



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:40 AM UTC

PDB ID : 8U0V / pdb_00008u0v
EMDB ID : EMD-41788
Title : S. cerevisiae Pex1/Pex6 with 1 mM ATP
Authors : Gardner, B.M.
Deposited on : 2023-08-29
Resolution : 3.89 Å(reported)
Based on initial model : .

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:

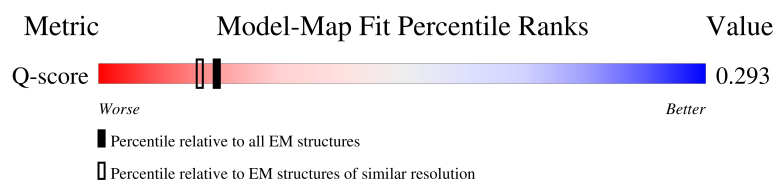
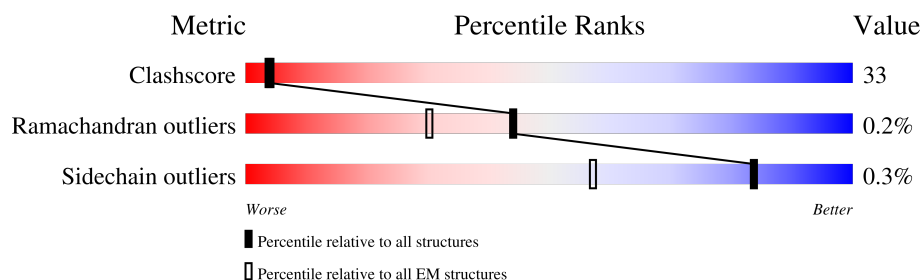
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.89 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	8712 (3.39 - 4.39)

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	A	1054	20% 43% 35% 22%
1	C	1054	15% 44% 34% 22%
1	E	1054	21% 50% 27% 22%
2	B	1044	13% 55% 43% .

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Mol	Chain	Length	Quality of chain
2	D	1044	
2	F	1044	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	1101	-	-	X	-
3	ATP	A	1102	-	-	X	-
3	ATP	B	1102	-	-	X	-
3	ATP	C	1101	-	-	X	-
3	ATP	C	1102	-	-	X	-
3	ATP	E	1101	-	-	X	-
3	ATP	F	1101	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 81859 atoms, of which 37662 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 Peroxisomal ATPase PEX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	821	Total	C	H	N	O	S	0	0
			13064	4121	6563	1113	1244	23		
1	C	821	Total	C	H	N	O	S	0	0
			12713	4121	6212	1113	1244	23		
1	E	821	Total	C	H	N	O	S	0	0
			12713	4121	6212	1113	1244	23		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1044	GLY	-	expression tag	UNP P24004
A	1045	SER	-	expression tag	UNP P24004
A	1046	SER	-	expression tag	UNP P24004
A	1047	ASP	-	expression tag	UNP P24004
A	1048	TYR	-	expression tag	UNP P24004
A	1049	LYS	-	expression tag	UNP P24004
A	1050	ASP	-	expression tag	UNP P24004
A	1051	ASP	-	expression tag	UNP P24004
A	1052	ASP	-	expression tag	UNP P24004
A	1053	ASP	-	expression tag	UNP P24004
A	1054	LYS	-	expression tag	UNP P24004
C	1044	GLY	-	expression tag	UNP P24004
C	1045	SER	-	expression tag	UNP P24004
C	1046	SER	-	expression tag	UNP P24004
C	1047	ASP	-	expression tag	UNP P24004
C	1048	TYR	-	expression tag	UNP P24004
C	1049	LYS	-	expression tag	UNP P24004
C	1050	ASP	-	expression tag	UNP P24004
C	1051	ASP	-	expression tag	UNP P24004
C	1052	ASP	-	expression tag	UNP P24004
C	1053	ASP	-	expression tag	UNP P24004
C	1054	LYS	-	expression tag	UNP P24004
E	1044	GLY	-	expression tag	UNP P24004
E	1045	SER	-	expression tag	UNP P24004

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1046	SER	-	expression tag	UNP P24004
E	1047	ASP	-	expression tag	UNP P24004
E	1048	TYR	-	expression tag	UNP P24004
E	1049	LYS	-	expression tag	UNP P24004
E	1050	ASP	-	expression tag	UNP P24004
E	1051	ASP	-	expression tag	UNP P24004
E	1052	ASP	-	expression tag	UNP P24004
E	1053	ASP	-	expression tag	UNP P24004
E	1054	LYS	-	expression tag	UNP P24004

- Molecule 2 is a protein called Peroxisomal ATPase PEX6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	1030	Total	C	H	N	O	S	1	0
			10551	5186	2419	1350	1551	45		
2	B	1030	Total	C	H	N	O	S	0	0
			16254	5183	8128	1349	1550	44		
2	D	1030	Total	C	H	N	O	S	0	0
			16254	5183	8128	1349	1550	44		

There are 42 discrepancies between the modelled and reference sequences:

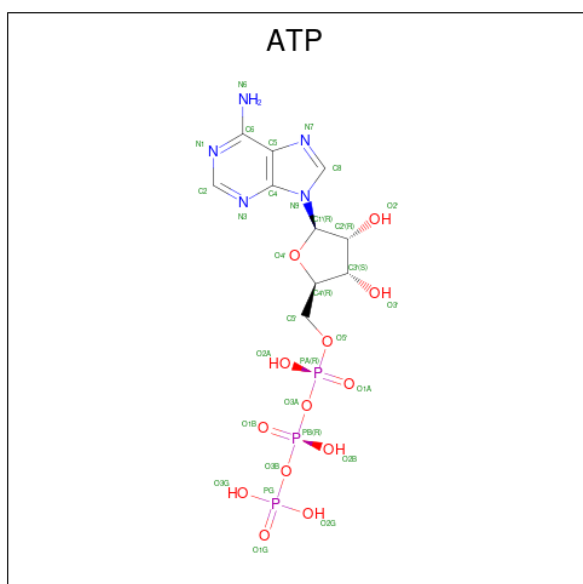
Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	initiating methionine	UNP P33760
F	-12	GLY	-	expression tag	UNP P33760
F	-11	SER	-	expression tag	UNP P33760
F	-10	SER	-	expression tag	UNP P33760
F	-9	HIS	-	expression tag	UNP P33760
F	-8	HIS	-	expression tag	UNP P33760
F	-7	HIS	-	expression tag	UNP P33760
F	-6	HIS	-	expression tag	UNP P33760
F	-5	HIS	-	expression tag	UNP P33760
F	-4	HIS	-	expression tag	UNP P33760
F	-3	SER	-	expression tag	UNP P33760
F	-2	GLN	-	expression tag	UNP P33760
F	-1	ASP	-	expression tag	UNP P33760
F	0	PRO	-	expression tag	UNP P33760
B	-13	MET	-	initiating methionine	UNP P33760
B	-12	GLY	-	expression tag	UNP P33760
B	-11	SER	-	expression tag	UNP P33760
B	-10	SER	-	expression tag	UNP P33760
B	-9	HIS	-	expression tag	UNP P33760

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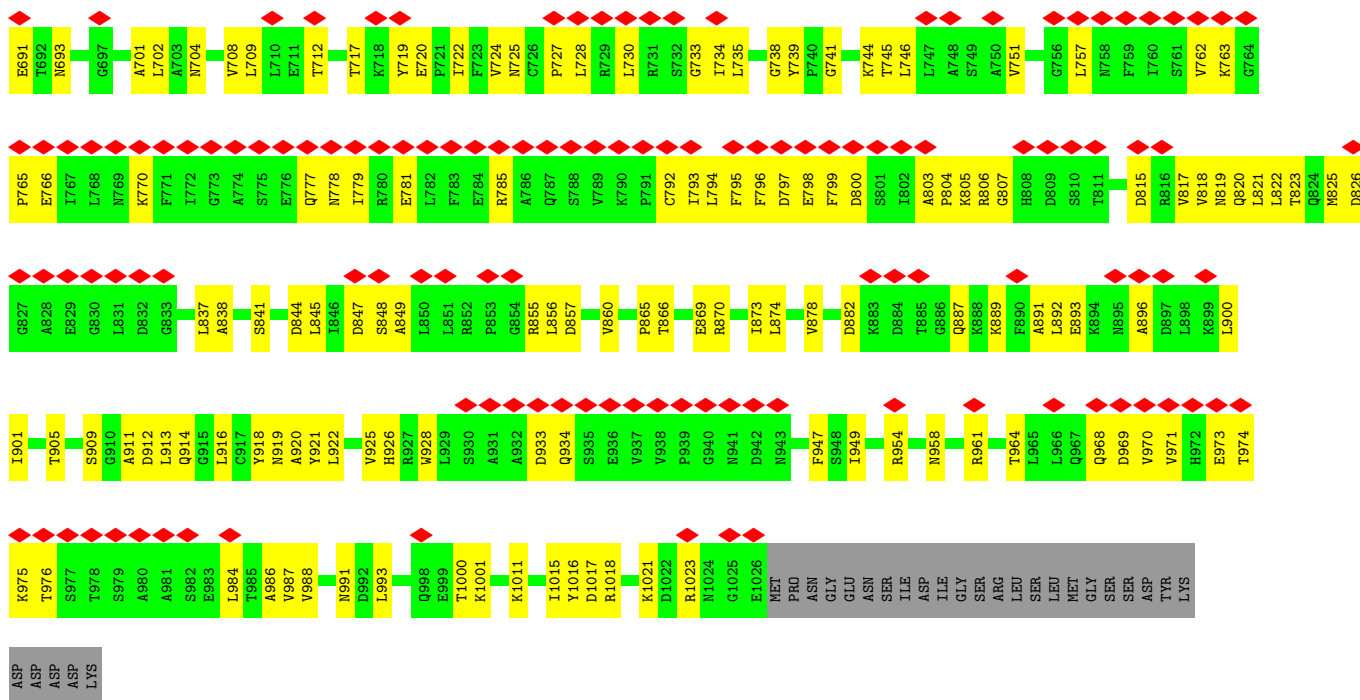
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P33760
B	-7	HIS	-	expression tag	UNP P33760
B	-6	HIS	-	expression tag	UNP P33760
B	-5	HIS	-	expression tag	UNP P33760
B	-4	HIS	-	expression tag	UNP P33760
B	-3	SER	-	expression tag	UNP P33760
B	-2	GLN	-	expression tag	UNP P33760
B	-1	ASP	-	expression tag	UNP P33760
B	0	PRO	-	expression tag	UNP P33760
D	-13	MET	-	initiating methionine	UNP P33760
D	-12	GLY	-	expression tag	UNP P33760
D	-11	SER	-	expression tag	UNP P33760
D	-10	SER	-	expression tag	UNP P33760
D	-9	HIS	-	expression tag	UNP P33760
D	-8	HIS	-	expression tag	UNP P33760
D	-7	HIS	-	expression tag	UNP P33760
D	-6	HIS	-	expression tag	UNP P33760
D	-5	HIS	-	expression tag	UNP P33760
D	-4	HIS	-	expression tag	UNP P33760
D	-3	SER	-	expression tag	UNP P33760
D	-2	GLN	-	expression tag	UNP P33760
D	-1	ASP	-	expression tag	UNP P33760
D	0	PRO	-	expression tag	UNP P33760

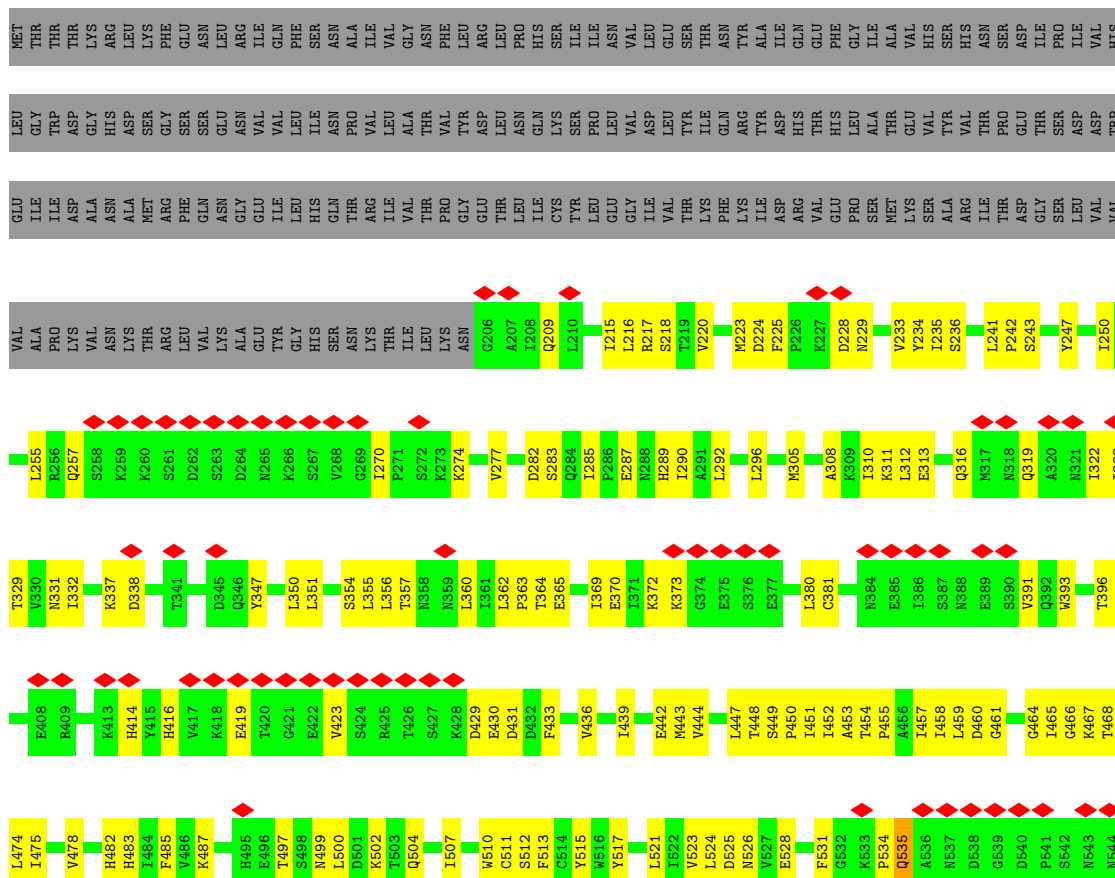
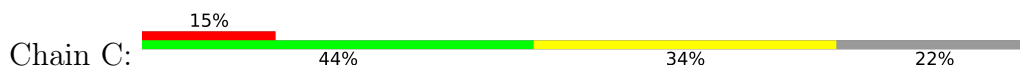
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

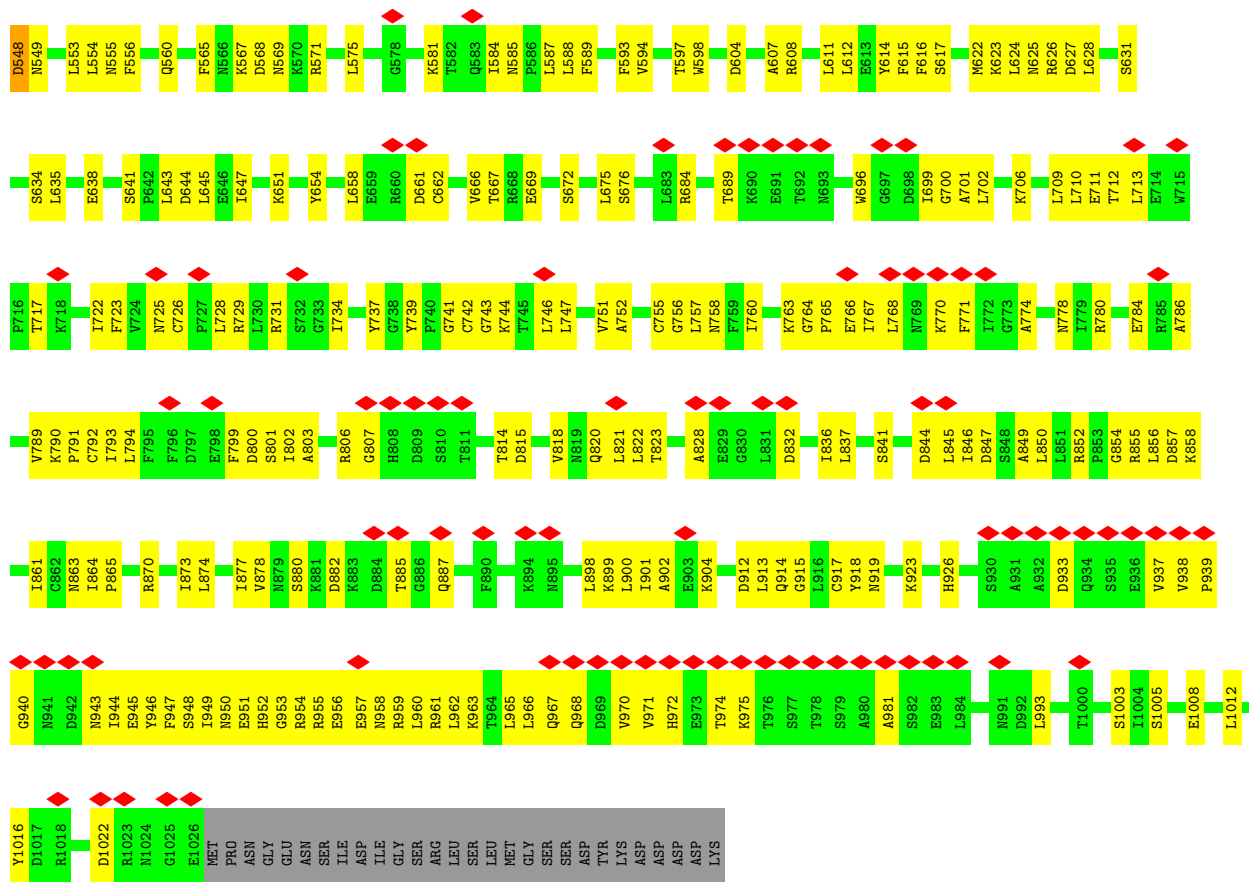


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0

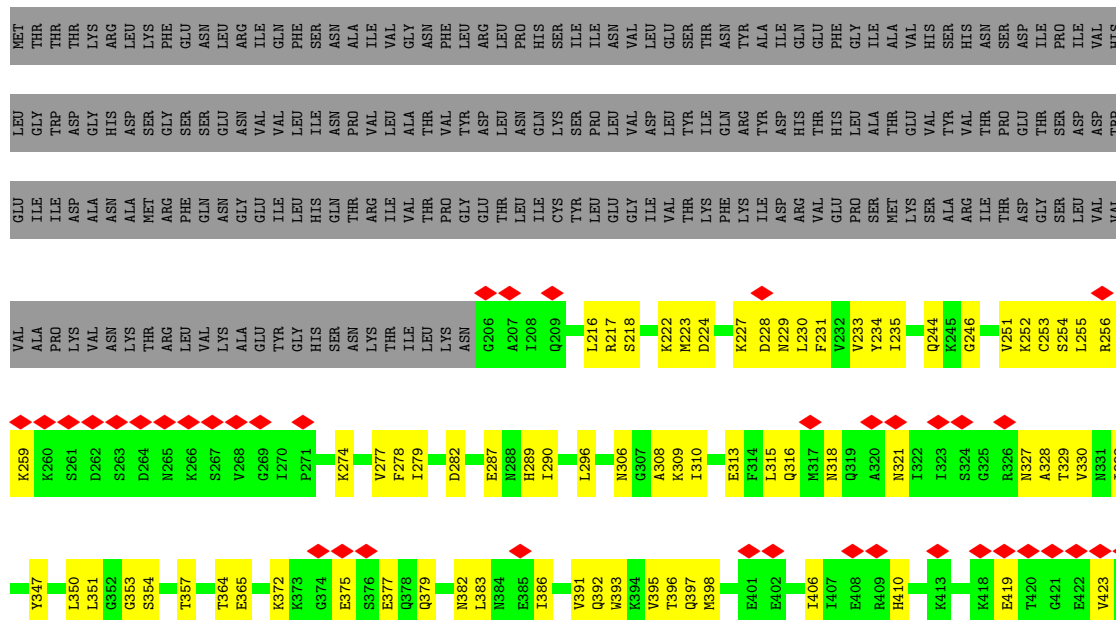


- Molecule 1: Peroxisomal ATPase PEX1

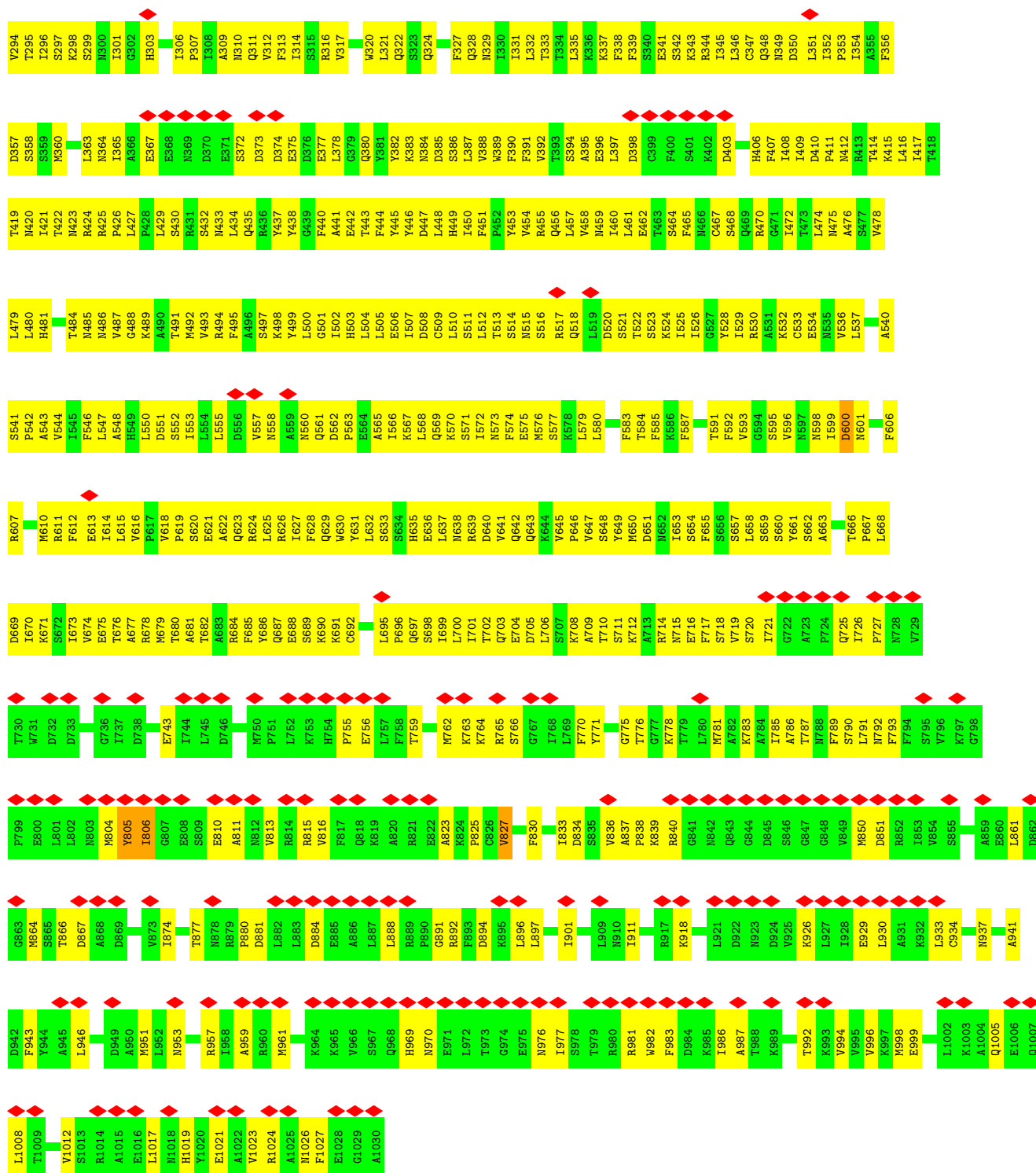


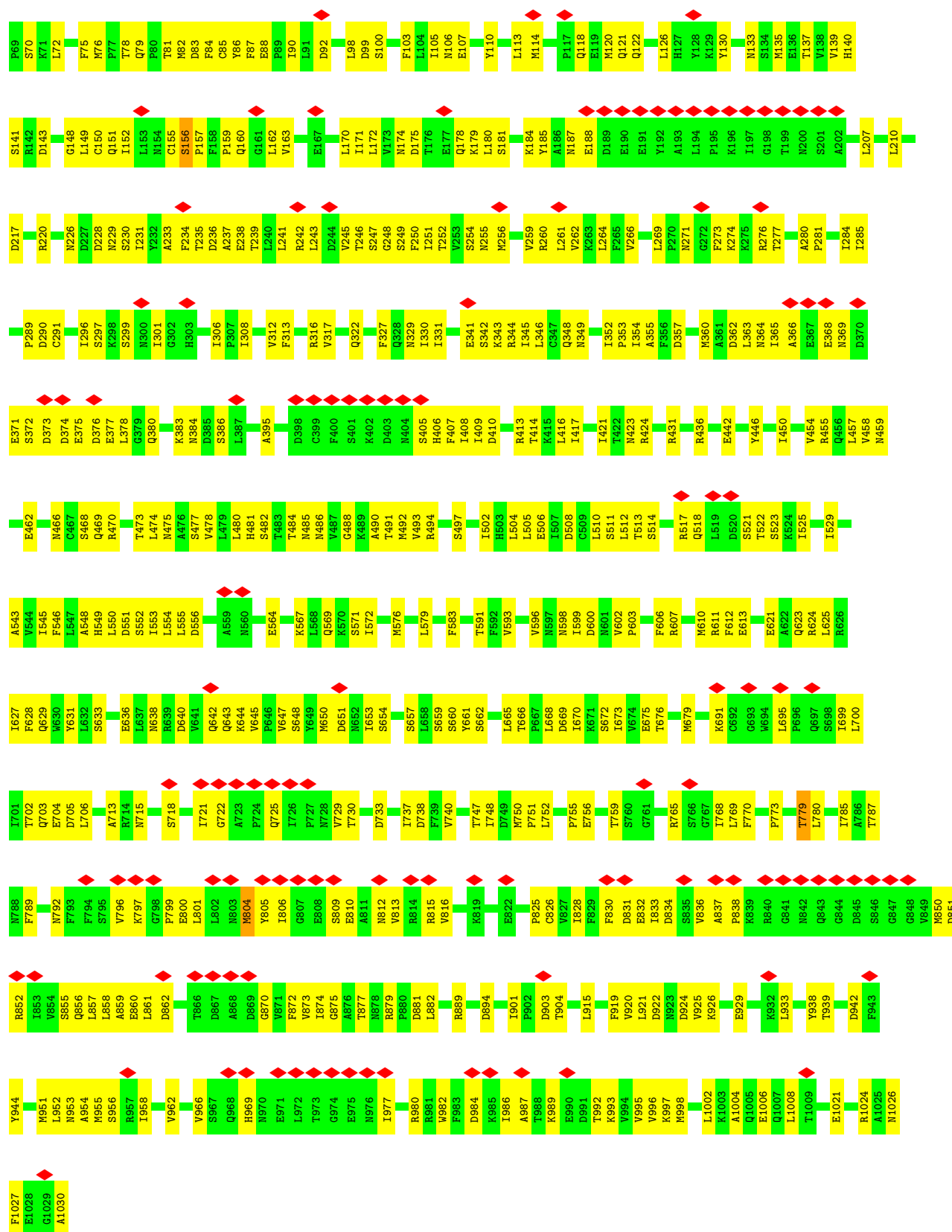


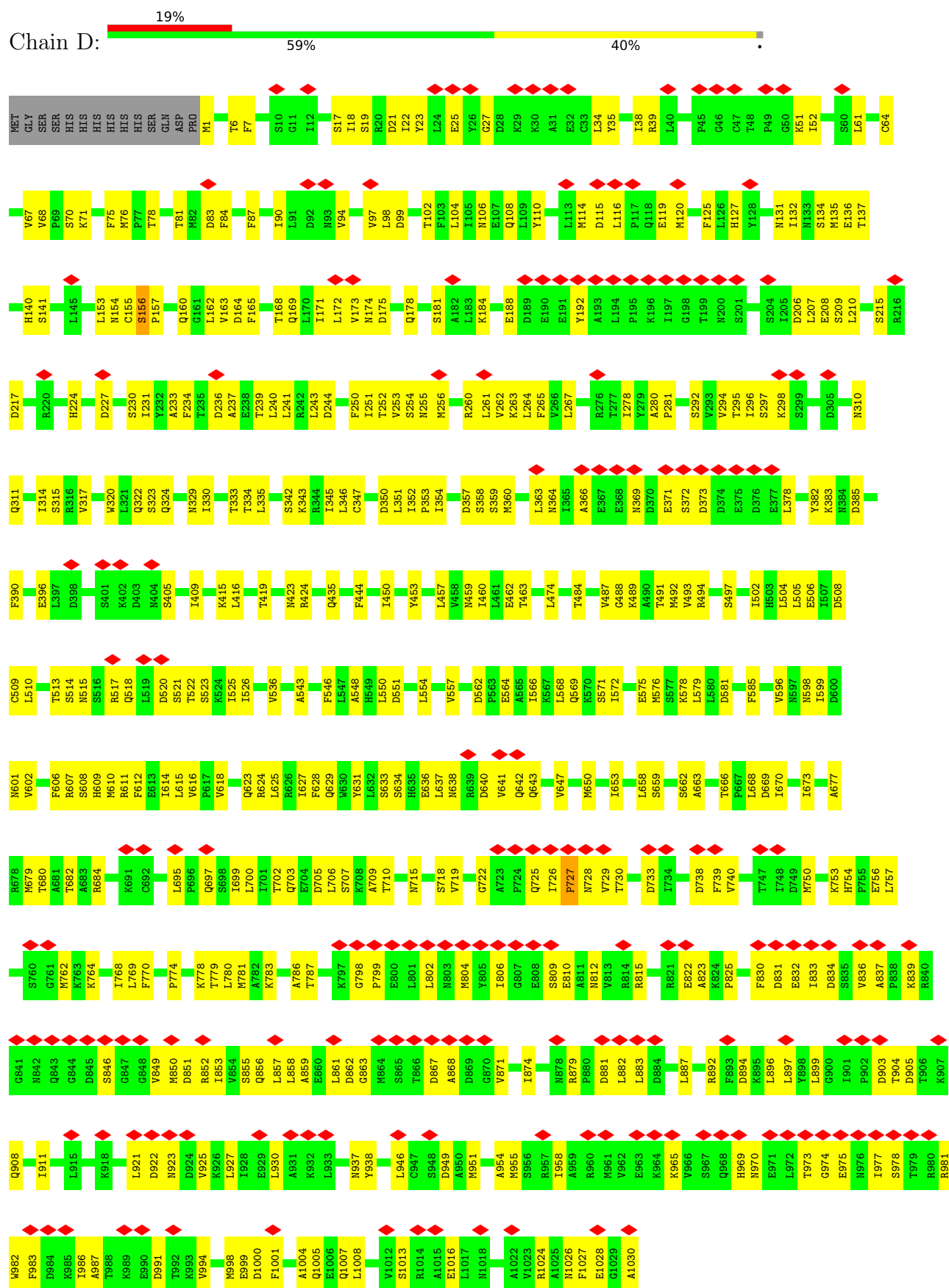
● Molecule 1: Peroxisomal ATPase PEX1











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	43478	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.487	Depositor
Minimum map value	-0.197	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.107	Depositor
Map size (Å)	322.0, 322.0, 322.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	A	0.14	0/6617	0.42	6/8934 (0.1%)
1	C	0.13	0/6617	0.36	2/8934 (0.0%)
1	E	0.13	0/6617	0.38	4/8934 (0.0%)
2	B	0.15	0/8294	0.36	0/11246
2	D	0.14	0/8294	0.34	0/11246
2	F	0.14	0/8300	0.39	2/11254 (0.0%)
All	All	0.14	0/44739	0.37	14/60548 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	548	ASP	CA-C-N	10.65	141.63	122.46
1	E	548	ASP	C-N-CA	10.65	141.63	122.46
1	A	265	ASN	CA-C-N	10.46	140.51	121.15
1	A	265	ASN	C-N-CA	10.46	140.51	121.15
2	F	805	TYR	CA-C-N	9.63	139.31	121.97
2	F	805	TYR	C-N-CA	9.63	139.31	121.97
1	C	548	ASP	CA-C-N	9.51	139.71	121.54
1	C	548	ASP	C-N-CA	9.51	139.71	121.54
1	A	256	ARG	CA-C-N	8.52	134.65	122.05
1	A	256	ARG	C-N-CA	8.52	134.65	122.05
1	E	543	ASN	CA-C-N	8.40	131.88	120.54
1	E	543	ASN	C-N-CA	8.40	131.88	120.54
1	A	389	GLU	CA-C-N	8.07	133.57	122.19
1	A	389	GLU	C-N-CA	8.07	133.57	122.19

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	A	6501	6563	6568	356	0
1	C	6501	6212	6568	398	0
1	E	6501	6212	6568	324	0
2	B	8126	8128	8130	425	0
2	D	8126	8128	8130	425	0
2	F	8132	2419	8134	1175	0
3	A	62	0	24	22	0
3	B	62	0	24	17	0
3	C	62	0	24	33	0
3	D	62	0	24	13	0
3	E	31	0	12	9	0
3	F	31	0	12	19	0
All	All	44197	37662	44218	2907	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 33.

All (2907) 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)
2:F:650:MET:HE1	2:F:702:THR:HA	1.33	1.11
2:F:544:VAL:HG23	2:F:591:THR:HG23	1.33	1.10
2:F:306:ILE:HD12	2:F:307:PRO:HD2	1.25	1.08
2:F:133:ASN:HB2	2:F:136:GLU:HB3	1.32	1.08
2:F:1:MET:HE1	2:F:3:ALA:HB2	1.36	1.06
2:F:31:ALA:HA	2:F:34:LEU:HD21	1.36	1.06
2:F:335:LEU:HD12	2:F:339:PHE:HE2	1.22	1.03
2:F:479:LEU:HB2	2:F:610:MET:HE3	1.39	1.03
2:F:12:ILE:HG23	2:F:72:LEU:HA	1.42	1.02
2:F:38:ILE:O	2:F:50:GLY:HA2	1.59	1.02
1:A:233:VAL:HG22	1:A:290:ILE:HD11	1.42	1.01
2:F:247:SER:HB2	2:F:266:VAL:HG23	1.40	1.01
2:B:360:MET:HE1	2:B:363:LEU:HD22	1.42	1.00
1:C:947:PHE:HB3	2:D:172:LEU:HD23	1.42	1.00
1:C:944:ILE:HD12	1:C:966:LEU:HD13	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:516:SER:HA	2:F:521:SER:HB2	1.43	0.98
2:F:429:LEU:HD22	2:F:499:TYR:HA	1.45	0.98
1:E:309:LYS:NZ	1:E:516:TRP:O	1.96	0.97
2:F:79:GLN:HB2	2:F:269:LEU:HD11	1.46	0.97
2:F:262:VAL:HG13	2:F:264:LEU:HD21	1.46	0.97
2:F:100:SER:HA	2:F:169:GLN:HB3	1.45	0.97
2:D:76:MET:SD	2:D:78:THR:OG1	2.23	0.95
1:E:964:THR:HA	1:E:968:GLN:HA	1.45	0.95
2:F:478:VAL:HG13	2:F:593:VAL:HG23	1.46	0.95
2:F:99:ASP:O	2:F:169:GLN:N	2.00	0.94
1:C:329:THR:OG1	1:C:372:LYS:O	1.85	0.94
1:C:961:ARG:HD2	2:D:171:ILE:HD11	1.49	0.94
1:E:949:ILE:HG12	1:E:951:GLU:OE1	1.67	0.94
2:F:251:ILE:HD13	2:F:264:LEU:HD23	1.48	0.94
2:F:114:MET:HE2	2:F:114:MET:HA	1.48	0.93
1:A:746:LEU:HD11	3:A:1101:ATP:H2'	1.51	0.92
1:C:431:ASP:O	1:C:469:ARG:NH2	2.01	0.92
2:D:71:LYS:NZ	2:D:188:GLU:OE1	2.04	0.91
2:F:103:PHE:HZ	2:F:170:LEU:HD12	1.34	0.90
2:F:328:GLN:HA	2:F:331:ILE:HD11	1.53	0.90
2:F:706:LEU:O	2:F:710:THR:HG23	1.72	0.90
2:B:457:LEU:HD13	2:B:492:MET:HE1	1.53	0.90
2:F:486:ASN:HD22	2:F:668:LEU:HD12	1.37	0.89
2:F:375:GLU:HA	2:F:378:LEU:HD13	1.53	0.89
2:F:104:LEU:HD11	2:F:175:ASP:HB2	1.54	0.89
2:F:261:LEU:HD12	2:F:262:VAL:H	1.36	0.89
1:A:357:THR:OG1	1:A:379:GLN:O	1.90	0.89
1:C:938:VAL:HG12	1:C:940:GLY:H	1.38	0.88
2:F:360:MET:HE1	2:F:363:LEU:HD23	1.55	0.88
1:C:700:GLY:O	3:C:1102:ATP:N6	2.07	0.88
2:F:457:LEU:HD23	2:F:492:MET:HE1	1.53	0.88
2:F:419:THR:HG22	2:F:420:ASN:H	1.39	0.88
2:F:643:GLN:OE1	2:F:643:GLN:N	2.07	0.87
2:D:366:ALA:O	2:D:369:ASN:ND2	2.07	0.87
2:B:482:SER:OG	2:B:484:THR:O	1.92	0.87
1:E:865:PRO:O	1:E:870:ARG:NH1	2.08	0.87
1:C:912:ASP:OD1	1:C:1003:SER:OG	1.92	0.87
2:B:341:GLU:OE2	2:B:344:ARG:NH2	2.08	0.87
2:F:653:ILE:HD11	2:F:658:LEU:HD21	1.57	0.86
1:C:1005:SER:OG	1:C:1008:GLU:OE1	1.91	0.86
2:B:643:GLN:OE1	2:B:644:LYS:N	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:509:CYS:O	2:D:513:THR:OG1	1.93	0.86
1:E:966:LEU:HD21	2:F:173:VAL:HG21	1.55	0.86
2:D:598:ASN:ND2	2:D:601:ASN:OD1	2.07	0.86
2:F:143:ASP:HB2	2:F:152:ILE:HD12	1.58	0.85
2:F:354:ILE:HG22	2:F:388:VAL:HG23	1.55	0.85
1:C:669:GLU:N	1:C:669:GLU:OE1	2.09	0.85
2:F:25:GLU:OE1	2:F:25:GLU:N	2.08	0.85
2:F:280:ALA:HB1	2:F:284:ILE:HD13	1.57	0.85
2:B:654:SER:O	2:B:657:SER:OG	1.92	0.85
2:F:97:VAL:HG22	2:F:162:LEU:HB3	1.56	0.84
2:F:522:THR:O	2:F:526:ILE:HG12	1.76	0.84
1:E:739:TYR:O	1:E:744:LYS:NZ	2.09	0.84
3:A:1101:ATP:O5'	2:B:889:ARG:NH2	2.10	0.84
2:F:409:ILE:HG23	2:F:414:THR:HG21	1.60	0.84
2:F:251:ILE:CD1	2:F:264:LEU:HD23	2.07	0.83
2:F:391:PHE:HD2	2:F:422:THR:HG21	1.41	0.83
1:C:743:GLY:N	3:C:1102:ATP:H5'1	1.93	0.83
2:F:516:SER:HA	2:F:521:SER:CB	2.06	0.83
1:E:351:LEU:O	1:E:354:SER:OG	1.97	0.83
2:F:104:LEU:HB3	2:F:151:GLN:HB3	1.60	0.83
2:F:162:LEU:HD12	2:F:163:VAL:H	1.43	0.83
2:F:678:ARG:O	2:F:682:THR:HG23	1.77	0.83
1:C:764:GLY:O	2:D:852:ARG:NH2	2.11	0.83
2:F:703:GLN:OE1	2:F:703:GLN:N	2.12	0.83
2:F:380:GLN:O	2:F:383:LYS:NZ	2.11	0.83
2:B:1:MET:N	2:B:87:PHE:O	2.11	0.83
2:B:329:ASN:ND2	2:B:364:ASN:OD1	2.10	0.83
2:F:132:ILE:HG23	2:F:137:THR:HG21	1.61	0.83
2:F:470:ARG:HH11	2:F:472:ILE:HD13	1.42	0.82
2:F:716:GLU:O	2:F:719:VAL:HG22	1.79	0.82
1:C:449:SER:OG	1:C:451:ILE:O	1.96	0.82
1:A:739:TYR:O	1:A:744:LYS:NZ	2.13	0.82
1:C:763:LYS:NZ	2:D:856:GLN:O	2.12	0.82
2:B:220:ARG:O	2:B:247:SER:OG	1.97	0.82
2:F:254:SER:HB3	2:F:259:VAL:HG13	1.58	0.82
2:D:134:SER:OG	2:D:135:MET:SD	2.38	0.82
2:F:144:ILE:CD1	2:F:151:GLN:HG2	2.09	0.82
1:E:826:ASP:OD2	1:E:855:ARG:NH2	2.12	0.82
2:F:491:THR:CG2	3:F:1101:ATP:H5'1	2.10	0.82
2:F:715:ASN:O	2:F:719:VAL:HG13	1.80	0.82
1:C:612:LEU:HD11	1:C:645:LEU:HD12	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:251:ILE:HG22	2:F:296:ILE:HD11	1.62	0.81
2:F:623:GLN:O	2:F:627:ILE:HG12	1.80	0.81
2:D:778:LYS:NZ	3:D:1602:ATP:O2B	2.13	0.81
1:E:595:SER:OG	1:E:596:GLU:OE1	1.97	0.81
1:E:882:ASP:OD2	1:E:885:THR:OG1	1.98	0.81
2:F:637:LEU:O	2:F:678:ARG:NH2	2.12	0.81
2:F:687:GLN:HB3	2:F:691:LYS:HZ2	1.45	0.81
2:D:181:SER:O	2:D:184:LYS:NZ	2.13	0.81
1:E:621:ILE:O	1:E:664:ASN:ND2	2.13	0.81
2:F:207:LEU:HD13	2:F:278:ILE:HG23	1.60	0.81
2:F:566:ILE:O	2:F:570:LYS:HG2	1.79	0.81
1:C:515:TYR:O	1:C:571:ARG:NH1	2.13	0.81
1:C:624:LEU:O	1:C:626:ARG:NH2	2.14	0.81
2:F:380:GLN:OE1	2:F:380:GLN:N	2.13	0.81
1:E:870:ARG:NE	1:E:902:ALA:O	2.13	0.81
2:F:144:ILE:HG13	2:F:183:LEU:HD21	1.62	0.81
2:F:621:GLU:N	2:F:621:GLU:OE2	2.14	0.81
2:B:704:GLU:OE1	2:B:704:GLU:N	2.14	0.81
2:F:335:LEU:HD12	2:F:339:PHE:CE2	2.12	0.81
2:F:566:ILE:HG22	2:F:570:LYS:HE3	1.63	0.81
2:F:681:ALA:HB1	2:F:699:ILE:HG22	1.63	0.81
1:C:641:SER:OG	1:C:644:ASP:OD1	1.98	0.81
2:F:109:LEU:HA	2:F:112:LYS:HZ1	1.45	0.80
2:F:310:ASN:O	2:F:415:LYS:N	2.11	0.80
2:F:957:ARG:NH2	2:F:999:GLU:OE2	2.14	0.80
2:B:246:THR:O	2:B:249:SER:OG	1.97	0.80
1:E:967:GLN:OE1	1:E:967:GLN:N	2.13	0.80
2:F:576:MET:HE3	2:F:576:MET:C	2.07	0.80
2:B:657:SER:O	2:B:660:SER:OG	1.96	0.80
2:B:175:ASP:OD2	2:B:179:LYS:N	2.14	0.80
2:F:284:ILE:H	2:F:284:ILE:HD12	1.46	0.80
2:F:503:HIS:HB2	2:F:543:ALA:HB2	1.61	0.80
1:C:852:ARG:NH1	3:B:1102:ATP:O3B	2.14	0.80
2:B:765:ARG:NH1	2:B:894:ASP:OD2	2.12	0.80
2:F:669:ASP:O	2:F:673:ILE:HG12	1.80	0.80
1:C:882:ASP:OD2	1:C:885:THR:OG1	1.99	0.80
1:C:316:GLN:O	1:C:319:GLN:NE2	2.15	0.80
2:F:575:GLU:OE1	2:F:575:GLU:N	2.14	0.80
2:D:520:ASP:OD1	2:D:523:SER:OG	1.99	0.80
1:C:870:ARG:O	1:C:874:LEU:HD22	1.81	0.79
2:B:621:GLU:OE2	2:B:659:SER:OG	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:338:PHE:O	2:F:344:ARG:NH2	2.14	0.79
2:F:433:ASN:ND2	2:F:442:GLU:OE2	2.14	0.79
2:B:256:MET:HE2	2:B:256:MET:O	1.82	0.79
1:A:363:PRO:O	1:A:366:GLN:NE2	2.16	0.79
1:C:957:GLU:O	1:C:961:ARG:HG2	1.81	0.79
2:F:100:SER:OG	2:F:156:SER:HB3	1.82	0.79
1:E:951:GLU:CG	2:F:169:GLN:HG2	2.13	0.79
2:F:144:ILE:HD11	2:F:151:GLN:HG2	1.63	0.79
2:F:446:TYR:HB3	2:F:451:PHE:HD2	1.46	0.79
2:F:557:VAL:CG1	2:F:566:ILE:HG23	2.13	0.79
2:F:102:THR:N	2:F:154:ASN:O	2.14	0.79
2:F:105:ILE:HG12	2:F:173:VAL:O	1.83	0.79
2:F:20:ARG:HA	2:F:57:LEU:HD11	1.65	0.79
2:F:104:LEU:HD21	2:F:180:LEU:HG	1.65	0.78
2:F:460:ILE:HD12	2:F:612:PHE:HE2	1.47	0.78
2:B:19:SER:OG	2:B:21:ASP:OD1	2.01	0.78
2:B:506:GLU:OE1	2:B:506:GLU:N	2.16	0.78
2:F:70:SER:OG	2:F:77:PRO:HD3	1.84	0.78
2:F:518:GLN:N	2:F:518:GLN:OE1	2.17	0.78
2:F:98:LEU:HD13	2:F:155:CYS:HB3	1.65	0.78
2:F:491:THR:HG21	3:F:1101:ATP:H5'1	1.65	0.78
1:E:958:ASN:HB2	1:E:960:LEU:HD12	1.66	0.78
2:B:118:GLN:OE1	2:B:121:GLN:NE2	2.17	0.78
1:C:429:ASP:OD1	1:C:430:GLU:N	2.17	0.78
1:A:548:ASP:O	1:A:551:SER:OG	2.00	0.77
2:B:491:THR:CG2	3:B:1101:ATP:H5'1	2.13	0.77
2:F:100:SER:CA	2:F:169:GLN:HB3	2.14	0.77
1:A:429:ASP:OD2	1:A:469:ARG:NE	2.17	0.77
1:E:638:GLU:OE1	1:E:638:GLU:N	2.18	0.77
2:F:127:HIS:ND1	2:F:132:ILE:O	2.17	0.77
1:A:633:LEU:O	1:A:637:THR:OG1	2.01	0.77
1:E:313:GLU:OE1	1:E:313:GLU:N	2.17	0.77
1:E:966:LEU:HD11	2:F:173:VAL:HG11	1.66	0.77
2:F:523:SER:HA	2:F:526:ILE:HD11	1.64	0.77
2:B:329:ASN:OD1	2:B:330:ILE:N	2.15	0.77
1:C:877:ILE:O	1:C:880:SER:OG	2.03	0.77
1:E:954:ARG:HD3	1:E:961:ARG:HH22	1.48	0.77
2:B:792:ASN:ND2	2:B:825:PRO:O	2.18	0.77
2:B:901:ILE:HD12	2:B:939:THR:HG22	1.67	0.77
2:D:718:SER:O	2:D:722:GLY:N	2.17	0.77
1:C:763:LYS:NZ	2:D:859:ALA:HB3	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:ASP:OD1	2:F:344:ARG:NH1	2.18	0.77
2:D:351:LEU:C	2:D:352:ILE:HD13	2.09	0.77
2:D:642:GLN:N	2:D:642:GLN:OE1	2.17	0.77
2:D:1026:ASN:OD1	2:D:1027:PHE:N	2.17	0.77
2:F:121:GLN:OE1	2:F:121:GLN:N	2.18	0.77
1:E:828:ALA:HB1	2:D:727:PRO:HG3	1.67	0.77
2:F:215:SER:OG	2:F:217:ASP:OD1	2.03	0.77
2:F:346:LEU:HD13	2:F:409:ILE:HG12	1.66	0.77
1:C:956:GLU:OE1	1:C:956:GLU:N	2.19	0.76
2:F:434:LEU:HD12	2:F:434:LEU:H	1.50	0.76
2:F:563:PRO:HA	2:F:566:ILE:HD12	1.67	0.76
2:F:622:ALA:O	2:F:626:ARG:HG2	1.85	0.76
1:E:699:ILE:O	1:E:706:LYS:NZ	2.17	0.76
2:F:475:ASN:HD21	2:F:611:ARG:HH21	1.33	0.76
2:D:70:SER:OG	2:D:75:PHE:O	2.03	0.76
1:A:443:MET:HA	1:A:443:MET:HE3	1.67	0.76
1:A:469:ARG:HH12	3:A:1102:ATP:H5'1	1.51	0.76
1:C:504:GLN:NE2	2:B:511:SER:O	2.18	0.76
1:E:828:ALA:HB3	2:D:725:GLN:NE2	2.01	0.76
2:F:255:ASN:ND2	2:F:291:CYS:SG	2.59	0.76
2:B:236:ASP:OD1	2:B:239:THR:OG1	2.00	0.76
2:B:518:GLN:O	2:B:521:SER:OG	2.01	0.76
2:B:376:ASP:OD2	2:B:377:GLU:N	2.19	0.76
1:A:567:LYS:NZ	2:F:383:LYS:HB2	1.99	0.76
1:E:951:GLU:OE2	2:F:170:LEU:N	2.18	0.76
1:E:398:MET:HE2	1:E:398:MET:N	2.01	0.76
1:E:654:TYR:OH	2:F:464:SER:HB3	1.86	0.76
1:C:611:LEU:HD11	3:C:1101:ATP:HN61	1.50	0.76
1:E:580:GLN:OE1	1:E:581:LYS:N	2.18	0.76
2:F:93:ASN:ND2	2:F:692:CYS:SG	2.59	0.76
2:F:506:GLU:OE1	2:F:506:GLU:N	2.19	0.76
2:B:926:LYS:NZ	2:B:998:MET:SD	2.59	0.76
2:F:226:ASN:O	2:F:342:SER:OG	2.04	0.76
2:D:682:THR:HA	2:D:699:ILE:HD11	1.68	0.76
1:A:606:HIS:O	1:A:610:LYS:NZ	2.19	0.75
1:A:947:PHE:CE2	2:B:172:LEU:HD21	2.21	0.75
2:F:50:GLY:H	2:F:697:GLN:HE21	1.34	0.75
2:F:951:MET:HE3	2:F:951:MET:HA	1.69	0.75
1:E:645:LEU:O	1:E:649:THR:HG23	1.86	0.75
2:F:103:PHE:CZ	2:F:170:LEU:HD12	2.21	0.75
2:F:621:GLU:HA	2:F:624:ARG:CZ	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:966:LEU:HD11	2:F:173:VAL:CG1	2.17	0.75
2:B:779:THR:OG1	3:B:1102:ATP:O1B	2.02	0.75
1:E:643:LEU:HD11	3:E:1101:ATP:H4'	1.69	0.75
2:F:576:MET:HE3	2:F:577:SER:N	2.02	0.75
2:D:104:LEU:HD21	2:D:153:LEU:HD11	1.68	0.75
1:A:503:THR:O	1:A:507:ILE:HD12	1.86	0.75
2:F:20:ARG:HD2	2:F:57:LEU:HD11	1.68	0.75
2:F:39:ARG:HH21	2:F:47:CYS:HA	1.52	0.75
2:F:146:THR:H	2:F:150:CYS:HB3	1.50	0.75
2:F:717:PHE:O	2:F:720:SER:OG	2.01	0.75
2:D:905:ASP:OD1	2:D:908:GLN:NE2	2.19	0.75
1:E:647:ILE:HD11	2:F:611:ARG:HD3	1.68	0.75
1:C:638:GLU:OE1	1:C:638:GLU:N	2.18	0.75
2:F:134:SER:HB2	2:F:165:PHE:CD1	2.22	0.75
2:F:191:GLU:OE1	2:F:191:GLU:N	2.15	0.75
1:A:819:ASN:O	1:A:823:THR:HG23	1.87	0.75
1:E:227:LYS:O	1:E:227:LYS:NZ	2.17	0.75
2:F:52:ILE:HG23	2:F:138:VAL:HG11	1.69	0.75
2:F:74:GLY:O	2:F:186:ALA:N	2.20	0.75
1:C:949:ILE:N	1:C:951:GLU:OE1	2.21	0.74
2:F:357:ASP:HB3	2:F:383:LYS:O	1.86	0.74
1:A:282:ASP:OD1	1:A:283:SER:N	2.19	0.74
2:F:320:TRP:HH2	2:F:532:LYS:HD2	1.52	0.74
2:F:306:ILE:CG1	2:F:408:ILE:HG12	2.18	0.74
2:F:457:LEU:HD23	2:F:492:MET:CE	2.17	0.74
2:F:460:ILE:HD12	2:F:612:PHE:CE2	2.21	0.74
2:B:235:THR:OG1	2:B:277:THR:O	2.03	0.74
1:E:256:ARG:NH2	1:E:258:SER:OG	2.20	0.74
2:F:274:LYS:O	2:F:277:THR:OG1	2.04	0.74
2:F:385:ASP:OD1	2:F:386:SER:N	2.21	0.74
2:F:26:TYR:CG	2:F:34:LEU:HD22	2.22	0.74
2:F:209:SER:HA	2:F:285:ILE:HD11	1.70	0.74
2:F:718:SER:HA	2:F:721:ILE:CG1	2.17	0.74
2:B:317:VAL:O	2:B:322:GLN:NE2	2.21	0.74
1:A:656:LEU:O	1:A:660:ARG:NH1	2.21	0.74
2:F:1026:ASN:OD1	2:F:1027:PHE:N	2.20	0.74
1:A:316:GLN:NE2	1:A:317:MET:O	2.21	0.74
2:F:23:TYR:CB	2:F:57:LEU:HD13	2.18	0.74
2:D:260:ARG:NE	2:D:350:ASP:OD2	2.20	0.74
1:C:865:PRO:O	1:C:870:ARG:NH1	2.21	0.73
1:E:244:GLN:O	1:E:279:ILE:N	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:718:SER:HA	2:F:721:ILE:HG13	1.70	0.73
1:E:852:ARG:NH1	3:D:1602:ATP:O2G	2.20	0.73
1:A:332:ILE:O	1:A:396:THR:OG1	2.04	0.73
1:C:216:LEU:HD23	1:C:290:ILE:HB	1.68	0.73
2:F:216:ARG:O	2:F:219:LEU:HG	1.87	0.73
2:F:329:ASN:O	2:F:333:THR:HG23	1.88	0.73
2:B:702:THR:OG1	2:B:705:ASP:OD2	2.04	0.73
2:F:358:SER:N	2:F:385:ASP:OD2	2.21	0.73
1:C:331:ASN:ND2	1:C:370:GLU:OE2	2.21	0.73
2:F:124:GLN:HG3	2:F:128:TYR:CE2	2.23	0.73
2:D:653:ILE:HG23	2:D:703:GLN:OE1	1.88	0.73
1:A:920:ALA:HB1	1:A:988:VAL:HG21	1.70	0.73
1:C:347:TYR:OH	1:C:365:GLU:OE2	2.05	0.73
1:C:469:ARG:NH1	1:C:469:ARG:O	2.21	0.73
1:C:949:ILE:HG12	2:D:172:LEU:HD22	1.70	0.73
2:F:491:THR:HG21	3:F:1101:ATP:H2'	1.70	0.73
2:F:508:ASP:OD1	2:F:510:LEU:N	2.20	0.73
2:F:666:THR:N	2:F:669:ASP:OD1	2.21	0.73
2:F:833:ILE:O	2:F:837:ALA:N	2.20	0.73
1:E:636:GLU:OE1	1:E:636:GLU:N	2.21	0.73
2:F:570:LYS:HA	2:F:573:ASN:HD21	1.53	0.73
2:F:661:TYR:O	2:F:714:ARG:NH2	2.15	0.73
2:F:687:GLN:O	2:F:691:LYS:HD3	1.89	0.73
2:F:792:ASN:ND2	2:F:823:ALA:O	2.21	0.73
2:D:867:ASP:OD1	2:D:868:ALA:N	2.22	0.73
1:A:564:ILE:HG21	1:A:572:ILE:HD13	1.70	0.72
1:C:947:PHE:CB	2:D:172:LEU:HD23	2.19	0.72
2:F:488:GLY:HA3	3:F:1101:ATP:C2	2.24	0.72
2:F:503:HIS:ND1	2:F:540:ALA:O	2.19	0.72
2:F:447:ASP:OD2	2:F:450:ILE:HD12	1.90	0.72
2:F:458:VAL:HA	2:F:461:LEU:CD1	2.19	0.72
2:F:677:ALA:HB1	2:F:701:ILE:CG2	2.18	0.72
1:A:725:ASN:ND2	2:F:992:THR:O	2.21	0.72
2:F:23:TYR:HB3	2:F:57:LEU:HD13	1.71	0.72
2:F:345:ILE:HG13	2:F:408:ILE:CD1	2.20	0.72
2:F:316:ARG:HB3	2:F:421:ILE:CD1	2.20	0.72
1:A:234:TYR:O	1:A:290:ILE:HD12	1.89	0.72
2:B:468:SER:OG	2:B:469:GLN:NE2	2.22	0.72
1:E:622:MET:C	1:E:622:MET:HE2	2.15	0.72
2:F:6:THR:HG23	2:F:67:VAL:HG22	1.70	0.72
2:F:635:HIS:CE1	2:F:636:GLU:HG2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:GLU:OE1	2:B:462:GLU:N	2.23	0.72
1:A:933:ASP:OD1	1:A:934:GLN:N	2.21	0.72
1:C:568:ASP:OD2	2:B:383:LYS:NZ	2.18	0.72
2:F:522:THR:HG22	2:F:572:ILE:HG22	1.72	0.72
1:C:209:GLN:OE1	1:C:316:GLN:NE2	2.22	0.72
2:F:461:LEU:H	2:F:461:LEU:HD12	1.54	0.72
1:C:423:VAL:HG12	2:D:585:PHE:CZ	2.25	0.72
1:A:252:LYS:NZ	2:F:364:ASN:O	2.21	0.71
1:C:712:THR:OG1	1:C:731:ARG:NH1	2.22	0.71
1:E:494:LEU:HD11	1:E:506:LEU:HD21	1.71	0.71
2:F:839:LYS:NZ	2:F:881:ASP:O	2.20	0.71
1:C:631:SER:O	1:C:634:SER:OG	2.05	0.71
2:B:99:ASP:OD1	2:B:100:SER:N	2.23	0.71
2:B:610:MET:N	2:B:610:MET:SD	2.62	0.71
2:B:810:GLU:N	2:B:810:GLU:OE1	2.23	0.71
2:D:236:ASP:OD1	2:D:237:ALA:N	2.24	0.71
1:A:596:GLU:OE1	1:A:598:TRP:NE1	2.23	0.71
1:C:546:GLN:NE2	1:C:548:ASP:OD1	2.23	0.71
1:A:564:ILE:O	1:A:568:ASP:N	2.21	0.71
1:C:713:LEU:O	1:C:717:THR:OG1	2.09	0.71
1:E:316:GLN:OE1	1:E:318:ASN:N	2.23	0.71
2:F:148:GLY:O	2:F:180:LEU:HB3	1.90	0.71
2:F:646:PRO:O	2:F:698:SER:OG	2.07	0.71
1:A:451:ILE:O	2:F:679:MET:HE1	1.90	0.71
2:B:82:MET:SD	2:B:83:ASP:N	2.63	0.71
2:D:684:ARG:NH2	2:D:705:ASP:OD2	2.23	0.71
2:F:537:LEU:HD21	2:F:587:PHE:CD1	2.26	0.71
2:F:102:THR:HB	2:F:154:ASN:H	1.55	0.71
2:F:190:GLU:HG3	2:F:193:ALA:H	1.56	0.71
1:A:745:THR:OG1	3:A:1101:ATP:O1A	2.08	0.71
2:F:250:PHE:HB3	2:F:261:LEU:HD11	1.73	0.71
2:F:489:LYS:HD2	2:F:595:SER:HB2	1.72	0.71
2:F:530:ARG:O	2:F:534:GLU:HG2	1.89	0.71
2:F:977:ILE:HD13	2:F:986:ILE:HD11	1.72	0.71
2:B:260:ARG:NH2	2:B:349:ASN:O	2.24	0.71
1:A:866:THR:OG1	1:A:869:GLU:OE1	2.08	0.70
2:D:99:ASP:O	2:D:169:GLN:N	2.22	0.70
1:C:746:LEU:HD11	3:C:1102:ATP:C2'	2.20	0.70
2:F:377:GLU:O	2:F:380:GLN:NE2	2.24	0.70
2:B:83:ASP:OD1	2:B:84:PHE:N	2.24	0.70
1:C:961:ARG:HD2	2:D:171:ILE:CD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:ILE:HD13	2:F:145:LEU:HA	1.74	0.70
2:F:82:MET:HA	2:F:268:LEU:HD13	1.72	0.70
2:F:489:LYS:O	2:F:493:VAL:HG23	1.91	0.70
2:B:636:GLU:OE1	2:B:636:GLU:N	2.23	0.70
2:F:216:ARG:NH2	2:F:223:PRO:O	2.25	0.70
2:B:360:MET:HE2	2:B:360:MET:HA	1.71	0.70
1:A:300:PHE:O	1:A:302:THR:HG23	1.91	0.70
1:C:746:LEU:HD11	3:C:1102:ATP:H2'	1.71	0.70
1:C:949:ILE:HD12	2:D:119:GLU:CG	2.22	0.70
2:F:563:PRO:HA	2:F:566:ILE:CD1	2.21	0.70
2:B:374:ASP:O	2:B:378:LEU:HD12	1.91	0.70
1:A:469:ARG:NH2	3:A:1102:ATP:H2'	2.06	0.70
1:C:944:ILE:HB	1:C:959:ARG:HH22	1.55	0.70
2:F:169:GLN:HE22	2:F:171:ILE:HG13	1.57	0.70
2:F:228:ASP:HB2	2:F:343:LYS:O	1.90	0.70
2:F:522:THR:HG22	2:F:572:ILE:CG2	2.22	0.70
2:B:492:MET:SD	2:B:493:VAL:N	2.65	0.70
2:B:770:PHE:N	2:B:875:GLY:O	2.23	0.70
1:A:309:LYS:NZ	1:A:516:TRP:O	2.24	0.70
1:E:647:ILE:CD1	2:F:611:ARG:HD3	2.22	0.70
2:B:413:ARG:NH1	2:B:413:ARG:O	2.25	0.70
1:A:237:ASP:N	1:A:282:ASP:O	2.24	0.70
1:A:435:THR:O	1:A:438:SER:OG	2.07	0.70
2:F:144:ILE:HD11	2:F:183:LEU:HD11	1.74	0.70
2:F:306:ILE:HG13	2:F:408:ILE:HG12	1.74	0.70
2:F:372:SER:O	2:F:375:GLU:HG2	1.91	0.70
2:F:478:VAL:CG1	2:F:593:VAL:HG23	2.21	0.70
1:A:922:LEU:HD11	2:B:765:ARG:HE	1.56	0.70
2:F:243:LEU:O	2:F:245:VAL:HG23	1.92	0.70
2:F:946:LEU:HD21	2:F:1005:GLN:HA	1.74	0.70
2:D:610:MET:N	2:D:610:MET:SD	2.65	0.70
1:C:224:ASP:OD1	1:C:234:TYR:OH	2.10	0.69
2:F:233:ALA:O	2:F:264:LEU:HA	1.92	0.69
2:B:130:TYR:OH	2:B:150:CYS:SG	2.49	0.69
2:B:446:TYR:CE2	2:B:454:VAL:HG21	2.26	0.69
2:D:810:GLU:OE1	2:D:810:GLU:N	2.24	0.69
1:C:933:ASP:HB2	1:C:939:PRO:HB3	1.74	0.69
1:A:468:THR:OG1	1:A:525:ASP:OD2	2.06	0.69
1:C:451:ILE:O	1:C:452:ILE:HD13	1.91	0.69
2:F:840:ARG:NE	2:F:851:ASP:OD1	2.26	0.69
2:D:315:SER:OG	2:D:419:THR:OG1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:OE1	1:A:389:GLU:N	2.25	0.69
1:E:964:THR:HA	1:E:968:GLN:CA	2.22	0.69
2:B:852:ARG:O	2:B:855:SER:OG	2.09	0.69
2:D:494:ARG:O	2:D:497:SER:OG	2.09	0.69
2:D:954:ALA:N	2:D:1000:ASP:OD2	2.26	0.69
2:D:969:HIS:O	2:D:973:THR:OG1	2.10	0.69
1:A:329:THR:OG1	1:A:372:LYS:O	2.06	0.69
1:A:567:LYS:HZ2	2:F:383:LYS:HB2	1.56	0.69
1:A:691:GLU:OE2	1:A:693:ASN:ND2	2.25	0.69
1:C:944:ILE:HD12	1:C:966:LEU:CD1	2.23	0.69
2:F:207:LEU:CD1	2:F:278:ILE:HG23	2.22	0.69
1:A:219:THR:HG21	1:A:285:ILE:HD11	1.73	0.69
2:F:20:ARG:HA	2:F:57:LEU:CD1	2.22	0.69
2:F:134:SER:HA	2:F:163:VAL:HG23	1.74	0.69
2:F:233:ALA:HB3	2:F:264:LEU:CD1	2.22	0.69
2:F:476:ALA:O	2:F:591:THR:OG1	2.01	0.69
1:A:442:GLU:OE1	1:A:442:GLU:N	2.23	0.69
2:F:213:THR:C	2:F:214:ILE:HD13	2.17	0.69
2:F:216:ARG:NH1	2:F:225:ILE:HD12	2.06	0.69
2:F:224:HIS:HB3	2:F:227:ASP:OD1	1.93	0.69
2:F:507:ILE:HG21	2:F:529:ILE:HD13	1.75	0.69
2:B:58:ASP:OD1	2:B:59:ASP:N	2.25	0.69
2:D:314:ILE:HD11	2:D:416:LEU:HD13	1.73	0.69
2:F:202:ALA:O	2:F:203:LEU:HD23	1.92	0.69
2:F:229:ASN:HA	2:F:232:TYR:CE1	2.28	0.69
2:F:653:ILE:CD1	2:F:658:LEU:HD21	2.22	0.69
2:D:756:GLU:OE1	2:D:756:GLU:N	2.24	0.69
2:F:137:THR:HB	2:F:163:VAL:HG21	1.75	0.69
1:E:469:ARG:NE	3:E:1101:ATP:H3'	2.07	0.69
1:E:218:SER:OG	1:E:308:ALA:N	2.26	0.68
1:E:621:ILE:HG22	1:E:664:ASN:HD21	1.59	0.68
2:F:38:ILE:O	2:F:50:GLY:CA	2.40	0.68
2:F:763:LYS:O	2:F:765:ARG:NH2	2.27	0.68
2:D:215:SER:OG	2:D:217:ASP:OD1	2.04	0.68
1:A:503:THR:OG1	1:A:553:LEU:HD11	1.93	0.68
1:A:638:GLU:N	1:A:638:GLU:OE1	2.26	0.68
2:F:256:MET:HE2	2:F:256:MET:O	1.94	0.68
2:F:235:THR:OG1	2:F:278:ILE:HA	1.92	0.68
2:F:486:ASN:HB3	2:F:668:LEU:HD12	1.75	0.68
2:F:864:MET:HA	2:F:864:MET:HE3	1.73	0.68
2:F:208:GLU:OE2	2:F:274:LYS:NZ	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:391:PHE:CD2	2:F:422:THR:HG21	2.26	0.68
1:C:622:MET:HE2	1:C:623:LYS:N	2.08	0.68
2:F:327:PHE:O	2:F:331:ILE:HG12	1.94	0.68
2:F:677:ALA:HB1	2:F:701:ILE:HG21	1.74	0.68
2:B:517:ARG:C	2:B:517:ARG:HE	2.02	0.68
1:E:785:ARG:O	1:E:788:SER:OG	2.10	0.68
2:D:726:ILE:HD12	2:D:787:THR:OG1	1.93	0.68
1:A:1011:LYS:O	1:A:1015:ILE:HG23	1.94	0.68
2:F:20:ARG:HD2	2:F:57:LEU:HD21	1.76	0.68
2:F:38:ILE:HD11	2:F:85:CYS:SG	2.33	0.68
2:F:726:ILE:HD11	2:F:787:THR:HA	1.76	0.68
2:D:329:ASN:O	2:D:333:THR:HG23	1.94	0.68
1:E:951:GLU:OE1	1:E:951:GLU:N	2.27	0.68
2:F:494:ARG:O	2:F:498:LYS:HG3	1.94	0.68
2:D:576:MET:HE2	2:D:576:MET:HA	1.76	0.68
1:A:216:LEU:HD13	1:A:235:ILE:HD13	1.75	0.68
1:A:887:GLN:N	1:A:887:GLN:OE1	2.27	0.68
1:C:218:SER:OG	1:C:308:ALA:N	2.26	0.68
1:E:938:VAL:HG22	1:E:939:PRO:HD2	1.76	0.68
2:B:633:SER:OG	2:B:636:GLU:OE1	2.09	0.68
1:C:722:ILE:HG22	2:B:992:THR:HG23	1.76	0.67
1:C:844:ASP:OD2	1:C:845:LEU:N	2.28	0.67
1:E:329:THR:OG1	1:E:372:LYS:O	2.09	0.67
2:F:372:SER:OG	2:F:374:ASP:OD2	2.11	0.67
2:F:648:SER:O	2:F:700:LEU:HA	1.95	0.67
1:E:983:GLU:OE1	1:E:983:GLU:N	2.26	0.67
2:B:801:LEU:HD21	2:B:813:VAL:HG22	1.76	0.67
1:A:425:ARG:NH1	1:A:430:GLU:OE2	2.26	0.67
2:F:254:SER:HB3	2:F:259:VAL:CG1	2.24	0.67
2:F:625:LEU:HD12	2:F:629:GLN:HE21	1.58	0.67
2:D:98:LEU:HD21	2:D:160:GLN:C	2.19	0.67
2:D:659:SER:O	2:D:662:SER:OG	2.11	0.67
2:D:946:LEU:HD21	2:D:1005:GLN:HA	1.74	0.67
1:C:338:ASP:O	1:C:338:ASP:OD1	2.13	0.67
1:C:585:ASN:OD1	1:C:587:LEU:N	2.27	0.67
2:F:240:LEU:HD12	2:F:266:VAL:HG22	1.75	0.67
2:F:328:GLN:HA	2:F:331:ILE:CD1	2.25	0.67
2:F:435:GLN:HE22	2:F:498:LYS:HE2	1.59	0.67
2:B:982:TRP:O	2:B:987:ALA:N	2.28	0.67
2:D:599:ILE:O	2:D:602:VAL:HG12	1.95	0.67
2:D:726:ILE:HD11	2:D:786:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ILE:CA	2:D:679:MET:HE1	2.25	0.67
2:F:457:LEU:CD2	2:F:492:MET:HE1	2.25	0.67
1:A:746:LEU:CD1	3:A:1101:ATP:H2'	2.25	0.67
1:C:699:ILE:HG22	3:C:1102:ATP:C2	2.30	0.67
2:F:6:THR:CG2	2:F:67:VAL:HG22	2.25	0.67
2:F:514:SER:HB2	2:F:524:LYS:NZ	2.10	0.67
2:F:565:ALA:O	2:F:568:LEU:HG	1.94	0.67
2:B:1021:GLU:OE1	2:B:1024:ARG:NH2	2.28	0.67
2:D:728:ASN:O	2:D:729:VAL:HG13	1.93	0.67
1:A:668:ARG:NH1	1:A:668:ARG:O	2.28	0.67
2:F:657:SER:HB3	2:F:661:TYR:HE1	1.60	0.67
1:E:649:THR:OG1	1:E:650:GLU:OE2	2.13	0.67
1:E:966:LEU:CD2	2:F:173:VAL:HG21	2.24	0.67
2:F:322:GLN:OE1	2:F:322:GLN:N	2.28	0.67
2:F:375:GLU:HA	2:F:378:LEU:CD1	2.23	0.67
2:B:485:ASN:OD1	2:B:486:ASN:N	2.27	0.67
1:A:658:LEU:HD12	2:B:459:ASN:ND2	2.10	0.67
1:E:959:ARG:HA	1:E:962:LEU:HB3	1.76	0.67
2:F:126:LEU:HD13	2:F:130:TYR:HE2	1.59	0.67
2:F:403:ASP:OD1	2:F:406:HIS:HB2	1.94	0.67
2:F:638:ASN:OD1	2:F:641:VAL:HG11	1.95	0.67
2:B:106:ASN:ND2	2:B:107:GLU:OE1	2.28	0.67
1:A:527:VAL:HG21	1:A:576:PHE:CD2	2.29	0.67
1:C:958:ASN:HA	1:C:961:ARG:NE	2.09	0.67
1:E:596:GLU:OE1	1:E:596:GLU:N	2.28	0.67
2:D:423:ASN:OD1	2:D:424:ARG:N	2.28	0.67
2:F:98:LEU:HD22	2:F:158:PHE:O	1.94	0.66
2:F:303:HIS:O	2:F:306:ILE:HG22	1.96	0.66
2:D:1024:ARG:NH1	2:D:1028:GLU:OE2	2.28	0.66
2:F:18:ILE:C	2:F:61:LEU:HD12	2.20	0.66
2:F:243:LEU:HD11	2:F:298:LYS:HB3	1.77	0.66
2:F:792:ASN:ND2	2:F:825:PRO:O	2.28	0.66
2:B:88:GLU:OE1	2:B:88:GLU:N	2.28	0.66
1:A:625:ASN:OD1	1:A:626:ARG:N	2.28	0.66
1:C:923:LYS:O	1:C:926:HIS:ND1	2.26	0.66
1:E:217:ARG:NH2	1:E:306:ASN:OD1	2.28	0.66
2:F:58:ASP:OD2	2:F:60:SER:OG	2.13	0.66
2:F:102:THR:HB	2:F:154:ASN:N	2.10	0.66
2:F:495:PHE:HA	2:F:498:LYS:HZ2	1.61	0.66
2:B:491:THR:HG21	3:B:1101:ATP:H5'1	1.77	0.66
2:D:491:THR:HG21	3:D:1601:ATP:H2'	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:CH2	2:F:365:ILE:HG12	2.30	0.66
2:B:29:LYS:HD3	2:B:29:LYS:N	2.09	0.66
2:B:120:MET:SD	2:B:121:GLN:N	2.68	0.66
2:D:127:HIS:ND1	2:D:132:ILE:O	2.29	0.66
1:C:350:LEU:HD23	1:C:351:LEU:HD22	1.76	0.66
2:F:79:GLN:CB	2:F:269:LEU:HD11	2.21	0.66
2:F:134:SER:HG	2:F:164:ASP:HA	1.61	0.66
2:B:436:ARG:NH2	2:B:636:GLU:OE2	2.27	0.66
2:B:488:GLY:HA3	3:B:1101:ATP:H2	1.59	0.66
2:D:634:SER:O	2:D:638:ASN:ND2	2.29	0.66
1:C:443:MET:HA	1:C:443:MET:HE3	1.77	0.66
1:C:746:LEU:HD11	3:C:1102:ATP:C3'	2.25	0.66
1:E:391:VAL:HG13	1:E:393:TRP:CZ2	2.31	0.66
1:E:454:THR:OG1	1:E:593:PHE:O	2.13	0.66
1:E:570:LYS:NZ	2:D:640:ASP:O	2.28	0.66
2:B:653:ILE:HG23	2:B:703:GLN:OE1	1.95	0.66
2:F:39:ARG:NE	2:F:47:CYS:HB2	2.11	0.66
2:F:459:ASN:HA	2:F:462:GLU:OE2	1.96	0.66
2:F:512:LEU:HG	2:F:528:TYR:CZ	2.31	0.66
2:B:828:ILE:HD12	2:B:828:ILE:O	1.95	0.66
1:E:958:ASN:HB2	1:E:960:LEU:CD1	2.24	0.66
2:F:488:GLY:HA3	3:F:1101:ATP:H2	1.59	0.66
2:D:353:PRO:O	2:D:354:ILE:HD13	1.96	0.66
1:E:954:ARG:CZ	1:E:956:GLU:HB2	2.26	0.66
2:F:352:ILE:HD13	2:F:390:PHE:HB3	1.78	0.66
2:F:454:VAL:O	2:F:458:VAL:HG13	1.95	0.66
2:B:226:ASN:O	2:B:342:SER:OG	2.12	0.66
1:C:757:LEU:HD22	1:C:791:PRO:O	1.96	0.65
2:F:126:LEU:HD13	2:F:130:TYR:CE2	2.31	0.65
2:F:668:LEU:HD21	3:F:1101:ATP:H4'	1.78	0.65
2:B:98:LEU:HD22	2:B:155:CYS:HB3	1.78	0.65
2:B:174:ASN:OD1	2:B:175:ASP:N	2.28	0.65
2:B:860:GLU:OE1	2:B:860:GLU:N	2.30	0.65
1:E:423:VAL:HG21	2:F:585:PHE:HZ	1.60	0.65
2:F:306:ILE:HD12	2:F:307:PRO:CD	2.13	0.65
2:F:328:GLN:O	2:F:332:LEU:HG	1.94	0.65
2:F:637:LEU:HG	2:F:678:ARG:HH21	1.61	0.65
1:C:247:TYR:O	1:C:312:LEU:HD23	1.95	0.65
2:F:175:ASP:HA	2:F:179:LYS:NZ	2.12	0.65
2:F:509:CYS:SG	2:F:553:ILE:HG13	2.37	0.65
2:B:718:SER:O	2:B:722:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:SER:OG	2:D:153:LEU:O	2.14	0.65
1:A:220:VAL:N	1:A:306:ASN:OD1	2.30	0.65
2:B:517:ARG:NE	2:B:517:ARG:O	2.29	0.65
1:A:849:ALA:O	1:A:855:ARG:NH2	2.30	0.65
2:F:4:SER:OG	2:F:65:SER:HA	1.96	0.65
2:F:447:ASP:OD2	2:F:626:ARG:NE	2.29	0.65
2:F:455:ARG:O	2:F:458:VAL:HG22	1.97	0.65
1:A:440:LYS:NZ	1:A:477:GLU:OE1	2.20	0.65
1:E:397:GLN:C	1:E:398:MET:HE2	2.21	0.65
2:F:81:THR:C	2:F:268:LEU:HD22	2.22	0.65
2:B:436:ARG:NE	2:B:442:GLU:OE2	2.29	0.65
2:F:298:LYS:HD2	2:F:298:LYS:C	2.22	0.65
2:F:316:ARG:HA	2:F:390:PHE:CD1	2.31	0.65
2:F:570:LYS:HA	2:F:573:ASN:ND2	2.11	0.65
1:C:792:CYS:SG	1:C:793:ILE:N	2.69	0.65
2:B:284:ILE:H	2:B:284:ILE:HD12	1.61	0.65
2:F:311:GLN:HB3	2:F:396:GLU:OE1	1.96	0.65
2:F:429:LEU:HD22	2:F:499:TYR:CA	2.23	0.65
2:B:521:SER:O	2:B:525:ILE:HD12	1.97	0.65
1:C:228:ASP:OD1	1:C:229:ASN:N	2.30	0.65
1:C:958:ASN:OD1	1:C:961:ARG:NH2	2.24	0.65
2:F:348:GLN:HE22	2:F:395:ALA:H	1.44	0.65
2:F:647:VAL:HG11	2:F:678:ARG:HH21	1.62	0.64
2:B:780:LEU:HD23	3:B:1102:ATP:O1A	1.97	0.64
1:A:806:ARG:CZ	1:A:818:VAL:HG21	2.27	0.64
1:C:324:SER:O	1:C:326:ARG:NH2	2.31	0.64
2:F:171:ILE:CG2	2:F:173:VAL:HG13	2.27	0.64
2:F:475:ASN:HB3	2:F:584:THR:HG21	1.79	0.64
2:F:479:LEU:CB	2:F:610:MET:HE3	2.23	0.64
2:D:1013:SER:OG	2:D:1016:GLU:OE2	2.11	0.64
1:A:218:SER:OG	1:A:308:ALA:N	2.30	0.64
1:E:739:TYR:CZ	1:E:1012:LEU:HD11	2.32	0.64
2:B:756:GLU:OE1	2:B:756:GLU:N	2.31	0.64
1:A:215:ILE:HD13	1:A:311:LYS:HA	1.79	0.64
1:E:948:SER:OG	2:F:172:LEU:HD13	1.98	0.64
2:F:481:HIS:O	2:F:615:LEU:HA	1.98	0.64
2:F:489:LYS:CE	2:F:595:SER:HB2	2.27	0.64
2:F:500:LEU:HB2	2:F:502:ILE:HG12	1.79	0.64
2:D:1026:ASN:O	2:D:1030:ALA:N	2.31	0.64
1:A:720:GLU:O	1:A:724:VAL:HG23	1.98	0.64
2:D:506:GLU:N	2:D:506:GLU:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:O	1:A:569:ASN:ND2	2.31	0.64
1:A:709:LEU:HD23	1:A:751:VAL:HG21	1.78	0.64
1:C:423:VAL:HG23	1:C:423:VAL:O	1.97	0.64
2:F:98:LEU:HD21	2:F:160:GLN:C	2.23	0.64
2:F:491:THR:HG23	3:F:1101:ATP:O1A	1.96	0.64
2:B:624:ARG:NE	2:B:662:SER:OG	2.30	0.64
1:E:515:TYR:HE2	2:D:360:MET:HE1	1.63	0.64
1:E:798:GLU:OE2	1:E:801:SER:OG	2.13	0.64
2:F:251:ILE:HB	2:F:264:LEU:CD2	2.28	0.64
2:F:516:SER:O	2:F:517:ARG:HD3	1.97	0.64
2:F:702:THR:OG1	2:F:705:ASP:OD2	2.15	0.64
1:A:334:TYR:HB2	1:A:367:ILE:HG22	1.80	0.64
2:F:175:ASP:HA	2:F:179:LYS:HZ3	1.62	0.64
2:F:502:ILE:HG22	2:F:543:ALA:HA	1.78	0.64
1:A:288:ASN:O	1:A:289:HIS:ND1	2.31	0.64
1:E:233:VAL:HG13	1:E:277:VAL:HG11	1.80	0.64
2:F:238:GLU:HA	2:F:241:LEU:CD2	2.28	0.64
2:F:254:SER:O	2:F:295:THR:OG1	2.16	0.64
2:F:274:LYS:N	2:F:279:TYR:OH	2.30	0.64
1:A:233:VAL:HG22	1:A:290:ILE:CD1	2.25	0.64
1:A:914:GLN:HG2	3:A:1101:ATP:H1'	1.79	0.63
1:E:956:GLU:HB3	1:E:961:ARG:NH1	2.13	0.63
2:F:345:ILE:C	2:F:346:LEU:HD12	2.23	0.63
2:F:347:CYS:O	2:F:392:VAL:HG11	1.97	0.63
2:F:562:ASP:O	2:F:566:ILE:HG13	1.98	0.63
2:F:505:LEU:HD21	2:F:536:VAL:HG11	1.80	0.63
2:F:680:THR:O	2:F:684:ARG:HG2	1.96	0.63
2:D:39:ARG:NH2	2:D:697:GLN:OE1	2.31	0.63
2:D:780:LEU:HD11	3:D:1602:ATP:H5'1	1.79	0.63
2:F:146:THR:HG21	2:F:149:LEU:HD12	1.81	0.63
1:A:728:LEU:HD22	2:F:918:LYS:HZ1	1.63	0.63
1:C:744:LYS:NZ	3:C:1102:ATP:O2B	2.26	0.63
2:F:20:ARG:O	2:F:24:LEU:HD23	1.98	0.63
2:F:210:LEU:HD11	2:F:281:PRO:HD3	1.80	0.63
2:F:262:VAL:HG13	2:F:264:LEU:CD2	2.25	0.63
2:F:286:ALA:O	2:F:289:PRO:HD3	1.98	0.63
2:F:688:GLU:HA	2:F:691:LYS:HE2	1.79	0.63
1:A:215:ILE:N	2:F:377:GLU:OE1	2.31	0.63
1:C:800:ASP:OD1	1:C:801:SER:N	2.31	0.63
1:E:533:LYS:O	1:E:535:GLN:NE2	2.31	0.63
2:F:175:ASP:OD1	2:F:179:LYS:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:673:ILE:HG21	2:F:710:THR:HG22	1.78	0.63
2:F:1021:GLU:OE1	2:F:1024:ARG:NH2	2.32	0.63
2:B:596:VAL:HG12	2:B:598:ASN:H	1.62	0.63
1:C:531:PHE:CG	1:C:554:LEU:HD13	2.34	0.63
1:E:951:GLU:HG2	2:F:169:GLN:HG2	1.80	0.63
2:F:314:ILE:CD1	2:F:392:VAL:HA	2.28	0.63
2:F:659:SER:O	2:F:662:SER:OG	2.11	0.63
2:B:322:GLN:N	2:B:322:GLN:OE1	2.29	0.63
2:D:762:MET:SD	2:D:764:LYS:NZ	2.71	0.63
1:C:469:ARG:HG2	1:C:469:ARG:HH11	1.63	0.63
2:F:144:ILE:CD1	2:F:183:LEU:HD11	2.28	0.63
2:F:251:ILE:HG23	2:F:297:SER:O	1.97	0.63
1:C:465:ILE:O	1:C:465:ILE:HG22	1.97	0.63
1:E:419:GLU:OE1	1:E:419:GLU:N	2.31	0.63
1:E:444:VAL:O	1:E:448:THR:OG1	2.16	0.63
1:E:800:ASP:CG	1:E:845:LEU:HD13	2.22	0.63
2:B:70:SER:OG	2:B:75:PHE:O	2.09	0.63
2:D:78:THR:HG21	2:D:192:TYR:CD2	2.34	0.63
2:D:624:ARG:NE	2:D:662:SER:OG	2.31	0.63
1:C:398:MET:N	1:C:398:MET:SD	2.71	0.63
1:C:430:GLU:N	1:C:430:GLU:OE1	2.31	0.63
2:F:210:LEU:HD11	2:F:281:PRO:CD	2.29	0.63
2:F:670:ILE:O	2:F:674:VAL:HG22	1.99	0.63
2:F:703:GLN:HA	2:F:706:LEU:HD13	1.81	0.63
2:F:778:LYS:O	2:F:781:MET:HE3	1.99	0.63
1:A:361:ILE:HG22	1:A:368:ILE:HD12	1.81	0.62
1:E:406:ILE:O	1:E:410:HIS:ND1	2.25	0.62
2:F:5:LEU:HD12	2:F:6:THR:N	2.14	0.62
2:F:234:PHE:O	2:F:278:ILE:HD12	1.99	0.62
2:F:360:MET:HE2	2:F:360:MET:HA	1.80	0.62
1:E:216:LEU:HD23	1:E:290:ILE:HB	1.81	0.62
2:F:234:PHE:CB	2:F:267:LEU:HD21	2.29	0.62
2:D:224:HIS:N	2:D:227:ASP:OD2	2.32	0.62
2:D:322:GLN:OE1	2:D:322:GLN:N	2.31	0.62
1:C:651:LYS:NZ	2:D:611:ARG:O	2.32	0.62
2:F:206:ASP:O	2:F:278:ILE:HG22	1.98	0.62
2:F:475:ASN:CB	2:F:584:THR:HG21	2.29	0.62
2:B:954:ALA:CB	2:B:996:VAL:HG12	2.28	0.62
2:D:804:MET:N	2:D:804:MET:SD	2.72	0.62
1:E:499:ASN:OD1	1:E:500:LEU:N	2.32	0.62
2:D:526:ILE:HG21	2:D:575:GLU:OE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:707:SER:O	2:D:710:THR:OG1	2.15	0.62
1:A:490:ASP:OD1	1:A:491:CYS:N	2.32	0.62
2:F:18:ILE:HG13	2:F:57:LEU:HA	1.81	0.62
2:F:162:LEU:HD12	2:F:163:VAL:N	2.14	0.62
2:F:191:GLU:H	2:F:191:GLU:CD	2.06	0.62
2:F:275:LYS:C	2:F:276:ARG:HG2	2.24	0.62
2:F:335:LEU:HD22	2:F:390:PHE:CE2	2.35	0.62
2:D:256:MET:N	2:D:256:MET:SD	2.73	0.62
1:A:633:LEU:HD23	1:A:671:PHE:CE2	2.34	0.62
1:C:257:GLN:OE1	2:B:364:ASN:ND2	2.33	0.62
1:C:356:LEU:O	1:C:381:CYS:N	2.32	0.62
2:F:572:ILE:HG13	2:F:573:ASN:N	2.15	0.62
2:B:251:ILE:HG21	2:B:296:ILE:HD11	1.82	0.62
2:B:477:SER:OG	2:B:611:ARG:N	2.30	0.62
1:E:647:ILE:HD11	2:F:611:ARG:HA	1.81	0.62
2:F:350:ASP:H	2:F:392:VAL:HB	1.63	0.62
2:D:358:SER:N	2:D:385:ASP:OD2	2.31	0.62
2:D:636:GLU:OE1	2:D:636:GLU:N	2.32	0.62
2:F:238:GLU:HA	2:F:241:LEU:HD21	1.82	0.62
2:F:555:LEU:O	2:F:569:GLN:HG2	1.99	0.62
2:F:122:GLN:O	2:F:126:LEU:HD23	1.99	0.62
2:F:248:GLY:C	2:F:263:LYS:HE2	2.25	0.62
2:F:410:ASP:OD1	2:F:412:ASN:N	2.33	0.62
2:F:448:LEU:O	2:F:455:ARG:NH2	2.31	0.62
2:F:457:LEU:HD12	2:F:457:LEU:O	1.99	0.62
2:F:550:LEU:HD21	2:F:606:PHE:HE2	1.64	0.62
2:F:104:LEU:HD23	2:F:151:GLN:HB2	1.81	0.62
2:F:557:VAL:HG13	2:F:566:ILE:HG23	1.81	0.62
2:F:621:GLU:HA	2:F:624:ARG:NE	2.13	0.62
1:C:696:TRP:CZ2	1:C:710:LEU:HD21	2.35	0.61
2:F:132:ILE:HG23	2:F:137:THR:CG2	2.29	0.61
2:F:233:ALA:CB	2:F:262:VAL:HG21	2.29	0.61
2:F:237:ALA:HB2	2:F:266:VAL:HG11	1.82	0.61
2:F:360:MET:HG2	2:F:382:TYR:HE1	1.64	0.61
2:F:409:ILE:HG23	2:F:414:THR:CG2	2.30	0.61
2:F:419:THR:HG22	2:F:420:ASN:N	2.12	0.61
2:D:35:TYR:HB2	2:D:90:ILE:HD11	1.80	0.61
1:C:507:ILE:HD11	1:C:556:PHE:CD2	2.36	0.61
1:C:953:GLY:HA2	1:C:955:ARG:HH11	1.65	0.61
1:E:947:PHE:CZ	2:F:174:ASN:HB3	2.35	0.61
2:F:34:LEU:HB2	2:F:55:CYS:SG	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:GLN:OE1	2:F:120:MET:HE1	2.00	0.61
2:F:238:GLU:O	2:F:241:LEU:HG	2.00	0.61
2:F:251:ILE:HB	2:F:264:LEU:HD23	1.82	0.61
2:F:311:GLN:O	2:F:396:GLU:HB2	2.00	0.61
2:F:704:GLU:OE1	2:F:704:GLU:N	2.29	0.61
1:A:218:SER:N	1:A:308:ALA:O	2.27	0.61
3:C:1102:ATP:H2'	3:C:1102:ATP:N3	2.15	0.61
1:C:954:ARG:HB2	2:D:169:GLN:HE22	1.66	0.61
2:F:76:MET:HE1	2:F:188:GLU:HB3	1.82	0.61
2:F:335:LEU:CD1	2:F:339:PHE:HE2	2.04	0.61
1:C:965:LEU:HD21	2:D:154:ASN:HD22	1.64	0.61
3:C:1101:ATP:H2'	3:C:1101:ATP:N3	2.15	0.61
2:F:35:TYR:CE1	2:F:54:HIS:HB2	2.35	0.61
2:F:109:LEU:HD23	2:F:112:LYS:CE	2.30	0.61
2:F:134:SER:HB2	2:F:165:PHE:CG	2.36	0.61
2:F:171:ILE:HG22	2:F:173:VAL:HG13	1.82	0.61
2:F:497:SER:HB3	2:F:504:LEU:HD13	1.81	0.61
2:F:573:ASN:OD1	2:F:574:PHE:N	2.33	0.61
2:D:243:LEU:O	2:D:298:LYS:NZ	2.27	0.61
1:A:973:GLU:HG3	1:A:974:THR:H	1.66	0.61
1:C:972:HIS:CE1	1:C:974:THR:HG22	2.35	0.61
2:F:78:THR:OG1	2:F:79:GLN:OE1	2.18	0.61
2:B:7:PHE:HD2	2:B:81:THR:HG21	1.65	0.61
2:D:837:ALA:HB1	2:D:887:LEU:HD11	1.81	0.61
1:A:1017:ASP:OD1	1:A:1021:LYS:NZ	2.34	0.61
1:C:850:LEU:HD12	1:C:856:LEU:HD11	1.82	0.61
1:C:945:GLU:HG2	2:D:174:ASN:HD22	1.66	0.61
1:E:827:GLY:O	1:E:829:GLU:N	2.34	0.61
2:D:38:ILE:HD12	2:D:38:ILE:O	2.01	0.61
1:A:466:GLY:HA2	3:A:1102:ATP:H5'2	1.83	0.61
2:F:228:ASP:HB3	2:F:345:ILE:CD1	2.29	0.61
2:B:779:THR:N	3:B:1102:ATP:O1B	2.28	0.61
2:D:351:LEU:O	2:D:352:ILE:HD13	1.99	0.61
2:D:492:MET:SD	2:D:616:VAL:HG21	2.41	0.61
2:D:497:SER:HB3	2:D:504:LEU:HD21	1.83	0.61
1:E:803:ALA:HA	1:E:818:VAL:HG22	1.82	0.61
2:F:447:ASP:OD1	2:F:450:ILE:HB	2.00	0.61
2:F:569:GLN:HA	2:F:572:ILE:HG12	1.82	0.61
2:B:248:GLY:N	2:B:264:LEU:O	2.29	0.61
2:D:508:ASP:HA	2:D:548:ALA:HB3	1.83	0.61
2:F:216:ARG:HH12	2:F:225:ILE:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:THR:O	2:F:296:ILE:HD12	2.00	0.61
2:F:350:ASP:N	2:F:392:VAL:HB	2.15	0.61
2:F:356:PHE:HA	2:F:384:ASN:OD1	2.01	0.61
2:F:360:MET:HG2	2:F:382:TYR:CE1	2.36	0.61
2:F:504:LEU:HD12	2:F:544:VAL:HG12	1.81	0.61
2:F:668:LEU:HD21	3:F:1101:ATP:C4'	2.31	0.61
2:B:450:ILE:O	2:B:623:GLN:NE2	2.33	0.61
2:B:954:ALA:HB2	2:B:996:VAL:HG12	1.82	0.61
1:C:282:ASP:OD1	1:C:283:SER:N	2.34	0.60
1:C:467:LYS:N	3:C:1101:ATP:O1B	2.34	0.60
1:E:965:LEU:HG	2:F:102:THR:HG21	1.83	0.60
2:F:18:ILE:HA	2:F:66:ILE:CD1	2.31	0.60
2:F:134:SER:OG	2:F:135:MET:HE2	2.00	0.60
2:F:416:LEU:O	2:F:417:ILE:HD13	2.01	0.60
2:F:620:SER:O	2:F:624:ARG:HG3	2.00	0.60
1:A:922:LEU:HD11	2:B:765:ARG:NE	2.15	0.60
1:C:255:LEU:HD13	1:C:513:PHE:CE1	2.36	0.60
1:E:951:GLU:HG3	2:F:169:GLN:HA	1.83	0.60
2:F:229:ASN:HA	2:F:232:TYR:HE1	1.62	0.60
2:F:486:ASN:ND2	2:F:668:LEU:HD12	2.13	0.60
2:B:668:LEU:HD21	3:B:1101:ATP:H4'	1.83	0.60
2:D:631:TYR:OH	3:D:1601:ATP:H8	1.84	0.60
1:A:466:GLY:CA	3:A:1102:ATP:H5'2	2.31	0.60
2:F:148:GLY:O	2:F:149:LEU:HD23	2.01	0.60
2:F:358:SER:H	2:F:385:ASP:CG	2.09	0.60
2:F:467:CYS:HA	2:F:470:ARG:NH1	2.15	0.60
1:A:252:LYS:NZ	2:F:364:ASN:OD1	2.35	0.60
1:A:545:GLY:C	2:F:555:LEU:HD11	2.26	0.60
1:E:494:LEU:HD21	1:E:506:LEU:CD2	2.31	0.60
1:E:495:HIS:NE2	2:F:567:LYS:HG2	2.16	0.60
2:F:107:GLU:HA	2:F:174:ASN:HD21	1.66	0.60
2:F:725:GLN:O	2:F:783:LYS:NZ	2.29	0.60
2:B:939:THR:OG1	2:B:942:ASP:OD1	2.12	0.60
1:A:650:GLU:OE2	2:B:474:LEU:HD12	2.00	0.60
2:F:31:ALA:CA	2:F:34:LEU:HD21	2.22	0.60
2:F:235:THR:HG23	2:F:277:THR:O	2.01	0.60
2:F:423:ASN:OD1	2:F:424:ARG:N	2.34	0.60
1:A:762:VAL:HG13	1:A:766:GLU:OE1	2.01	0.60
2:F:426:PRO:HG2	2:F:501:GLY:C	2.26	0.60
2:F:445:TYR:HD1	2:F:495:PHE:HE2	1.50	0.60
2:B:673:ILE:HD11	2:B:713:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASP:OD1	1:A:663:ASP:O	2.19	0.60
1:A:825:MET:HE1	1:A:855:ARG:NH2	2.16	0.60
1:C:746:LEU:HD11	3:C:1102:ATP:H3'	1.83	0.60
1:E:396:THR:OG1	1:E:398:MET:HE1	2.02	0.60
2:F:647:VAL:HG11	2:F:678:ARG:NH2	2.16	0.60
1:A:588:LEU:HD12	1:A:589:PHE:N	2.16	0.60
1:E:794:LEU:O	1:E:837:LEU:N	2.33	0.60
2:F:234:PHE:HB2	2:F:267:LEU:HD21	1.82	0.60
2:F:261:LEU:HD12	2:F:262:VAL:N	2.13	0.60
2:B:826:CYS:N	2:B:870:GLY:O	2.35	0.60
1:A:244:GLN:O	1:A:279:ILE:HG22	2.01	0.60
1:A:612:LEU:HD21	1:A:645:LEU:HD12	1.83	0.60
1:A:974:THR:O	1:A:976:THR:HG23	2.02	0.60
1:C:728:LEU:HD21	2:B:919:PHE:CZ	2.36	0.60
1:C:806:ARG:NE	1:C:847:ASP:OD2	2.35	0.60
1:E:350:LEU:HD23	1:E:350:LEU:O	2.01	0.60
1:E:810:SER:O	2:D:846:SER:OG	2.20	0.60
1:E:836:ILE:C	1:E:837:LEU:HD22	2.27	0.60
2:F:250:PHE:C	2:F:251:ILE:HD12	2.27	0.60
2:B:238:GLU:OE2	2:B:242:ARG:NH2	2.35	0.60
1:A:449:SER:OG	1:A:451:ILE:O	2.20	0.60
1:A:949:ILE:HB	2:B:170:LEU:HD21	1.84	0.60
1:E:852:ARG:NH2	3:D:1602:ATP:O3A	2.33	0.60
2:F:387:LEU:HD12	2:F:438:TYR:HE2	1.67	0.60
2:F:558:ASN:OD1	2:F:560:ASN:N	2.35	0.60
1:C:949:ILE:HD12	2:D:119:GLU:HG2	1.82	0.59
2:F:20:ARG:CD	2:F:57:LEU:HD21	2.32	0.59
2:F:449:HIS:HA	2:F:455:ARG:NH2	2.16	0.59
2:F:565:ALA:HA	2:F:568:LEU:CD2	2.32	0.59
2:F:658:LEU:H	2:F:658:LEU:HD22	1.67	0.59
2:B:1004:ALA:O	2:B:1008:LEU:N	2.35	0.59
1:A:466:GLY:N	3:A:1102:ATP:O2B	2.35	0.59
1:C:958:ASN:HA	1:C:961:ARG:HE	1.67	0.59
1:E:874:LEU:CB	1:E:898:LEU:HD13	2.32	0.59
2:F:240:LEU:O	2:F:244:ASP:N	2.35	0.59
2:F:310:ASN:ND2	2:F:398:ASP:OD1	2.34	0.59
2:F:569:GLN:NE2	2:F:572:ILE:HD11	2.16	0.59
1:A:443:MET:HE1	1:A:598:TRP:CE2	2.37	0.59
1:A:804:PRO:O	1:A:806:ARG:NH1	2.35	0.59
1:E:434:ILE:HD12	1:E:434:ILE:H	1.66	0.59
2:F:488:GLY:N	3:F:1101:ATP:O2B	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:568:LEU:O	2:F:572:ILE:HG23	2.02	0.59
2:B:178:GLN:O	2:B:181:SER:OG	2.20	0.59
2:B:550:LEU:HD21	2:B:554:LEU:HD22	1.84	0.59
1:C:241:LEU:HD12	1:C:242:PRO:HD2	1.84	0.59
1:C:474:LEU:HD23	1:C:475:ILE:N	2.17	0.59
2:F:74:GLY:C	2:F:185:TYR:HB3	2.27	0.59
2:F:75:PHE:HA	2:F:186:ALA:O	2.02	0.59
2:F:219:LEU:HD12	2:F:223:PRO:HG3	1.83	0.59
2:F:569:GLN:CD	2:F:572:ILE:HD11	2.26	0.59
2:F:686:TYR:O	2:F:690:LYS:HG2	2.01	0.59
2:B:668:LEU:CD2	3:B:1101:ATP:H4'	2.32	0.59
2:B:922:ASP:O	2:B:925:VAL:HG22	2.02	0.59
2:D:236:ASP:O	2:D:239:THR:OG1	2.19	0.59
2:D:239:THR:O	2:D:243:LEU:HD22	2.03	0.59
1:A:803:ALA:HB1	1:A:818:VAL:HG22	1.84	0.59
2:F:81:THR:O	2:F:268:LEU:HD22	2.01	0.59
2:F:647:VAL:HG21	2:F:678:ARG:HE	1.67	0.59
2:D:554:LEU:H	2:D:554:LEU:HD12	1.68	0.59
1:E:377:GLU:N	1:E:377:GLU:OE1	2.36	0.59
1:E:658:LEU:HD22	2:F:459:ASN:HB3	1.84	0.59
1:E:901:ILE:CG1	1:E:993:LEU:HD21	2.32	0.59
2:F:133:ASN:HB2	2:F:136:GLU:CB	2.20	0.59
2:D:450:ILE:O	2:D:623:GLN:NE2	2.33	0.59
1:C:954:ARG:HB3	1:C:957:GLU:OE1	2.03	0.59
1:E:901:ILE:HG12	1:E:993:LEU:HD21	1.85	0.59
2:F:2:LYS:HE2	2:F:84:PHE:CB	2.33	0.59
2:F:238:GLU:O	2:F:242:ARG:HG3	2.02	0.59
2:F:702:THR:N	2:F:705:ASP:OD2	2.34	0.59
1:A:669:GLU:OE1	1:A:669:GLU:N	2.34	0.59
1:A:734:ILE:O	1:A:837:LEU:HD12	2.02	0.59
1:C:914:GLN:OE1	3:C:1102:ATP:O2'	2.13	0.59
1:E:938:VAL:CG2	1:E:939:PRO:HD2	2.32	0.59
2:F:106:ASN:HD21	2:F:109:LEU:HG	1.66	0.59
2:F:224:HIS:HB3	2:F:227:ASP:CG	2.27	0.59
2:F:702:THR:O	2:F:706:LEU:HD12	2.03	0.59
2:B:475:ASN:O	2:B:611:ARG:NH1	2.35	0.59
2:B:551:ASP:OD1	2:B:552:SER:N	2.36	0.59
2:D:615:LEU:HD23	2:D:616:VAL:N	2.17	0.59
1:A:608:ARG:NH2	1:A:637:THR:O	2.36	0.59
1:E:255:LEU:O	1:E:256:ARG:NH1	2.36	0.59
2:F:20:ARG:HD2	2:F:57:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:255:ASN:OD1	2:F:256:MET:HG3	2.02	0.59
2:F:429:LEU:CD2	2:F:499:TYR:HA	2.28	0.59
2:D:90:ILE:HD12	2:D:90:ILE:O	2.02	0.59
1:A:712:THR:HG21	1:A:734:ILE:HD13	1.84	0.59
1:C:821:LEU:CD2	1:C:850:LEU:HD11	2.32	0.59
1:E:874:LEU:HB3	1:E:898:LEU:HD13	1.85	0.59
2:F:119:GLU:O	2:F:123:ILE:HG12	2.02	0.59
2:F:206:ASP:CG	2:F:277:THR:HG22	2.28	0.59
2:B:958:ILE:O	2:B:962:VAL:HG23	2.03	0.58
2:D:546:PHE:HE2	2:D:548:ALA:HB2	1.68	0.58
1:A:500:LEU:HD21	2:F:514:SER:HA	1.85	0.58
1:A:874:LEU:O	1:A:878:VAL:HG22	2.03	0.58
2:F:441:ALA:HA	2:F:639:ARG:NH1	2.18	0.58
2:F:488:GLY:HA2	3:F:1101:ATP:PA	2.43	0.58
2:F:625:LEU:HD12	2:F:629:GLN:NE2	2.17	0.58
2:B:477:SER:O	2:B:612:PHE:N	2.32	0.58
2:D:489:LYS:O	2:D:493:VAL:HG23	2.03	0.58
1:A:515:TYR:O	1:A:571:ARG:NH1	2.36	0.58
1:E:460:ASP:OD2	1:E:581:LYS:N	2.36	0.58
1:E:554:LEU:O	1:E:558:ILE:HG22	2.04	0.58
1:E:944:ILE:C	1:E:945:GLU:HG3	2.28	0.58
2:F:5:LEU:HD23	2:F:82:MET:HG2	1.84	0.58
2:F:625:LEU:O	2:F:629:GLN:HG2	2.03	0.58
2:F:705:ASP:HA	2:F:708:LYS:NZ	2.18	0.58
2:F:759:THR:O	2:F:759:THR:HG22	2.03	0.58
2:D:310:ASN:O	2:D:415:LYS:N	2.32	0.58
2:D:557:VAL:HG11	2:D:566:ILE:HG23	1.84	0.58
1:A:362:LEU:O	1:A:366:GLN:N	2.36	0.58
1:A:825:MET:HE1	1:A:855:ARG:CZ	2.33	0.58
1:C:728:LEU:HD21	2:B:919:PHE:CE1	2.38	0.58
1:E:228:ASP:OD1	1:E:229:ASN:N	2.36	0.58
1:E:452:ILE:HA	2:D:679:MET:HE1	1.85	0.58
1:E:452:ILE:HD11	1:E:573:ARG:NE	2.17	0.58
1:E:962:LEU:O	1:E:967:GLN:NE2	2.34	0.58
2:F:20:ARG:HG2	2:F:59:ASP:HA	1.85	0.58
2:F:114:MET:HE2	2:F:114:MET:CA	2.30	0.58
2:F:269:LEU:HD12	2:F:269:LEU:H	1.66	0.58
2:F:551:ASP:OD1	2:F:552:SER:N	2.36	0.58
2:B:141:SER:N	2:B:159:PRO:O	2.36	0.58
2:B:666:THR:N	2:B:669:ASP:OD1	2.36	0.58
2:D:699:ILE:O	2:D:700:LEU:HD22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:C	1:A:275:ILE:HD12	2.28	0.58
1:C:709:LEU:CD1	1:C:710:LEU:HD22	2.32	0.58
1:C:841:SER:O	1:C:1016:TYR:OH	2.16	0.58
2:F:206:ASP:OD1	2:F:277:THR:HA	2.03	0.58
2:F:571:SER:O	2:F:575:GLU:OE1	2.21	0.58
2:F:685:PHE:CZ	2:F:695:LEU:HD22	2.38	0.58
2:B:251:ILE:HD13	2:B:264:LEU:HB2	1.85	0.58
2:B:289:PRO:O	2:B:431:ARG:NH1	2.30	0.58
2:D:903:ASP:OD1	2:D:904:THR:N	2.36	0.58
1:A:478:VAL:CG2	1:A:484:ILE:HD13	2.33	0.58
2:F:1019:HIS:O	2:F:1023:VAL:HG23	2.03	0.58
2:B:828:ILE:HD12	2:B:828:ILE:C	2.28	0.58
2:D:641:VAL:O	2:D:641:VAL:HG13	2.02	0.58
1:C:739:TYR:CE2	1:C:1012:LEU:HD11	2.38	0.58
2:F:78:THR:OG1	2:F:187:ASN:OD1	2.06	0.58
2:F:183:LEU:C	2:F:184:LYS:HD3	2.29	0.58
2:F:205:ILE:HD11	2:F:276:ARG:C	2.28	0.58
2:F:703:GLN:HA	2:F:706:LEU:CD1	2.34	0.58
2:F:706:LEU:HD12	2:F:706:LEU:H	1.69	0.58
2:B:504:LEU:HD11	2:B:506:GLU:HB3	1.85	0.58
2:B:508:ASP:HA	2:B:548:ALA:HB3	1.85	0.58
2:D:208:GLU:OE2	2:D:209:SER:N	2.36	0.58
1:C:742:CYS:N	3:C:1102:ATP:O2B	2.36	0.58
1:E:805:LYS:N	1:E:845:LEU:O	2.37	0.58
2:F:105:ILE:HD11	2:F:110:TYR:HB2	1.84	0.58
2:F:926:LYS:O	2:F:998:MET:HE1	2.03	0.58
2:D:633:SER:OG	2:D:636:GLU:OE1	2.22	0.58
1:C:362:LEU:HD11	1:C:364:THR:OG1	2.02	0.58
2:F:26:TYR:CD2	2:F:34:LEU:HD22	2.39	0.58
2:F:311:GLN:CD	2:F:417:ILE:HG12	2.28	0.58
2:F:312:VAL:O	2:F:416:LEU:HD13	2.03	0.58
2:F:348:GLN:HE22	2:F:395:ALA:N	2.01	0.58
2:F:444:PHE:HA	2:F:630:TRP:CE2	2.39	0.58
2:B:517:ARG:C	2:B:517:ARG:NE	2.61	0.58
2:D:780:LEU:HD11	3:D:1602:ATP:H2'	1.85	0.58
1:A:918:TYR:OH	2:B:765:ARG:N	2.36	0.58
1:E:257:GLN:OE1	1:E:257:GLN:N	2.32	0.58
2:F:491:THR:HG23	3:F:1101:ATP:H5'1	1.86	0.58
2:B:28:ASP:OD1	2:B:29:LYS:N	2.37	0.58
2:B:185:TYR:N	2:B:188:GLU:OE1	2.35	0.58
1:C:803:ALA:HA	1:C:818:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:959:ARG:HG3	1:E:963:LYS:CB	2.34	0.57
2:F:235:THR:HG22	2:F:236:ASP:N	2.18	0.57
2:F:489:LYS:CD	2:F:595:SER:HB2	2.33	0.57
2:F:618:VAL:CG1	2:F:619:PRO:HD2	2.34	0.57
2:F:717:PHE:O	2:F:721:ILE:HG12	2.04	0.57
2:D:230:SER:C	2:D:231:ILE:HD13	2.29	0.57
1:E:512:SER:HB2	2:D:363:LEU:HD21	1.85	0.57
2:F:135:MET:C	2:F:162:LEU:HD11	2.29	0.57
2:F:681:ALA:HB1	2:F:699:ILE:CG2	2.33	0.57
2:B:564:GLU:N	2:B:564:GLU:OE1	2.37	0.57
1:A:469:ARG:HH22	3:A:1102:ATP:H2'	1.67	0.57
1:C:696:TRP:CH2	1:C:710:LEU:HD21	2.39	0.57
1:C:746:LEU:CD1	3:C:1102:ATP:H2'	2.35	0.57
1:C:765:PRO:HA	2:D:852:ARG:HH21	1.67	0.57
2:F:619:PRO:HA	2:F:623:GLN:OE1	2.05	0.57
2:B:938:TYR:OH	2:B:1008:LEU:HD22	2.04	0.57
1:A:469:ARG:CZ	3:A:1102:ATP:H2'	2.34	0.57
1:A:733:GLY:C	1:A:734:ILE:HD12	2.30	0.57
1:C:725:ASN:ND2	2:B:992:THR:HG22	2.19	0.57
2:F:90:ILE:O	2:F:90:ILE:HG13	2.03	0.57
2:F:96:PRO:O	2:F:162:LEU:N	2.28	0.57
2:F:194:LEU:H	2:F:194:LEU:HD12	1.68	0.57
2:F:446:TYR:HB3	2:F:451:PHE:CD2	2.33	0.57
2:F:901:ILE:HD11	2:F:937:ASN:O	2.04	0.57
2:B:255:ASN:O	2:B:256:MET:SD	2.62	0.57
1:A:757:LEU:HD13	1:A:793:ILE:HD11	1.86	0.57
1:C:947:PHE:N	2:D:172:LEU:O	2.37	0.57
1:C:965:LEU:O	1:C:968:GLN:HG3	2.04	0.57
2:F:353:PRO:HB3	2:F:389:TRP:CZ3	2.39	0.57
2:F:233:ALA:HB3	2:F:262:VAL:HG21	1.86	0.57
2:F:275:LYS:HB2	2:F:276:ARG:NH1	2.20	0.57
2:B:217:ASP:O	2:B:220:ARG:NH2	2.33	0.57
2:D:973:THR:OG1	2:D:975:GLU:OE1	2.16	0.57
1:C:414:HIS:O	1:C:416:HIS:ND1	2.36	0.57
1:E:935:SER:O	1:E:936:GLU:HG2	2.05	0.57
2:F:479:LEU:HD23	2:F:479:LEU:C	2.30	0.57
2:F:537:LEU:HD21	2:F:587:PHE:CG	2.38	0.57
2:F:648:SER:O	2:F:701:ILE:HD12	2.04	0.57
2:D:1:MET:HE2	2:D:1:MET:N	2.20	0.57
1:A:701:ALA:C	1:A:702:LEU:HD12	2.30	0.57
1:C:220:VAL:O	1:C:220:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:ILE:CG2	2:F:72:LEU:HA	2.27	0.57
2:F:133:ASN:N	2:F:137:THR:OG1	2.28	0.57
2:F:492:MET:SD	2:F:493:VAL:N	2.78	0.57
1:C:874:LEU:HD13	1:C:913:LEU:HD11	1.87	0.57
2:F:20:ARG:HD2	2:F:57:LEU:CG	2.35	0.57
2:F:118:GLN:HB3	2:F:120:MET:CE	2.35	0.57
2:B:769:LEU:HD23	2:B:770:PHE:N	2.20	0.57
2:D:518:GLN:N	2:D:521:SER:OG	2.38	0.57
2:F:275:LYS:HB2	2:F:276:ARG:CZ	2.35	0.57
2:F:320:TRP:CH2	2:F:532:LYS:HD2	2.38	0.57
2:D:17:SER:OG	2:D:61:LEU:HD11	2.05	0.57
1:A:797:ASP:OD1	1:A:798:GLU:N	2.38	0.56
1:E:954:ARG:HD3	1:E:961:ARG:NH2	2.18	0.56
2:B:231:ILE:O	2:B:231:ILE:HG22	2.05	0.56
2:D:164:ASP:O	2:D:168:THR:HG22	2.04	0.56
2:D:174:ASN:OD1	2:D:175:ASP:N	2.37	0.56
1:E:624:LEU:HA	1:E:666:VAL:HG12	1.87	0.56
1:E:793:ILE:HG23	1:E:837:LEU:HD23	1.87	0.56
2:F:38:ILE:HD12	2:F:87:PHE:HA	1.86	0.56
2:F:168:THR:O	2:F:170:LEU:HD22	2.05	0.56
2:F:248:GLY:O	2:F:263:LYS:HE2	2.05	0.56
2:B:261:LEU:HD23	2:B:262:VAL:N	2.19	0.56
2:D:505:LEU:HD12	2:D:505:LEU:N	2.21	0.56
2:D:647:VAL:HA	2:D:699:ILE:HG22	1.86	0.56
1:C:553:LEU:H	1:C:553:LEU:HD12	1.70	0.56
1:C:643:LEU:CD1	1:C:647:ILE:HD11	2.35	0.56
1:C:763:LYS:HZ3	2:D:859:ALA:HB3	1.70	0.56
1:E:251:VAL:HG23	1:E:251:VAL:O	2.04	0.56
1:E:903:GLU:OE1	1:E:903:GLU:N	2.36	0.56
2:F:43:TYR:CB	2:F:273:PHE:HZ	2.17	0.56
2:F:109:LEU:HD23	2:F:112:LYS:HE2	1.86	0.56
2:F:316:ARG:HB3	2:F:421:ILE:HD12	1.86	0.56
2:F:429:LEU:HD23	2:F:430:SER:H	1.70	0.56
2:F:481:HIS:CG	2:F:599:ILE:HB	2.41	0.56
2:F:671:LYS:HA	2:F:674:VAL:CG2	2.35	0.56
2:D:353:PRO:C	2:D:354:ILE:HD13	2.31	0.56
2:D:830:PHE:HB2	2:D:833:ILE:HG22	1.86	0.56
1:A:443:MET:HE1	1:A:598:TRP:NE1	2.20	0.56
1:A:633:LEU:HD23	1:A:671:PHE:HE2	1.70	0.56
1:E:500:LEU:HD13	1:E:553:LEU:HD21	1.88	0.56
2:F:894:ASP:OD1	2:F:894:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:MET:N	2:B:163:VAL:O	2.34	0.56
2:B:650:MET:HA	2:B:650:MET:HE3	1.88	0.56
2:D:115:ASP:OD1	2:D:115:ASP:N	2.36	0.56
1:A:233:VAL:CG2	1:A:290:ILE:HD11	2.28	0.56
1:A:735:LEU:HD13	1:A:838:ALA:HB3	1.88	0.56
1:C:316:GLN:N	1:C:316:GLN:OE1	2.38	0.56
2:F:139:VAL:HG23	2:F:152:ILE:HD13	1.88	0.56
2:F:243:LEU:O	2:F:243:LEU:HG	2.04	0.56
2:F:311:GLN:OE1	2:F:417:ILE:HG12	2.04	0.56
2:F:347:CYS:N	2:F:350:ASP:OD2	2.35	0.56
2:F:576:MET:SD	2:F:580:LEU:HD23	2.45	0.56
2:F:579:LEU:HD23	2:F:580:LEU:HD22	1.86	0.56
2:B:313:PHE:CD1	2:B:417:ILE:HG22	2.41	0.56
1:A:970:VAL:HG13	1:A:970:VAL:O	2.06	0.56
1:C:821:LEU:HD23	1:C:850:LEU:HD11	1.87	0.56
1:E:452:ILE:HD11	1:E:573:ARG:HE	1.70	0.56
2:F:553:ILE:HG22	2:F:572:ILE:HD12	1.87	0.56
2:B:122:GLN:O	2:B:126:LEU:HD22	2.06	0.56
2:D:564:GLU:OE1	2:D:564:GLU:N	2.38	0.56
1:A:654:TYR:OH	2:B:474:LEU:O	2.23	0.56
1:A:745:THR:N	3:A:1101:ATP:O1B	2.38	0.56
1:A:799:PHE:HE2	1:A:803:ALA:HB3	1.69	0.56
1:C:949:ILE:HG23	2:D:119:GLU:CG	2.35	0.56
1:E:330:VAL:HG13	1:E:332:ILE:HD11	1.86	0.56
2:B:545:ILE:HD12	2:B:591:THR:O	2.05	0.56
1:A:431:ASP:OD1	3:A:1102:ATP:N6	2.35	0.56
1:C:305:MET:HE1	1:C:517:TYR:CZ	2.40	0.56
2:F:271:ASN:CG	2:F:272:GLY:H	2.14	0.56
2:F:316:ARG:CZ	2:F:421:ILE:HD11	2.35	0.56
2:F:350:ASP:C	2:F:351:LEU:HD23	2.31	0.56
2:F:387:LEU:HD23	2:F:387:LEU:C	2.30	0.56
2:B:79:GLN:HB3	2:B:269:LEU:HD22	1.88	0.56
2:B:858:LEU:O	2:B:862:ASP:OD1	2.24	0.56
2:D:627:ILE:HG22	2:D:670:ILE:HG21	1.88	0.56
1:C:465:ILE:N	3:C:1101:ATP:O2B	2.39	0.56
1:C:965:LEU:CD2	2:D:102:THR:HG21	2.36	0.56
1:E:497:THR:HG23	1:E:502:LYS:HE3	1.88	0.56
1:E:621:ILE:HD13	2:F:472:ILE:HG12	1.86	0.56
2:F:313:PHE:HB2	2:F:394:SER:OG	2.06	0.56
2:F:429:LEU:HD23	2:F:430:SER:N	2.21	0.56
2:F:771:TYR:HE2	2:F:896:LEU:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:MET:C	2:B:162:LEU:HD11	2.31	0.56
2:B:353:PRO:O	2:B:354:ILE:HD13	2.06	0.56
1:C:616:PHE:HB3	1:C:622:MET:SD	2.45	0.56
1:E:755:CYS:SG	1:E:756:GLY:N	2.79	0.56
1:E:963:LYS:HA	1:E:967:GLN:NE2	2.21	0.56
2:F:98:LEU:HD12	2:F:139:VAL:HG13	1.88	0.56
2:F:306:ILE:HG12	2:F:408:ILE:HG12	1.85	0.56
2:F:348:GLN:NE2	2:F:394:SER:HA	2.21	0.56
2:D:230:SER:O	2:D:231:ILE:HD13	2.05	0.56
1:E:493:THR:HA	2:F:574:PHE:HE2	1.71	0.55
1:E:971:VAL:CG2	1:E:974:THR:HA	2.36	0.55
2:F:62:PRO:HG2	2:F:65:SER:OG	2.06	0.55
1:A:500:LEU:HD23	1:A:501:ASP:H	1.70	0.55
1:A:763:LYS:HD2	2:B:859:ALA:HB1	1.88	0.55
1:C:356:LEU:CD1	1:C:360:LEU:HD21	2.36	0.55
1:E:544:ASN:N	1:E:544:ASN:OD1	2.39	0.55
2:F:100:SER:HB2	2:F:169:GLN:OE1	2.06	0.55
2:F:372:SER:HB3	2:F:375:GLU:OE2	2.05	0.55
2:F:810:GLU:OE1	2:F:810:GLU:N	2.35	0.55
2:B:962:VAL:O	2:B:966:VAL:HG23	2.05	0.55
2:D:35:TYR:CB	2:D:90:ILE:HD11	2.35	0.55
1:C:863:ASN:OD1	1:C:864:ILE:N	2.38	0.55
2:F:20:ARG:HD3	2:F:59:ASP:HB2	1.89	0.55
2:F:23:TYR:CD2	2:F:57:LEU:HD22	2.41	0.55
2:F:101:VAL:HA	2:F:155:CYS:HA	1.88	0.55
2:F:316:ARG:HD2	2:F:322:GLN:CG	2.36	0.55
1:A:545:GLY:HA3	2:F:555:LEU:HD11	1.88	0.55
1:E:951:GLU:OE2	2:F:169:GLN:HG2	2.06	0.55
2:F:145:LEU:HD12	2:F:150:CYS:SG	2.47	0.55
2:F:146:THR:CG2	2:F:149:LEU:HD12	2.37	0.55
2:B:229:ASN:OD1	2:B:230:SER:N	2.40	0.55
2:B:812:ASN:O	2:B:816:VAL:HG12	2.07	0.55
1:A:709:LEU:HG	1:A:751:VAL:HG11	1.88	0.55
1:A:734:ILE:HG21	1:A:860:VAL:HG23	1.87	0.55
1:C:362:LEU:HD12	1:C:363:PRO:HD2	1.88	0.55
1:C:955:ARG:HA	1:C:958:ASN:HB2	1.88	0.55
2:F:39:ARG:CZ	2:F:41:PRO:HA	2.35	0.55
2:F:104:LEU:HD13	2:F:179:LYS:HE2	1.89	0.55
2:B:602:VAL:O	2:B:607:ARG:NE	2.38	0.55
1:A:487:LYS:HA	1:A:487:LYS:HE2	1.88	0.55
1:A:494:LEU:HD21	1:A:510:TRP:CH2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LEU:HD13	1:C:360:LEU:HD21	1.89	0.55
1:E:790:LYS:HB3	1:E:791:PRO:HD2	1.88	0.55
2:F:254:SER:CB	2:F:259:VAL:HG13	2.32	0.55
2:D:643:GLN:N	2:D:643:GLN:OE1	2.39	0.55
1:A:464:GLY:O	1:A:641:SER:OG	2.23	0.55
1:E:246:GLY:HA2	1:E:315:LEU:HD12	1.88	0.55
2:F:2:LYS:HE2	2:F:84:PHE:HB2	1.88	0.55
2:F:3:ALA:HA	2:F:64:CYS:SG	2.46	0.55
2:F:216:ARG:HH12	2:F:225:ILE:HD12	1.70	0.55
2:F:250:PHE:O	2:F:299:SER:HB3	2.07	0.55
1:A:735:LEU:CD1	1:A:838:ALA:HB3	2.37	0.55
1:C:857:ASP:OD1	1:C:858:LYS:N	2.38	0.55
1:E:840:THR:HG21	1:E:846:ILE:HD11	1.89	0.55
2:F:217:ASP:OD1	2:F:217:ASP:N	2.39	0.55
2:F:218:LEU:HA	2:F:220:ARG:HH12	1.72	0.55
2:F:756:GLU:OE1	2:F:756:GLU:N	2.36	0.55
2:B:348:GLN:OE1	2:B:349:ASN:N	2.38	0.55
2:B:492:MET:SD	2:B:493:VAL:HG23	2.47	0.55
2:D:453:TYR:CD2	2:D:492:MET:HE1	2.41	0.55
1:A:365:GLU:O	1:A:367:ILE:HG23	2.07	0.55
1:C:215:ILE:N	2:B:377:GLU:OE1	2.35	0.55
1:C:612:LEU:CD1	1:C:645:LEU:HD12	2.36	0.55
2:F:20:ARG:NE	2:F:57:LEU:HD21	2.21	0.55
2:F:23:TYR:CG	2:F:57:LEU:HD22	2.41	0.55
2:F:104:LEU:HD23	2:F:151:GLN:CB	2.37	0.55
2:F:120:MET:SD	2:F:120:MET:N	2.67	0.55
2:F:215:SER:HB3	2:F:218:LEU:CD2	2.36	0.55
2:B:228:ASP:OD1	2:B:230:SER:N	2.39	0.55
1:A:528:GLU:OE1	1:A:528:GLU:N	2.35	0.55
1:C:739:TYR:CD2	1:C:864:ILE:HG23	2.42	0.55
1:E:949:ILE:HD12	1:E:957:GLU:OE2	2.07	0.55
2:F:9:LEU:HD11	2:F:76:MET:HB2	1.89	0.55
2:F:102:THR:HB	2:F:153:LEU:HB3	1.89	0.55
2:F:486:ASN:HB3	2:F:668:LEU:CD1	2.36	0.55
2:B:969:HIS:HE1	2:B:977:ILE:HD12	1.72	0.55
1:E:347:TYR:O	1:E:351:LEU:N	2.40	0.54
2:F:19:SER:H	2:F:66:ILE:HD13	1.72	0.54
2:F:137:THR:HB	2:F:163:VAL:CG2	2.36	0.54
2:F:146:THR:HG21	2:F:149:LEU:HB2	1.89	0.54
2:F:811:ALA:O	2:F:815:ARG:HG2	2.07	0.54
2:B:598:ASN:OD1	2:B:600:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:OG	1:A:307:GLY:N	2.39	0.54
1:A:326:ARG:O	1:A:327:ASN:OD1	2.25	0.54
1:C:836:ILE:C	1:C:837:LEU:HD22	2.32	0.54
2:F:97:VAL:HG22	2:F:162:LEU:CB	2.31	0.54
2:F:135:MET:CA	2:F:162:LEU:HD11	2.38	0.54
2:F:786:ALA:O	2:F:790:SER:N	2.40	0.54
2:F:343:LYS:HD2	2:F:343:LYS:N	2.22	0.54
2:F:429:LEU:HD21	2:F:499:TYR:CD1	2.42	0.54
2:F:557:VAL:HG11	2:F:566:ILE:HG23	1.87	0.54
2:F:675:GLU:OE1	2:F:675:GLU:HA	2.05	0.54
2:B:85:CYS:SG	2:B:86:TYR:N	2.80	0.54
2:D:23:TYR:O	2:D:27:GLY:N	2.40	0.54
1:C:709:LEU:HD11	1:C:710:LEU:HD22	1.88	0.54
2:F:18:ILE:HG21	2:F:55:CYS:SG	2.47	0.54
2:F:301:ILE:HD13	2:F:403:ASP:OD2	2.06	0.54
2:F:316:ARG:HB3	2:F:421:ILE:HD11	1.88	0.54
2:F:651:ASP:OD2	2:F:651:ASP:C	2.50	0.54
2:F:743:GLU:HG2	2:F:897:LEU:HD21	1.88	0.54
2:D:135:MET:SD	2:D:135:MET:N	2.80	0.54
2:D:850:MET:SD	2:D:851:ASP:N	2.80	0.54
2:F:39:ARG:C	2:F:39:ARG:HD3	2.32	0.54
2:F:345:ILE:HG13	2:F:408:ILE:HD11	1.89	0.54
2:F:457:LEU:O	2:F:460:ILE:HG12	2.07	0.54
2:F:884:ASP:OD1	2:F:884:ASP:N	2.39	0.54
2:B:327:PHE:O	2:B:330:ILE:HG22	2.08	0.54
2:D:1:MET:N	2:D:87:PHE:O	2.40	0.54
1:E:287:GLU:O	1:E:289:HIS:ND1	2.38	0.54
2:F:217:ASP:OD1	2:F:218:LEU:HD22	2.07	0.54
2:F:448:LEU:CD1	2:F:455:ARG:HA	2.38	0.54
2:D:450:ILE:O	2:D:450:ILE:HG22	2.07	0.54
1:A:738:GLY:O	1:A:1016:TYR:OH	2.26	0.54
1:C:223:MET:N	1:C:223:MET:SD	2.80	0.54
1:C:499:ASN:OD1	1:C:500:LEU:N	2.41	0.54
2:F:23:TYR:HB2	2:F:57:LEU:HD13	1.90	0.54
2:F:120:MET:HA	2:F:123:ILE:HD11	1.87	0.54
2:F:637:LEU:HG	2:F:647:VAL:CG1	2.38	0.54
2:B:207:LEU:HD21	2:B:285:ILE:HG13	1.89	0.54
2:B:505:LEU:O	2:B:546:PHE:N	2.40	0.54
2:B:643:GLN:CD	2:B:645:VAL:HG12	2.32	0.54
2:B:797:LYS:N	2:B:800:GLU:OE2	2.41	0.54
1:C:799:PHE:O	1:C:799:PHE:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:937:VAL:CG1	1:E:938:VAL:N	2.71	0.54
2:F:169:GLN:NE2	2:F:171:ILE:HG13	2.23	0.54
2:F:250:PHE:CB	2:F:261:LEU:HD11	2.38	0.54
2:F:273:PHE:HB3	2:F:279:TYR:CZ	2.42	0.54
2:F:618:VAL:HG13	2:F:619:PRO:HD2	1.90	0.54
1:A:588:LEU:HD13	1:A:594:VAL:CG1	2.38	0.54
1:A:631:SER:O	1:A:635:LEU:HG	2.08	0.54
1:A:901:ILE:HG21	1:A:993:LEU:HD21	1.89	0.54
2:F:76:MET:HG2	2:F:78:THR:HG23	1.90	0.54
2:F:275:LYS:O	2:F:276:ARG:HG2	2.08	0.54
2:F:311:GLN:NE2	2:F:415:LYS:HB2	2.22	0.54
2:F:486:ASN:HD22	2:F:668:LEU:CD1	2.15	0.54
2:F:568:LEU:HD12	2:F:569:GLN:N	2.23	0.54
2:F:569:GLN:OE1	2:F:572:ILE:HD11	2.08	0.54
2:B:366:ALA:HB3	2:B:368:GLU:OE1	2.07	0.54
2:D:207:LEU:N	2:D:292:SER:O	2.41	0.54
1:A:566:ASN:OD1	2:F:671:LYS:NZ	2.35	0.54
1:A:825:MET:SD	1:A:826:ASP:N	2.81	0.54
1:C:938:VAL:HG12	1:C:940:GLY:N	2.16	0.54
2:F:354:ILE:CG2	2:F:388:VAL:HG23	2.33	0.54
2:F:667:PRO:HG2	3:F:1101:ATP:C2	2.42	0.54
2:B:148:GLY:O	2:B:149:LEU:HD22	2.08	0.54
2:D:453:TYR:HD2	2:D:492:MET:HE1	1.72	0.54
2:D:725:GLN:NE2	2:D:725:GLN:O	2.39	0.54
1:A:614:TYR:O	1:A:617:SER:OG	2.17	0.53
1:A:763:LYS:NZ	2:B:862:ASP:OD2	2.41	0.53
1:E:613:GLU:OE2	1:E:614:TYR:N	2.41	0.53
3:E:1101:ATP:N3	3:E:1101:ATP:H5'2	2.22	0.53
2:F:6:THR:HG22	2:F:66:ILE:O	2.08	0.53
2:F:450:ILE:HG22	2:F:450:ILE:O	2.08	0.53
2:F:518:GLN:HB2	2:F:520:ASP:OD1	2.08	0.53
2:F:654:SER:O	2:F:658:LEU:HD22	2.07	0.53
2:F:671:LYS:O	2:F:674:VAL:HG23	2.09	0.53
2:B:135:MET:HG3	2:B:135:MET:O	2.08	0.53
2:B:243:LEU:O	2:B:245:VAL:HG13	2.09	0.53
2:D:809:SER:OG	2:D:810:GLU:OE1	2.27	0.53
1:C:710:LEU:O	1:C:711:GLU:C	2.49	0.53
1:C:729:ARG:O	2:B:944:TYR:OH	2.19	0.53
1:C:836:ILE:O	1:C:837:LEU:HD22	2.08	0.53
1:E:775:SER:OG	1:E:816:ARG:NH2	2.41	0.53
1:E:948:SER:OG	2:F:172:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1026:GLU:OE1	2:D:1007:GLN:NE2	2.41	0.53
2:F:836:VAL:O	2:F:836:VAL:HG12	2.07	0.53
2:B:52:ILE:O	2:B:140:HIS:NE2	2.38	0.53
1:E:730:LEU:HD12	1:E:731:ARG:O	2.09	0.53
2:F:207:LEU:HD13	2:F:278:ILE:CG2	2.35	0.53
2:F:624:ARG:HB2	2:F:659:SER:OG	2.08	0.53
1:C:323:ILE:HG23	1:C:373:LYS:HD2	1.90	0.53
1:C:469:ARG:NH1	1:C:469:ARG:HG2	2.24	0.53
1:E:780:ARG:NH1	1:E:781:GLU:OE2	2.41	0.53
1:E:955:ARG:NH1	1:E:956:GLU:HA	2.24	0.53
2:F:23:TYR:CD2	2:F:24:LEU:HD22	2.44	0.53
2:F:156:SER:OG	2:F:157:PRO:HA	2.09	0.53
2:F:352:ILE:HB	2:F:390:PHE:HB2	1.91	0.53
2:B:410:ASP:O	2:B:414:THR:OG1	2.27	0.53
1:A:494:LEU:HD11	1:A:510:TRP:HH2	1.73	0.53
1:A:503:THR:C	1:A:507:ILE:HD12	2.33	0.53
1:A:909:SER:N	1:A:912:ASP:OD2	2.41	0.53
1:C:614:TYR:O	1:C:617:SER:OG	2.07	0.53
1:E:469:ARG:HB2	3:E:1101:ATP:H5'1	1.91	0.53
1:E:567:LYS:NZ	2:D:357:ASP:OD2	2.37	0.53
2:F:100:SER:CB	2:F:169:GLN:HB3	2.38	0.53
2:F:310:ASN:OD1	2:F:311:GLN:N	2.40	0.53
2:F:337:LYS:CE	2:F:375:GLU:HB3	2.37	0.53
2:F:806:ILE:HG23	2:F:806:ILE:O	2.08	0.53
2:B:473:THR:C	2:B:474:LEU:HD22	2.32	0.53
1:C:944:ILE:HG21	1:C:962:LEU:HB3	1.89	0.53
2:F:20:ARG:CA	2:F:57:LEU:HD11	2.37	0.53
2:F:415:LYS:O	2:F:416:LEU:HD22	2.09	0.53
2:F:657:SER:O	2:F:661:TYR:HD1	1.91	0.53
2:B:35:TYR:HB2	2:B:90:ILE:HD11	1.91	0.53
2:D:320:TRP:O	2:D:324:GLN:NE2	2.40	0.53
2:D:562:ASP:OD1	2:D:564:GLU:N	2.42	0.53
1:C:322:ILE:CG1	1:C:380:LEU:HD23	2.38	0.53
1:C:608:ARG:NH2	1:C:634:SER:O	2.40	0.53
1:C:764:GLY:O	1:C:767:ILE:HD12	2.09	0.53
2:F:352:ILE:HD12	2:F:390:PHE:O	2.09	0.53
2:F:726:ILE:HG23	2:F:726:ILE:O	2.09	0.53
2:D:83:ASP:OD1	2:D:84:PHE:N	2.42	0.53
2:D:637:LEU:H	2:D:637:LEU:HD12	1.74	0.53
1:A:516:TRP:CD2	2:F:363:LEU:HD21	2.44	0.53
1:A:870:ARG:NE	1:A:905:THR:OG1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLU:O	1:C:289:HIS:ND1	2.35	0.53
1:C:455:PRO:HG3	1:C:565:PHE:CD2	2.44	0.53
1:C:949:ILE:CG1	2:D:172:LEU:HD22	2.37	0.53
1:E:654:TYR:CE1	2:F:460:ILE:HG23	2.44	0.53
1:E:951:GLU:CD	2:F:169:GLN:HG2	2.32	0.53
2:F:20:ARG:HD2	2:F:57:LEU:CD2	2.39	0.53
2:F:22:ILE:HG23	2:F:87:PHE:CE2	2.44	0.53
2:F:35:TYR:OH	2:F:136:GLU:O	2.25	0.53
2:F:51:LYS:HD3	2:F:73:PHE:CE2	2.44	0.53
2:F:408:ILE:O	2:F:409:ILE:HD13	2.09	0.53
2:F:546:PHE:CD1	2:F:593:VAL:HG13	2.44	0.53
1:A:469:ARG:NH1	3:A:1102:ATP:H2'	2.24	0.53
1:C:767:ILE:HD12	1:C:767:ILE:H	1.74	0.53
1:C:949:ILE:HG23	2:D:119:GLU:HG3	1.90	0.53
1:E:959:ARG:HG3	1:E:963:LYS:HB2	1.90	0.53
1:E:966:LEU:HA	2:F:153:LEU:HD21	1.89	0.53
2:F:98:LEU:HD11	2:F:161:GLY:N	2.23	0.53
2:D:576:MET:HE1	2:D:579:LEU:HD22	1.89	0.53
1:A:651:LYS:NZ	2:B:611:ARG:O	2.42	0.53
1:C:814:THR:O	1:C:818:VAL:HG23	2.09	0.53
1:E:469:ARG:CD	3:E:1101:ATP:H3'	2.38	0.53
1:E:469:ARG:HD3	3:E:1101:ATP:H3'	1.91	0.53
1:E:960:LEU:HD12	1:E:960:LEU:H	1.74	0.53
2:F:148:GLY:HA2	2:F:183:LEU:HB3	1.90	0.53
2:F:159:PRO:HG2	2:F:160:GLN:OE1	2.09	0.53
2:F:185:TYR:O	2:F:188:GLU:HG3	2.09	0.53
2:F:486:ASN:O	2:F:666:THR:HB	2.08	0.53
2:F:793:PHE:HD1	2:F:827:VAL:HG13	1.74	0.53
2:B:82:MET:SD	2:B:84:PHE:N	2.78	0.53
2:D:754:HIS:CD2	2:D:757:LEU:HD13	2.43	0.53
1:A:778:ASN:HA	1:A:781:GLU:OE1	2.09	0.52
1:C:468:THR:HG21	3:C:1101:ATP:O1G	2.09	0.52
1:E:826:ASP:OD1	2:D:779:THR:HG21	2.09	0.52
2:F:281:PRO:O	2:F:285:ILE:HD12	2.09	0.52
2:F:429:LEU:HD11	2:F:499:TYR:HD1	1.74	0.52
2:F:521:SER:O	2:F:525:ILE:HD13	2.09	0.52
2:B:79:GLN:CD	2:B:237:ALA:HB3	2.34	0.52
2:B:642:GLN:OE1	2:B:642:GLN:HA	2.09	0.52
1:A:391:VAL:HG13	1:A:393:TRP:CZ3	2.44	0.52
1:A:635:LEU:HD13	2:F:981:ARG:HD2	1.90	0.52
1:A:800:ASP:N	1:A:800:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ASP:OD1	1:E:430:GLU:N	2.42	0.52
1:E:444:VAL:O	1:E:448:THR:N	2.33	0.52
2:F:509:CYS:SG	2:F:552:SER:HB3	2.49	0.52
2:F:514:SER:CB	2:F:524:LYS:HD3	2.38	0.52
1:A:535:GLN:N	1:A:538:ASP:OD1	2.43	0.52
1:A:878:VAL:HB	1:A:892:LEU:HD13	1.91	0.52
1:C:755:CYS:SG	1:C:756:GLY:N	2.82	0.52
1:C:954:ARG:HD3	2:D:169:GLN:NE2	2.24	0.52
2:F:184:LYS:HB3	2:F:188:GLU:OE2	2.08	0.52
2:F:458:VAL:HA	2:F:461:LEU:HD13	1.90	0.52
2:F:507:ILE:HG21	2:F:529:ILE:CD1	2.39	0.52
2:B:1:MET:N	2:B:1:MET:HE2	2.24	0.52
1:A:219:THR:CG2	1:A:285:ILE:HD11	2.39	0.52
1:A:825:MET:HE1	1:A:855:ARG:NH1	2.25	0.52
2:F:18:ILE:HA	2:F:66:ILE:HD13	1.90	0.52
2:F:453:TYR:HB2	2:F:614:ILE:HD11	1.92	0.52
2:B:280:ALA:HB1	2:B:284:ILE:HD13	1.92	0.52
2:B:773:PRO:HB2	2:B:901:ILE:HD11	1.89	0.52
2:D:682:THR:CA	2:D:699:ILE:HD11	2.39	0.52
1:A:219:THR:N	1:A:290:ILE:O	2.42	0.52
1:C:611:LEU:CD1	3:C:1101:ATP:HN61	2.19	0.52
2:F:51:LYS:HD3	2:F:73:PHE:HE2	1.74	0.52
2:F:71:LYS:HD2	2:F:185:TYR:CE2	2.45	0.52
2:F:98:LEU:HD21	2:F:160:GLN:O	2.09	0.52
2:F:213:THR:HA	2:F:437:TYR:HE1	1.75	0.52
2:F:378:LEU:H	2:F:378:LEU:HD12	1.74	0.52
2:B:969:HIS:CE1	2:B:977:ILE:HD12	2.44	0.52
2:D:106:ASN:O	2:D:110:TYR:N	2.33	0.52
2:D:518:GLN:N	2:D:518:GLN:OE1	2.42	0.52
1:A:210:LEU:HD11	1:A:247:TYR:CE2	2.45	0.52
1:E:955:ARG:HH11	1:E:955:ARG:C	2.17	0.52
2:F:169:GLN:HE22	2:F:171:ILE:CG1	2.23	0.52
2:F:474:LEU:HD12	2:F:475:ASN:N	2.25	0.52
2:F:488:GLY:HA2	3:F:1101:ATP:O1A	2.09	0.52
2:F:491:THR:CG2	3:F:1101:ATP:H2'	2.38	0.52
2:D:311:GLN:O	2:D:396:GLU:N	2.40	0.52
1:A:728:LEU:HD22	2:F:918:LYS:NZ	2.24	0.52
1:C:622:MET:HE2	1:C:623:LYS:CA	2.40	0.52
1:E:329:THR:HG22	1:E:392:GLN:HB2	1.92	0.52
2:F:98:LEU:HG	2:F:161:GLY:HA3	1.91	0.52
2:F:106:ASN:OD1	2:F:108:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:ASP:OD2	2:F:180:LEU:HB2	2.09	0.52
2:F:348:GLN:HE22	2:F:394:SER:HA	1.74	0.52
2:F:484:THR:HG22	2:F:485:ASN:O	2.10	0.52
2:F:489:LYS:HG3	3:F:1101:ATP:O1B	2.10	0.52
2:D:251:ILE:HG22	2:D:297:SER:O	2.10	0.52
2:D:922:ASP:OD1	2:D:923:ASN:N	2.42	0.52
1:A:330:VAL:HG23	1:A:371:ILE:HD11	1.91	0.52
1:A:709:LEU:HD23	1:A:751:VAL:CG2	2.40	0.52
1:E:254:SER:O	2:D:364:ASN:ND2	2.42	0.52
1:E:451:ILE:C	2:D:679:MET:HE1	2.34	0.52
2:F:106:ASN:ND2	2:F:109:LEU:HG	2.25	0.52
2:F:374:ASP:O	2:F:378:LEU:HD12	2.10	0.52
1:A:244:GLN:C	1:A:279:ILE:HG22	2.35	0.52
1:C:313:GLU:N	1:C:313:GLU:OE1	2.43	0.52
1:C:560:GLN:OE1	1:C:560:GLN:HA	2.08	0.52
1:E:950:ASN:HD21	2:F:123:ILE:HG21	1.75	0.52
2:F:92:ASP:OD2	2:F:93:ASN:N	2.43	0.52
2:F:438:TYR:HB3	2:F:440:PHE:CZ	2.45	0.52
2:F:686:TYR:HA	2:F:689:SER:OG	2.10	0.52
2:D:120:MET:SD	2:D:120:MET:N	2.71	0.52
2:D:237:ALA:O	2:D:241:LEU:HD22	2.10	0.52
2:D:557:VAL:CG1	2:D:566:ILE:HG23	2.40	0.52
2:D:726:ILE:HD11	2:D:786:ALA:CB	2.40	0.52
1:A:389:GLU:O	1:A:391:VAL:HG12	2.09	0.52
1:A:793:ILE:N	1:A:793:ILE:HD12	2.26	0.52
1:A:947:PHE:CZ	2:B:172:LEU:HD21	2.44	0.52
1:E:955:ARG:HD3	1:E:955:ARG:H	1.74	0.52
2:F:382:TYR:C	2:F:383:LYS:HD2	2.34	0.52
2:F:387:LEU:CD1	2:F:438:TYR:HE2	2.22	0.52
2:B:569:GLN:HA	2:B:572:ILE:HG22	1.92	0.52
2:D:21:ASP:OD1	2:D:22:ILE:N	2.43	0.52
2:D:98:LEU:O	2:D:168:THR:OG1	2.24	0.52
2:D:575:GLU:OE1	2:D:575:GLU:N	2.42	0.52
1:C:774:ALA:O	1:C:778:ASN:N	2.39	0.51
2:F:1:MET:C	2:F:1:MET:HE2	2.35	0.51
2:F:9:LEU:HD11	2:F:76:MET:CB	2.40	0.51
2:F:18:ILE:HG13	2:F:18:ILE:O	2.10	0.51
2:F:26:TYR:CB	2:F:34:LEU:HD22	2.39	0.51
2:F:598:ASN:OD1	2:F:601:ASN:N	2.32	0.51
2:D:98:LEU:HD22	2:D:155:CYS:CB	2.39	0.51
1:A:545:GLY:CA	2:F:555:LEU:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:ASP:OD1	1:C:887:GLN:N	2.43	0.51
2:F:8:SER:O	2:F:69:PRO:HA	2.10	0.51
2:F:40:LEU:HD12	2:F:40:LEU:N	2.25	0.51
2:F:467:CYS:HB2	2:F:472:ILE:HB	1.92	0.51
2:F:514:SER:HB2	2:F:524:LYS:HZ1	1.75	0.51
2:F:552:SER:O	2:F:555:LEU:HD23	2.10	0.51
2:B:13:TYR:OH	2:B:139:VAL:HG23	2.11	0.51
2:B:376:ASP:OD2	2:B:376:ASP:C	2.53	0.51
2:D:135:MET:C	2:D:162:LEU:HD11	2.35	0.51
1:C:448:THR:HG21	1:C:482:HIS:CE1	2.45	0.51
1:C:474:LEU:HD23	1:C:474:LEU:C	2.36	0.51
1:C:625:ASN:H	1:C:628:LEU:HD12	1.76	0.51
1:C:915:GLY:O	1:C:919:ASN:ND2	2.43	0.51
1:C:946:TYR:CG	1:C:962:LEU:HD11	2.45	0.51
2:F:234:PHE:O	2:F:235:THR:OG1	2.23	0.51
2:F:324:GLN:HB2	2:F:327:PHE:HD2	1.75	0.51
2:F:470:ARG:NH1	2:F:472:ILE:HD13	2.19	0.51
2:F:516:SER:OG	2:F:517:ARG:NH1	2.43	0.51
2:F:523:SER:HA	2:F:526:ILE:CD1	2.36	0.51
2:B:78:THR:OG1	2:B:187:ASN:OD1	2.05	0.51
2:D:726:ILE:HG23	2:D:787:THR:OG1	2.10	0.51
2:D:806:ILE:CG2	2:D:849:VAL:HG13	2.40	0.51
2:D:822:GLU:OE1	2:D:823:ALA:N	2.43	0.51
1:A:641:SER:N	1:A:644:ASP:OD2	2.36	0.51
1:C:709:LEU:HD13	1:C:751:VAL:HG11	1.93	0.51
2:F:196:LYS:O	2:F:196:LYS:HD3	2.10	0.51
2:F:425:ARG:HG2	2:F:426:PRO:HD2	1.92	0.51
2:F:429:LEU:HD22	2:F:499:TYR:O	2.10	0.51
2:F:901:ILE:HD11	2:F:937:ASN:C	2.36	0.51
2:D:488:GLY:N	3:D:1601:ATP:O2B	2.44	0.51
2:D:839:LYS:N	2:D:882:LEU:O	2.43	0.51
1:C:760:ILE:O	1:C:760:ILE:HG22	2.09	0.51
1:E:625:ASN:OD1	1:E:626:ARG:N	2.43	0.51
1:E:956:GLU:HG2	1:E:958:ASN:OD1	2.10	0.51
2:F:104:LEU:CD1	2:F:179:LYS:HE2	2.41	0.51
2:F:135:MET:HE1	2:F:164:ASP:OD1	2.10	0.51
2:F:316:ARG:O	2:F:421:ILE:HD12	2.11	0.51
2:F:351:LEU:HD11	2:F:424:ARG:NH1	2.24	0.51
2:F:458:VAL:C	2:F:460:ILE:H	2.19	0.51
2:B:105:ILE:HG21	2:B:113:LEU:HD12	1.91	0.51
2:D:102:THR:HG1	2:D:153:LEU:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:ARG:NH1	2:D:169:GLN:OE1	2.41	0.51
2:F:72:LEU:HD22	2:F:73:PHE:CE1	2.44	0.51
2:F:230:SER:C	2:F:231:ILE:HD13	2.36	0.51
2:F:345:ILE:HA	2:F:408:ILE:HD13	1.93	0.51
2:F:387:LEU:HD12	2:F:438:TYR:CE2	2.44	0.51
2:F:687:GLN:HA	2:F:690:LYS:NZ	2.25	0.51
2:D:977:ILE:HG23	2:D:981:ARG:HG3	1.92	0.51
1:A:327:ASN:OD1	1:A:327:ASN:O	2.28	0.51
1:A:817:VAL:O	1:A:821:LEU:HG	2.11	0.51
1:C:311:LYS:NZ	2:B:373:ASP:OD1	2.42	0.51
1:C:955:ARG:HD3	1:C:955:ARG:H	1.75	0.51
2:F:82:MET:HE1	2:F:270:PRO:HD3	1.93	0.51
2:F:676:THR:O	2:F:679:MET:HB2	2.11	0.51
2:B:850:MET:SD	2:B:851:ASP:N	2.84	0.51
2:B:881:ASP:OD1	2:B:882:LEU:N	2.42	0.51
2:D:106:ASN:OD1	2:D:108:GLN:N	2.44	0.51
1:E:468:THR:OG1	3:E:1101:ATP:O1A	2.28	0.51
2:F:43:TYR:HB3	2:F:273:PHE:HZ	1.75	0.51
2:F:118:GLN:HB3	2:F:120:MET:HE1	1.92	0.51
2:F:120:MET:HE2	2:F:121:GLN:OE1	2.11	0.51
2:F:445:TYR:CD1	2:F:495:PHE:HE2	2.28	0.51
2:F:646:PRO:O	2:F:699:ILE:HD12	2.11	0.51
2:F:785:ILE:HG23	2:F:789:PHE:CE2	2.46	0.51
2:D:514:SER:OG	2:D:515:ASN:OD1	2.26	0.51
2:D:978:SER:O	2:D:982:TRP:N	2.38	0.51
1:C:466:GLY:HA3	3:C:1101:ATP:C2	2.46	0.51
1:C:743:GLY:CA	3:C:1102:ATP:H5'1	2.40	0.51
2:F:7:PHE:HB3	2:F:70:SER:HB3	1.92	0.51
2:F:26:TYR:CE2	2:F:34:LEU:HB3	2.46	0.51
2:F:444:PHE:HA	2:F:630:TRP:CZ2	2.46	0.51
2:F:467:CYS:O	2:F:472:ILE:N	2.35	0.51
2:F:641:VAL:HG23	2:F:643:GLN:CD	2.36	0.51
2:B:360:MET:O	2:B:360:MET:SD	2.69	0.51
2:D:515:ASN:OD1	2:D:515:ASN:N	2.42	0.51
1:A:298:ASP:OD1	1:A:299:ALA:N	2.44	0.51
1:C:631:SER:O	1:C:635:LEU:HG	2.11	0.51
1:C:807:GLY:N	1:C:815:ASP:OD1	2.40	0.51
1:E:474:LEU:HD23	1:E:474:LEU:C	2.36	0.51
1:E:702:LEU:HD11	1:E:862:CYS:HB2	1.91	0.51
2:F:20:ARG:CD	2:F:57:LEU:HD11	2.39	0.51
2:F:448:LEU:HD12	2:F:455:ARG:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:867:ASP:OD1	2:D:867:ASP:C	2.53	0.51
1:C:643:LEU:HD12	1:C:647:ILE:HD11	1.93	0.50
1:C:675:LEU:HD23	1:C:675:LEU:C	2.36	0.50
1:E:829:GLU:OE1	2:D:725:GLN:NE2	2.44	0.50
2:F:207:LEU:HD12	2:F:278:ILE:O	2.11	0.50
2:F:600:ASP:HA	2:F:607:ARG:NH2	2.27	0.50
2:D:572:ILE:O	2:D:575:GLU:OE1	2.29	0.50
2:D:754:HIS:CG	2:D:757:LEU:HD13	2.46	0.50
1:C:770:LYS:HE3	2:D:804:MET:SD	2.52	0.50
1:C:954:ARG:HD3	2:D:169:GLN:CD	2.36	0.50
2:F:39:ARG:NH1	2:F:41:PRO:HA	2.25	0.50
2:F:217:ASP:O	2:F:220:ARG:NH1	2.38	0.50
2:D:35:TYR:HB3	2:D:52:ILE:HD11	1.93	0.50
2:D:416:LEU:C	2:D:416:LEU:HD12	2.35	0.50
1:A:719:TYR:CE2	2:F:959:ALA:HB1	2.47	0.50
2:F:203:LEU:O	2:F:296:ILE:HG22	2.12	0.50
2:F:557:VAL:HG11	2:F:566:ILE:HA	1.94	0.50
2:F:571:SER:O	2:F:572:ILE:C	2.54	0.50
2:F:677:ALA:HB1	2:F:701:ILE:HG23	1.92	0.50
2:B:155:CYS:O	2:B:157:PRO:HD2	2.11	0.50
2:B:271:ASN:OD1	2:B:273:PHE:N	2.44	0.50
2:B:343:LYS:HD3	2:B:408:ILE:HD11	1.92	0.50
2:D:363:LEU:N	2:D:363:LEU:HD23	2.26	0.50
2:D:633:SER:O	2:D:637:LEU:HD12	2.11	0.50
1:C:347:TYR:O	1:C:351:LEU:N	2.44	0.50
1:C:515:TYR:OH	1:C:567:LYS:NZ	2.40	0.50
1:C:737:TYR:CE2	1:C:861:ILE:HD13	2.46	0.50
1:E:274:LYS:NZ	1:E:313:GLU:OE2	2.44	0.50
1:E:382:ASN:O	1:E:386:ILE:HG22	2.12	0.50
1:E:800:ASP:OD2	1:E:840:THR:OG1	2.27	0.50
1:E:947:PHE:CE2	2:F:174:ASN:HB3	2.46	0.50
2:F:39:ARG:HG2	2:F:48:THR:O	2.10	0.50
2:F:57:LEU:HD12	2:F:58:ASP:H	1.76	0.50
2:F:481:HIS:NE2	2:F:615:LEU:HB3	2.26	0.50
2:F:620:SER:H	2:F:623:GLN:CD	2.20	0.50
1:A:250:ILE:HG22	1:A:310:ILE:HG22	1.93	0.50
1:A:882:ASP:OD1	1:A:889:LYS:HA	2.11	0.50
1:C:357:THR:O	1:C:360:LEU:HD23	2.12	0.50
1:C:763:LYS:HZ2	2:D:859:ALA:HB3	1.74	0.50
2:F:11:GLY:O	2:F:69:PRO:HB3	2.12	0.50
2:F:146:THR:CG2	2:F:149:LEU:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:346:LEU:HD13	2:F:409:ILE:CG1	2.39	0.50
2:B:478:VAL:HG12	2:B:612:PHE:CB	2.42	0.50
2:D:97:VAL:HG22	2:D:162:LEU:HB3	1.94	0.50
2:D:951:MET:CA	2:D:951:MET:HE3	2.42	0.50
1:C:355:LEU:C	1:C:356:LEU:HD22	2.36	0.50
1:C:450:PRO:O	1:C:451:ILE:HD13	2.11	0.50
1:C:943:ASN:O	1:C:944:ILE:HD13	2.11	0.50
1:E:507:ILE:HD11	1:E:556:PHE:HD2	1.76	0.50
2:F:189:ASP:OD1	2:F:189:ASP:N	2.44	0.50
2:F:449:HIS:HA	2:F:455:ARG:HH21	1.76	0.50
2:F:480:LEU:HD12	2:F:480:LEU:N	2.27	0.50
2:F:613:GLU:N	2:F:613:GLU:OE1	2.44	0.50
2:F:937:ASN:CB	2:F:1017:LEU:HD11	2.40	0.50
2:B:490:ALA:N	3:B:1101:ATP:O1B	2.40	0.50
2:B:650:MET:HE1	2:B:700:LEU:HD12	1.93	0.50
2:D:373:ASP:OD1	2:D:373:ASP:N	2.43	0.50
2:D:839:LYS:NZ	2:D:881:ASP:O	2.40	0.50
1:A:458:ILE:HD11	1:A:594:VAL:HG11	1.94	0.50
1:A:547:TRP:O	1:A:552:LYS:NZ	2.44	0.50
1:A:921:TYR:O	1:A:925:VAL:HG23	2.12	0.50
1:E:451:ILE:HD11	2:D:643:GLN:HE22	1.76	0.50
1:E:845:LEU:H	1:E:845:LEU:HD12	1.77	0.50
1:E:922:LEU:HD23	2:F:762:MET:HE2	1.92	0.50
2:F:80:PRO:O	2:F:269:LEU:HD12	2.11	0.50
2:F:453:TYR:CE2	2:F:454:VAL:HG23	2.46	0.50
2:B:17:SER:HB3	2:B:67:VAL:HG12	1.93	0.50
2:B:180:LEU:H	2:B:180:LEU:HD12	1.76	0.50
2:B:650:MET:CE	2:B:700:LEU:HD12	2.41	0.50
2:B:702:THR:OG1	2:B:704:GLU:OE2	2.29	0.50
1:A:440:LYS:HZ1	1:A:473:GLU:HB3	1.76	0.50
1:C:452:ILE:HA	2:B:679:MET:HE3	1.94	0.50
1:C:758:ASN:ND2	1:C:790:LYS:O	2.45	0.50
1:E:891:ALA:C	1:E:987:VAL:HG13	2.37	0.50
1:E:954:ARG:CD	1:E:961:ARG:HH22	2.23	0.50
2:F:133:ASN:O	2:F:137:THR:N	2.44	0.50
2:F:378:LEU:O	2:F:382:TYR:N	2.37	0.50
2:D:102:THR:OG1	2:D:153:LEU:N	2.38	0.50
2:D:335:LEU:HD21	2:D:390:PHE:CE2	2.46	0.50
2:D:879:ARG:HD2	2:D:882:LEU:HD23	1.94	0.50
1:A:531:PHE:HB3	1:A:554:LEU:HD13	1.93	0.50
1:A:922:LEU:O	1:A:926:HIS:ND1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:THR:OG1	1:C:593:PHE:O	2.22	0.50
2:F:17:SER:OG	2:F:67:VAL:HB	2.12	0.50
2:B:929:GLU:O	2:B:933:LEU:HD23	2.12	0.50
2:D:484:THR:HG21	2:D:618:VAL:HG22	1.93	0.50
2:D:668:LEU:O	2:D:668:LEU:HD12	2.10	0.50
1:A:391:VAL:HG13	1:A:393:TRP:CE3	2.47	0.49
1:A:450:PRO:O	1:A:570:LYS:NZ	2.42	0.49
1:C:215:ILE:HG22	1:C:216:LEU:H	1.76	0.49
1:C:585:ASN:OD1	1:C:587:LEU:HB3	2.12	0.49
1:C:938:VAL:CG2	1:C:963:LYS:HZ1	2.25	0.49
2:F:230:SER:O	2:F:231:ILE:HD13	2.11	0.49
2:F:335:LEU:O	2:F:339:PHE:HD2	1.95	0.49
2:B:35:TYR:HB3	2:B:52:ILE:HD11	1.94	0.49
2:B:79:GLN:NE2	2:B:237:ALA:HB3	2.27	0.49
2:B:457:LEU:HD13	2:B:492:MET:CE	2.36	0.49
2:B:494:ARG:O	2:B:497:SER:OG	2.22	0.49
2:D:522:THR:O	2:D:526:ILE:HG12	2.12	0.49
2:D:625:LEU:HD12	2:D:629:GLN:NE2	2.27	0.49
2:D:628:PHE:CE1	2:D:670:ILE:HG23	2.47	0.49
2:D:951:MET:HE3	2:D:951:MET:HA	1.94	0.49
1:A:356:LEU:HD23	1:A:356:LEU:N	2.27	0.49
1:A:398:MET:HE1	1:A:406:ILE:HD12	1.93	0.49
1:A:585:ASN:OD1	1:A:587:LEU:HD23	2.11	0.49
1:E:451:ILE:HD11	2:D:643:GLN:NE2	2.27	0.49
1:E:490:ASP:OD1	1:E:491:CYS:N	2.44	0.49
2:F:259:VAL:O	2:F:260:ARG:HD3	2.12	0.49
2:F:655:PHE:HA	2:F:658:LEU:HD23	1.94	0.49
2:B:706:LEU:N	2:B:706:LEU:HD12	2.26	0.49
2:D:975:GLU:OE1	2:D:975:GLU:N	2.41	0.49
1:A:438:SER:O	1:A:442:GLU:OE1	2.31	0.49
1:C:567:LYS:HE2	2:B:383:LYS:O	2.11	0.49
1:C:627:ASP:N	1:C:627:ASP:OD1	2.46	0.49
1:E:954:ARG:NH2	1:E:956:GLU:HB2	2.28	0.49
2:F:102:THR:OG1	2:F:154:ASN:HB2	2.12	0.49
2:F:169:GLN:O	2:F:170:LEU:HD13	2.11	0.49
2:F:235:THR:CG2	2:F:236:ASP:N	2.75	0.49
2:F:470:ARG:HB3	2:F:472:ILE:CD1	2.42	0.49
2:F:770:PHE:CE2	2:F:781:MET:HE1	2.46	0.49
2:B:647:VAL:HG12	2:B:699:ILE:CG2	2.42	0.49
1:A:468:THR:N	3:A:1102:ATP:O1B	2.40	0.49
1:A:561:VAL:HG21	1:A:593:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ILE:H	1:C:439:ILE:HD12	1.78	0.49
1:C:952:HIS:O	1:C:954:ARG:NE	2.45	0.49
2:F:16[A]:CYS:SG	2:F:69:PRO:HD3	2.52	0.49
2:F:153:LEU:HG	2:F:154:ASN:OD1	2.13	0.49
2:B:155:CYS:O	2:B:156:SER:HB3	2.12	0.49
2:B:254:SER:HB3	2:B:259:VAL:HG23	1.94	0.49
2:B:492:MET:HE2	2:B:492:MET:C	2.37	0.49
2:B:882:LEU:O	2:B:882:LEU:HD12	2.12	0.49
2:D:156:SER:CB	2:D:157:PRO:CD	2.91	0.49
2:D:251:ILE:HG21	2:D:296:ILE:HD11	1.94	0.49
1:C:768:LEU:HD23	1:C:768:LEU:C	2.37	0.49
2:F:18:ILE:HD11	2:F:23:TYR:HB2	1.95	0.49
2:F:228:ASP:HB3	2:F:345:ILE:HD12	1.93	0.49
2:D:673:ILE:HG13	2:D:709:ALA:HB1	1.94	0.49
1:A:928:TRP:HB2	1:A:986:ALA:HB2	1.94	0.49
1:C:800:ASP:HA	1:C:846:ILE:HG23	1.94	0.49
1:C:960:LEU:C	1:C:960:LEU:HD23	2.38	0.49
1:E:512:SER:O	2:D:363:LEU:HD11	2.12	0.49
2:F:100:SER:HB2	2:F:169:GLN:CD	2.37	0.49
2:F:201:SER:O	2:F:297:SER:HA	2.12	0.49
2:F:616:VAL:HG13	2:F:616:VAL:O	2.12	0.49
2:F:953:ASN:O	2:F:957:ARG:HG2	2.12	0.49
2:B:374:ASP:O	2:B:377:GLU:N	2.43	0.49
2:B:508:ASP:OD1	2:B:511:SER:N	2.46	0.49
2:D:22:ILE:HD11	2:D:64:CYS:HA	1.94	0.49
2:D:730:THR:N	2:D:733:ASP:OD2	2.45	0.49
1:A:330:VAL:HG12	1:A:391:VAL:HG22	1.94	0.49
1:C:322:ILE:HG12	1:C:380:LEU:HD23	1.93	0.49
1:E:230:LEU:HD22	1:E:354:SER:OG	2.13	0.49
1:E:581:LYS:HZ1	1:E:597:THR:CB	2.25	0.49
1:E:614:TYR:O	1:E:617:SER:OG	2.17	0.49
2:F:2:LYS:CE	2:F:84:PHE:HB2	2.42	0.49
2:F:17:SER:O	2:F:66:ILE:HG23	2.13	0.49
2:F:206:ASP:OD1	2:F:277:THR:HG22	2.11	0.49
2:F:435:GLN:NE2	2:F:498:LYS:HE2	2.27	0.49
2:F:487:VAL:HG22	2:F:487:VAL:O	2.12	0.49
2:B:140:HIS:N	2:B:143:ASP:OD2	2.44	0.49
2:B:181:SER:O	2:B:184:LYS:NZ	2.45	0.49
2:B:237:ALA:HB2	2:B:266:VAL:HG11	1.94	0.49
2:D:240:LEU:O	2:D:244:ASP:N	2.44	0.49
1:E:258:SER:O	1:E:259:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:TYR:O	2:F:114:MET:HB3	2.12	0.49
2:F:238:GLU:HA	2:F:241:LEU:HG	1.93	0.49
2:F:335:LEU:HA	2:F:354:ILE:CD1	2.43	0.49
2:F:351:LEU:HD11	2:F:424:ARG:CZ	2.42	0.49
2:F:408:ILE:C	2:F:409:ILE:HD13	2.37	0.49
2:F:451:PHE:HE1	2:F:623:GLN:HB3	1.76	0.49
2:F:492:MET:SD	2:F:492:MET:C	2.95	0.49
2:F:830:PHE:HB3	2:F:833:ILE:HG22	1.94	0.49
2:B:480:LEU:HD21	2:B:492:MET:SD	2.53	0.49
2:B:512:LEU:O	2:B:513:THR:C	2.56	0.49
2:D:261:LEU:HD12	2:D:262:VAL:N	2.27	0.49
2:D:666:THR:N	2:D:669:ASP:OD2	2.43	0.49
1:E:321:ASN:C	1:E:321:ASN:OD1	2.55	0.49
1:E:965:LEU:HG	2:F:154:ASN:OD1	2.13	0.49
2:F:13:TYR:HE1	2:F:145:LEU:HD22	1.78	0.49
2:F:21:ASP:OD2	2:F:64:CYS:N	2.46	0.49
2:F:35:TYR:HE1	2:F:54:HIS:HB2	1.78	0.49
2:F:811:ALA:HB1	2:F:815:ARG:HE	1.78	0.49
2:B:598:ASN:OD1	2:B:598:ASN:C	2.56	0.49
2:D:98:LEU:HD22	2:D:155:CYS:HB3	1.94	0.49
2:D:551:ASP:OD2	2:D:551:ASP:C	2.55	0.49
1:A:357:THR:O	1:A:360:LEU:HD13	2.12	0.49
1:A:531:PHE:CG	1:A:554:LEU:HD13	2.47	0.49
1:A:794:LEU:HD11	1:A:796:PHE:CE1	2.48	0.49
1:A:841:SER:O	1:A:1016:TYR:OH	2.17	0.49
1:C:547:TRP:C	1:C:549:ASN:H	2.21	0.49
1:C:901:ILE:HG12	1:C:993:LEU:HD21	1.95	0.49
1:C:965:LEU:HD21	2:D:154:ASN:ND2	2.27	0.49
1:E:587:LEU:HD12	1:E:587:LEU:H	1.78	0.49
2:F:4:SER:HG	2:F:65:SER:HA	1.77	0.49
2:F:109:LEU:HD23	2:F:112:LYS:NZ	2.28	0.49
2:F:285:ILE:HG22	2:F:427:LEU:HD23	1.95	0.49
2:F:341:GLU:OE1	2:F:342:SER:HB3	2.13	0.49
2:F:367:GLU:OE1	2:F:367:GLU:N	2.40	0.49
2:F:663:ALA:O	2:F:714:ARG:NH2	2.46	0.49
2:B:378:LEU:HD12	2:B:378:LEU:H	1.78	0.49
2:D:38:ILE:HD12	2:D:38:ILE:C	2.37	0.49
2:D:90:ILE:HD12	2:D:90:ILE:C	2.38	0.49
1:A:799:PHE:HD1	1:A:838:ALA:HB1	1.78	0.48
1:C:684:ARG:NH2	2:D:607:ARG:HG3	2.28	0.48
1:C:741:GLY:C	3:C:1102:ATP:H5'2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:937:VAL:O	1:C:937:VAL:HG12	2.13	0.48
1:C:961:ARG:O	1:C:962:LEU:C	2.56	0.48
1:E:836:ILE:O	1:E:837:LEU:HD22	2.13	0.48
2:F:44:GLY:HA3	2:F:212:CYS:SG	2.53	0.48
2:F:456:GLN:OE1	2:F:457:LEU:N	2.46	0.48
2:B:780:LEU:HD23	3:B:1102:ATP:PA	2.53	0.48
2:D:21:ASP:O	2:D:25:GLU:HG3	2.13	0.48
2:D:255:ASN:HD21	2:D:294:VAL:HG22	1.78	0.48
1:A:436:VAL:HA	1:A:439:ILE:HD12	1.94	0.48
1:C:949:ILE:HD12	2:D:119:GLU:CB	2.44	0.48
1:E:971:VAL:HG22	1:E:974:THR:HA	1.95	0.48
2:F:1:MET:HE1	2:F:3:ALA:CB	2.25	0.48
2:F:52:ILE:CG2	2:F:138:VAL:HG21	2.43	0.48
2:F:446:TYR:HD2	2:F:454:VAL:HG11	1.77	0.48
2:F:550:LEU:HD21	2:F:606:PHE:CE2	2.47	0.48
2:D:650:MET:HE1	2:D:702:THR:HG22	1.95	0.48
1:A:891:ALA:O	1:A:987:VAL:HG23	2.12	0.48
1:E:334:TYR:OH	1:E:337:LYS:O	2.31	0.48
1:E:445:ASN:O	1:E:449:SER:N	2.46	0.48
2:F:419:THR:CG2	2:F:420:ASN:H	2.19	0.48
2:F:448:LEU:HB3	2:F:455:ARG:HE	1.77	0.48
2:F:548:ALA:HA	2:F:595:SER:OG	2.12	0.48
2:F:606:PHE:CD1	2:F:606:PHE:C	2.89	0.48
2:B:475:ASN:OD1	2:B:611:ARG:NH1	2.44	0.48
2:B:730:THR:OG1	2:B:733:ASP:OD2	2.30	0.48
2:D:460:ILE:HD11	2:D:612:PHE:CE2	2.48	0.48
1:A:525:ASP:OD1	1:A:526:ASN:N	2.46	0.48
1:A:704:ASN:O	1:A:708:VAL:HG23	2.13	0.48
1:C:356:LEU:HD12	1:C:369:ILE:HG21	1.94	0.48
1:C:675:LEU:HD23	1:C:675:LEU:O	2.13	0.48
1:E:327:ASN:OD1	1:E:329:THR:HG23	2.14	0.48
1:E:557:PHE:HE1	1:E:561:VAL:HG11	1.78	0.48
1:E:584:ILE:CG2	1:E:588:LEU:HD21	2.43	0.48
1:E:652:ILE:HD11	1:E:674:SER:CB	2.43	0.48
1:E:825:MET:SD	1:E:825:MET:N	2.85	0.48
2:F:97:VAL:HG13	2:F:162:LEU:O	2.13	0.48
2:F:446:TYR:OH	2:F:492:MET:HA	2.13	0.48
2:F:640:ASP:HA	2:F:642:GLN:HE22	1.78	0.48
2:B:299:SER:OG	2:B:301:ILE:HG22	2.13	0.48
2:B:423:ASN:OD1	2:B:424:ARG:N	2.45	0.48
2:B:554:LEU:HD12	2:B:554:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:504:LEU:C	2:D:505:LEU:HD12	2.38	0.48
1:A:217:ARG:NH1	1:A:518:GLY:O	2.46	0.48
1:A:233:VAL:HG13	1:A:279:ILE:HD12	1.94	0.48
1:A:567:LYS:HZ1	2:F:383:LYS:HB2	1.74	0.48
1:A:588:LEU:HD13	1:A:594:VAL:HG13	1.95	0.48
1:C:396:THR:OG1	1:C:397:GLN:N	2.45	0.48
2:F:72:LEU:HD23	2:F:72:LEU:C	2.38	0.48
2:F:135:MET:HE1	2:F:164:ASP:CG	2.39	0.48
2:F:251:ILE:HG22	2:F:296:ILE:CD1	2.38	0.48
2:B:508:ASP:OD2	2:B:549:HIS:ND1	2.47	0.48
2:B:750:MET:O	2:B:750:MET:HE3	2.13	0.48
1:A:969:ASP:OD1	1:A:969:ASP:N	2.43	0.48
1:E:557:PHE:CE1	1:E:561:VAL:HG11	2.49	0.48
1:E:933:ASP:OD1	1:E:939:PRO:HD3	2.13	0.48
2:F:26:TYR:HA	2:F:91:LEU:HD21	1.95	0.48
2:F:341:GLU:HB3	2:F:344:ARG:NH2	2.28	0.48
2:D:254:SER:OG	2:D:295:THR:HG23	2.12	0.48
2:D:462:GLU:OE2	2:D:463:THR:N	2.47	0.48
2:D:514:SER:OG	2:D:515:ASN:N	2.41	0.48
1:A:746:LEU:HD11	3:A:1101:ATP:C2'	2.34	0.48
1:C:469:ARG:NH2	1:C:473:GLU:OE1	2.46	0.48
1:C:628:LEU:HD11	1:C:667:THR:HA	1.95	0.48
1:C:850:LEU:HB3	1:C:856:LEU:HD13	1.96	0.48
1:C:948:SER:HA	1:C:951:GLU:OE2	2.14	0.48
1:E:375:GLU:HA	1:E:375:GLU:OE2	2.13	0.48
1:E:937:VAL:HG12	1:E:938:VAL:N	2.29	0.48
2:F:18:ILE:HA	2:F:66:ILE:HD12	1.96	0.48
2:F:114:MET:SD	2:F:114:MET:O	2.72	0.48
2:F:132:ILE:HG23	2:F:137:THR:CB	2.43	0.48
2:F:238:GLU:HA	2:F:241:LEU:CG	2.44	0.48
2:F:335:LEU:HD22	2:F:390:PHE:CZ	2.48	0.48
2:F:364:ASN:HB2	2:F:367:GLU:OE2	2.13	0.48
2:F:497:SER:OG	2:F:504:LEU:HD22	2.14	0.48
2:F:983:PHE:HA	2:F:987:ALA:HB2	1.94	0.48
2:D:317:VAL:HG23	2:D:390:PHE:CA	2.43	0.48
2:D:806:ILE:HG23	2:D:849:VAL:HG13	1.96	0.48
1:C:647:ILE:HG23	2:D:611:ARG:HD3	1.94	0.48
1:E:966:LEU:HA	2:F:153:LEU:CD2	2.44	0.48
2:F:209:SER:OG	2:F:432:SER:HA	2.14	0.48
2:F:481:HIS:CB	2:F:599:ILE:HB	2.44	0.48
2:F:688:GLU:OE2	2:F:696:PRO:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TYR:O	2:B:114:MET:SD	2.72	0.48
2:B:233:ALA:HB2	2:B:262:VAL:HG21	1.94	0.48
2:B:572:ILE:HD11	2:B:576:MET:CE	2.44	0.48
2:D:116:LEU:HD22	2:D:125:PHE:HZ	1.77	0.48
1:A:452:ILE:HA	2:F:679:MET:CE	2.44	0.48
1:C:469:ARG:HD2	3:C:1101:ATP:N3	2.29	0.48
1:E:739:TYR:CE1	1:E:1012:LEU:HD11	2.49	0.48
1:E:778:ASN:O	1:E:782:LEU:HD23	2.13	0.48
1:E:874:LEU:HD13	1:E:898:LEU:HB3	1.96	0.48
2:F:20:ARG:HG3	2:F:59:ASP:OD1	2.13	0.48
2:F:101:VAL:HG12	2:F:102:THR:N	2.29	0.48
2:F:231:ILE:HG22	2:F:262:VAL:HA	1.96	0.48
2:F:243:LEU:HD11	2:F:298:LYS:N	2.29	0.48
2:F:497:SER:CB	2:F:504:LEU:HD13	2.43	0.48
2:F:629:GLN:HE22	2:F:655:PHE:HB3	1.79	0.48
2:F:650:MET:SD	2:F:650:MET:N	2.78	0.48
2:B:312:VAL:HG11	2:B:409:ILE:CD1	2.43	0.48
2:B:691:LYS:C	2:B:691:LYS:HD3	2.39	0.48
2:B:850:MET:SD	2:B:850:MET:C	2.97	0.48
1:A:290:ILE:HG21	1:A:310:ILE:HD11	1.96	0.48
1:A:567:LYS:NZ	2:F:383:LYS:O	2.43	0.48
1:A:947:PHE:CE2	2:B:172:LEU:HD11	2.49	0.48
1:A:974:THR:O	1:A:975:LYS:HG3	2.13	0.48
1:C:460:ASP:OD1	1:C:461:GLY:N	2.47	0.48
1:C:587:LEU:O	1:C:587:LEU:HD12	2.14	0.48
1:E:971:VAL:HG22	1:E:974:THR:CB	2.44	0.48
2:F:73:PHE:HB2	2:F:75:PHE:CE1	2.49	0.48
2:F:79:GLN:O	2:F:269:LEU:HD13	2.14	0.48
2:F:107:GLU:HA	2:F:174:ASN:ND2	2.29	0.48
2:F:107:GLU:CD	2:F:174:ASN:HD21	2.22	0.48
2:F:316:ARG:HB2	2:F:390:PHE:HE1	1.79	0.48
2:F:348:GLN:HG3	2:F:349:ASN:OD1	2.14	0.48
2:F:946:LEU:HG	2:F:1008:LEU:HD13	1.95	0.48
2:D:739:PHE:CE2	2:D:740:VAL:HG13	2.49	0.48
1:A:433:PHE:HE1	1:A:435:THR:HG1	1.59	0.47
1:A:870:ARG:HG2	1:A:913:LEU:HD11	1.96	0.47
1:C:322:ILE:HD11	1:C:380:LEU:HD23	1.95	0.47
1:C:820:GLN:HG2	2:B:799:PRO:HB2	1.95	0.47
1:E:235:ILE:O	1:E:282:ASP:N	2.47	0.47
2:F:103:PHE:HE2	2:F:170:LEU:HB3	1.79	0.47
2:F:164:ASP:O	2:F:168:THR:HB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:LEU:C	2:F:183:LEU:HD23	2.38	0.47
2:F:314:ILE:HD13	2:F:392:VAL:HA	1.94	0.47
2:F:415:LYS:N	2:F:415:LYS:HD3	2.28	0.47
2:F:611:ARG:C	2:F:612:PHE:HD1	2.22	0.47
1:A:492:GLU:OE2	1:A:493:THR:OG1	2.31	0.47
1:C:524:LEU:HD12	1:C:524:LEU:N	2.29	0.47
1:E:731:ARG:NH2	2:D:949:ASP:OD2	2.47	0.47
2:F:20:ARG:CG	2:F:59:ASP:HA	2.44	0.47
2:F:755:PRO:O	2:F:759:THR:N	2.46	0.47
2:B:478:VAL:CG2	2:B:593:VAL:HG12	2.45	0.47
2:D:568:LEU:O	2:D:571:SER:OG	2.29	0.47
2:D:715:ASN:O	2:D:718:SER:OG	2.27	0.47
1:A:527:VAL:HG21	1:A:576:PHE:CE2	2.48	0.47
1:A:799:PHE:CD1	1:A:838:ALA:HB1	2.49	0.47
1:C:743:GLY:H	3:C:1102:ATP:H5'1	1.74	0.47
1:C:844:ASP:OD2	1:C:844:ASP:C	2.58	0.47
1:C:914:GLN:OE1	3:C:1102:ATP:H1'	2.15	0.47
1:C:944:ILE:HG23	1:C:966:LEU:CD1	2.43	0.47
1:C:971:VAL:HG13	1:C:971:VAL:O	2.14	0.47
1:E:719:TYR:HB3	2:D:955:MET:HE1	1.96	0.47
1:E:735:LEU:C	1:E:736:LEU:HD12	2.39	0.47
2:F:38:ILE:HD12	2:F:86:TYR:O	2.14	0.47
2:F:134:SER:OG	2:F:164:ASP:HA	2.14	0.47
2:F:137:THR:O	2:F:162:LEU:HD12	2.13	0.47
2:F:214:ILE:HD13	2:F:214:ILE:N	2.27	0.47
2:F:234:PHE:HB3	2:F:267:LEU:HD21	1.95	0.47
2:F:360:MET:SD	2:F:360:MET:O	2.72	0.47
2:F:426:PRO:HG2	2:F:501:GLY:O	2.14	0.47
2:F:654:SER:OG	2:F:657:SER:OG	2.13	0.47
2:D:551:ASP:HB2	2:D:596:VAL:HG13	1.95	0.47
2:D:726:ILE:HG21	2:D:787:THR:HG23	1.97	0.47
2:D:850:MET:SD	2:D:850:MET:N	2.87	0.47
1:A:815:ASP:O	1:A:819:ASN:OD1	2.31	0.47
1:A:1015:ILE:O	1:A:1018:ARG:NH2	2.46	0.47
1:C:611:LEU:HD11	3:C:1101:ATP:N6	2.26	0.47
1:E:423:VAL:HG23	1:E:423:VAL:O	2.14	0.47
1:E:584:ILE:HG22	1:E:588:LEU:HD21	1.96	0.47
2:F:5:LEU:HD12	2:F:6:THR:H	1.77	0.47
2:F:209:SER:HB3	2:F:285:ILE:HD13	1.96	0.47
2:F:216:ARG:HH21	2:F:223:PRO:HD2	1.79	0.47
2:F:241:LEU:HD12	2:F:242:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:343:LYS:HZ1	2:F:411:PRO:HD2	1.79	0.47
2:F:508:ASP:OD1	2:F:508:ASP:C	2.57	0.47
2:F:930:LEU:HG	2:F:998:MET:HE3	1.96	0.47
2:D:21:ASP:OD2	2:D:64:CYS:N	2.37	0.47
2:D:323:SER:HB3	2:D:536:VAL:HG12	1.97	0.47
2:D:715:ASN:C	2:D:715:ASN:OD1	2.56	0.47
1:A:357:THR:CG2	1:A:360:LEU:HD11	2.45	0.47
1:A:607:ALA:O	1:A:611:LEU:HG	2.15	0.47
1:A:857:ASP:O	1:A:1023:ARG:NH2	2.47	0.47
1:A:971:VAL:HG22	1:A:975:LYS:HZ2	1.80	0.47
2:F:407:PHE:CD2	2:F:409:ILE:HD11	2.49	0.47
2:F:435:GLN:OE1	2:F:442:GLU:HA	2.13	0.47
2:F:526:ILE:O	2:F:529:ILE:HG22	2.15	0.47
2:F:533:CYS:SG	2:F:583:PHE:HE2	2.37	0.47
2:F:1012:VAL:HG21	2:F:1017:LEU:HD21	1.97	0.47
2:B:699:ILE:C	2:B:700:LEU:HD22	2.39	0.47
2:D:781:MET:HE2	2:D:781:MET:HA	1.95	0.47
1:A:246:GLY:HA2	1:A:315:LEU:HG	1.97	0.47
1:A:451:ILE:C	2:F:679:MET:HE1	2.39	0.47
1:A:825:MET:HE2	1:A:856:LEU:HG	1.96	0.47
1:A:954:ARG:O	1:A:958:ASN:ND2	2.47	0.47
1:C:357:THR:H	1:C:360:LEU:HD23	1.78	0.47
1:C:844:ASP:OD2	1:C:845:LEU:HG	2.15	0.47
1:E:252:LYS:NZ	1:E:253:CYS:O	2.43	0.47
2:F:52:ILE:HG21	2:F:138:VAL:HG21	1.96	0.47
2:F:81:THR:HG22	2:F:269:LEU:HB2	1.95	0.47
2:F:190:GLU:CG	2:F:193:ALA:H	2.25	0.47
2:F:233:ALA:HB3	2:F:264:LEU:HD11	1.95	0.47
2:F:311:GLN:HE21	2:F:415:LYS:HB2	1.79	0.47
2:F:762:MET:HE3	2:F:763:LYS:H	1.79	0.47
2:B:513:THR:O	2:B:514:SER:OG	2.32	0.47
2:D:663:ALA:HB1	2:D:825:PRO:CD	2.44	0.47
2:D:911:ILE:HG23	3:D:1602:ATP:N6	2.29	0.47
1:A:494:LEU:HD21	1:A:510:TRP:CZ3	2.50	0.47
1:A:544:ASN:C	1:A:544:ASN:OD1	2.58	0.47
1:A:574:VAL:HG22	1:A:575:LEU:N	2.30	0.47
1:C:487:LYS:HZ3	1:C:510:TRP:CD1	2.32	0.47
1:E:230:LEU:HD21	1:E:351:LEU:HA	1.96	0.47
1:E:357:THR:OG1	1:E:379:GLN:O	2.24	0.47
1:E:495:HIS:CE1	2:F:567:LYS:HG2	2.49	0.47
1:E:622:MET:HE2	1:E:623:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:PHE:CZ	2:F:89:PRO:HB3	2.50	0.47
2:F:357:ASP:OD1	2:F:357:ASP:N	2.42	0.47
2:F:470:ARG:O	2:F:470:ARG:HG2	2.14	0.47
2:F:494:ARG:O	2:F:498:LYS:CG	2.63	0.47
2:F:568:LEU:HD12	2:F:568:LEU:C	2.40	0.47
2:F:631:TYR:OH	2:F:671:LYS:HD2	2.15	0.47
2:F:699:ILE:C	2:F:700:LEU:HD22	2.39	0.47
2:B:446:TYR:HE2	2:B:454:VAL:HG21	1.79	0.47
2:B:606:PHE:O	2:B:610:MET:SD	2.73	0.47
2:B:672:SER:O	2:B:676:THR:OG1	2.20	0.47
2:D:251:ILE:CG2	2:D:296:ILE:HD11	2.45	0.47
2:D:571:SER:O	2:D:575:GLU:OE1	2.33	0.47
2:D:802:LEU:CD2	2:D:853:ILE:HD13	2.44	0.47
1:A:717:THR:HG21	1:A:757:LEU:HD11	1.97	0.47
1:C:216:LEU:HD21	1:C:235:ILE:CD1	2.45	0.47
1:C:944:ILE:HG23	1:C:966:LEU:HD11	1.97	0.47
1:E:491:CYS:SG	1:E:530:LEU:N	2.87	0.47
2:F:87:PHE:HZ	2:F:89:PRO:HB3	1.80	0.47
2:F:182:ALA:HA	2:F:184:LYS:HZ2	1.79	0.47
2:F:286:ALA:HA	2:F:427:LEU:HD11	1.97	0.47
2:F:599:ILE:HG12	2:F:607:ARG:CZ	2.45	0.47
2:F:877:THR:HG21	2:F:880:PRO:HA	1.96	0.47
2:B:729:VAL:H	2:B:787:THR:HG21	1.80	0.47
2:B:1008:LEU:HD23	2:B:1008:LEU:C	2.40	0.47
2:D:628:PHE:HE1	2:D:670:ILE:HG23	1.78	0.47
2:D:925:VAL:O	2:D:925:VAL:HG23	2.15	0.47
1:C:944:ILE:HB	1:C:959:ARG:HH12	1.79	0.47
1:C:947:PHE:CZ	2:D:114:MET:SD	3.08	0.47
1:E:821:LEU:O	1:E:825:MET:SD	2.73	0.47
2:F:36:GLY:O	2:F:52:ILE:HD12	2.15	0.47
2:F:599:ILE:HG12	2:F:607:ARG:NH1	2.30	0.47
2:F:951:MET:HE1	2:F:996:VAL:CG2	2.45	0.47
2:B:135:MET:O	2:B:162:LEU:HD21	2.14	0.47
2:D:38:ILE:HD11	2:D:51:LYS:HB3	1.97	0.47
2:D:378:LEU:O	2:D:382:TYR:N	2.46	0.47
2:D:951:MET:HE3	2:D:951:MET:O	2.15	0.47
1:C:450:PRO:C	1:C:451:ILE:HD13	2.40	0.47
1:C:658:LEU:HD12	2:D:459:ASN:ND2	2.30	0.47
1:E:224:ASP:OD1	1:E:234:TYR:OH	2.32	0.47
1:E:561:VAL:HG21	1:E:593:PHE:CZ	2.50	0.47
2:F:354:ILE:HG22	2:F:388:VAL:CG2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:LEU:HD23	2:B:457:LEU:C	2.40	0.47
2:B:952:LEU:HD23	2:B:952:LEU:C	2.40	0.47
2:D:487:VAL:O	2:D:487:VAL:HG12	2.15	0.47
1:C:643:LEU:O	1:C:647:ILE:HG12	2.15	0.46
1:C:661:ASP:OD1	1:C:662:CYS:N	2.46	0.46
1:C:765:PRO:HG3	2:D:856:GLN:HA	1.96	0.46
1:C:967:GLN:HA	1:C:970:VAL:CG2	2.46	0.46
1:E:497:THR:O	1:E:497:THR:HG22	2.15	0.46
2:F:5:LEU:N	2:F:83:ASP:O	2.47	0.46
2:F:51:LYS:NZ	2:F:72:LEU:HD21	2.30	0.46
2:F:262:VAL:O	2:F:264:LEU:HD22	2.15	0.46
2:F:666:THR:O	2:F:670:ILE:HG12	2.15	0.46
2:F:717:PHE:C	2:F:717:PHE:CD2	2.93	0.46
2:F:891:GLY:O	2:F:892:ARG:NH2	2.48	0.46
2:D:673:ILE:HD11	2:D:710:THR:HG23	1.95	0.46
2:D:983:PHE:CD1	2:D:987:ALA:HB2	2.51	0.46
1:C:469:ARG:HD2	3:C:1101:ATP:H2'	1.96	0.46
1:C:525:ASP:OD1	1:C:526:ASN:N	2.49	0.46
1:E:554:LEU:O	1:E:554:LEU:HD23	2.15	0.46
1:E:922:LEU:O	1:E:925:VAL:HG22	2.15	0.46
1:E:946:TYR:OH	1:E:949:ILE:HG13	2.15	0.46
2:F:813:VAL:HA	2:F:816:VAL:HG12	1.97	0.46
2:B:627:ILE:HG23	2:B:670:ILE:HG21	1.97	0.46
2:D:330:ILE:O	2:D:334:THR:OG1	2.32	0.46
2:D:459:ASN:C	2:D:459:ASN:OD1	2.59	0.46
2:D:896:LEU:O	2:D:896:LEU:HG	2.14	0.46
1:A:459:LEU:HD23	1:A:575:LEU:HD11	1.98	0.46
1:A:494:LEU:HD11	1:A:510:TRP:CH2	2.50	0.46
1:A:504:GLN:NE2	2:F:511:SER:O	2.41	0.46
1:A:662:CYS:HB2	1:A:665:VAL:HG12	1.97	0.46
1:A:777:GLN:O	1:A:781:GLU:OE1	2.34	0.46
1:A:991:ASN:C	1:A:991:ASN:OD1	2.58	0.46
1:C:419:GLU:OE1	1:C:419:GLU:N	2.45	0.46
1:C:608:ARG:O	1:C:612:LEU:HD22	2.15	0.46
1:E:253:CYS:SG	1:E:255:LEU:HD21	2.55	0.46
1:E:450:PRO:C	1:E:451:ILE:HD13	2.41	0.46
2:F:109:LEU:HA	2:F:112:LYS:NZ	2.22	0.46
2:F:353:PRO:HB3	2:F:389:TRP:CH2	2.50	0.46
2:F:465:PHE:O	2:F:468:SER:OG	2.29	0.46
2:F:505:LEU:HB2	2:F:544:VAL:O	2.15	0.46
2:B:120:MET:SD	2:B:120:MET:C	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ASN:O	2:B:369:ASN:ND2	2.49	0.46
2:D:513:THR:HG22	2:D:525:ILE:CD1	2.45	0.46
2:D:856:GLN:O	2:D:857:LEU:C	2.58	0.46
1:A:373:LYS:O	1:A:375:GLU:N	2.48	0.46
1:A:947:PHE:HE2	2:B:172:LEU:HD11	1.79	0.46
1:C:401:GLU:N	1:C:401:GLU:OE2	2.49	0.46
1:C:523:VAL:HG23	1:C:575:LEU:HD22	1.96	0.46
1:C:622:MET:HE2	1:C:622:MET:C	2.39	0.46
1:E:310:ILE:HG23	1:E:310:ILE:O	2.15	0.46
1:E:924:SER:HB3	1:E:988:VAL:HG12	1.96	0.46
1:E:970:VAL:HG23	1:E:974:THR:HB	1.97	0.46
2:F:182:ALA:HA	2:F:184:LYS:NZ	2.30	0.46
2:F:373:ASP:N	2:F:373:ASP:OD1	2.49	0.46
2:F:641:VAL:O	2:F:641:VAL:HG13	2.16	0.46
1:A:357:THR:HG1	1:A:380:LEU:HA	1.81	0.46
1:E:223:MET:SD	1:E:223:MET:N	2.88	0.46
2:F:81:THR:HB	2:F:269:LEU:O	2.15	0.46
2:F:316:ARG:HB2	2:F:390:PHE:CE1	2.51	0.46
2:F:322:GLN:NE2	2:F:389:TRP:H	2.13	0.46
2:F:343:LYS:HD2	2:F:343:LYS:H	1.80	0.46
2:F:657:SER:O	2:F:661:TYR:CD1	2.68	0.46
2:F:951:MET:HE1	2:F:996:VAL:HG22	1.98	0.46
2:B:106:ASN:ND2	2:B:178:GLN:OE1	2.48	0.46
2:B:953:ASN:O	2:B:956:SER:OG	2.26	0.46
2:D:18:ILE:C	2:D:61:LEU:HD12	2.40	0.46
2:D:206:ASP:O	2:D:278:ILE:HG22	2.15	0.46
2:D:347:CYS:HA	2:D:405:SER:O	2.15	0.46
2:D:606:PHE:O	2:D:610:MET:SD	2.73	0.46
2:D:859:ALA:O	2:D:863:GLY:N	2.42	0.46
1:A:806:ARG:NH1	1:A:818:VAL:HG21	2.31	0.46
1:C:458:ILE:HG21	1:C:581:LYS:HE3	1.97	0.46
1:C:458:ILE:HG22	1:C:594:VAL:HG11	1.98	0.46
1:C:923:LYS:C	1:C:926:HIS:HD1	2.20	0.46
1:E:557:PHE:CD1	1:E:557:PHE:C	2.93	0.46
2:F:2:LYS:HD3	2:F:84:PHE:CD1	2.51	0.46
2:F:23:TYR:HE1	2:F:31:ALA:HB1	1.81	0.46
2:F:485:ASN:HB3	3:F:1101:ATP:O3G	2.16	0.46
2:F:485:ASN:HB2	2:F:486:ASN:OD1	2.15	0.46
2:F:530:ARG:HG3	2:F:534:GLU:OE2	2.15	0.46
2:F:641:VAL:HG23	2:F:643:GLN:HG2	1.97	0.46
2:F:678:ARG:HG2	2:F:678:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:789:PHE:O	2:F:791:LEU:HD12	2.16	0.46
2:B:2:LYS:HD2	2:B:84:PHE:CD2	2.50	0.46
1:A:719:TYR:CZ	2:F:959:ALA:HB1	2.51	0.46
1:C:786:ALA:HB2	1:C:794:LEU:HD21	1.97	0.46
1:E:224:ASP:OD1	1:E:224:ASP:N	2.49	0.46
1:E:619:ASN:O	1:E:622:MET:HG3	2.15	0.46
2:F:442:GLU:O	2:F:630:TRP:HZ2	1.99	0.46
2:B:252:THR:OG1	2:B:297:SER:OG	2.34	0.46
1:A:214:VAL:HG12	1:A:215:ILE:N	2.30	0.46
1:A:500:LEU:O	1:A:504:GLN:HG3	2.16	0.46
1:A:558:ILE:O	1:A:562:THR:HG22	2.16	0.46
1:C:233:VAL:HG23	1:C:277:VAL:HG21	1.97	0.46
1:E:253:CYS:O	1:E:253:CYS:SG	2.73	0.46
1:E:582:THR:OG1	1:E:583:GLN:NE2	2.49	0.46
1:E:627:ASP:OD1	1:E:628:LEU:N	2.48	0.46
2:F:82:MET:N	2:F:82:MET:SD	2.89	0.46
2:F:486:ASN:O	2:F:667:PRO:HD2	2.16	0.46
2:F:489:LYS:HE2	2:F:595:SER:HB2	1.97	0.46
2:F:551:ASP:HB3	2:F:596:VAL:HG22	1.97	0.46
2:F:697:GLN:OE1	2:F:697:GLN:HA	2.16	0.46
2:B:478:VAL:HG12	2:B:612:PHE:HB3	1.98	0.46
2:B:555:LEU:N	2:B:555:LEU:HD23	2.30	0.46
2:B:662:SER:HA	2:B:665:LEU:HD12	1.97	0.46
2:D:34:LEU:HD23	2:D:35:TYR:N	2.31	0.46
2:D:251:ILE:HD12	2:D:264:LEU:HB2	1.96	0.46
2:D:317:VAL:HG23	2:D:390:PHE:HA	1.97	0.46
2:D:513:THR:O	2:D:514:SER:OG	2.33	0.46
2:D:699:ILE:C	2:D:700:LEU:HD22	2.41	0.46
2:D:1004:ALA:O	2:D:1008:LEU:N	2.48	0.46
1:A:434:ILE:HD12	1:A:610:LYS:NZ	2.31	0.46
1:A:465:ILE:HD13	1:A:641:SER:HB2	1.97	0.46
1:A:503:THR:O	1:A:506:LEU:N	2.49	0.46
1:C:475:ILE:HA	1:C:478:VAL:HG12	1.98	0.46
1:C:511:CYS:SG	1:C:512:SER:N	2.89	0.46
1:E:468:THR:OG1	3:E:1101:ATP:O1B	2.24	0.46
2:F:255:ASN:O	2:F:256:MET:SD	2.74	0.46
2:F:443:THR:CB	2:F:498:LYS:HZ3	2.29	0.46
2:F:514:SER:OG	2:F:524:LYS:HD3	2.15	0.46
2:F:515:ASN:HA	2:F:517:ARG:HH21	1.81	0.46
2:F:961:MET:SD	2:F:961:MET:C	2.99	0.46
2:D:251:ILE:HD11	2:D:264:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:O	1:A:223:MET:C	2.59	0.46
1:A:226:PRO:HD3	1:A:234:TYR:OH	2.16	0.46
1:C:464:GLY:N	3:C:1101:ATP:O2B	2.49	0.46
1:C:701:ALA:C	1:C:702:LEU:HD12	2.41	0.46
1:C:731:ARG:NH2	2:B:952:LEU:HD13	2.31	0.46
1:E:450:PRO:O	1:E:451:ILE:HD13	2.16	0.46
2:F:489:LYS:HA	2:F:492:MET:HG3	1.97	0.46
2:F:500:LEU:HB2	2:F:502:ILE:CG1	2.46	0.46
2:F:637:LEU:HG	2:F:647:VAL:HG11	1.97	0.46
2:F:775:GLY:HA3	2:F:941:ALA:HB2	1.97	0.46
2:F:1026:ASN:OD1	2:F:1026:ASN:C	2.59	0.46
2:B:546:PHE:CD1	2:B:593:VAL:HG23	2.50	0.46
2:B:556:ASP:N	2:B:556:ASP:OD1	2.49	0.46
2:B:647:VAL:HG12	2:B:699:ILE:HB	1.98	0.46
2:B:806:ILE:H	2:B:806:ILE:HD12	1.80	0.46
2:D:602:VAL:CG1	2:D:607:ARG:HE	2.28	0.46
1:A:805:LYS:N	1:A:845:LEU:O	2.47	0.45
1:C:487:LYS:HZ3	1:C:510:TRP:CG	2.34	0.45
1:C:528:GLU:OE1	1:C:584:ILE:N	2.49	0.45
1:E:453:ALA:N	2:D:679:MET:CE	2.79	0.45
2:F:140:HIS:HB2	2:F:143:ASP:OD2	2.15	0.45
2:F:286:ALA:HA	2:F:427:LEU:HD21	1.97	0.45
2:F:616:VAL:O	2:F:616:VAL:CG1	2.65	0.45
2:F:649:TYR:CE2	2:F:653:ILE:HG21	2.52	0.45
2:F:708:LYS:O	2:F:711:SER:OG	2.22	0.45
2:B:837:ALA:N	2:B:838:PRO:CD	2.79	0.45
2:D:264:LEU:HD12	2:D:265:PHE:O	2.16	0.45
2:D:444:PHE:CD2	3:D:1601:ATP:N6	2.84	0.45
2:D:868:ALA:HB1	2:D:871:VAL:HG11	1.99	0.45
1:C:224:ASP:OD1	1:C:225:PHE:N	2.50	0.45
1:C:451:ILE:HG23	1:C:569:ASN:ND2	2.31	0.45
1:C:468:THR:HG22	1:C:525:ASP:OD1	2.17	0.45
1:C:768:LEU:HD11	2:D:806:ILE:HD12	1.97	0.45
1:E:397:GLN:CA	1:E:398:MET:HE2	2.45	0.45
1:E:547:TRP:O	1:E:547:TRP:CG	2.70	0.45
1:E:607:ALA:O	1:E:611:LEU:HD23	2.17	0.45
1:E:956:GLU:HB3	1:E:961:ARG:CZ	2.46	0.45
2:F:82:MET:CE	2:F:270:PRO:HD3	2.46	0.45
2:F:671:LYS:HA	2:F:674:VAL:HG22	1.97	0.45
2:B:210:LEU:HD12	2:B:281:PRO:N	2.31	0.45
2:B:755:PRO:O	2:B:759:THR:OG1	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:LEU:HG	2:D:153:LEU:HD21	1.97	0.45
2:D:250:PHE:C	2:D:251:ILE:HG13	2.41	0.45
2:D:357:ASP:OD1	2:D:359:SER:OG	2.31	0.45
1:C:332:ILE:HG23	1:C:369:ILE:CD1	2.46	0.45
1:C:472:LYS:HA	1:C:475:ILE:HG12	1.98	0.45
1:C:722:ILE:HG13	2:B:955:MET:CE	2.46	0.45
1:C:806:ARG:HD2	1:C:818:VAL:HG11	1.99	0.45
1:E:702:LEU:O	1:E:706:LYS:N	2.41	0.45
2:F:109:LEU:CA	2:F:112:LYS:HZ1	2.24	0.45
2:F:317:VAL:HG21	2:F:389:TRP:HB3	1.99	0.45
2:F:350:ASP:HB2	2:F:392:VAL:HG21	1.98	0.45
2:F:489:LYS:O	2:F:492:MET:HG3	2.15	0.45
2:F:982:TRP:O	2:F:987:ALA:N	2.47	0.45
2:B:599:ILE:HG22	2:B:607:ARG:NH1	2.32	0.45
2:D:173:VAL:HG22	2:D:174:ASN:N	2.32	0.45
1:C:799:PHE:CD1	1:C:799:PHE:C	2.94	0.45
1:C:802:ILE:HA	2:D:852:ARG:HH12	1.80	0.45
1:E:561:VAL:HG21	1:E:593:PHE:HZ	1.81	0.45
1:E:622:MET:HE2	1:E:623:LYS:HA	1.98	0.45
2:F:135:MET:HA	2:F:162:LEU:HD11	1.98	0.45
2:D:7:PHE:HA	2:D:68:VAL:O	2.17	0.45
2:D:210:LEU:N	2:D:280:ALA:O	2.44	0.45
1:A:440:LYS:HA	1:A:443:MET:HG2	1.98	0.45
1:E:353:GLY:N	1:E:383:LEU:HD22	2.32	0.45
2:F:107:GLU:HA	2:F:174:ASN:OD1	2.17	0.45
2:B:137:THR:O	2:B:162:LEU:HD12	2.16	0.45
2:D:114:MET:SD	2:D:114:MET:O	2.74	0.45
2:D:581:ASP:OD1	2:D:609:HIS:NE2	2.36	0.45
2:D:855:SER:O	2:D:856:GLN:C	2.58	0.45
1:A:675:LEU:C	1:A:675:LEU:HD23	2.41	0.45
1:A:765:PRO:HB3	2:B:856:GLN:OE1	2.17	0.45
1:C:270:ILE:HG23	1:C:270:ILE:O	2.17	0.45
1:C:647:ILE:HD13	1:C:647:ILE:N	2.32	0.45
1:C:790:LYS:O	1:C:791:PRO:C	2.59	0.45
1:C:953:GLY:C	1:C:954:ARG:HD2	2.42	0.45
1:E:971:VAL:HG22	1:E:974:THR:HB	1.98	0.45
2:F:30:LYS:O	2:F:31:ALA:HB3	2.16	0.45
2:F:97:VAL:HG22	2:F:162:LEU:CG	2.47	0.45
2:F:516:SER:C	2:F:517:ARG:HD3	2.40	0.45
2:F:565:ALA:HA	2:F:568:LEU:HD23	1.99	0.45
2:F:599:ILE:HG12	2:F:607:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:776:THR:OG1	2:F:778:LYS:NZ	2.47	0.45
2:F:1012:VAL:CG2	2:F:1017:LEU:HD21	2.47	0.45
2:B:21:ASP:OD2	2:B:64:CYS:N	2.48	0.45
2:D:550:LEU:CD2	2:D:554:LEU:HD13	2.46	0.45
1:C:534:PRO:C	1:C:535:GLN:CD	2.85	0.45
1:C:729:ARG:NH1	1:C:854:GLY:O	2.42	0.45
1:E:924:SER:CB	1:E:988:VAL:HG12	2.47	0.45
2:F:5:LEU:CD1	2:F:68:VAL:HG12	2.47	0.45
2:F:766:SER:OG	2:F:891:GLY:O	2.26	0.45
2:B:384:ASN:O	2:B:384:ASN:OD1	2.34	0.45
1:A:313:GLU:OE1	1:A:313:GLU:N	2.50	0.45
1:A:825:MET:HE2	1:A:856:LEU:HD11	1.99	0.45
1:A:1001:LYS:HB2	2:B:1030:ALA:HB3	1.99	0.45
1:E:277:VAL:HG12	1:E:278:PHE:O	2.17	0.45
2:F:7:PHE:HE2	2:F:82:MET:SD	2.39	0.45
2:F:12:ILE:HG23	2:F:72:LEU:CA	2.29	0.45
2:B:274:LYS:O	2:B:277:THR:HG22	2.16	0.45
2:D:264:LEU:HD12	2:D:265:PHE:N	2.32	0.45
2:D:346:LEU:HD11	2:D:409:ILE:HG22	1.99	0.45
2:D:522:THR:HG23	2:D:523:SER:N	2.32	0.45
1:C:899:LYS:O	1:C:902:ALA:HB3	2.17	0.45
1:C:947:PHE:HB2	2:D:172:LEU:HG	1.98	0.45
1:C:956:GLU:HG2	1:C:957:GLU:N	2.32	0.45
1:E:353:GLY:H	1:E:383:LEU:HD22	1.82	0.45
2:F:38:ILE:HD12	2:F:38:ILE:HA	1.82	0.45
2:F:146:THR:N	2:F:150:CYS:HB3	2.26	0.45
2:F:343:LYS:NZ	2:F:410:ASP:OD2	2.34	0.45
2:F:451:PHE:HE1	2:F:623:GLN:CB	2.30	0.45
2:F:456:GLN:CD	2:F:456:GLN:C	2.85	0.45
2:F:503:HIS:HB2	2:F:543:ALA:CB	2.41	0.45
2:F:668:LEU:CD2	3:F:1101:ATP:H4'	2.45	0.45
2:F:673:ILE:HG23	2:F:709:ALA:CB	2.47	0.45
2:D:140:HIS:CG	2:D:160:GLN:HB3	2.52	0.45
2:D:857:LEU:O	2:D:858:LEU:C	2.59	0.45
2:D:1026:ASN:OD1	2:D:1026:ASN:C	2.60	0.45
1:A:984:LEU:O	1:A:984:LEU:HD23	2.15	0.45
1:C:285:ILE:HD11	1:C:289:HIS:C	2.42	0.45
1:C:701:ALA:O	1:C:706:LYS:NZ	2.45	0.45
1:C:803:ALA:O	1:C:846:ILE:HG22	2.17	0.45
1:C:954:ARG:HD2	1:C:954:ARG:N	2.32	0.45
1:E:231:PHE:HA	1:E:296:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:531:PHE:HB3	1:E:554:LEU:HD12	1.98	0.45
2:F:135:MET:HA	2:F:162:LEU:HD21	1.98	0.45
2:F:210:LEU:HD11	2:F:281:PRO:CG	2.47	0.45
2:F:219:LEU:O	2:F:220:ARG:NH2	2.50	0.45
2:F:446:TYR:CD2	2:F:454:VAL:HG21	2.52	0.45
2:B:72:LEU:HD12	2:B:72:LEU:O	2.17	0.45
2:B:828:ILE:CD1	2:B:873:VAL:HG23	2.47	0.45
2:D:252:THR:O	2:D:296:ILE:HD12	2.17	0.45
1:A:243:SER:OG	1:A:315:LEU:O	2.26	0.44
1:C:236:SER:HA	1:C:285:ILE:HG23	1.98	0.44
1:C:684:ARG:NH2	2:D:608:SER:HA	2.32	0.44
1:C:726:CYS:CB	2:B:951:MET:HE2	2.46	0.44
1:C:771:PHE:HB3	2:B:804:MET:SD	2.57	0.44
2:F:70:SER:CB	2:F:77:PRO:HD3	2.48	0.44
2:F:97:VAL:HG22	2:F:162:LEU:HD23	1.99	0.44
2:B:838:PRO:O	2:B:850:MET:HE3	2.16	0.44
2:D:156:SER:HB3	2:D:157:PRO:CD	2.47	0.44
2:D:261:LEU:HD12	2:D:261:LEU:C	2.42	0.44
1:A:909:SER:O	1:A:912:ASP:N	2.50	0.44
1:A:928:TRP:CH2	1:A:984:LEU:HD21	2.52	0.44
1:C:828:ALA:N	2:B:725:GLN:OE1	2.50	0.44
1:C:917:CYS:SG	1:C:918:TYR:N	2.90	0.44
1:E:654:TYR:HE1	2:F:460:ILE:HA	1.81	0.44
1:E:957:GLU:OE1	1:E:957:GLU:HA	2.17	0.44
1:E:1006:THR:O	1:E:1010:VAL:HG22	2.17	0.44
2:F:137:THR:O	2:F:163:VAL:HG22	2.17	0.44
2:F:217:ASP:C	2:F:220:ARG:HH22	2.25	0.44
2:F:273:PHE:HB3	2:F:279:TYR:CE2	2.52	0.44
2:F:836:VAL:HA	2:F:850:MET:HE1	1.98	0.44
2:B:103:PHE:N	2:B:103:PHE:CD1	2.84	0.44
2:B:306:ILE:HG22	2:B:408:ILE:HG22	1.99	0.44
2:B:695:LEU:HD23	2:B:695:LEU:H	1.81	0.44
2:B:966:VAL:HG13	2:B:982:TRP:NE1	2.32	0.44
2:B:1026:ASN:OD1	2:B:1027:PHE:N	2.51	0.44
2:D:160:GLN:OE1	2:D:160:GLN:N	2.51	0.44
2:D:357:ASP:OD2	2:D:383:LYS:N	2.49	0.44
2:D:502:ILE:HG22	2:D:543:ALA:HA	1.98	0.44
1:A:363:PRO:HG3	1:A:411:LEU:HD11	1.99	0.44
1:A:968:GLN:NE2	2:B:651:ASP:O	2.43	0.44
1:C:292:LEU:HB3	1:C:296:LEU:HD12	1.99	0.44
1:C:485:PHE:O	1:C:521:LEU:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:THR:HG23	1:E:502:LYS:CE	2.47	0.44
1:E:507:ILE:HD11	1:E:556:PHE:CD2	2.52	0.44
1:E:558:ILE:HG23	1:E:559:ASN:H	1.81	0.44
1:E:955:ARG:HD3	1:E:955:ARG:N	2.30	0.44
2:F:100:SER:O	2:F:156:SER:N	2.35	0.44
2:F:219:LEU:HD12	2:F:223:PRO:CG	2.47	0.44
2:F:254:SER:HB2	2:F:259:VAL:HG22	1.99	0.44
2:F:639:ARG:CZ	2:F:639:ARG:HB2	2.47	0.44
2:B:82:MET:N	2:B:269:LEU:O	2.40	0.44
2:B:327:PHE:O	2:B:331:ILE:HG13	2.17	0.44
2:D:132:ILE:HA	2:D:137:THR:HG21	1.99	0.44
2:D:136:GLU:OE1	2:D:137:THR:HG23	2.17	0.44
2:D:251:ILE:CG2	2:D:297:SER:O	2.66	0.44
2:D:768:ILE:HD13	2:D:874:ILE:HG13	2.00	0.44
2:D:822:GLU:CD	2:D:822:GLU:C	2.85	0.44
1:C:483:HIS:O	1:C:483:HIS:ND1	2.50	0.44
1:C:898:LEU:H	1:C:898:LEU:HD12	1.83	0.44
1:C:914:GLN:OE1	3:C:1102:ATP:C2'	2.65	0.44
1:E:950:ASN:OD1	2:F:119:GLU:HB3	2.17	0.44
2:F:20:ARG:HE	2:F:57:LEU:HD21	1.82	0.44
2:F:137:THR:O	2:F:163:VAL:HG13	2.16	0.44
2:F:378:LEU:HD12	2:F:378:LEU:N	2.31	0.44
2:F:970:ASN:ND2	2:F:976:ASN:OD1	2.51	0.44
2:B:170:LEU:HD23	2:B:170:LEU:H	1.83	0.44
2:D:251:ILE:CD1	2:D:264:LEU:HD23	2.48	0.44
2:D:265:PHE:N	2:D:265:PHE:CD2	2.84	0.44
2:D:663:ALA:HB1	2:D:825:PRO:HD2	2.00	0.44
2:D:998:MET:HA	2:D:1001:PHE:CD1	2.52	0.44
1:A:819:ASN:HA	1:A:822:LEU:HD12	1.99	0.44
1:A:916:LEU:HA	1:A:919:ASN:ND2	2.33	0.44
1:C:741:GLY:O	3:C:1102:ATP:H5'2	2.17	0.44
1:C:947:PHE:CD2	2:D:114:MET:HE3	2.52	0.44
1:C:974:THR:OG1	1:C:975:LYS:N	2.50	0.44
1:E:788:SER:OG	1:E:789:VAL:HG13	2.17	0.44
2:F:224:HIS:HE1	2:F:226:ASN:HB2	1.83	0.44
2:F:280:ALA:O	2:F:285:ILE:HD11	2.16	0.44
2:F:341:GLU:OE2	2:F:342:SER:N	2.51	0.44
2:F:475:ASN:ND2	2:F:611:ARG:HH21	2.09	0.44
2:B:235:THR:HG22	2:B:264:LEU:HD11	1.99	0.44
2:B:603:PRO:O	2:B:607:ARG:HG3	2.17	0.44
2:D:634:SER:HA	2:D:637:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:738:ASP:OD1	2:D:739:PHE:N	2.51	0.44
2:D:861:LEU:HD12	2:D:861:LEU:O	2.17	0.44
1:A:335:PHE:CD2	1:A:403:VAL:HG13	2.53	0.44
1:C:215:ILE:O	2:B:377:GLU:OE2	2.35	0.44
1:C:523:VAL:C	1:C:524:LEU:HD12	2.42	0.44
1:E:925:VAL:HG12	1:E:986:ALA:HB3	2.00	0.44
2:F:17:SER:CB	2:F:61:LEU:HD11	2.47	0.44
2:F:504:LEU:HD12	2:F:504:LEU:HA	1.81	0.44
2:B:236:ASP:OD2	2:B:276:ARG:N	2.47	0.44
2:B:488:GLY:CA	3:B:1101:ATP:H2	2.27	0.44
2:B:492:MET:SD	2:B:492:MET:C	3.00	0.44
2:D:798:GLY:CA	2:D:836:VAL:HG11	2.47	0.44
2:D:851:ASP:O	2:D:855:SER:OG	2.36	0.44
1:A:495:HIS:NE2	2:B:567:LYS:O	2.48	0.44
1:A:509:GLU:O	1:A:512:SER:OG	2.35	0.44
1:C:470:LEU:C	1:C:470:LEU:HD23	2.42	0.44
1:C:497:THR:HG23	1:C:502:LYS:HE2	2.00	0.44
1:C:965:LEU:HD21	2:D:102:THR:HG21	2.00	0.44
1:E:382:ASN:OD1	1:E:383:LEU:N	2.50	0.44
1:E:612:LEU:HD21	1:E:645:LEU:HD12	1.99	0.44
1:E:944:ILE:O	1:E:944:ILE:HG22	2.16	0.44
1:E:1019:PHE:O	1:E:1023:ARG:N	2.40	0.44
2:F:3:ALA:HA	2:F:64:CYS:HG	1.83	0.44
2:F:251:ILE:HD12	2:F:251:ILE:N	2.33	0.44
2:F:481:HIS:ND1	2:F:599:ILE:HB	2.33	0.44
2:F:785:ILE:HG23	2:F:789:PHE:CD2	2.53	0.44
2:B:126:LEU:HD22	2:B:126:LEU:H	1.82	0.44
2:B:362:ASP:C	2:B:363:LEU:HD12	2.43	0.44
2:D:7:PHE:CD2	2:D:81:THR:HG21	2.52	0.44
2:D:830:PHE:CB	2:D:833:ILE:HG22	2.48	0.44
2:D:937:ASN:OD1	2:D:938:TYR:N	2.51	0.44
1:A:413:LYS:O	1:A:416:HIS:ND1	2.51	0.44
1:C:739:TYR:CD2	1:C:1012:LEU:HD11	2.52	0.44
1:E:233:VAL:HB	1:E:290:ILE:HD11	1.99	0.44
1:E:586:PRO:O	1:E:587:LEU:C	2.61	0.44
1:E:956:GLU:OE2	1:E:958:ASN:N	2.51	0.44
2:F:39:ARG:CZ	2:F:47:CYS:HB2	2.48	0.44
2:F:50:GLY:N	2:F:697:GLN:HE21	2.11	0.44
2:F:252:THR:HG23	2:F:297:SER:OG	2.18	0.44
2:F:311:GLN:NE2	2:F:417:ILE:HG12	2.33	0.44
2:F:341:GLU:CD	2:F:342:SER:HB3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:470:ARG:C	2:F:472:ILE:HD12	2.43	0.44
2:F:641:VAL:HG22	2:F:643:GLN:O	2.18	0.44
2:B:40:LEU:N	2:B:40:LEU:HD12	2.32	0.44
2:B:139:VAL:HG22	2:B:140:HIS:N	2.33	0.44
2:B:455:ARG:HA	2:B:458:VAL:HG22	2.00	0.44
2:D:261:LEU:HD21	2:D:345:ILE:HG21	2.00	0.44
2:D:294:VAL:HG12	2:D:295:THR:N	2.32	0.44
1:A:807:GLY:O	2:F:804:MET:HE2	2.18	0.44
1:C:457:ILE:HD11	1:C:575:LEU:CD1	2.48	0.44
1:C:739:TYR:CD2	1:C:1012:LEU:HD21	2.53	0.44
1:C:758:ASN:HD22	1:C:789:VAL:HG23	1.83	0.44
1:C:780:ARG:O	1:C:784:GLU:HG2	2.18	0.44
2:F:146:THR:HB	2:F:150:CYS:N	2.33	0.44
2:F:464:SER:HA	2:F:467:CYS:SG	2.58	0.44
2:F:507:ILE:HD12	2:F:507:ILE:N	2.33	0.44
2:F:620:SER:N	2:F:623:GLN:OE1	2.49	0.44
2:F:704:GLU:H	2:F:704:GLU:CD	2.20	0.44
2:F:705:ASP:HA	2:F:708:LYS:HZ3	1.82	0.44
2:B:84:PHE:CD2	2:B:85:CYS:N	2.86	0.44
2:B:371:GLU:O	2:B:372:SER:C	2.61	0.44
2:B:828:ILE:HD11	2:B:873:VAL:HG23	2.00	0.44
2:D:627:ILE:CG2	2:D:670:ILE:HG21	2.48	0.44
2:D:762:MET:C	2:D:762:MET:HE2	2.43	0.44
1:A:250:ILE:HG23	1:A:300:PHE:CD1	2.53	0.43
1:A:467:LYS:N	3:A:1102:ATP:O1B	2.51	0.43
1:A:491:CYS:SG	1:A:527:VAL:HA	2.58	0.43
1:A:741:GLY:O	3:A:1101:ATP:H5'2	2.17	0.43
1:E:470:LEU:HD23	1:E:470:LEU:C	2.43	0.43
1:E:568:ASP:OD1	1:E:569:ASN:N	2.51	0.43
1:E:699:ILE:O	1:E:699:ILE:HG23	2.18	0.43
2:F:18:ILE:CG2	2:F:55:CYS:HB2	2.48	0.43
2:F:414:THR:C	2:F:415:LYS:HD3	2.43	0.43
2:F:494:ARG:HA	2:F:497:SER:OG	2.18	0.43
2:F:684:ARG:CZ	2:F:684:ARG:HB2	2.47	0.43
2:B:151:GLN:NE2	2:B:152:ILE:O	2.50	0.43
2:B:353:PRO:C	2:B:354:ILE:HD13	2.42	0.43
2:B:579:LEU:HD11	2:B:583:PHE:CE2	2.52	0.43
2:B:986:ILE:O	2:B:986:ILE:HG22	2.18	0.43
2:B:995:VAL:HG12	2:B:997:LYS:HZ2	1.83	0.43
2:D:19:SER:N	2:D:61:LEU:HD12	2.32	0.43
2:D:231:ILE:HG22	2:D:262:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:882:LEU:C	2:D:882:LEU:HD12	2.43	0.43
1:A:301:PHE:CD2	1:A:301:PHE:O	2.72	0.43
1:A:382:ASN:OD1	1:A:383:LEU:N	2.52	0.43
1:A:452:ILE:HD11	1:A:573:ARG:CZ	2.47	0.43
1:C:401:GLU:CD	1:C:402:GLU:N	2.76	0.43
1:C:874:LEU:HA	1:C:877:ILE:HG12	2.00	0.43
1:E:612:LEU:HD21	1:E:645:LEU:CD1	2.48	0.43
1:E:951:GLU:HG2	1:E:954:ARG:HB3	2.00	0.43
1:E:966:LEU:HB2	1:E:967:GLN:OE1	2.18	0.43
2:F:52:ILE:HG23	2:F:138:VAL:CG1	2.44	0.43
2:B:233:ALA:C	2:B:234:PHE:HD1	2.26	0.43
2:B:502:ILE:HG22	2:B:543:ALA:HA	2.00	0.43
2:B:571:SER:OG	2:B:572:ILE:N	2.52	0.43
2:B:750:MET:HB3	2:B:751:PRO:HD3	2.00	0.43
2:B:813:VAL:HG11	2:B:856:GLN:HB3	2.00	0.43
2:D:104:LEU:CD2	2:D:153:LEU:HD11	2.44	0.43
1:C:452:ILE:HA	2:B:679:MET:CE	2.49	0.43
1:C:654:TYR:CZ	2:D:474:LEU:HD12	2.53	0.43
1:C:672:SER:O	1:C:676:SER:OG	2.37	0.43
1:C:877:ILE:HD13	1:C:913:LEU:CD2	2.48	0.43
2:F:233:ALA:HB2	2:F:262:VAL:HG21	1.98	0.43
2:F:447:ASP:CG	2:F:450:ILE:HD12	2.43	0.43
2:F:547:LEU:HD23	2:F:550:LEU:HD13	2.00	0.43
2:F:612:PHE:HD1	2:F:612:PHE:N	2.17	0.43
2:F:838:PRO:CD	2:F:850:MET:HE3	2.49	0.43
2:F:911:ILE:HG21	2:F:943:PHE:CD2	2.53	0.43
2:B:780:LEU:HG	3:B:1102:ATP:H2'	2.00	0.43
2:B:809:SER:HA	2:B:812:ASN:OD1	2.17	0.43
2:B:874:ILE:O	2:B:874:ILE:HG13	2.18	0.43
2:D:210:LEU:HD12	2:D:281:PRO:N	2.33	0.43
2:D:489:LYS:O	2:D:492:MET:HG2	2.18	0.43
2:D:739:PHE:CZ	2:D:740:VAL:HG13	2.52	0.43
1:A:444:VAL:O	1:A:448:THR:OG1	2.25	0.43
1:A:779:ILE:CD1	1:A:817:VAL:HG13	2.49	0.43
1:C:292:LEU:HD12	1:C:292:LEU:N	2.33	0.43
1:C:568:ASP:OD1	1:C:569:ASN:N	2.51	0.43
1:C:855:ARG:NH2	3:B:1102:ATP:O2G	2.51	0.43
1:E:777:GLN:C	1:E:777:GLN:OE1	2.62	0.43
2:F:237:ALA:HB2	2:F:266:VAL:CG1	2.46	0.43
2:F:513:THR:O	2:F:525:ILE:HD11	2.18	0.43
2:F:687:GLN:HA	2:F:690:LYS:HZ3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ASP:OD1	2:B:228:ASP:C	2.61	0.43
2:B:312:VAL:HG11	2:B:409:ILE:HD12	1.99	0.43
2:B:522:THR:HG23	2:B:523:SER:N	2.34	0.43
2:D:894:ASP:OD1	2:D:894:ASP:N	2.44	0.43
1:A:548:ASP:OD1	1:A:550:ALA:HB3	2.18	0.43
1:E:551:SER:O	1:E:554:LEU:N	2.51	0.43
1:E:613:GLU:C	1:E:613:GLU:CD	2.87	0.43
2:F:208:GLU:OE1	2:F:208:GLU:HA	2.18	0.43
2:F:458:VAL:O	2:F:462:GLU:OE1	2.37	0.43
2:F:467:CYS:HA	2:F:470:ARG:HH12	1.81	0.43
2:F:488:GLY:HA2	3:F:1101:ATP:C5'	2.48	0.43
2:F:866:THR:HG23	2:F:867:ASP:N	2.33	0.43
2:B:316:ARG:HB2	2:B:421:ILE:HD12	2.00	0.43
2:B:517:ARG:O	2:B:518:GLN:C	2.61	0.43
2:B:894:ASP:OD1	2:B:894:ASP:N	2.39	0.43
2:D:254:SER:O	2:D:295:THR:HG22	2.19	0.43
1:A:825:MET:HE2	1:A:856:LEU:CG	2.49	0.43
1:C:873:ILE:HG21	1:C:913:LEU:HD13	2.01	0.43
1:E:444:VAL:C	1:E:448:THR:HG1	2.21	0.43
1:E:622:MET:HE2	1:E:623:LYS:CA	2.48	0.43
2:F:13:TYR:CE1	2:F:145:LEU:HD22	2.53	0.43
2:B:834:ASP:OD2	2:B:877:THR:HG23	2.17	0.43
2:B:920:VAL:O	2:B:920:VAL:HG12	2.18	0.43
2:B:924:ASP:O	2:B:926:LYS:NZ	2.45	0.43
2:D:510:LEU:HD12	2:D:510:LEU:O	2.19	0.43
1:A:660:ARG:NE	1:A:660:ARG:HA	2.34	0.43
1:A:1000:THR:HG22	1:A:1001:LYS:N	2.33	0.43
1:C:709:LEU:CD1	1:C:751:VAL:HG11	2.48	0.43
1:E:451:ILE:O	2:D:679:MET:HE1	2.19	0.43
2:F:21:ASP:O	2:F:25:GLU:OE1	2.36	0.43
2:F:82:MET:HE3	2:F:82:MET:H	1.84	0.43
2:F:209:SER:CB	2:F:285:ILE:HD13	2.48	0.43
2:F:236:ASP:O	2:F:239:THR:OG1	2.33	0.43
2:F:328:GLN:HA	2:F:331:ILE:CG1	2.48	0.43
2:F:425:ARG:HH21	2:F:502:ILE:HD11	1.84	0.43
2:F:480:LEU:CD1	2:F:593:VAL:HG22	2.48	0.43
2:F:541:SER:OG	2:F:542:PRO:HA	2.18	0.43
2:F:569:GLN:HE22	2:F:572:ILE:HD11	1.84	0.43
2:B:491:THR:HG23	3:B:1101:ATP:H5'1	1.96	0.43
2:B:624:ARG:HE	2:B:662:SER:HG	1.65	0.43
2:D:921:LEU:HB3	2:D:925:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ALA:HB3	1:A:873:ILE:HD11	1.99	0.43
1:A:781:GLU:O	1:A:785:ARG:HG3	2.18	0.43
1:C:525:ASP:OD1	1:C:525:ASP:C	2.61	0.43
1:E:256:ARG:HA	1:E:256:ARG:NE	2.32	0.43
1:E:954:ARG:HE	1:E:956:GLU:H	1.66	0.43
2:F:218:LEU:HA	2:F:220:ARG:NH1	2.34	0.43
2:F:312:VAL:HG13	2:F:394:SER:O	2.18	0.43
2:F:555:LEU:H	2:F:569:GLN:NE2	2.16	0.43
2:F:892:ARG:NE	2:F:892:ARG:HA	2.33	0.43
2:D:342:SER:OG	2:D:343:LYS:N	2.52	0.43
1:A:439:ILE:O	1:A:442:GLU:OE1	2.37	0.43
1:A:632:ASP:O	1:A:633:LEU:C	2.62	0.43
1:A:844:ASP:OD1	1:A:844:ASP:N	2.52	0.43
1:A:847:ASP:OD1	1:A:848:SER:N	2.51	0.43
1:C:436:VAL:CG1	1:C:439:ILE:HD13	2.49	0.43
1:C:588:LEU:HD12	1:C:589:PHE:N	2.34	0.43
1:E:456:ALA:HA	1:E:574:VAL:HG13	2.01	0.43
1:E:469:ARG:CZ	3:E:1101:ATP:H3'	2.48	0.43
1:E:632:ASP:C	1:E:632:ASP:OD2	2.62	0.43
1:E:652:ILE:HD11	1:E:674:SER:OG	2.19	0.43
2:F:156:SER:HA	2:F:157:PRO:C	2.44	0.43
2:F:182:ALA:O	2:F:184:LYS:HD3	2.19	0.43
2:F:309:ALA:HA	2:F:397:LEU:HD23	1.99	0.43
2:F:344:ARG:O	2:F:408:ILE:HA	2.19	0.43
2:F:352:ILE:HD11	2:F:392:VAL:HG23	2.01	0.43
2:F:612:PHE:N	2:F:612:PHE:CD1	2.87	0.43
2:F:827:VAL:HG23	2:F:874:ILE:HD13	2.00	0.43
2:B:241:LEU:C	2:B:241:LEU:HD23	2.43	0.43
2:D:658:LEU:HD13	2:D:706:LEU:HD23	2.01	0.43
2:D:862:ASP:OD2	2:D:892:ARG:NH2	2.52	0.43
1:C:451:ILE:O	2:B:679:MET:HE1	2.19	0.43
1:C:689:THR:O	1:C:689:THR:OG1	2.37	0.43
1:E:730:LEU:HD12	1:E:730:LEU:C	2.44	0.43
2:F:343:LYS:N	2:F:343:LYS:CD	2.81	0.43
2:B:290:ASP:OD1	2:B:291:CYS:N	2.51	0.43
2:B:384:ASN:OD1	2:B:384:ASN:C	2.62	0.43
2:B:624:ARG:O	2:B:627:ILE:HG22	2.18	0.43
2:D:217:ASP:OD1	2:D:217:ASP:N	2.51	0.43
2:D:435:GLN:OE1	2:D:435:GLN:HA	2.19	0.43
2:D:457:LEU:HD12	2:D:614:ILE:HD11	2.01	0.43
2:D:462:GLU:OE2	2:D:462:GLU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:ASP:CG	2:D:609:HIS:HE2	2.22	0.43
1:A:233:VAL:HG23	1:A:292:LEU:HD23	2.01	0.42
1:C:252:LYS:O	2:B:365:ILE:HD12	2.19	0.42
1:C:515:TYR:OH	2:B:357:ASP:OD2	2.36	0.42
1:C:873:ILE:CG2	1:C:913:LEU:HD13	2.49	0.42
1:E:251:VAL:HG22	1:E:309:LYS:O	2.19	0.42
1:E:433:PHE:CD1	1:E:611:LEU:HD11	2.54	0.42
1:E:654:TYR:HH	2:F:464:SER:HB3	1.83	0.42
2:F:134:SER:OG	2:F:135:MET:CE	2.67	0.42
2:F:224:HIS:CE1	2:F:226:ASN:HB2	2.53	0.42
2:F:245:VAL:HG12	2:F:246:THR:N	2.34	0.42
2:F:316:ARG:NE	2:F:421:ILE:HD11	2.34	0.42
2:F:426:PRO:HD3	2:F:503:HIS:CD2	2.54	0.42
2:F:576:MET:HE3	2:F:577:SER:CA	2.49	0.42
2:B:236:ASP:O	2:B:239:THR:OG1	2.36	0.42
2:B:416:LEU:C	2:B:416:LEU:HD12	2.44	0.42
2:B:602:VAL:O	2:B:607:ARG:NH2	2.52	0.42
2:B:748:ILE:HG21	2:B:789:PHE:CD2	2.54	0.42
2:B:752:LEU:HD21	2:B:872:PHE:HZ	1.84	0.42
2:B:796:VAL:HG21	2:B:816:VAL:HG21	2.01	0.42
1:A:250:ILE:HG23	1:A:300:PHE:CE1	2.54	0.42
1:A:557:PHE:CZ	1:A:561:VAL:HG11	2.54	0.42
1:A:770:LYS:HG2	2:B:805:TYR:HB3	2.01	0.42
1:A:806:ARG:NE	1:A:806:ARG:HA	2.34	0.42
1:C:643:LEU:HD11	1:C:647:ILE:HD11	2.02	0.42
1:C:944:ILE:HG12	1:C:963:LYS:HZ1	1.84	0.42
2:F:97:VAL:CG2	2:F:162:LEU:HD23	2.49	0.42
2:F:235:THR:HG21	2:F:239:THR:HG21	2.02	0.42
2:F:285:ILE:HG22	2:F:427:LEU:CD2	2.48	0.42
2:F:781:MET:SD	2:F:781:MET:C	3.03	0.42
2:F:836:VAL:O	2:F:836:VAL:CG1	2.67	0.42
2:B:638:ASN:OD1	2:B:647:VAL:HG22	2.18	0.42
2:B:706:LEU:HD12	2:B:706:LEU:H	1.84	0.42
2:D:757:LEU:H	2:D:757:LEU:HD12	1.84	0.42
1:A:251:VAL:HB	2:F:365:ILE:HD11	2.00	0.42
1:C:467:LYS:HG2	3:C:1101:ATP:O1B	2.19	0.42
2:F:76:MET:SD	2:F:76:MET:N	2.88	0.42
2:F:273:PHE:CD2	2:F:273:PHE:N	2.87	0.42
2:B:857:LEU:HD12	2:B:861:LEU:HD13	2.01	0.42
2:D:137:THR:O	2:D:163:VAL:HG23	2.19	0.42
2:D:323:SER:HB3	2:D:536:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:911:ILE:HG23	3:D:1602:ATP:HN61	1.84	0.42
1:A:451:ILE:HG23	2:F:679:MET:CE	2.49	0.42
1:A:516:TRP:CG	2:F:363:LEU:HD21	2.54	0.42
1:A:733:GLY:N	1:A:857:ASP:OD2	2.53	0.42
1:C:443:MET:O	1:C:444:VAL:C	2.63	0.42
1:C:555:ASN:ND2	2:B:510:LEU:HD23	2.35	0.42
1:E:819:ASN:HB3	2:D:832:GLU:OE2	2.19	0.42
1:E:823:THR:HG23	2:D:831:ASP:OD2	2.19	0.42
2:F:120:MET:HA	2:F:123:ILE:CD1	2.49	0.42
2:F:133:ASN:HD22	2:F:136:GLU:HG2	1.84	0.42
2:F:251:ILE:HD13	2:F:264:LEU:HB2	2.01	0.42
2:B:377:GLU:O	2:B:380:GLN:HG3	2.20	0.42
2:D:119:GLU:OE2	2:D:120:MET:N	2.53	0.42
2:D:517:ARG:O	2:D:517:ARG:NH1	2.43	0.42
2:D:958:ILE:HD11	2:D:994:VAL:HA	2.01	0.42
1:A:500:LEU:HD11	2:F:514:SER:H	1.84	0.42
1:A:643:LEU:HB2	3:A:1102:ATP:H4'	2.01	0.42
1:A:651:LYS:NZ	2:B:612:PHE:HA	2.35	0.42
1:A:779:ILE:HD11	1:A:817:VAL:HG13	2.01	0.42
1:C:469:ARG:C	1:C:469:ARG:HD3	2.45	0.42
1:C:666:VAL:HG22	1:C:667:THR:N	2.35	0.42
1:C:944:ILE:CB	1:C:959:ARG:HH22	2.26	0.42
2:F:426:PRO:HG3	2:F:503:HIS:CD2	2.55	0.42
2:F:480:LEU:HD23	2:F:489:LYS:HB2	2.01	0.42
2:F:650:MET:N	2:F:700:LEU:HD12	2.34	0.42
2:B:20:ARG:N	2:B:58:ASP:O	2.52	0.42
2:B:715:ASN:O	2:B:718:SER:OG	2.30	0.42
2:B:737:ILE:HG22	2:B:740:VAL:HG23	2.02	0.42
2:B:903:ASP:OD1	2:B:904:THR:HG23	2.19	0.42
2:B:921:LEU:HB3	2:B:925:VAL:HG11	2.00	0.42
2:D:557:VAL:HG11	2:D:566:ILE:HA	2.01	0.42
2:D:575:GLU:HA	2:D:578:LYS:HB3	2.02	0.42
1:A:209:GLN:H	1:A:209:GLN:CD	2.28	0.42
1:A:431:ASP:CG	3:A:1102:ATP:HN61	2.26	0.42
1:A:458:ILE:HB	1:A:597:THR:HG23	2.01	0.42
1:A:911:ALA:O	1:A:914:GLN:NE2	2.53	0.42
1:C:568:ASP:N	2:B:640:ASP:OD2	2.53	0.42
1:C:948:SER:HA	1:C:951:GLU:CD	2.43	0.42
2:F:98:LEU:HD11	2:F:160:GLN:HA	2.01	0.42
2:F:324:GLN:HB2	2:F:327:PHE:CD2	2.55	0.42
1:A:961:ARG:HA	1:A:964:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:965:LEU:O	2:F:153:LEU:HD21	2.18	0.42
2:F:146:THR:OG1	2:F:150:CYS:HB2	2.19	0.42
2:F:337:LYS:HE2	2:F:375:GLU:HB3	2.01	0.42
2:F:380:GLN:O	2:F:383:LYS:CE	2.67	0.42
2:F:385:ASP:OD1	2:F:385:ASP:C	2.63	0.42
2:F:449:HIS:CA	2:F:455:ARG:HH21	2.33	0.42
2:F:764:LYS:NZ	2:F:866:THR:O	2.52	0.42
2:B:133:ASN:N	2:B:137:THR:OG1	2.52	0.42
2:B:747:THR:HG21	2:B:768:ILE:HD11	2.02	0.42
2:D:509:CYS:SG	2:D:550:LEU:HA	2.60	0.42
2:D:634:SER:C	2:D:638:ASN:HD22	2.27	0.42
2:D:965:LYS:NZ	2:D:991:ASP:OD1	2.53	0.42
1:A:484:ILE:O	1:A:486:VAL:HG13	2.19	0.42
1:C:433:PHE:HE2	1:C:469:ARG:HE	1.66	0.42
1:C:746:LEU:O	1:C:747:LEU:C	2.61	0.42
1:E:396:THR:HG1	1:E:398:MET:HE1	1.85	0.42
1:E:558:ILE:O	1:E:559:ASN:C	2.60	0.42
1:E:567:LYS:HE2	2:D:383:LYS:O	2.20	0.42
1:E:820:GLN:N	2:D:799:PRO:HG3	2.35	0.42
2:F:243:LEU:HD11	2:F:298:LYS:CB	2.49	0.42
2:F:316:ARG:HD2	2:F:322:GLN:HG3	2.02	0.42
2:F:346:LEU:CD1	2:F:409:ILE:HG12	2.44	0.42
2:F:461:LEU:HB2	2:F:500:LEU:CD1	2.50	0.42
2:F:628:PHE:O	2:F:632:LEU:HD23	2.20	0.42
2:F:929:GLU:OE2	2:F:933:LEU:HD11	2.19	0.42
2:F:934:CYS:N	2:F:1005:GLN:OE1	2.53	0.42
2:B:255:ASN:OD1	2:B:256:MET:N	2.53	0.42
2:B:407:PHE:HE1	2:B:409:ILE:HD11	1.85	0.42
2:D:6:THR:CG2	2:D:67:VAL:HG22	2.50	0.42
2:D:550:LEU:HD21	2:D:554:LEU:HD13	2.01	0.42
2:D:970:ASN:O	2:D:974:GLY:N	2.48	0.42
1:A:208:ILE:HG21	1:A:315:LEU:HB3	2.01	0.42
1:A:622:MET:HE1	1:A:653:PHE:HB2	2.01	0.42
1:A:730:LEU:C	1:A:730:LEU:HD12	2.45	0.42
1:A:792:CYS:SG	1:A:793:ILE:N	2.92	0.42
1:C:250:ILE:HG22	1:C:310:ILE:HD12	2.02	0.42
1:C:337:LYS:O	1:C:338:ASP:HB3	2.19	0.42
1:C:443:MET:O	1:C:447:LEU:HD23	2.19	0.42
1:E:452:ILE:N	1:E:452:ILE:HD12	2.35	0.42
1:E:938:VAL:O	1:E:939:PRO:C	2.63	0.42
1:E:963:LYS:HD2	1:E:964:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:ILE:O	2:F:165:PHE:HZ	2.03	0.42
2:F:139:VAL:O	2:F:160:GLN:HA	2.20	0.42
2:F:316:ARG:HA	2:F:390:PHE:HD1	1.82	0.42
2:F:446:TYR:CE2	2:F:454:VAL:HG21	2.55	0.42
2:F:561:GLN:N	2:F:561:GLN:OE1	2.53	0.42
2:B:67:VAL:HG13	2:B:67:VAL:O	2.19	0.42
2:B:250:PHE:HB3	2:B:261:LEU:HD21	2.02	0.42
2:B:673:ILE:HD11	2:B:713:ALA:CB	2.47	0.42
2:D:371:GLU:O	2:D:372:SER:C	2.63	0.42
1:A:451:ILE:HD11	2:F:678:ARG:HH11	1.85	0.42
1:A:521:LEU:HD23	1:A:521:LEU:O	2.20	0.42
1:A:882:ASP:OD1	1:A:889:LYS:CG	2.68	0.42
1:C:255:LEU:HD13	1:C:513:PHE:CZ	2.54	0.42
1:C:351:LEU:O	1:C:354:SER:OG	2.38	0.42
1:C:654:TYR:CE1	2:D:474:LEU:HD12	2.54	0.42
1:C:710:LEU:O	1:C:713:LEU:N	2.53	0.42
1:C:949:ILE:HG23	2:D:119:GLU:HG2	1.99	0.42
2:F:87:PHE:CE2	2:F:89:PRO:HD3	2.54	0.42
2:F:343:LYS:HA	2:F:343:LYS:HE3	2.02	0.42
2:F:709:ALA:HA	2:F:712:LYS:HG2	2.01	0.42
2:B:170:LEU:O	2:B:171:ILE:HD13	2.20	0.42
2:B:308:ILE:HA	2:B:408:ILE:HG23	2.02	0.42
2:B:345:ILE:HD12	2:B:345:ILE:N	2.35	0.42
2:B:466:ASN:O	2:B:470:ARG:N	2.53	0.42
2:B:828:ILE:HD13	2:B:830:PHE:CE2	2.55	0.42
2:D:695:LEU:HD23	2:D:695:LEU:H	1.84	0.42
1:A:290:ILE:HG12	1:A:310:ILE:HD11	2.02	0.41
1:A:330:VAL:HG22	1:A:330:VAL:O	2.20	0.41
1:A:478:VAL:HG22	1:A:484:ILE:HD13	2.00	0.41
1:C:241:LEU:HD11	1:C:243:SER:O	2.19	0.41
1:C:347:TYR:HH	1:C:365:GLU:CD	2.19	0.41
1:C:443:MET:HE1	1:C:598:TRP:CE3	2.55	0.41
1:C:453:ALA:HA	2:B:675:GLU:OE1	2.19	0.41
1:C:723:PHE:CG	2:B:955:MET:HE1	2.55	0.41
1:C:852:ARG:NH1	3:B:1102:ATP:PB	2.93	0.41
1:E:916:LEU:HD13	1:E:997:CYS:HA	2.02	0.41
2:F:7:PHE:CE1	2:F:68:VAL:HG13	2.55	0.41
2:F:45:PRO:HD3	2:F:212:CYS:HB2	2.01	0.41
2:F:98:LEU:HD11	2:F:160:GLN:C	2.45	0.41
2:F:166:THR:OG1	2:F:167:GLU:OE2	2.35	0.41
2:F:316:ARG:NH2	2:F:421:ILE:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:387:LEU:HD23	2:F:388:VAL:N	2.35	0.41
2:F:451:PHE:CE1	2:F:623:GLN:HG2	2.55	0.41
2:B:140:HIS:HA	2:B:160:GLN:HA	2.02	0.41
2:B:647:VAL:HG12	2:B:699:ILE:HG21	2.02	0.41
2:B:812:ASN:HA	2:B:815:ARG:HG2	2.02	0.41
2:B:833:ILE:O	2:B:836:VAL:HG22	2.19	0.41
2:D:514:SER:HG	2:D:515:ASN:H	1.62	0.41
1:A:357:THR:HG22	1:A:360:LEU:HD11	2.01	0.41
1:A:484:ILE:HD12	1:A:484:ILE:N	2.34	0.41
1:A:632:ASP:O	1:A:635:LEU:N	2.53	0.41
1:C:360:LEU:O	1:C:360:LEU:HD12	2.20	0.41
1:E:770:LYS:HE3	2:F:805:TYR:HB2	2.02	0.41
2:F:254:SER:CB	2:F:259:VAL:HG22	2.51	0.41
2:F:324:GLN:OE1	2:F:324:GLN:N	2.53	0.41
2:F:455:ARG:HA	2:F:458:VAL:HG22	2.02	0.41
2:F:592:PHE:CD1	2:F:593:VAL:N	2.88	0.41
2:F:599:ILE:O	2:F:607:ARG:NH2	2.53	0.41
2:F:633:SER:OG	2:F:636:GLU:HB2	2.20	0.41
2:F:645:VAL:HG13	2:F:698:SER:HA	2.02	0.41
2:F:888:LEU:HD13	2:F:896:LEU:HD11	2.01	0.41
2:B:355:ALA:HA	2:B:386:SER:O	2.20	0.41
2:B:806:ILE:HD12	2:B:806:ILE:N	2.35	0.41
2:D:1:MET:HE2	2:D:1:MET:CA	2.50	0.41
2:D:233:ALA:C	2:D:234:PHE:CD1	2.98	0.41
2:D:562:ASP:OD1	2:D:562:ASP:C	2.63	0.41
2:D:575:GLU:OE1	2:D:575:GLU:CA	2.68	0.41
2:D:853:ILE:O	2:D:856:GLN:HB2	2.20	0.41
1:A:360:LEU:HD12	1:A:360:LEU:N	2.35	0.41
1:A:651:LYS:CE	2:B:611:ARG:O	2.68	0.41
1:A:825:MET:HE2	1:A:856:LEU:CD1	2.50	0.41
1:C:504:GLN:HG2	1:C:556:PHE:CD2	2.55	0.41
1:C:734:ILE:O	1:C:837:LEU:HD13	2.20	0.41
1:E:483:HIS:O	1:E:483:HIS:ND1	2.49	0.41
1:E:515:TYR:OH	1:E:567:LYS:NZ	2.54	0.41
1:E:772:ILE:HB	2:D:804:MET:HA	2.02	0.41
2:F:1:MET:O	2:F:86:TYR:HA	2.20	0.41
2:F:39:ARG:NH2	2:F:47:CYS:HA	2.28	0.41
2:F:251:ILE:O	2:F:262:VAL:HG12	2.20	0.41
2:F:346:LEU:HD12	2:F:346:LEU:N	2.35	0.41
2:F:508:ASP:HB3	2:F:511:SER:OG	2.20	0.41
2:F:659:SER:HA	2:F:662:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:861:LEU:HB3	2:F:892:ARG:HE	1.86	0.41
2:B:363:LEU:HD12	2:B:363:LEU:N	2.35	0.41
2:B:738:ASP:N	2:B:738:ASP:OD1	2.50	0.41
2:D:488:GLY:CA	3:D:1601:ATP:H5'1	2.50	0.41
2:D:769:LEU:O	2:D:897:LEU:N	2.54	0.41
1:A:274:LYS:C	1:A:274:LYS:CD	2.93	0.41
1:A:458:ILE:C	1:A:459:LEU:HD22	2.45	0.41
1:A:727:PRO:HG2	2:F:918:LYS:HZ3	1.86	0.41
1:A:746:LEU:HD11	3:A:1101:ATP:H5'1	2.03	0.41
1:C:347:TYR:O	1:C:351:LEU:HD23	2.19	0.41
1:C:458:ILE:HG23	1:C:597:THR:HB	2.01	0.41
1:E:434:ILE:HA	1:E:437:ASN:ND2	2.35	0.41
2:F:90:ILE:HD12	2:F:93:ASN:O	2.21	0.41
2:F:235:THR:HG22	2:F:239:THR:OG1	2.21	0.41
2:F:351:LEU:HA	2:F:390:PHE:O	2.20	0.41
2:F:592:PHE:CD1	2:F:592:PHE:C	2.98	0.41
2:F:678:ARG:HG2	2:F:678:ARG:NH1	2.34	0.41
2:B:721:ILE:O	2:B:721:ILE:HG22	2.20	0.41
2:B:785:ILE:HD11	2:B:789:PHE:CZ	2.55	0.41
2:D:34:LEU:HD23	2:D:35:TYR:C	2.46	0.41
1:A:794:LEU:HD12	1:A:795:PHE:N	2.36	0.41
1:A:893:GLU:CB	1:A:896:ALA:HB2	2.51	0.41
1:A:900:LEU:N	1:A:900:LEU:HD23	2.35	0.41
1:C:247:TYR:CD2	1:C:274:LYS:HG3	2.56	0.41
1:C:766:GLU:CD	1:C:766:GLU:C	2.87	0.41
1:C:950:ASN:ND2	2:D:165:PHE:O	2.53	0.41
1:C:1022:ASP:OD1	1:C:1022:ASP:C	2.64	0.41
1:E:1023:ARG:O	1:E:1024:ASN:C	2.63	0.41
2:F:260:ARG:HH21	2:F:350:ASP:HA	1.85	0.41
2:F:657:SER:O	2:F:660:SER:N	2.54	0.41
2:B:7:PHE:CD2	2:B:81:THR:HG21	2.50	0.41
2:B:481:HIS:HA	2:B:596:VAL:O	2.20	0.41
2:B:525:ILE:O	2:B:529:ILE:HG22	2.20	0.41
2:D:178:GLN:O	2:D:181:SER:OG	2.35	0.41
2:D:262:VAL:HG22	2:D:263:LYS:O	2.20	0.41
2:D:569:GLN:HA	2:D:572:ILE:HG22	2.01	0.41
2:D:802:LEU:HD21	2:D:853:ILE:HD13	2.03	0.41
1:A:646:GLU:OE2	1:A:646:GLU:C	2.64	0.41
1:A:779:ILE:HG21	1:A:820:GLN:HG3	2.03	0.41
1:A:865:PRO:O	1:A:870:ARG:NH1	2.50	0.41
1:A:882:ASP:OD1	1:A:889:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:PHE:CD2	2:B:955:MET:HE1	2.55	0.41
1:E:497:THR:HG23	1:E:502:LYS:HB3	2.02	0.41
1:E:646:GLU:O	1:E:650:GLU:HG2	2.19	0.41
2:F:19:SER:OG	2:F:21:ASP:OD1	2.20	0.41
2:F:21:ASP:OD1	2:F:22:ILE:N	2.54	0.41
2:F:192:TYR:CE2	2:F:194:LEU:HG	2.55	0.41
2:F:238:GLU:C	2:F:241:LEU:HG	2.46	0.41
2:F:969:HIS:HB3	2:F:982:TRP:HZ2	1.84	0.41
2:B:831:ASP:OD2	2:B:832:GLU:HG2	2.20	0.41
2:B:1002:LEU:O	2:B:1006:GLU:HG2	2.20	0.41
2:D:127:HIS:O	2:D:131:ASN:N	2.38	0.41
2:D:206:ASP:C	2:D:206:ASP:OD1	2.62	0.41
2:D:250:PHE:CD1	2:D:250:PHE:N	2.87	0.41
1:A:255:LEU:N	2:F:364:ASN:OD1	2.54	0.41
1:A:372:LYS:HB2	1:A:376:SER:O	2.20	0.41
1:C:217:ARG:NH1	1:C:517:TYR:O	2.50	0.41
1:C:604:ASP:OD1	1:C:607:ALA:N	2.43	0.41
2:F:72:LEU:HD22	2:F:73:PHE:CZ	2.56	0.41
2:F:73:PHE:HB2	2:F:75:PHE:CD1	2.56	0.41
2:F:145:LEU:HB2	2:F:150:CYS:HB3	2.02	0.41
2:F:284:ILE:HD12	2:F:284:ILE:N	2.26	0.41
2:F:478:VAL:O	2:F:593:VAL:HA	2.19	0.41
2:B:82:MET:SD	2:B:82:MET:C	3.03	0.41
2:B:610:MET:HE3	2:B:610:MET:HA	2.02	0.41
2:B:879:ARG:O	2:B:879:ARG:HG3	2.20	0.41
2:D:812:ASN:O	2:D:815:ARG:HG2	2.21	0.41
2:D:999:GLU:OE1	2:D:999:GLU:N	2.51	0.41
1:C:799:PHE:O	1:C:802:ILE:HG22	2.20	0.41
1:E:707:ASP:OD1	1:E:707:ASP:N	2.52	0.41
2:F:316:ARG:HD2	2:F:322:GLN:HB3	2.02	0.41
2:F:457:LEU:HD12	2:F:457:LEU:C	2.46	0.41
2:F:491:THR:HG21	3:F:1101:ATP:C2'	2.44	0.41
2:F:503:HIS:HD1	2:F:540:ALA:C	2.23	0.41
2:B:625:LEU:HD12	2:B:629:GLN:OE1	2.21	0.41
2:B:628:PHE:O	2:B:629:GLN:C	2.64	0.41
2:D:253:VAL:O	2:D:253:VAL:HG23	2.20	0.41
2:D:770:PHE:HE2	2:D:899:LEU:HD22	1.85	0.41
1:A:371:ILE:HG23	1:A:381:CYS:SG	2.61	0.41
1:A:452:ILE:CA	2:F:679:MET:CE	2.98	0.41
1:A:594:VAL:O	1:A:594:VAL:HG23	2.20	0.41
1:A:600:LEU:HD12	1:A:600:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:649:THR:HG22	2.20	0.41
1:A:652:ILE:HA	1:A:655:ASP:OD1	2.21	0.41
1:A:820:GLN:O	1:A:820:GLN:NE2	2.53	0.41
1:C:255:LEU:HB3	1:C:513:PHE:HE1	1.86	0.41
1:C:442:GLU:O	1:C:443:MET:C	2.63	0.41
1:C:723:PHE:CE1	2:B:955:MET:SD	3.14	0.41
1:C:965:LEU:N	1:C:965:LEU:HD12	2.35	0.41
1:C:981:ALA:O	2:D:757:LEU:HG	2.21	0.41
1:E:395:VAL:O	1:E:396:THR:HG23	2.21	0.41
1:E:828:ALA:HB2	2:D:783:LYS:CD	2.51	0.41
1:E:852:ARG:HD2	2:D:774:PRO:HB2	2.03	0.41
2:F:9:LEU:HA	2:F:9:LEU:HD12	1.84	0.41
2:F:13:TYR:CD2	2:F:132:ILE:HG12	2.56	0.41
2:F:36:GLY:C	2:F:52:ILE:HD12	2.46	0.41
2:F:45:PRO:CD	2:F:212:CYS:HB2	2.51	0.41
2:F:129:LYS:HB2	2:F:129:LYS:HE2	1.87	0.41
2:F:133:ASN:HD22	2:F:136:GLU:CG	2.34	0.41
2:F:317:VAL:HG23	2:F:390:PHE:CA	2.51	0.41
2:F:342:SER:OG	2:F:343:LYS:N	2.54	0.41
2:F:475:ASN:HB2	2:F:584:THR:HG21	2.02	0.41
2:F:523:SER:HA	2:F:526:ILE:CG1	2.51	0.41
2:F:637:LEU:HG	2:F:647:VAL:HG13	2.03	0.41
2:F:687:GLN:OE1	2:F:690:LYS:HE2	2.21	0.41
2:F:834:ASP:N	2:F:834:ASP:OD1	2.53	0.41
2:B:37:THR:HG22	2:B:38:ILE:N	2.36	0.41
2:B:75:PHE:CD2	2:B:269:LEU:HD23	2.56	0.41
2:B:76:MET:HG2	2:B:78:THR:HG23	2.02	0.41
2:B:92:ASP:OD1	2:B:92:ASP:N	2.53	0.41
2:B:374:ASP:O	2:B:375:GLU:C	2.62	0.41
2:D:750:MET:HA	2:D:753:LYS:HG2	2.03	0.41
2:D:850:MET:O	2:D:851:ASP:C	2.63	0.41
2:D:922:ASP:O	2:D:925:VAL:HG22	2.21	0.41
1:A:401:GLU:OE1	1:A:402:GLU:N	2.54	0.41
1:A:462:LYS:O	1:A:465:ILE:HG12	2.21	0.41
1:A:474:LEU:O	1:A:475:ILE:C	2.64	0.41
1:C:743:GLY:HA2	3:C:1102:ATP:H5'1	2.02	0.41
2:F:9:LEU:HD13	2:F:77:PRO:HD2	2.03	0.41
2:F:76:MET:CE	2:F:188:GLU:HB3	2.51	0.41
2:F:264:LEU:HD22	2:F:264:LEU:N	2.35	0.41
2:F:284:ILE:H	2:F:284:ILE:CD1	2.22	0.41
2:F:351:LEU:HD23	2:F:351:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:937:ASN:HB2	2:F:1017:LEU:HD11	2.02	0.41
2:B:545:ILE:HD12	2:B:545:ILE:H	1.85	0.41
2:B:551:ASP:OD1	2:B:551:ASP:C	2.64	0.41
2:B:599:ILE:O	2:B:607:ARG:NH1	2.54	0.41
2:B:599:ILE:HD11	2:B:613:GLU:OE2	2.21	0.41
2:B:647:VAL:O	2:B:648:SER:OG	2.36	0.41
2:B:980:ARG:O	2:B:984:ASP:OD2	2.38	0.41
2:B:989:LYS:O	2:B:993:LYS:N	2.49	0.41
2:D:728:ASN:OD1	2:D:728:ASN:N	2.52	0.41
2:D:927:LEU:HD23	2:D:930:LEU:HD12	2.03	0.41
1:A:567:LYS:NZ	2:F:383:LYS:CB	2.78	0.40
1:A:719:TYR:HB3	1:A:722:ILE:HD12	2.03	0.40
1:A:987:VAL:O	1:A:987:VAL:HG13	2.21	0.40
1:E:321:ASN:OD1	1:E:321:ASN:O	2.39	0.40
1:E:482:HIS:C	1:E:483:HIS:CG	2.99	0.40
1:E:652:ILE:HD13	1:E:652:ILE:HA	1.95	0.40
2:F:9:LEU:CD1	2:F:76:MET:HB2	2.51	0.40
2:F:642:GLN:CD	2:F:642:GLN:N	2.78	0.40
2:F:705:ASP:HA	2:F:708:LYS:HZ1	1.85	0.40
2:F:864:MET:N	2:F:864:MET:SD	2.94	0.40
2:B:346:LEU:HD23	2:B:352:ILE:HD11	2.04	0.40
2:B:405:SER:OG	2:B:406:HIS:ND1	2.50	0.40
2:B:599:ILE:O	2:B:602:VAL:HG12	2.20	0.40
2:B:715:ASN:C	2:B:715:ASN:OD1	2.63	0.40
2:D:98:LEU:HD22	2:D:155:CYS:HB2	2.02	0.40
2:D:104:LEU:CG	2:D:153:LEU:HD21	2.51	0.40
2:D:834:ASP:OD1	2:D:883:LEU:HD21	2.20	0.40
1:A:436:VAL:HG22	1:A:600:LEU:HD11	2.04	0.40
1:A:487:LYS:HD3	1:A:487:LYS:C	2.46	0.40
1:A:722:ILE:HG23	2:F:994:VAL:HG22	2.03	0.40
1:C:752:ALA:O	1:C:756:GLY:N	2.53	0.40
1:C:900:LEU:HG	1:C:904:LYS:HD2	2.01	0.40
1:C:965:LEU:HD12	1:C:965:LEU:H	1.87	0.40
1:E:364:THR:HG23	1:E:365:GLU:N	2.36	0.40
1:E:459:LEU:HD23	1:E:459:LEU:C	2.46	0.40
2:F:207:LEU:HD22	2:F:294:VAL:HG21	2.02	0.40
2:F:317:VAL:HB	2:F:389:TRP:CB	2.51	0.40
2:F:317:VAL:O	2:F:322:GLN:HG2	2.22	0.40
2:F:352:ILE:HD12	2:F:352:ILE:N	2.36	0.40
2:F:515:ASN:HA	2:F:517:ARG:NH2	2.36	0.40
2:F:686:TYR:C	2:F:690:LYS:HZ3	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:PHE:HD1	2:B:234:PHE:N	2.20	0.40
2:B:457:LEU:HD23	2:B:458:VAL:N	2.37	0.40
2:B:606:PHE:CE1	2:B:610:MET:SD	3.14	0.40
2:B:915:LEU:HD11	3:B:1102:ATP:N7	2.37	0.40
2:D:137:THR:O	2:D:162:LEU:HD12	2.21	0.40
1:A:451:ILE:CD1	2:F:678:ARG:HH11	2.34	0.40
1:C:360:LEU:HD12	1:C:360:LEU:C	2.46	0.40
1:C:874:LEU:O	1:C:878:VAL:HG22	2.22	0.40
1:C:901:ILE:CG1	1:C:993:LEU:HD21	2.52	0.40
1:E:870:ARG:O	1:E:874:LEU:HG	2.21	0.40
2:F:19:SER:N	2:F:61:LEU:HD12	2.37	0.40
2:F:119:GLU:HA	2:F:122:GLN:NE2	2.36	0.40
2:F:257:GLY:O	2:F:259:VAL:HG23	2.22	0.40
2:B:52:ILE:HG21	2:B:160:GLN:OE1	2.22	0.40
2:D:925:VAL:HG12	2:D:1001:PHE:HE1	1.85	0.40
2:D:982:TRP:O	2:D:986:ILE:HB	2.21	0.40
1:A:644:ASP:O	1:A:647:ILE:HG22	2.22	0.40
1:C:322:ILE:CD1	1:C:380:LEU:HD23	2.51	0.40
1:C:391:VAL:HG23	1:C:393:TRP:CZ2	2.57	0.40
1:C:822:LEU:HD12	1:C:850:LEU:HD22	2.03	0.40
1:C:944:ILE:HG12	1:C:963:LYS:NZ	2.36	0.40
1:E:328:ALA:HB3	1:E:391:VAL:HA	2.03	0.40
1:E:452:ILE:N	2:D:679:MET:HE1	2.36	0.40
2:F:76:MET:HE1	2:F:188:GLU:CB	2.50	0.40
2:F:79:GLN:OE1	2:F:79:GLN:N	2.54	0.40
2:F:317:VAL:HG23	2:F:390:PHE:C	2.46	0.40
2:F:321:LEU:O	2:F:324:GLN:HG2	2.22	0.40
2:F:335:LEU:CD1	2:F:339:PHE:CE2	2.91	0.40
2:F:504:LEU:HG	2:F:506:GLU:CD	2.46	0.40
2:F:650:MET:SD	2:F:700:LEU:HD12	2.61	0.40
2:F:699:ILE:O	2:F:700:LEU:HD22	2.22	0.40
2:B:233:ALA:O	2:B:264:LEU:HA	2.21	0.40
2:B:261:LEU:HD23	2:B:262:VAL:H	1.85	0.40
2:B:657:SER:O	2:B:661:TYR:CD1	2.74	0.40
2:B:752:LEU:HD21	2:B:872:PHE:CZ	2.56	0.40
2:D:94:VAL:HG13	2:D:94:VAL:O	2.22	0.40
2:D:508:ASP:HB2	2:D:548:ALA:HB3	2.03	0.40
2:D:677:ALA:HA	2:D:680:THR:HG22	2.04	0.40
1:A:684:ARG:HH12	2:B:607:ARG:HD2	1.86	0.40
1:A:974:THR:C	1:A:975:LYS:HG3	2.47	0.40
1:C:215:ILE:HG22	1:C:216:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:LYS:HD3	1:C:567:LYS:O	2.22	0.40
1:C:615:PHE:CZ	3:C:1101:ATP:C8	3.10	0.40
1:C:823:THR:HG21	2:B:797:LYS:HG2	2.03	0.40
1:C:847:ASP:OD2	1:C:849:ALA:HB3	2.21	0.40
1:C:873:ILE:HG12	3:C:1102:ATP:HN61	1.86	0.40
1:C:938:VAL:HG13	1:C:939:PRO:HD2	2.04	0.40
1:E:222:LYS:NZ	1:E:223:MET:O	2.48	0.40
1:E:965:LEU:C	2:F:153:LEU:HD21	2.46	0.40
1:E:968:GLN:OE1	1:E:968:GLN:N	2.52	0.40
2:F:1:MET:HE2	2:F:2:LYS:C	2.46	0.40
2:F:143:ASP:O	2:F:152:ILE:N	2.48	0.40
2:F:251:ILE:CB	2:F:264:LEU:HD23	2.50	0.40
2:F:337:LYS:HE2	2:F:375:GLU:CB	2.51	0.40
2:F:699:ILE:HD12	2:F:699:ILE:H	1.87	0.40
2:B:5:LEU:HD11	2:B:68:VAL:HG12	2.03	0.40
2:B:105:ILE:HG22	2:B:106:ASN:N	2.37	0.40
2:B:180:LEU:HD12	2:B:180:LEU:N	2.36	0.40
2:B:228:ASP:OD1	2:B:230:SER:OG	2.33	0.40
2:B:312:VAL:HG12	2:B:395:ALA:HB1	2.04	0.40
2:B:553:ILE:HB	2:B:554:LEU:HD12	2.03	0.40
2:D:488:GLY:HA2	3:D:1601:ATP:H5'1	2.02	0.40
2:D:715:ASN:O	2:D:719:VAL:HG23	2.21	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	A	819/1054 (78%)	737 (90%)	79 (10%)	3 (0%)	30	64
1	C	819/1054 (78%)	745 (91%)	73 (9%)	1 (0%)	48	80
1	E	819/1054 (78%)	741 (90%)	78 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1028/1044 (98%)	944 (92%)	83 (8%)	1 (0%)	48	80
2	D	1028/1044 (98%)	956 (93%)	70 (7%)	2 (0%)	43	74
2	F	1029/1044 (99%)	972 (94%)	55 (5%)	2 (0%)	43	74
All	All	5542/6294 (88%)	5095 (92%)	438 (8%)	9 (0%)	44	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	806	ILE
2	B	156	SER
2	D	156	SER
1	A	536	ALA
1	C	535	GLN
2	D	727	PRO
1	A	423	VAL
2	F	727	PRO
1	A	417	VAL

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	A	729/939 (78%)	728 (100%)	1 (0%)	88	89
1	C	729/939 (78%)	726 (100%)	3 (0%)	84	83
1	E	729/939 (78%)	724 (99%)	5 (1%)	76	78
2	B	922/935 (99%)	919 (100%)	3 (0%)	86	85
2	D	922/935 (99%)	921 (100%)	1 (0%)	88	89
2	F	923/935 (99%)	921 (100%)	2 (0%)	87	87
All	All	4954/5622 (88%)	4939 (100%)	15 (0%)	84	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	508	MET
1	C	459	LEU
1	C	469	ARG
1	C	832	ASP
1	E	448	THR
1	E	452	ILE
1	E	521	LEU
1	E	544	ASN
1	E	547	TRP
2	F	600	ASP
2	F	827	VAL
2	B	631	TYR
2	B	779	THR
2	B	804	MET
2	D	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	358	ASN
1	A	808	HIS
1	A	967	GLN
1	C	758	ASN
1	C	875	GLN
1	C	968	GLN
1	E	265	ASN
1	E	583	GLN
1	E	606	HIS
1	E	758	ASN
2	F	127	HIS
2	F	133	ASN
2	F	178	GLN
2	F	200	ASN
2	F	255	ASN
2	F	369	ASN
2	F	569	GLN
2	F	597	ASN
2	F	629	GLN
2	F	642	GLN
2	F	697	GLN
2	B	131	ASN
2	B	384	ASN

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Mol	Chain	Res	Type
2	B	469	GLN
2	B	518	GLN
2	B	635	HIS
2	D	369	ASN
2	D	560	ASN
2	D	629	GLN
2	D	725	GLN
2	D	970	ASN
2	D	1007	GLN
2	D	1018	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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	1102	-	32,33,33	0.35	0	48,52,52	0.29	0
3	ATP	C	1101	-	32,33,33	0.35	0	48,52,52	0.30	0
3	ATP	B	1101	-	32,33,33	0.29	0	48,52,52	0.30	0
3	ATP	D	1602	-	32,33,33	0.30	0	48,52,52	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	1101	-	32,33,33	0.27	0	48,52,52	0.28	0
3	ATP	C	1102	-	32,33,33	0.31	0	48,52,52	0.44	0
3	ATP	F	1101	-	32,33,33	0.31	0	48,52,52	0.27	0
3	ATP	E	1101	-	32,33,33	0.29	0	48,52,52	0.27	0
3	ATP	B	1102	-	32,33,33	0.40	0	48,52,52	0.32	0
3	ATP	D	1601	-	32,33,33	0.37	0	48,52,52	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1102	-	-	5/22/38/38	0/3/3/3
3	ATP	C	1101	-	-	12/22/38/38	0/3/3/3
3	ATP	B	1101	-	-	7/22/38/38	0/3/3/3
3	ATP	D	1602	-	-	7/22/38/38	0/3/3/3
3	ATP	A	1101	-	-	5/22/38/38	0/3/3/3
3	ATP	C	1102	-	-	9/22/38/38	0/3/3/3
3	ATP	F	1101	-	-	6/22/38/38	0/3/3/3
3	ATP	E	1101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	1102	-	-	8/22/38/38	0/3/3/3
3	ATP	D	1601	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	ATP	O4'-C1'-N9-C8
3	A	1101	ATP	O4'-C1'-N9-C4
3	A	1102	ATP	O4'-C1'-N9-C8
3	A	1102	ATP	O4'-C1'-N9-C4
3	C	1101	ATP	PB-O3B-PG-O3G
3	C	1101	ATP	C5'-O5'-PA-O1A
3	C	1101	ATP	C5'-O5'-PA-O3A
3	C	1102	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	1102	ATP	C5'-O5'-PA-O3A
3	E	1101	ATP	C5'-O5'-PA-O1A
3	E	1101	ATP	C5'-O5'-PA-O2A
3	E	1101	ATP	C5'-O5'-PA-O3A
3	E	1101	ATP	O4'-C4'-C5'-O5'
3	B	1102	ATP	C5'-O5'-PA-O1A
3	D	1601	ATP	PB-O3B-PG-O3G
3	D	1601	ATP	C5'-O5'-PA-O1A
3	D	1601	ATP	C5'-O5'-PA-O3A
3	D	1602	ATP	C5'-O5'-PA-O2A
3	D	1602	ATP	C5'-O5'-PA-O3A
3	D	1602	ATP	O4'-C1'-N9-C8
3	D	1602	ATP	O4'-C1'-N9-C4
3	E	1101	ATP	C3'-C4'-C5'-O5'
3	B	1102	ATP	O4'-C4'-C5'-O5'
3	C	1101	ATP	O4'-C4'-C5'-O5'
3	C	1102	ATP	O4'-C4'-C5'-O5'
3	A	1101	ATP	C3'-C4'-C5'-O5'
3	C	1101	ATP	C3'-C4'-C5'-O5'
3	B	1102	ATP	C3'-C4'-C5'-O5'
3	A	1101	ATP	O4'-C4'-C5'-O5'
3	D	1602	ATP	O4'-C4'-C5'-O5'
3	C	1101	ATP	PB-O3B-PG-O1G
3	C	1101	ATP	PG-O3B-PB-O1B
3	A	1102	ATP	O4'-C4'-C5'-O5'
3	F	1101	ATP	O4'-C4'-C5'-O5'
3	D	1602	ATP	C3'-C4'-C5'-O5'
3	B	1101	ATP	O4'-C1'-N9-C4
3	C	1102	ATP	C2'-C1'-N9-C4
3	B	1101	ATP	O4'-C1'-N9-C8
3	A	1101	ATP	PG-O3B-PB-O1B
3	C	1102	ATP	PG-O3B-PB-O1B
3	B	1102	ATP	PA-O3A-PB-O1B
3	C	1101	ATP	C5'-O5'-PA-O2A
3	C	1102	ATP	C5'-O5'-PA-O2A
3	D	1601	ATP	C5'-O5'-PA-O2A
3	C	1101	ATP	C2'-C1'-N9-C8
3	C	1102	ATP	C2'-C1'-N9-C8
3	C	1101	ATP	PG-O3B-PB-O2B
3	C	1101	ATP	C2'-C1'-N9-C4
3	A	1102	ATP	C3'-C4'-C5'-O5'
3	B	1101	ATP	PG-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
3	F	1101	ATP	O4'-C1'-N9-C4
3	B	1102	ATP	PB-O3B-PG-O1G
3	F	1101	ATP	O4'-C1'-N9-C8
3	D	1601	ATP	O4'-C1'-N9-C8
3	C	1101	ATP	C4'-C5'-O5'-PA
3	F	1101	ATP	C3'-C4'-C5'-O5'
3	D	1601	ATP	O4'-C1'-N9-C4
3	F	1101	ATP	PA-O3A-PB-O1B
3	B	1101	ATP	PA-O3A-PB-O1B
3	C	1102	ATP	C3'-C4'-C5'-O5'
3	B	1101	ATP	PB-O3B-PG-O3G
3	B	1102	ATP	PB-O3B-PG-O2G
3	B	1102	ATP	PB-O3B-PG-O3G
3	C	1102	ATP	O4'-C1'-N9-C8
3	F	1101	ATP	PA-O3A-PB-O2B
3	B	1101	ATP	PG-O3B-PB-O1B
3	B	1101	ATP	PA-O3A-PB-O2B
3	B	1102	ATP	PA-O3A-PB-O2B
3	D	1602	ATP	PB-O3A-PA-O2A
3	A	1102	ATP	PA-O3A-PB-O2B

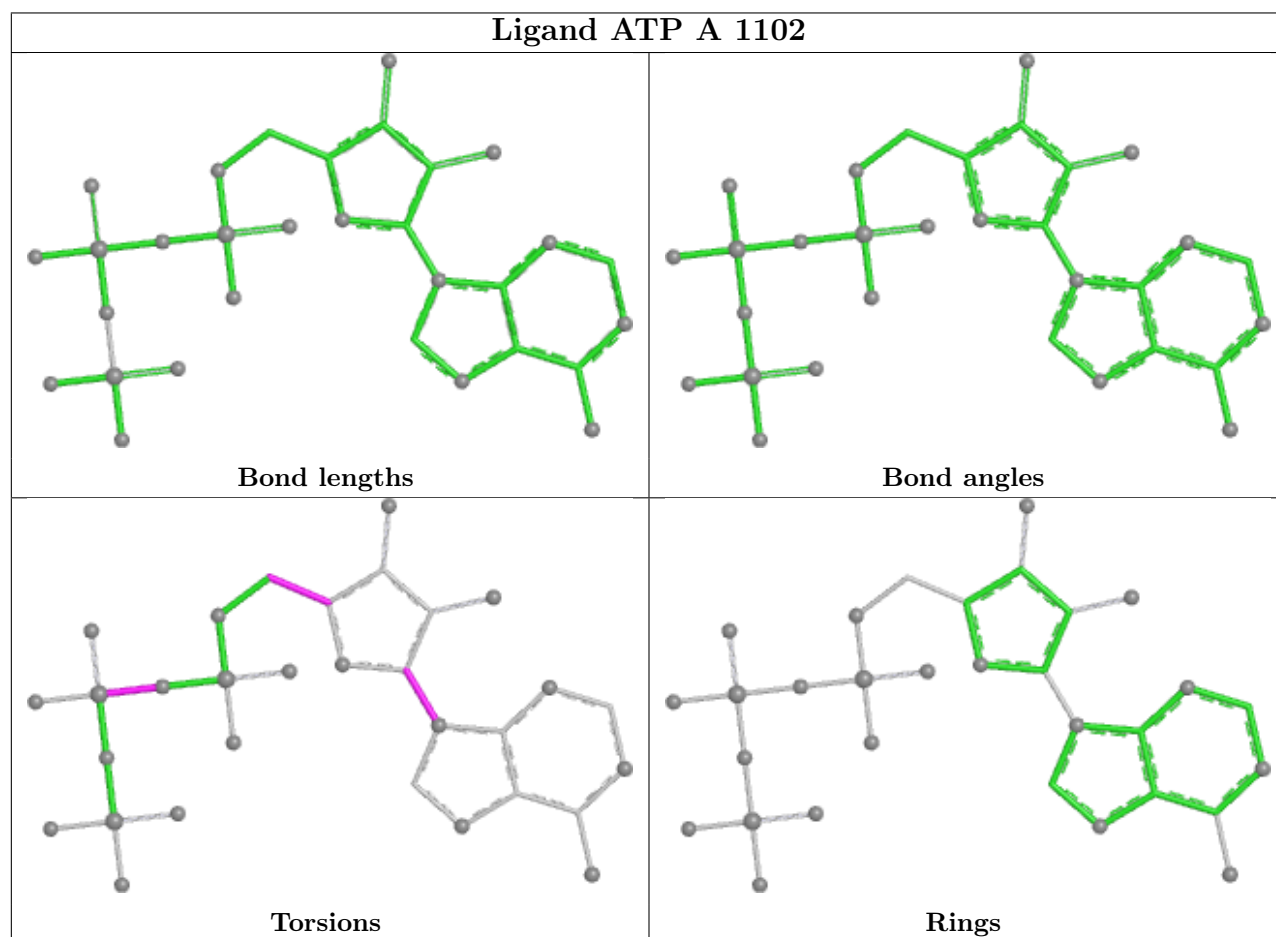
There are no ring outliers.

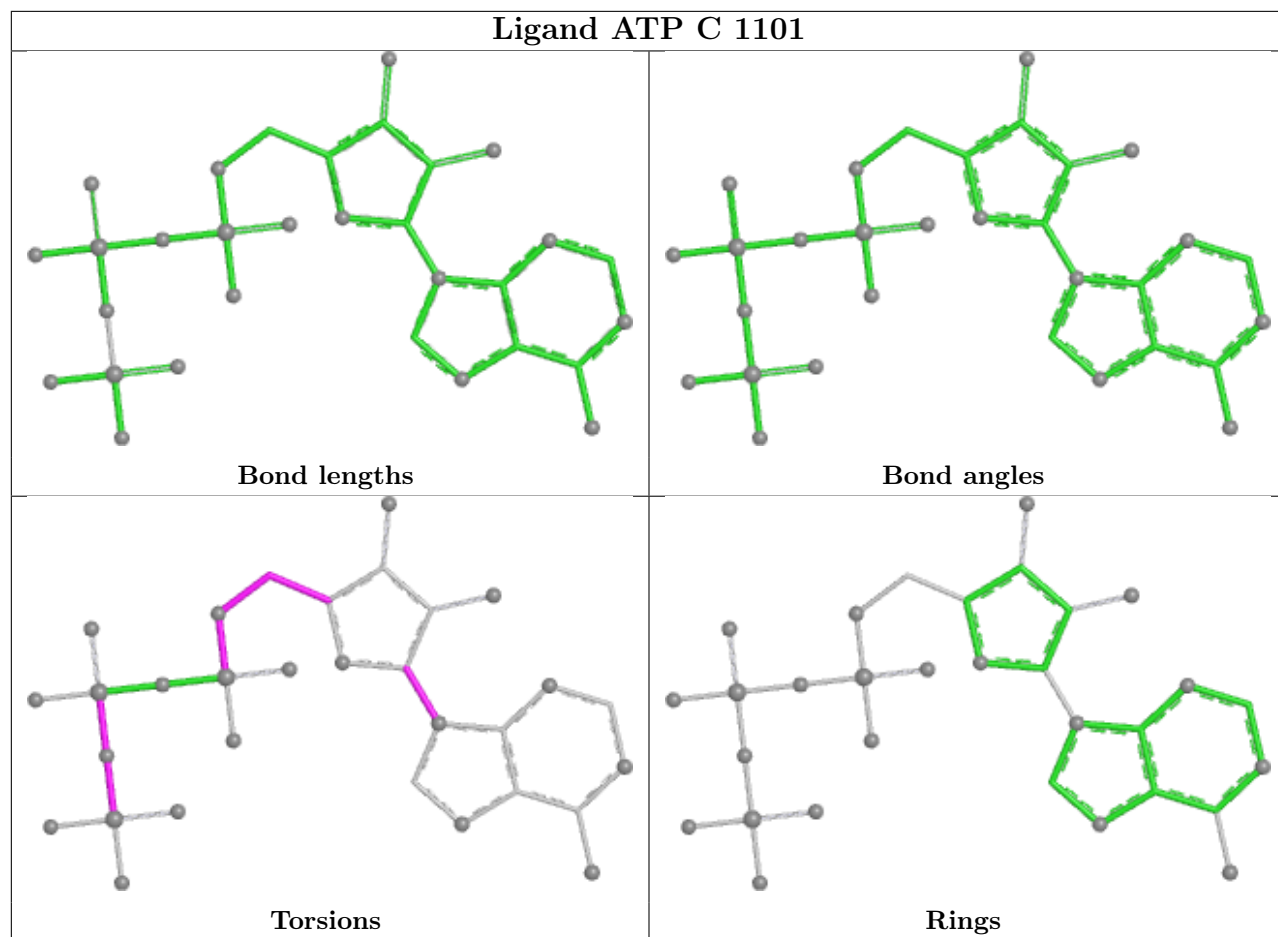
10 monomers are involved in 113 short contacts:

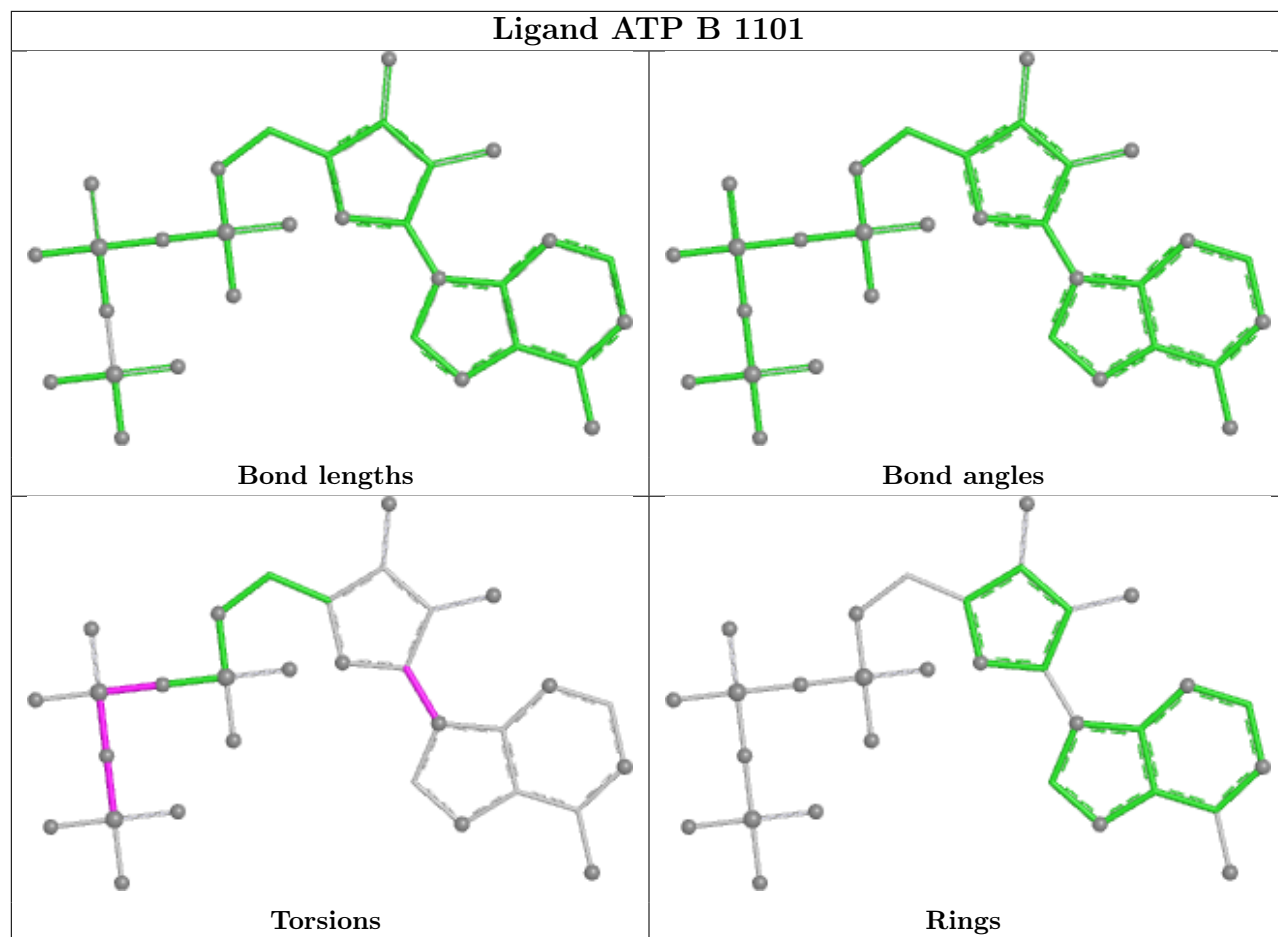
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	ATP	13	0
3	C	1101	ATP	13	0
3	B	1101	ATP	8	0
3	D	1602	ATP	7	0
3	A	1101	ATP	9	0
3	C	1102	ATP	20	0
3	F	1101	ATP	19	0
3	E	1101	ATP	9	0
3	B	1102	ATP	9	0
3	D	1601	ATP	6	0

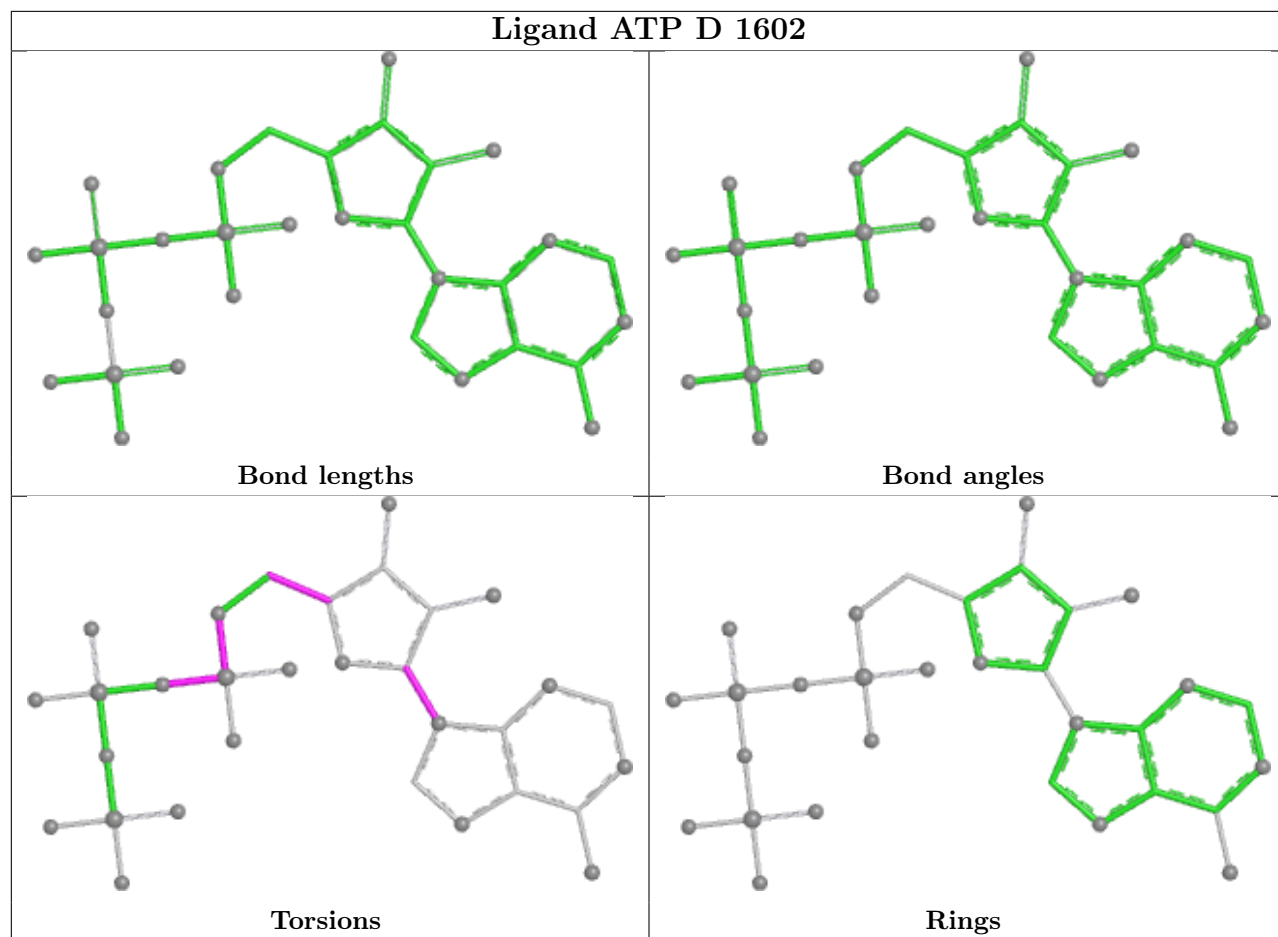
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

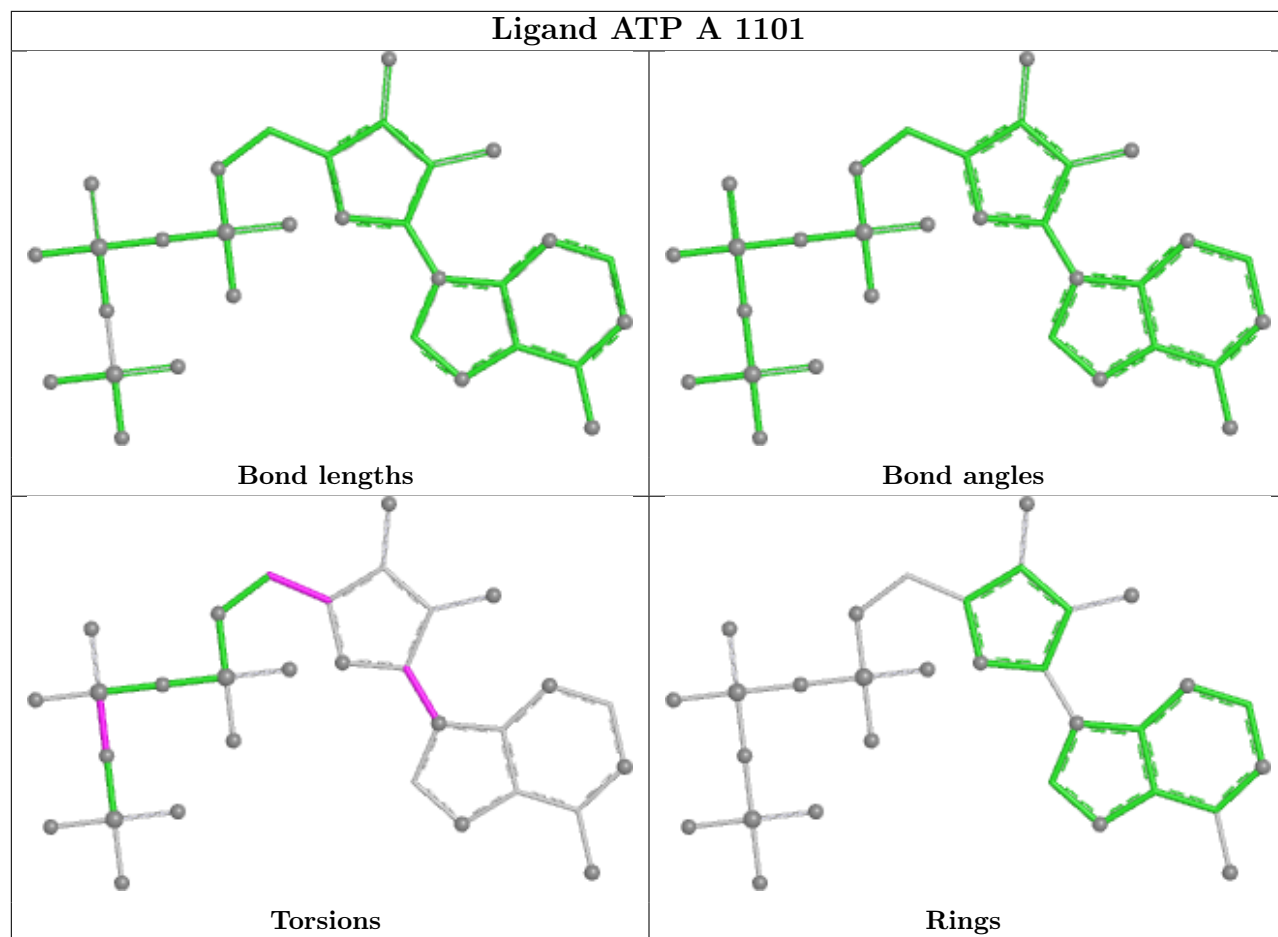
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

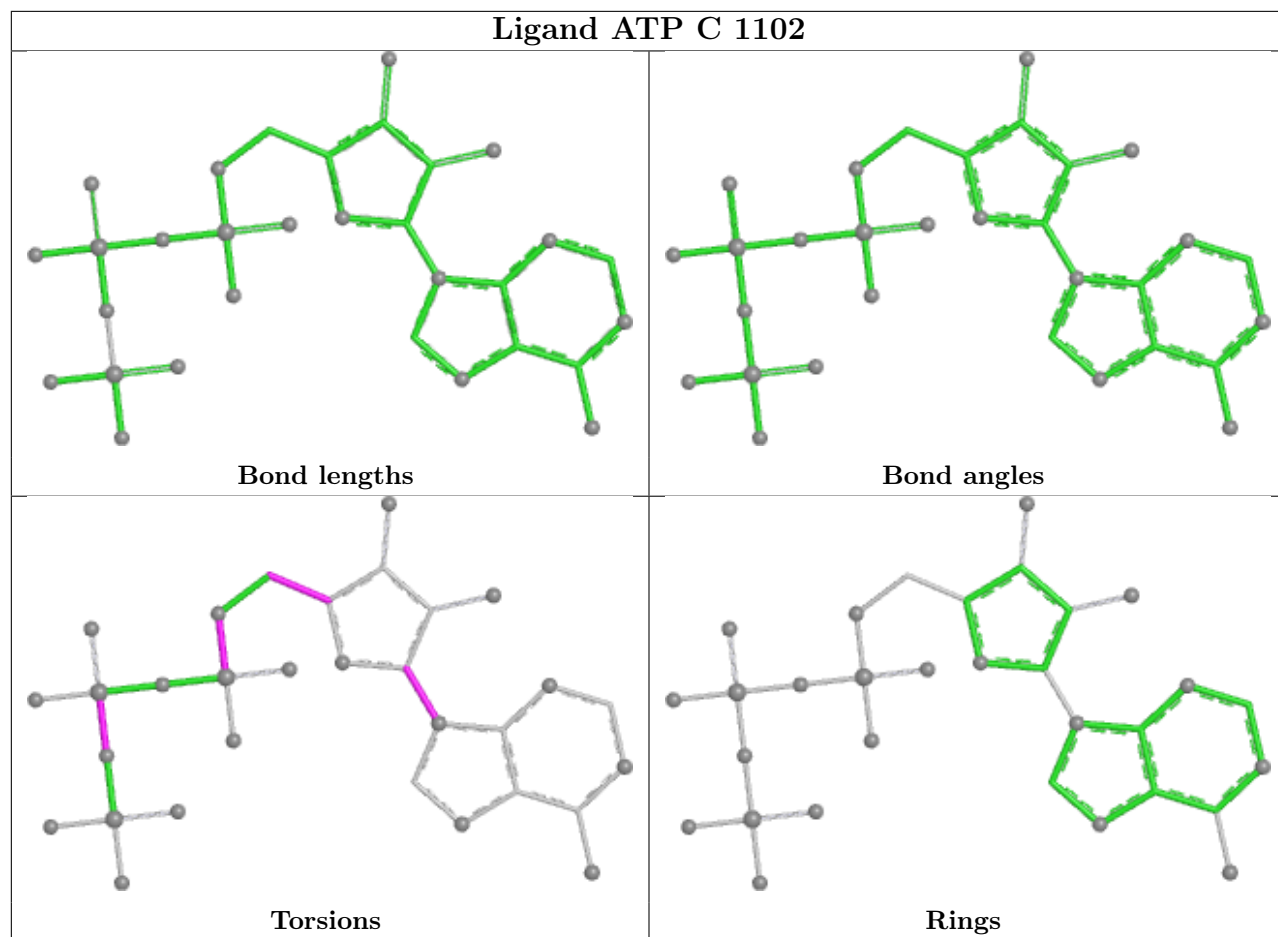


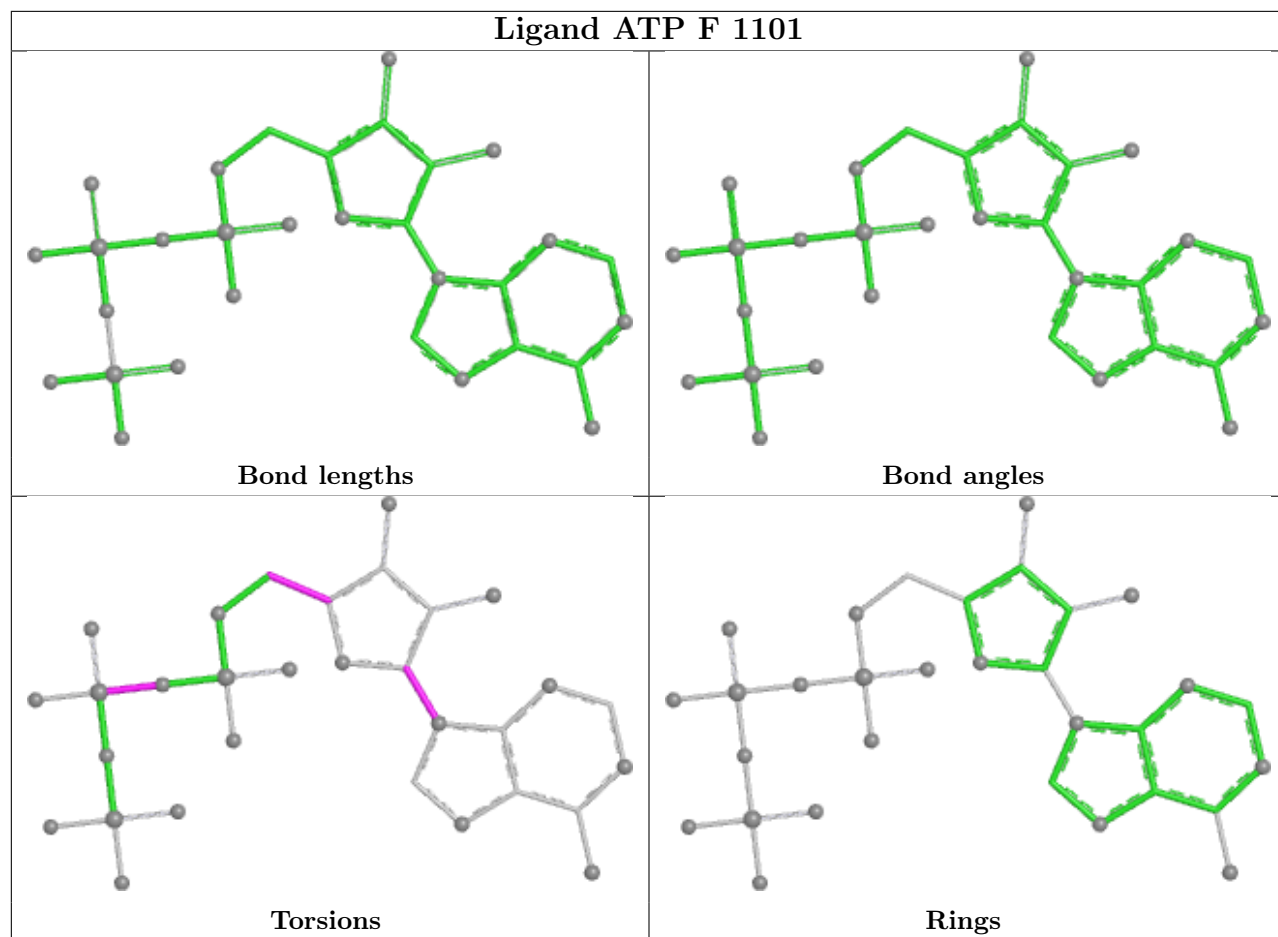


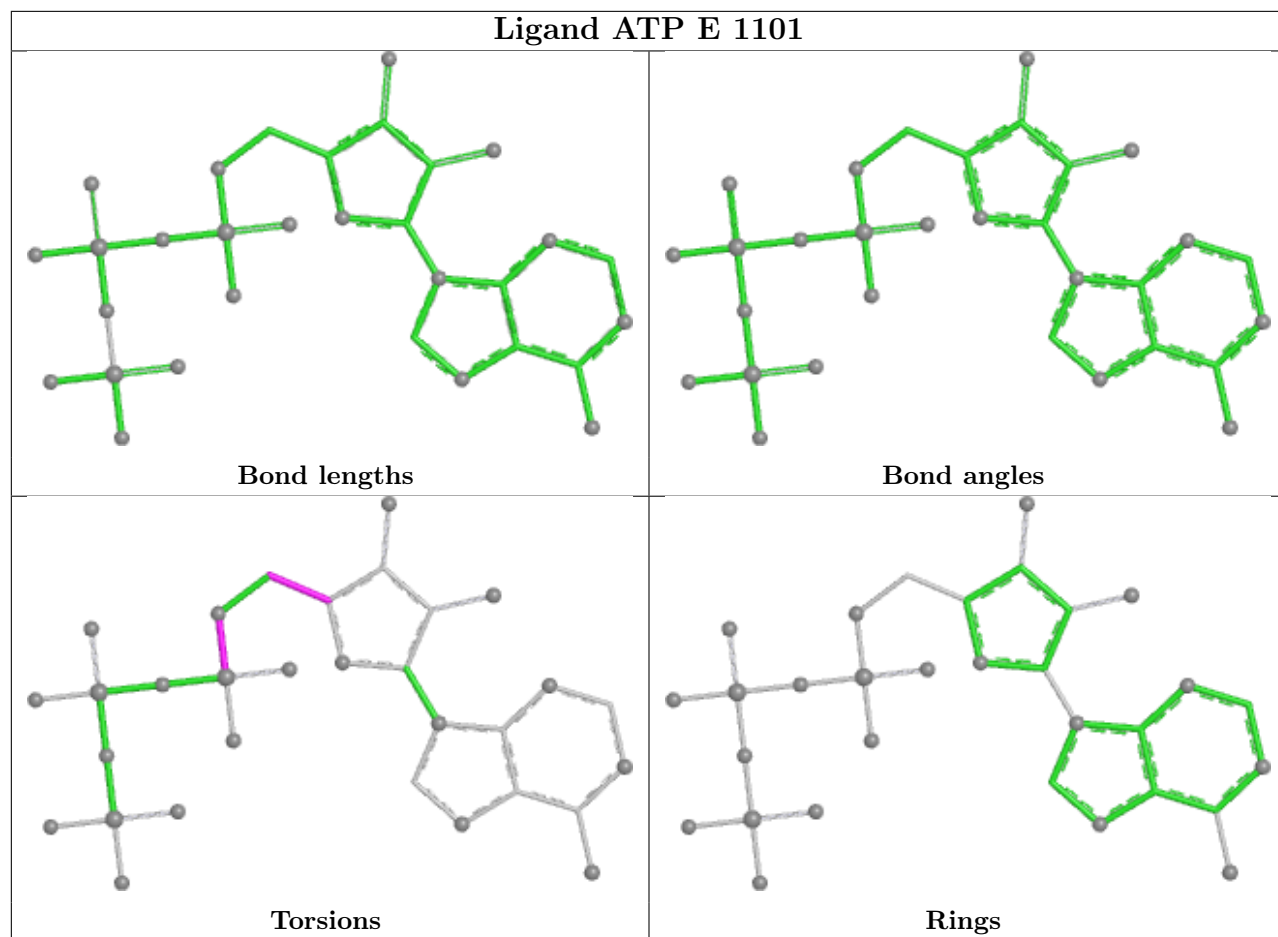


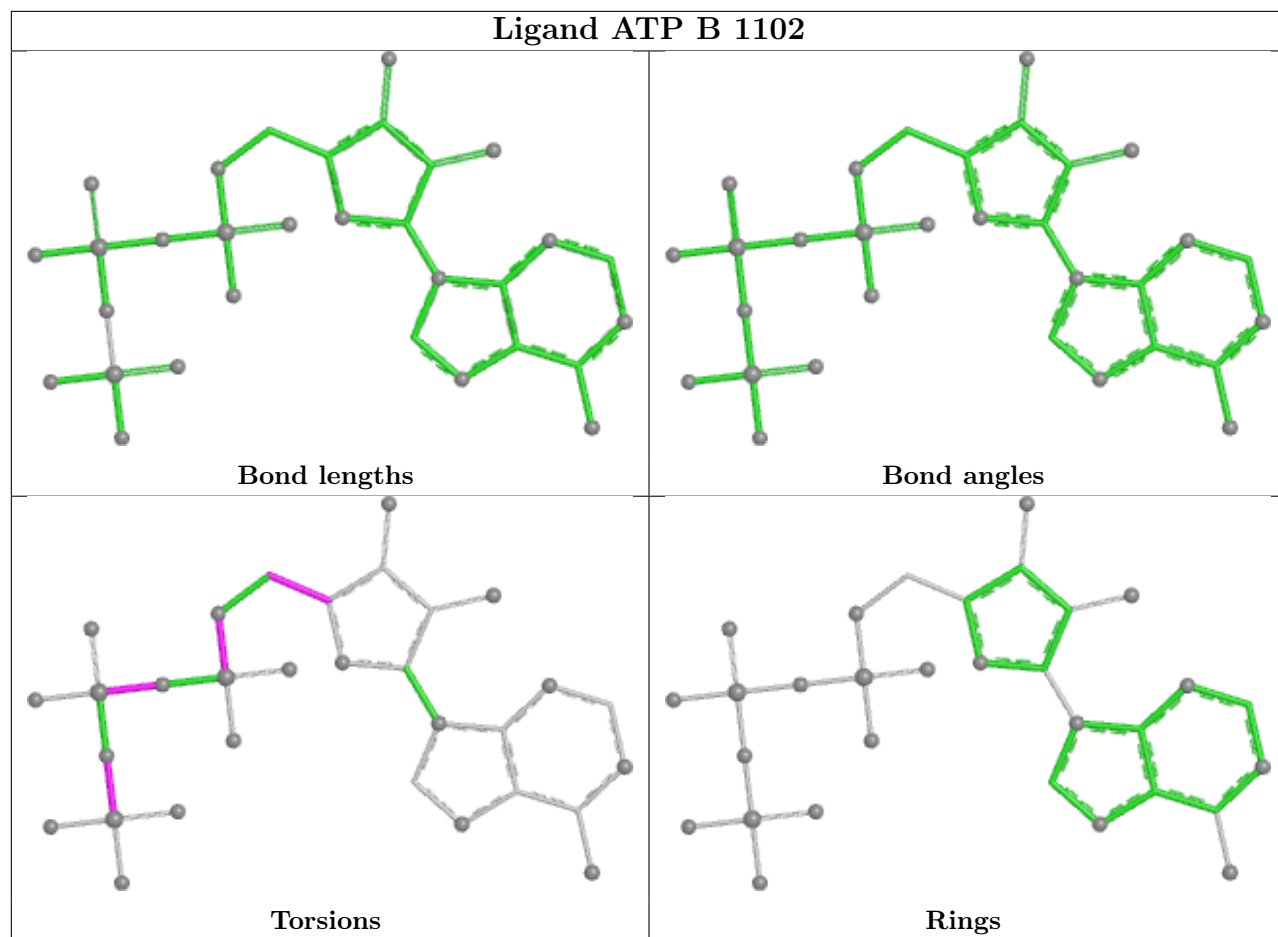


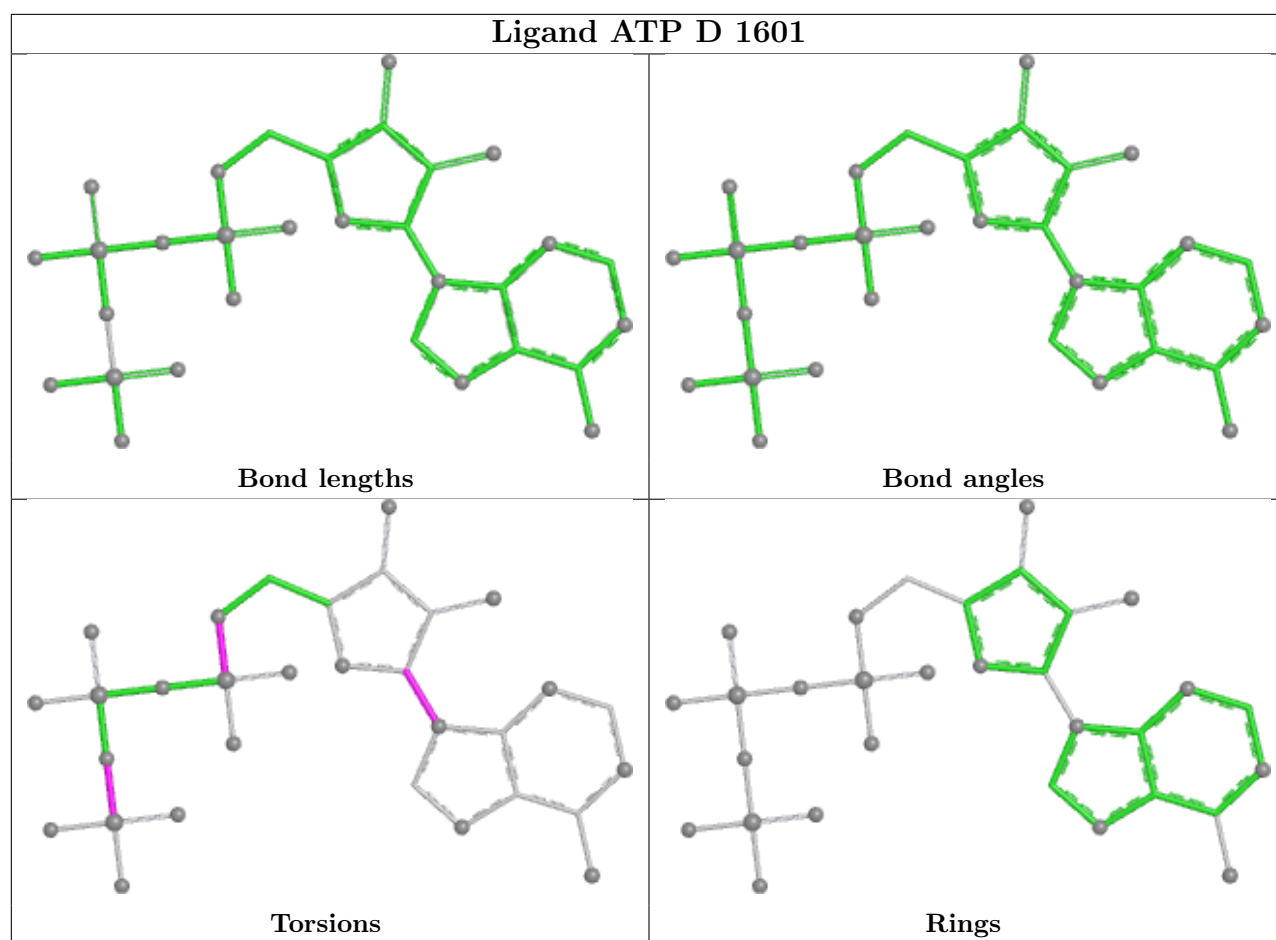












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

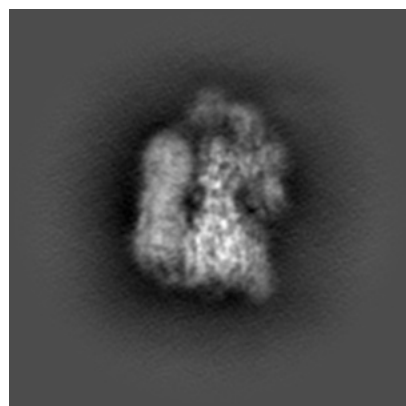
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41788. These allow visual inspection of the internal detail of the map and identification of artifacts.

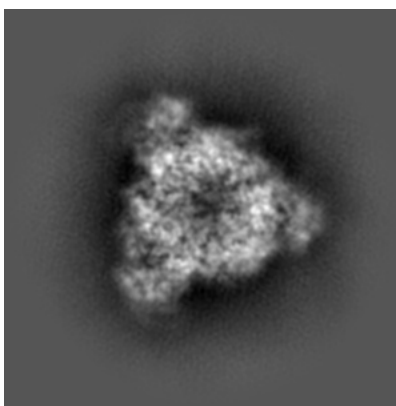
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

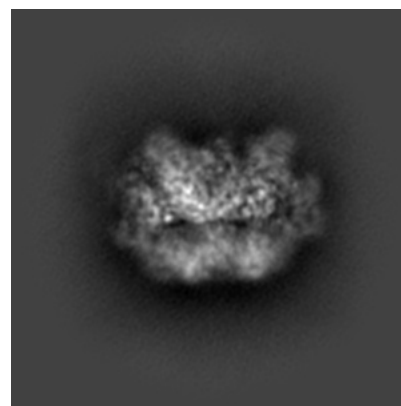
6.1.1 Primary map



X

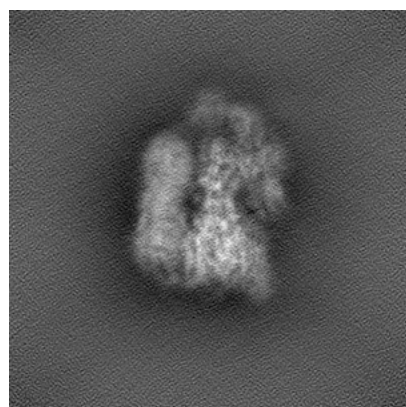


Y

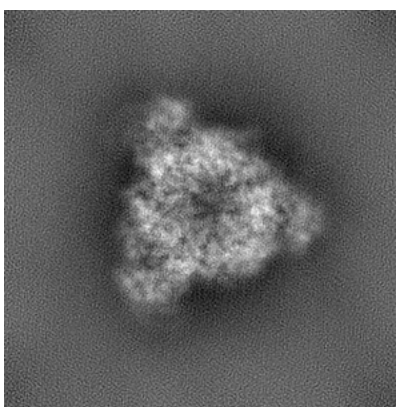


Z

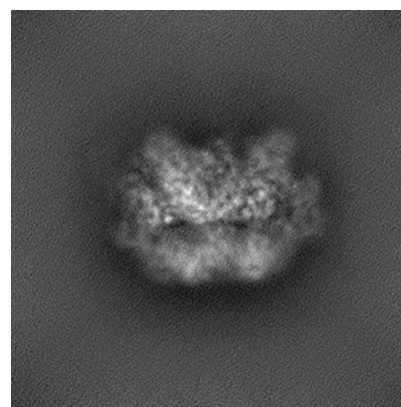
6.1.2 Raw map



X



Y

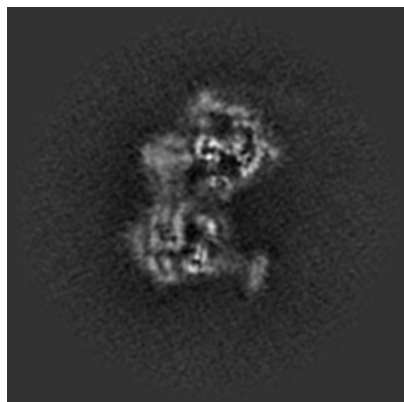


Z

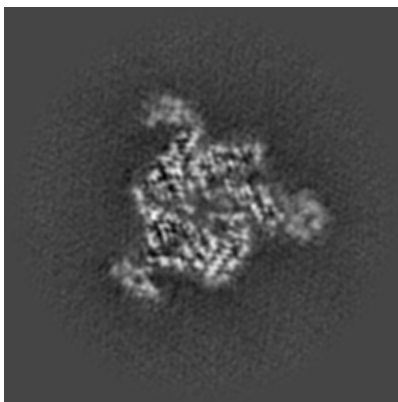
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

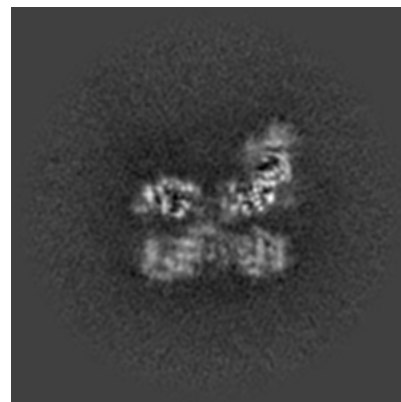
6.2.1 Primary map



X Index: 140

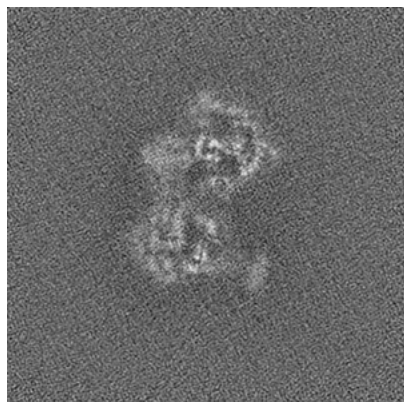


Y Index: 140

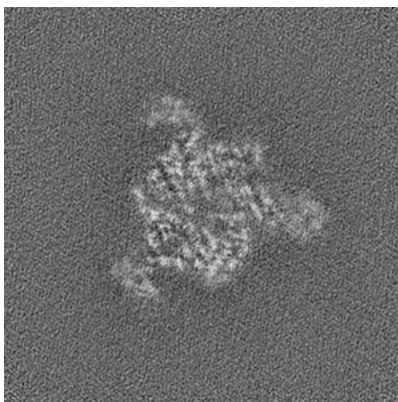


Z Index: 140

6.2.2 Raw map



X Index: 140



Y Index: 140

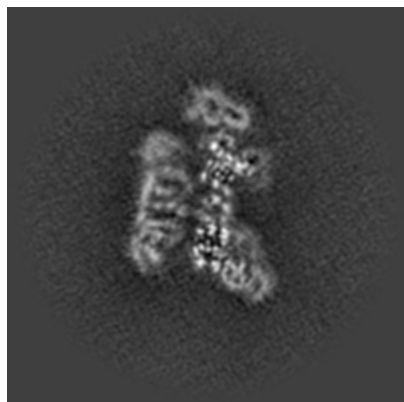


Z Index: 140

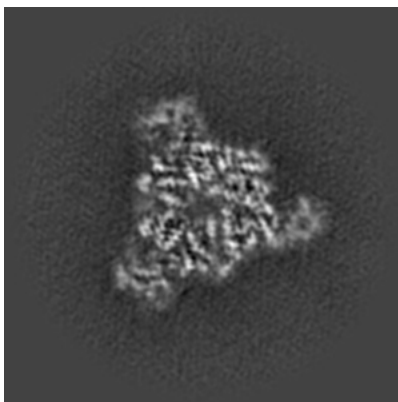
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

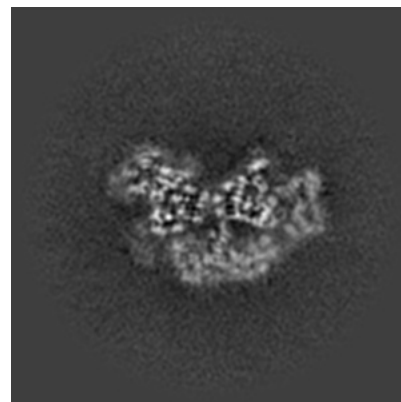
6.3.1 Primary map



X Index: 125

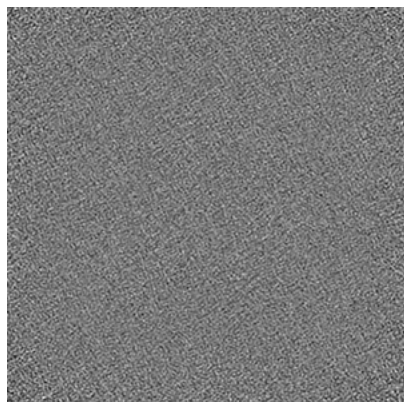


Y Index: 146

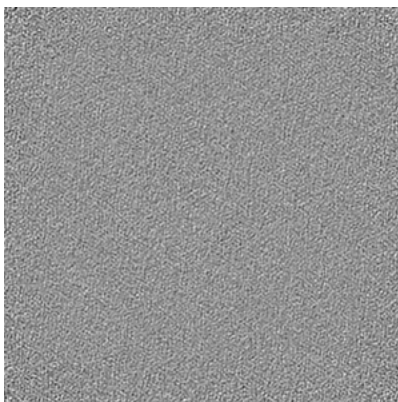


Z Index: 117

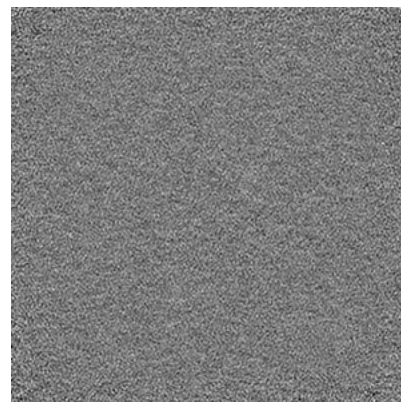
6.3.2 Raw map



X Index: 0



Y Index: 0

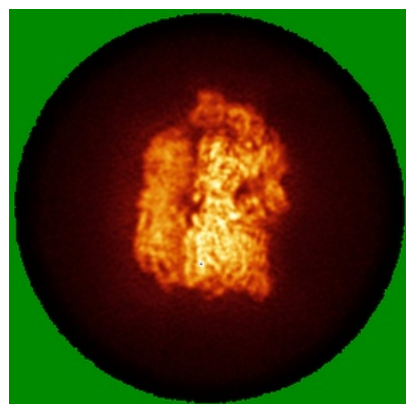


Z Index: 0

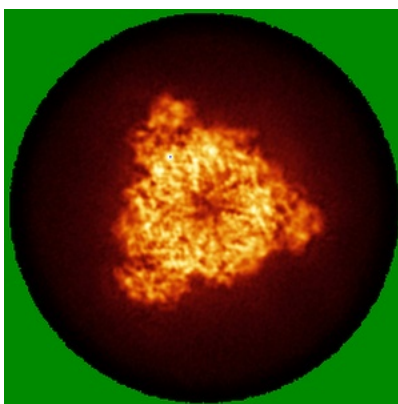
The images above show the largest variance slices of the map in three orthogonal directions.

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

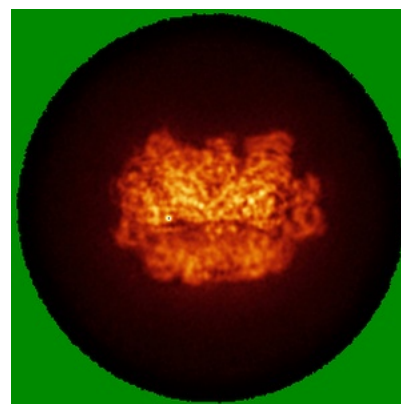
6.4.1 Primary map



X

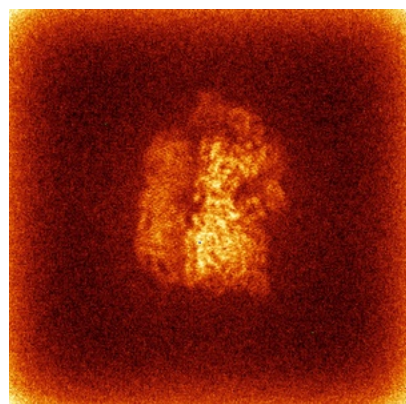


Y

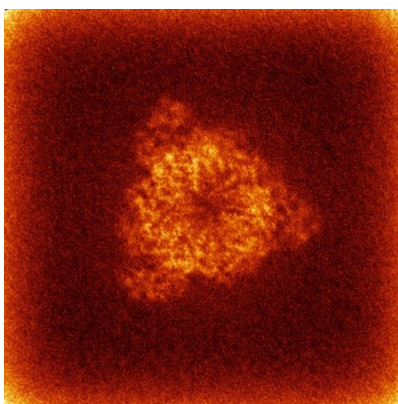


Z

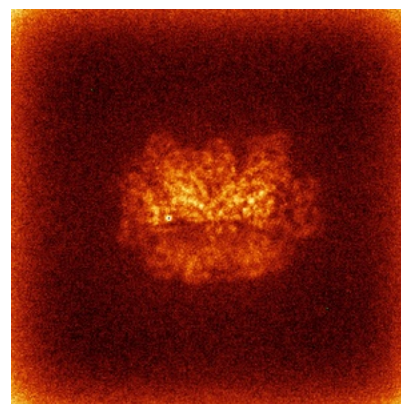
6.4.2 Raw map



X



Y



Z

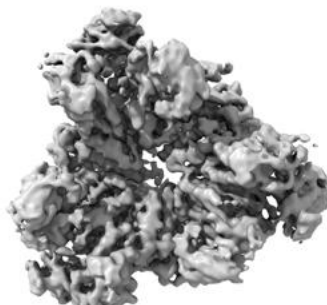
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

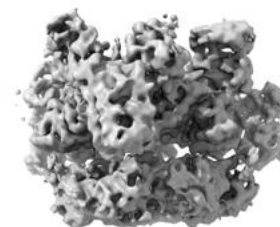
6.5.1 Primary map



X



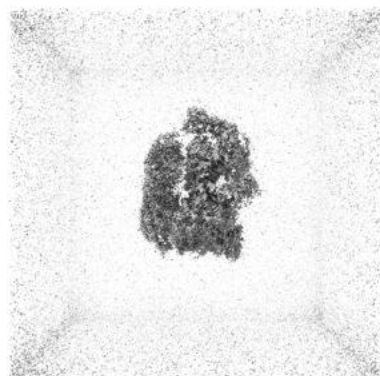
Y



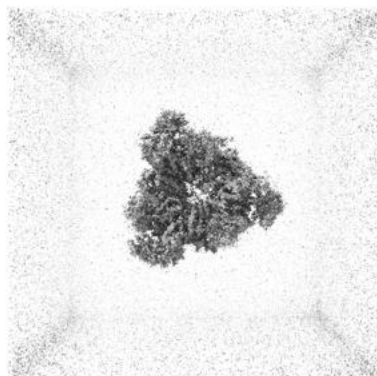
Z

The images above show the 3D surface view of the map at the recommended contour level 0.107. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

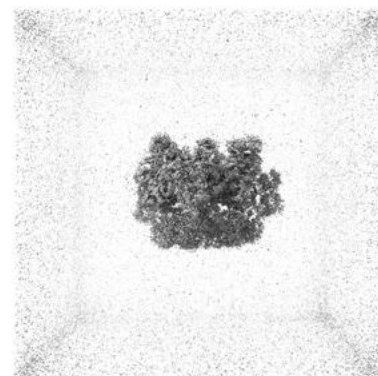
6.5.2 Raw map



X



Y



Z

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

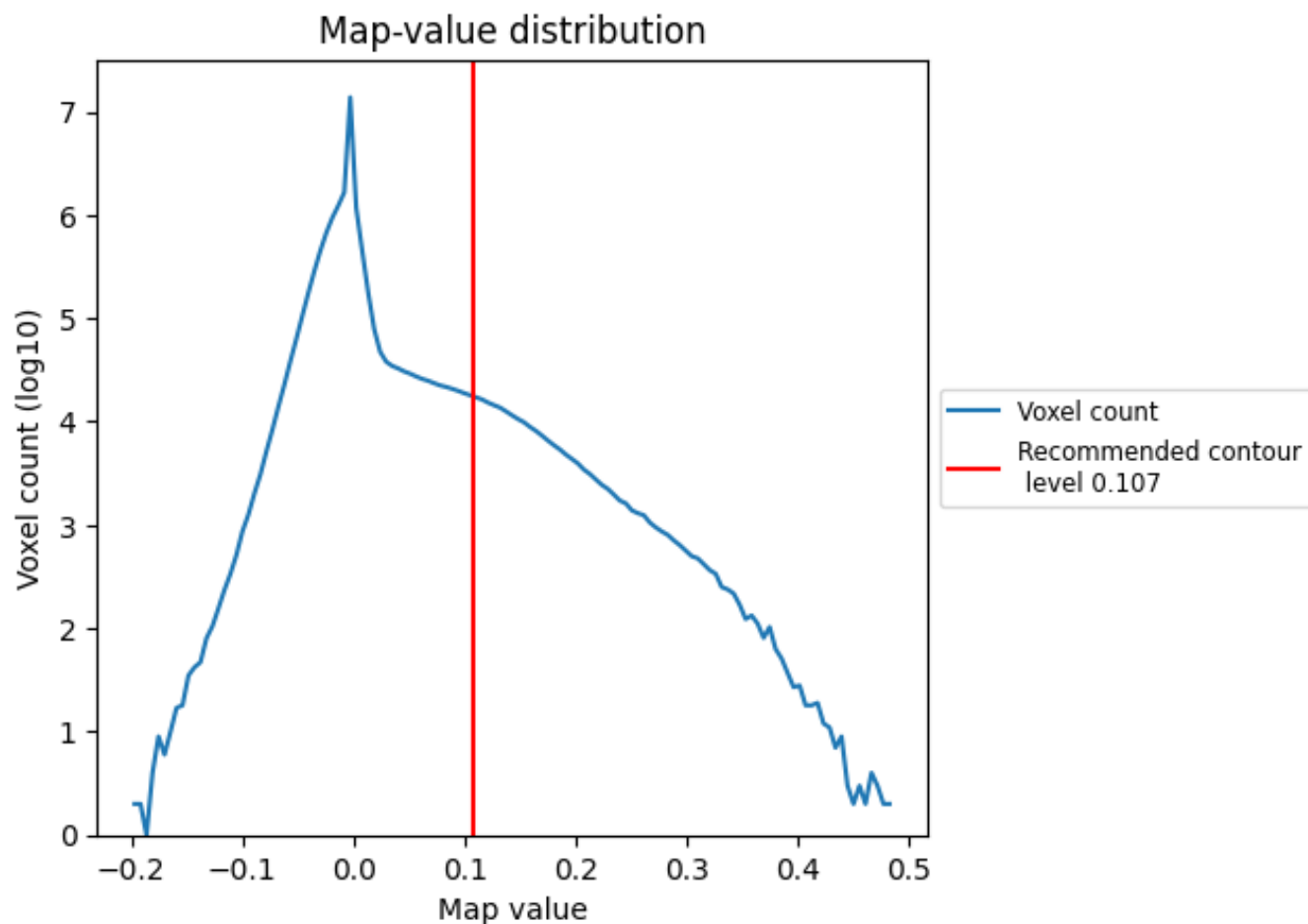
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

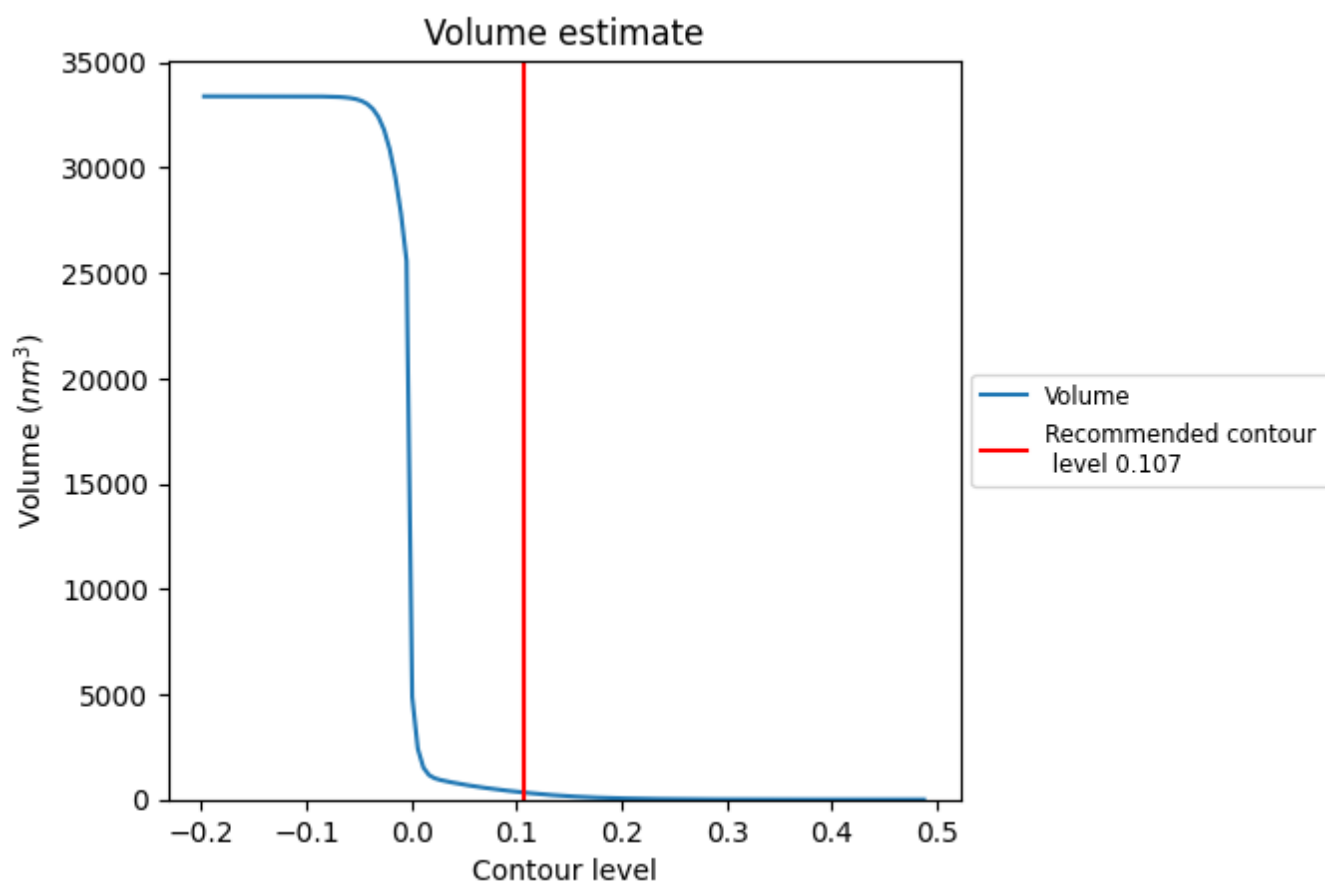
This section contains the results of statistical analysis of the map.

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.

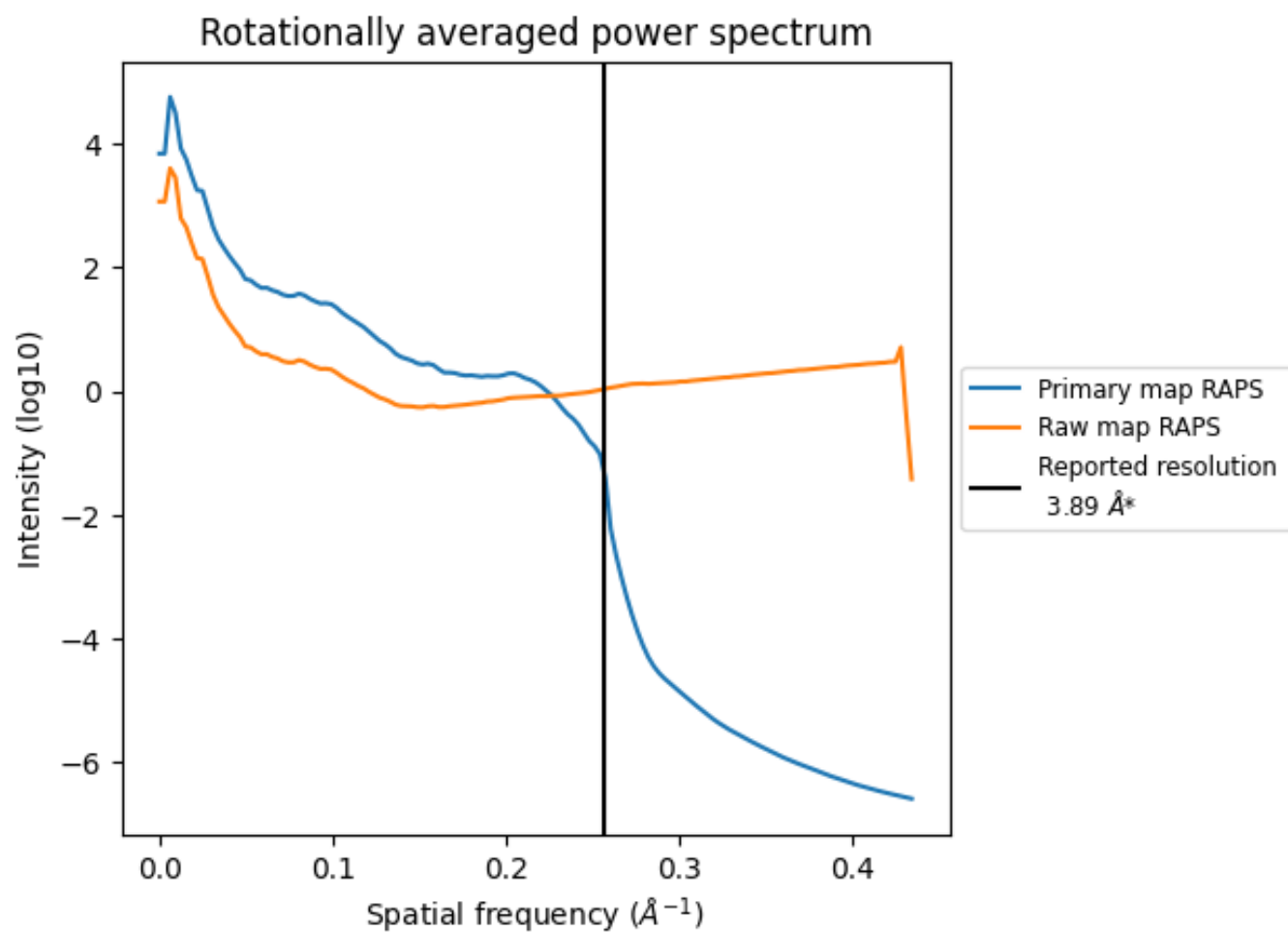
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 335 nm³; this corresponds to an approximate mass of 303 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 ⓘ

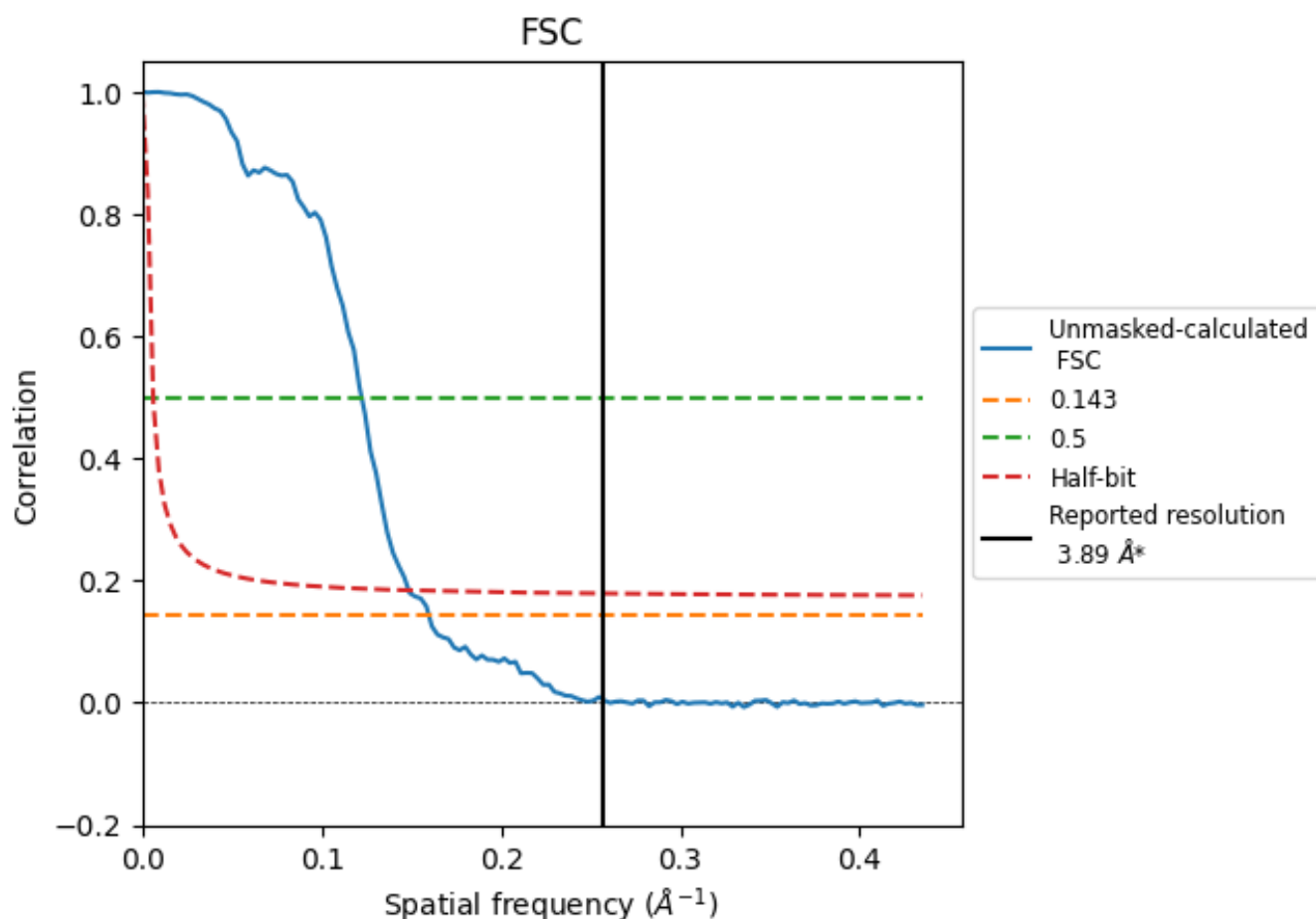


*Reported resolution corresponds to spatial frequency of 0.257 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.257 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

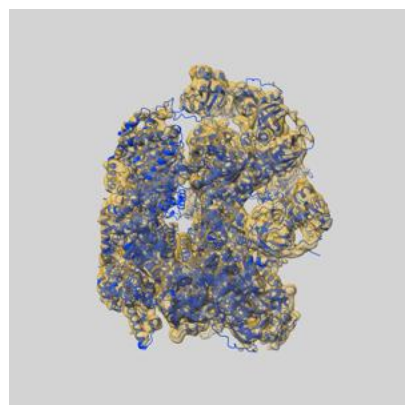
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.26	8.18	6.73

*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 6.26 differs from the reported value 3.89 by more than 10 %

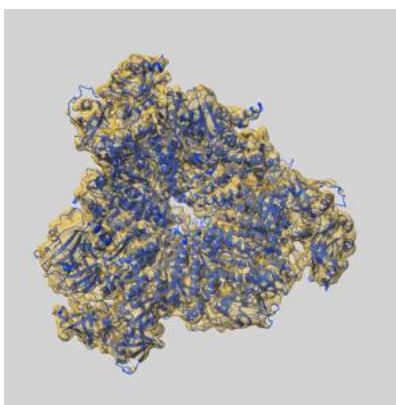
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41788 and PDB model 8U0V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

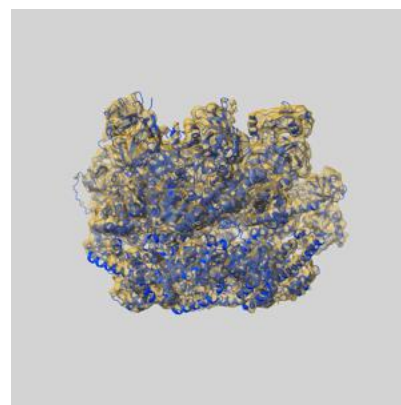
9.1 Map-model overlay [i](#)



X



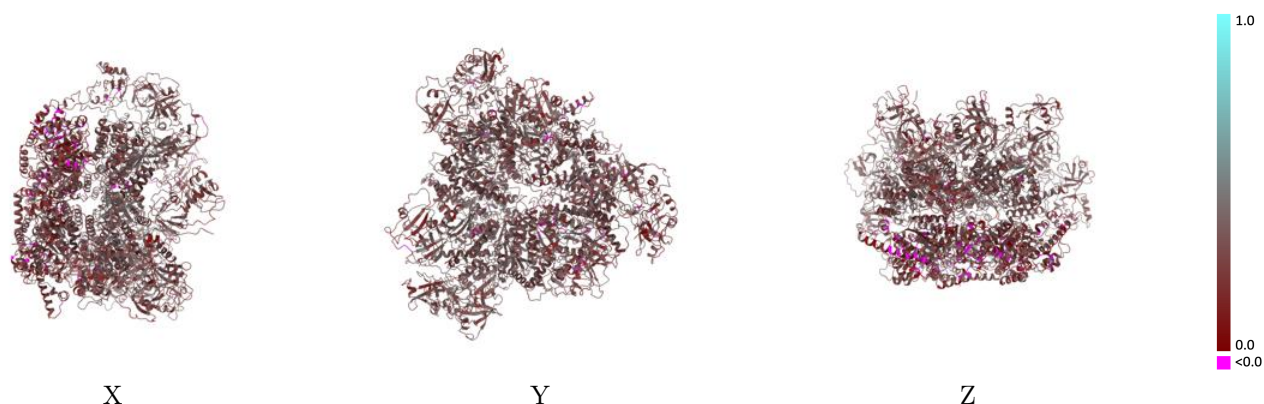
Y



Z

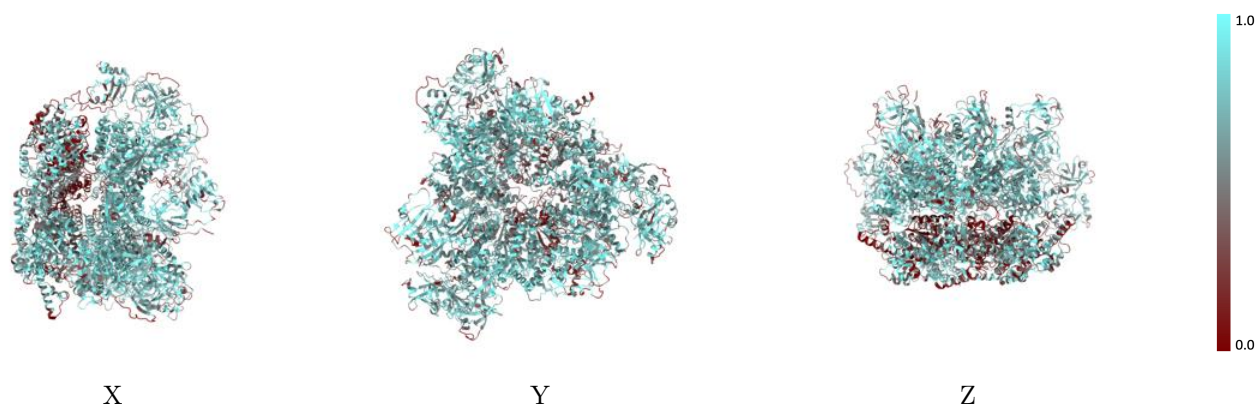
The images above show the 3D surface view of the map at the recommended contour level 0.107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



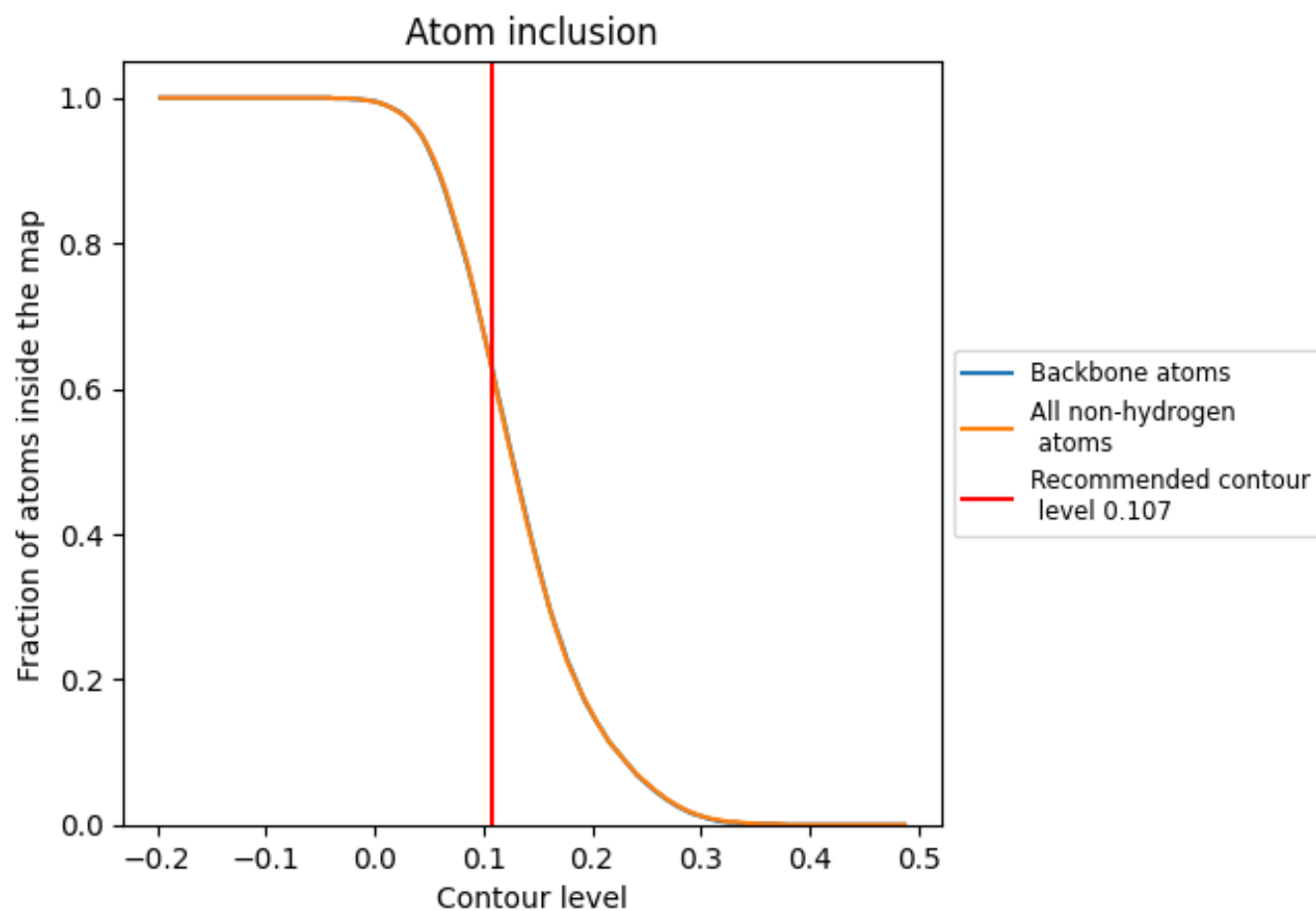
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.107).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (0.107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6330	0.2930
A	0.6040	0.2900
B	0.6750	0.3150
C	0.6430	0.3060
D	0.6530	0.2950
E	0.5930	0.2830
F	0.6170	0.2700

1.0

0.0

<0.0