG22	2.02	0.41
10:Y:14:VAL:HG21	10:Y:19:GLN:OE1	2.21	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
19:k:58:ARG:CD	22:n:34:ARG:HG3	2.48	0.41
20:l:88:PRO:HB2	22:n:86:PRO:CB	2.51	0.41
20:l:152:SER:HA	23:o:5:LEU:CD2	2.46	0.41
21:m:124:LYS:O	21:m:126:ASN:N	2.54	0.41
1:D:71:ILE:HG13	1:D:72:LEU:N	2.34	0.41
2:J:165:ILE:HG23	6:N:42:PRO:CG	2.37	0.41
4:L:231:PRO:O	4:L:234:PRO:HD2	2.20	0.41
4:L:286:LEU:HG	4:L:290:ILE:HD11	2.01	0.41
4:L:546:LEU:HD22	21:m:72:ARG:NH2	2.35	0.41
5:M:247:SER:OG	5:M:304:GLN:NE2	2.53	0.41
5:M:319:HIS:HA	5:M:322:THR:CG2	2.44	0.41
5:M:350:MET:HE3	5:M:350:MET:HB2	1.80	0.41
26:M:503:CDL:H632	26:M:503:CDL:H602	1.94	0.41
13:e:34:HIS:HB3	16:h:189:ASN:ND2	2.35	0.41
13:e:41:ILE:CG2	16:h:179:ILE:CD1	2.92	0.41
15:g:140:PHE:HB3	24:p:75:THR:CG2	2.50	0.41
15:g:145:ILE:CG2	24:p:160:LYS:HE2	2.39	0.41
16:h:175:GLU:HB2	16:h:178:PHE:CE2	2.55	0.41
20:l:48:ARG:NH2	20:l:64:PRO:HD2	2.36	0.41
20:l:122:THR:HG22	20:l:124:VAL:H	1.85	0.41
4:L:258:PHE:O	4:L:261:VAL:HG22	2.20	0.41
4:L:477:ILE:HG13	23:o:91:GLU:OE1	2.21	0.41
4:L:533:ILE:HG12	25:L:702:3PE:H3A2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:4:ILE:CD1	5:M:41:LEU:HD21	2.51	0.41
5:M:177:MET:HE3	5:M:177:MET:HB3	1.70	0.41
5:M:270:ILE:HD12	5:M:395:LEU:HD22	2.02	0.41
6:N:168:GLY:HA3	6:N:181:TYR:CE1	2.56	0.41
6:N:191:LEU:HG	6:N:191:LEU:O	2.20	0.41
6:N:338:PRO:HB3	26:d:201:CDL:H732	2.02	0.41
7:O:354:LEU:HD12	7:O:354:LEU:HA	1.95	0.41
13:e:32:ARG:NH1	13:e:67:LEU:HA	2.35	0.41
13:e:41:ILE:CG1	16:h:174:PRO:HB2	2.51	0.41
14:f:16:VAL:O	14:f:17:PRO:C	2.63	0.41
24:p:132:PHE:O	24:p:136:THR:OG1	2.17	0.41
4:L:13:ILE:HD11	25:i:201:3PE:H2B1	2.02	0.41
4:L:149:ILE:HG21	5:M:364:LEU:HD21	2.02	0.41
4:L:389:PHE:CE1	18:j:79:ALA:HB1	2.56	0.41
4:L:482:MET:CE	4:L:486:LEU:HB3	2.51	0.41
5:M:210:TYR:HB2	5:M:268:GLY:HA3	2.02	0.41
5:M:270:ILE:HD11	5:M:395:LEU:HA	2.03	0.41
5:M:301:ILE:HG22	5:M:301:ILE:O	2.19	0.41
5:M:329:LEU:HD23	5:M:437:MET:CE	2.49	0.41
6:N:159:ILE:HB	6:N:278:MET:HE1	2.01	0.41
7:O:52:LYS:HD3	7:O:152:SER:O	2.20	0.41
7:O:90:GLY:H	7:O:93:TYR:HB2	1.85	0.41
7:O:105:ASP:OD1	7:O:106:ILE:N	2.54	0.41
7:O:262:GLU:O	7:O:265:ASP:HB3	2.21	0.41
7:O:287:ASP:HB3	7:O:290:THR:HG23	2.02	0.41
24:p:71:VAL:HB	24:p:72:PRO:CD	2.50	0.41
24:p:73:ASP:OD1	24:p:73:ASP:N	2.54	0.41
24:p:91:GLN:O	24:p:91:GLN:HG2	2.21	0.41
3:K:30:LEU:HD22	3:K:78:LEU:HD13	2.03	0.41
4:L:253:VAL:HB	4:L:310:LEU:CD1	2.50	0.41
4:L:364:LYS:O	18:j:47:PHE:HZ	2.03	0.41
4:L:368:PHE:HB3	4:L:445:GLU:OE1	2.20	0.41
26:L:703:CDL:H512	26:L:703:CDL:H711	2.02	0.41
5:M:22:LYS:HE3	5:M:26:ASN:HD21	1.86	0.41
5:M:49:TYR:CD1	5:M:60:PRO:HD2	2.55	0.41
5:M:164:LEU:HB3	5:M:174:LEU:HD11	2.03	0.41
5:M:178:ILE:O	5:M:179:LEU:C	2.60	0.41
5:M:216:LEU:CG	5:M:220:HIS:CE1	2.88	0.41
5:M:250:LEU:HD12	5:M:250:LEU:C	2.39	0.41
26:M:503:CDL:H1	26:M:503:CDL:OA7	2.20	0.41
6:N:324:LEU:HD11	12:d:64:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:229:VAL:HG13	7:O:229:VAL:O	2.21	0.41
7:O:263:ALA:C	7:O:265:ASP:N	2.77	0.41
9:X:167:PHE:HD2	9:X:170:TRP:HE1	1.65	0.41
13:e:49:GLY:O	13:e:52:ALA:N	2.54	0.41
19:k:49:ASP:OD2	22:n:38:ARG:HG3	2.21	0.41
19:k:81:PHE:O	19:k:85:VAL:HG23	2.21	0.41
20:l:63:GLU:O	20:l:64:PRO:C	2.63	0.41
22:n:70:GLU:OE1	29:n:201:EHZ:O1	2.38	0.41
2:J:124:LEU:CD2	2:J:125:MET:HG2	2.50	0.41
2:J:135:LEU:O	2:J:136:GLU:HB3	2.21	0.41
4:L:58:ASN:HA	4:L:58:ASN:HD22	1.65	0.41
4:L:68:TRP:CE3	4:L:76:LEU:CD2	3.04	0.41
4:L:321:GLN:NE2	4:L:324:LEU:HD13	2.36	0.41
4:L:598:ILE:HD11	6:N:153:ILE:CD1	2.51	0.41
5:M:160:LEU:O	5:M:164:LEU:HD13	2.21	0.41
5:M:248:ILE:HG13	5:M:249:ILE:H	1.85	0.41
5:M:307:TRP:HB2	21:m:129:TYR:O	2.21	0.41
25:M:501:3PE:H241	10:Y:135:TRP:CZ3	2.55	0.41
6:N:109:ALA:O	6:N:112:HIS:ND1	2.52	0.41
6:N:125:HIS:CE1	6:N:129:ILE:HD11	2.56	0.41
6:N:307:THR:CG2	6:N:308:ASN:N	2.79	0.41
6:N:331:ILE:HD12	6:N:335:MET:HE3	2.03	0.41
7:O:256:LEU:HD21	7:O:276:LEU:HD23	2.03	0.41
8:U:128:PHE:CZ	8:U:148:ILE:CD1	3.04	0.41
10:Y:51:THR:HG23	10:Y:52:LEU:N	2.35	0.41
12:d:25:LYS:HE3	12:d:27:ASN:OD1	2.21	0.41
12:d:45:ASP:O	12:d:46:ASN:C	2.62	0.41
13:e:49:GLY:HA2	13:e:52:ALA:HB3	2.02	0.41
13:e:65:GLU:CD	13:e:71:LYS:HB2	2.46	0.41
15:g:121:GLU:OE2	24:p:10:TYR:CE2	2.74	0.41
17:i:29:SER:O	17:i:32:GLU:HB2	2.21	0.41
17:i:106:PRO:HD2	23:o:64:ILE:HG21	2.03	0.41
20:l:44:THR:HG23	20:l:46:GLU:HG2	2.03	0.41
21:m:50:GLN:O	21:m:50:GLN:HG2	2.21	0.41
21:m:82:PRO:HB2	25:m:201:3PE:H12	2.02	0.41
23:o:71:ARG:NH1	23:o:72:ASP:OD1	2.54	0.41
24:p:40:VAL:O	24:p:44:PRO:HG2	2.21	0.41
4:L:3:ILE:HG22	4:L:49:LEU:CD2	2.51	0.41
5:M:6:LEU:O	5:M:7:PRO:C	2.60	0.41
5:M:303:ILE:HG13	5:M:385:LEU:HD23	2.03	0.41
6:N:146:TYR:CG	6:N:147:PRO:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:175:MET:O	6:N:176:ARG:C	2.63	0.41
6:N:224:SER:HB2	6:N:229:SER:HB2	2.01	0.41
7:O:104:LEU:HD23	7:O:104:LEU:HA	1.90	0.41
7:O:263:ALA:C	7:O:265:ASP:H	2.29	0.41
7:O:332:ARG:O	7:O:338:LYS:HA	2.21	0.41
15:g:112:MET:HE3	15:g:115:TRP:CE3	2.56	0.41
26:h:201:CDL:HB61	17:i:84:TYR:CE2	2.56	0.41
17:i:26:GLN:HA	22:n:118:TYR:HE1	1.86	0.41
17:i:93:LYS:HB3	17:i:94:PRO:HD2	2.03	0.41
18:j:47:PHE:O	18:j:48:PRO:C	2.62	0.41
19:k:57:TRP:HA	19:k:60:MET:HB3	2.02	0.41
22:n:139:GLN:O	22:n:140:LEU:C	2.64	0.41
1:D:47:PHE:CG	6:N:227:ILE:HD11	2.57	0.40
25:D:501:3PE:H322	25:D:501:3PE:H351	1.72	0.40
2:J:159:LEU:CD2	3:K:69:CYS:SG	3.09	0.40
2:J:164:PHE:CE2	6:N:8:ILE:CG1	2.90	0.40
4:L:67:HIS:C	25:L:705:3PE:HN1	2.29	0.40
4:L:358:LYS:CG	22:n:80:TYR:CE1	2.86	0.40
4:L:424:MET:HE2	4:L:502:LEU:CA	2.51	0.40
4:L:427:ILE:CD1	19:k:69:PHE:HE1	2.34	0.40
25:L:702:3PE:H232	20:l:116:ARG:HA	2.03	0.40
5:M:173:THR:HB	16:h:143:GLU:OE2	2.20	0.40
25:M:502:3PE:H321	25:M:502:3PE:H352	1.92	0.40
6:N:22:SER:HB2	13:e:6:ILE:HG22	2.03	0.40
11:c:35:VAL:HG23	11:c:36:ASN:N	2.36	0.40
15:g:63:ASN:OD1	22:n:106:TYR:HE1	2.04	0.40
20:l:159:LYS:HE3	20:l:161:TYR:CE1	2.56	0.40
21:m:59:HIS:O	21:m:60:ILE:C	2.64	0.40
22:n:157:ALA:O	22:n:158:ARG:HB2	2.21	0.40
22:n:167:TRP:CD1	22:n:167:TRP:H	2.38	0.40
23:o:52:THR:O	23:o:53:LEU:C	2.62	0.40
2:J:10:SER:O	2:J:14:VAL:HG23	2.21	0.40
4:L:52:LEU:O	4:L:53:MET:C	2.63	0.40
4:L:210:LEU:O	4:L:211:ILE:C	2.62	0.40
26:L:703:CDL:H352	16:h:72:LYS:HA	2.03	0.40
5:M:158:ILE:HG21	6:N:283:ALA:HB1	2.03	0.40
5:M:428:PRO:HD3	22:n:106:TYR:CG	2.56	0.40
6:N:215:MET:HE3	6:N:215:MET:HB3	1.96	0.40
7:O:219:GLN:NE2	7:O:219:GLN:HA	2.35	0.40
7:O:221:LYS:HG3	7:O:221:LYS:O	2.21	0.40
8:U:93:ILE:CG1	8:U:110:LEU:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:5:LYS:C	10:Y:7:PHE:N	2.77	0.40
20:l:122:THR:CG2	20:l:129:MET:HE1	2.45	0.40
20:l:129:MET:HE3	20:l:129:MET:HB2	1.90	0.40
22:n:41:ALA:C	22:n:43:LEU:N	2.78	0.40
23:o:39:MET:CE	23:o:58:TYR:HA	2.48	0.40
1:D:61:TRP:CD1	1:D:61:TRP:N	2.89	0.40
2:J:136:GLU:O	2:J:137:GLY:C	2.58	0.40
4:L:324:LEU:HB3	4:L:395:ILE:CD1	2.51	0.40
4:L:399:ILE:HG22	4:L:409:LEU:CD1	2.51	0.40
4:L:400:ASN:HD22	4:L:409:LEU:HD11	1.85	0.40
4:L:466:PHE:HB3	18:j:68:TRP:CZ2	2.45	0.40
5:M:53:SER:O	5:M:54:ASN:C	2.63	0.40
5:M:197:LEU:O	5:M:201:MET:HB2	2.21	0.40
5:M:259:TYR:HB2	5:M:260:PRO:HD3	2.03	0.40
5:M:394:ILE:O	5:M:398:ILE:HG13	2.22	0.40
5:M:398:ILE:HD11	25:M:502:3PE:H2I3	2.02	0.40
6:N:106:LEU:HD21	6:N:138:PRO:HB2	2.03	0.40
7:O:170:LEU:CD2	7:O:184:VAL:HG13	2.51	0.40
7:O:268:LYS:HA	7:O:271:GLU:OE1	2.21	0.40
7:O:276:LEU:HD12	7:O:276:LEU:C	2.46	0.40
16:h:148:GLU:O	16:h:152:LYS:HG3	2.21	0.40
17:i:11:ARG:NE	22:n:154:LEU:HB2	2.37	0.40
2:J:22:LYS:NZ	3:K:21:MET:C	2.79	0.40
4:L:22:SER:HA	4:L:27:ILE:CG2	2.52	0.40
4:L:210:LEU:HD12	4:L:270:ASN:HD21	1.86	0.40
4:L:364:LYS:HE2	19:k:67:ILE:HD12	1.90	0.40
4:L:371:SER:O	4:L:374:VAL:HG12	2.21	0.40
5:M:3:LYS:HD3	14:f:20:PHE:HE1	1.86	0.40
5:M:17:LEU:HD13	14:f:11:TRP:HH2	1.86	0.40
5:M:435:THR:HG23	5:M:436:LEU:N	2.36	0.40
6:N:59:TYR:O	6:N:63:GLN:HG2	2.21	0.40
6:N:139:LEU:HD23	6:N:139:LEU:HA	1.86	0.40
7:O:153:THR:OG1	7:O:154:GLY:N	2.55	0.40
10:Y:64:THR:O	10:Y:68:ILE:HG23	2.20	0.40
13:e:81:LYS:HB3	13:e:81:LYS:HE2	1.77	0.40
16:h:87:THR:O	16:h:91:ILE:HG13	2.22	0.40
17:i:32:GLU:OE2	22:n:117:ASP:N	2.55	0.40
17:i:99:SER:O	17:i:100:SER:C	2.64	0.40
18:j:71:TRP:HZ3	18:j:72:ARG:NH2	2.19	0.40
21:m:28:GLU:HG2	21:m:31:ARG:NH2	2.37	0.40
21:m:124:LYS:HG2	21:m:125:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:43:TRP:HB3	24:p:44:PRO:HD3	2.03	0.40
4:L:67:HIS:HD2	4:L:76:LEU:O	2.05	0.40
4:L:277:MET:HG3	4:L:318:GLY:HA3	2.04	0.40
4:L:381:THR:HG22	4:L:420:ALA:HA	2.04	0.40
5:M:218:LYS:HE3	5:M:218:LYS:HB3	1.58	0.40
5:M:437:MET:O	5:M:438:ALA:C	2.62	0.40
6:N:122:ILE:CD1	6:N:127:GLY:HA2	2.52	0.40
6:N:132:THR:HB	6:N:209:ILE:HG12	2.03	0.40
6:N:211:LEU:CD2	6:N:333:SER:HB2	2.45	0.40
6:N:223:ASN:OD1	6:N:223:ASN:O	2.39	0.40
6:N:297:ILE:O	6:N:298:TYR:C	2.63	0.40
12:d:93:TYR:HD2	16:h:156:VAL:HG13	1.86	0.40
12:d:100:ASP:OD2	16:h:163:ARG:NH2	2.55	0.40
14:f:10:HIS:HB3	14:f:13:HIS:HD2	1.85	0.40
17:i:4:TYR:HB2	17:i:9:LYS:HE2	2.04	0.40
17:i:18:LEU:CD2	22:n:125:TRP:HH2	2.34	0.40
19:k:56:ALA:O	19:k:60:MET:N	2.53	0.40
21:m:37:LEU:CA	21:m:40:ARG:HG2	2.50	0.40
24:p:45:VAL:O	24:p:46:THR:C	2.64	0.40
24:p:128:GLU:OE2	24:p:128:GLU:N	2.51	0.40
24:p:167:ARG:O	24:p:171:ARG:NE	2.53	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%)	36 (90%)	4 (10%)	0	100	100
2	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
3	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
4	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
6	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	68
7	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
8	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
9	X	25/172 (14%)	23 (92%)	2 (8%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
13	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
14	f	49/57 (86%)	49 (100%)	0	0	100	100
15	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
16	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
17	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
18	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
19	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
20	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
21	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
22	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	56
23	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
24	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
All	All	3750/4813 (78%)	3569 (95%)	179 (5%)	2 (0%)	49	79

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	37/395 (9%)	37 (100%)	0	100	100
2	J	124/138 (90%)	123 (99%)	1 (1%)	73	82
3	K	86/88 (98%)	86 (100%)	0	100	100
4	L	549/550 (100%)	547 (100%)	2 (0%)	84	86
5	M	415/415 (100%)	414 (100%)	1 (0%)	87	89
6	N	307/308 (100%)	306 (100%)	1 (0%)	86	88
7	O	282/309 (91%)	282 (100%)	0	100	100
8	U	80/135 (59%)	80 (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	91/94 (97%)	91 (100%)	0	100	100
14	f	47/53 (89%)	47 (100%)	0	100	100
15	g	90/129 (70%)	90 (100%)	0	100	100
16	h	123/162 (76%)	123 (100%)	0	100	100
17	i	86/120 (72%)	86 (100%)	0	100	100
18	j	62/87 (71%)	62 (100%)	0	100	100
19	k	54/78 (69%)	54 (100%)	0	100	100
20	l	140/161 (87%)	140 (100%)	0	100	100
21	m	112/114 (98%)	111 (99%)	1 (1%)	70	81
22	n	162/164 (99%)	161 (99%)	1 (1%)	78	84
23	o	111/121 (92%)	111 (100%)	0	100	100
24	p	152/158 (96%)	152 (100%)	0	100	100
All	All	3385/4214 (80%)	3378 (100%)	7 (0%)	85	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	136	GLU
4	L	3	ILE
4	L	69	VAL
5	M	218	LYS

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Mol	Chain	Res	Type
6	N	159	ILE
21	m	49	LEU
22	n	98	LYS

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

Mol	Chain	Res	Type
1	D	60	HIS
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	226	GLN
4	L	264	HIS
4	L	269	ASN
4	L	296	ASN
4	L	321	GLN
4	L	354	GLN
4	L	400	ASN
4	L	446	ASN
4	L	452	ASN
4	L	579	ASN
5	M	26	ASN
5	M	51	ASN
5	M	81	GLN
5	M	92	GLN
5	M	170	HIS
5	M	175	ASN
5	M	213	HIS
5	M	279	GLN
5	M	293	HIS
5	M	304	GLN
5	M	374	ASN
5	M	415	GLN

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Mol	Chain	Res	Type
6	N	120	GLN
6	N	134	GLN
6	N	273	ASN
6	N	289	ASN
6	N	310	ASN
6	N	317	GLN
7	O	80	GLN
7	O	132	GLN
7	O	175	ASN
7	O	219	GLN
7	O	286	GLN
7	O	292	HIS
7	O	299	GLN
7	O	306	ASN
7	O	323	GLN
10	Y	21	HIS
10	Y	91	ASN
12	d	59	HIS
12	d	79	GLN
12	d	88	HIS
14	f	10	HIS
14	f	13	HIS
15	g	113	GLN
16	h	109	HIS
16	h	170	GLN
17	i	74	HIS
17	i	83	HIS
18	j	41	GLN
19	k	39	GLN
19	k	66	ASN
20	l	83	GLN
20	l	91	GLN
20	l	106	HIS
21	m	75	ASN
21	m	79	ASN
22	n	12	HIS
22	n	13	GLN
22	n	14	GLN
22	n	53	ASN
22	n	62	GLN
22	n	74	ASN
22	n	76	HIS

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Mol	Chain	Res	Type
22	n	139	GLN
23	o	4	HIS
23	o	61	HIS
24	p	67	GLN
24	p	91	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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.17	7 (9%)
28	ADP	O	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
25	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.15	3 (7%)
25	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.07	2 (4%)
25	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.06	3 (7%)
25	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	3PE	m	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.16	3 (6%)
26	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.22	7 (10%)
26	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.16	6 (8%)
25	3PE	J	201	-	45,45,50	0.98	2 (4%)	48,50,55	1.07	3 (6%)
26	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.15	6 (7%)
26	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.15	7 (8%)
29	EHZ	n	201	-	29,31,37	1.82	7 (24%)	37,41,47	1.65	5 (13%)
25	3PE	D	501	-	37,37,50	1.07	2 (5%)	40,42,55	1.09	3 (7%)
25	3PE	L	702	-	48,48,50	0.93	2 (4%)	51,53,55	1.11	3 (5%)
25	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.15	4 (7%)

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
26	CDL	Y	201	-	-	15/81/81/110	-
28	ADP	O	401	-	-	2/16/32/32	0/3/3/3
25	3PE	i	201	-	-	9/43/43/54	-
25	3PE	L	701	-	-	10/43/43/54	-
25	3PE	M	501	-	-	10/40/40/54	-
25	3PE	L	705	-	-	13/47/47/54	-
25	3PE	m	201	-	-	10/44/44/54	-
26	CDL	d	201	-	-	27/75/75/110	-
26	CDL	h	201	-	-	19/78/78/110	-
25	3PE	J	201	-	-	13/49/49/54	-
26	CDL	L	703	-	-	20/83/83/110	-
26	CDL	M	503	-	-	24/92/92/110	-
29	EHZ	n	201	-	-	22/39/39/45	-
25	3PE	D	501	-	-	8/41/41/54	-
25	3PE	L	702	-	-	13/52/52/54	-
25	3PE	M	502	-	-	14/52/52/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C12-N1	5.28	1.45	1.33
29	n	201	EHZ	C15-N2	4.93	1.45	1.33
28	O	401	ADP	C5-C4	4.50	1.47	1.39
26	Y	201	CDL	OA8-CA7	4.31	1.45	1.33
25	M	501	3PE	O31-C31	4.31	1.45	1.33
25	J	201	3PE	O31-C31	4.30	1.45	1.33
25	D	501	3PE	O31-C31	4.27	1.45	1.33
26	L	703	CDL	OB8-CB7	4.27	1.45	1.33
25	L	705	3PE	O31-C31	4.27	1.45	1.33
25	M	502	3PE	O31-C31	4.26	1.45	1.33
25	i	201	3PE	O31-C31	4.26	1.45	1.33
26	d	201	CDL	OB8-CB7	4.25	1.45	1.33
26	M	503	CDL	OA8-CA7	4.24	1.45	1.33
25	m	201	3PE	O31-C31	4.21	1.45	1.33
26	M	503	CDL	OB8-CB7	4.20	1.45	1.33
26	d	201	CDL	OA8-CA7	4.20	1.45	1.33
26	h	201	CDL	OB8-CB7	4.18	1.45	1.33
26	h	201	CDL	OA8-CA7	4.17	1.45	1.33
25	L	701	3PE	O21-C21	4.15	1.46	1.34
25	L	702	3PE	O31-C31	4.14	1.45	1.33
26	M	503	CDL	OB6-CB5	4.12	1.45	1.34
25	L	701	3PE	O31-C31	4.11	1.45	1.33
26	L	703	CDL	OA8-CA7	4.10	1.45	1.33
26	h	201	CDL	OB6-CB5	4.10	1.45	1.34
26	Y	201	CDL	OB8-CB7	4.09	1.45	1.33
26	d	201	CDL	OB6-CB5	4.08	1.45	1.34
26	h	201	CDL	OA6-CA5	4.08	1.45	1.34
25	M	501	3PE	O21-C21	4.07	1.45	1.34
25	i	201	3PE	O21-C21	4.06	1.45	1.34
26	M	503	CDL	OA6-CA5	4.06	1.45	1.34
26	L	703	CDL	OB6-CB5	4.05	1.45	1.34
26	Y	201	CDL	OB6-CB5	4.04	1.45	1.34
26	Y	201	CDL	OA6-CA5	4.04	1.45	1.34
25	J	201	3PE	O21-C21	4.02	1.45	1.34
25	m	201	3PE	O21-C21	4.01	1.45	1.34
25	D	501	3PE	O21-C21	4.00	1.45	1.34
25	L	705	3PE	O21-C21	4.00	1.45	1.34
25	M	502	3PE	O21-C21	3.99	1.45	1.34
25	L	702	3PE	O21-C21	3.98	1.45	1.34
26	d	201	CDL	OA6-CA5	3.94	1.45	1.34
26	L	703	CDL	OA6-CA5	3.89	1.45	1.34
29	n	201	EHZ	P1-O7	2.78	1.65	1.54
28	O	401	ADP	C5-C6	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	201	EHZ	C9-S1	2.59	1.82	1.76
29	n	201	EHZ	O4-C15	-2.48	1.18	1.23
29	n	201	EHZ	O3-C12	-2.32	1.18	1.23
28	O	401	ADP	C5-N7	-2.30	1.34	1.39
28	O	401	ADP	C8-N7	2.26	1.36	1.31
29	n	201	EHZ	P1-OP3	-2.24	1.46	1.54
28	O	401	ADP	C4-N9	-2.03	1.33	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	O	401	ADP	C5-C4-N3	-5.66	118.92	126.72
29	n	201	EHZ	C8-C9-S1	5.50	120.50	113.56
26	M	503	CDL	OA6-CA5-C11	4.62	121.47	111.48
28	O	401	ADP	N3-C4-N9	4.57	134.94	127.17
26	L	703	CDL	OB6-CB5-C51	4.22	120.61	111.48
26	h	201	CDL	OB6-CB5-C51	4.20	120.57	111.48
25	M	502	3PE	O21-C21-C22	4.13	120.42	111.48
26	d	201	CDL	OA6-CA5-C11	4.11	120.37	111.48
26	Y	201	CDL	OA6-CA5-C11	4.07	120.28	111.48
25	L	701	3PE	O21-C21-C22	4.02	120.17	111.48
25	J	201	3PE	O21-C21-C22	3.97	120.06	111.48
26	d	201	CDL	OB6-CB5-C51	3.96	120.05	111.48
26	M	503	CDL	OB6-CB5-C51	3.96	120.05	111.48
25	L	702	3PE	O21-C21-C22	3.92	119.96	111.48
26	Y	201	CDL	OB6-CB5-C51	3.90	119.91	111.48
25	m	201	3PE	O21-C21-C22	3.90	119.91	111.48
25	L	705	3PE	O21-C21-C22	3.86	119.83	111.48
25	i	201	3PE	O21-C21-C22	3.81	119.72	111.48
28	O	401	ADP	C2-N3-C4	3.69	120.86	111.83
26	h	201	CDL	OA6-CA5-C11	3.64	119.35	111.48
26	L	703	CDL	OA6-CA5-C11	3.62	119.32	111.48
25	D	501	3PE	O21-C21-C22	3.60	119.27	111.48
25	M	501	3PE	O21-C21-C22	3.59	119.25	111.48
28	O	401	ADP	N3-C2-N1	-3.30	123.59	128.58
28	O	401	ADP	C4-C5-N7	-3.29	106.82	110.58
25	M	502	3PE	O31-C31-C32	3.05	121.12	111.83
25	M	502	3PE	C2-O21-C21	-3.01	110.58	117.80
26	d	201	CDL	CA4-OA6-CA5	-2.96	110.72	117.80
25	L	702	3PE	C2-O21-C21	-2.94	110.75	117.80
25	L	705	3PE	O31-C31-C32	2.92	120.74	111.83
28	O	401	ADP	C4-N9-C8	2.90	108.78	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	i	201	3PE	C2-O21-C21	-2.89	110.88	117.80
26	M	503	CDL	OA8-CA7-C31	2.88	120.61	111.83
26	d	201	CDL	OA8-CA7-C31	2.87	120.60	111.83
25	m	201	3PE	O31-C31-C32	2.86	120.55	111.83
25	J	201	3PE	C2-O21-C21	-2.83	111.03	117.80
25	m	201	3PE	C2-O21-C21	-2.83	111.03	117.80
29	n	201	EHZ	O2-C9-C8	-2.81	119.31	123.74
26	Y	201	CDL	OA8-CA7-C31	2.77	120.27	111.83
25	L	702	3PE	O31-C31-C32	2.76	120.24	111.83
26	h	201	CDL	OB8-CB7-C71	2.71	120.11	111.83
29	n	201	EHZ	C10-S1-C9	2.71	109.85	101.84
29	n	201	EHZ	OP3-P1-O9	-2.70	100.33	110.83
25	J	201	3PE	O31-C31-C32	2.69	120.03	111.83
26	Y	201	CDL	CA4-OA6-CA5	-2.67	111.39	117.80
26	Y	201	CDL	OB8-CB7-C71	2.67	119.96	111.83
25	i	201	3PE	O31-C31-C32	2.65	119.91	111.83
26	L	703	CDL	CB4-OB6-CB5	-2.65	111.46	117.80
26	L	703	CDL	OA8-CA7-C31	2.63	119.86	111.83
26	h	201	CDL	OA8-CA7-C31	2.61	119.79	111.83
26	L	703	CDL	OB8-CB7-C71	2.58	119.72	111.83
26	d	201	CDL	OB8-CB7-C71	2.57	119.66	111.83
25	L	705	3PE	C2-O21-C21	-2.56	111.66	117.80
25	M	501	3PE	O31-C31-C32	2.51	119.47	111.83
25	D	501	3PE	O31-C31-C32	2.49	119.42	111.83
28	O	401	ADP	C5-N7-C8	2.49	107.36	103.45
26	L	703	CDL	CA4-OA6-CA5	-2.48	111.86	117.80
26	M	503	CDL	OB8-CB7-C71	2.39	119.12	111.83
29	n	201	EHZ	C5-C6-C7	-2.36	108.17	114.68
25	M	501	3PE	C2-O21-C21	-2.34	112.21	117.80
26	Y	201	CDL	CB4-OB6-CB5	-2.33	112.23	117.80
25	L	701	3PE	O31-C31-C32	2.28	118.78	111.83
26	d	201	CDL	CB4-OB6-CB5	-2.28	112.34	117.80
26	h	201	CDL	CA4-OA6-CA5	-2.25	112.41	117.80
26	M	503	CDL	CA4-OA6-CA5	-2.16	112.63	117.80
28	O	401	ADP	C6-C5-N7	2.15	136.24	132.09
28	O	401	ADP	N9-C8-N7	-2.14	110.90	113.94
26	M	503	CDL	OA6-CA5-OA7	-2.12	118.75	123.70
25	D	501	3PE	C2-O21-C21	-2.09	112.80	117.80
26	Y	201	CDL	OB8-CB7-OB9	-2.07	118.44	123.63
26	d	201	CDL	OA6-CA5-OA7	-2.06	118.89	123.70
28	O	401	ADP	C3'-C2'-C1'	2.06	105.36	101.46
25	M	502	3PE	O21-C21-O22	-2.06	118.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	201	CDL	OA8-CA7-OA9	-2.04	118.53	123.63
26	M	503	CDL	CB4-OB6-CB5	-2.01	112.99	117.80

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D	501	3PE	C1-O11-P-O14
25	J	201	3PE	C1-O11-P-O12
25	J	201	3PE	C1-O11-P-O13
25	J	201	3PE	C1-O11-P-O14
25	L	701	3PE	C1-O11-P-O12
25	L	701	3PE	C1-O11-P-O13
25	L	701	3PE	C22-C21-O21-C2
25	L	702	3PE	C1-O11-P-O12
25	L	702	3PE	C1-O11-P-O13
25	L	702	3PE	C1-O11-P-O14
25	L	702	3PE	C11-O13-P-O11
25	L	702	3PE	C11-O13-P-O12
25	L	702	3PE	C11-O13-P-O14
25	L	702	3PE	O22-C21-O21-C2
25	L	702	3PE	C22-C21-O21-C2
25	L	705	3PE	C1-O11-P-O12
25	L	705	3PE	C1-O11-P-O13
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	L	705	3PE	O22-C21-O21-C2
25	L	705	3PE	C22-C21-O21-C2
25	M	501	3PE	C1-O11-P-O12
25	M	501	3PE	C11-O13-P-O11
25	M	501	3PE	C11-O13-P-O12
25	M	502	3PE	C1-O11-P-O13
25	M	502	3PE	C1-O11-P-O14
25	M	502	3PE	C32-C31-O31-C3
25	M	502	3PE	C22-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	C2-C1-O11-P
25	i	201	3PE	C22-C21-O21-C2
25	m	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
25	m	201	3PE	C11-O13-P-O12
26	L	703	CDL	CA3-OA5-PA1-OA2
26	L	703	CDL	CA3-OA5-PA1-OA3
26	L	703	CDL	CA3-OA5-PA1-OA4
26	L	703	CDL	CB2-OB2-PB2-OB4
26	L	703	CDL	CB2-OB2-PB2-OB5
26	L	703	CDL	CB3-OB5-PB2-OB2
26	L	703	CDL	CB3-OB5-PB2-OB3
26	L	703	CDL	C51-CB5-OB6-CB4
26	M	503	CDL	CA2-OA2-PA1-OA3
26	M	503	CDL	CA2-OA2-PA1-OA4
26	M	503	CDL	CA2-OA2-PA1-OA5
26	M	503	CDL	CA3-OA5-PA1-OA2
26	M	503	CDL	C11-CA5-OA6-CA4
26	M	503	CDL	CB2-OB2-PB2-OB3
26	M	503	CDL	CB2-OB2-PB2-OB4
26	M	503	CDL	CB2-OB2-PB2-OB5
26	M	503	CDL	CB3-OB5-PB2-OB2
26	M	503	CDL	CB3-OB5-PB2-OB3
26	M	503	CDL	CB3-OB5-PB2-OB4
26	M	503	CDL	C51-CB5-OB6-CB4
26	Y	201	CDL	CA2-OA2-PA1-OA3
26	Y	201	CDL	CA2-OA2-PA1-OA4
26	Y	201	CDL	CA2-OA2-PA1-OA5
26	Y	201	CDL	CB3-OB5-PB2-OB2
26	Y	201	CDL	CB3-OB5-PB2-OB4
26	d	201	CDL	CA2-OA2-PA1-OA3
26	d	201	CDL	CA2-OA2-PA1-OA4
26	d	201	CDL	CA2-OA2-PA1-OA5
26	d	201	CDL	CA3-OA5-PA1-OA2
26	d	201	CDL	CB2-OB2-PB2-OB4
26	d	201	CDL	CB2-OB2-PB2-OB5
26	d	201	CDL	CB3-OB5-PB2-OB2
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-OA4
26	h	201	CDL	CB3-OB5-PB2-OB2
26	h	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	C51-CB5-OB6-CB4
29	n	201	EHZ	O1-C7-C8-C9
29	n	201	EHZ	C7-C8-C9-S1

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Mol	Chain	Res	Type	Atoms
29	n	201	EHZ	C10-C11-N1-C12
29	n	201	EHZ	C15-C16-C17-C18
29	n	201	EHZ	C15-C16-C17-C19
29	n	201	EHZ	C15-C16-C17-C20
29	n	201	EHZ	O5-C16-C17-C18
29	n	201	EHZ	O5-C16-C17-C19
29	n	201	EHZ	O5-C16-C17-C20
29	n	201	EHZ	O2-C9-S1-C10
29	n	201	EHZ	C8-C9-S1-C10
29	n	201	EHZ	C20-O6-P1-O7
29	n	201	EHZ	C20-O6-P1-O9
29	n	201	EHZ	C20-O6-P1-OP3
25	M	502	3PE	O32-C31-O31-C3
25	m	201	3PE	O32-C31-O31-C3
25	m	201	3PE	C32-C31-O31-C3
25	D	501	3PE	O22-C21-O21-C2
25	L	701	3PE	O22-C21-O21-C2
25	M	502	3PE	O22-C21-O21-C2
26	L	703	CDL	OB7-CB5-OB6-CB4
26	M	503	CDL	OA7-CA5-OA6-CA4
26	h	201	CDL	OB7-CB5-OB6-CB4
25	M	501	3PE	C2-C3-O31-C31
25	D	501	3PE	C22-C21-O21-C2
25	i	201	3PE	C32-C31-O31-C3
25	i	201	3PE	O22-C21-O21-C2
26	M	503	CDL	OB7-CB5-OB6-CB4
26	L	703	CDL	C11-CA5-OA6-CA4
25	i	201	3PE	O32-C31-O31-C3
26	Y	201	CDL	C31-CA7-OA8-CA6
26	Y	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	OB9-CB7-OB8-CB6
26	Y	201	CDL	OB9-CB7-OB8-CB6
25	m	201	3PE	C22-C21-O21-C2
26	Y	201	CDL	OA9-CA7-OA8-CA6
26	h	201	CDL	CA4-CA3-OA5-PA1
26	d	201	CDL	O1-C1-CB2-OB2
26	L	703	CDL	OA7-CA5-OA6-CA4
26	L	703	CDL	C71-CB7-OB8-CB6
26	d	201	CDL	C11-CA5-OA6-CA4
25	m	201	3PE	O22-C21-O21-C2
26	d	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
26	d	201	CDL	C54-C55-C56-C57
26	d	201	CDL	OA7-CA5-OA6-CA4
26	L	703	CDL	OB9-CB7-OB8-CB6
26	d	201	CDL	C71-CB7-OB8-CB6
25	J	201	3PE	C32-C31-O31-C3
25	M	501	3PE	C32-C31-O31-C3
26	L	703	CDL	C11-C12-C13-C14
25	M	501	3PE	C32-C33-C34-C35
26	M	503	CDL	C71-CB7-OB8-CB6
26	M	503	CDL	C62-C63-C64-C65
26	d	201	CDL	C31-CA7-OA8-CA6
25	M	501	3PE	C23-C24-C25-C26
25	J	201	3PE	O32-C31-O31-C3
26	d	201	CDL	OB9-CB7-OB8-CB6
26	h	201	CDL	C14-C15-C16-C17
26	L	703	CDL	C31-CA7-OA8-CA6
25	M	501	3PE	O32-C31-O31-C3
25	J	201	3PE	C22-C21-O21-C2
25	J	201	3PE	O22-C21-O21-C2
25	M	502	3PE	C2-C3-O31-C31
26	M	503	CDL	OB9-CB7-OB8-CB6
26	d	201	CDL	OA9-CA7-OA8-CA6
26	L	703	CDL	OA9-CA7-OA8-CA6
25	J	201	3PE	C2A-C2B-C2C-C2D
25	L	702	3PE	C24-C25-C26-C27
25	L	705	3PE	C3C-C3D-C3E-C3F
25	i	201	3PE	C27-C28-C29-C2A
26	L	703	CDL	C74-C75-C76-C77
25	L	702	3PE	C28-C29-C2A-C2B
26	h	201	CDL	C18-C19-C20-C21
29	n	201	EHZ	C3-C4-C5-C6
29	n	201	EHZ	C5-C6-C7-O1
25	D	501	3PE	C24-C25-C26-C27
29	n	201	EHZ	C6-C7-C8-C9
25	L	701	3PE	C3-C2-O21-C21
26	h	201	CDL	CB3-CB4-OB6-CB5
25	L	705	3PE	C27-C28-C29-C2A
25	L	705	3PE	C32-C31-O31-C3
26	M	503	CDL	C31-CA7-OA8-CA6
29	n	201	EHZ	O4-C15-C16-O5
26	d	201	CDL	C51-CB5-OB6-CB4
25	L	705	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
26	M	503	CDL	OA9-CA7-OA8-CA6
25	L	701	3PE	C36-C37-C38-C39
25	L	701	3PE	C1-O11-P-O14
25	L	705	3PE	C1-O11-P-O14
25	M	501	3PE	C1-O11-P-O13
25	M	501	3PE	C1-O11-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-O12
25	M	502	3PE	C11-O13-P-O14
25	m	201	3PE	C1-O11-P-O13
25	m	201	3PE	C11-O13-P-O11
25	m	201	3PE	C11-O13-P-O14
26	L	703	CDL	CB3-OB5-PB2-OB4
26	M	503	CDL	CA3-OA5-PA1-OA3
26	d	201	CDL	CA3-OA5-PA1-OA3
26	d	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	CA3-OA5-PA1-OA2
26	h	201	CDL	CB3-OB5-PB2-OB4
25	L	702	3PE	C33-C34-C35-C36
25	L	701	3PE	C2-C1-O11-P
26	Y	201	CDL	C1-CA2-OA2-PA1
26	L	703	CDL	C32-C33-C34-C35
25	M	502	3PE	C2D-C2E-C2F-C2G
29	n	201	EHZ	C5-C6-C7-C8
26	h	201	CDL	CB4-CB3-OB5-PB2
25	L	705	3PE	C36-C37-C38-C39
26	d	201	CDL	OB7-CB5-OB6-CB4
29	n	201	EHZ	C7-C8-C9-O2
26	Y	201	CDL	C55-C56-C57-C58
25	J	201	3PE	C36-C37-C38-C39
29	n	201	EHZ	C2-C3-C4-C5
25	D	501	3PE	C32-C31-O31-C3
25	D	501	3PE	O32-C31-O31-C3
26	M	503	CDL	C58-C59-C60-C61
26	M	503	CDL	CB4-CB3-OB5-PB2
25	m	201	3PE	C3-C2-O21-C21
26	Y	201	CDL	C56-C57-C58-C59
26	M	503	CDL	C36-C37-C38-C39
26	L	703	CDL	CA3-CA4-CA6-OA8
26	M	503	CDL	CB3-CB4-CB6-OB8
25	J	201	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
25	M	502	3PE	C34-C35-C36-C37
25	J	201	3PE	O21-C2-C3-O31
25	L	702	3PE	C2-C1-O11-P
28	O	401	ADP	C4'-C5'-O5'-PA
25	M	502	3PE	C32-C33-C34-C35
25	J	201	3PE	C38-C39-C3A-C3B
26	d	201	CDL	CB4-CB3-OB5-PB2
25	D	501	3PE	C32-C33-C34-C35
26	Y	201	CDL	OA7-CA5-OA6-CA4
25	J	201	3PE	O11-C1-C2-C3
26	Y	201	CDL	C11-CA5-OA6-CA4
25	L	702	3PE	C26-C27-C28-C29
25	D	501	3PE	C34-C35-C36-C37
28	O	401	ADP	O4'-C4'-C5'-O5'
26	d	201	CDL	C32-C31-CA7-OA8
26	d	201	CDL	C57-C58-C59-C60
26	d	201	CDL	C1-CB2-OB2-PB2
25	L	701	3PE	C22-C23-C24-C25
26	d	201	CDL	C56-C57-C58-C59
26	h	201	CDL	C11-C12-C13-C14
29	n	201	EHZ	N2-C15-C16-O5
26	d	201	CDL	C34-C35-C36-C37
26	h	201	CDL	C16-C17-C18-C19
26	Y	201	CDL	C54-C55-C56-C57
25	L	701	3PE	O32-C31-O31-C3
26	d	201	CDL	C32-C31-CA7-OA9

There are no ring outliers.

16 monomers are involved in 111 short contacts:

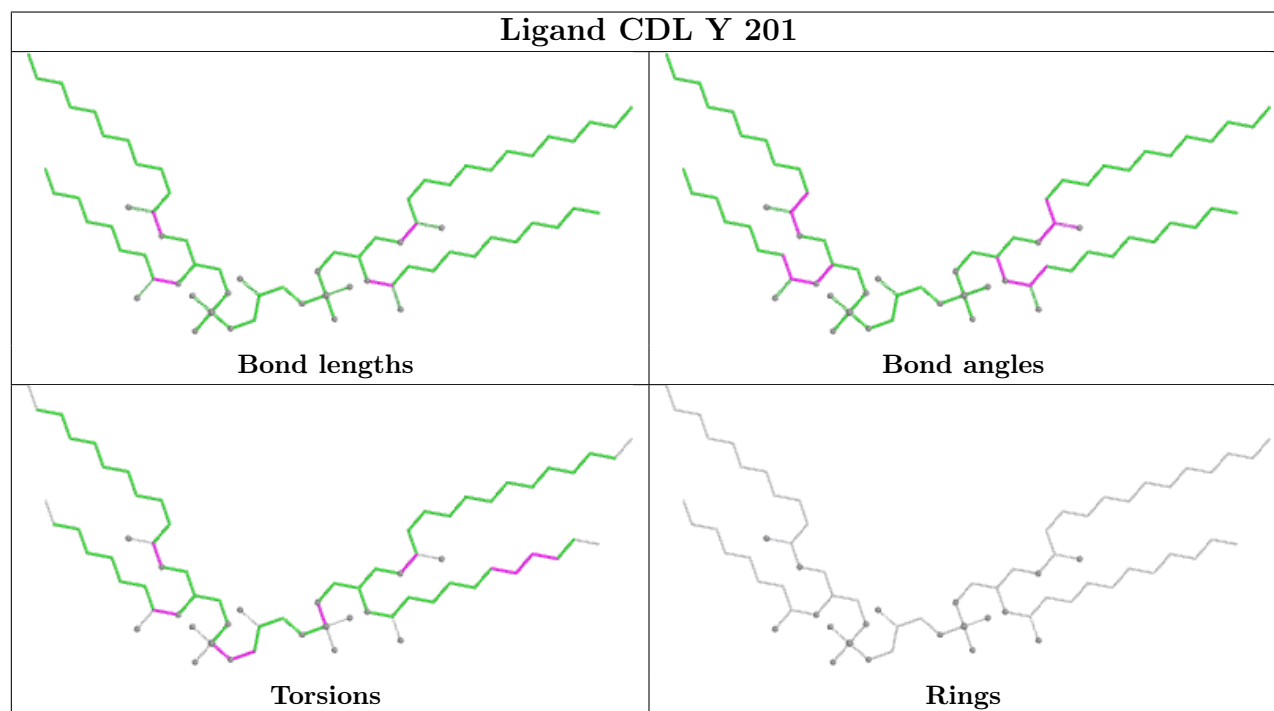
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	201	CDL	5	0
28	O	401	ADP	3	0
25	i	201	3PE	11	0
25	L	701	3PE	5	0
25	M	501	3PE	10	0
25	L	705	3PE	4	0
25	m	201	3PE	9	0
26	d	201	CDL	8	0
26	h	201	CDL	13	0
25	J	201	3PE	1	0
26	L	703	CDL	12	0

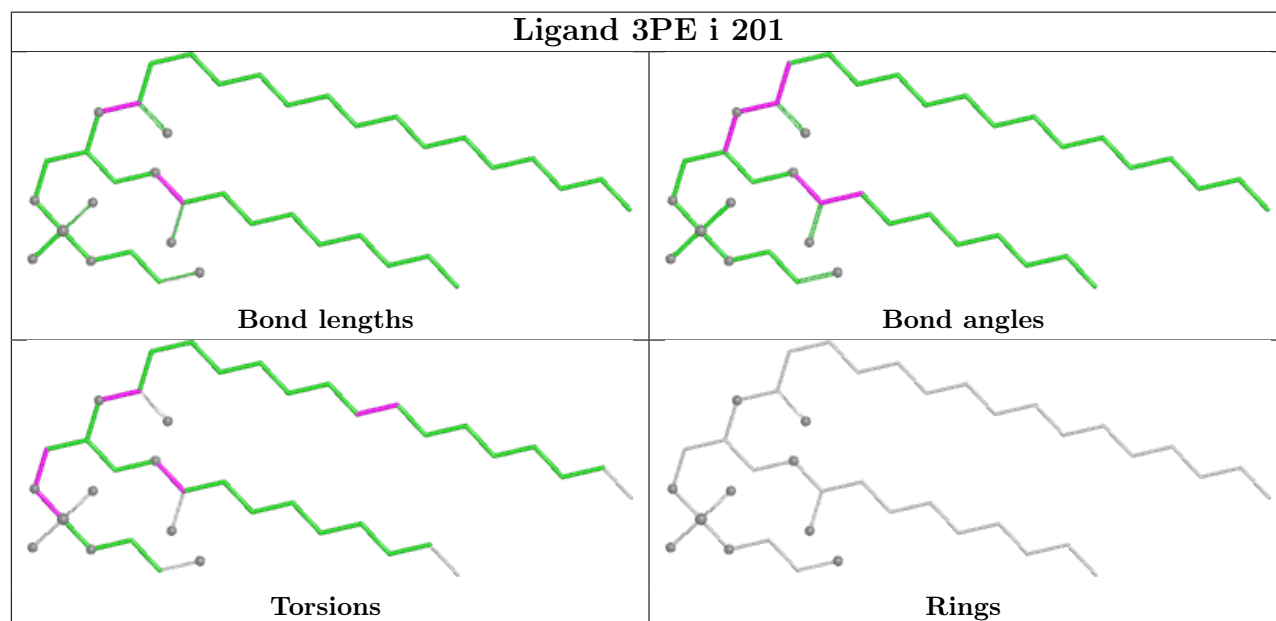
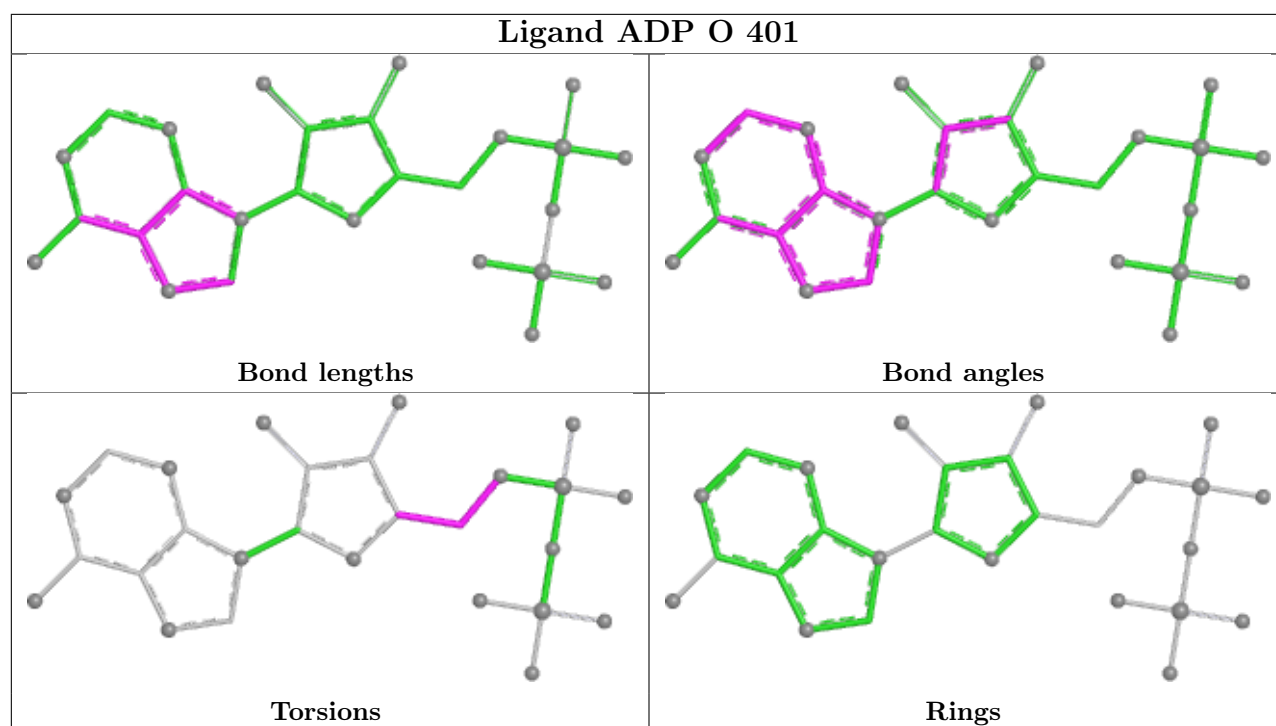
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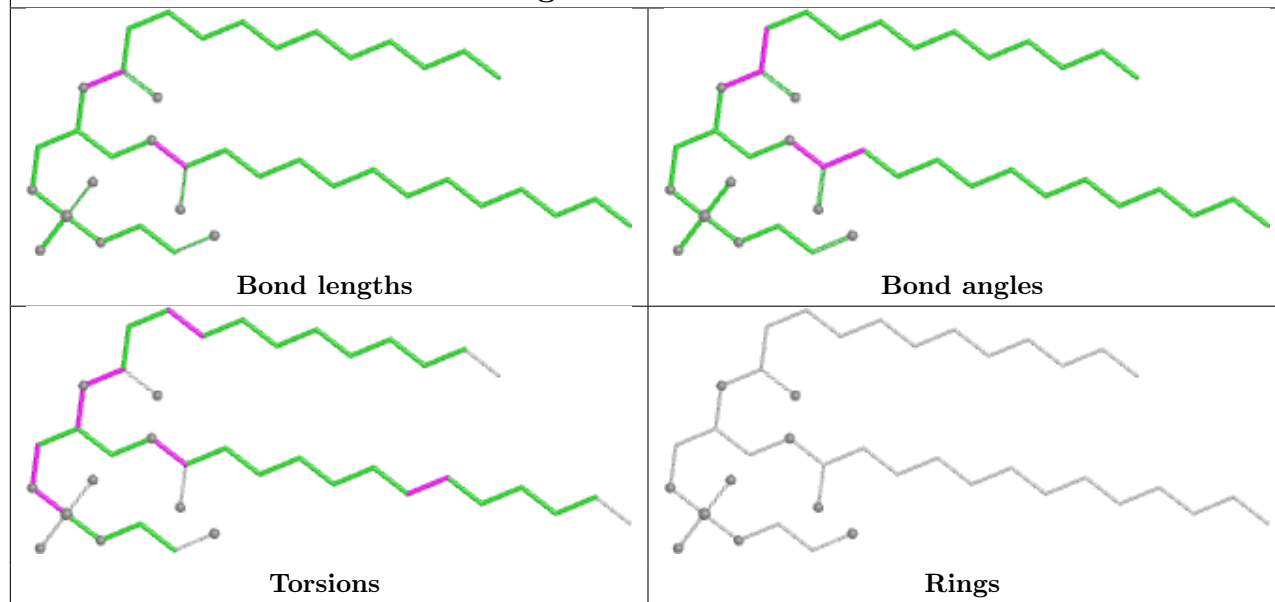
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	M	503	CDL	12	0
29	n	201	EHZ	1	0
25	D	501	3PE	6	0
25	L	702	3PE	9	0
25	M	502	3PE	5	0

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.

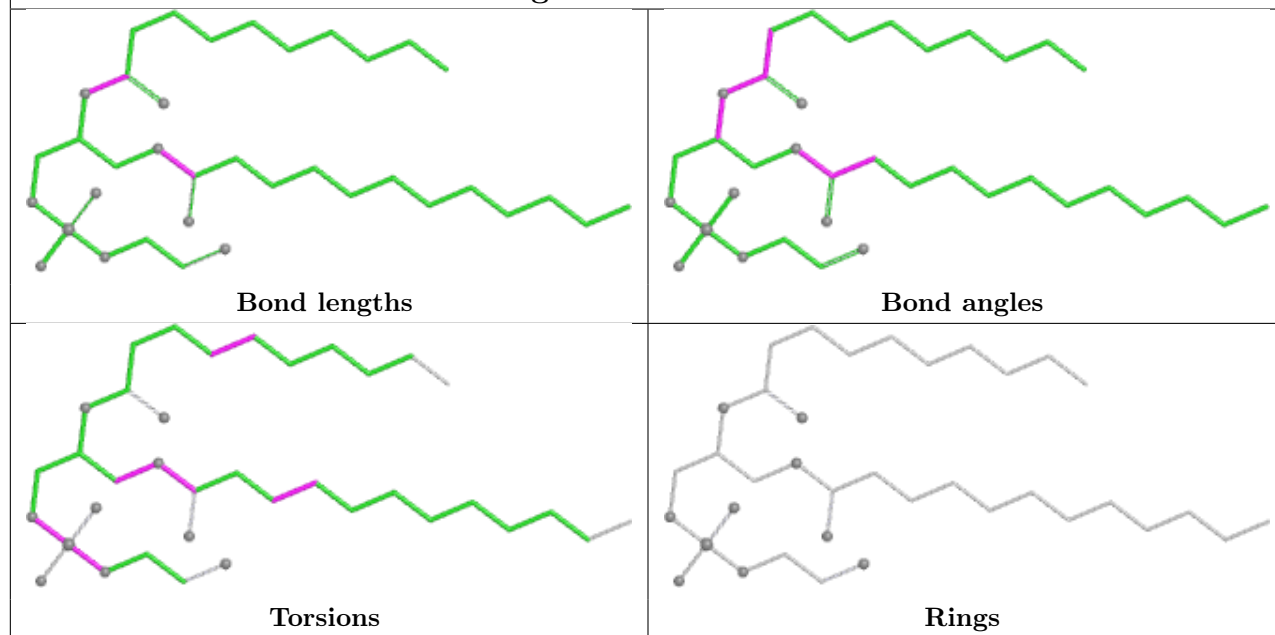


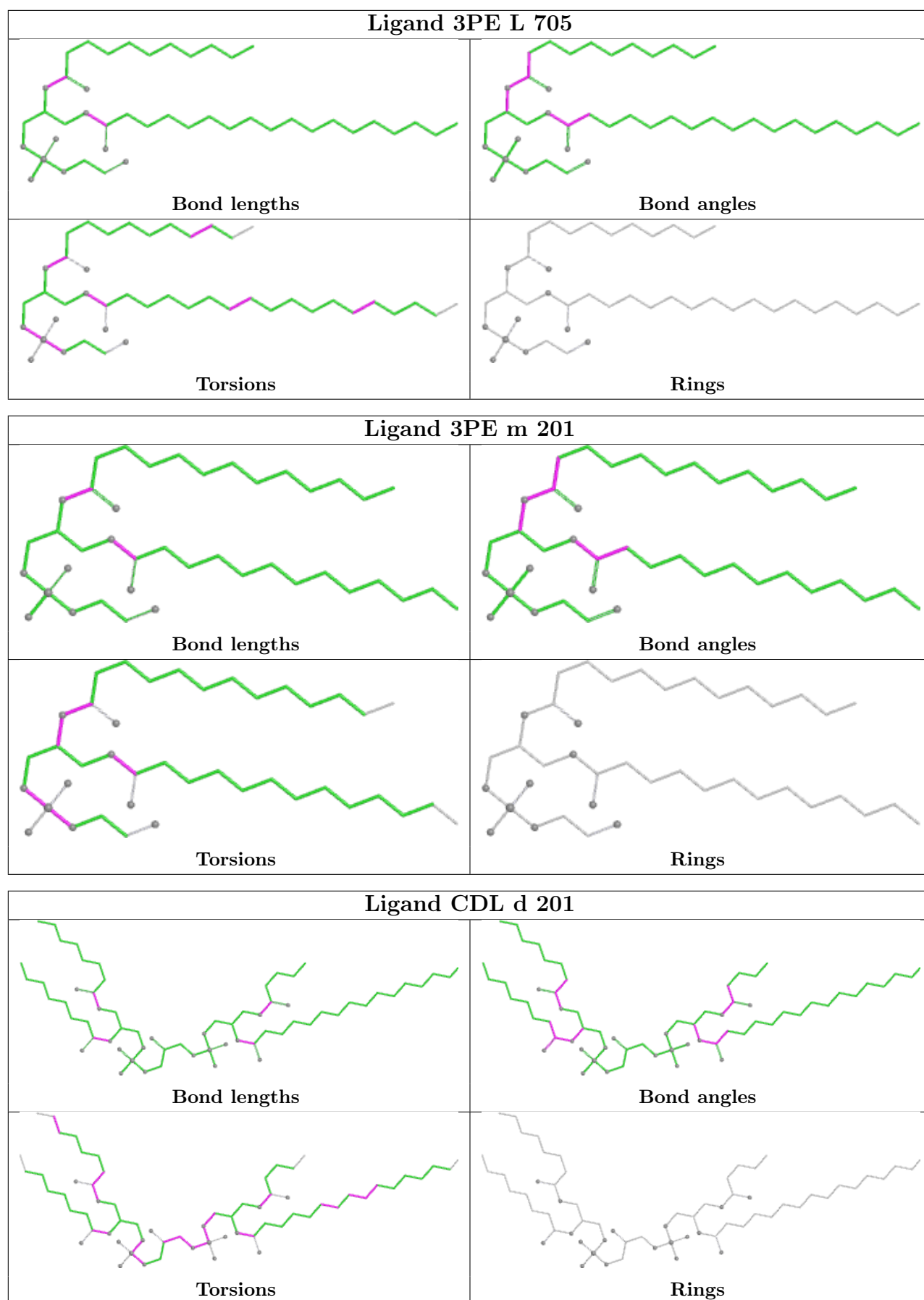


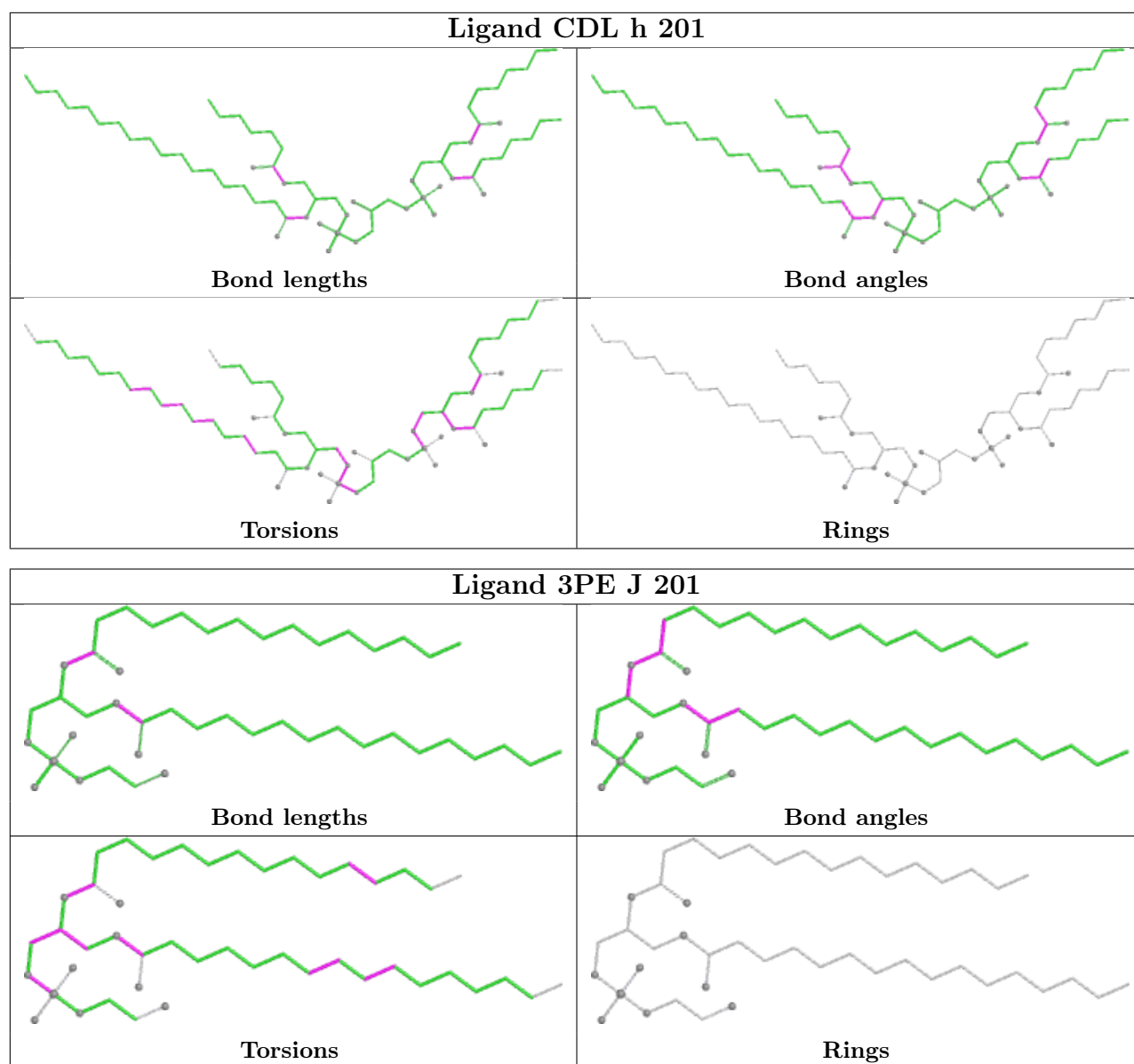
Ligand 3PE L 701

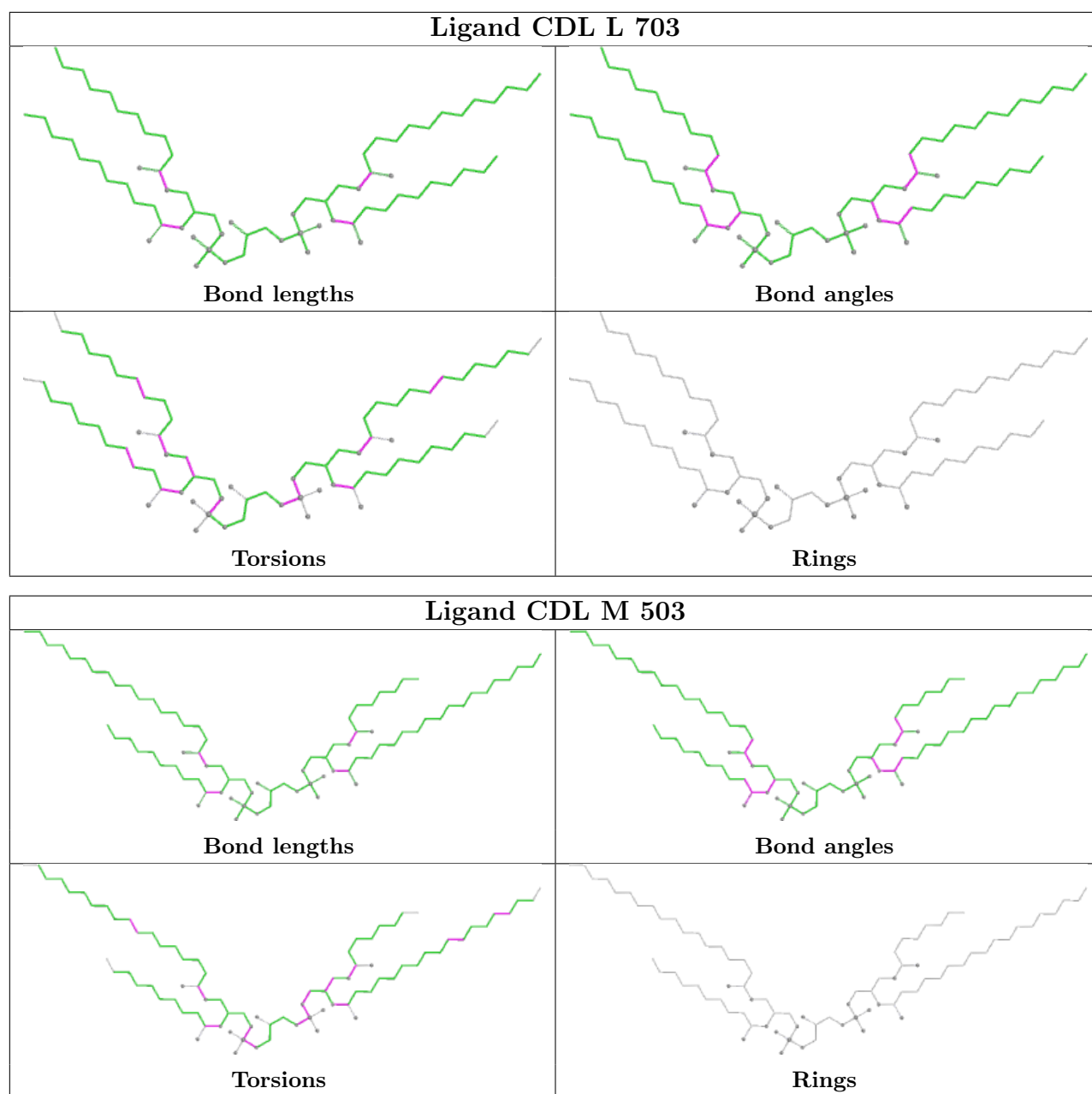


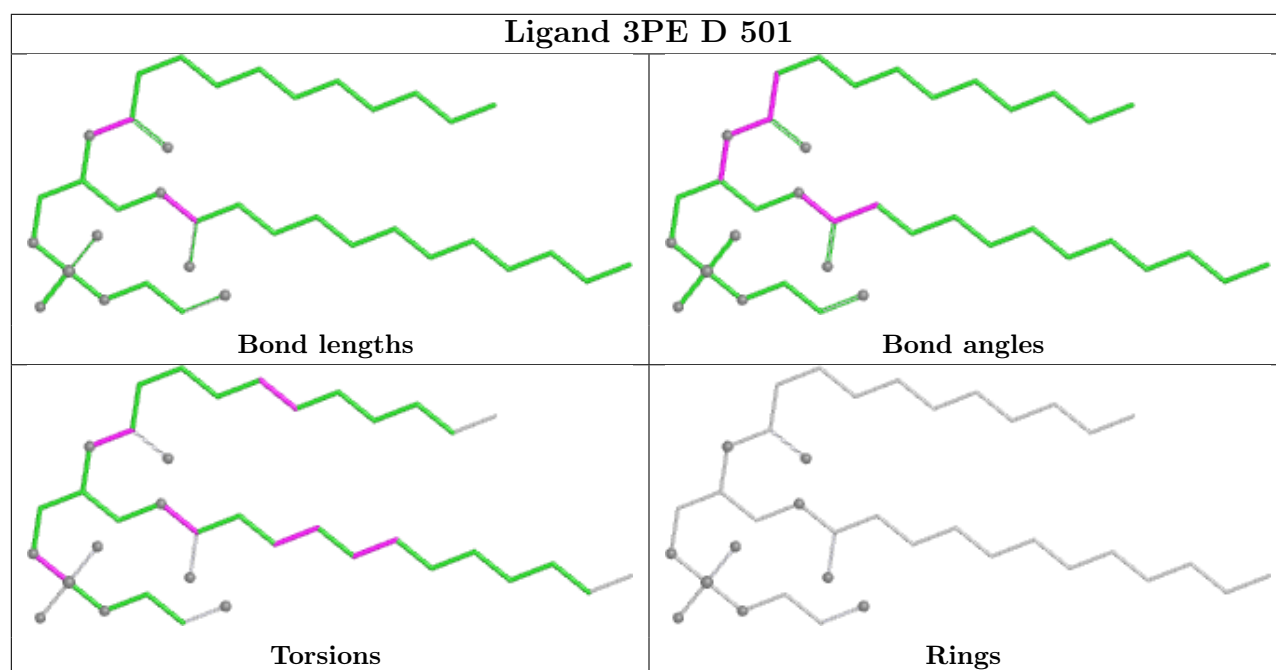
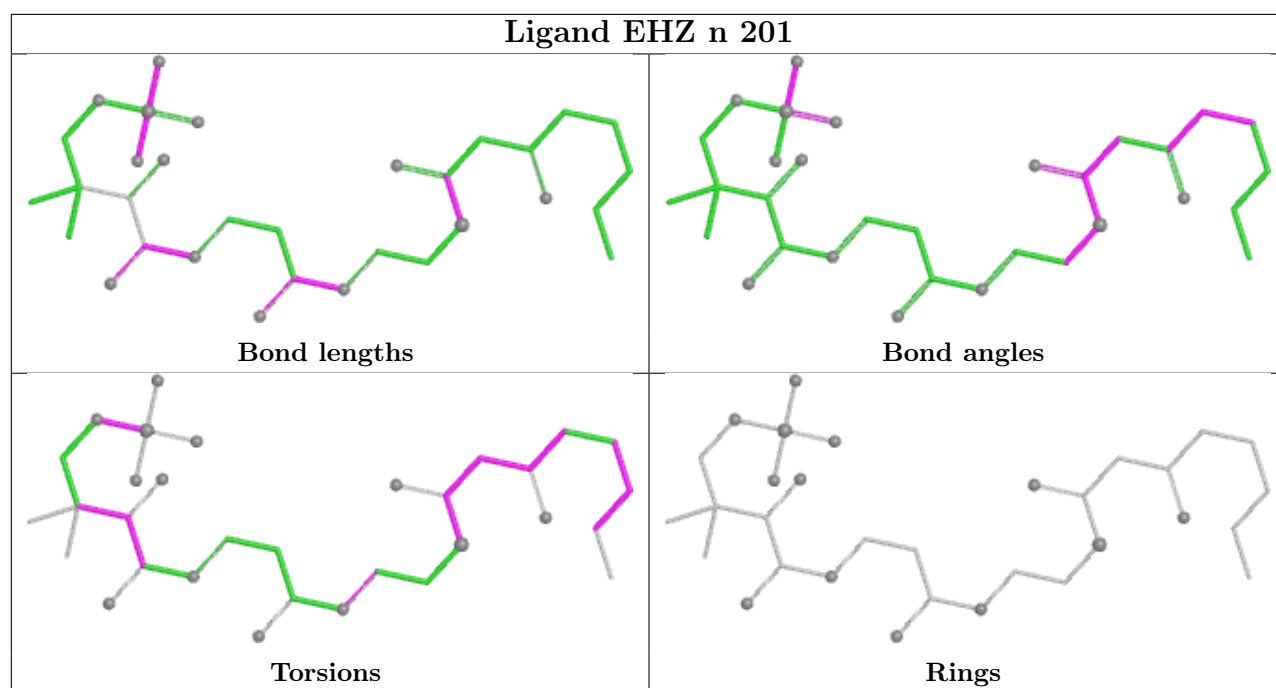
Ligand 3PE M 501

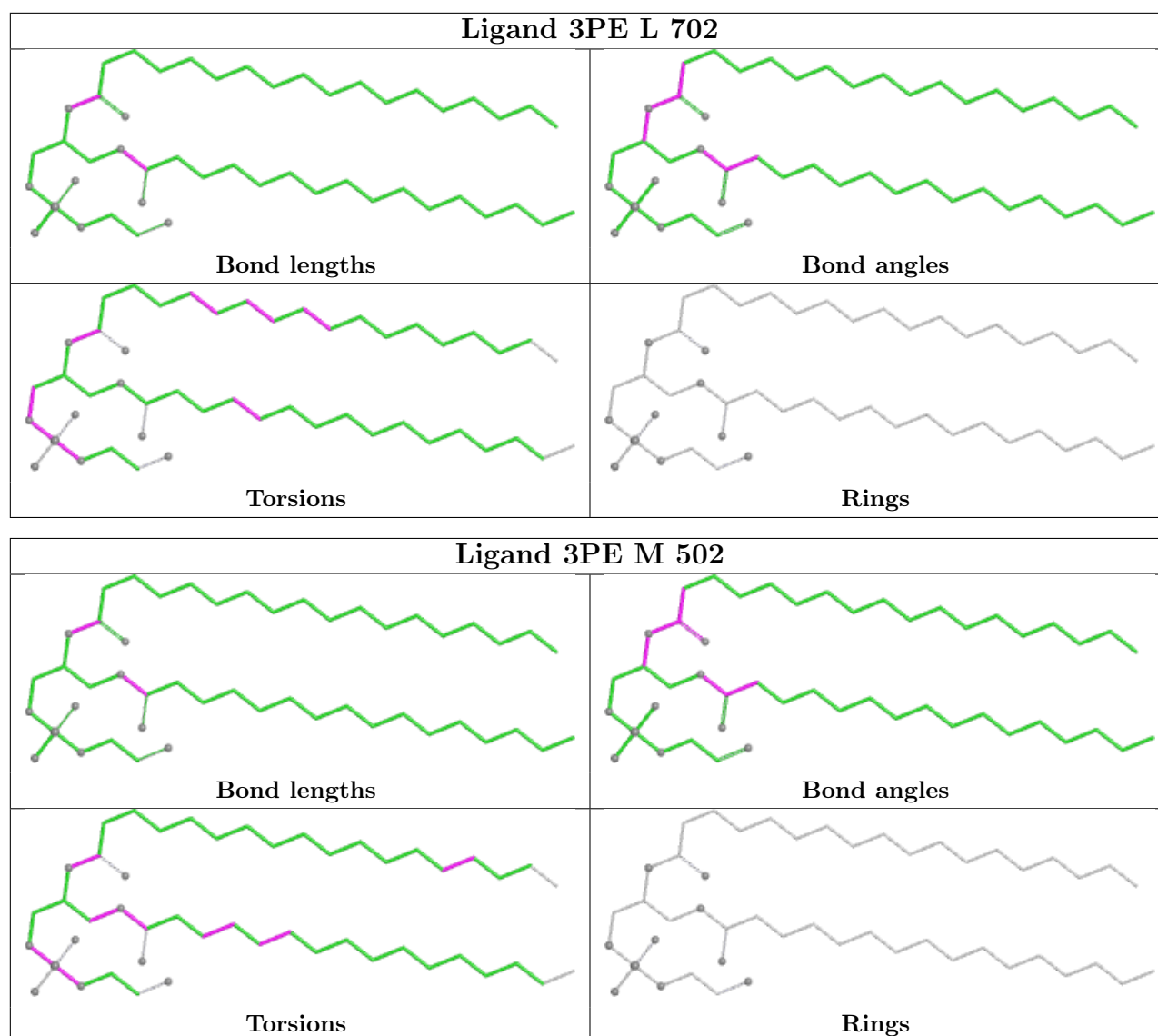












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

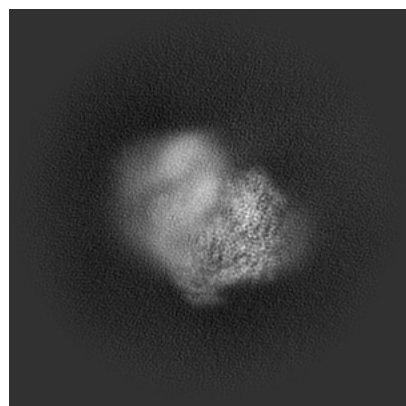
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35354. These allow visual inspection of the internal detail of the map and identification of artifacts.

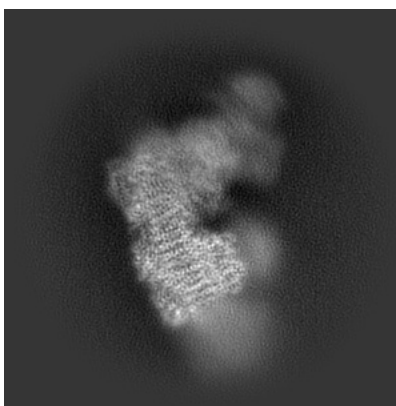
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

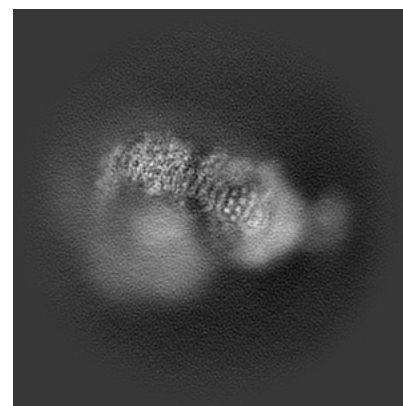
6.1.1 Primary map



X

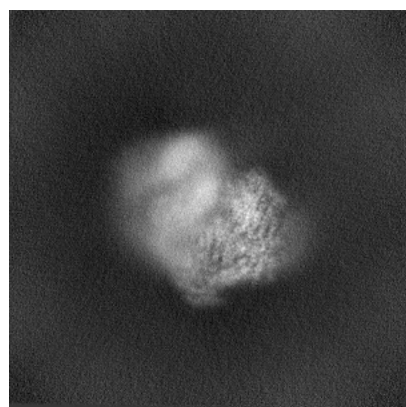


Y



Z

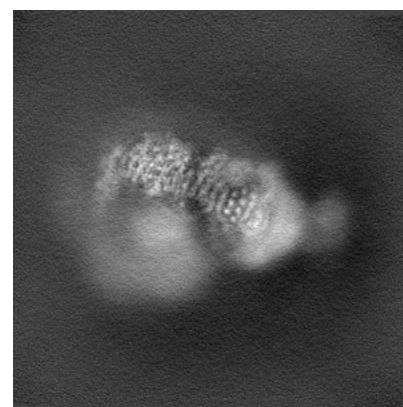
6.1.2 Raw map



X



Y

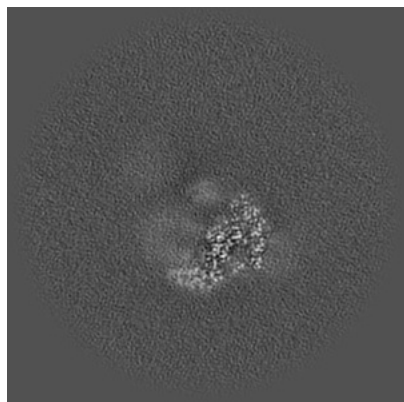


Z

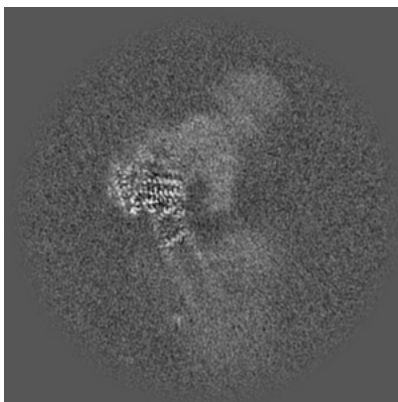
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

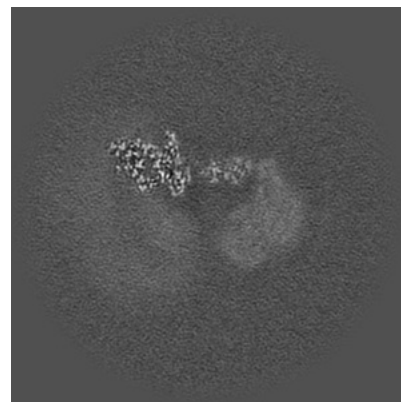
6.2.1 Primary map



X Index: 256

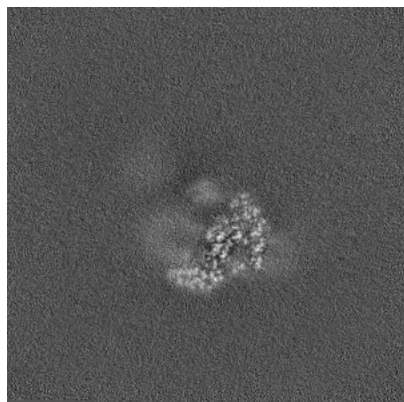


Y Index: 256

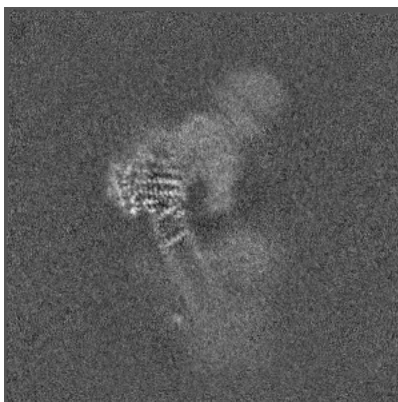


Z Index: 256

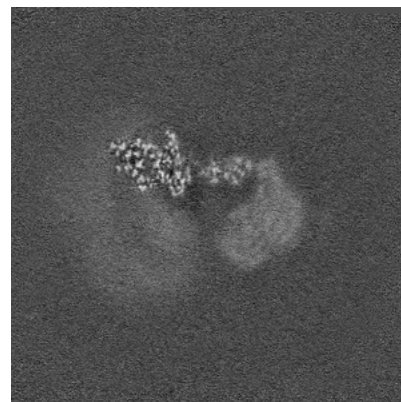
6.2.2 Raw map



X Index: 256



Y Index: 256

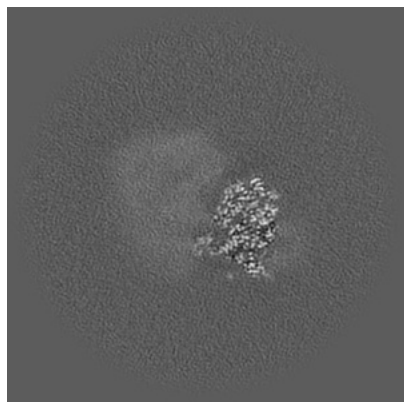


Z Index: 256

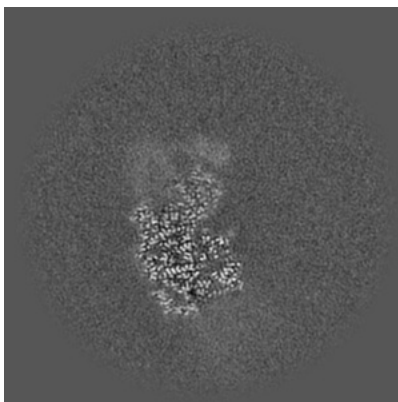
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

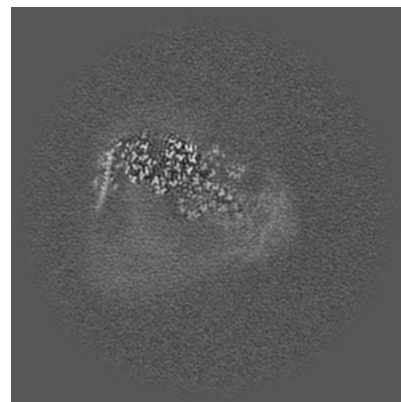
6.3.1 Primary map



X Index: 211

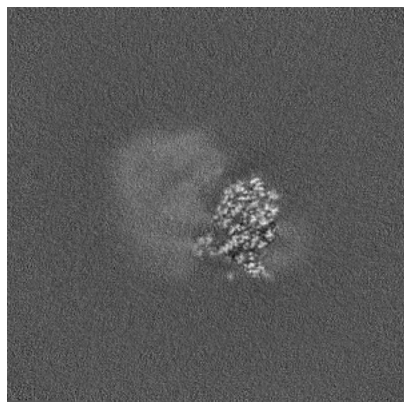


Y Index: 300

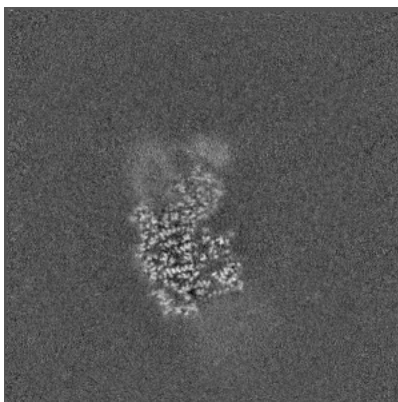


Z Index: 224

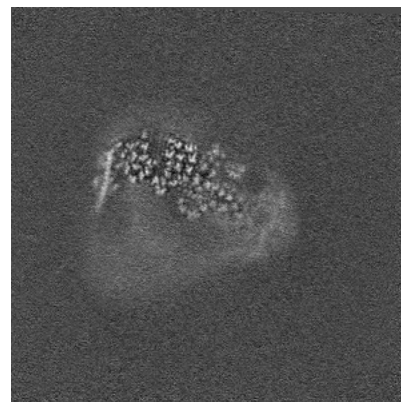
6.3.2 Raw map



X Index: 211



Y Index: 300

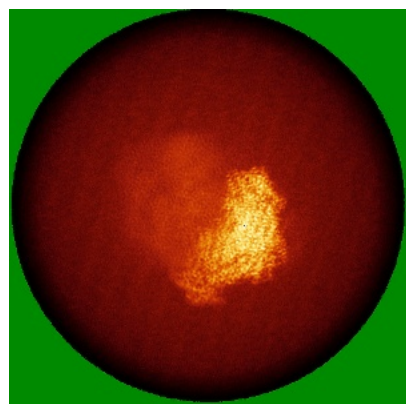


Z Index: 224

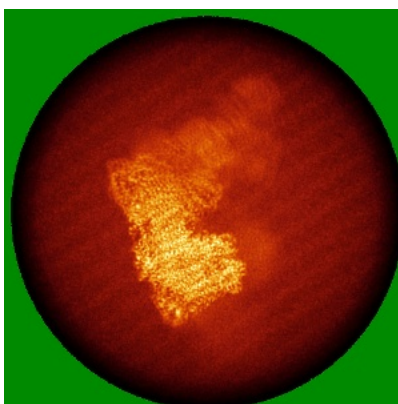
The images above show the largest variance slices of the map in three orthogonal directions.

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

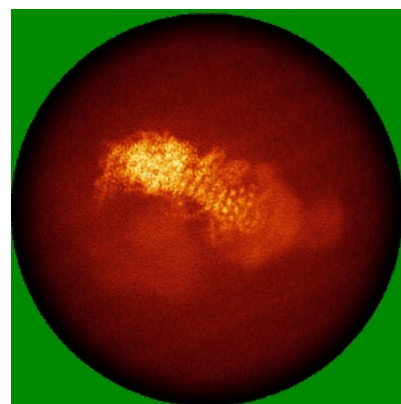
6.4.1 Primary map



X

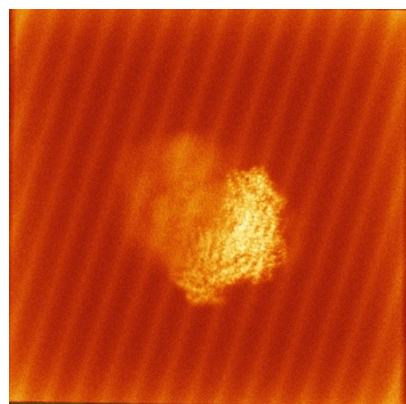


Y

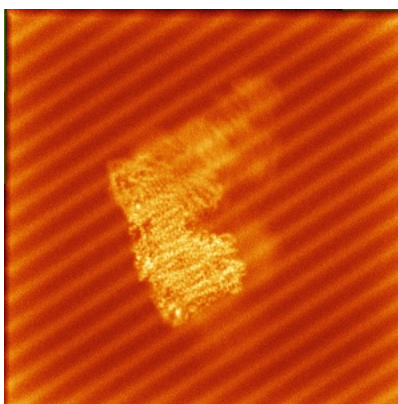


Z

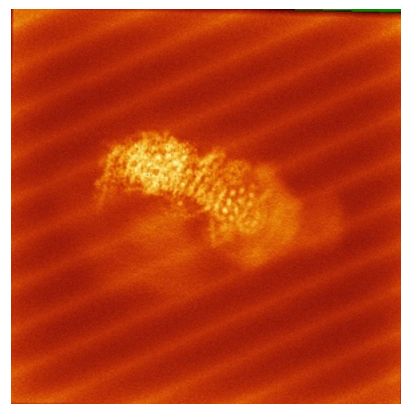
6.4.2 Raw map



X



Y

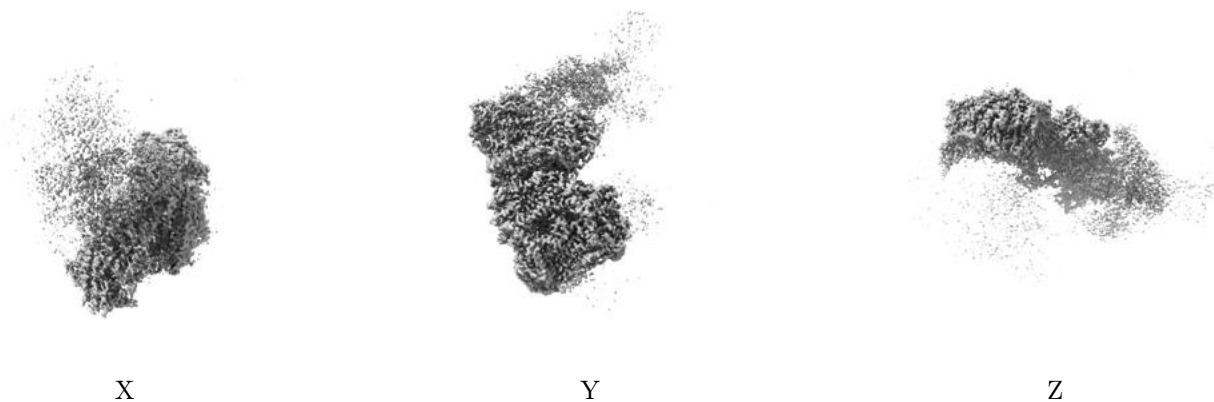


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

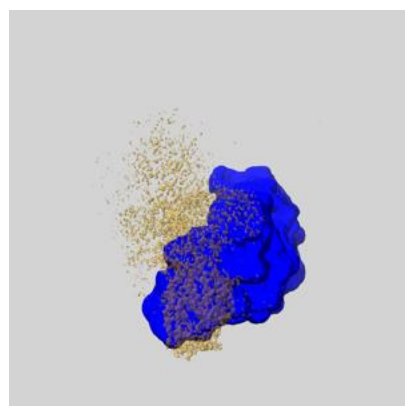
6.6 Mask visualisation [i](#)

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

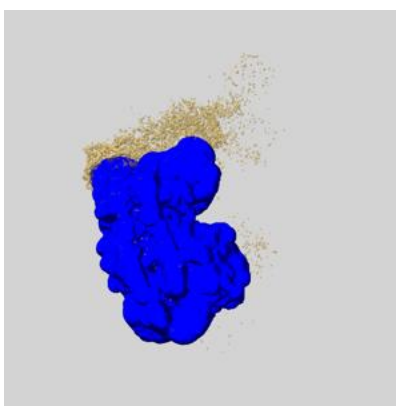
A mask typically either:

- 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_35354_msk_1.map [i](#)



X



Y

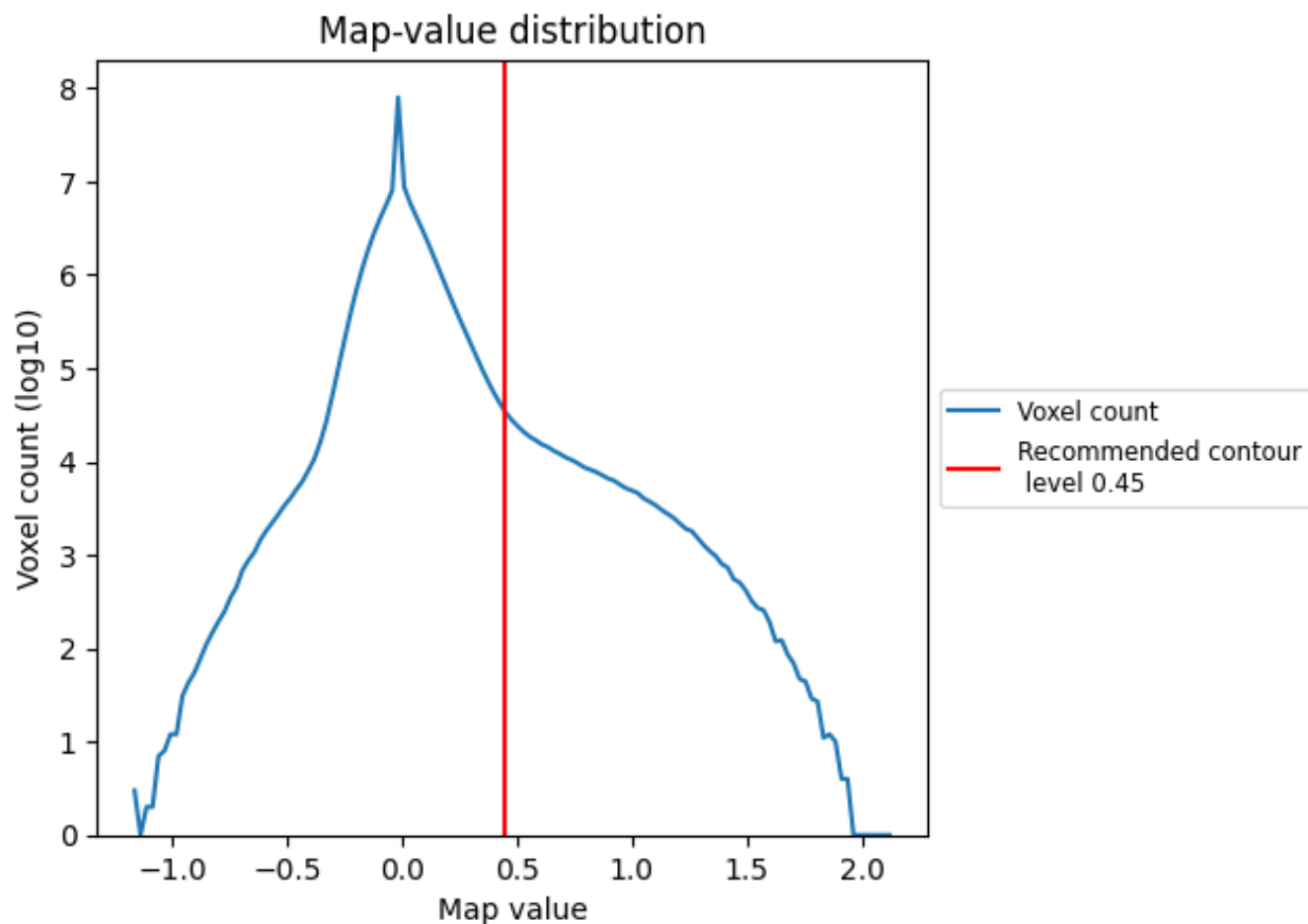


Z

7 Map analysis [i](#)

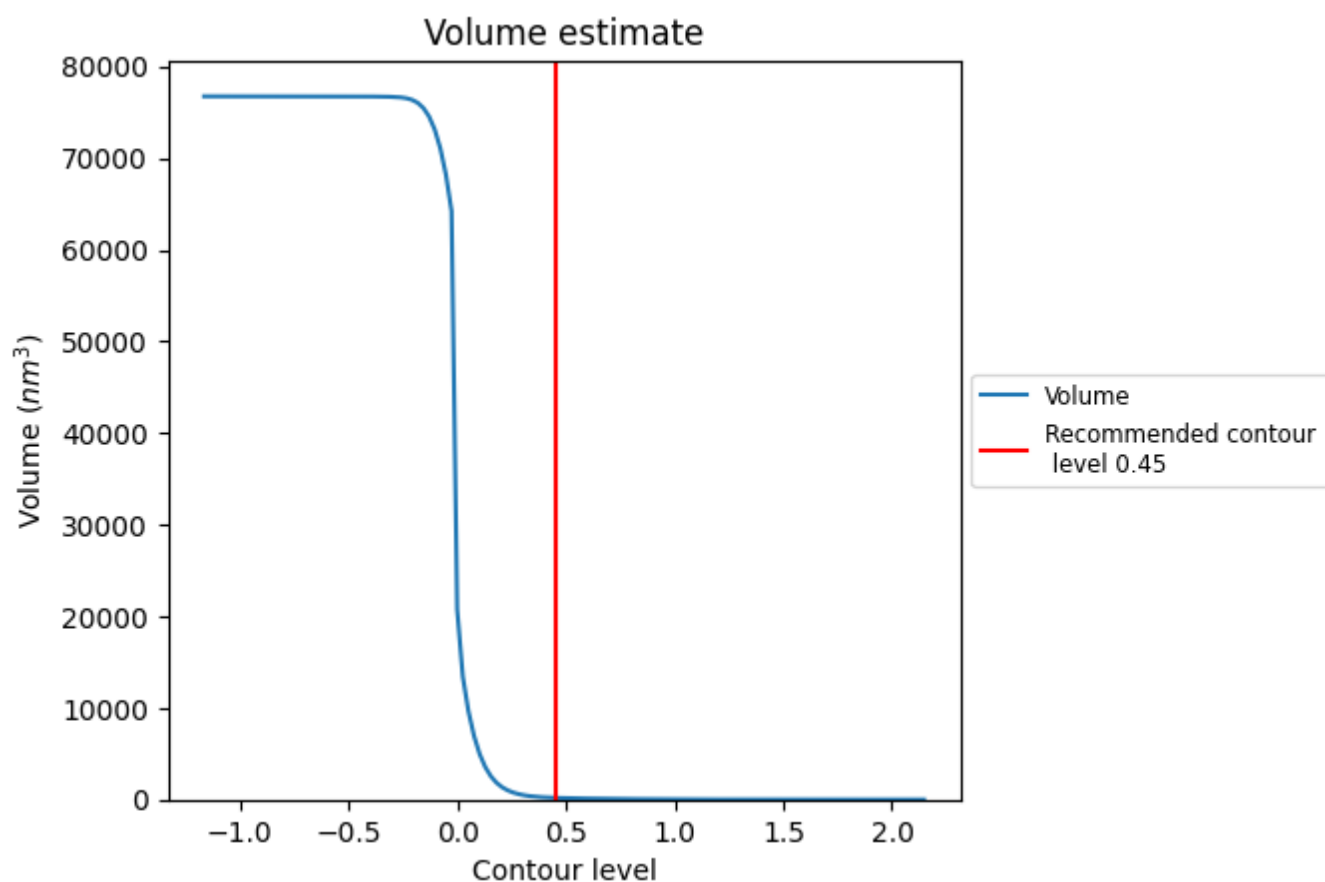
This section contains the results of statistical analysis of the map.

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.

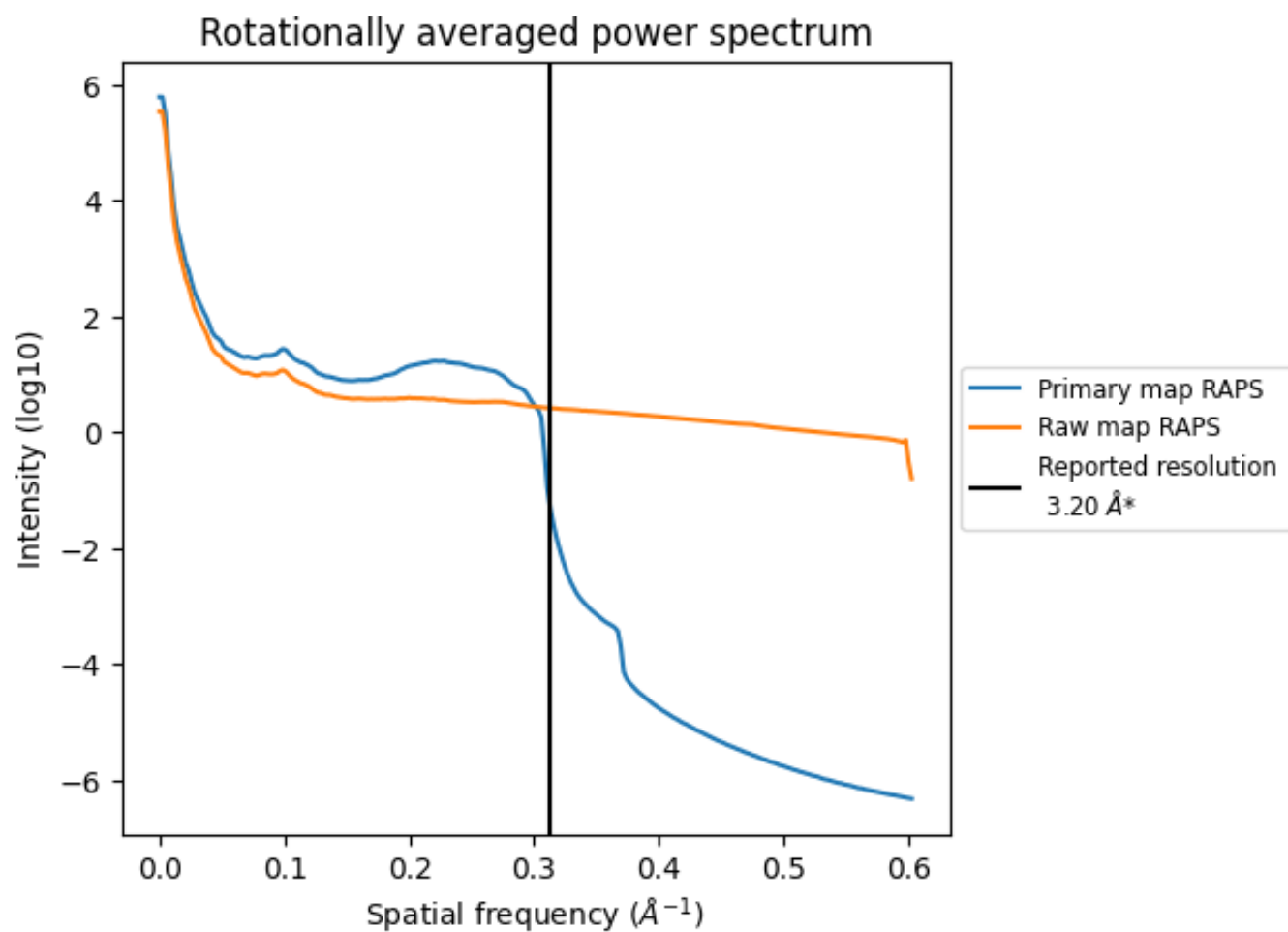
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 171 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 ⓘ

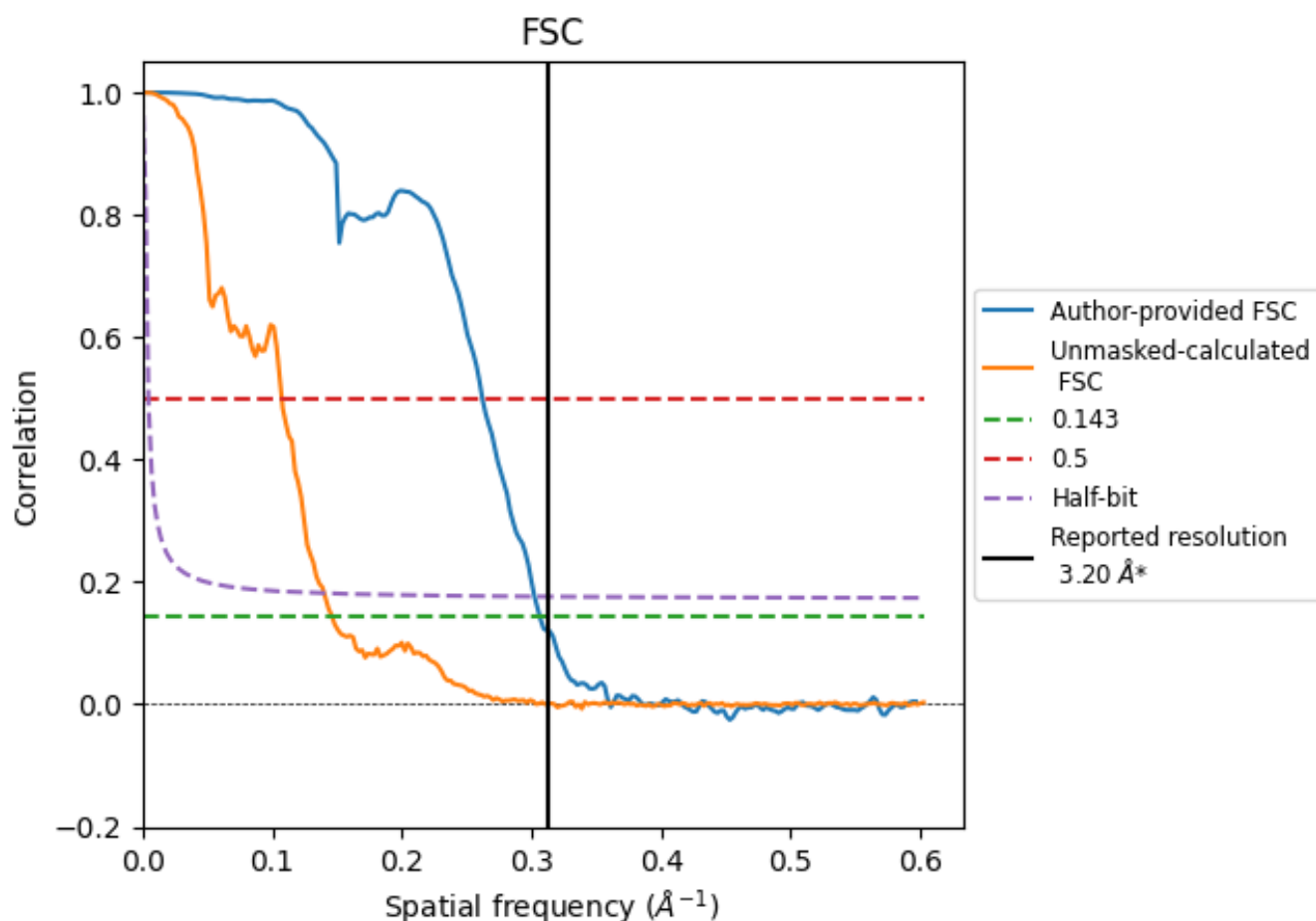


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

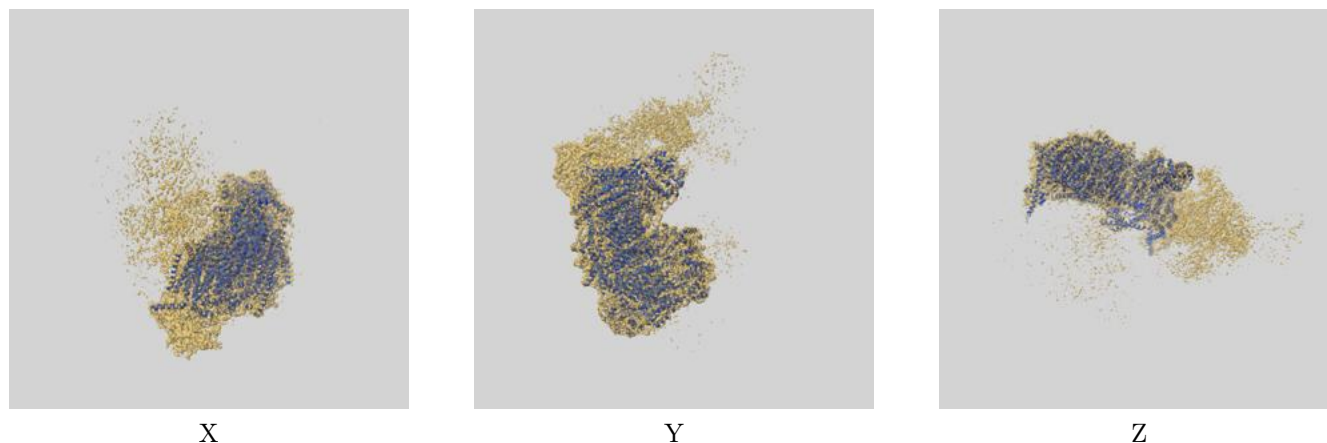
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.81	3.31
Unmasked-calculated*	6.84	9.31	7.14

*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 6.84 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

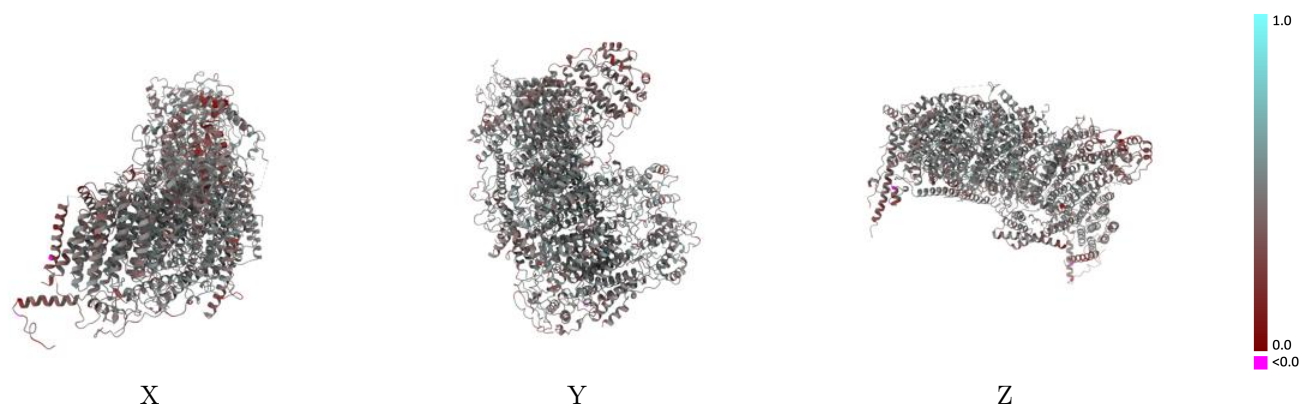
This section contains information regarding the fit between EMDB map EMD-35354 and PDB model 8IC4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

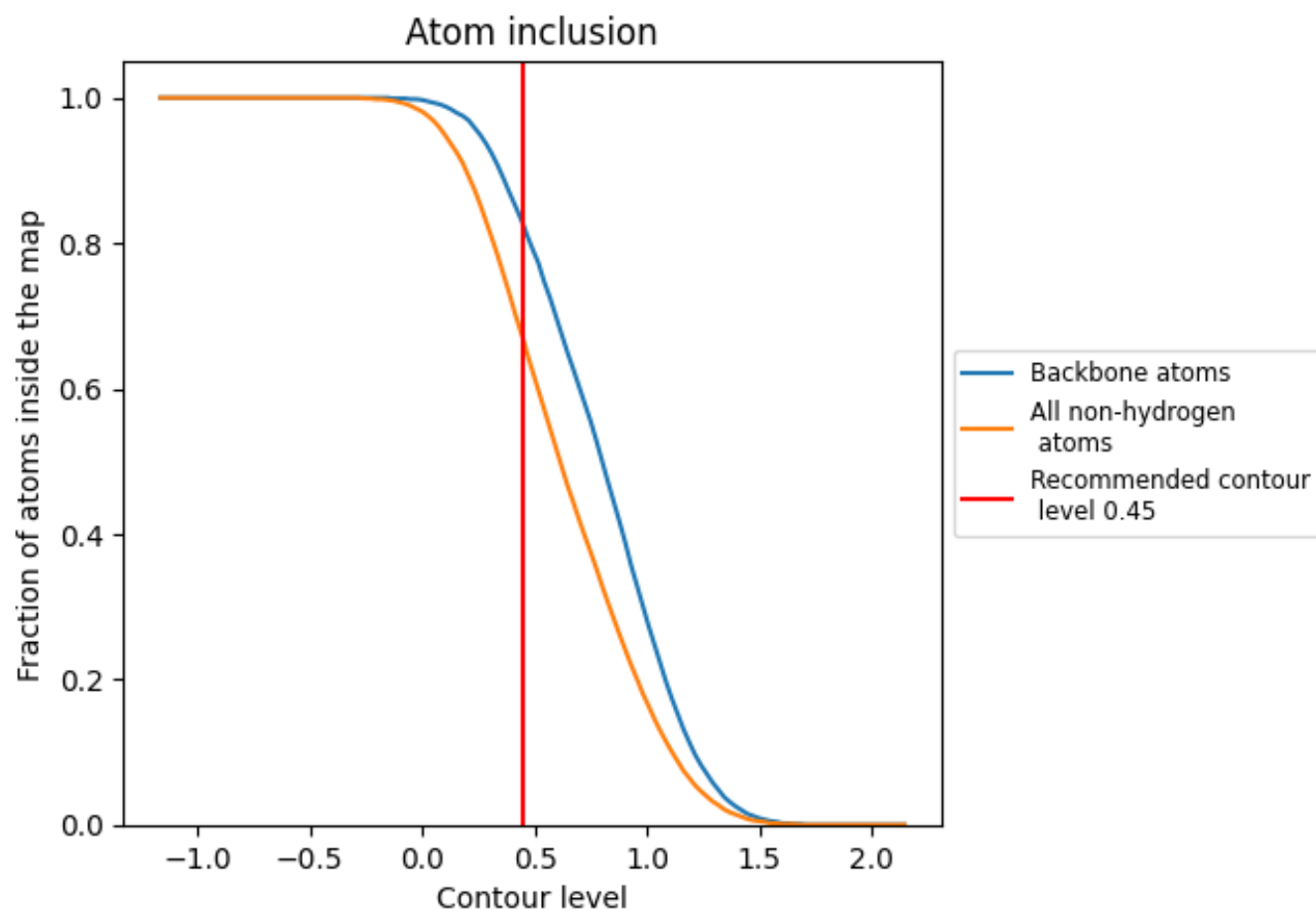


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 67% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.4500
D	 0.4170	 0.4180
J	 0.4460	 0.4010
K	 0.6210	 0.4630
L	 0.6960	 0.4680
M	 0.7040	 0.4860
N	 0.6940	 0.4770
O	 0.5680	 0.3830
U	 0.7420	 0.4720
X	 0.7450	 0.4480
Y	 0.4880	 0.4150
c	 0.5820	 0.4040
d	 0.7030	 0.4670
e	 0.6030	 0.3850
f	 0.6640	 0.4600
g	 0.7100	 0.4560
h	 0.7180	 0.4630
i	 0.7060	 0.4560
j	 0.6920	 0.4160
k	 0.7520	 0.4620
l	 0.7480	 0.4710
m	 0.6850	 0.4550
n	 0.7610	 0.4750
o	 0.6540	 0.4080
p	 0.7070	 0.4380

