



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2024 – 01:18 AM JST

PDB ID : 8JFL  
EMDB ID : EMD-36213  
Title : PhK holoenzyme in active state, muscle isoform  
Authors : Yang, X.K.; Xiao, J.Y.  
Deposited on : 2023-05-18  
Resolution : 2.90 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

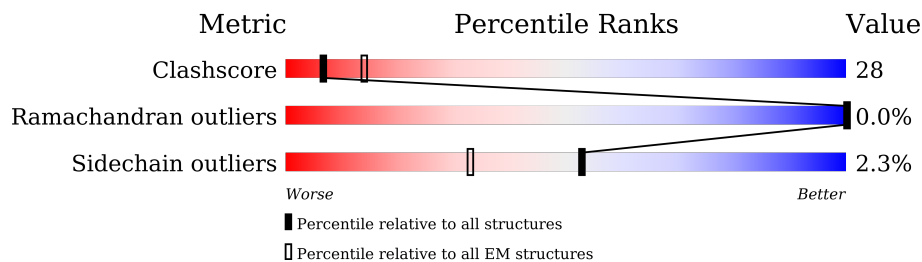
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.




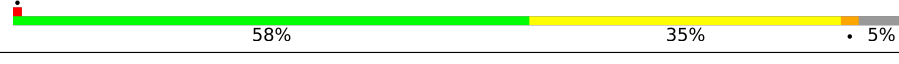


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1223	 50% 28% 21%
1	E	1223	 51% 28% 21%
1	I	1223	 51% 28% 21%
1	M	1223	 51% 27% 21%
2	C	387	 88%
2	G	387	 88%
2	K	387	 88%
2	O	387	 88%

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Mol	Chain	Length	Quality of chain
3	B	1093	
3	F	1093	
3	J	1093	
3	N	1093	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FAR	A	1301	-	-	X	-
4	FAR	B	1101	-	-	X	-
4	FAR	E	1301	-	-	X	-
4	FAR	F	1101	-	-	X	-
4	FAR	F	1103	-	-	X	-
4	FAR	I	1301	-	-	X	-
4	FAR	M	1301	-	-	X	-
4	FAR	N	1101	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 65884 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 Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	970	Total 7673	C 4891	N 1295	O 1442	S 45	0	0
1	E	970	Total 7673	C 4891	N 1295	O 1442	S 45	0	0
1	M	970	Total 7673	C 4891	N 1295	O 1442	S 45	0	0
1	I	970	Total 7673	C 4891	N 1295	O 1442	S 45	0	0

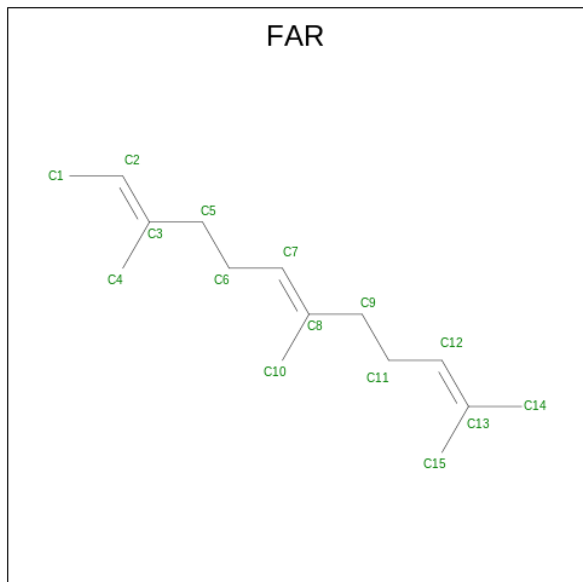
- Molecule 2 is a protein called Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	48	Total 402	C 263	N 75	O 64	0	0
2	G	48	Total 402	C 263	N 75	O 64	0	0
2	O	48	Total 402	C 263	N 75	O 64	0	0
2	K	48	Total 402	C 263	N 75	O 64	0	0

- Molecule 3 is a protein called Phosphorylase b kinase regulatory subunit beta.

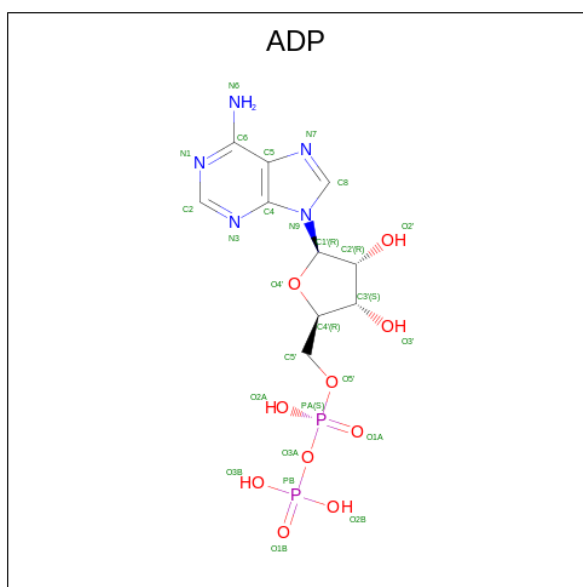
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	1033	Total 8339	C 5338	N 1423	O 1541	S 37	0	0
3	F	1033	Total 8339	C 5338	N 1423	O 1541	S 37	0	0
3	J	1033	Total 8339	C 5338	N 1423	O 1541	S 37	0	0
3	N	1033	Total 8339	C 5338	N 1423	O 1541	S 37	0	0

- Molecule 4 is FARNESYL (three-letter code: FAR) (formula:  $C_{15}H_{26}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 15 15	0
4	E	1	Total C 15 15	0
4	M	1	Total C 15 15	0
4	I	1	Total C 15 15	0
4	B	1	Total C 15 15	0
4	F	1	Total C 15 15	0
4	F	1	Total C 15 15	0
4	N	1	Total C 15 15	0

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

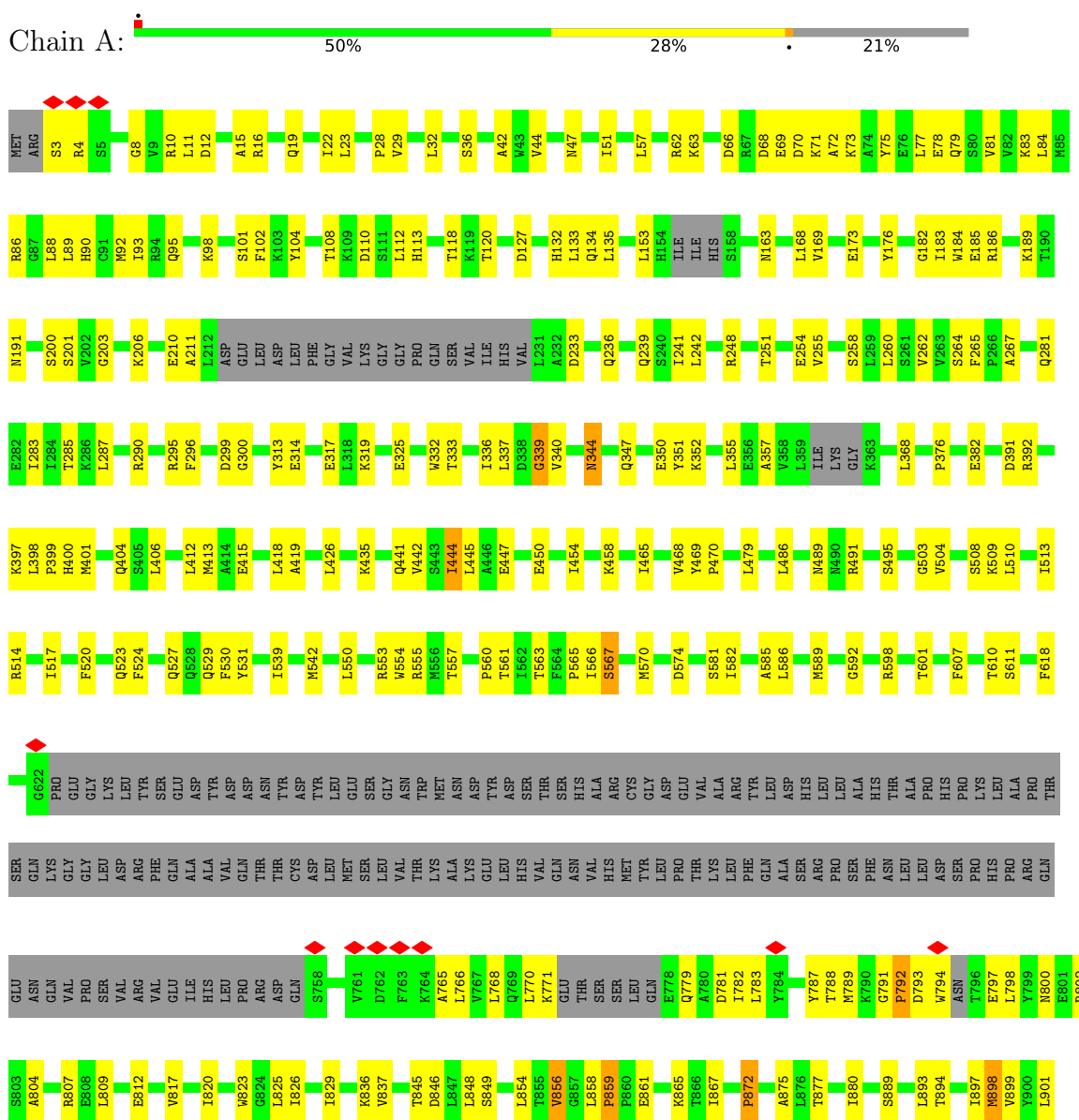


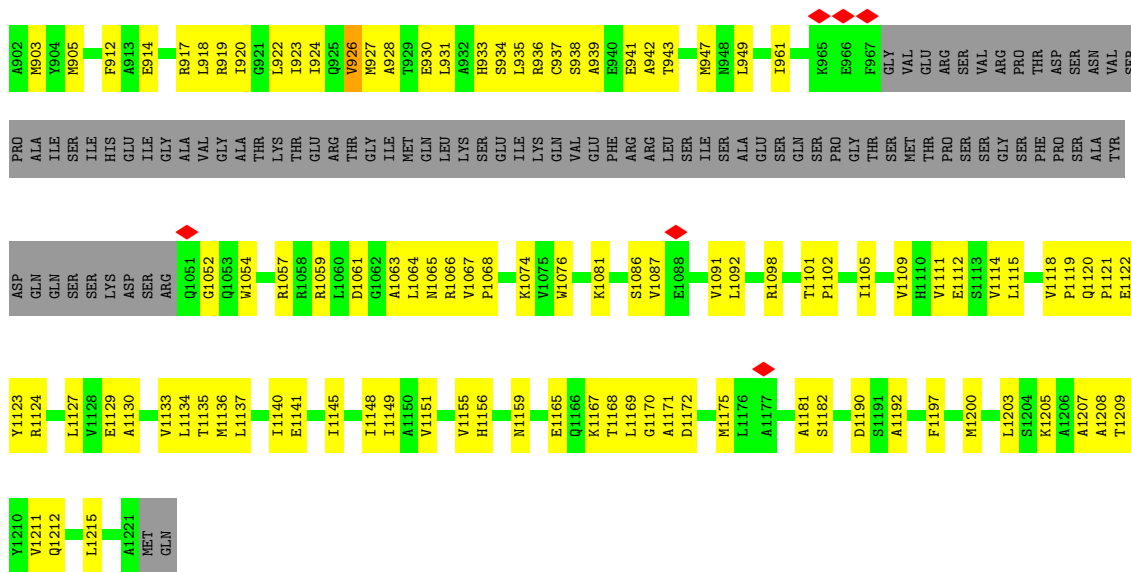
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	N	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 3 Residue-property plots

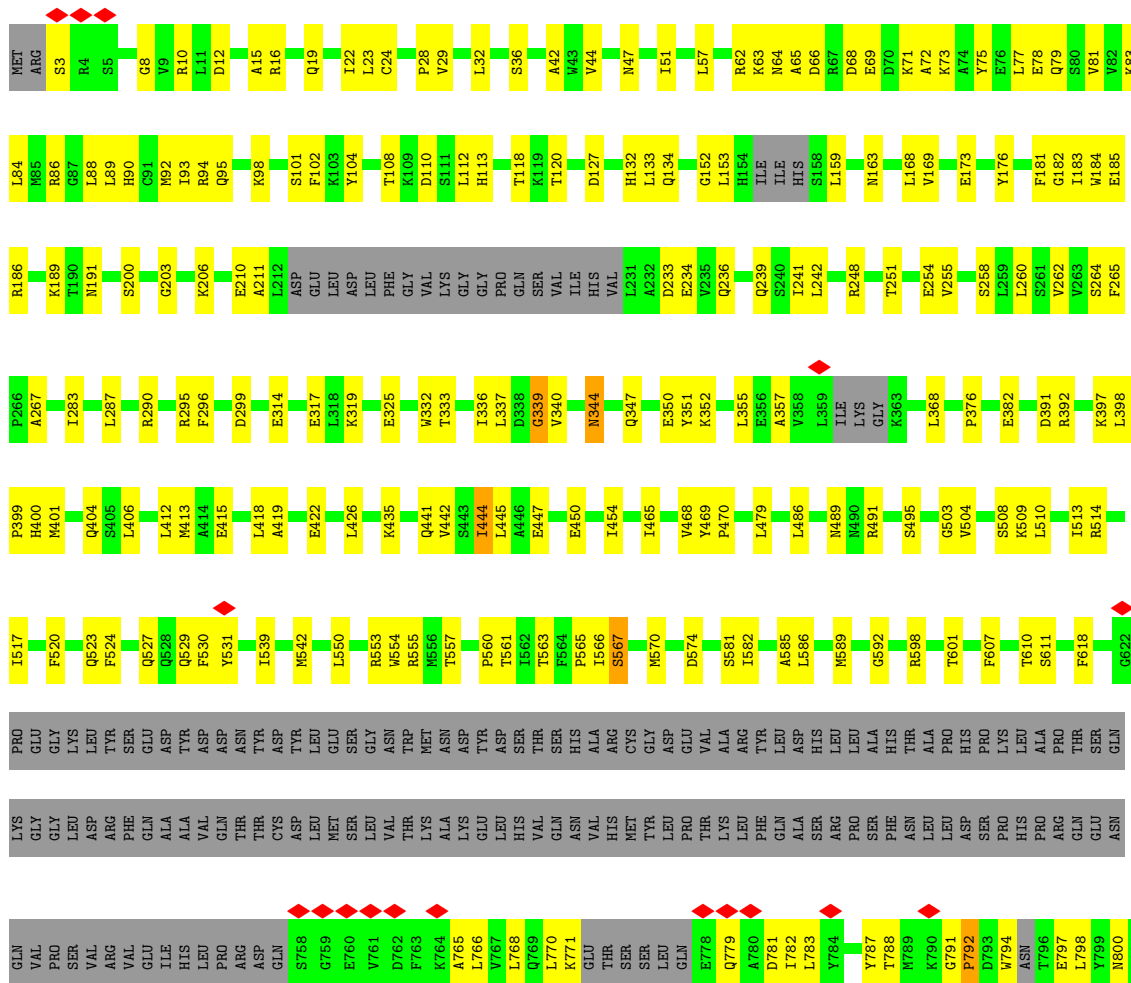
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform



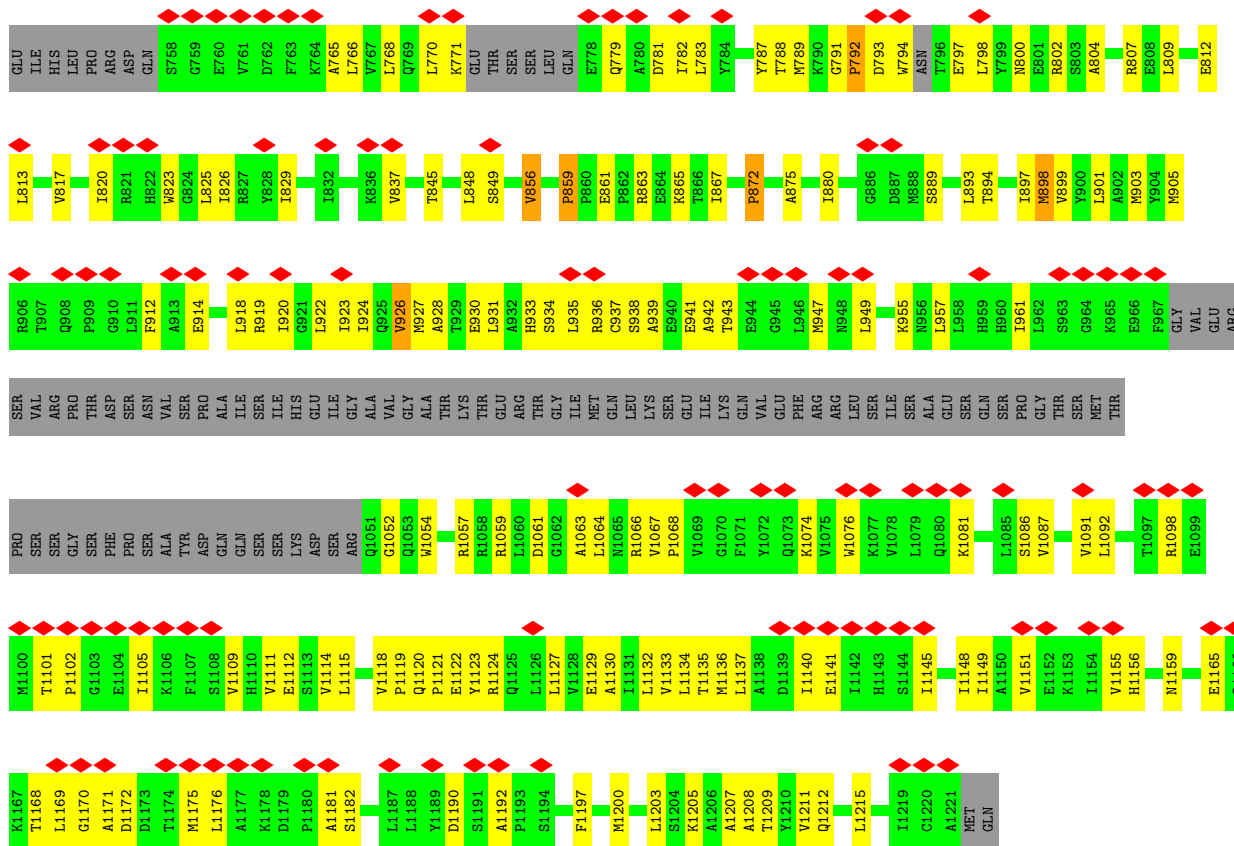


• Molecule 1: Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform

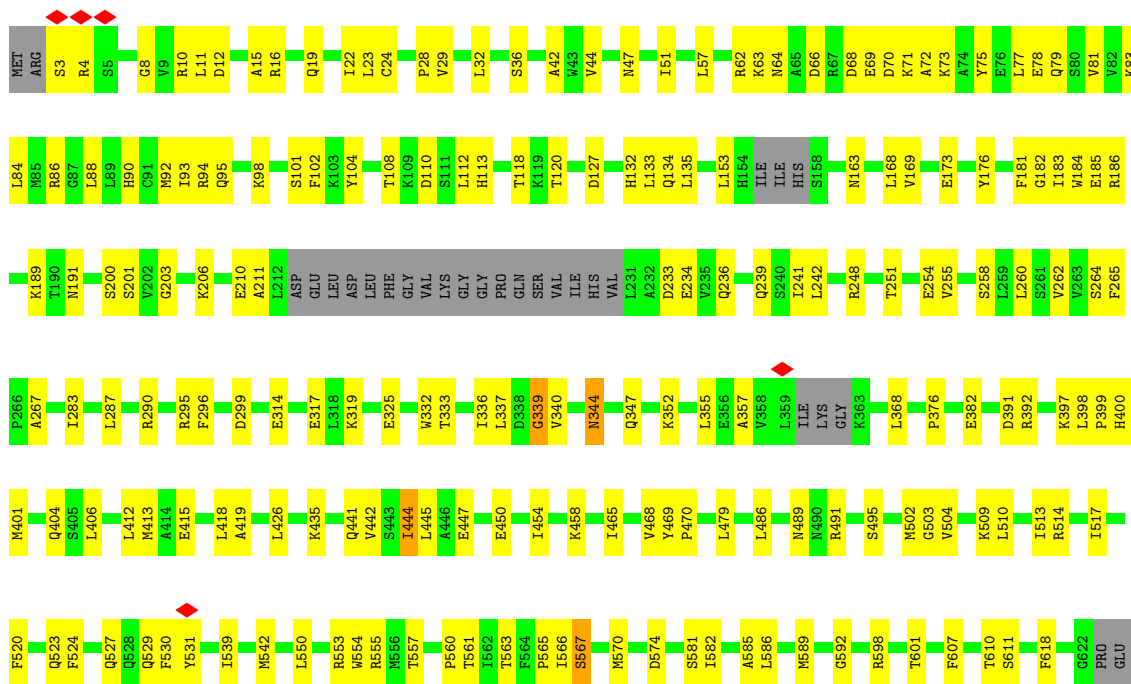


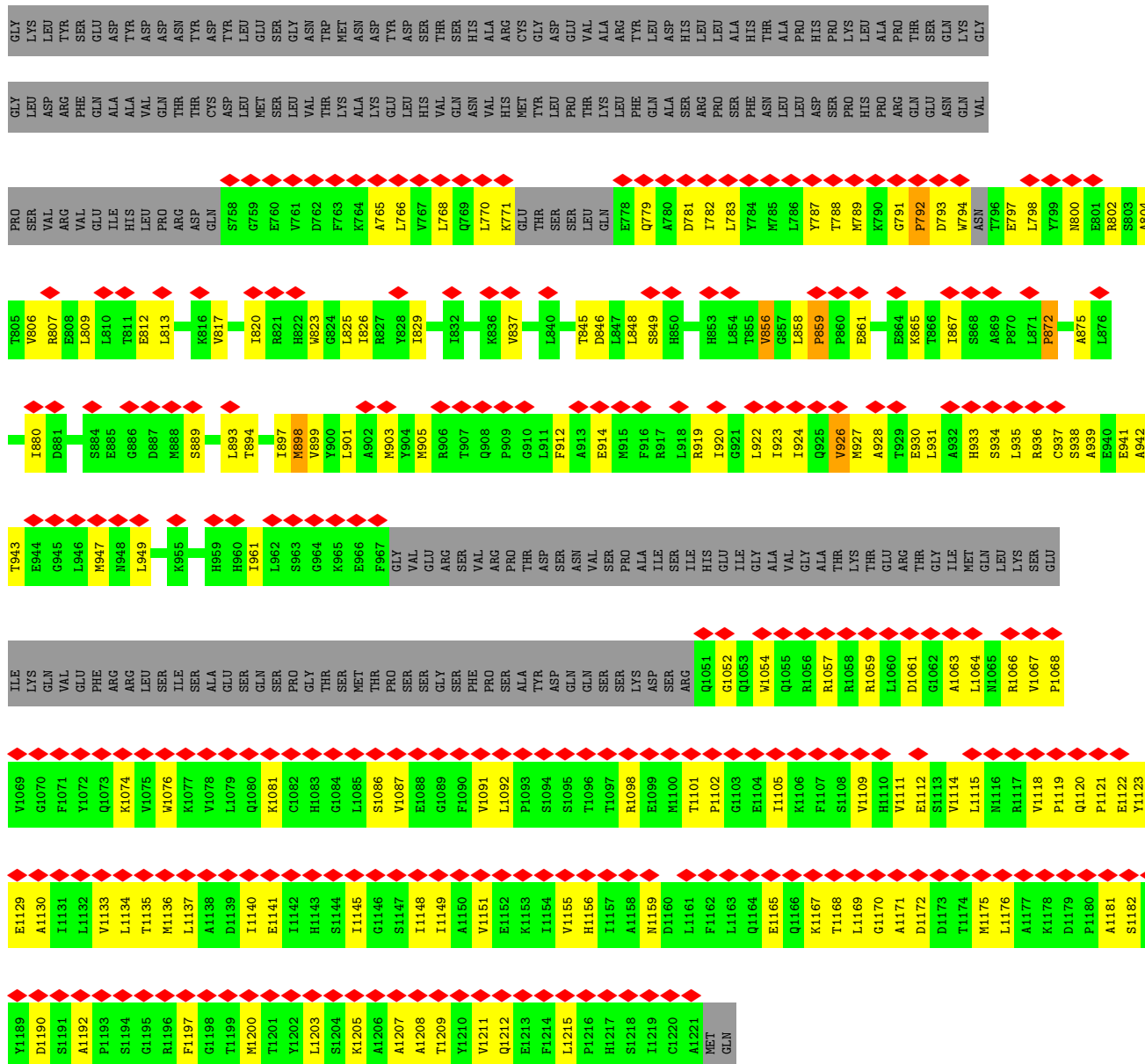






• Molecule 1: Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform





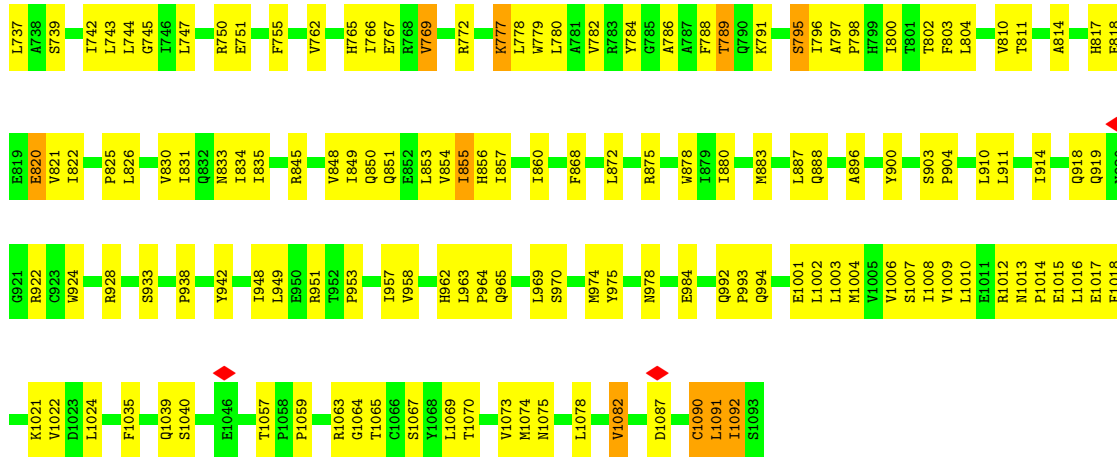
● Molecule 2: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform



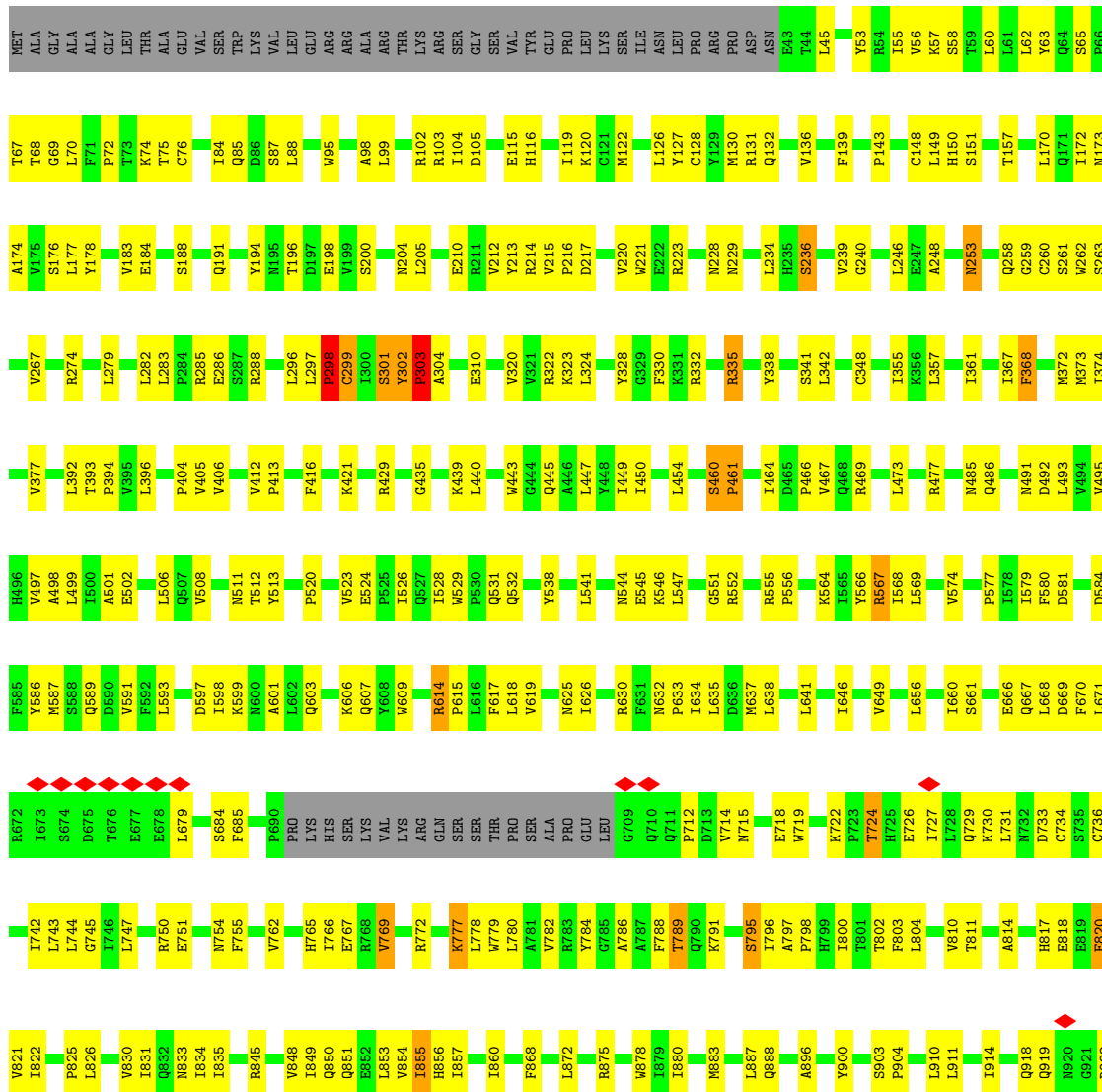






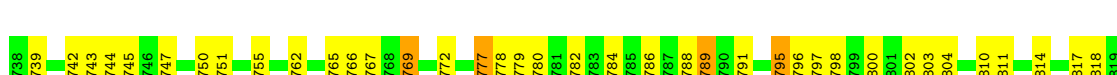
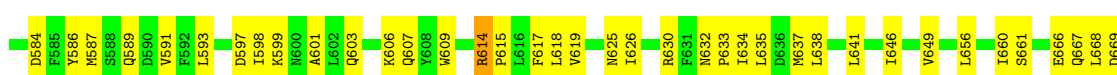
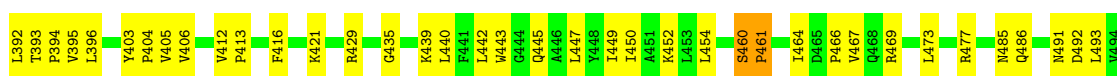
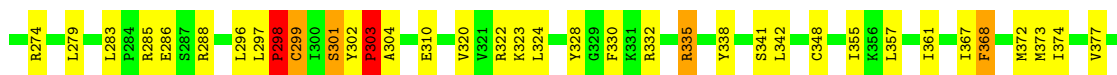
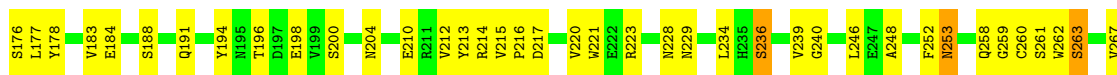
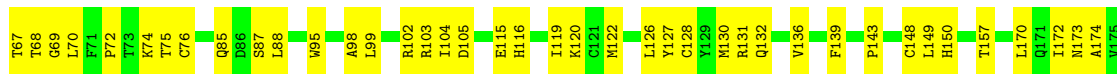
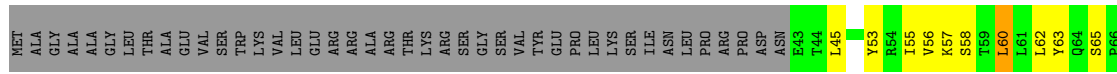


• Molecule 3: Phosphorylase b kinase regulatory subunit beta





• Molecule 3: Phosphorylase b kinase regulatory subunit beta





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432047	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.761	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	481.50003, 481.50003, 481.50003	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	1/7826 (0.0%)	0.63	8/10595 (0.1%)
1	E	0.54	1/7826 (0.0%)	0.63	9/10595 (0.1%)
1	I	0.54	1/7826 (0.0%)	0.63	8/10595 (0.1%)
1	M	0.54	1/7826 (0.0%)	0.63	8/10595 (0.1%)
2	C	0.92	0/411	0.95	1/557 (0.2%)
2	G	0.91	0/411	0.95	1/557 (0.2%)
2	K	0.91	0/411	0.95	1/557 (0.2%)
2	O	0.91	0/411	0.95	1/557 (0.2%)
3	B	0.81	12/8527 (0.1%)	1.05	25/11556 (0.2%)
3	F	0.80	11/8527 (0.1%)	1.04	22/11556 (0.2%)
3	J	0.80	11/8527 (0.1%)	1.04	21/11556 (0.2%)
3	N	0.80	11/8527 (0.1%)	1.04	21/11556 (0.2%)
All	All	0.69	49/67056 (0.1%)	0.87	126/90832 (0.1%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	284	PRO	N-CD	9.48	1.61	1.47
3	N	301	SER	CA-CB	-7.16	1.42	1.52
3	F	301	SER	CA-CB	-7.13	1.42	1.52
3	B	301	SER	CA-CB	-7.12	1.42	1.52
3	J	301	SER	CA-CB	-7.09	1.42	1.52
3	B	263	SER	CA-CB	-6.51	1.43	1.52
3	J	263	SER	CA-CB	-6.49	1.43	1.52
3	F	263	SER	CA-CB	-6.49	1.43	1.52
3	N	263	SER	CA-CB	-6.47	1.43	1.52
1	M	792	PRO	N-CD	-5.62	1.40	1.47
3	N	65	SER	CA-CB	-5.61	1.44	1.52
3	B	65	SER	CA-CB	-5.60	1.44	1.52
3	J	65	SER	CA-CB	-5.60	1.44	1.52
1	A	792	PRO	N-CD	-5.60	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	792	PRO	N-CD	-5.58	1.40	1.47
3	F	65	SER	CA-CB	-5.57	1.44	1.52
1	I	792	PRO	N-CD	-5.57	1.40	1.47
3	F	58	SER	CA-CB	-5.56	1.44	1.52
3	J	188	SER	CA-CB	-5.54	1.44	1.52
3	B	188	SER	CA-CB	-5.54	1.44	1.52
3	F	188	SER	CA-CB	-5.54	1.44	1.52
3	N	188	SER	CA-CB	-5.53	1.44	1.52
3	B	58	SER	CA-CB	-5.53	1.44	1.52
3	N	58	SER	CA-CB	-5.52	1.44	1.52
3	J	58	SER	CA-CB	-5.52	1.44	1.52
3	B	200	SER	CA-CB	-5.44	1.44	1.52
3	J	200	SER	CA-CB	-5.43	1.44	1.52
3	F	200	SER	CA-CB	-5.42	1.44	1.52
3	N	200	SER	CA-CB	-5.41	1.44	1.52
3	N	661	SER	CA-CB	-5.38	1.44	1.52
3	J	661	SER	CA-CB	-5.38	1.44	1.52
3	F	661	SER	CA-CB	-5.37	1.45	1.52
3	B	661	SER	CA-CB	-5.36	1.45	1.52
3	F	795	SER	CA-CB	-5.28	1.45	1.52
3	J	795	SER	CA-CB	-5.28	1.45	1.52
3	B	795	SER	CA-CB	-5.27	1.45	1.52
3	N	795	SER	CA-CB	-5.25	1.45	1.52
3	F	87	SER	CA-CB	-5.22	1.45	1.52
3	N	87	SER	CA-CB	-5.22	1.45	1.52
3	J	87	SER	CA-CB	-5.20	1.45	1.52
3	N	236	SER	CA-CB	-5.18	1.45	1.52
3	B	87	SER	CA-CB	-5.17	1.45	1.52
3	J	236	SER	CA-CB	-5.15	1.45	1.52
3	F	236	SER	CA-CB	-5.15	1.45	1.52
3	B	236	SER	CA-CB	-5.13	1.45	1.52
3	N	176	SER	CA-CB	-5.11	1.45	1.52
3	J	176	SER	CA-CB	-5.10	1.45	1.52
3	B	176	SER	CA-CB	-5.08	1.45	1.52
3	F	176	SER	CA-CB	-5.07	1.45	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	PRO	N-CA-CB	-9.50	91.90	103.30
3	J	303	PRO	N-CA-CB	-9.49	91.91	103.30
3	F	303	PRO	N-CA-CB	-9.49	91.91	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	303	PRO	N-CA-CB	-9.45	91.96	103.30
3	B	284	PRO	N-CA-C	-9.15	88.32	112.10
3	F	283	LEU	N-CA-C	8.50	133.94	111.00
3	N	253	ASN	N-CA-C	-8.08	89.18	111.00
3	F	1091	LEU	CB-CA-C	7.73	124.89	110.20
3	B	283	LEU	CB-CG-CD2	-7.56	98.15	111.00
3	N	303	PRO	N-CA-C	7.53	131.67	112.10
3	B	303	PRO	N-CA-C	7.52	131.64	112.10
3	F	303	PRO	N-CA-C	7.52	131.64	112.10
3	J	303	PRO	N-CA-C	7.51	131.63	112.10
1	M	872	PRO	CA-N-CD	-7.49	101.02	111.50
1	I	872	PRO	CA-N-CD	-7.46	101.06	111.50
1	E	872	PRO	CA-N-CD	-7.45	101.07	111.50
1	A	872	PRO	CA-N-CD	-7.45	101.07	111.50
3	F	302	TYR	CB-CA-C	-7.39	95.62	110.40
3	B	302	TYR	CB-CA-C	-7.37	95.66	110.40
3	N	302	TYR	CB-CA-C	-7.36	95.68	110.40
3	J	302	TYR	CB-CA-C	-7.36	95.69	110.40
3	B	777	LYS	CB-CA-C	7.11	124.61	110.40
3	N	777	LYS	CB-CA-C	7.10	124.61	110.40
3	J	777	LYS	CB-CA-C	7.10	124.60	110.40
3	F	777	LYS	CB-CA-C	7.09	124.57	110.40
1	I	347	GLN	N-CA-C	-7.08	91.88	111.00
1	E	347	GLN	N-CA-C	-7.08	91.89	111.00
1	A	347	GLN	N-CA-C	-7.06	91.93	111.00
1	M	347	GLN	N-CA-C	-7.06	91.94	111.00
1	E	856	VAL	N-CA-C	6.83	129.44	111.00
1	A	856	VAL	N-CA-C	6.82	129.42	111.00
1	M	856	VAL	N-CA-C	6.82	129.42	111.00
1	I	856	VAL	N-CA-C	6.82	129.41	111.00
3	F	368	PHE	CB-CA-C	6.67	123.74	110.40
3	B	368	PHE	CB-CA-C	6.66	123.72	110.40
3	N	368	PHE	CB-CA-C	6.65	123.70	110.40
3	J	368	PHE	CB-CA-C	6.64	123.68	110.40
3	B	283	LEU	N-CA-C	6.48	128.49	111.00
2	K	375	PRO	N-CA-C	-6.42	95.42	112.10
2	C	375	PRO	N-CA-C	-6.41	95.43	112.10
2	O	375	PRO	N-CA-C	-6.40	95.45	112.10
2	G	375	PRO	N-CA-C	-6.39	95.48	112.10
1	E	859	PRO	N-CA-C	6.33	128.55	112.10
1	I	859	PRO	N-CA-C	6.32	128.54	112.10
1	A	859	PRO	N-CA-C	6.32	128.54	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	859	PRO	N-CA-C	6.31	128.51	112.10
3	F	513	TYR	CB-CA-C	6.08	122.56	110.40
3	F	204	ASN	CB-CA-C	6.07	122.55	110.40
3	N	204	ASN	CB-CA-C	6.07	122.54	110.40
3	J	513	TYR	CB-CA-C	6.06	122.53	110.40
3	B	204	ASN	CB-CA-C	6.06	122.53	110.40
3	B	513	TYR	CB-CA-C	6.06	122.52	110.40
3	J	204	ASN	CB-CA-C	6.05	122.51	110.40
3	N	513	TYR	CB-CA-C	6.05	122.49	110.40
3	J	299	CYS	CB-CA-C	-5.86	98.69	110.40
3	B	299	CYS	CB-CA-C	-5.85	98.71	110.40
3	N	299	CYS	CB-CA-C	-5.84	98.71	110.40
3	F	299	CYS	CB-CA-C	-5.82	98.76	110.40
3	B	254	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	E	861	GLU	N-CA-C	5.66	126.29	111.00
1	M	861	GLU	N-CA-C	5.66	126.29	111.00
1	I	861	GLU	N-CA-C	5.66	126.28	111.00
1	A	861	GLU	N-CA-C	5.66	126.27	111.00
3	B	332	ARG	CB-CG-CD	-5.64	96.93	111.60
3	F	332	ARG	CB-CG-CD	-5.63	96.95	111.60
3	J	332	ARG	CB-CG-CD	-5.63	96.95	111.60
3	N	332	ARG	CB-CG-CD	-5.63	96.96	111.60
3	B	461	PRO	N-CA-CB	-5.61	96.43	102.60
3	J	461	PRO	N-CA-CB	-5.61	96.43	102.60
3	F	461	PRO	N-CA-CB	-5.60	96.44	102.60
3	N	335	ARG	CB-CA-C	5.60	121.59	110.40
3	N	461	PRO	N-CA-CB	-5.59	96.45	102.60
3	J	335	ARG	CB-CA-C	5.59	121.58	110.40
3	B	335	ARG	CB-CA-C	5.59	121.58	110.40
3	B	254	LEU	CA-CB-CG	5.59	128.15	115.30
3	F	335	ARG	CB-CA-C	5.55	121.50	110.40
3	N	229	ASN	CB-CA-C	-5.53	99.34	110.40
3	J	229	ASN	CB-CA-C	-5.52	99.35	110.40
3	B	229	ASN	CB-CA-C	-5.51	99.37	110.40
3	F	229	ASN	CB-CA-C	-5.50	99.40	110.40
1	M	444	ILE	N-CA-C	-5.43	96.34	111.00
1	A	444	ILE	N-CA-C	-5.43	96.34	111.00
1	I	444	ILE	N-CA-C	-5.42	96.36	111.00
1	E	444	ILE	N-CA-C	-5.42	96.37	111.00
3	B	116	HIS	CB-CA-C	5.42	121.24	110.40
3	F	116	HIS	CB-CA-C	5.42	121.23	110.40
3	J	116	HIS	CB-CA-C	5.41	121.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	116	HIS	CB-CA-C	5.41	121.22	110.40
3	N	818	GLU	O-C-N	5.40	131.34	122.70
3	J	818	GLU	O-C-N	5.39	131.33	122.70
3	B	900	TYR	CB-CA-C	5.38	121.16	110.40
3	F	818	GLU	O-C-N	5.38	131.31	122.70
3	B	818	GLU	O-C-N	5.37	131.30	122.70
3	N	900	TYR	CB-CA-C	5.37	121.14	110.40
3	F	900	TYR	CB-CA-C	5.35	121.11	110.40
3	J	900	TYR	CB-CA-C	5.35	121.09	110.40
3	F	298	PRO	N-CA-CB	-5.33	96.74	102.60
1	M	339	GLY	N-CA-C	-5.32	99.79	113.10
1	A	339	GLY	N-CA-C	-5.32	99.81	113.10
3	J	298	PRO	N-CA-CB	-5.31	96.76	102.60
1	I	339	GLY	N-CA-C	-5.30	99.84	113.10
1	E	339	GLY	N-CA-C	-5.30	99.84	113.10
3	B	298	PRO	N-CA-CB	-5.30	96.77	102.60
3	N	298	PRO	N-CA-CB	-5.29	96.78	102.60
1	E	344	ASN	N-CA-C	5.21	125.08	111.00
1	I	344	ASN	N-CA-C	5.20	125.04	111.00
1	A	344	ASN	N-CA-C	5.20	125.03	111.00
1	M	344	ASN	N-CA-C	5.19	125.03	111.00
3	J	253	ASN	N-CA-C	-5.14	97.12	111.00
3	N	555	ARG	CB-CA-C	-5.13	100.14	110.40
3	F	555	ARG	CB-CA-C	-5.12	100.17	110.40
3	J	555	ARG	CB-CA-C	-5.12	100.17	110.40
3	B	555	ARG	CB-CA-C	-5.11	100.17	110.40
1	E	1176	LEU	CA-CB-CG	5.10	127.02	115.30
3	F	789	THR	CB-CA-C	-5.10	97.84	111.60
3	B	789	THR	CB-CA-C	-5.10	97.84	111.60
3	J	789	THR	CB-CA-C	-5.08	97.87	111.60
3	N	789	THR	CB-CA-C	-5.08	97.88	111.60
3	J	614	ARG	CB-CA-C	5.05	120.50	110.40
3	B	301	SER	CB-CA-C	-5.05	100.51	110.10
3	J	301	SER	CB-CA-C	-5.04	100.52	110.10
3	F	614	ARG	CB-CA-C	5.04	120.47	110.40
3	F	301	SER	CB-CA-C	-5.03	100.55	110.10
3	B	614	ARG	CB-CA-C	5.02	120.43	110.40
3	N	301	SER	CB-CA-C	-5.01	100.58	110.10
3	N	614	ARG	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7673	0	7689	394	0
1	E	7673	0	7689	444	0
1	I	7673	0	7689	399	0
1	M	7673	0	7689	389	0
2	C	402	0	417	65	0
2	G	402	0	417	66	0
2	K	402	0	417	68	0
2	O	402	0	417	68	0
3	B	8339	0	8330	608	0
3	F	8339	0	8328	648	0
3	J	8339	0	8330	587	0
3	N	8339	0	8329	561	0
4	A	15	0	23	18	0
4	B	15	0	23	19	0
4	E	15	0	23	17	0
4	F	30	0	49	66	0
4	I	15	0	23	18	0
4	M	15	0	23	17	0
4	N	15	0	24	40	0
5	B	27	0	12	3	0
5	F	27	0	12	2	0
5	J	27	0	12	3	0
5	N	27	0	12	2	0
All	All	65884	0	65977	3654	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 28.

All (3654) 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:E:28:PRO:HG2	3:F:547:LEU:CD2	1.26	1.64
3:N:974:MET:CE	3:N:975:TYR:CZ	1.82	1.63
4:F:1101:FAR:C15	3:J:1013:ASN:HD21	1.04	1.61
1:E:28:PRO:CG	3:F:547:LEU:HD21	1.14	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:974:MET:CE	3:B:975:TYR:CZ	1.82	1.59
3:F:965:GLN:HG2	3:F:969:LEU:CD1	1.14	1.59
3:J:974:MET:CE	3:J:975:TYR:CZ	1.82	1.58
3:N:965:GLN:HG2	3:N:969:LEU:CD1	1.14	1.58
1:I:1211:VAL:CG2	4:I:1301:FAR:H101	1.33	1.58
3:F:974:MET:CE	3:F:975:TYR:CZ	1.82	1.57
3:B:965:GLN:HG2	3:B:969:LEU:CD1	1.14	1.55
3:J:965:GLN:HG2	3:J:969:LEU:CD1	1.14	1.55
3:F:1013:ASN:HD21	4:F:1103:FAR:C15	0.97	1.54
1:E:1211:VAL:CG2	4:E:1301:FAR:H101	1.33	1.53
1:A:1211:VAL:CG2	4:A:1301:FAR:H101	1.33	1.52
1:I:28:PRO:CG	3:J:547:LEU:HD21	1.36	1.52
3:B:1092:ILE:HD11	3:N:1001:GLU:CG	1.08	1.51
3:F:1009:VAL:HA	4:F:1103:FAR:C14	1.38	1.51
1:M:1211:VAL:CG2	4:M:1301:FAR:H101	1.33	1.50
3:J:965:GLN:CG	3:J:969:LEU:HD11	1.40	1.50
2:G:332:ILE:HD13	2:G:340:LEU:CD1	1.41	1.49
2:C:332:ILE:HD13	2:C:340:LEU:CD1	1.41	1.49
4:F:1101:FAR:C14	3:J:1009:VAL:HA	1.42	1.49
3:J:974:MET:HE3	3:J:975:TYR:CZ	1.40	1.49
1:I:28:PRO:HG2	3:J:547:LEU:CD2	1.42	1.48
3:B:965:GLN:CG	3:B:969:LEU:CD1	1.89	1.47
3:F:965:GLN:CG	3:F:969:LEU:CD1	1.89	1.47
3:B:965:GLN:CG	3:B:969:LEU:HD11	1.40	1.47
3:J:744:LEU:HD22	3:J:765:HIS:CD2	1.50	1.47
3:F:974:MET:HE3	3:F:975:TYR:CZ	1.39	1.45
2:O:332:ILE:HD13	2:O:340:LEU:CD1	1.41	1.45
2:K:332:ILE:HD13	2:K:340:LEU:CD1	1.41	1.45
3:F:744:LEU:HD22	3:F:765:HIS:CD2	1.50	1.45
3:J:965:GLN:CG	3:J:969:LEU:CD1	1.89	1.45
1:E:120:THR:HG22	3:F:131:ARG:CZ	1.44	1.43
3:B:744:LEU:HD22	3:B:765:HIS:CD2	1.50	1.43
3:N:965:GLN:CG	3:N:969:LEU:HD11	1.40	1.43
3:F:965:GLN:CG	3:F:969:LEU:HD11	1.40	1.43
3:N:744:LEU:HD22	3:N:765:HIS:CD2	1.50	1.42
1:E:28:PRO:CG	3:F:547:LEU:CD2	1.87	1.41
1:A:788:THR:O	1:A:792:PRO:CD	1.69	1.41
3:B:1092:ILE:CD1	3:N:1001:GLU:HG2	0.93	1.41
1:M:788:THR:O	1:M:792:PRO:CD	1.69	1.40
3:N:965:GLN:CG	3:N:969:LEU:CD1	1.89	1.40
1:E:66:ASP:CB	3:B:667:GLN:HE22	1.32	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:PRO:CG	3:N:547:LEU:HD21	1.49	1.39
4:F:1101:FAR:H151	3:J:1013:ASN:ND2	1.07	1.39
1:A:28:PRO:CG	3:B:547:LEU:HD21	1.50	1.39
1:I:28:PRO:CG	3:J:547:LEU:CD2	1.96	1.37
1:I:788:THR:O	1:I:792:PRO:CD	1.69	1.37
1:E:788:THR:O	1:E:792:PRO:CD	1.69	1.37
3:N:974:MET:HE3	3:N:975:TYR:OH	1.21	1.35
3:F:1001:GLU:HG2	3:J:1092:ILE:CD1	0.88	1.35
3:B:974:MET:HE3	3:B:975:TYR:OH	1.19	1.33
3:F:1001:GLU:CG	3:J:1092:ILE:HD11	0.86	1.33
3:N:974:MET:HE3	3:N:975:TYR:CZ	1.47	1.33
1:E:93:ILE:HG22	3:F:67:THR:CG2	1.57	1.32
1:M:28:PRO:HG2	3:N:547:LEU:CD2	1.58	1.32
3:J:361:ILE:HD11	3:J:421:LYS:CE	1.60	1.31
1:I:788:THR:O	1:I:792:PRO:HD2	1.23	1.31
1:E:788:THR:O	1:E:792:PRO:HD2	1.23	1.31
1:A:28:PRO:CG	3:B:547:LEU:CD2	2.07	1.30
3:J:974:MET:HE2	3:J:975:TYR:CE2	1.67	1.30
1:M:28:PRO:CG	3:N:547:LEU:CD2	2.07	1.29
3:B:361:ILE:HD11	3:B:421:LYS:CE	1.60	1.29
3:F:361:ILE:HD11	3:F:421:LYS:CE	1.60	1.29
3:F:974:MET:HE3	3:F:975:TYR:OH	1.25	1.29
3:B:223:ARG:HD3	3:B:228:ASN:OD1	1.30	1.29
4:F:1101:FAR:H143	3:J:1009:VAL:CA	1.60	1.29
3:N:361:ILE:HD11	3:N:421:LYS:CE	1.60	1.28
3:N:223:ARG:HD3	3:N:228:ASN:OD1	1.30	1.28
4:B:1101:FAR:C15	3:N:1013:ASN:HD21	1.46	1.27
3:F:974:MET:HE2	3:F:975:TYR:CE2	1.67	1.27
3:N:974:MET:HE2	3:N:975:TYR:CE2	1.68	1.27
1:M:788:THR:O	1:M:792:PRO:HD2	1.23	1.26
3:B:974:MET:HE2	3:B:975:TYR:CE2	1.70	1.26
1:E:63:LYS:C	3:B:567:ARG:HH22	1.37	1.26
3:B:974:MET:HE3	3:B:975:TYR:CZ	1.53	1.26
3:B:1013:ASN:HD21	4:N:1101:FAR:C15	1.47	1.26
1:I:93:ILE:HG22	3:J:67:THR:CG2	1.65	1.26
3:B:579:ILE:CD1	3:B:601:ALA:HB2	1.65	1.26
3:F:579:ILE:CD1	3:F:601:ALA:HB2	1.65	1.25
3:J:579:ILE:CD1	3:J:601:ALA:HB2	1.65	1.25
3:B:1093:SER:O	3:N:924:TRP:CH2	1.89	1.25
3:J:974:MET:HE3	3:J:975:TYR:OH	1.24	1.25
3:F:223:ARG:HD3	3:F:228:ASN:OD1	1.30	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:THR:HG23	3:F:511:ASN:OD1	1.34	1.25
3:F:1001:GLU:HG2	3:J:1092:ILE:CG1	1.67	1.25
3:F:1013:ASN:ND2	4:F:1103:FAR:H151	0.95	1.25
3:N:579:ILE:CD1	3:N:601:ALA:HB2	1.65	1.25
3:J:223:ARG:HD3	3:J:228:ASN:OD1	1.30	1.25
1:I:28:PRO:CB	3:J:547:LEU:HD21	1.66	1.24
1:A:28:PRO:CB	3:B:547:LEU:HD21	1.68	1.23
1:E:66:ASP:CB	3:B:667:GLN:NE2	2.00	1.23
1:I:557:THR:HG23	3:N:511:ASN:OD1	1.38	1.23
1:A:28:PRO:HG2	3:B:547:LEU:CD2	1.62	1.23
1:A:788:THR:O	1:A:792:PRO:HD2	1.23	1.23
3:B:974:MET:CE	3:B:975:TYR:CE2	2.23	1.22
1:M:557:THR:HG23	3:J:511:ASN:OD1	1.38	1.22
1:M:28:PRO:CB	3:N:547:LEU:HD21	1.70	1.22
3:B:74:LYS:HD3	3:B:439:LYS:NZ	1.53	1.22
3:B:1013:ASN:ND2	4:N:1101:FAR:H151	1.51	1.22
3:F:744:LEU:CD2	3:F:765:HIS:CD2	2.23	1.21
3:J:74:LYS:HD3	3:J:439:LYS:NZ	1.53	1.21
1:M:768:LEU:HD23	1:M:802:ARG:NH2	1.55	1.21
3:B:744:LEU:CD2	3:B:765:HIS:CD2	2.23	1.21
3:J:744:LEU:CD2	3:J:765:HIS:CD2	2.23	1.21
3:F:1009:VAL:CA	4:F:1103:FAR:H143	1.70	1.21
1:E:768:LEU:HD23	1:E:802:ARG:NH2	1.54	1.21
1:A:768:LEU:HD23	1:A:802:ARG:NH2	1.55	1.20
3:B:1092:ILE:HD11	3:N:1001:GLU:CD	1.60	1.20
3:F:974:MET:CE	3:F:975:TYR:CE2	2.23	1.20
3:N:744:LEU:CD2	3:N:765:HIS:CD2	2.23	1.20
3:F:74:LYS:HD3	3:F:439:LYS:NZ	1.53	1.20
3:F:1001:GLU:CB	3:J:1092:ILE:HD11	1.70	1.20
3:N:74:LYS:HD3	3:N:439:LYS:NZ	1.53	1.20
1:I:768:LEU:HD23	1:I:802:ARG:NH2	1.55	1.19
1:A:1211:VAL:CG2	4:A:1301:FAR:C10	2.20	1.19
1:M:1211:VAL:CG2	4:M:1301:FAR:C10	2.20	1.19
2:K:332:ILE:CD1	2:K:340:LEU:CD1	2.21	1.18
3:N:974:MET:CE	3:N:975:TYR:CE2	2.23	1.18
2:C:332:ILE:CD1	2:C:340:LEU:CD1	2.21	1.18
1:I:1211:VAL:CG2	4:I:1301:FAR:C10	2.20	1.18
1:E:1211:VAL:CG2	4:E:1301:FAR:C10	2.20	1.18
2:O:332:ILE:CD1	2:O:340:LEU:CD1	2.21	1.17
1:E:120:THR:CG2	3:F:131:ARG:CZ	2.21	1.17
3:B:974:MET:HE2	3:B:975:TYR:CZ	1.52	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:LEU:CD2	1:A:802:ARG:HH21	1.58	1.16
2:G:332:ILE:CD1	2:G:340:LEU:CD1	2.21	1.16
3:B:261:SER:HB2	3:B:669:ASP:OD2	1.44	1.16
3:B:1090:CYS:SG	4:B:1101:FAR:C1	1.07	1.16
3:J:261:SER:HB2	3:J:669:ASP:OD2	1.44	1.16
3:J:974:MET:CE	3:J:975:TYR:CE2	2.23	1.15
3:B:1092:ILE:CD1	3:N:1001:GLU:CG	1.83	1.15
3:F:261:SER:HB2	3:F:669:ASP:OD2	1.44	1.15
3:N:974:MET:HE2	3:N:975:TYR:CZ	1.59	1.15
1:E:768:LEU:CD2	1:E:802:ARG:HH21	1.58	1.15
1:I:768:LEU:CD2	1:I:802:ARG:HH21	1.59	1.15
3:F:924:TRP:CH2	3:J:1093:SER:O	2.00	1.15
1:M:93:ILE:HG22	3:N:67:THR:CG2	1.75	1.14
1:E:28:PRO:CB	3:F:547:LEU:HD21	1.77	1.14
2:C:332:ILE:HB	2:C:340:LEU:HD11	1.18	1.14
1:M:768:LEU:CD2	1:M:802:ARG:HH21	1.59	1.14
3:N:261:SER:HB2	3:N:669:ASP:OD2	1.44	1.14
1:E:28:PRO:HB2	3:F:130:MET:CE	1.77	1.13
1:E:62:ARG:NH1	3:F:258:GLN:OE1	1.78	1.13
2:O:332:ILE:CD1	2:O:340:LEU:HD13	1.78	1.13
1:I:120:THR:HG22	3:J:131:ARG:CZ	1.77	1.13
2:G:332:ILE:HB	2:G:340:LEU:HD11	1.18	1.12
3:B:579:ILE:HD11	3:B:601:ALA:HB2	1.23	1.12
3:F:361:ILE:CD1	3:F:421:LYS:HE3	1.78	1.12
2:G:332:ILE:CD1	2:G:340:LEU:HD13	1.79	1.12
2:K:332:ILE:CD1	2:K:340:LEU:HD13	1.78	1.12
1:A:93:ILE:HG22	3:B:67:THR:HG22	1.20	1.12
3:B:1009:VAL:HA	4:N:1101:FAR:C14	1.78	1.12
3:B:1090:CYS:SG	4:B:1101:FAR:H13	0.88	1.12
3:J:143:PRO:HB2	3:J:215:VAL:HG21	1.31	1.12
1:E:120:THR:HG22	3:F:131:ARG:NE	1.62	1.12
2:O:332:ILE:HB	2:O:340:LEU:HD11	1.19	1.11
1:I:66:ASP:CB	3:N:667:GLN:HE22	1.61	1.11
3:N:361:ILE:CD1	3:N:421:LYS:HE3	1.79	1.11
3:B:361:ILE:CD1	3:B:421:LYS:HE3	1.78	1.11
3:F:1090:CYS:SG	4:F:1101:FAR:C1	1.01	1.11
4:F:1103:FAR:C1	3:J:1090:CYS:SG	1.01	1.11
3:J:361:ILE:CD1	3:J:421:LYS:HE3	1.79	1.11
3:N:1090:CYS:SG	4:N:1101:FAR:C1	1.01	1.11
1:A:62:ARG:NH1	3:B:258:GLN:OE1	1.82	1.10
1:I:28:PRO:HG2	3:J:547:LEU:HD23	1.23	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:974:MET:HE2	3:F:975:TYR:CZ	1.67	1.10
1:M:93:ILE:HG22	3:N:67:THR:HG22	1.11	1.10
3:F:965:GLN:HG3	3:F:969:LEU:HD11	1.24	1.10
3:F:143:PRO:HB2	3:F:215:VAL:HG21	1.32	1.10
1:A:768:LEU:CD2	1:A:802:ARG:NH2	2.15	1.10
3:B:965:GLN:HG3	3:B:969:LEU:HD11	1.24	1.10
1:A:28:PRO:HG2	3:B:547:LEU:HD23	1.33	1.09
2:C:332:ILE:CD1	2:C:340:LEU:HD13	1.78	1.09
1:M:768:LEU:CD2	1:M:802:ARG:NH2	2.15	1.09
2:G:332:ILE:HD13	2:G:340:LEU:HD12	1.34	1.09
1:M:66:ASP:CB	3:J:667:GLN:HE22	1.65	1.09
3:B:1009:VAL:HA	4:N:1101:FAR:H143	1.14	1.09
1:E:28:PRO:HG2	3:F:547:LEU:HD23	1.34	1.09
1:E:491:ARG:HG2	3:F:62:LEU:HD11	1.32	1.09
4:F:1103:FAR:H13	3:J:1090:CYS:SG	0.83	1.09
3:N:579:ILE:HD11	3:N:601:ALA:HB2	1.23	1.09
3:N:965:GLN:HG3	3:N:969:LEU:HD11	1.24	1.09
1:I:93:ILE:CG2	3:J:67:THR:HG22	1.81	1.09
3:N:526:ILE:HD13	3:N:660:ILE:HD12	1.16	1.09
1:E:93:ILE:HG22	3:F:67:THR:HG22	1.12	1.08
3:J:579:ILE:HD11	3:J:601:ALA:HB2	1.23	1.08
3:N:143:PRO:HB2	3:N:215:VAL:HG21	1.32	1.08
3:F:579:ILE:HD11	3:F:601:ALA:HB2	1.23	1.08
3:F:526:ILE:HD13	3:F:660:ILE:CD1	1.83	1.08
3:F:526:ILE:HD13	3:F:660:ILE:HD12	1.16	1.08
3:J:526:ILE:HD13	3:J:660:ILE:HD12	1.16	1.08
1:M:28:PRO:HG2	3:N:547:LEU:HD23	1.31	1.08
1:I:768:LEU:CD2	1:I:802:ARG:NH2	2.15	1.08
1:A:788:THR:O	1:A:792:PRO:CG	2.01	1.08
1:I:62:ARG:NH1	3:J:258:GLN:OE1	1.86	1.07
1:I:788:THR:O	1:I:792:PRO:CG	2.01	1.07
3:B:526:ILE:HD13	3:B:660:ILE:CD1	1.83	1.07
3:B:1092:ILE:HD12	3:N:1001:GLU:HG2	1.11	1.07
1:A:1137:LEU:HD13	4:A:1301:FAR:H61	1.29	1.07
1:E:768:LEU:CD2	1:E:802:ARG:NH2	2.15	1.07
1:M:788:THR:O	1:M:792:PRO:CG	2.01	1.07
3:B:526:ILE:HD13	3:B:660:ILE:HD12	1.16	1.07
1:A:93:ILE:HG22	3:B:67:THR:CG2	1.84	1.07
1:E:120:THR:HG21	3:F:131:ARG:NH2	1.68	1.07
1:E:1137:LEU:HD13	4:E:1301:FAR:H61	1.29	1.07
1:M:1120:GLN:HE21	1:M:1181:ALA:CB	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1001:GLU:HA	3:J:1092:ILE:HD12	1.18	1.07
4:F:1101:FAR:H151	3:J:1013:ASN:CG	1.74	1.07
1:A:1120:GLN:HE21	1:A:1181:ALA:CB	1.68	1.07
1:E:28:PRO:HB2	3:F:130:MET:HE1	1.31	1.07
1:I:1137:LEU:HD13	4:I:1301:FAR:H61	1.29	1.07
3:J:526:ILE:HD13	3:J:660:ILE:CD1	1.83	1.07
3:N:526:ILE:HD13	3:N:660:ILE:CD1	1.84	1.06
2:K:332:ILE:HB	2:K:340:LEU:HD11	1.18	1.06
3:N:965:GLN:CG	3:N:969:LEU:HD12	1.69	1.06
1:M:1137:LEU:HD13	4:M:1301:FAR:H61	1.29	1.06
4:B:1101:FAR:C14	3:N:1009:VAL:HA	1.85	1.06
1:E:491:ARG:HG3	3:F:62:LEU:CD1	1.85	1.06
1:E:788:THR:O	1:E:792:PRO:CG	2.01	1.06
3:B:143:PRO:HB2	3:B:215:VAL:HG21	1.32	1.06
3:N:1015:GLU:OE1	4:N:1101:FAR:H62	1.56	1.06
1:A:435:LYS:HD3	1:A:555:ARG:HD2	1.38	1.05
1:A:1211:VAL:HG21	4:A:1301:FAR:C10	1.85	1.05
3:J:965:GLN:HG3	3:J:969:LEU:HD11	1.24	1.05
1:M:120:THR:HG22	3:N:131:ARG:CZ	1.86	1.05
4:F:1103:FAR:C2	3:J:1090:CYS:SG	2.44	1.05
3:N:1090:CYS:SG	4:N:1101:FAR:C2	2.44	1.05
1:A:1120:GLN:NE2	1:A:1181:ALA:HB3	1.72	1.05
1:E:120:THR:CG2	3:F:131:ARG:NH2	2.19	1.05
1:E:1120:GLN:HE21	1:E:1181:ALA:CB	1.68	1.05
1:M:1120:GLN:NE2	1:M:1181:ALA:HB3	1.72	1.05
1:I:1120:GLN:HE21	1:I:1181:ALA:CB	1.68	1.05
1:A:66:ASP:CB	3:F:667:GLN:HE22	1.69	1.05
3:B:1015:GLU:OE1	3:N:1012:ARG:NH1	1.90	1.05
3:J:853:LEU:CD1	3:J:880:ILE:HG13	1.87	1.05
3:F:1001:GLU:CB	3:J:1092:ILE:CD1	2.32	1.04
1:I:1120:GLN:NE2	1:I:1181:ALA:HB3	1.72	1.04
3:B:853:LEU:CD1	3:B:880:ILE:HG13	1.87	1.04
1:A:68:ASP:OD1	3:B:259:GLY:O	1.75	1.04
3:F:853:LEU:CD1	3:F:880:ILE:HG13	1.87	1.04
3:N:853:LEU:CD1	3:N:880:ILE:HG13	1.87	1.04
1:E:435:LYS:HD3	1:E:555:ARG:HD2	1.38	1.04
1:E:1120:GLN:NE2	1:E:1181:ALA:HB3	1.72	1.04
1:M:435:LYS:HD3	1:M:555:ARG:HD2	1.38	1.04
1:E:1120:GLN:NE2	1:E:1181:ALA:CB	2.21	1.04
1:A:1120:GLN:OE1	1:A:1182:SER:HB3	1.58	1.03
1:M:93:ILE:CG2	3:N:67:THR:HG22	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1120:GLN:OE1	1:M:1182:SER:HB3	1.58	1.03
1:I:435:LYS:HD3	1:I:555:ARG:HD2	1.38	1.03
1:A:28:PRO:HB2	3:B:547:LEU:HD21	1.40	1.03
1:I:1120:GLN:NE2	1:I:1181:ALA:CB	2.21	1.03
2:K:332:ILE:HD13	2:K:340:LEU:HD12	1.34	1.03
2:C:332:ILE:HD13	2:C:340:LEU:HD12	1.34	1.03
1:A:1120:GLN:NE2	1:A:1181:ALA:CB	2.21	1.03
1:E:75:TYR:OH	3:F:191:GLN:CG	2.07	1.03
1:M:1120:GLN:NE2	1:M:1181:ALA:CB	2.21	1.03
3:N:1090:CYS:SG	4:N:1101:FAR:H13	0.83	1.03
1:E:66:ASP:HB3	3:B:667:GLN:HE22	0.87	1.02
1:E:491:ARG:CG	3:F:62:LEU:HD11	1.89	1.02
1:E:491:ARG:CG	3:F:62:LEU:CD1	2.36	1.02
2:O:332:ILE:HD13	2:O:340:LEU:HD12	1.34	1.02
4:B:1101:FAR:H143	3:N:1009:VAL:HA	1.37	1.02
3:J:625:ASN:O	3:J:634:ILE:HD12	1.60	1.02
3:B:965:GLN:CG	3:B:969:LEU:HD12	1.69	1.02
3:J:143:PRO:HB2	3:J:215:VAL:CG2	1.89	1.02
3:J:173:ASN:OD1	3:J:174:ALA:N	1.92	1.02
3:N:173:ASN:OD1	3:N:174:ALA:N	1.92	1.02
3:B:1093:SER:O	3:N:924:TRP:CZ2	2.12	1.02
1:I:113:HIS:NE2	1:I:127:ASP:OD1	1.92	1.02
3:F:143:PRO:HB2	3:F:215:VAL:CG2	1.89	1.02
3:N:143:PRO:HB2	3:N:215:VAL:CG2	1.89	1.02
1:A:113:HIS:NE2	1:A:127:ASP:OD1	1.92	1.02
2:C:332:ILE:HB	2:C:340:LEU:CD1	1.89	1.02
1:E:1120:GLN:OE1	1:E:1182:SER:HB3	1.58	1.02
2:G:332:ILE:HB	2:G:340:LEU:CD1	1.89	1.02
1:M:783:LEU:O	1:M:787:TYR:HD2	1.43	1.02
1:I:1211:VAL:HG21	4:I:1301:FAR:C10	1.85	1.02
1:M:28:PRO:HB2	3:N:547:LEU:HD21	1.42	1.01
2:K:332:ILE:HB	2:K:340:LEU:CD1	1.89	1.01
3:B:625:ASN:O	3:B:634:ILE:HD12	1.60	1.01
1:M:113:HIS:NE2	1:M:127:ASP:OD1	1.92	1.01
1:I:783:LEU:O	1:I:787:TYR:HD2	1.42	1.01
3:B:173:ASN:OD1	3:B:174:ALA:N	1.92	1.01
1:E:28:PRO:HG3	3:F:547:LEU:CD2	1.84	1.01
1:I:66:ASP:HB3	3:N:667:GLN:HE22	1.21	1.01
3:B:143:PRO:HB2	3:B:215:VAL:CG2	1.89	1.01
3:F:173:ASN:OD1	3:F:174:ALA:N	1.92	1.01
3:F:625:ASN:O	3:F:634:ILE:HD12	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1015:GLU:OE2	4:N:1101:FAR:H41	1.60	1.01
1:A:1211:VAL:HG23	4:A:1301:FAR:H101	1.43	1.01
1:E:783:LEU:O	1:E:787:TYR:HD2	1.42	1.01
3:F:1015:GLU:OE2	4:F:1101:FAR:C4	2.09	1.01
3:N:625:ASN:O	3:N:634:ILE:HD12	1.59	1.01
2:O:332:ILE:HB	2:O:340:LEU:CD1	1.89	1.00
1:M:1211:VAL:HG21	4:M:1301:FAR:C10	1.85	1.00
1:M:1211:VAL:HG23	4:M:1301:FAR:H101	1.43	1.00
3:B:744:LEU:HD21	3:B:765:HIS:HB3	1.40	1.00
3:F:1090:CYS:SG	4:F:1101:FAR:C2	2.49	1.00
1:A:783:LEU:O	1:A:787:TYR:HD2	1.42	1.00
3:F:744:LEU:HD21	3:F:765:HIS:HB3	1.40	1.00
3:F:1009:VAL:HA	4:F:1103:FAR:H141	1.40	1.00
3:J:974:MET:HE2	3:J:975:TYR:CZ	1.65	1.00
1:I:1120:GLN:OE1	1:I:1182:SER:HB3	1.58	1.00
1:E:113:HIS:NE2	1:E:127:ASP:OD1	1.92	1.00
3:F:1015:GLU:OE1	4:F:1101:FAR:H62	1.60	1.00
1:E:63:LYS:C	3:B:567:ARG:NH2	2.14	0.99
3:B:485:ASN:ND2	3:F:105:ASP:OD1	1.95	0.99
3:F:1015:GLU:OE2	4:F:1101:FAR:H41	1.59	0.99
3:N:744:LEU:HD21	3:N:765:HIS:HB3	1.40	0.99
3:N:744:LEU:CD2	3:N:765:HIS:CG	2.46	0.99
3:F:1082:VAL:HG21	3:J:1060:LEU:HD23	1.45	0.99
1:A:783:LEU:O	1:A:787:TYR:CD2	2.16	0.99
3:J:223:ARG:HD3	3:J:228:ASN:CG	1.83	0.99
1:I:93:ILE:HG22	3:J:67:THR:HG22	1.01	0.99
3:F:283:LEU:HD21	3:F:307:LEU:HG	1.44	0.99
3:B:223:ARG:HD3	3:B:228:ASN:CG	1.83	0.99
1:E:491:ARG:HG3	3:F:62:LEU:HD12	1.41	0.98
3:B:744:LEU:CD2	3:B:765:HIS:CG	2.46	0.98
3:F:74:LYS:HD3	3:F:439:LYS:HZ3	1.28	0.98
3:J:485:ASN:ND2	3:N:105:ASP:OD1	1.96	0.98
1:M:783:LEU:O	1:M:787:TYR:CD2	2.16	0.98
3:N:1015:GLU:OE2	4:N:1101:FAR:C4	2.10	0.98
1:A:66:ASP:HB3	3:F:667:GLN:HE22	1.29	0.98
1:E:872:PRO:HD2	1:E:875:ALA:HB3	1.45	0.98
1:I:1211:VAL:HG23	4:I:1301:FAR:H101	1.43	0.98
1:E:783:LEU:O	1:E:787:TYR:CD2	2.16	0.98
3:F:223:ARG:HD3	3:F:228:ASN:CG	1.84	0.98
3:J:744:LEU:CD2	3:J:765:HIS:CG	2.46	0.98
4:F:1101:FAR:C15	3:J:1013:ASN:ND2	1.82	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1001:GLU:HG2	3:J:1092:ILE:HD12	1.46	0.98
1:E:66:ASP:HB2	3:B:667:GLN:NE2	1.78	0.98
1:E:93:ILE:HG22	3:F:67:THR:HG23	1.46	0.98
1:I:783:LEU:O	1:I:787:TYR:CD2	2.16	0.98
3:F:965:GLN:CG	3:F:969:LEU:HD12	1.69	0.98
3:J:744:LEU:HD21	3:J:765:HIS:HB3	1.40	0.98
2:O:332:ILE:HD13	2:O:340:LEU:HD13	0.98	0.98
3:F:1013:ASN:HD21	4:F:1103:FAR:H152	1.29	0.98
2:C:332:ILE:HD13	2:C:340:LEU:HD13	0.98	0.98
1:A:93:ILE:CG2	3:B:67:THR:HG22	1.94	0.97
2:G:332:ILE:HD13	2:G:340:LEU:HD13	0.98	0.97
3:B:1090:CYS:SG	4:B:1101:FAR:C2	2.50	0.97
1:A:872:PRO:HD2	1:A:875:ALA:HB3	1.45	0.97
2:C:332:ILE:CB	2:C:340:LEU:HD11	1.95	0.97
1:E:1211:VAL:HG23	4:E:1301:FAR:C10	1.93	0.97
3:B:744:LEU:HD22	3:B:765:HIS:HD2	1.29	0.97
3:F:1004:MET:CB	3:J:1092:ILE:HG21	1.94	0.97
3:N:744:LEU:HD22	3:N:765:HIS:HD2	1.29	0.97
3:B:74:LYS:HD3	3:B:439:LYS:HZ1	1.23	0.97
3:N:625:ASN:O	3:N:634:ILE:CD1	2.12	0.97
3:F:1001:GLU:CA	3:J:1092:ILE:HD12	1.94	0.97
2:O:332:ILE:CB	2:O:340:LEU:HD11	1.95	0.97
3:F:1090:CYS:SG	4:F:1101:FAR:H13	0.96	0.97
3:N:74:LYS:HD3	3:N:439:LYS:HZ1	1.27	0.97
1:M:1211:VAL:HG23	4:M:1301:FAR:C10	1.93	0.97
3:B:625:ASN:O	3:B:634:ILE:CD1	2.12	0.97
3:N:223:ARG:HD3	3:N:228:ASN:CG	1.84	0.97
3:B:1012:ARG:NH1	4:N:1101:FAR:H7	1.78	0.97
3:F:744:LEU:CD2	3:F:765:HIS:CG	2.46	0.97
1:E:79:GLN:NE2	3:F:194:TYR:CE1	2.32	0.97
2:K:332:ILE:HD13	2:K:340:LEU:HD13	0.98	0.97
1:I:872:PRO:HD2	1:I:875:ALA:HB3	1.45	0.96
3:F:625:ASN:O	3:F:634:ILE:CD1	2.12	0.96
3:F:1009:VAL:CA	4:F:1103:FAR:C14	2.34	0.96
1:E:1211:VAL:HG23	4:E:1301:FAR:H101	1.43	0.96
1:M:441:GLN:NE2	1:M:607:PHE:HB3	1.80	0.96
1:I:63:LYS:C	3:N:567:ARG:HH22	1.67	0.96
3:B:413:PRO:HG2	3:B:416:PHE:HD2	1.27	0.96
1:E:83:LYS:HE3	3:F:198:GLU:OE1	1.65	0.96
1:I:441:GLN:NE2	1:I:607:PHE:HB3	1.80	0.96
2:K:332:ILE:CB	2:K:340:LEU:HD11	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLN:NE2	1:A:607:PHE:HB3	1.80	0.96
1:M:771:LYS:HG3	1:M:802:ARG:NH1	1.81	0.96
3:F:1013:ASN:CG	4:F:1103:FAR:H151	1.86	0.96
1:E:419:ALA:HB1	3:B:524:GLU:OE1	1.64	0.96
1:E:1211:VAL:HG21	4:E:1301:FAR:C10	1.85	0.96
1:A:771:LYS:HG3	1:A:802:ARG:NH1	1.81	0.96
1:E:441:GLN:NE2	1:E:607:PHE:HB3	1.80	0.96
1:I:28:PRO:HB2	3:J:547:LEU:HD21	1.45	0.96
3:N:413:PRO:HG2	3:N:416:PHE:HD2	1.27	0.96
1:I:771:LYS:HG3	1:I:802:ARG:NH1	1.81	0.96
1:E:83:LYS:HD2	3:F:198:GLU:OE1	1.65	0.96
2:G:332:ILE:CB	2:G:340:LEU:HD11	1.94	0.96
3:F:413:PRO:HG2	3:F:416:PHE:HD2	1.27	0.96
3:J:625:ASN:O	3:J:634:ILE:CD1	2.12	0.96
3:B:1013:ASN:HD21	4:N:1101:FAR:H151	1.04	0.96
1:A:120:THR:HG22	3:B:131:ARG:CZ	1.94	0.95
1:M:62:ARG:NH1	3:N:258:GLN:OE1	1.98	0.95
3:J:965:GLN:CG	3:J:969:LEU:HD12	1.69	0.95
3:N:261:SER:CB	3:N:669:ASP:OD2	2.15	0.95
1:E:93:ILE:CG2	3:F:67:THR:HG22	1.96	0.95
1:I:28:PRO:HG3	3:J:547:LEU:CD2	1.95	0.95
3:J:261:SER:CB	3:J:669:ASP:OD2	2.15	0.95
1:E:771:LYS:HG3	1:E:802:ARG:NH1	1.81	0.95
4:B:1101:FAR:C15	3:N:1013:ASN:ND2	2.28	0.95
3:F:1001:GLU:CD	3:J:1092:ILE:HD11	1.87	0.95
3:J:413:PRO:HG2	3:J:416:PHE:HD2	1.27	0.95
3:B:1092:ILE:CG1	3:N:1001:GLU:HG2	1.96	0.95
3:J:105:ASP:OD1	3:N:485:ASN:ND2	1.99	0.94
3:F:261:SER:CB	3:F:669:ASP:OD2	2.15	0.94
1:A:1211:VAL:HG23	4:A:1301:FAR:C10	1.93	0.94
3:B:261:SER:CB	3:B:669:ASP:OD2	2.15	0.94
1:A:75:TYR:OH	3:B:191:GLN:HB3	1.68	0.94
3:B:579:ILE:CD1	3:B:601:ALA:CB	2.46	0.94
1:E:1211:VAL:HG21	4:E:1301:FAR:H101	0.95	0.93
1:M:872:PRO:HD2	1:M:875:ALA:HB3	1.45	0.93
3:F:283:LEU:HD23	3:F:307:LEU:HD21	1.50	0.93
3:J:579:ILE:CD1	3:J:601:ALA:CB	2.46	0.93
3:B:103:ARG:NH2	3:F:477:ARG:CZ	2.31	0.93
1:M:66:ASP:HB3	3:J:667:GLN:HE22	1.32	0.93
3:F:579:ILE:CD1	3:F:601:ALA:CB	2.46	0.93
3:J:223:ARG:CD	3:J:228:ASN:OD1	2.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:744:LEU:HD22	3:J:765:HIS:HD2	1.29	0.93
1:M:1211:VAL:HG21	4:M:1301:FAR:H101	0.95	0.93
3:N:223:ARG:CD	3:N:228:ASN:OD1	2.17	0.93
3:F:1001:GLU:HA	3:J:1092:ILE:CD1	1.99	0.92
3:N:579:ILE:CD1	3:N:601:ALA:CB	2.46	0.92
3:B:1093:SER:O	3:N:1059:PRO:HG3	1.69	0.92
3:F:223:ARG:CD	3:F:228:ASN:OD1	2.17	0.92
3:F:744:LEU:HD22	3:F:765:HIS:HD2	1.29	0.92
1:A:1211:VAL:HG21	4:A:1301:FAR:H101	0.95	0.92
1:I:1211:VAL:HG21	4:I:1301:FAR:H101	0.95	0.92
3:B:1009:VAL:CA	4:N:1101:FAR:H143	1.99	0.92
1:E:28:PRO:HG3	3:F:547:LEU:HD21	1.46	0.91
1:I:66:ASP:CB	3:N:667:GLN:NE2	2.33	0.91
3:B:803:PHE:CD2	3:B:810:VAL:HG22	2.05	0.91
1:E:93:ILE:CG2	3:F:67:THR:CG2	2.47	0.91
3:B:974:MET:CE	3:B:975:TYR:OH	2.00	0.91
3:F:744:LEU:HD21	3:F:765:HIS:CB	2.00	0.91
1:E:66:ASP:HB3	3:B:667:GLN:NE2	1.73	0.91
3:F:803:PHE:CD2	3:F:810:VAL:HG22	2.05	0.91
3:B:744:LEU:HD21	3:B:765:HIS:CB	2.00	0.91
3:J:74:LYS:HD3	3:J:439:LYS:HZ1	1.13	0.91
3:J:803:PHE:CD2	3:J:810:VAL:HG22	2.05	0.91
3:N:744:LEU:HD21	3:N:765:HIS:CB	2.00	0.91
1:I:93:ILE:CG2	3:J:67:THR:CG2	2.45	0.91
3:B:223:ARG:CD	3:B:228:ASN:OD1	2.17	0.91
3:B:942:TYR:OH	3:B:984:GLU:OE2	1.88	0.91
3:F:75:THR:HG21	3:F:440:LEU:HB2	1.52	0.91
1:A:63:LYS:C	3:F:567:ARG:HH22	1.72	0.91
1:I:1211:VAL:HG23	4:I:1301:FAR:C10	1.92	0.91
3:F:361:ILE:CD1	3:F:421:LYS:CE	2.44	0.91
3:F:74:LYS:HD3	3:F:439:LYS:HZ1	1.29	0.91
3:N:361:ILE:CD1	3:N:421:LYS:CE	2.44	0.91
3:B:795:SER:OG	3:B:855:ILE:CD1	2.19	0.90
3:F:1004:MET:HG3	3:J:1092:ILE:CG2	2.02	0.90
3:N:942:TYR:OH	3:N:984:GLU:OE2	1.88	0.90
3:F:942:TYR:OH	3:F:984:GLU:OE2	1.88	0.90
3:J:75:THR:HG21	3:J:440:LEU:HB2	1.52	0.90
3:N:803:PHE:CD2	3:N:810:VAL:HG22	2.05	0.90
3:J:103:ARG:NH2	3:N:477:ARG:CZ	2.34	0.90
3:F:795:SER:OG	3:F:855:ILE:CD1	2.19	0.90
3:B:477:ARG:CZ	3:F:103:ARG:NH2	2.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:744:LEU:HD21	3:J:765:HIS:CB	2.00	0.90
3:J:942:TYR:OH	3:J:984:GLU:OE2	1.88	0.90
3:B:974:MET:HE2	3:B:975:TYR:CE1	2.05	0.90
1:A:445:LEU:HD12	1:A:563:THR:HG23	1.54	0.89
3:N:795:SER:OG	3:N:855:ILE:CD1	2.19	0.89
3:N:74:LYS:HD3	3:N:439:LYS:HZ3	1.30	0.89
1:A:28:PRO:HG3	3:B:547:LEU:CD2	1.98	0.89
1:I:68:ASP:OD1	3:J:259:GLY:O	1.90	0.89
3:F:1004:MET:HB2	3:J:1092:ILE:HG21	1.52	0.89
1:A:29:VAL:HG11	3:B:131:ARG:CG	2.02	0.89
3:B:361:ILE:CD1	3:B:421:LYS:CE	2.44	0.89
3:N:1090:CYS:HG	4:N:1101:FAR:C1	0.72	0.89
1:I:1137:LEU:CD1	4:I:1301:FAR:H61	2.03	0.89
3:N:822:ILE:HG23	3:N:826:LEU:HD12	1.55	0.89
1:I:445:LEU:HD12	1:I:563:THR:HG23	1.54	0.89
1:M:1137:LEU:CD1	4:M:1301:FAR:H61	2.02	0.89
3:B:75:THR:HG21	3:B:440:LEU:HB2	1.52	0.89
1:A:1137:LEU:CD1	4:A:1301:FAR:H61	2.03	0.89
1:I:28:PRO:HB2	3:J:130:MET:CE	2.04	0.88
3:J:795:SER:OG	3:J:855:ILE:CD1	2.19	0.88
3:B:1008:ILE:CG2	3:B:1012:ARG:NE	2.36	0.88
1:M:445:LEU:HD12	1:M:563:THR:HG23	1.54	0.88
1:I:79:GLN:NE2	3:J:194:TYR:CE1	2.41	0.88
3:N:75:THR:HG21	3:N:440:LEU:HB2	1.52	0.88
1:M:28:PRO:HG3	3:N:547:LEU:CD2	2.01	0.88
3:J:477:ARG:CZ	3:N:103:ARG:NH2	2.36	0.88
1:A:29:VAL:HG11	3:B:131:ARG:HG3	1.55	0.88
1:E:1137:LEU:CD1	4:E:1301:FAR:H61	2.03	0.88
3:B:74:LYS:HD3	3:B:439:LYS:HZ3	1.35	0.88
1:E:445:LEU:HD12	1:E:563:THR:HG23	1.54	0.88
3:B:105:ASP:OD1	3:F:485:ASN:ND2	2.07	0.88
3:B:1015:GLU:CD	3:N:1012:ARG:HH12	1.76	0.88
1:A:79:GLN:NE2	3:B:194:TYR:CE1	2.42	0.88
3:J:822:ILE:HG23	3:J:826:LEU:HD12	1.55	0.88
1:E:75:TYR:OH	3:F:191:GLN:OE1	1.90	0.88
3:B:822:ILE:HG23	3:B:826:LEU:HD12	1.55	0.88
1:E:83:LYS:CD	3:F:198:GLU:OE1	2.22	0.87
3:B:1012:ARG:HH12	4:N:1101:FAR:H7	1.35	0.87
3:F:974:MET:HE3	3:F:975:TYR:CE1	2.08	0.87
3:F:1009:VAL:HA	4:F:1103:FAR:H143	0.88	0.87
3:J:361:ILE:CD1	3:J:421:LYS:CE	2.44	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1004:MET:CB	3:J:1092:ILE:CG2	2.52	0.87
3:N:974:MET:CE	3:N:975:TYR:OH	2.00	0.87
1:A:68:ASP:CG	3:B:259:GLY:O	2.13	0.87
3:F:974:MET:CE	3:F:975:TYR:CE1	2.58	0.87
3:N:361:ILE:HD11	3:N:421:LYS:HE3	0.88	0.87
1:M:68:ASP:OD1	3:N:259:GLY:O	1.93	0.87
3:J:974:MET:HE3	3:J:975:TYR:CE1	2.10	0.87
2:K:332:ILE:CD1	2:K:340:LEU:HD12	1.99	0.87
3:B:361:ILE:HD11	3:B:421:LYS:HE3	0.88	0.87
3:B:656:LEU:HG	3:B:660:ILE:HD11	1.57	0.87
3:N:335:ARG:HB3	3:N:355:ILE:HG23	1.56	0.87
3:N:656:LEU:HG	3:N:660:ILE:HD11	1.57	0.87
3:B:1090:CYS:SG	4:B:1101:FAR:H11	1.16	0.86
3:F:853:LEU:HD11	3:F:880:ILE:HG13	1.57	0.86
3:J:974:MET:CE	3:J:975:TYR:CE1	2.58	0.86
3:F:361:ILE:HD11	3:F:421:LYS:HE3	0.88	0.86
1:A:1172:ASP:HB3	1:A:1175:MET:HB2	1.55	0.86
2:C:359:VAL:HG21	2:C:367:ARG:HG2	1.58	0.86
1:E:63:LYS:O	3:B:567:ARG:NH2	2.09	0.86
1:E:1120:GLN:HE21	1:E:1181:ALA:HB3	1.31	0.86
1:I:75:TYR:OH	3:J:191:GLN:HB3	1.76	0.86
3:J:361:ILE:HD11	3:J:421:LYS:HE3	0.88	0.86
3:J:656:LEU:HG	3:J:660:ILE:HD11	1.57	0.86
3:B:1012:ARG:HD2	4:N:1101:FAR:H142	1.58	0.86
3:F:335:ARG:HB3	3:F:355:ILE:HG23	1.56	0.86
3:B:798:PRO:HA	5:B:1102:ADP:O2B	1.75	0.85
2:O:359:VAL:HG21	2:O:367:ARG:HG2	1.58	0.85
3:F:822:ILE:HG23	3:F:826:LEU:HD12	1.55	0.85
1:A:557:THR:CG2	3:F:511:ASN:OD1	2.22	0.85
1:E:83:LYS:CE	3:F:198:GLU:OE1	2.24	0.85
1:M:441:GLN:HE22	1:M:607:PHE:HB3	1.41	0.85
3:F:656:LEU:HG	3:F:660:ILE:HD11	1.57	0.85
1:E:94:ARG:NH1	3:F:157:THR:HA	1.92	0.85
1:M:66:ASP:CB	3:J:667:GLN:NE2	2.40	0.85
3:B:335:ARG:HB3	3:B:355:ILE:HG23	1.56	0.85
3:J:335:ARG:HB3	3:J:355:ILE:HG23	1.56	0.85
1:I:771:LYS:HG3	1:I:802:ARG:HH12	1.41	0.85
2:K:359:VAL:HG21	2:K:367:ARG:HG2	1.58	0.85
3:J:853:LEU:HD11	3:J:880:ILE:HG13	1.57	0.85
1:I:771:LYS:CG	1:I:802:ARG:NH1	2.40	0.85
1:A:441:GLN:HE22	1:A:607:PHE:HB3	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1013:ASN:ND2	4:F:1103:FAR:C15	1.80	0.85
3:N:974:MET:CE	3:N:975:TYR:CE1	2.58	0.85
1:A:771:LYS:CG	1:A:802:ARG:NH1	2.40	0.84
1:M:771:LYS:CG	1:M:802:ARG:NH1	2.40	0.84
1:E:29:VAL:HG11	3:F:131:ARG:HG3	1.58	0.84
1:M:771:LYS:HD2	1:M:802:ARG:NH1	1.93	0.84
3:B:574:VAL:HG21	3:B:656:LEU:HD21	1.60	0.84
1:A:771:LYS:HG3	1:A:802:ARG:HH12	1.41	0.84
1:M:29:VAL:HG11	3:N:131:ARG:HG3	1.59	0.84
1:M:63:LYS:C	3:J:567:ARG:HH22	1.80	0.84
3:F:1001:GLU:CG	3:J:1092:ILE:CD1	1.74	0.84
4:F:1103:FAR:H11	3:J:1090:CYS:SG	1.15	0.84
1:E:441:GLN:HE22	1:E:607:PHE:HB3	1.41	0.84
1:E:1172:ASP:HB3	1:E:1175:MET:HB2	1.57	0.84
2:O:332:ILE:CD1	2:O:340:LEU:HD12	1.99	0.84
1:I:771:LYS:HD2	1:I:802:ARG:NH1	1.93	0.84
3:N:853:LEU:HD11	3:N:880:ILE:HG13	1.57	0.84
1:M:771:LYS:HG3	1:M:802:ARG:HH12	1.41	0.84
1:A:771:LYS:HD2	1:A:802:ARG:NH1	1.93	0.84
1:I:441:GLN:HE22	1:I:607:PHE:HB3	1.41	0.84
3:F:1013:ASN:HD21	4:F:1101:FAR:C15	1.90	0.84
4:F:1103:FAR:H12A	3:J:1090:CYS:SG	1.46	0.84
3:J:526:ILE:CD1	3:J:660:ILE:HD12	2.06	0.84
3:N:1090:CYS:SG	4:N:1101:FAR:H11	1.14	0.84
1:M:29:VAL:HG11	3:N:131:ARG:CG	2.08	0.84
3:F:283:LEU:CD2	3:F:307:LEU:HG	2.07	0.84
3:F:1070:THR:HG21	4:F:1103:FAR:H91	1.60	0.84
1:M:93:ILE:CG2	3:N:67:THR:CG2	2.53	0.83
1:E:771:LYS:CG	1:E:802:ARG:NH1	2.40	0.83
3:B:853:LEU:HD11	3:B:880:ILE:HG13	1.57	0.83
3:F:526:ILE:CD1	3:F:660:ILE:HD12	2.06	0.83
1:E:771:LYS:HD2	1:E:802:ARG:NH1	1.93	0.83
2:G:332:ILE:CD1	2:G:340:LEU:HD12	1.99	0.83
3:N:172:ILE:HG21	3:N:212:VAL:CG2	2.08	0.83
3:N:574:VAL:HG21	3:N:656:LEU:HD21	1.60	0.83
1:E:75:TYR:OH	3:F:191:GLN:CD	2.16	0.83
3:J:172:ILE:HG21	3:J:212:VAL:CG2	2.08	0.83
1:I:1120:GLN:HE21	1:I:1181:ALA:HB3	1.30	0.83
3:B:172:ILE:HG21	3:B:212:VAL:CG2	2.08	0.83
4:F:1101:FAR:C14	3:J:1009:VAL:CA	2.37	0.83
3:J:413:PRO:HG2	3:J:416:PHE:CD2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:75:TYR:OH	3:N:191:GLN:HB3	1.79	0.83
3:F:172:ILE:HG21	3:F:212:VAL:CG2	2.08	0.83
3:J:965:GLN:HG2	3:J:969:LEU:HD12	0.83	0.83
3:B:965:GLN:HG2	3:B:969:LEU:HD12	0.83	0.83
3:B:974:MET:CE	3:B:975:TYR:CE1	2.58	0.83
3:N:413:PRO:HG2	3:N:416:PHE:CD2	2.13	0.83
3:N:526:ILE:CD1	3:N:660:ILE:HD12	2.06	0.83
1:I:29:VAL:HG11	3:J:131:ARG:HG3	1.61	0.82
1:I:79:GLN:NE2	3:J:194:TYR:CD1	2.46	0.82
1:A:79:GLN:HB3	3:B:194:TYR:HB3	1.61	0.82
1:A:419:ALA:HB1	3:F:524:GLU:OE1	1.79	0.82
1:I:83:LYS:HD2	3:J:198:GLU:OE1	1.77	0.82
3:F:574:VAL:HG21	3:F:656:LEU:HD21	1.59	0.82
1:M:1120:GLN:HE21	1:M:1181:ALA:HB1	1.44	0.82
3:F:1004:MET:CG	3:J:1092:ILE:HG21	2.09	0.82
3:F:1059:PRO:HG3	3:J:1093:SER:O	1.80	0.82
3:B:143:PRO:CB	3:B:215:VAL:HG21	2.10	0.82
3:N:965:GLN:HG2	3:N:969:LEU:HD12	0.83	0.82
3:B:413:PRO:HG2	3:B:416:PHE:CD2	2.13	0.82
3:J:656:LEU:HG	3:J:660:ILE:CD1	2.10	0.82
2:G:359:VAL:HG21	2:G:367:ARG:HG2	1.58	0.82
1:I:120:THR:CG2	3:J:131:ARG:NH2	2.43	0.82
3:F:413:PRO:HG2	3:F:416:PHE:CD2	2.13	0.82
3:J:574:VAL:HG21	3:J:656:LEU:HD21	1.60	0.82
1:A:1120:GLN:HE21	1:A:1181:ALA:HB1	1.43	0.82
3:F:965:GLN:HG2	3:F:969:LEU:HD12	0.83	0.82
1:A:66:ASP:CB	3:F:667:GLN:NE2	2.41	0.81
3:F:744:LEU:HD21	3:F:765:HIS:CG	2.14	0.81
1:A:29:VAL:CG1	3:B:131:ARG:HG3	2.10	0.81
2:C:332:ILE:CD1	2:C:340:LEU:HD12	1.99	0.81
3:B:656:LEU:HG	3:B:660:ILE:CD1	2.10	0.81
1:E:28:PRO:HG3	3:F:547:LEU:CG	2.11	0.81
1:E:75:TYR:OH	3:F:191:GLN:HB3	1.81	0.81
1:E:1120:GLN:HE21	1:E:1181:ALA:HB1	1.43	0.81
1:M:771:LYS:CD	1:M:802:ARG:NH1	2.44	0.81
1:M:1211:VAL:CB	4:M:1301:FAR:H101	2.10	0.81
1:I:1211:VAL:CB	4:I:1301:FAR:H101	2.10	0.81
3:N:143:PRO:CB	3:N:215:VAL:HG21	2.10	0.81
3:N:579:ILE:HD11	3:N:601:ALA:CB	2.09	0.81
1:E:804:ALA:HB1	1:E:809:LEU:HD11	1.62	0.81
1:M:804:ALA:HB1	1:M:809:LEU:HD11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:712:PRO:HD3	3:B:780:LEU:HD23	1.62	0.81
3:B:744:LEU:HD21	3:B:765:HIS:CG	2.14	0.81
3:F:974:MET:CE	3:F:975:TYR:OH	2.00	0.81
1:I:804:ALA:HB1	1:I:809:LEU:HD11	1.62	0.81
3:N:656:LEU:HG	3:N:660:ILE:CD1	2.10	0.81
1:A:290:ARG:O	1:A:352:LYS:NZ	2.14	0.81
3:B:1008:ILE:HG21	3:B:1012:ARG:CZ	2.10	0.81
1:E:771:LYS:CD	1:E:802:ARG:NH1	2.44	0.81
1:I:771:LYS:CD	1:I:802:ARG:NH1	2.44	0.81
1:A:804:ALA:HB1	1:A:809:LEU:HD11	1.62	0.81
1:E:290:ARG:O	1:E:352:LYS:NZ	2.14	0.81
1:I:290:ARG:O	1:I:352:LYS:NZ	2.14	0.81
1:I:1120:GLN:HE21	1:I:1181:ALA:HB1	1.44	0.81
3:F:1001:GLU:CA	3:J:1092:ILE:CD1	2.56	0.81
4:F:1103:FAR:H12A	3:J:1090:CYS:HG	0.83	0.81
3:N:712:PRO:HD3	3:N:780:LEU:HD23	1.62	0.81
1:A:771:LYS:CD	1:A:802:ARG:NH1	2.44	0.81
1:A:1211:VAL:CB	4:A:1301:FAR:H101	2.10	0.81
3:J:803:PHE:CD2	3:J:810:VAL:CG2	2.64	0.81
1:E:79:GLN:NE2	3:F:194:TYR:CD1	2.46	0.80
3:F:656:LEU:HG	3:F:660:ILE:CD1	2.10	0.80
3:F:803:PHE:CD2	3:F:810:VAL:CG2	2.64	0.80
3:J:712:PRO:HD3	3:J:780:LEU:HD23	1.62	0.80
1:A:79:GLN:NE2	3:B:194:TYR:CD1	2.49	0.80
1:E:64:ASN:N	3:B:567:ARG:NH2	2.29	0.80
1:M:290:ARG:O	1:M:352:LYS:NZ	2.14	0.80
3:B:1090:CYS:HG	4:B:1101:FAR:C1	1.01	0.80
1:M:435:LYS:HD3	1:M:555:ARG:CD	2.12	0.80
3:N:803:PHE:CD2	3:N:810:VAL:CG2	2.64	0.80
4:F:1101:FAR:H141	3:J:1009:VAL:HA	1.62	0.80
3:J:143:PRO:CB	3:J:215:VAL:HG21	2.10	0.80
1:E:771:LYS:HG3	1:E:802:ARG:HH12	1.41	0.80
3:J:744:LEU:HD21	3:J:765:HIS:CG	2.14	0.80
1:M:557:THR:CG2	3:J:511:ASN:OD1	2.28	0.80
3:F:1004:MET:HG3	3:J:1092:ILE:HG21	1.62	0.80
1:A:1120:GLN:HE21	1:A:1181:ALA:HB3	1.30	0.80
1:E:1211:VAL:CB	4:E:1301:FAR:H101	2.11	0.80
1:I:435:LYS:HD3	1:I:555:ARG:CD	2.12	0.80
3:B:803:PHE:CD2	3:B:810:VAL:CG2	2.64	0.80
3:F:143:PRO:CB	3:F:215:VAL:HG21	2.10	0.79
1:A:435:LYS:HD3	1:A:555:ARG:CD	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ASN:CA	3:B:567:ARG:NH2	2.46	0.79
1:I:29:VAL:HG11	3:J:131:ARG:CG	2.12	0.79
1:A:1209:THR:HG23	2:C:334:ILE:HD13	1.65	0.79
1:E:788:THR:C	1:E:792:PRO:HD2	2.03	0.79
1:M:79:GLN:NE2	3:N:194:TYR:CE1	2.50	0.79
3:B:714:VAL:HG11	3:B:743:LEU:HG	1.64	0.79
3:F:712:PRO:HD3	3:F:780:LEU:HD23	1.62	0.79
3:N:1090:CYS:HG	4:N:1101:FAR:C2	1.89	0.79
1:A:771:LYS:CG	1:A:802:ARG:HH12	1.96	0.79
1:I:788:THR:C	1:I:792:PRO:HD2	2.03	0.79
3:F:579:ILE:HD11	3:F:601:ALA:CB	2.10	0.79
3:N:714:VAL:HG11	3:N:743:LEU:HG	1.64	0.79
3:F:826:LEU:HD22	3:F:830:VAL:HG11	1.65	0.79
3:N:826:LEU:HD22	3:N:830:VAL:HG11	1.65	0.79
1:E:75:TYR:OH	3:F:191:GLN:CB	2.31	0.79
3:B:826:LEU:HD22	3:B:830:VAL:HG11	1.65	0.79
3:J:74:LYS:HD3	3:J:439:LYS:HZ3	1.45	0.79
1:I:28:PRO:HB2	3:J:130:MET:HE1	1.64	0.78
3:J:826:LEU:HD22	3:J:830:VAL:HG11	1.65	0.78
1:A:788:THR:C	1:A:792:PRO:HD2	2.03	0.78
1:M:788:THR:C	1:M:792:PRO:HD2	2.03	0.78
1:M:79:GLN:HB3	3:N:194:TYR:HB3	1.66	0.78
1:E:435:LYS:HD3	1:E:555:ARG:CD	2.12	0.78
1:M:771:LYS:CG	1:M:802:ARG:HH12	1.96	0.78
1:I:66:ASP:HB2	3:N:667:GLN:NE2	1.99	0.78
3:N:974:MET:HE2	3:N:975:TYR:CE1	2.15	0.78
1:I:557:THR:CG2	3:N:511:ASN:OD1	2.28	0.78
3:J:974:MET:CE	3:J:975:TYR:OH	1.99	0.78
1:A:28:PRO:HB2	3:B:130:MET:CE	2.14	0.78
3:F:714:VAL:HG11	3:F:743:LEU:HG	1.64	0.78
1:E:28:PRO:HB2	3:F:130:MET:HE2	1.63	0.78
1:E:771:LYS:CG	1:E:802:ARG:HH12	1.96	0.78
1:E:1209:THR:HG23	2:G:334:ILE:HD13	1.65	0.78
1:M:1209:THR:HG23	2:O:334:ILE:HD13	1.65	0.78
1:I:419:ALA:HB1	3:N:524:GLU:OE1	1.83	0.78
3:B:1092:ILE:CD1	3:N:1001:GLU:CB	2.62	0.78
1:E:64:ASN:N	3:B:567:ARG:HH22	1.80	0.77
3:J:714:VAL:HG11	3:J:743:LEU:HG	1.64	0.77
3:B:486:GLN:NE2	3:B:492:ASP:OD1	2.18	0.77
3:B:1013:ASN:CG	4:N:1101:FAR:H151	2.05	0.77
3:N:486:GLN:NE2	3:N:492:ASP:OD1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:PRO:HB2	3:N:130:MET:CE	2.15	0.77
1:I:79:GLN:HB3	3:J:194:TYR:HB3	1.67	0.77
1:I:771:LYS:CG	1:I:802:ARG:HH12	1.96	0.77
3:F:283:LEU:CD2	3:F:307:LEU:CG	2.63	0.77
3:J:523:VAL:HG23	3:J:523:VAL:O	1.85	0.77
3:N:744:LEU:HD21	3:N:765:HIS:CG	2.14	0.77
1:M:441:GLN:NE2	1:M:561:THR:OG1	2.17	0.77
1:A:28:PRO:CG	3:B:547:LEU:HD23	1.96	0.77
3:F:223:ARG:HH22	3:F:338:TYR:HA	1.50	0.77
1:M:66:ASP:HB2	3:J:667:GLN:HE22	1.48	0.77
2:O:332:ILE:CB	2:O:340:LEU:CD1	2.61	0.77
3:F:486:GLN:NE2	3:F:492:ASP:OD1	2.18	0.77
3:F:1082:VAL:HG21	3:J:1060:LEU:CD2	2.15	0.77
1:M:419:ALA:HB1	3:J:524:GLU:OE1	1.84	0.76
1:I:163:ASN:HB2	1:I:489:ASN:ND2	2.00	0.76
3:J:579:ILE:HD11	3:J:601:ALA:CB	2.10	0.76
3:F:1004:MET:CG	3:J:1092:ILE:CG2	2.64	0.76
1:I:120:THR:CG2	3:J:131:ARG:CZ	2.61	0.76
3:B:1092:ILE:HD12	3:N:1001:GLU:HA	1.67	0.76
3:J:486:GLN:NE2	3:J:492:ASP:OD1	2.18	0.76
3:J:486:GLN:HE22	3:J:492:ASP:C	1.89	0.76
3:N:587:MET:HE1	3:N:855:ILE:CG1	2.15	0.76
3:B:1008:ILE:CG2	3:B:1012:ARG:CZ	2.62	0.76
3:F:486:GLN:HE22	3:F:492:ASP:C	1.89	0.76
3:J:223:ARG:HH22	3:J:338:TYR:HA	1.50	0.76
3:N:223:ARG:HH22	3:N:338:TYR:HA	1.50	0.76
1:M:66:ASP:HB2	3:J:667:GLN:NE2	2.00	0.76
3:B:579:ILE:HD11	3:B:601:ALA:CB	2.10	0.76
3:F:924:TRP:HH2	3:J:1093:SER:O	1.67	0.76
1:E:163:ASN:HB2	1:E:489:ASN:ND2	2.00	0.76
1:M:794:TRP:O	1:M:798:LEU:HD12	1.86	0.76
1:I:794:TRP:O	1:I:798:LEU:HD12	1.86	0.76
3:N:486:GLN:HE22	3:N:492:ASP:C	1.89	0.76
1:E:794:TRP:O	1:E:798:LEU:HD12	1.86	0.76
3:B:1012:ARG:HH22	4:N:1101:FAR:H41	1.48	0.76
3:B:1013:ASN:HD21	4:B:1101:FAR:C15	1.98	0.76
3:B:1013:ASN:ND2	4:N:1101:FAR:C15	2.23	0.76
3:B:1090:CYS:HG	4:B:1101:FAR:H12A	0.62	0.76
1:A:68:ASP:OD2	3:B:259:GLY:O	2.04	0.76
1:E:66:ASP:CA	3:B:667:GLN:NE2	2.48	0.76
3:B:1008:ILE:HG22	3:B:1012:ARG:NE	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1103:FAR:H13	3:J:1090:CYS:CB	2.14	0.76
1:I:1209:THR:HG23	2:K:334:ILE:HD13	1.65	0.76
3:B:486:GLN:HE22	3:B:492:ASP:C	1.89	0.76
1:I:75:TYR:OH	3:J:191:GLN:CG	2.33	0.76
3:B:223:ARG:HH22	3:B:338:TYR:HA	1.50	0.75
1:A:163:ASN:HB2	1:A:489:ASN:ND2	2.00	0.75
2:O:332:ILE:CG1	2:O:340:LEU:CD1	2.64	0.75
3:F:184:GLU:HG2	3:F:466:PRO:HD2	1.68	0.75
1:I:120:THR:HG22	3:J:131:ARG:NE	2.00	0.75
3:J:853:LEU:HD12	3:J:880:ILE:HG13	1.69	0.75
1:M:163:ASN:HB2	1:M:489:ASN:ND2	2.00	0.75
3:F:1015:GLU:CD	4:F:1101:FAR:H41	2.05	0.75
1:A:93:ILE:CG2	3:B:67:THR:CG2	2.60	0.75
2:C:332:ILE:CG1	2:C:340:LEU:CD1	2.64	0.75
2:K:332:ILE:CG1	2:K:340:LEU:CD1	2.64	0.75
3:B:853:LEU:CD1	3:B:880:ILE:CG1	2.64	0.75
1:E:382:GLU:OE1	1:E:382:GLU:N	2.20	0.75
2:G:332:ILE:CG1	2:G:340:LEU:CD1	2.64	0.75
1:M:29:VAL:CG1	3:N:131:ARG:HG3	2.15	0.75
3:B:526:ILE:CD1	3:B:660:ILE:HD12	2.06	0.75
1:E:28:PRO:HG3	3:F:547:LEU:HG	1.69	0.74
1:E:441:GLN:NE2	1:E:561:THR:OG1	2.17	0.74
1:M:1120:GLN:HE21	1:M:1181:ALA:HB3	1.31	0.74
1:I:120:THR:HG22	3:J:131:ARG:NH2	2.01	0.74
3:B:566:TYR:HE1	3:B:666:GLU:OE1	1.70	0.74
3:F:523:VAL:HG23	3:F:523:VAL:O	1.85	0.74
3:F:523:VAL:HG21	3:F:528:ILE:HD11	1.69	0.74
1:E:422:GLU:OE2	3:B:525:PRO:HG3	1.86	0.74
1:A:794:TRP:O	1:A:798:LEU:HD12	1.86	0.74
1:M:120:THR:CG2	3:N:131:ARG:NH2	2.51	0.74
3:J:853:LEU:CD1	3:J:880:ILE:CG1	2.64	0.74
3:N:184:GLU:HG2	3:N:466:PRO:HD2	1.68	0.74
1:M:382:GLU:OE1	1:M:382:GLU:N	2.20	0.74
2:O:375:PRO:HD2	2:O:378:VAL:HG13	1.70	0.74
3:B:523:VAL:HG21	3:B:528:ILE:HD11	1.69	0.74
3:B:523:VAL:HG23	3:B:523:VAL:O	1.85	0.74
4:F:1103:FAR:C15	3:J:1013:ASN:HD21	2.00	0.74
3:N:172:ILE:HG21	3:N:212:VAL:HG22	1.69	0.74
3:J:184:GLU:HG2	3:J:466:PRO:HD2	1.68	0.74
3:N:853:LEU:CD1	3:N:880:ILE:CG1	2.64	0.74
1:A:441:GLN:NE2	1:A:561:THR:OG1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:375:PRO:HD2	2:C:378:VAL:HG13	1.70	0.74
3:B:948:ILE:HD11	3:B:1007:SER:HA	1.70	0.74
3:F:283:LEU:HD21	3:F:307:LEU:CG	2.17	0.74
3:F:1018:PHE:CD2	3:F:1022:VAL:HG22	2.23	0.74
3:J:1018:PHE:CD2	3:J:1022:VAL:HG22	2.23	0.74
3:N:948:ILE:HD11	3:N:1007:SER:HA	1.70	0.74
3:N:1013:ASN:HD21	4:N:1101:FAR:C15	2.00	0.74
3:B:853:LEU:HD12	3:B:880:ILE:HG13	1.69	0.74
3:J:74:LYS:CD	3:J:439:LYS:HZ1	1.98	0.74
3:B:184:GLU:HG2	3:B:466:PRO:HD2	1.68	0.74
3:F:1002:LEU:HD23	3:F:1024:LEU:HD22	1.70	0.74
3:J:566:TYR:HE1	3:J:666:GLU:OE1	1.70	0.74
3:B:974:MET:HE1	3:B:975:TYR:CE2	2.23	0.74
3:N:1018:PHE:CD2	3:N:1022:VAL:HG22	2.23	0.74
2:K:375:PRO:HD2	2:K:378:VAL:HG13	1.70	0.73
3:F:498:ALA:HB3	3:F:618:LEU:HD23	1.70	0.73
3:F:853:LEU:CD1	3:F:880:ILE:CG1	2.64	0.73
3:J:523:VAL:HG21	3:J:528:ILE:HD11	1.69	0.73
3:N:523:VAL:HG23	3:N:523:VAL:O	1.85	0.73
3:F:566:TYR:HE1	3:F:666:GLU:OE1	1.69	0.73
1:A:75:TYR:OH	3:B:191:GLN:CB	2.34	0.73
3:N:523:VAL:HG21	3:N:528:ILE:HD11	1.69	0.73
1:E:68:ASP:OD1	3:F:259:GLY:O	2.07	0.73
1:I:382:GLU:N	1:I:382:GLU:OE1	2.20	0.73
3:J:1002:LEU:HD23	3:J:1024:LEU:HD22	1.70	0.73
1:M:79:GLN:NE2	3:N:194:TYR:CD1	2.55	0.73
3:F:579:ILE:HD13	3:F:601:ALA:HB2	1.69	0.73
3:J:795:SER:OG	3:J:855:ILE:HD13	1.87	0.73
3:B:172:ILE:HG21	3:B:212:VAL:HG22	1.69	0.73
3:B:1018:PHE:CD2	3:B:1022:VAL:HG22	2.23	0.73
1:A:75:TYR:OH	3:B:191:GLN:CG	2.37	0.73
1:A:901:LEU:HD22	1:A:912:PHE:HZ	1.53	0.73
3:B:795:SER:OG	3:B:855:ILE:HD13	1.87	0.73
3:J:498:ALA:HB3	3:J:618:LEU:HD23	1.70	0.73
3:N:566:TYR:HE1	3:N:666:GLU:OE1	1.70	0.73
1:A:382:GLU:N	1:A:382:GLU:OE1	2.20	0.73
1:A:1208:ALA:HB3	2:C:334:ILE:HG12	1.71	0.73
3:B:587:MET:HE1	3:B:855:ILE:CG1	2.18	0.73
3:B:965:GLN:CD	3:B:969:LEU:CD1	2.56	0.73
4:B:1101:FAR:H141	3:N:1009:VAL:HA	1.66	0.73
3:F:172:ILE:HG21	3:F:212:VAL:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1208:ALA:HB3	2:G:334:ILE:HG12	1.71	0.73
3:J:948:ILE:HD11	3:J:1007:SER:HA	1.70	0.73
3:F:965:GLN:CD	3:F:969:LEU:CD1	2.56	0.73
3:F:795:SER:OG	3:F:855:ILE:HD13	1.87	0.72
2:G:375:PRO:HD2	2:G:378:VAL:HG13	1.70	0.72
3:B:1002:LEU:HD23	3:B:1024:LEU:HD22	1.70	0.72
3:F:853:LEU:HD12	3:F:880:ILE:HG13	1.69	0.72
3:J:508:VAL:O	3:J:512:THR:HG23	1.89	0.72
3:N:965:GLN:CD	3:N:969:LEU:CD1	2.56	0.72
1:A:79:GLN:HB3	3:B:194:TYR:CB	2.18	0.72
3:F:173:ASN:ND2	3:F:220:VAL:HA	2.04	0.72
3:J:965:GLN:CD	3:J:969:LEU:CD1	2.56	0.72
3:N:173:ASN:ND2	3:N:220:VAL:HA	2.04	0.72
2:C:332:ILE:CB	2:C:340:LEU:CD1	2.61	0.72
1:M:901:LEU:HD22	1:M:912:PHE:HZ	1.53	0.72
3:F:283:LEU:HD23	3:F:307:LEU:CD2	2.18	0.72
3:N:795:SER:OG	3:N:855:ILE:HD13	1.87	0.72
3:N:1002:LEU:HD23	3:N:1024:LEU:HD22	1.70	0.72
2:G:332:ILE:CB	2:G:340:LEU:CD1	2.61	0.72
2:K:332:ILE:CB	2:K:340:LEU:CD1	2.61	0.72
3:F:508:VAL:O	3:F:512:THR:HG23	1.89	0.72
3:F:1090:CYS:SG	4:F:1101:FAR:H11	1.17	0.72
3:N:853:LEU:HD12	3:N:880:ILE:HG13	1.69	0.72
1:E:901:LEU:HD22	1:E:912:PHE:HZ	1.53	0.72
1:I:29:VAL:CG1	3:J:131:ARG:HG3	2.18	0.72
1:I:901:LEU:HD22	1:I:912:PHE:HZ	1.53	0.72
3:F:948:ILE:HD11	3:F:1007:SER:HA	1.70	0.72
3:N:1090:CYS:CB	4:N:1101:FAR:H13	2.14	0.72
1:A:1209:THR:CG2	2:C:334:ILE:HD13	2.20	0.72
1:M:1081:LYS:HB3	4:M:1301:FAR:H143	1.72	0.72
3:B:498:ALA:HB3	3:B:618:LEU:HD23	1.70	0.72
3:J:173:ASN:ND2	3:J:220:VAL:HA	2.04	0.72
1:A:1081:LYS:HB3	4:A:1301:FAR:H143	1.72	0.72
1:M:120:THR:HG22	3:N:131:ARG:NH2	2.05	0.72
3:B:223:ARG:HD3	3:B:228:ASN:ND2	2.05	0.72
3:B:508:VAL:O	3:B:512:THR:HG23	1.89	0.72
1:E:94:ARG:HH12	3:F:157:THR:CA	2.03	0.72
1:I:1081:LYS:HB3	4:I:1301:FAR:H143	1.72	0.72
3:B:173:ASN:ND2	3:B:220:VAL:HA	2.04	0.72
1:M:1209:THR:CG2	2:O:334:ILE:HD13	2.20	0.72
3:J:172:ILE:HG21	3:J:212:VAL:HG22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:579:ILE:HD13	3:J:601:ALA:HB2	1.69	0.72
1:E:1209:THR:CG2	2:G:334:ILE:HD13	2.20	0.71
1:M:83:LYS:HD2	3:N:198:GLU:OE1	1.90	0.71
1:M:872:PRO:CD	1:M:875:ALA:HB3	2.20	0.71
1:I:441:GLN:NE2	1:I:561:THR:OG1	2.17	0.71
3:N:508:VAL:O	3:N:512:THR:HG23	1.89	0.71
1:A:779:GLN:HB3	1:A:782:ILE:HG12	1.73	0.71
3:N:974:MET:HE3	3:N:975:TYR:CE1	2.20	0.71
1:E:64:ASN:HA	3:B:567:ARG:NH2	2.05	0.71
1:E:75:TYR:OH	3:F:191:GLN:HG3	1.88	0.71
1:I:1209:THR:CG2	2:K:334:ILE:HD13	2.20	0.71
3:F:495:VAL:HG13	3:F:615:PRO:HB2	1.72	0.71
3:J:322:ARG:HH11	3:J:323:LYS:HE2	1.56	0.71
1:A:28:PRO:HB2	3:B:130:MET:HE1	1.71	0.71
1:A:66:ASP:HB2	3:F:667:GLN:NE2	2.05	0.71
3:B:495:VAL:HG13	3:B:615:PRO:HB2	1.72	0.71
3:J:587:MET:HE1	3:J:855:ILE:HD12	1.72	0.71
1:M:779:GLN:HB3	1:M:782:ILE:HG12	1.73	0.71
1:I:28:PRO:HG2	3:J:547:LEU:HD21	1.12	0.71
3:J:223:ARG:HD3	3:J:228:ASN:ND2	2.05	0.71
1:M:290:ARG:NH2	1:M:391:ASP:OD1	2.23	0.71
1:I:1208:ALA:HB3	2:K:334:ILE:HG12	1.71	0.71
3:N:498:ALA:HB3	3:N:618:LEU:HD23	1.70	0.71
3:F:172:ILE:HD13	3:F:212:VAL:HG22	1.73	0.71
4:F:1101:FAR:C10	3:J:1070:THR:OG1	2.38	0.71
1:E:779:GLN:HB3	1:E:782:ILE:HG12	1.73	0.71
3:B:172:ILE:HD13	3:B:212:VAL:HG22	1.73	0.71
3:F:965:GLN:HG2	3:F:969:LEU:CG	2.18	0.71
1:A:83:LYS:HD2	3:B:198:GLU:OE1	1.91	0.70
1:E:66:ASP:HB2	3:B:667:GLN:CD	2.10	0.70
1:E:422:GLU:OE2	3:B:525:PRO:CG	2.38	0.70
3:J:495:VAL:HG13	3:J:615:PRO:HB2	1.72	0.70
1:A:524:PHE:HE1	1:A:539:ILE:HG23	1.56	0.70
1:E:66:ASP:HA	3:B:667:GLN:NE2	2.06	0.70
1:E:491:ARG:HD3	3:F:62:LEU:HG	1.73	0.70
1:M:1172:ASP:HB3	1:M:1175:MET:HB2	1.73	0.70
1:I:75:TYR:OH	3:J:191:GLN:CB	2.39	0.70
1:I:120:THR:HG21	3:J:131:ARG:NH2	2.06	0.70
3:B:566:TYR:CE1	3:B:666:GLU:OE1	2.45	0.70
3:F:223:ARG:HD3	3:F:228:ASN:ND2	2.05	0.70
3:F:1013:ASN:HA	3:J:1012:ARG:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1208:ALA:HB3	2:O:334:ILE:HG12	1.71	0.70
1:I:779:GLN:HB3	1:I:782:ILE:HG12	1.73	0.70
3:J:566:TYR:CE1	3:J:666:GLU:OE1	2.44	0.70
3:N:495:VAL:HG13	3:N:615:PRO:HB2	1.72	0.70
3:N:566:TYR:CE1	3:N:666:GLU:OE1	2.45	0.70
1:A:1136:MET:HE1	2:C:347:ILE:HA	1.74	0.70
1:E:1081:LYS:HB3	4:E:1301:FAR:H143	1.72	0.70
1:I:68:ASP:CG	3:J:259:GLY:O	2.28	0.70
3:F:322:ARG:HH11	3:F:323:LYS:HE2	1.56	0.70
3:F:1090:CYS:SG	4:F:1101:FAR:H12A	1.29	0.70
3:N:223:ARG:HD3	3:N:228:ASN:ND2	2.05	0.70
1:E:872:PRO:CD	1:E:875:ALA:HB3	2.20	0.70
1:M:68:ASP:CG	3:N:259:GLY:O	2.28	0.70
3:J:172:ILE:HD13	3:J:212:VAL:HG22	1.73	0.70
3:J:274:ARG:HH22	3:J:802:THR:HA	1.57	0.70
3:J:491:ASN:HD21	3:J:607:GLN:HA	1.57	0.70
3:N:322:ARG:HH11	3:N:323:LYS:HE2	1.56	0.70
3:N:593:LEU:HD21	3:N:856:HIS:HE1	1.57	0.70
1:A:78:GLU:HB3	1:A:153:LEU:HD21	1.74	0.70
1:A:1120:GLN:NE2	1:A:1181:ALA:HB1	2.03	0.70
1:I:79:GLN:HB3	3:J:194:TYR:CB	2.21	0.70
3:B:593:LEU:HD21	3:B:856:HIS:HE1	1.57	0.70
3:B:1012:ARG:HB2	4:N:1101:FAR:C14	2.21	0.70
3:J:593:LEU:HD21	3:J:856:HIS:HE1	1.57	0.70
1:E:768:LEU:HD22	1:E:802:ARG:NH2	2.07	0.70
3:B:491:ASN:HD21	3:B:607:GLN:HA	1.57	0.70
3:F:491:ASN:HD21	3:F:607:GLN:HA	1.57	0.70
1:A:69:GLU:HG3	3:B:262:TRP:CZ3	2.26	0.70
1:M:1200:MET:HA	1:M:1203:LEU:HD12	1.74	0.70
3:B:322:ARG:HH11	3:B:323:LYS:HE2	1.56	0.70
3:N:172:ILE:HD13	3:N:212:VAL:HG22	1.73	0.70
1:E:94:ARG:NH2	3:F:157:THR:O	2.23	0.70
1:E:557:THR:HG23	3:B:511:ASN:OD1	1.92	0.70
1:E:1200:MET:HA	1:E:1203:LEU:HD12	1.74	0.70
1:M:524:PHE:HE1	1:M:539:ILE:HG23	1.57	0.70
1:M:768:LEU:HD22	1:M:802:ARG:NH2	2.07	0.70
1:E:28:PRO:HG2	3:F:547:LEU:HD21	0.79	0.69
3:B:1092:ILE:HD11	3:N:1001:GLU:CB	2.13	0.69
3:F:1015:GLU:HG3	3:J:1012:ARG:HH22	1.56	0.69
1:A:872:PRO:CD	1:A:875:ALA:HB3	2.20	0.69
1:I:1200:MET:HA	1:I:1203:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1101:FAR:H91	3:J:1070:THR:HG21	1.74	0.69
1:A:1200:MET:HA	1:A:1203:LEU:HD12	1.74	0.69
3:B:274:ARG:HH22	3:B:802:THR:HA	1.57	0.69
1:E:524:PHE:HE1	1:E:539:ILE:HG23	1.57	0.69
3:F:274:ARG:HH22	3:F:802:THR:HA	1.57	0.69
1:A:68:ASP:OD2	3:B:260:CYS:HA	1.92	0.69
1:I:163:ASN:CB	1:I:489:ASN:ND2	2.56	0.69
3:F:566:TYR:CE1	3:F:666:GLU:OE1	2.44	0.69
3:N:274:ARG:HH22	3:N:802:THR:HA	1.57	0.69
1:A:163:ASN:CB	1:A:489:ASN:ND2	2.56	0.69
3:B:1093:SER:O	3:N:924:TRP:HH2	1.67	0.69
3:F:1004:MET:CE	3:J:1091:LEU:HB2	2.23	0.69
3:J:214:ARG:HA	3:J:825:PRO:HG2	1.75	0.69
1:E:290:ARG:NH2	1:E:391:ASP:OD1	2.23	0.69
1:M:78:GLU:HB3	1:M:153:LEU:HD21	1.74	0.69
1:M:254:GLU:OE1	1:M:1101:THR:OG1	2.11	0.69
1:I:524:PHE:HE1	1:I:539:ILE:HG23	1.56	0.69
3:B:88:LEU:HD21	3:B:178:TYR:HA	1.75	0.69
3:B:214:ARG:NH2	5:B:1102:ADP:O3B	2.25	0.69
3:F:214:ARG:HA	3:F:825:PRO:HG2	1.75	0.69
3:F:1082:VAL:CG2	3:J:1060:LEU:CD2	2.71	0.69
3:N:214:ARG:HA	3:N:825:PRO:HG2	1.75	0.69
1:M:163:ASN:CB	1:M:489:ASN:ND2	2.56	0.69
3:B:579:ILE:HD13	3:B:601:ALA:HB2	1.69	0.69
1:E:1136:MET:HE1	2:G:347:ILE:HA	1.76	0.69
1:M:1136:MET:HE1	2:O:347:ILE:HA	1.75	0.69
1:I:872:PRO:CD	1:I:875:ALA:HB3	2.20	0.69
3:J:591:VAL:HG21	3:J:634:ILE:HG13	1.75	0.69
3:N:88:LEU:HD21	3:N:178:TYR:HA	1.75	0.69
3:J:965:GLN:HG2	3:J:969:LEU:CG	2.18	0.68
3:N:491:ASN:HD21	3:N:607:GLN:HA	1.57	0.68
1:I:1136:MET:HE1	2:K:347:ILE:HA	1.76	0.68
3:B:965:GLN:HG2	3:B:969:LEU:CG	2.18	0.68
3:B:1013:ASN:OD1	4:B:1101:FAR:C13	2.41	0.68
3:B:1090:CYS:SG	4:B:1101:FAR:H12A	1.50	0.68
3:F:593:LEU:HD21	3:F:856:HIS:HE1	1.57	0.68
1:M:413:MET:HG2	1:M:418:LEU:HB3	1.76	0.68
3:B:1008:ILE:HG22	3:B:1012:ARG:CD	2.23	0.68
3:F:591:VAL:HG21	3:F:634:ILE:HG13	1.75	0.68
1:A:69:GLU:HG3	3:B:262:TRP:HZ3	1.58	0.68
3:F:744:LEU:O	3:F:766:ILE:HD11	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:786:ALA:HB3	3:N:848:VAL:HG11	1.76	0.68
1:A:445:LEU:HD12	1:A:563:THR:CG2	2.24	0.68
1:A:923:ILE:O	1:A:927:MET:HG3	1.94	0.68
1:E:78:GLU:HB3	1:E:153:LEU:HD21	1.74	0.68
1:M:28:PRO:HG2	3:N:547:LEU:HD21	1.29	0.68
1:M:1109:VAL:HA	1:M:1112:GLU:HG2	1.75	0.68
3:B:786:ALA:HB3	3:B:848:VAL:HG11	1.75	0.68
1:A:120:THR:HG22	3:B:131:ARG:NH2	2.09	0.68
1:A:447:GLU:OE1	1:A:567:SER:HA	1.94	0.68
1:E:163:ASN:CB	1:E:489:ASN:ND2	2.56	0.68
1:E:445:LEU:HD12	1:E:563:THR:CG2	2.24	0.68
3:B:214:ARG:HA	3:B:825:PRO:HG2	1.75	0.68
3:J:786:ALA:HB3	3:J:848:VAL:HG11	1.75	0.68
3:N:587:MET:HE1	3:N:855:ILE:HG13	1.75	0.68
3:N:744:LEU:O	3:N:766:ILE:HD11	1.94	0.68
1:A:254:GLU:OE1	1:A:1101:THR:OG1	2.11	0.68
1:A:1109:VAL:HA	1:A:1112:GLU:HG2	1.75	0.68
1:M:68:ASP:OD2	3:N:259:GLY:O	2.11	0.68
1:M:445:LEU:HD12	1:M:563:THR:CG2	2.24	0.68
1:I:78:GLU:HB3	1:I:153:LEU:HD21	1.74	0.68
3:F:406:VAL:H	3:F:445:GLN:HE22	1.42	0.68
4:F:1101:FAR:H143	3:J:1009:VAL:HA	0.71	0.68
3:N:1013:ASN:OD1	4:N:1101:FAR:C13	2.41	0.68
1:A:290:ARG:NH2	1:A:391:ASP:OD1	2.23	0.68
1:E:75:TYR:HH	3:F:191:GLN:CD	1.94	0.68
1:M:447:GLU:OE1	1:M:567:SER:HA	1.94	0.68
3:F:938:PRO:HG2	3:J:1092:ILE:HB	1.76	0.68
3:N:965:GLN:HG2	3:N:969:LEU:CG	2.18	0.68
1:A:66:ASP:HB2	3:F:667:GLN:HE22	1.56	0.68
1:A:413:MET:HG2	1:A:418:LEU:HB3	1.76	0.68
1:E:254:GLU:OE1	1:E:1101:THR:OG1	2.11	0.68
1:E:1120:GLN:NE2	1:E:1181:ALA:HB1	2.03	0.68
3:N:591:VAL:HG21	3:N:634:ILE:HG13	1.75	0.68
1:A:768:LEU:HD22	1:A:802:ARG:NH2	2.07	0.67
1:E:447:GLU:OE1	1:E:567:SER:HA	1.94	0.67
1:I:413:MET:HG2	1:I:418:LEU:HB3	1.76	0.67
1:I:447:GLU:OE1	1:I:567:SER:HA	1.94	0.67
3:J:88:LEU:HD21	3:J:178:TYR:HA	1.75	0.67
1:A:1209:THR:HG23	2:C:334:ILE:CG2	2.25	0.67
1:E:1109:VAL:HA	1:E:1112:GLU:HG2	1.75	0.67
1:M:28:PRO:HB2	3:N:130:MET:HE2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1092:LEU:HB2	1:I:1114:VAL:HG11	1.76	0.67
3:J:744:LEU:O	3:J:766:ILE:HD11	1.94	0.67
1:E:1092:LEU:HB2	1:E:1114:VAL:HG11	1.76	0.67
4:F:1103:FAR:C13	3:J:1013:ASN:OD1	2.42	0.67
1:E:29:VAL:HG11	3:F:131:ARG:CG	2.22	0.67
1:M:1209:THR:HG23	2:O:334:ILE:CG2	2.25	0.67
3:F:405:VAL:HG21	3:F:435:GLY:HA3	1.77	0.67
4:F:1101:FAR:H142	3:J:1012:ARG:HB2	1.76	0.67
3:J:405:VAL:HG21	3:J:435:GLY:HA3	1.77	0.67
3:N:579:ILE:HD13	3:N:601:ALA:HB2	1.69	0.67
1:A:10:ARG:NH1	1:A:415:GLU:OE1	2.28	0.67
1:E:28:PRO:HB2	3:F:547:LEU:HD21	1.73	0.67
1:I:63:LYS:C	3:N:567:ARG:NH2	2.44	0.67
1:I:254:GLU:OE1	1:I:1101:THR:OG1	2.11	0.67
1:I:290:ARG:NH2	1:I:391:ASP:OD1	2.23	0.67
1:I:1209:THR:HG23	2:K:334:ILE:CG2	2.25	0.67
3:F:974:MET:HE2	3:F:975:TYR:CD2	2.29	0.67
1:I:1109:VAL:HA	1:I:1112:GLU:HG2	1.75	0.67
3:B:591:VAL:HG21	3:B:634:ILE:HG13	1.75	0.67
3:B:853:LEU:HD11	3:B:880:ILE:CG1	2.24	0.67
3:F:88:LEU:HD21	3:F:178:TYR:HA	1.75	0.67
3:F:587:MET:HE1	3:F:855:ILE:CG1	2.23	0.67
3:F:875:ARG:HB2	3:F:878:TRP:HB2	1.77	0.67
1:E:10:ARG:NH1	1:E:415:GLU:OE1	2.28	0.67
1:E:923:ILE:O	1:E:927:MET:HG3	1.94	0.67
1:M:923:ILE:O	1:M:927:MET:HG3	1.94	0.67
1:M:1092:LEU:HB2	1:M:1114:VAL:HG11	1.76	0.67
3:B:744:LEU:O	3:B:766:ILE:HD11	1.94	0.67
3:F:786:ALA:HB3	3:F:848:VAL:HG11	1.75	0.67
1:E:1209:THR:HG23	2:G:334:ILE:CG2	2.25	0.67
3:J:406:VAL:H	3:J:445:GLN:HE22	1.42	0.67
1:E:29:VAL:CG1	3:F:131:ARG:HG3	2.25	0.67
1:M:10:ARG:NH1	1:M:415:GLU:OE1	2.28	0.67
3:J:853:LEU:HD11	3:J:880:ILE:CG1	2.24	0.67
3:N:405:VAL:HG21	3:N:435:GLY:HA3	1.77	0.67
3:N:974:MET:HE2	3:N:975:TYR:CD2	2.29	0.67
1:M:79:GLN:HB3	3:N:194:TYR:CB	2.25	0.67
1:I:923:ILE:O	1:I:927:MET:HG3	1.94	0.67
3:N:406:VAL:H	3:N:445:GLN:HE22	1.42	0.67
1:M:1120:GLN:NE2	1:M:1181:ALA:HB1	2.03	0.66
1:I:10:ARG:NH1	1:I:415:GLU:OE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:777:LYS:HG2	3:B:779:TRP:CZ2	2.30	0.66
3:F:724:THR:C	3:F:726:GLU:H	1.98	0.66
3:F:1090:CYS:HG	4:F:1101:FAR:C2	2.01	0.66
3:J:875:ARG:HB2	3:J:878:TRP:HB2	1.77	0.66
3:F:883:MET:HE1	3:F:911:LEU:HB2	1.77	0.66
3:N:1015:GLU:CD	4:N:1101:FAR:H41	2.16	0.66
1:E:413:MET:HG2	1:E:418:LEU:HB3	1.76	0.66
3:B:493:LEU:HD21	3:B:615:PRO:HG2	1.77	0.66
3:F:586:TYR:HB3	3:F:782:VAL:HG12	1.78	0.66
3:F:1091:LEU:HB2	3:J:1004:MET:HE1	1.77	0.66
1:M:75:TYR:OH	3:N:191:GLN:CG	2.43	0.66
3:J:777:LYS:HG2	3:J:779:TRP:CZ2	2.30	0.66
3:N:586:TYR:HB3	3:N:782:VAL:HG12	1.77	0.66
1:I:93:ILE:HG22	3:J:67:THR:HG23	1.70	0.66
1:I:445:LEU:HD12	1:I:563:THR:CG2	2.24	0.66
3:B:143:PRO:CB	3:B:215:VAL:CG2	2.71	0.66
3:F:777:LYS:HG2	3:F:779:TRP:CZ2	2.30	0.66
1:I:28:PRO:HB2	3:J:130:MET:HE2	1.76	0.66
1:I:893:LEU:HD11	1:I:947:MET:HE3	1.77	0.66
3:B:405:VAL:HG21	3:B:435:GLY:HA3	1.77	0.66
3:J:586:TYR:HB3	3:J:782:VAL:HG12	1.78	0.66
1:A:120:THR:CG2	3:B:131:ARG:NH2	2.58	0.66
1:I:28:PRO:CG	3:J:547:LEU:HD23	1.93	0.66
1:I:75:TYR:OH	3:J:191:GLN:OE1	2.13	0.66
3:B:279:LEU:HG	3:B:283:LEU:HD22	1.76	0.66
3:B:586:TYR:HB3	3:B:782:VAL:HG12	1.78	0.66
3:N:724:THR:C	3:N:726:GLU:H	1.98	0.66
3:N:875:ARG:HB2	3:N:878:TRP:HB2	1.77	0.66
1:M:859:PRO:HB2	1:M:1119:PRO:HA	1.78	0.66
3:J:974:MET:HE2	3:J:975:TYR:CD2	2.29	0.66
2:C:335:ARG:O	2:C:336:ASP:OD1	2.14	0.66
1:M:120:THR:CG2	3:N:131:ARG:CZ	2.71	0.66
1:I:28:PRO:HG3	3:J:547:LEU:CG	2.25	0.66
4:F:1101:FAR:H51	3:J:1008:ILE:HG21	1.76	0.66
3:N:777:LYS:HG2	3:N:779:TRP:CZ2	2.30	0.66
1:A:859:PRO:HB2	1:A:1119:PRO:HA	1.78	0.65
1:E:28:PRO:CB	3:F:130:MET:HE1	2.19	0.65
2:G:335:ARG:O	2:G:336:ASP:OD1	2.14	0.65
2:O:335:ARG:O	2:O:336:ASP:OD1	2.14	0.65
3:F:593:LEU:HD21	3:F:856:HIS:CE1	2.31	0.65
1:A:1092:LEU:HB2	1:A:1114:VAL:HG11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:724:THR:HB	3:B:726:GLU:H	1.61	0.65
1:A:75:TYR:HH	3:B:191:GLN:HB3	1.60	0.65
2:K:335:ARG:O	2:K:336:ASP:OD1	2.14	0.65
4:B:1101:FAR:H143	3:N:1009:VAL:CA	2.20	0.65
3:J:724:THR:HB	3:J:726:GLU:H	1.61	0.65
1:I:768:LEU:HD22	1:I:802:ARG:NH2	2.07	0.65
3:B:1090:CYS:CB	4:B:1101:FAR:H13	2.19	0.65
3:N:724:THR:HB	3:N:726:GLU:H	1.61	0.65
1:M:771:LYS:CD	1:M:802:ARG:HH11	2.10	0.65
3:B:406:VAL:H	3:B:445:GLN:HE22	1.42	0.65
3:F:587:MET:HE1	3:F:855:ILE:HD12	1.77	0.65
4:F:1101:FAR:H102	3:J:1070:THR:OG1	1.97	0.65
3:J:493:LEU:HD21	3:J:615:PRO:HG2	1.77	0.65
3:J:853:LEU:HD12	3:J:880:ILE:CG1	2.26	0.65
3:N:853:LEU:HD11	3:N:880:ILE:CG1	2.24	0.65
1:I:445:LEU:O	1:I:565:PRO:HA	1.97	0.65
3:B:460:SER:HB2	3:F:477:ARG:NH2	2.11	0.65
3:B:1009:VAL:HA	4:N:1101:FAR:H141	1.77	0.65
1:A:29:VAL:HG11	3:B:131:ARG:HG2	1.79	0.65
1:A:163:ASN:HB2	1:A:489:ASN:HD21	1.62	0.65
1:M:872:PRO:HD2	1:M:872:PRO:O	1.97	0.65
3:B:875:ARG:HB2	3:B:878:TRP:HB2	1.77	0.65
1:M:445:LEU:O	1:M:565:PRO:HA	1.97	0.65
1:I:859:PRO:HB2	1:I:1119:PRO:HA	1.79	0.65
3:F:143:PRO:HB2	3:F:215:VAL:HG22	1.79	0.65
3:J:724:THR:C	3:J:726:GLU:H	1.98	0.65
1:A:893:LEU:HD11	1:A:947:MET:HE3	1.79	0.65
1:E:872:PRO:HD2	1:E:872:PRO:O	1.97	0.65
1:M:113:HIS:HA	1:M:132:HIS:HB3	1.79	0.65
1:I:83:LYS:CD	3:J:198:GLU:OE1	2.45	0.65
3:F:625:ASN:HB3	3:F:634:ILE:CD1	2.27	0.65
3:J:593:LEU:HD21	3:J:856:HIS:CE1	2.31	0.65
1:E:79:GLN:HB3	3:F:194:TYR:CB	2.28	0.64
1:I:771:LYS:CD	1:I:802:ARG:HH11	2.10	0.64
3:B:593:LEU:HD21	3:B:856:HIS:CE1	2.31	0.64
3:B:625:ASN:HB3	3:B:634:ILE:CD1	2.27	0.64
3:F:853:LEU:HD12	3:F:880:ILE:CG1	2.26	0.64
1:A:445:LEU:O	1:A:565:PRO:HA	1.97	0.64
1:A:1137:LEU:HD13	4:A:1301:FAR:C6	2.19	0.64
1:E:62:ARG:CZ	3:F:258:GLN:OE1	2.44	0.64
1:E:113:HIS:HA	1:E:132:HIS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:LEU:O	1:E:565:PRO:HA	1.97	0.64
1:E:768:LEU:HD23	1:E:802:ARG:HH21	1.24	0.64
1:M:75:TYR:OH	3:N:191:GLN:CB	2.45	0.64
1:I:113:HIS:HA	1:I:132:HIS:HB3	1.79	0.64
3:B:724:THR:C	3:B:726:GLU:H	1.98	0.64
3:B:853:LEU:HD12	3:B:880:ILE:CG1	2.26	0.64
3:F:724:THR:HB	3:F:726:GLU:H	1.61	0.64
3:N:883:MET:HE1	3:N:911:LEU:HB2	1.78	0.64
1:M:28:PRO:CG	3:N:547:LEU:HD23	1.98	0.64
1:M:163:ASN:HB2	1:M:489:ASN:HD21	1.62	0.64
3:N:493:LEU:HD21	3:N:615:PRO:HG2	1.77	0.64
3:N:625:ASN:HB3	3:N:634:ILE:CD1	2.27	0.64
1:M:893:LEU:HD11	1:M:947:MET:HE3	1.78	0.64
3:F:493:LEU:HD21	3:F:615:PRO:HG2	1.77	0.64
3:N:593:LEU:HD21	3:N:856:HIS:CE1	2.31	0.64
3:J:625:ASN:HB3	3:J:634:ILE:CD1	2.27	0.64
1:A:113:HIS:HA	1:A:132:HIS:HB3	1.79	0.64
1:M:68:ASP:OD2	3:N:260:CYS:HA	1.98	0.64
1:M:69:GLU:HG3	3:N:262:TRP:CZ3	2.33	0.64
3:B:587:MET:HE1	3:B:855:ILE:HG13	1.80	0.64
1:M:69:GLU:HG3	3:N:262:TRP:HZ3	1.61	0.64
1:I:931:LEU:HD11	1:I:949:LEU:HD11	1.80	0.64
3:J:223:ARG:HB3	3:J:228:ASN:OD1	1.98	0.64
3:N:172:ILE:HG21	3:N:212:VAL:HG21	1.80	0.64
3:N:853:LEU:HD12	3:N:880:ILE:CG1	2.26	0.64
1:A:63:LYS:C	3:F:567:ARG:NH2	2.49	0.64
1:I:768:LEU:HD23	1:I:802:ARG:HH21	1.24	0.64
3:F:625:ASN:O	3:F:634:ILE:HD11	1.98	0.64
1:E:893:LEU:HD11	1:E:947:MET:HE3	1.79	0.64
3:F:1070:THR:OG1	4:F:1103:FAR:H102	1.97	0.64
1:E:859:PRO:HB2	1:E:1119:PRO:HA	1.78	0.64
3:J:883:MET:HE1	3:J:911:LEU:HB2	1.79	0.64
1:E:931:LEU:HD11	1:E:949:LEU:HD11	1.80	0.63
3:B:223:ARG:HB3	3:B:228:ASN:OD1	1.98	0.63
2:O:332:ILE:CG1	2:O:340:LEU:HD13	2.28	0.63
1:I:28:PRO:HG3	3:J:547:LEU:HG	1.79	0.63
1:I:176:TYR:HB2	1:I:241:ILE:HD13	1.81	0.63
3:F:924:TRP:CZ2	3:J:1093:SER:O	2.51	0.63
1:A:872:PRO:HD2	1:A:872:PRO:O	1.97	0.63
1:M:176:TYR:HB2	1:M:241:ILE:HD13	1.81	0.63
3:B:800:ILE:O	3:B:804:LEU:HG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:467:VAL:HG12	3:F:469:ARG:HG2	1.81	0.63
3:J:556:PRO:HD2	5:J:1101:ADP:O1A	1.99	0.63
3:J:800:ILE:O	3:J:804:LEU:HG	1.99	0.63
1:A:817:VAL:HA	1:A:820:ILE:HG12	1.81	0.63
3:N:223:ARG:HB3	3:N:228:ASN:OD1	1.98	0.63
1:A:69:GLU:CG	3:B:262:TRP:CZ3	2.82	0.63
1:A:176:TYR:HB2	1:A:241:ILE:HD13	1.81	0.63
2:G:349:ALA:O	2:G:353:ARG:HG3	1.99	0.63
3:F:223:ARG:HB3	3:F:228:ASN:OD1	1.98	0.63
1:E:24:CYS:O	3:F:546:LYS:HD3	1.99	0.63
1:I:817:VAL:HA	1:I:820:ILE:HG12	1.81	0.63
1:I:872:PRO:HD2	1:I:872:PRO:O	1.97	0.63
1:I:930:GLU:HA	1:I:933:HIS:CD2	2.34	0.63
3:B:467:VAL:HG12	3:B:469:ARG:HG2	1.81	0.63
3:F:556:PRO:HD2	5:F:1102:ADP:O2A	1.99	0.63
3:N:467:VAL:HG12	3:N:469:ARG:HG2	1.81	0.63
3:J:467:VAL:HG12	3:J:469:ARG:HG2	1.81	0.63
3:N:556:PRO:HD2	5:N:1102:ADP:O1A	1.99	0.63
3:N:800:ILE:O	3:N:804:LEU:HG	1.99	0.63
1:A:19:GLN:HA	1:A:23:LEU:HB2	1.81	0.63
1:M:19:GLN:HA	1:M:23:LEU:HB2	1.81	0.63
1:I:163:ASN:HB2	1:I:489:ASN:HD21	1.61	0.63
3:N:625:ASN:O	3:N:634:ILE:HD11	1.98	0.63
1:A:771:LYS:CD	1:A:802:ARG:HH11	2.10	0.63
1:E:72:ALA:HB2	3:F:260:CYS:HB2	1.80	0.63
1:E:120:THR:CG2	3:F:131:ARG:NE	2.50	0.63
1:E:163:ASN:HB2	1:E:489:ASN:HD21	1.62	0.63
1:E:771:LYS:CD	1:E:802:ARG:HH11	2.10	0.63
1:M:450:GLU:O	1:M:454:ILE:HG13	1.99	0.63
1:M:931:LEU:HD11	1:M:949:LEU:HD11	1.80	0.63
2:O:349:ALA:O	2:O:353:ARG:HG3	1.99	0.63
3:F:853:LEU:HD11	3:F:880:ILE:CG1	2.24	0.63
3:N:143:PRO:CB	3:N:215:VAL:CG2	2.71	0.63
1:E:817:VAL:HA	1:E:820:ILE:HG12	1.81	0.62
3:B:143:PRO:HB2	3:B:215:VAL:HG22	1.79	0.62
3:B:172:ILE:HG21	3:B:212:VAL:HG21	1.80	0.62
1:E:450:GLU:O	1:E:454:ILE:HG13	1.99	0.62
1:M:817:VAL:HA	1:M:820:ILE:HG12	1.81	0.62
2:K:349:ALA:O	2:K:353:ARG:HG3	1.99	0.62
3:B:1012:ARG:HB2	4:N:1101:FAR:H141	1.81	0.62
3:F:800:ILE:O	3:F:804:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:172:ILE:HG21	3:J:212:VAL:HG21	1.80	0.62
3:N:283:LEU:HA	3:N:285:ARG:H	1.64	0.62
2:C:349:ALA:O	2:C:353:ARG:HG3	1.99	0.62
2:G:332:ILE:CG1	2:G:340:LEU:HD13	2.28	0.62
3:B:587:MET:HE1	3:B:855:ILE:HD12	1.82	0.62
3:F:223:ARG:NH2	3:F:338:TYR:HA	2.14	0.62
3:F:279:LEU:O	3:F:283:LEU:HB2	2.00	0.62
1:A:768:LEU:HD23	1:A:802:ARG:HH21	1.24	0.62
1:M:444:ILE:HG12	1:M:586:LEU:HD22	1.82	0.62
1:I:68:ASP:OD2	3:J:259:GLY:O	2.16	0.62
1:I:444:ILE:HG12	1:I:586:LEU:HD22	1.81	0.62
1:I:1137:LEU:HD13	4:I:1301:FAR:C6	2.19	0.62
3:F:143:PRO:CB	3:F:215:VAL:CG2	2.71	0.62
3:J:625:ASN:O	3:J:634:ILE:HD11	1.98	0.62
3:N:223:ARG:NH2	3:N:338:TYR:HA	2.14	0.62
3:N:288:ARG:HH11	3:N:978:ASN:HD21	1.48	0.62
3:F:172:ILE:HG21	3:F:212:VAL:HG21	1.80	0.62
3:J:288:ARG:HH11	3:J:978:ASN:HD21	1.48	0.62
1:A:899:VAL:O	1:A:903:MET:HG3	2.00	0.62
1:A:930:GLU:HA	1:A:933:HIS:CD2	2.34	0.62
1:E:28:PRO:CG	3:F:547:LEU:HD23	2.02	0.62
1:I:19:GLN:HA	1:I:23:LEU:HB2	1.81	0.62
1:I:450:GLU:O	1:I:454:ILE:HG13	1.99	0.62
1:E:444:ILE:HG12	1:E:586:LEU:HD22	1.81	0.62
1:E:930:GLU:HA	1:E:933:HIS:CD2	2.34	0.62
1:M:491:ARG:HG3	3:N:62:LEU:CD1	2.30	0.62
1:I:72:ALA:HB2	3:J:260:CYS:HB2	1.81	0.62
1:I:83:LYS:HE3	3:J:198:GLU:OE1	2.00	0.62
1:I:899:VAL:O	1:I:903:MET:HG3	2.00	0.62
3:B:223:ARG:NH2	3:B:338:TYR:HA	2.14	0.62
1:A:450:GLU:O	1:A:454:ILE:HG13	1.99	0.62
1:E:176:TYR:HB2	1:E:241:ILE:HD13	1.81	0.62
1:M:930:GLU:HA	1:M:933:HIS:CD2	2.34	0.62
1:I:491:ARG:HG3	3:J:62:LEU:CD1	2.29	0.62
1:I:1127:LEU:HD22	1:I:1151:VAL:HG12	1.81	0.62
3:N:1015:GLU:OE2	4:N:1101:FAR:H42	1.99	0.62
1:A:444:ILE:HG12	1:A:586:LEU:HD22	1.81	0.62
1:E:899:VAL:O	1:E:903:MET:HG3	2.00	0.62
3:B:1060:LEU:HD23	3:N:1082:VAL:HG21	1.80	0.62
3:F:724:THR:C	3:F:726:GLU:N	2.54	0.62
1:A:69:GLU:CG	3:B:262:TRP:HZ3	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:SER:OG	1:A:1148:ILE:HG22	2.00	0.61
1:A:1127:LEU:HD22	1:A:1151:VAL:HG12	1.81	0.61
1:E:1127:LEU:HD22	1:E:1151:VAL:HG12	1.81	0.61
1:M:899:VAL:O	1:M:903:MET:HG3	2.00	0.61
3:B:310:GLU:OE2	3:B:473:LEU:HB2	2.00	0.61
3:N:974:MET:HE1	3:N:975:TYR:CE2	2.27	0.61
1:E:791:GLY:H	1:E:792:PRO:HD2	1.66	0.61
3:J:143:PRO:CB	3:J:215:VAL:CG2	2.71	0.61
3:J:172:ILE:O	3:J:172:ILE:HG22	2.00	0.61
1:E:19:GLN:HA	1:E:23:LEU:HB2	1.81	0.61
3:F:288:ARG:HH11	3:F:978:ASN:HD21	1.48	0.61
3:F:974:MET:HE1	3:F:975:TYR:CE2	2.32	0.61
1:I:791:GLY:H	1:I:792:PRO:HD2	1.66	0.61
3:J:223:ARG:NH2	3:J:338:TYR:HA	2.14	0.61
1:E:94:ARG:HH12	3:F:157:THR:HA	1.60	0.61
1:E:1086:SER:OG	1:E:1148:ILE:HG22	2.00	0.61
1:I:1086:SER:OG	1:I:1148:ILE:HG22	2.00	0.61
3:B:883:MET:HE1	3:B:911:LEU:HB2	1.83	0.61
3:J:310:GLU:OE2	3:J:473:LEU:HB2	2.00	0.61
1:A:931:LEU:HD11	1:A:949:LEU:HD11	1.80	0.61
1:M:1086:SER:OG	1:M:1148:ILE:HG22	2.00	0.61
3:B:724:THR:C	3:B:726:GLU:N	2.54	0.61
3:F:172:ILE:HG22	3:F:172:ILE:O	2.00	0.61
3:F:974:MET:HE2	3:F:975:TYR:CE1	2.27	0.61
1:M:768:LEU:HD22	1:M:802:ARG:HH21	1.60	0.61
3:B:460:SER:CB	3:F:477:ARG:HH22	2.14	0.61
3:F:283:LEU:HD23	3:F:307:LEU:CG	2.31	0.61
3:F:1070:THR:OG1	4:F:1103:FAR:C10	2.48	0.61
4:F:1103:FAR:C1	3:J:1090:CYS:HG	1.10	0.61
3:J:872:LEU:HB3	3:J:984:GLU:OE2	2.01	0.61
3:N:1090:CYS:HG	4:N:1101:FAR:H12A	0.44	0.61
1:I:491:ARG:HG3	3:J:62:LEU:HD12	1.83	0.61
3:F:1004:MET:HE2	3:J:1092:ILE:HG22	1.81	0.61
3:J:727:ILE:HG22	3:J:747:LEU:HD11	1.83	0.61
3:N:310:GLU:OE2	3:N:473:LEU:HB2	2.00	0.61
1:E:93:ILE:HG21	3:F:66:PRO:C	2.21	0.60
1:M:791:GLY:H	1:M:792:PRO:HD2	1.66	0.60
1:A:28:PRO:HG2	3:B:547:LEU:HD21	1.34	0.60
1:E:72:ALA:CB	3:F:260:CYS:HB2	2.31	0.60
1:E:1208:ALA:CB	2:G:334:ILE:HG12	2.32	0.60
1:M:926:VAL:HG23	1:M:1059:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1301:FAR:H2	2:O:330:ARG:HG3	1.83	0.60
3:N:172:ILE:HG22	3:N:172:ILE:O	2.00	0.60
1:A:95:GLN:HE22	1:A:113:HIS:CG	2.19	0.60
1:M:1127:LEU:HD22	1:M:1151:VAL:HG12	1.81	0.60
3:B:811:THR:OG1	3:B:875:ARG:HA	2.02	0.60
3:N:727:ILE:HG22	3:N:747:LEU:HD11	1.83	0.60
1:A:961:ILE:HG22	1:A:1064:LEU:HD21	1.84	0.60
1:M:961:ILE:HG22	1:M:1064:LEU:HD21	1.84	0.60
3:B:477:ARG:NH1	3:F:103:ARG:NH2	2.49	0.60
3:J:724:THR:C	3:J:726:GLU:N	2.54	0.60
3:N:724:THR:C	3:N:726:GLU:N	2.54	0.60
2:K:332:ILE:CG1	2:K:340:LEU:HD13	2.28	0.60
1:I:928:ALA:HB1	1:I:943:THR:HG22	1.84	0.60
4:I:1301:FAR:H2	2:K:330:ARG:HG3	1.83	0.60
3:F:587:MET:HE1	3:F:855:ILE:CD1	2.32	0.60
3:F:811:THR:OG1	3:F:875:ARG:HA	2.02	0.60
1:I:961:ILE:HG22	1:I:1064:LEU:HD21	1.84	0.60
1:I:1120:GLN:NE2	1:I:1181:ALA:HB1	2.03	0.60
3:B:172:ILE:O	3:B:172:ILE:HG22	2.00	0.60
3:F:1004:MET:HB3	3:J:1092:ILE:CG2	2.32	0.60
4:F:1101:FAR:H101	3:J:1070:THR:OG1	2.01	0.60
1:A:926:VAL:HG23	1:A:1059:ARG:HG2	1.83	0.60
1:M:120:THR:HG22	3:N:131:ARG:NE	2.15	0.60
1:M:928:ALA:HB1	1:M:943:THR:HG22	1.84	0.60
3:B:974:MET:HE2	3:B:975:TYR:CD2	2.32	0.60
3:F:283:LEU:HB3	3:F:312:LEU:HD13	1.83	0.60
3:F:310:GLU:OE2	3:F:473:LEU:HB2	2.01	0.60
1:M:95:GLN:HE22	1:M:113:HIS:CG	2.19	0.60
3:F:1013:ASN:ND2	4:F:1101:FAR:C15	2.59	0.60
1:E:928:ALA:HB1	1:E:943:THR:HG22	1.84	0.60
1:I:491:ARG:HG2	3:J:62:LEU:HD11	1.84	0.60
3:F:1013:ASN:OD1	4:F:1101:FAR:C13	2.50	0.60
1:A:928:ALA:HB1	1:A:943:THR:HG22	1.84	0.59
1:E:926:VAL:HG23	1:E:1059:ARG:HG2	1.83	0.59
1:I:491:ARG:CG	3:J:62:LEU:HD11	2.32	0.59
3:B:625:ASN:O	3:B:634:ILE:HD11	1.98	0.59
3:B:625:ASN:HB3	3:B:634:ILE:HD13	1.84	0.59
3:N:143:PRO:HB2	3:N:215:VAL:HG22	1.79	0.59
3:N:795:SER:OG	3:N:855:ILE:HD11	2.02	0.59
1:I:95:GLN:HE22	1:I:113:HIS:CG	2.19	0.59
3:N:811:THR:OG1	3:N:875:ARG:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLY:H	1:A:792:PRO:HD2	1.66	0.59
1:E:28:PRO:CG	3:F:547:LEU:CG	2.70	0.59
1:M:120:THR:HG21	3:N:131:ARG:NH2	2.16	0.59
1:I:1208:ALA:CB	2:K:334:ILE:HG12	2.32	0.59
3:J:177:LEU:HD11	3:J:303:PRO:HG3	1.84	0.59
3:N:803:PHE:CG	3:N:810:VAL:CG2	2.86	0.59
1:A:1208:ALA:CB	2:C:334:ILE:HG12	2.32	0.59
1:E:1168:THR:C	1:E:1170:GLY:N	2.52	0.59
1:I:1215:LEU:HB3	2:K:330:ARG:HH22	1.67	0.59
3:B:872:LEU:HB3	3:B:984:GLU:OE2	2.01	0.59
3:F:177:LEU:HD11	3:F:303:PRO:HG3	1.84	0.59
3:F:795:SER:OG	3:F:855:ILE:HD11	2.02	0.59
3:F:872:LEU:HB3	3:F:984:GLU:OE2	2.01	0.59
3:J:803:PHE:CG	3:J:810:VAL:CG2	2.85	0.59
3:N:872:LEU:HB3	3:N:984:GLU:OE2	2.01	0.59
1:A:75:TYR:OH	3:B:191:GLN:OE1	2.21	0.59
4:A:1301:FAR:H2	2:C:330:ARG:HG3	1.83	0.59
1:E:95:GLN:HE22	1:E:113:HIS:CG	2.19	0.59
3:F:727:ILE:HG22	3:F:747:LEU:HD11	1.83	0.59
2:C:332:ILE:CG1	2:C:340:LEU:HD13	2.28	0.59
1:E:1081:LYS:CB	4:E:1301:FAR:H143	2.33	0.59
2:K:356:GLY:O	2:K:359:VAL:HG12	2.03	0.59
3:B:587:MET:HE1	3:B:855:ILE:CD1	2.33	0.59
3:F:803:PHE:CG	3:F:810:VAL:CG2	2.86	0.59
3:F:1091:LEU:HB2	3:J:1004:MET:CE	2.32	0.59
3:J:132:GLN:HE22	3:J:150:HIS:CG	2.20	0.59
3:J:587:MET:HE1	3:J:855:ILE:CD1	2.32	0.59
3:J:974:MET:HE2	3:J:975:TYR:CE1	2.26	0.59
3:N:625:ASN:HB3	3:N:634:ILE:HD13	1.84	0.59
1:E:352:LYS:HD2	1:E:352:LYS:O	2.03	0.59
1:E:445:LEU:CD1	1:E:563:THR:HG23	2.30	0.59
1:E:1215:LEU:HB3	2:G:330:ARG:HH22	1.67	0.59
1:M:491:ARG:CG	3:N:62:LEU:HD11	2.32	0.59
2:O:356:GLY:O	2:O:359:VAL:HG12	2.03	0.59
1:I:445:LEU:CD1	1:I:563:THR:HG23	2.30	0.59
1:E:961:ILE:HG22	1:E:1064:LEU:HD21	1.84	0.59
1:I:926:VAL:HG23	1:I:1059:ARG:HG2	1.83	0.59
3:B:803:PHE:CG	3:B:810:VAL:CG2	2.86	0.59
3:F:1015:GLU:CG	3:J:1012:ARG:HH22	2.15	0.59
1:M:352:LYS:HD2	1:M:352:LYS:O	2.03	0.59
3:B:283:LEU:HB3	3:B:312:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:491:ARG:HG3	3:N:62:LEU:HD12	1.84	0.59
1:I:1081:LYS:CB	4:I:1301:FAR:H143	2.32	0.59
3:J:493:LEU:HD21	3:J:615:PRO:CG	2.33	0.59
1:A:1081:LYS:CB	4:A:1301:FAR:H143	2.32	0.58
1:M:1208:ALA:CB	2:O:334:ILE:HG12	2.32	0.58
3:B:529:TRP:CD1	3:B:684:SER:HB3	2.39	0.58
3:B:727:ILE:HG22	3:B:747:LEU:HD11	1.83	0.58
3:J:587:MET:HE1	3:J:855:ILE:CG1	2.33	0.58
3:J:811:THR:OG1	3:J:875:ARG:HA	2.02	0.58
3:N:132:GLN:HE22	3:N:150:HIS:CG	2.20	0.58
3:N:501:ALA:O	3:N:520:PRO:HD3	2.03	0.58
2:C:356:GLY:O	2:C:359:VAL:HG12	2.03	0.58
1:M:930:GLU:OE2	1:M:933:HIS:NE2	2.36	0.58
3:F:68:THR:HB	3:F:70:LEU:HD12	1.86	0.58
3:F:501:ALA:O	3:F:520:PRO:HD3	2.03	0.58
3:F:1004:MET:HG3	3:J:1092:ILE:HG22	1.84	0.58
3:J:460:SER:HB2	3:N:477:ARG:NH2	2.18	0.58
1:A:894:THR:HA	1:A:920:ILE:HG21	1.85	0.58
1:E:75:TYR:CD1	3:F:258:GLN:HB2	2.38	0.58
1:M:768:LEU:HD23	1:M:802:ARG:HH21	1.24	0.58
1:M:1215:LEU:HB3	2:O:330:ARG:HH22	1.67	0.58
1:I:352:LYS:HD2	1:I:352:LYS:O	2.03	0.58
3:B:132:GLN:HE22	3:B:150:HIS:CG	2.20	0.58
3:N:53:TYR:CZ	3:N:57:LYS:HG3	2.39	0.58
3:N:177:LEU:HD11	3:N:303:PRO:HG3	1.84	0.58
1:A:1120:GLN:HE22	1:A:1182:SER:N	2.02	0.58
1:A:1168:THR:C	1:A:1170:GLY:N	2.52	0.58
1:E:509:LYS:HG2	1:E:554:TRP:HH2	1.69	0.58
1:E:926:VAL:HG13	1:E:961:ILE:HD12	1.86	0.58
1:E:930:GLU:OE2	1:E:933:HIS:NE2	2.36	0.58
4:E:1301:FAR:H2	2:G:330:ARG:HG3	1.83	0.58
1:M:1081:LYS:CB	4:M:1301:FAR:H143	2.33	0.58
1:I:163:ASN:CB	1:I:489:ASN:HD21	2.16	0.58
3:F:132:GLN:HE22	3:F:150:HIS:CG	2.20	0.58
3:J:53:TYR:CZ	3:J:57:LYS:HG3	2.39	0.58
3:N:586:TYR:CB	3:N:782:VAL:HG12	2.33	0.58
1:A:352:LYS:O	1:A:352:LYS:HD2	2.03	0.58
1:A:930:GLU:OE2	1:A:933:HIS:NE2	2.35	0.58
2:G:356:GLY:O	2:G:359:VAL:HG12	2.03	0.58
3:B:493:LEU:HD21	3:B:615:PRO:CG	2.33	0.58
3:B:795:SER:OG	3:B:855:ILE:HD11	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:625:ASN:HB3	3:F:634:ILE:HD13	1.84	0.58
3:J:68:THR:HB	3:J:70:LEU:HD12	1.86	0.58
3:N:493:LEU:HD21	3:N:615:PRO:CG	2.33	0.58
3:N:529:TRP:CD1	3:N:684:SER:HB3	2.39	0.58
1:E:1120:GLN:HE22	1:E:1182:SER:N	2.02	0.58
1:I:1209:THR:HG23	2:K:334:ILE:HG23	1.86	0.58
3:B:501:ALA:O	3:B:520:PRO:HD3	2.03	0.58
3:F:148:CYS:HB3	3:F:170:LEU:HD13	1.86	0.58
3:F:734:CYS:SG	3:F:743:LEU:HD12	2.44	0.58
3:F:780:LEU:HG	3:F:784:TYR:CE2	2.39	0.58
3:J:143:PRO:HB2	3:J:215:VAL:HG22	1.79	0.58
3:J:501:ALA:O	3:J:520:PRO:HD3	2.03	0.58
3:N:734:CYS:SG	3:N:743:LEU:HD12	2.44	0.58
1:A:1215:LEU:HB3	2:C:330:ARG:HH22	1.67	0.58
2:C:359:VAL:HG21	2:C:367:ARG:CG	2.32	0.58
1:M:894:THR:HA	1:M:920:ILE:HG21	1.85	0.58
1:I:930:GLU:OE2	1:I:933:HIS:NE2	2.35	0.58
3:B:1012:ARG:HB2	4:N:1101:FAR:H142	1.85	0.58
3:J:586:TYR:CB	3:J:782:VAL:HG12	2.34	0.58
3:J:625:ASN:HB3	3:J:634:ILE:HD13	1.84	0.58
3:J:630:ARG:HE	3:J:777:LYS:HE3	1.68	0.58
1:M:509:LYS:HG2	1:M:554:TRP:HH2	1.69	0.58
1:I:926:VAL:HG13	1:I:961:ILE:HD12	1.86	0.58
3:B:126:LEU:HB2	3:B:178:TYR:OH	2.03	0.58
3:B:328:TYR:CD2	3:B:429:ARG:HD2	2.39	0.58
3:F:126:LEU:HB2	3:F:178:TYR:OH	2.04	0.58
3:F:493:LEU:HD21	3:F:615:PRO:CG	2.33	0.58
3:F:731:LEU:HD21	3:F:744:LEU:HB2	1.86	0.58
1:A:509:LYS:HG2	1:A:554:TRP:HH2	1.69	0.58
1:E:75:TYR:CD1	3:F:258:GLN:CB	2.87	0.58
1:M:265:PHE:CD2	1:M:337:LEU:HD13	2.39	0.58
1:M:445:LEU:CD1	1:M:563:THR:HG23	2.30	0.58
1:M:1209:THR:HG23	2:O:334:ILE:HG23	1.86	0.58
3:B:279:LEU:O	3:B:283:LEU:HB2	2.04	0.58
3:J:328:TYR:CD2	3:J:429:ARG:HD2	2.39	0.58
3:N:126:LEU:HB2	3:N:178:TYR:OH	2.03	0.58
1:A:163:ASN:CB	1:A:489:ASN:HD21	2.16	0.58
1:A:926:VAL:HG13	1:A:961:ILE:HD12	1.86	0.58
1:E:65:ALA:N	3:B:567:ARG:HH21	2.01	0.58
1:E:93:ILE:CG2	3:F:67:THR:HG23	2.23	0.58
1:E:265:PHE:CD2	1:E:337:LEU:HD13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:926:VAL:HG13	1:M:961:ILE:HD12	1.86	0.58
1:I:1168:THR:C	1:I:1170:GLY:N	2.52	0.58
3:F:630:ARG:HE	3:F:777:LYS:HE3	1.68	0.58
3:J:98:ALA:HB1	3:J:115:GLU:HG3	1.86	0.58
3:J:731:LEU:HD21	3:J:744:LEU:HB2	1.86	0.58
3:J:780:LEU:HG	3:J:784:TYR:CE2	2.39	0.58
3:N:173:ASN:OD1	3:N:173:ASN:C	2.42	0.58
3:N:328:TYR:CD2	3:N:429:ARG:HD2	2.39	0.58
1:A:265:PHE:CD2	1:A:337:LEU:HD13	2.39	0.57
1:E:251:THR:HA	1:E:1105:ILE:HG13	1.86	0.57
2:K:359:VAL:HG21	2:K:367:ARG:CG	2.32	0.57
3:B:53:TYR:CZ	3:B:57:LYS:HG3	2.39	0.57
3:B:148:CYS:HB3	3:B:170:LEU:HD13	1.86	0.57
3:B:477:ARG:NH2	3:F:460:SER:HB2	2.18	0.57
3:B:1060:LEU:HB3	3:N:1082:VAL:HG23	1.85	0.57
3:F:173:ASN:OD1	3:F:173:ASN:C	2.42	0.57
3:F:586:TYR:CB	3:F:782:VAL:HG12	2.33	0.57
3:J:45:LEU:HD23	3:J:104:ILE:HG13	1.86	0.57
1:A:28:PRO:HB2	3:B:130:MET:HE2	1.86	0.57
1:M:206:LYS:NZ	1:M:210:GLU:OE2	2.37	0.57
1:I:509:LYS:HG2	1:I:554:TRP:HH2	1.69	0.57
3:B:586:TYR:CB	3:B:782:VAL:HG12	2.33	0.57
3:F:53:TYR:CZ	3:F:57:LYS:HG3	2.39	0.57
3:N:780:LEU:HG	3:N:784:TYR:CE2	2.39	0.57
1:E:1137:LEU:HD13	4:E:1301:FAR:C6	2.19	0.57
1:E:1140:ILE:H	1:E:1140:ILE:HD12	1.70	0.57
1:M:28:PRO:HB2	3:N:130:MET:HE1	1.85	0.57
1:M:922:LEU:HD22	1:M:1121:PRO:HG3	1.86	0.57
1:M:1120:GLN:HE22	1:M:1182:SER:N	2.02	0.57
1:I:1081:LYS:HB3	4:I:1301:FAR:C14	2.35	0.57
1:I:1140:ILE:HD12	1:I:1140:ILE:H	1.69	0.57
3:B:734:CYS:SG	3:B:743:LEU:HD12	2.44	0.57
3:N:45:LEU:HD23	3:N:104:ILE:HG13	1.87	0.57
3:N:98:ALA:HB1	3:N:115:GLU:HG3	1.86	0.57
3:N:587:MET:HE1	3:N:855:ILE:HD12	1.85	0.57
1:E:75:TYR:CZ	3:F:191:GLN:OE1	2.57	0.57
1:M:1137:LEU:HD13	4:M:1301:FAR:C6	2.19	0.57
1:I:1120:GLN:HE22	1:I:1182:SER:N	2.02	0.57
3:B:74:LYS:CD	3:B:439:LYS:HZ1	2.07	0.57
3:F:328:TYR:CD2	3:F:429:ARG:HD2	2.39	0.57
3:J:529:TRP:CD1	3:J:684:SER:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:630:ARG:HE	3:N:777:LYS:HE3	1.68	0.57
3:N:731:LEU:HD21	3:N:744:LEU:HB2	1.86	0.57
1:A:206:LYS:NZ	1:A:210:GLU:OE2	2.37	0.57
1:I:265:PHE:CD2	1:I:337:LEU:HD13	2.39	0.57
2:K:350:TYR:O	2:K:354:ILE:HG13	2.05	0.57
3:B:45:LEU:HD23	3:B:104:ILE:HG13	1.86	0.57
3:B:68:THR:HB	3:B:70:LEU:HD12	1.86	0.57
3:B:853:LEU:HD12	3:B:880:ILE:CD1	2.35	0.57
3:F:45:LEU:HD23	3:F:104:ILE:HG13	1.86	0.57
3:F:98:ALA:HB1	3:F:115:GLU:HG3	1.86	0.57
3:F:625:ASN:C	3:F:634:ILE:CD1	2.73	0.57
3:J:63:TYR:O	3:J:72:PRO:HD3	2.05	0.57
3:J:625:ASN:C	3:J:634:ILE:CD1	2.73	0.57
3:N:625:ASN:C	3:N:634:ILE:CD1	2.73	0.57
1:E:1208:ALA:HB1	2:G:334:ILE:HG13	1.86	0.57
1:M:1140:ILE:H	1:M:1140:ILE:HD12	1.69	0.57
2:O:359:VAL:HG21	2:O:367:ARG:CG	2.32	0.57
1:I:922:LEU:HD22	1:I:1121:PRO:HG3	1.87	0.57
3:J:126:LEU:HB2	3:J:178:TYR:OH	2.03	0.57
3:J:173:ASN:OD1	3:J:173:ASN:C	2.42	0.57
3:N:68:THR:HB	3:N:70:LEU:HD12	1.86	0.57
1:I:93:ILE:CG2	3:J:67:THR:HG23	2.31	0.57
1:I:1208:ALA:HB1	2:K:334:ILE:HG13	1.86	0.57
3:B:392:LEU:HG	3:B:396:LEU:HG	1.87	0.57
3:F:361:ILE:CD1	3:F:421:LYS:HE2	2.35	0.57
3:N:853:LEU:HD12	3:N:880:ILE:CD1	2.35	0.57
1:A:1208:ALA:HB1	2:C:334:ILE:HG13	1.86	0.57
1:A:1209:THR:HG23	2:C:334:ILE:HG23	1.86	0.57
1:M:1200:MET:CE	2:O:351:ALA:HA	2.35	0.57
3:B:98:ALA:HB1	3:B:115:GLU:HG3	1.86	0.57
3:B:177:LEU:HD11	3:B:303:PRO:HG3	1.84	0.57
3:B:630:ARG:HE	3:B:777:LYS:HE3	1.68	0.57
3:B:742:ILE:HA	3:B:788:PHE:HE2	1.70	0.57
3:F:948:ILE:HD11	3:F:1007:SER:CA	2.35	0.57
1:A:72:ALA:HB2	3:B:260:CYS:HB2	1.87	0.57
3:F:392:LEU:HG	3:F:396:LEU:HG	1.87	0.57
3:F:938:PRO:CG	3:J:1092:ILE:HB	2.35	0.57
3:J:586:TYR:HA	3:J:589:GLN:HE22	1.70	0.57
3:J:853:LEU:HD12	3:J:880:ILE:CD1	2.35	0.57
3:N:63:TYR:O	3:N:72:PRO:HD3	2.05	0.57
1:A:445:LEU:CD1	1:A:563:THR:HG23	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:LEU:HD22	1:A:802:ARG:HH21	1.60	0.57
1:E:1209:THR:HG23	2:G:334:ILE:HG23	1.86	0.57
2:O:350:TYR:O	2:O:354:ILE:HG13	2.05	0.57
3:B:780:LEU:HG	3:B:784:TYR:CE2	2.39	0.57
3:F:63:TYR:O	3:F:72:PRO:HD3	2.05	0.57
3:J:734:CYS:SG	3:J:743:LEU:HD12	2.44	0.57
3:N:392:LEU:HG	3:N:396:LEU:HG	1.87	0.57
2:C:350:TYR:O	2:C:354:ILE:HG13	2.05	0.56
1:E:163:ASN:CB	1:E:489:ASN:HD21	2.16	0.56
1:E:1200:MET:CE	2:G:351:ALA:HA	2.35	0.56
3:J:148:CYS:HB3	3:J:170:LEU:HD13	1.86	0.56
3:J:574:VAL:HG23	3:J:618:LEU:HD11	1.87	0.56
1:A:51:ILE:HD13	1:A:84:LEU:HD13	1.87	0.56
1:A:251:THR:HA	1:A:1105:ILE:HG13	1.86	0.56
1:A:491:ARG:HG3	3:B:62:LEU:CD1	2.36	0.56
1:A:922:LEU:HD22	1:A:1121:PRO:HG3	1.87	0.56
1:A:1205:LYS:HG3	2:C:337:PRO:HG2	1.87	0.56
1:E:29:VAL:HG13	3:F:130:MET:HB2	1.87	0.56
1:E:29:VAL:HG22	3:F:130:MET:HB3	1.87	0.56
1:E:90:HIS:HD2	3:F:67:THR:O	1.88	0.56
2:G:359:VAL:HG21	2:G:367:ARG:CG	2.32	0.56
1:M:29:VAL:HG11	3:N:131:ARG:HG2	1.87	0.56
1:M:1205:LYS:HG3	2:O:337:PRO:HG2	1.87	0.56
1:I:894:THR:HA	1:I:920:ILE:HG21	1.85	0.56
3:B:236:SER:HB2	3:B:296:LEU:HD21	1.87	0.56
3:B:784:TYR:CD1	3:B:845:ARG:HD3	2.41	0.56
1:A:1200:MET:CE	2:C:351:ALA:HA	2.35	0.56
1:E:894:THR:HA	1:E:920:ILE:HG21	1.85	0.56
1:M:51:ILE:HD13	1:M:84:LEU:HD13	1.87	0.56
1:M:163:ASN:CB	1:M:489:ASN:HD21	2.16	0.56
1:M:251:THR:HA	1:M:1105:ILE:HG13	1.86	0.56
1:M:1208:ALA:HB2	4:M:1301:FAR:H51	1.88	0.56
1:M:1208:ALA:HB1	2:O:334:ILE:HG13	1.86	0.56
1:I:206:LYS:NZ	1:I:210:GLU:OE2	2.37	0.56
1:I:251:THR:HA	1:I:1105:ILE:HG13	1.85	0.56
1:I:1200:MET:CE	2:K:351:ALA:HA	2.35	0.56
3:B:393:THR:HB	3:B:394:PRO:HD3	1.87	0.56
3:B:731:LEU:HD21	3:B:744:LEU:HB2	1.86	0.56
3:B:1063:ARG:NH1	3:N:1079:GLU:HG2	2.19	0.56
3:B:1078:LEU:HD22	3:N:1067:SER:HB2	1.85	0.56
3:F:393:THR:HB	3:F:394:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:529:TRP:CD1	3:F:684:SER:HB3	2.38	0.56
3:F:586:TYR:HA	3:F:589:GLN:HE22	1.70	0.56
3:F:742:ILE:HA	3:F:788:PHE:HE2	1.70	0.56
3:F:853:LEU:HD12	3:F:880:ILE:CD1	2.35	0.56
3:F:1002:LEU:CD2	3:F:1024:LEU:HD22	2.35	0.56
3:N:148:CYS:HB3	3:N:170:LEU:HD13	1.86	0.56
3:N:587:MET:HE1	3:N:855:ILE:CD1	2.34	0.56
3:N:668:LEU:HG	3:N:670:PHE:CE2	2.41	0.56
1:A:1081:LYS:HB3	4:A:1301:FAR:C14	2.35	0.56
1:A:1208:ALA:HB2	4:A:1301:FAR:H51	1.88	0.56
1:E:922:LEU:HD22	1:E:1121:PRO:HG3	1.86	0.56
3:B:63:TYR:O	3:B:72:PRO:HD3	2.05	0.56
3:B:625:ASN:C	3:B:634:ILE:CD1	2.73	0.56
3:J:392:LEU:HG	3:J:396:LEU:HG	1.87	0.56
3:J:784:TYR:CD1	3:J:845:ARG:HD3	2.40	0.56
3:N:586:TYR:HA	3:N:589:GLN:HE22	1.70	0.56
3:N:742:ILE:HA	3:N:788:PHE:HE2	1.70	0.56
3:B:574:VAL:HG23	3:B:618:LEU:HD11	1.87	0.56
3:B:730:LYS:HB2	3:B:743:LEU:HD13	1.88	0.56
3:B:948:ILE:HD11	3:B:1007:SER:CA	2.35	0.56
3:F:574:VAL:HG23	3:F:618:LEU:HD11	1.87	0.56
3:F:850:GLN:HG3	3:F:880:ILE:CD1	2.36	0.56
3:N:393:THR:HB	3:N:394:PRO:HD3	1.88	0.56
1:A:397:LYS:HE3	1:A:400:HIS:HD2	1.71	0.56
1:M:1081:LYS:HB3	4:M:1301:FAR:C14	2.35	0.56
1:I:51:ILE:HD13	1:I:84:LEU:HD13	1.87	0.56
1:I:1208:ALA:HB2	4:I:1301:FAR:H51	1.88	0.56
3:J:236:SER:HB2	3:J:296:LEU:HD21	1.87	0.56
3:J:393:THR:HB	3:J:394:PRO:HD3	1.88	0.56
3:J:668:LEU:HG	3:J:670:PHE:CE2	2.40	0.56
3:J:974:MET:HE1	3:J:975:TYR:CE2	2.32	0.56
3:N:574:VAL:HG23	3:N:618:LEU:HD11	1.87	0.56
1:A:1140:ILE:HD12	1:A:1140:ILE:H	1.69	0.56
3:F:730:LYS:HB2	3:F:743:LEU:HD13	1.88	0.56
3:F:784:TYR:CD1	3:F:845:ARG:HD3	2.41	0.56
3:F:918:GLN:HE22	3:F:922:ARG:HH11	1.54	0.56
3:J:298:PRO:O	3:J:301:SER:O	2.24	0.56
3:J:948:ILE:HD11	3:J:1007:SER:CA	2.35	0.56
1:E:79:GLN:HB3	3:F:194:TYR:HB3	1.87	0.56
1:M:574:ASP:OD1	1:M:574:ASP:N	2.39	0.56
3:B:173:ASN:OD1	3:B:173:ASN:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:668:LEU:HG	3:B:670:PHE:CE2	2.41	0.56
3:F:668:LEU:HG	3:F:670:PHE:CE2	2.40	0.56
3:J:730:LYS:HB2	3:J:743:LEU:HD13	1.88	0.56
3:N:730:LYS:HB2	3:N:743:LEU:HD13	1.88	0.56
3:N:850:GLN:HG3	3:N:880:ILE:CD1	2.36	0.56
3:N:1002:LEU:CD2	3:N:1024:LEU:HD22	2.35	0.56
1:A:788:THR:O	1:A:792:PRO:HG2	2.03	0.56
1:E:86:ARG:HH22	3:F:120:LYS:HG3	1.69	0.56
1:E:419:ALA:CB	3:B:524:GLU:OE1	2.47	0.56
1:E:491:ARG:CD	3:F:62:LEU:HG	2.36	0.56
3:B:1092:ILE:HD12	3:N:1001:GLU:CA	2.35	0.56
3:B:1092:ILE:HD12	3:N:1001:GLU:CG	1.94	0.56
3:F:298:PRO:O	3:F:301:SER:O	2.24	0.56
3:J:477:ARG:NH2	3:N:460:SER:HB2	2.21	0.56
3:J:742:ILE:HA	3:J:788:PHE:HE2	1.70	0.56
3:J:751:GLU:HB3	3:J:755:PHE:CG	2.41	0.56
3:J:953:PRO:HD2	3:J:1018:PHE:O	2.06	0.56
3:N:953:PRO:HD2	3:N:1018:PHE:O	2.06	0.56
3:B:598:ILE:CD1	3:B:637:MET:SD	2.94	0.56
3:B:918:GLN:HE22	3:B:922:ARG:HH11	1.54	0.56
3:F:115:GLU:O	3:F:119:ILE:HD12	2.06	0.56
3:F:236:SER:HB2	3:F:296:LEU:HD21	1.87	0.56
3:F:283:LEU:CD2	3:F:307:LEU:HD21	2.31	0.56
3:F:953:PRO:HD2	3:F:1018:PHE:O	2.06	0.56
3:J:1002:LEU:CD2	3:J:1024:LEU:HD22	2.35	0.56
3:N:236:SER:HB2	3:N:296:LEU:HD21	1.87	0.56
3:N:598:ILE:CD1	3:N:637:MET:SD	2.94	0.56
1:E:68:ASP:CG	3:F:259:GLY:O	2.45	0.55
1:M:397:LYS:HE3	1:M:400:HIS:HD2	1.71	0.55
3:B:586:TYR:HA	3:B:589:GLN:HE22	1.70	0.55
3:B:850:GLN:HG3	3:B:880:ILE:CD1	2.36	0.55
3:F:598:ILE:CD1	3:F:637:MET:SD	2.94	0.55
3:F:751:GLU:HB3	3:F:755:PHE:CG	2.41	0.55
3:J:115:GLU:O	3:J:119:ILE:HD12	2.06	0.55
3:J:598:ILE:CD1	3:J:637:MET:SD	2.94	0.55
3:N:298:PRO:O	3:N:301:SER:O	2.24	0.55
3:N:784:TYR:CD1	3:N:845:ARG:HD3	2.41	0.55
1:A:339:GLY:HA2	1:A:344:ASN:HB2	1.89	0.55
1:A:919:ARG:HE	1:A:922:LEU:HD12	1.70	0.55
1:M:919:ARG:HE	1:M:922:LEU:HD12	1.70	0.55
1:I:397:LYS:HE3	1:I:400:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:298:PRO:O	3:B:301:SER:O	2.24	0.55
3:B:1018:PHE:CD2	3:B:1022:VAL:CG2	2.90	0.55
3:F:1082:VAL:CG2	3:J:1060:LEU:HD22	2.36	0.55
3:F:1091:LEU:HD23	3:J:944:ARG:NH1	2.22	0.55
4:F:1101:FAR:C14	3:J:1012:ARG:HB2	2.36	0.55
3:J:795:SER:OG	3:J:855:ILE:HD11	2.02	0.55
3:J:948:ILE:HD12	3:J:1010:LEU:HD12	1.89	0.55
1:E:51:ILE:HD13	1:E:84:LEU:HD13	1.87	0.55
1:M:339:GLY:HA2	1:M:344:ASN:HB2	1.89	0.55
1:I:1205:LYS:HG3	2:K:337:PRO:HG2	1.87	0.55
3:B:751:GLU:HB3	3:B:755:PHE:CG	2.41	0.55
2:G:350:TYR:O	2:G:354:ILE:HG13	2.05	0.55
1:M:1168:THR:C	1:M:1170:GLY:N	2.52	0.55
3:B:949:LEU:HD22	3:B:963:LEU:CD2	2.37	0.55
3:B:953:PRO:HD2	3:B:1018:PHE:O	2.06	0.55
3:N:115:GLU:O	3:N:119:ILE:HD12	2.06	0.55
1:E:206:LYS:NZ	1:E:210:GLU:OE2	2.37	0.55
1:E:919:ARG:HE	1:E:922:LEU:HD12	1.70	0.55
3:J:850:GLN:HG3	3:J:880:ILE:CD1	2.36	0.55
1:M:1200:MET:HE1	2:O:354:ILE:HD12	1.88	0.55
1:I:339:GLY:HA2	1:I:344:ASN:HB2	1.89	0.55
3:F:283:LEU:CD2	3:F:307:LEU:CD2	2.83	0.55
1:A:610:THR:HG22	3:F:635:LEU:CD2	2.37	0.55
1:E:397:LYS:HE3	1:E:400:HIS:HD2	1.71	0.55
1:E:1197:PHE:HE2	2:G:373:ASN:O	1.90	0.55
1:M:491:ARG:HG2	3:N:62:LEU:HD11	1.88	0.55
1:I:919:ARG:HE	1:I:922:LEU:HD12	1.70	0.55
3:B:367:ILE:HD11	3:B:447:LEU:HD12	1.89	0.55
3:B:477:ARG:HH22	3:F:460:SER:CB	2.20	0.55
3:F:213:TYR:O	3:F:234:LEU:HD21	2.07	0.55
3:F:569:LEU:HD13	3:F:679:LEU:HB3	1.89	0.55
3:F:948:ILE:HD12	3:F:1010:LEU:HD12	1.89	0.55
3:J:918:GLN:HE22	3:J:922:ARG:HH11	1.54	0.55
1:A:574:ASP:N	1:A:574:ASP:OD1	2.39	0.55
1:E:152:GLY:HA3	3:B:661:SER:OG	2.07	0.55
1:E:809:LEU:HA	1:E:812:GLU:HB3	1.89	0.55
1:I:809:LEU:HA	1:I:812:GLU:HB3	1.89	0.55
1:I:1171:ALA:HB2	2:K:377:ALA:HB2	1.88	0.55
3:B:115:GLU:O	3:B:119:ILE:HD12	2.06	0.55
3:F:751:GLU:HB3	3:F:755:PHE:CB	2.37	0.55
3:F:1018:PHE:CD2	3:F:1022:VAL:CG2	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:948:ILE:HD12	3:N:1010:LEU:HD12	1.89	0.55
1:A:1197:PHE:HE2	2:C:373:ASN:O	1.90	0.55
1:E:86:ARG:HH12	3:F:120:LYS:HZ3	1.53	0.55
1:E:788:THR:O	1:E:792:PRO:HG2	2.03	0.55
1:I:1208:ALA:CB	2:K:334:ILE:CG1	2.85	0.55
3:N:361:ILE:CD1	3:N:421:LYS:HE2	2.35	0.55
3:N:949:LEU:HD22	3:N:963:LEU:CD2	2.37	0.55
1:E:64:ASN:CA	3:B:567:ARG:HH21	2.19	0.55
1:M:1087:VAL:HG21	1:M:1115:LEU:HD12	1.89	0.55
1:M:1197:PHE:HE2	2:O:373:ASN:O	1.90	0.55
3:F:587:MET:HE1	3:F:855:ILE:HG13	1.87	0.55
3:N:751:GLU:HB3	3:N:755:PHE:CB	2.37	0.55
3:N:751:GLU:HB3	3:N:755:PHE:CG	2.41	0.55
3:N:948:ILE:HD11	3:N:1007:SER:CA	2.35	0.55
1:E:1208:ALA:HB2	4:E:1301:FAR:H51	1.88	0.54
1:M:1074:LYS:HE2	2:O:353:ARG:NH2	2.23	0.54
3:F:949:LEU:HD22	3:F:963:LEU:CD2	2.37	0.54
1:A:71:LYS:HD2	3:B:258:GLN:NE2	2.22	0.54
1:A:1087:VAL:HG21	1:A:1115:LEU:HD12	1.89	0.54
1:E:29:VAL:HG13	3:F:130:MET:CB	2.37	0.54
3:F:949:LEU:HD22	3:F:963:LEU:HD21	1.90	0.54
3:J:45:LEU:HD23	3:J:104:ILE:CG1	2.37	0.54
3:J:949:LEU:HD22	3:J:963:LEU:CD2	2.37	0.54
1:E:610:THR:HG22	3:B:635:LEU:CD2	2.38	0.54
1:E:936:ARG:H	1:E:936:ARG:HD2	1.72	0.54
1:E:1087:VAL:HG21	1:E:1115:LEU:HD12	1.89	0.54
1:E:1208:ALA:CB	2:G:334:ILE:CG1	2.85	0.54
1:I:574:ASP:N	1:I:574:ASP:OD1	2.39	0.54
3:F:1059:PRO:HG3	3:J:1093:SER:C	2.27	0.54
3:N:213:TYR:O	3:N:234:LEU:HD21	2.07	0.54
3:N:367:ILE:HD11	3:N:447:LEU:HD12	1.89	0.54
1:E:1081:LYS:HB3	4:E:1301:FAR:C14	2.35	0.54
1:M:809:LEU:HA	1:M:812:GLU:HB3	1.89	0.54
1:I:69:GLU:HG3	3:J:262:TRP:CZ3	2.43	0.54
1:I:1087:VAL:HG21	1:I:1115:LEU:HD12	1.89	0.54
3:J:569:LEU:HD13	3:J:679:LEU:HB3	1.89	0.54
1:M:75:TYR:HH	3:N:191:GLN:CD	2.11	0.54
1:I:1074:LYS:HE2	2:K:353:ARG:NH2	2.23	0.54
3:B:213:TYR:O	3:B:234:LEU:HD21	2.07	0.54
3:B:361:ILE:CD1	3:B:421:LYS:HE2	2.35	0.54
3:F:965:GLN:O	3:F:969:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:949:LEU:HD22	3:J:963:LEU:HD21	1.90	0.54
1:A:491:ARG:CG	3:B:62:LEU:HD11	2.38	0.54
1:A:1171:ALA:HB2	2:C:377:ALA:HB2	1.88	0.54
1:E:1205:LYS:HG3	2:G:337:PRO:HG2	1.87	0.54
1:M:1171:ALA:HB2	2:O:377:ALA:HB2	1.88	0.54
1:M:1208:ALA:CB	2:O:334:ILE:CG1	2.85	0.54
3:B:751:GLU:HB3	3:B:755:PHE:CB	2.37	0.54
3:F:45:LEU:HD23	3:F:104:ILE:CG1	2.37	0.54
3:J:751:GLU:HB3	3:J:755:PHE:CB	2.37	0.54
3:J:1018:PHE:CD2	3:J:1022:VAL:CG2	2.90	0.54
3:N:737:LEU:HD21	3:N:772:ARG:NH2	2.23	0.54
1:A:1074:LYS:HE2	2:C:353:ARG:NH2	2.23	0.54
1:A:1208:ALA:CB	2:C:334:ILE:CG1	2.85	0.54
1:I:491:ARG:CG	3:J:62:LEU:CD1	2.85	0.54
1:I:936:ARG:H	1:I:936:ARG:HD2	1.72	0.54
3:B:45:LEU:HD23	3:B:104:ILE:CG1	2.37	0.54
3:B:948:ILE:HD12	3:B:1010:LEU:HD12	1.89	0.54
3:F:1092:ILE:HG21	3:J:1001:GLU:HG2	1.89	0.54
3:J:965:GLN:O	3:J:969:LEU:HG	2.08	0.54
3:N:965:GLN:O	3:N:969:LEU:HG	2.07	0.54
1:E:1200:MET:CE	2:G:354:ILE:HD12	2.38	0.54
1:M:1127:LEU:CD2	1:M:1151:VAL:HG12	2.38	0.54
2:K:359:VAL:CG2	2:K:367:ARG:HG2	2.36	0.54
3:F:587:MET:CE	3:F:855:ILE:HG13	2.38	0.54
3:J:213:TYR:O	3:J:234:LEU:HD21	2.07	0.54
1:A:809:LEU:HA	1:A:812:GLU:HB3	1.89	0.54
1:E:339:GLY:HA2	1:E:344:ASN:HB2	1.89	0.54
1:E:1171:ALA:HB2	2:G:377:ALA:HB2	1.88	0.54
1:I:1197:PHE:HE2	2:K:373:ASN:O	1.90	0.54
3:B:737:LEU:HD21	3:B:772:ARG:NH2	2.23	0.54
3:B:1002:LEU:CD2	3:B:1024:LEU:HD22	2.35	0.54
3:B:1092:ILE:HG21	3:N:1004:MET:CB	2.38	0.54
3:F:374:ILE:HG23	3:F:454:LEU:HD12	1.89	0.54
3:F:1015:GLU:CD	3:J:1012:ARG:HH22	2.11	0.54
1:A:1127:LEU:CD2	1:A:1151:VAL:HG12	2.38	0.54
1:A:1200:MET:CE	2:C:354:ILE:HD12	2.38	0.54
1:E:574:ASP:OD1	1:E:574:ASP:N	2.39	0.54
1:E:1074:LYS:HE2	2:G:353:ARG:NH2	2.23	0.54
1:M:936:ARG:H	1:M:936:ARG:HD2	1.72	0.54
1:I:75:TYR:HH	3:J:191:GLN:CD	2.10	0.54
3:F:1015:GLU:HG3	3:J:1012:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:569:LEU:HD13	3:N:679:LEU:HB3	1.89	0.54
3:N:918:GLN:HE22	3:N:922:ARG:HH11	1.54	0.54
3:N:949:LEU:HD22	3:N:963:LEU:HD21	1.90	0.54
1:I:68:ASP:OD2	3:J:260:CYS:HA	2.08	0.53
3:B:342:LEU:CD2	3:B:421:LYS:NZ	2.72	0.53
3:B:374:ILE:HG23	3:B:454:LEU:HD12	1.89	0.53
3:B:965:GLN:O	3:B:969:LEU:HG	2.08	0.53
3:F:283:LEU:O	3:F:284:PRO:C	2.45	0.53
3:F:367:ILE:HD11	3:F:447:LEU:HD12	1.89	0.53
1:A:783:LEU:O	1:A:787:TYR:CE2	2.61	0.53
1:A:936:ARG:H	1:A:936:ARG:HD2	1.72	0.53
2:C:329:THR:O	2:C:332:ILE:HG13	2.09	0.53
1:E:939:ALA:O	1:E:943:THR:HG23	2.09	0.53
1:M:823:TRP:CE3	1:M:826:ILE:HD12	2.43	0.53
2:K:329:THR:O	2:K:332:ILE:HG13	2.09	0.53
3:J:374:ILE:HG23	3:J:454:LEU:HD12	1.89	0.53
3:J:587:MET:CE	3:J:855:ILE:HG13	2.38	0.53
3:N:45:LEU:HD23	3:N:104:ILE:CG1	2.38	0.53
3:N:374:ILE:HG23	3:N:454:LEU:HD12	1.89	0.53
1:E:376:PRO:HD3	1:E:392:ARG:HA	1.91	0.53
1:E:783:LEU:O	1:E:787:TYR:CE2	2.61	0.53
1:M:783:LEU:O	1:M:787:TYR:CE2	2.61	0.53
3:F:342:LEU:CD2	3:F:421:LYS:NZ	2.72	0.53
3:N:1018:PHE:CD2	3:N:1022:VAL:CG2	2.90	0.53
2:O:329:THR:O	2:O:332:ILE:HG13	2.09	0.53
1:I:376:PRO:HD3	1:I:392:ARG:HA	1.91	0.53
3:J:477:ARG:NH1	3:N:103:ARG:NH2	2.57	0.53
3:N:568:ILE:HG12	3:N:668:LEU:HD22	1.91	0.53
1:A:51:ILE:HG13	1:A:81:VAL:HG22	1.91	0.53
1:E:491:ARG:CG	3:F:62:LEU:HD12	2.20	0.53
1:E:768:LEU:HD22	1:E:802:ARG:HH21	1.60	0.53
1:M:63:LYS:C	3:J:567:ARG:NH2	2.57	0.53
1:M:939:ALA:O	1:M:943:THR:HG23	2.09	0.53
3:B:288:ARG:HH11	3:B:978:ASN:HD21	1.57	0.53
3:B:568:ILE:HG12	3:B:668:LEU:HD22	1.91	0.53
3:F:737:LEU:HD21	3:F:772:ARG:NH2	2.23	0.53
3:F:1015:GLU:OE2	4:F:1101:FAR:H42	2.05	0.53
3:J:460:SER:CB	3:N:477:ARG:HH22	2.21	0.53
1:A:791:GLY:N	1:A:792:PRO:HD2	2.24	0.53
1:A:939:ALA:O	1:A:943:THR:HG23	2.09	0.53
2:G:375:PRO:HD2	2:G:378:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:ILE:HG13	1:M:81:VAL:HG22	1.91	0.53
1:I:75:TYR:HH	3:J:191:GLN:HB3	1.73	0.53
1:I:823:TRP:CE3	1:I:826:ILE:HD12	2.43	0.53
1:I:1200:MET:CE	2:K:354:ILE:HD12	2.38	0.53
2:K:338:TYR:CE1	2:K:344:ARG:HG3	2.44	0.53
3:B:850:GLN:O	3:B:854:VAL:HG23	2.09	0.53
3:F:1004:MET:CG	3:J:1092:ILE:HG22	2.37	0.53
3:N:342:LEU:CD2	3:N:421:LYS:NZ	2.72	0.53
1:E:823:TRP:CE3	1:E:826:ILE:HD12	2.43	0.53
1:E:1127:LEU:CD2	1:E:1151:VAL:HG12	2.38	0.53
1:M:1200:MET:CE	2:O:354:ILE:HD12	2.38	0.53
1:I:783:LEU:O	1:I:787:TYR:CE2	2.61	0.53
3:B:949:LEU:HD22	3:B:963:LEU:HD21	1.90	0.53
3:F:1004:MET:HE1	3:J:1091:LEU:HB2	1.90	0.53
3:J:367:ILE:HD11	3:J:447:LEU:HD12	1.89	0.53
1:A:823:TRP:CE3	1:A:826:ILE:HD12	2.43	0.53
2:G:329:THR:O	2:G:332:ILE:HG13	2.09	0.53
1:M:93:ILE:HG22	3:N:67:THR:HG23	1.78	0.53
1:I:69:GLU:HG3	3:J:262:TRP:HZ3	1.74	0.53
1:I:1127:LEU:CD2	1:I:1151:VAL:HG12	2.38	0.53
3:B:587:MET:CE	3:B:855:ILE:HG13	2.38	0.53
3:F:1091:LEU:HD12	3:J:939:THR:CG2	2.39	0.53
3:J:361:ILE:CD1	3:J:421:LYS:HE2	2.35	0.53
1:M:57:LEU:HB3	1:M:77:LEU:HD13	1.91	0.53
1:M:314:GLU:N	1:M:317:GLU:OE2	2.40	0.53
1:M:791:GLY:N	1:M:792:PRO:HD2	2.24	0.53
3:B:279:LEU:O	3:B:283:LEU:HD22	2.09	0.53
3:F:1082:VAL:HG23	3:J:1060:LEU:HB3	1.91	0.53
3:J:320:VAL:O	3:J:324:LEU:HB2	2.09	0.53
3:N:587:MET:CE	3:N:855:ILE:HG13	2.38	0.53
3:N:850:GLN:O	3:N:854:VAL:HG23	2.09	0.53
3:N:965:GLN:CD	3:N:969:LEU:HD11	2.22	0.53
1:M:69:GLU:CG	3:N:262:TRP:CZ3	2.92	0.52
1:I:101:SER:OG	1:I:110:ASP:OD2	2.27	0.52
1:I:189:LYS:HG3	1:I:296:PHE:HE2	1.74	0.52
3:B:569:LEU:HD13	3:B:679:LEU:HB3	1.89	0.52
3:B:1013:ASN:ND2	4:B:1101:FAR:C15	2.68	0.52
1:A:57:LEU:HB3	1:A:77:LEU:HD13	1.91	0.52
1:E:189:LYS:HG3	1:E:296:PHE:HE2	1.74	0.52
3:F:320:VAL:O	3:F:324:LEU:HB2	2.10	0.52
3:F:564:LYS:HE3	3:F:666:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:342:LEU:CD2	3:J:421:LYS:NZ	2.72	0.52
3:J:737:LEU:HD21	3:J:772:ARG:NH2	2.23	0.52
1:A:504:VAL:O	1:A:508:SER:OG	2.20	0.52
1:M:376:PRO:HD3	1:M:392:ARG:HA	1.91	0.52
1:I:939:ALA:O	1:I:943:THR:HG23	2.09	0.52
3:N:320:VAL:O	3:N:324:LEU:HB2	2.09	0.52
1:A:1169:LEU:HD12	2:C:375:PRO:HG2	1.92	0.52
1:M:1169:LEU:HD12	2:O:375:PRO:HG2	1.92	0.52
1:I:75:TYR:OH	3:J:191:GLN:CD	2.47	0.52
1:I:880:ILE:HD11	1:I:898:MET:HE1	1.91	0.52
3:B:1093:SER:C	3:N:1059:PRO:HG3	2.28	0.52
3:F:486:GLN:NE2	3:F:492:ASP:O	2.41	0.52
3:F:574:VAL:CG2	3:F:618:LEU:HD11	2.40	0.52
3:F:1014:PRO:HD2	3:J:1012:ARG:CZ	2.39	0.52
3:F:1015:GLU:OE1	4:F:1101:FAR:C6	2.47	0.52
3:J:564:LYS:HE3	3:J:666:GLU:OE1	2.09	0.52
3:N:127:TYR:CZ	3:N:131:ARG:HD2	2.44	0.52
3:N:564:LYS:HE3	3:N:666:GLU:OE1	2.10	0.52
3:N:1013:ASN:ND2	4:N:1101:FAR:C15	2.68	0.52
1:A:781:ASP:HA	1:A:825:LEU:HD21	1.91	0.52
1:E:422:GLU:OE2	3:B:525:PRO:HB3	2.10	0.52
1:M:69:GLU:CG	3:N:262:TRP:HZ3	2.23	0.52
1:M:300:GLY:O	1:M:313:TYR:OH	2.21	0.52
2:O:338:TYR:CE1	2:O:344:ARG:HG3	2.44	0.52
3:B:814:ALA:HB3	3:B:817:HIS:HB2	1.92	0.52
3:F:568:ILE:HG12	3:F:668:LEU:HD22	1.91	0.52
3:F:1082:VAL:CG2	3:J:1060:LEU:HD23	2.25	0.52
3:J:127:TYR:CZ	3:J:131:ARG:HD2	2.44	0.52
3:J:568:ILE:HG12	3:J:668:LEU:HD22	1.91	0.52
3:N:751:GLU:HB3	3:N:755:PHE:HB2	1.91	0.52
1:E:51:ILE:HG13	1:E:81:VAL:HG22	1.91	0.52
2:G:338:TYR:CE1	2:G:344:ARG:HG3	2.44	0.52
1:M:72:ALA:HB2	3:N:260:CYS:HB2	1.91	0.52
3:B:751:GLU:HB3	3:B:755:PHE:HB2	1.91	0.52
3:B:965:GLN:CD	3:B:969:LEU:HD11	2.22	0.52
3:J:850:GLN:O	3:J:854:VAL:HG23	2.09	0.52
1:M:42:ALA:HB1	1:M:47:ASN:HD21	1.75	0.52
1:M:75:TYR:HH	3:N:191:GLN:HB3	1.75	0.52
1:I:781:ASP:HA	1:I:825:LEU:HD21	1.91	0.52
3:B:127:TYR:CZ	3:B:131:ARG:HD2	2.44	0.52
3:B:1008:ILE:HG21	4:N:1101:FAR:H51	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1062:LYS:HE2	3:N:1019:GLN:HE22	1.74	0.52
3:F:70:LEU:HD11	3:F:128:CYS:SG	2.50	0.52
3:J:751:GLU:HB3	3:J:755:PHE:HB2	1.91	0.52
3:N:70:LEU:HD11	3:N:128:CYS:SG	2.50	0.52
1:M:491:ARG:CG	3:N:62:LEU:CD1	2.87	0.52
1:M:1120:GLN:HE22	1:M:1181:ALA:HB3	1.71	0.52
1:M:1192:ALA:HB3	2:O:372:GLU:HB2	1.92	0.52
3:F:850:GLN:O	3:F:854:VAL:HG23	2.09	0.52
3:F:853:LEU:HD12	3:F:880:ILE:HD11	1.92	0.52
3:J:103:ARG:NH2	3:N:477:ARG:NH1	2.57	0.52
1:A:42:ALA:HB1	1:A:47:ASN:HD21	1.75	0.52
2:C:338:TYR:CE1	2:C:344:ARG:HG3	2.44	0.52
1:E:781:ASP:HA	1:E:825:LEU:HD21	1.91	0.52
2:G:359:VAL:CG2	2:G:367:ARG:HG2	2.36	0.52
1:M:28:PRO:HG3	3:N:547:LEU:CG	2.40	0.52
1:M:189:LYS:HG3	1:M:296:PHE:HE2	1.74	0.52
1:M:781:ASP:HA	1:M:825:LEU:HD21	1.91	0.52
3:B:460:SER:CB	3:F:477:ARG:NH2	2.72	0.52
3:B:784:TYR:CE1	3:B:845:ARG:HD3	2.45	0.52
3:F:962:HIS:HE1	3:F:1021:LYS:HD3	1.75	0.52
3:N:814:ALA:HB3	3:N:817:HIS:HB2	1.92	0.52
3:N:1015:GLU:OE1	4:N:1101:FAR:C6	2.45	0.52
1:A:1192:ALA:HB3	2:C:372:GLU:HB2	1.92	0.52
1:E:880:ILE:HD11	1:E:898:MET:HE1	1.92	0.52
1:I:791:GLY:N	1:I:792:PRO:HD2	2.24	0.52
3:B:69:GLY:HA3	3:B:120:LYS:HG2	1.92	0.52
3:B:962:HIS:HE1	3:B:1021:LYS:HD3	1.75	0.52
3:N:574:VAL:CG2	3:N:618:LEU:HD11	2.40	0.52
1:A:1205:LYS:HG3	2:C:337:PRO:CG	2.40	0.51
1:E:90:HIS:CD2	3:F:67:THR:O	2.62	0.51
1:E:1169:LEU:HD12	2:G:375:PRO:HG2	1.91	0.51
1:M:880:ILE:HD11	1:M:898:MET:HE1	1.91	0.51
1:M:1205:LYS:HG3	2:O:337:PRO:CG	2.40	0.51
3:B:591:VAL:CG2	3:B:634:ILE:HG13	2.40	0.51
3:F:69:GLY:HA3	3:F:120:LYS:HG2	1.92	0.51
3:J:70:LEU:HD11	3:J:128:CYS:SG	2.50	0.51
3:J:853:LEU:HD12	3:J:880:ILE:HD11	1.92	0.51
3:N:69:GLY:HA3	3:N:120:LYS:HG2	1.92	0.51
1:E:94:ARG:HH12	3:F:157:THR:HB	1.74	0.51
1:E:486:LEU:HD13	1:E:618:PHE:CD1	2.46	0.51
1:M:486:LEU:HD13	1:M:618:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:ALA:HB1	1:I:47:ASN:HD21	1.75	0.51
1:I:51:ILE:HG13	1:I:81:VAL:HG22	1.91	0.51
1:I:486:LEU:HD13	1:I:618:PHE:CD1	2.46	0.51
3:B:800:ILE:HD12	3:B:831:ILE:HD13	1.93	0.51
3:F:127:TYR:CZ	3:F:131:ARG:HD2	2.44	0.51
3:J:274:ARG:HH22	3:J:802:THR:CA	2.22	0.51
3:J:574:VAL:CG2	3:J:618:LEU:HD11	2.40	0.51
3:J:962:HIS:CE1	3:J:1021:LYS:HD3	2.45	0.51
3:N:274:ARG:HH22	3:N:802:THR:CA	2.22	0.51
1:A:880:ILE:HD11	1:A:898:MET:HE1	1.92	0.51
1:I:57:LEU:HB3	1:I:77:LEU:HD13	1.91	0.51
3:B:564:LYS:HE3	3:B:666:GLU:OE1	2.09	0.51
3:B:574:VAL:CG2	3:B:618:LEU:HD11	2.40	0.51
3:B:962:HIS:CE1	3:B:1021:LYS:HD3	2.45	0.51
3:F:274:ARG:HH22	3:F:802:THR:CA	2.22	0.51
3:F:544:ASN:HD22	3:F:547:LEU:HG	1.76	0.51
3:J:183:VAL:HG11	3:J:248:ALA:HB1	1.92	0.51
3:N:122:MET:HE3	3:N:178:TYR:CE1	2.46	0.51
1:E:42:ALA:HB1	1:E:47:ASN:HD21	1.75	0.51
1:I:69:GLU:O	1:I:73:LYS:HG3	2.11	0.51
3:F:210:GLU:HA	3:F:246:LEU:HD11	1.93	0.51
3:F:962:HIS:CE1	3:F:1021:LYS:HD3	2.45	0.51
1:A:376:PRO:HD3	1:A:392:ARG:HA	1.91	0.51
1:E:817:VAL:HG23	1:E:826:ILE:HG12	1.92	0.51
1:I:1169:LEU:HD12	2:K:375:PRO:HG2	1.91	0.51
3:B:70:LEU:HD11	3:B:128:CYS:SG	2.50	0.51
3:B:320:VAL:O	3:B:324:LEU:HB2	2.10	0.51
3:B:632:ASN:HB2	3:B:633:PRO:HD3	1.93	0.51
3:N:183:VAL:HG11	3:N:248:ALA:HB1	1.92	0.51
1:A:314:GLU:N	1:A:317:GLU:OE2	2.40	0.51
3:B:210:GLU:HA	3:B:246:LEU:HD11	1.93	0.51
3:B:577:PRO:HD2	3:B:580:PHE:HD2	1.76	0.51
3:F:183:VAL:HG11	3:F:248:ALA:HB1	1.92	0.51
3:F:724:THR:HB	3:F:726:GLU:HB2	1.92	0.51
3:J:69:GLY:HA3	3:J:120:LYS:HG2	1.92	0.51
3:J:830:VAL:O	3:J:834:ILE:HG13	2.11	0.51
3:J:962:HIS:HE1	3:J:1021:LYS:HD3	1.75	0.51
3:N:849:ILE:HG23	3:N:880:ILE:HD13	1.92	0.51
1:A:90:HIS:HA	1:A:93:ILE:HB	1.93	0.51
1:M:872:PRO:CD	1:M:872:PRO:O	2.58	0.51
2:O:375:PRO:HD2	2:O:378:VAL:CG1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:357:ALA:HB2	1:I:398:LEU:HD11	1.93	0.51
3:F:726:GLU:C	3:F:729:GLN:H	2.14	0.51
3:J:210:GLU:HA	3:J:246:LEU:HD11	1.93	0.51
3:J:849:ILE:HG23	3:J:880:ILE:HD13	1.92	0.51
3:N:210:GLU:HA	3:N:246:LEU:HD11	1.93	0.51
1:E:57:LEU:HB3	1:E:77:LEU:HD13	1.91	0.51
1:E:69:GLU:O	1:E:73:LYS:HG3	2.11	0.51
1:E:357:ALA:HB2	1:E:398:LEU:HD11	1.93	0.51
1:E:848:LEU:HD11	1:E:867:ILE:HG22	1.93	0.51
1:E:1200:MET:HE1	2:G:354:ILE:HD12	1.93	0.51
1:I:872:PRO:CD	1:I:872:PRO:O	2.58	0.51
3:B:283:LEU:HD23	3:B:307:LEU:HD21	1.92	0.51
3:B:486:GLN:NE2	3:B:492:ASP:O	2.41	0.51
1:M:90:HIS:HA	1:M:93:ILE:HB	1.93	0.51
1:I:1156:HIS:O	1:I:1159:ASN:N	2.44	0.51
1:I:1192:ALA:HB3	2:K:372:GLU:HB2	1.92	0.51
1:I:1205:LYS:HG3	2:K:337:PRO:CG	2.40	0.51
3:F:523:VAL:O	3:F:523:VAL:CG2	2.56	0.51
3:F:745:GLY:HA2	3:F:766:ILE:HD11	1.93	0.51
3:F:751:GLU:HB3	3:F:755:PHE:HB2	1.91	0.51
3:F:814:ALA:HB3	3:F:817:HIS:HB2	1.92	0.51
3:J:598:ILE:HD13	3:J:637:MET:SD	2.51	0.51
3:J:784:TYR:CE1	3:J:845:ARG:HD3	2.45	0.51
3:N:486:GLN:NE2	3:N:492:ASP:O	2.41	0.51
3:N:784:TYR:CE1	3:N:845:ARG:HD3	2.45	0.51
3:N:853:LEU:HD12	3:N:880:ILE:HD11	1.92	0.51
3:N:962:HIS:HE1	3:N:1021:LYS:HD3	1.75	0.51
1:A:189:LYS:HG3	1:A:296:PHE:HE2	1.74	0.51
1:A:486:LEU:HD13	1:A:618:PHE:CD1	2.46	0.51
1:A:1156:HIS:O	1:A:1159:ASN:N	2.44	0.51
3:B:183:VAL:HG11	3:B:248:ALA:HB1	1.92	0.51
3:B:556:PRO:HB2	5:B:1102:ADP:C8	2.46	0.51
3:B:830:VAL:O	3:B:834:ILE:HG13	2.11	0.51
3:F:74:LYS:CD	3:F:439:LYS:HZ1	2.14	0.51
3:F:342:LEU:HD22	3:F:421:LYS:NZ	2.26	0.51
3:J:342:LEU:HD23	3:J:357:LEU:HB3	1.93	0.51
3:J:591:VAL:CG2	3:J:634:ILE:HG13	2.40	0.51
3:J:724:THR:HB	3:J:726:GLU:HB2	1.93	0.51
3:N:598:ILE:HD12	3:N:637:MET:SD	2.51	0.51
3:N:632:ASN:HB2	3:N:633:PRO:HD3	1.93	0.51
1:E:314:GLU:N	1:E:317:GLU:OE2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1156:HIS:O	1:E:1159:ASN:N	2.44	0.50
1:E:1172:ASP:HB3	1:E:1175:MET:CB	2.35	0.50
1:M:441:GLN:OE1	1:M:607:PHE:CD1	2.64	0.50
1:I:848:LEU:HD11	1:I:867:ILE:HG22	1.93	0.50
3:F:283:LEU:CD2	3:F:307:LEU:HD11	2.42	0.50
3:N:577:PRO:HD2	3:N:580:PHE:HD2	1.76	0.50
3:N:830:VAL:O	3:N:834:ILE:HG13	2.11	0.50
1:M:1086:SER:OG	1:M:1148:ILE:CG2	2.60	0.50
1:I:441:GLN:OE1	1:I:607:PHE:CD1	2.64	0.50
3:B:726:GLU:C	3:B:729:GLN:H	2.14	0.50
3:B:1060:LEU:CD2	3:N:1082:VAL:HG21	2.41	0.50
3:F:784:TYR:CE1	3:F:845:ARG:HD3	2.45	0.50
3:F:830:VAL:O	3:F:834:ILE:HG13	2.11	0.50
3:F:1009:VAL:CA	4:F:1103:FAR:H141	2.25	0.50
3:J:477:ARG:HH22	3:N:460:SER:CB	2.23	0.50
3:J:544:ASN:HD22	3:J:547:LEU:HG	1.75	0.50
3:J:577:PRO:HD2	3:J:580:PHE:HD2	1.76	0.50
3:J:625:ASN:HB3	3:J:634:ILE:HD11	1.94	0.50
3:N:800:ILE:HD12	3:N:831:ILE:HD13	1.93	0.50
1:M:1156:HIS:O	1:M:1159:ASN:N	2.43	0.50
1:I:1208:ALA:HB1	2:K:334:ILE:CG1	2.42	0.50
3:B:849:ILE:HG23	3:B:880:ILE:HD13	1.92	0.50
3:F:598:ILE:HD12	3:F:637:MET:SD	2.51	0.50
3:J:715:ASN:HB3	3:J:718:GLU:HG2	1.94	0.50
3:J:1023:ASP:HB3	3:J:1026:ARG:HB2	1.92	0.50
3:J:1090:CYS:HB3	3:J:1093:SER:HB2	1.94	0.50
3:N:342:LEU:HD22	3:N:421:LYS:NZ	2.26	0.50
3:N:342:LEU:HD23	3:N:357:LEU:HB3	1.94	0.50
1:A:441:GLN:OE1	1:A:607:PHE:CD1	2.64	0.50
1:A:1209:THR:HG23	2:C:334:ILE:HG21	1.93	0.50
1:E:1192:ALA:HB3	2:G:372:GLU:HB2	1.92	0.50
1:E:1205:LYS:HG3	2:G:337:PRO:CG	2.41	0.50
1:M:69:GLU:O	1:M:73:LYS:HG3	2.11	0.50
1:I:83:LYS:CE	3:J:198:GLU:OE1	2.59	0.50
1:I:264:SER:OG	1:I:265:PHE:N	2.44	0.50
2:K:375:PRO:HD2	2:K:378:VAL:CG1	2.38	0.50
3:B:724:THR:HB	3:B:726:GLU:HB2	1.92	0.50
3:B:853:LEU:HD12	3:B:880:ILE:HD11	1.92	0.50
3:B:1023:ASP:HB3	3:B:1026:ARG:HB2	1.92	0.50
3:B:1090:CYS:HB3	3:B:1093:SER:HB2	1.94	0.50
3:F:577:PRO:HD2	3:F:580:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:719:TRP:CE3	3:F:722:LYS:HE2	2.47	0.50
3:N:962:HIS:CE1	3:N:1021:LYS:HD3	2.45	0.50
1:A:69:GLU:O	1:A:73:LYS:HG3	2.11	0.50
1:A:491:ARG:HG3	3:B:62:LEU:HD12	1.92	0.50
1:A:817:VAL:HG23	1:A:826:ILE:HG12	1.92	0.50
1:E:791:GLY:N	1:E:792:PRO:HD2	2.24	0.50
1:E:1208:ALA:HB1	2:G:334:ILE:CG1	2.42	0.50
1:M:101:SER:OG	1:M:110:ASP:OD2	2.27	0.50
1:M:357:ALA:HB2	1:M:398:LEU:HD11	1.93	0.50
1:I:90:HIS:HA	1:I:93:ILE:HB	1.93	0.50
1:I:817:VAL:HG23	1:I:826:ILE:HG12	1.92	0.50
3:B:544:ASN:HD22	3:B:547:LEU:HG	1.76	0.50
3:J:579:ILE:HD12	3:J:601:ALA:CB	2.41	0.50
3:J:598:ILE:HD12	3:J:637:MET:SD	2.51	0.50
3:J:800:ILE:HD12	3:J:831:ILE:HD13	1.93	0.50
3:J:814:ALA:HB3	3:J:817:HIS:HB2	1.92	0.50
3:N:715:ASN:HB3	3:N:718:GLU:HG2	1.94	0.50
1:A:319:LYS:HE3	1:A:1098:ARG:HA	1.94	0.50
1:A:937:CYS:SG	1:A:942:ALA:HB2	2.52	0.50
2:C:375:PRO:HD2	2:C:378:VAL:CG1	2.38	0.50
1:M:1209:THR:HG23	2:O:334:ILE:HG21	1.93	0.50
1:I:1200:MET:HE1	2:K:351:ALA:HA	1.93	0.50
3:B:274:ARG:HH22	3:B:802:THR:CA	2.22	0.50
3:B:342:LEU:HD22	3:B:421:LYS:NZ	2.26	0.50
3:B:944:ARG:NH1	3:N:1091:LEU:HD23	2.27	0.50
3:F:342:LEU:HD23	3:F:357:LEU:HB3	1.94	0.50
3:F:579:ILE:HD12	3:F:601:ALA:CB	2.41	0.50
3:F:625:ASN:HB3	3:F:634:ILE:HD11	1.94	0.50
3:F:715:ASN:HB3	3:F:718:GLU:HG2	1.94	0.50
3:F:1004:MET:HB2	3:J:1092:ILE:CG2	2.28	0.50
3:J:719:TRP:CE3	3:J:722:LYS:HE2	2.47	0.50
3:N:1004:MET:O	3:N:1008:ILE:HG12	2.12	0.50
1:E:93:ILE:HG21	3:F:67:THR:N	2.27	0.50
1:M:1122:GLU:O	1:M:1123:TYR:C	2.48	0.50
3:F:499:LEU:HD23	3:F:619:VAL:HB	1.94	0.50
3:J:726:GLU:C	3:J:729:GLN:H	2.14	0.50
1:A:92:MET:HG2	1:A:112:LEU:HD13	1.94	0.50
1:A:300:GLY:O	1:A:313:TYR:OH	2.21	0.50
1:E:1129:GLU:O	1:E:1133:VAL:HG13	2.12	0.50
3:B:103:ARG:NH2	3:F:477:ARG:NE	2.60	0.50
3:B:406:VAL:H	3:B:445:GLN:NE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:625:ASN:HB3	3:B:634:ILE:HD11	1.94	0.50
3:F:122:MET:HE3	3:F:178:TYR:CE1	2.47	0.50
3:F:591:VAL:CG2	3:F:634:ILE:HG13	2.40	0.50
3:F:632:ASN:HB2	3:F:633:PRO:HD3	1.93	0.50
3:F:849:ILE:HG23	3:F:880:ILE:HD13	1.92	0.50
3:N:598:ILE:HD13	3:N:637:MET:SD	2.51	0.50
3:N:726:GLU:C	3:N:729:GLN:H	2.14	0.50
1:E:92:MET:HG2	1:E:112:LEU:HD13	1.94	0.50
1:E:845:THR:O	1:E:849:SER:HB3	2.12	0.50
1:E:937:CYS:SG	1:E:942:ALA:HB2	2.52	0.50
1:M:937:CYS:SG	1:M:942:ALA:HB2	2.52	0.50
1:I:22:ILE:HG12	1:I:401:MET:HG2	1.94	0.50
3:F:579:ILE:HG23	3:F:597:ASP:HB3	1.94	0.50
3:F:598:ILE:HD13	3:F:637:MET:SD	2.51	0.50
3:F:800:ILE:HD12	3:F:831:ILE:HD13	1.93	0.50
3:J:342:LEU:HD22	3:J:421:LYS:NZ	2.26	0.50
3:N:625:ASN:HB3	3:N:634:ILE:HD11	1.94	0.50
1:A:28:PRO:HG3	3:B:547:LEU:CG	2.42	0.49
1:A:101:SER:OG	1:A:110:ASP:OD2	2.27	0.49
1:E:299:ASP:H	1:E:325:GLU:HG2	1.77	0.49
1:M:22:ILE:HG12	1:M:401:MET:HG2	1.94	0.49
3:B:413:PRO:CG	3:B:416:PHE:HD2	2.13	0.49
3:B:598:ILE:HD12	3:B:637:MET:SD	2.51	0.49
3:B:598:ILE:HD13	3:B:637:MET:SD	2.51	0.49
3:B:857:ILE:HG12	3:B:868:PHE:HZ	1.77	0.49
3:F:1091:LEU:C	3:J:938:PRO:HB3	2.33	0.49
3:J:499:LEU:HD23	3:J:619:VAL:HB	1.94	0.49
3:J:856:HIS:O	3:J:860:ILE:HG12	2.12	0.49
1:A:872:PRO:CD	1:A:872:PRO:O	2.58	0.49
1:E:94:ARG:HH12	3:F:157:THR:CB	2.24	0.49
1:E:441:GLN:OE1	1:E:607:PHE:CD1	2.64	0.49
1:M:817:VAL:HG23	1:M:826:ILE:HG12	1.92	0.49
1:M:848:LEU:HD11	1:M:867:ILE:HG22	1.93	0.49
1:I:92:MET:HG2	1:I:112:LEU:HD13	1.94	0.49
1:I:94:ARG:HH12	3:J:157:THR:HB	1.76	0.49
3:J:745:GLY:HA2	3:J:766:ILE:HD11	1.93	0.49
3:N:724:THR:HB	3:N:726:GLU:HB2	1.93	0.49
1:E:90:HIS:HA	1:E:93:ILE:HB	1.93	0.49
1:E:186:ARG:HE	1:E:191:ASN:HD21	1.60	0.49
1:E:264:SER:OG	1:E:265:PHE:N	2.44	0.49
1:E:1086:SER:OG	1:E:1148:ILE:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1122:GLU:O	1:E:1123:TYR:C	2.48	0.49
1:M:845:THR:O	1:M:849:SER:HB3	2.12	0.49
1:I:937:CYS:SG	1:I:942:ALA:HB2	2.52	0.49
3:B:342:LEU:HD23	3:B:357:LEU:HB3	1.93	0.49
3:B:811:THR:HG22	3:B:821:VAL:HG22	1.95	0.49
3:B:856:HIS:O	3:B:860:ILE:HG12	2.12	0.49
1:A:357:ALA:HB2	1:A:398:LEU:HD11	1.93	0.49
1:A:848:LEU:HD11	1:A:867:ILE:HG22	1.93	0.49
1:A:897:ILE:O	1:A:901:LEU:HG	2.13	0.49
1:A:1086:SER:OG	1:A:1148:ILE:CG2	2.60	0.49
1:M:28:PRO:HG3	3:N:547:LEU:HG	1.95	0.49
1:M:319:LYS:HE3	1:M:1098:ARG:HA	1.94	0.49
1:I:1209:THR:HG23	2:K:334:ILE:HG21	1.93	0.49
3:B:719:TRP:CE3	3:B:722:LYS:HE2	2.47	0.49
3:F:797:ALA:HB3	3:F:798:PRO:HD3	1.94	0.49
3:F:857:ILE:HG12	3:F:868:PHE:HZ	1.77	0.49
3:J:632:ASN:HB2	3:J:633:PRO:HD3	1.93	0.49
3:J:951:ARG:O	3:J:1017:GLU:HG3	2.13	0.49
3:N:745:GLY:HA2	3:N:766:ILE:HD11	1.93	0.49
1:E:22:ILE:HG12	1:E:401:MET:HG2	1.94	0.49
1:M:1208:ALA:HB1	2:O:334:ILE:CG1	2.42	0.49
1:I:314:GLU:N	1:I:317:GLU:OE2	2.40	0.49
1:I:845:THR:O	1:I:849:SER:HB3	2.12	0.49
3:B:103:ARG:NH2	3:F:477:ARG:NH1	2.58	0.49
3:F:730:LYS:HB2	3:F:743:LEU:CD1	2.43	0.49
3:F:1090:CYS:CB	4:F:1101:FAR:H13	2.24	0.49
3:N:406:VAL:H	3:N:445:GLN:NE2	2.10	0.49
3:N:413:PRO:CG	3:N:416:PHE:HD2	2.13	0.49
3:N:544:ASN:HD22	3:N:547:LEU:HG	1.76	0.49
3:N:951:ARG:O	3:N:1017:GLU:HG3	2.13	0.49
1:A:83:LYS:CD	3:B:198:GLU:OE1	2.60	0.49
1:A:120:THR:HG21	3:B:131:ARG:NH2	2.27	0.49
1:E:1120:GLN:HE22	1:E:1181:ALA:C	2.16	0.49
3:F:541:LEU:HD13	3:F:670:PHE:CD2	2.48	0.49
3:F:1004:MET:HE2	3:J:1091:LEU:HB2	1.95	0.49
3:J:730:LYS:HB2	3:J:743:LEU:CD1	2.43	0.49
3:J:797:ALA:HB3	3:J:798:PRO:HD3	1.94	0.49
3:J:857:ILE:HG12	3:J:868:PHE:HZ	1.77	0.49
1:A:22:ILE:HG12	1:A:401:MET:HG2	1.94	0.49
1:A:1200:MET:HE1	2:C:351:ALA:HA	1.94	0.49
1:M:93:ILE:CG2	3:N:67:THR:HG23	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:359:VAL:CG2	2:O:367:ARG:HG2	2.36	0.49
1:I:72:ALA:CB	3:J:260:CYS:HB2	2.41	0.49
1:I:1120:GLN:HE22	1:I:1181:ALA:C	2.16	0.49
1:I:1122:GLU:O	1:I:1123:TYR:C	2.48	0.49
1:I:1129:GLU:O	1:I:1133:VAL:HG13	2.12	0.49
3:B:285:ARG:HH22	3:B:977:MET:HB2	1.76	0.49
3:B:734:CYS:SG	3:B:743:LEU:CD1	3.01	0.49
3:B:951:ARG:O	3:B:1017:GLU:HG3	2.13	0.49
3:F:856:HIS:O	3:F:860:ILE:HG12	2.12	0.49
3:F:1004:MET:O	3:F:1008:ILE:HG12	2.12	0.49
3:J:579:ILE:HG23	3:J:597:ASP:HB3	1.94	0.49
3:N:719:TRP:CE3	3:N:722:LYS:HE2	2.47	0.49
1:I:1086:SER:OG	1:I:1148:ILE:CG2	2.60	0.49
3:B:183:VAL:CG1	3:B:467:VAL:HG21	2.43	0.49
3:B:283:LEU:HD21	3:B:307:LEU:HG	1.95	0.49
3:B:526:ILE:HG21	3:B:660:ILE:CD1	2.43	0.49
3:B:730:LYS:HB2	3:B:743:LEU:CD1	2.43	0.49
3:B:745:GLY:HA2	3:B:766:ILE:HD11	1.93	0.49
3:B:835:ILE:HD13	3:B:851:GLN:HG3	1.95	0.49
3:B:1092:ILE:HG21	3:N:1004:MET:HG3	1.95	0.49
3:F:173:ASN:HD21	3:F:220:VAL:HA	1.77	0.49
3:F:1015:GLU:OE1	4:F:1101:FAR:H41	2.12	0.49
3:N:734:CYS:SG	3:N:743:LEU:CD1	3.01	0.49
3:N:811:THR:HG22	3:N:821:VAL:HG22	1.95	0.49
1:M:264:SER:OG	1:M:265:PHE:N	2.44	0.49
1:M:1129:GLU:O	1:M:1133:VAL:HG13	2.12	0.49
1:I:1054:TRP:CZ2	2:K:370:LEU:HA	2.48	0.49
1:I:1120:GLN:HE22	1:I:1181:ALA:HB3	1.71	0.49
3:B:715:ASN:HB3	3:B:718:GLU:HG2	1.94	0.49
3:B:888:GLN:HA	3:B:896:ALA:HB2	1.95	0.49
3:B:1004:MET:O	3:B:1008:ILE:HG12	2.12	0.49
3:F:330:PHE:HB2	3:F:368:PHE:HB2	1.95	0.49
3:J:1004:MET:O	3:J:1008:ILE:HG12	2.12	0.49
3:N:183:VAL:CG1	3:N:467:VAL:HG21	2.43	0.49
3:N:541:LEU:HD13	3:N:670:PHE:CD2	2.48	0.49
3:N:591:VAL:CG2	3:N:634:ILE:HG13	2.40	0.49
3:N:857:ILE:HG12	3:N:868:PHE:HZ	1.76	0.49
1:A:264:SER:OG	1:A:265:PHE:N	2.44	0.49
1:E:75:TYR:HH	3:F:191:GLN:HB3	1.73	0.49
1:M:83:LYS:CD	3:N:198:GLU:OE1	2.60	0.49
1:M:897:ILE:O	1:M:901:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1120:GLN:HE22	1:M:1181:ALA:CB	2.21	0.49
1:I:71:LYS:HD2	3:J:258:GLN:NE2	2.28	0.49
1:I:585:ALA:O	1:I:589:MET:HG3	2.13	0.49
3:B:1009:VAL:CA	4:N:1101:FAR:C14	2.71	0.49
3:J:132:GLN:HE22	3:J:150:HIS:HB2	1.78	0.49
3:J:486:GLN:NE2	3:J:492:ASP:O	2.41	0.49
3:N:330:PHE:HB2	3:N:368:PHE:HB2	1.95	0.49
3:N:499:LEU:HD23	3:N:619:VAL:HB	1.94	0.49
3:N:835:ILE:HD13	3:N:851:GLN:HG3	1.95	0.49
3:N:856:HIS:O	3:N:860:ILE:HG12	2.12	0.49
1:A:95:GLN:HE22	1:A:113:HIS:CD2	2.32	0.48
1:A:299:ASP:H	1:A:325:GLU:HG2	1.77	0.48
1:A:585:ALA:O	1:A:589:MET:HG3	2.13	0.48
1:A:1122:GLU:O	1:A:1123:TYR:C	2.48	0.48
1:A:1129:GLU:O	1:A:1133:VAL:HG13	2.12	0.48
1:E:1092:LEU:HD21	1:E:1111:VAL:HG22	1.95	0.48
3:B:132:GLN:HE22	3:B:150:HIS:HB2	1.78	0.48
3:F:74:LYS:CD	3:F:439:LYS:HZ3	2.13	0.48
3:F:183:VAL:CG1	3:F:467:VAL:HG21	2.43	0.48
3:F:283:LEU:HD23	3:F:307:LEU:HD11	1.94	0.48
3:F:526:ILE:HG21	3:F:660:ILE:CD1	2.43	0.48
3:J:223:ARG:NE	3:J:228:ASN:HD21	2.11	0.48
3:J:526:ILE:HG21	3:J:660:ILE:CD1	2.43	0.48
3:J:734:CYS:SG	3:J:743:LEU:CD1	3.01	0.48
3:N:577:PRO:HD2	3:N:580:PHE:CD2	2.48	0.48
1:A:186:ARG:NE	1:A:191:ASN:HD21	2.12	0.48
1:A:340:VAL:HG11	1:A:413:MET:HB3	1.95	0.48
1:A:610:THR:HG22	3:F:635:LEU:HD21	1.95	0.48
1:E:15:ALA:HA	1:E:57:LEU:HD21	1.95	0.48
1:E:893:LEU:HD13	1:E:924:ILE:HD12	1.95	0.48
1:M:585:ALA:O	1:M:589:MET:HG3	2.13	0.48
1:M:788:THR:O	1:M:792:PRO:HG2	2.03	0.48
1:I:299:ASP:H	1:I:325:GLU:HG2	1.77	0.48
1:I:788:THR:O	1:I:792:PRO:HG2	2.03	0.48
3:B:499:LEU:HD23	3:B:619:VAL:HB	1.94	0.48
3:B:579:ILE:HG23	3:B:597:ASP:HB3	1.94	0.48
3:F:413:PRO:CG	3:F:416:PHE:HD2	2.13	0.48
3:J:330:PHE:HB2	3:J:368:PHE:HB2	1.95	0.48
3:J:888:GLN:HA	3:J:896:ALA:HB2	1.95	0.48
3:N:579:ILE:HG23	3:N:597:ASP:HB3	1.94	0.48
1:A:1091:VAL:HG13	1:A:1148:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:ARG:NE	1:M:191:ASN:HD21	2.12	0.48
1:M:299:ASP:H	1:M:325:GLU:HG2	1.77	0.48
1:I:186:ARG:HE	1:I:191:ASN:HD21	1.60	0.48
1:I:340:VAL:HG11	1:I:413:MET:HB3	1.95	0.48
3:B:223:ARG:HD3	3:B:228:ASN:HD21	1.78	0.48
3:B:564:LYS:HG2	3:B:609:TRP:HH2	1.79	0.48
3:F:132:GLN:HE22	3:F:150:HIS:HB2	1.78	0.48
3:F:586:TYR:HB2	3:F:782:VAL:HG11	1.95	0.48
3:J:577:PRO:HD2	3:J:580:PHE:CD2	2.48	0.48
3:J:586:TYR:HB2	3:J:782:VAL:HG11	1.95	0.48
3:N:962:HIS:CD2	3:N:964:PRO:HB3	2.49	0.48
1:A:44:VAL:HG22	1:A:88:LEU:HD22	1.95	0.48
1:A:845:THR:O	1:A:849:SER:HB3	2.12	0.48
1:A:1208:ALA:HB1	2:C:334:ILE:CG1	2.42	0.48
1:E:104:TYR:OH	1:E:495:SER:O	2.31	0.48
1:I:893:LEU:HD13	1:I:924:ILE:HD12	1.95	0.48
3:B:223:ARG:NE	3:B:228:ASN:HD21	2.11	0.48
3:F:577:PRO:HD2	3:F:580:PHE:CD2	2.48	0.48
3:F:919:GLN:N	3:F:919:GLN:OE1	2.47	0.48
3:J:406:VAL:H	3:J:445:GLN:NE2	2.10	0.48
3:N:888:GLN:HA	3:N:896:ALA:HB2	1.95	0.48
3:N:1013:ASN:OD1	4:N:1101:FAR:C15	2.61	0.48
1:A:186:ARG:HE	1:A:191:ASN:HD21	1.60	0.48
1:E:340:VAL:HG11	1:E:413:MET:HB3	1.95	0.48
1:E:872:PRO:CD	1:E:872:PRO:O	2.58	0.48
1:E:1091:VAL:HG13	1:E:1148:ILE:HG21	1.95	0.48
1:E:1209:THR:HG23	2:G:334:ILE:HG21	1.93	0.48
1:M:83:LYS:HE3	3:N:198:GLU:OE1	2.12	0.48
1:M:104:TYR:OH	1:M:495:SER:O	2.31	0.48
3:B:577:PRO:HD2	3:B:580:PHE:CD2	2.48	0.48
3:B:939:THR:HG23	3:N:1091:LEU:HD12	1.95	0.48
3:F:223:ARG:NE	3:F:228:ASN:HD21	2.11	0.48
3:F:887:LEU:HG	3:F:910:LEU:HD21	1.95	0.48
3:F:888:GLN:HA	3:F:896:ALA:HB2	1.95	0.48
3:F:951:ARG:O	3:F:1017:GLU:HG3	2.13	0.48
3:J:1008:ILE:HG22	3:J:1012:ARG:HD2	1.96	0.48
1:A:1208:ALA:O	2:C:330:ARG:HD3	2.14	0.48
1:E:68:ASP:OD2	3:F:259:GLY:O	2.32	0.48
1:M:92:MET:HG2	1:M:112:LEU:HD13	1.94	0.48
1:M:95:GLN:HE22	1:M:113:HIS:CD2	2.32	0.48
1:M:186:ARG:HE	1:M:191:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1120:GLN:HE22	1:M:1181:ALA:C	2.16	0.48
1:I:1092:LEU:HD21	1:I:1111:VAL:HG22	1.95	0.48
3:B:285:ARG:HG2	3:B:291:ASN:HA	1.96	0.48
3:B:541:LEU:HD13	3:B:670:PHE:CD2	2.48	0.48
3:F:962:HIS:CD2	3:F:964:PRO:HB3	2.49	0.48
3:N:526:ILE:HG21	3:N:660:ILE:CD1	2.43	0.48
3:N:797:ALA:HB3	3:N:798:PRO:HD3	1.94	0.48
1:E:290:ARG:NH1	1:E:391:ASP:OD1	2.47	0.48
1:M:340:VAL:HG11	1:M:413:MET:HB3	1.95	0.48
3:B:105:ASP:O	3:F:614:ARG:NH2	2.46	0.48
3:B:283:LEU:O	3:B:316:THR:OG1	2.24	0.48
3:B:330:PHE:HB2	3:B:368:PHE:HB2	1.95	0.48
3:B:1016:LEU:HD23	3:B:1082:VAL:HG12	1.96	0.48
3:F:734:CYS:SG	3:F:743:LEU:CD1	3.01	0.48
3:F:1008:ILE:HG22	3:F:1012:ARG:HD2	1.96	0.48
3:J:811:THR:HG22	3:J:821:VAL:HG22	1.95	0.48
3:J:962:HIS:CD2	3:J:964:PRO:HB3	2.49	0.48
3:N:1016:LEU:HD23	3:N:1082:VAL:HG12	1.96	0.48
1:E:186:ARG:NE	1:E:191:ASN:HD21	2.12	0.48
1:E:1054:TRP:CZ2	2:G:370:LEU:HA	2.48	0.48
1:E:1208:ALA:O	2:G:330:ARG:HD3	2.14	0.48
1:M:1208:ALA:O	2:O:330:ARG:HD3	2.14	0.48
1:I:1091:VAL:HG11	1:I:1148:ILE:HD13	1.96	0.48
3:B:797:ALA:HB3	3:B:798:PRO:HD3	1.94	0.48
3:F:136:VAL:HG23	3:F:149:LEU:HD21	1.96	0.48
3:F:564:LYS:HG2	3:F:609:TRP:HH2	1.78	0.48
3:N:730:LYS:HB2	3:N:743:LEU:CD1	2.43	0.48
1:A:1054:TRP:CZ2	2:C:370:LEU:HA	2.48	0.48
1:E:236:GLN:HA	1:E:239:GLN:HB3	1.95	0.48
1:E:1091:VAL:HG11	1:E:1148:ILE:HD13	1.96	0.48
1:I:186:ARG:NE	1:I:191:ASN:HD21	2.12	0.48
1:I:897:ILE:O	1:I:901:LEU:HG	2.13	0.48
3:B:919:GLN:OE1	3:B:919:GLN:N	2.47	0.48
3:N:586:TYR:HB2	3:N:782:VAL:HG11	1.95	0.48
3:N:1002:LEU:HD13	3:N:1069:LEU:HD22	1.96	0.48
1:A:236:GLN:HA	1:A:239:GLN:HB3	1.95	0.48
1:E:319:LYS:HE3	1:E:1098:ARG:HA	1.94	0.48
1:E:809:LEU:O	1:E:813:LEU:N	2.37	0.48
1:E:1127:LEU:HD23	1:E:1155:VAL:HG21	1.96	0.48
1:M:332:TRP:HH2	1:M:352:LYS:HZ2	1.58	0.48
1:M:1054:TRP:CZ2	2:O:370:LEU:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1091:VAL:HG13	1:M:1148:ILE:HG21	1.95	0.48
1:I:75:TYR:OH	3:J:191:GLN:HG3	2.12	0.48
1:I:104:TYR:OH	1:I:495:SER:O	2.31	0.48
1:I:524:PHE:HB2	1:I:542:MET:SD	2.54	0.48
3:B:173:ASN:HD21	3:B:220:VAL:HA	1.77	0.48
3:B:962:HIS:CD2	3:B:964:PRO:HB3	2.49	0.48
4:F:1101:FAR:H151	3:J:1013:ASN:OD1	2.12	0.48
3:J:541:LEU:HD13	3:J:670:PHE:CD2	2.48	0.48
3:J:1002:LEU:HD13	3:J:1069:LEU:HD22	1.96	0.48
3:N:74:LYS:CD	3:N:439:LYS:HZ1	2.12	0.48
3:N:523:VAL:O	3:N:523:VAL:CG2	2.56	0.48
3:N:712:PRO:HD3	3:N:780:LEU:CD2	2.40	0.48
1:A:15:ALA:HA	1:A:57:LEU:HD21	1.95	0.47
1:E:28:PRO:HB3	3:F:197:ASP:HB3	1.95	0.47
1:E:897:ILE:O	1:E:901:LEU:HG	2.13	0.47
1:M:236:GLN:HA	1:M:239:GLN:HB3	1.95	0.47
1:I:15:ALA:HA	1:I:57:LEU:HD21	1.95	0.47
1:I:236:GLN:HA	1:I:239:GLN:HB3	1.95	0.47
3:B:477:ARG:CZ	3:F:103:ARG:HH21	2.22	0.47
3:B:778:LEU:O	3:B:782:VAL:HG23	2.14	0.47
3:B:1008:ILE:HG22	3:B:1012:ARG:HD2	1.94	0.47
3:B:1092:ILE:CD1	3:N:1001:GLU:CD	2.54	0.47
3:F:778:LEU:O	3:F:782:VAL:HG23	2.14	0.47
4:F:1103:FAR:C15	3:J:1013:ASN:OD1	2.62	0.47
3:J:183:VAL:CG1	3:J:467:VAL:HG21	2.43	0.47
3:J:523:VAL:O	3:J:523:VAL:CG2	2.56	0.47
3:J:835:ILE:HD13	3:J:851:GLN:HG3	1.95	0.47
3:J:887:LEU:HG	3:J:910:LEU:HD21	1.95	0.47
3:N:173:ASN:HD21	3:N:220:VAL:HA	1.77	0.47
3:N:564:LYS:HG2	3:N:609:TRP:HH2	1.78	0.47
1:E:422:GLU:OE2	3:B:525:PRO:CB	2.62	0.47
1:E:422:GLU:CD	3:B:525:PRO:HG3	2.34	0.47
1:E:1200:MET:HE1	2:G:351:ALA:HA	1.96	0.47
1:I:69:GLU:CG	3:J:262:TRP:CZ3	2.97	0.47
1:I:319:LYS:HE3	1:I:1098:ARG:HA	1.94	0.47
1:I:1054:TRP:HZ2	2:K:370:LEU:HA	1.80	0.47
1:I:1091:VAL:HG13	1:I:1148:ILE:HG21	1.95	0.47
3:B:887:LEU:HG	3:B:910:LEU:HD21	1.95	0.47
3:N:136:VAL:HG23	3:N:149:LEU:HD21	1.96	0.47
3:N:223:ARG:NE	3:N:228:ASN:HD21	2.11	0.47
3:N:835:ILE:HG21	3:N:851:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LYS:HG3	1:A:802:ARG:HH11	1.75	0.47
1:A:1120:GLN:HE22	1:A:1181:ALA:HB3	1.71	0.47
1:E:1068:PRO:HG3	2:G:354:ILE:HG23	1.96	0.47
1:M:71:LYS:HD2	3:N:258:GLN:NE2	2.28	0.47
1:M:1054:TRP:HZ2	2:O:370:LEU:HA	1.80	0.47
3:B:221:TRP:CH2	3:B:368:PHE:HZ	2.32	0.47
3:B:367:ILE:HD11	3:B:443:TRP:CD1	2.49	0.47
3:B:1002:LEU:HD13	3:B:1069:LEU:HD22	1.96	0.47
3:F:373:MET:O	3:F:377:VAL:HG23	2.15	0.47
3:F:811:THR:HG22	3:F:821:VAL:HG22	1.95	0.47
3:J:297:LEU:HD21	3:J:372:MET:HG2	1.96	0.47
3:J:564:LYS:HG2	3:J:609:TRP:HH2	1.79	0.47
3:J:835:ILE:HG21	3:J:851:GLN:HE21	1.79	0.47
3:J:919:GLN:OE1	3:J:919:GLN:N	2.47	0.47
3:J:1016:LEU:HD23	3:J:1082:VAL:HG12	1.96	0.47
3:N:878:TRP:HE3	3:N:933:SER:HA	1.79	0.47
1:E:44:VAL:HG22	1:E:88:LEU:HD22	1.95	0.47
1:E:75:TYR:HB2	3:F:258:GLN:HB3	1.95	0.47
1:M:524:PHE:HB2	1:M:542:MET:SD	2.54	0.47
3:B:136:VAL:HG23	3:B:149:LEU:HD21	1.96	0.47
3:B:373:MET:O	3:B:377:VAL:HG23	2.15	0.47
3:F:367:ILE:HD11	3:F:443:TRP:CD1	2.49	0.47
3:J:136:VAL:HG23	3:J:149:LEU:HD21	1.96	0.47
3:J:223:ARG:HD3	3:J:228:ASN:HD21	1.78	0.47
3:J:803:PHE:CE2	3:J:810:VAL:HG22	2.49	0.47
3:N:132:GLN:HE22	3:N:150:HIS:HB2	1.78	0.47
3:N:177:LEU:CD1	3:N:303:PRO:HG3	2.45	0.47
3:N:283:LEU:HA	3:N:285:ARG:N	2.29	0.47
3:N:367:ILE:HD11	3:N:443:TRP:CD1	2.49	0.47
1:A:893:LEU:HD13	1:A:924:ILE:HD12	1.95	0.47
1:A:1054:TRP:HZ2	2:C:370:LEU:HA	1.79	0.47
1:M:1091:VAL:HG11	1:M:1148:ILE:HD13	1.96	0.47
1:M:1092:LEU:HD21	1:M:1111:VAL:HG22	1.95	0.47
1:I:794:TRP:O	1:I:798:LEU:CD1	2.61	0.47
3:B:297:LEU:HD21	3:B:372:MET:HG2	1.96	0.47
3:F:297:LEU:HD21	3:F:372:MET:HG2	1.96	0.47
3:F:835:ILE:HG21	3:F:851:GLN:HE21	1.79	0.47
3:F:878:TRP:HE3	3:F:933:SER:HA	1.79	0.47
3:J:173:ASN:HD21	3:J:220:VAL:HA	1.77	0.47
1:A:1092:LEU:HD21	1:A:1111:VAL:HG22	1.95	0.47
1:A:1200:MET:HE1	2:C:354:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:585:ALA:O	1:E:589:MET:HG3	2.13	0.47
1:M:44:VAL:HG22	1:M:88:LEU:HD22	1.95	0.47
1:M:1061:ASP:OD2	2:O:357:HIS:CE1	2.68	0.47
1:I:63:LYS:O	3:N:567:ARG:NH2	2.30	0.47
1:I:69:GLU:CG	3:J:262:TRP:HZ3	2.28	0.47
3:B:586:TYR:HB2	3:B:782:VAL:HG11	1.95	0.47
3:F:283:LEU:CD2	3:F:307:LEU:CD1	2.92	0.47
3:F:1002:LEU:HD13	3:F:1069:LEU:HD22	1.96	0.47
3:F:1091:LEU:HG	3:J:939:THR:O	2.14	0.47
3:N:887:LEU:HG	3:N:910:LEU:HD21	1.95	0.47
1:A:104:TYR:OH	1:A:495:SER:O	2.31	0.47
1:A:1068:PRO:HG3	2:C:354:ILE:HG23	1.96	0.47
1:A:1120:GLN:HE22	1:A:1181:ALA:C	2.16	0.47
1:E:32:LEU:HD12	1:E:118:THR:HA	1.96	0.47
1:E:93:ILE:HG21	3:F:67:THR:CA	2.45	0.47
1:E:1054:TRP:HZ2	2:G:370:LEU:HA	1.79	0.47
1:M:15:ALA:HA	1:M:57:LEU:HD21	1.95	0.47
1:M:893:LEU:HD13	1:M:924:ILE:HD12	1.95	0.47
1:M:923:ILE:O	1:M:926:VAL:HG12	2.15	0.47
1:I:32:LEU:HD12	1:I:118:THR:HA	1.96	0.47
1:I:95:GLN:HE22	1:I:113:HIS:CD2	2.32	0.47
1:I:290:ARG:NH1	1:I:391:ASP:OD1	2.47	0.47
1:I:923:ILE:O	1:I:926:VAL:HG12	2.15	0.47
1:I:1061:ASP:OD2	2:K:357:HIS:CE1	2.68	0.47
1:I:1208:ALA:O	2:K:330:ARG:HD3	2.14	0.47
3:B:526:ILE:HD13	3:B:660:ILE:HD13	1.90	0.47
3:F:177:LEU:CD1	3:F:303:PRO:HG3	2.45	0.47
3:F:221:TRP:CH2	3:F:368:PHE:HZ	2.32	0.47
3:F:406:VAL:H	3:F:445:GLN:NE2	2.10	0.47
3:J:172:ILE:O	3:J:172:ILE:CG2	2.62	0.47
3:J:177:LEU:CD1	3:J:303:PRO:HG3	2.45	0.47
3:J:221:TRP:CH2	3:J:368:PHE:HZ	2.32	0.47
3:J:586:TYR:HB2	3:J:782:VAL:CG1	2.45	0.47
3:J:789:THR:HG22	3:J:789:THR:O	2.15	0.47
3:N:172:ILE:O	3:N:172:ILE:CG2	2.62	0.47
3:N:373:MET:O	3:N:377:VAL:HG23	2.15	0.47
3:N:374:ILE:HG23	3:N:454:LEU:CD1	2.45	0.47
3:N:538:TYR:HB3	3:N:552:ARG:HD3	1.97	0.47
3:N:545:GLU:HG2	3:N:545:GLU:O	2.15	0.47
3:N:586:TYR:HB2	3:N:782:VAL:CG1	2.45	0.47
3:N:1008:ILE:HG22	3:N:1012:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:PHE:HB2	1:A:542:MET:SD	2.54	0.47
1:A:938:SER:OG	1:A:941:GLU:CG	2.63	0.47
1:M:32:LEU:HD12	1:M:118:THR:HA	1.96	0.47
1:M:248:ARG:HA	1:M:254:GLU:O	2.15	0.47
1:M:938:SER:OG	1:M:941:GLU:CG	2.63	0.47
1:I:44:VAL:HG22	1:I:88:LEU:HD22	1.95	0.47
3:B:177:LEU:CD1	3:B:303:PRO:HG3	2.45	0.47
3:B:523:VAL:O	3:B:523:VAL:CG2	2.56	0.47
3:B:538:TYR:HB3	3:B:552:ARG:HD3	1.97	0.47
3:B:878:TRP:HE3	3:B:933:SER:HA	1.79	0.47
3:F:726:GLU:HA	3:F:729:GLN:CB	2.45	0.47
3:F:835:ILE:HD13	3:F:851:GLN:HG3	1.95	0.47
3:F:1091:LEU:HD23	3:J:944:ARG:HH11	1.80	0.47
1:A:1061:ASP:OD2	2:C:357:HIS:CE1	2.68	0.47
1:E:524:PHE:HB2	1:E:542:MET:SD	2.54	0.47
1:E:788:THR:O	1:E:792:PRO:HG3	2.09	0.47
1:M:290:ARG:NH1	1:M:391:ASP:OD1	2.47	0.47
3:B:374:ILE:HG23	3:B:454:LEU:CD1	2.45	0.47
3:B:545:GLU:O	3:B:545:GLU:HG2	2.15	0.47
3:J:727:ILE:HG21	3:J:747:LEU:HG	1.97	0.47
3:N:778:LEU:O	3:N:782:VAL:HG23	2.14	0.47
1:A:83:LYS:HE3	3:B:198:GLU:OE1	2.15	0.47
1:A:290:ARG:NH1	1:A:391:ASP:OD1	2.47	0.47
1:A:923:ILE:O	1:A:926:VAL:HG12	2.15	0.47
1:A:1120:GLN:HE22	1:A:1181:ALA:CB	2.21	0.47
1:A:1127:LEU:HD23	1:A:1155:VAL:HG21	1.96	0.47
1:M:333:THR:O	1:M:337:LEU:HG	2.15	0.47
1:M:817:VAL:HG21	1:M:829:ILE:HD12	1.97	0.47
1:I:1068:PRO:HG3	2:K:354:ILE:HG23	1.96	0.47
3:B:532:GLN:H	3:B:532:GLN:HG3	1.51	0.47
3:B:586:TYR:CB	3:B:782:VAL:CG1	2.93	0.47
3:B:1002:LEU:O	3:B:1006:VAL:HG23	2.15	0.47
3:B:1008:ILE:HG21	3:B:1012:ARG:NH2	2.29	0.47
3:F:172:ILE:O	3:F:172:ILE:CG2	2.62	0.47
3:F:545:GLU:HG2	3:F:545:GLU:O	2.15	0.47
3:J:586:TYR:CB	3:J:782:VAL:CG1	2.93	0.47
3:J:726:GLU:HA	3:J:729:GLN:CB	2.45	0.47
3:N:1002:LEU:O	3:N:1006:VAL:HG23	2.15	0.47
1:A:846:ASP:O	1:A:849:SER:OG	2.23	0.46
1:E:510:LEU:HD23	1:E:517:ILE:HG21	1.97	0.46
1:M:1127:LEU:HD22	1:M:1151:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:726:GLU:HA	3:B:729:GLN:CB	2.45	0.46
3:B:1071:LYS:HE2	3:N:1075:ASN:HA	1.96	0.46
3:F:625:ASN:C	3:F:634:ILE:HD12	2.34	0.46
3:F:1002:LEU:O	3:F:1006:VAL:HG23	2.15	0.46
3:F:1016:LEU:HD23	3:F:1082:VAL:HG12	1.96	0.46
3:J:367:ILE:HD11	3:J:443:TRP:CD1	2.49	0.46
3:N:726:GLU:HA	3:N:729:GLN:CB	2.45	0.46
3:N:789:THR:O	3:N:789:THR:HG22	2.15	0.46
1:A:163:ASN:CG	1:A:489:ASN:HD21	2.18	0.46
1:A:817:VAL:HG21	1:A:829:ILE:HD12	1.97	0.46
1:E:260:LEU:HG	1:E:283:ILE:HD13	1.98	0.46
1:M:771:LYS:HG3	1:M:802:ARG:HH11	1.75	0.46
1:M:794:TRP:O	1:M:798:LEU:CD1	2.61	0.46
1:I:333:THR:O	1:I:337:LEU:HG	2.15	0.46
1:I:1200:MET:HE1	2:K:354:ILE:HD12	1.98	0.46
3:B:586:TYR:HB2	3:B:782:VAL:CG1	2.45	0.46
3:B:835:ILE:HG21	3:B:851:GLN:HE21	1.79	0.46
3:B:1092:ILE:HG21	3:N:1004:MET:HB2	1.97	0.46
3:F:586:TYR:CB	3:F:782:VAL:CG1	2.93	0.46
3:J:283:LEU:HA	3:J:285:ARG:H	1.80	0.46
3:J:373:MET:O	3:J:377:VAL:HG23	2.15	0.46
3:N:221:TRP:CH2	3:N:368:PHE:HZ	2.32	0.46
3:N:335:ARG:NH1	3:N:970:SER:O	2.48	0.46
3:N:586:TYR:CB	3:N:782:VAL:CG1	2.93	0.46
3:N:1090:CYS:SG	4:N:1101:FAR:H12A	1.46	0.46
1:A:914:GLU:HG3	1:A:1066:ARG:HG3	1.98	0.46
4:A:1301:FAR:H43	2:C:333:VAL:HG21	1.98	0.46
1:E:95:GLN:HE22	1:E:113:HIS:CD2	2.31	0.46
1:E:248:ARG:HA	1:E:254:GLU:O	2.15	0.46
1:E:504:VAL:O	1:E:508:SER:OG	2.20	0.46
1:E:923:ILE:O	1:E:926:VAL:HG12	2.15	0.46
1:I:531:TYR:HB2	1:I:823:TRP:HZ3	1.81	0.46
1:I:1127:LEU:HD22	1:I:1151:VAL:CG1	2.45	0.46
3:F:223:ARG:HD3	3:F:228:ASN:HD21	1.78	0.46
3:F:374:ILE:HG23	3:F:454:LEU:CD1	2.45	0.46
3:F:450:ILE:HG23	3:F:464:ILE:CD1	2.46	0.46
3:F:538:TYR:HB3	3:F:552:ARG:HD3	1.97	0.46
3:F:1001:GLU:CG	3:J:1092:ILE:CG1	2.57	0.46
3:F:1078:LEU:HD22	3:J:1067:SER:HA	1.97	0.46
3:J:374:ILE:HG23	3:J:454:LEU:CD1	2.45	0.46
3:J:545:GLU:O	3:J:545:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:778:LEU:O	3:J:782:VAL:HG23	2.14	0.46
1:A:69:GLU:HG2	3:B:262:TRP:CH2	2.50	0.46
1:A:531:TYR:HB2	1:A:823:TRP:HZ3	1.81	0.46
1:E:333:THR:O	1:E:337:LEU:HG	2.15	0.46
1:M:914:GLU:HG3	1:M:1066:ARG:HG3	1.98	0.46
1:I:397:LYS:HE3	1:I:400:HIS:CD2	2.51	0.46
3:B:1004:MET:CE	3:N:1091:LEU:HB2	2.45	0.46
3:J:538:TYR:HB3	3:J:552:ARG:HD3	1.97	0.46
3:J:878:TRP:HE3	3:J:933:SER:HA	1.79	0.46
3:J:1002:LEU:O	3:J:1006:VAL:HG23	2.15	0.46
3:N:727:ILE:HG21	3:N:747:LEU:HG	1.97	0.46
1:A:914:GLU:HB2	1:A:1067:VAL:O	2.16	0.46
1:E:101:SER:OG	1:E:110:ASP:OD2	2.27	0.46
1:E:938:SER:OG	1:E:941:GLU:CG	2.63	0.46
1:E:1061:ASP:OD2	2:G:357:HIS:CE1	2.68	0.46
1:M:94:ARG:HH12	3:N:157:THR:HB	1.81	0.46
1:I:66:ASP:HB2	3:N:667:GLN:HE22	1.52	0.46
1:I:260:LEU:HG	1:I:283:ILE:HD13	1.98	0.46
3:B:45:LEU:CD2	3:B:104:ILE:HG13	2.46	0.46
3:F:803:PHE:CE2	3:F:810:VAL:HG22	2.49	0.46
3:N:297:LEU:HD21	3:N:372:MET:HG2	1.96	0.46
3:N:396:LEU:HD21	3:N:406:VAL:HG22	1.97	0.46
3:N:450:ILE:HG23	3:N:464:ILE:CD1	2.46	0.46
3:N:919:GLN:N	3:N:919:GLN:OE1	2.47	0.46
1:A:32:LEU:HD12	1:A:118:THR:HA	1.96	0.46
1:A:1091:VAL:HG11	1:A:1148:ILE:HD13	1.96	0.46
1:E:771:LYS:HG3	1:E:802:ARG:HH11	1.75	0.46
1:M:531:TYR:HB2	1:M:823:TRP:HZ3	1.81	0.46
1:I:98:LYS:NZ	1:I:127:ASP:OD2	2.39	0.46
3:B:335:ARG:NH1	3:B:970:SER:O	2.48	0.46
3:B:396:LEU:HD21	3:B:406:VAL:HG22	1.97	0.46
3:B:450:ILE:HG23	3:B:464:ILE:CD1	2.46	0.46
3:B:789:THR:HG22	3:B:789:THR:O	2.15	0.46
3:F:586:TYR:HB2	3:F:782:VAL:CG1	2.45	0.46
3:F:727:ILE:HG21	3:F:747:LEU:HG	1.97	0.46
3:N:1035:PHE:CZ	3:N:1039:GLN:HG3	2.51	0.46
1:A:333:THR:O	1:A:337:LEU:HG	2.15	0.46
1:A:539:ILE:HG21	1:A:570:MET:HE2	1.97	0.46
1:E:163:ASN:CG	1:E:489:ASN:HD21	2.18	0.46
1:E:539:ILE:HG21	1:E:570:MET:HE2	1.97	0.46
1:M:901:LEU:HD22	1:M:912:PHE:CZ	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:GLN:HB2	3:J:194:TYR:O	2.15	0.46
1:I:510:LEU:HD23	1:I:517:ILE:HG21	1.97	0.46
1:I:938:SER:OG	1:I:941:GLU:CG	2.63	0.46
1:I:1127:LEU:HD23	1:I:1155:VAL:HG21	1.96	0.46
3:B:172:ILE:O	3:B:172:ILE:CG2	2.62	0.46
3:B:1057:THR:CG2	3:B:1064:GLY:HA2	2.46	0.46
3:B:1092:ILE:HD12	3:N:1001:GLU:CB	2.40	0.46
3:F:789:THR:O	3:F:789:THR:HG22	2.15	0.46
3:N:584:ASP:HB2	3:N:791:LYS:HE3	1.98	0.46
1:A:10:ARG:NH1	1:A:10:ARG:HB3	2.31	0.46
1:A:79:GLN:NE2	3:B:194:TYR:CZ	2.82	0.46
1:A:200:SER:HA	1:A:262:VAL:HG21	1.98	0.46
1:M:397:LYS:HE3	1:M:400:HIS:CD2	2.51	0.46
1:I:248:ARG:HA	1:I:254:GLU:O	2.15	0.46
3:F:335:ARG:NH1	3:F:970:SER:O	2.49	0.46
3:F:1035:PHE:CZ	3:F:1039:GLN:HG3	2.51	0.46
4:F:1101:FAR:C5	3:J:1008:ILE:HG13	2.46	0.46
3:J:335:ARG:NH1	3:J:970:SER:O	2.48	0.46
3:J:584:ASP:HB2	3:J:791:LYS:HE3	1.98	0.46
1:A:248:ARG:HA	1:A:254:GLU:O	2.15	0.46
1:A:1081:LYS:CB	4:A:1301:FAR:C14	2.94	0.46
1:E:184:TRP:O	1:E:185:GLU:HG2	2.16	0.46
1:E:771:LYS:NZ	1:E:802:ARG:HD3	2.31	0.46
1:E:1127:LEU:HD22	1:E:1151:VAL:CG1	2.45	0.46
1:M:163:ASN:CG	1:M:489:ASN:HD21	2.18	0.46
1:I:817:VAL:HG21	1:I:829:ILE:HD12	1.97	0.46
1:I:914:GLU:HG3	1:I:1066:ARG:HG3	1.98	0.46
3:B:826:LEU:HD22	3:B:830:VAL:CG1	2.43	0.46
3:B:1013:ASN:OD1	4:B:1101:FAR:C15	2.64	0.46
1:M:72:ALA:CB	3:N:262:TRP:CZ2	2.99	0.46
1:M:184:TRP:O	1:M:185:GLU:HG2	2.16	0.46
1:M:1068:PRO:HG3	2:O:354:ILE:HG23	1.96	0.46
1:I:914:GLU:HB2	1:I:1067:VAL:O	2.16	0.46
3:B:1004:MET:HE1	3:N:1091:LEU:HB2	1.97	0.46
3:F:584:ASP:HB2	3:F:791:LYS:HE3	1.98	0.46
3:J:1057:THR:CG2	3:J:1064:GLY:HA2	2.46	0.46
3:N:342:LEU:HD22	3:N:421:LYS:HZ1	1.80	0.46
3:N:736:CYS:HB3	3:N:739:SER:H	1.81	0.46
1:A:108:THR:HG22	1:A:133:LEU:HD23	1.98	0.45
1:A:211:ALA:HB1	1:A:426:LEU:HD13	1.99	0.45
1:A:1207:ALA:O	1:A:1211:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:VAL:HG21	1:E:829:ILE:HD12	1.97	0.45
1:M:72:ALA:HB3	3:N:262:TRP:CZ2	2.51	0.45
1:M:809:LEU:O	1:M:813:LEU:N	2.37	0.45
4:M:1301:FAR:H43	2:O:333:VAL:HG21	1.98	0.45
1:I:163:ASN:CG	1:I:489:ASN:HD21	2.18	0.45
1:I:184:TRP:O	1:I:185:GLU:HG2	2.16	0.45
1:I:400:HIS:O	1:I:404:GLN:N	2.43	0.45
3:B:584:ASP:HB2	3:B:791:LYS:HE3	1.98	0.45
3:B:849:ILE:HG23	3:B:880:ILE:CD1	2.46	0.45
3:F:76:CYS:O	3:F:76:CYS:SG	2.74	0.45
3:F:298:PRO:O	3:F:303:PRO:HD2	2.16	0.45
3:J:76:CYS:O	3:J:76:CYS:SG	2.74	0.45
3:J:342:LEU:CD2	3:J:421:LYS:HZ1	2.29	0.45
3:J:587:MET:HE2	3:J:855:ILE:HG13	1.97	0.45
1:A:510:LEU:HD23	1:A:517:ILE:HG21	1.97	0.45
1:M:922:LEU:HD23	1:M:922:LEU:HA	1.81	0.45
3:B:76:CYS:O	3:B:76:CYS:SG	2.74	0.45
3:B:223:ARG:CZ	3:B:228:ASN:HD21	2.29	0.45
3:B:939:THR:CG2	3:N:1091:LEU:HD12	2.45	0.45
3:B:1035:PHE:CZ	3:B:1039:GLN:HG3	2.51	0.45
3:F:342:LEU:CD2	3:F:421:LYS:HZ2	2.29	0.45
3:F:714:VAL:HG11	3:F:743:LEU:CG	2.41	0.45
3:F:857:ILE:HG12	3:F:868:PHE:CZ	2.52	0.45
3:J:736:CYS:HB3	3:J:739:SER:H	1.81	0.45
3:J:857:ILE:HG12	3:J:868:PHE:CZ	2.52	0.45
3:J:1035:PHE:CZ	3:J:1039:GLN:HG3	2.51	0.45
3:N:803:PHE:CE2	3:N:810:VAL:HG22	2.49	0.45
1:A:1127:LEU:HD22	1:A:1151:VAL:CG1	2.45	0.45
1:E:531:TYR:HB2	1:E:823:TRP:HZ3	1.81	0.45
1:E:1134:LEU:HD11	1:E:1149:ILE:HG21	1.99	0.45
1:M:200:SER:HA	1:M:262:VAL:HG21	1.98	0.45
1:M:510:LEU:HD23	1:M:517:ILE:HG21	1.97	0.45
1:M:1127:LEU:HD23	1:M:1155:VAL:HG21	1.96	0.45
4:I:1301:FAR:H43	2:K:333:VAL:HG21	1.98	0.45
3:B:298:PRO:O	3:B:303:PRO:HD2	2.16	0.45
3:B:477:ARG:NH1	3:F:103:ARG:HH22	2.14	0.45
3:F:796:ILE:HD11	3:F:851:GLN:O	2.17	0.45
3:F:1091:LEU:O	3:J:938:PRO:HB3	2.16	0.45
3:J:450:ILE:HG23	3:J:464:ILE:CD1	2.46	0.45
1:E:112:LEU:HD11	1:E:168:LEU:HD21	1.98	0.45
1:E:794:TRP:O	1:E:798:LEU:CD1	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:ARG:NH1	1:M:10:ARG:HB3	2.31	0.45
1:M:788:THR:O	1:M:792:PRO:HG3	2.09	0.45
3:B:355:ILE:HD13	3:B:355:ILE:HA	1.77	0.45
3:B:883:MET:HG3	3:B:914:ILE:HD13	1.99	0.45
3:F:396:LEU:HD21	3:F:406:VAL:HG22	1.97	0.45
3:F:800:ILE:HD13	3:F:822:ILE:HD12	1.99	0.45
3:J:45:LEU:CD2	3:J:104:ILE:HG13	2.46	0.45
3:J:849:ILE:HG23	3:J:880:ILE:CD1	2.46	0.45
3:J:857:ILE:HG23	3:J:868:PHE:CZ	2.51	0.45
3:N:883:MET:HG3	3:N:914:ILE:HD13	1.99	0.45
1:A:491:ARG:HG2	3:B:62:LEU:HD11	1.97	0.45
1:E:914:GLU:HB2	1:E:1067:VAL:O	2.16	0.45
1:M:504:VAL:HG22	1:M:550:LEU:HG	1.98	0.45
1:M:539:ILE:HG21	1:M:570:MET:HE2	1.98	0.45
1:M:914:GLU:HB2	1:M:1067:VAL:O	2.16	0.45
1:I:435:LYS:HE2	1:I:435:LYS:HB3	1.80	0.45
1:I:1052:GLY:HA2	1:I:1190:ASP:OD2	2.16	0.45
3:B:523:VAL:HG21	3:B:528:ILE:CD1	2.43	0.45
3:F:223:ARG:CZ	3:F:228:ASN:HD21	2.29	0.45
3:J:342:LEU:HD22	3:J:421:LYS:HZ1	1.80	0.45
3:J:413:PRO:CG	3:J:416:PHE:HD2	2.13	0.45
3:J:826:LEU:HD22	3:J:830:VAL:CG1	2.43	0.45
3:N:942:TYR:CZ	3:N:984:GLU:OE2	2.69	0.45
1:A:794:TRP:O	1:A:798:LEU:CD1	2.61	0.45
1:A:934:SER:O	1:A:935:LEU:HB2	2.17	0.45
2:C:359:VAL:CG2	2:C:367:ARG:HG2	2.36	0.45
1:E:108:THR:HG22	1:E:133:LEU:HD23	1.98	0.45
1:E:938:SER:OG	1:E:941:GLU:HG3	2.17	0.45
1:E:1081:LYS:CB	4:E:1301:FAR:C14	2.94	0.45
1:M:211:ALA:HB1	1:M:426:LEU:HD13	1.99	0.45
1:M:260:LEU:HG	1:M:283:ILE:HD13	1.98	0.45
2:O:374:THR:OG1	2:O:379:LEU:HB2	2.16	0.45
1:I:10:ARG:NH1	1:I:10:ARG:HB3	2.31	0.45
1:I:539:ILE:HG21	1:I:570:MET:HE2	1.98	0.45
3:B:727:ILE:HG21	3:B:747:LEU:HG	1.97	0.45
3:B:803:PHE:CE2	3:B:810:VAL:HG22	2.49	0.45
3:F:45:LEU:CD2	3:F:104:ILE:HG13	2.46	0.45
3:F:1092:ILE:HG13	4:F:1101:FAR:H11	1.97	0.45
3:N:45:LEU:CD2	3:N:104:ILE:HG13	2.46	0.45
3:N:342:LEU:CD2	3:N:421:LYS:HZ1	2.29	0.45
3:N:526:ILE:HD13	3:N:660:ILE:HD13	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:796:ILE:HD11	3:N:851:GLN:O	2.17	0.45
3:N:857:ILE:HG12	3:N:868:PHE:CZ	2.52	0.45
1:A:93:ILE:HG22	3:B:67:THR:HG23	1.86	0.45
1:A:938:SER:OG	1:A:941:GLU:HG3	2.17	0.45
1:A:1052:GLY:HA2	1:A:1190:ASP:OD2	2.16	0.45
1:E:64:ASN:CA	3:B:567:ARG:HH22	2.21	0.45
1:E:66:ASP:HB2	3:B:667:GLN:OE1	2.16	0.45
1:E:200:SER:HA	1:E:262:VAL:HG21	1.98	0.45
1:E:491:ARG:HD3	3:F:62:LEU:CG	2.45	0.45
1:E:504:VAL:HG22	1:E:550:LEU:HG	1.98	0.45
1:M:435:LYS:HE2	1:M:435:LYS:HB3	1.80	0.45
3:B:634:ILE:HG22	3:B:638:LEU:CD1	2.47	0.45
3:B:736:CYS:HB3	3:B:739:SER:H	1.81	0.45
3:B:1012:ARG:NH2	4:N:1101:FAR:H41	2.26	0.45
3:F:223:ARG:CD	3:F:228:ASN:ND2	2.79	0.45
3:F:712:PRO:HD3	3:F:780:LEU:CD2	2.41	0.45
3:J:69:GLY:CA	3:J:120:LYS:HG2	2.47	0.45
3:J:396:LEU:HD21	3:J:406:VAL:HG22	1.97	0.45
3:N:76:CYS:O	3:N:76:CYS:SG	2.74	0.45
3:N:298:PRO:O	3:N:303:PRO:HD2	2.16	0.45
3:N:849:ILE:HG23	3:N:880:ILE:CD1	2.46	0.45
3:N:1057:THR:CG2	3:N:1064:GLY:HA2	2.46	0.45
1:A:57:LEU:HD13	1:A:412:LEU:HD11	1.99	0.45
1:A:184:TRP:O	1:A:185:GLU:HG2	2.16	0.45
1:A:479:LEU:HB2	1:A:520:PHE:CD2	2.52	0.45
1:E:337:LEU:CD1	1:E:406:LEU:HD22	2.47	0.45
1:E:479:LEU:HB2	1:E:520:PHE:CD2	2.52	0.45
1:E:1052:GLY:HA2	1:E:1190:ASP:OD2	2.16	0.45
1:M:771:LYS:NZ	1:M:802:ARG:HD3	2.31	0.45
1:I:112:LEU:HD11	1:I:168:LEU:HD21	1.98	0.45
1:I:200:SER:HA	1:I:262:VAL:HG21	1.98	0.45
1:I:504:VAL:HG22	1:I:550:LEU:HG	1.98	0.45
1:I:1120:GLN:HA	1:I:1121:PRO:HD3	1.89	0.45
3:B:69:GLY:CA	3:B:120:LYS:HG2	2.47	0.45
3:B:279:LEU:HG	3:B:283:LEU:CD2	2.44	0.45
3:B:742:ILE:HD11	3:B:784:TYR:CZ	2.52	0.45
3:B:857:ILE:HG23	3:B:868:PHE:CZ	2.51	0.45
3:B:958:VAL:HG22	3:B:1024:LEU:HD12	1.99	0.45
3:F:742:ILE:HD11	3:F:784:TYR:CZ	2.52	0.45
3:J:98:ALA:O	3:J:102:ARG:HG3	2.17	0.45
3:J:223:ARG:CZ	3:J:228:ASN:HD21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:742:ILE:HD11	3:N:784:TYR:CZ	2.52	0.45
3:N:958:VAL:HG22	3:N:1024:LEU:HD12	1.99	0.45
1:A:86:ARG:O	1:A:90:HIS:ND1	2.50	0.45
1:A:765:ALA:HB1	1:A:768:LEU:CD1	2.47	0.45
1:E:10:ARG:NH1	1:E:10:ARG:HB3	2.31	0.45
1:E:400:HIS:O	1:E:404:GLN:N	2.43	0.45
1:E:435:LYS:HB3	1:E:435:LYS:HE2	1.80	0.45
1:E:914:GLU:HG3	1:E:1066:ARG:HG3	1.98	0.45
1:E:934:SER:O	1:E:935:LEU:HB2	2.17	0.45
3:B:342:LEU:CD2	3:B:421:LYS:HZ2	2.29	0.45
3:F:122:MET:HE3	3:F:122:MET:HB3	1.88	0.45
3:F:849:ILE:HG23	3:F:880:ILE:CD1	2.46	0.45
3:F:1057:THR:CG2	3:F:1064:GLY:HA2	2.46	0.45
3:J:742:ILE:HD11	3:J:784:TYR:CZ	2.52	0.45
3:J:903:SER:O	3:J:904:PRO:C	2.56	0.45
3:J:989:ASN:HD22	3:J:989:ASN:HA	1.63	0.45
3:N:69:GLY:CA	3:N:120:LYS:HG2	2.47	0.45
3:N:98:ALA:O	3:N:102:ARG:HG3	2.17	0.45
3:N:223:ARG:CZ	3:N:228:ASN:HD21	2.29	0.45
3:N:857:ILE:HG23	3:N:868:PHE:CZ	2.51	0.45
1:A:28:PRO:HG3	3:B:547:LEU:HG	1.99	0.45
1:E:211:ALA:HB1	1:E:426:LEU:HD13	1.98	0.45
1:M:112:LEU:HD11	1:M:168:LEU:HD21	1.98	0.45
1:M:1052:GLY:HA2	1:M:1190:ASP:OD2	2.16	0.45
2:O:382:LEU:HD13	2:O:382:LEU:HA	1.76	0.45
1:I:108:THR:HG22	1:I:133:LEU:HD23	1.98	0.45
1:I:1134:LEU:HD11	1:I:1149:ILE:HG21	1.99	0.45
3:B:216:PRO:HG3	3:B:234:LEU:HD11	1.99	0.45
3:B:779:TRP:HA	3:B:782:VAL:HG23	1.99	0.45
3:F:240:GLY:HA3	3:F:299:CYS:SG	2.57	0.45
3:F:857:ILE:HG23	3:F:868:PHE:CZ	2.51	0.45
3:N:452:LYS:HD2	3:N:452:LYS:HA	1.72	0.45
3:N:903:SER:O	3:N:904:PRO:C	2.56	0.45
1:A:72:ALA:HB3	3:B:262:TRP:CZ2	2.52	0.44
1:A:337:LEU:CD1	1:A:406:LEU:HD22	2.47	0.44
1:A:1197:PHE:CZ	2:C:375:PRO:HG3	2.53	0.44
1:E:66:ASP:HA	3:B:667:GLN:HE21	1.82	0.44
1:E:1207:ALA:O	1:E:1211:VAL:HG23	2.17	0.44
1:M:1081:LYS:CB	4:M:1301:FAR:C14	2.94	0.44
1:I:233:ASP:OD2	1:I:503:GLY:N	2.50	0.44
1:I:771:LYS:NZ	1:I:802:ARG:HD3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1207:ALA:O	1:I:1211:VAL:HG23	2.17	0.44
3:B:342:LEU:HD21	3:B:421:LYS:HZ2	1.82	0.44
3:B:857:ILE:HG12	3:B:868:PHE:CZ	2.52	0.44
3:J:298:PRO:O	3:J:303:PRO:HD2	2.16	0.44
3:J:634:ILE:HG22	3:J:638:LEU:CD1	2.47	0.44
1:A:260:LEU:HG	1:A:283:ILE:HD13	1.97	0.44
1:E:765:ALA:HB1	1:E:768:LEU:CD1	2.47	0.44
4:E:1301:FAR:H43	2:G:333:VAL:HG21	1.98	0.44
1:M:108:THR:HG22	1:M:133:LEU:HD23	1.98	0.44
1:M:938:SER:OG	1:M:941:GLU:HG3	2.17	0.44
1:I:479:LEU:HB2	1:I:520:PHE:CD2	2.52	0.44
1:I:788:THR:O	1:I:792:PRO:HG3	2.09	0.44
3:B:98:ALA:O	3:B:102:ARG:HG3	2.17	0.44
3:B:284:PRO:HD3	3:B:312:LEU:HD21	2.00	0.44
3:B:477:ARG:NH2	3:F:460:SER:CB	2.80	0.44
3:J:103:ARG:HH21	3:N:477:ARG:CZ	2.28	0.44
3:J:122:MET:HE3	3:J:178:TYR:CE1	2.52	0.44
3:J:240:GLY:HA3	3:J:299:CYS:SG	2.57	0.44
3:J:497:VAL:HA	3:J:617:PHE:O	2.17	0.44
3:J:587:MET:HE1	3:J:855:ILE:HG13	1.99	0.44
3:J:795:SER:C	3:J:798:PRO:HD2	2.38	0.44
3:J:796:ILE:HD11	3:J:851:GLN:O	2.17	0.44
3:J:883:MET:HG3	3:J:914:ILE:HD13	1.99	0.44
3:N:497:VAL:HA	3:N:617:PHE:O	2.17	0.44
3:N:556:PRO:HB2	5:N:1102:ADP:C8	2.52	0.44
3:N:779:TRP:HA	3:N:782:VAL:HG23	1.99	0.44
1:A:69:GLU:HG2	3:B:262:TRP:CZ3	2.51	0.44
2:C:382:LEU:HD13	2:C:382:LEU:HA	1.76	0.44
1:E:169:VAL:O	1:E:173:GLU:HB2	2.17	0.44
1:E:1074:LYS:HG2	1:E:1135:THR:HG21	1.99	0.44
1:E:1120:GLN:HE22	1:E:1181:ALA:CB	2.21	0.44
1:M:57:LEU:HD13	1:M:412:LEU:HD11	1.99	0.44
1:M:262:VAL:HA	1:M:267:ALA:HB3	2.00	0.44
1:M:1207:ALA:O	1:M:1211:VAL:HG23	2.17	0.44
1:I:337:LEU:CD1	1:I:406:LEU:HD22	2.47	0.44
3:B:780:LEU:HD12	3:B:780:LEU:HA	1.84	0.44
3:F:98:ALA:O	3:F:102:ARG:HG3	2.17	0.44
3:F:883:MET:HG3	3:F:914:ILE:HD13	1.99	0.44
3:J:958:VAL:HG22	3:J:1024:LEU:HD12	1.99	0.44
3:N:811:THR:HA	3:N:820:GLU:O	2.18	0.44
1:A:112:LEU:HD11	1:A:168:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ALA:HA	1:A:1133:VAL:HG22	2.00	0.44
1:E:1054:TRP:HA	1:E:1057:ARG:HG3	2.00	0.44
2:G:374:THR:OG1	2:G:379:LEU:HB2	2.17	0.44
1:M:98:LYS:HE3	1:M:127:ASP:OD1	2.18	0.44
1:M:337:LEU:CD1	1:M:406:LEU:HD22	2.47	0.44
1:M:1130:ALA:HA	1:M:1133:VAL:HG22	2.00	0.44
1:I:465:ILE:O	1:I:468:VAL:HG12	2.18	0.44
3:B:103:ARG:HH21	3:F:477:ARG:CZ	2.26	0.44
3:B:477:ARG:HD3	3:F:103:ARG:CZ	2.48	0.44
3:B:497:VAL:HA	3:B:617:PHE:O	2.17	0.44
3:B:796:ILE:HD11	3:B:851:GLN:O	2.17	0.44
3:F:139:PHE:CD1	3:F:143:PRO:HA	2.53	0.44
3:F:223:ARG:CD	3:F:228:ASN:HD21	2.31	0.44
3:J:223:ARG:CD	3:J:228:ASN:HD21	2.31	0.44
3:J:304:ALA:O	3:J:469:ARG:HB3	2.18	0.44
3:J:942:TYR:CZ	3:J:984:GLU:OE2	2.70	0.44
3:J:1059:PRO:HA	3:J:1065:THR:OG1	2.17	0.44
3:N:304:ALA:O	3:N:469:ARG:HB3	2.18	0.44
1:A:169:VAL:O	1:A:173:GLU:HB2	2.17	0.44
1:A:189:LYS:C	1:A:191:ASN:N	2.71	0.44
1:A:771:LYS:NZ	1:A:802:ARG:HD3	2.31	0.44
1:E:86:ARG:O	1:E:90:HIS:ND1	2.50	0.44
1:M:86:ARG:O	1:M:90:HIS:ND1	2.50	0.44
1:M:1200:MET:HE1	2:O:351:ALA:HA	1.99	0.44
1:I:262:VAL:HA	1:I:267:ALA:HB3	2.00	0.44
1:I:1081:LYS:CB	4:I:1301:FAR:C14	2.94	0.44
3:B:223:ARG:CD	3:B:228:ASN:HD21	2.31	0.44
3:B:730:LYS:O	3:B:733:ASP:N	2.46	0.44
3:F:69:GLY:CA	3:F:120:LYS:HG2	2.47	0.44
3:F:737:LEU:HD22	3:F:769:VAL:HG22	2.00	0.44
4:F:1103:FAR:C15	3:J:1013:ASN:ND2	2.69	0.44
3:J:737:LEU:HD22	3:J:769:VAL:HG22	2.00	0.44
3:J:811:THR:HA	3:J:820:GLU:O	2.18	0.44
3:N:74:LYS:CD	3:N:439:LYS:HZ3	2.16	0.44
3:N:240:GLY:HA3	3:N:299:CYS:SG	2.57	0.44
3:N:998:ILE:HD13	3:N:998:ILE:HA	1.84	0.44
1:A:93:ILE:CG2	3:B:67:THR:HG23	2.45	0.44
1:A:504:VAL:HG22	1:A:550:LEU:HG	1.98	0.44
1:E:98:LYS:HE3	1:E:127:ASP:OD1	2.18	0.44
1:M:934:SER:O	1:M:935:LEU:HB2	2.17	0.44
1:I:86:ARG:O	1:I:90:HIS:ND1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:809:LEU:O	1:I:813:LEU:N	2.38	0.44
1:I:938:SER:OG	1:I:941:GLU:HG3	2.17	0.44
3:B:304:ALA:O	3:B:469:ARG:HB3	2.18	0.44
3:B:452:LYS:HD2	3:B:452:LYS:HA	1.72	0.44
3:F:216:PRO:HG3	3:F:234:LEU:HD11	1.99	0.44
3:F:958:VAL:HG22	3:F:1024:LEU:HD12	1.99	0.44
3:F:1063:ARG:HD2	3:F:1063:ARG:HA	1.82	0.44
3:F:1074:MET:HE3	3:J:1074:MET:HG3	1.99	0.44
3:J:800:ILE:HD13	3:J:822:ILE:HD12	1.99	0.44
3:N:216:PRO:HG3	3:N:234:LEU:HD11	1.99	0.44
3:N:634:ILE:HG22	3:N:638:LEU:CD1	2.47	0.44
1:A:3:SER:O	1:A:8:GLY:N	2.51	0.44
1:A:788:THR:O	1:A:792:PRO:HG3	2.09	0.44
1:M:169:VAL:O	1:M:173:GLU:HB2	2.17	0.44
1:M:479:LEU:HB2	1:M:520:PHE:CD2	2.52	0.44
1:M:1134:LEU:HD11	1:M:1149:ILE:HG21	1.99	0.44
1:M:1197:PHE:CZ	2:O:375:PRO:HG3	2.52	0.44
1:I:858:LEU:HD23	1:I:858:LEU:HA	1.80	0.44
1:I:934:SER:O	1:I:935:LEU:HB2	2.17	0.44
3:B:240:GLY:HA3	3:B:299:CYS:SG	2.57	0.44
3:B:714:VAL:HG11	3:B:743:LEU:CG	2.41	0.44
3:B:1059:PRO:HA	3:B:1065:THR:OG1	2.17	0.44
3:F:736:CYS:HB3	3:F:739:SER:H	1.82	0.44
3:F:1090:CYS:HG	4:F:1101:FAR:C1	1.13	0.44
3:F:1091:LEU:HD12	3:J:939:THR:HG23	1.98	0.44
3:J:361:ILE:CG1	3:J:421:LYS:CE	2.96	0.44
3:N:569:LEU:HD22	3:N:679:LEU:HD22	2.00	0.44
3:N:1059:PRO:HA	3:N:1065:THR:OG1	2.18	0.44
1:A:98:LYS:HE3	1:A:127:ASP:OD1	2.18	0.44
2:C:333:VAL:O	2:C:337:PRO:HG3	2.18	0.44
1:E:62:ARG:NH2	3:F:258:GLN:OE1	2.50	0.44
1:E:1067:VAL:HG12	1:E:1124:ARG:NH2	2.33	0.44
2:G:352:PHE:O	2:G:353:ARG:C	2.55	0.44
1:M:3:SER:O	1:M:8:GLY:N	2.51	0.44
1:I:98:LYS:HE3	1:I:127:ASP:OD1	2.18	0.44
1:I:901:LEU:HD22	1:I:912:PHE:CZ	2.43	0.44
1:I:1074:LYS:HG2	1:I:1135:THR:HG21	1.99	0.44
3:B:139:PHE:CD1	3:B:143:PRO:HA	2.53	0.44
3:B:1092:ILE:CG2	3:N:1004:MET:HG3	2.48	0.44
3:F:1075:ASN:HA	3:J:1071:LYS:HE2	2.00	0.44
3:J:105:ASP:O	3:N:614:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:556:PRO:HB2	5:J:1101:ADP:C8	2.52	0.44
1:A:75:TYR:OH	3:B:191:GLN:CD	2.56	0.44
1:A:233:ASP:OD2	1:A:503:GLY:N	2.50	0.44
1:A:262:VAL:HA	1:A:267:ALA:HB3	2.00	0.44
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.88	0.44
1:A:1134:LEU:HD11	1:A:1149:ILE:HG21	1.99	0.44
1:M:189:LYS:C	1:M:191:ASN:N	2.71	0.44
1:M:765:ALA:HB1	1:M:768:LEU:CD1	2.47	0.44
1:M:1200:MET:HE3	2:O:351:ALA:HA	1.98	0.44
1:I:337:LEU:HD11	1:I:406:LEU:HD22	2.00	0.44
1:I:765:ALA:HB1	1:I:768:LEU:CD1	2.47	0.44
3:B:755:PHE:O	3:B:762:VAL:HG13	2.18	0.44
3:B:795:SER:C	3:B:798:PRO:HD2	2.38	0.44
3:F:744:LEU:HD21	3:F:765:HIS:CD2	2.32	0.44
3:F:1059:PRO:HA	3:F:1065:THR:OG1	2.17	0.44
3:N:223:ARG:CD	3:N:228:ASN:ND2	2.79	0.44
1:A:1074:LYS:HG2	1:A:1135:THR:HG21	1.99	0.43
1:E:527:GLN:HB3	1:E:529:GLN:HE22	1.83	0.43
1:E:1197:PHE:CZ	2:G:375:PRO:HG3	2.53	0.43
2:G:333:VAL:O	2:G:337:PRO:HG3	2.18	0.43
1:M:465:ILE:O	1:M:468:VAL:HG12	2.18	0.43
1:I:24:CYS:O	3:J:546:LYS:HD3	2.18	0.43
1:I:768:LEU:HD22	1:I:802:ARG:HH21	1.60	0.43
1:I:1197:PHE:CZ	2:K:375:PRO:HG3	2.52	0.43
2:K:333:VAL:O	2:K:337:PRO:HG3	2.18	0.43
3:B:800:ILE:HD13	3:B:822:ILE:HD12	1.99	0.43
4:B:1101:FAR:H91	3:N:1070:THR:HG21	2.00	0.43
3:F:497:VAL:HA	3:F:617:PHE:O	2.17	0.43
3:F:556:PRO:HB2	5:F:1102:ADP:C8	2.52	0.43
3:F:795:SER:C	3:F:798:PRO:HD2	2.38	0.43
3:F:1012:ARG:HD3	3:J:1013:ASN:HA	2.00	0.43
3:J:139:PHE:CD1	3:J:143:PRO:HA	2.53	0.43
3:J:183:VAL:HG12	3:J:467:VAL:HG21	2.00	0.43
3:J:569:LEU:HD22	3:J:679:LEU:HD22	2.00	0.43
3:N:223:ARG:CD	3:N:228:ASN:HD21	2.31	0.43
3:N:1092:ILE:HG23	4:N:1101:FAR:H11	2.00	0.43
1:A:79:GLN:HB2	3:B:194:TYR:O	2.19	0.43
1:A:491:ARG:CG	3:B:62:LEU:CD1	2.96	0.43
2:C:352:PHE:O	2:C:353:ARG:C	2.55	0.43
1:E:337:LEU:HD11	1:E:406:LEU:HD22	2.00	0.43
1:E:397:LYS:HE3	1:E:400:HIS:CD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:ILE:O	1:E:468:VAL:HG12	2.18	0.43
1:E:1215:LEU:O	2:G:330:ARG:NH2	2.52	0.43
2:G:333:VAL:HG13	2:G:343:LEU:HD21	2.00	0.43
1:M:100:GLU:OE2	1:M:495:SER:OG	2.30	0.43
1:M:527:GLN:HB3	1:M:529:GLN:HE22	1.83	0.43
1:I:3:SER:O	1:I:8:GLY:N	2.51	0.43
1:I:211:ALA:HB1	1:I:426:LEU:HD13	1.99	0.43
1:I:441:GLN:HG2	1:I:560:PRO:O	2.18	0.43
3:B:599:LYS:HG2	3:B:646:ILE:HG12	2.00	0.43
3:B:811:THR:HA	3:B:820:GLU:O	2.18	0.43
3:B:903:SER:O	3:B:904:PRO:C	2.56	0.43
3:F:304:ALA:O	3:F:469:ARG:HB3	2.18	0.43
3:F:780:LEU:HD12	3:F:780:LEU:HA	1.84	0.43
3:J:714:VAL:HG11	3:J:743:LEU:CG	2.41	0.43
3:J:924:TRP:CE2	3:J:1059:PRO:HD3	2.53	0.43
3:N:139:PHE:CD1	3:N:143:PRO:HA	2.53	0.43
3:N:523:VAL:HG21	3:N:528:ILE:CD1	2.43	0.43
1:A:1054:TRP:HA	1:A:1057:ARG:HG3	2.00	0.43
1:E:469:TYR:CG	1:E:470:PRO:HA	2.54	0.43
1:E:1130:ALA:HA	1:E:1133:VAL:HG22	2.00	0.43
1:M:441:GLN:HG2	1:M:560:PRO:O	2.18	0.43
1:M:1215:LEU:O	2:O:330:ARG:NH2	2.51	0.43
1:I:57:LEU:HD13	1:I:412:LEU:HD11	1.99	0.43
1:I:169:VAL:O	1:I:173:GLU:HB2	2.17	0.43
1:I:1054:TRP:HA	1:I:1057:ARG:HG3	2.00	0.43
1:I:1130:ALA:HA	1:I:1133:VAL:HG22	2.00	0.43
2:K:374:THR:OG1	2:K:379:LEU:HB2	2.17	0.43
3:F:132:GLN:HE22	3:F:150:HIS:CB	2.32	0.43
3:F:342:LEU:HD21	3:F:421:LYS:HZ2	1.82	0.43
3:F:634:ILE:HG22	3:F:638:LEU:CD1	2.47	0.43
3:F:903:SER:O	3:F:904:PRO:C	2.56	0.43
3:F:942:TYR:CZ	3:F:984:GLU:OE2	2.69	0.43
3:N:170:LEU:O	3:N:217:ASP:HB2	2.19	0.43
3:N:924:TRP:CE2	3:N:1059:PRO:HD3	2.53	0.43
1:A:825:LEU:O	1:A:829:ILE:HG13	2.19	0.43
1:E:513:ILE:HG22	1:E:514:ARG:HG3	2.01	0.43
1:E:797:GLU:HG2	1:E:807:ARG:HD2	2.00	0.43
1:E:1120:GLN:HE22	1:E:1181:ALA:HB3	1.71	0.43
1:M:337:LEU:HD11	1:M:406:LEU:HD22	2.00	0.43
1:M:1054:TRP:HA	1:M:1057:ARG:HG3	2.00	0.43
1:I:797:GLU:HG2	1:I:807:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1067:VAL:HG12	1:I:1124:ARG:NH2	2.33	0.43
2:K:333:VAL:HG13	2:K:343:LEU:HD21	2.01	0.43
3:B:103:ARG:HH22	3:F:477:ARG:NH1	2.16	0.43
3:B:361:ILE:CG1	3:B:421:LYS:CE	2.96	0.43
3:J:279:LEU:HG	3:J:283:LEU:HD12	2.00	0.43
3:N:599:LYS:HG2	3:N:646:ILE:HG12	2.00	0.43
1:E:3:SER:O	1:E:8:GLY:N	2.51	0.43
1:E:93:ILE:HG21	3:F:67:THR:HA	2.00	0.43
1:E:134:GLN:HG2	1:E:182:GLY:O	2.19	0.43
1:E:262:VAL:HA	1:E:267:ALA:HB3	2.00	0.43
2:O:352:PHE:CD1	2:O:352:PHE:C	2.92	0.43
1:I:57:LEU:HD12	1:I:57:LEU:HA	1.79	0.43
1:I:66:ASP:HA	3:N:667:GLN:NE2	2.34	0.43
1:I:458:LYS:HD3	1:I:458:LYS:HA	1.76	0.43
1:I:846:ASP:O	1:I:849:SER:OG	2.23	0.43
1:I:1215:LEU:O	2:K:330:ARG:NH2	2.52	0.43
2:K:382:LEU:HD13	2:K:382:LEU:HA	1.76	0.43
3:B:569:LEU:HD22	3:B:679:LEU:HD22	2.00	0.43
3:B:737:LEU:HD22	3:B:769:VAL:HG22	2.00	0.43
3:F:568:ILE:HG23	3:F:671:LEU:CD1	2.49	0.43
3:F:811:THR:HA	3:F:820:GLU:O	2.18	0.43
3:F:1001:GLU:HG2	3:J:1092:ILE:HG13	1.85	0.43
3:J:132:GLN:HE22	3:J:150:HIS:CB	2.31	0.43
3:N:183:VAL:HG12	3:N:467:VAL:HG21	2.00	0.43
3:N:1057:THR:HG22	3:N:1064:GLY:HA2	2.00	0.43
1:A:120:THR:HG22	3:B:131:ARG:NE	2.28	0.43
1:A:184:TRP:CD2	1:A:295:ARG:HD2	2.54	0.43
1:A:465:ILE:O	1:A:468:VAL:HG12	2.18	0.43
1:A:513:ILE:HG22	1:A:514:ARG:HG3	2.01	0.43
1:A:854:LEU:O	1:A:867:ILE:N	2.38	0.43
1:E:57:LEU:HD13	1:E:412:LEU:HD11	1.99	0.43
1:E:557:THR:HG22	3:B:514:GLY:HA2	2.00	0.43
1:E:566:ILE:HA	1:E:570:MET:SD	2.59	0.43
1:E:825:LEU:O	1:E:829:ILE:HG13	2.19	0.43
1:M:1067:VAL:HG12	1:M:1124:ARG:NH2	2.33	0.43
1:I:924:ILE:HD13	1:I:924:ILE:HA	1.89	0.43
3:B:170:LEU:O	3:B:217:ASP:HB2	2.19	0.43
3:B:924:TRP:CE2	3:B:1059:PRO:HD3	2.53	0.43
3:J:779:TRP:HA	3:J:782:VAL:HG23	2.00	0.43
3:N:714:VAL:HG13	3:N:719:TRP:CD1	2.54	0.43
3:N:744:LEU:HG	3:N:766:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:949:LEU:CD2	3:N:963:LEU:HG	2.49	0.43
1:A:901:LEU:HD22	1:A:912:PHE:CZ	2.43	0.43
1:M:184:TRP:CD2	1:M:295:ARG:HD2	2.54	0.43
1:M:797:GLU:HG2	1:M:807:ARG:HD2	2.00	0.43
1:M:918:LEU:HD13	1:M:918:LEU:HA	1.91	0.43
1:M:1074:LYS:HG2	1:M:1135:THR:HG21	1.99	0.43
2:K:352:PHE:C	2:K:352:PHE:CD1	2.92	0.43
3:B:122:MET:HE3	3:B:122:MET:HB3	1.80	0.43
3:B:1057:THR:HG22	3:B:1064:GLY:HA2	2.00	0.43
3:N:800:ILE:HD13	3:N:822:ILE:HD12	1.99	0.43
1:A:72:ALA:CB	3:B:260:CYS:HB2	2.49	0.43
1:A:75:TYR:OH	3:B:191:GLN:HG3	2.17	0.43
1:A:79:GLN:HB3	3:B:194:TYR:CG	2.54	0.43
1:A:89:LEU:O	1:A:93:ILE:N	2.43	0.43
1:A:441:GLN:HG2	1:A:560:PRO:O	2.18	0.43
1:E:203:GLY:HA2	1:E:242:LEU:HD11	2.01	0.43
1:E:523:GLN:O	1:E:527:GLN:HG3	2.19	0.43
1:M:203:GLY:HA2	1:M:242:LEU:HD11	2.01	0.43
1:M:825:LEU:O	1:M:829:ILE:HG13	2.19	0.43
1:M:1132:LEU:O	1:M:1136:MET:N	2.46	0.43
2:O:352:PHE:O	2:O:353:ARG:C	2.55	0.43
1:I:184:TRP:CE2	1:I:295:ARG:HD2	2.54	0.43
1:I:523:GLN:O	1:I:527:GLN:HG3	2.19	0.43
3:B:223:ARG:CD	3:B:228:ASN:ND2	2.79	0.43
3:B:714:VAL:HG13	3:B:719:TRP:CD1	2.54	0.43
3:B:744:LEU:HG	3:B:766:ILE:HG13	2.01	0.43
3:B:938:PRO:HB3	3:N:1091:LEU:O	2.18	0.43
3:B:949:LEU:CD2	3:B:963:LEU:HG	2.49	0.43
3:F:744:LEU:HG	3:F:766:ILE:HG13	2.01	0.43
3:F:924:TRP:CE2	3:F:1059:PRO:HD3	2.53	0.43
3:F:949:LEU:CD2	3:F:963:LEU:HG	2.49	0.43
3:J:744:LEU:HG	3:J:766:ILE:HG13	2.01	0.43
3:N:279:LEU:HG	3:N:283:LEU:CD1	2.49	0.43
3:N:795:SER:C	3:N:798:PRO:HD2	2.38	0.43
1:A:71:LYS:HD2	3:B:258:GLN:HE22	1.83	0.43
1:A:183:ILE:HD13	1:A:258:SER:HB2	2.00	0.43
1:A:397:LYS:HE3	1:A:400:HIS:CD2	2.51	0.43
1:A:1208:ALA:HB3	2:C:334:ILE:CG1	2.46	0.43
2:G:382:LEU:HD13	2:G:382:LEU:HA	1.76	0.43
1:M:183:ILE:HD13	1:M:258:SER:HB2	2.00	0.43
1:M:1067:VAL:HG12	1:M:1124:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:GLN:HG2	1:I:182:GLY:O	2.19	0.43
1:I:469:TYR:CG	1:I:470:PRO:HA	2.54	0.43
1:I:1067:VAL:HG12	1:I:1124:ARG:HH22	1.84	0.43
1:I:1118:VAL:HG21	1:I:1127:LEU:HD12	2.01	0.43
3:B:132:GLN:HE22	3:B:150:HIS:CB	2.31	0.43
3:F:214:ARG:HB2	3:F:825:PRO:HB2	2.01	0.43
3:F:576:TYR:HA	3:F:577:PRO:HD3	1.84	0.43
3:F:1014:PRO:HD2	3:J:1012:ARG:NE	2.34	0.43
3:J:216:PRO:HG3	3:J:234:LEU:HD11	1.99	0.43
3:J:477:ARG:CZ	3:N:103:ARG:HH21	2.28	0.43
3:J:714:VAL:HG13	3:J:719:TRP:CD1	2.54	0.43
3:J:755:PHE:O	3:J:762:VAL:HG13	2.18	0.43
3:J:1057:THR:HG22	3:J:1064:GLY:HA2	2.00	0.43
3:N:568:ILE:HG23	3:N:671:LEU:CD1	2.49	0.43
3:N:737:LEU:HD22	3:N:769:VAL:HG22	2.00	0.43
1:A:797:GLU:HG2	1:A:807:ARG:HD2	2.00	0.43
1:E:184:TRP:CE2	1:E:295:ARG:HD2	2.54	0.43
1:E:441:GLN:HG2	1:E:560:PRO:O	2.18	0.43
1:E:1200:MET:HE3	2:G:351:ALA:HA	2.01	0.43
1:M:523:GLN:O	1:M:527:GLN:HG3	2.19	0.43
2:O:333:VAL:HG13	2:O:343:LEU:HD21	2.00	0.43
1:I:610:THR:HG22	3:N:635:LEU:CD2	2.48	0.43
1:I:770:LEU:HD22	1:I:787:TYR:CE2	2.54	0.43
1:I:1172:ASP:O	1:I:1175:MET:HG2	2.19	0.43
3:F:1004:MET:CB	3:J:1092:ILE:HG22	2.44	0.43
3:F:1009:VAL:CB	4:F:1103:FAR:H143	2.42	0.43
3:N:714:VAL:HG11	3:N:743:LEU:CG	2.41	0.43
1:A:337:LEU:HD11	1:A:406:LEU:HD22	2.00	0.42
1:A:770:LEU:HD22	1:A:787:TYR:CE2	2.54	0.42
1:A:1215:LEU:O	2:C:330:ARG:NH2	2.52	0.42
1:E:189:LYS:C	1:E:191:ASN:N	2.71	0.42
1:M:184:TRP:CE2	1:M:295:ARG:HD2	2.54	0.42
1:M:441:GLN:HG3	1:M:561:THR:HG23	2.01	0.42
1:M:469:TYR:CG	1:M:470:PRO:HA	2.54	0.42
1:I:203:GLY:HA2	1:I:242:LEU:HD11	2.01	0.42
1:I:1141:GLU:OE2	1:I:1215:LEU:HD21	2.19	0.42
3:B:568:ILE:HG23	3:B:671:LEU:CD1	2.49	0.42
3:B:992:GLN:HA	3:B:993:PRO:HD3	1.89	0.42
3:F:532:GLN:H	3:F:532:GLN:HG3	1.51	0.42
3:F:569:LEU:HD22	3:F:679:LEU:HD22	2.00	0.42
3:F:593:LEU:HD12	3:F:593:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:606:LYS:HD3	3:F:649:VAL:HG22	2.01	0.42
3:F:714:VAL:HG13	3:F:719:TRP:CD1	2.54	0.42
3:J:214:ARG:HB2	3:J:825:PRO:HB2	2.01	0.42
3:J:789:THR:HG21	3:J:791:LYS:NZ	2.34	0.42
3:N:355:ILE:HD13	3:N:355:ILE:HA	1.78	0.42
3:N:630:ARG:HE	3:N:777:LYS:CE	2.32	0.42
3:N:755:PHE:O	3:N:762:VAL:HG13	2.18	0.42
1:A:203:GLY:HA2	1:A:242:LEU:HD11	2.01	0.42
1:A:1067:VAL:HG12	1:A:1124:ARG:NH2	2.33	0.42
1:E:102:PHE:HB2	1:E:110:ASP:O	2.19	0.42
1:E:184:TRP:CD2	1:E:295:ARG:HD2	2.54	0.42
1:E:441:GLN:HG3	1:E:561:THR:HG23	2.01	0.42
1:E:442:VAL:HG22	1:E:601:THR:HG22	2.02	0.42
1:E:800:ASN:ND2	1:E:809:LEU:HD13	2.34	0.42
1:M:71:LYS:HD2	3:N:258:GLN:HE22	1.83	0.42
1:M:770:LEU:HD22	1:M:787:TYR:CE2	2.54	0.42
1:M:903:MET:HE2	1:M:955:LYS:HE2	2.01	0.42
2:O:333:VAL:O	2:O:337:PRO:HG3	2.18	0.42
1:I:94:ARG:NH1	3:J:157:THR:HA	2.34	0.42
1:I:102:PHE:HB2	1:I:110:ASP:O	2.19	0.42
1:I:332:TRP:HH2	1:I:352:LYS:HZ2	1.64	0.42
3:B:497:VAL:HG21	3:B:641:LEU:HD22	2.01	0.42
3:F:726:GLU:HA	3:F:729:GLN:HB2	2.01	0.42
3:F:755:PHE:O	3:F:762:VAL:HG13	2.18	0.42
3:F:779:TRP:HA	3:F:782:VAL:HG23	1.99	0.42
3:F:786:ALA:CB	3:F:848:VAL:HG11	2.47	0.42
3:F:1078:LEU:HD11	3:J:1070:THR:CG2	2.48	0.42
3:J:460:SER:CB	3:N:477:ARG:NH2	2.79	0.42
3:J:599:LYS:HG2	3:J:646:ILE:HG12	2.00	0.42
3:J:928:ARG:HH12	3:J:1065:THR:HG21	1.84	0.42
3:J:949:LEU:CD2	3:J:963:LEU:HG	2.49	0.42
3:N:214:ARG:HB2	3:N:825:PRO:HB2	2.00	0.42
3:N:789:THR:HG21	3:N:791:LYS:NZ	2.35	0.42
1:A:442:VAL:HG22	1:A:601:THR:HG22	2.02	0.42
1:A:469:TYR:CG	1:A:470:PRO:HA	2.54	0.42
1:A:566:ILE:HA	1:A:570:MET:SD	2.59	0.42
1:M:102:PHE:HB2	1:M:110:ASP:O	2.19	0.42
1:M:368:LEU:HA	1:M:399:PRO:HB3	2.01	0.42
1:M:1118:VAL:HG21	1:M:1127:LEU:HD12	2.01	0.42
1:M:1141:GLU:OE2	1:M:1215:LEU:HD21	2.19	0.42
1:I:441:GLN:HG3	1:I:561:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:442:VAL:HG22	1:I:601:THR:HG22	2.02	0.42
1:I:527:GLN:HB3	1:I:529:GLN:HE22	1.83	0.42
1:I:856:VAL:HG22	1:I:865:LYS:O	2.20	0.42
1:I:905:MET:HG2	1:I:912:PHE:CD2	2.55	0.42
3:B:216:PRO:HG3	3:B:234:LEU:CD1	2.50	0.42
3:J:95:TRP:CE2	3:J:99:LEU:HD11	2.55	0.42
3:N:60:LEU:HD23	3:N:60:LEU:HA	1.90	0.42
2:C:352:PHE:C	2:C:352:PHE:CD1	2.92	0.42
1:E:233:ASP:OD2	1:E:503:GLY:N	2.50	0.42
1:E:934:SER:HG	1:E:967:PHE:HD2	1.67	0.42
1:E:1120:GLN:HA	1:E:1121:PRO:HD3	1.89	0.42
1:M:442:VAL:HG22	1:M:601:THR:HG22	2.02	0.42
1:I:566:ILE:HA	1:I:570:MET:SD	2.59	0.42
2:K:352:PHE:O	2:K:353:ARG:C	2.55	0.42
3:B:361:ILE:CG1	3:B:421:LYS:HE3	2.44	0.42
3:F:95:TRP:CE2	3:F:99:LEU:HD11	2.55	0.42
3:F:599:LYS:HG2	3:F:646:ILE:HG12	2.00	0.42
3:J:122:MET:HE3	3:J:122:MET:HB3	1.84	0.42
3:J:282:LEU:HD23	3:J:282:LEU:HA	1.91	0.42
3:J:568:ILE:HG23	3:J:671:LEU:CD1	2.49	0.42
3:J:630:ARG:HE	3:J:777:LYS:CE	2.32	0.42
3:N:132:GLN:HE22	3:N:150:HIS:CB	2.32	0.42
1:A:441:GLN:O	1:A:561:THR:HA	2.20	0.42
1:A:527:GLN:HB3	1:A:529:GLN:HE22	1.83	0.42
1:A:856:VAL:HG22	1:A:865:LYS:O	2.20	0.42
1:A:1141:GLU:OE2	1:A:1215:LEU:HD21	2.19	0.42
1:M:255:VAL:HG13	1:M:287:LEU:HD11	2.02	0.42
1:M:419:ALA:CB	3:J:524:GLU:OE1	2.63	0.42
1:M:513:ILE:HG22	1:M:514:ARG:HG3	2.01	0.42
2:O:340:LEU:HA	2:O:340:LEU:HD23	1.85	0.42
1:I:184:TRP:CD2	1:I:295:ARG:HD2	2.54	0.42
1:I:513:ILE:HG22	1:I:514:ARG:HG3	2.01	0.42
1:I:582:ILE:O	1:I:586:LEU:HG	2.20	0.42
1:I:800:ASN:ND2	1:I:809:LEU:HD13	2.34	0.42
1:I:825:LEU:O	1:I:829:ILE:HG13	2.19	0.42
1:I:1076:TRP:CZ2	1:I:1102:PRO:HD3	2.55	0.42
3:B:214:ARG:HB2	3:B:825:PRO:HB2	2.01	0.42
3:B:579:ILE:HD12	3:B:601:ALA:CB	2.41	0.42
3:B:614:ARG:HA	3:B:615:PRO:HD3	1.92	0.42
3:B:928:ARG:HH12	3:B:1065:THR:HG21	1.85	0.42
3:F:183:VAL:HG12	3:F:467:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:789:THR:HG21	3:F:791:LYS:NZ	2.35	0.42
3:F:928:ARG:HH12	3:F:1065:THR:HG21	1.84	0.42
3:J:216:PRO:HG3	3:J:234:LEU:CD1	2.50	0.42
3:J:580:PHE:CZ	3:J:598:ILE:HG12	2.55	0.42
1:E:582:ILE:O	1:E:586:LEU:HG	2.20	0.42
1:E:903:MET:HE2	1:E:955:LYS:HE2	2.02	0.42
1:E:1076:TRP:CZ2	1:E:1102:PRO:HD3	2.55	0.42
1:E:1118:VAL:HG21	1:E:1127:LEU:HD12	2.01	0.42
1:I:66:ASP:CA	3:N:667:GLN:NE2	2.81	0.42
1:I:183:ILE:HD13	1:I:258:SER:HB2	2.00	0.42
3:B:103:ARG:CZ	3:F:477:ARG:CD	2.98	0.42
3:B:580:PHE:CZ	3:B:598:ILE:HG12	2.55	0.42
3:B:942:TYR:CZ	3:B:984:GLU:OE2	2.70	0.42
3:B:957:ILE:CG1	3:B:962:HIS:ND1	2.83	0.42
3:F:1057:THR:HG22	3:F:1064:GLY:HA2	2.00	0.42
3:J:205:LEU:HD23	3:J:205:LEU:HA	1.85	0.42
1:A:184:TRP:CE2	1:A:295:ARG:HD2	2.54	0.42
1:A:236:GLN:HG3	1:A:553:ARG:HB3	2.02	0.42
1:A:400:HIS:O	1:A:404:GLN:N	2.43	0.42
1:A:441:GLN:HG3	1:A:561:THR:HG23	2.01	0.42
1:E:183:ILE:HD13	1:E:258:SER:HB2	2.00	0.42
1:E:856:VAL:HG22	1:E:865:LYS:O	2.20	0.42
1:M:1076:TRP:CZ2	1:M:1102:PRO:HD3	2.55	0.42
1:I:1205:LYS:O	1:I:1209:THR:OG1	2.31	0.42
3:F:580:PHE:CZ	3:F:598:ILE:HG12	2.55	0.42
3:J:170:LEU:O	3:J:217:ASP:HB2	2.19	0.42
3:J:523:VAL:HG21	3:J:528:ILE:CD1	2.43	0.42
3:J:606:LYS:HD3	3:J:649:VAL:HG22	2.02	0.42
3:N:95:TRP:CE2	3:N:99:LEU:HD11	2.55	0.42
3:N:497:VAL:HG21	3:N:641:LEU:HD22	2.01	0.42
3:N:502:GLU:HG3	3:N:685:PHE:HZ	1.85	0.42
1:A:134:GLN:HG2	1:A:182:GLY:O	2.19	0.42
1:A:435:LYS:HE2	1:A:435:LYS:HB3	1.80	0.42
1:A:1118:VAL:HG21	1:A:1127:LEU:HD12	2.01	0.42
1:E:854:LEU:O	1:E:867:ILE:N	2.38	0.42
1:M:441:GLN:O	1:M:561:THR:HA	2.20	0.42
1:M:566:ILE:HA	1:M:570:MET:SD	2.59	0.42
1:I:922:LEU:HD13	1:I:1063:ALA:HA	2.02	0.42
3:B:630:ARG:HE	3:B:777:LYS:CE	2.32	0.42
3:F:992:GLN:HA	3:F:993:PRO:HD3	1.89	0.42
3:J:103:ARG:NH2	3:N:477:ARG:NE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:212:VAL:HG12	3:J:239:VAL:HG22	2.01	0.42
3:J:957:ILE:CG1	3:J:962:HIS:ND1	2.83	0.42
1:A:789:MET:O	1:A:793:ASP:HB2	2.20	0.42
1:A:1076:TRP:CZ2	1:A:1102:PRO:HD3	2.55	0.42
1:E:905:MET:HG2	1:E:912:PHE:CD2	2.55	0.42
1:M:856:VAL:HG22	1:M:865:LYS:O	2.20	0.42
1:I:771:LYS:HG3	1:I:802:ARG:HH11	1.75	0.42
3:B:88:LEU:CD2	3:B:178:TYR:HA	2.48	0.42
3:B:618:LEU:HD21	3:B:656:LEU:HD11	2.02	0.42
3:F:216:PRO:HG3	3:F:234:LEU:CD1	2.49	0.42
3:F:361:ILE:CG1	3:F:421:LYS:CE	2.96	0.42
3:F:957:ILE:CG1	3:F:962:HIS:ND1	2.83	0.42
3:F:1013:ASN:OD1	4:F:1101:FAR:C15	2.68	0.42
3:J:412:VAL:HG22	3:J:429:ARG:HG2	2.02	0.42
3:N:412:VAL:HG22	3:N:429:ARG:HG2	2.02	0.42
3:N:579:ILE:HD12	3:N:601:ALA:CB	2.41	0.42
3:N:614:ARG:HA	3:N:615:PRO:HD3	1.92	0.42
3:N:989:ASN:HD22	3:N:989:ASN:HA	1.63	0.42
1:A:858:LEU:HD23	1:A:858:LEU:HA	1.80	0.42
1:A:1067:VAL:HG12	1:A:1124:ARG:HH22	1.84	0.42
2:C:333:VAL:HG13	2:C:343:LEU:HD21	2.01	0.42
1:E:71:LYS:HD2	3:F:258:GLN:NE2	2.35	0.42
1:E:79:GLN:HB3	3:F:194:TYR:CG	2.55	0.42
1:E:236:GLN:HE21	1:E:553:ARG:HB3	1.85	0.42
1:E:441:GLN:O	1:E:561:THR:HA	2.20	0.42
1:E:1057:ARG:H	1:E:1057:ARG:HG2	1.61	0.42
1:E:1205:LYS:O	1:E:1209:THR:OG1	2.31	0.42
1:M:236:GLN:HG3	1:M:553:ARG:HB3	2.02	0.42
1:M:400:HIS:O	1:M:404:GLN:N	2.43	0.42
1:M:905:MET:HG2	1:M:912:PHE:CD2	2.55	0.42
1:I:368:LEU:HA	1:I:399:PRO:HB3	2.01	0.42
1:I:502:MET:O	1:I:523:GLN:NE2	2.50	0.42
3:B:212:VAL:HG12	3:B:239:VAL:HG22	2.01	0.42
3:B:637:MET:HG3	3:B:646:ILE:CD1	2.50	0.42
3:B:974:MET:HE3	3:B:975:TYR:CE1	2.31	0.42
3:F:173:ASN:ND2	3:F:220:VAL:CA	2.80	0.42
3:F:1006:VAL:HG22	3:F:1073:VAL:HG21	2.02	0.42
3:F:1016:LEU:HD11	4:F:1101:FAR:H92	2.02	0.42
3:J:618:LEU:HD21	3:J:656:LEU:HD11	2.02	0.42
3:N:361:ILE:CG1	3:N:421:LYS:CE	2.96	0.42
3:N:580:PHE:CZ	3:N:598:ILE:HG12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:606:LYS:HD3	3:N:649:VAL:HG22	2.02	0.42
1:E:1141:GLU:OE2	1:E:1215:LEU:HD21	2.19	0.41
1:M:134:GLN:HG2	1:M:182:GLY:O	2.19	0.41
1:M:332:TRP:HZ3	1:M:355:LEU:HD21	1.85	0.41
1:I:236:GLN:HE21	1:I:553:ARG:HB3	1.85	0.41
1:I:236:GLN:HG3	1:I:553:ARG:HB3	2.02	0.41
3:B:541:LEU:O	3:B:551:GLY:HA2	2.21	0.41
3:B:726:GLU:HA	3:B:729:GLN:HB2	2.01	0.41
3:F:170:LEU:O	3:F:217:ASP:HB2	2.19	0.41
3:F:173:ASN:HD22	3:F:220:VAL:CA	2.33	0.41
3:F:618:LEU:HD21	3:F:656:LEU:HD11	2.02	0.41
3:J:103:ARG:HH22	3:N:477:ARG:NH1	2.18	0.41
3:J:355:ILE:HD13	3:J:355:ILE:HA	1.78	0.41
3:J:965:GLN:CD	3:J:969:LEU:HD12	2.31	0.41
3:N:216:PRO:HG3	3:N:234:LEU:CD1	2.50	0.41
3:N:618:LEU:HD21	3:N:656:LEU:HD11	2.02	0.41
3:N:957:ILE:CG1	3:N:962:HIS:ND1	2.83	0.41
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.81	0.41
1:A:368:LEU:HA	1:A:399:PRO:HB3	2.01	0.41
1:A:523:GLN:O	1:A:527:GLN:HG3	2.19	0.41
1:E:765:ALA:O	1:E:766:LEU:HD23	2.20	0.41
2:G:333:VAL:HG13	2:G:343:LEU:CD2	2.50	0.41
1:M:800:ASN:ND2	1:M:809:LEU:HD13	2.34	0.41
3:B:173:ASN:HD22	3:B:220:VAL:CA	2.33	0.41
3:B:502:GLU:HG3	3:B:685:PHE:HZ	1.85	0.41
3:B:789:THR:HG21	3:B:791:LYS:NZ	2.35	0.41
3:B:1063:ARG:HA	3:B:1063:ARG:HD2	1.82	0.41
3:B:1067:SER:HB2	3:N:1078:LEU:HD22	2.02	0.41
3:F:283:LEU:HD23	3:F:307:LEU:CD1	2.51	0.41
3:F:541:LEU:O	3:F:551:GLY:HA2	2.21	0.41
3:F:994:GLN:H	3:F:994:GLN:HG2	1.53	0.41
3:F:1074:MET:HG3	3:J:1074:MET:CE	2.49	0.41
3:J:1006:VAL:HG22	3:J:1073:VAL:HG21	2.02	0.41
3:N:56:VAL:CG2	3:N:449:ILE:HG13	2.51	0.41
3:N:212:VAL:HG12	3:N:239:VAL:HG22	2.01	0.41
3:N:637:MET:HG3	3:N:646:ILE:CD1	2.50	0.41
3:N:826:LEU:HD22	3:N:830:VAL:CG1	2.43	0.41
3:N:1063:ARG:HD2	3:N:1063:ARG:HA	1.82	0.41
1:A:102:PHE:HB2	1:A:110:ASP:O	2.19	0.41
1:E:368:LEU:HA	1:E:399:PRO:HB3	2.01	0.41
1:E:530:PHE:CD2	1:E:837:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:770:LEU:HD22	1:E:787:TYR:CE2	2.54	0.41
1:E:922:LEU:HD13	1:E:1063:ALA:HA	2.02	0.41
1:E:938:SER:HG	1:E:941:GLU:HB2	1.84	0.41
1:E:1145:ILE:HG23	1:E:1215:LEU:HD13	2.03	0.41
1:M:530:PHE:CD2	1:M:837:VAL:HG22	2.55	0.41
1:M:1120:GLN:HA	1:M:1121:PRO:HD3	1.89	0.41
1:I:1208:ALA:CB	4:I:1301:FAR:H51	2.50	0.41
3:B:122:MET:HE3	3:B:178:TYR:CE1	2.56	0.41
3:B:454:LEU:HD23	3:B:454:LEU:HA	1.90	0.41
3:B:1003:LEU:HD21	3:B:1024:LEU:HD11	2.01	0.41
3:B:1015:GLU:CD	3:N:1012:ARG:NH1	2.38	0.41
3:F:405:VAL:HA	3:F:445:GLN:HE22	1.86	0.41
3:F:413:PRO:CG	3:F:416:PHE:CD2	2.95	0.41
3:J:246:LEU:HB3	3:J:267:VAL:HG11	2.02	0.41
3:J:497:VAL:HG21	3:J:641:LEU:HD22	2.02	0.41
3:N:223:ARG:CB	3:N:228:ASN:OD1	2.68	0.41
3:N:246:LEU:HB3	3:N:267:VAL:HG11	2.02	0.41
3:N:413:PRO:CG	3:N:416:PHE:CD2	2.95	0.41
3:N:928:ARG:HH12	3:N:1065:THR:HG21	1.84	0.41
1:E:89:LEU:O	1:E:93:ILE:N	2.43	0.41
1:E:94:ARG:HG3	3:F:67:THR:HG21	2.03	0.41
1:E:153:LEU:HD23	1:E:153:LEU:HA	1.94	0.41
2:G:352:PHE:CD1	2:G:352:PHE:C	2.92	0.41
1:M:1134:LEU:HD23	1:M:1134:LEU:HA	1.90	0.41
1:I:62:ARG:CZ	3:J:258:GLN:OE1	2.62	0.41
1:I:255:VAL:HG13	1:I:287:LEU:HD11	2.02	0.41
1:I:441:GLN:O	1:I:561:THR:HA	2.20	0.41
1:I:765:ALA:O	1:I:766:LEU:HD23	2.20	0.41
1:I:1208:ALA:O	2:K:334:ILE:HD11	2.21	0.41
3:B:95:TRP:CE2	3:B:99:LEU:HD11	2.55	0.41
3:B:183:VAL:HG12	3:B:467:VAL:HG21	2.00	0.41
3:F:212:VAL:HG12	3:F:239:VAL:HG22	2.01	0.41
3:F:637:MET:HG3	3:F:646:ILE:CD1	2.50	0.41
3:F:646:ILE:O	3:F:646:ILE:HG23	2.21	0.41
3:F:737:LEU:HD21	3:F:772:ARG:CZ	2.51	0.41
3:F:878:TRP:CE3	3:F:933:SER:HA	2.55	0.41
3:N:361:ILE:CG1	3:N:421:LYS:HE3	2.44	0.41
3:N:541:LEU:O	3:N:551:GLY:HA2	2.20	0.41
1:A:68:ASP:O	1:A:69:GLU:C	2.58	0.41
1:A:905:MET:HG2	1:A:912:PHE:CD2	2.55	0.41
1:A:1145:ILE:HD11	1:A:1149:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:ASN:O	2:C:367:ARG:HB2	2.21	0.41
1:E:159:LEU:HD22	3:F:113:GLU:OE1	2.21	0.41
1:E:332:TRP:HZ3	1:E:355:LEU:HD21	1.84	0.41
1:E:928:ALA:CB	1:E:943:THR:HG22	2.50	0.41
1:E:1067:VAL:HG12	1:E:1124:ARG:HH22	1.84	0.41
1:M:332:TRP:O	1:M:336:ILE:HG13	2.21	0.41
1:M:922:LEU:HD13	1:M:1063:ALA:HA	2.02	0.41
1:M:927:MET:HE3	1:M:957:LEU:HB3	2.02	0.41
1:M:1208:ALA:O	2:O:334:ILE:HD11	2.21	0.41
2:O:333:VAL:HG13	2:O:343:LEU:CD2	2.50	0.41
1:I:789:MET:O	1:I:793:ASP:HB2	2.20	0.41
3:B:342:LEU:HD22	3:B:421:LYS:HZ1	1.86	0.41
3:B:413:PRO:CG	3:B:416:PHE:CD2	2.95	0.41
3:F:56:VAL:CG2	3:F:449:ILE:HG13	2.51	0.41
3:J:55:ILE:HD13	3:J:404:PRO:HD2	2.03	0.41
3:J:56:VAL:CG2	3:J:449:ILE:HG13	2.51	0.41
3:J:223:ARG:CD	3:J:228:ASN:ND2	2.79	0.41
3:J:502:GLU:HG3	3:J:685:PHE:HZ	1.85	0.41
3:J:646:ILE:HG23	3:J:646:ILE:O	2.21	0.41
3:J:726:GLU:HA	3:J:729:GLN:HB2	2.01	0.41
3:J:737:LEU:HD21	3:J:772:ARG:CZ	2.51	0.41
3:J:1010:LEU:HD23	3:J:1010:LEU:HA	1.90	0.41
3:N:223:ARG:HD3	3:N:228:ASN:HD21	1.78	0.41
1:A:765:ALA:O	1:A:766:LEU:HD23	2.20	0.41
1:E:83:LYS:HD3	3:F:195:ASN:OD1	2.21	0.41
1:E:236:GLN:HG3	1:E:553:ARG:HB3	2.02	0.41
2:G:359:VAL:HG21	2:G:367:ARG:CD	2.51	0.41
1:M:75:TYR:OH	3:N:191:GLN:OE1	2.27	0.41
1:M:765:ALA:O	1:M:766:LEU:HD23	2.20	0.41
1:M:928:ALA:CB	1:M:943:THR:HG22	2.50	0.41
1:I:64:ASN:N	3:N:567:ARG:NH2	2.68	0.41
2:K:341:ARG:O	2:K:342:PRO:C	2.57	0.41
3:B:56:VAL:CG2	3:B:449:ILE:HG13	2.51	0.41
3:B:246:LEU:HB3	3:B:267:VAL:HG11	2.02	0.41
3:F:45:LEU:HG	3:F:104:ILE:HD11	2.02	0.41
3:F:181:TYR:HH	3:F:302:TYR:HH	1.69	0.41
3:F:965:GLN:CD	3:F:969:LEU:HD11	2.22	0.41
3:F:1003:LEU:HD21	3:F:1024:LEU:HD11	2.02	0.41
3:J:603:GLN:HA	3:J:649:VAL:HG21	2.03	0.41
3:J:712:PRO:HD3	3:J:780:LEU:CD2	2.41	0.41
3:N:576:TYR:HA	3:N:577:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.76	0.41
1:A:582:ILE:O	1:A:586:LEU:HG	2.20	0.41
1:I:332:TRP:HZ3	1:I:355:LEU:HD21	1.85	0.41
1:I:530:PHE:CD2	1:I:837:VAL:HG22	2.55	0.41
3:F:614:ARG:HA	3:F:615:PRO:HD3	1.92	0.41
3:F:656:LEU:HD12	3:F:656:LEU:HA	1.92	0.41
3:F:796:ILE:O	3:F:800:ILE:HG13	2.21	0.41
3:J:173:ASN:HD22	3:J:220:VAL:CA	2.33	0.41
3:J:614:ARG:HA	3:J:615:PRO:HD3	1.92	0.41
3:N:591:VAL:HG21	3:N:634:ILE:CG1	2.49	0.41
3:N:603:GLN:HA	3:N:649:VAL:HG21	2.03	0.41
1:A:255:VAL:HG13	1:A:287:LEU:HD11	2.02	0.41
1:A:332:TRP:HZ3	1:A:355:LEU:HD21	1.85	0.41
1:A:530:PHE:CD2	1:A:837:VAL:HG22	2.55	0.41
1:A:1208:ALA:CB	4:A:1301:FAR:H51	2.51	0.41
1:A:1208:ALA:O	2:C:334:ILE:HD11	2.21	0.41
1:E:12:ASP:O	1:E:16:ARG:HG3	2.21	0.41
1:E:64:ASN:C	3:B:567:ARG:HH21	2.24	0.41
1:M:12:ASP:O	1:M:16:ARG:HG3	2.21	0.41
1:I:189:LYS:C	1:I:191:ASN:N	2.71	0.41
3:B:45:LEU:HG	3:B:104:ILE:HD11	2.02	0.41
3:B:55:ILE:HD13	3:B:404:PRO:HD2	2.03	0.41
3:B:412:VAL:HG22	3:B:429:ARG:HG2	2.02	0.41
3:B:606:LYS:HD3	3:B:649:VAL:HG22	2.01	0.41
3:B:796:ILE:O	3:B:800:ILE:HG13	2.21	0.41
3:F:55:ILE:HD13	3:F:404:PRO:HD2	2.03	0.41
3:F:60:LEU:HD23	3:F:60:LEU:HA	1.90	0.41
3:F:279:LEU:HG	3:F:283:LEU:HD22	2.02	0.41
3:F:630:ARG:HE	3:F:777:LYS:CE	2.32	0.41
3:J:45:LEU:HG	3:J:104:ILE:HD11	2.02	0.41
3:J:173:ASN:ND2	3:J:220:VAL:CA	2.80	0.41
3:J:730:LYS:O	3:J:733:ASP:N	2.46	0.41
3:J:796:ILE:HD13	3:J:796:ILE:HA	1.87	0.41
3:N:55:ILE:HD13	3:N:404:PRO:HD2	2.03	0.41
3:N:173:ASN:HD22	3:N:220:VAL:CA	2.33	0.41
1:A:4:ARG:NH2	1:A:70:ASP:OD2	2.54	0.41
1:A:12:ASP:O	1:A:16:ARG:HG3	2.21	0.41
1:A:72:ALA:CB	3:B:262:TRP:CZ2	3.04	0.41
1:A:419:ALA:CB	3:F:524:GLU:OE1	2.61	0.41
1:A:800:ASN:ND2	1:A:809:LEU:HD13	2.34	0.41
1:A:836:LYS:HD3	1:A:877:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LEU:HD13	1:A:1063:ALA:HA	2.02	0.41
1:A:1145:ILE:HG23	1:A:1215:LEU:HD13	2.03	0.41
2:C:333:VAL:HG13	2:C:343:LEU:CD2	2.50	0.41
1:E:68:ASP:O	1:E:69:GLU:C	2.58	0.41
1:E:592:GLY:O	1:E:598:ARG:HA	2.21	0.41
1:E:1208:ALA:O	2:G:334:ILE:HD11	2.21	0.41
1:M:135:LEU:HB2	1:M:201:SER:HB3	2.03	0.41
1:M:173:GLU:HG2	1:M:234:GLU:HG2	2.03	0.41
1:M:236:GLN:HE21	1:M:553:ARG:HB3	1.85	0.41
1:M:582:ILE:O	1:M:586:LEU:HG	2.20	0.41
1:M:789:MET:O	1:M:793:ASP:HB2	2.20	0.41
1:I:12:ASP:O	1:I:16:ARG:HG3	2.21	0.41
1:I:28:PRO:CG	3:J:547:LEU:CG	2.81	0.41
1:I:314:GLU:O	1:I:317:GLU:HG2	2.21	0.41
3:B:529:TRP:CZ2	3:B:682:PHE:HB3	2.56	0.41
3:B:576:TYR:HA	3:B:577:PRO:HD3	1.84	0.41
3:B:957:ILE:HG12	3:B:962:HIS:ND1	2.36	0.41
3:B:1012:ARG:CD	4:N:1101:FAR:H142	2.41	0.41
3:F:246:LEU:HB3	3:F:267:VAL:HG11	2.02	0.41
3:F:279:LEU:CD1	3:F:283:LEU:HD13	2.51	0.41
3:F:412:VAL:HG22	3:F:429:ARG:HG2	2.02	0.41
3:F:497:VAL:HG21	3:F:641:LEU:HD22	2.01	0.41
3:F:730:LYS:O	3:F:733:ASP:N	2.46	0.41
3:J:532:GLN:H	3:J:532:GLN:HG3	1.51	0.41
3:J:754:ASN:O	3:J:755:PHE:C	2.59	0.41
3:J:1003:LEU:HD21	3:J:1024:LEU:HD11	2.02	0.41
3:N:529:TRP:CZ2	3:N:682:PHE:HB3	2.56	0.41
3:N:625:ASN:C	3:N:634:ILE:HD12	2.34	0.41
3:N:722:LYS:HB3	3:N:724:THR:OG1	2.21	0.41
3:N:796:ILE:O	3:N:800:ILE:HG13	2.21	0.41
3:N:878:TRP:CE3	3:N:933:SER:HA	2.55	0.41
3:N:1003:LEU:HD21	3:N:1024:LEU:HD11	2.01	0.41
1:A:135:LEU:HB2	1:A:201:SER:HB3	2.03	0.41
1:A:592:GLY:O	1:A:598:ARG:HA	2.21	0.41
1:A:917:ARG:HB3	1:A:1065:ASN:HD22	1.86	0.41
1:E:79:GLN:HB3	3:F:194:TYR:CA	2.51	0.41
1:E:332:TRP:O	1:E:336:ILE:HG13	2.21	0.41
1:E:924:ILE:HD13	1:E:924:ILE:HA	1.90	0.41
1:M:233:ASP:OD2	1:M:503:GLY:N	2.50	0.41
1:M:610:THR:HG22	3:J:635:LEU:CD2	2.51	0.41
1:M:1145:ILE:HD11	1:M:1149:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:LEU:HD23	1:I:11:LEU:HA	1.81	0.41
1:I:71:LYS:HD2	3:J:258:GLN:HE22	1.85	0.41
1:I:1145:ILE:HG23	1:I:1215:LEU:HD13	2.03	0.41
2:K:359:VAL:HG21	2:K:367:ARG:CD	2.51	0.41
3:B:103:ARG:CZ	3:F:477:ARG:HD3	2.50	0.41
3:F:523:VAL:HG21	3:F:528:ILE:CD1	2.43	0.41
3:J:405:VAL:HA	3:J:445:GLN:HE22	1.86	0.41
3:J:526:ILE:HD13	3:J:660:ILE:HD13	1.90	0.41
3:J:541:LEU:O	3:J:551:GLY:HA2	2.20	0.41
3:N:60:LEU:HD23	3:N:442:LEU:HD22	2.03	0.41
3:N:714:VAL:HG21	3:N:743:LEU:HD11	2.03	0.41
2:C:340:LEU:HD23	2:C:340:LEU:HA	1.85	0.40
1:E:79:GLN:HB2	3:F:194:TYR:O	2.21	0.40
1:E:255:VAL:HG13	1:E:287:LEU:HD11	2.02	0.40
1:E:798:LEU:O	1:E:806:VAL:HG23	2.21	0.40
1:M:314:GLU:O	1:M:317:GLU:HG2	2.21	0.40
1:I:4:ARG:NH2	1:I:70:ASP:OD2	2.54	0.40
1:I:64:ASN:CA	3:N:567:ARG:NH2	2.84	0.40
1:I:592:GLY:O	1:I:598:ARG:HA	2.21	0.40
1:I:1145:ILE:HD11	1:I:1149:ILE:HD11	2.03	0.40
3:B:84:ILE:HG12	3:B:151:SER:O	2.22	0.40
3:B:405:VAL:HA	3:B:445:GLN:HE22	1.86	0.40
3:B:714:VAL:HG21	3:B:743:LEU:HD11	2.03	0.40
3:B:878:TRP:CE3	3:B:933:SER:HA	2.55	0.40
3:B:1093:SER:C	3:N:924:TRP:CZ2	2.90	0.40
3:F:60:LEU:HD11	3:F:446:ALA:HB2	2.03	0.40
3:F:283:LEU:HD21	3:F:307:LEU:CD1	2.51	0.40
3:F:1091:LEU:N	3:F:1091:LEU:HD22	2.36	0.40
3:J:279:LEU:HD11	3:J:283:LEU:HD11	2.01	0.40
3:J:413:PRO:CG	3:J:416:PHE:CD2	2.95	0.40
3:J:637:MET:HG3	3:J:646:ILE:CD1	2.50	0.40
3:N:392:LEU:HA	3:N:395:VAL:HG22	2.03	0.40
3:N:730:LYS:O	3:N:733:ASP:N	2.46	0.40
1:A:350:GLU:HG2	1:A:351:TYR:N	2.37	0.40
1:A:918:LEU:HD13	1:A:918:LEU:HA	1.91	0.40
1:E:51:ILE:HG12	1:E:81:VAL:HA	2.03	0.40
1:E:314:GLU:O	1:E:317:GLU:HG2	2.21	0.40
1:E:804:ALA:HB1	1:E:809:LEU:CD1	2.43	0.40
1:E:918:LEU:HD13	1:E:918:LEU:HA	1.91	0.40
1:E:929:THR:HG21	1:E:1059:ARG:HD2	2.03	0.40
1:M:1205:LYS:CG	2:O:337:PRO:CG	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:LEU:HB2	1:I:201:SER:HB3	2.03	0.40
1:I:332:TRP:O	1:I:336:ILE:HG13	2.21	0.40
2:K:333:VAL:HG13	2:K:343:LEU:CD2	2.50	0.40
3:B:60:LEU:HD11	3:B:446:ALA:HB2	2.03	0.40
3:B:252:PHE:HD2	3:B:254:LEU:HD23	1.86	0.40
3:B:302:TYR:OH	3:B:464:ILE:HD11	2.21	0.40
3:B:392:LEU:HA	3:B:395:VAL:HG22	2.03	0.40
3:B:625:ASN:C	3:B:634:ILE:HD12	2.34	0.40
3:B:722:LYS:HB3	3:B:724:THR:OG1	2.21	0.40
3:B:737:LEU:HD21	3:B:772:ARG:CZ	2.51	0.40
3:F:173:ASN:HD22	3:F:220:VAL:HA	1.84	0.40
3:F:342:LEU:CD2	3:F:421:LYS:HZ1	2.34	0.40
3:F:724:THR:CB	3:F:726:GLU:HB2	2.51	0.40
3:J:84:ILE:HG12	3:J:151:SER:O	2.22	0.40
3:J:302:TYR:OH	3:J:464:ILE:HD11	2.21	0.40
3:J:722:LYS:HB3	3:J:724:THR:OG1	2.21	0.40
3:N:45:LEU:HG	3:N:104:ILE:HD11	2.02	0.40
3:N:403:TYR:HA	3:N:404:PRO:HD3	1.95	0.40
3:N:405:VAL:HA	3:N:445:GLN:HE22	1.86	0.40
3:N:724:THR:CB	3:N:726:GLU:HB2	2.51	0.40
3:N:737:LEU:HD21	3:N:772:ARG:CZ	2.51	0.40
1:A:281:GLN:O	1:A:285:THR:OG1	2.33	0.40
1:A:441:GLN:CD	1:A:607:PHE:CG	2.95	0.40
1:E:1209:THR:CG2	2:G:334:ILE:HG21	2.52	0.40
1:M:51:ILE:HG12	1:M:81:VAL:HA	2.03	0.40
1:M:350:GLU:HG2	1:M:351:TYR:N	2.37	0.40
1:M:550:LEU:HD23	1:M:550:LEU:HA	1.88	0.40
1:M:863:ARG:H	1:M:863:ARG:HG3	1.52	0.40
1:I:68:ASP:O	1:I:69:GLU:C	2.58	0.40
1:I:173:GLU:HG2	1:I:234:GLU:HG2	2.03	0.40
2:K:376:LYS:HA	2:K:379:LEU:HB3	2.04	0.40
3:B:60:LEU:HD23	3:B:442:LEU:HD22	2.03	0.40
3:B:283:LEU:HB3	3:B:312:LEU:CD1	2.48	0.40
3:B:646:ILE:HG23	3:B:646:ILE:O	2.21	0.40
3:B:720:LYS:HE3	3:B:720:LYS:HB2	1.92	0.40
3:F:502:GLU:HG3	3:F:685:PHE:HZ	1.85	0.40
3:F:671:LEU:HD22	3:F:680:PRO:HG3	2.02	0.40
3:F:722:LYS:HB3	3:F:724:THR:OG1	2.21	0.40
3:F:795:SER:HG	3:F:855:ILE:CD1	2.31	0.40
3:J:556:PRO:HB2	5:J:1101:ADP:H8	1.87	0.40
3:N:646:ILE:HG23	3:N:646:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:726:GLU:HA	3:N:729:GLN:HB2	2.02	0.40
3:N:1006:VAL:HG22	3:N:1073:VAL:HG21	2.02	0.40
1:A:51:ILE:HG12	1:A:81:VAL:HA	2.03	0.40
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.94	0.40
1:A:332:TRP:O	1:A:336:ILE:HG13	2.21	0.40
1:E:28:PRO:O	3:F:130:MET:SD	2.79	0.40
1:E:133:LEU:O	1:E:181:PHE:HB2	2.22	0.40
1:E:173:GLU:HG2	1:E:234:GLU:HG2	2.03	0.40
1:M:68:ASP:O	1:M:69:GLU:C	2.58	0.40
1:M:1145:ILE:HG23	1:M:1215:LEU:HD13	2.02	0.40
2:O:359:VAL:HG21	2:O:367:ARG:CD	2.51	0.40
1:I:133:LEU:O	1:I:181:PHE:HB2	2.22	0.40
1:I:788:THR:C	1:I:792:PRO:CD	2.70	0.40
1:I:798:LEU:O	1:I:806:VAL:HG23	2.22	0.40
1:I:1167:LYS:O	1:I:1170:GLY:HA2	2.21	0.40
2:K:366:ASN:O	2:K:367:ARG:HB2	2.21	0.40
3:B:671:LEU:HD22	3:B:680:PRO:HG3	2.02	0.40
3:F:84:ILE:HG12	3:F:151:SER:O	2.22	0.40
3:F:223:ARG:CB	3:F:228:ASN:OD1	2.68	0.40
3:J:506:LEU:CD1	3:J:626:ILE:HG12	2.51	0.40
3:J:786:ALA:CB	3:J:848:VAL:HG11	2.47	0.40
3:N:263:SER:O	3:N:263:SER:OG	2.40	0.40
3:N:506:LEU:CD1	3:N:626:ILE:HG12	2.51	0.40
1:A:176:TYR:HB2	1:A:241:ILE:CD1	2.50	0.40
1:A:1167:LYS:O	1:A:1170:GLY:HA2	2.21	0.40
1:E:350:GLU:HG2	1:E:351:TYR:N	2.37	0.40
1:E:441:GLN:CD	1:E:607:PHE:CG	2.95	0.40
1:E:1065:ASN:ND2	1:E:1116:ASN:HD22	2.20	0.40
1:E:1167:LYS:O	1:E:1170:GLY:HA2	2.21	0.40
1:M:4:ARG:NH2	1:M:70:ASP:OD2	2.54	0.40
1:M:441:GLN:CD	1:M:607:PHE:CG	2.95	0.40
1:M:933:HIS:O	1:M:936:ARG:HG3	2.22	0.40
2:O:376:LYS:HA	2:O:379:LEU:HB3	2.04	0.40
1:I:355:LEU:HD12	1:I:355:LEU:O	2.22	0.40
1:I:922:LEU:HD23	1:I:922:LEU:HA	1.81	0.40
1:I:1209:THR:CG2	2:K:334:ILE:HG21	2.52	0.40
3:F:454:LEU:HD23	3:F:454:LEU:HA	1.90	0.40
3:F:529:TRP:CZ2	3:F:682:PHE:HB3	2.56	0.40
3:J:260:CYS:SG	3:J:261:SER:N	2.94	0.40
3:J:477:ARG:NH2	3:N:460:SER:CB	2.82	0.40
3:N:342:LEU:HD21	3:N:421:LYS:HZ2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:532:GLN:H	3:N:532:GLN:HG3	1.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	954/1223 (78%)	912 (96%)	42 (4%)	0	100	100
1	E	954/1223 (78%)	914 (96%)	40 (4%)	0	100	100
1	I	954/1223 (78%)	912 (96%)	42 (4%)	0	100	100
1	M	954/1223 (78%)	913 (96%)	41 (4%)	0	100	100
2	C	44/387 (11%)	43 (98%)	1 (2%)	0	100	100
2	G	44/387 (11%)	42 (96%)	2 (4%)	0	100	100
2	K	44/387 (11%)	42 (96%)	2 (4%)	0	100	100
2	O	44/387 (11%)	42 (96%)	2 (4%)	0	100	100
3	B	1029/1093 (94%)	992 (96%)	36 (4%)	1 (0%)	51	82
3	F	1029/1093 (94%)	995 (97%)	34 (3%)	0	100	100
3	J	1029/1093 (94%)	994 (97%)	35 (3%)	0	100	100
3	N	1029/1093 (94%)	993 (96%)	36 (4%)	0	100	100
All	All	8108/10812 (75%)	7794 (96%)	313 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	283	LEU

### 5.3.2 Protein sidechains [i](#)

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	844/1068 (79%)	835 (99%)	9 (1%)	73	92
1	E	844/1068 (79%)	834 (99%)	10 (1%)	71	91
1	I	844/1068 (79%)	834 (99%)	10 (1%)	71	91
1	M	844/1068 (79%)	834 (99%)	10 (1%)	71	91
2	C	41/349 (12%)	37 (90%)	4 (10%)	8	24
2	G	41/349 (12%)	37 (90%)	4 (10%)	8	24
2	K	41/349 (12%)	37 (90%)	4 (10%)	8	24
2	O	41/349 (12%)	37 (90%)	4 (10%)	8	24
3	B	924/975 (95%)	896 (97%)	28 (3%)	41	75
3	F	924/975 (95%)	898 (97%)	26 (3%)	43	76
3	J	924/975 (95%)	897 (97%)	27 (3%)	42	76
3	N	924/975 (95%)	896 (97%)	28 (3%)	41	75
All	All	7236/9568 (76%)	7072 (98%)	164 (2%)	53	80

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	567	SER
1	A	581	SER
1	A	611	SER
1	A	889	SER
1	A	898	MET
1	A	926	VAL
1	A	1165	GLU
1	A	1212	GLN
2	C	338	TYR
2	C	374	THR
2	C	378	VAL
2	C	382	LEU
1	E	36	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	567	SER
1	E	581	SER
1	E	611	SER
1	E	889	SER
1	E	898	MET
1	E	926	VAL
1	E	1165	GLU
1	E	1176	LEU
1	E	1212	GLN
2	G	338	TYR
2	G	374	THR
2	G	378	VAL
2	G	382	LEU
1	M	36	SER
1	M	567	SER
1	M	581	SER
1	M	611	SER
1	M	889	SER
1	M	898	MET
1	M	926	VAL
1	M	1165	GLU
1	M	1176	LEU
1	M	1212	GLN
2	O	338	TYR
2	O	374	THR
2	O	378	VAL
2	O	382	LEU
1	I	36	SER
1	I	567	SER
1	I	581	SER
1	I	611	SER
1	I	889	SER
1	I	898	MET
1	I	926	VAL
1	I	1165	GLU
1	I	1176	LEU
1	I	1212	GLN
2	K	338	TYR
2	K	374	THR
2	K	378	VAL
2	K	382	LEU
3	B	60	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B	85	GLN
3	B	196	THR
3	B	282	LEU
3	B	285	ARG
3	B	286	GLU
3	B	298	PRO
3	B	303	PRO
3	B	341	SER
3	B	348	CYS
3	B	460	SER
3	B	461	PRO
3	B	531	GLN
3	B	567	ARG
3	B	581	ASP
3	B	724	THR
3	B	750	ARG
3	B	767	GLU
3	B	769	VAL
3	B	820	GLU
3	B	833	ASN
3	B	855	ILE
3	B	1040	SER
3	B	1067	SER
3	B	1082	VAL
3	B	1087	ASP
3	B	1090	CYS
3	B	1092	ILE
3	F	60	LEU
3	F	85	GLN
3	F	196	THR
3	F	286	GLU
3	F	298	PRO
3	F	303	PRO
3	F	341	SER
3	F	348	CYS
3	F	460	SER
3	F	461	PRO
3	F	531	GLN
3	F	567	ARG
3	F	581	ASP
3	F	724	THR
3	F	750	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	767	GLU
3	F	769	VAL
3	F	820	GLU
3	F	833	ASN
3	F	855	ILE
3	F	1040	SER
3	F	1067	SER
3	F	1082	VAL
3	F	1087	ASP
3	F	1090	CYS
3	F	1092	ILE
3	J	60	LEU
3	J	85	GLN
3	J	196	THR
3	J	253	ASN
3	J	286	GLU
3	J	298	PRO
3	J	303	PRO
3	J	341	SER
3	J	348	CYS
3	J	460	SER
3	J	461	PRO
3	J	531	GLN
3	J	567	ARG
3	J	581	ASP
3	J	724	THR
3	J	750	ARG
3	J	767	GLU
3	J	769	VAL
3	J	820	GLU
3	J	833	ASN
3	J	855	ILE
3	J	1040	SER
3	J	1067	SER
3	J	1082	VAL
3	J	1087	ASP
3	J	1090	CYS
3	J	1092	ILE
3	N	60	LEU
3	N	85	GLN
3	N	196	THR
3	N	252	PHE

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Mol	Chain	Res	Type
3	N	253	ASN
3	N	286	GLU
3	N	298	PRO
3	N	303	PRO
3	N	341	SER
3	N	348	CYS
3	N	460	SER
3	N	461	PRO
3	N	531	GLN
3	N	567	ARG
3	N	581	ASP
3	N	724	THR
3	N	750	ARG
3	N	767	GLU
3	N	769	VAL
3	N	820	GLU
3	N	833	ASN
3	N	855	ILE
3	N	1040	SER
3	N	1067	SER
3	N	1082	VAL
3	N	1087	ASP
3	N	1090	CYS
3	N	1092	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	163	ASN
1	A	236	GLN
1	A	243	ASN
1	A	400	HIS
1	A	441	GLN
1	A	489	ASN
1	A	529	GLN
1	A	1065	ASN
1	A	1120	GLN
1	E	47	ASN
1	E	163	ASN
1	E	236	GLN
1	E	243	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	400	HIS
1	E	427	ASN
1	E	441	GLN
1	E	489	ASN
1	E	1065	ASN
1	E	1120	GLN
1	M	47	ASN
1	M	163	ASN
1	M	236	GLN
1	M	243	ASN
1	M	400	HIS
1	M	441	GLN
1	M	489	ASN
1	M	529	GLN
1	M	1065	ASN
1	M	1120	GLN
2	O	357	HIS
1	I	47	ASN
1	I	163	ASN
1	I	236	GLN
1	I	243	ASN
1	I	400	HIS
1	I	441	GLN
1	I	489	ASN
1	I	529	GLN
1	I	1065	ASN
1	I	1120	GLN
3	B	132	GLN
3	B	171	GLN
3	B	315	GLN
3	B	445	GLN
3	B	491	ASN
3	B	507	GLN
3	B	516	GLN
3	B	522	GLN
3	B	589	GLN
3	B	607	GLN
3	B	625	ASN
3	B	667	GLN
3	B	710	GLN
3	B	711	GLN
3	B	740	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	B	765	HIS
3	B	809	GLN
3	B	840	ASN
3	B	856	HIS
3	B	901	GLN
3	B	909	GLN
3	B	918	GLN
3	B	935	ASN
3	B	978	ASN
3	B	989	ASN
3	B	1019	GLN
3	F	132	GLN
3	F	171	GLN
3	F	315	GLN
3	F	445	GLN
3	F	491	ASN
3	F	516	GLN
3	F	544	ASN
3	F	589	GLN
3	F	607	GLN
3	F	625	ASN
3	F	667	GLN
3	F	710	GLN
3	F	711	GLN
3	F	740	GLN
3	F	765	HIS
3	F	809	GLN
3	F	840	ASN
3	F	856	HIS
3	F	901	GLN
3	F	909	GLN
3	F	918	GLN
3	F	935	ASN
3	F	978	ASN
3	F	989	ASN
3	F	1019	GLN
3	J	132	GLN
3	J	171	GLN
3	J	315	GLN
3	J	427	GLN
3	J	445	GLN
3	J	491	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	J	516	GLN
3	J	544	ASN
3	J	589	GLN
3	J	607	GLN
3	J	625	ASN
3	J	667	GLN
3	J	710	GLN
3	J	711	GLN
3	J	740	GLN
3	J	765	HIS
3	J	809	GLN
3	J	840	ASN
3	J	856	HIS
3	J	901	GLN
3	J	909	GLN
3	J	918	GLN
3	J	935	ASN
3	J	978	ASN
3	J	989	ASN
3	J	1013	ASN
3	J	1019	GLN
3	N	132	GLN
3	N	171	GLN
3	N	315	GLN
3	N	427	GLN
3	N	445	GLN
3	N	491	ASN
3	N	516	GLN
3	N	544	ASN
3	N	589	GLN
3	N	607	GLN
3	N	625	ASN
3	N	667	GLN
3	N	710	GLN
3	N	711	GLN
3	N	740	GLN
3	N	765	HIS
3	N	809	GLN
3	N	840	ASN
3	N	856	HIS
3	N	901	GLN
3	N	909	GLN

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Mol	Chain	Res	Type
3	N	918	GLN
3	N	935	ASN
3	N	978	ASN
3	N	989	ASN
3	N	1019	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FAR	N	1101	4	14,14,14	0.30	0	16,16,16	0.32	0
5	ADP	F	1102	-	24,29,29	0.66	0	29,45,45	0.71	1 (3%)
4	FAR	E	1301	-	14,14,14	0.36	0	16,16,16	1.66	5 (31%)
5	ADP	N	1102	-	24,29,29	0.66	0	29,45,45	0.71	1 (3%)
4	FAR	F	1101	-	14,14,14	0.30	0	16,16,16	0.32	0
5	ADP	J	1101	-	24,29,29	0.65	0	29,45,45	0.71	1 (3%)
4	FAR	A	1301	-	14,14,14	0.36	0	16,16,16	1.66	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAR	I	1301	-	14,14,14	0.36	0	16,16,16	1.66	5 (31%)
4	FAR	B	1101	4	14,14,14	0.30	0	16,16,16	0.32	0
4	FAR	F	1103	-	14,14,14	0.30	0	16,16,16	0.31	0
4	FAR	M	1301	-	14,14,14	0.36	0	16,16,16	1.65	5 (31%)
5	ADP	B	1102	-	24,29,29	0.65	0	29,45,45	0.71	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAR	N	1101	4	-	4/14/14/14	-
5	ADP	F	1102	-	-	2/12/32/32	0/3/3/3
4	FAR	E	1301	-	-	2/14/14/14	-
5	ADP	N	1102	-	-	2/12/32/32	0/3/3/3
4	FAR	F	1101	-	-	4/14/14/14	-
5	ADP	J	1101	-	-	2/12/32/32	0/3/3/3
4	FAR	A	1301	-	-	2/14/14/14	-
4	FAR	I	1301	-	-	2/14/14/14	-
4	FAR	B	1101	4	-	4/14/14/14	-
4	FAR	F	1103	-	-	4/14/14/14	-
4	FAR	M	1301	-	-	2/14/14/14	-
5	ADP	B	1102	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1301	FAR	C4-C3-C5	3.27	120.77	115.27
4	E	1301	FAR	C4-C3-C5	3.26	120.76	115.27
4	A	1301	FAR	C4-C3-C5	3.25	120.74	115.27
4	M	1301	FAR	C4-C3-C5	3.22	120.68	115.27
4	M	1301	FAR	C1-C2-C3	-2.66	120.46	126.57
4	I	1301	FAR	C1-C2-C3	-2.66	120.47	126.57
4	A	1301	FAR	C1-C2-C3	-2.66	120.47	126.57
4	E	1301	FAR	C1-C2-C3	-2.65	120.47	126.57
4	E	1301	FAR	C6-C7-C8	-2.37	121.96	127.66

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1301	FAR	C6-C7-C8	-2.36	121.97	127.66
4	M	1301	FAR	C6-C7-C8	-2.36	121.97	127.66
4	I	1301	FAR	C15-C13-C14	2.35	119.80	114.60
4	E	1301	FAR	C15-C13-C14	2.35	119.80	114.60
4	M	1301	FAR	C15-C13-C14	2.35	119.80	114.60
4	A	1301	FAR	C6-C7-C8	-2.35	122.00	127.66
4	A	1301	FAR	C15-C13-C14	2.34	119.77	114.60
5	B	1102	ADP	C5-C6-N6	2.17	123.65	120.35
5	N	1102	ADP	C5-C6-N6	2.16	123.63	120.35
5	J	1101	ADP	C5-C6-N6	2.14	123.61	120.35
5	F	1102	ADP	C5-C6-N6	2.14	123.60	120.35
4	E	1301	FAR	C4-C3-C2	-2.09	119.68	123.81
4	A	1301	FAR	C4-C3-C2	-2.08	119.70	123.81
4	I	1301	FAR	C4-C3-C2	-2.07	119.71	123.81
4	M	1301	FAR	C4-C3-C2	-2.07	119.72	123.81

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1102	ADP	O4'-C4'-C5'-O5'
5	F	1102	ADP	O4'-C4'-C5'-O5'
5	J	1101	ADP	O4'-C4'-C5'-O5'
5	N	1102	ADP	O4'-C4'-C5'-O5'
5	B	1102	ADP	C3'-C4'-C5'-O5'
5	F	1102	ADP	C3'-C4'-C5'-O5'
5	J	1101	ADP	C3'-C4'-C5'-O5'
5	N	1102	ADP	C3'-C4'-C5'-O5'
4	B	1101	FAR	C3-C5-C6-C7
4	F	1101	FAR	C3-C5-C6-C7
4	F	1103	FAR	C3-C5-C6-C7
4	N	1101	FAR	C3-C5-C6-C7
4	A	1301	FAR	C10-C8-C9-C11
4	E	1301	FAR	C10-C8-C9-C11
4	M	1301	FAR	C10-C8-C9-C11
4	I	1301	FAR	C10-C8-C9-C11
4	A	1301	FAR	C7-C8-C9-C11
4	E	1301	FAR	C7-C8-C9-C11
4	M	1301	FAR	C7-C8-C9-C11
4	I	1301	FAR	C7-C8-C9-C11
4	B	1101	FAR	C10-C8-C9-C11
4	F	1101	FAR	C10-C8-C9-C11

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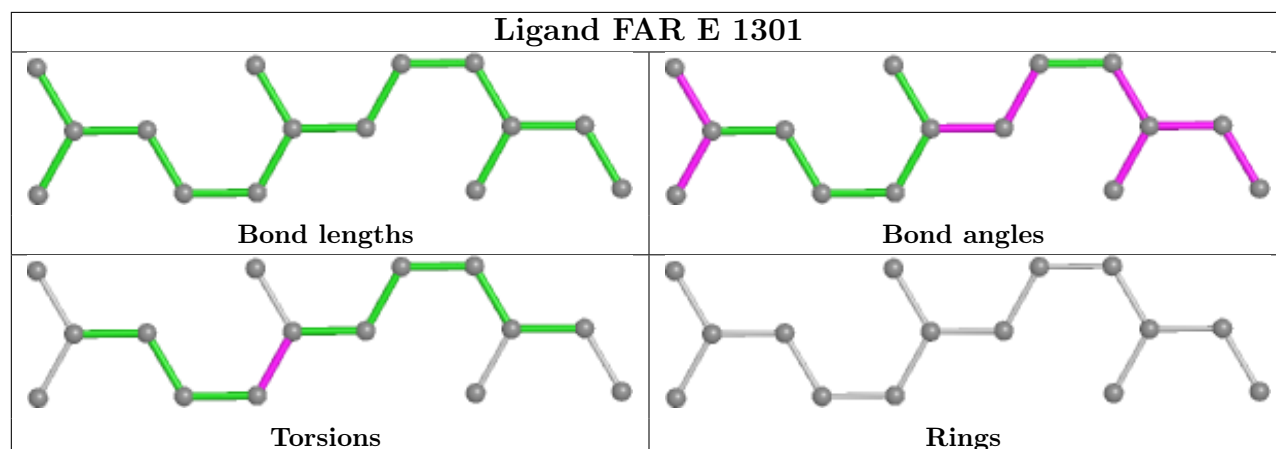
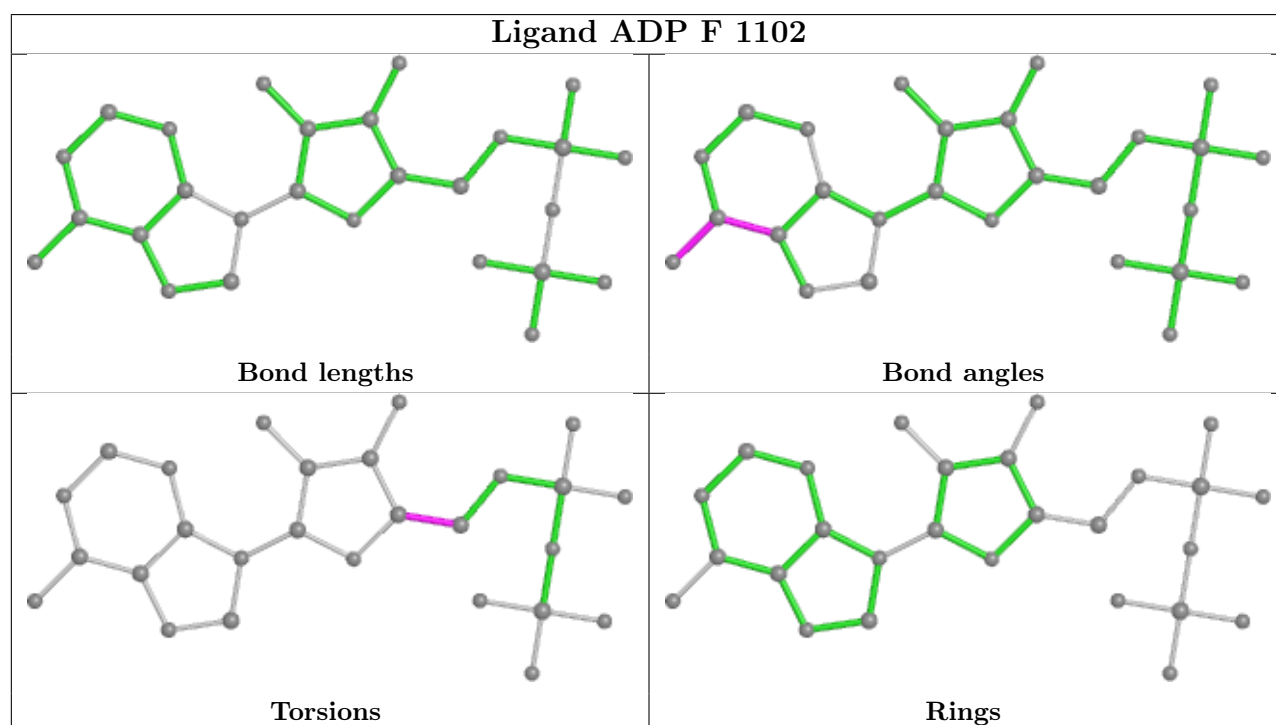
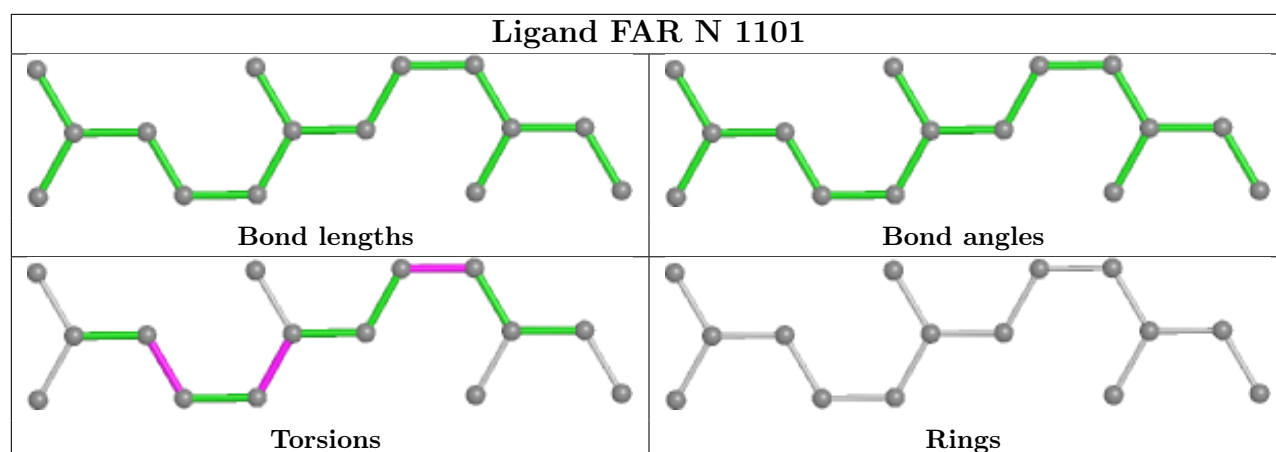
Mol	Chain	Res	Type	Atoms
4	F	1103	FAR	C10-C8-C9-C11
4	N	1101	FAR	C10-C8-C9-C11
4	F	1101	FAR	C7-C8-C9-C11
4	N	1101	FAR	C7-C8-C9-C11
4	B	1101	FAR	C7-C8-C9-C11
4	F	1103	FAR	C7-C8-C9-C11
4	B	1101	FAR	C9-C11-C12-C13
4	F	1101	FAR	C9-C11-C12-C13
4	F	1103	FAR	C9-C11-C12-C13
4	N	1101	FAR	C9-C11-C12-C13

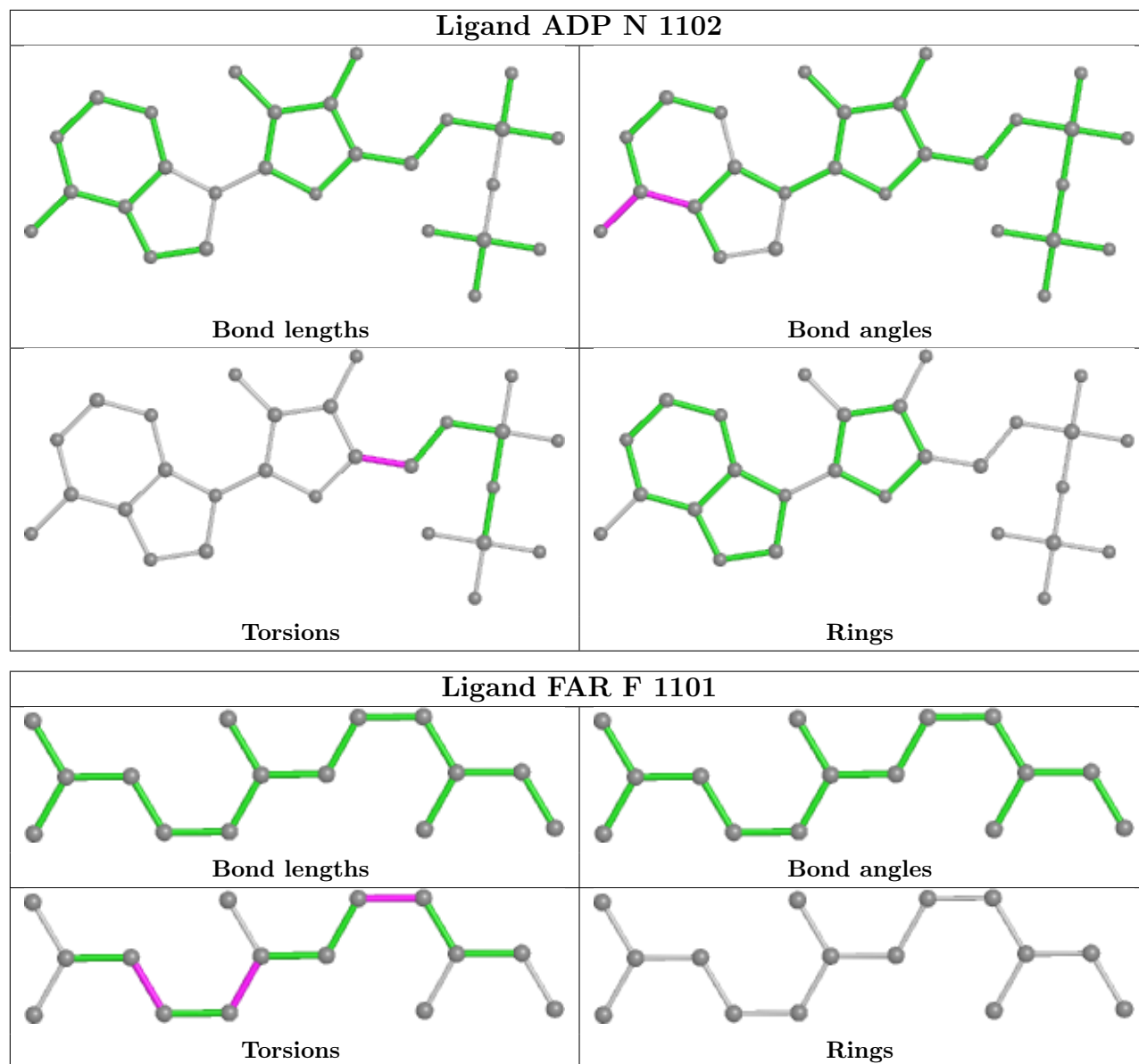
There are no ring outliers.

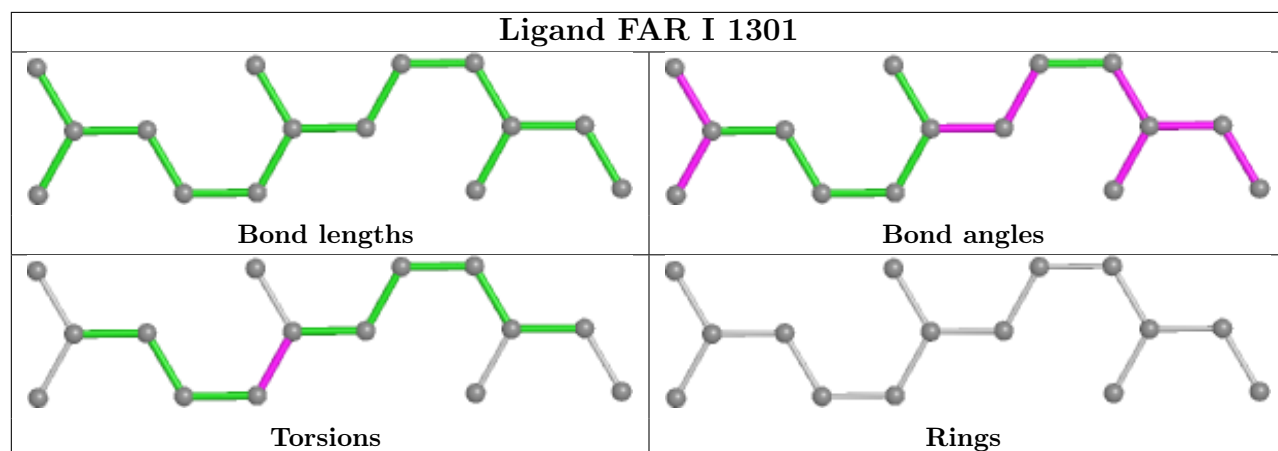
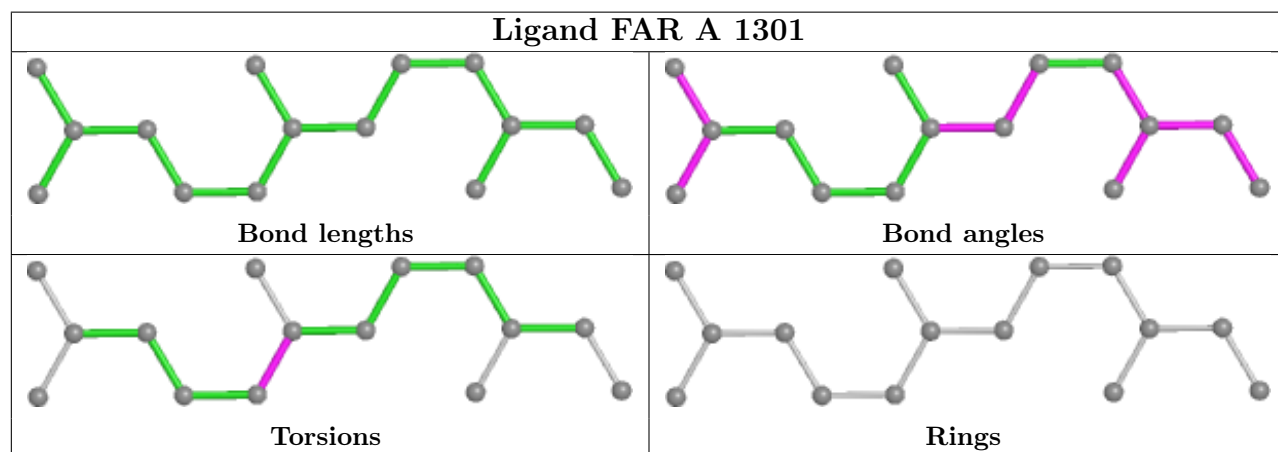
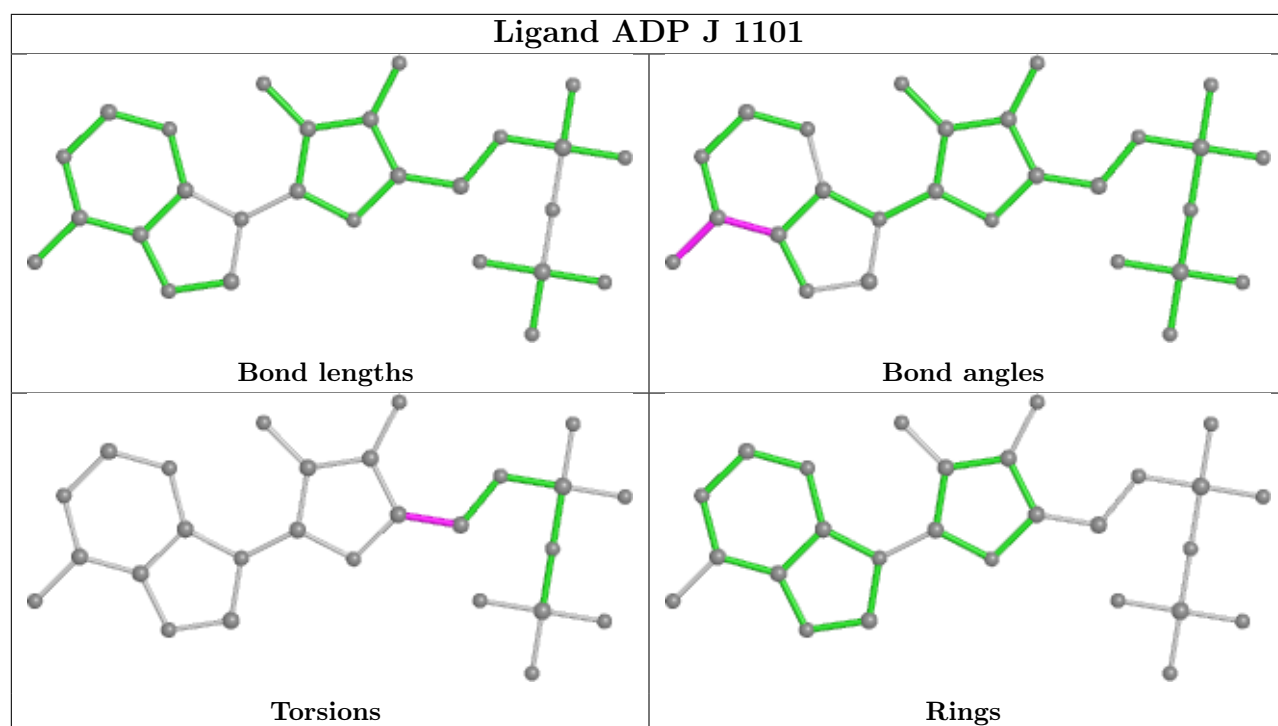
12 monomers are involved in 205 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1101	FAR	40	0
5	F	1102	ADP	2	0
4	E	1301	FAR	17	0
5	N	1102	ADP	2	0
4	F	1101	FAR	39	0
5	J	1101	ADP	3	0
4	A	1301	FAR	18	0
4	I	1301	FAR	18	0
4	B	1101	FAR	19	0
4	F	1103	FAR	27	0
4	M	1301	FAR	17	0
5	B	1102	ADP	3	0

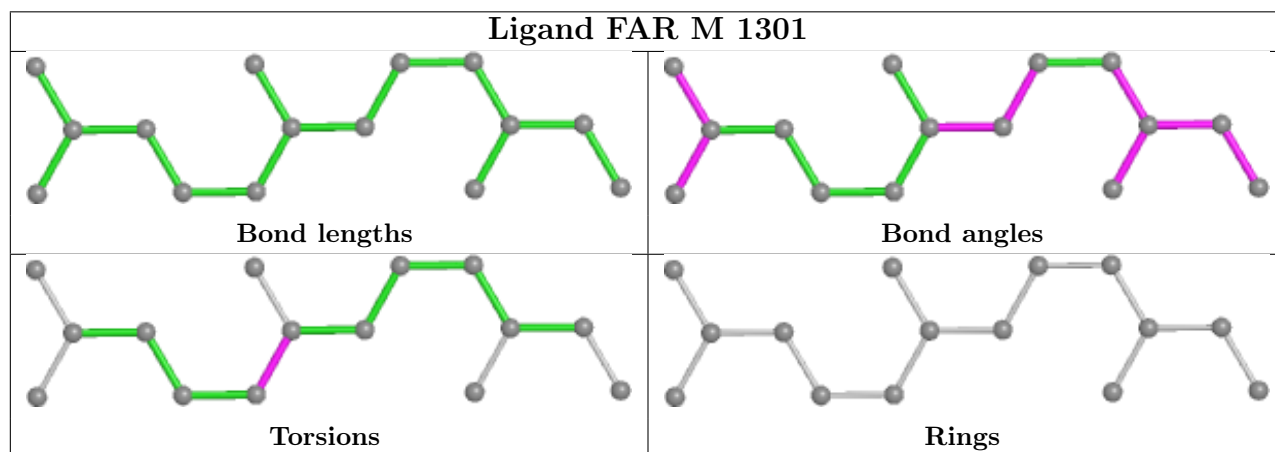
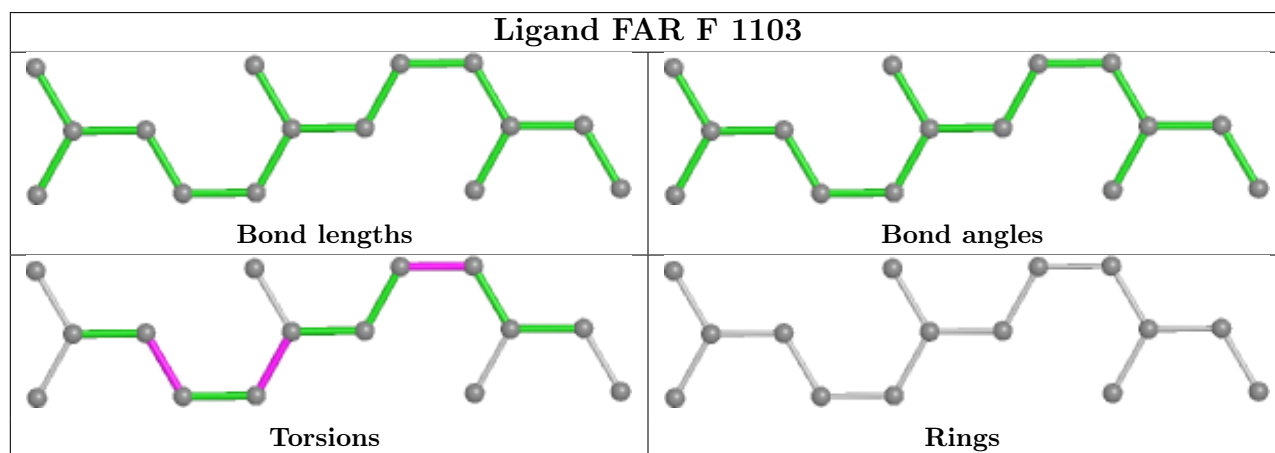
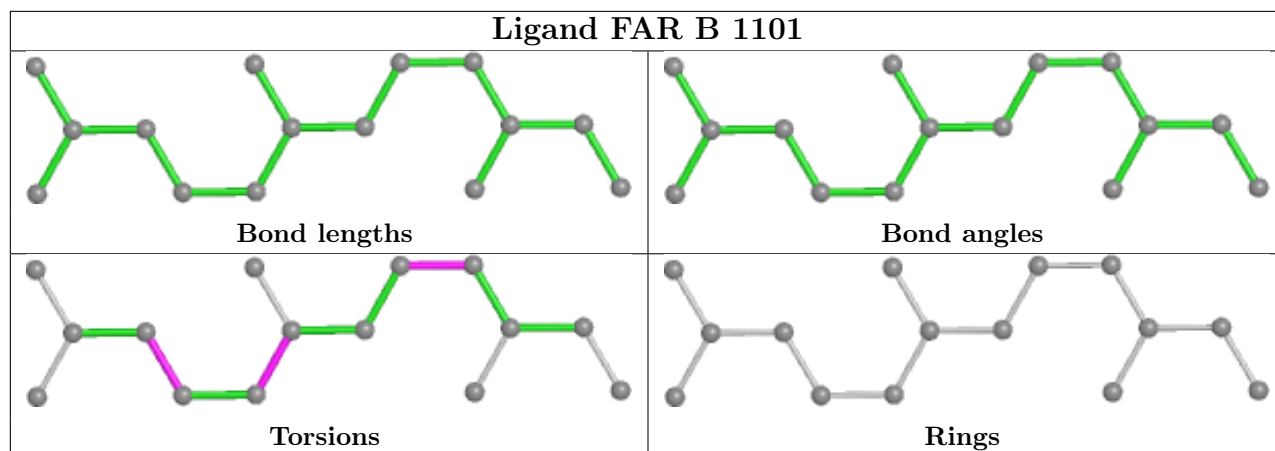
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

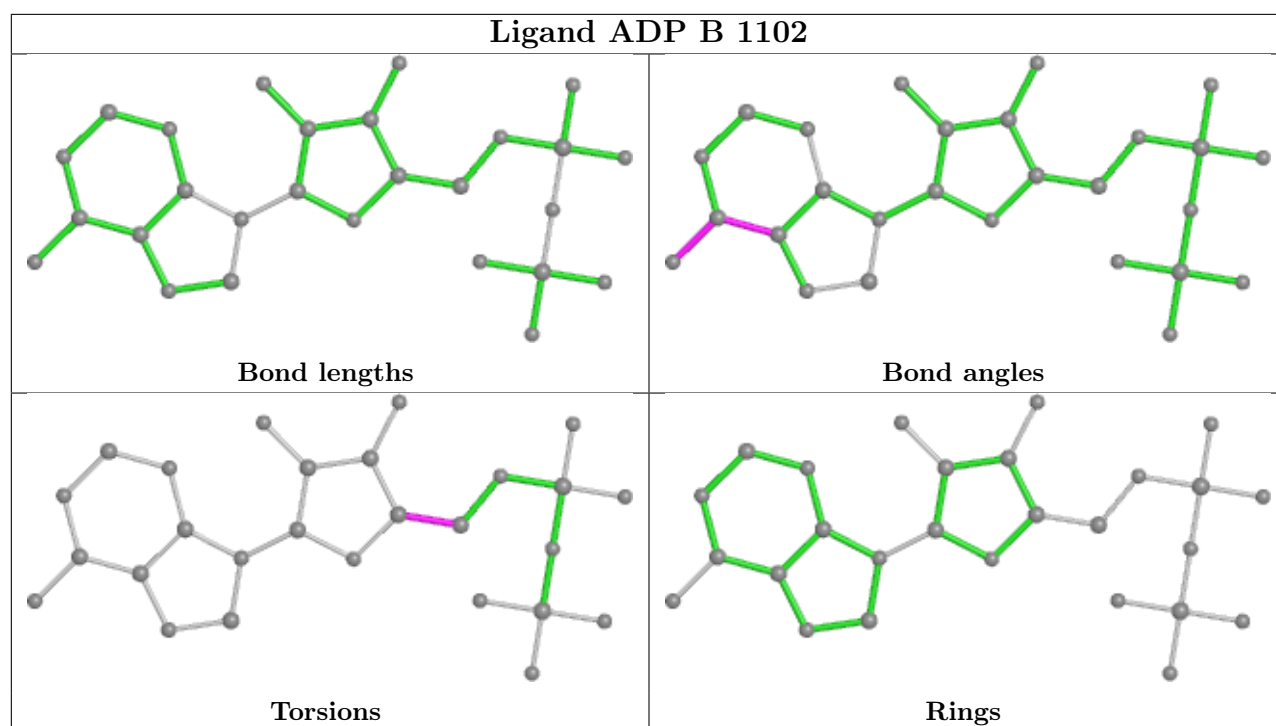












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

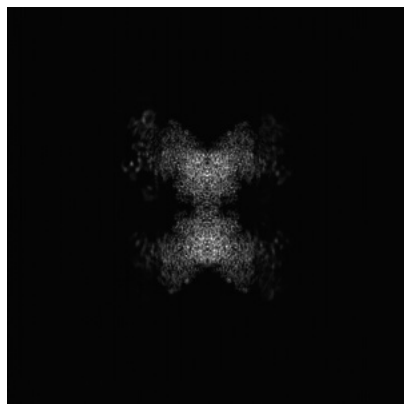
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36213. These allow visual inspection of the internal detail of the map and identification of artifacts.

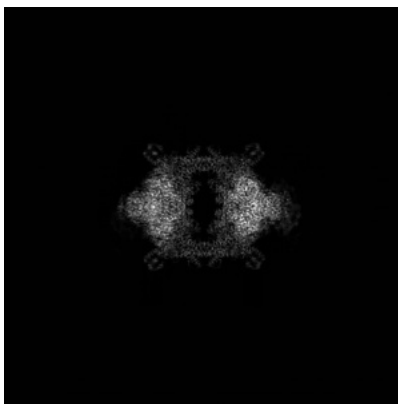
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

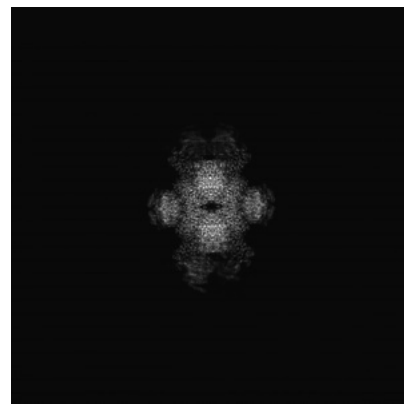
#### 6.1.1 Primary map



X

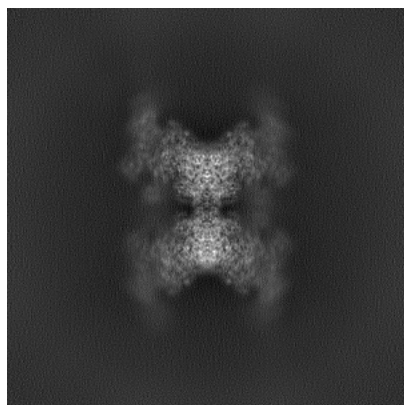


Y

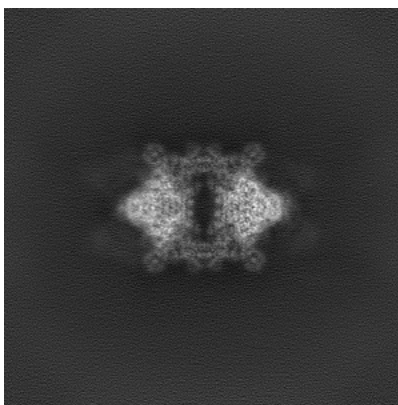


Z

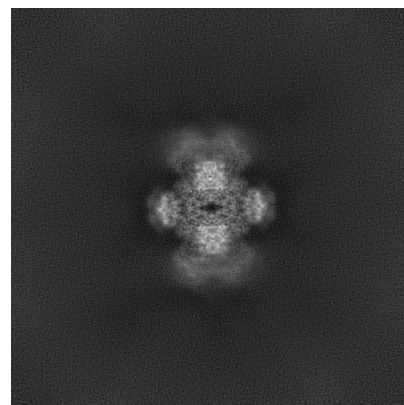
#### 6.1.2 Raw map



X



Y



Z

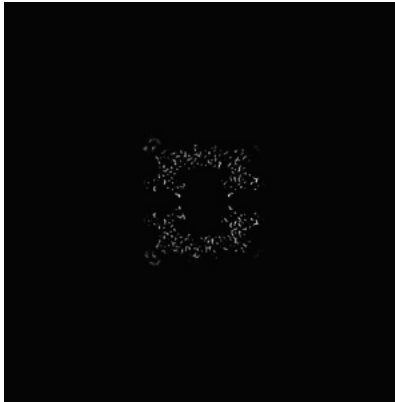
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

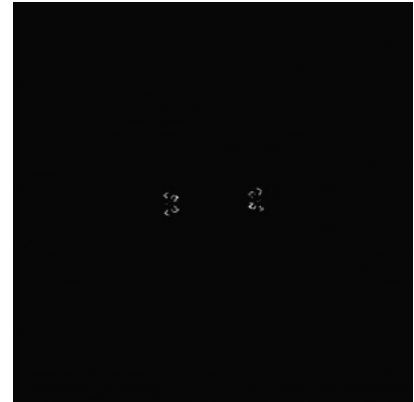
### 6.2.1 Primary map



X Index: 225

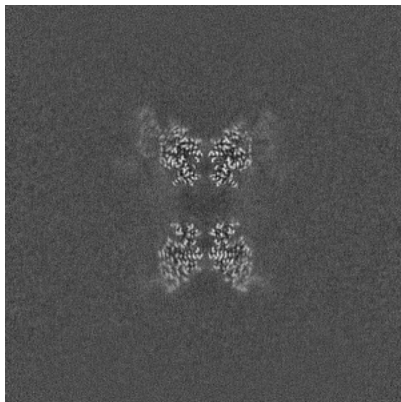


Y Index: 225

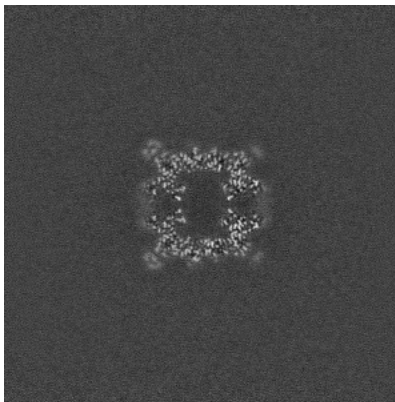


Z Index: 225

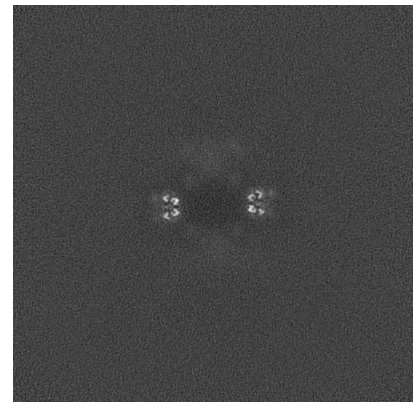
### 6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

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: 225

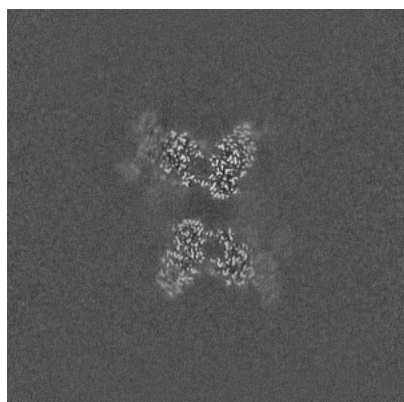


Y Index: 233

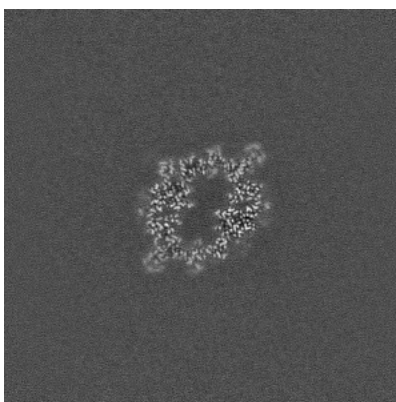


Z Index: 269

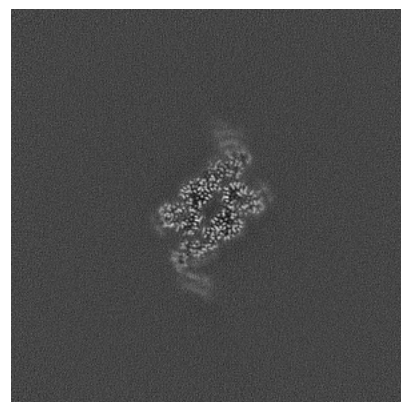
### 6.3.2 Raw map



X Index: 219



Y Index: 233

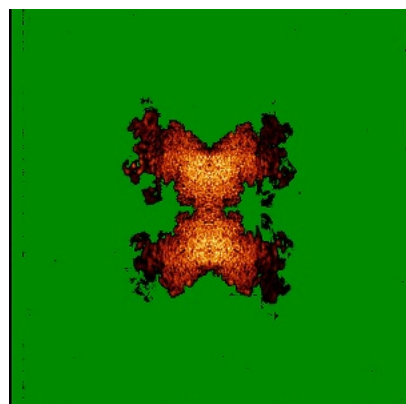


Z Index: 269

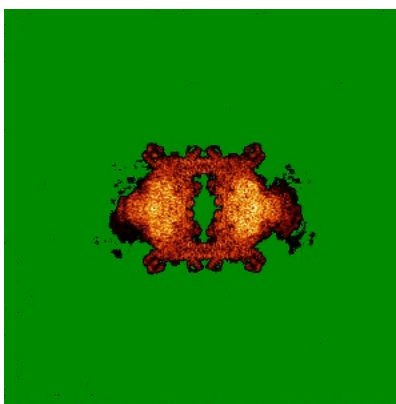
The images above show the largest variance slices of the map in three orthogonal directions.

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

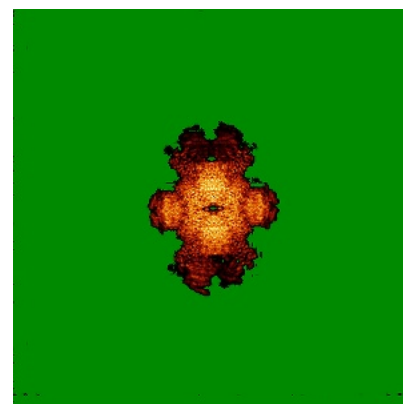
### 6.4.1 Primary map



X

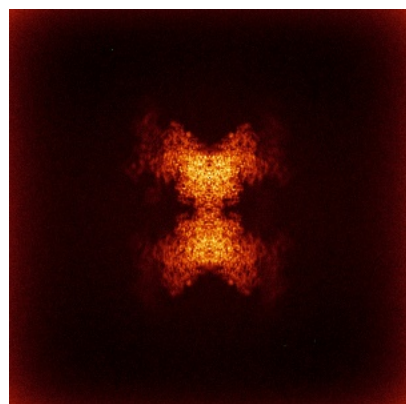


Y

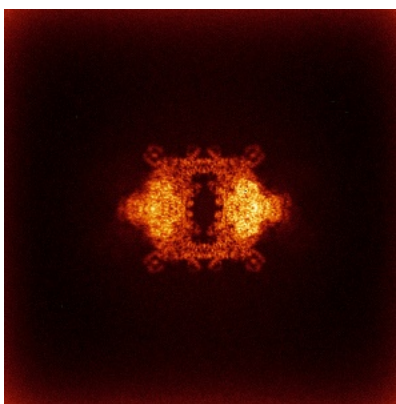


Z

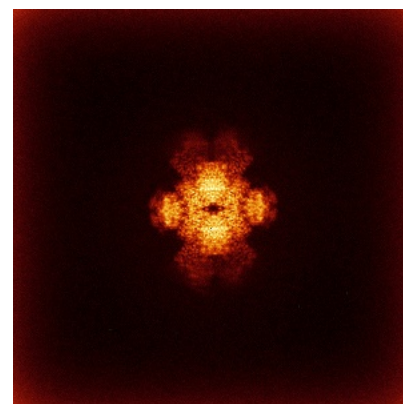
### 6.4.2 Raw map



X



Y

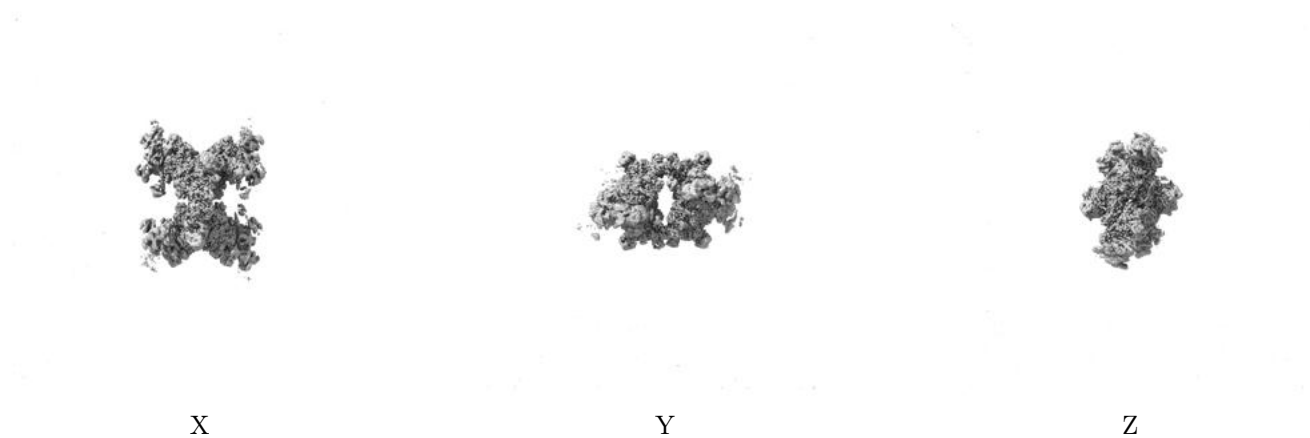


Z

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.

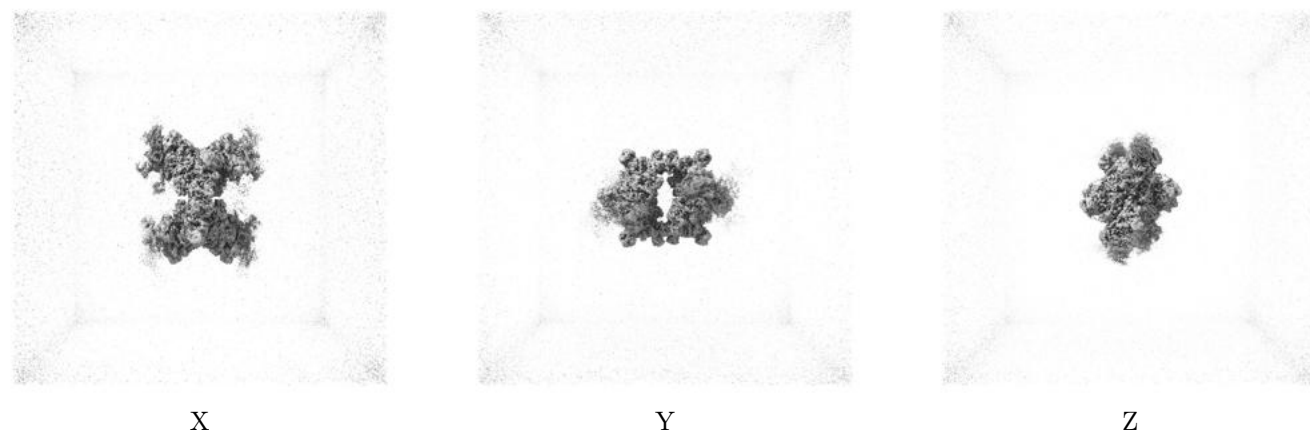
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

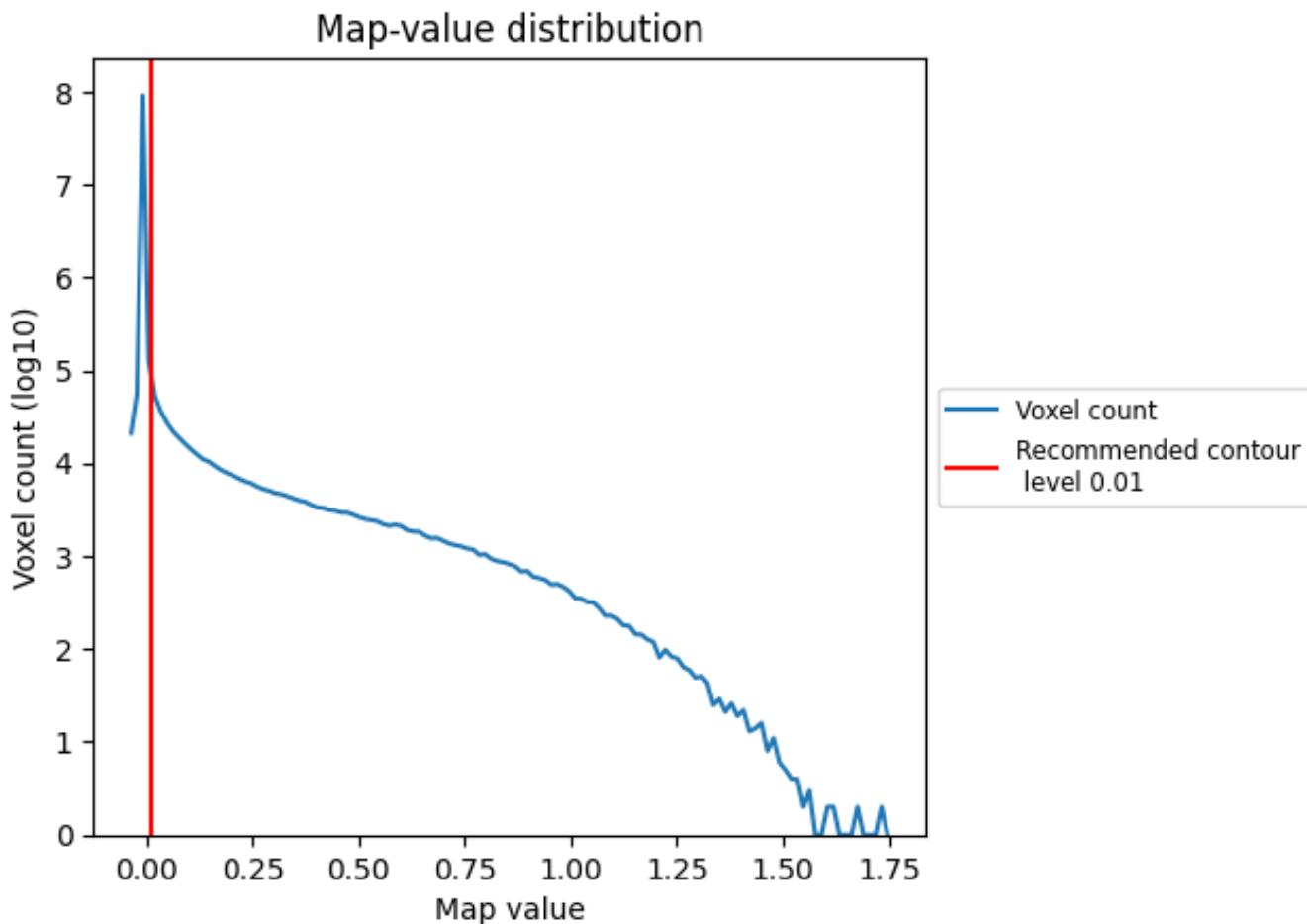
## 6.6 Mask visualisation [i](#)

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.

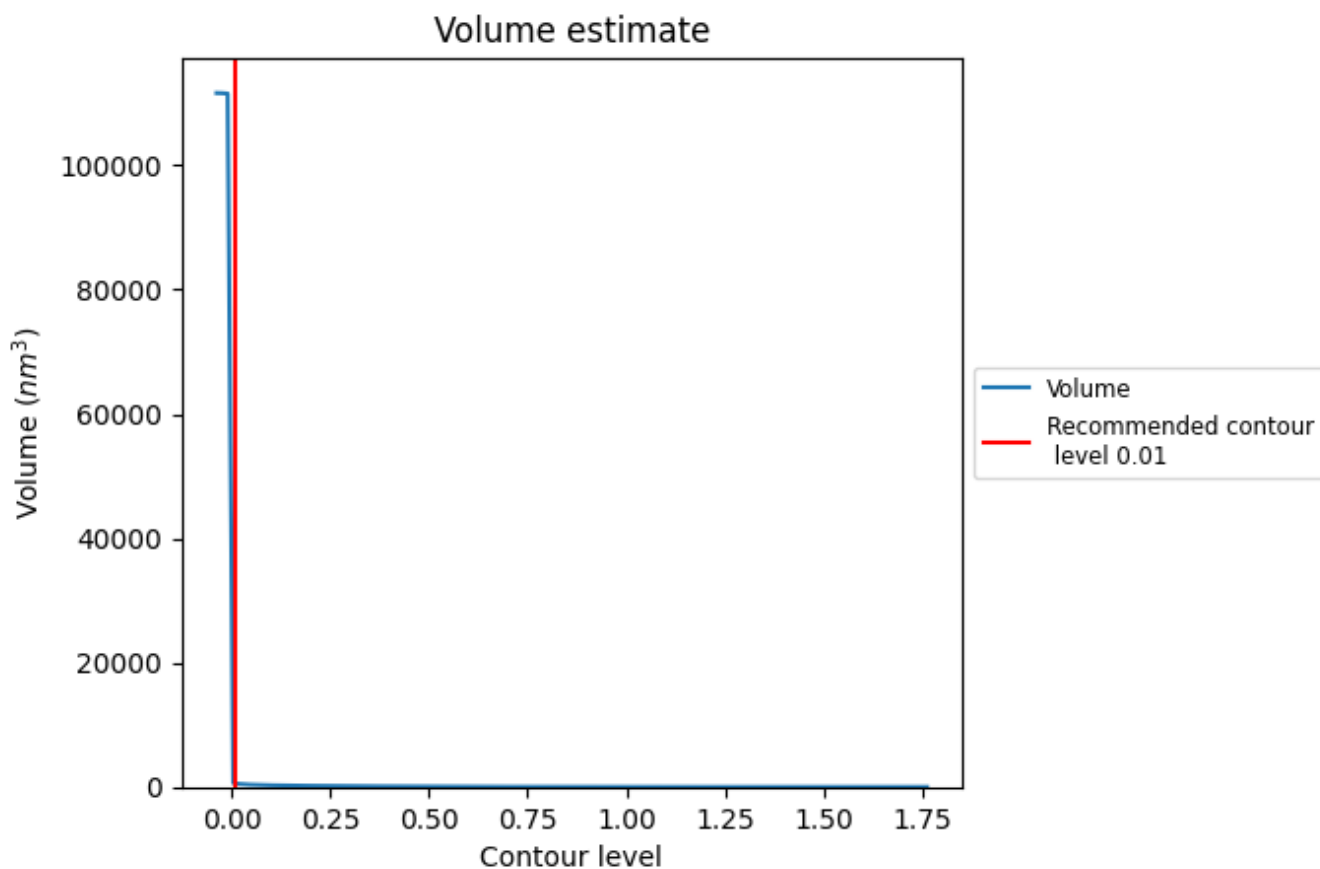
### 7.1 Map-value distribution [i](#)



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.



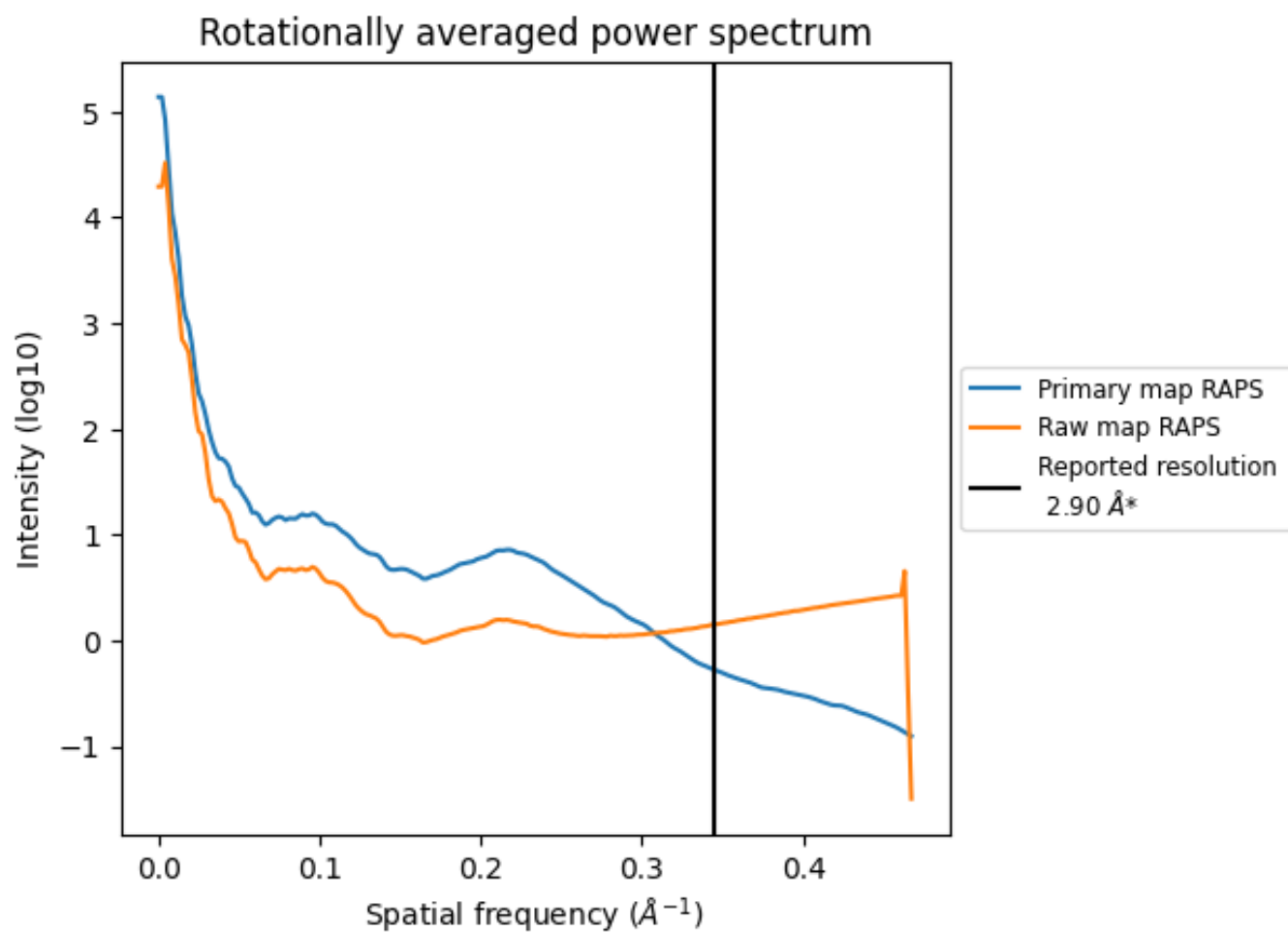
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $587 \text{ nm}^3$ ; this corresponds to an approximate mass of 531 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 i

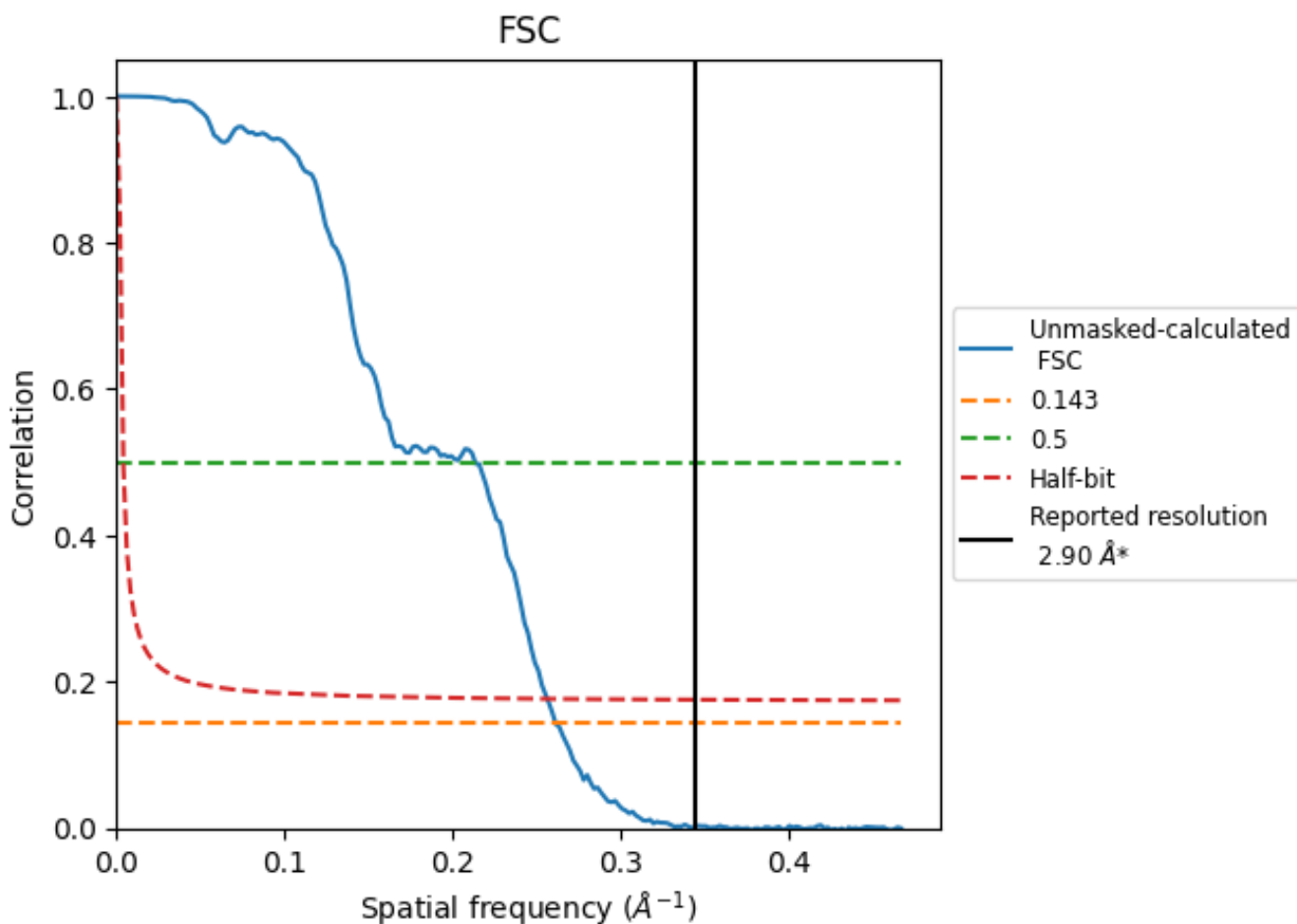


\*Reported resolution corresponds to spatial frequency of  $0.345 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

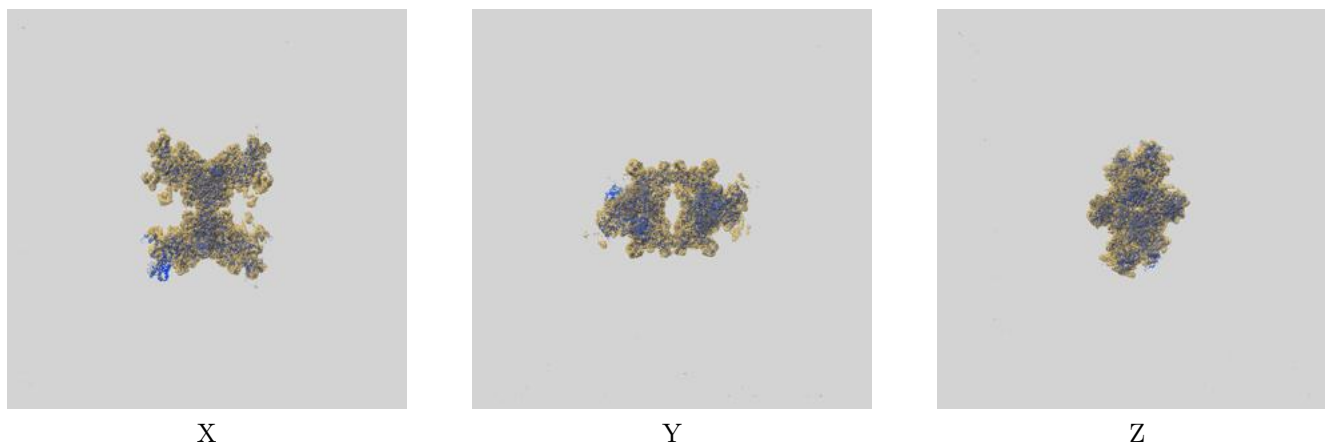
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.68	3.90

\*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 3.82 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

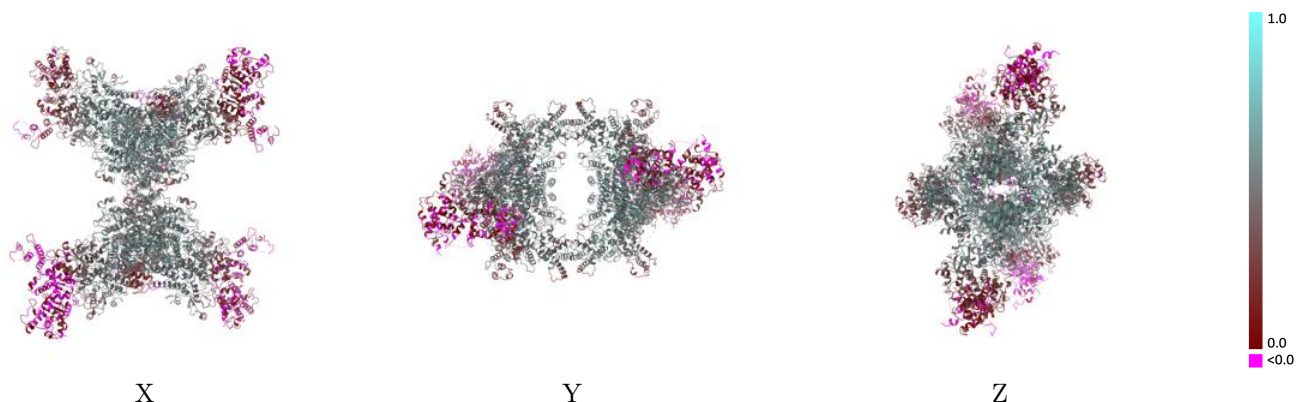
This section contains information regarding the fit between EMDB map EMD-36213 and PDB model 8JFL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



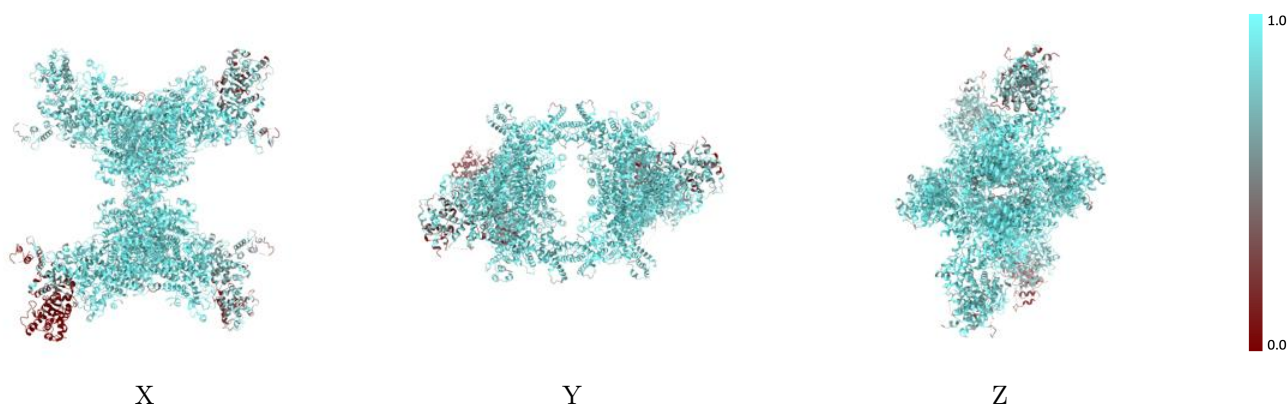
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



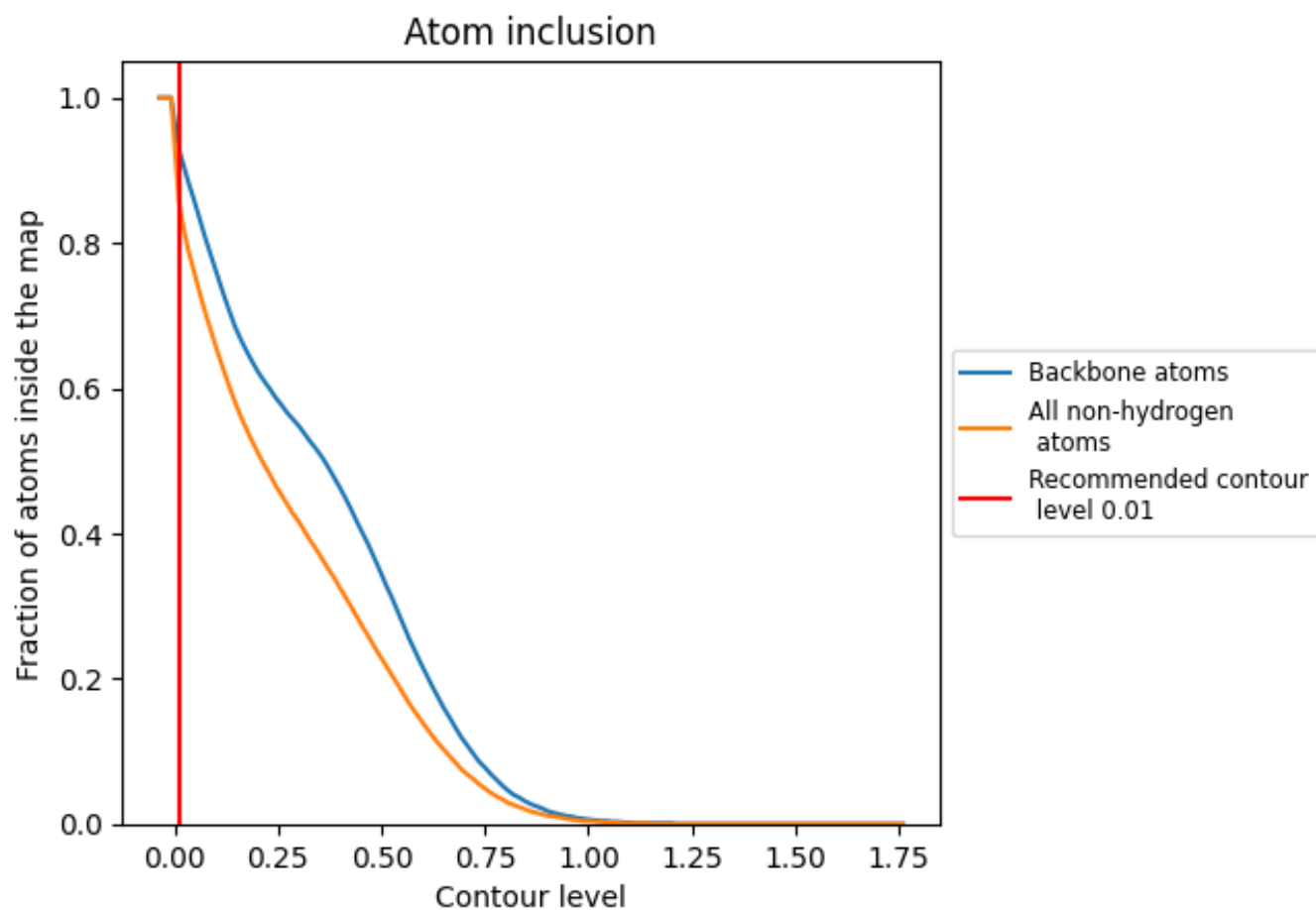
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3960
A	 0.8740	 0.3650
B	 0.9460	 0.5160
C	 0.7660	 0.1280
E	 0.8190	 0.3100
F	 0.9430	 0.5030
G	 0.5570	 0.0650
I	 0.6550	 0.2370
J	 0.9420	 0.4910
K	 0.0100	 0.0640
M	 0.7910	 0.2870
N	 0.9390	 0.4870
O	 0.4480	 0.0450

