



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:05 AM UTC

PDB ID : 8HR7 / pdb_00008hr7
EMDB ID : EMD-34962
Title : Structure of RdrA-RdrB complex
Authors : Gao, Y.
Deposited on : 2022-12-15
Resolution : 3.96 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

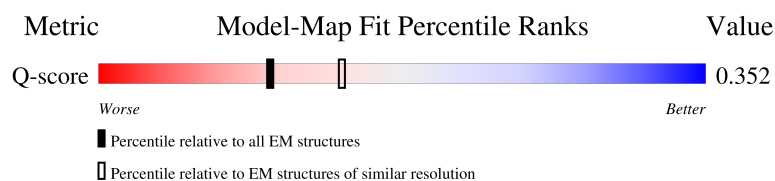
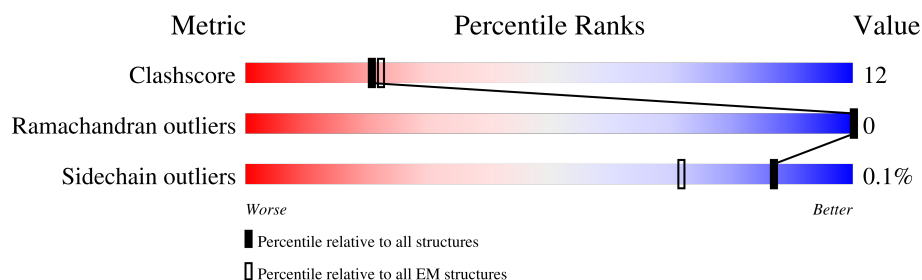
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.96 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	7646 (3.46 - 4.46)

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	947	11% 62% 26% 12%
1	O	947	11% 60% 28% 12%
1	P	947	8% 62% 26% 12%
1	Q	947	9% 63% 26% 12%

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Mol	Chain	Length	Quality of chain
1	R	947	
1	S	947	
1	T	947	
2	B	799	
2	C	799	
2	D	799	
2	E	799	
2	F	799	
2	G	799	
2	I	799	
2	J	799	
2	K	799	
2	L	799	
2	M	799	
2	N	799	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 121662 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Archaeal ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	O	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	P	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	Q	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	R	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	S	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0
1	T	834	Total 6657	C 4220	N 1148	O 1258	S 31	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	636	ARG	LEU	conflict	UNP A0A8H9B1T2
A	940	LEU	SER	conflict	UNP A0A8H9B1T2
O	636	ARG	LEU	conflict	UNP A0A8H9B1T2
O	940	LEU	SER	conflict	UNP A0A8H9B1T2
P	636	ARG	LEU	conflict	UNP A0A8H9B1T2
P	940	LEU	SER	conflict	UNP A0A8H9B1T2
Q	636	ARG	LEU	conflict	UNP A0A8H9B1T2
Q	940	LEU	SER	conflict	UNP A0A8H9B1T2
R	636	ARG	LEU	conflict	UNP A0A8H9B1T2
R	940	LEU	SER	conflict	UNP A0A8H9B1T2
S	636	ARG	LEU	conflict	UNP A0A8H9B1T2
S	940	LEU	SER	conflict	UNP A0A8H9B1T2
T	636	ARG	LEU	conflict	UNP A0A8H9B1T2
T	940	LEU	SER	conflict	UNP A0A8H9B1T2

- Molecule 2 is a protein called Adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	C	774	Total	C	N	O	S	0	0
			6244	3999	1087	1126	32		
2	D	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	E	770	Total	C	N	O	S	0	0
			6217	3983	1080	1122	32		
2	F	775	Total	C	N	O	S	0	0
			6239	3997	1085	1125	32		
2	G	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	I	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	J	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	K	779	Total	C	N	O	S	0	0
			6273	4021	1089	1131	32		
2	L	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		
2	M	786	Total	C	N	O	S	0	0
			6361	4073	1102	1154	32		
2	N	776	Total	C	N	O	S	0	0
			6247	4001	1086	1128	32		

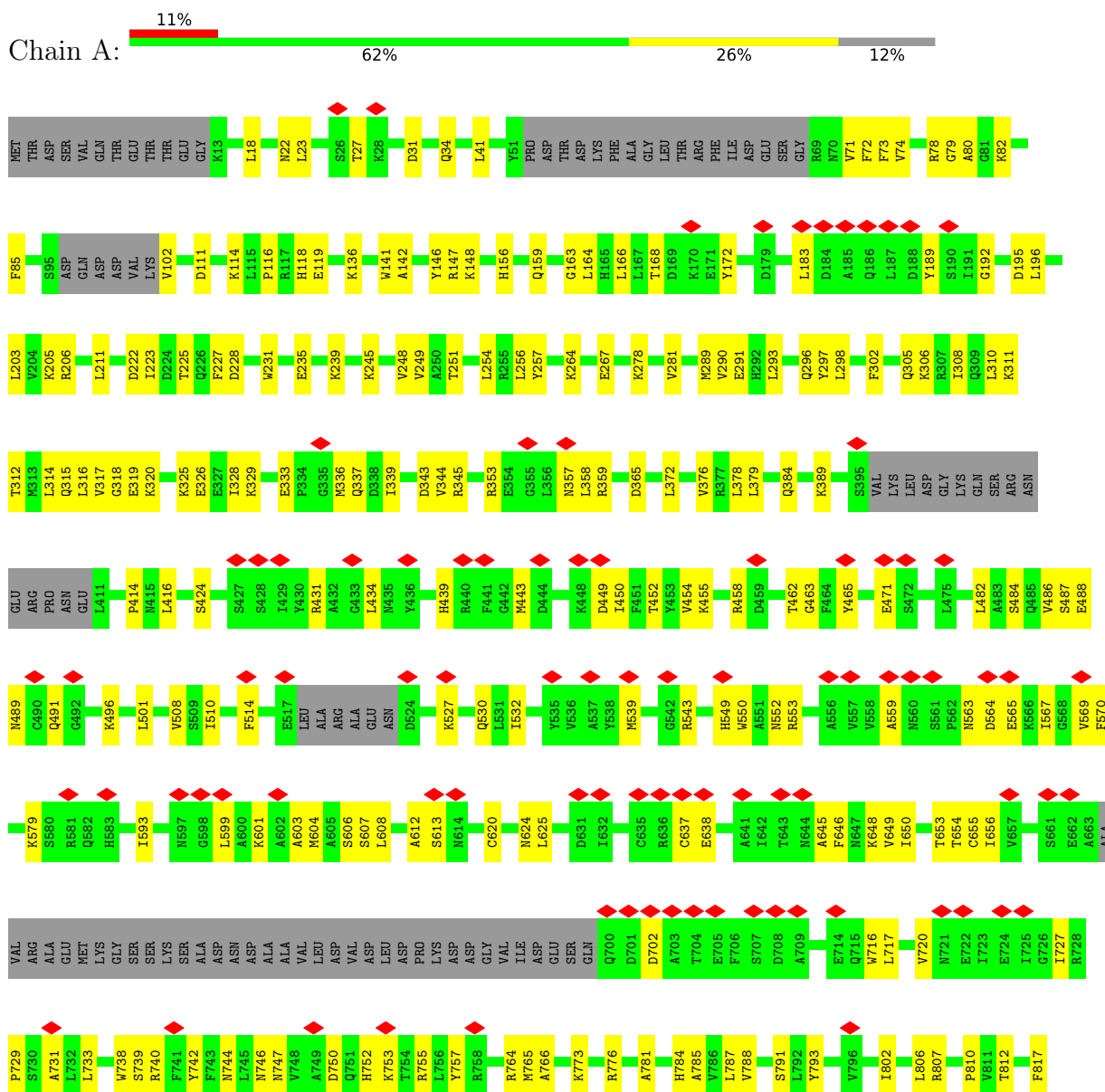
There are 12 discrepancies between the modelled and reference sequences:

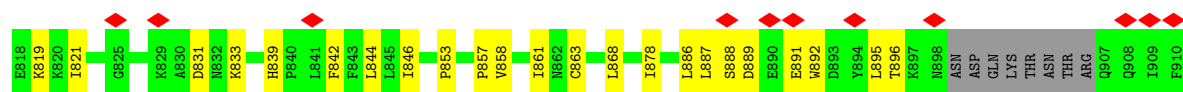
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	THR	ILE	conflict	UNP A0A8E2SFD7
C	274	THR	ILE	conflict	UNP A0A8E2SFD7
D	274	THR	ILE	conflict	UNP A0A8E2SFD7
E	274	THR	ILE	conflict	UNP A0A8E2SFD7
F	274	THR	ILE	conflict	UNP A0A8E2SFD7
G	274	THR	ILE	conflict	UNP A0A8E2SFD7
I	274	THR	ILE	conflict	UNP A0A8E2SFD7
J	274	THR	ILE	conflict	UNP A0A8E2SFD7
K	274	THR	ILE	conflict	UNP A0A8E2SFD7
L	274	THR	ILE	conflict	UNP A0A8E2SFD7
M	274	THR	ILE	conflict	UNP A0A8E2SFD7
N	274	THR	ILE	conflict	UNP A0A8E2SFD7

3 Residue-property plots

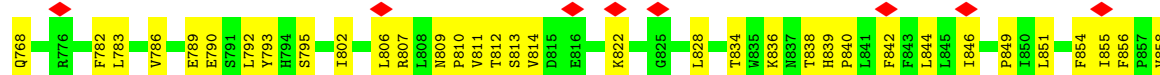
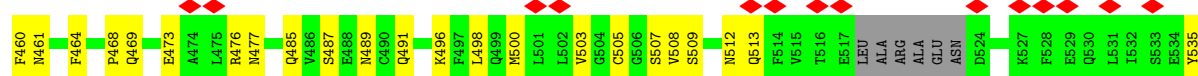
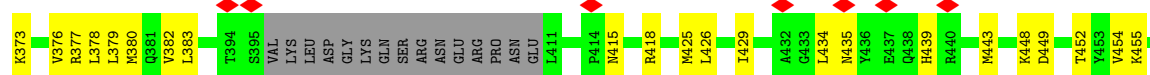
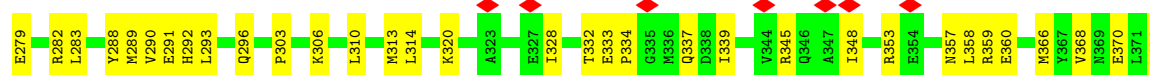
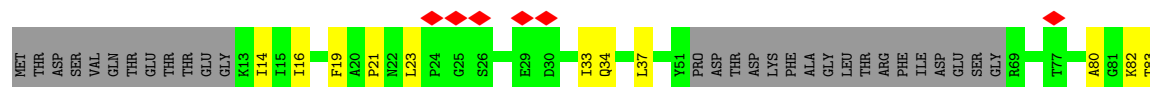
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

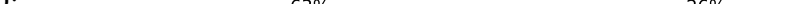
• Molecule 1: Archaeal ATPase



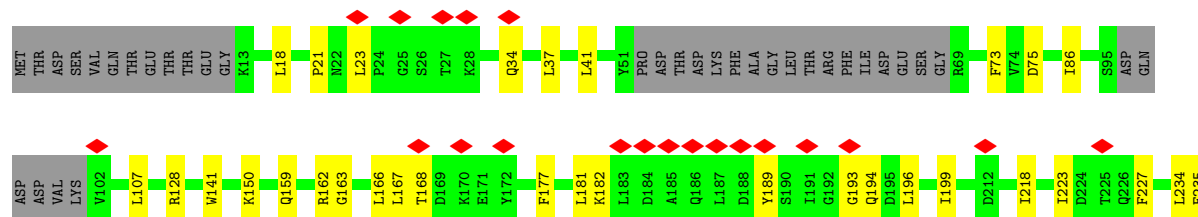


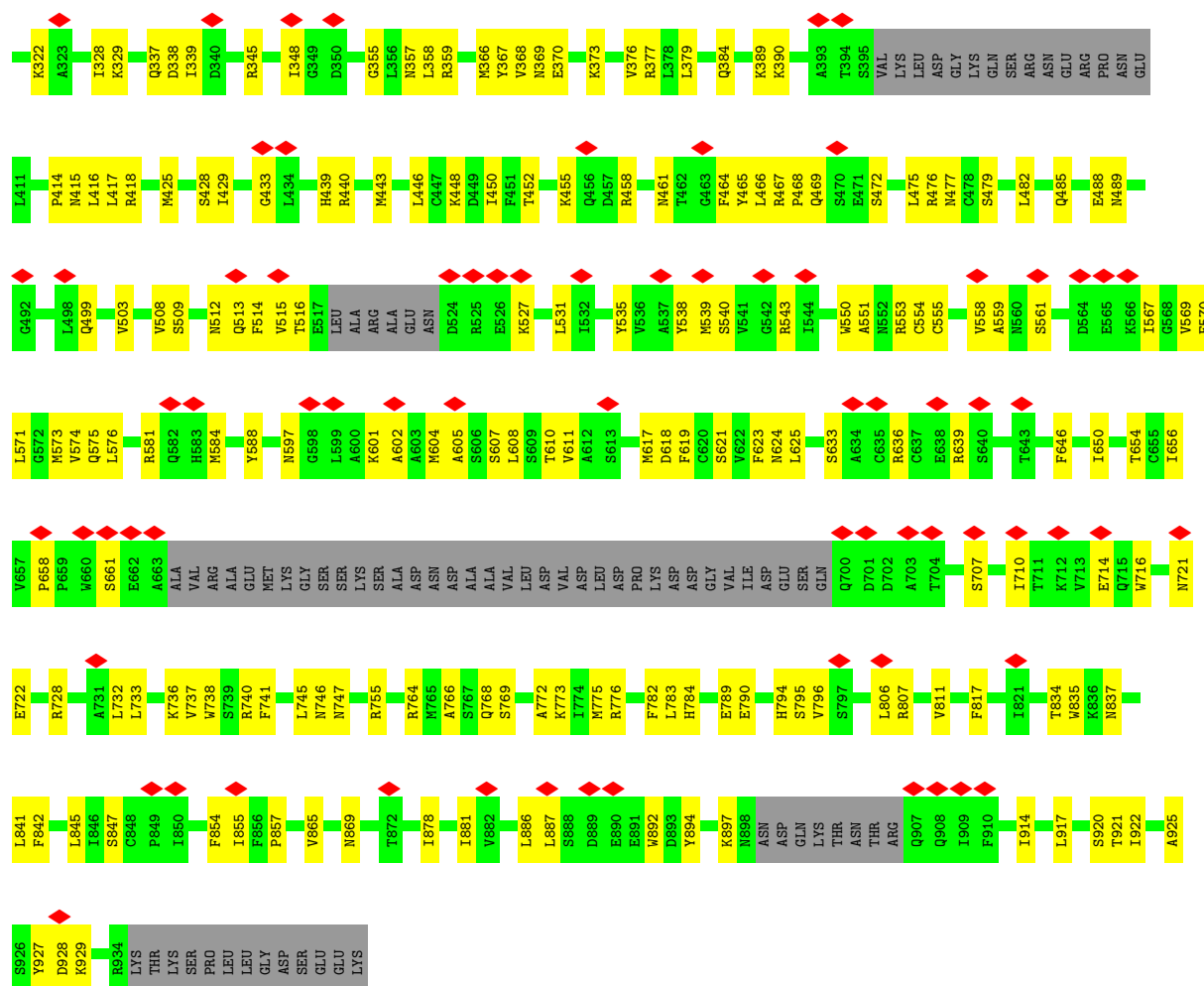
• Molecule 1: Archaeal ATPase



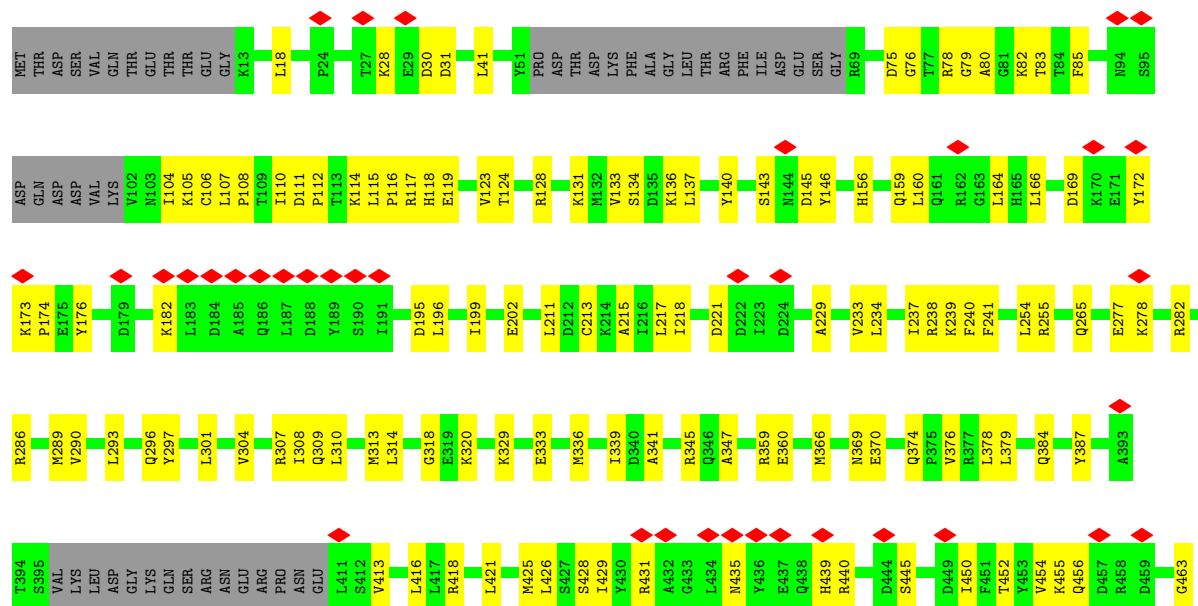
Chain Q: 

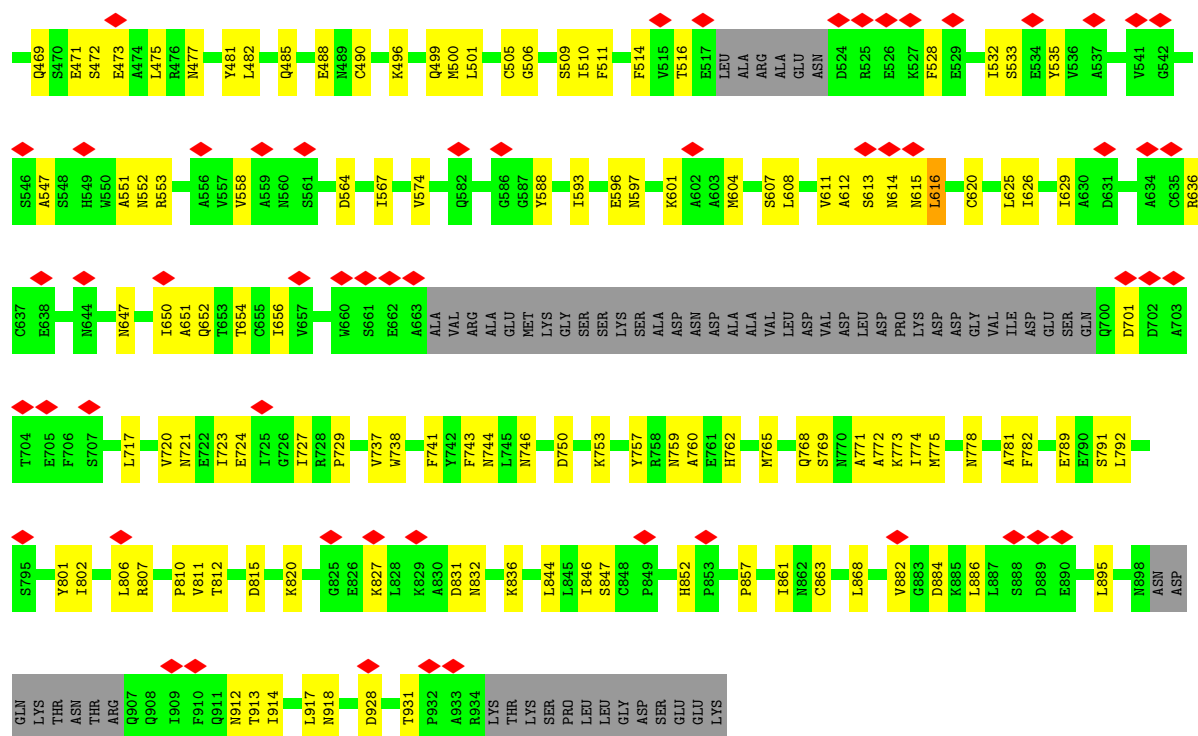
- Molecule 1: Archaeal ATPase





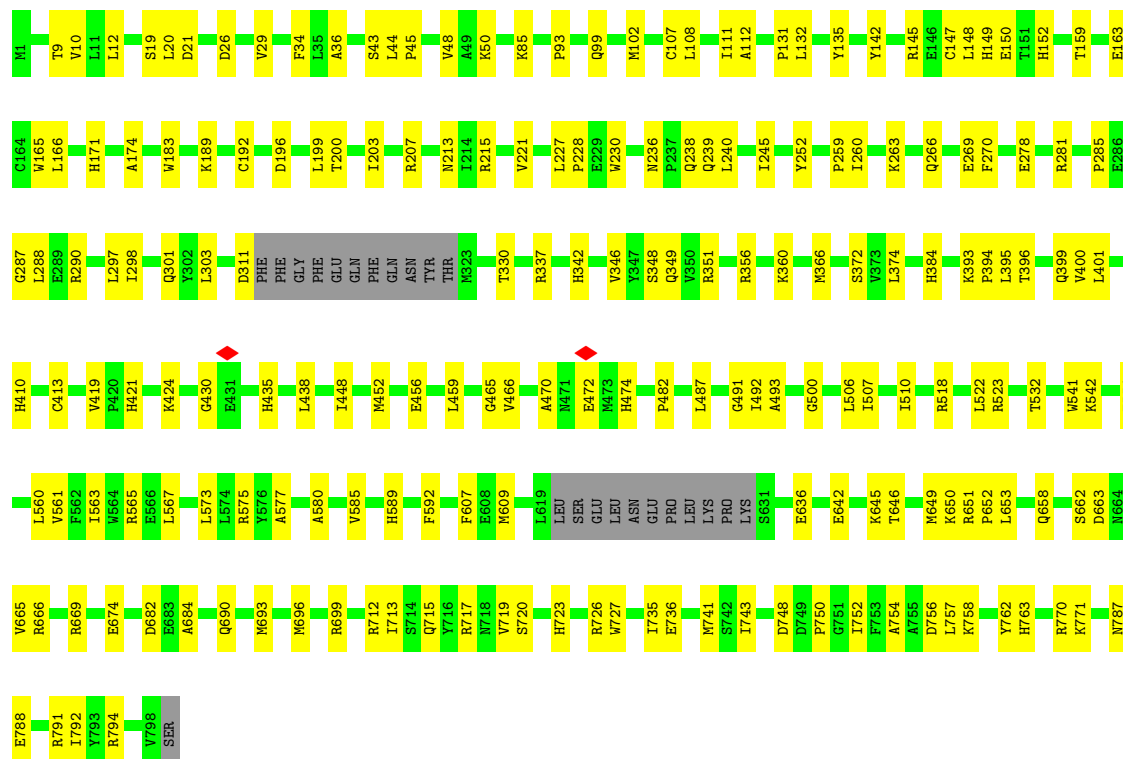
● Molecule 1: Archaeal ATPase



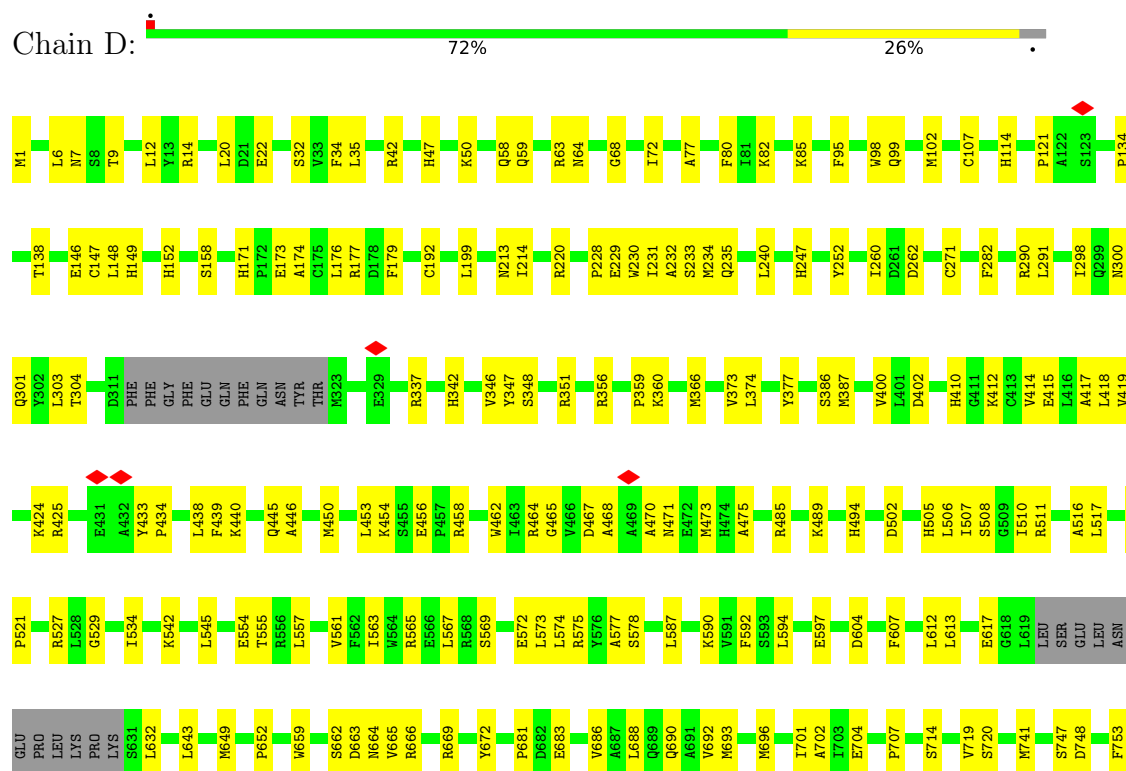


• Molecule 2: Adenosine deaminase

Chain B: 73% 24% .

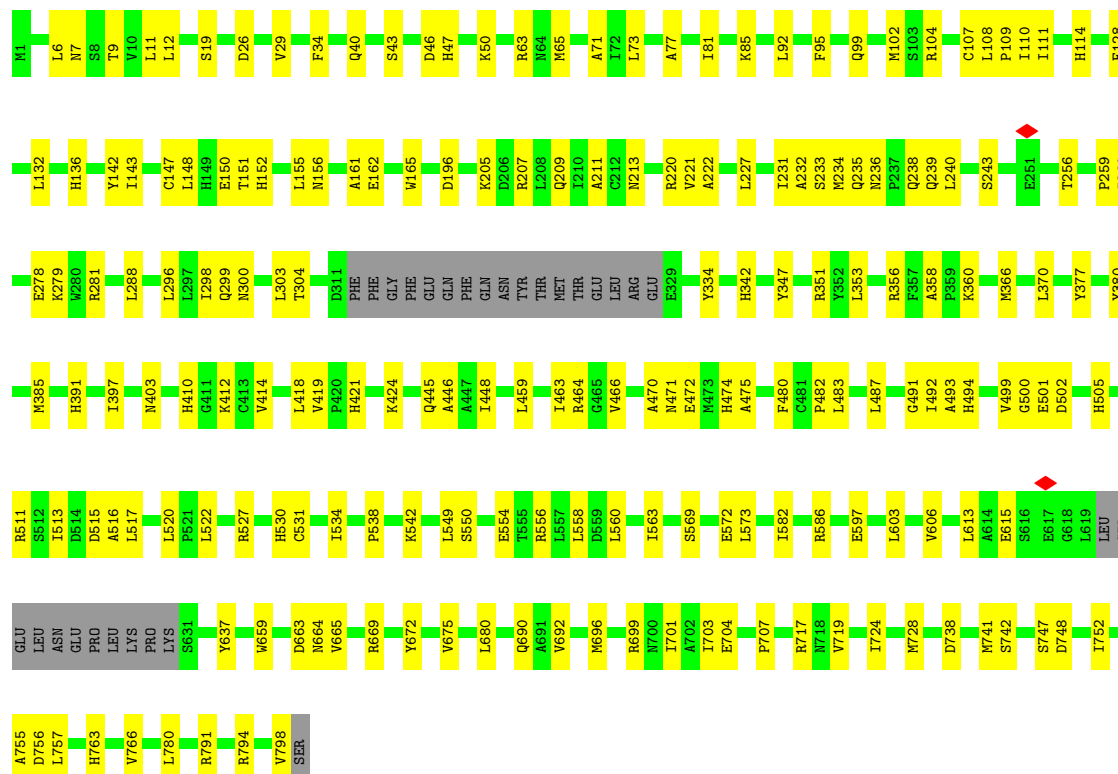


• Molecule 2: Adenosine deaminase



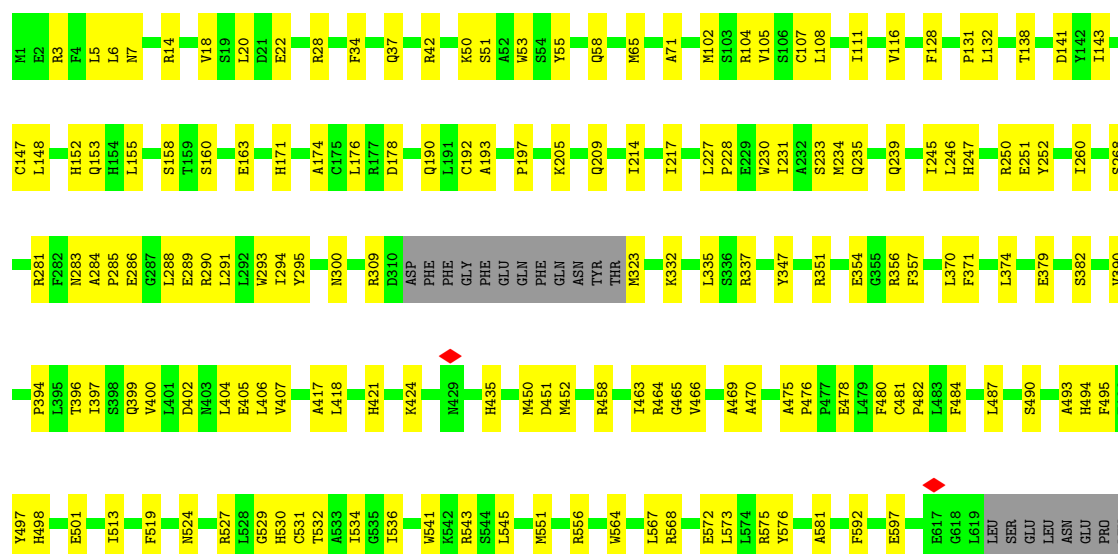
- Molecule 2: Adenosine deaminase

Chain E: 72% 24% .



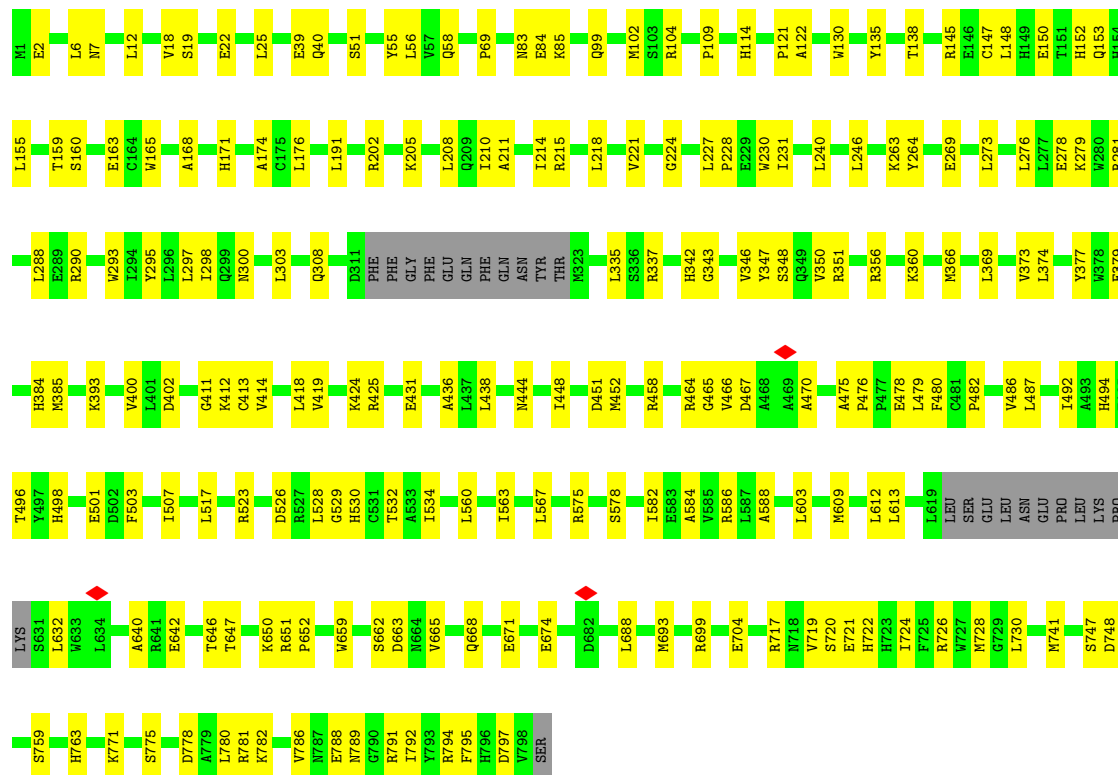
- Molecule 2: Adenosine deaminase

Chain F:  71% 26% .

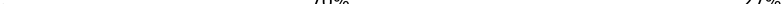


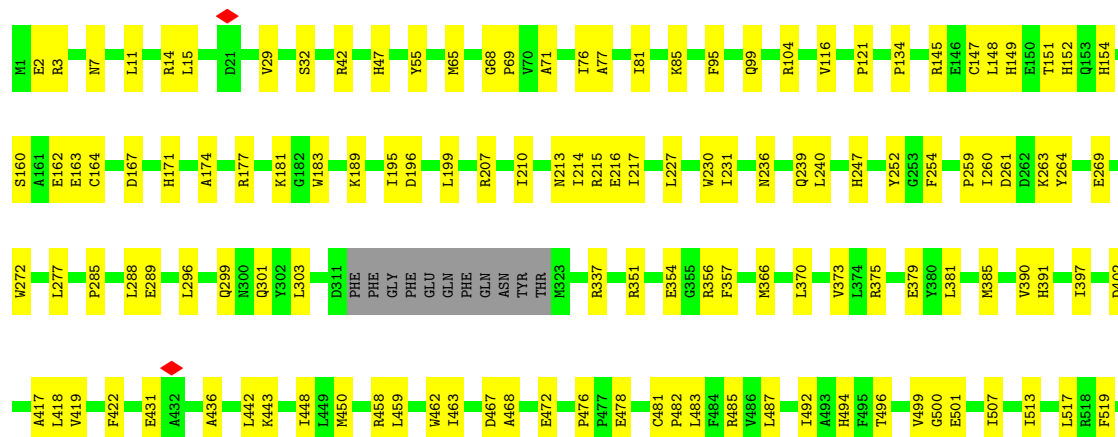
- Molecule 2: Adenosine deaminase

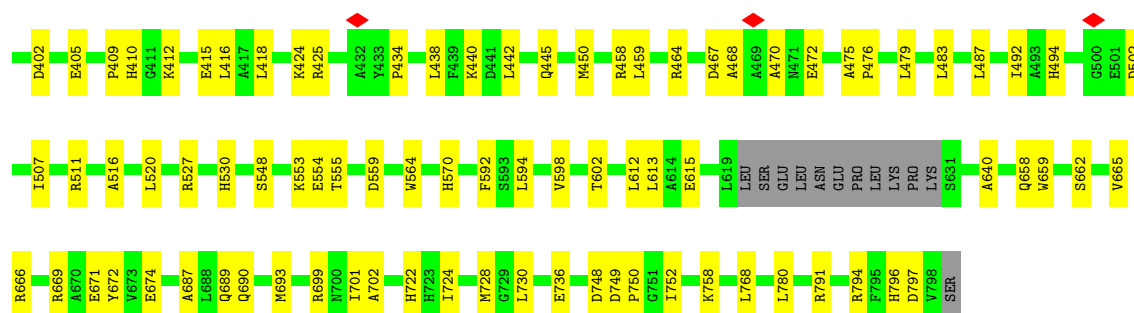
Chain G:  72% 26% .



- Molecule 2: Adenosine deaminase

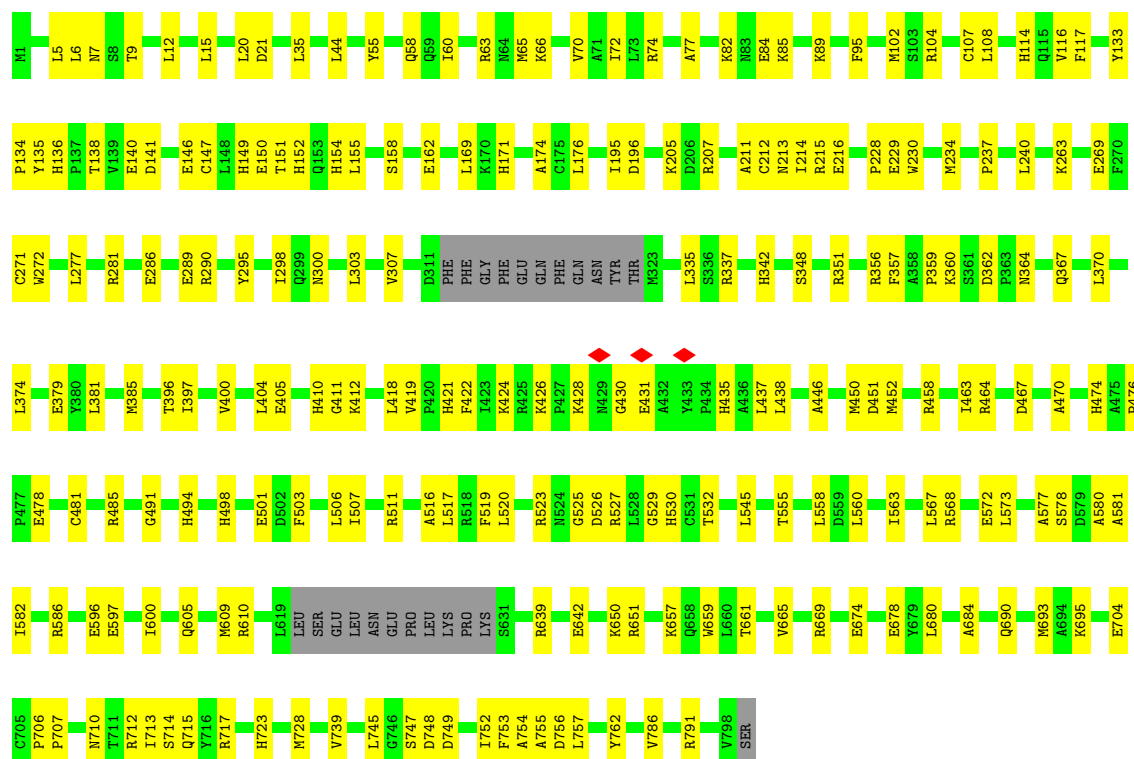
Chain I:  70% 27% .





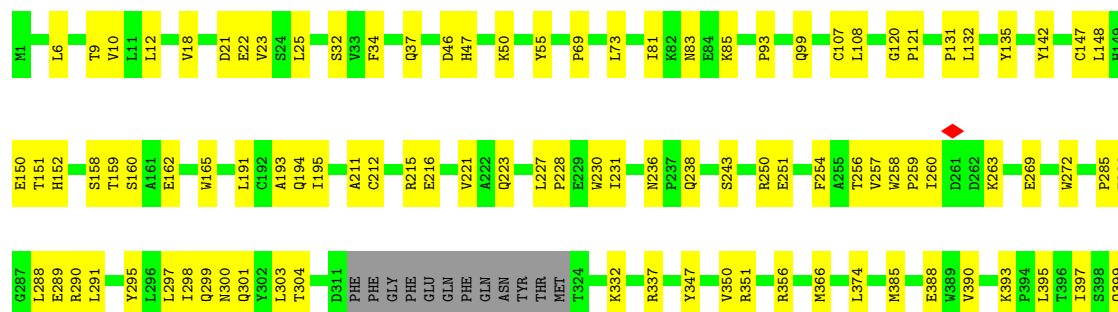
• Molecule 2: Adenosine deaminase

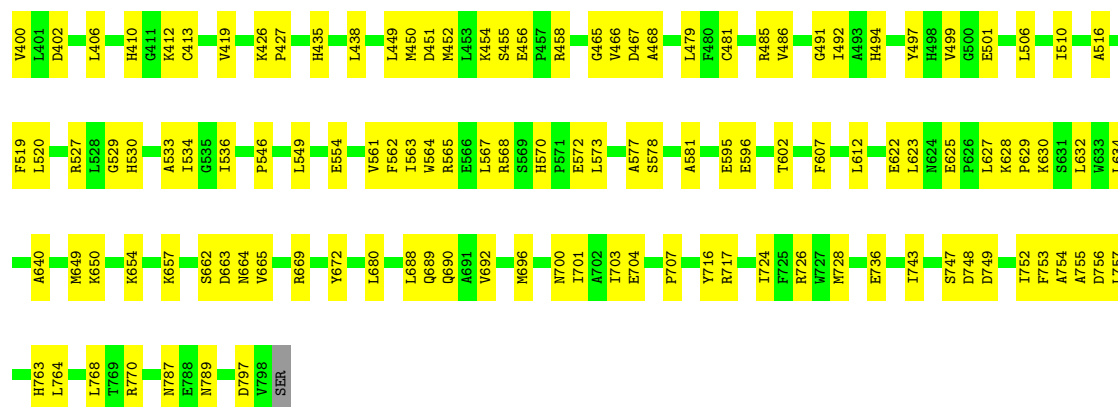
Chain L: 70% 27% .



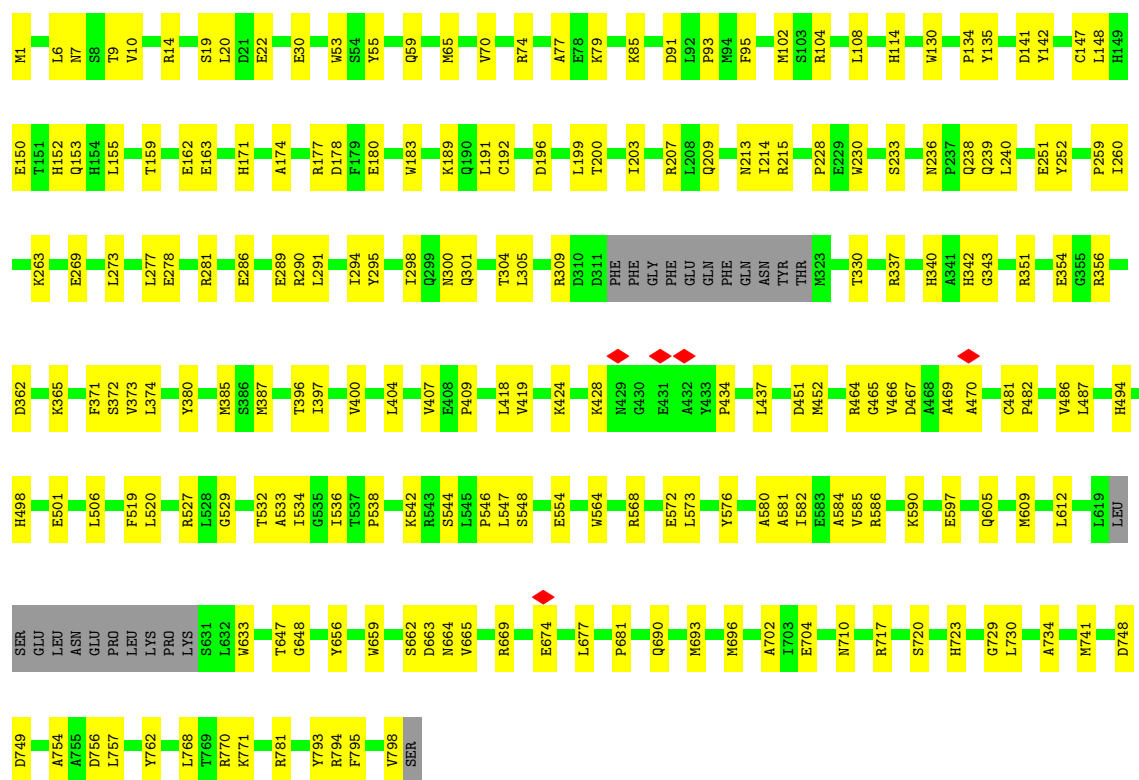
• Molecule 2: Adenosine deaminase

Chain M: 71% 27% .





• Molecule 2: Adenosine deaminase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	432.63998, 432.63998, 432.63998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/6771	0.32	0/9131
1	O	0.14	0/6771	0.31	0/9131
1	P	0.14	0/6771	0.32	0/9131
1	Q	0.13	0/6771	0.31	0/9131
1	R	0.14	0/6771	0.33	0/9131
1	S	0.15	0/6771	0.32	0/9131
1	T	0.14	0/6771	0.29	0/9131
2	B	0.10	0/6403	0.28	0/8683
2	C	0.09	0/6400	0.27	0/8678
2	D	0.10	0/6403	0.27	0/8683
2	E	0.09	0/6373	0.25	0/8641
2	F	0.12	0/6395	0.29	0/8672
2	G	0.10	0/6403	0.26	0/8683
2	I	0.09	0/6403	0.27	0/8683
2	J	0.11	0/6403	0.29	0/8683
2	K	0.09	0/6431	0.29	0/8720
2	L	0.10	0/6403	0.27	0/8683
2	M	0.10	0/6520	0.28	0/8840
2	N	0.10	0/6403	0.27	0/8683
All	All	0.12	0/124337	0.29	0/168249

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6657	0	6680	203	0
1	O	6657	0	6680	218	0
1	P	6657	0	6680	208	0
1	Q	6657	0	6680	188	0
1	R	6657	0	6680	193	0
1	S	6657	0	6680	249	0
1	T	6657	0	6680	210	0
2	B	6247	0	6183	136	0
2	C	6244	0	6189	154	0
2	D	6247	0	6183	144	0
2	E	6217	0	6171	130	0
2	F	6239	0	6179	152	0
2	G	6247	0	6183	136	0
2	I	6247	0	6183	145	0
2	J	6247	0	6183	136	0
2	K	6273	0	6204	121	0
2	L	6247	0	6183	153	0
2	M	6361	0	6331	152	0
2	N	6247	0	6183	134	0
All	All	121662	0	121115	2903	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 12.

All (2903) 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)
1:A:599:LEU:HD22	1:A:911:GLN:CB	1.60	1.29
1:S:570:PHE:CE1	1:S:617:MET:HE1	1.78	1.18
1:S:573:MET:SD	1:S:619:PHE:HB3	1.84	1.17
1:A:599:LEU:CD2	1:A:911:GLN:HB3	1.76	1.14
1:S:555:CYS:SG	1:S:573:MET:HE1	1.89	1.11
1:O:656:ILE:HD13	1:P:461:ASN:ND2	1.66	1.10
1:R:431:ARG:HG3	1:T:282:ARG:HH22	0.99	1.07
1:S:571:LEU:HG	1:S:623:PHE:HE2	1.21	1.05
1:O:656:ILE:HD13	1:P:461:ASN:HD21	0.88	1.04
1:R:431:ARG:HG3	1:T:282:ARG:NH2	1.74	1.03
1:R:431:ARG:CG	1:T:282:ARG:HH22	1.71	1.02
1:S:570:PHE:O	1:S:573:MET:HG2	1.58	1.02
1:O:656:ILE:CD1	1:P:461:ASN:HD21	1.73	1.00
1:P:176:TYR:O	1:P:180:ALA:N	2.00	0.95
1:A:599:LEU:HD22	1:A:911:GLN:HB3	0.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ASN:ND2	1:P:181:LEU:HD21	1.83	0.93
1:S:573:MET:CE	1:S:621:SER:HB2	1.98	0.93
1:S:570:PHE:CE1	1:S:617:MET:CE	2.54	0.90
1:A:747:ASN:OD1	1:T:616:LEU:HG	1.71	0.90
1:S:571:LEU:CG	1:S:623:PHE:HE2	1.85	0.90
1:Q:280:SER:O	1:Q:283:LEU:HG	1.71	0.88
1:S:559:ALA:HA	1:S:570:PHE:CD2	2.10	0.87
1:R:654:THR:HG22	1:S:461:ASN:HB2	1.57	0.86
1:A:656:ILE:HD12	1:O:512:ASN:HD22	1.42	0.84
2:F:541:TRP:O	2:F:545:LEU:HD12	1.77	0.84
2:C:163:GLU:HG2	2:C:266:GLN:NE2	1.93	0.84
1:O:127:ALA:HA	1:P:181:LEU:HD13	1.59	0.83
1:P:720:VAL:HG23	1:P:844:LEU:HD13	1.61	0.83
1:T:552:ASN:HD21	1:T:611:VAL:HG22	1.43	0.82
1:S:573:MET:HE2	1:S:621:SER:HB2	1.59	0.82
1:R:654:THR:HG23	1:R:656:ILE:HD11	1.61	0.81
1:A:599:LEU:HD22	1:A:911:GLN:HB2	1.62	0.81
1:O:656:ILE:HD11	1:P:461:ASN:OD1	1.81	0.81
1:P:768:GLN:HG2	1:P:931:THR:HG21	1.62	0.80
2:I:693:MET:HG2	2:I:741:MET:HE1	1.62	0.79
2:K:385:MET:HB3	2:K:387:MET:HE1	1.63	0.79
1:S:570:PHE:HE1	1:S:617:MET:HE1	1.47	0.79
1:R:654:THR:HG22	1:S:461:ASN:CB	2.12	0.78
1:S:540:SER:HB2	1:S:543:ARG:HD2	1.65	0.78
2:F:551:MET:HE3	2:F:675:VAL:HG11	1.64	0.78
1:T:769:SER:HA	1:T:773:LYS:HD2	1.66	0.77
2:D:433:TYR:HA	2:D:666:ARG:HH12	1.47	0.77
2:K:69:PRO:HG2	2:K:292:LEU:HB3	1.66	0.77
1:O:612:ALA:HB3	1:O:655:CYS:O	1.84	0.77
2:F:147:CYS:HB2	2:F:351:ARG:HB2	1.66	0.76
1:S:571:LEU:HG	1:S:623:PHE:CE2	2.14	0.76
1:T:79:GLY:H	1:T:82:LYS:HE3	1.51	0.76
1:A:543:ARG:HD3	1:O:469:GLN:HB2	1.67	0.76
1:R:783:LEU:HD22	1:R:846:ILE:HG12	1.65	0.76
1:T:490:CYS:HB3	1:T:729:PRO:HG2	1.66	0.76
1:P:18:LEU:HD12	1:P:384:GLN:HA	1.68	0.76
2:C:42:ARG:HH22	2:D:42:ARG:H	1.30	0.76
1:A:656:ILE:CD1	1:O:512:ASN:HD22	1.98	0.75
1:P:649:VAL:HA	1:P:653:THR:OG1	1.86	0.75
1:S:559:ALA:HA	1:S:570:PHE:CE2	2.22	0.75
2:F:541:TRP:O	2:F:545:LEU:CD1	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:359:PRO:HB2	2:K:445:GLN:HE21	1.50	0.75
1:P:656:ILE:N	1:P:656:ILE:HD12	2.02	0.75
1:O:34:GLN:HB2	1:O:37:LEU:HB2	1.68	0.74
2:M:516:ALA:HA	2:M:520:LEU:HD23	1.69	0.74
2:C:431:GLU:HG3	2:C:436:ALA:HB3	1.69	0.74
1:A:649:VAL:HA	1:A:653:THR:HB	1.69	0.73
1:O:130:ASN:HD22	1:P:181:LEU:HD11	1.53	0.73
2:C:163:GLU:CG	2:C:266:GLN:NE2	2.51	0.73
1:P:162:ARG:HH21	1:P:180:ALA:N	1.87	0.73
2:D:424:LYS:HD3	2:D:475:ALA:HB3	1.70	0.73
2:L:713:ILE:HG23	2:L:715:GLN:H	1.54	0.73
2:K:65:MET:HE3	2:K:71:ALA:HA	1.69	0.73
2:G:218:LEU:HD12	2:G:276:LEU:HD11	1.69	0.73
1:R:277:GLU:O	1:R:286:ARG:NH2	2.22	0.73
1:P:654:THR:HG21	1:Q:465:TYR:OH	1.88	0.72
1:A:431:ARG:HE	1:P:282:ARG:HH22	1.35	0.72
2:D:171:HIS:HB3	2:D:174:ALA:HB3	1.69	0.72
2:K:19:SER:O	2:K:290:ARG:NH1	2.22	0.72
1:A:650:ILE:HD12	1:O:807:ARG:H	1.55	0.72
1:O:370:GLU:HA	1:O:373:LYS:HE2	1.72	0.72
1:S:571:LEU:CG	1:S:623:PHE:CE2	2.73	0.72
1:P:784:HIS:NE2	1:P:808:LEU:O	2.22	0.72
1:R:446:LEU:HD22	1:R:485:GLN:HG3	1.70	0.72
2:K:7:ASN:HD22	2:K:104:ARG:HB3	1.54	0.71
1:P:648:LYS:HG3	1:P:649:VAL:HG23	1.72	0.71
2:B:285:PRO:HG2	2:B:288:LEU:HB2	1.73	0.71
2:B:410:HIS:HE1	2:B:413:CYS:HB2	1.54	0.71
1:O:656:ILE:CD1	1:P:461:ASN:OD1	2.38	0.71
1:A:806:LEU:HD22	1:T:593:ILE:HG12	1.71	0.71
2:F:390:VAL:HG23	2:F:406:LEU:HD11	1.71	0.71
2:I:147:CYS:HB2	2:I:351:ARG:HG2	1.73	0.71
2:I:431:GLU:HG3	2:I:436:ALA:HB3	1.72	0.71
1:O:130:ASN:HB3	1:P:181:LEU:HD11	1.72	0.71
1:O:429:ILE:HG23	1:O:434:LEU:HB3	1.72	0.71
1:R:755:ARG:HD3	1:R:767:SER:HA	1.71	0.71
1:A:784:HIS:HD1	1:A:810:PRO:HD3	1.55	0.71
2:E:227:LEU:HD13	2:E:231:ILE:HG21	1.72	0.71
2:E:424:LYS:HD3	2:E:475:ALA:HB3	1.73	0.71
1:O:656:ILE:CD1	1:P:461:ASN:ND2	2.41	0.71
1:A:452:THR:HA	1:A:455:LYS:HE2	1.71	0.70
2:J:693:MET:HG2	2:J:741:MET:HE3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:385:MET:HB3	2:N:387:MET:HE1	1.73	0.70
2:F:250:ARG:NH2	2:F:252:TYR:OH	2.24	0.70
2:J:424:LYS:HD3	2:J:475:ALA:HB3	1.73	0.70
1:A:733:LEU:HD13	1:A:793:TYR:HB2	1.73	0.70
1:O:320:LYS:HD3	1:O:345:ARG:HH21	1.56	0.70
1:Q:861:ILE:HG13	1:Q:895:LEU:HD21	1.72	0.70
2:B:374:LEU:HB3	2:B:400:VAL:HG11	1.73	0.70
2:L:426:LYS:HA	2:L:474:HIS:HD2	1.56	0.70
1:O:552:ASN:ND2	1:O:655:CYS:SG	2.64	0.70
2:I:65:MET:HE2	2:I:71:ALA:HA	1.72	0.70
2:B:171:HIS:HB3	2:B:174:ALA:HB3	1.72	0.69
2:J:111:ILE:HD12	2:J:132:LEU:HD21	1.74	0.69
2:M:99:GLN:HG3	2:M:763:HIS:HD1	1.58	0.69
2:B:750:PRO:HB2	2:B:752:ILE:HG12	1.74	0.69
2:C:85:LYS:NZ	2:I:524:ASN:O	2.25	0.69
2:D:696:MET:HG3	2:D:701:ILE:HB	1.73	0.69
2:I:227:LEU:HD13	2:I:231:ILE:HG21	1.73	0.69
2:F:469:ALA:HB2	2:F:498:HIS:HB3	1.74	0.69
2:L:6:LEU:O	2:L:300:ASN:ND2	2.25	0.69
2:B:342:HIS:ND1	2:B:348:SER:HB3	2.08	0.69
2:J:213:ASN:ND2	2:J:240:LEU:O	2.26	0.69
2:L:195:ILE:O	2:L:196:ASP:OD1	2.10	0.69
2:N:582:ILE:HG22	2:N:586:ARG:HH12	1.57	0.69
1:O:744:ASN:OD1	1:O:747:ASN:ND2	2.25	0.69
1:Q:266:TYR:HE1	1:Q:290:VAL:HG21	1.58	0.69
1:R:747:ASN:O	1:R:751:GLN:NE2	2.26	0.69
1:Q:151:GLU:HA	1:Q:154:GLN:HB2	1.75	0.69
1:R:415:ASN:OD1	1:R:418:ARG:NH1	2.25	0.69
2:D:707:PRO:HG3	2:D:747:SER:HA	1.73	0.69
2:J:20:LEU:HD12	2:J:287:GLY:HA2	1.75	0.69
2:L:335:LEU:HD13	2:L:379:GLU:HG3	1.73	0.69
2:N:7:ASN:HD22	2:N:104:ARG:HB3	1.58	0.69
2:B:719:VAL:HG21	2:B:763:HIS:HE2	1.57	0.68
1:S:571:LEU:HG	1:S:571:LEU:O	1.93	0.68
1:A:720:VAL:HG12	1:A:844:LEU:HD22	1.73	0.68
2:G:612:LEU:HG	2:G:640:ALA:HB1	1.75	0.68
2:J:147:CYS:HB2	2:J:351:ARG:HB2	1.75	0.68
2:L:501:GLU:OE2	2:L:530:HIS:ND1	2.22	0.68
2:L:213:ASN:ND2	2:L:240:LEU:O	2.25	0.68
1:R:775:MET:HA	1:R:778:ASN:HB2	1.76	0.68
1:R:652:GLN:HB2	1:S:736:LYS:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:GLY:HA3	2:C:89:LYS:HE2	1.75	0.68
2:N:196:ASP:OD2	2:N:301:GLN:NE2	2.26	0.68
2:M:22:GLU:O	2:M:290:ARG:NH2	2.24	0.68
1:O:186:GLN:HG2	1:O:187:LEU:HG	1.76	0.68
2:B:213:ASN:ND2	2:B:240:LEU:O	2.27	0.68
1:A:114:LYS:HE2	1:O:239:LYS:HA	1.75	0.68
1:S:728:ARG:HB3	1:S:795:SER:HB2	1.76	0.68
1:P:389:LYS:HG3	1:P:416:LEU:HD22	1.75	0.68
2:G:719:VAL:HG21	2:G:763:HIS:HE2	1.59	0.67
2:C:651:ARG:NH1	2:F:597:GLU:OE2	2.27	0.67
2:D:663:ASP:OD1	2:D:664:ASN:N	2.27	0.67
2:L:82:LYS:NZ	2:L:84:GLU:OE1	2.27	0.67
1:R:654:THR:CG2	1:S:461:ASN:HB2	2.24	0.67
1:S:509:SER:O	1:S:513:GLN:NE2	2.26	0.67
1:A:746:ASN:ND2	1:T:613:SER:O	2.27	0.67
2:B:430:GLY:H	2:B:666:ARG:HH22	1.41	0.67
1:O:201:GLU:HG2	1:O:243:SER:HB3	1.76	0.67
1:T:616:LEU:N	1:T:616:LEU:HD22	2.08	0.67
2:C:216:GLU:OE2	2:C:263:LYS:NZ	2.26	0.67
2:I:236:ASN:HB3	2:I:239:GLN:HG3	1.75	0.67
2:I:707:PRO:HG3	2:I:747:SER:HA	1.75	0.67
2:C:527:ARG:NH2	2:C:793:TYR:O	2.28	0.67
1:Q:17:ASN:HA	1:Q:331:LYS:HB3	1.76	0.67
1:S:575:GLN:HG3	1:S:617:MET:HG3	1.76	0.67
2:G:221:VAL:HG21	2:G:288:LEU:HD21	1.75	0.67
2:L:374:LEU:HB3	2:L:400:VAL:HG11	1.75	0.67
2:M:356:ARG:NH1	2:M:467:ASP:OD2	2.28	0.67
2:M:634:LEU:HD21	1:S:154:GLN:NE2	2.10	0.67
2:E:471:ASN:ND2	2:E:502:ASP:OD2	2.27	0.67
1:A:183:LEU:HD22	1:T:131:LYS:HE2	1.77	0.66
1:A:329:LYS:NZ	1:A:343:ASP:OD1	2.28	0.66
1:A:389:LYS:HB3	1:A:416:LEU:HD22	1.77	0.66
2:C:356:ARG:NH1	2:C:467:ASP:OD2	2.27	0.66
1:Q:810:PRO:HG3	1:Q:817:PHE:HB2	1.76	0.66
1:A:296:GLN:HG3	1:T:78:ARG:HB3	1.78	0.66
2:K:213:ASN:ND2	2:K:240:LEU:O	2.28	0.66
2:N:428:LYS:HG3	2:N:437:LEU:HB3	1.77	0.66
1:A:486:VAL:HG21	1:A:731:ALA:HB2	1.76	0.66
2:B:245:ILE:HG22	2:B:252:TYR:HB2	1.78	0.66
1:Q:738:TRP:CD1	1:Q:741:PHE:HB3	2.31	0.66
2:C:37:GLN:NE2	2:C:41:ALA:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:565:ARG:O	2:M:568:ARG:NH1	2.28	0.66
2:D:214:ILE:HG12	2:D:291:LEU:HD12	1.77	0.66
2:K:130:TRP:HE1	2:K:340:HIS:HA	1.60	0.66
2:L:146:GLU:OE2	2:L:149:HIS:NE2	2.25	0.66
1:S:34:GLN:HE22	1:S:311:LYS:H	1.44	0.66
1:S:555:CYS:HA	1:S:558:VAL:HG22	1.78	0.66
1:T:418:ARG:NH1	1:T:481:TYR:O	2.29	0.66
1:A:314:LEU:HB3	1:A:372:LEU:HB3	1.77	0.66
2:C:373:VAL:HG11	2:C:418:LEU:HD21	1.77	0.66
2:M:9:THR:HG22	2:M:301:GLN:HE22	1.59	0.66
1:P:255:ARG:HH22	1:Q:285:GLU:HG3	1.60	0.66
1:Q:578:ARG:HG3	1:Q:618:ASP:HB2	1.78	0.66
1:A:471:GLU:HG3	1:T:440:ARG:HH22	1.61	0.65
2:D:720:SER:HB2	2:D:771:LYS:HD2	1.78	0.65
2:F:233:SER:O	2:F:239:GLN:NE2	2.28	0.65
1:Q:448:LYS:HB2	1:Q:542:GLY:HA3	1.78	0.65
1:O:509:SER:O	1:O:513:GLN:NE2	2.28	0.65
1:A:599:LEU:CG	1:A:911:GLN:HB3	2.25	0.65
2:C:176:LEU:HD22	2:C:205:LYS:HG3	1.78	0.65
1:R:196:LEU:HD23	1:R:199:ILE:HD11	1.77	0.65
1:R:431:ARG:CB	1:T:282:ARG:HH22	2.08	0.65
1:T:254:LEU:HD22	1:T:307:ARG:HH21	1.61	0.65
2:G:191:LEU:HD11	2:G:308:GLN:HG3	1.79	0.65
1:O:130:ASN:OD1	1:O:153:TRP:NE1	2.29	0.65
1:Q:437:GLU:HB3	1:Q:440:ARG:HB2	1.77	0.65
1:Q:511:PHE:HZ	1:Q:532:ILE:HG12	1.60	0.65
1:R:163:GLY:HA3	1:R:196:LEU:HD21	1.77	0.65
2:B:163:GLU:OE2	2:B:266:GLN:HG3	1.95	0.65
2:N:19:SER:O	2:N:290:ARG:NH1	2.29	0.65
2:G:424:LYS:HD2	2:G:475:ALA:HB3	1.78	0.65
2:I:154:HIS:O	2:I:337:ARG:NH1	2.29	0.65
1:P:802:ILE:O	1:P:807:ARG:NH2	2.30	0.65
1:A:414:PRO:HB2	1:A:488:GLU:HG2	1.79	0.65
1:A:431:ARG:NH1	1:O:291:GLU:OE1	2.30	0.65
2:K:7:ASN:HD21	2:K:304:THR:HG21	1.61	0.65
2:M:158:SER:O	2:M:337:ARG:NH2	2.30	0.65
1:S:370:GLU:OE1	1:S:476:ARG:NH1	2.30	0.65
1:A:648:LYS:O	1:A:653:THR:N	2.28	0.65
2:D:410:HIS:HE1	2:D:412:LYS:HE3	1.61	0.65
2:K:147:CYS:HB2	2:K:351:ARG:HB2	1.78	0.65
1:A:886:LEU:O	1:A:912:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:553:ARG:HH11	1:R:655:CYS:HA	1.62	0.65
1:A:887:LEU:HG	1:A:891:GLU:HG3	1.79	0.64
2:B:215:ARG:NH2	2:B:263:LYS:O	2.30	0.64
1:S:515:VAL:HG12	1:S:531:LEU:HD21	1.79	0.64
2:I:738:ASP:OD1	2:I:739:VAL:N	2.29	0.64
2:E:6:LEU:O	2:E:300:ASN:ND2	2.30	0.64
2:G:794:ARG:NH1	2:J:141:ASP:OD1	2.29	0.64
1:P:374:GLN:NE2	1:P:473:GLU:OE2	2.29	0.64
2:L:364:ASN:OD1	2:L:367:GLN:NE2	2.25	0.64
2:N:162:GLU:HG3	2:N:754:ALA:HB2	1.79	0.64
2:D:517:LEU:HD11	2:D:696:MET:HB2	1.78	0.64
2:I:11:LEU:HD11	2:I:29:VAL:HG23	1.80	0.64
1:A:747:ASN:HA	1:T:616:LEU:HD21	1.79	0.64
2:C:563:ILE:HG23	2:C:567:LEU:HD12	1.80	0.64
2:G:466:VAL:HG21	2:G:487:LEU:HD13	1.79	0.64
2:D:14:ARG:HH11	2:D:32:SER:HB2	1.62	0.64
2:L:84:GLU:HG3	2:L:85:LYS:H	1.60	0.64
1:Q:156:HIS:HA	1:Q:159:GLN:HE21	1.63	0.64
1:R:833:LYS:HB3	1:R:838:THR:HG21	1.80	0.64
2:L:710:ASN:ND2	2:L:749:ASP:O	2.29	0.64
2:E:472:GLU:OE2	2:E:500:GLY:N	2.31	0.64
2:G:482:PRO:HG2	2:G:613:LEU:HD13	1.79	0.64
2:G:788:GLU:OE1	2:G:791:ARG:NH1	2.30	0.64
2:L:20:LEU:HA	2:L:290:ARG:HH21	1.63	0.64
1:S:573:MET:HB3	1:S:621:SER:HA	1.80	0.64
1:A:569:VAL:HG11	1:A:753:LYS:HA	1.79	0.64
2:F:7:ASN:ND2	2:F:104:ARG:O	2.31	0.64
2:G:374:LEU:HB3	2:G:400:VAL:HG11	1.80	0.64
2:K:442:LEU:HB3	2:K:483:LEU:HD21	1.79	0.64
2:L:171:HIS:HB3	2:L:174:ALA:HB3	1.80	0.64
1:P:350:ASP:OD1	1:P:353:ARG:NH2	2.31	0.64
1:S:345:ARG:NH2	1:S:369:ASN:OD1	2.31	0.64
1:S:573:MET:SD	1:S:619:PHE:CB	2.75	0.64
1:A:318:GLY:O	1:A:345:ARG:NH1	2.31	0.63
2:E:466:VAL:HG21	2:E:487:LEU:HD13	1.78	0.63
2:E:471:ASN:HB3	2:E:474:HIS:HB2	1.80	0.63
1:T:123:VAL:HG12	1:T:164:LEU:HD21	1.78	0.63
1:T:234:LEU:HD22	1:T:301:LEU:HD21	1.78	0.63
1:T:774:ILE:O	1:T:778:ASN:ND2	2.31	0.63
2:E:522:LEU:O	2:E:699:ARG:NH2	2.31	0.63
2:G:717:ARG:HH21	2:I:717:ARG:HH11	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:374:LEU:HB3	2:M:400:VAL:HG11	1.80	0.63
2:M:466:VAL:HG23	2:M:492:ILE:HG21	1.80	0.63
1:O:578:ARG:HD3	1:O:618:ASP:HB2	1.80	0.63
1:P:762:HIS:HA	1:P:859:GLY:HA2	1.81	0.63
2:F:153:GLN:HE22	2:F:155:LEU:HD23	1.63	0.63
1:O:130:ASN:CG	1:P:181:LEU:HD21	2.22	0.63
1:T:552:ASN:HD21	1:T:611:VAL:CG2	2.10	0.63
1:A:559:ALA:HA	1:A:570:PHE:HE2	1.63	0.63
2:D:260:ILE:HD11	1:R:141:TRP:HB2	1.80	0.63
2:G:210:ILE:HG12	2:G:240:LEU:HB2	1.81	0.63
2:M:83:ASN:HD21	2:M:121:PRO:HD3	1.63	0.63
1:P:473:GLU:HA	1:P:476:ARG:HB2	1.79	0.63
1:Q:123:VAL:HG12	1:Q:164:LEU:HD21	1.78	0.63
1:Q:280:SER:HA	1:Q:283:LEU:CD2	2.29	0.63
1:R:439:HIS:HB2	1:S:314:LEU:HD23	1.80	0.63
1:S:440:ARG:NH2	1:T:473:GLU:OE1	2.30	0.63
2:J:466:VAL:HG23	2:J:492:ILE:HG21	1.79	0.63
2:J:590:LYS:O	2:J:668:GLN:NE2	2.30	0.63
1:Q:359:ARG:NH2	1:Q:792:LEU:O	2.29	0.63
1:A:656:ILE:HG12	1:O:461:ASN:OD1	1.99	0.63
2:B:466:VAL:HG23	2:B:492:ILE:HG21	1.79	0.63
2:C:227:LEU:HD13	2:C:231:ILE:HG13	1.81	0.63
1:R:639:ARG:NH1	1:R:714:GLU:OE1	2.32	0.63
1:S:262:ARG:O	1:S:266:TYR:CD2	2.52	0.63
1:T:616:LEU:HD22	1:T:616:LEU:H	1.63	0.63
2:K:192:CYS:HB3	2:K:199:LEU:HD23	1.81	0.63
1:O:107:LEU:HD11	1:O:128:ARG:HB3	1.81	0.63
1:P:19:PHE:HE2	1:P:334:PRO:HD3	1.64	0.63
2:K:750:PRO:HB2	2:K:752:ILE:HG12	1.80	0.63
1:R:18:LEU:O	1:R:384:GLN:NE2	2.32	0.63
2:G:534:ILE:O	2:G:726:ARG:NH2	2.32	0.63
1:S:567:ILE:HG23	1:S:569:VAL:HG12	1.80	0.63
2:C:285:PRO:HG2	2:C:288:LEU:HB2	1.80	0.62
2:F:402:ASP:OD1	2:F:458:ARG:NH1	2.32	0.62
2:I:7:ASN:ND2	2:I:104:ARG:O	2.29	0.62
2:I:485:ARG:HE	2:I:639:ARG:HH22	1.47	0.62
2:B:147:CYS:HB2	2:B:351:ARG:HB2	1.81	0.62
2:G:529:GLY:HA2	2:G:704:GLU:HB3	1.82	0.62
2:G:335:LEU:HD13	2:G:379:GLU:HG3	1.81	0.62
2:M:390:VAL:HG23	2:M:406:LEU:HD11	1.79	0.62
1:Q:745:LEU:HD22	1:Q:778:ASN:HD22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:402:ASP:OD1	2:G:458:ARG:NH1	2.32	0.62
2:K:69:PRO:HG3	2:K:293:TRP:CD1	2.34	0.62
1:A:744:ASN:HD22	1:A:785:ALA:HB2	1.64	0.62
2:M:724:ILE:HG13	2:M:728:MET:HE2	1.81	0.62
2:N:362:ASP:HB3	2:N:365:LYS:HB2	1.81	0.62
1:R:453:TYR:O	1:R:456:GLN:NE2	2.30	0.62
1:S:747:ASN:HB3	1:S:811:VAL:HG22	1.80	0.62
1:A:656:ILE:HD11	1:O:460:PHE:HB2	1.82	0.62
1:O:464:PHE:HB3	1:O:508:VAL:HG11	1.80	0.62
1:S:465:TYR:O	1:S:467:ARG:NH1	2.33	0.62
1:A:337:GLN:HG3	1:A:339:ILE:H	1.64	0.62
2:E:147:CYS:HB2	2:E:351:ARG:HB2	1.81	0.62
2:J:228:PRO:HB2	2:J:230:TRP:HD1	1.64	0.62
2:N:434:PRO:HG2	2:N:669:ARG:HH21	1.64	0.62
1:P:752:HIS:HA	1:P:755:ARG:HB2	1.82	0.62
2:J:424:LYS:O	2:J:425:ARG:NH1	2.32	0.62
2:M:259:PRO:HG2	2:M:260:ILE:HD12	1.82	0.62
1:Q:117:ARG:HB2	1:R:168:THR:HG22	1.82	0.62
2:M:159:THR:HG22	2:M:337:ARG:HA	1.81	0.62
1:O:656:ILE:CD1	1:P:461:ASN:CG	2.73	0.62
1:P:578:ARG:HG3	1:P:618:ASP:HB2	1.81	0.62
1:S:253:ASP:OD2	1:S:255:ARG:NH1	2.31	0.62
2:F:111:ILE:HD12	2:F:132:LEU:HD21	1.81	0.62
1:O:608:LEU:HD22	1:O:650:ILE:HG12	1.81	0.62
1:Q:569:VAL:HG21	1:Q:774:ILE:HD13	1.81	0.62
2:B:791:ARG:HA	2:B:794:ARG:HB3	1.82	0.61
1:P:647:ASN:HB2	1:Q:806:LEU:HD23	1.82	0.61
1:S:571:LEU:HD21	1:S:623:PHE:CE2	2.35	0.61
2:F:3:ARG:HD2	2:F:104:ARG:HG3	1.82	0.61
2:J:374:LEU:HB3	2:J:400:VAL:HG11	1.81	0.61
2:K:405:GLU:OE1	2:K:458:ARG:NH1	2.32	0.61
1:S:605:ALA:HB1	1:T:806:LEU:HD21	1.82	0.61
1:T:106:CYS:HB3	1:T:217:LEU:HD23	1.83	0.61
1:O:473:GLU:OE2	1:O:476:ARG:NH1	2.33	0.61
1:O:783:LEU:HB3	1:O:846:ILE:HG22	1.81	0.61
2:G:227:LEU:HB3	2:G:231:ILE:HD13	1.82	0.61
2:J:690:GLN:NE2	2:J:736:GLU:O	2.32	0.61
1:R:177:PHE:HE1	1:R:181:LEU:HD22	1.66	0.61
2:G:693:MET:HG2	2:G:741:MET:HE1	1.82	0.61
1:O:130:ASN:ND2	1:P:181:LEU:CD2	2.62	0.61
1:O:279:GLU:HB3	1:O:282:ARG:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:41:LEU:HD13	1:R:308:ILE:HG13	1.81	0.61
1:S:452:THR:HA	1:S:455:LYS:HG3	1.82	0.61
1:A:378:LEU:HG	1:A:424:SER:HB2	1.83	0.61
2:M:529:GLY:HA2	2:M:704:GLU:HB3	1.82	0.61
1:O:128:ARG:HG3	1:P:192:GLY:H	1.64	0.61
1:O:762:HIS:HA	1:O:859:GLY:HA2	1.82	0.61
2:C:592:PHE:O	2:C:658:GLN:NE2	2.34	0.61
2:D:686:VAL:HG13	2:D:690:GLN:HE21	1.66	0.61
2:L:516:ALA:HA	2:L:520:LEU:HD13	1.82	0.61
1:T:636:ARG:NH1	1:T:724:GLU:OE2	2.33	0.61
2:B:342:HIS:CE1	2:B:348:SER:N	2.69	0.61
2:C:147:CYS:HB2	2:C:351:ARG:HB2	1.82	0.61
2:G:431:GLU:HG3	2:G:436:ALA:HB3	1.82	0.61
2:M:467:ASP:OD1	2:M:468:ALA:N	2.33	0.61
2:N:374:LEU:HB3	2:N:400:VAL:HG11	1.83	0.61
2:N:534:ILE:HD12	2:N:741:MET:HE1	1.81	0.61
2:N:690:GLN:HA	2:N:693:MET:HB2	1.82	0.61
1:O:235:GLU:OE1	1:O:238:ARG:NH1	2.34	0.61
1:Q:375:PRO:HB3	1:R:296:GLN:HE22	1.65	0.61
2:B:163:GLU:HG3	2:B:266:GLN:HE21	1.65	0.61
2:D:374:LEU:HB3	2:D:400:VAL:HG11	1.81	0.61
2:G:7:ASN:ND2	2:G:104:ARG:O	2.34	0.61
2:L:478:GLU:OE2	2:L:610:ARG:NH1	2.34	0.61
1:Q:466:LEU:HD13	1:Q:731:ALA:HB1	1.81	0.61
2:D:467:ASP:OD1	2:D:468:ALA:N	2.34	0.61
2:K:227:LEU:HD13	2:K:231:ILE:HG21	1.82	0.61
1:P:353:ARG:NH1	1:P:360:GLU:OE2	2.33	0.61
2:F:356:ARG:NH2	2:F:704:GLU:OE2	2.34	0.60
2:I:370:LEU:HD21	2:I:463:ILE:HD11	1.83	0.60
2:L:356:ARG:NH2	2:L:704:GLU:OE2	2.33	0.60
1:S:509:SER:HB2	1:S:738:TRP:HE1	1.65	0.60
1:A:608:LEU:O	1:A:624:ASN:ND2	2.33	0.60
2:B:163:GLU:HG2	2:B:166:LEU:HD12	1.83	0.60
2:D:232:ALA:O	2:D:235:GLN:NE2	2.34	0.60
1:Q:755:ARG:HH11	1:Q:767:SER:HA	1.66	0.60
1:R:311:LYS:HG2	1:R:316:LEU:HD12	1.83	0.60
1:S:633:SER:HA	1:S:636:ARG:HG2	1.82	0.60
2:G:424:LYS:HZ3	2:G:470:ALA:HB3	1.65	0.60
2:I:507:ILE:HD12	2:I:563:ILE:HD11	1.83	0.60
1:O:647:ASN:O	1:O:652:GLN:NE2	2.33	0.60
1:Q:559:ALA:HA	1:Q:570:PHE:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:516:THR:O	1:S:527:LYS:NZ	2.34	0.60
1:A:305:GLN:HG2	1:A:306:LYS:HD3	1.84	0.60
2:L:481:CYS:SG	2:L:485:ARG:NH2	2.74	0.60
2:C:19:SER:O	2:C:290:ARG:NH1	2.34	0.60
2:E:491:GLY:HA2	2:I:121:PRO:HB2	1.83	0.60
2:M:152:HIS:HD2	2:M:356:ARG:HG3	1.67	0.60
1:P:764:ARG:O	1:P:863:CYS:N	2.30	0.60
1:Q:747:ASN:HB3	1:Q:811:VAL:HG11	1.82	0.60
1:A:727:ILE:HG22	1:A:729:PRO:HD3	1.82	0.60
2:B:401:LEU:HD12	2:B:456:GLU:HG2	1.84	0.60
2:D:271:CYS:HG	1:R:141:TRP:CG	2.19	0.60
2:D:597:GLU:OE2	2:I:651:ARG:NH1	2.34	0.60
1:R:357:ASN:OD1	1:R:728:ARG:NH1	2.35	0.60
2:E:108:LEU:HD23	2:E:162:GLU:HG2	1.84	0.60
2:I:356:ARG:NH1	2:I:467:ASP:OD2	2.34	0.60
2:N:466:VAL:HG21	2:N:487:LEU:HD13	1.83	0.60
1:O:415:ASN:OD1	1:O:418:ARG:NH2	2.34	0.60
2:J:385:MET:SD	2:J:410:HIS:NE2	2.72	0.60
1:O:288:TYR:O	1:O:292:HIS:ND1	2.32	0.60
1:Q:78:ARG:HH21	1:R:293:LEU:HD23	1.66	0.60
1:Q:320:LYS:HE3	1:Q:345:ARG:HE	1.66	0.60
1:Q:769:SER:HA	1:Q:773:LYS:HD2	1.84	0.60
1:R:455:LYS:HD2	1:R:532:ILE:HD13	1.82	0.60
1:T:366:MET:HA	1:T:369:ASN:HB2	1.82	0.60
1:T:647:ASN:O	1:T:652:GLN:NE2	2.35	0.60
1:A:79:GLY:H	1:A:82:LYS:HZ1	1.49	0.60
2:B:108:LEU:HD21	2:B:269:GLU:HG2	1.82	0.60
2:E:692:VAL:O	2:E:696:MET:N	2.32	0.60
2:F:572:GLU:HG3	2:F:573:LEU:HD12	1.84	0.60
2:J:183:TRP:O	2:J:189:LYS:NZ	2.34	0.60
2:L:597:GLU:O	2:L:651:ARG:NH2	2.34	0.60
2:G:102:MET:HA	2:G:102:MET:HE3	1.83	0.60
1:R:128:ARG:HA	1:S:192:GLY:HA3	1.83	0.60
1:T:435:ASN:HD21	1:T:440:ARG:HB3	1.67	0.60
2:L:639:ARG:HA	2:L:642:GLU:HG2	1.83	0.59
2:M:223:GLN:HG3	1:P:147:ARG:HH22	1.67	0.59
1:S:573:MET:HE2	1:S:621:SER:CB	2.32	0.59
2:B:26:ASP:HA	2:B:29:VAL:HG12	1.83	0.59
1:O:107:LEU:HD23	1:O:218:ILE:HD13	1.84	0.59
1:Q:128:ARG:HD3	1:R:193:GLY:HA3	1.83	0.59
1:Q:863:CYS:HA	1:Q:868:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:530:HIS:NE2	2:K:748:ASP:OD2	2.32	0.59
1:T:511:PHE:HZ	1:T:532:ILE:HG12	1.67	0.59
1:A:291:GLU:HG2	1:T:431:ARG:HD2	1.84	0.59
1:A:314:LEU:HD21	1:T:439:HIS:HB2	1.85	0.59
1:A:599:LEU:HD13	1:A:911:GLN:CD	2.27	0.59
2:C:171:HIS:HB3	2:C:174:ALA:HB3	1.85	0.59
2:E:672:TYR:H	2:F:58:GLN:HE22	1.49	0.59
2:I:529:GLY:HA2	2:I:704:GLU:HB2	1.83	0.59
1:O:856:PHE:HD2	1:O:887:LEU:HD11	1.67	0.59
1:R:569:VAL:HG23	1:R:574:VAL:HG22	1.84	0.59
2:G:147:CYS:HB2	2:G:351:ARG:HB2	1.83	0.59
2:M:690:GLN:NE2	2:M:736:GLU:O	2.35	0.59
1:P:17:ASN:HA	1:P:331:LYS:HB3	1.83	0.59
1:S:414:PRO:HB2	1:S:488:GLU:HB2	1.85	0.59
2:G:153:GLN:O	2:G:356:ARG:N	2.35	0.59
2:K:374:LEU:HD12	2:K:397:ILE:HD11	1.83	0.59
1:Q:808:LEU:HD23	1:Q:816:GLU:HG2	1.84	0.59
1:S:78:ARG:HG2	1:T:296:GLN:HG2	1.84	0.59
2:E:9:THR:HG21	2:E:196:ASP:HB3	1.85	0.59
2:F:529:GLY:HA2	2:F:704:GLU:HB2	1.84	0.59
2:E:527:ARG:NH2	2:E:704:GLU:OE2	2.36	0.59
2:G:728:MET:HE1	2:G:786:VAL:HG21	1.84	0.59
2:I:596:GLU:OE2	2:I:651:ARG:NH2	2.35	0.59
2:M:650:LYS:HG3	2:M:654:LYS:HZ1	1.67	0.59
1:R:426:LEU:HD23	1:S:254:LEU:HD11	1.83	0.59
1:A:78:ARG:HH12	1:O:293:LEU:HD23	1.67	0.59
1:A:550:TRP:HA	1:A:553:ARG:HH22	1.68	0.59
2:B:93:PRO:HG3	2:B:770:ARG:HH12	1.67	0.59
2:C:501:GLU:OE2	2:C:530:HIS:ND1	2.36	0.59
2:C:402:ASP:OD1	2:C:458:ARG:NH1	2.36	0.59
2:E:360:LYS:HB2	2:E:366:MET:HB3	1.85	0.59
2:K:592:PHE:HB2	2:K:594:LEU:HD22	1.85	0.59
1:O:727:ILE:HG22	1:O:729:PRO:HD3	1.85	0.59
1:T:112:PRO:HG3	1:T:233:VAL:HG21	1.84	0.59
2:B:585:VAL:O	2:B:589:HIS:ND1	2.30	0.58
1:Q:105:LYS:HE2	1:Q:213:CYS:HB3	1.85	0.58
1:T:567:ILE:HG21	1:T:753:LYS:HD3	1.84	0.58
2:C:424:LYS:O	2:C:425:ARG:NH1	2.36	0.58
2:D:471:ASN:ND2	2:D:502:ASP:OD2	2.35	0.58
2:F:543:ARG:HD3	2:F:717:ARG:HH21	1.67	0.58
2:J:390:VAL:HG23	2:J:406:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:858:VAL:HG13	1:O:913:THR:HG21	1.83	0.58
1:R:762:HIS:HA	1:R:859:GLY:HA2	1.86	0.58
2:C:209:GLN:O	2:C:213:ASN:ND2	2.36	0.58
2:C:467:ASP:OD1	2:C:468:ALA:N	2.35	0.58
2:D:529:GLY:HA2	2:D:704:GLU:HB2	1.84	0.58
2:G:215:ARG:NE	2:G:269:GLU:OE1	2.36	0.58
2:L:108:LEU:HD21	2:L:269:GLU:HG2	1.83	0.58
2:M:481:CYS:HB3	2:M:485:ARG:HH12	1.68	0.58
1:T:616:LEU:H	1:T:616:LEU:CD2	2.16	0.58
2:F:374:LEU:HB3	2:F:400:VAL:HG11	1.83	0.58
2:M:662:SER:OG	2:M:664:ASN:OD1	2.22	0.58
2:C:111:ILE:HD12	2:C:132:LEU:HD11	1.84	0.58
1:O:130:ASN:HD22	1:P:181:LEU:CD1	2.16	0.58
1:O:503:VAL:O	1:O:507:SER:OG	2.22	0.58
1:S:571:LEU:CD2	1:S:623:PHE:CE2	2.87	0.58
2:C:522:LEU:O	2:C:699:ARG:NH2	2.37	0.58
2:D:213:ASN:ND2	2:D:240:LEU:O	2.36	0.58
2:G:278:GLU:OE1	2:G:281:ARG:NH2	2.34	0.58
1:S:555:CYS:HA	1:S:558:VAL:CG2	2.34	0.58
1:S:574:VAL:HG11	1:S:922:ILE:CD1	2.34	0.58
1:S:604:MET:HE3	1:S:608:LEU:HD21	1.85	0.58
1:T:329:LYS:NZ	1:T:339:ILE:O	2.36	0.58
2:G:373:VAL:HG11	2:G:418:LEU:HD11	1.86	0.58
1:P:457:ASP:HA	1:P:475:LEU:HD21	1.84	0.58
2:N:180:GLU:HA	2:N:183:TRP:HB3	1.85	0.58
1:P:105:LYS:HD3	1:P:213:CYS:HB3	1.86	0.58
1:Q:735:GLY:O	1:Q:739:SER:OG	2.20	0.58
1:S:611:VAL:CG2	1:S:619:PHE:HE2	2.17	0.58
2:J:228:PRO:HB2	2:J:230:TRP:CD1	2.38	0.58
2:J:671:GLU:OE2	2:K:58:GLN:NE2	2.36	0.58
2:M:236:ASN:ND2	2:M:238:GLN:OE1	2.37	0.58
2:N:794:ARG:HH22	2:N:798:VAL:HG22	1.69	0.58
1:P:128:ARG:HG3	1:P:131:LYS:HE2	1.86	0.58
1:R:34:GLN:HB3	1:R:37:LEU:HB2	1.84	0.58
1:R:331:LYS:HE2	1:R:334:PRO:HA	1.84	0.58
2:J:234:MET:HA	2:J:239:GLN:HE22	1.69	0.58
2:N:527:ARG:NH1	2:N:793:TYR:O	2.37	0.58
2:F:689:GLN:OE1	2:F:726:ARG:NH1	2.35	0.57
2:M:486:VAL:HG23	2:M:632:LEU:HB3	1.86	0.57
1:P:330:VAL:HG13	1:P:344:VAL:HG12	1.85	0.57
1:Q:425:MET:SD	1:Q:477:ASN:HB3	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:358:LEU:HD21	1:S:732:LEU:HB3	1.84	0.57
2:B:491:GLY:HA3	2:G:122:ALA:HB2	1.86	0.57
2:C:162:GLU:HA	2:C:303:LEU:HD11	1.86	0.57
2:E:34:PHE:HB3	2:F:190:GLN:HE21	1.69	0.57
2:G:99:GLN:NE2	2:G:759:SER:OG	2.37	0.57
2:G:778:ASP:OD1	2:G:781:ARG:NH2	2.37	0.57
2:I:99:GLN:HG3	2:I:763:HIS:HD1	1.67	0.57
2:I:152:HIS:CG	2:I:748:ASP:HB3	2.38	0.57
2:J:422:PHE:N	2:J:467:ASP:O	2.32	0.57
1:O:142:ALA:HB2	1:O:147:ARG:HH21	1.67	0.57
1:P:886:LEU:O	1:P:912:ASN:ND2	2.38	0.57
1:R:786:VAL:HB	1:R:841:LEU:HD21	1.85	0.57
1:S:202:GLU:HA	1:S:205:LYS:HG2	1.85	0.57
2:D:418:LEU:N	2:D:462:TRP:O	2.37	0.57
2:G:160:SER:OG	2:G:163:GLU:OE1	2.22	0.57
2:G:160:SER:N	2:G:163:GLU:OE2	2.30	0.57
2:I:472:GLU:HB2	2:I:500:GLY:H	1.68	0.57
2:M:426:LYS:HD3	2:M:427:PRO:HD2	1.85	0.57
1:R:757:TYR:HB3	1:R:930:ASP:HA	1.85	0.57
1:A:654:THR:CG2	1:O:743:PHE:HB2	2.34	0.57
1:A:765:MET:O	1:A:773:LYS:NZ	2.37	0.57
2:C:478:GLU:OE2	2:C:610:ARG:NH2	2.37	0.57
2:E:213:ASN:ND2	2:E:240:LEU:O	2.38	0.57
2:E:466:VAL:HG23	2:E:492:ILE:HG21	1.85	0.57
2:I:534:ILE:HA	2:I:689:GLN:HG2	1.85	0.57
2:N:269:GLU:OE2	2:N:295:TYR:OH	2.21	0.57
1:P:755:ARG:NH1	1:P:766:ALA:O	2.38	0.57
1:R:636:ARG:HD2	1:R:717:LEU:HD21	1.86	0.57
1:R:758:ARG:NH2	1:R:926:SER:O	2.37	0.57
1:S:639:ARG:NH2	1:S:714:GLU:OE1	2.37	0.57
1:A:450:ILE:HG12	1:A:482:LEU:HD13	1.86	0.57
2:B:424:LYS:HB2	2:B:438:LEU:HD21	1.86	0.57
2:G:609:MET:HG2	2:G:612:LEU:HD13	1.85	0.57
2:N:22:GLU:O	2:N:290:ARG:NH2	2.33	0.57
1:O:359:ARG:NE	1:O:792:LEU:O	2.37	0.57
1:Q:538:TYR:O	1:Q:553:ARG:NH1	2.37	0.57
1:S:573:MET:SD	1:S:621:SER:HB2	2.44	0.57
1:S:865:VAL:O	1:S:869:ASN:ND2	2.37	0.57
2:N:209:GLN:O	2:N:213:ASN:ND2	2.37	0.57
1:Q:438:GLN:HG3	1:R:309:GLN:HG2	1.87	0.57
1:T:744:ASN:HB3	1:T:781:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:VAL:O	2:B:384:HIS:NE2	2.34	0.57
2:D:485:ARG:HG3	2:D:521:PRO:HG3	1.86	0.57
2:F:6:LEU:O	2:F:300:ASN:ND2	2.31	0.57
2:M:152:HIS:CD2	2:M:356:ARG:HG3	2.39	0.57
1:P:78:ARG:HH12	1:Q:289:MET:HE1	1.70	0.57
1:Q:348:ILE:HG22	1:Q:368:VAL:HG22	1.87	0.57
1:S:538:TYR:OH	1:S:656:ILE:O	2.23	0.57
1:A:278:LYS:O	1:A:278:LYS:HG2	2.05	0.57
2:B:230:TRP:CD1	2:B:230:TRP:H	2.23	0.57
2:D:433:TYR:HA	2:D:666:ARG:NH1	2.19	0.57
2:I:517:LEU:HD11	2:I:696:MET:HE1	1.85	0.57
1:O:353:ARG:NH1	1:O:360:GLU:OE1	2.38	0.57
2:E:445:GLN:HA	2:E:448:ILE:HD12	1.86	0.57
2:J:424:LYS:HA	2:J:438:LEU:HD11	1.87	0.57
2:L:586:ARG:HD2	2:N:605:GLN:HE21	1.69	0.57
2:M:23:VAL:HG23	2:M:286:GLU:HG3	1.86	0.57
2:M:228:PRO:HG2	2:M:230:TRP:CE2	2.39	0.57
1:P:289:MET:HE3	1:P:293:LEU:HG	1.86	0.57
1:P:570:PHE:HB2	1:P:573:MET:HB3	1.87	0.57
1:Q:332:THR:HG21	1:Q:342:ILE:HD11	1.86	0.57
1:R:776:ARG:HG2	1:R:780:LEU:HD12	1.87	0.57
1:A:791:SER:HB2	1:A:839:HIS:HE1	1.70	0.57
2:D:220:ARG:HD2	2:D:228:PRO:HG3	1.85	0.57
2:F:18:VAL:HG11	2:F:28:ARG:HH22	1.70	0.57
2:F:176:LEU:HD11	2:F:205:LYS:HD3	1.87	0.57
2:G:22:GLU:O	2:G:290:ARG:NH2	2.36	0.57
2:G:720:SER:HB2	2:G:771:LYS:HG3	1.86	0.57
2:N:548:SER:OG	2:N:674:GLU:OE2	2.21	0.57
1:Q:330:VAL:HG23	1:Q:344:VAL:HG12	1.85	0.57
1:Q:370:GLU:OE2	1:Q:477:ASN:ND2	2.38	0.57
1:R:168:THR:O	1:S:172:TYR:OH	2.22	0.57
1:S:114:LYS:HA	1:T:239:LYS:HD2	1.85	0.57
1:T:182:LYS:HZ1	1:T:199:ILE:HD13	1.69	0.57
2:B:410:HIS:CE1	2:B:413:CYS:HB2	2.39	0.56
2:B:696:MET:HG3	2:B:741:MET:HE1	1.86	0.56
2:G:210:ILE:HG23	2:G:240:LEU:HD12	1.87	0.56
2:K:146:GLU:OE2	2:K:791:ARG:NH1	2.38	0.56
2:C:193:ALA:HB1	2:D:35:LEU:HD21	1.87	0.56
2:C:466:VAL:HG21	2:C:487:LEU:HD13	1.86	0.56
2:G:668:GLN:NE2	2:G:671:GLU:OE1	2.38	0.56
2:I:152:HIS:CD2	2:I:356:ARG:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:551:MET:HE2	2:J:675:VAL:HG21	1.86	0.56
1:P:90:VAL:HG23	1:P:106:CYS:HB2	1.86	0.56
1:Q:482:LEU:HD23	1:Q:485:GLN:HE21	1.69	0.56
1:Q:502:LEU:HA	1:Q:738:TRP:HZ3	1.69	0.56
1:T:159:GLN:HB2	1:T:182:LYS:HZ3	1.70	0.56
2:C:42:ARG:NH2	2:D:42:ARG:H	2.02	0.56
2:C:69:PRO:HD2	2:C:289:GLU:HG2	1.87	0.56
2:E:794:ARG:HH22	2:E:798:VAL:HG12	1.71	0.56
2:J:7:ASN:ND2	2:J:104:ARG:O	2.38	0.56
2:J:748:ASP:OD1	2:J:749:ASP:N	2.37	0.56
2:K:440:LYS:NZ	2:K:615:GLU:OE2	2.38	0.56
2:L:560:LEU:HD12	2:L:580:ALA:HA	1.87	0.56
2:N:469:ALA:HB2	2:N:498:HIS:HB3	1.86	0.56
1:O:348:ILE:HD13	1:O:383:LEU:HD13	1.86	0.56
2:J:116:VAL:O	2:J:281:ARG:NH2	2.38	0.56
2:K:371:PHE:HA	2:K:397:ILE:HD13	1.86	0.56
2:K:402:ASP:OD1	2:K:458:ARG:NH2	2.38	0.56
2:L:215:ARG:NH1	2:L:269:GLU:OE1	2.38	0.56
1:T:18:LEU:HD13	1:T:384:GLN:HA	1.88	0.56
2:C:152:HIS:CG	2:C:748:ASP:HB3	2.40	0.56
2:C:210:ILE:O	2:C:214:ILE:HG12	2.04	0.56
2:L:428:LYS:HG3	2:L:437:LEU:HD22	1.88	0.56
2:L:578:SER:OG	2:N:568:ARG:NH1	2.38	0.56
2:N:501:GLU:HG3	2:N:532:THR:HB	1.87	0.56
1:P:854:PHE:HE1	1:P:914:ILE:HG13	1.71	0.56
1:Q:355:GLY:HA3	1:Q:417:LEU:HD13	1.88	0.56
1:Q:424:SER:HA	1:R:304:VAL:HG21	1.88	0.56
1:R:227:PHE:HD2	1:R:260:LEU:HD13	1.70	0.56
1:A:637:CYS:SG	1:A:638:GLU:N	2.78	0.56
2:D:233:SER:HB3	2:D:247:HIS:HB2	1.87	0.56
2:E:233:SER:O	2:E:239:GLN:NE2	2.38	0.56
1:O:121:ILE:HG12	1:O:233:VAL:HG22	1.87	0.56
1:Q:865:VAL:O	1:Q:869:ASN:ND2	2.38	0.56
1:R:624:ASN:O	1:R:628:ALA:N	2.37	0.56
1:S:721:ASN:OD1	1:S:722:GLU:N	2.39	0.56
1:T:320:LYS:HG2	1:T:345:ARG:HH21	1.71	0.56
1:A:604:MET:HE1	1:A:917:LEU:HD12	1.87	0.56
1:A:755:ARG:NH1	1:A:766:ALA:O	2.37	0.56
2:F:102:MET:HA	2:F:102:MET:HE3	1.87	0.56
2:I:213:ASN:ND2	2:I:240:LEU:O	2.38	0.56
2:J:140:GLU:OE2	2:J:758:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:469:GLN:HA	1:O:476:ARG:HE	1.70	0.56
1:S:34:GLN:NE2	1:S:311:LYS:O	2.39	0.56
2:F:192:CYS:SG	2:F:193:ALA:N	2.78	0.56
2:J:58:GLN:O	2:J:62:GLN:HG3	2.06	0.56
2:J:507:ILE:HG21	2:J:563:ILE:HD11	1.88	0.56
2:L:211:ALA:HB2	2:L:298:ILE:HG21	1.87	0.56
2:M:227:LEU:HG	2:M:231:ILE:HD13	1.88	0.56
2:M:451:ASP:OD1	2:M:452:MET:N	2.39	0.56
2:M:649:MET:HA	2:M:649:MET:HE3	1.86	0.56
1:R:234:LEU:HD22	1:R:301:LEU:HD21	1.87	0.56
1:S:262:ARG:O	1:S:266:TYR:HD2	1.87	0.56
1:S:429:ILE:O	1:S:433:GLY:N	2.38	0.56
2:G:728:MET:HB3	2:G:730:LEU:HD13	1.88	0.56
2:D:563:ILE:HG23	2:D:567:LEU:HD12	1.87	0.56
2:E:501:GLU:OE2	2:E:530:HIS:HB3	2.06	0.56
2:F:748:ASP:OD1	2:F:749:ASP:N	2.38	0.56
2:I:710:ASN:HA	2:I:751:GLY:HA3	1.86	0.56
2:L:357:PHE:HE1	2:L:418:LEU:HB3	1.70	0.56
2:N:177:ARG:NH2	2:N:178:ASP:OD1	2.39	0.56
1:Q:205:LYS:HE3	1:Q:245:LYS:HE3	1.88	0.56
1:Q:538:TYR:OH	1:Q:656:ILE:O	2.23	0.56
1:S:367:TYR:OH	1:S:467:ARG:NH2	2.39	0.56
1:T:366:MET:O	1:T:370:GLU:N	2.30	0.56
1:A:156:HIS:HE2	1:A:206:ARG:HG3	1.70	0.55
2:F:592:PHE:HE1	2:F:659:TRP:HB2	1.70	0.55
2:L:44:LEU:HD21	2:M:546:PRO:HD3	1.87	0.55
1:O:539:MET:CE	1:O:557:VAL:HG21	2.36	0.55
1:P:309:GLN:NE2	1:P:310:LEU:O	2.38	0.55
1:P:721:ASN:OD1	1:P:722:GLU:N	2.39	0.55
1:R:472:SER:HB3	1:R:475:LEU:HB2	1.88	0.55
1:S:485:GLN:O	1:S:489:ASN:ND2	2.39	0.55
1:S:554:CYS:SG	1:S:571:LEU:HD22	2.46	0.55
2:C:543:ARG:NH2	2:C:721:GLU:OE2	2.39	0.55
2:C:671:GLU:OE1	2:D:58:GLN:NE2	2.40	0.55
2:G:148:LEU:HB2	2:G:350:VAL:HG22	1.86	0.55
1:A:192:GLY:O	1:T:128:ARG:NH1	2.40	0.55
1:A:608:LEU:HD22	1:A:650:ILE:HG22	1.87	0.55
2:E:11:LEU:HD11	2:E:29:VAL:HG23	1.87	0.55
2:I:522:LEU:O	2:I:699:ARG:NH2	2.39	0.55
2:N:286:GLU:HA	2:N:289:GLU:HB3	1.88	0.55
1:R:527:LYS:HG2	1:R:531:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:790:GLU:HB2	1:R:794:HIS:HE1	1.71	0.55
1:A:887:LEU:HD23	1:A:892:TRP:HE3	1.70	0.55
2:G:214:ILE:HG21	2:G:295:TYR:HB2	1.88	0.55
2:M:630:LYS:HB3	1:S:158:ALA:HB2	1.88	0.55
1:O:658:PRO:O	1:O:661:SER:OG	2.22	0.55
1:O:802:ILE:O	1:O:807:ARG:NH2	2.39	0.55
1:R:549:HIS:HA	1:R:552:ASN:HD21	1.71	0.55
1:T:159:GLN:HB2	1:T:182:LYS:NZ	2.21	0.55
1:A:654:THR:HG21	1:O:743:PHE:HB2	1.88	0.55
2:L:507:ILE:HG21	2:L:563:ILE:HD11	1.88	0.55
1:O:574:VAL:HB	1:O:620:CYS:HB2	1.89	0.55
1:Q:313:MET:HE2	1:Q:376:VAL:HG13	1.89	0.55
1:S:574:VAL:CG1	1:S:922:ILE:HG12	2.36	0.55
1:S:611:VAL:HG23	1:S:619:PHE:HE2	1.70	0.55
1:T:313:MET:HE2	1:T:379:LEU:HD22	1.88	0.55
1:A:195:ASP:OD2	1:T:128:ARG:NH2	2.39	0.55
2:F:14:ARG:NH1	2:F:28:ARG:O	2.39	0.55
2:I:285:PRO:HG2	2:I:288:LEU:HB2	1.88	0.55
2:J:421:HIS:ND1	2:J:421:HIS:O	2.40	0.55
2:N:464:ARG:O	2:N:494:HIS:HB2	2.07	0.55
1:O:783:LEU:HD22	1:O:846:ILE:HA	1.88	0.55
1:P:717:LEU:HA	1:P:720:VAL:HG12	1.88	0.55
1:R:75:ASP:N	1:R:308:ILE:O	2.34	0.55
1:R:819:LYS:HA	1:R:822:LYS:HE2	1.87	0.55
1:S:107:LEU:HA	1:S:132:MET:HE1	1.88	0.55
1:A:146:TYR:OH	2:L:21:ASP:O	2.25	0.55
2:D:173:GLU:O	2:D:177:ARG:NH1	2.40	0.55
2:D:373:VAL:HG11	2:D:418:LEU:HD21	1.88	0.55
2:E:719:VAL:HG11	2:E:763:HIS:CE1	2.41	0.55
2:J:579:ASP:OD1	2:L:568:ARG:NH1	2.39	0.55
1:T:278:LYS:O	1:T:278:LYS:HG2	2.07	0.55
1:T:413:VAL:HA	1:T:416:LEU:HG	1.89	0.55
2:B:507:ILE:HG21	2:B:563:ILE:HD11	1.89	0.55
2:G:152:HIS:CD2	2:G:356:ARG:HG3	2.41	0.55
2:I:354:GLU:N	2:I:354:GLU:OE2	2.40	0.55
1:Q:282:ARG:NH2	1:Q:285:GLU:OE1	2.33	0.55
1:Q:599:LEU:HD23	1:Q:912:ASN:HA	1.89	0.55
1:R:418:ARG:NE	1:R:485:GLN:OE1	2.40	0.55
1:S:512:ASN:O	1:S:516:THR:OG1	2.24	0.55
1:T:636:ARG:NH1	1:T:721:ASN:OD1	2.40	0.55
2:B:142:TYR:OH	2:B:787:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:GLU:OE1	2:C:281:ARG:NH2	2.40	0.55
2:E:690:GLN:NE2	2:E:738:ASP:OD1	2.30	0.55
2:J:456:GLU:OE2	2:J:458:ARG:NH2	2.38	0.55
2:B:493:ALA:O	2:B:523:ARG:NH2	2.40	0.55
2:J:121:PRO:O	2:J:124:GLN:NE2	2.32	0.55
2:J:756:ASP:OD1	2:J:757:LEU:N	2.40	0.55
1:R:73:PHE:HE2	1:R:254:LEU:HD12	1.72	0.55
2:J:211:ALA:HB2	2:J:298:ILE:HG21	1.89	0.54
2:M:455:SER:OG	2:M:456:GLU:OE1	2.26	0.54
2:D:659:TRP:HA	2:D:665:VAL:HG11	1.90	0.54
2:F:788:GLU:OE1	2:F:791:ARG:NH1	2.40	0.54
1:O:452:THR:HA	1:O:455:LYS:HE2	1.90	0.54
1:Q:570:PHE:HB2	1:Q:573:MET:HB2	1.90	0.54
1:R:21:PRO:HB2	1:R:23:LEU:HD13	1.87	0.54
1:S:581:ARG:HH21	1:S:584:MET:HE3	1.72	0.54
1:T:117:ARG:HH22	1:T:229:ALA:HA	1.71	0.54
2:C:40:GLN:O	2:D:42:ARG:NH2	2.40	0.54
2:C:214:ILE:HD12	2:C:291:LEU:HD11	1.89	0.54
2:M:6:LEU:O	2:M:300:ASN:ND2	2.40	0.54
1:O:713:VAL:HA	1:O:849:PRO:HG2	1.88	0.54
1:Q:105:LYS:HE3	1:Q:211:LEU:HB3	1.88	0.54
1:Q:738:TRP:HD1	1:Q:741:PHE:HB3	1.68	0.54
1:A:501:LEU:HD23	1:A:738:TRP:HE3	1.72	0.54
1:A:656:ILE:HG12	1:O:461:ASN:CG	2.32	0.54
2:B:758:LYS:HE2	2:B:762:TYR:HE2	1.71	0.54
2:C:518:ARG:NH2	2:C:608:GLU:OE1	2.40	0.54
2:D:152:HIS:CD2	2:D:356:ARG:HG3	2.42	0.54
2:E:582:ILE:HD11	2:K:564:TRP:HH2	1.72	0.54
2:F:530:HIS:CE1	2:F:706:PRO:HB3	2.42	0.54
2:G:155:LEU:O	2:G:337:ARG:NH2	2.40	0.54
2:G:176:LEU:HD22	2:G:205:LYS:HG3	1.90	0.54
2:G:466:VAL:HG23	2:G:492:ILE:HG21	1.90	0.54
2:L:659:TRP:HA	2:L:665:VAL:HG11	1.90	0.54
1:O:733:LEU:HD13	1:O:793:TYR:HB2	1.89	0.54
1:P:107:LEU:HD11	1:P:128:ARG:HB3	1.89	0.54
1:P:225:THR:HG23	1:Q:297:TYR:HE1	1.72	0.54
1:A:189:TYR:HB2	1:T:131:LYS:NZ	2.22	0.54
1:Q:390:LYS:HA	1:Q:416:LEU:HD11	1.89	0.54
1:R:569:VAL:HG13	1:R:753:LYS:HE2	1.90	0.54
1:S:80:ALA:HA	1:S:376:VAL:HB	1.90	0.54
1:S:558:VAL:HG11	1:S:571:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:658:PRO:O	1:S:661:SER:OG	2.25	0.54
1:S:783:LEU:HB3	1:S:842:PHE:HE1	1.73	0.54
1:T:765:MET:O	1:T:773:LYS:NZ	2.40	0.54
2:B:45:PRO:HG2	2:B:48:VAL:HB	1.89	0.54
2:C:725:PHE:HB3	2:C:730:LEU:HD12	1.90	0.54
2:F:178:ASP:OD2	2:F:323:MET:N	2.40	0.54
2:N:7:ASN:HD21	2:N:304:THR:HG21	1.72	0.54
1:O:290:VAL:HA	1:O:293:LEU:HD12	1.90	0.54
1:O:581:ARG:HH21	1:O:923:VAL:HG22	1.73	0.54
1:O:614:ASN:OD1	1:O:615:ASN:N	2.40	0.54
1:R:775:MET:HE2	1:R:917:LEU:HD22	1.90	0.54
1:A:372:LEU:HA	1:A:379:LEU:HD11	1.88	0.54
2:C:58:GLN:NE2	2:D:672:TYR:O	2.40	0.54
2:D:158:SER:O	2:D:337:ARG:NH2	2.40	0.54
2:D:260:ILE:HG22	2:D:262:ASP:H	1.73	0.54
2:D:561:VAL:HG11	2:D:607:PHE:CD2	2.42	0.54
2:E:511:ARG:NH1	2:E:515:ASP:OD2	2.40	0.54
2:M:481:CYS:SG	2:M:519:PHE:HB3	2.48	0.54
1:O:173:LYS:HB2	1:O:176:TYR:CD2	2.43	0.54
1:Q:49:ILE:HG22	1:Q:214:LYS:HE2	1.90	0.54
1:Q:227:PHE:HD2	1:Q:260:LEU:HD13	1.73	0.54
1:R:654:THR:CG2	1:S:461:ASN:CB	2.86	0.54
1:T:265:GLN:HB2	1:T:290:VAL:HG13	1.89	0.54
2:B:19:SER:O	2:B:290:ARG:NH1	2.41	0.54
2:E:278:GLU:OE1	2:E:281:ARG:NH2	2.41	0.54
2:I:443:LYS:NZ	2:I:615:GLU:OE2	2.41	0.54
2:M:142:TYR:HE2	2:M:787:ASN:HD22	1.56	0.54
1:P:740:ARG:HB2	1:P:785:ALA:HB1	1.90	0.54
2:C:191:LEU:HD11	2:C:308:GLN:HB3	1.88	0.54
2:J:214:ILE:HG12	2:J:291:LEU:HD22	1.90	0.54
2:L:527:ARG:NH2	2:L:704:GLU:OE2	2.34	0.54
2:M:223:GLN:NE2	2:M:259:PRO:HD3	2.23	0.54
2:M:654:LYS:HA	2:M:657:LYS:NZ	2.23	0.54
1:O:485:GLN:O	1:O:489:ASN:ND2	2.41	0.54
1:O:834:THR:HG21	1:O:836:LYS:HE2	1.88	0.54
1:P:34:GLN:HE22	1:P:310:LEU:HB3	1.73	0.54
1:P:502:LEU:HB3	1:P:550:TRP:HZ3	1.73	0.54
1:Q:69:ARG:NH2	1:Q:242:ASN:OD1	2.40	0.54
1:Q:748:VAL:HG12	1:Q:811:VAL:HG13	1.89	0.54
1:S:554:CYS:SG	1:S:571:LEU:CD2	2.96	0.54
1:T:304:VAL:HA	1:T:307:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:GLU:HB2	2:C:757:LEU:HD22	1.89	0.54
2:C:614:ALA:HB2	2:C:660:LEU:HD13	1.89	0.54
2:E:152:HIS:CD2	2:E:356:ARG:HG3	2.43	0.54
2:G:152:HIS:CG	2:G:748:ASP:HB3	2.42	0.54
1:Q:255:ARG:NH2	1:Q:259:GLN:OE1	2.40	0.54
1:Q:381:GLN:HE22	1:Q:424:SER:HB2	1.73	0.54
1:R:319:GLU:HB3	1:R:322:LYS:HB3	1.90	0.54
1:S:86:ILE:HD11	1:S:251:THR:HB	1.90	0.54
1:S:303:PRO:HB2	1:S:306:LYS:HG2	1.89	0.54
1:A:579:LYS:NZ	1:O:750:ASP:O	2.36	0.53
2:C:543:ARG:HH22	2:C:717:ARG:H	1.55	0.53
2:J:154:HIS:O	2:J:337:ARG:NH1	2.41	0.53
2:M:435:HIS:HB2	2:M:479:LEU:HD11	1.89	0.53
2:M:622:GLU:OE1	2:M:623:LEU:N	2.41	0.53
1:O:839:HIS:HB3	1:O:842:PHE:HB3	1.89	0.53
1:P:277:GLU:OE1	1:P:286:ARG:NH1	2.41	0.53
1:A:239:LYS:HG2	1:T:114:LYS:HG2	1.89	0.53
1:A:320:LYS:HD3	1:A:345:ARG:HH21	1.73	0.53
1:A:764:ARG:O	1:A:863:CYS:N	2.33	0.53
2:D:146:GLU:OE2	2:D:149:HIS:NE2	2.36	0.53
2:J:84:GLU:HG3	2:J:89:LYS:HB2	1.89	0.53
2:J:527:ARG:HG2	2:J:702:ALA:HB3	1.90	0.53
2:N:65:MET:HE1	2:N:74:ARG:HH11	1.74	0.53
1:O:539:MET:HE1	1:O:557:VAL:CG2	2.38	0.53
1:O:879:ASP:OD2	1:O:885:LYS:NZ	2.41	0.53
1:P:201:GLU:OE2	1:P:205:LYS:NZ	2.37	0.53
1:P:656:ILE:HD12	1:P:656:ILE:H	1.70	0.53
1:S:112:PRO:HB3	1:S:121:ILE:HD11	1.90	0.53
1:S:443:MET:HE2	1:S:499:GLN:HG3	1.90	0.53
1:A:163:GLY:HA3	1:A:196:LEU:HD13	1.89	0.53
2:C:416:LEU:HD21	2:C:418:LEU:HG	1.89	0.53
2:K:155:LEU:HD23	2:K:337:ARG:HD2	1.90	0.53
2:M:770:ARG:HH11	2:M:770:ARG:HG3	1.73	0.53
2:C:690:GLN:HA	2:C:693:MET:HG3	1.89	0.53
2:D:534:ILE:HG21	2:D:692:VAL:HG11	1.90	0.53
2:E:63:ARG:HB2	2:E:65:MET:HG2	1.90	0.53
2:F:234:MET:HA	2:F:234:MET:HE3	1.90	0.53
2:I:116:VAL:HG21	2:I:277:LEU:HB2	1.90	0.53
2:K:362:ASP:HB3	2:K:365:LYS:HB2	1.91	0.53
1:O:104:ILE:HG12	1:O:215:ALA:HB3	1.91	0.53
2:N:130:TRP:HE1	2:N:340:HIS:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:547:LEU:HD12	2:N:677:LEU:HB3	1.90	0.53
1:Q:93:LEU:HD22	1:Q:106:CYS:HB3	1.91	0.53
1:A:147:ARG:HB3	1:A:148:LYS:HZ2	1.74	0.53
1:A:593:ILE:HD11	1:O:806:LEU:HD13	1.91	0.53
2:C:569:SER:HB3	2:F:575:ARG:HG2	1.90	0.53
2:D:9:THR:HG22	2:D:301:GLN:HE21	1.73	0.53
2:E:150:GLU:OE2	2:E:747:SER:N	2.34	0.53
2:E:211:ALA:HB2	2:E:298:ILE:HG21	1.90	0.53
2:N:6:LEU:O	2:N:300:ASN:ND2	2.32	0.53
1:O:448:LYS:O	1:O:452:THR:N	2.40	0.53
1:P:165:HIS:O	1:P:168:THR:OG1	2.25	0.53
1:P:652:GLN:HG2	1:Q:789:GLU:OE2	2.09	0.53
1:Q:856:PHE:HA	1:Q:861:ILE:HD11	1.90	0.53
1:T:501:LEU:HD13	1:T:737:VAL:HG23	1.91	0.53
2:F:55:TYR:HD1	2:F:58:GLN:HE21	1.56	0.53
2:L:228:PRO:O	2:L:229:GLU:HG3	2.09	0.53
1:O:259:GLN:OE1	1:O:262:ARG:NH2	2.42	0.53
1:R:234:LEU:HD12	1:R:261:ILE:HD11	1.91	0.53
1:A:189:TYR:HB2	1:T:131:LYS:HZ2	1.73	0.53
2:C:162:GLU:OE2	2:C:299:GLN:NE2	2.42	0.53
2:C:453:LEU:HA	2:C:459:LEU:HD23	1.91	0.53
2:D:563:ILE:HG12	2:D:688:LEU:HD11	1.89	0.53
2:E:719:VAL:HG11	2:E:763:HIS:HE1	1.74	0.53
2:E:756:ASP:OD1	2:E:757:LEU:N	2.41	0.53
2:F:143:ILE:HG12	2:F:148:LEU:HD21	1.90	0.53
2:G:12:LEU:HD12	2:G:297:LEU:HB3	1.89	0.53
2:I:148:LEU:HB3	2:I:757:LEU:HD23	1.91	0.53
2:M:554:GLU:HB3	2:M:669:ARG:HB3	1.90	0.53
1:O:14:ILE:HB	1:O:328:ILE:HG12	1.89	0.53
1:Q:217:LEU:HD13	1:Q:247:VAL:HG13	1.89	0.53
1:S:170:LYS:CD	1:S:171:GLU:OE2	2.57	0.53
1:S:569:VAL:HG13	1:S:569:VAL:O	2.09	0.53
1:S:573:MET:SD	1:S:619:PHE:CD1	3.02	0.53
2:E:111:ILE:HG21	2:E:128:PHE:CD2	2.43	0.53
1:Q:206:ARG:O	1:Q:210:ILE:HG12	2.09	0.53
1:S:597:ASN:O	1:S:601:LYS:N	2.36	0.53
2:D:176:LEU:HD12	2:D:179:PHE:HB3	1.91	0.53
2:I:501:GLU:OE2	2:I:530:HIS:ND1	2.42	0.53
2:I:533:ALA:O	2:I:689:GLN:NE2	2.42	0.53
2:J:5:LEU:HD22	2:J:72:ILE:HD11	1.91	0.53
2:L:693:MET:HB3	2:L:739:VAL:HB	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:766:ALA:HB1	1:O:812:THR:HB	1.90	0.53
1:R:330:VAL:HG13	1:R:344:VAL:HG12	1.90	0.53
1:A:455:LYS:HD2	1:A:532:ILE:HG12	1.90	0.52
2:C:527:ARG:NH1	2:C:744:CYS:SG	2.82	0.52
2:G:501:GLU:HG3	2:G:532:THR:HB	1.91	0.52
2:G:530:HIS:NE2	2:G:748:ASP:OD2	2.40	0.52
2:N:356:ARG:HD3	2:N:419:VAL:HB	1.91	0.52
2:N:356:ARG:NH1	2:N:467:ASP:OD2	2.42	0.52
1:O:130:ASN:HD22	1:P:181:LEU:CG	2.22	0.52
1:O:152:GLN:O	1:O:156:HIS:ND1	2.26	0.52
1:O:278:LYS:O	1:O:278:LYS:HG2	2.09	0.52
1:O:337:GLN:HB2	1:O:339:ILE:HG12	1.90	0.52
1:Q:149:GLN:HA	1:Q:152:GLN:CD	2.33	0.52
1:T:75:ASP:O	1:T:310:LEU:N	2.40	0.52
1:A:439:HIS:HD2	1:O:314:LEU:HD23	1.73	0.52
1:A:888:SER:OG	1:A:889:ASP:N	2.42	0.52
2:F:791:ARG:O	2:F:794:ARG:NH1	2.36	0.52
2:G:356:ARG:NH1	2:G:467:ASP:OD2	2.42	0.52
2:K:381:LEU:HD12	2:K:385:MET:HG3	1.92	0.52
1:O:205:LYS:HA	1:O:245:LYS:HZ1	1.73	0.52
1:Q:117:ARG:HH22	1:Q:229:ALA:HB2	1.74	0.52
1:R:594:ASP:OD1	1:R:594:ASP:N	2.42	0.52
2:B:9:THR:HG21	2:B:196:ASP:HB2	1.91	0.52
2:B:575:ARG:HD2	2:D:569:SER:HB3	1.91	0.52
2:F:116:VAL:O	2:F:281:ARG:NH2	2.36	0.52
2:J:58:GLN:NE2	2:K:672:TYR:O	2.42	0.52
2:K:149:HIS:CE1	2:K:791:ARG:HB2	2.44	0.52
2:K:285:PRO:HG2	2:K:288:LEU:HB2	1.92	0.52
2:L:176:LEU:HD22	2:L:205:LYS:HG3	1.91	0.52
1:P:758:ARG:HA	1:P:927:TYR:HB3	1.92	0.52
1:S:733:LEU:O	1:S:737:VAL:HG13	2.09	0.52
1:T:318:GLY:O	1:T:345:ARG:NH1	2.43	0.52
2:K:153:GLN:O	2:K:356:ARG:N	2.40	0.52
2:K:570:HIS:HE1	2:K:687:ALA:HB1	1.74	0.52
2:L:529:GLY:HA2	2:L:704:GLU:HB2	1.92	0.52
1:O:846:ILE:HD11	1:O:881:ILE:HG21	1.92	0.52
1:A:527:LYS:HA	1:A:530:GLN:HG2	1.92	0.52
2:C:659:TRP:HA	2:C:665:VAL:HG11	1.91	0.52
2:D:489:LYS:HE3	2:D:632:LEU:HD12	1.90	0.52
1:P:552:ASN:ND2	1:P:653:THR:HG21	2.24	0.52
1:P:856:PHE:HB2	1:P:887:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:540:SER:HA	1:Q:543:ARG:CZ	2.39	0.52
1:Q:910:PHE:HD2	1:Q:915:THR:HG22	1.75	0.52
1:R:347:ALA:O	1:R:387:TYR:OH	2.27	0.52
1:T:452:THR:HA	1:T:455:LYS:HD3	1.90	0.52
2:E:410:HIS:CE1	2:E:412:LYS:HB2	2.44	0.52
2:F:729:GLY:HA2	2:F:734:ALA:HB2	1.91	0.52
2:L:581:ALA:HB1	2:L:600:ILE:HG12	1.92	0.52
2:N:207:ARG:HB3	2:N:298:ILE:HD11	1.92	0.52
1:O:162:ARG:O	1:O:165:HIS:NE2	2.42	0.52
1:P:277:GLU:HB2	1:P:286:ARG:HH12	1.74	0.52
1:P:658:PRO:O	1:P:661:SER:OG	2.22	0.52
1:Q:73:PHE:HE2	1:Q:254:LEU:HB2	1.75	0.52
1:T:612:ALA:HB1	1:T:616:LEU:HD13	1.91	0.52
1:T:886:LEU:O	1:T:912:ASN:ND2	2.43	0.52
1:A:608:LEU:HA	1:A:620:CYS:HA	1.91	0.52
2:C:155:LEU:O	2:C:337:ARG:NH1	2.42	0.52
2:C:311:ASP:OD2	2:C:712:ARG:NH1	2.42	0.52
2:F:450:MET:SD	2:F:490:SER:OG	2.61	0.52
2:F:464:ARG:HH21	2:F:494:HIS:CE1	2.28	0.52
2:G:6:LEU:O	2:G:300:ASN:ND2	2.39	0.52
1:O:535:TYR:O	1:O:539:MET:HB2	2.10	0.52
1:P:816:GLU:HA	1:P:819:LYS:HE2	1.91	0.52
1:R:497:PHE:O	1:R:501:LEU:N	2.39	0.52
1:R:540:SER:HA	1:R:543:ARG:HH11	1.74	0.52
2:C:7:ASN:HD22	2:C:104:ARG:HG3	1.75	0.52
2:F:102:MET:HE1	2:F:107:CYS:HB3	1.91	0.52
1:P:513:GLN:OE1	1:P:742:TYR:OH	2.28	0.52
1:R:234:LEU:HD11	1:R:257:TYR:HD2	1.75	0.52
1:T:78:ARG:NH2	1:T:255:ARG:HH22	2.08	0.52
1:T:564:ASP:N	1:T:564:ASP:OD1	2.43	0.52
2:B:466:VAL:HG21	2:B:487:LEU:HD13	1.91	0.52
2:D:425:ARG:H	2:D:438:LEU:HD13	1.74	0.52
2:I:501:GLU:OE1	2:I:501:GLU:N	2.43	0.52
2:J:517:LEU:HD13	2:J:695:LYS:HG3	1.91	0.52
2:M:510:ILE:HG21	2:M:688:LEU:HB3	1.92	0.52
1:O:353:ARG:O	1:O:358:LEU:N	2.40	0.52
1:R:159:GLN:OE1	1:R:189:TYR:OH	2.27	0.52
1:T:807:ARG:HG3	1:T:820:LYS:HE3	1.92	0.52
1:A:740:ARG:HH21	1:T:652:GLN:HB3	1.75	0.52
2:B:342:HIS:ND1	2:B:348:SER:CB	2.73	0.52
2:B:690:GLN:HA	2:B:693:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:157:GLY:O	2:K:337:ARG:NH2	2.43	0.52
2:L:435:HIS:HD2	2:L:438:LEU:HD23	1.75	0.52
2:N:424:LYS:HB2	2:N:470:ALA:HB3	1.92	0.52
1:O:226:GLN:HA	1:P:268:ASN:HD21	1.75	0.52
1:O:581:ARG:HE	1:O:923:VAL:HG22	1.75	0.52
1:Q:224:ASP:HB3	1:Q:256:LEU:HG	1.92	0.52
1:Q:444:ASP:N	1:Q:444:ASP:OD1	2.43	0.52
1:R:843:PHE:O	1:R:847:SER:OG	2.25	0.52
1:S:425:MET:HE2	1:S:428:SER:HB2	1.92	0.52
1:S:914:ILE:HG21	1:S:917:LEU:HB2	1.92	0.52
1:T:613:SER:HB3	1:T:656:ILE:HA	1.91	0.52
1:T:846:ILE:O	1:T:852:HIS:NE2	2.40	0.52
1:A:172:TYR:H	1:T:118:HIS:HB3	1.74	0.51
1:A:454:VAL:HG11	1:A:508:VAL:HG21	1.92	0.51
2:D:649:MET:HE2	2:D:652:PRO:HG2	1.92	0.51
2:F:730:LEU:HD11	2:F:768:LEU:HD22	1.92	0.51
2:I:216:GLU:OE2	2:I:263:LYS:NZ	2.38	0.51
2:K:613:LEU:HG	2:K:615:GLU:H	1.73	0.51
2:M:748:ASP:OD1	2:M:749:ASP:N	2.38	0.51
1:O:448:LYS:HB2	1:O:542:GLY:HA3	1.91	0.51
1:P:510:ILE:HD11	1:P:558:VAL:HG12	1.92	0.51
1:R:235:GLU:OE1	1:R:238:ARG:NH1	2.43	0.51
1:A:861:ILE:HG21	1:A:896:THR:HG22	1.93	0.51
2:D:797:ASP:OD1	2:D:798:VAL:N	2.42	0.51
2:I:716:TYR:OH	2:I:723:HIS:ND1	2.34	0.51
2:J:27:GLU:OE2	2:K:186:GLN:NE2	2.41	0.51
2:J:99:GLN:HG3	2:J:763:HIS:ND1	2.25	0.51
2:M:356:ARG:HD3	2:M:419:VAL:HB	1.92	0.51
2:N:91:ASP:OD2	2:N:93:PRO:HD2	2.10	0.51
2:N:213:ASN:ND2	2:N:240:LEU:O	2.43	0.51
1:P:465:TYR:OH	1:P:739:SER:OG	2.27	0.51
1:R:415:ASN:HA	1:R:418:ARG:HH11	1.75	0.51
1:S:106:CYS:HA	1:S:217:LEU:HB3	1.91	0.51
1:T:329:LYS:HE3	1:T:341:ALA:HB3	1.93	0.51
2:D:534:ILE:HD12	2:D:741:MET:HE1	1.93	0.51
2:G:523:ARG:N	2:G:526:ASP:OD2	2.44	0.51
2:M:165:TRP:HB2	2:M:303:LEU:HD21	1.93	0.51
2:M:221:VAL:HG21	2:M:288:LEU:HD13	1.91	0.51
2:N:148:LEU:HD13	2:N:757:LEU:HG	1.93	0.51
1:O:227:PHE:HB2	1:O:260:LEU:HD12	1.92	0.51
1:P:854:PHE:CE1	1:P:914:ILE:HG13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:612:LEU:HD11	2:D:643:LEU:HD11	1.91	0.51
2:G:789:ASN:HA	2:G:792:ILE:HB	1.93	0.51
2:J:60:ILE:HD12	2:J:71:ALA:HB1	1.91	0.51
2:J:360:LYS:H	2:J:366:MET:HE2	1.75	0.51
2:K:167:ASP:HA	2:K:170:LYS:HE2	1.92	0.51
2:L:77:ALA:HB1	2:L:114:HIS:HB2	1.92	0.51
2:L:752:ILE:HD11	2:L:755:ALA:HB2	1.92	0.51
1:O:114:LYS:HD3	1:P:239:LYS:HG2	1.92	0.51
1:P:928:ASP:OD1	1:P:929:LYS:N	2.43	0.51
1:R:539:MET:HA	1:R:553:ARG:HG2	1.92	0.51
1:T:765:MET:HB2	1:T:768:GLN:HG3	1.92	0.51
2:C:5:LEU:HD22	2:C:293:TRP:HZ2	1.75	0.51
2:D:686:VAL:O	2:D:690:GLN:HG2	2.11	0.51
2:D:789:ASN:HD22	2:D:792:ILE:HG13	1.75	0.51
2:F:394:PRO:HB3	2:F:399:GLN:HB2	1.92	0.51
2:F:435:HIS:CD2	2:F:475:ALA:HB2	2.46	0.51
2:K:379:GLU:O	2:K:382:SER:OG	2.28	0.51
2:N:690:GLN:HG2	2:N:693:MET:HE3	1.91	0.51
1:O:366:MET:HE1	1:O:469:GLN:CD	2.36	0.51
1:O:563:ASN:ND2	1:O:569:VAL:O	2.44	0.51
1:Q:524:ASP:HB3	1:Q:527:LYS:HB3	1.93	0.51
1:S:237:ILE:HG22	1:S:301:LEU:HD11	1.93	0.51
1:A:289:MET:SD	1:T:255:ARG:NE	2.67	0.51
2:C:215:ARG:NH2	2:C:268:SER:OG	2.44	0.51
2:D:792:ILE:HA	2:N:141:ASP:OD2	2.11	0.51
2:F:556:ARG:HH22	2:F:679:TYR:HE2	1.59	0.51
2:F:680:LEU:HB3	2:F:684:ALA:HB3	1.92	0.51
2:I:527:ARG:HG2	2:I:702:ALA:HB3	1.93	0.51
2:J:689:GLN:O	2:J:693:MET:HG3	2.11	0.51
2:K:145:ARG:HE	2:L:791:ARG:HH21	1.58	0.51
2:L:572:GLU:HG2	2:L:573:LEU:HD12	1.92	0.51
2:M:533:ALA:O	2:M:689:GLN:NE2	2.44	0.51
1:O:202:GLU:HA	1:O:205:LYS:HG2	1.91	0.51
1:O:538:TYR:CE2	1:O:539:MET:SD	3.04	0.51
1:T:136:LYS:NZ	1:T:140:TYR:OH	2.43	0.51
1:T:857:PRO:HA	1:T:913:THR:HG23	1.92	0.51
1:A:166:LEU:HD21	1:T:116:PRO:HD3	1.93	0.51
2:B:554:GLU:HB2	2:B:669:ARG:HB3	1.93	0.51
2:F:309:ARG:NH1	2:F:309:ARG:O	2.40	0.51
2:F:347:TYR:OH	2:K:409:PRO:O	2.21	0.51
2:F:451:ASP:OD1	2:F:452:MET:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:451:ASP:OD1	2:J:452:MET:N	2.43	0.51
2:K:690:GLN:NE2	2:K:736:GLU:O	2.44	0.51
2:L:152:HIS:CD2	2:L:356:ARG:HD3	2.46	0.51
2:M:707:PRO:HG3	2:M:747:SER:HA	1.93	0.51
2:N:85:LYS:HD3	2:N:135:TYR:CZ	2.46	0.51
1:O:789:GLU:OE1	1:O:789:GLU:N	2.42	0.51
1:O:828:LEU:HD21	1:O:838:THR:HG21	1.92	0.51
1:P:490:CYS:HB3	1:P:729:PRO:HG2	1.93	0.51
1:P:647:ASN:ND2	1:Q:806:LEU:HA	2.26	0.51
1:P:765:MET:HB3	1:P:768:GLN:HG3	1.92	0.51
1:P:786:VAL:O	1:P:790:GLU:HB3	2.11	0.51
1:T:861:ILE:HG13	1:T:895:LEU:HD21	1.92	0.51
2:B:360:LYS:HB2	2:B:366:MET:HB2	1.92	0.51
2:B:649:MET:HG2	2:B:650:LYS:H	1.76	0.51
2:C:102:MET:HE3	2:C:102:MET:HA	1.93	0.51
2:C:666:ARG:HD2	2:C:669:ARG:HH21	1.75	0.51
2:J:5:LEU:HD11	2:J:53:TRP:HZ3	1.76	0.51
2:J:450:MET:HE2	2:J:450:MET:HA	1.92	0.51
2:K:88:PRO:HG3	2:K:126:TYR:CZ	2.46	0.51
2:L:728:MET:HE1	2:L:786:VAL:HG21	1.93	0.51
2:N:108:LEU:HD21	2:N:269:GLU:HG2	1.93	0.51
1:R:227:PHE:HZ	1:S:269:TYR:HD1	1.59	0.51
1:S:116:PRO:HG2	1:S:119:GLU:HB2	1.92	0.51
1:T:815:ASP:OD1	1:T:815:ASP:N	2.42	0.51
1:A:716:TRP:HZ2	1:A:844:LEU:HA	1.75	0.51
2:F:705:CYS:SG	2:F:724:ILE:HD12	2.51	0.51
2:G:346:VAL:O	2:G:384:HIS:NE2	2.31	0.51
2:K:207:ARG:NH1	2:K:301:GLN:OE1	2.44	0.51
2:K:216:GLU:OE2	2:K:263:LYS:NZ	2.38	0.51
2:L:745:LEU:HG	2:L:757:LEU:HD11	1.92	0.51
2:M:303:LEU:HB3	2:M:753:PHE:CE1	2.45	0.51
2:N:506:LEU:HD13	2:N:536:ILE:HD11	1.91	0.51
1:O:256:LEU:HD11	1:P:293:LEU:HD21	1.92	0.51
1:R:163:GLY:HA2	1:R:166:LEU:HB2	1.93	0.51
1:S:14:ILE:HB	1:S:328:ILE:HG12	1.92	0.51
1:A:784:HIS:ND1	1:A:810:PRO:HD3	2.26	0.51
2:B:424:LYS:HG2	2:B:470:ALA:HB3	1.93	0.51
2:D:788:GLU:OE2	2:D:791:ARG:NH2	2.44	0.51
2:G:642:GLU:O	2:G:646:THR:HG23	2.11	0.51
2:K:111:ILE:HG22	2:K:270:PHE:HE1	1.76	0.51
2:M:93:PRO:HA	2:M:770:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:454:VAL:HG23	1:R:463:GLY:HA3	1.92	0.51
1:R:570:PHE:N	1:R:573:MET:O	2.32	0.51
1:T:418:ARG:NH2	1:T:485:GLN:OE1	2.44	0.51
1:A:750:ASP:OD2	1:T:615:ASN:CB	2.59	0.50
1:A:868:LEU:HD11	1:A:896:THR:HB	1.92	0.50
2:E:222:ALA:O	2:E:279:LYS:NZ	2.43	0.50
2:F:370:LEU:HD11	2:F:463:ILE:HD11	1.93	0.50
2:G:18:VAL:HG11	2:G:25:LEU:HD21	1.92	0.50
2:G:19:SER:O	2:G:290:ARG:NH1	2.45	0.50
2:G:717:ARG:HD2	2:I:543:ARG:HG2	1.93	0.50
2:L:426:LYS:HA	2:L:474:HIS:CD2	2.43	0.50
2:N:527:ARG:HG2	2:N:702:ALA:HB3	1.92	0.50
1:O:888:SER:O	1:O:892:TRP:NE1	2.44	0.50
1:P:762:HIS:ND1	1:P:762:HIS:O	2.44	0.50
1:S:570:PHE:CD1	1:S:617:MET:CE	2.94	0.50
1:S:576:LEU:HD22	1:S:920:SER:HB2	1.93	0.50
2:C:213:ASN:ND2	2:C:240:LEU:O	2.44	0.50
2:C:551:MET:HE1	2:C:675:VAL:HG21	1.93	0.50
2:D:464:ARG:O	2:D:494:HIS:HB2	2.11	0.50
2:J:719:VAL:HG21	2:J:763:HIS:HE2	1.75	0.50
2:K:150:GLU:OE1	2:K:151:THR:N	2.43	0.50
1:O:19:PHE:CE2	1:O:334:PRO:HD3	2.46	0.50
1:O:372:LEU:HA	1:O:379:LEU:HD22	1.93	0.50
1:P:77:THR:HB	1:P:80:ALA:HB3	1.93	0.50
1:Q:552:ASN:OD1	1:Q:553:ARG:N	2.44	0.50
1:T:196:LEU:HB3	1:T:240:PHE:HE1	1.75	0.50
1:A:489:ASN:HB3	1:A:496:LYS:HE3	1.93	0.50
2:B:149:HIS:CE1	2:B:791:ARG:HD3	2.46	0.50
2:B:727:TRP:HB3	2:B:743:ILE:HD11	1.92	0.50
2:C:641:ARG:HH12	2:C:657:LYS:NZ	2.09	0.50
2:F:356:ARG:HB3	2:F:421:HIS:HD2	1.77	0.50
2:J:261:ASP:OD1	2:J:262:ASP:N	2.44	0.50
2:J:349:GLN:HG3	2:J:350:VAL:HG23	1.92	0.50
2:L:215:ARG:NH2	2:L:263:LYS:O	2.44	0.50
2:L:396:THR:O	2:L:400:VAL:HG23	2.12	0.50
2:L:424:LYS:HB3	2:L:470:ALA:HB3	1.92	0.50
2:M:18:VAL:HG11	2:M:25:LEU:HD11	1.93	0.50
1:Q:863:CYS:HB3	1:Q:868:LEU:HD22	1.94	0.50
1:R:446:LEU:HD23	1:R:500:MET:HE3	1.93	0.50
1:S:18:LEU:HD13	1:S:384:GLN:HA	1.93	0.50
1:A:359:ARG:NH2	1:A:791:SER:O	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:396:THR:O	2:J:400:VAL:HG23	2.12	0.50
2:K:425:ARG:H	2:K:438:LEU:HD12	1.75	0.50
2:L:422:PHE:N	2:L:467:ASP:O	2.39	0.50
2:N:330:THR:O	2:N:372:SER:HB2	2.12	0.50
2:N:662:SER:HB3	2:N:665:VAL:HB	1.93	0.50
1:O:161:GLN:OE1	1:P:178:SER:OG	2.28	0.50
1:Q:859:GLY:HA3	1:Q:918:ASN:HD22	1.76	0.50
1:S:610:THR:OG1	1:S:618:ASP:OD1	2.27	0.50
1:T:237:ILE:HA	1:T:241:PHE:HB2	1.92	0.50
1:T:914:ILE:HB	1:T:917:LEU:HB2	1.93	0.50
1:A:235:GLU:OE2	1:A:297:TYR:OH	2.27	0.50
2:D:228:PRO:O	2:D:229:GLU:HG2	2.12	0.50
2:E:221:VAL:HG21	2:E:288:LEU:HD13	1.94	0.50
2:I:548:SER:OG	2:I:674:GLU:OE1	2.29	0.50
1:O:426:LEU:HD13	1:P:254:LEU:HD11	1.94	0.50
1:S:121:ILE:HG13	1:S:233:VAL:HG22	1.94	0.50
1:S:318:GLY:O	1:S:345:ARG:NH1	2.33	0.50
2:D:152:HIS:CG	2:D:748:ASP:HB3	2.46	0.50
2:D:446:ALA:O	2:D:450:MET:HG2	2.11	0.50
2:G:663:ASP:OD1	2:G:663:ASP:N	2.44	0.50
2:M:147:CYS:HB2	2:M:351:ARG:HB2	1.93	0.50
1:O:654:THR:HG23	1:O:654:THR:O	2.12	0.50
1:P:162:ARG:NH2	1:P:180:ALA:CA	2.75	0.50
1:S:755:ARG:NH1	1:S:766:ALA:O	2.45	0.50
1:A:316:LEU:HD22	1:A:326:GLU:OE1	2.12	0.50
2:I:210:ILE:HA	2:I:213:ASN:HD22	1.76	0.50
2:K:138:THR:HG22	2:K:780:LEU:HD22	1.92	0.50
2:M:756:ASP:OD1	2:M:757:LEU:N	2.43	0.50
2:N:141:ASP:OD1	2:N:142:TYR:N	2.45	0.50
1:O:468:PRO:O	1:O:476:ARG:HG3	2.12	0.50
1:O:553:ARG:NH1	1:O:654:THR:O	2.44	0.50
1:P:319:GLU:HB2	1:P:322:LYS:HB2	1.94	0.50
1:P:588:TYR:HB3	1:P:921:THR:HG22	1.93	0.50
1:A:567:ILE:HG22	1:A:569:VAL:HG12	1.94	0.50
2:I:160:SER:HB2	2:I:754:ALA:HA	1.94	0.50
2:I:604:ASP:O	2:I:608:GLU:HG2	2.12	0.50
2:I:662:SER:HB2	2:I:665:VAL:HB	1.94	0.50
2:J:530:HIS:NE2	2:J:748:ASP:OD2	2.39	0.50
1:P:858:VAL:HG13	1:P:913:THR:HG21	1.93	0.50
1:R:318:GLY:O	1:R:345:ARG:NH1	2.45	0.50
2:D:360:LYS:N	2:D:366:MET:SD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:ASP:OD1	2:K:794:ARG:NH1	2.43	0.50
2:K:487:LEU:HB3	2:K:492:ILE:HG13	1.93	0.50
2:M:625:GLU:OE2	2:M:628:LYS:NZ	2.44	0.50
2:N:102:MET:HA	2:N:102:MET:HE3	1.92	0.50
1:O:610:THR:O	1:O:655:CYS:SG	2.67	0.50
1:P:423:GLY:HA2	1:P:426:LEU:HB2	1.93	0.50
1:P:471:GLU:O	1:P:476:ARG:NH2	2.45	0.50
1:R:727:ILE:HG12	1:R:729:PRO:HD3	1.93	0.50
1:T:277:GLU:OE1	1:T:282:ARG:HD2	2.12	0.50
1:A:251:THR:O	1:A:257:TYR:OH	2.27	0.49
2:E:493:ALA:HB1	2:I:85:LYS:HA	1.93	0.49
2:I:160:SER:OG	2:I:163:GLU:OE1	2.27	0.49
2:K:3:ARG:HD3	2:K:104:ARG:HG3	1.94	0.49
2:K:80:PHE:HD2	2:K:98:TRP:HB2	1.77	0.49
2:L:70:VAL:HG23	2:L:277:LEU:HD22	1.94	0.49
2:L:228:PRO:HB2	2:L:230:TRP:NE1	2.27	0.49
2:N:710:ASN:ND2	2:N:749:ASP:O	2.45	0.49
1:O:103:ASN:OD1	1:O:105:LYS:NZ	2.39	0.49
1:P:32:LEU:HD22	1:P:38:ARG:HH11	1.77	0.49
1:P:348:ILE:HG22	1:P:383:LEU:HD13	1.93	0.49
1:S:776:ARG:NE	1:S:855:ILE:O	2.43	0.49
1:S:928:ASP:OD1	1:S:929:LYS:N	2.45	0.49
1:A:71:VAL:HG22	1:A:248:VAL:HB	1.94	0.49
1:A:192:GLY:HA3	1:T:128:ARG:HA	1.92	0.49
2:E:724:ILE:HG12	2:E:728:MET:HE2	1.94	0.49
2:E:791:ARG:HH12	2:I:145:ARG:HH11	1.60	0.49
2:F:690:GLN:NE2	2:F:736:GLU:O	2.44	0.49
2:G:424:LYS:HD3	2:G:480:PHE:HZ	1.77	0.49
2:I:366:MET:HG3	2:I:448:ILE:HG21	1.94	0.49
2:J:647:THR:HA	2:N:590:LYS:HE2	1.94	0.49
2:K:6:LEU:O	2:K:300:ASN:ND2	2.25	0.49
2:N:183:TRP:O	2:N:189:LYS:NZ	2.42	0.49
1:Q:114:LYS:O	1:Q:115:LEU:HD12	2.12	0.49
1:Q:446:LEU:HD21	1:Q:486:VAL:HG22	1.94	0.49
1:T:616:LEU:N	1:T:616:LEU:CD2	2.73	0.49
1:T:750:ASP:HA	1:T:753:LYS:HE3	1.94	0.49
1:A:764:ARG:HB3	1:A:863:CYS:HB2	1.92	0.49
2:C:617:GLU:O	2:C:657:LYS:NZ	2.35	0.49
2:E:572:GLU:HG2	2:E:573:LEU:HG	1.93	0.49
2:F:649:MET:HE2	2:F:649:MET:HA	1.94	0.49
2:M:83:ASN:HD21	2:M:120:GLY:HA2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:200:THR:H	2:N:203:ILE:HB	1.77	0.49
1:O:237:ILE:HA	1:O:241:PHE:HD2	1.76	0.49
1:P:431:ARG:HA	1:R:282:ARG:HH12	1.76	0.49
1:P:788:VAL:HG23	1:P:802:ILE:HG21	1.93	0.49
1:R:223:ILE:HD12	1:R:227:PHE:HB2	1.94	0.49
1:T:116:PRO:HG2	1:T:119:GLU:HB2	1.93	0.49
2:D:6:LEU:O	2:D:300:ASN:ND2	2.29	0.49
2:E:161:ALA:HB1	2:E:303:LEU:HD12	1.93	0.49
2:F:464:ARG:O	2:F:494:HIS:HB2	2.12	0.49
2:I:151:THR:HA	2:I:354:GLU:OE1	2.13	0.49
2:J:285:PRO:HG2	2:J:288:LEU:HB2	1.93	0.49
2:L:155:LEU:O	2:L:337:ARG:NH2	2.45	0.49
2:L:657:LYS:O	2:L:661:THR:OG1	2.29	0.49
2:N:233:SER:O	2:N:239:GLN:NE2	2.31	0.49
1:S:173:LYS:HD2	1:S:176:TYR:HE2	1.78	0.49
1:S:741:PHE:O	1:S:745:LEU:HG	2.13	0.49
1:S:834:THR:OG1	1:S:837:ASN:OD1	2.30	0.49
1:A:738:TRP:O	1:A:742:TYR:N	2.44	0.49
1:A:889:ASP:N	1:A:889:ASP:OD1	2.45	0.49
2:D:138:THR:HG22	2:D:780:LEU:HD22	1.95	0.49
2:D:282:PHE:HE2	1:S:152:GLN:HG3	1.78	0.49
2:L:5:LEU:HD22	2:L:72:ILE:HG13	1.95	0.49
1:Q:93:LEU:HD21	1:Q:104:ILE:HG13	1.95	0.49
1:Q:852:HIS:HD2	1:Q:855:ILE:HD12	1.77	0.49
1:S:198:GLU:O	1:S:201:GLU:HG2	2.13	0.49
1:S:228:ASP:OD1	1:S:229:ALA:N	2.45	0.49
1:A:656:ILE:HD11	1:O:460:PHE:CB	2.42	0.49
2:B:649:MET:HG2	2:B:650:LYS:N	2.28	0.49
2:C:3:ARG:NH1	2:C:100:THR:O	2.33	0.49
2:G:717:ARG:HD3	2:I:544:SER:HB3	1.95	0.49
2:J:643:LEU:O	2:J:647:THR:HG22	2.12	0.49
2:K:356:ARG:NH1	2:K:467:ASP:OD2	2.45	0.49
2:K:476:PRO:HG2	2:K:479:LEU:HB2	1.93	0.49
2:M:251:GLU:HA	1:P:186:GLN:HB2	1.94	0.49
1:O:231:TRP:HE3	1:O:260:LEU:HD21	1.77	0.49
1:O:536:VAL:HA	1:O:541:VAL:HG12	1.95	0.49
1:P:162:ARG:CZ	1:P:180:ALA:HA	2.43	0.49
1:P:426:LEU:HD22	1:Q:254:LEU:HD22	1.93	0.49
1:P:887:LEU:HB3	1:P:892:TRP:HB2	1.95	0.49
1:Q:257:TYR:O	1:Q:261:ILE:HG12	2.13	0.49
1:Q:443:MET:N	1:Q:443:MET:SD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:738:TRP:HD1	1:Q:738:TRP:O	1.96	0.49
1:T:202:GLU:N	1:T:202:GLU:OE2	2.46	0.49
1:T:378:LEU:HD21	1:T:425:MET:SD	2.52	0.49
1:T:612:ALA:CB	1:T:616:LEU:HA	2.43	0.49
1:A:78:ARG:HD3	1:O:296:GLN:HB2	1.93	0.49
2:B:93:PRO:HB3	2:B:770:ARG:HH22	1.77	0.49
2:B:651:ARG:HB3	2:B:652:PRO:HD3	1.93	0.49
2:D:693:MET:SD	2:D:741:MET:HE3	2.52	0.49
2:F:228:PRO:HB2	2:F:230:TRP:CZ3	2.48	0.49
2:J:69:PRO:HD2	2:J:289:GLU:HG2	1.94	0.49
1:O:108:PRO:HB2	1:P:191:ILE:HG22	1.95	0.49
1:R:440:ARG:HH11	1:S:373:LYS:HG2	1.78	0.49
1:R:553:ARG:NH1	1:R:655:CYS:HA	2.28	0.49
1:S:254:LEU:HA	1:S:257:TYR:HB2	1.95	0.49
1:S:555:CYS:CA	1:S:558:VAL:HG22	2.42	0.49
1:A:599:LEU:CB	1:A:911:GLN:HB3	2.42	0.49
1:A:645:ALA:HA	1:A:648:LYS:HZ3	1.76	0.49
2:D:592:PHE:HB2	2:D:594:LEU:HD23	1.95	0.49
2:E:672:TYR:O	2:F:58:GLN:NE2	2.46	0.49
2:I:481:CYS:SG	2:I:519:PHE:HB3	2.53	0.49
2:J:176:LEU:HD11	2:J:205:LYS:HB2	1.95	0.49
2:L:381:LEU:HD22	2:L:385:MET:HE3	1.94	0.49
2:N:532:THR:HG23	2:N:723:HIS:CE1	2.48	0.49
1:Q:280:SER:HA	1:Q:283:LEU:HD23	1.94	0.49
1:Q:552:ASN:HD22	1:Q:649:VAL:HG23	1.78	0.49
1:R:720:VAL:HG22	1:R:844:LEU:HD22	1.94	0.49
1:R:842:PHE:HE2	1:R:881:ILE:HG12	1.77	0.49
1:S:446:LEU:HD21	1:S:485:GLN:HE22	1.77	0.49
1:A:858:VAL:HG12	1:A:895:LEU:HD22	1.95	0.49
2:B:99:GLN:HG3	2:B:763:HIS:ND1	2.28	0.49
2:B:674:GLU:HB2	2:N:55:TYR:CZ	2.48	0.49
2:C:785:GLU:HA	2:C:788:GLU:HG2	1.95	0.49
2:E:152:HIS:CG	2:E:748:ASP:HB3	2.48	0.49
2:F:357:PHE:HE2	2:F:418:LEU:HB3	1.78	0.49
2:G:647:THR:O	2:G:650:LYS:NZ	2.45	0.49
2:J:14:ARG:HH11	2:J:32:SER:HB2	1.77	0.49
2:M:108:LEU:HD21	2:M:269:GLU:HG2	1.93	0.49
2:M:211:ALA:HB2	2:M:298:ILE:HG21	1.95	0.49
2:N:278:GLU:OE1	2:N:281:ARG:NH2	2.37	0.49
2:N:481:CYS:SG	2:N:519:PHE:HB3	2.52	0.49
1:R:314:LEU:HA	1:R:317:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:30:ASP:OD1	1:T:31:ASP:N	2.46	0.49
1:T:277:GLU:O	1:T:286:ARG:NH1	2.46	0.49
1:T:771:ALA:HB3	1:T:918:ASN:HA	1.95	0.49
2:F:466:VAL:HG21	2:F:487:LEU:HD13	1.94	0.49
2:G:560:LEU:HB3	2:G:584:ALA:HB2	1.95	0.49
2:G:717:ARG:N	2:G:721:GLU:OE2	2.46	0.49
2:L:359:PRO:HG3	2:L:422:PHE:HD1	1.78	0.49
2:M:46:ASP:OD1	2:M:47:HIS:N	2.46	0.49
2:N:663:ASP:OD1	2:N:664:ASN:N	2.45	0.49
1:O:159:GLN:HA	1:O:162:ARG:HG2	1.94	0.49
1:Q:776:ARG:HD2	1:Q:860:GLY:O	2.13	0.49
1:R:438:GLN:NE2	1:S:310:LEU:O	2.45	0.49
1:R:452:THR:HA	1:R:455:LYS:HE2	1.94	0.49
1:T:196:LEU:HB3	1:T:240:PHE:CE1	2.47	0.49
1:A:72:PHE:HA	1:A:306:LYS:HB3	1.95	0.48
2:D:386:SER:C	2:D:387:MET:HE2	2.37	0.48
2:J:451:ASP:HA	2:J:454:LYS:HG2	1.94	0.48
2:L:85:LYS:HD2	2:L:135:TYR:CZ	2.49	0.48
1:R:563:ASN:HB2	1:R:567:ILE:HG22	1.94	0.48
1:S:168:THR:HG21	1:T:172:TYR:HD2	1.77	0.48
1:S:170:LYS:HE2	1:S:171:GLU:OE2	2.13	0.48
1:A:136:LYS:HG3	1:A:211:LEU:HD23	1.94	0.48
2:B:85:LYS:HD2	2:B:135:TYR:CZ	2.47	0.48
2:B:111:ILE:HG12	2:B:132:LEU:HD11	1.95	0.48
2:C:563:ILE:HG12	2:C:688:LEU:HD21	1.96	0.48
2:L:405:GLU:OE1	2:L:458:ARG:NH1	2.46	0.48
2:M:107:CYS:N	2:M:162:GLU:OE2	2.41	0.48
1:O:332:THR:OG1	1:O:333:GLU:OE1	2.26	0.48
1:O:425:MET:SD	1:O:477:ASN:HB3	2.53	0.48
1:P:255:ARG:HH11	1:Q:289:MET:HE3	1.78	0.48
1:P:857:PRO:HA	1:P:913:THR:HG23	1.95	0.48
1:Q:117:ARG:NE	1:Q:226:GLN:OE1	2.46	0.48
1:Q:810:PRO:HB3	1:Q:816:GLU:HB2	1.96	0.48
1:R:414:PRO:HB2	1:R:488:GLU:HB2	1.95	0.48
1:R:762:HIS:ND1	1:R:762:HIS:O	2.46	0.48
1:S:122:LEU:HA	1:S:125:VAL:HG12	1.96	0.48
1:S:277:GLU:HB3	1:S:286:ARG:HH22	1.78	0.48
2:C:25:LEU:HD11	2:C:290:ARG:CZ	2.43	0.48
2:C:595:GLU:HA	2:M:649:MET:HE1	1.94	0.48
2:M:366:MET:HE1	2:M:449:LEU:HB2	1.95	0.48
2:N:192:CYS:HB3	2:N:199:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:500:MET:O	1:O:505:CYS:N	2.46	0.48
1:Q:585:PRO:HG2	1:Q:758:ARG:HD3	1.95	0.48
1:T:41:LEU:HD21	1:T:308:ILE:HG13	1.95	0.48
1:T:145:ASP:OD1	1:T:146:TYR:N	2.46	0.48
1:T:347:ALA:O	1:T:387:TYR:OH	2.31	0.48
1:T:744:ASN:HD21	1:T:810:PRO:HD2	1.77	0.48
1:T:811:VAL:HG12	1:T:812:THR:HG23	1.95	0.48
1:T:928:ASP:OD1	1:T:928:ASP:N	2.46	0.48
1:A:484:SER:O	1:A:487:SER:OG	2.31	0.48
2:G:360:LYS:HB2	2:G:366:MET:HB2	1.96	0.48
2:G:503:PHE:O	2:I:47:HIS:NE2	2.45	0.48
2:I:402:ASP:OD1	2:I:458:ARG:NH1	2.47	0.48
2:L:63:ARG:HB3	2:L:65:MET:HE3	1.95	0.48
1:T:743:PHE:HA	1:T:746:ASN:HD21	1.78	0.48
1:A:740:ARG:HH22	1:T:651:ALA:HB1	1.78	0.48
2:B:150:GLU:HG2	2:B:757:LEU:HD22	1.94	0.48
2:F:693:MET:HG2	2:F:741:MET:CE	2.43	0.48
2:I:69:PRO:HD2	2:I:289:GLU:OE2	2.13	0.48
2:M:797:ASP:N	2:M:797:ASP:OD1	2.46	0.48
2:N:451:ASP:OD1	2:N:452:MET:N	2.46	0.48
1:O:313:MET:HE2	1:O:379:LEU:HD11	1.94	0.48
1:S:74:VAL:O	1:S:82:LYS:NZ	2.47	0.48
2:E:207:ARG:HB3	2:E:298:ILE:HD12	1.96	0.48
2:E:659:TRP:HA	2:E:665:VAL:HG11	1.96	0.48
2:F:497:TYR:O	2:F:529:GLY:N	2.39	0.48
2:G:451:ASP:OD1	2:G:452:MET:N	2.47	0.48
2:J:3:ARG:HH21	2:J:104:ARG:HG3	1.78	0.48
2:M:419:VAL:HG13	2:M:465:GLY:C	2.38	0.48
2:N:150:GLU:HG2	2:N:153:GLN:HB2	1.94	0.48
1:S:772:ALA:HB1	1:S:857:PRO:HB2	1.96	0.48
1:T:156:HIS:O	1:T:160:LEU:HD23	2.13	0.48
1:T:717:LEU:HA	1:T:720:VAL:HG12	1.94	0.48
2:B:152:HIS:ND1	2:B:748:ASP:OD2	2.46	0.48
2:D:792:ILE:HD13	2:N:141:ASP:OD2	2.13	0.48
2:E:150:GLU:HB3	2:E:353:LEU:HD12	1.95	0.48
2:E:232:ALA:O	2:E:235:GLN:NE2	2.46	0.48
2:E:505:HIS:CD2	2:E:549:LEU:HD12	2.49	0.48
2:E:597:GLU:HG2	2:K:602:THR:HG21	1.95	0.48
2:F:285:PRO:HG2	2:F:288:LEU:HB2	1.95	0.48
2:G:487:LEU:HB3	2:G:492:ILE:HG13	1.96	0.48
2:J:102:MET:N	2:J:102:MET:HE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:446:ALA:O	2:L:450:MET:N	2.44	0.48
2:L:523:ARG:N	2:L:526:ASP:OD2	2.46	0.48
1:O:764:ARG:N	1:O:768:GLN:OE1	2.46	0.48
1:P:80:ALA:HA	1:P:376:VAL:HB	1.96	0.48
1:A:564:ASP:N	1:A:564:ASP:OD1	2.47	0.48
2:B:342:HIS:CE1	2:B:348:SER:CA	2.96	0.48
2:C:410:HIS:CE1	2:C:412:LYS:HD2	2.48	0.48
2:E:7:ASN:ND2	2:E:104:ARG:O	2.46	0.48
2:E:370:LEU:HD11	2:E:463:ILE:HD11	1.95	0.48
2:F:710:ASN:ND2	2:F:749:ASP:O	2.35	0.48
2:L:58:GLN:NE2	2:M:672:TYR:O	2.33	0.48
2:N:419:VAL:HG21	2:N:795:PHE:HD2	1.78	0.48
1:O:16:ILE:HG21	1:O:380:MET:HE1	1.94	0.48
1:O:426:LEU:HG	1:O:429:ILE:HD12	1.96	0.48
1:Q:846:ILE:O	1:Q:852:HIS:NE2	2.46	0.48
1:R:512:ASN:O	1:R:516:THR:OG1	2.32	0.48
1:S:835:TRP:CG	1:S:881:ILE:HD11	2.49	0.48
1:T:238:ARG:HD2	1:T:297:TYR:HE1	1.79	0.48
1:T:775:MET:HA	1:T:778:ASN:HD22	1.78	0.48
1:A:918:ASN:OD1	1:A:919:SER:N	2.47	0.48
2:E:663:ASP:OD1	2:E:664:ASN:N	2.47	0.48
2:I:450:MET:HE1	2:I:487:LEU:HD13	1.95	0.48
2:I:748:ASP:OD1	2:I:749:ASP:N	2.42	0.48
2:J:513:ILE:HG13	2:J:534:ILE:HG23	1.96	0.48
2:K:14:ARG:NH1	2:K:31:SER:OG	2.31	0.48
2:K:553:LYS:HE3	2:K:671:GLU:HG2	1.95	0.48
1:O:237:ILE:HA	1:O:241:PHE:CD2	2.48	0.48
1:Q:113:THR:HG21	1:R:238:ARG:HH22	1.78	0.48
1:Q:817:PHE:O	1:Q:821:ILE:HG12	2.14	0.48
1:R:350:ASP:OD1	1:R:353:ARG:NH1	2.46	0.48
1:R:502:LEU:HD11	1:R:626:ILE:HB	1.96	0.48
1:S:317:VAL:HG21	1:S:345:ARG:HB2	1.96	0.48
1:S:425:MET:O	1:S:425:MET:HG3	2.14	0.48
1:T:359:ARG:HH22	1:T:791:SER:C	2.22	0.48
1:T:435:ASN:HD22	1:T:445:SER:HB2	1.78	0.48
2:B:435:HIS:NE2	2:B:474:HIS:O	2.45	0.48
2:F:690:GLN:HA	2:F:693:MET:HE3	1.96	0.48
2:J:134:PRO:HD2	2:J:762:TYR:HD2	1.78	0.48
2:J:563:ILE:HG12	2:J:688:LEU:HD11	1.96	0.48
2:J:680:LEU:HD12	2:J:684:ALA:HB1	1.95	0.48
2:L:511:ARG:HH21	2:L:555:THR:HG23	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:743:ILE:H	2:M:789:ASN:HD22	1.61	0.48
1:P:237:ILE:HG23	1:P:301:LEU:HD11	1.96	0.48
1:Q:262:ARG:NE	1:R:277:GLU:OE2	2.47	0.48
1:R:543:ARG:HD3	1:S:469:GLN:HG3	1.95	0.48
1:R:836:LYS:NZ	1:R:837:ASN:OD1	2.39	0.48
1:R:856:PHE:HA	1:R:861:ILE:HD11	1.95	0.48
1:S:70:ASN:HD22	1:S:244:ARG:HA	1.79	0.48
1:S:450:ILE:HG23	1:S:466:LEU:HD11	1.95	0.48
1:A:34:GLN:NE2	1:A:311:LYS:O	2.46	0.47
2:B:430:GLY:H	2:B:666:ARG:NH2	2.08	0.47
2:C:450:MET:SD	2:C:490:SER:OG	2.70	0.47
2:D:192:CYS:HB3	2:D:199:LEU:HD23	1.96	0.47
2:F:234:MET:SD	2:F:245:ILE:HD12	2.54	0.47
2:G:39:GLU:O	2:I:42:ARG:NH1	2.46	0.47
2:I:492:ILE:HG22	2:I:494:HIS:H	1.78	0.47
2:L:498:HIS:NE2	2:L:501:GLU:OE2	2.47	0.47
1:P:440:ARG:HD2	1:Q:373:LYS:HD2	1.96	0.47
1:Q:348:ILE:HD11	1:Q:383:LEU:HD22	1.95	0.47
2:C:385:MET:HE2	2:C:413:CYS:SG	2.55	0.47
2:C:543:ARG:NH2	2:C:715:GLN:O	2.28	0.47
2:D:567:LEU:HB3	2:D:577:ALA:HB2	1.96	0.47
2:G:2:GLU:HG3	2:G:56:LEU:HD11	1.95	0.47
2:G:211:ALA:HB2	2:G:298:ILE:HG21	1.96	0.47
2:M:627:LEU:HD23	1:S:154:GLN:NE2	2.29	0.47
1:O:875:ASN:ND2	1:O:892:TRP:HZ3	2.12	0.47
1:Q:421:LEU:HD22	1:Q:425:MET:HE3	1.97	0.47
1:R:358:LEU:HD11	1:R:732:LEU:HD12	1.96	0.47
1:R:790:GLU:HB2	1:R:794:HIS:CE1	2.48	0.47
1:S:355:GLY:HA3	1:S:417:LEU:HD13	1.96	0.47
1:A:18:LEU:HD13	1:A:384:GLN:HA	1.96	0.47
1:A:791:SER:HB2	1:A:839:HIS:CE1	2.48	0.47
2:C:60:ILE:HD12	2:C:71:ALA:HB1	1.96	0.47
2:C:408:GLU:OE2	2:E:347:TYR:OH	2.30	0.47
2:E:752:ILE:HD11	2:E:755:ALA:HB2	1.96	0.47
2:F:379:GLU:OE1	2:F:382:SER:OG	2.32	0.47
2:I:151:THR:O	2:I:356:ARG:NH2	2.47	0.47
2:I:261:ASP:N	2:I:261:ASP:OD1	2.47	0.47
2:M:629:PRO:HB3	1:S:157:LEU:HB3	1.96	0.47
2:M:629:PRO:HG3	1:S:161:GLN:HE21	1.78	0.47
2:N:65:MET:HE1	2:N:74:ARG:NH1	2.30	0.47
2:N:720:SER:HB2	2:N:771:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:612:ALA:O	1:S:746:ASN:ND2	2.47	0.47
1:A:80:ALA:HA	1:A:376:VAL:HB	1.96	0.47
2:C:85:LYS:H	2:C:85:LYS:HD2	1.79	0.47
2:C:464:ARG:O	2:C:494:HIS:HB2	2.13	0.47
2:D:303:LEU:HB3	2:D:753:PHE:CE1	2.49	0.47
2:E:142:TYR:HB2	2:E:780:LEU:HD21	1.96	0.47
2:E:342:HIS:ND1	2:E:380:TYR:OH	2.37	0.47
2:I:702:ALA:HB2	2:I:793:TYR:CD2	2.49	0.47
2:J:152:HIS:ND1	2:J:748:ASP:OD2	2.47	0.47
2:L:356:ARG:HB3	2:L:421:HIS:CD2	2.49	0.47
2:M:288:LEU:HD23	2:M:291:LEU:HD12	1.97	0.47
1:Q:16:ILE:HG22	1:Q:31:ASP:HA	1.96	0.47
1:R:568:GLY:N	1:R:923:VAL:O	2.47	0.47
1:S:551:ALA:O	1:S:555:CYS:N	2.39	0.47
1:A:599:LEU:HB2	1:A:911:GLN:HB3	1.97	0.47
2:B:148:LEU:HD13	2:B:757:LEU:HG	1.94	0.47
2:D:346:VAL:HG13	2:D:347:TYR:HD1	1.79	0.47
2:D:456:GLU:OE1	2:D:458:ARG:NH2	2.48	0.47
2:J:342:HIS:HE1	2:J:384:HIS:CE1	2.32	0.47
2:J:607:PHE:HB3	2:J:610:ARG:HE	1.78	0.47
2:L:20:LEU:HD21	2:L:237:PRO:HG3	1.97	0.47
2:L:464:ARG:O	2:L:494:HIS:HB2	2.15	0.47
2:M:21:ASP:OD1	2:M:21:ASP:N	2.42	0.47
1:O:85:PHE:CD2	1:O:310:LEU:HD21	2.50	0.47
1:O:594:ASP:OD1	1:O:594:ASP:N	2.48	0.47
1:O:855:ILE:HG22	1:O:856:PHE:CE1	2.50	0.47
1:Q:289:MET:HE2	1:Q:289:MET:HA	1.97	0.47
1:Q:653:THR:O	1:Q:653:THR:HG23	2.14	0.47
1:Q:701:ASP:OD1	1:Q:701:ASP:N	2.46	0.47
1:S:539:MET:HA	1:S:553:ARG:HD2	1.96	0.47
1:T:452:THR:O	1:T:456:GLN:NE2	2.46	0.47
2:G:152:HIS:HE1	2:G:498:HIS:HD2	1.62	0.47
2:G:674:GLU:HG2	2:I:55:TYR:CZ	2.48	0.47
2:I:164:CYS:HA	2:I:167:ASP:HB2	1.97	0.47
2:M:99:GLN:HG3	2:M:763:HIS:ND1	2.28	0.47
2:N:286:GLU:CD	2:N:290:ARG:HH21	2.22	0.47
2:N:756:ASP:OD1	2:N:757:LEU:N	2.46	0.47
1:O:21:PRO:HB2	1:O:23:LEU:HG	1.97	0.47
1:Q:757:TYR:HH	1:Q:767:SER:HG	1.62	0.47
1:S:465:TYR:HB3	1:S:467:ARG:HH11	1.79	0.47
1:T:75:ASP:HB3	1:T:309:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:320:LYS:HD3	1:T:345:ARG:HE	1.80	0.47
1:T:509:SER:HB2	1:T:738:TRP:HE1	1.80	0.47
1:A:831:ASP:OD2	1:A:833:LYS:NZ	2.43	0.47
2:B:330:THR:O	2:B:372:SER:HB2	2.15	0.47
2:B:642:GLU:O	2:B:646:THR:HG23	2.15	0.47
2:C:591:VAL:HA	2:C:668:GLN:HG2	1.95	0.47
2:D:7:ASN:HD21	2:D:304:THR:HG21	1.80	0.47
2:D:152:HIS:HD2	2:D:356:ARG:HG3	1.78	0.47
2:E:234:MET:HE1	2:E:240:LEU:HD21	1.97	0.47
2:E:717:ARG:HE	2:F:717:ARG:HH22	1.62	0.47
2:F:424:LYS:HD3	2:F:480:PHE:HZ	1.79	0.47
2:F:690:GLN:HA	2:F:693:MET:HB2	1.96	0.47
2:F:784:ALA:O	2:F:788:GLU:HG2	2.14	0.47
2:G:130:TRP:NE1	2:G:343:GLY:HA2	2.29	0.47
2:I:163:GLU:OE1	2:I:163:GLU:N	2.42	0.47
2:I:259:PRO:HG2	2:I:260:ILE:HD12	1.96	0.47
2:J:483:LEU:O	2:J:486:VAL:HG12	2.15	0.47
2:K:170:LYS:HG2	2:K:264:TYR:CD2	2.50	0.47
2:K:511:ARG:HH21	2:K:555:THR:HG23	1.80	0.47
2:N:251:GLU:OE2	2:N:252:TYR:N	2.47	0.47
1:O:603:ALA:HB1	1:O:854:PHE:CE2	2.49	0.47
1:O:764:ARG:O	1:O:863:CYS:N	2.48	0.47
1:P:41:LEU:HD12	1:P:308:ILE:HD12	1.96	0.47
1:P:93:LEU:HD12	1:P:217:LEU:HD22	1.95	0.47
1:P:162:ARG:HH22	1:P:176:TYR:HB3	1.80	0.47
1:P:176:TYR:O	1:P:180:ALA:CB	2.62	0.47
1:Q:502:LEU:HA	1:Q:738:TRP:CZ3	2.49	0.47
1:Q:648:LYS:HD2	1:Q:652:GLN:HE21	1.78	0.47
1:R:422:TYR:O	1:R:426:LEU:HB2	2.15	0.47
1:S:737:VAL:HA	1:S:789:GLU:OE1	2.15	0.47
1:S:775:MET:HE1	1:S:854:PHE:HB3	1.97	0.47
1:S:784:HIS:HD1	1:S:817:PHE:HD1	1.63	0.47
1:T:511:PHE:HB2	1:T:535:TYR:CE1	2.49	0.47
1:T:791:SER:HB3	1:T:802:ILE:HD11	1.95	0.47
1:A:267:GLU:HB3	1:O:272:THR:HG21	1.96	0.47
2:B:145:ARG:HD2	2:J:791:ARG:NE	2.30	0.47
2:B:421:HIS:ND1	2:B:421:HIS:O	2.47	0.47
2:C:424:LYS:HD2	2:C:475:ALA:HB3	1.96	0.47
2:D:147:CYS:HB2	2:D:351:ARG:HB2	1.96	0.47
2:D:557:LEU:HB2	2:D:587:LEU:HD22	1.97	0.47
2:G:202:ARG:HH12	2:G:205:LYS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:475:ALA:HB1	2:G:479:LEU:HD13	1.97	0.47
2:I:195:ILE:HG13	2:I:196:ASP:N	2.30	0.47
2:M:258:TRP:HZ3	2:M:272:TRP:HB2	1.80	0.47
2:N:290:ARG:O	2:N:294:ILE:HD12	2.15	0.47
1:O:19:PHE:HE2	1:O:334:PRO:HD3	1.78	0.47
1:O:160:LEU:HD22	1:O:199:ILE:HG22	1.96	0.47
1:O:626:ILE:HG12	1:O:782:PHE:CE1	2.50	0.47
1:O:889:ASP:HA	1:O:892:TRP:CD1	2.49	0.47
1:P:423:GLY:HA2	1:P:426:LEU:HD12	1.97	0.47
1:Q:428:SER:OG	1:Q:474:ALA:O	2.33	0.47
1:Q:466:LEU:HD23	1:Q:482:LEU:HB3	1.96	0.47
1:S:45:ILE:HG13	1:S:72:PHE:CE2	2.50	0.47
1:S:574:VAL:HG11	1:S:922:ILE:HD11	1.97	0.47
2:B:102:MET:SD	2:B:107:CYS:HB3	2.54	0.47
2:D:148:LEU:HD23	2:D:787:ASN:ND2	2.30	0.47
2:E:40:GLN:O	2:F:42:ARG:NH1	2.48	0.47
2:E:538:PRO:O	2:E:542:LYS:HG3	2.14	0.47
2:F:138:THR:HG22	2:F:780:LEU:HD22	1.96	0.47
2:G:582:ILE:O	2:G:586:ARG:HG2	2.15	0.47
2:I:397:ILE:HD11	2:I:459:LEU:HD21	1.96	0.47
2:J:483:LEU:O	2:J:487:LEU:HD23	2.14	0.47
2:K:467:ASP:OD1	2:K:468:ALA:N	2.47	0.47
2:M:612:LEU:HB3	2:M:640:ALA:HB1	1.96	0.47
1:O:723:ILE:HB	1:O:844:LEU:HD11	1.96	0.47
1:Q:318:GLY:O	1:Q:345:ARG:NH1	2.44	0.47
1:Q:428:SER:OG	1:Q:478:CYS:SG	2.68	0.47
1:Q:738:TRP:CD1	1:Q:738:TRP:O	2.68	0.47
1:R:254:LEU:HD21	1:R:298:LEU:HD13	1.97	0.47
1:T:612:ALA:HB1	1:T:616:LEU:HA	1.96	0.47
1:T:847:SER:HB3	1:T:882:VAL:HG22	1.95	0.47
1:A:552:ASN:HB3	1:A:655:CYS:SG	2.55	0.47
2:B:12:LEU:HB2	2:B:297:LEU:HB3	1.95	0.47
2:C:228:PRO:HB2	2:C:230:TRP:NE1	2.30	0.47
2:D:102:MET:HE2	2:D:102:MET:HA	1.95	0.47
2:F:501:GLU:OE2	2:F:530:HIS:HB3	2.15	0.47
2:G:58:GLN:NE2	2:I:672:TYR:O	2.48	0.47
2:I:645:LYS:O	2:I:650:LYS:NZ	2.44	0.47
2:J:218:LEU:HD12	2:J:276:LEU:HD11	1.97	0.47
2:K:659:TRP:HA	2:K:665:VAL:HG11	1.96	0.47
2:L:176:LEU:HD13	2:L:205:LYS:HB2	1.96	0.47
1:P:359:ARG:NH2	1:P:791:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:431:ARG:CB	1:T:282:ARG:NH2	2.76	0.47
1:R:539:MET:HE1	1:R:550:TRP:NE1	2.30	0.47
1:S:110:ILE:HG22	1:S:128:ARG:HE	1.80	0.47
1:S:133:VAL:HG11	1:S:153:TRP:CZ2	2.50	0.47
1:A:312:THR:N	1:A:315:GLN:OE1	2.37	0.46
1:A:317:VAL:HG12	1:A:345:ARG:HH11	1.80	0.46
2:D:20:LEU:HD23	2:D:290:ARG:HD2	1.96	0.46
2:D:85:LYS:HD3	2:M:494:HIS:NE2	2.29	0.46
2:E:499:VAL:HG21	2:E:513:ILE:HD13	1.97	0.46
2:G:165:TRP:HB2	2:G:303:LEU:HD21	1.97	0.46
2:I:171:HIS:HB3	2:I:174:ALA:HB3	1.97	0.46
2:J:342:HIS:ND1	2:J:380:TYR:OH	2.28	0.46
2:L:370:LEU:HD11	2:L:463:ILE:HD11	1.96	0.46
2:M:402:ASP:OD1	2:M:458:ARG:NH1	2.47	0.46
1:P:312:THR:N	1:P:315:GLN:OE1	2.40	0.46
1:P:437:GLU:HB2	1:P:440:ARG:HB3	1.96	0.46
1:Q:94:ASN:ND2	1:Q:106:CYS:SG	2.87	0.46
1:R:107:LEU:HD12	1:R:218:ILE:HG22	1.96	0.46
1:R:632:ILE:HA	1:R:642:ILE:HG22	1.97	0.46
2:B:21:ASP:OD1	2:B:21:ASP:N	2.49	0.46
2:C:163:GLU:CD	2:C:266:GLN:HE21	2.21	0.46
2:I:483:LEU:O	2:I:487:LEU:HD23	2.15	0.46
2:N:20:LEU:HD11	2:N:291:LEU:HD21	1.97	0.46
1:O:639:ARG:NH1	1:O:714:GLU:HB3	2.31	0.46
1:P:133:VAL:HG11	1:P:153:TRP:CE2	2.50	0.46
1:P:162:ARG:NE	1:P:180:ALA:HA	2.30	0.46
1:S:716:TRP:NE1	1:S:847:SER:OG	2.42	0.46
2:B:34:PHE:CZ	2:B:50:LYS:HA	2.50	0.46
2:D:592:PHE:HA	2:D:665:VAL:HG22	1.97	0.46
2:F:158:SER:O	2:F:337:ARG:NH2	2.47	0.46
2:F:484:PHE:HB3	2:F:495:PHE:CE2	2.50	0.46
2:G:517:LEU:O	2:G:699:ARG:NH1	2.46	0.46
2:I:68:GLY:HA3	2:I:289:GLU:OE2	2.16	0.46
1:P:303:PRO:HB2	1:P:306:LYS:HG2	1.97	0.46
1:R:75:ASP:O	1:R:310:LEU:HG	2.15	0.46
1:R:278:LYS:O	1:R:278:LYS:HG2	2.15	0.46
1:R:446:LEU:HB3	1:R:500:MET:HE1	1.96	0.46
1:S:740:ARG:HG3	1:S:789:GLU:HB3	1.97	0.46
2:B:522:LEU:O	2:B:699:ARG:NH2	2.37	0.46
2:E:152:HIS:HD2	2:E:356:ARG:HG3	1.80	0.46
2:I:551:MET:HE2	2:I:556:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:654:LYS:HA	2:I:657:LYS:HG2	1.97	0.46
2:L:12:LEU:HD21	2:L:298:ILE:HD13	1.97	0.46
2:L:511:ARG:HD3	2:L:558:LEU:HB3	1.98	0.46
1:O:131:LYS:HE3	1:P:192:GLY:HA2	1.98	0.46
1:P:652:GLN:HA	1:Q:740:ARG:HD3	1.97	0.46
1:P:763:GLY:H	1:P:770:ASN:ND2	2.14	0.46
1:R:297:TYR:HA	1:R:300:LYS:HG2	1.98	0.46
1:S:231:TRP:HB2	1:S:260:LEU:HD11	1.97	0.46
1:S:611:VAL:HG23	1:S:619:PHE:CE2	2.49	0.46
2:B:239:GLN:HE21	2:B:245:ILE:HD11	1.81	0.46
2:B:560:LEU:HD12	2:B:580:ALA:HA	1.97	0.46
2:C:7:ASN:HD21	2:C:304:THR:HG21	1.81	0.46
2:D:377:TYR:OH	2:D:414:VAL:O	2.29	0.46
2:D:419:VAL:HG13	2:D:465:GLY:C	2.41	0.46
2:G:384:HIS:ND1	2:G:413:CYS:SG	2.89	0.46
2:I:599:SER:OG	2:I:602:THR:OG1	2.23	0.46
2:J:551:MET:HE3	2:J:556:ARG:HA	1.97	0.46
2:K:410:HIS:ND1	2:K:412:LYS:HB2	2.31	0.46
2:M:256:THR:OG1	2:M:257:VAL:N	2.49	0.46
1:P:370:GLU:HA	1:P:373:LYS:HG2	1.97	0.46
1:P:747:ASN:HB3	1:P:811:VAL:HG13	1.96	0.46
1:S:794:HIS:ND1	1:S:796:VAL:HG22	2.30	0.46
1:T:105:LYS:NZ	1:T:213:CYS:HB3	2.30	0.46
1:T:863:CYS:HA	1:T:868:LEU:HD21	1.97	0.46
1:A:702:ASP:OD1	1:A:702:ASP:N	2.48	0.46
2:F:131:PRO:HB3	2:F:754:ALA:HB1	1.98	0.46
2:G:464:ARG:NE	2:G:795:PHE:O	2.34	0.46
2:I:3:ARG:NH2	2:I:104:ARG:HE	2.13	0.46
2:J:567:LEU:HD21	2:J:688:LEU:HG	1.97	0.46
2:M:696:MET:HE1	2:M:703:ILE:HD11	1.97	0.46
2:N:152:HIS:CD2	2:N:356:ARG:HG3	2.50	0.46
1:P:740:ARG:HB3	1:P:809:ASN:HD21	1.81	0.46
1:Q:131:LYS:HG3	1:R:193:GLY:H	1.81	0.46
1:S:46:ARG:HE	1:S:104:ILE:HD13	1.81	0.46
1:S:278:LYS:HG2	1:S:278:LYS:O	2.15	0.46
1:A:454:VAL:HG13	1:A:463:GLY:HA3	1.97	0.46
2:B:236:ASN:HD21	2:B:238:GLN:HB3	1.79	0.46
2:D:342:HIS:CE1	2:D:348:SER:HB3	2.51	0.46
2:F:713:ILE:HG23	2:F:715:GLN:H	1.81	0.46
2:G:155:LEU:HD23	2:G:337:ARG:HG2	1.98	0.46
2:I:303:LEU:HB3	2:I:753:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:516:ALA:HA	2:J:520:LEU:HD13	1.98	0.46
2:K:393:LYS:HD3	2:K:393:LYS:HA	1.77	0.46
2:M:497:TYR:CD1	2:M:499:VAL:HB	2.50	0.46
2:N:373:VAL:HG11	2:N:418:LEU:HD21	1.96	0.46
1:O:545:GLU:OE2	1:O:549:HIS:ND1	2.42	0.46
1:P:716:TRP:HE3	1:P:717:LEU:HD22	1.80	0.46
1:Q:789:GLU:HB3	1:Q:793:TYR:HD2	1.81	0.46
1:R:893:ASP:OD1	1:R:897:LYS:NZ	2.45	0.46
1:S:41:LEU:HD12	1:S:308:ILE:HG21	1.97	0.46
1:A:443:MET:SD	1:A:496:LYS:HD3	2.56	0.46
2:B:542:LYS:NZ	2:B:682:ASP:OD2	2.49	0.46
2:C:519:PHE:CE2	2:C:610:ARG:HD3	2.51	0.46
2:E:236:ASN:ND2	2:E:238:GLN:HB2	2.31	0.46
2:I:215:ARG:HH21	2:I:269:GLU:HB3	1.80	0.46
2:L:212:CYS:O	2:L:216:GLU:HG2	2.15	0.46
1:O:138:LYS:O	1:O:141:TRP:NE1	2.49	0.46
1:Q:69:ARG:NH2	1:Q:238:ARG:O	2.48	0.46
1:Q:254:LEU:HD21	1:Q:298:LEU:HD13	1.98	0.46
1:Q:500:MET:SD	1:Q:734:ILE:HD13	2.56	0.46
1:R:572:GLY:HA3	1:R:745:LEU:HD21	1.97	0.46
1:S:69:ARG:NH2	1:S:238:ARG:O	2.49	0.46
1:S:168:THR:HG21	1:T:172:TYR:CD2	2.50	0.46
1:S:236:SER:HA	1:S:240:PHE:HD2	1.81	0.46
1:A:603:ALA:HB2	1:A:853:PRO:HG2	1.97	0.46
2:B:311:ASP:OD1	2:B:712:ARG:NH1	2.48	0.46
2:D:121:PRO:HB2	2:M:491:GLY:HA2	1.98	0.46
2:E:151:THR:HB	2:E:527:ARG:NH2	2.31	0.46
2:K:450:MET:HE3	2:K:487:LEU:HD23	1.98	0.46
2:L:307:VAL:O	2:L:712:ARG:NH2	2.49	0.46
2:L:478:GLU:HB3	2:L:519:PHE:CD2	2.51	0.46
2:N:481:CYS:HB2	2:N:482:PRO:HD3	1.98	0.46
1:O:448:LYS:HD3	1:O:542:GLY:HA3	1.97	0.46
1:O:786:VAL:HG12	1:O:790:GLU:HB3	1.97	0.46
1:S:143:SER:OG	1:S:144:ASN:N	2.49	0.46
1:T:143:SER:H	1:T:146:TYR:HB3	1.81	0.46
1:T:505:CYS:HB3	1:T:738:TRP:CG	2.51	0.46
1:T:528:PHE:O	1:T:532:ILE:HG13	2.16	0.46
2:I:2:GLU:HG3	2:I:76:ILE:HG12	1.98	0.46
2:K:594:LEU:HD11	2:K:598:VAL:HB	1.97	0.46
2:L:532:THR:HG23	2:L:723:HIS:CD2	2.51	0.46
2:M:570:HIS:CE1	2:M:573:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:572:GLU:HG2	2:N:573:LEU:HG	1.98	0.46
1:O:539:MET:HE1	1:O:557:VAL:HG21	1.98	0.46
1:R:622:VAL:HG23	1:R:625:LEU:HD12	1.98	0.46
1:R:701:ASP:N	1:R:701:ASP:OD1	2.48	0.46
1:S:367:TYR:CZ	1:S:468:PRO:HD3	2.51	0.46
1:T:124:THR:O	1:T:128:ARG:HG2	2.16	0.46
1:T:514:PHE:CE2	1:T:558:VAL:HG22	2.51	0.46
2:B:788:GLU:O	2:B:792:ILE:HG13	2.16	0.45
2:C:138:THR:HG22	2:C:780:LEU:HD22	1.98	0.45
2:C:437:LEU:HA	2:C:440:LYS:HD2	1.98	0.45
2:D:572:GLU:HG2	2:D:573:LEU:HD22	1.98	0.45
2:D:578:SER:HB2	2:I:568:ARG:HD2	1.98	0.45
2:E:741:MET:HG2	2:E:742:SER:H	1.81	0.45
2:I:356:ARG:HA	2:I:419:VAL:O	2.16	0.45
2:K:143:ILE:HG21	2:K:758:LYS:HE2	1.99	0.45
2:K:472:GLU:HB3	2:K:502:ASP:OD1	2.16	0.45
2:L:356:ARG:HA	2:L:419:VAL:O	2.16	0.45
1:O:83:THR:H	1:O:377:ARG:NH2	2.14	0.45
1:O:917:LEU:O	1:O:920:SER:OG	2.32	0.45
1:P:539:MET:SD	1:P:550:TRP:NE1	2.67	0.45
1:P:794:HIS:CE1	1:P:796:VAL:HG13	2.51	0.45
1:R:421:LEU:HD22	1:R:425:MET:HE1	1.97	0.45
1:S:134:SER:O	1:S:138:LYS:HG2	2.16	0.45
1:T:238:ARG:HD2	1:T:297:TYR:CE1	2.52	0.45
1:T:727:ILE:HG13	1:T:729:PRO:HD3	1.98	0.45
2:C:476:PRO:HB2	2:C:478:GLU:OE1	2.16	0.45
2:F:22:GLU:OE2	2:F:290:ARG:NH1	2.44	0.45
2:F:227:LEU:HD13	2:F:231:ILE:HG21	1.98	0.45
2:G:651:ARG:HB3	2:G:652:PRO:HD3	1.98	0.45
2:K:722:HIS:ND1	2:K:724:ILE:HG22	2.31	0.45
2:L:7:ASN:ND2	2:L:104:ARG:O	2.50	0.45
2:M:10:VAL:HG13	2:M:32:SER:OG	2.16	0.45
2:M:752:ILE:HD11	2:M:755:ALA:HB2	1.98	0.45
2:N:30:GLU:HG2	2:N:53:TRP:NE1	2.31	0.45
1:O:123:VAL:HG21	1:P:177:PHE:CE2	2.51	0.45
1:O:206:ARG:HD3	1:O:206:ARG:HA	1.65	0.45
1:P:713:VAL:HG12	1:P:849:PRO:HG2	1.97	0.45
1:R:373:LYS:HG3	1:R:374:GLN:HE21	1.82	0.45
1:R:444:ASP:OD1	1:R:445:SER:N	2.50	0.45
1:S:602:ALA:HB1	1:S:646:PHE:CD2	2.51	0.45
1:S:764:ARG:N	1:S:768:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:806:LEU:C	1:S:807:ARG:HD2	2.42	0.45
1:T:604:MET:O	1:T:608:LEU:N	2.50	0.45
1:A:650:ILE:HG21	1:O:806:LEU:HD23	1.98	0.45
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.86	0.45
2:B:532:THR:HG23	2:B:723:HIS:CE1	2.51	0.45
2:B:567:LEU:HB3	2:B:577:ALA:HB2	1.98	0.45
2:C:85:LYS:HD3	2:C:135:TYR:CE2	2.51	0.45
2:C:730:LEU:HD23	2:C:782:LYS:HE2	1.97	0.45
2:F:214:ILE:HG23	2:F:291:LEU:HG	1.97	0.45
2:J:446:ALA:O	2:J:450:MET:HG2	2.17	0.45
2:L:154:HIS:CE1	2:L:748:ASP:HB2	2.51	0.45
2:M:385:MET:HE2	2:M:413:CYS:SG	2.56	0.45
2:N:155:LEU:O	2:N:337:ARG:NH2	2.50	0.45
1:O:348:ILE:HG22	1:O:368:VAL:HG22	1.97	0.45
1:O:656:ILE:HD11	1:P:461:ASN:CG	2.37	0.45
1:Q:197:SER:O	1:Q:201:GLU:HG2	2.16	0.45
1:A:111:ASP:HB3	1:A:114:LYS:HB3	1.98	0.45
1:A:559:ALA:HA	1:A:570:PHE:CE2	2.46	0.45
2:C:22:GLU:O	2:C:290:ARG:NH2	2.44	0.45
2:C:741:MET:HE3	2:C:741:MET:HB2	1.79	0.45
2:D:424:LYS:H	2:D:470:ALA:HB2	1.81	0.45
2:D:613:LEU:O	2:D:617:GLU:N	2.42	0.45
2:E:554:GLU:HB2	2:E:669:ARG:HD2	1.99	0.45
2:G:55:TYR:CZ	2:I:674:GLU:HG2	2.51	0.45
2:I:77:ALA:HA	2:I:81:ILE:HD13	1.99	0.45
2:L:234:MET:HE2	2:L:234:MET:HB3	1.83	0.45
2:L:680:LEU:HB3	2:L:684:ALA:HB3	1.98	0.45
2:N:159:THR:OG1	2:N:163:GLU:OE2	2.21	0.45
1:R:381:GLN:NE2	1:S:305:GLN:OE1	2.43	0.45
1:T:104:ILE:HD12	1:T:215:ALA:HB3	1.98	0.45
1:T:418:ARG:CZ	1:T:485:GLN:HB2	2.46	0.45
1:T:421:LEU:HD21	1:T:481:TYR:HA	1.98	0.45
1:T:511:PHE:HB2	1:T:535:TYR:CZ	2.52	0.45
2:B:690:GLN:NE2	2:B:736:GLU:O	2.49	0.45
2:B:756:ASP:OD1	2:B:757:LEU:N	2.49	0.45
2:C:174:ALA:HA	2:C:177:ARG:HE	1.82	0.45
2:C:196:ASP:OD1	2:C:199:LEU:HB2	2.17	0.45
2:C:554:GLU:HB2	2:C:669:ARG:HD2	1.98	0.45
2:F:290:ARG:O	2:F:294:ILE:HD12	2.16	0.45
2:F:396:THR:HG22	2:F:399:GLN:OE1	2.17	0.45
2:K:85:LYS:HZ1	2:L:525:GLY:HA3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:794:ARG:HB2	2:K:796:HIS:HD2	1.80	0.45
2:N:147:CYS:HB2	2:N:351:ARG:HB2	1.99	0.45
2:N:152:HIS:CG	2:N:748:ASP:HB3	2.52	0.45
1:P:350:ASP:O	1:P:354:GLU:HG2	2.16	0.45
1:S:464:PHE:CD1	1:S:508:VAL:HG11	2.52	0.45
1:S:535:TYR:O	1:S:539:MET:HG2	2.17	0.45
1:T:75:ASP:OD1	1:T:76:GLY:N	2.50	0.45
1:A:320:LYS:HE2	1:A:365:ASP:HB3	1.98	0.45
2:B:482:PRO:HA	2:B:636:GLU:OE2	2.17	0.45
2:B:506:LEU:HB2	2:B:541:TRP:CD2	2.52	0.45
2:D:247:HIS:HB3	2:D:252:TYR:CD2	2.51	0.45
2:F:424:LYS:HB2	2:F:470:ALA:HB3	1.99	0.45
2:G:444:ASN:O	2:G:448:ILE:HG13	2.16	0.45
2:I:481:CYS:HB2	2:I:482:PRO:HD3	1.98	0.45
2:J:259:PRO:HG2	2:J:260:ILE:HD12	1.99	0.45
1:Q:353:ARG:HA	1:Q:358:LEU:HB2	1.98	0.45
1:R:162:ARG:HH12	1:R:194:GLN:HB3	1.82	0.45
1:S:156:HIS:NE2	1:S:187:LEU:HD11	2.31	0.45
1:S:370:GLU:HA	1:S:373:LYS:HE2	1.99	0.45
1:S:448:LYS:HE2	1:T:471:GLU:HG3	1.98	0.45
1:S:576:LEU:HA	1:S:921:THR:O	2.17	0.45
1:A:166:LEU:HG	1:T:116:PRO:HG3	1.97	0.45
2:G:69:PRO:HD3	2:G:293:TRP:CD2	2.51	0.45
2:G:150:GLU:OE2	2:G:747:SER:N	2.42	0.45
2:K:121:PRO:HB2	2:L:491:GLY:HA2	1.97	0.45
2:K:507:ILE:HG22	2:K:559:ASP:OD1	2.17	0.45
2:L:60:ILE:HG23	2:L:65:MET:HG3	1.99	0.45
2:L:84:GLU:HG3	2:L:85:LYS:N	2.31	0.45
1:O:227:PHE:CZ	1:P:268:ASN:HB3	2.52	0.45
1:O:811:VAL:HG12	1:O:812:THR:HG23	1.99	0.45
1:P:654:THR:CG2	1:Q:465:TYR:OH	2.62	0.45
1:Q:237:ILE:HA	1:Q:241:PHE:CD2	2.52	0.45
1:Q:569:VAL:HG23	1:Q:574:VAL:HG22	1.99	0.45
1:S:28:LYS:H	1:S:31:ASP:HB2	1.81	0.45
1:S:366:MET:HE1	1:S:468:PRO:HD2	1.99	0.45
1:T:496:LYS:O	1:T:500:MET:HG2	2.16	0.45
1:A:613:SER:O	1:O:746:ASN:ND2	2.33	0.45
2:B:200:THR:HG23	2:B:203:ILE:HD12	1.99	0.45
2:E:356:ARG:HB3	2:E:421:HIS:HD2	1.82	0.45
2:E:464:ARG:O	2:E:494:HIS:HB2	2.17	0.45
2:E:707:PRO:HG3	2:E:747:SER:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:748:ASP:OD1	2:E:748:ASP:N	2.47	0.45
2:G:171:HIS:HB3	2:G:174:ALA:HB3	1.98	0.45
2:I:151:THR:HG21	2:I:744:CYS:HB2	1.99	0.45
2:K:68:GLY:H	2:K:71:ALA:HB3	1.82	0.45
2:K:191:LEU:HD21	2:K:308:GLN:HB3	1.99	0.45
2:K:360:LYS:HG3	2:K:369:LEU:HD22	1.99	0.45
2:M:435:HIS:HB3	2:M:438:LEU:HB3	1.98	0.45
2:N:191:LEU:HD21	2:N:309:ARG:HA	1.99	0.45
1:S:159:GLN:OE1	1:S:189:TYR:OH	2.30	0.45
1:S:769:SER:HA	1:S:773:LYS:HD2	1.98	0.45
1:T:82:LYS:HG3	1:T:83:THR:H	1.81	0.45
1:T:160:LEU:O	1:T:164:LEU:HB2	2.17	0.45
1:T:237:ILE:HA	1:T:241:PHE:HD2	1.82	0.45
1:A:27:THR:HG23	1:A:31:ASP:HB3	1.98	0.45
1:A:147:ARG:NH1	2:L:66:LYS:HG3	2.32	0.45
1:A:319:GLU:CD	1:A:320:LYS:H	2.25	0.45
2:B:131:PRO:HB3	2:B:754:ALA:HB1	1.98	0.45
2:E:696:MET:SD	2:E:701:ILE:HB	2.56	0.45
2:G:797:ASP:OD1	2:G:797:ASP:N	2.49	0.45
2:K:339:LYS:HA	2:K:342:HIS:CD2	2.52	0.45
2:L:476:PRO:HB2	2:L:478:GLU:CD	2.42	0.45
2:L:690:GLN:HA	2:L:693:MET:HG3	1.99	0.45
1:O:750:ASP:OD1	1:O:750:ASP:N	2.48	0.45
1:P:741:PHE:CE1	1:P:785:ALA:HB3	2.51	0.45
1:R:553:ARG:NH1	1:R:654:THR:O	2.50	0.45
1:R:797:SER:OG	1:R:798:ASP:N	2.49	0.45
1:S:357:ASN:ND2	1:S:728:ARG:HG2	2.32	0.45
1:S:878:ILE:HG21	1:S:886:LEU:HD22	1.99	0.45
1:A:74:VAL:HB	1:A:310:LEU:HD21	1.98	0.45
1:A:750:ASP:OD2	1:T:615:ASN:HB2	2.16	0.45
2:D:507:ILE:HG21	2:D:563:ILE:HD11	1.99	0.45
2:G:159:THR:OG1	2:G:163:GLU:OE2	2.24	0.45
2:G:748:ASP:OD1	2:G:749:ASP:N	2.45	0.45
2:I:476:PRO:HB2	2:I:478:GLU:OE1	2.16	0.45
2:J:214:ILE:HG23	2:J:291:LEU:HB3	1.99	0.45
2:M:534:ILE:O	2:M:726:ARG:NH1	2.50	0.45
1:O:93:LEU:HD12	1:O:217:LEU:HD22	1.99	0.45
1:O:359:ARG:HG3	1:O:795:SER:HA	1.99	0.45
1:P:78:ARG:HH21	1:Q:292:HIS:CG	2.34	0.45
1:P:227:PHE:HD2	1:P:260:LEU:HB2	1.82	0.45
1:Q:356:LEU:HB2	1:Q:358:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:503:VAL:HG22	1:R:550:TRP:CG	2.52	0.45
1:S:76:GLY:HA3	1:S:310:LEU:HD12	1.99	0.45
1:S:390:LYS:HA	1:S:416:LEU:HD13	1.99	0.45
1:T:588:TYR:OH	1:T:757:TYR:O	2.31	0.45
1:A:549:HIS:NE2	1:A:653:THR:HG23	2.32	0.44
1:A:752:HIS:HA	1:A:755:ARG:HG3	1.99	0.44
1:A:802:ILE:HG21	1:A:807:ARG:HE	1.81	0.44
2:B:200:THR:H	2:B:203:ILE:HB	1.82	0.44
2:C:163:GLU:HG2	2:C:266:GLN:HE22	1.77	0.44
2:E:231:ILE:HA	2:E:234:MET:HB2	1.99	0.44
2:F:108:LEU:HD13	2:F:128:PHE:HD2	1.82	0.44
2:F:171:HIS:HB3	2:F:174:ALA:HB3	1.99	0.44
2:F:718:ASN:OD1	2:F:720:SER:N	2.47	0.44
2:K:127:SER:H	2:K:129:ARG:HH12	1.66	0.44
2:M:158:SER:OG	2:M:159:THR:N	2.48	0.44
2:N:580:ALA:O	2:N:584:ALA:N	2.48	0.44
1:O:16:ILE:HD11	1:O:33:ILE:HD11	1.99	0.44
1:P:738:TRP:HA	1:P:741:PHE:CD2	2.52	0.44
1:Q:467:ARG:NH1	1:Q:732:LEU:HD13	2.32	0.44
1:R:590:LYS:HG2	1:R:591:PHE:H	1.82	0.44
1:S:165:HIS:HB3	1:T:174:PRO:HB3	1.98	0.44
1:S:559:ALA:HA	1:S:570:PHE:HD2	1.75	0.44
1:S:574:VAL:CG1	1:S:922:ILE:CD1	2.95	0.44
1:T:496:LYS:O	1:T:499:GLN:HG2	2.16	0.44
1:T:547:ALA:O	1:T:551:ALA:N	2.39	0.44
1:T:772:ALA:HA	1:T:917:LEU:HD22	1.99	0.44
1:A:358:LEU:HD12	1:A:359:ARG:H	1.81	0.44
1:A:565:GLU:HB3	1:A:567:ILE:HG13	1.99	0.44
2:B:573:LEU:HD13	2:B:684:ALA:HA	1.98	0.44
2:C:215:ARG:HE	2:C:269:GLU:HG2	1.82	0.44
2:F:233:SER:HB2	2:F:245:ILE:HD11	1.99	0.44
2:I:183:TRP:O	2:I:189:LYS:NZ	2.39	0.44
2:I:240:LEU:HD22	2:I:254:PHE:CZ	2.52	0.44
2:I:690:GLN:HA	2:I:693:MET:HB2	1.99	0.44
2:K:247:HIS:H	2:K:252:TYR:HE2	1.66	0.44
2:L:478:GLU:HB3	2:L:519:PHE:HD2	1.82	0.44
2:L:707:PRO:HG3	2:L:747:SER:HA	2.00	0.44
2:M:152:HIS:ND1	2:M:748:ASP:OD2	2.49	0.44
2:M:159:THR:OG1	2:M:160:SER:N	2.50	0.44
1:P:564:ASP:OD2	1:P:753:LYS:NZ	2.39	0.44
1:P:647:ASN:HD21	1:Q:807:ARG:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:784:HIS:CG	1:P:810:PRO:HD3	2.52	0.44
1:Q:18:LEU:HG	1:Q:330:VAL:HG13	1.99	0.44
1:Q:370:GLU:HA	1:Q:373:LYS:HE2	1.99	0.44
1:R:431:ARG:CG	1:T:282:ARG:NH2	2.51	0.44
1:R:584:MET:HG3	1:R:584:MET:O	2.17	0.44
1:R:878:ILE:HD12	1:R:886:LEU:HD12	1.98	0.44
1:S:170:LYS:HD3	1:S:171:GLU:OE2	2.17	0.44
1:T:114:LYS:O	1:T:115:LEU:HD12	2.17	0.44
1:T:506:GLY:O	1:T:510:ILE:HG12	2.16	0.44
2:D:59:GLN:HE22	2:D:63:ARG:NH1	2.15	0.44
2:D:402:ASP:OD1	2:D:458:ARG:NH1	2.50	0.44
2:D:565:ARG:NH1	2:D:604:ASP:OD2	2.50	0.44
2:F:176:LEU:HD21	2:F:205:LYS:HB2	1.98	0.44
2:F:205:LYS:NZ	2:F:209:GLN:HE21	2.15	0.44
2:L:151:THR:HB	2:L:527:ARG:NH2	2.32	0.44
2:N:1:MET:HA	2:N:1:MET:HE2	1.99	0.44
2:N:486:VAL:HG11	2:N:633:TRP:CZ3	2.53	0.44
1:P:890:GLU:HG2	1:P:891:GLU:N	2.32	0.44
1:R:514:PHE:HZ	1:R:571:LEU:HD22	1.82	0.44
1:S:208:CYS:O	1:S:212:ASP:N	2.50	0.44
1:A:41:LEU:HD22	1:A:308:ILE:HG13	1.98	0.44
1:A:817:PHE:CE2	1:A:821:ILE:HD11	2.53	0.44
2:C:69:PRO:O	2:C:73:LEU:HG	2.18	0.44
2:E:77:ALA:HB1	2:E:114:HIS:HB2	1.99	0.44
2:E:299:GLN:O	2:E:303:LEU:HD23	2.17	0.44
2:E:517:LEU:HD21	2:E:696:MET:HE1	1.99	0.44
2:E:534:ILE:HG21	2:E:692:VAL:HG11	2.00	0.44
2:F:568:ARG:NH1	2:M:578:SER:OG	2.51	0.44
2:I:390:VAL:HG12	2:I:391:HIS:CD2	2.53	0.44
2:I:422:PHE:HB3	2:I:442:LEU:HD22	1.99	0.44
2:I:789:ASN:O	2:I:789:ASN:ND2	2.50	0.44
2:L:9:THR:HB	2:L:196:ASP:OD1	2.18	0.44
2:L:451:ASP:OD1	2:L:452:MET:N	2.50	0.44
2:M:410:HIS:CE1	2:M:412:LYS:HD2	2.52	0.44
2:M:564:TRP:CD1	2:M:581:ALA:HB2	2.53	0.44
1:P:162:ARG:NH2	1:P:176:TYR:O	2.50	0.44
1:Q:359:ARG:HG2	1:Q:360:GLU:N	2.33	0.44
1:R:771:ALA:HA	1:R:774:ILE:HD12	1.98	0.44
1:S:348:ILE:HG23	1:S:368:VAL:HG13	1.99	0.44
1:S:415:ASN:OD1	1:S:418:ARG:NH2	2.46	0.44
1:S:472:SER:HB3	1:S:475:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:168:THR:OG1	2.29	0.44
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.85	0.44
2:B:221:VAL:HG22	2:B:227:LEU:HD21	1.98	0.44
2:B:278:GLU:OE1	2:B:281:ARG:NH2	2.50	0.44
2:B:713:ILE:HG22	2:B:715:GLN:HG2	1.99	0.44
2:C:452:MET:O	2:C:452:MET:HE3	2.17	0.44
2:C:553:LYS:NZ	2:C:668:GLN:OE1	2.49	0.44
2:D:228:PRO:HB2	2:D:230:TRP:CE2	2.53	0.44
2:D:234:MET:HE2	2:D:240:LEU:HD21	2.00	0.44
2:D:473:MET:HE2	2:D:473:MET:HB2	1.93	0.44
2:E:582:ILE:O	2:E:586:ARG:HG3	2.17	0.44
2:F:152:HIS:CD2	2:F:356:ARG:HD2	2.53	0.44
2:G:360:LYS:HE3	2:G:369:LEU:HD22	1.99	0.44
2:J:22:GLU:OE1	2:J:24:SER:OG	2.34	0.44
2:J:434:PRO:HG2	2:J:435:HIS:CE1	2.52	0.44
2:M:563:ILE:HD11	2:M:680:LEU:HD11	2.00	0.44
2:N:564:TRP:CD1	2:N:581:ALA:HB2	2.52	0.44
2:N:696:MET:HB3	2:N:741:MET:HE2	1.99	0.44
1:O:454:VAL:HG21	1:O:508:VAL:HG21	1.99	0.44
1:O:473:GLU:HB2	1:P:288:TYR:CE1	2.52	0.44
1:P:296:GLN:HE21	1:P:300:LYS:HB3	1.81	0.44
1:P:313:MET:HG3	1:P:379:LEU:HD23	1.98	0.44
1:Q:752:HIS:HE1	1:Q:777:PHE:HD2	1.64	0.44
1:R:320:LYS:HE3	1:R:365:ASP:HB3	1.99	0.44
1:R:431:ARG:HH21	1:R:474:ALA:HB3	1.83	0.44
1:R:765:MET:H	1:R:768:GLN:HB2	1.81	0.44
1:S:313:MET:HG3	1:S:379:LEU:HD22	1.99	0.44
2:B:43:SER:O	2:N:544:SER:OG	2.27	0.44
2:B:693:MET:HA	2:B:741:MET:HE2	2.00	0.44
2:C:311:ASP:OD1	2:C:311:ASP:N	2.51	0.44
2:C:544:SER:O	2:C:545:LEU:HD22	2.17	0.44
2:E:99:GLN:HG3	2:E:763:HIS:CD2	2.53	0.44
2:F:465:GLY:HA2	2:F:494:HIS:O	2.18	0.44
2:G:567:LEU:HD21	2:G:688:LEU:HD22	1.99	0.44
2:I:210:ILE:O	2:I:214:ILE:HG12	2.17	0.44
2:K:424:LYS:H	2:K:470:ALA:HB2	1.82	0.44
2:M:497:TYR:O	2:M:529:GLY:N	2.48	0.44
1:O:539:MET:CE	1:O:557:VAL:CG2	2.96	0.44
1:P:19:PHE:CE2	1:P:334:PRO:HD3	2.49	0.44
1:Q:757:TYR:CZ	1:Q:932:PRO:HD3	2.53	0.44
1:Q:776:ARG:NH2	1:Q:871:GLU:OE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:23:LEU:HD21	1:S:69:ARG:HA	2.00	0.44
1:R:86:ILE:HD11	1:R:251:THR:HB	1.98	0.44
1:R:929:LYS:HG2	1:R:930:ASP:H	1.81	0.44
1:S:503:VAL:HA	1:S:550:TRP:NE1	2.33	0.44
1:T:516:THR:HG23	1:T:528:PHE:HE1	1.83	0.44
1:A:717:LEU:HA	1:A:720:VAL:HG22	2.00	0.44
2:C:179:PHE:O	2:C:183:TRP:N	2.51	0.44
2:E:81:ILE:HD12	2:E:132:LEU:HD12	2.00	0.44
2:F:791:ARG:HE	2:L:141:ASP:CG	2.25	0.44
2:I:719:VAL:HG11	2:I:767:VAL:HG21	1.99	0.44
2:J:133:TYR:HB3	2:J:762:TYR:CE2	2.53	0.44
2:K:359:PRO:HB2	2:K:445:GLN:NE2	2.26	0.44
2:K:797:ASP:N	2:K:797:ASP:OD1	2.49	0.44
2:L:135:TYR:CE2	2:L:140:GLU:HG3	2.52	0.44
2:M:150:GLU:HB2	2:M:757:LEU:HD22	1.99	0.44
2:M:501:GLU:OE1	2:M:530:HIS:ND1	2.41	0.44
2:N:214:ILE:HG21	2:N:295:TYR:HB2	1.99	0.44
1:O:566:LYS:HD3	1:O:566:LYS:HA	1.83	0.44
1:P:116:PRO:HG2	1:P:119:GLU:HB2	2.00	0.44
1:P:133:VAL:HG11	1:P:153:TRP:CZ2	2.52	0.44
1:R:628:ALA:O	1:R:632:ILE:HG12	2.17	0.44
1:S:290:VAL:HA	1:S:293:LEU:HD12	2.00	0.44
1:S:439:HIS:HB2	1:T:314:LEU:HD23	1.98	0.44
1:T:425:MET:HB3	1:T:428:SER:HB3	1.99	0.44
1:A:569:VAL:O	1:A:570:PHE:HD1	2.01	0.44
2:B:236:ASN:ND2	2:B:238:GLN:HB3	2.32	0.44
2:F:246:LEU:HD23	2:F:246:LEU:H	1.83	0.44
2:G:246:LEU:HD23	2:G:246:LEU:H	1.82	0.44
2:I:567:LEU:HB3	2:I:577:ALA:HB2	1.99	0.44
2:I:778:ASP:HA	2:I:781:ARG:HH11	1.82	0.44
2:K:475:ALA:HB1	2:K:479:LEU:HD23	2.00	0.44
2:K:554:GLU:HB3	2:K:669:ARG:HD2	2.00	0.44
2:L:410:HIS:CE1	2:L:412:LYS:HB2	2.52	0.44
2:L:650:LYS:HA	2:L:650:LYS:HD2	1.85	0.44
2:L:748:ASP:OD1	2:L:749:ASP:N	2.48	0.44
1:P:112:PRO:HG3	1:P:233:VAL:HG21	1.99	0.44
1:Q:438:GLN:HG2	1:R:309:GLN:HE21	1.82	0.44
1:Q:445:SER:OG	1:Q:449:ASP:OD2	2.36	0.44
1:Q:838:THR:HG23	1:Q:839:HIS:ND1	2.32	0.44
1:R:549:HIS:HA	1:R:552:ASN:ND2	2.30	0.44
2:B:523:ARG:NH1	2:G:84:GLU:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:LEU:HB3	2:C:72:ILE:HD13	2.00	0.44
2:C:149:HIS:CE1	2:C:791:ARG:HB2	2.53	0.44
2:C:554:GLU:OE1	2:C:669:ARG:NH1	2.50	0.44
2:C:756:ASP:OD1	2:C:757:LEU:N	2.49	0.44
2:D:64:ASN:HD21	1:S:144:ASN:HA	1.82	0.44
2:E:92:LEU:HD21	2:E:136:HIS:HD2	1.83	0.44
2:F:205:LYS:HZ3	2:F:209:GLN:HB2	1.83	0.44
2:J:207:ARG:HB3	2:J:298:ILE:HD12	1.99	0.44
2:J:209:GLN:O	2:J:213:ASN:ND2	2.51	0.44
2:L:35:LEU:HD21	2:M:193:ALA:HB1	1.99	0.44
2:L:381:LEU:HD23	2:L:381:LEU:HA	1.86	0.44
2:N:93:PRO:HG3	2:N:770:ARG:HH12	1.81	0.44
2:N:481:CYS:SG	2:N:520:LEU:HD23	2.58	0.44
2:N:781:ARG:HA	2:N:781:ARG:HD2	1.86	0.44
1:P:748:VAL:HA	1:P:752:HIS:HD2	1.83	0.44
1:P:776:ARG:HB3	1:P:857:PRO:HG2	2.00	0.44
1:Q:146:TYR:HA	1:Q:149:GLN:NE2	2.32	0.44
1:Q:366:MET:HE1	1:Q:467:ARG:HD3	2.00	0.44
1:Q:473:GLU:OE1	1:R:288:TYR:OH	2.34	0.44
1:R:355:GLY:HA2	1:R:413:VAL:HG12	2.00	0.44
1:R:507:SER:O	1:R:535:TYR:OH	2.28	0.44
1:T:333:GLU:HB2	1:T:336:MET:HG2	1.99	0.44
1:T:741:PHE:CE1	1:T:782:PHE:HB2	2.53	0.44
1:T:831:ASP:OD1	1:T:832:ASN:N	2.48	0.44
1:A:744:ASN:ND2	1:A:781:ALA:O	2.51	0.43
2:B:159:THR:HG22	2:B:337:ARG:HA	2.00	0.43
2:C:613:LEU:HD23	2:C:613:LEU:H	1.83	0.43
2:C:654:LYS:HE2	2:C:654:LYS:HB3	1.84	0.43
2:D:80:PHE:CD2	2:D:98:TRP:HE3	2.35	0.43
2:D:714:SER:O	2:D:714:SER:OG	2.34	0.43
2:F:679:TYR:HD1	2:F:680:LEU:HG	1.83	0.43
2:G:51:SER:OG	2:I:550:SER:O	2.25	0.43
2:J:481:CYS:HB3	2:J:485:ARG:HH22	1.83	0.43
2:K:548:SER:OG	2:K:674:GLU:OE2	2.30	0.43
2:L:89:LYS:HD2	2:L:133:TYR:O	2.18	0.43
2:L:717:ARG:HE	2:M:717:ARG:CZ	2.31	0.43
2:M:85:LYS:HD2	2:M:135:TYR:OH	2.18	0.43
1:O:737:VAL:HA	1:O:789:GLU:OE2	2.18	0.43
1:Q:622:VAL:HG23	1:Q:625:LEU:HD12	2.00	0.43
1:R:303:PRO:HB2	1:R:306:LYS:HG2	2.00	0.43
1:A:254:LEU:HD23	1:T:426:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:LEU:HD12	1:T:650:ILE:HD12	1.99	0.43
2:B:10:VAL:HG12	2:B:36:ALA:HB2	1.99	0.43
2:B:85:LYS:HE2	2:J:494:HIS:CE1	2.53	0.43
2:C:42:ARG:HH12	2:D:42:ARG:HB2	1.82	0.43
2:C:44:LEU:HD12	2:C:44:LEU:HA	1.91	0.43
2:E:410:HIS:HE1	2:E:412:LYS:HB2	1.82	0.43
2:G:722:HIS:ND1	2:G:724:ILE:HG22	2.33	0.43
2:J:347:TYR:HD1	2:J:412:LYS:HB3	1.83	0.43
2:J:481:CYS:SG	2:J:519:PHE:HB3	2.58	0.43
2:M:215:ARG:NH2	2:M:263:LYS:O	2.45	0.43
1:O:744:ASN:HD21	1:O:810:PRO:HD2	1.83	0.43
1:O:747:ASN:HD21	1:O:809:ASN:HB3	1.83	0.43
1:Q:718:LYS:HD3	1:Q:718:LYS:HA	1.84	0.43
1:Q:888:SER:HB2	1:Q:891:GLU:HG2	2.00	0.43
1:R:107:LEU:HD22	1:R:128:ARG:HB3	1.99	0.43
1:S:543:ARG:HA	1:T:469:GLN:HB3	1.98	0.43
1:T:107:LEU:HG	1:T:108:PRO:HD2	2.00	0.43
1:A:439:HIS:CD2	1:O:314:LEU:HD23	2.51	0.43
2:B:19:SER:OG	2:B:20:LEU:N	2.51	0.43
2:B:152:HIS:CD2	2:B:356:ARG:HG3	2.53	0.43
2:B:472:GLU:HB2	2:B:500:GLY:H	1.83	0.43
2:C:523:ARG:HH11	2:E:85:LYS:HD3	1.82	0.43
2:D:439:PHE:HD2	2:D:440:LYS:HE2	1.82	0.43
2:E:424:LYS:NZ	2:E:470:ALA:H	2.16	0.43
2:F:493:ALA:HB1	2:L:85:LYS:HA	1.99	0.43
2:I:450:MET:HG3	2:I:633:TRP:CH2	2.54	0.43
2:K:152:HIS:ND1	2:K:748:ASP:OD2	2.51	0.43
2:L:600:ILE:H	2:L:600:ILE:HD12	1.83	0.43
2:N:9:THR:HG21	2:N:196:ASP:HB2	2.00	0.43
2:N:554:GLU:HG3	2:N:669:ARG:HD2	2.00	0.43
1:O:92:SER:O	1:O:95:SER:OG	2.37	0.43
1:O:572:GLY:O	1:O:573:MET:HE2	2.17	0.43
1:P:426:LEU:O	1:P:429:ILE:HG12	2.17	0.43
1:P:654:THR:HG23	1:P:654:THR:O	2.18	0.43
1:P:835:TRP:HB3	1:P:843:PHE:CZ	2.53	0.43
1:Q:738:TRP:HA	1:Q:741:PHE:HB2	2.01	0.43
1:Q:783:LEU:HD11	1:Q:845:LEU:HB3	2.01	0.43
1:Q:789:GLU:HB3	1:Q:793:TYR:CD2	2.53	0.43
1:R:256:LEU:HD13	1:S:289:MET:HE3	2.00	0.43
1:R:274:LEU:HB3	1:S:276:GLN:NE2	2.32	0.43
1:R:336:MET:HE1	1:R:341:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:659:PRO:HB3	1:S:516:THR:HB	2.01	0.43
1:S:85:PHE:O	1:S:89:VAL:HG23	2.18	0.43
1:S:152:GLN:O	1:S:156:HIS:ND1	2.49	0.43
1:S:205:LYS:HZ3	1:S:245:LYS:HD2	1.83	0.43
1:T:107:LEU:HD22	1:T:218:ILE:HG22	1.99	0.43
1:A:333:GLU:H	1:A:336:MET:HE2	1.82	0.43
2:C:95:PHE:CE1	2:C:134:PRO:HD3	2.52	0.43
2:E:34:PHE:HZ	2:E:50:LYS:HA	1.83	0.43
2:E:511:ARG:HD2	2:E:558:LEU:HB3	2.00	0.43
2:F:20:LEU:N	2:F:235:GLN:O	2.48	0.43
2:F:205:LYS:HZ3	2:F:209:GLN:HE21	1.64	0.43
2:G:40:GLN:HG3	2:G:104:ARG:HH21	1.84	0.43
2:G:528:LEU:O	2:G:704:GLU:N	2.41	0.43
2:I:149:HIS:CE1	2:I:791:ARG:HB2	2.53	0.43
2:I:217:ILE:HG12	2:I:230:TRP:HH2	1.84	0.43
2:J:148:LEU:HD21	2:J:761:PHE:CD2	2.54	0.43
2:J:169:LEU:HD22	2:J:212:CYS:HB2	2.01	0.43
2:J:424:LYS:H	2:J:470:ALA:CB	2.32	0.43
2:K:69:PRO:HB2	2:K:292:LEU:HD23	1.99	0.43
2:M:151:THR:HB	2:M:527:ARG:NH2	2.34	0.43
2:M:567:LEU:HB3	2:M:577:ALA:HB2	1.99	0.43
2:N:236:ASN:ND2	2:N:238:GLN:HB2	2.33	0.43
2:N:371:PHE:HB2	2:N:397:ILE:HG13	2.01	0.43
2:N:538:PRO:O	2:N:542:LYS:HG3	2.19	0.43
1:P:775:MET:HE2	1:P:854:PHE:CE2	2.53	0.43
1:Q:367:TYR:OH	1:Q:467:ARG:NH2	2.48	0.43
1:Q:743:PHE:HA	1:Q:746:ASN:HD21	1.84	0.43
1:Q:911:GLN:HE21	1:Q:912:ASN:ND2	2.17	0.43
1:R:431:ARG:NH2	1:R:472:SER:OG	2.51	0.43
1:R:772:ALA:HB2	1:R:918:ASN:HB3	2.00	0.43
1:S:337:GLN:OE1	1:S:339:ILE:HG12	2.19	0.43
1:S:558:VAL:HG21	1:S:571:LEU:HB2	2.00	0.43
1:T:173:LYS:HB2	1:T:176:TYR:CD1	2.54	0.43
1:A:539:MET:O	1:A:539:MET:HE3	2.19	0.43
2:B:165:TRP:HB2	2:B:303:LEU:HD21	2.01	0.43
2:B:396:THR:HG23	2:B:399:GLN:H	1.84	0.43
2:D:453:LEU:HD23	2:D:453:LEU:HA	1.88	0.43
2:E:556:ARG:HD3	2:E:675:VAL:HG21	2.00	0.43
2:F:476:PRO:HG2	2:F:478:GLU:HG3	2.01	0.43
2:F:478:GLU:HB3	2:F:519:PHE:CD2	2.52	0.43
2:F:536:ILE:HG21	2:F:541:TRP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:263:LYS:HE2	2:I:264:TYR:CZ	2.53	0.43
2:I:756:ASP:OD1	2:I:757:LEU:N	2.51	0.43
2:M:212:CYS:O	2:M:216:GLU:HG2	2.18	0.43
2:N:130:TRP:CE2	2:N:343:GLY:HA2	2.53	0.43
2:N:729:GLY:HA2	2:N:734:ALA:HB2	2.00	0.43
1:O:132:MET:HA	1:O:135:ASP:HB2	1.99	0.43
1:P:425:MET:SD	1:P:425:MET:N	2.91	0.43
1:P:604:MET:HG2	1:P:914:ILE:HD12	2.00	0.43
1:S:389:LYS:HG2	1:S:416:LEU:HD22	2.01	0.43
1:T:614:ASN:ND2	1:T:614:ASN:C	2.75	0.43
1:A:141:TRP:CG	1:A:142:ALA:N	2.86	0.43
1:A:755:ARG:HH12	1:A:812:THR:HG23	1.83	0.43
1:A:787:LEU:HD23	1:A:817:PHE:HE1	1.82	0.43
2:B:561:VAL:HG11	2:B:607:PHE:CD2	2.53	0.43
2:C:588:ALA:HB2	2:C:603:LEU:HD11	1.99	0.43
2:C:642:GLU:HA	2:C:645:LYS:HB2	2.00	0.43
2:D:68:GLY:O	2:D:72:ILE:HG13	2.19	0.43
2:F:524:ASN:OD1	2:F:700:ASN:HB3	2.18	0.43
2:I:545:LEU:HD12	2:I:546:PRO:HD2	2.00	0.43
2:J:230:TRP:CE3	2:J:245:ILE:HG12	2.53	0.43
2:J:424:LYS:H	2:J:470:ALA:HB2	1.83	0.43
2:J:437:LEU:HA	2:J:440:LYS:HG2	2.01	0.43
2:K:689:GLN:O	2:K:693:MET:HG3	2.19	0.43
2:L:147:CYS:HB2	2:L:351:ARG:HB2	2.00	0.43
1:S:782:PHE:CE1	1:S:845:LEU:HD13	2.53	0.43
1:T:289:MET:O	1:T:293:LEU:N	2.40	0.43
1:T:574:VAL:HB	1:T:620:CYS:HB3	2.01	0.43
2:C:381:LEU:HD23	2:C:381:LEU:HA	1.86	0.43
2:C:503:PHE:HE2	2:C:532:THR:HG23	1.83	0.43
2:D:99:GLN:HG3	2:D:763:HIS:ND1	2.33	0.43
2:D:516:ALA:O	2:D:520:LEU:HB2	2.18	0.43
2:E:563:ILE:HD13	2:E:680:LEU:HD11	1.99	0.43
2:F:575:ARG:NH2	2:F:576:TYR:OH	2.51	0.43
2:G:109:PRO:HA	2:G:273:LEU:HD21	2.00	0.43
2:G:224:GLY:HA2	2:G:279:LYS:HE3	2.00	0.43
2:I:750:PRO:C	2:I:752:ILE:H	2.26	0.43
2:J:143:ILE:HG13	2:J:758:LYS:HE2	2.01	0.43
2:J:159:THR:HG22	2:J:337:ARG:HA	2.00	0.43
2:J:659:TRP:HD1	2:J:660:LEU:HD12	1.83	0.43
2:K:212:CYS:O	2:K:216:GLU:HG2	2.18	0.43
2:K:214:ILE:HG21	2:K:295:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:674:GLU:HB2	2:M:55:TYR:CZ	2.54	0.43
2:M:561:VAL:HG11	2:M:607:PHE:CD2	2.54	0.43
2:M:562:PHE:HE2	2:M:688:LEU:HD23	1.82	0.43
2:N:215:ARG:NH1	2:N:263:LYS:O	2.49	0.43
1:P:160:LEU:HD12	1:P:196:LEU:HD22	2.00	0.43
1:Q:929:LYS:HD3	1:Q:930:ASP:O	2.19	0.43
1:R:787:LEU:HA	1:R:790:GLU:HG2	2.01	0.43
1:S:741:PHE:CE1	1:S:745:LEU:HD21	2.53	0.43
1:A:72:PHE:O	1:A:249:VAL:HA	2.19	0.43
2:B:419:VAL:HG13	2:B:465:GLY:C	2.44	0.43
2:B:662:SER:HB3	2:B:665:VAL:HB	2.00	0.43
2:C:354:GLU:OE2	2:C:356:ARG:NE	2.50	0.43
2:D:542:LYS:HA	2:D:545:LEU:HD12	2.00	0.43
2:D:575:ARG:HB3	2:I:569:SER:HB3	2.01	0.43
2:I:357:PHE:HE1	2:I:418:LEU:HB3	1.84	0.43
2:K:699:ARG:HB2	2:K:701:ILE:HG12	1.99	0.43
2:L:162:GLU:HG3	2:L:754:ALA:HB2	2.01	0.43
2:N:771:LYS:HD3	2:N:771:LYS:HA	1.81	0.43
1:O:105:LYS:HG2	1:O:213:CYS:HB3	2.00	0.43
1:Q:255:ARG:NH1	1:Q:259:GLN:HG2	2.34	0.43
1:Q:607:SER:HB2	1:Q:625:LEU:HG	2.00	0.43
1:T:450:ILE:HG12	1:T:482:LEU:HD13	2.00	0.43
2:B:112:ALA:HA	2:B:270:PHE:HE1	1.83	0.43
2:B:207:ARG:NH1	2:B:301:GLN:OE1	2.50	0.43
2:B:649:MET:HG2	2:B:652:PRO:HD2	2.00	0.43
2:D:82:LYS:HB3	2:D:82:LYS:HE2	1.77	0.43
2:G:486:VAL:HG23	2:G:632:LEU:HB3	2.01	0.43
2:L:133:TYR:HB3	2:L:762:TYR:CE2	2.54	0.43
2:L:150:GLU:HG3	2:L:757:LEU:HD22	2.00	0.43
2:L:596:GLU:OE1	2:L:596:GLU:N	2.51	0.43
2:M:81:ILE:HD12	2:M:132:LEU:HD12	2.01	0.43
2:M:250:ARG:NH2	1:P:206:ARG:HH12	2.17	0.43
2:M:595:GLU:OE1	2:M:595:GLU:N	2.52	0.43
2:M:764:LEU:O	2:M:768:LEU:HG	2.18	0.43
2:N:342:HIS:HB2	2:N:380:TYR:HE2	1.84	0.43
1:O:473:GLU:HB2	1:P:288:TYR:HE1	1.84	0.43
1:O:538:TYR:HE2	1:O:539:MET:SD	2.42	0.43
1:P:801:TYR:HE2	1:P:833:LYS:HD2	1.84	0.43
1:Q:790:GLU:O	1:Q:794:HIS:HB2	2.18	0.43
1:S:29:GLU:H	1:S:29:GLU:CD	2.26	0.43
1:S:39:ASP:OD1	1:S:40:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:329:LYS:HE2	1:S:329:LYS:HB3	1.90	0.43
1:T:80:ALA:HA	1:T:376:VAL:HB	2.01	0.43
1:T:111:ASP:HB2	1:T:221:ASP:HB2	2.00	0.43
1:A:316:LEU:HD23	1:A:325:LYS:HD2	2.01	0.43
1:A:462:THR:HA	1:A:465:TYR:CD2	2.54	0.43
2:B:609:MET:HE1	2:B:653:LEU:HA	2.01	0.43
2:B:791:ARG:HH22	2:G:145:ARG:HD2	1.84	0.43
2:C:543:ARG:NH2	2:C:717:ARG:HG2	2.34	0.43
2:D:719:VAL:HG21	2:D:763:HIS:HE2	1.83	0.43
2:E:143:ILE:HG12	2:E:148:LEU:HD21	2.01	0.43
2:E:209:GLN:CD	2:E:243:SER:HB3	2.44	0.43
2:E:424:LYS:HE3	2:E:480:PHE:CE2	2.54	0.43
2:F:22:GLU:OE1	2:F:22:GLU:N	2.50	0.43
2:F:663:ASP:OD1	2:F:664:ASN:N	2.51	0.43
2:G:588:ALA:HB2	2:G:603:LEU:HD11	2.00	0.43
2:J:404:LEU:O	2:J:407:VAL:HG12	2.19	0.43
2:J:750:PRO:HB2	2:J:752:ILE:HG12	2.00	0.43
2:K:34:PHE:O	2:K:37:GLN:HG3	2.19	0.43
2:K:464:ARG:O	2:K:494:HIS:HB2	2.19	0.43
2:L:207:ARG:HB3	2:L:298:ILE:HD12	2.00	0.43
2:M:393:LYS:HB3	2:M:395:LEU:HD23	2.01	0.43
2:M:654:LYS:HA	2:M:657:LYS:HZ3	1.84	0.43
1:P:69:ARG:NH2	1:P:242:ASN:OD1	2.52	0.43
1:S:531:LEU:O	1:S:535:TYR:N	2.47	0.43
1:T:753:LYS:HE3	1:T:753:LYS:HB2	1.77	0.43
1:A:290:VAL:HA	1:A:293:LEU:HB2	2.00	0.42
1:A:353:ARG:O	1:A:357:ASN:N	2.52	0.42
2:C:752:ILE:HD11	2:C:755:ALA:HB2	2.01	0.42
2:D:34:PHE:CZ	2:D:50:LYS:HD2	2.54	0.42
2:D:454:LYS:HE2	2:D:454:LYS:HB3	1.81	0.42
2:D:574:LEU:HD23	2:D:574:LEU:HA	1.89	0.42
2:E:19:SER:OG	2:E:235:GLN:O	2.28	0.42
2:E:516:ALA:O	2:E:520:LEU:HB2	2.18	0.42
2:F:283:ASN:OD1	2:F:284:ALA:N	2.52	0.42
2:F:371:PHE:HB2	2:F:397:ILE:HG13	2.00	0.42
2:G:138:THR:HG22	2:G:780:LEU:HD22	1.99	0.42
2:I:199:LEU:HD11	2:I:301:GLN:HE22	1.84	0.42
2:K:724:ILE:O	2:K:728:MET:HG2	2.18	0.42
2:M:332:LYS:N	2:M:332:LYS:HD2	2.34	0.42
2:M:397:ILE:H	2:M:397:ILE:HD12	1.83	0.42
2:N:70:VAL:HG23	2:N:277:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:95:PHE:CE1	2:N:134:PRO:HD3	2.54	0.42
1:P:554:CYS:O	1:P:558:VAL:HG13	2.19	0.42
1:Q:539:MET:HE3	1:Q:550:TRP:NE1	2.34	0.42
1:R:372:LEU:HA	1:R:379:LEU:HD22	2.01	0.42
1:S:128:ARG:HH22	1:T:195:ASP:HB2	1.83	0.42
1:S:322:LYS:HA	1:S:322:LYS:HD2	1.82	0.42
2:B:165:TRP:HH2	2:B:298:ILE:HG22	1.84	0.42
2:C:419:VAL:HG13	2:C:465:GLY:C	2.44	0.42
2:C:658:GLN:O	2:C:662:SER:HB2	2.19	0.42
2:D:1:MET:SD	2:D:1:MET:N	2.92	0.42
2:E:12:LEU:HD21	2:E:207:ARG:HD2	2.00	0.42
2:E:391:HIS:O	2:E:403:ASN:ND2	2.30	0.42
2:E:471:ASN:OD1	2:E:472:GLU:N	2.50	0.42
2:F:5:LEU:HD11	2:F:53:TRP:HZ3	1.83	0.42
2:F:417:ALA:HB1	2:F:464:ARG:HG3	2.00	0.42
2:G:476:PRO:HB2	2:G:478:GLU:OE1	2.18	0.42
2:G:730:LEU:HD11	2:G:782:LYS:HD3	2.01	0.42
2:I:375:ARG:NH1	2:I:379:GLU:HB2	2.33	0.42
2:K:349:GLN:OE1	2:K:758:LYS:HE3	2.19	0.42
2:L:356:ARG:HB3	2:L:421:HIS:HD2	1.84	0.42
2:M:506:LEU:O	2:M:510:ILE:HG12	2.19	0.42
2:M:596:GLU:H	2:M:596:GLU:CD	2.27	0.42
2:M:703:ILE:HB	2:M:743:ILE:HD13	2.01	0.42
2:N:55:TYR:O	2:N:59:GLN:HG3	2.19	0.42
2:N:305:LEU:O	2:N:309:ARG:HG3	2.19	0.42
1:O:435:ASN:ND2	1:O:449:ASP:OD2	2.50	0.42
1:O:597:ASN:ND2	1:O:910:PHE:O	2.52	0.42
1:P:37:LEU:HD23	1:P:37:LEU:HA	1.87	0.42
1:Q:133:VAL:HG11	1:Q:153:TRP:CE2	2.54	0.42
1:Q:467:ARG:HA	1:Q:468:PRO:HD3	1.88	0.42
1:R:654:THR:HG22	1:R:654:THR:O	2.19	0.42
1:S:414:PRO:O	1:S:418:ARG:N	2.45	0.42
1:T:313:MET:HE1	1:T:376:VAL:HG22	2.00	0.42
1:T:759:ASN:HB2	1:T:931:THR:HG23	2.01	0.42
1:T:760:ALA:HB1	1:T:769:SER:O	2.18	0.42
1:A:328:ILE:HG22	1:A:344:VAL:HG21	2.01	0.42
2:B:419:VAL:HG22	2:B:465:GLY:H	1.84	0.42
2:C:556:ARG:HE	2:C:560:LEU:HD21	1.85	0.42
2:C:791:ARG:O	2:C:794:ARG:NH1	2.43	0.42
2:D:231:ILE:O	2:D:234:MET:HG3	2.19	0.42
2:D:415:GLU:HG2	2:D:796:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:681:PRO:HB2	2:D:683:GLU:OE1	2.19	0.42
2:E:65:MET:CE	2:E:71:ALA:HA	2.50	0.42
2:E:102:MET:SD	2:E:107:CYS:HB3	2.60	0.42
2:E:220:ARG:CZ	2:E:256:THR:HB	2.49	0.42
2:F:354:GLU:HB2	2:F:417:ALA:O	2.19	0.42
2:F:421:HIS:ND1	2:F:421:HIS:O	2.51	0.42
2:F:513:ILE:HD12	2:F:534:ILE:HG23	2.02	0.42
2:F:527:ARG:HG2	2:F:702:ALA:HB3	2.02	0.42
2:G:385:MET:HE2	2:G:413:CYS:SG	2.59	0.42
2:G:419:VAL:HG13	2:G:465:GLY:C	2.44	0.42
2:I:678:GLU:OE1	2:I:678:GLU:N	2.52	0.42
2:J:375:ARG:HA	2:J:375:ARG:HD2	1.89	0.42
2:J:511:ARG:HH21	2:J:555:THR:HG23	1.85	0.42
2:J:655:LEU:O	2:J:659:TRP:N	2.45	0.42
2:K:416:LEU:HD21	2:K:418:LEU:HD21	2.00	0.42
2:L:136:HIS:ND1	2:L:138:THR:HG22	2.34	0.42
2:N:171:HIS:HB3	2:N:174:ALA:HB3	2.01	0.42
2:N:529:GLY:HA2	2:N:704:GLU:HB3	2.01	0.42
2:N:656:TYR:HA	2:N:659:TRP:HB3	2.00	0.42
1:O:82:LYS:HA	1:O:82:LYS:HD2	1.71	0.42
1:P:776:ARG:NH2	1:P:855:ILE:O	2.36	0.42
1:Q:439:HIS:CE1	1:R:314:LEU:HD12	2.54	0.42
1:R:427:SER:HB2	1:S:294:GLU:OE1	2.19	0.42
1:R:451:PHE:O	1:R:455:LYS:HG3	2.20	0.42
1:S:254:LEU:O	1:S:258:SER:N	2.44	0.42
1:A:73:PHE:HB2	1:A:302:PHE:HD2	1.84	0.42
1:A:116:PRO:HB2	1:A:119:GLU:HB2	2.00	0.42
1:A:563:ASN:ND2	1:A:567:ILE:O	2.47	0.42
2:B:393:LYS:HD3	2:B:393:LYS:HA	1.82	0.42
2:G:85:LYS:HD2	2:G:135:TYR:CZ	2.54	0.42
2:G:263:LYS:HE2	2:G:264:TYR:CZ	2.54	0.42
2:G:662:SER:HB2	2:G:665:VAL:HB	2.00	0.42
2:I:247:HIS:HB3	2:I:252:TYR:CE2	2.54	0.42
2:J:66:LYS:HD3	2:J:66:LYS:HA	1.77	0.42
2:J:133:TYR:HB3	2:J:762:TYR:HE2	1.84	0.42
2:K:170:LYS:HG2	2:K:264:TYR:CG	2.54	0.42
2:L:714:SER:O	2:L:714:SER:OG	2.38	0.42
2:M:536:ILE:HG12	2:M:716:TYR:OH	2.19	0.42
2:M:561:VAL:O	2:M:565:ARG:HG3	2.19	0.42
1:P:78:ARG:HG3	1:P:224:ASP:OD2	2.19	0.42
1:P:524:ASP:OD1	1:P:525:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:611:VAL:O	1:P:616:LEU:HD13	2.18	0.42
1:Q:114:LYS:HE3	1:R:239:LYS:O	2.20	0.42
1:R:631:ASP:OD1	1:R:632:ILE:N	2.50	0.42
1:R:856:PHE:HB3	1:R:895:LEU:HD11	2.02	0.42
1:S:894:TYR:HA	1:S:897:LYS:HB2	2.01	0.42
1:T:136:LYS:HE2	1:T:211:LEU:HA	2.01	0.42
1:A:74:VAL:HG12	1:A:308:ILE:HB	2.02	0.42
2:C:596:GLU:OE1	2:C:651:ARG:NH2	2.50	0.42
2:D:473:MET:HE1	2:D:502:ASP:CG	2.44	0.42
2:D:561:VAL:HG11	2:D:607:PHE:HD2	1.83	0.42
2:F:50:LYS:HE2	2:F:50:LYS:HB2	1.90	0.42
2:F:193:ALA:HA	2:F:197:PRO:HA	2.00	0.42
2:F:649:MET:SD	2:F:652:PRO:HG2	2.59	0.42
2:G:168:ALA:HB1	2:G:208:LEU:HD11	2.01	0.42
2:I:162:GLU:OE2	2:I:299:GLN:NE2	2.53	0.42
2:L:485:ARG:HD2	2:L:639:ARG:HH21	1.84	0.42
2:L:517:LEU:HD21	2:L:695:LYS:HB3	2.01	0.42
2:M:12:LEU:HD12	2:M:297:LEU:HB3	2.01	0.42
2:M:688:LEU:O	2:M:692:VAL:HG23	2.20	0.42
2:N:419:VAL:HG13	2:N:465:GLY:C	2.44	0.42
1:O:576:LEU:HD12	1:O:618:ASP:OD2	2.19	0.42
1:O:639:ARG:NH1	1:O:711:THR:HA	2.35	0.42
1:P:765:MET:HG3	1:P:766:ALA:N	2.34	0.42
1:P:787:LEU:HB2	1:P:842:PHE:CZ	2.54	0.42
1:R:856:PHE:O	1:R:913:THR:HG23	2.19	0.42
1:S:223:ILE:HG22	1:S:227:PHE:HA	2.01	0.42
1:S:337:GLN:CD	1:S:338:ASP:H	2.28	0.42
1:T:485:GLN:NE2	1:T:488:GLU:OE1	2.52	0.42
1:T:720:VAL:HA	1:T:844:LEU:CD1	2.49	0.42
1:A:601:LYS:HG3	1:O:806:LEU:HD12	2.00	0.42
1:A:819:LYS:HB2	1:A:819:LYS:HE3	1.91	0.42
2:B:12:LEU:HD21	2:B:298:ILE:HG13	2.02	0.42
2:B:663:ASP:OD1	2:B:663:ASP:N	2.52	0.42
2:J:763:HIS:O	2:J:767:VAL:HG12	2.19	0.42
2:K:82:LYS:HD3	2:K:83:ASN:O	2.20	0.42
2:K:594:LEU:HD23	2:K:594:LEU:H	1.85	0.42
2:L:70:VAL:O	2:L:74:ARG:HG3	2.20	0.42
2:L:286:GLU:HA	2:L:289:GLU:HB3	2.02	0.42
2:L:430:GLY:C	2:L:431:GLU:HG3	2.44	0.42
2:L:545:LEU:HD23	2:L:545:LEU:HA	1.92	0.42
2:M:572:GLU:OE1	2:M:572:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:70:VAL:HG12	2:N:289:GLU:OE2	2.19	0.42
1:O:378:LEU:O	1:O:382:VAL:HG23	2.20	0.42
1:P:227:PHE:CD2	1:P:260:LEU:HB2	2.55	0.42
1:P:359:ARG:HB2	1:P:795:SER:HA	2.01	0.42
1:P:450:ILE:HD12	1:P:466:LEU:HD11	2.01	0.42
1:P:470:SER:HB2	1:P:476:ARG:HG3	2.02	0.42
1:P:608:LEU:HB3	1:P:650:ILE:HG22	2.01	0.42
1:Q:467:ARG:HH12	1:Q:732:LEU:HD13	1.84	0.42
1:Q:559:ALA:HA	1:Q:570:PHE:CE2	2.52	0.42
1:Q:872:THR:O	1:Q:876:LYS:HG2	2.19	0.42
1:Q:879:ASP:HA	1:Q:882:VAL:HG12	2.02	0.42
1:S:359:ARG:HH21	1:S:794:HIS:HB3	1.83	0.42
1:T:511:PHE:CZ	1:T:532:ILE:HG12	2.51	0.42
1:T:723:ILE:HD11	1:T:836:LYS:HB2	2.00	0.42
1:A:223:ILE:HD11	1:A:257:TYR:HE1	1.85	0.42
2:E:385:MET:HE2	2:E:410:HIS:NE2	2.34	0.42
2:E:615:GLU:OE1	2:E:637:TYR:OH	2.32	0.42
2:F:532:THR:HG23	2:F:723:HIS:CD2	2.55	0.42
2:J:187:GLU:OE1	2:J:187:GLU:N	2.50	0.42
2:J:217:ILE:HD11	2:J:230:TRP:HH2	1.84	0.42
2:K:14:ARG:HB3	2:K:28:ARG:HE	1.84	0.42
2:K:370:LEU:HD21	2:K:459:LEU:HD11	2.01	0.42
2:L:158:SER:O	2:L:337:ARG:NH1	2.49	0.42
2:L:503:PHE:CE2	2:L:506:LEU:HA	2.55	0.42
2:M:347:TYR:CE1	2:M:412:LYS:HD3	2.54	0.42
2:N:273:LEU:HD23	2:N:273:LEU:HA	1.91	0.42
1:O:539:MET:HE2	1:O:557:VAL:HG21	2.01	0.42
1:P:123:VAL:HG12	1:P:164:LEU:HD21	2.02	0.42
1:P:231:TRP:CZ2	1:P:264:LYS:HD2	2.54	0.42
1:R:227:PHE:HZ	1:S:269:TYR:CD1	2.37	0.42
1:R:431:ARG:NH2	1:R:474:ALA:HB3	2.33	0.42
1:S:133:VAL:HG23	1:S:210:ILE:HG21	2.01	0.42
1:S:650:ILE:HD12	1:T:807:ARG:H	1.85	0.42
1:T:133:VAL:O	1:T:137:LEU:HD23	2.20	0.42
1:A:488:GLU:O	1:A:491:GLN:HG2	2.19	0.42
1:A:757:TYR:HE1	1:A:929:LYS:HE3	1.84	0.42
1:A:842:PHE:O	1:A:846:ILE:HG22	2.20	0.42
2:E:356:ARG:HD3	2:E:419:VAL:HB	2.02	0.42
2:E:672:TYR:N	2:F:58:GLN:HE22	2.15	0.42
2:F:332:LYS:HD2	2:F:335:LEU:HD23	2.01	0.42
2:F:354:GLU:O	2:F:354:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:789:ASN:HD22	2:I:792:ILE:HB	1.85	0.42
2:J:148:LEU:HD13	2:J:757:LEU:HG	2.02	0.42
2:J:601:THR:HG21	2:N:585:VAL:HG21	2.01	0.42
2:K:351:ARG:O	2:K:415:GLU:N	2.50	0.42
2:K:730:LEU:HD21	2:K:768:LEU:HD22	2.02	0.42
2:L:15:LEU:HD13	2:L:290:ARG:HG3	2.00	0.42
2:M:664:ASN:OD1	2:M:665:VAL:N	2.53	0.42
1:Q:312:THR:HG22	1:Q:313:MET:H	1.84	0.42
1:R:162:ARG:HD2	1:R:163:GLY:N	2.35	0.42
1:R:460:PHE:HD2	1:R:512:ASN:HB2	1.85	0.42
1:R:771:ALA:O	1:R:775:MET:HG2	2.20	0.42
1:S:79:GLY:O	1:S:377:ARG:HG2	2.20	0.42
1:S:285:GLU:HG2	1:S:286:ARG:N	2.33	0.42
1:T:789:GLU:HA	1:T:792:LEU:HB2	2.02	0.42
1:A:606:SER:HB3	1:A:646:PHE:CD1	2.55	0.42
2:C:111:ILE:HD11	2:C:126:TYR:HE2	1.85	0.42
2:C:359:PRO:HG2	2:C:445:GLN:HE21	1.85	0.42
2:C:404:LEU:HB3	2:C:462:TRP:CZ2	2.54	0.42
2:E:155:LEU:HD12	2:E:334:TYR:HD1	1.85	0.42
2:F:214:ILE:HA	2:F:217:ILE:HG22	2.02	0.42
2:G:496:THR:HB	2:G:795:PHE:HZ	1.84	0.42
2:I:467:ASP:OD1	2:I:468:ALA:N	2.53	0.42
2:I:791:ARG:HA	2:I:794:ARG:HB3	2.01	0.42
2:L:756:ASP:OD1	2:L:757:LEU:N	2.52	0.42
2:M:12:LEU:HD11	2:M:298:ILE:HD13	2.01	0.42
2:M:696:MET:O	2:M:700:ASN:N	2.53	0.42
2:N:717:ARG:HA	2:N:717:ARG:HD3	1.86	0.42
1:O:303:PRO:HB2	1:O:306:LYS:HG2	2.01	0.42
1:O:498:LEU:HD13	1:O:629:ILE:HG23	2.02	0.42
1:P:32:LEU:HD22	1:P:38:ARG:NH1	2.34	0.42
1:Q:845:LEU:HD23	1:Q:845:LEU:HA	1.93	0.42
1:S:551:ALA:HB3	1:S:624:ASN:OD1	2.20	0.42
1:S:790:GLU:OE1	1:S:841:LEU:HB2	2.18	0.42
1:T:701:ASP:N	1:T:701:ASP:OD1	2.52	0.42
1:T:882:VAL:HG12	1:T:884:ASP:H	1.85	0.42
1:A:914:ILE:HG12	1:A:917:LEU:HB2	2.01	0.42
2:C:797:ASP:OD1	2:C:798:VAL:N	2.53	0.42
2:E:73:LEU:HD13	2:E:110:ILE:HD13	2.02	0.42
2:F:494:HIS:CE1	2:L:85:LYS:HD3	2.54	0.42
2:G:424:LYS:HD3	2:G:480:PHE:CZ	2.54	0.42
2:G:659:TRP:HA	2:G:665:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:GLN:HG3	2:J:62:GLN:NE2	2.35	0.42
2:J:529:GLY:HA2	2:J:704:GLU:HB2	2.02	0.42
2:J:548:SER:OG	2:J:674:GLU:OE2	2.36	0.42
2:K:658:GLN:HG2	2:K:665:VAL:HG21	2.02	0.42
2:K:748:ASP:OD1	2:K:749:ASP:N	2.52	0.42
2:M:195:ILE:HD13	2:M:304:THR:HG22	2.00	0.42
2:M:465:GLY:HA2	2:M:494:HIS:O	2.19	0.42
2:N:501:GLU:OE1	2:N:533:ALA:HB2	2.20	0.42
2:N:609:MET:O	2:N:612:LEU:HG	2.20	0.42
1:O:813:SER:OG	1:O:814:VAL:N	2.53	0.42
1:P:496:LYS:O	1:P:500:MET:HE3	2.20	0.42
1:P:575:GLN:CD	1:P:923:VAL:HG12	2.45	0.42
1:P:838:THR:HG23	1:P:839:HIS:CD2	2.55	0.42
1:Q:642:ILE:HD12	1:Q:710:ILE:HG23	2.02	0.42
1:R:150:LYS:HA	1:R:150:LYS:HD2	1.85	0.42
1:S:707:SER:HA	1:S:710:ILE:HB	2.02	0.42
1:S:728:ARG:H	1:S:794:HIS:CE1	2.38	0.42
1:T:425:MET:O	1:T:429:ILE:HG12	2.19	0.42
1:T:472:SER:HB3	1:T:475:LEU:HB2	2.02	0.42
1:T:596:GLU:HG2	1:T:914:ILE:HG23	2.02	0.42
1:T:626:ILE:HA	1:T:629:ILE:HG22	2.01	0.42
1:A:434:LEU:HD12	1:A:449:ASP:HB3	2.01	0.41
2:C:142:TYR:CG	2:C:780:LEU:HD11	2.55	0.41
2:C:163:GLU:CG	2:C:266:GLN:HE21	2.32	0.41
2:C:450:MET:HA	2:C:453:LEU:HB3	2.02	0.41
2:D:77:ALA:HB1	2:D:114:HIS:HB2	2.01	0.41
2:D:505:HIS:O	2:D:508:SER:OG	2.25	0.41
2:E:7:ASN:HD21	2:E:304:THR:HG21	1.84	0.41
2:E:95:PHE:HD2	2:E:766:VAL:HG21	1.85	0.41
2:E:482:PRO:HG2	2:E:613:LEU:HD13	2.02	0.41
2:F:233:SER:OG	2:F:247:HIS:ND1	2.52	0.41
2:F:402:ASP:O	2:F:405:GLU:HG2	2.20	0.41
2:G:393:LYS:HD3	2:G:393:LYS:HA	1.76	0.41
2:G:507:ILE:HG21	2:G:563:ILE:HD11	2.02	0.41
2:I:14:ARG:HH11	2:I:32:SER:HB2	1.84	0.41
2:I:606:VAL:HA	2:I:609:MET:HE2	2.02	0.41
2:J:155:LEU:HA	2:J:337:ARG:HH12	1.85	0.41
2:J:342:HIS:HD2	2:J:343:GLY:O	2.03	0.41
2:L:102:MET:SD	2:L:107:CYS:HB3	2.60	0.41
2:L:665:VAL:O	2:L:669:ARG:HG3	2.20	0.41
2:M:148:LEU:HB2	2:M:350:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:259:PRO:HG2	2:N:260:ILE:HD12	2.02	0.41
1:O:727:ILE:HG13	1:O:840:PRO:HG2	2.01	0.41
1:P:162:ARG:HH21	1:P:180:ALA:CA	2.33	0.41
1:P:769:SER:HA	1:P:773:LYS:HD2	2.01	0.41
1:Q:575:GLN:HA	1:Q:618:ASP:O	2.20	0.41
1:S:255:ARG:NH1	1:S:255:ARG:HB3	2.35	0.41
1:A:18:LEU:HD22	1:A:384:GLN:HB2	2.02	0.41
1:A:74:VAL:HG11	1:A:85:PHE:HE2	1.85	0.41
2:B:717:ARG:HD2	2:N:717:ARG:HH21	1.84	0.41
2:C:294:ILE:O	2:C:298:ILE:HG12	2.20	0.41
2:D:359:PRO:O	2:D:445:GLN:NE2	2.54	0.41
2:E:531:CYS:HB2	2:E:703:ILE:HD13	2.02	0.41
2:E:569:SER:HB3	2:G:575:ARG:HB3	2.01	0.41
2:F:567:LEU:HD21	2:F:688:LEU:HG	2.02	0.41
2:G:342:HIS:ND1	2:G:348:SER:HB3	2.35	0.41
2:I:678:GLU:HG2	2:I:678:GLU:O	2.20	0.41
2:J:234:MET:HE3	2:J:234:MET:HB3	1.96	0.41
2:K:79:LYS:HG2	2:K:80:PHE:CE1	2.55	0.41
2:K:592:PHE:HE1	2:K:659:TRP:HB2	1.84	0.41
2:M:347:TYR:CE2	2:N:409:PRO:HG2	2.54	0.41
2:N:354:GLU:CD	2:N:527:ARG:HH22	2.27	0.41
2:N:576:TYR:OH	2:N:681:PRO:HG2	2.20	0.41
1:Q:312:THR:HG22	1:Q:313:MET:N	2.35	0.41
1:T:607:SER:HB2	1:T:625:LEU:HD21	2.02	0.41
1:A:231:TRP:CD2	1:A:264:LYS:HG3	2.55	0.41
2:B:228:PRO:HD2	2:B:230:TRP:HE1	1.85	0.41
2:C:303:LEU:HB3	2:C:753:PHE:CE1	2.55	0.41
2:C:360:LYS:O	2:C:366:MET:HE3	2.20	0.41
2:D:659:TRP:NE1	2:D:669:ARG:HH11	2.19	0.41
2:E:397:ILE:HD11	2:E:459:LEU:HD13	2.03	0.41
2:E:560:LEU:HD23	2:E:560:LEU:HA	1.90	0.41
2:E:582:ILE:HD11	2:K:564:TRP:CH2	2.55	0.41
2:F:481:CYS:HB3	2:F:482:PRO:HD3	2.03	0.41
2:G:40:GLN:O	2:I:42:ARG:NH2	2.53	0.41
2:I:95:PHE:CD2	2:I:134:PRO:HG3	2.55	0.41
2:J:464:ARG:O	2:J:494:HIS:HB2	2.21	0.41
2:K:123:SER:O	2:K:123:SER:OG	2.31	0.41
2:L:55:TYR:O	2:L:58:GLN:HG2	2.20	0.41
2:L:152:HIS:CG	2:L:748:ASP:HB3	2.55	0.41
2:M:243:SER:HA	2:M:254:PHE:HD2	1.84	0.41
2:N:77:ALA:HB1	2:N:114:HIS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:ALA:HB1	1:O:376:VAL:HG23	2.02	0.41
1:O:439:HIS:HB2	1:P:314:LEU:HD23	2.03	0.41
1:O:439:HIS:HE1	1:P:373:LYS:HD3	1.85	0.41
1:O:487:SER:O	1:O:491:GLN:HB2	2.20	0.41
1:P:839:HIS:O	1:P:843:PHE:HD2	2.03	0.41
1:R:162:ARG:O	1:R:166:LEU:HD23	2.20	0.41
1:S:122:LEU:HA	1:S:122:LEU:HD12	1.86	0.41
1:T:454:VAL:HG22	1:T:463:GLY:HA3	2.02	0.41
2:B:356:ARG:HB3	2:B:421:HIS:HD2	1.85	0.41
2:B:506:LEU:O	2:B:510:ILE:HG12	2.20	0.41
2:B:726:ARG:HE	2:B:735:ILE:HG12	1.84	0.41
2:D:22:GLU:OE1	2:D:22:GLU:N	2.32	0.41
2:E:155:LEU:HD12	2:E:334:TYR:CD1	2.56	0.41
2:F:725:PHE:HB2	2:F:733:GLU:HG2	2.02	0.41
2:G:356:ARG:HD3	2:G:419:VAL:HB	2.01	0.41
2:I:487:LEU:HD12	2:I:492:ILE:HG13	2.02	0.41
2:K:293:TRP:O	2:K:297:LEU:HG	2.20	0.41
2:M:131:PRO:HB3	2:M:754:ALA:HB1	2.02	0.41
2:N:130:TRP:NE1	2:N:343:GLY:HA2	2.36	0.41
2:N:404:LEU:O	2:N:407:VAL:HG12	2.20	0.41
1:P:656:ILE:N	1:P:656:ILE:CD1	2.73	0.41
1:Q:266:TYR:CD2	1:R:273:LEU:HA	2.55	0.41
1:R:264:LYS:HA	1:R:264:LYS:HD2	1.83	0.41
1:R:367:TYR:CD2	1:R:480:ILE:HG22	2.56	0.41
1:R:444:ASP:HB2	1:R:542:GLY:C	2.46	0.41
1:R:716:TRP:HE3	1:R:849:PRO:HG3	1.85	0.41
1:S:448:LYS:HE3	1:S:452:THR:HG21	2.03	0.41
1:S:571:LEU:HD21	1:S:623:PHE:CD2	2.56	0.41
1:T:110:ILE:HG22	1:T:128:ARG:HE	1.85	0.41
1:A:458:ARG:NH2	1:T:533:SER:HB3	2.35	0.41
2:B:20:LEU:HD22	2:B:287:GLY:HA2	2.02	0.41
2:B:183:TRP:O	2:B:189:LYS:NZ	2.48	0.41
2:B:642:GLU:O	2:B:645:LYS:HG3	2.21	0.41
2:C:130:TRP:NE1	2:C:343:GLY:HA2	2.36	0.41
2:C:134:PRO:HG2	2:C:762:TYR:CD1	2.55	0.41
2:C:531:CYS:HB2	2:C:703:ILE:HD13	2.02	0.41
2:E:165:TRP:HB2	2:E:303:LEU:HD21	2.02	0.41
2:F:214:ILE:HG21	2:F:295:TYR:HB2	2.02	0.41
2:G:347:TYR:CG	2:G:412:LYS:HE3	2.55	0.41
2:I:177:ARG:HH12	2:I:181:LYS:HD2	1.85	0.41
2:I:207:ARG:HA	2:I:210:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:269:GLU:HA	2:I:272:TRP:HB3	2.02	0.41
2:I:381:LEU:HD23	2:I:381:LEU:HA	1.90	0.41
2:I:724:ILE:O	2:I:728:MET:HG2	2.20	0.41
2:J:82:LYS:HA	2:J:82:LYS:HE3	2.02	0.41
2:J:356:ARG:HA	2:J:419:VAL:O	2.20	0.41
2:K:80:PHE:CD2	2:K:98:TRP:HB2	2.56	0.41
2:L:397:ILE:H	2:L:397:ILE:HG13	1.72	0.41
2:N:228:PRO:HG2	2:N:230:TRP:CZ2	2.56	0.41
1:O:279:GLU:O	1:O:283:LEU:HD13	2.20	0.41
1:O:626:ILE:HD11	1:O:741:PHE:HE2	1.84	0.41
1:P:525:ARG:NH1	1:P:525:ARG:O	2.53	0.41
1:S:455:LYS:O	1:S:458:ARG:NH1	2.54	0.41
1:A:118:HIS:CG	1:O:171:GLU:HA	2.56	0.41
1:A:228:ASP:N	1:A:228:ASP:OD1	2.52	0.41
1:A:846:ILE:HD11	1:A:878:ILE:HD12	2.01	0.41
2:C:259:PRO:HG2	2:C:260:ILE:HD12	2.01	0.41
2:C:351:ARG:O	2:C:415:GLU:N	2.51	0.41
2:C:610:ARG:HA	2:C:656:TYR:CZ	2.55	0.41
2:D:12:LEU:HD11	2:D:298:ILE:HG12	2.02	0.41
2:D:102:MET:SD	2:D:107:CYS:HB3	2.61	0.41
2:D:527:ARG:HG2	2:D:702:ALA:HB3	2.02	0.41
2:D:690:GLN:HA	2:D:693:MET:HB2	2.01	0.41
2:D:693:MET:HA	2:D:741:MET:HE2	2.02	0.41
2:F:564:TRP:CD1	2:F:581:ALA:HB2	2.55	0.41
2:F:693:MET:HG2	2:F:741:MET:HE3	2.02	0.41
2:I:236:ASN:N	2:I:239:GLN:OE1	2.52	0.41
2:K:612:LEU:HD22	2:K:640:ALA:HB1	2.03	0.41
2:L:400:VAL:HG12	2:L:404:LEU:HD23	2.02	0.41
2:L:678:GLU:OE2	2:L:678:GLU:N	2.41	0.41
2:M:269:GLU:OE2	2:M:295:TYR:OH	2.27	0.41
1:O:930:ASP:N	1:O:930:ASP:OD1	2.43	0.41
1:P:716:TRP:HE1	1:P:847:SER:HB2	1.85	0.41
1:S:204:VAL:HG21	1:S:246:LEU:HD21	2.03	0.41
1:S:204:VAL:HG21	1:S:246:LEU:HD11	2.01	0.41
1:S:514:PHE:CD1	1:S:561:SER:HB3	2.55	0.41
1:T:166:LEU:HA	1:T:169:ASP:HB2	2.02	0.41
1:T:374:GLN:NE2	1:T:477:ASN:OD1	2.53	0.41
2:D:417:ALA:HB1	2:D:464:ARG:HG3	2.03	0.41
2:D:590:LYS:HD3	2:I:647:THR:HA	2.01	0.41
2:E:26:ASP:OD1	2:E:26:ASP:N	2.53	0.41
2:E:205:LYS:HA	2:E:205:LYS:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:LEU:HD22	2:F:293:TRP:HZ2	1.85	0.41
2:F:245:ILE:HG23	2:F:252:TYR:HB2	2.02	0.41
2:F:286:GLU:HA	2:F:289:GLU:HB3	2.03	0.41
2:F:713:ILE:HG13	2:F:715:GLN:OE1	2.21	0.41
2:G:464:ARG:O	2:G:494:HIS:HB2	2.21	0.41
2:J:162:GLU:O	2:J:165:TRP:HB3	2.20	0.41
2:J:576:TYR:OH	2:J:681:PRO:HG2	2.20	0.41
2:K:516:ALA:O	2:K:520:LEU:HB2	2.21	0.41
2:L:342:HIS:CE1	2:L:348:SER:HB3	2.55	0.41
2:L:582:ILE:O	2:L:586:ARG:HD3	2.20	0.41
2:N:434:PRO:HG2	2:N:669:ARG:NH2	2.31	0.41
1:P:733:LEU:O	1:P:737:VAL:HG13	2.19	0.41
1:Q:35:LYS:HZ2	1:Q:38:ARG:HD3	1.86	0.41
1:R:425:MET:SD	1:R:480:ILE:HD11	2.61	0.41
1:R:723:ILE:HG22	1:R:840:PRO:HB3	2.02	0.41
1:S:925:ALA:C	1:S:927:TYR:H	2.28	0.41
1:T:614:ASN:C	1:T:614:ASN:HD22	2.28	0.41
1:A:82:LYS:HD2	1:A:222:ASP:HB3	2.03	0.41
1:A:159:GLN:OE1	1:A:189:TYR:OH	2.20	0.41
2:B:649:MET:CG	2:B:652:PRO:HD2	2.51	0.41
2:C:107:CYS:HA	2:C:110:ILE:HD12	2.02	0.41
2:C:597:GLU:OE1	2:M:602:THR:OG1	2.37	0.41
2:D:149:HIS:CE1	2:D:791:ARG:HB2	2.56	0.41
2:D:662:SER:O	2:D:666:ARG:HG3	2.20	0.41
2:E:43:SER:HA	2:F:714:SER:HB2	2.02	0.41
2:E:111:ILE:HD12	2:E:132:LEU:HD21	2.03	0.41
2:E:550:SER:O	2:F:51:SER:OG	2.28	0.41
2:F:160:SER:N	2:F:163:GLU:OE2	2.42	0.41
2:F:251:GLU:H	2:F:251:GLU:CD	2.28	0.41
2:G:351:ARG:NE	2:G:411:GLY:HA2	2.36	0.41
2:G:425:ARG:H	2:G:438:LEU:HD11	1.84	0.41
2:I:417:ALA:HB2	2:I:796:HIS:CD2	2.56	0.41
2:I:499:VAL:HG21	2:I:513:ILE:HD13	2.02	0.41
2:I:789:ASN:HD22	2:I:789:ASN:C	2.28	0.41
2:L:214:ILE:HG21	2:L:295:TYR:HB2	2.03	0.41
2:L:303:LEU:HB3	2:L:753:PHE:CZ	2.56	0.41
2:L:516:ALA:O	2:L:520:LEU:HB2	2.20	0.41
2:M:34:PHE:O	2:M:37:GLN:HG3	2.21	0.41
2:N:134:PRO:HG2	2:N:762:TYR:CD1	2.56	0.41
2:N:730:LEU:HD21	2:N:768:LEU:HD22	2.01	0.41
1:O:701:ASP:OD1	1:O:701:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:822:LYS:HD2	1:O:822:LYS:HA	1.89	0.41
1:P:616:LEU:HD21	1:Q:746:ASN:CG	2.46	0.41
1:P:744:ASN:HA	1:P:747:ASN:OD1	2.21	0.41
1:Q:266:TYR:HD2	1:R:273:LEU:HA	1.84	0.41
1:Q:303:PRO:HB2	1:Q:306:LYS:HG2	2.02	0.41
1:Q:511:PHE:CZ	1:Q:532:ILE:HG12	2.49	0.41
1:Q:639:ARG:HB3	1:Q:642:ILE:HD11	2.03	0.41
1:R:167:LEU:O	1:R:168:THR:OG1	2.26	0.41
1:R:801:TYR:HB3	1:R:824:ILE:HG12	2.02	0.41
1:T:277:GLU:HB3	1:T:282:ARG:HG3	2.03	0.41
1:A:156:HIS:HB3	1:A:203:LEU:HD12	2.03	0.41
1:A:183:LEU:HD11	1:T:134:SER:HB3	2.02	0.41
1:A:225:THR:OG1	1:O:238:ARG:NH2	2.54	0.41
1:A:788:VAL:HG13	1:A:807:ARG:HD3	2.02	0.41
2:B:394:PRO:O	2:B:395:LEU:HG	2.21	0.41
2:B:720:SER:HB2	2:B:771:LYS:HG2	2.02	0.41
2:C:234:MET:HE3	2:C:240:LEU:HD11	2.03	0.41
2:D:247:HIS:HB3	2:D:252:TYR:HD2	1.86	0.41
2:D:511:ARG:HH21	2:D:555:THR:HG23	1.85	0.41
2:D:554:GLU:HG3	2:D:555:THR:N	2.35	0.41
2:E:46:ASP:OD1	2:E:47:HIS:N	2.54	0.41
2:E:109:PRO:HG3	2:E:296:LEU:HD11	2.02	0.41
2:E:259:PRO:HG2	2:E:260:ILE:HD12	2.02	0.41
2:E:418:LEU:HB2	2:E:463:ILE:HD13	2.03	0.41
2:F:65:MET:HE1	2:F:71:ALA:HA	2.03	0.41
2:G:228:PRO:HB2	2:G:230:TRP:CD1	2.56	0.41
2:G:775:SER:OG	2:G:778:ASP:OD2	2.37	0.41
2:J:95:PHE:CE1	2:J:134:PRO:HD3	2.55	0.41
2:J:134:PRO:HD2	2:J:762:TYR:CD2	2.54	0.41
2:J:418:LEU:HB2	2:J:463:ILE:HD13	2.03	0.41
2:J:565:ARG:NH1	2:J:604:ASP:OD1	2.50	0.41
2:K:108:LEU:HD13	2:K:269:GLU:HG2	2.03	0.41
2:K:360:LYS:HD3	2:K:365:LYS:HB3	2.02	0.41
2:L:351:ARG:HG3	2:L:411:GLY:O	2.20	0.41
2:L:424:LYS:HG3	2:L:438:LEU:HD21	2.03	0.41
2:L:530:HIS:HA	2:L:706:PRO:HD3	2.03	0.41
2:L:717:ARG:H	2:L:717:ARG:HG2	1.73	0.41
2:M:12:LEU:HD13	2:M:301:GLN:HG3	2.02	0.41
2:M:69:PRO:O	2:M:73:LEU:HG	2.21	0.41
2:M:299:GLN:O	2:M:303:LEU:HD23	2.20	0.41
2:M:388:GLU:HG2	1:Q:141:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:450:MET:O	2:M:454:LYS:HG3	2.20	0.41
2:M:696:MET:HG3	2:M:701:ILE:HB	2.02	0.41
1:O:160:LEU:O	1:O:164:LEU:N	2.54	0.41
1:O:755:ARG:HH11	1:O:767:SER:HA	1.85	0.41
1:P:69:ARG:HH22	1:P:238:ARG:HA	1.86	0.41
1:P:131:LYS:HD2	1:Q:192:GLY:H	1.84	0.41
1:P:133:VAL:O	1:P:137:LEU:HD23	2.21	0.41
1:P:543:ARG:HG2	1:Q:469:GLN:O	2.21	0.41
1:P:576:LEU:HD22	1:P:920:SER:HB2	2.03	0.41
1:P:639:ARG:HB3	1:P:642:ILE:HD12	2.03	0.41
1:P:787:LEU:HB2	1:P:842:PHE:HZ	1.86	0.41
1:Q:38:ARG:HH21	1:Q:92:SER:HB2	1.85	0.41
1:Q:740:ARG:HH12	1:Q:807:ARG:HG2	1.86	0.41
1:Q:741:PHE:CZ	1:Q:745:LEU:HD11	2.56	0.41
1:R:73:PHE:CE2	1:R:254:LEU:HD12	2.52	0.41
1:S:195:ASP:HB2	1:S:198:GLU:OE2	2.21	0.41
1:S:366:MET:O	1:S:370:GLU:HG2	2.20	0.41
1:S:527:LYS:HE2	1:S:531:LEU:HD22	2.03	0.41
1:T:82:LYS:HG3	1:T:83:THR:N	2.36	0.41
1:T:359:ARG:HG2	1:T:360:GLU:H	1.86	0.41
1:T:553:ARG:NH1	1:T:654:THR:O	2.54	0.41
1:T:597:ASN:O	1:T:601:LYS:N	2.37	0.41
1:T:720:VAL:HA	1:T:844:LEU:HD13	2.02	0.41
1:T:914:ILE:HG13	1:T:917:LEU:HD12	2.01	0.41
2:C:5:LEU:HD11	2:C:53:TRP:HZ3	1.86	0.41
2:C:9:THR:HG21	2:C:196:ASP:HB3	2.03	0.41
2:C:471:ASN:OD1	2:C:473:MET:N	2.54	0.41
2:F:34:PHE:O	2:F:37:GLN:HG3	2.21	0.41
2:G:227:LEU:HA	2:G:228:PRO:HD3	1.93	0.41
2:I:564:TRP:O	2:I:568:ARG:HB2	2.21	0.41
2:J:129:ARG:HB3	2:J:130:TRP:CE3	2.56	0.41
2:J:477:PRO:O	2:J:520:LEU:HD11	2.20	0.41
2:K:425:ARG:H	2:K:438:LEU:CD1	2.33	0.41
2:L:95:PHE:CG	2:L:134:PRO:HG3	2.56	0.41
2:L:116:VAL:O	2:L:281:ARG:NH2	2.54	0.41
2:L:567:LEU:HB3	2:L:577:ALA:HB2	2.02	0.41
2:N:79:LYS:HE2	2:N:79:LYS:HB2	1.95	0.41
1:P:787:LEU:O	1:P:790:GLU:HG2	2.21	0.41
1:Q:303:PRO:O	1:Q:307:ARG:HG3	2.21	0.41
1:Q:313:MET:HE3	1:Q:379:LEU:HD11	2.02	0.41
1:Q:826:GLU:HG3	1:Q:827:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:227:PHE:HD1	1:S:260:LEU:HD13	1.86	0.41
1:S:654:THR:HA	1:T:743:PHE:CE2	2.56	0.41
1:A:102:VAL:O	1:A:102:VAL:HG13	2.21	0.40
2:B:148:LEU:N	2:B:349:GLN:O	2.50	0.40
2:C:466:VAL:HG23	2:C:492:ILE:HG21	2.02	0.40
2:C:503:PHE:O	2:D:47:HIS:NE2	2.53	0.40
2:C:651:ARG:HB3	2:C:652:PRO:HD3	2.03	0.40
2:C:764:LEU:HD23	2:C:764:LEU:HA	1.89	0.40
2:D:506:LEU:O	2:D:510:ILE:HG13	2.22	0.40
2:D:788:GLU:O	2:D:792:ILE:HG12	2.21	0.40
2:I:15:LEU:HD23	2:I:15:LEU:HA	1.93	0.40
2:I:418:LEU:N	2:I:462:TRP:O	2.55	0.40
2:I:642:GLU:HG2	2:I:643:LEU:N	2.36	0.40
2:L:717:ARG:HG3	2:M:717:ARG:HH22	1.86	0.40
2:N:236:ASN:N	2:N:239:GLN:OE1	2.53	0.40
2:N:396:THR:O	2:N:400:VAL:HG23	2.21	0.40
1:O:357:ASN:HB3	1:O:728:ARG:HB2	2.04	0.40
1:O:565:GLU:HG2	1:O:567:ILE:HG13	2.03	0.40
1:Q:864:SER:HB2	1:Q:867:ALA:H	1.86	0.40
1:R:273:LEU:O	1:R:286:ARG:NH1	2.54	0.40
1:R:427:SER:HA	1:R:430:TYR:HD2	1.86	0.40
1:S:145:ASP:HB2	1:S:148:LYS:HE3	2.03	0.40
1:S:887:LEU:HD12	1:S:892:TRP:HD1	1.86	0.40
1:S:929:LYS:HE2	1:S:929:LYS:HB3	1.88	0.40
1:T:41:LEU:HD12	1:T:85:PHE:HE2	1.85	0.40
1:A:136:LYS:HB3	1:A:136:LYS:HE3	1.89	0.40
1:A:739:SER:HA	1:A:742:TYR:HB3	2.03	0.40
1:A:776:ARG:HB2	1:A:857:PRO:HG2	2.03	0.40
2:B:245:ILE:HD12	2:B:245:ILE:HA	2.00	0.40
2:C:158:SER:O	2:C:337:ARG:NH2	2.53	0.40
2:C:176:LEU:HD13	2:C:205:LYS:HB2	2.02	0.40
2:E:156:ASN:OD1	2:E:358:ALA:N	2.54	0.40
2:F:108:LEU:HA	2:F:128:PHE:HE2	1.86	0.40
2:F:404:LEU:O	2:F:407:VAL:HG12	2.21	0.40
2:G:83:ASN:OD1	2:G:114:HIS:NE2	2.53	0.40
2:I:296:LEU:HD23	2:I:296:LEU:HA	1.92	0.40
2:I:381:LEU:O	2:I:385:MET:N	2.51	0.40
2:J:37:GLN:NE2	2:J:44:LEU:HB3	2.36	0.40
2:M:399:GLN:OE1	1:R:182:LYS:NZ	2.52	0.40
2:M:663:ASP:OD1	2:M:663:ASP:N	2.54	0.40
1:O:443:MET:HE3	1:O:496:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:491:GLN:HA	1:O:729:PRO:HD2	2.03	0.40
1:P:443:MET:SD	1:P:496:LYS:HD3	2.61	0.40
1:P:884:ASP:OD1	1:P:884:ASP:N	2.50	0.40
1:R:426:LEU:HA	1:R:429:ILE:HB	2.03	0.40
1:S:255:ARG:HB3	1:S:255:ARG:CZ	2.51	0.40
1:T:304:VAL:HA	1:T:307:ARG:CG	2.51	0.40
1:T:801:TYR:HD1	1:T:827:LYS:HB3	1.86	0.40
1:A:510:ILE:HG13	1:A:514:PHE:HD2	1.86	0.40
1:A:612:ALA:HB1	1:O:746:ASN:HD21	1.86	0.40
1:A:654:THR:OG1	1:O:743:PHE:HB2	2.20	0.40
2:B:44:LEU:HD21	2:N:546:PRO:HD3	2.03	0.40
2:B:152:HIS:HD2	2:B:356:ARG:HG3	1.86	0.40
2:B:401:LEU:HD11	2:B:459:LEU:HD23	2.02	0.40
2:B:518:ARG:HD2	2:B:565:ARG:NH2	2.36	0.40
2:B:592:PHE:O	2:B:658:GLN:NE2	2.51	0.40
2:D:95:PHE:CD2	2:D:134:PRO:HG3	2.57	0.40
2:D:228:PRO:HB2	2:D:230:TRP:NE1	2.37	0.40
2:D:434:PRO:N	2:D:666:ARG:HH22	2.19	0.40
2:F:531:CYS:HB2	2:F:703:ILE:HD13	2.04	0.40
2:G:578:SER:O	2:G:582:ILE:HG12	2.21	0.40
2:I:2:GLU:OE1	2:I:2:GLU:N	2.54	0.40
2:I:696:MET:SD	2:I:701:ILE:HB	2.62	0.40
2:J:659:TRP:HA	2:J:665:VAL:HG11	2.03	0.40
2:J:788:GLU:O	2:J:792:ILE:HG13	2.21	0.40
2:K:434:PRO:HG3	2:K:666:ARG:HD2	2.03	0.40
2:K:662:SER:HB2	2:K:665:VAL:HB	2.03	0.40
2:L:74:ARG:HD2	2:L:117:PHE:CE1	2.56	0.40
2:L:360:LYS:HD3	2:L:362:ASP:H	1.86	0.40
2:L:605:GLN:O	2:L:609:MET:HG3	2.21	0.40
2:M:546:PRO:HG2	2:M:549:LEU:HD23	2.02	0.40
1:O:105:LYS:HA	1:O:105:LYS:HD3	1.75	0.40
1:O:289:MET:O	1:O:293:LEU:HG	2.22	0.40
1:O:729:PRO:HA	1:O:733:LEU:HD23	2.02	0.40
1:O:851:LEU:O	1:O:855:ILE:HG13	2.21	0.40
1:P:220:PHE:HB2	1:P:250:ALA:HA	2.02	0.40
1:P:426:LEU:HD23	1:P:430:TYR:HE2	1.86	0.40
1:R:234:LEU:HD21	1:R:257:TYR:CE2	2.56	0.40
1:R:536:VAL:HA	1:R:541:VAL:HG22	2.04	0.40
1:S:479:SER:HA	1:S:482:LEU:HB2	2.02	0.40
1:T:28:LYS:HA	1:T:28:LYS:HD2	1.96	0.40
1:T:762:HIS:O	1:T:762:HIS:ND1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:ND1	1:A:118:HIS:O	2.54	0.40
1:A:320:LYS:HD3	1:A:345:ARG:NH2	2.35	0.40
2:B:259:PRO:HG2	2:B:260:ILE:HD12	2.03	0.40
2:B:491:GLY:HA2	2:G:121:PRO:HB2	2.04	0.40
2:C:89:LYS:HD2	2:C:133:TYR:O	2.22	0.40
2:E:377:TYR:OH	2:E:414:VAL:O	2.32	0.40
2:E:446:ALA:HB2	2:E:483:LEU:HD11	2.02	0.40
2:E:603:LEU:HA	2:E:606:VAL:HG12	2.03	0.40
2:F:105:VAL:HG23	2:F:300:ASN:ND2	2.37	0.40
2:F:230:TRP:HB3	2:F:252:TYR:HD2	1.87	0.40
2:F:541:TRP:O	2:F:545:LEU:HD11	2.18	0.40
2:G:377:TYR:OH	2:G:414:VAL:O	2.33	0.40
2:I:373:VAL:HG11	2:I:418:LEU:HD21	2.03	0.40
2:I:496:THR:HB	2:I:795:PHE:HZ	1.87	0.40
2:I:778:ASP:HA	2:I:781:ARG:NH1	2.36	0.40
2:J:165:TRP:HB2	2:J:303:LEU:HD21	2.04	0.40
2:J:534:ILE:HD12	2:J:741:MET:HE1	2.02	0.40
2:J:647:THR:HG23	2:J:649:MET:SD	2.61	0.40
2:J:651:ARG:NH1	2:N:597:GLU:OE2	2.55	0.40
2:K:245:ILE:HG13	2:K:246:LEU:N	2.36	0.40
2:K:410:HIS:CE1	2:K:412:LYS:HB2	2.57	0.40
2:L:169:LEU:HD11	2:L:212:CYS:HB2	2.03	0.40
2:M:34:PHE:CZ	2:M:50:LYS:HA	2.57	0.40
2:M:191:LEU:O	2:M:194:GLN:HB3	2.20	0.40
2:M:747:SER:O	2:M:747:SER:OG	2.36	0.40
2:N:10:VAL:O	2:N:14:ARG:HG3	2.20	0.40
1:O:727:ILE:HD11	1:O:840:PRO:HB2	2.03	0.40
1:P:414:PRO:HB2	1:P:488:GLU:HG2	2.04	0.40
1:Q:443:MET:HE2	1:Q:496:LYS:HB3	2.03	0.40
1:Q:764:ARG:H	1:Q:764:ARG:HD3	1.87	0.40
1:R:824:ILE:O	1:R:828:LEU:HG	2.22	0.40
1:S:73:PHE:CE2	1:S:75:ASP:HB2	2.57	0.40
1:S:231:TRP:CD1	1:S:264:LYS:HE3	2.57	0.40
1:S:607:SER:HB2	1:S:625:LEU:HG	2.04	0.40
1:A:23:LEU:HD12	1:O:244:ARG:NH2	2.37	0.40
1:A:205:LYS:HD3	1:A:245:LYS:HE3	2.02	0.40
1:A:227:PHE:CZ	1:A:256:LEU:HB3	2.56	0.40
1:A:607:SER:HB2	1:A:625:LEU:HD21	2.04	0.40
2:B:192:CYS:HB3	2:B:199:LEU:HD23	2.03	0.40
2:B:342:HIS:ND1	2:B:348:SER:CA	2.85	0.40
2:B:448:ILE:O	2:B:452:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:ARG:HH11	2:C:104:ARG:HB2	1.86	0.40
2:D:424:LYS:H	2:D:470:ALA:CB	2.34	0.40
2:F:260:ILE:HG21	2:F:268:SER:HB3	2.03	0.40
2:F:494:HIS:CD2	2:F:795:PHE:HD1	2.40	0.40
2:G:412:LYS:HA	2:G:412:LYS:HD2	1.93	0.40
2:I:771:LYS:HA	2:I:771:LYS:HD3	1.89	0.40
2:J:651:ARG:NH1	2:J:655:LEU:HD11	2.36	0.40
2:K:527:ARG:HG2	2:K:702:ALA:HB3	2.03	0.40
2:L:271:CYS:SG	2:L:272:TRP:N	2.94	0.40
2:M:285:PRO:O	2:M:289:GLU:HB2	2.22	0.40
2:N:647:THR:OG1	2:N:648:GLY:N	2.53	0.40
1:O:198:GLU:HA	1:O:201:GLU:OE1	2.22	0.40
1:P:454:VAL:O	1:P:458:ARG:N	2.48	0.40
1:P:873:SER:O	1:P:876:LYS:HG3	2.22	0.40
1:R:878:ILE:HG13	1:R:879:ASP:N	2.37	0.40
1:S:218:ILE:HG23	1:S:248:VAL:HG23	2.02	0.40
1:S:425:MET:SD	1:S:477:ASN:HB3	2.61	0.40
1:S:588:TYR:HB3	1:S:921:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	820/947 (87%)	784 (96%)	36 (4%)	0	100	100
1	O	820/947 (87%)	785 (96%)	35 (4%)	0	100	100
1	P	820/947 (87%)	786 (96%)	34 (4%)	0	100	100
1	Q	820/947 (87%)	790 (96%)	30 (4%)	0	100	100
1	R	820/947 (87%)	781 (95%)	39 (5%)	0	100	100
1	S	820/947 (87%)	790 (96%)	30 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	820/947 (87%)	785 (96%)	35 (4%)	0	100	100
2	B	770/799 (96%)	740 (96%)	30 (4%)	0	100	100
2	C	768/799 (96%)	744 (97%)	24 (3%)	0	100	100
2	D	770/799 (96%)	745 (97%)	25 (3%)	0	100	100
2	E	764/799 (96%)	735 (96%)	29 (4%)	0	100	100
2	F	769/799 (96%)	746 (97%)	23 (3%)	0	100	100
2	G	770/799 (96%)	744 (97%)	26 (3%)	0	100	100
2	I	770/799 (96%)	745 (97%)	25 (3%)	0	100	100
2	J	770/799 (96%)	751 (98%)	19 (2%)	0	100	100
2	K	773/799 (97%)	748 (97%)	25 (3%)	0	100	100
2	L	770/799 (96%)	744 (97%)	26 (3%)	0	100	100
2	M	782/799 (98%)	760 (97%)	22 (3%)	0	100	100
2	N	770/799 (96%)	748 (97%)	22 (3%)	0	100	100
All	All	14986/16217 (92%)	14451 (96%)	535 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	737/835 (88%)	735 (100%)	2 (0%)	86	85
1	O	737/835 (88%)	737 (100%)	0	100	100
1	P	737/835 (88%)	735 (100%)	2 (0%)	86	85
1	Q	737/835 (88%)	737 (100%)	0	100	100
1	R	737/835 (88%)	734 (100%)	3 (0%)	84	84
1	S	737/835 (88%)	736 (100%)	1 (0%)	88	89
1	T	737/835 (88%)	736 (100%)	1 (0%)	88	89
2	B	670/706 (95%)	670 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	671/706 (95%)	671 (100%)	0	100	100
2	D	670/706 (95%)	670 (100%)	0	100	100
2	E	670/706 (95%)	670 (100%)	0	100	100
2	F	669/706 (95%)	669 (100%)	0	100	100
2	G	670/706 (95%)	670 (100%)	0	100	100
2	I	670/706 (95%)	670 (100%)	0	100	100
2	J	670/706 (95%)	670 (100%)	0	100	100
2	K	672/706 (95%)	672 (100%)	0	100	100
2	L	670/706 (95%)	670 (100%)	0	100	100
2	M	690/706 (98%)	690 (100%)	0	100	100
2	N	670/706 (95%)	670 (100%)	0	100	100
All	All	13221/14317 (92%)	13212 (100%)	9 (0%)	87	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	281	VAL
1	P	384	GLN
1	P	656	ILE
1	R	279	GLU
1	R	281	VAL
1	R	656	ILE
1	S	281	VAL
1	T	616	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	87	ASN
1	A	265	GLN
1	A	384	GLN
1	A	715	GLN
1	A	721	ASN
1	A	912	ASN
2	B	58	GLN

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Mol	Chain	Res	Type
2	B	62	GLN
2	B	153	GLN
2	B	236	ASN
2	B	238	GLN
2	B	266	GLN
2	B	308	GLN
2	B	399	GLN
2	B	410	HIS
2	B	789	ASN
2	C	7	ASN
2	C	114	HIS
2	C	213	ASN
2	C	248	ASN
2	C	266	GLN
2	C	445	GLN
2	C	474	HIS
2	C	494	HIS
2	C	664	ASN
2	C	787	ASN
2	C	796	HIS
2	D	7	ASN
2	D	64	ASN
2	D	152	HIS
2	D	186	GLN
2	D	190	GLN
2	D	223	GLN
2	D	445	GLN
2	D	570	HIS
2	E	136	HIS
2	E	209	GLN
2	E	213	ASN
2	E	235	GLN
2	E	238	GLN
2	E	668	GLN
2	E	710	ASN
2	F	58	GLN
2	F	213	ASN
2	F	700	ASN
2	F	789	ASN
2	G	40	GLN
2	G	152	HIS
2	G	213	ASN

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Mol	Chain	Res	Type
2	G	308	GLN
2	G	340	HIS
2	G	658	GLN
2	G	787	ASN
2	I	213	ASN
2	J	37	GLN
2	J	62	GLN
2	J	266	GLN
2	J	710	ASN
2	J	787	ASN
2	K	7	ASN
2	K	62	GLN
2	K	149	HIS
2	K	190	GLN
2	K	209	GLN
2	K	213	ASN
2	K	239	GLN
2	K	248	ASN
2	K	391	HIS
2	K	435	HIS
2	K	589	HIS
2	K	796	HIS
2	L	154	HIS
2	L	171	HIS
2	L	190	GLN
2	L	384	HIS
2	L	421	HIS
2	L	445	GLN
2	L	474	HIS
2	M	7	ASN
2	M	83	ASN
2	M	236	ASN
2	M	266	GLN
2	M	301	GLN
2	M	570	HIS
2	N	7	ASN
2	N	37	GLN
2	N	153	GLN
2	N	213	ASN
2	N	236	ASN
2	N	238	GLN
2	N	391	HIS

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Mol	Chain	Res	Type
2	N	435	HIS
2	N	444	ASN
2	N	530	HIS
2	N	605	GLN
1	O	296	GLN
1	O	485	GLN
1	O	489	ASN
1	O	512	ASN
1	O	552	ASN
1	O	583	HIS
1	O	744	ASN
1	O	747	ASN
1	O	908	GLN
1	O	912	ASN
1	P	70	ASN
1	P	265	GLN
1	P	296	GLN
1	P	346	GLN
1	P	489	ASN
1	P	530	GLN
1	P	647	ASN
1	Q	22	ASN
1	Q	159	GLN
1	Q	439	HIS
1	Q	485	GLN
1	Q	597	ASN
1	Q	912	ASN
1	R	22	ASN
1	R	94	ASN
1	R	296	GLN
1	R	337	GLN
1	R	369	ASN
1	R	751	GLN
1	R	809	ASN
1	S	34	GLN
1	S	70	ASN
1	S	130	ASN
1	S	268	ASN
1	S	346	GLN
1	S	357	ASN
1	S	549	HIS
1	S	552	ASN

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Mol	Chain	Res	Type
1	S	592	ASN
1	T	186	GLN
1	T	194	GLN
1	T	226	GLN
1	T	276	GLN
1	T	296	GLN
1	T	374	GLN
1	T	419	ASN
1	T	435	ASN
1	T	461	ASN
1	T	477	ASN
1	T	552	ASN
1	T	614	ASN
1	T	744	ASN
1	T	778	ASN
1	T	862	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

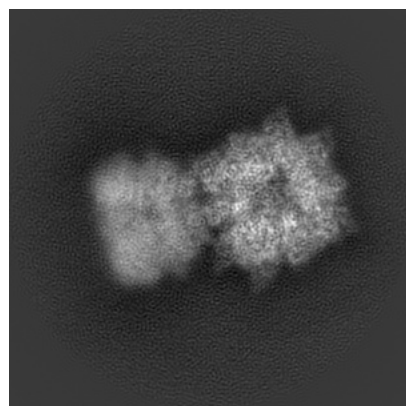
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34962. These allow visual inspection of the internal detail of the map and identification of artifacts.

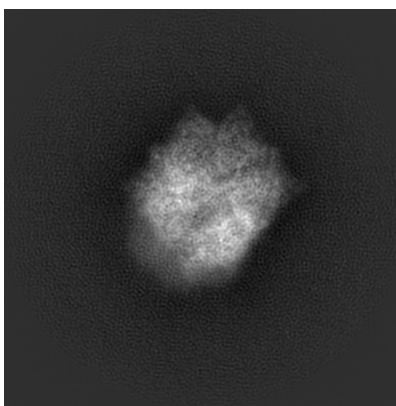
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

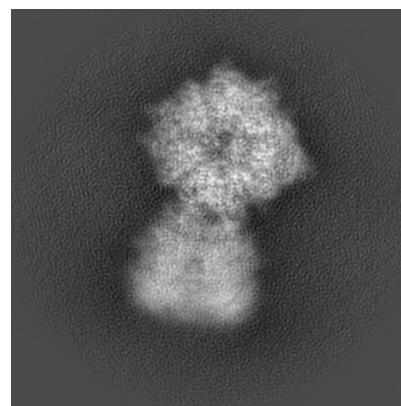
6.1.1 Primary map



X

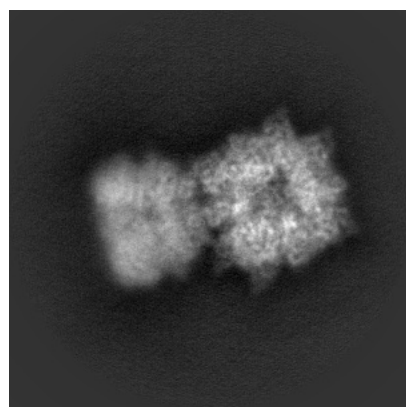


Y

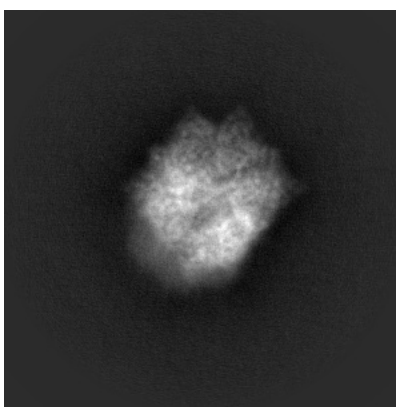


Z

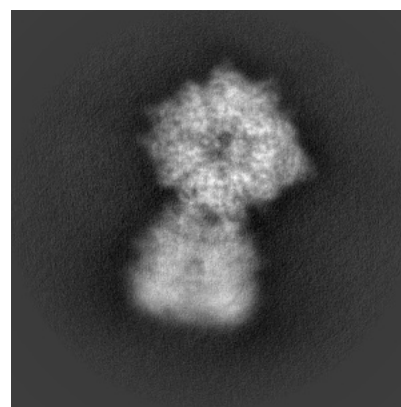
6.1.2 Raw map



X



Y

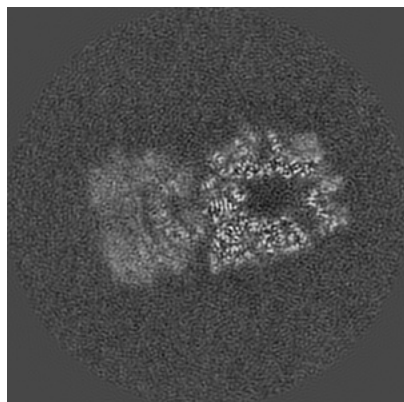


Z

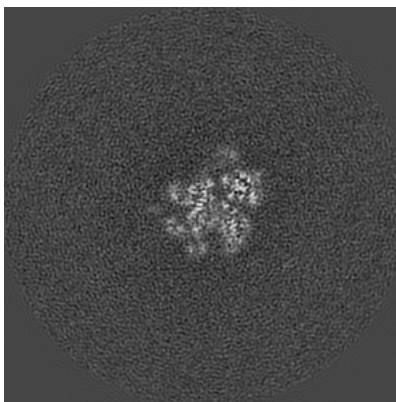
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

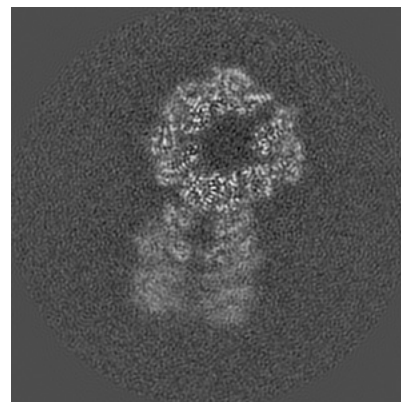
6.2.1 Primary map



X Index: 208

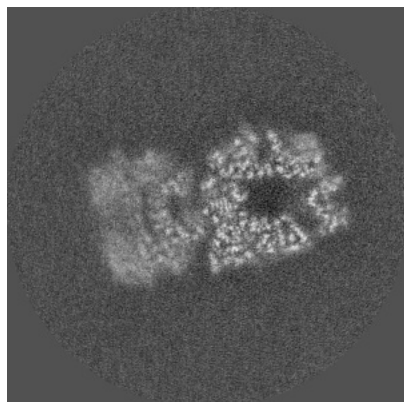


Y Index: 208

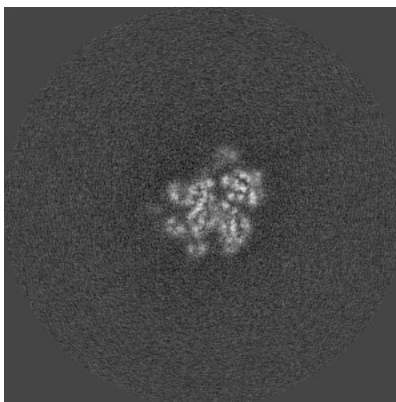


Z Index: 208

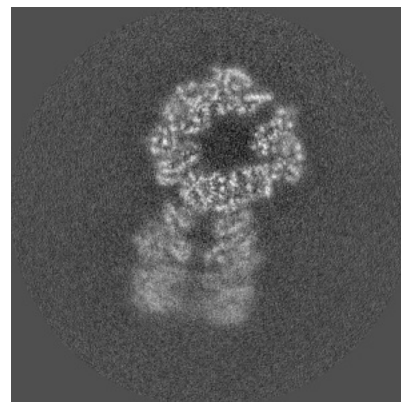
6.2.2 Raw map



X Index: 208



Y Index: 208

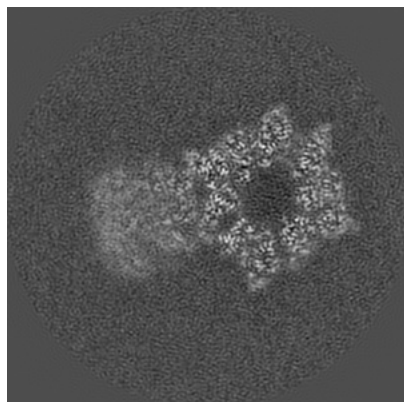


Z Index: 208

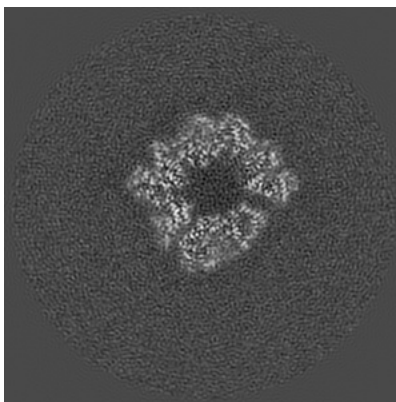
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

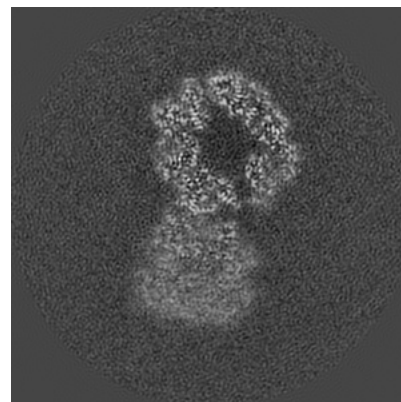
6.3.1 Primary map



X Index: 228

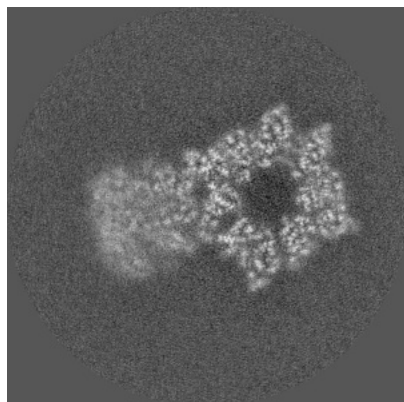


Y Index: 269

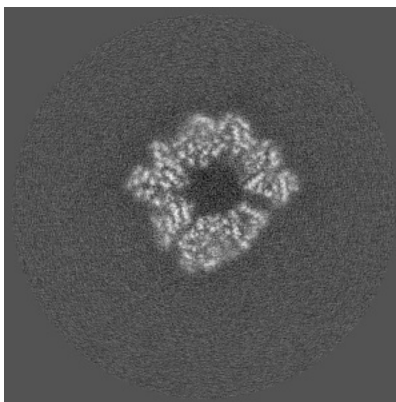


Z Index: 227

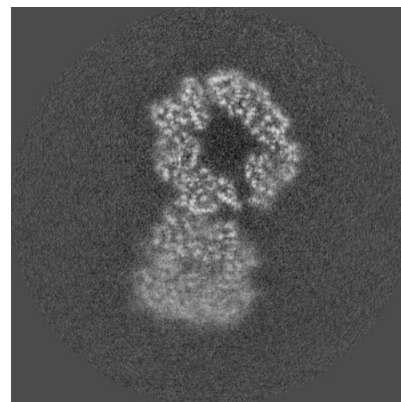
6.3.2 Raw map



X Index: 228



Y Index: 269

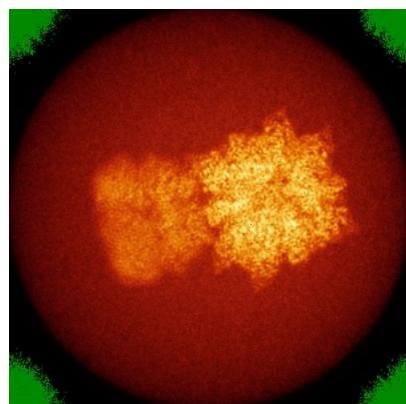


Z Index: 227

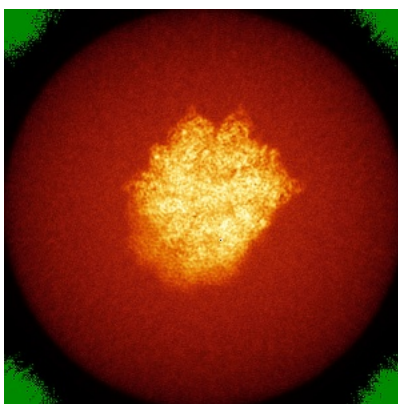
The images above show the largest variance slices of the map in three orthogonal directions.

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

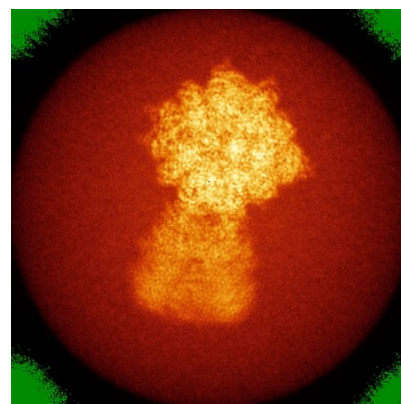
6.4.1 Primary map



X

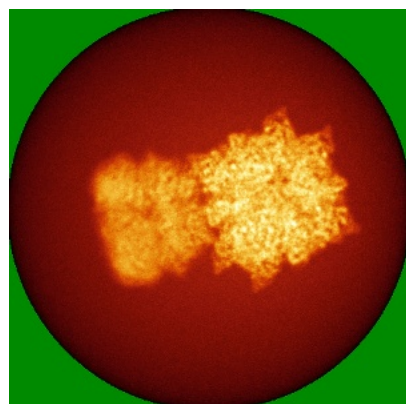


Y

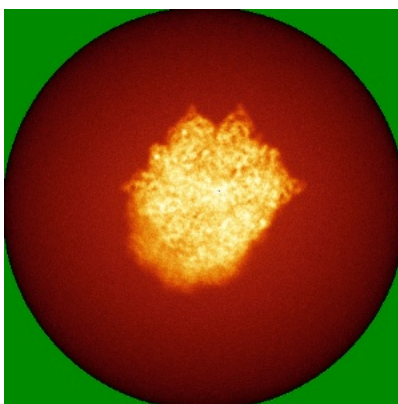


Z

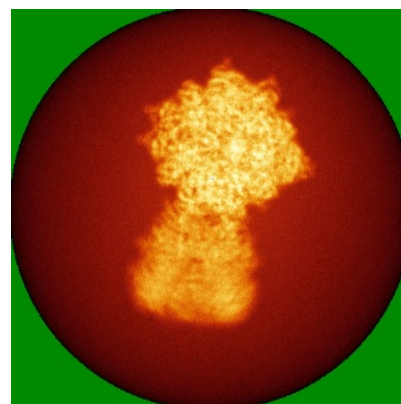
6.4.2 Raw map



X



Y

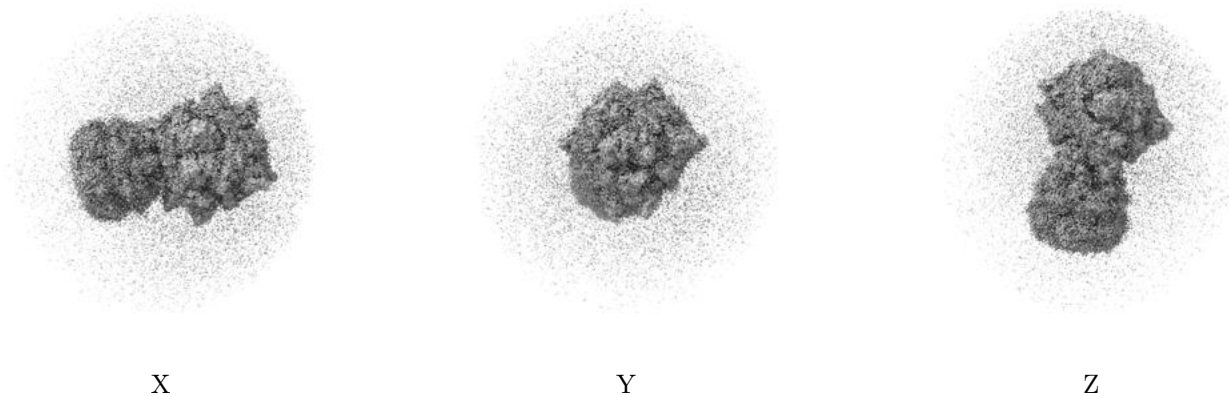


Z

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

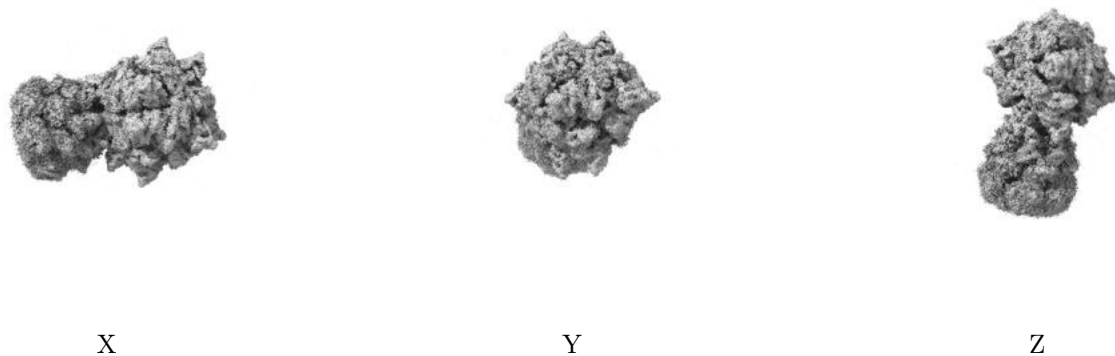
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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



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.

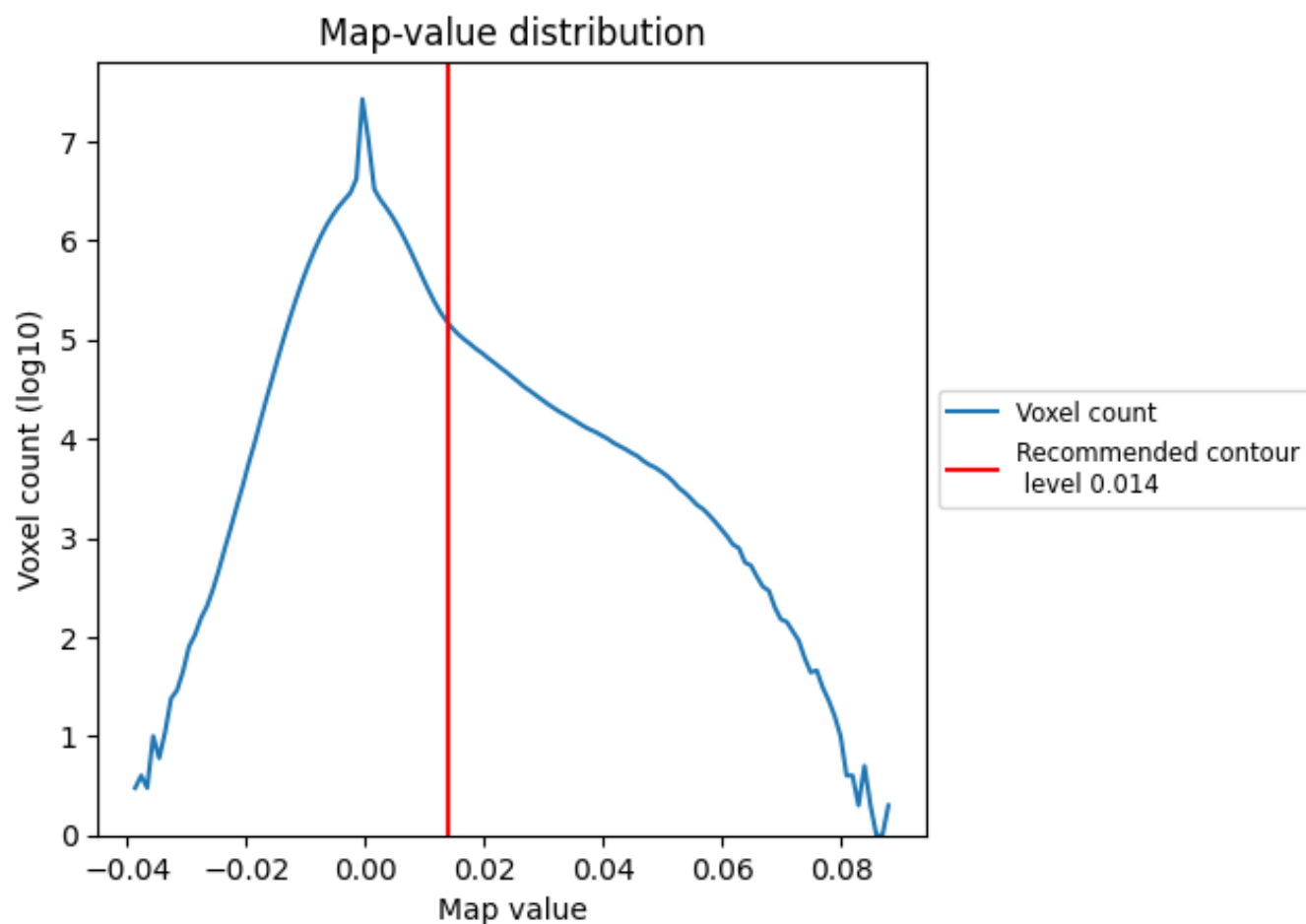
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

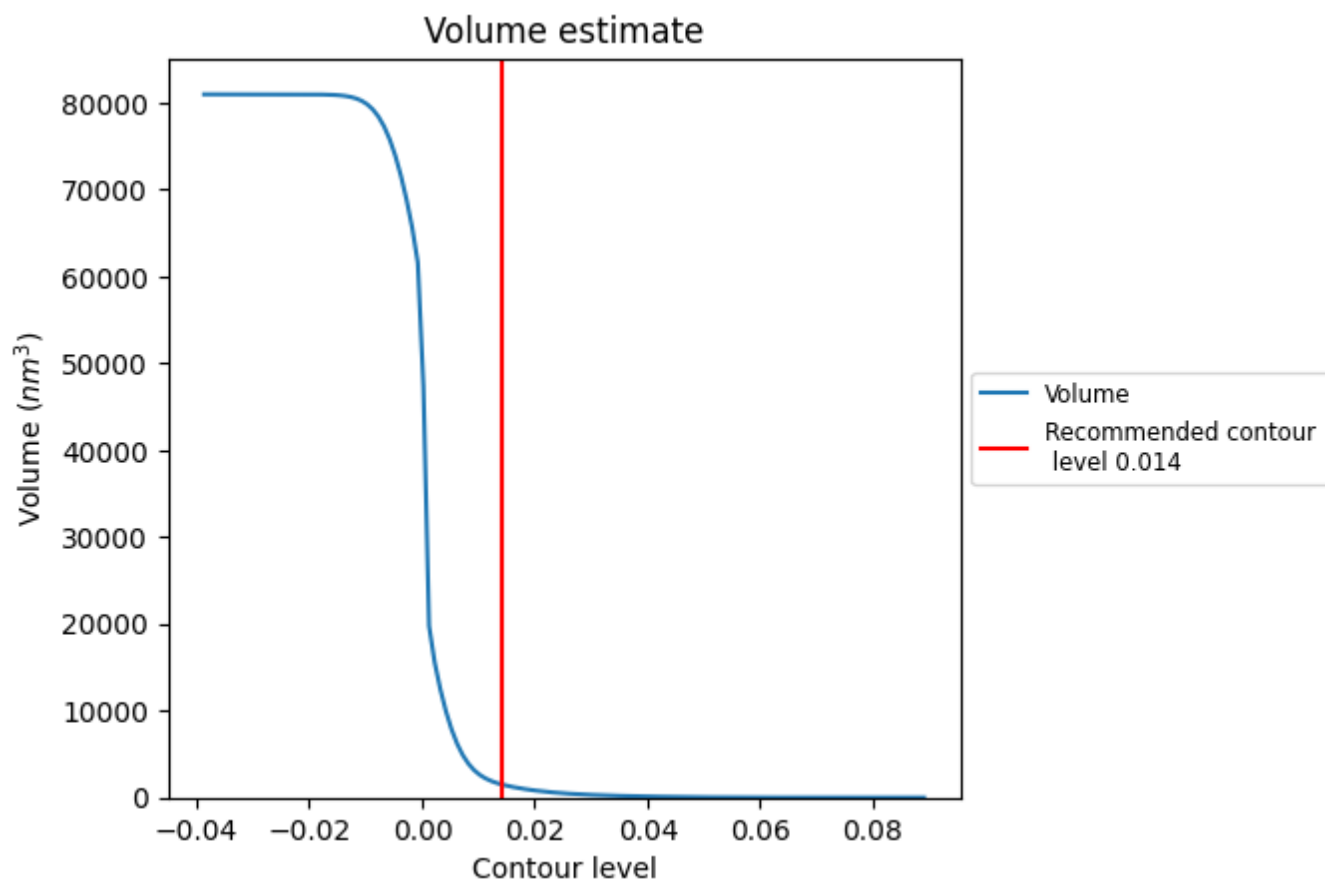
This section contains the results of statistical analysis of the map.

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.

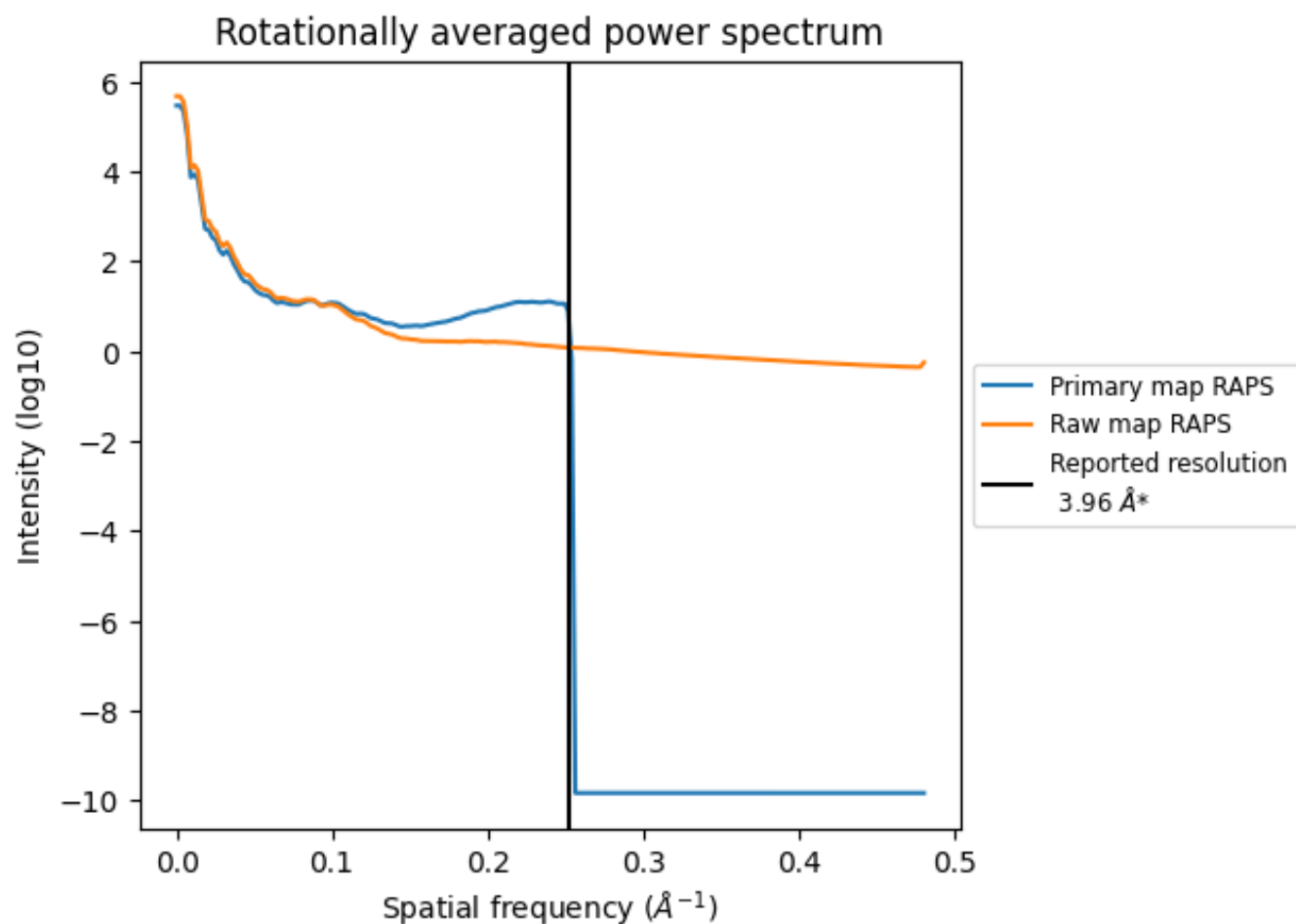
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1538 nm³; this corresponds to an approximate mass of 1389 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 ⓘ

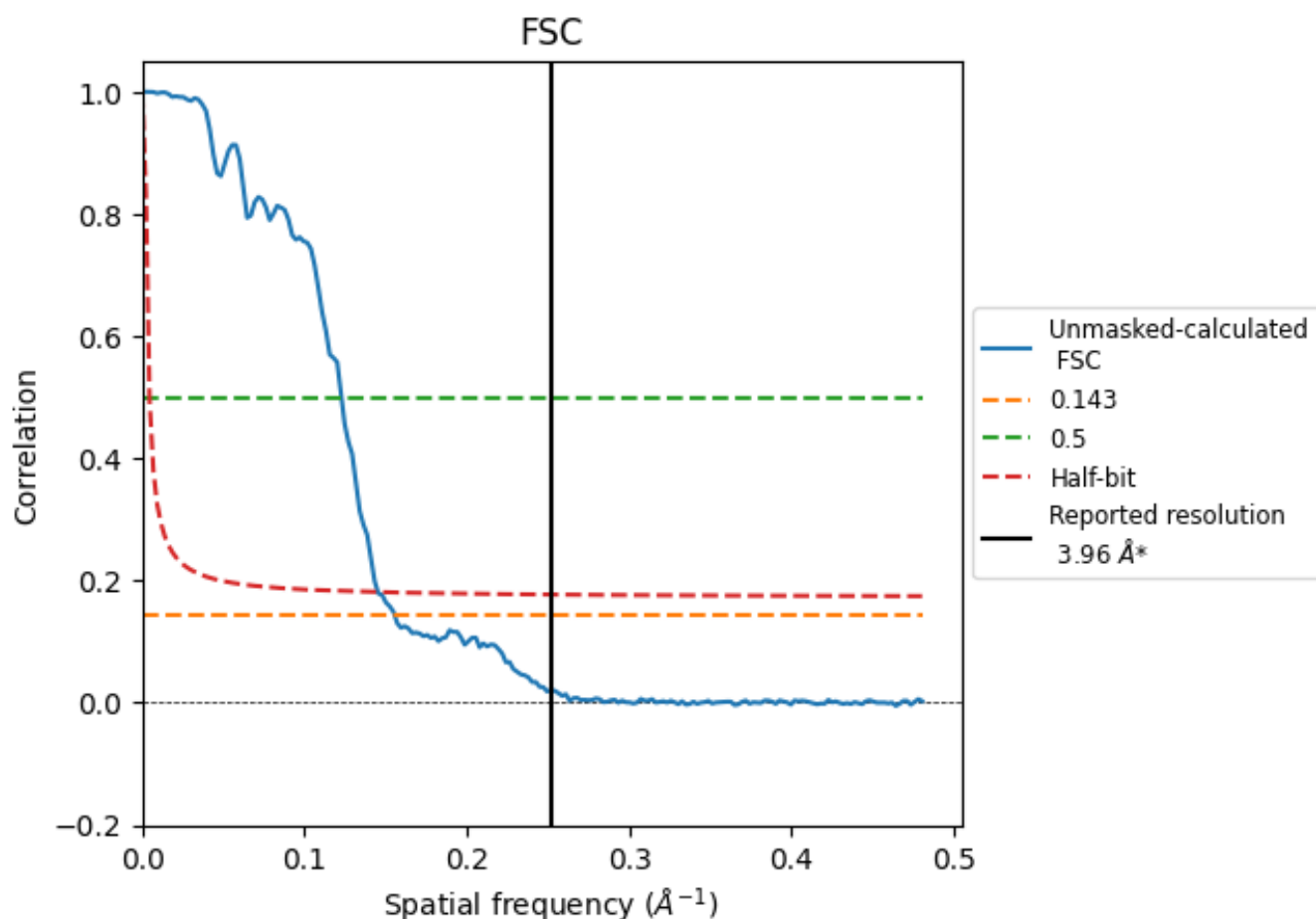


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.43	8.14	6.88

*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 6.43 differs from the reported value 3.96 by more than 10 %

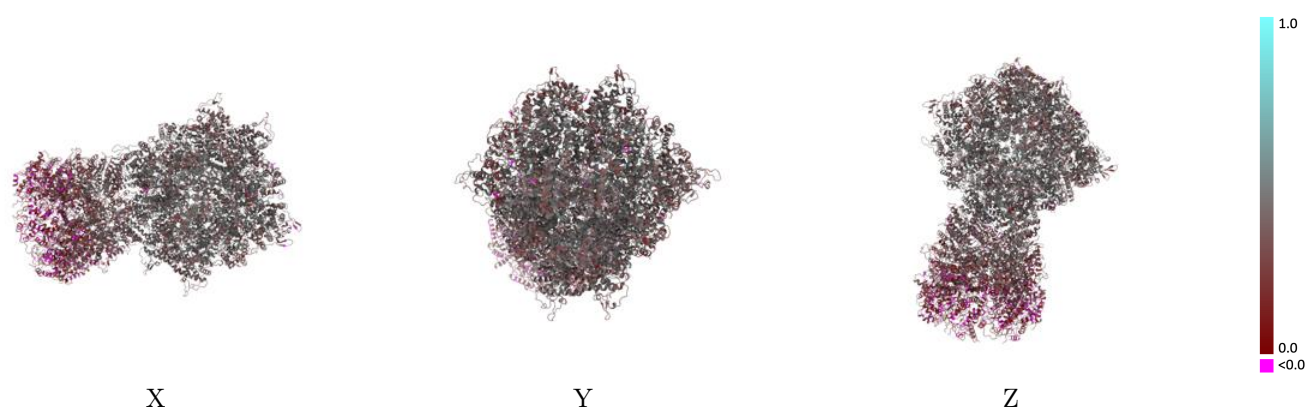
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34962 and PDB model 8HR7. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

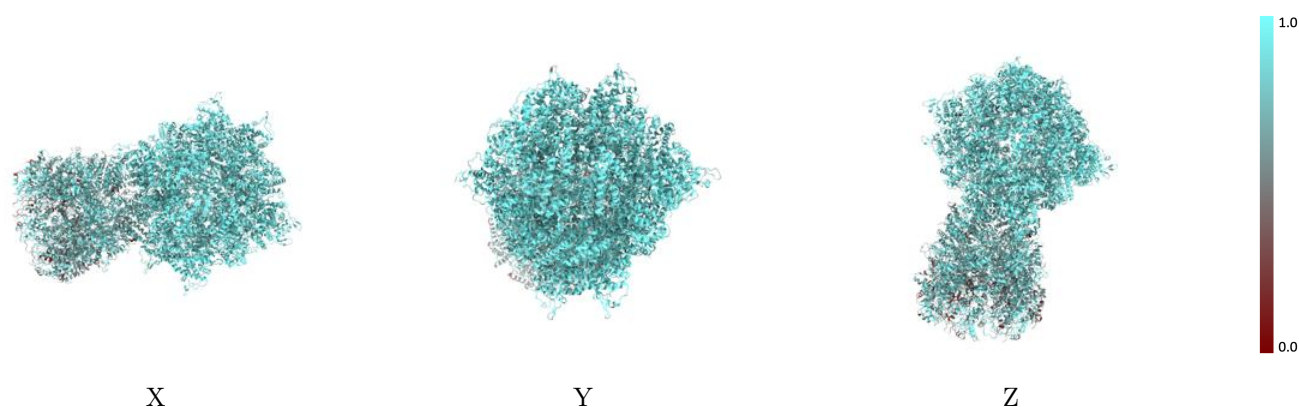
This section was not generated.

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



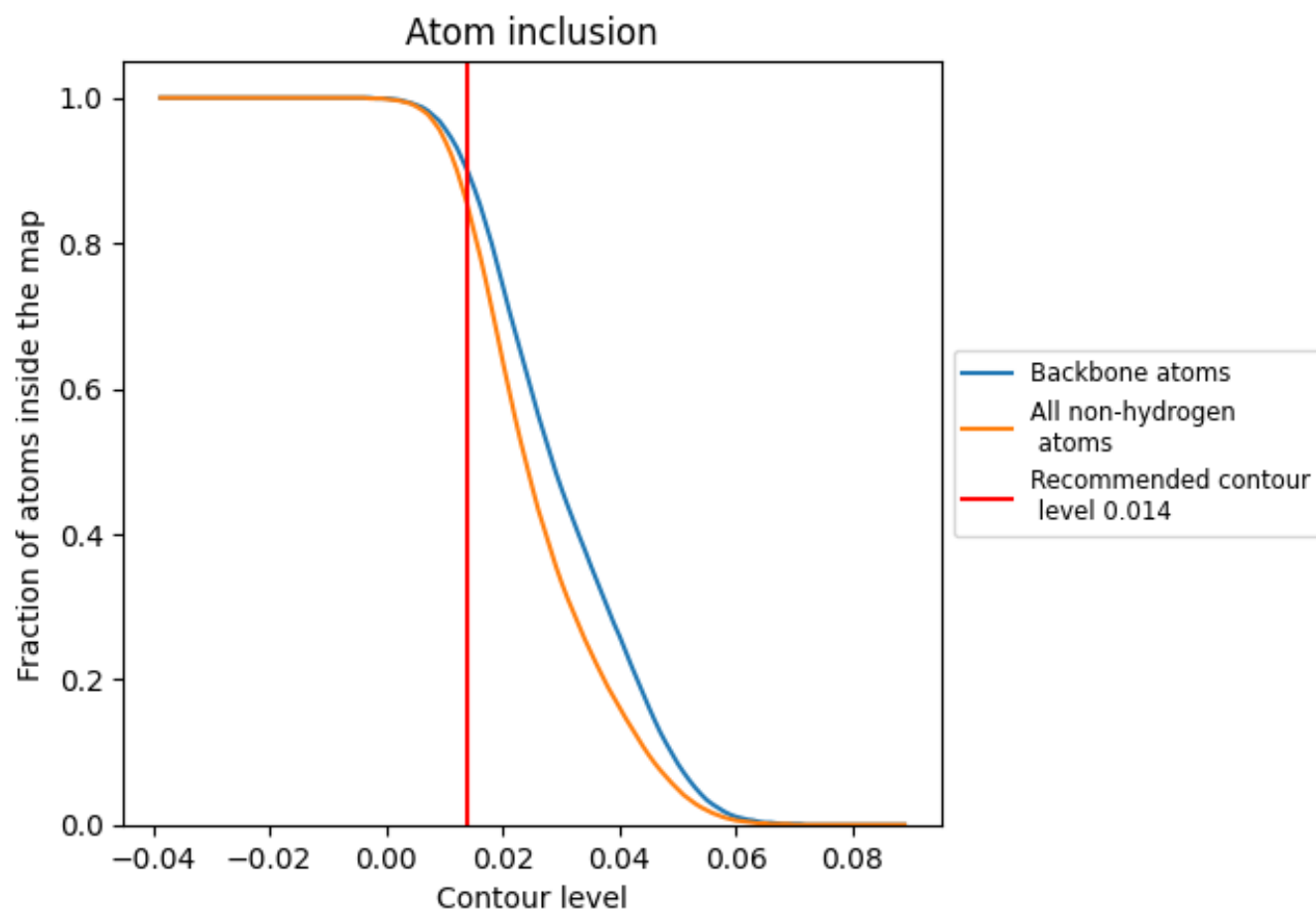
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.3520
A	 0.7460	 0.2330
B	 0.9180	 0.4130
C	 0.9240	 0.4250
D	 0.9200	 0.4270
E	 0.9250	 0.4220
F	 0.9220	 0.4230
G	 0.9200	 0.4170
I	 0.9230	 0.4200
J	 0.9150	 0.4130
K	 0.9190	 0.4130
L	 0.9320	 0.4320
M	 0.9140	 0.4390
N	 0.9190	 0.4260
O	 0.7380	 0.2290
P	 0.7460	 0.2470
Q	 0.7420	 0.2450
R	 0.7240	 0.2420
S	 0.7550	 0.2350
T	 0.7550	 0.2390

