



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:32 am GMT

PDB ID : 3J3R  
EMDB ID: : EMD-5610  
Title : Structural dynamics of the MecA-ClpC complex revealed by cryo-EM  
Authors : Liu, J.; Mei, Z.; Li, N.; Qi, Y.; Xu, Y.; Shi, Y.; Wang, F.; Lei, J.; Gao, N.  
Deposited on : 2013-04-18  
Resolution : 9.40 Å(reported)  
Based on PDB ID : 3PXI

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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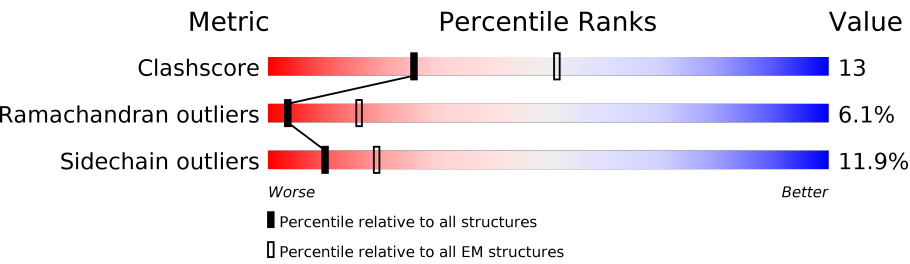
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

# 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 9.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	218	<div><div>28%11%57%</div></div>
1	2	218	<div><div>29%11%57%</div></div>
1	3	218	<div><div>31%11%57%</div></div>
1	4	218	<div><div>32%10%57%</div></div>
1	5	218	<div><div>28%12%57%</div></div>
1	6	218	<div><div>30%10%57%</div></div>
2	A	810	<div><div>65%27%6%</div></div>
2	B	810	<div><div>65%25%7%</div></div>
2	C	810	<div><div>67%26%6%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	810	<div><div></div><div>67%24%7% ..</div></div>
2	E	810	<div><div></div><div>66%25%7% ..</div></div>
2	F	810	<div><div></div><div>64%27%6% ..</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41838 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 Adapter protein MecA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	2	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	3	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	4	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	5	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	6	94	Total	C	N	O	S	0	0
			777	498	123	154	2		

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	B	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	C	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	D	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	E	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	F	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

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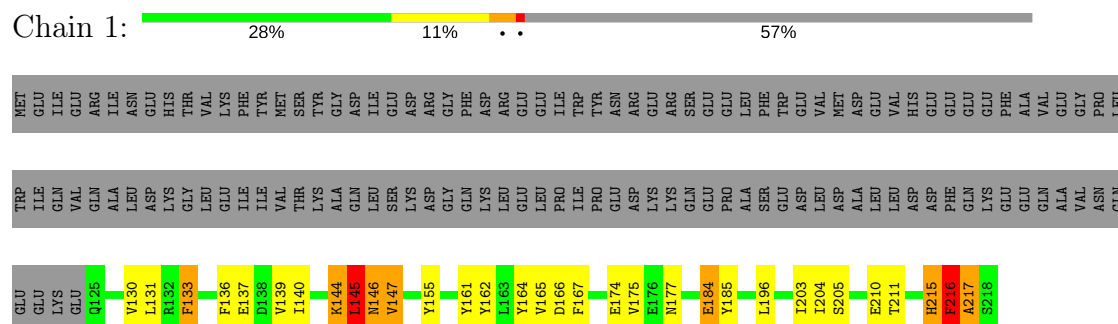
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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
E	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
E	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
F	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
F	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

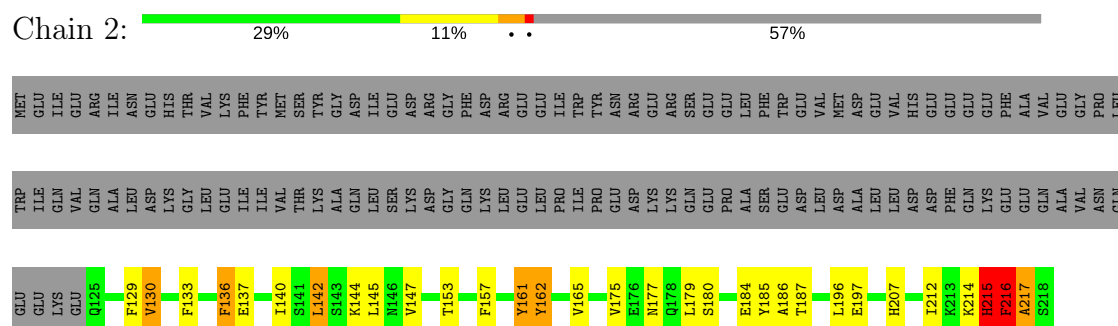
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

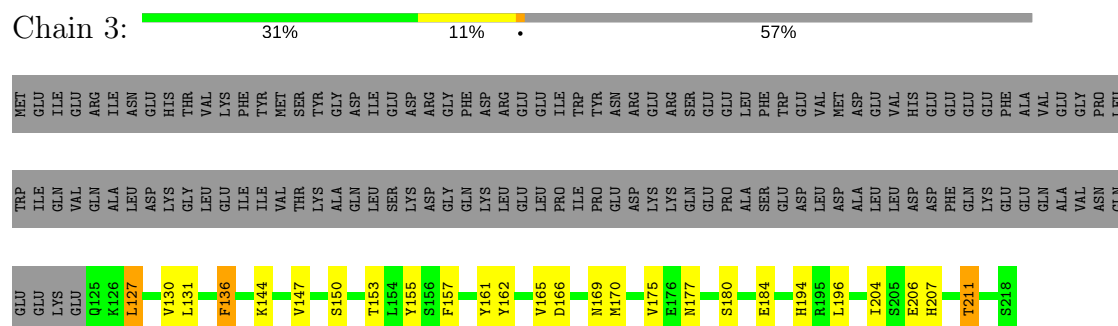
#### • Molecule 1: Adapter protein MecA 1



#### • Molecule 1: Adapter protein MecA 1



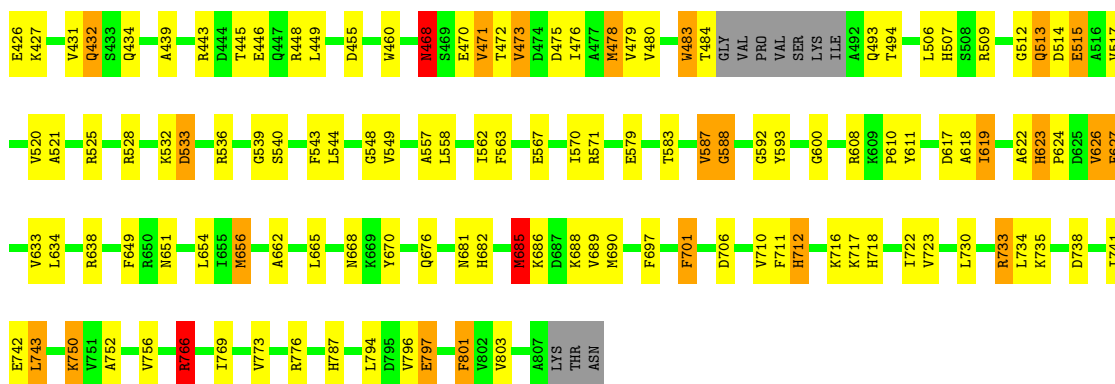
#### • Molecule 1: Adapter protein MecA 1



#### • Molecule 1: Adapter protein MecA 1

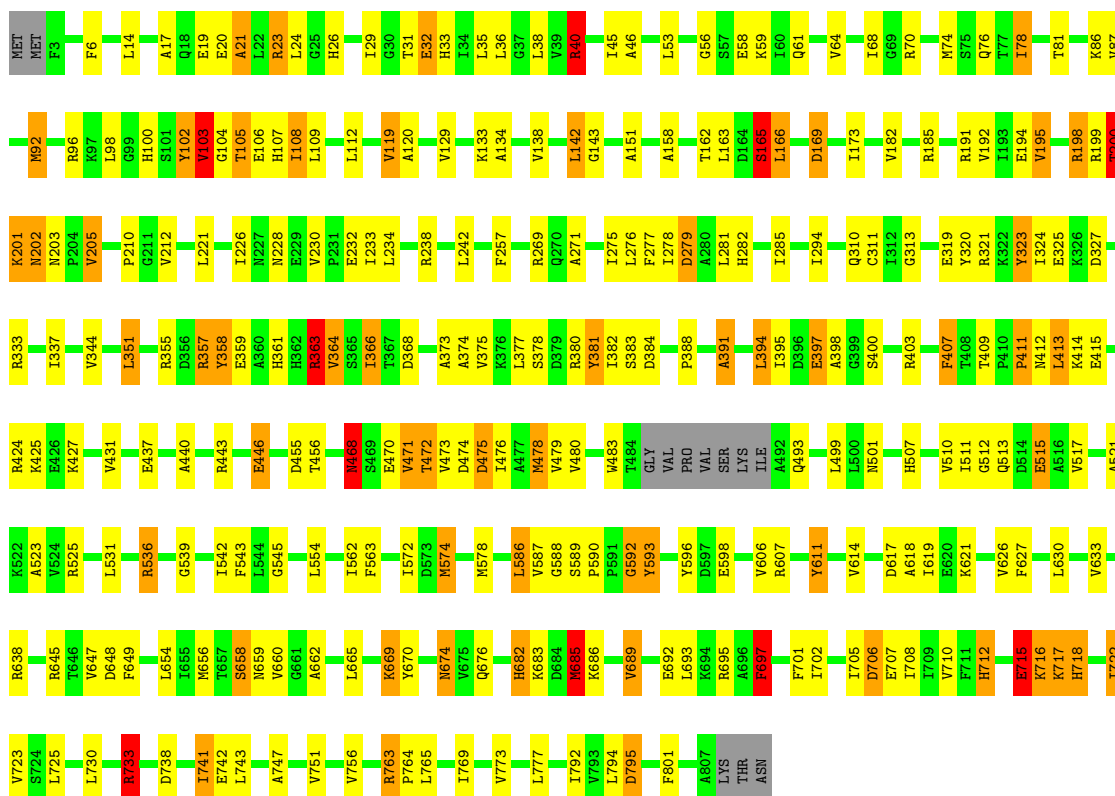






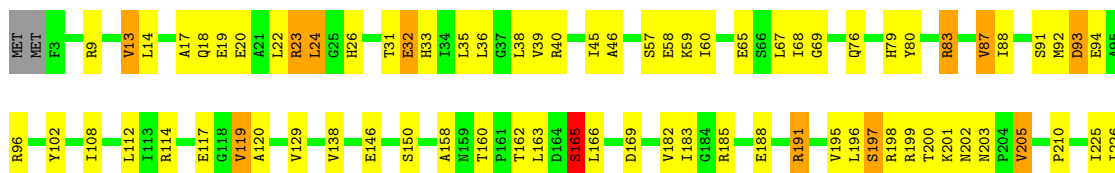
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain B: 65% 25% 7% ..

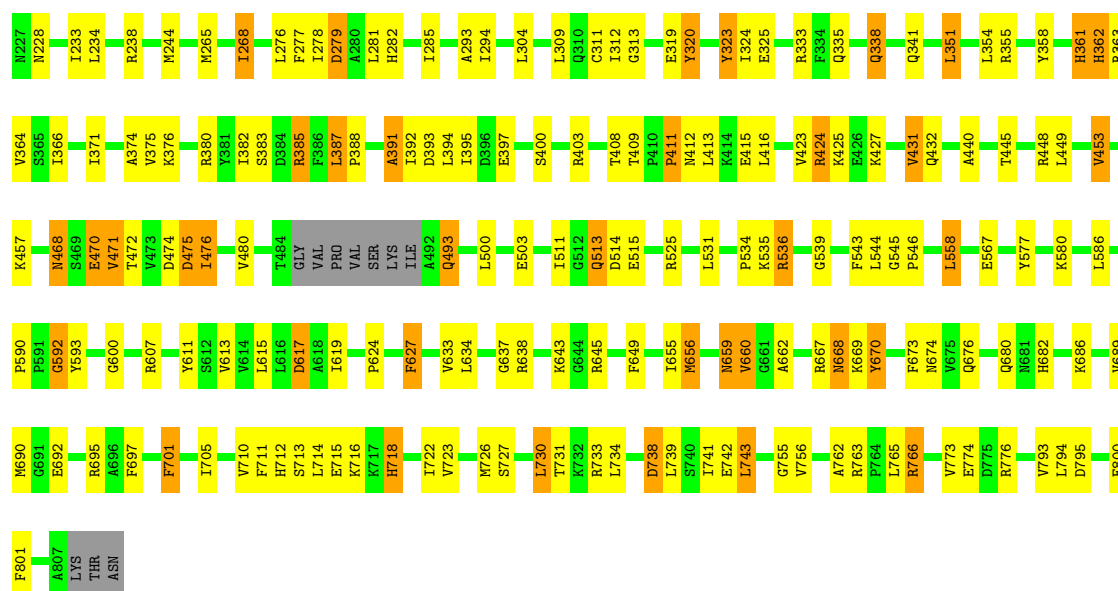


• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain C: 67% 26% 6% ..

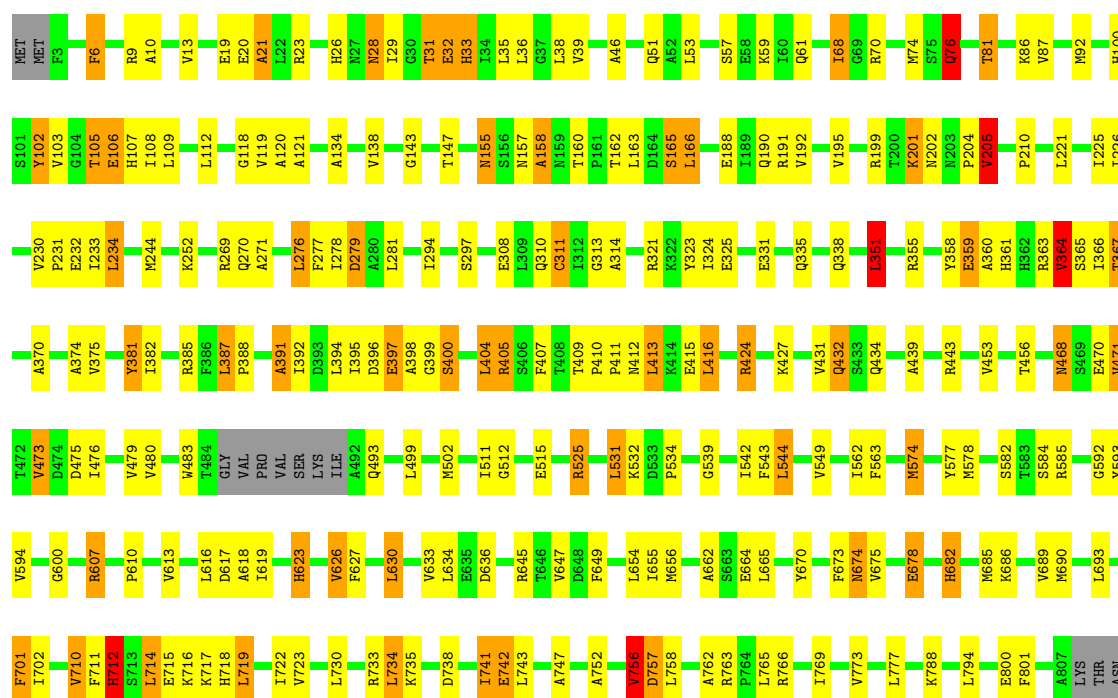






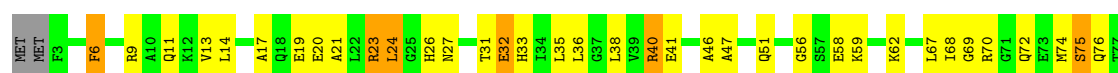
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

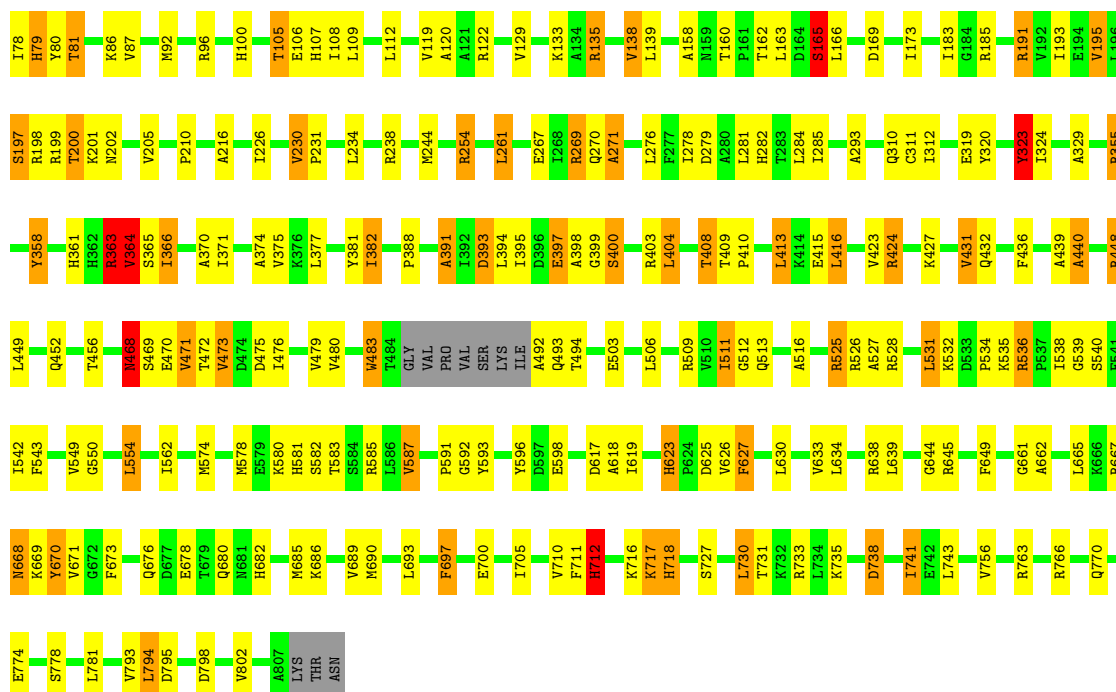
Chain D: 67% 24% 7% ..



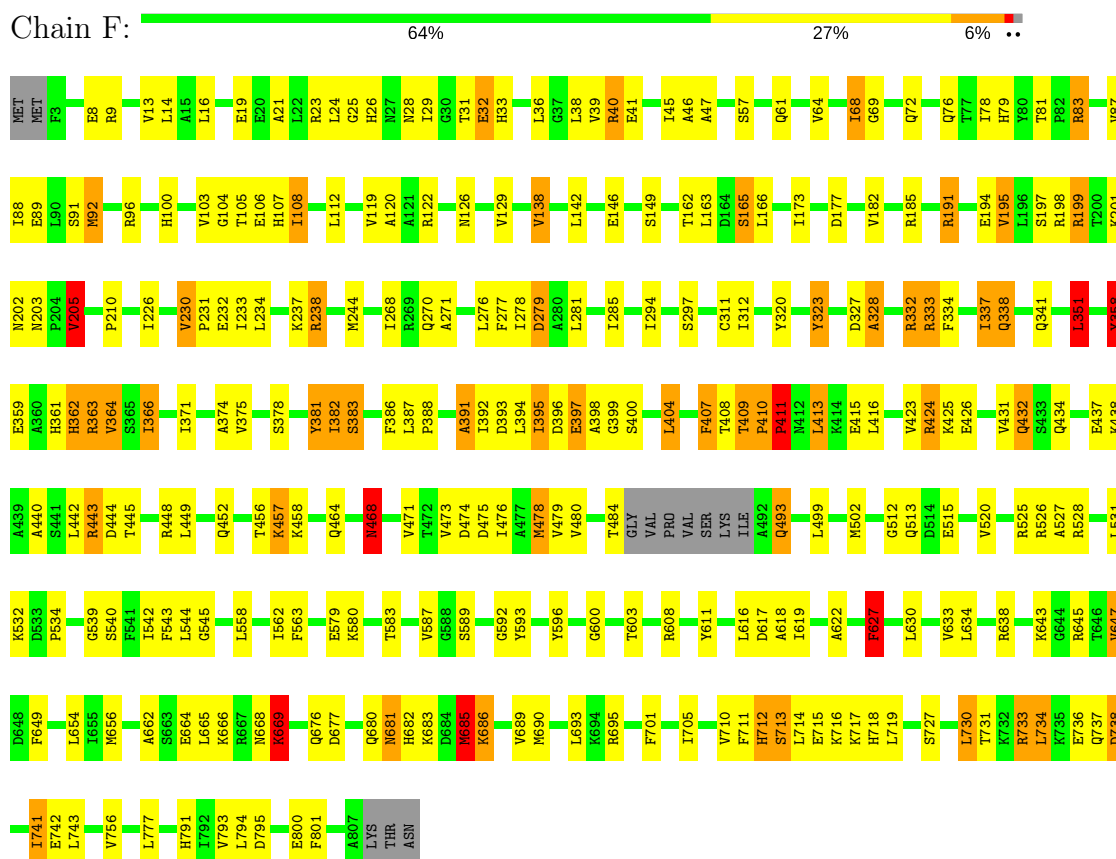
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain E: 66% 25% 7% ..





• Molecule 2: Negative regulator of genetic competence ClpC/MecB



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26037	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each defocus group on 3D level	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI Eagle 4k*4k CCD	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	1	1.00	0/791	1.33	7/1064 (0.7%)
1	2	0.99	0/791	1.32	7/1064 (0.7%)
1	3	0.99	0/791	1.30	2/1064 (0.2%)
1	4	0.99	0/791	1.33	2/1064 (0.2%)
1	5	0.99	0/791	1.28	4/1064 (0.4%)
1	6	1.00	0/791	1.37	5/1064 (0.5%)
2	A	1.00	0/6265	1.29	30/8436 (0.4%)
2	B	1.00	0/6265	1.29	33/8436 (0.4%)
2	C	0.99	0/6265	1.30	26/8436 (0.3%)
2	D	1.00	0/6265	1.28	32/8436 (0.4%)
2	E	1.01	0/6265	1.32	40/8436 (0.5%)
2	F	1.00	0/6265	1.30	36/8436 (0.4%)
All	All	1.00	0/42336	1.30	224/57000 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
1	2	0	3
1	3	0	2
1	4	0	4
1	5	0	3
1	6	0	4
2	A	0	9
2	B	0	15
2	C	0	17
2	D	0	13
2	E	0	17
2	F	0	19
All	All	0	109

There are no bond length outliers.

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	358	TYR	CB-CG-CD2	-10.16	114.90	121.00
2	A	801	PHE	CB-CG-CD1	-8.94	114.55	120.80
1	4	162	TYR	CB-CG-CD1	-8.93	115.64	121.00
2	F	358	TYR	CB-CG-CD1	8.86	126.32	121.00
2	E	697	PHE	CB-CG-CD2	8.79	126.95	120.80
2	C	670	TYR	CB-CG-CD2	8.70	126.22	121.00
1	4	162	TYR	CB-CG-CD2	8.51	126.11	121.00
2	E	697	PHE	CB-CG-CD1	-8.31	114.98	120.80
2	E	670	TYR	CB-CG-CD1	-8.27	116.04	121.00
2	B	685	MET	CG-SD-CE	-8.10	87.24	100.20
2	A	593	TYR	CB-CG-CD1	-8.05	116.17	121.00
2	C	670	TYR	CB-CG-CD1	-8.02	116.19	121.00
2	B	697	PHE	CB-CG-CD1	-8.02	115.19	120.80
2	B	6	PHE	CB-CG-CD1	-7.93	115.25	120.80
2	C	543	PHE	CB-CG-CD1	7.84	126.29	120.80
2	E	158	ALA	C-N-CA	7.69	140.92	121.70
2	B	697	PHE	CB-CG-CD2	7.65	126.16	120.80
2	C	543	PHE	CB-CG-CD2	-7.58	115.50	120.80
2	E	6	PHE	CB-CG-CD1	-7.54	115.52	120.80
1	1	216	PHE	CB-CG-CD2	-7.47	115.57	120.80
2	C	656	MET	CG-SD-CE	-7.47	88.25	100.20
2	F	593	TYR	CB-CG-CD2	-7.42	116.55	121.00
2	A	165	SER	C-N-CA	7.41	140.22	121.70
2	B	6	PHE	CB-CG-CD2	7.36	125.95	120.80
2	E	670	TYR	CB-CG-CD2	7.33	125.40	121.00
1	6	217	ALA	N-CA-CB	7.30	120.32	110.10
2	A	801	PHE	CB-CG-CD2	7.29	125.90	120.80
1	6	215	HIS	CA-CB-CG	7.28	125.98	113.60
2	F	165	SER	C-N-CA	7.23	139.78	121.70
1	2	216	PHE	CB-CG-CD2	-7.23	115.74	120.80
2	A	257	PHE	CB-CG-CD2	7.18	125.83	120.80
2	A	158	ALA	C-N-CA	7.16	139.61	121.70
2	D	364	VAL	C-N-CA	7.12	139.50	121.70
2	A	656	MET	CG-SD-CE	-7.09	88.85	100.20
2	B	165	SER	C-N-CA	7.09	139.43	121.70
2	E	197	SER	N-CA-CB	7.06	121.08	110.50
2	B	102	TYR	CB-CG-CD1	-6.94	116.84	121.00
2	C	158	ALA	C-N-CA	6.89	138.94	121.70
2	E	6	PHE	CB-CG-CD2	6.88	125.62	120.80
2	B	539	GLY	N-CA-C	-6.88	95.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	102	TYR	CB-CG-CD2	6.85	125.11	121.00
2	E	673	PHE	CB-CG-CD2	6.79	125.55	120.80
2	F	593	TYR	CB-CG-CD1	6.77	125.06	121.00
2	E	165	SER	C-N-CA	6.75	138.57	121.70
2	E	539	GLY	N-CA-C	-6.71	96.32	113.10
2	C	165	SER	C-N-CA	6.69	138.42	121.70
2	A	593	TYR	CB-CG-CD2	6.68	125.01	121.00
2	F	669	LYS	N-CA-CB	6.66	122.59	110.60
1	6	216	PHE	CB-CG-CD2	-6.63	116.16	120.80
2	E	323	TYR	CB-CG-CD1	6.60	124.96	121.00
2	A	539	GLY	N-CA-C	-6.60	96.61	113.10
2	C	102	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	1	166	ASP	N-CA-C	-6.57	93.27	111.00
1	1	216	PHE	CB-CG-CD1	6.57	125.40	120.80
2	D	165	SER	C-N-CA	6.51	137.99	121.70
2	C	358	TYR	CB-CG-CD1	6.51	124.91	121.00
2	F	383	SER	N-CA-CB	6.50	120.25	110.50
2	E	440	ALA	CB-CA-C	-6.47	100.40	110.10
1	2	215	HIS	CA-CB-CG	6.46	124.59	113.60
1	1	217	ALA	N-CA-CB	6.43	119.11	110.10
2	E	667	ARG	C-N-CA	6.43	137.79	121.70
2	E	323	TYR	CB-CG-CD2	-6.43	117.14	121.00
2	B	543	PHE	CB-CG-CD2	-6.43	116.30	120.80
2	B	543	PHE	CB-CG-CD1	6.39	125.27	120.80
2	D	543	PHE	CB-CG-CD1	6.37	125.26	120.80
2	B	158	ALA	C-N-CA	6.36	137.59	121.70
2	E	543	PHE	CB-CG-CD1	6.34	125.24	120.80
2	B	674	ASN	N-CA-C	-6.34	93.89	111.00
2	F	685	MET	CG-SD-CE	-6.33	90.06	100.20
2	F	596	TYR	CB-CG-CD1	-6.28	117.23	121.00
2	A	257	PHE	CB-CG-CD1	-6.25	116.43	120.80
1	1	162	TYR	CB-CG-CD2	6.23	124.74	121.00
2	E	717	LYS	N-CA-CB	6.20	121.76	110.60
2	D	244	MET	CG-SD-CE	-6.18	90.31	100.20
2	B	205	VAL	N-CA-C	-6.16	94.36	111.00
2	E	673	PHE	CB-CG-CD1	-6.16	116.49	120.80
2	E	543	PHE	CB-CG-CD2	-6.15	116.49	120.80
2	D	31	THR	CA-CB-CG2	-6.14	103.81	112.40
2	E	743	LEU	N-CA-C	-6.14	94.43	111.00
2	C	539	GLY	N-CA-C	-6.12	97.81	113.10
2	F	539	GLY	N-CA-C	-6.11	97.82	113.10
2	C	701	PHE	CB-CG-CD2	-6.06	116.56	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	543	PHE	CB-CG-CD2	-6.06	116.56	120.80
2	D	543	PHE	CB-CG-CD2	-6.06	116.56	120.80
2	C	738	ASP	N-CA-CB	6.05	121.49	110.60
2	F	563	PHE	CB-CG-CD1	-6.05	116.57	120.80
1	2	217	ALA	N-CA-CB	6.04	118.56	110.10
2	D	539	GLY	N-CA-C	-6.04	98.00	113.10
2	B	398	ALA	C-N-CA	6.03	134.97	122.30
2	F	323	TYR	CB-CG-CD1	-6.02	117.39	121.00
2	E	408	THR	N-CA-C	-6.01	94.77	111.00
2	B	468	ASN	N-CA-C	6.01	127.22	111.00
2	C	743	LEU	N-CA-C	-6.00	94.80	111.00
2	B	102	TYR	CB-CG-CD2	5.99	124.60	121.00
2	F	543	PHE	CB-CG-CD2	-5.98	116.61	120.80
2	B	200	THR	N-CA-CB	5.95	121.61	110.30
2	B	21	ALA	CB-CA-C	-5.94	101.19	110.10
1	5	157	PHE	CB-CG-CD2	-5.93	116.65	120.80
2	D	92	MET	CG-SD-CE	-5.93	90.71	100.20
1	5	155	TYR	CA-CB-CG	-5.87	102.24	113.40
2	C	440	ALA	CB-CA-C	-5.86	101.31	110.10
2	B	40	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	D	358	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	A	200	THR	N-CA-CB	5.83	121.37	110.30
2	D	358	TYR	CB-CG-CD1	5.80	124.48	121.00
2	A	543	PHE	CB-CG-CD1	5.77	124.84	120.80
2	A	366	ILE	C-N-CA	5.77	136.12	121.70
1	1	133	PHE	CB-CG-CD1	-5.75	116.77	120.80
2	F	323	TYR	CB-CG-CD2	5.74	124.44	121.00
2	F	738	ASP	N-CA-CB	5.73	120.92	110.60
2	E	483	TRP	CB-CG-CD2	-5.73	119.15	126.60
2	B	394	LEU	CB-CA-C	5.73	121.08	110.20
2	E	536	ARG	N-CA-C	-5.72	95.56	111.00
1	2	161	TYR	CA-CB-CG	-5.71	102.55	113.40
1	1	162	TYR	CB-CG-CD1	-5.69	117.58	121.00
2	C	361	HIS	C-N-CA	5.67	135.88	121.70
2	C	358	TYR	CB-CG-CD2	-5.67	117.60	121.00
2	F	543	PHE	CB-CG-CD1	5.67	124.77	120.80
2	B	200	THR	CA-CB-CG2	-5.66	104.47	112.40
2	D	483	TRP	CB-CG-CD2	-5.66	119.25	126.60
2	E	364	VAL	C-N-CA	5.66	135.84	121.70
2	A	21	ALA	N-CA-CB	5.65	118.02	110.10
1	5	157	PHE	CB-CG-CD1	5.65	124.75	120.80
2	D	158	ALA	CB-CA-C	-5.63	101.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	PHE	CB-CG-CD2	5.63	124.74	120.80
2	E	200	THR	N-CA-CB	5.63	120.99	110.30
1	6	214	LYS	C-N-CA	5.62	135.75	121.70
2	C	393	ASP	CB-CA-C	-5.62	99.17	110.40
2	A	323	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	E	802	VAL	N-CA-C	-5.61	95.86	111.00
2	D	21	ALA	N-CA-CB	5.60	117.94	110.10
2	B	412	ASN	C-N-CA	5.60	135.69	121.70
2	C	659	ASN	N-CA-CB	5.59	120.67	110.60
2	D	381	TYR	CB-CG-CD1	-5.59	117.64	121.00
2	E	200	THR	CA-CB-CG2	-5.58	104.59	112.40
2	A	685	MET	CG-SD-CE	-5.57	91.28	100.20
2	A	383	SER	N-CA-CB	5.57	118.85	110.50
2	C	423	VAL	CA-CB-CG1	-5.56	102.56	110.90
2	D	674	ASN	N-CA-C	-5.54	96.04	111.00
2	E	79	HIS	N-CA-C	-5.53	96.06	111.00
1	3	166	ASP	N-CA-C	-5.50	96.16	111.00
2	F	364	VAL	CA-CB-CG1	-5.49	102.67	110.90
2	F	408	THR	C-N-CA	5.48	135.39	121.70
2	F	669	LYS	N-CA-C	-5.48	96.21	111.00
1	2	214	LYS	C-N-CA	5.47	135.37	121.70
1	6	216	PHE	CB-CG-CD1	5.46	124.62	120.80
2	F	502	MET	CG-SD-CE	-5.45	91.48	100.20
2	F	596	TYR	CB-CG-CD2	5.45	124.27	121.00
2	A	627	PHE	CB-CG-CD2	-5.45	116.99	120.80
2	F	79	HIS	N-CA-C	-5.45	96.29	111.00
2	E	627	PHE	CB-CG-CD2	-5.41	117.01	120.80
2	F	743	LEU	N-CA-C	-5.40	96.42	111.00
2	A	364	VAL	C-N-CA	5.40	135.19	121.70
2	B	327	ASP	C-N-CA	5.37	135.11	121.70
2	D	204	PRO	N-CA-C	-5.35	98.19	112.10
2	E	483	TRP	CB-CG-CD1	5.35	133.96	127.00
2	F	205	VAL	N-CA-C	-5.35	96.56	111.00
2	E	738	ASP	N-CA-CB	5.34	120.21	110.60
2	F	364	VAL	N-CA-C	-5.32	96.65	111.00
1	3	150	SER	N-CA-C	-5.31	96.65	111.00
2	E	366	ILE	C-N-CA	5.31	134.97	121.70
2	D	323	TYR	CB-CG-CD1	-5.30	117.82	121.00
2	C	627	PHE	CB-CG-CD2	-5.30	117.09	120.80
2	B	383	SER	N-CA-CB	5.29	118.43	110.50
1	2	207	HIS	N-CA-C	-5.27	96.77	111.00
2	F	366	ILE	N-CA-CB	5.27	122.92	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	279	ASP	CB-CG-OD2	5.26	123.04	118.30
2	B	658	SER	N-CA-CB	5.25	118.38	110.50
2	B	279	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	364	VAL	C-N-CA	5.24	134.81	121.70
2	A	733	ARG	NE-CZ-NH2	5.24	122.92	120.30
2	C	440	ALA	N-CA-CB	5.24	117.43	110.10
2	E	794	LEU	N-CA-C	-5.24	96.87	111.00
2	B	617	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	279	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	93	ASP	CB-CA-C	5.22	120.85	110.40
2	B	669	LYS	N-CA-C	-5.22	96.91	111.00
2	F	617	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	407	PHE	CB-CG-CD1	-5.22	117.15	120.80
2	F	563	PHE	CB-CG-CD2	5.22	124.45	120.80
2	D	617	ASP	CB-CG-OD2	5.21	122.99	118.30
2	D	323	TYR	CB-CG-CD2	5.21	124.12	121.00
2	E	382	ILE	C-N-CA	5.21	134.72	121.70
2	A	279	ASP	CB-CG-OD2	5.20	122.98	118.30
2	D	279	ASP	CB-CG-OD2	5.20	122.98	118.30
1	2	216	PHE	CB-CG-CD1	5.19	124.44	120.80
2	E	617	ASP	CB-CG-OD2	5.18	122.97	118.30
2	A	617	ASP	CB-CG-OD2	5.18	122.96	118.30
1	5	155	TYR	CB-CG-CD1	-5.18	117.89	121.00
2	F	279	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	351	LEU	CB-CG-CD2	5.18	119.80	111.00
2	E	70	ARG	C-N-CA	5.17	133.17	122.30
2	A	624	PRO	N-CA-C	5.17	125.55	112.10
2	F	540	SER	N-CA-C	-5.17	97.05	111.00
2	A	201	LYS	N-CA-C	-5.15	97.09	111.00
2	C	617	ASP	CB-CG-OD2	5.15	122.93	118.30
2	F	411	PRO	CA-N-CD	-5.14	104.30	111.50
2	A	743	LEU	CB-CA-C	-5.14	100.43	110.20
2	D	160	THR	CA-C-N	5.13	131.47	117.10
2	D	270	GLN	C-N-CA	5.13	134.53	121.70
2	A	540	SER	N-CA-C	-5.13	97.16	111.00
2	A	364	VAL	O-C-N	-5.12	114.50	122.70
2	D	434	GLN	C-N-CA	5.12	134.51	121.70
2	D	434	GLN	N-CA-CB	5.12	119.82	110.60
2	D	710	VAL	CA-CB-CG1	-5.12	103.22	110.90
2	F	328	ALA	N-CA-CB	5.12	117.27	110.10
2	F	351	LEU	CB-CG-CD2	5.12	119.70	111.00
2	F	382	ILE	C-N-CA	5.11	134.48	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	LYS	C-N-CA	5.09	134.43	121.70
2	A	341	GLN	N-CA-C	-5.09	97.26	111.00
2	D	757	ASP	N-CA-CB	5.09	119.76	110.60
2	F	627	PHE	CB-CG-CD2	-5.09	117.24	120.80
2	D	502	MET	CG-SD-CE	-5.09	92.06	100.20
2	B	382	ILE	C-N-CA	5.08	134.40	121.70
2	E	323	TYR	CA-CB-CG	5.08	123.05	113.40
2	E	439	ALA	N-CA-CB	5.08	117.21	110.10
2	A	412	ASN	C-N-CA	5.06	134.35	121.70
2	E	270	GLN	C-N-CA	5.05	134.33	121.70
2	D	382	ILE	C-N-CA	5.05	134.33	121.70
2	C	627	PHE	CB-CG-CD1	5.04	124.33	120.80
2	F	341	GLN	N-CA-C	-5.03	97.42	111.00
2	D	205	VAL	N-CA-C	-5.03	97.43	111.00
2	D	21	ALA	CB-CA-C	-5.02	102.57	110.10
2	B	40	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (109) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	155	TYR	Sidechain
1	1	161	TYR	Sidechain
1	1	185	TYR	Sidechain
1	2	161	TYR	Sidechain
1	2	215	HIS	Sidechain
1	2	216	PHE	Sidechain
1	3	155	TYR	Sidechain
1	3	161	TYR	Sidechain
1	4	161	TYR	Sidechain
1	4	162	TYR	Sidechain
1	4	185	TYR	Sidechain
1	4	215	HIS	Sidechain
1	5	155	TYR	Sidechain
1	5	161	TYR	Sidechain
1	5	185	TYR	Sidechain
1	6	161	TYR	Sidechain
1	6	162	TYR	Sidechain
1	6	199	TYR	Sidechain
1	6	215	HIS	Sidechain
2	A	210	PRO	Peptide
2	A	33	HIS	Sidechain

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Mol	Chain	Res	Type	Group
2	A	399	GLY	Mainchain
2	A	409	THR	Peptide
2	A	468	ASN	Peptide
2	A	592	GLY	Peptide
2	A	716	LYS	Peptide
2	A	756	VAL	Peptide
2	A	766	ARG	Sidechain
2	B	102	TYR	Sidechain
2	B	210	PRO	Peptide
2	B	357	ARG	Sidechain
2	B	358	TYR	Sidechain
2	B	363	ARG	Sidechain
2	B	409	THR	Peptide
2	B	468	ASN	Peptide
2	B	592	GLY	Peptide
2	B	596	TYR	Sidechain
2	B	611	TYR	Sidechain
2	B	716	LYS	Mainchain,Peptide
2	B	733	ARG	Sidechain
2	B	756	VAL	Peptide
2	B	96	ARG	Sidechain
2	C	210	PRO	Peptide
2	C	320	TYR	Sidechain
2	C	355	ARG	Sidechain
2	C	380	ARG	Sidechain
2	C	409	THR	Peptide
2	C	424	ARG	Sidechain
2	C	468	ASN	Peptide
2	C	525	ARG	Sidechain
2	C	536	ARG	Sidechain
2	C	577	TYR	Sidechain
2	C	592	GLY	Peptide
2	C	611	TYR	Sidechain
2	C	697	PHE	Sidechain
2	C	713	SER	Peptide
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	766	ARG	Sidechain
2	D	210	PRO	Peptide
2	D	33	HIS	Sidechain
2	D	381	TYR	Sidechain
2	D	409	THR	Peptide

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Mol	Chain	Res	Type	Group
2	D	424	ARG	Sidechain
2	D	468	ASN	Peptide
2	D	592	GLY	Peptide
2	D	593	TYR	Sidechain
2	D	682	HIS	Sidechain
2	D	712	HIS	Sidechain
2	D	716	LYS	Peptide
2	D	756	VAL	Peptide
2	D	766	ARG	Sidechain
2	E	210	PRO	Peptide
2	E	358	TYR	Sidechain
2	E	363	ARG	Sidechain
2	E	40	ARG	Sidechain
2	E	409	THR	Peptide
2	E	424	ARG	Sidechain
2	E	468	ASN	Peptide
2	E	525	ARG	Sidechain
2	E	592	GLY	Peptide
2	E	593	TYR	Sidechain
2	E	627	PHE	Sidechain
2	E	716	LYS	Mainchain,Peptide
2	E	733	ARG	Sidechain
2	E	756	VAL	Peptide
2	E	766	ARG	Sidechain
2	E	96	ARG	Sidechain
2	F	210	PRO	Peptide
2	F	238	ARG	Sidechain
2	F	320	TYR	Sidechain
2	F	358	TYR	Sidechain
2	F	381	TYR	Sidechain
2	F	407	PHE	Sidechain
2	F	409	THR	Mainchain,Peptide
2	F	424	ARG	Sidechain
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	600	GLY	Peptide
2	F	627	PHE	Sidechain
2	F	716	LYS	Mainchain,Peptide
2	F	756	VAL	Peptide
2	F	791	HIS	Sidechain
2	F	83	ARG	Sidechain
2	F	96	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	777	0	758	17	0
1	2	777	0	758	17	0
1	3	777	0	758	7	0
1	4	777	0	758	11	0
1	5	777	0	758	15	0
1	6	777	0	758	17	0
2	A	6196	0	6289	190	0
2	B	6196	0	6289	202	0
2	C	6196	0	6289	169	0
2	D	6196	0	6289	166	0
2	E	6196	0	6289	156	0
2	F	6196	0	6289	175	0
All	All	41838	0	42282	1061	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 13.

All (1061) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:281:LEU:CD1	2:D:313:GLY:CA	1.78	1.61
2:E:278:ILE:HB	2:E:281:LEU:CD2	1.29	1.60
2:D:281:LEU:CD1	2:D:313:GLY:HA2	1.14	1.59
2:B:281:LEU:HD11	2:B:313:GLY:CA	1.34	1.58
2:A:278:ILE:HB	2:A:281:LEU:CD2	1.33	1.55
2:B:281:LEU:CD1	2:B:313:GLY:CA	1.88	1.51
2:A:278:ILE:CG2	2:A:281:LEU:HD23	1.38	1.50
2:D:278:ILE:HB	2:D:281:LEU:CD2	1.38	1.49
2:A:278:ILE:CB	2:A:281:LEU:HD21	1.39	1.48
2:D:278:ILE:CG2	2:D:281:LEU:HD23	1.39	1.48
2:A:281:LEU:CD1	2:A:313:GLY:HA2	1.41	1.48
2:A:278:ILE:CB	2:A:281:LEU:CD2	1.89	1.47
2:C:278:ILE:CG2	2:C:281:LEU:HD23	1.43	1.47
2:A:619:ILE:HG23	2:A:627:PHE:CE1	1.48	1.45
2:B:281:LEU:CD1	2:B:313:GLY:HA2	1.46	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:ILE:HB	2:C:281:LEU:CD2	1.47	1.43
2:E:278:ILE:CB	2:E:281:LEU:HD21	1.53	1.37
2:D:278:ILE:CB	2:D:281:LEU:HD21	1.53	1.37
2:F:278:ILE:HB	2:F:281:LEU:CD2	1.54	1.35
2:A:278:ILE:CG2	2:A:281:LEU:CD2	2.00	1.35
2:A:281:LEU:CD1	2:A:313:GLY:CA	2.04	1.35
2:D:278:ILE:CB	2:D:281:LEU:CD2	2.06	1.33
2:D:281:LEU:HD12	2:D:313:GLY:CA	1.46	1.33
2:B:619:ILE:CD1	2:B:656:MET:HB3	1.57	1.32
2:E:278:ILE:CB	2:E:281:LEU:CD2	2.05	1.32
2:E:619:ILE:HD13	2:E:630:LEU:CD1	1.60	1.30
2:D:281:LEU:HD11	2:D:313:GLY:CA	1.47	1.30
2:C:278:ILE:CB	2:C:281:LEU:CD2	2.10	1.30
2:B:619:ILE:HD12	2:B:656:MET:CB	1.62	1.29
2:F:278:ILE:CG2	2:F:281:LEU:HD23	1.63	1.29
2:C:619:ILE:HG23	2:C:627:PHE:CE1	1.69	1.26
2:C:278:ILE:CB	2:C:281:LEU:HD21	1.65	1.23
2:A:281:LEU:HD12	2:A:313:GLY:CA	1.65	1.23
2:E:278:ILE:CG2	2:E:281:LEU:HD23	1.72	1.19
2:B:281:LEU:CD1	2:B:313:GLY:HA3	1.59	1.18
2:C:278:ILE:CG2	2:C:281:LEU:CD2	2.20	1.18
2:F:619:ILE:HD11	2:F:656:MET:HB3	1.23	1.18
2:D:278:ILE:CG2	2:D:281:LEU:CD2	2.20	1.18
2:B:277:PHE:CE2	2:B:279:ASP:OD1	1.97	1.17
2:A:619:ILE:CG2	2:A:627:PHE:CZ	2.29	1.16
2:B:619:ILE:HG21	2:B:701:PHE:CZ	1.79	1.16
2:F:278:ILE:CB	2:F:281:LEU:HD21	1.74	1.16
2:F:619:ILE:HG23	2:F:627:PHE:CE1	1.80	1.16
2:B:278:ILE:HG22	2:B:281:LEU:HD23	1.22	1.15
2:A:619:ILE:HD11	2:A:656:MET:CB	1.74	1.15
2:C:619:ILE:HG21	2:C:701:PHE:CE2	1.82	1.14
2:A:619:ILE:CG2	2:A:627:PHE:CE1	2.30	1.14
2:F:278:ILE:CB	2:F:281:LEU:CD2	2.25	1.14
2:D:281:LEU:CD1	2:D:313:GLY:HA3	1.76	1.14
2:A:281:LEU:HD11	2:A:313:GLY:CA	1.73	1.13
2:B:281:LEU:HD12	2:B:313:GLY:HA3	1.16	1.12
2:A:619:ILE:CD1	2:A:656:MET:HB3	1.79	1.11
2:E:619:ILE:HD13	2:E:630:LEU:HD11	1.28	1.11
2:C:619:ILE:HD11	2:C:656:MET:CG	1.81	1.10
2:D:619:ILE:HD13	2:D:630:LEU:HD11	1.13	1.10
2:C:619:ILE:HD11	2:C:656:MET:HG2	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:278:ILE:O	2:F:281:LEU:HG	1.52	1.09
2:A:281:LEU:HD12	2:A:313:GLY:HA3	1.31	1.08
2:D:278:ILE:HG22	2:D:281:LEU:HD23	1.26	1.07
2:B:278:ILE:CG2	2:B:281:LEU:HD23	1.84	1.07
2:C:619:ILE:HG21	2:C:701:PHE:HE2	0.89	1.05
2:F:278:ILE:HG22	2:F:281:LEU:HD23	1.32	1.05
2:F:277:PHE:CE2	2:F:279:ASP:OD1	2.10	1.05
2:C:619:ILE:CG2	2:C:627:PHE:CE1	2.40	1.04
2:B:619:ILE:CG2	2:B:701:PHE:CZ	2.40	1.04
2:E:619:ILE:CD1	2:E:630:LEU:HD11	1.87	1.04
2:A:619:ILE:HG22	2:A:627:PHE:HZ	1.24	1.02
2:C:278:ILE:HG22	2:C:281:LEU:HD23	1.06	1.02
2:E:278:ILE:HG22	2:E:281:LEU:HD23	1.39	1.02
2:D:278:ILE:HG21	2:D:281:LEU:HD23	1.40	1.02
2:D:616:LEU:HB3	2:D:619:ILE:HD11	1.42	1.02
2:A:619:ILE:HG23	2:A:627:PHE:CZ	1.93	1.01
2:E:619:ILE:CD1	2:E:630:LEU:CD1	2.38	1.01
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.38	1.01
2:A:278:ILE:HG22	2:A:281:LEU:CD2	1.75	1.00
2:A:278:ILE:HB	2:A:281:LEU:HD22	1.44	0.99
2:C:277:PHE:CE2	2:C:279:ASP:OD1	2.14	0.99
2:B:278:ILE:O	2:B:281:LEU:CD2	2.11	0.99
2:E:619:ILE:HD13	2:E:630:LEU:HD12	1.42	0.98
2:F:619:ILE:HG23	2:F:627:PHE:CZ	1.98	0.98
2:D:619:ILE:CG2	2:D:701:PHE:CE2	2.48	0.97
2:F:278:ILE:CG2	2:F:281:LEU:CD2	2.43	0.96
2:B:278:ILE:HB	2:B:281:LEU:CD2	1.94	0.96
2:D:619:ILE:HG23	2:D:627:PHE:CE1	2.01	0.95
2:A:278:ILE:CA	2:A:281:LEU:HD21	1.96	0.95
2:A:281:LEU:HD11	2:A:313:GLY:HA2	0.95	0.94
2:C:619:ILE:CG2	2:C:701:PHE:HE2	1.80	0.94
2:D:281:LEU:HD12	2:D:313:GLY:HA3	1.37	0.94
2:D:619:ILE:HG21	2:D:701:PHE:CE2	2.02	0.94
2:B:619:ILE:CD1	2:B:656:MET:CB	2.31	0.93
2:A:278:ILE:O	2:A:281:LEU:HG	1.67	0.93
2:B:619:ILE:HG23	2:B:627:PHE:CE1	2.03	0.93
2:D:619:ILE:HD13	2:D:630:LEU:CD1	1.99	0.92
2:B:281:LEU:HD12	2:B:313:GLY:CA	1.75	0.92
2:D:619:ILE:HG22	2:D:701:PHE:HE2	1.34	0.91
2:B:619:ILE:CD1	2:B:656:MET:CG	2.48	0.91
2:D:277:PHE:CE2	2:D:279:ASP:OD2	2.24	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:CG2	2:B:701:PHE:HZ	1.82	0.89
2:B:281:LEU:HD11	2:B:313:GLY:HA2	0.89	0.88
2:E:278:ILE:CG2	2:E:281:LEU:CD2	2.40	0.88
2:A:619:ILE:HD13	2:A:701:PHE:CZ	2.08	0.87
2:F:619:ILE:HD11	2:F:656:MET:CB	2.05	0.87
2:A:281:LEU:CD1	2:A:313:GLY:HA3	1.93	0.86
2:A:278:ILE:O	2:A:281:LEU:CG	2.24	0.86
2:F:619:ILE:CG2	2:F:627:PHE:CZ	2.58	0.86
2:C:281:LEU:HD11	2:C:313:GLY:HA2	1.57	0.86
2:F:278:ILE:O	2:F:281:LEU:CG	2.24	0.86
2:C:278:ILE:HB	2:C:281:LEU:HD21	0.88	0.85
2:E:574:MET:HG3	2:E:619:ILE:HD11	1.57	0.85
2:D:619:ILE:HG22	2:D:619:ILE:O	1.75	0.85
2:F:278:ILE:HB	2:F:281:LEU:HD21	0.89	0.84
2:B:278:ILE:O	2:B:281:LEU:HD21	1.75	0.84
2:C:278:ILE:HG22	2:C:281:LEU:CD2	1.99	0.84
2:F:542:ILE:HD12	2:F:619:ILE:CD1	2.08	0.83
2:D:619:ILE:CD1	2:D:630:LEU:HD11	2.05	0.83
2:F:619:ILE:HG23	2:F:627:PHE:HE1	1.33	0.83
2:B:619:ILE:O	2:B:619:ILE:HG22	1.76	0.83
2:D:278:ILE:O	2:D:281:LEU:HG	1.78	0.83
2:C:281:LEU:CD1	2:C:313:GLY:HA2	2.08	0.83
2:A:278:ILE:O	2:A:281:LEU:CD2	2.27	0.82
2:B:278:ILE:CB	2:B:281:LEU:CD2	2.56	0.82
2:A:278:ILE:HG22	2:A:281:LEU:HD23	0.82	0.82
2:B:278:ILE:HB	2:B:281:LEU:HD21	1.61	0.82
2:B:277:PHE:CD2	2:B:279:ASP:OD1	2.32	0.82
2:D:619:ILE:CD1	2:D:656:MET:HG3	2.10	0.81
2:D:281:LEU:HD12	2:D:313:GLY:C	2.01	0.81
2:B:619:ILE:HG23	2:B:627:PHE:HE1	1.42	0.81
2:D:619:ILE:HG22	2:D:701:PHE:CE2	2.14	0.81
2:F:278:ILE:CB	2:F:281:LEU:HD23	2.05	0.81
2:D:619:ILE:HG23	2:D:627:PHE:HE1	1.43	0.80
2:A:278:ILE:HB	2:A:281:LEU:HD21	0.80	0.80
2:B:281:LEU:CG	2:B:313:GLY:HA2	2.11	0.80
2:E:574:MET:HG3	2:E:619:ILE:CD1	2.11	0.80
2:E:278:ILE:O	2:E:281:LEU:HG	1.80	0.79
2:A:619:ILE:HG22	2:A:627:PHE:CZ	2.04	0.79
2:F:619:ILE:CG2	2:F:627:PHE:HZ	1.96	0.79
2:B:277:PHE:HE2	2:B:279:ASP:OD1	1.66	0.78
2:C:26:HIS:CG	2:C:33:HIS:CE1	2.71	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:ILE:HB	2:E:281:LEU:HD22	1.58	0.78
2:C:203:ASN:HD22	2:C:281:LEU:HD11	1.46	0.78
2:D:619:ILE:CG2	2:D:701:PHE:HE2	1.93	0.78
2:C:281:LEU:CD1	2:C:313:GLY:CA	2.62	0.77
2:A:619:ILE:HD11	2:A:656:MET:HB3	0.85	0.77
2:C:619:ILE:HD11	2:C:656:MET:SD	2.24	0.76
2:C:619:ILE:HD13	2:C:701:PHE:CE2	2.20	0.76
2:B:281:LEU:HD11	2:B:313:GLY:N	2.00	0.76
2:D:351:LEU:HD22	2:D:392:ILE:HG23	1.68	0.76
2:C:281:LEU:HD11	2:C:313:GLY:CA	2.16	0.75
2:A:26:HIS:CG	2:A:33:HIS:CE1	2.75	0.75
2:A:619:ILE:HG23	2:A:627:PHE:HE1	0.90	0.74
2:C:278:ILE:O	2:C:281:LEU:HG	1.88	0.74
2:B:278:ILE:CG2	2:B:281:LEU:CD2	2.65	0.74
1:2:140:ILE:HD13	2:B:443:ARG:HG3	1.68	0.74
2:C:619:ILE:CD1	2:C:656:MET:SD	2.76	0.74
2:B:619:ILE:HG21	2:B:701:PHE:CE1	2.21	0.74
2:E:619:ILE:HG22	2:E:619:ILE:O	1.87	0.73
2:A:233:ILE:HG23	2:F:361:HIS:HA	1.70	0.73
2:B:394:LEU:HD13	2:B:480:VAL:HG22	1.70	0.73
2:C:93:ASP:HB3	2:D:158:ALA:H	1.53	0.73
2:D:619:ILE:HD12	2:D:656:MET:HG3	1.69	0.73
2:F:542:ILE:HD12	2:F:619:ILE:HD13	1.71	0.73
2:D:619:ILE:HG21	2:D:701:PHE:CZ	2.24	0.73
2:D:10:ALA:HB1	2:D:108:ILE:HD11	1.70	0.73
2:F:351:LEU:HD22	2:F:392:ILE:HG23	1.70	0.73
2:C:619:ILE:CD1	2:C:656:MET:CG	2.65	0.72
2:C:278:ILE:HG21	2:C:281:LEU:HD23	1.62	0.72
2:B:619:ILE:CD1	2:B:656:MET:HG2	2.19	0.72
2:A:278:ILE:O	2:A:281:LEU:HD21	1.89	0.72
2:A:665:LEU:HD23	2:A:685:MET:HB3	1.71	0.72
2:E:574:MET:CG	2:E:619:ILE:HD11	2.19	0.72
2:C:733:ARG:HH12	2:D:531:LEU:HD13	1.54	0.72
2:C:277:PHE:CD2	2:C:279:ASP:OD1	2.43	0.71
2:D:616:LEU:CB	2:D:619:ILE:HD11	2.18	0.71
2:B:682:HIS:CD2	2:B:712:HIS:CE1	2.79	0.71
2:C:281:LEU:HD12	2:C:313:GLY:HA3	1.73	0.71
2:A:619:ILE:CG2	2:A:627:PHE:HE1	1.83	0.71
2:B:278:ILE:O	2:B:281:LEU:HG	1.91	0.71
2:A:278:ILE:C	2:A:281:LEU:HD21	2.10	0.70
2:B:513:GLN:H	2:B:718:HIS:CD2	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:277:PHE:CD2	2:F:279:ASP:OD1	2.45	0.70
2:E:278:ILE:HB	2:E:281:LEU:HD21	0.71	0.70
2:B:588:GLY:H	2:C:593:TYR:H	1.38	0.70
2:E:278:ILE:CA	2:E:281:LEU:HD21	2.22	0.70
2:F:278:ILE:HG21	2:F:281:LEU:HD23	1.71	0.69
2:B:682:HIS:CD2	2:B:712:HIS:HE1	2.10	0.69
2:E:398:ALA:HB1	2:E:475:ASP:CG	2.12	0.69
2:F:619:ILE:CD1	2:F:656:MET:HB3	2.13	0.69
2:B:278:ILE:O	2:B:281:LEU:CG	2.39	0.69
2:C:619:ILE:HG23	2:C:627:PHE:CD1	2.25	0.69
2:A:619:ILE:HD13	2:A:701:PHE:HZ	1.57	0.69
2:D:281:LEU:HD11	2:D:313:GLY:HA2	0.69	0.68
2:D:32:GLU:HB3	2:D:119:VAL:HG12	1.75	0.68
2:F:24:LEU:HD23	2:F:69:GLY:HA2	1.74	0.68
2:A:665:LEU:HD23	2:A:685:MET:CB	2.24	0.68
2:B:619:ILE:HG22	2:B:701:PHE:HZ	1.59	0.68
2:A:24:LEU:HD22	2:A:64:VAL:HG12	1.75	0.68
2:D:619:ILE:CG2	2:D:627:PHE:CE1	2.75	0.68
2:A:278:ILE:CG2	2:A:281:LEU:HD22	2.19	0.68
2:E:278:ILE:O	2:E:281:LEU:CG	2.42	0.67
2:A:619:ILE:HD13	2:A:701:PHE:CE2	2.29	0.67
2:B:278:ILE:CB	2:B:281:LEU:HD23	2.22	0.67
2:B:374:ALA:HA	2:B:476:ILE:HG21	1.76	0.67
2:B:619:ILE:CG2	2:B:619:ILE:O	2.42	0.67
2:E:278:ILE:O	2:E:281:LEU:CD2	2.43	0.67
2:E:506:LEU:HD13	2:E:554:LEU:HD11	1.77	0.67
2:D:665:LEU:HD23	2:D:685:MET:HB2	1.77	0.67
2:F:619:ILE:HG22	2:F:627:PHE:HZ	1.59	0.66
1:1:140:ILE:HD13	2:A:443:ARG:HG3	1.77	0.66
2:B:619:ILE:HD11	2:B:656:MET:CG	2.24	0.66
2:B:36:LEU:HD22	2:B:40:ARG:HH22	1.60	0.66
2:C:619:ILE:HD13	2:C:701:PHE:CZ	2.31	0.66
2:B:511:ILE:HD12	2:B:722:ILE:HA	1.78	0.66
2:B:619:ILE:HD13	2:B:656:MET:HG2	1.77	0.66
2:C:278:ILE:HB	2:C:281:LEU:HD22	1.71	0.66
2:B:100:HIS:CD2	2:B:107:HIS:CE1	2.83	0.66
2:C:203:ASN:ND2	2:C:281:LEU:HD11	2.11	0.66
2:F:281:LEU:HD11	2:F:312:ILE:O	1.85	0.66
2:F:277:PHE:HE2	2:F:279:ASP:OD1	1.73	0.66
2:F:351:LEU:HD11	2:F:391:ALA:HB1	1.79	0.65
2:D:619:ILE:CG2	2:D:619:ILE:O	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:394:LEU:HD13	2:F:480:VAL:HG22	1.78	0.65
2:A:619:ILE:CG2	2:A:627:PHE:HZ	1.80	0.65
2:B:361:HIS:HA	2:C:233:ILE:HG23	1.77	0.65
2:C:278:ILE:O	2:C:281:LEU:CD2	2.44	0.65
2:D:394:LEU:HD13	2:D:480:VAL:HG22	1.80	0.64
2:C:615:LEU:HG	2:C:617:ASP:OD1	1.97	0.64
2:A:278:ILE:C	2:A:281:LEU:CD2	2.65	0.64
2:F:665:LEU:HD21	2:F:710:VAL:HG13	1.80	0.64
1:2:137:GLU:HA	1:2:140:ILE:HD12	1.80	0.64
2:D:395:ILE:HA	2:D:476:ILE:HD12	1.79	0.64
2:A:619:ILE:HG21	2:A:701:PHE:CE2	2.34	0.63
1:4:130:VAL:HG13	1:4:196:LEU:HD11	1.80	0.63
2:C:203:ASN:ND2	2:C:281:LEU:CD1	2.61	0.63
2:F:476:ILE:O	2:F:480:VAL:HG23	1.99	0.62
2:D:351:LEU:HD11	2:D:391:ALA:HB1	1.80	0.62
2:A:476:ILE:O	2:A:480:VAL:HG23	1.98	0.62
2:B:26:HIS:HB2	2:B:33:HIS:CE1	2.34	0.62
2:C:619:ILE:HG22	2:C:627:PHE:CZ	2.34	0.62
2:C:619:ILE:HG23	2:C:627:PHE:HE1	1.52	0.62
2:C:203:ASN:HD22	2:C:281:LEU:CD1	2.11	0.62
2:F:278:ILE:O	2:F:281:LEU:CD2	2.47	0.62
2:A:611:TYR:HA	2:A:651:ASN:HB3	1.82	0.62
2:D:38:LEU:HD21	2:D:108:ILE:HB	1.81	0.62
2:D:277:PHE:HE2	2:D:279:ASP:OD2	1.81	0.62
2:D:374:ALA:HB2	2:D:395:ILE:HG23	1.80	0.62
2:E:38:LEU:HD22	2:E:46:ALA:CB	2.30	0.62
1:1:137:GLU:HA	1:1:140:ILE:HD12	1.81	0.61
2:B:512:GLY:HA3	2:B:718:HIS:CG	2.35	0.61
2:C:619:ILE:HD12	2:C:656:MET:HB3	1.81	0.61
2:A:36:LEU:HD12	2:A:64:VAL:HG11	1.83	0.61
2:C:281:LEU:HD12	2:C:313:GLY:CA	2.28	0.61
2:A:619:ILE:HG21	2:A:701:PHE:HE2	1.63	0.61
2:A:278:ILE:CB	2:A:281:LEU:HD22	2.09	0.61
2:D:714:LEU:HD22	2:D:718:HIS:HB2	1.83	0.61
2:D:747:ALA:HB1	2:D:794:LEU:HD23	1.81	0.61
2:D:26:HIS:HA	2:D:68:ILE:HD12	1.82	0.61
1:2:140:ILE:HD13	2:B:443:ARG:CG	2.31	0.61
1:6:204:ILE:HG21	1:6:208:ALA:HA	1.82	0.60
2:F:544:LEU:HB2	2:F:689:VAL:HG13	1.83	0.60
2:E:511:ILE:H	2:E:511:ILE:HD13	1.65	0.60
2:A:730:LEU:HD12	2:A:769:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:ILE:O	2:C:281:LEU:CG	2.49	0.60
2:C:39:VAL:HG13	2:C:57:SER:HA	1.82	0.60
2:E:413:LEU:HD23	2:E:416:LEU:HG	1.84	0.60
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.83	0.60
2:B:203:ASN:HD22	2:B:281:LEU:HD13	1.67	0.60
2:B:374:ALA:CA	2:B:476:ILE:HG21	2.32	0.60
2:B:619:ILE:HD13	2:B:630:LEU:HD13	1.83	0.60
2:D:733:ARG:HH11	2:E:534:PRO:HD2	1.66	0.60
2:F:92:MET:HA	2:F:103:VAL:HG22	1.83	0.60
2:D:21:ALA:HB2	2:D:29:ILE:CG2	2.31	0.60
2:E:661:GLY:HA3	2:E:689:VAL:HG13	1.83	0.60
2:E:404:LEU:HD22	2:F:194:GLU:HG2	1.83	0.60
2:A:26:HIS:CD2	2:A:68:ILE:HB	2.37	0.59
2:B:476:ILE:O	2:B:480:VAL:HG23	2.01	0.59
2:D:28:ASN:HD22	2:D:81:THR:HG23	1.66	0.59
2:E:41:GLU:HG2	2:E:47:ALA:HB2	1.83	0.59
2:E:395:ILE:HA	2:E:476:ILE:HD12	1.84	0.59
2:E:56:GLY:H	2:E:59:LYS:HD3	1.67	0.59
2:F:499:LEU:HD22	2:F:525:ARG:HA	1.84	0.59
2:A:544:LEU:HB3	2:A:689:VAL:HG11	1.84	0.59
1:6:204:ILE:HG23	2:F:434:GLN:HE22	1.67	0.59
2:D:542:ILE:HD11	2:D:702:ILE:HG22	1.83	0.59
2:A:278:ILE:HG21	2:A:281:LEU:CD2	2.22	0.59
2:C:278:ILE:CA	2:C:281:LEU:HD21	2.33	0.59
2:C:619:ILE:HG22	2:C:627:PHE:CE1	2.37	0.59
2:C:93:ASP:HB3	2:D:157:ASN:H	1.67	0.58
2:A:587:VAL:HG12	2:A:588:GLY:H	1.66	0.58
2:B:26:HIS:CD2	2:B:68:ILE:HB	2.38	0.58
2:D:730:LEU:HD22	2:D:741:ILE:HD11	1.86	0.58
2:F:374:ALA:HB1	2:F:391:ALA:O	2.03	0.58
2:B:619:ILE:HD12	2:B:656:MET:HB3	0.69	0.58
2:D:685:MET:SD	2:D:712:HIS:CD2	2.97	0.58
2:A:670:TYR:H	2:A:681:ASN:HD21	1.50	0.58
2:C:731:THR:HG22	2:C:742:GLU:HA	1.86	0.58
2:D:278:ILE:HG21	2:D:281:LEU:CD2	2.16	0.58
2:E:476:ILE:O	2:E:480:VAL:HG23	2.03	0.58
1:4:204:ILE:HG21	1:4:211:THR:HB	1.85	0.58
2:D:387:LEU:HD22	2:D:387:LEU:H	1.68	0.58
2:F:100:HIS:CG	2:F:107:HIS:CE1	2.92	0.58
2:A:100:HIS:CG	2:A:107:HIS:CE1	2.91	0.58
2:B:697:PHE:CE1	2:B:702:ILE:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:730:LEU:HD12	2:C:774:GLU:HG2	1.84	0.58
1:1:140:ILE:HG22	1:1:144:LYS:HZ2	1.68	0.57
2:D:741:ILE:HG21	2:E:531:LEU:HD21	1.86	0.57
2:B:472:THR:H	2:B:475:ASP:HB2	1.69	0.57
2:C:394:LEU:CD1	2:C:480:VAL:HG22	2.34	0.57
2:C:449:LEU:O	2:C:453:VAL:HG23	2.04	0.57
2:A:471:VAL:HG22	2:A:476:ILE:HD11	1.85	0.57
2:A:665:LEU:HD21	2:A:689:VAL:CG2	2.35	0.57
2:D:38:LEU:HD22	2:D:46:ALA:CB	2.33	0.57
2:B:56:GLY:H	2:B:59:LYS:HD3	1.70	0.57
2:D:355:ARG:HH21	2:D:364:VAL:HG12	1.70	0.57
2:E:36:LEU:HD22	2:E:40:ARG:HE	1.69	0.57
2:F:426:GLU:HB3	2:F:442:LEU:HD13	1.87	0.57
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.86	0.57
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.38	0.57
2:D:278:ILE:HB	2:D:281:LEU:HD21	0.61	0.56
1:1:140:ILE:HD13	2:A:443:ARG:CG	2.35	0.56
1:5:141:SER:HA	2:E:27:ASN:HD21	1.70	0.56
2:E:374:ALA:HB1	2:E:391:ALA:O	2.05	0.56
2:D:278:ILE:O	2:D:281:LEU:CG	2.51	0.56
2:F:603:THR:HG23	2:F:647:VAL:HG11	1.87	0.56
2:C:619:ILE:CD1	2:C:656:MET:HB3	2.36	0.56
2:E:281:LEU:HD11	2:E:312:ILE:O	2.05	0.56
1:4:149:GLY:H	1:4:207:HIS:CE1	2.24	0.56
2:A:665:LEU:HD21	2:A:689:VAL:HG21	1.88	0.56
2:D:281:LEU:HD12	2:D:314:ALA:N	2.20	0.56
1:2:216:PHE:CD1	2:B:443:ARG:HB2	2.39	0.56
2:D:26:HIS:CG	2:D:33:HIS:CE1	2.93	0.56
2:D:714:LEU:HD11	2:D:756:VAL:O	2.06	0.56
1:6:147:VAL:HG13	1:6:148:ASN:H	1.71	0.56
2:D:665:LEU:HD11	2:D:689:VAL:HG11	1.87	0.56
2:E:100:HIS:CG	2:E:107:HIS:CE1	2.93	0.56
2:C:545:GLY:HA3	2:C:711:PHE:HB2	1.86	0.56
2:E:398:ALA:HB3	2:E:476:ILE:HD13	1.88	0.56
2:E:554:LEU:HD23	2:E:711:PHE:CZ	2.40	0.56
2:D:26:HIS:HB2	2:D:33:HIS:CE1	2.41	0.56
2:B:619:ILE:CG2	2:B:627:PHE:CE1	2.85	0.56
2:E:26:HIS:CD2	2:E:68:ILE:HB	2.41	0.56
2:E:619:ILE:CG2	2:E:619:ILE:O	2.54	0.56
2:B:21:ALA:HB2	2:B:29:ILE:CG1	2.36	0.55
2:F:41:GLU:HG2	2:F:47:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:HIS:CG	2:B:319:GLU:HB3	2.41	0.55
2:B:743:LEU:HD11	2:B:773:VAL:HG11	1.88	0.55
2:C:351:LEU:HD11	2:C:391:ALA:HB1	1.88	0.55
2:E:100:HIS:CG	2:E:107:HIS:HE1	2.23	0.55
2:E:665:LEU:HD21	2:E:710:VAL:CG1	2.36	0.55
2:B:741:ILE:HD12	2:B:742:GLU:N	2.21	0.55
2:A:100:HIS:CG	2:A:107:HIS:HE1	2.25	0.55
2:C:282:HIS:CD2	2:C:319:GLU:HB3	2.42	0.55
2:C:730:LEU:HD11	2:C:773:VAL:HG11	1.88	0.55
2:D:100:HIS:CG	2:D:107:HIS:HE1	2.23	0.55
2:E:278:ILE:O	2:E:281:LEU:HD21	2.05	0.55
2:F:278:ILE:HG22	2:F:281:LEU:CD2	2.21	0.55
2:D:281:LEU:CG	2:D:313:GLY:HA2	2.21	0.55
2:E:26:HIS:HB2	2:E:33:HIS:HE1	1.71	0.55
2:C:544:LEU:HB2	2:C:689:VAL:HG13	1.87	0.55
2:B:741:ILE:HD13	2:B:777:LEU:HD11	1.88	0.55
2:C:385:ARG:HH21	2:D:321:ARG:HH12	1.53	0.55
2:D:364:VAL:HG13	2:D:399:GLY:HA3	1.88	0.55
2:D:515:GLU:CD	2:D:712:HIS:CD2	2.81	0.55
2:F:24:LEU:HD22	2:F:64:VAL:HG12	1.87	0.55
2:E:528:ARG:HE	2:E:562:ILE:HA	1.71	0.54
2:F:26:HIS:CG	2:F:68:ILE:HD12	2.42	0.54
2:C:278:ILE:O	2:C:281:LEU:HD21	2.06	0.54
1:6:179:LEU:HD23	2:F:122:ARG:HE	1.72	0.54
2:A:79:HIS:CG	2:A:80:TYR:H	2.25	0.54
2:B:278:ILE:CB	2:B:281:LEU:HD21	2.28	0.54
2:F:520:VAL:CG1	2:F:558:LEU:HD21	2.37	0.54
2:C:351:LEU:HD22	2:C:392:ILE:HG23	1.89	0.54
2:E:685:MET:SD	2:E:712:HIS:CE1	3.01	0.54
2:F:394:LEU:HD22	2:F:480:VAL:HA	1.89	0.54
1:5:130:VAL:HG13	1:5:196:LEU:HD11	1.90	0.54
2:C:20:GLU:HB3	2:C:33:HIS:CE1	2.43	0.54
2:F:9:ARG:HB3	2:F:105:THR:H	1.71	0.54
2:C:374:ALA:HB1	2:C:391:ALA:O	2.07	0.54
2:F:363:ARG:HH21	2:F:468:ASN:HA	1.72	0.54
2:F:45:ILE:H	2:F:45:ILE:HD12	1.73	0.54
2:A:39:VAL:HG11	2:A:60:ILE:HD12	1.88	0.54
2:B:282:HIS:CD2	2:B:319:GLU:HB3	2.43	0.54
2:C:45:ILE:H	2:C:45:ILE:HD12	1.72	0.54
2:D:719:LEU:H	2:D:719:LEU:HD23	1.73	0.54
2:F:665:LEU:HD23	2:F:685:MET:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:471:VAL:O	2:A:471:VAL:HG22	2.08	0.54
2:A:685:MET:HB2	2:A:712:HIS:CD2	2.42	0.54
2:C:387:LEU:HD22	2:C:387:LEU:H	1.72	0.54
1:4:136:PHE:CZ	2:D:431:VAL:HG11	2.43	0.54
2:D:633:VAL:HG13	2:D:649:PHE:CG	2.42	0.54
2:E:394:LEU:HD22	2:E:480:VAL:HA	1.89	0.54
1:5:185:TYR:HA	2:E:81:THR:HG21	1.90	0.54
2:F:686:LYS:HA	2:F:710:VAL:HG11	1.88	0.54
2:C:362:HIS:H	2:C:362:HIS:CD2	2.24	0.53
2:C:94:GLU:HG3	2:C:114:ARG:HE	1.73	0.53
1:3:196:LEU:H	1:3:196:LEU:HD23	1.72	0.53
2:B:38:LEU:HD21	2:B:108:ILE:HB	1.91	0.53
2:B:36:LEU:HD21	2:B:61:GLN:HA	1.91	0.53
2:C:416:LEU:HB3	2:C:453:VAL:HG22	1.90	0.53
2:E:665:LEU:HD13	2:E:711:PHE:O	2.08	0.53
2:E:730:LEU:HD13	2:E:774:GLU:HG2	1.89	0.53
1:2:216:PHE:CZ	2:B:431:VAL:CG2	2.91	0.53
1:6:132:ARG:HB3	1:6:162:TYR:CE1	2.42	0.53
2:A:515:GLU:HG2	2:A:712:HIS:CE1	2.44	0.53
2:A:633:VAL:HG13	2:A:649:PHE:CG	2.43	0.53
2:D:686:LYS:HA	2:D:710:VAL:HG21	1.91	0.53
2:B:542:ILE:HD11	2:B:702:ILE:HG22	1.90	0.53
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.43	0.53
2:F:230:VAL:HG22	2:F:231:PRO:HD2	1.91	0.53
2:A:21:ALA:HB2	2:A:29:ILE:CG2	2.38	0.53
2:A:512:GLY:HA3	2:A:718:HIS:CG	2.43	0.53
2:C:660:VAL:HG11	2:C:695:ARG:HH21	1.73	0.53
2:A:431:VAL:HG13	2:A:439:ALA:HB1	1.90	0.53
2:B:203:ASN:HD22	2:B:281:LEU:CD1	2.22	0.53
2:B:20:GLU:HB2	2:B:33:HIS:CG	2.44	0.53
2:D:773:VAL:HG13	2:D:794:LEU:HD22	1.91	0.53
2:B:413:LEU:HD13	2:B:456:THR:HG21	1.90	0.53
2:D:619:ILE:HG23	2:D:627:PHE:CD1	2.42	0.53
2:F:733:ARG:HE	2:F:734:LEU:HD23	1.74	0.53
2:A:723:VAL:HG11	2:A:752:ALA:HB2	1.90	0.53
2:D:741:ILE:HD13	2:D:777:LEU:CD1	2.40	0.52
2:E:135:ARG:HH21	2:E:139:LEU:HB2	1.75	0.52
2:C:727:SER:O	2:C:731:THR:HG23	2.09	0.52
1:2:130:VAL:HG12	1:2:196:LEU:HD12	1.90	0.52
2:A:26:HIS:CG	2:A:33:HIS:HE1	2.27	0.52
2:A:374:ALA:HB1	2:A:391:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:HD11	2:B:656:MET:HG3	1.90	0.52
2:D:397:GLU:HB3	2:D:479:VAL:HB	1.91	0.52
2:E:394:LEU:HD21	2:E:483:TRP:CE2	2.44	0.52
1:1:216:PHE:CD1	2:A:443:ARG:HB2	2.44	0.52
2:B:38:LEU:HD22	2:B:46:ALA:CB	2.40	0.52
2:C:24:LEU:CD1	2:C:69:GLY:H	2.22	0.52
2:A:521:ALA:HB1	2:A:525:ARG:HH21	1.74	0.52
2:C:351:LEU:CD1	2:C:391:ALA:HB1	2.38	0.52
2:E:100:HIS:CD2	2:E:107:HIS:HE1	2.27	0.52
2:A:387:LEU:HD22	2:A:387:LEU:H	1.75	0.52
2:E:198:ARG:HD3	2:E:201:LYS:HB3	1.91	0.52
2:A:188:GLU:O	2:A:192:VAL:HG23	2.10	0.52
2:B:619:ILE:HG22	2:B:701:PHE:CZ	2.35	0.52
2:B:478:MET:SD	2:B:479:VAL:HG13	2.49	0.52
2:D:619:ILE:HD12	2:D:656:MET:CG	2.40	0.52
2:A:282:HIS:CG	2:A:319:GLU:HB3	2.45	0.51
2:E:633:VAL:HG13	2:E:649:PHE:CG	2.45	0.51
2:F:26:HIS:CG	2:F:33:HIS:CE1	2.97	0.51
2:D:324:ILE:HD12	2:D:331:GLU:HA	1.93	0.51
2:F:100:HIS:CD2	2:F:107:HIS:HE2	2.29	0.51
2:B:109:LEU:HD23	2:B:138:VAL:HG22	1.93	0.51
2:B:26:HIS:HA	2:B:68:ILE:HD12	1.92	0.51
2:B:355:ARG:HH22	2:B:368:ASP:HA	1.76	0.51
2:C:371:ILE:O	2:C:374:ALA:HB3	2.10	0.51
2:F:100:HIS:CD2	2:F:107:HIS:NE2	2.79	0.51
2:F:513:GLN:H	2:F:718:HIS:CD2	2.28	0.51
2:B:763:ARG:H	2:B:764:PRO:HD2	1.76	0.51
2:D:400:SER:HB3	2:E:198:ARG:HE	1.76	0.51
1:4:180:SER:HB3	2:D:119:VAL:HG13	1.92	0.51
2:A:351:LEU:HD22	2:A:392:ILE:HB	1.91	0.51
2:B:45:ILE:H	2:B:45:ILE:HD12	1.75	0.51
2:A:766:ARG:HE	2:B:536:ARG:HH12	1.59	0.51
2:B:763:ARG:H	2:B:764:PRO:CD	2.23	0.51
2:C:660:VAL:HG13	2:C:692:GLU:HB3	1.92	0.51
2:E:371:ILE:O	2:E:374:ALA:HB3	2.11	0.51
2:E:404:LEU:HD22	2:F:194:GLU:CG	2.41	0.51
2:C:31:THR:HB	2:C:120:ALA:H	1.75	0.51
2:C:755:GLY:HA3	2:C:765:LEU:HD21	1.93	0.51
2:F:31:THR:HB	2:F:120:ALA:H	1.76	0.51
2:B:38:LEU:HD13	2:B:109:LEU:HA	1.93	0.51
2:E:9:ARG:HB3	2:E:105:THR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:O	2:B:17:ALA:HB3	2.11	0.50
2:B:521:ALA:HB1	2:B:525:ARG:HH21	1.76	0.50
2:A:361:HIS:CD2	2:B:233:ILE:HD13	2.46	0.50
2:C:686:LYS:HA	2:C:710:VAL:HG11	1.92	0.50
2:D:21:ALA:HB2	2:D:29:ILE:HG23	1.93	0.50
2:F:38:LEU:HD22	2:F:46:ALA:CB	2.42	0.50
2:A:38:LEU:CD1	2:A:112:LEU:HD11	2.41	0.50
2:A:31:THR:HG22	2:A:120:ALA:HB2	1.93	0.50
2:B:142:LEU:HD23	2:B:143:GLY:H	1.75	0.50
2:D:630:LEU:HD13	2:D:701:PHE:CZ	2.46	0.50
2:D:633:VAL:HG13	2:D:649:PHE:CD2	2.46	0.50
2:E:513:GLN:H	2:E:718:HIS:CD2	2.29	0.50
1:1:184:GLU:HA	2:A:119:VAL:HG21	1.93	0.50
2:C:79:HIS:CG	2:C:80:TYR:H	2.29	0.50
2:E:202:ASN:HB2	2:E:310:GLN:HA	1.91	0.50
2:E:261:LEU:HD11	2:E:284:LEU:HD21	1.93	0.50
2:E:581:HIS:CD2	2:E:585:ARG:HE	2.30	0.50
2:F:619:ILE:HD13	2:F:701:PHE:HE2	1.76	0.50
2:A:268:ILE:HD13	2:A:309:LEU:HA	1.94	0.50
2:F:413:LEU:HD22	2:F:456:THR:OG1	2.11	0.50
1:6:184:GLU:HG3	2:F:81:THR:HG21	1.93	0.50
2:B:24:LEU:CD1	2:B:61:GLN:HE22	2.25	0.50
2:C:472:THR:H	2:C:475:ASP:HB2	1.76	0.50
2:D:773:VAL:HG22	2:D:794:LEU:HD22	1.94	0.50
2:E:685:MET:CE	2:E:712:HIS:CE1	2.94	0.50
2:F:669:LYS:HA	2:F:681:ASN:HB3	1.93	0.50
2:F:741:ILE:HD13	2:F:777:LEU:HD11	1.94	0.50
1:6:154:LEU:HD12	1:6:162:TYR:O	2.10	0.50
2:A:95:ALA:HB2	2:A:103:VAL:HG13	1.94	0.50
1:2:216:PHE:CZ	2:B:431:VAL:HG22	2.47	0.50
2:C:281:LEU:CD1	2:C:313:GLY:HA3	2.32	0.50
2:E:191:ARG:HH12	2:E:198:ARG:HH22	1.59	0.50
1:5:162:TYR:CD1	1:5:196:LEU:HD21	2.47	0.49
2:A:413:LEU:HD23	2:A:416:LEU:HG	1.92	0.49
2:B:723:VAL:HG22	2:B:765:LEU:HD13	1.92	0.49
2:C:225:ILE:HD11	2:C:234:LEU:HD22	1.92	0.49
2:C:26:HIS:HA	2:C:68:ILE:HD12	1.94	0.49
2:D:398:ALA:HB1	2:D:475:ASP:CG	2.32	0.49
2:F:191:ARG:O	2:F:195:VAL:HG23	2.12	0.49
2:F:32:GLU:HG3	2:F:64:VAL:HG13	1.94	0.49
1:3:130:VAL:HG13	1:3:196:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:420:LEU:HA	2:A:449:LEU:HD13	1.93	0.49
2:B:397:GLU:HB3	2:B:479:VAL:HB	1.94	0.49
2:E:23:ARG:HH11	2:E:24:LEU:HG	1.77	0.49
1:2:142:LEU:HD23	1:2:185:TYR:CD2	2.47	0.49
2:B:363:ARG:NH1	2:B:471:VAL:HG23	2.26	0.49
2:B:715:GLU:OE1	2:B:718:HIS:CD2	2.65	0.49
2:C:94:GLU:CG	2:C:114:ARG:HE	2.26	0.49
2:F:544:LEU:HD13	2:F:689:VAL:CG1	2.42	0.49
1:3:127:LEU:HA	1:3:175:VAL:HG11	1.93	0.49
2:B:35:LEU:HD13	2:B:112:LEU:CD1	2.42	0.49
2:A:619:ILE:CD1	2:A:701:PHE:HZ	2.23	0.49
2:A:685:MET:O	2:A:710:VAL:HG11	2.12	0.49
2:E:285:ILE:HG13	2:E:323:TYR:CD1	2.47	0.49
2:A:191:ARG:O	2:A:195:VAL:HG23	2.13	0.49
2:B:545:GLY:H	2:B:659:ASN:HB3	1.78	0.49
2:D:512:GLY:HA3	2:D:718:HIS:CD2	2.48	0.49
2:A:478:MET:SD	2:A:479:VAL:HG13	2.53	0.49
2:A:633:VAL:HG11	2:A:654:LEU:CD2	2.43	0.49
2:D:730:LEU:HG	2:D:733:ARG:HH21	1.78	0.49
2:E:285:ILE:HG13	2:E:323:TYR:CE1	2.48	0.49
2:A:355:ARG:HA	2:A:358:TYR:CE2	2.48	0.49
1:1:216:PHE:CZ	2:A:427:LYS:HG2	2.47	0.49
2:A:528:ARG:HE	2:A:651:ASN:HD21	1.60	0.49
2:C:83:ARG:HA	2:C:83:ARG:HE	1.77	0.49
2:D:427:LYS:HG3	2:D:443:ARG:HA	1.94	0.49
2:F:619:ILE:HG21	2:F:701:PHE:HE2	1.78	0.49
2:A:773:VAL:HG22	2:A:801:PHE:HE1	1.78	0.49
2:B:24:LEU:HD13	2:B:61:GLN:HE22	1.78	0.49
2:C:558:LEU:HD12	2:C:655:ILE:HD11	1.94	0.49
2:D:476:ILE:O	2:D:480:VAL:HG23	2.13	0.49
2:D:734:LEU:HD13	2:D:741:ILE:HG23	1.94	0.49
2:C:23:ARG:HH12	2:C:65:GLU:HG2	1.77	0.48
2:C:20:GLU:HG3	2:C:40:ARG:HH22	1.78	0.48
2:F:276:LEU:O	2:F:311:CYS:HA	2.13	0.48
2:A:533:ASP:HB2	2:A:536:ARG:HH11	1.78	0.48
2:C:730:LEU:HD11	2:C:773:VAL:CG1	2.43	0.48
2:D:794:LEU:HD21	2:D:801:PHE:CE1	2.47	0.48
2:E:193:ILE:HG21	2:E:230:VAL:HG21	1.94	0.48
2:A:198:ARG:HD3	2:F:397:GLU:HA	1.95	0.48
2:B:589:SER:H	2:C:592:GLY:HA2	1.78	0.48
2:D:544:LEU:HD21	2:D:693:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:PHE:HB2	2:D:103:VAL:H	1.78	0.48
2:E:183:ILE:H	2:E:216:ALA:HB1	1.77	0.48
2:C:690:MET:SD	2:C:710:VAL:HG22	2.52	0.48
1:4:203:ILE:HA	2:D:432:GLN:HA	1.95	0.48
2:E:370:ALA:CB	2:E:471:VAL:HG13	2.42	0.48
2:F:46:ALA:HB2	2:F:105:THR:O	2.13	0.48
1:5:154:LEU:HB2	1:5:208:ALA:HB1	1.95	0.48
2:C:403:ARG:HH21	2:D:232:GLU:HB3	1.79	0.48
2:F:21:ALA:HB2	2:F:29:ILE:HG12	1.95	0.48
2:F:437:GLU:HA	2:F:440:ALA:HB3	1.96	0.48
2:A:750:LYS:HB2	2:A:796:VAL:HG21	1.94	0.48
2:B:21:ALA:HB2	2:B:29:ILE:HD11	1.96	0.48
2:B:619:ILE:HG23	2:B:627:PHE:CD1	2.48	0.48
2:D:585:ARG:HH11	2:E:623:HIS:CE1	2.32	0.48
1:5:147:VAL:HG13	1:5:148:ASN:H	1.79	0.48
2:F:106:GLU:HG2	2:F:107:HIS:H	1.78	0.48
1:5:215:HIS:HB2	2:E:440:ALA:HB2	1.95	0.48
2:B:202:ASN:HB2	2:B:311:CYS:H	1.79	0.48
2:C:511:ILE:HG21	2:C:722:ILE:HG12	1.95	0.48
2:E:26:HIS:HB2	2:E:33:HIS:CE1	2.48	0.48
2:E:278:ILE:HG21	2:E:281:LEU:HD23	1.86	0.48
2:F:112:LEU:HD13	2:F:120:ALA:HB1	1.96	0.48
2:F:478:MET:SD	2:F:479:VAL:HG13	2.53	0.48
2:A:548:GLY:O	2:A:722:ILE:HD13	2.14	0.48
2:B:233:ILE:HD12	2:B:234:LEU:HG	1.96	0.48
2:B:685:MET:HB2	2:B:712:HIS:CD2	2.48	0.48
2:F:685:MET:HB2	2:F:712:HIS:CD2	2.49	0.48
2:F:9:ARG:HB2	2:F:104:GLY:HA2	1.96	0.48
2:A:378:SER:OG	2:A:394:LEU:HD12	2.14	0.48
2:B:32:GLU:OE2	2:B:33:HIS:CG	2.67	0.48
2:D:205:VAL:HB	2:D:335:GLN:H	1.79	0.48
2:E:619:ILE:HD11	2:E:630:LEU:HD11	1.89	0.48
2:E:665:LEU:HD23	2:E:685:MET:HB3	1.95	0.48
2:F:619:ILE:HD13	2:F:701:PHE:CE2	2.49	0.48
1:6:152:THR:CG2	1:6:209:LEU:H	2.27	0.47
2:B:374:ALA:HB1	2:B:391:ALA:O	2.14	0.47
2:B:46:ALA:HB2	2:B:105:THR:O	2.14	0.47
2:E:403:ARG:HH22	2:F:232:GLU:HB3	1.78	0.47
2:E:682:HIS:HA	2:E:685:MET:CE	2.44	0.47
1:1:164:TYR:HB2	1:1:196:LEU:HD21	1.96	0.47
2:A:183:ILE:H	2:A:216:ALA:HB1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:LEU:O	2:A:47:ALA:HB2	2.14	0.47
2:B:46:ALA:HB1	2:B:109:LEU:HB2	1.95	0.47
2:E:35:LEU:HD13	2:E:112:LEU:CD1	2.45	0.47
2:F:665:LEU:HD11	2:F:689:VAL:CG2	2.44	0.47
1:2:180:SER:O	2:B:119:VAL:HG13	2.15	0.47
2:A:26:HIS:CD2	2:A:33:HIS:CE1	3.02	0.47
1:1:203:ILE:HA	2:A:432:GLN:HA	1.97	0.47
2:E:14:LEU:O	2:E:17:ALA:HB3	2.14	0.47
2:F:106:GLU:HA	2:F:138:VAL:HG11	1.96	0.47
2:E:361:HIS:CD2	2:F:233:ILE:HD13	2.49	0.47
2:D:607:ARG:HG3	2:D:645:ARG:HE	1.80	0.47
2:E:423:VAL:HG21	2:E:449:LEU:CD1	2.44	0.47
2:F:387:LEU:H	2:F:387:LEU:HD22	1.80	0.47
1:2:129:PHE:CZ	1:2:179:LEU:HD22	2.49	0.47
2:A:46:ALA:HB1	2:A:109:LEU:HB2	1.97	0.47
2:A:79:HIS:CG	2:A:80:TYR:N	2.83	0.47
2:C:202:ASN:HB3	2:C:311:CYS:H	1.80	0.47
2:C:743:LEU:HD22	2:C:773:VAL:HG21	1.97	0.47
2:E:31:THR:HB	2:E:120:ALA:H	1.80	0.47
2:B:378:SER:HB2	2:B:394:LEU:HD12	1.97	0.47
2:C:14:LEU:HD22	2:C:88:ILE:HG12	1.97	0.47
2:C:619:ILE:CD1	2:C:656:MET:CB	2.93	0.47
2:D:613:VAL:CG1	2:D:655:ILE:HD12	2.45	0.47
2:D:623:HIS:HB3	2:D:626:VAL:H	1.79	0.47
2:E:320:TYR:CZ	2:E:324:ILE:HD12	2.49	0.47
2:A:231:PRO:HA	2:F:407:PHE:CE2	2.49	0.47
2:A:398:ALA:HB3	2:A:476:ILE:HD13	1.95	0.47
2:B:275:ILE:HG23	2:B:310:GLN:HE21	1.78	0.47
2:B:587:VAL:HG13	2:C:592:GLY:HA3	1.96	0.47
2:D:574:MET:HA	2:D:577:TYR:CD2	2.50	0.47
1:1:215:HIS:O	1:1:216:PHE:CD1	2.68	0.47
2:A:622:ALA:HA	2:A:626:VAL:HG21	1.97	0.47
2:A:358:TYR:CE1	2:B:200:THR:HG23	2.51	0.47
2:B:523:ALA:HB1	2:B:706:ASP:HB3	1.97	0.47
1:4:154:LEU:HB2	1:4:208:ALA:HB1	1.97	0.46
2:A:14:LEU:HD21	2:A:108:ILE:HD12	1.95	0.46
2:A:570:ILE:HG22	2:A:571:ARG:H	1.79	0.46
2:D:20:GLU:HB2	2:D:33:HIS:CG	2.50	0.46
2:D:689:VAL:HG12	2:D:710:VAL:HG12	1.97	0.46
2:F:205:VAL:H	2:F:337:ILE:HD13	1.80	0.46
2:A:276:LEU:O	2:A:311:CYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:513:GLN:HG3	2:A:712:HIS:H	1.81	0.46
2:D:276:LEU:O	2:D:311:CYS:HA	2.15	0.46
2:D:35:LEU:HD13	2:D:112:LEU:CD1	2.45	0.46
2:D:723:VAL:HG21	2:D:752:ALA:HA	1.97	0.46
2:E:370:ALA:HB1	2:E:471:VAL:HG13	1.97	0.46
1:4:130:VAL:CG1	1:4:196:LEU:HD11	2.45	0.46
1:5:139:VAL:HG12	1:5:212:ILE:HG21	1.98	0.46
2:A:26:HIS:CG	2:A:68:ILE:HD12	2.50	0.46
2:B:53:LEU:HD11	2:B:134:ALA:HA	1.98	0.46
2:D:374:ALA:HB1	2:D:391:ALA:O	2.15	0.46
2:E:46:ALA:HB2	2:E:105:THR:O	2.14	0.46
2:F:238:ARG:HH22	2:F:270:GLN:HG3	1.78	0.46
2:F:338:GLN:H	2:F:338:GLN:CD	2.18	0.46
2:F:26:HIS:HB2	2:F:33:HIS:HE1	1.80	0.46
2:B:513:GLN:HA	2:B:712:HIS:HB2	1.97	0.46
2:C:32:GLU:OE2	2:C:33:HIS:CG	2.68	0.46
2:F:682:HIS:CD2	2:F:712:HIS:HE1	2.33	0.46
2:F:665:LEU:HD23	2:F:685:MET:HB3	1.96	0.46
2:D:682:HIS:CE1	2:D:712:HIS:CE1	3.04	0.46
2:E:574:MET:HG3	2:E:619:ILE:CG1	2.45	0.46
2:A:112:LEU:HD13	2:A:120:ALA:HB1	1.98	0.46
2:A:665:LEU:HD22	2:A:711:PHE:O	2.16	0.46
2:B:92:MET:HA	2:B:103:VAL:HG13	1.98	0.46
2:C:26:HIS:CD2	2:C:68:ILE:HD12	2.51	0.46
2:E:355:ARG:HH21	2:E:395:ILE:HG21	1.80	0.46
2:E:669:LYS:O	2:E:678:GLU:HA	2.15	0.46
2:F:285:ILE:HD12	2:F:323:TYR:CE2	2.51	0.46
1:1:147:VAL:HG21	1:1:210:GLU:HG3	1.97	0.46
2:B:31:THR:HB	2:B:120:ALA:H	1.80	0.46
2:B:542:ILE:HG13	2:B:693:LEU:HD21	1.96	0.46
2:C:445:THR:HG23	2:C:448:ARG:HH21	1.80	0.46
2:C:776:ARG:HH11	2:C:794:LEU:HD11	1.81	0.46
2:F:28:ASN:HB2	2:F:81:THR:HG22	1.97	0.46
1:5:165:VAL:HG11	1:5:182:LEU:HD13	1.97	0.46
2:A:106:GLU:HG2	2:A:107:HIS:H	1.80	0.46
2:A:682:HIS:CE1	2:A:712:HIS:CE1	3.04	0.46
2:B:199:ARG:HA	2:B:202:ASN:HB3	1.98	0.46
2:C:743:LEU:HD13	2:C:773:VAL:CG2	2.46	0.46
2:D:367:THR:H	2:D:370:ALA:HB3	1.81	0.46
2:E:665:LEU:HD11	2:E:689:VAL:HG21	1.97	0.46
2:F:36:LEU:HD22	2:F:40:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:31:THR:HB	2:A:120:ALA:H	1.81	0.46
2:A:95:ALA:CB	2:A:103:VAL:HG22	2.46	0.46
2:B:427:LYS:HD2	2:B:446:GLU:HB2	1.98	0.46
2:F:364:VAL:CG1	2:F:399:GLY:HA3	2.46	0.46
2:F:665:LEU:HD13	2:F:711:PHE:H	1.82	0.46
1:6:184:GLU:CG	2:F:81:THR:HG21	2.46	0.45
2:A:396:ASP:CG	2:B:199:ARG:H	2.20	0.45
2:B:276:LEU:O	2:B:311:CYS:HA	2.16	0.45
2:B:515:GLU:HG2	2:B:712:HIS:CD2	2.52	0.45
2:D:118:GLY:H	2:D:121:ALA:HB3	1.81	0.45
1:4:141:SER:HA	2:D:76:GLN:HE22	1.81	0.45
2:F:665:LEU:HD23	2:F:685:MET:HB2	1.97	0.45
1:6:216:PHE:CD1	2:F:443:ARG:HB2	2.51	0.45
2:A:730:LEU:HD12	2:A:769:ILE:CG2	2.46	0.45
2:B:374:ALA:N	2:B:476:ILE:HG21	2.31	0.45
2:B:531:LEU:N	2:B:531:LEU:HD22	2.30	0.45
2:C:633:VAL:HG13	2:C:649:PHE:CD1	2.51	0.45
2:D:278:ILE:HG22	2:D:281:LEU:CD2	2.14	0.45
2:F:544:LEU:HD11	2:F:693:LEU:HD22	1.99	0.45
2:A:403:ARG:HH22	2:B:232:GLU:HB3	1.80	0.45
2:A:520:VAL:HG11	2:A:558:LEU:HD11	1.99	0.45
2:B:364:VAL:HG22	2:B:471:VAL:HG11	1.97	0.45
2:C:26:HIS:HB2	2:C:33:HIS:CE1	2.51	0.45
2:C:730:LEU:HD12	2:C:774:GLU:CG	2.46	0.45
2:C:361:HIS:HA	2:D:233:ILE:HG23	1.98	0.45
2:D:394:LEU:HD22	2:D:480:VAL:HG22	1.98	0.45
1:1:204:ILE:HG21	1:1:211:THR:HB	1.98	0.45
2:A:733:ARG:HH11	2:A:766:ARG:CZ	2.28	0.45
2:C:17:ALA:HA	2:C:33:HIS:HB3	1.97	0.45
2:D:722:ILE:HD13	2:D:762:ALA:HB3	1.98	0.45
2:E:476:ILE:HA	2:E:479:VAL:HG22	1.99	0.45
2:E:512:GLY:HA2	2:E:718:HIS:CG	2.51	0.45
2:F:545:GLY:HA2	2:F:665:LEU:HD12	1.99	0.45
2:A:135:ARG:HH21	2:A:139:LEU:HD21	1.82	0.45
2:B:743:LEU:HD21	2:B:773:VAL:HG21	1.99	0.45
2:A:427:LYS:HD2	2:A:446:GLU:HB2	1.98	0.45
2:C:304:LEU:HG	2:C:309:LEU:HD23	1.98	0.45
2:E:254:ARG:HE	2:E:254:ARG:HA	1.81	0.45
2:F:202:ASN:HD22	2:F:333:ARG:HA	1.81	0.45
2:A:197:SER:HA	2:A:233:ILE:HG21	1.99	0.45
2:A:371:ILE:HA	2:A:395:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:LYS:H	2:B:717:LYS:HG2	1.81	0.45
2:D:613:VAL:HG13	2:D:655:ILE:HD12	1.98	0.45
2:A:278:ILE:CA	2:A:281:LEU:CD2	2.74	0.45
2:A:21:ALA:HB2	2:A:29:ILE:HG23	1.97	0.45
2:C:182:VAL:HG12	2:C:183:ILE:H	1.82	0.45
2:D:413:LEU:HD22	2:D:456:THR:OG1	2.16	0.45
2:D:562:ILE:HG23	2:D:563:PHE:CD1	2.52	0.45
2:E:361:HIS:HE1	2:F:199:ARG:HH11	1.65	0.45
2:B:587:VAL:HG11	2:B:593:TYR:CE2	2.52	0.45
2:D:431:VAL:HG22	2:D:439:ALA:HB1	1.99	0.45
2:E:527:ALA:HB1	2:E:538:ILE:HB	1.99	0.45
2:E:682:HIS:HA	2:E:685:MET:HE2	1.98	0.45
2:F:100:HIS:CG	2:F:107:HIS:HE1	2.35	0.45
2:B:192:VAL:CG1	2:B:221:LEU:HD21	2.47	0.45
2:B:98:LEU:HD13	2:B:142:LEU:HD13	1.99	0.45
2:C:203:ASN:ND2	2:C:281:LEU:HD13	2.32	0.45
2:C:395:ILE:HA	2:C:476:ILE:HD11	1.98	0.45
2:C:715:GLU:OE2	2:C:718:HIS:CE1	2.69	0.45
2:E:278:ILE:C	2:E:281:LEU:HD21	2.38	0.45
2:E:516:ALA:HB2	2:E:711:PHE:CG	2.52	0.45
2:E:393:ASP:OD1	2:F:332:ARG:HA	2.17	0.45
2:F:410:PRO:HB2	2:F:457:LYS:HA	1.98	0.45
2:B:320:TYR:CE1	2:B:324:ILE:HG21	2.53	0.44
2:B:545:GLY:HA2	2:B:665:LEU:HD22	1.98	0.44
2:D:188:GLU:O	2:D:192:VAL:HG23	2.17	0.44
2:E:540:SER:HB2	2:E:705:ILE:HA	1.97	0.44
2:E:727:SER:O	2:E:731:THR:HG23	2.17	0.44
2:F:351:LEU:HD12	2:F:371:ILE:HG23	1.99	0.44
2:F:38:LEU:CD1	2:F:112:LEU:HD11	2.47	0.44
1:6:203:ILE:HA	2:F:432:GLN:HA	1.99	0.44
2:B:21:ALA:HA	2:B:33:HIS:CE1	2.53	0.44
2:C:14:LEU:O	2:C:17:ALA:HB3	2.18	0.44
2:D:230:VAL:HG22	2:D:231:PRO:HD2	1.99	0.44
2:D:385:ARG:CZ	2:E:324:ILE:HD11	2.47	0.44
2:E:781:LEU:HD13	2:F:531:LEU:HD21	1.99	0.44
2:A:14:LEU:HD22	2:A:88:ILE:HG12	1.98	0.44
2:B:20:GLU:HB2	2:B:33:HIS:CD2	2.52	0.44
2:B:377:LEU:HB2	2:B:480:VAL:HG21	2.00	0.44
2:B:545:GLY:H	2:B:659:ASN:CB	2.30	0.44
2:C:165:SER:HB2	2:C:166:LEU:HB3	1.99	0.44
2:C:268:ILE:HG12	2:C:309:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:ALA:CA	2:E:476:ILE:HG21	2.48	0.44
2:E:377:LEU:HD11	2:E:492:ALA:HB1	1.98	0.44
2:E:542:ILE:HG21	2:E:693:LEU:HD13	1.99	0.44
1:5:126:LYS:H	1:5:126:LYS:HD3	1.83	0.44
2:B:499:LEU:HB3	2:B:525:ARG:HB2	1.99	0.44
2:B:633:VAL:HG13	2:B:649:PHE:CG	2.52	0.44
2:C:91:SER:HB2	2:C:108:ILE:HA	1.99	0.44
2:C:31:THR:HG22	2:C:120:ALA:HB2	1.99	0.44
2:C:24:LEU:HG	2:C:33:HIS:HE2	1.82	0.44
2:E:320:TYR:CE1	2:E:324:ILE:HD12	2.52	0.44
2:F:682:HIS:CD2	2:F:712:HIS:CE1	3.06	0.44
1:5:181:ILE:HG12	2:E:67:LEU:HA	1.99	0.44
1:6:131:LEU:HD22	1:6:183:LEU:HD21	1.99	0.44
2:A:394:LEU:HD21	2:A:483:TRP:CE3	2.52	0.44
2:A:685:MET:SD	2:A:712:HIS:CG	3.11	0.44
2:B:100:HIS:CG	2:B:107:HIS:CE1	3.05	0.44
2:B:198:ARG:HD3	2:B:201:LYS:HB3	2.00	0.44
2:B:606:VAL:HG11	2:B:649:PHE:CD1	2.52	0.44
2:D:404:LEU:HB3	2:D:405:ARG:HH21	1.82	0.44
2:D:471:VAL:O	2:D:476:ILE:HD11	2.18	0.44
2:E:619:ILE:HG21	2:E:630:LEU:HD12	1.99	0.44
2:B:285:ILE:HG13	2:B:323:TYR:CD2	2.53	0.44
2:D:38:LEU:HD22	2:D:46:ALA:HB1	2.00	0.44
2:E:413:LEU:HD22	2:E:456:THR:OG1	2.18	0.44
1:5:211:THR:HG21	2:E:436:PHE:CD1	2.53	0.44
2:F:364:VAL:HG13	2:F:399:GLY:HA3	2.00	0.44
2:C:197:SER:HB3	2:C:233:ILE:HB	1.99	0.44
2:C:285:ILE:HG13	2:C:323:TYR:CD2	2.53	0.44
2:C:723:VAL:HG22	2:C:765:LEU:HD22	1.99	0.44
2:E:31:THR:HG22	2:E:120:ALA:HB2	1.99	0.44
2:F:616:LEU:HD13	2:F:630:LEU:HD22	1.99	0.44
2:F:619:ILE:HG21	2:F:701:PHE:CE2	2.52	0.44
1:1:145:LEU:HD21	2:A:27:ASN:HD22	1.83	0.44
2:B:363:ARG:HD2	2:B:403:ARG:H	1.83	0.44
2:C:191:ARG:NH1	2:C:198:ARG:HH22	2.16	0.44
2:C:619:ILE:HD11	2:C:656:MET:CB	2.45	0.44
2:C:776:ARG:HH11	2:C:794:LEU:CD1	2.31	0.44
2:D:630:LEU:HD13	2:D:701:PHE:CE1	2.53	0.44
2:D:773:VAL:HG22	2:D:794:LEU:CD2	2.47	0.44
2:F:458:LYS:HE2	2:F:458:LYS:HA	2.00	0.44
2:A:743:LEU:HD11	2:A:773:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:438:LYS:O	2:F:442:LEU:HD12	2.17	0.44
1:2:162:TYR:CD1	1:2:196:LEU:HD11	2.54	0.43
1:6:162:TYR:CE1	1:6:191:ILE:HD12	2.53	0.43
2:A:10:ALA:HB1	2:A:108:ILE:HD11	1.99	0.43
2:A:361:HIS:CE1	2:B:199:ARG:HD2	2.52	0.43
2:B:689:VAL:HG23	2:B:710:VAL:HG12	2.01	0.43
2:C:96:ARG:HB2	2:D:158:ALA:HB2	1.99	0.43
1:6:177:ASN:HA	2:F:126:ASN:HD21	1.83	0.43
2:A:410:PRO:HA	2:A:460:TRP:CG	2.53	0.43
2:A:544:LEU:HB3	2:A:689:VAL:CG1	2.47	0.43
2:B:374:ALA:CB	2:B:395:ILE:HG23	2.48	0.43
2:C:682:HIS:CE1	2:C:712:HIS:CE1	3.06	0.43
2:D:619:ILE:HG21	2:D:630:LEU:CD1	2.48	0.43
2:F:28:ASN:CB	2:F:81:THR:HG22	2.49	0.43
2:F:741:ILE:HD13	2:F:777:LEU:CD1	2.47	0.43
2:A:38:LEU:HD11	2:A:112:LEU:HD11	2.00	0.43
2:A:195:VAL:HA	2:A:198:ARG:NE	2.33	0.43
2:A:26:HIS:HB2	2:A:33:HIS:CE1	2.53	0.43
2:A:20:GLU:HB2	2:A:33:HIS:CG	2.53	0.43
2:C:87:VAL:HG21	2:C:112:LEU:HD22	2.01	0.43
2:D:741:ILE:HD12	2:D:742:GLU:N	2.33	0.43
2:F:689:VAL:HB	2:F:710:VAL:HG22	2.00	0.43
2:A:776:ARG:HH21	2:A:794:LEU:CD1	2.31	0.43
2:C:205:VAL:HG23	2:C:313:GLY:HA3	2.00	0.43
2:C:513:GLN:H	2:C:718:HIS:CD2	2.36	0.43
2:D:46:ALA:HB2	2:D:105:THR:O	2.18	0.43
2:D:106:GLU:HG2	2:D:107:HIS:CD2	2.53	0.43
2:F:371:ILE:O	2:F:374:ALA:HB3	2.18	0.43
2:B:381:TYR:HA	2:B:611:TYR:CZ	2.53	0.43
2:B:619:ILE:HG21	2:B:701:PHE:HZ	1.40	0.43
2:B:794:LEU:HD11	2:B:801:PHE:CD1	2.53	0.43
2:C:276:LEU:O	2:C:311:CYS:HA	2.18	0.43
2:C:265:MET:SD	2:C:309:LEU:HD22	2.58	0.43
2:D:38:LEU:HD13	2:D:109:LEU:HA	1.99	0.43
2:F:794:LEU:HD21	2:F:801:PHE:CD1	2.54	0.43
1:1:167:PHE:CD2	1:1:175:VAL:HG13	2.53	0.43
2:B:665:LEU:HD21	2:B:689:VAL:HG11	2.00	0.43
2:B:665:LEU:HD21	2:B:689:VAL:CG1	2.49	0.43
2:C:282:HIS:CG	2:C:319:GLU:HB3	2.53	0.43
2:D:100:HIS:CG	2:D:107:HIS:CE1	3.04	0.43
1:5:179:LEU:HD23	2:E:122:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:448:ARG:HH21	2:E:449:LEU:HD23	1.83	0.43
2:E:578:MET:HG2	2:E:581:HIS:CD2	2.53	0.43
2:F:14:LEU:HD22	2:F:88:ILE:HG12	2.01	0.43
2:A:201:LYS:HE3	2:F:397:GLU:CG	2.49	0.43
2:A:520:VAL:CG1	2:A:558:LEU:HD21	2.48	0.43
2:B:26:HIS:HB2	2:B:33:HIS:HE1	1.82	0.43
2:B:692:GLU:HA	2:B:695:ARG:HE	1.84	0.43
2:D:225:ILE:HG12	2:D:234:LEU:HD22	2.01	0.43
2:D:39:VAL:HG13	2:D:57:SER:HA	1.99	0.43
2:E:106:GLU:HG2	2:E:107:HIS:CD2	2.54	0.43
2:E:668:ASN:HA	2:E:712:HIS:CE1	2.54	0.43
2:C:278:ILE:HG21	2:C:281:LEU:CD2	2.29	0.43
2:E:58:GLU:CD	2:E:58:GLU:H	2.22	0.43
2:A:730:LEU:HD11	2:A:773:VAL:HG11	1.99	0.43
2:B:351:LEU:N	2:B:351:LEU:HD23	2.34	0.43
2:B:437:GLU:HA	2:B:440:ALA:HB3	1.99	0.43
1:3:184:GLU:HA	2:C:119:VAL:HG21	2.00	0.43
2:C:26:HIS:CG	2:C:68:ILE:HD12	2.54	0.43
2:E:165:SER:HB2	2:E:166:LEU:HB3	2.00	0.43
2:E:682:HIS:CE1	2:E:712:HIS:CD2	3.06	0.43
2:F:26:HIS:HB2	2:F:33:HIS:CE1	2.53	0.43
2:F:404:LEU:HA	2:F:404:LEU:HD13	1.84	0.43
2:A:633:VAL:HG11	2:A:654:LEU:HD22	2.01	0.43
2:B:574:MET:HB3	2:B:626:VAL:HG13	2.01	0.43
2:C:633:VAL:HG13	2:C:649:PHE:CG	2.53	0.43
2:E:199:ARG:HA	2:E:202:ASN:HB3	2.00	0.43
2:F:25:GLY:HA2	2:F:72:GLN:O	2.19	0.43
2:F:445:THR:HB	2:F:448:ARG:HH21	1.84	0.43
2:A:377:LEU:HD23	2:A:380:ARG:HH21	1.84	0.42
2:B:21:ALA:CB	2:B:29:ILE:HD11	2.48	0.42
2:B:281:LEU:HG	2:B:313:GLY:HA2	2.00	0.42
2:A:366:ILE:HB	2:A:367:THR:HA	2.00	0.42
2:A:49:ALA:O	2:A:53:LEU:HD22	2.20	0.42
2:B:195:VAL:HA	2:B:198:ARG:NE	2.34	0.42
2:B:510:VAL:HG21	2:B:554:LEU:HD13	2.01	0.42
2:C:741:ILE:HD12	2:C:742:GLU:H	1.84	0.42
2:F:91:SER:HB3	2:F:108:ILE:HA	2.00	0.42
2:F:685:MET:SD	2:F:712:HIS:CG	3.12	0.42
2:F:91:SER:CB	2:F:108:ILE:HA	2.49	0.42
2:A:355:ARG:HH12	2:A:370:ALA:HB3	1.84	0.42
2:B:100:HIS:CD2	2:B:107:HIS:HE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ALA:HB1	2:B:29:ILE:CG2	2.48	0.42
2:B:38:LEU:HD22	2:B:46:ALA:HB1	2.01	0.42
2:B:705:ILE:HG21	2:B:708:ILE:HD13	2.02	0.42
2:C:26:HIS:CD2	2:C:33:HIS:CE1	3.07	0.42
2:C:374:ALA:HB1	2:C:391:ALA:HA	2.01	0.42
2:E:363:ARG:HH11	2:E:399:GLY:HA2	1.84	0.42
2:E:397:GLU:HB3	2:E:479:VAL:HB	2.01	0.42
2:A:100:HIS:CD2	2:A:107:HIS:NE2	2.88	0.42
2:A:665:LEU:HD23	2:A:685:MET:HB2	1.99	0.42
2:B:562:ILE:HB	2:B:563:PHE:CD2	2.54	0.42
2:B:747:ALA:HB2	2:B:795:ASP:HA	2.01	0.42
2:C:667:ARG:HG2	2:C:668:ASN:HD22	1.84	0.42
2:E:106:GLU:HA	2:E:138:VAL:HG11	2.01	0.42
2:E:32:GLU:HB3	2:E:119:VAL:HG12	2.01	0.42
2:E:404:LEU:HA	2:F:231:PRO:HD3	2.01	0.42
2:A:237:LYS:HE2	2:F:361:HIS:CE1	2.54	0.42
2:F:362:HIS:CD2	2:F:362:HIS:H	2.37	0.42
2:F:484:THR:HG23	2:F:562:ILE:O	2.20	0.42
2:A:100:HIS:CD2	2:A:107:HIS:CE1	3.07	0.42
1:2:216:PHE:CZ	2:B:431:VAL:HG21	2.55	0.42
2:B:682:HIS:CG	2:B:712:HIS:HE1	2.37	0.42
2:C:474:ASP:HB3	2:C:493:GLN:HG3	2.01	0.42
2:C:511:ILE:O	2:C:511:ILE:HG22	2.20	0.42
2:C:794:LEU:HD21	2:C:801:PHE:CD1	2.55	0.42
2:D:9:ARG:HB3	2:D:105:THR:HG23	2.01	0.42
2:E:195:VAL:HA	2:E:198:ARG:HD2	2.02	0.42
2:F:32:GLU:HB3	2:F:119:VAL:HG12	2.00	0.42
1:3:136:PHE:CE2	2:C:431:VAL:HG21	2.54	0.42
2:A:100:HIS:CD2	2:A:107:HIS:HE2	2.38	0.42
2:A:203:ASN:HA	2:A:204:PRO:HD2	1.90	0.42
2:A:36:LEU:HG	2:A:60:ILE:HG22	2.01	0.42
2:A:515:GLU:OE2	2:A:712:HIS:CD2	2.73	0.42
2:A:787:HIS:CE1	2:B:373:ALA:HA	2.54	0.42
2:B:278:ILE:C	2:B:281:LEU:CD2	2.84	0.42
2:B:515:GLU:HG3	2:B:515:GLU:H	1.50	0.42
2:D:715:GLU:HB2	2:D:718:HIS:CD2	2.55	0.42
2:F:38:LEU:HD12	2:F:112:LEU:HD11	2.02	0.42
2:E:741:ILE:HG21	2:F:531:LEU:HD13	2.00	0.42
2:F:682:HIS:CG	2:F:712:HIS:HE1	2.38	0.42
2:C:35:LEU:HG	2:C:60:ILE:HD13	2.01	0.42
2:C:733:ARG:HD3	2:D:534:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:PHE:HA	2:D:102:TYR:HA	2.02	0.42
2:D:670:TYR:CE2	2:D:758:LEU:HA	2.55	0.42
2:E:503:GLU:H	2:E:525:ARG:HH21	1.68	0.42
2:E:79:HIS:CG	2:E:80:TYR:H	2.37	0.42
2:A:619:ILE:O	2:A:619:ILE:HG22	2.20	0.42
2:B:364:VAL:HG13	2:B:366:ILE:O	2.19	0.42
2:D:192:VAL:CG1	2:D:221:LEU:HD21	2.50	0.42
2:F:515:GLU:CD	2:F:515:GLU:H	2.23	0.42
2:F:633:VAL:HG13	2:F:649:PHE:CG	2.54	0.42
1:6:152:THR:HG23	1:6:209:LEU:H	1.85	0.42
2:B:715:GLU:HG2	2:B:718:HIS:CE1	2.55	0.42
1:2:184:GLU:HA	2:B:119:VAL:HG21	2.02	0.42
2:B:194:GLU:HG3	2:B:195:VAL:H	1.85	0.42
2:C:197:SER:O	2:C:233:ILE:HG21	2.20	0.42
2:C:205:VAL:HB	2:C:335:GLN:H	1.84	0.42
2:C:320:TYR:CE1	2:C:324:ILE:HG21	2.55	0.42
2:C:624:PRO:HA	2:C:627:PHE:CD2	2.55	0.42
2:E:72:GLN:HG2	2:E:75:SER:H	1.85	0.42
2:F:395:ILE:HA	2:F:476:ILE:HD12	2.02	0.42
2:F:39:VAL:HG13	2:F:57:SER:HA	2.02	0.42
2:A:506:LEU:HD21	2:A:558:LEU:HD23	2.01	0.41
2:A:750:LYS:CB	2:A:796:VAL:HG21	2.50	0.41
2:A:14:LEU:CD2	2:A:88:ILE:HG12	2.50	0.41
2:C:196:LEU:HD21	2:C:312:ILE:HG12	2.02	0.41
2:C:513:GLN:HG3	2:C:712:HIS:H	1.84	0.41
2:D:191:ARG:HH21	2:D:338:GLN:HE22	1.67	0.41
2:D:360:ALA:O	2:D:361:HIS:CD2	2.73	0.41
2:D:364:VAL:HG11	2:D:396:ASP:HA	2.02	0.41
2:F:398:ALA:HB1	2:F:475:ASP:CG	2.41	0.41
2:A:507:HIS:CD2	2:A:517:VAL:HG11	2.55	0.41
2:B:614:VAL:HB	2:B:654:LEU:HD12	2.02	0.41
2:B:730:LEU:HD13	2:B:769:ILE:HG22	2.02	0.41
1:3:180:SER:HB2	2:C:67:LEU:HD22	2.02	0.41
2:D:361:HIS:CD2	2:E:197:SER:C	2.93	0.41
2:E:665:LEU:HD22	2:E:712:HIS:HA	2.02	0.41
2:E:400:SER:HB2	2:F:197:SER:HB3	2.02	0.41
2:F:278:ILE:CA	2:F:281:LEU:HD21	2.46	0.41
2:A:619:ILE:CD1	2:A:701:PHE:CZ	2.90	0.41
2:A:513:GLN:H	2:A:718:HIS:CE1	2.37	0.41
2:B:715:GLU:HB3	2:B:717:LYS:HG2	2.02	0.41
2:C:338:GLN:CD	2:C:338:GLN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:397:GLU:HB3	2:F:479:VAL:HG21	2.02	0.41
2:F:734:LEU:CD2	2:F:741:ILE:HG13	2.50	0.41
2:B:103:VAL:HB	2:B:104:GLY:H	1.73	0.41
2:B:473:VAL:HG23	2:B:474:ASP:H	1.86	0.41
2:C:18:GLN:HE22	2:C:79:HIS:HA	1.86	0.41
2:E:526:ARG:HD2	2:E:532:LYS:HZ2	1.84	0.41
2:E:574:MET:HB2	2:E:619:ILE:CG1	2.50	0.41
2:E:668:ASN:HA	2:E:712:HIS:HE1	1.85	0.41
2:F:423:VAL:HG21	2:F:449:LEU:CD1	2.51	0.41
2:F:665:LEU:HD22	2:F:712:HIS:N	2.36	0.41
2:A:201:LYS:HZ2	2:A:335:GLN:HG2	1.86	0.41
2:A:445:THR:HB	2:A:448:ARG:HH21	1.85	0.41
2:B:733:ARG:HA	2:C:535:LYS:HZ2	1.86	0.41
2:F:665:LEU:HD11	2:F:689:VAL:HG21	2.03	0.41
2:A:773:VAL:HG13	2:A:794:LEU:HD21	2.03	0.41
2:B:36:LEU:HD11	2:B:64:VAL:HG11	2.02	0.41
1:2:216:PHE:HA	2:B:440:ALA:HA	2.02	0.41
2:B:607:ARG:HG2	2:B:645:ARG:HE	1.86	0.41
2:B:741:ILE:HA	2:B:792:ILE:O	2.19	0.41
2:C:38:LEU:HD22	2:C:46:ALA:CB	2.50	0.41
2:E:38:LEU:HD21	2:E:108:ILE:HB	2.03	0.41
2:E:398:ALA:HB3	2:E:476:ILE:CD1	2.50	0.41
2:F:203:ASN:HB2	2:F:334:PHE:HA	2.02	0.41
2:F:31:THR:HG22	2:F:120:ALA:HB2	2.02	0.41
2:F:351:LEU:HD21	2:F:391:ALA:CB	2.50	0.41
2:A:282:HIS:H	2:A:315:THR:HG22	1.85	0.41
2:B:278:ILE:C	2:B:281:LEU:HD21	2.39	0.41
2:D:665:LEU:HD13	2:D:711:PHE:O	2.21	0.41
2:E:230:VAL:HG22	2:E:231:PRO:HD2	2.03	0.41
2:E:778:SER:HB3	2:F:526:ARG:HA	2.03	0.41
2:F:234:LEU:HA	2:F:237:LYS:HG2	2.02	0.41
2:F:730:LEU:HD23	2:F:731:THR:N	2.35	0.41
1:5:164:TYR:HB2	1:5:196:LEU:HD12	2.03	0.41
2:A:46:ALA:HB2	2:A:105:THR:O	2.20	0.41
2:A:282:HIS:CD2	2:A:319:GLU:HB3	2.56	0.41
2:A:515:GLU:CD	2:A:712:HIS:CD2	2.93	0.41
2:B:511:ILE:HD11	2:B:725:LEU:HD22	2.02	0.41
2:C:203:ASN:HA	2:C:311:CYS:O	2.21	0.41
2:D:416:LEU:HB3	2:D:453:VAL:HG22	2.03	0.41
2:D:670:TYR:CD1	2:D:678:GLU:HB3	2.55	0.41
2:F:36:LEU:HD21	2:F:61:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:512:GLY:HA3	2:F:718:HIS:CG	2.56	0.41
2:F:515:GLU:CD	2:F:712:HIS:CD2	2.94	0.41
2:F:715:GLU:HB2	2:F:717:LYS:HG2	2.03	0.41
2:B:397:GLU:HB3	2:B:479:VAL:CB	2.50	0.41
2:C:24:LEU:HD11	2:C:65:GLU:HA	2.02	0.41
2:D:394:LEU:HD13	2:D:480:VAL:CG2	2.49	0.41
2:D:53:LEU:HD11	2:D:134:ALA:HA	2.02	0.41
2:E:282:HIS:CG	2:E:319:GLU:HB3	2.56	0.41
2:E:574:MET:CB	2:E:619:ILE:HG12	2.51	0.41
2:E:623:HIS:CD2	2:E:625:ASP:HB3	2.56	0.41
2:A:195:VAL:HG11	2:A:204:PRO:HA	2.02	0.41
2:B:58:GLU:CD	2:B:58:GLU:H	2.24	0.41
2:D:743:LEU:HD11	2:D:773:VAL:HG11	2.02	0.41
2:D:747:ALA:HB1	2:D:794:LEU:CD2	2.50	0.41
2:E:633:VAL:HG22	2:E:639:LEU:HG	2.03	0.41
2:F:713:SER:HB2	2:F:714:LEU:H	1.58	0.41
1:2:136:PHE:CE2	2:B:431:VAL:HG21	2.56	0.41
1:3:204:ILE:HG21	1:3:211:THR:HB	2.03	0.41
2:A:355:ARG:HA	2:A:358:TYR:CZ	2.56	0.41
2:C:58:GLU:CD	2:C:58:GLU:H	2.23	0.41
2:C:619:ILE:CG2	2:C:627:PHE:CD1	2.95	0.41
2:D:499:LEU:HB2	2:D:525:ARG:HA	2.03	0.41
2:E:202:ASN:HD22	2:E:311:CYS:H	1.69	0.41
1:1:133:PHE:CB	1:1:139:VAL:HG22	2.51	0.40
1:1:147:VAL:HG22	1:1:147:VAL:O	2.21	0.40
1:4:167:PHE:CD2	1:4:175:VAL:HG22	2.56	0.40
2:A:509:ARG:HB3	2:A:557:ALA:HB2	2.03	0.40
2:C:613:VAL:CG1	2:C:655:ILE:HD12	2.52	0.40
2:D:31:THR:HB	2:D:120:ALA:HB2	2.03	0.40
2:E:269:ARG:C	2:E:271:ALA:H	2.23	0.40
2:F:100:HIS:CD2	2:F:107:HIS:CE1	3.09	0.40
1:5:203:ILE:HG23	2:E:431:VAL:HB	2.02	0.40
1:6:181:ILE:O	1:6:184:GLU:HG2	2.22	0.40
2:A:18:GLN:O	2:A:21:ALA:HB3	2.20	0.40
2:B:165:SER:HB2	2:B:166:LEU:HB3	2.03	0.40
2:B:507:HIS:HA	2:B:517:VAL:HG21	2.03	0.40
2:B:23:ARG:HH21	2:B:70:ARG:HD3	1.86	0.40
2:D:351:LEU:HA	2:D:392:ILE:HG22	2.03	0.40
2:D:36:LEU:HD21	2:D:61:GLN:HB2	2.03	0.40
2:E:276:LEU:O	2:E:311:CYS:HA	2.21	0.40
2:F:499:LEU:HD21	2:F:528:ARG:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:203:ILE:HG22	1:4:204:ILE:HG12	2.03	0.40
2:A:194:GLU:HB3	2:A:198:ARG:HH21	1.86	0.40
2:B:394:LEU:HD21	2:B:483:TRP:CE2	2.57	0.40
2:C:536:ARG:HA	2:C:637:GLY:HA3	2.02	0.40
2:D:723:VAL:HG23	2:D:765:LEU:HD13	2.03	0.40
2:E:46:ALA:HB1	2:E:109:LEU:HB2	2.03	0.40
2:F:474:ASP:HA	2:F:493:GLN:H	1.86	0.40
1:2:133:PHE:CE2	1:2:186:ALA:HB2	2.57	0.40
1:6:203:ILE:HG23	2:F:431:VAL:O	2.21	0.40
2:C:79:HIS:CG	2:C:80:TYR:N	2.89	0.40
2:D:281:LEU:HD11	2:D:313:GLY:N	2.22	0.40
1:1:130:VAL:HG11	1:1:196:LEU:HD13	2.04	0.40
1:2:130:VAL:HG12	1:2:196:LEU:CD1	2.52	0.40
2:A:24:LEU:HD23	2:A:65:GLU:HA	2.04	0.40
2:A:484:THR:HG22	2:A:563:PHE:HB3	2.03	0.40
2:A:776:ARG:HH21	2:A:794:LEU:HD12	1.87	0.40
2:C:9:ARG:O	2:C:13:VAL:HG13	2.21	0.40
2:D:542:ILE:HD13	2:D:656:MET:HB2	2.03	0.40
2:F:198:ARG:HH11	2:F:201:LYS:HD3	1.86	0.40
2:F:527:ALA:HA	2:F:532:LYS:HB3	2.04	0.40
2:F:622:ALA:HB3	2:F:627:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	92/218 (42%)	73 (79%)	11 (12%)	8 (9%)	1	15
1	2	92/218 (42%)	76 (83%)	11 (12%)	5 (5%)	2	25
1	3	92/218 (42%)	79 (86%)	8 (9%)	5 (5%)	2	25
1	4	92/218 (42%)	77 (84%)	12 (13%)	3 (3%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	92/218 (42%)	77 (84%)	11 (12%)	4 (4%)	3	29
1	6	92/218 (42%)	77 (84%)	8 (9%)	7 (8%)	1	18
2	A	794/810 (98%)	640 (81%)	102 (13%)	52 (6%)	1	22
2	B	794/810 (98%)	635 (80%)	114 (14%)	45 (6%)	2	24
2	C	794/810 (98%)	627 (79%)	119 (15%)	48 (6%)	2	23
2	D	794/810 (98%)	627 (79%)	115 (14%)	52 (6%)	1	22
2	E	794/810 (98%)	632 (80%)	118 (15%)	44 (6%)	2	25
2	F	794/810 (98%)	640 (81%)	105 (13%)	49 (6%)	2	22
All	All	5316/6168 (86%)	4260 (80%)	734 (14%)	322 (6%)	3	22

All (322) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	217	ALA
1	2	147	VAL
1	2	217	ALA
1	3	147	VAL
1	4	147	VAL
1	6	146	ASN
1	6	207	HIS
1	6	217	ALA
2	A	129	VAL
2	A	229	GLU
2	A	468	ASN
2	A	471	VAL
2	A	472	THR
2	A	473	VAL
2	A	532	LYS
2	A	579	GLU
2	A	587	VAL
2	A	623	HIS
2	B	129	VAL
2	B	230	VAL
2	B	333	ARG
2	B	366	ILE
2	B	411	PRO
2	B	468	ASN
2	B	493	GLN
2	B	658	SER

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Mol	Chain	Res	Type
2	B	660	VAL
2	B	662	ALA
2	B	674	ASN
2	B	697	PHE
2	B	738	ASP
2	B	763	ARG
2	C	146	GLU
2	C	362	HIS
2	C	383	SER
2	C	411	PRO
2	C	468	ASN
2	C	471	VAL
2	C	493	GLN
2	C	580	LYS
2	C	660	VAL
2	C	668	ASN
2	C	669	LYS
2	C	739	LEU
2	D	70	ARG
2	D	271	ALA
2	D	364	VAL
2	D	365	SER
2	D	366	ILE
2	D	468	ASN
2	D	473	VAL
2	D	532	LYS
2	D	582	SER
2	D	712	HIS
2	D	717	LYS
2	E	129	VAL
2	E	329	ALA
2	E	365	SER
2	E	366	ILE
2	E	468	ASN
2	E	472	THR
2	E	473	VAL
2	E	493	GLN
2	E	587	VAL
2	E	618	ALA
2	E	668	ASN
2	E	712	HIS
2	E	738	ASP

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Mol	Chain	Res	Type
2	F	129	VAL
2	F	199	ARG
2	F	294	ILE
2	F	332	ARG
2	F	362	HIS
2	F	366	ILE
2	F	383	SER
2	F	409	THR
2	F	411	PRO
2	F	468	ASN
2	F	471	VAL
2	F	493	GLN
2	F	587	VAL
2	F	668	ASN
2	F	669	LYS
2	F	712	HIS
2	F	713	SER
2	F	738	ASP
1	1	147	VAL
1	2	144	LYS
1	2	216	PHE
1	3	170	MET
1	5	146	ASN
2	A	6	PHE
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	327	ASP
2	A	363	ARG
2	A	366	ILE
2	A	384	ASP
2	A	391	ALA
2	A	413	LEU
2	A	493	GLN
2	A	610	PRO
2	A	668	ASN
2	A	738	ASP
2	B	163	LEU
2	B	165	SER
2	B	201	LYS
2	B	375	VAL
2	B	391	ALA

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Mol	Chain	Res	Type
2	B	413	LEU
2	C	129	VAL
2	C	165	SER
2	C	201	LYS
2	C	293	ALA
2	C	294	ILE
2	C	333	ARG
2	C	363	ARG
2	C	366	ILE
2	C	391	ALA
2	C	470	GLU
2	C	662	ALA
2	C	674	ASN
2	C	738	ASP
2	D	165	SER
2	D	201	LYS
2	D	294	ILE
2	D	411	PRO
2	D	412	ASN
2	D	470	GLU
2	D	493	GLN
2	D	618	ALA
2	D	662	ALA
2	D	673	PHE
2	D	714	LEU
2	D	738	ASP
2	D	756	VAL
2	D	757	ASP
2	D	788	LYS
2	E	165	SER
2	E	375	VAL
2	E	391	ALA
2	E	408	THR
2	E	413	LEU
2	E	580	LYS
2	E	582	SER
2	E	671	VAL
2	F	163	LEU
2	F	165	SER
2	F	327	ASP
2	F	375	VAL
2	F	386	PHE

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Mol	Chain	Res	Type
2	F	662	ALA
1	1	144	LYS
1	1	177	ASN
1	1	216	PHE
1	2	177	ASN
1	3	144	LYS
1	3	177	ASN
1	3	207	HIS
1	4	144	LYS
1	4	177	ASN
1	5	147	VAL
1	5	177	ASN
1	6	177	ASN
2	A	333	ARG
2	A	410	PRO
2	A	434	GLN
2	A	588	GLY
2	A	618	ALA
2	A	662	ALA
2	A	690	MET
2	A	712	HIS
2	A	717	LYS
2	B	470	GLU
2	B	578	MET
2	B	590	PRO
2	B	592	GLY
2	B	715	GLU
2	B	717	LYS
2	C	163	LEU
2	C	375	VAL
2	C	586	LEU
2	C	600	GLY
2	C	643	LYS
2	C	673	PHE
2	D	143	GLY
2	D	162	THR
2	D	163	LEU
2	D	202	ASN
2	D	363	ARG
2	D	391	ALA
2	D	413	LEU
2	E	163	LEU

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Mol	Chain	Res	Type
2	E	293	ALA
2	E	382	ILE
2	E	388	PRO
2	E	410	PRO
2	E	550	GLY
2	E	591	PRO
2	E	662	ALA
2	E	717	LYS
2	F	146	GLU
2	F	166	LEU
2	F	391	ALA
2	F	410	PRO
2	F	413	LEU
2	F	534	PRO
2	F	618	ALA
1	1	146	ASN
1	5	144	LYS
1	6	144	LYS
1	6	147	VAL
2	A	152	ALA
2	A	157	ASN
2	A	162	THR
2	A	177	ASP
2	A	226	ILE
2	A	388	PRO
2	A	400	SER
2	A	470	GLU
2	A	686	LYS
2	A	797	GLU
2	B	151	ALA
2	B	162	THR
2	B	166	LEU
2	B	212	VAL
2	B	226	ILE
2	B	271	ALA
2	B	388	PRO
2	B	471	VAL
2	B	618	ALA
2	B	670	TYR
2	C	117	GLU
2	C	150	SER
2	C	162	THR

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Mol	Chain	Res	Type
2	C	388	PRO
2	C	400	SER
2	C	413	LEU
2	C	659	ASN
2	D	76	GLN
2	D	166	LEU
2	D	226	ILE
2	D	375	VAL
2	D	388	PRO
2	D	400	SER
2	D	610	PRO
2	D	675	VAL
2	E	162	THR
2	E	169	ASP
2	E	226	ILE
2	E	271	ALA
2	E	400	SER
2	E	471	VAL
2	E	686	LYS
2	F	226	ILE
2	F	271	ALA
2	F	328	ALA
2	F	382	ILE
2	F	388	PRO
2	F	400	SER
2	F	583	THR
2	F	643	LYS
2	F	686	LYS
1	1	145	LEU
1	1	205	SER
1	6	216	PHE
2	A	151	ALA
2	A	364	VAL
2	A	375	VAL
2	A	533	ASP
2	A	600	GLY
2	B	169	ASP
2	B	294	ILE
2	B	384	ASP
2	B	400	SER
2	C	226	ILE
2	C	382	ILE

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Mol	Chain	Res	Type
2	C	408	THR
2	C	412	ASN
2	C	546	PRO
2	D	147	THR
2	D	155	ASN
2	D	359	GLU
2	D	410	PRO
2	D	584	SER
2	D	674	ASN
2	D	690	MET
2	E	583	THR
2	F	149	SER
2	F	580	LYS
2	A	169	ASP
2	A	212	VAL
2	A	619	ILE
2	B	76	GLN
2	B	103	VAL
2	B	586	LEU
2	C	228	ASN
2	C	762	ALA
2	E	69	GLY
2	E	323	TYR
2	E	469	SER
2	E	623	HIS
2	F	162	THR
2	F	177	ASP
2	F	333	ARG
2	B	182	VAL
2	D	600	GLY
2	F	182	VAL
2	F	473	VAL
2	F	589	SER
2	A	549	VAL
2	B	78	ILE
2	D	511	ILE
2	C	534	PRO
2	E	364	VAL
2	D	68	ILE
2	D	471	VAL
2	E	644	GLY
2	F	68	ILE

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Mol	Chain	Res	Type
2	C	453	VAL
2	C	590	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	88/201 (44%)	80 (91%)	8 (9%)	11	38
1	2	88/201 (44%)	75 (85%)	13 (15%)	3	20
1	3	88/201 (44%)	77 (88%)	11 (12%)	5	26
1	4	88/201 (44%)	82 (93%)	6 (7%)	18	51
1	5	88/201 (44%)	77 (88%)	11 (12%)	5	26
1	6	88/201 (44%)	83 (94%)	5 (6%)	24	56
2	A	666/685 (97%)	587 (88%)	79 (12%)	6	27
2	B	666/685 (97%)	581 (87%)	85 (13%)	5	25
2	C	666/685 (97%)	590 (89%)	76 (11%)	7	28
2	D	666/685 (97%)	593 (89%)	73 (11%)	7	30
2	E	666/685 (97%)	577 (87%)	89 (13%)	4	24
2	F	666/685 (97%)	584 (88%)	82 (12%)	5	26
All	All	4524/5316 (85%)	3986 (88%)	538 (12%)	10	27

All (538) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	131	LEU
1	1	136	PHE
1	1	145	LEU
1	1	146	ASN
1	1	165	VAL
1	1	174	GLU
1	1	184	GLU
1	1	215	HIS

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Mol	Chain	Res	Type
1	2	130	VAL
1	2	136	PHE
1	2	142	LEU
1	2	145	LEU
1	2	153	THR
1	2	157	PHE
1	2	162	TYR
1	2	165	VAL
1	2	175	VAL
1	2	187	THR
1	2	197	GLU
1	2	212	ILE
1	2	215	HIS
1	3	127	LEU
1	3	131	LEU
1	3	136	PHE
1	3	153	THR
1	3	157	PHE
1	3	162	TYR
1	3	165	VAL
1	3	169	ASN
1	3	194	HIS
1	3	206	GLU
1	3	211	THR
1	4	136	PHE
1	4	137	GLU
1	4	154	LEU
1	4	165	VAL
1	4	176	GLU
1	4	206	GLU
1	5	126	LYS
1	5	136	PHE
1	5	142	LEU
1	5	147	VAL
1	5	151	LYS
1	5	157	PHE
1	5	164	TYR
1	5	176	GLU
1	5	187	THR
1	5	202	LEU
1	5	207	HIS
1	6	136	PHE

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Mol	Chain	Res	Type
1	6	147	VAL
1	6	165	VAL
1	6	166	ASP
1	6	207	HIS
2	A	16	LEU
2	A	19	GLU
2	A	22	LEU
2	A	23	ARG
2	A	32	GLU
2	A	73	GLU
2	A	76	GLN
2	A	83	ARG
2	A	87	VAL
2	A	89	GLU
2	A	105	THR
2	A	108	ILE
2	A	119	VAL
2	A	138	VAL
2	A	146	GLU
2	A	173	ILE
2	A	185	ARG
2	A	191	ARG
2	A	195	VAL
2	A	198	ARG
2	A	200	THR
2	A	205	VAL
2	A	223	GLN
2	A	230	VAL
2	A	257	PHE
2	A	260	ARG
2	A	269	ARG
2	A	270	GLN
2	A	311	CYS
2	A	323	TYR
2	A	324	ILE
2	A	341	GLN
2	A	355	ARG
2	A	358	TYR
2	A	362	HIS
2	A	363	ARG
2	A	364	VAL
2	A	381	TYR

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Mol	Chain	Res	Type
2	A	387	LEU
2	A	395	ILE
2	A	396	ASP
2	A	397	GLU
2	A	415	GLU
2	A	416	LEU
2	A	424	ARG
2	A	426	GLU
2	A	432	GLN
2	A	455	ASP
2	A	468	ASN
2	A	473	VAL
2	A	475	ASP
2	A	478	MET
2	A	483	TRP
2	A	494	THR
2	A	513	GLN
2	A	514	ASP
2	A	515	GLU
2	A	562	ILE
2	A	567	GLU
2	A	583	THR
2	A	608	ARG
2	A	623	HIS
2	A	626	VAL
2	A	634	LEU
2	A	638	ARG
2	A	676	GLN
2	A	685	MET
2	A	688	LYS
2	A	697	PHE
2	A	701	PHE
2	A	706	ASP
2	A	734	LEU
2	A	735	LYS
2	A	741	ILE
2	A	742	GLU
2	A	750	LYS
2	A	766	ARG
2	A	797	GLU
2	A	803	VAL
2	B	19	GLU

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Mol	Chain	Res	Type
2	B	23	ARG
2	B	32	GLU
2	B	40	ARG
2	B	74	MET
2	B	78	ILE
2	B	81	THR
2	B	86	LYS
2	B	87	VAL
2	B	92	MET
2	B	103	VAL
2	B	105	THR
2	B	106	GLU
2	B	108	ILE
2	B	119	VAL
2	B	133	LYS
2	B	142	LEU
2	B	169	ASP
2	B	173	ILE
2	B	185	ARG
2	B	191	ARG
2	B	195	VAL
2	B	198	ARG
2	B	200	THR
2	B	202	ASN
2	B	205	VAL
2	B	228	ASN
2	B	238	ARG
2	B	242	LEU
2	B	257	PHE
2	B	269	ARG
2	B	321	ARG
2	B	323	TYR
2	B	325	GLU
2	B	337	ILE
2	B	344	VAL
2	B	351	LEU
2	B	357	ARG
2	B	358	TYR
2	B	359	GLU
2	B	363	ARG
2	B	380	ARG
2	B	381	TYR

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Mol	Chain	Res	Type
2	B	397	GLU
2	B	407	PHE
2	B	411	PRO
2	B	414	LYS
2	B	415	GLU
2	B	424	ARG
2	B	425	LYS
2	B	446	GLU
2	B	455	ASP
2	B	472	THR
2	B	475	ASP
2	B	478	MET
2	B	501	ASN
2	B	515	GLU
2	B	536	ARG
2	B	572	ILE
2	B	574	MET
2	B	586	LEU
2	B	593	TYR
2	B	598	GLU
2	B	621	LYS
2	B	638	ARG
2	B	647	VAL
2	B	648	ASP
2	B	669	LYS
2	B	676	GLN
2	B	682	HIS
2	B	683	LYS
2	B	685	MET
2	B	686	LYS
2	B	689	VAL
2	B	697	PHE
2	B	706	ASP
2	B	707	GLU
2	B	712	HIS
2	B	715	GLU
2	B	718	HIS
2	B	722	ILE
2	B	733	ARG
2	B	741	ILE
2	B	751	VAL
2	B	795	ASP

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Mol	Chain	Res	Type
2	C	13	VAL
2	C	19	GLU
2	C	22	LEU
2	C	23	ARG
2	C	24	LEU
2	C	32	GLU
2	C	36	LEU
2	C	59	LYS
2	C	76	GLN
2	C	83	ARG
2	C	87	VAL
2	C	92	MET
2	C	119	VAL
2	C	138	VAL
2	C	160	THR
2	C	169	ASP
2	C	185	ARG
2	C	188	GLU
2	C	191	ARG
2	C	195	VAL
2	C	197	SER
2	C	199	ARG
2	C	200	THR
2	C	205	VAL
2	C	238	ARG
2	C	244	MET
2	C	268	ILE
2	C	323	TYR
2	C	325	GLU
2	C	338	GLN
2	C	341	GLN
2	C	351	LEU
2	C	354	LEU
2	C	364	VAL
2	C	376	LYS
2	C	385	ARG
2	C	387	LEU
2	C	397	GLU
2	C	411	PRO
2	C	415	GLU
2	C	424	ARG
2	C	425	LYS

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Mol	Chain	Res	Type
2	C	427	LYS
2	C	431	VAL
2	C	432	GLN
2	C	457	LYS
2	C	470	GLU
2	C	471	VAL
2	C	475	ASP
2	C	476	ILE
2	C	500	LEU
2	C	503	GLU
2	C	513	GLN
2	C	514	ASP
2	C	515	GLU
2	C	531	LEU
2	C	558	LEU
2	C	567	GLU
2	C	607	ARG
2	C	634	LEU
2	C	638	ARG
2	C	645	ARG
2	C	670	TYR
2	C	676	GLN
2	C	680	GLN
2	C	705	ILE
2	C	714	LEU
2	C	718	HIS
2	C	726	MET
2	C	730	LEU
2	C	734	LEU
2	C	763	ARG
2	C	766	ARG
2	C	793	VAL
2	C	795	ASP
2	C	800	GLU
2	D	6	PHE
2	D	13	VAL
2	D	19	GLU
2	D	23	ARG
2	D	28	ASN
2	D	32	GLU
2	D	51	GLN
2	D	59	LYS

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Mol	Chain	Res	Type
2	D	74	MET
2	D	76	GLN
2	D	81	THR
2	D	86	LYS
2	D	87	VAL
2	D	102	TYR
2	D	105	THR
2	D	106	GLU
2	D	138	VAL
2	D	155	ASN
2	D	166	LEU
2	D	190	GLN
2	D	195	VAL
2	D	199	ARG
2	D	205	VAL
2	D	234	LEU
2	D	252	LYS
2	D	269	ARG
2	D	276	LEU
2	D	297	SER
2	D	308	GLU
2	D	310	GLN
2	D	311	CYS
2	D	325	GLU
2	D	351	LEU
2	D	359	GLU
2	D	364	VAL
2	D	367	THR
2	D	387	LEU
2	D	397	GLU
2	D	404	LEU
2	D	405	ARG
2	D	407	PHE
2	D	415	GLU
2	D	416	LEU
2	D	424	ARG
2	D	432	GLN
2	D	473	VAL
2	D	525	ARG
2	D	531	LEU
2	D	544	LEU
2	D	549	VAL

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Mol	Chain	Res	Type
2	D	574	MET
2	D	578	MET
2	D	594	VAL
2	D	607	ARG
2	D	623	HIS
2	D	626	VAL
2	D	630	LEU
2	D	634	LEU
2	D	636	ASP
2	D	647	VAL
2	D	654	LEU
2	D	664	GLU
2	D	678	GLU
2	D	701	PHE
2	D	719	LEU
2	D	734	LEU
2	D	735	LYS
2	D	741	ILE
2	D	742	GLU
2	D	756	VAL
2	D	763	ARG
2	D	769	ILE
2	D	800	GLU
2	E	6	PHE
2	E	11	GLN
2	E	13	VAL
2	E	19	GLU
2	E	20	GLU
2	E	23	ARG
2	E	24	LEU
2	E	32	GLU
2	E	51	GLN
2	E	62	LYS
2	E	74	MET
2	E	75	SER
2	E	76	GLN
2	E	78	ILE
2	E	81	THR
2	E	86	LYS
2	E	87	VAL
2	E	92	MET
2	E	105	THR

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Mol	Chain	Res	Type
2	E	133	LYS
2	E	135	ARG
2	E	138	VAL
2	E	160	THR
2	E	173	ILE
2	E	185	ARG
2	E	191	ARG
2	E	195	VAL
2	E	200	THR
2	E	205	VAL
2	E	230	VAL
2	E	234	LEU
2	E	238	ARG
2	E	244	MET
2	E	254	ARG
2	E	261	LEU
2	E	267	GLU
2	E	269	ARG
2	E	323	TYR
2	E	355	ARG
2	E	358	TYR
2	E	363	ARG
2	E	364	VAL
2	E	381	TYR
2	E	393	ASP
2	E	397	GLU
2	E	404	LEU
2	E	415	GLU
2	E	416	LEU
2	E	424	ARG
2	E	427	LYS
2	E	431	VAL
2	E	432	GLN
2	E	448	ARG
2	E	452	GLN
2	E	468	ASN
2	E	470	GLU
2	E	473	VAL
2	E	494	THR
2	E	509	ARG
2	E	511	ILE
2	E	531	LEU

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Mol	Chain	Res	Type
2	E	535	LYS
2	E	536	ARG
2	E	549	VAL
2	E	554	LEU
2	E	587	VAL
2	E	596	TYR
2	E	598	GLU
2	E	626	VAL
2	E	634	LEU
2	E	638	ARG
2	E	645	ARG
2	E	670	TYR
2	E	676	GLN
2	E	680	GLN
2	E	690	MET
2	E	697	PHE
2	E	700	GLU
2	E	712	HIS
2	E	718	HIS
2	E	730	LEU
2	E	735	LYS
2	E	741	ILE
2	E	763	ARG
2	E	770	GLN
2	E	793	VAL
2	E	794	LEU
2	E	795	ASP
2	E	798	ASP
2	F	8	GLU
2	F	13	VAL
2	F	16	LEU
2	F	19	GLU
2	F	23	ARG
2	F	32	GLU
2	F	40	ARG
2	F	76	GLN
2	F	78	ILE
2	F	83	ARG
2	F	87	VAL
2	F	89	GLU
2	F	92	MET
2	F	108	ILE

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Mol	Chain	Res	Type
2	F	138	VAL
2	F	142	LEU
2	F	173	ILE
2	F	185	ARG
2	F	191	ARG
2	F	195	VAL
2	F	205	VAL
2	F	230	VAL
2	F	244	MET
2	F	268	ILE
2	F	297	SER
2	F	337	ILE
2	F	338	GLN
2	F	351	LEU
2	F	358	TYR
2	F	359	GLU
2	F	363	ARG
2	F	378	SER
2	F	381	TYR
2	F	393	ASP
2	F	395	ILE
2	F	396	ASP
2	F	397	GLU
2	F	404	LEU
2	F	411	PRO
2	F	415	GLU
2	F	416	LEU
2	F	424	ARG
2	F	425	LYS
2	F	432	GLN
2	F	443	ARG
2	F	444	ASP
2	F	452	GLN
2	F	457	LYS
2	F	464	GLN
2	F	478	MET
2	F	579	GLU
2	F	608	ARG
2	F	611	TYR
2	F	634	LEU
2	F	638	ARG
2	F	645	ARG

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Mol	Chain	Res	Type
2	F	647	VAL
2	F	654	LEU
2	F	664	GLU
2	F	666	LYS
2	F	669	LYS
2	F	676	GLN
2	F	677	ASP
2	F	680	GLN
2	F	681	ASN
2	F	683	LYS
2	F	685	MET
2	F	690	MET
2	F	695	ARG
2	F	705	ILE
2	F	719	LEU
2	F	727	SER
2	F	730	LEU
2	F	733	ARG
2	F	734	LEU
2	F	736	GLU
2	F	737	GLN
2	F	741	ILE
2	F	742	GLU
2	F	793	VAL
2	F	795	ASP
2	F	800	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	194	HIS
1	4	207	HIS
1	6	207	HIS
2	A	11	GLN
2	A	28	ASN
2	A	33	HIS
2	A	76	GLN
2	A	100	HIS
2	A	137	GLN
2	A	352	GLN
2	A	361	HIS
2	A	712	HIS

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Mol	Chain	Res	Type
2	A	787	HIS
2	B	26	HIS
2	B	100	HIS
2	B	107	HIS
2	B	310	GLN
2	B	434	GLN
2	B	507	HIS
2	B	681	ASN
2	B	682	HIS
2	B	712	HIS
2	B	718	HIS
2	B	791	HIS
2	C	33	HIS
2	C	352	GLN
2	C	362	HIS
2	C	447	GLN
2	C	468	ASN
2	C	513	GLN
2	C	668	ASN
2	C	718	HIS
2	D	76	GLN
2	D	79	HIS
2	D	107	HIS
2	D	228	ASN
2	D	338	GLN
2	D	361	HIS
2	D	452	GLN
2	D	464	GLN
2	D	581	HIS
2	D	674	ASN
2	D	682	HIS
2	E	27	ASN
2	E	76	GLN
2	E	107	HIS
2	E	202	ASN
2	E	361	HIS
2	E	581	HIS
2	E	623	HIS
2	E	712	HIS
2	E	718	HIS
2	E	729	GLN
2	F	26	HIS

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Mol	Chain	Res	Type
2	F	33	HIS
2	F	76	GLN
2	F	79	HIS
2	F	100	HIS
2	F	362	HIS
2	F	434	GLN
2	F	601	GLN
2	F	682	HIS
2	F	712	HIS
2	F	772	HIS

### 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 carbohydrates in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.