



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:33 am GMT

PDB ID : 3J3T
EMDB ID: : EMD-5607
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 : 9.00 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

A user guide is available at

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

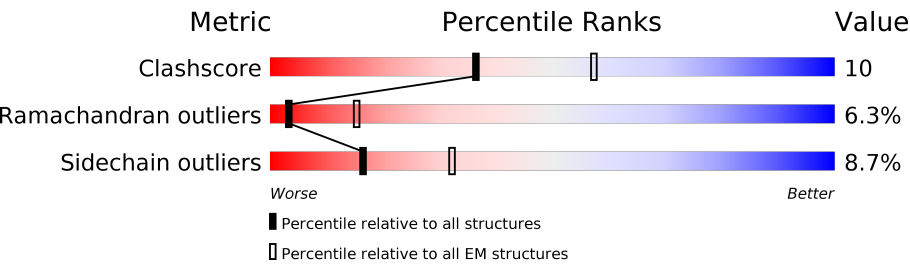
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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 9.00 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 ≥ 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	29% 11% . 57%
1	2	218	25% 13% . . 57%
1	3	218	26% 11% 5% 57%
1	4	218	27% 13% . . 57%
1	5	218	28% 11% . . 57%
1	6	218	29% 11% . . 57%
2	A	810	71% 23% . .
2	B	810	70% 23% 5% . .
2	C	810	72% 22% 5% .

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Mol	Chain	Length	Quality of chain
2	D	810	<div><div></div><div>70%</div><div>24%</div><div>• •</div></div>
2	E	810	<div><div></div><div>72%</div><div>22%</div><div>5% •</div></div>
2	F	810	<div><div></div><div>70%</div><div>24%</div><div>• ••</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41862 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
			6200	3850	1120	1215	15		
2	B	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	C	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	D	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	E	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	F	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		

There are 6 discrepancies between the modelled and reference sequences:

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

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

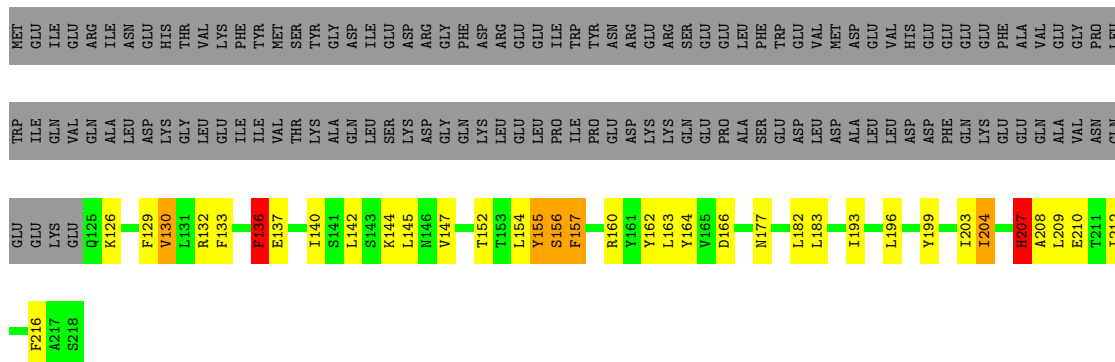
- Molecule 1: Adapter protein MecA 1





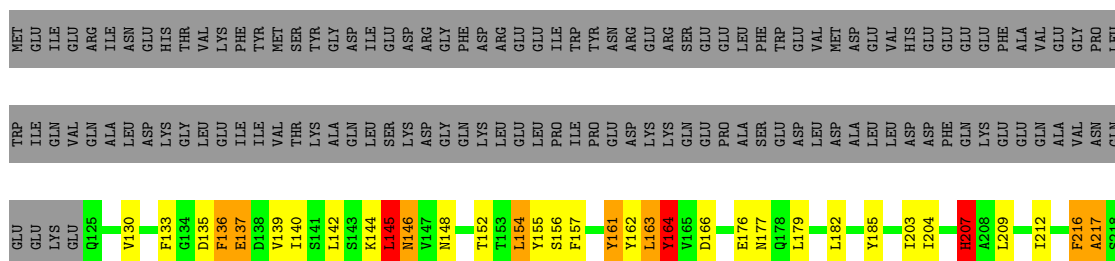
- Molecule 1: Adapter protein MecA 1

Chain 4: 27% 13% 57%



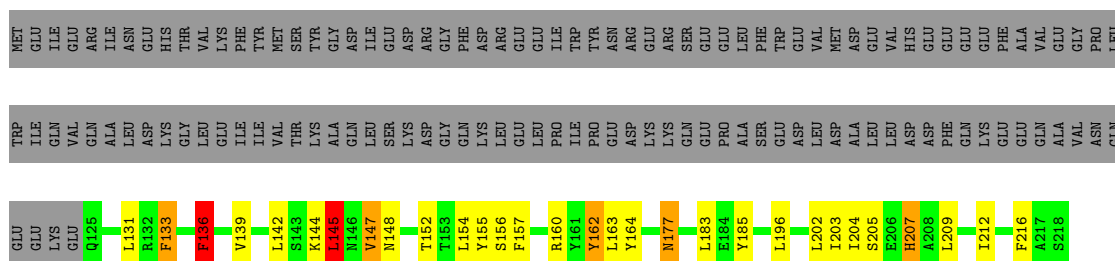
- Molecule 1: Adapter protein MecA 1

Chain 5: 28% 11% 57%



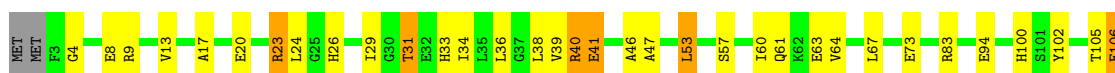
- Molecule 1: Adapter protein MecA 1

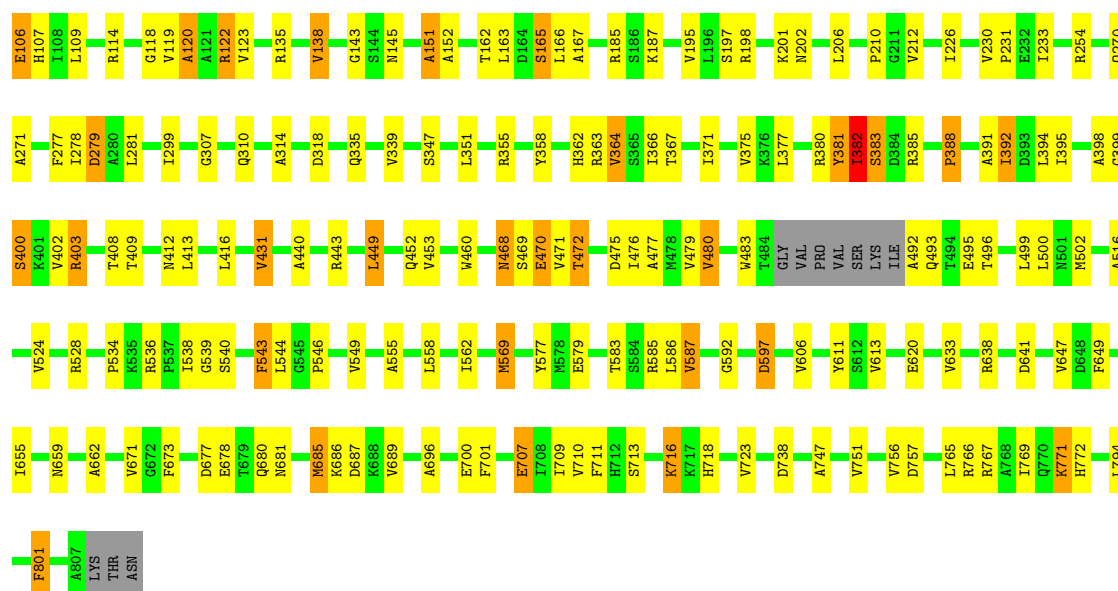
Chain 6: 29% 11% 57%



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

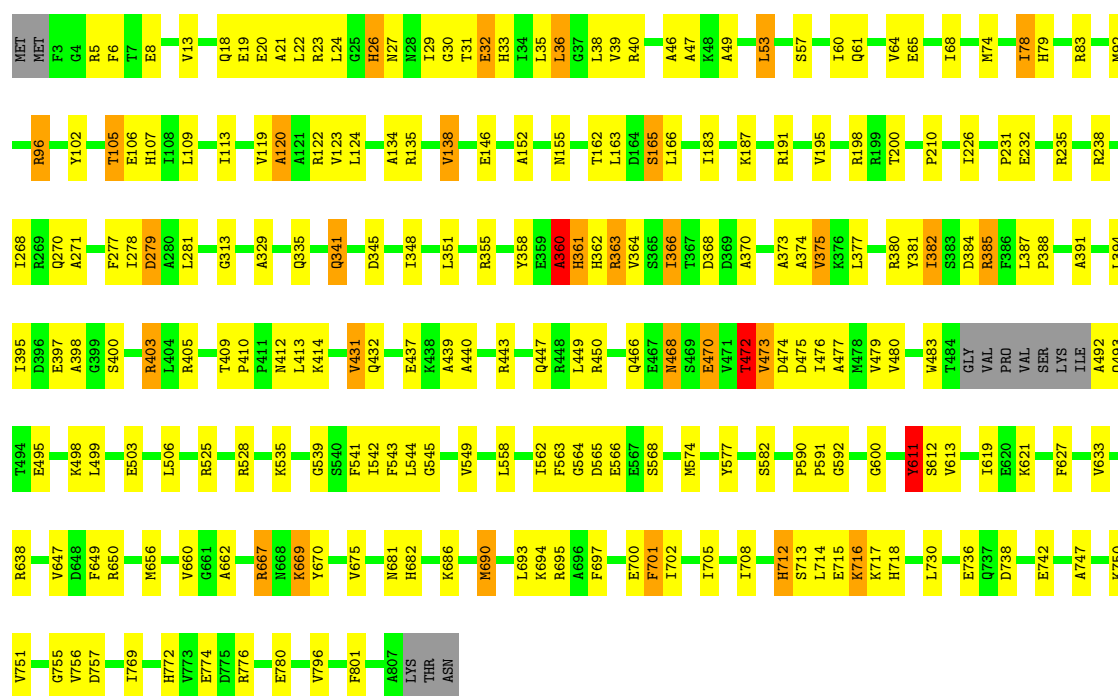
Chain A: 71% 23%





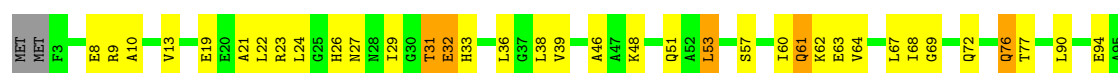
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

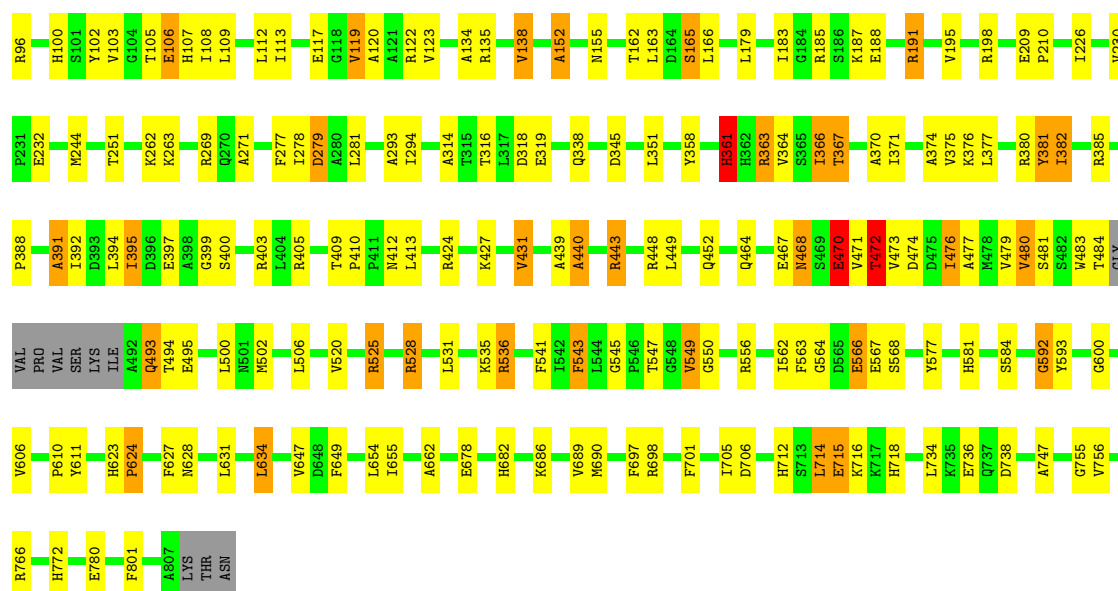
Chain D: 70% 24%



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

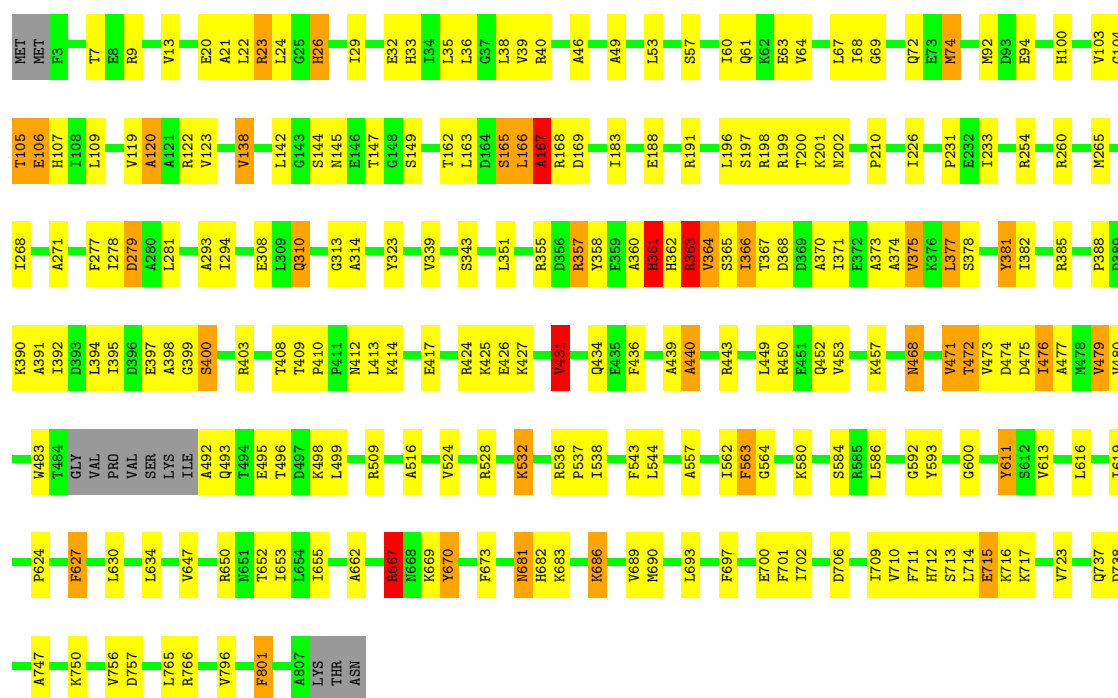
Chain E: 72% 22% 5%





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

Chain F: 70% 24%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	45514	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)	3000	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	1.01	0/791	1.34	8/1064 (0.8%)
1	2	1.03	0/791	1.47	15/1064 (1.4%)
1	3	1.05	0/791	1.42	12/1064 (1.1%)
1	4	1.03	0/791	1.43	11/1064 (1.0%)
1	5	1.02	0/791	1.36	11/1064 (1.0%)
1	6	1.03	0/791	1.31	5/1064 (0.5%)
2	A	0.97	0/6269	1.23	17/8441 (0.2%)
2	B	0.98	0/6269	1.26	28/8441 (0.3%)
2	C	0.97	0/6269	1.22	20/8441 (0.2%)
2	D	0.97	0/6269	1.24	20/8441 (0.2%)
2	E	0.97	0/6269	1.21	12/8441 (0.1%)
2	F	0.97	0/6269	1.24	26/8441 (0.3%)
All	All	0.98	0/42360	1.25	185/57030 (0.3%)

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	1
1	2	0	2
1	3	0	4
1	4	0	1
1	5	0	3
1	6	0	1
2	A	0	20
2	B	0	14
2	C	0	12
2	D	0	17
2	E	0	16
2	F	0	14
All	All	0	105

There are no bond length outliers.

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	611	TYR	CB-CG-CD1	-12.10	113.74	121.00
1	2	216	PHE	CB-CG-CD1	10.40	128.08	120.80
1	2	216	PHE	CB-CG-CD2	-9.32	114.28	120.80
2	D	611	TYR	CB-CG-CD2	8.74	126.24	121.00
2	F	358	TYR	CB-CG-CD2	-8.64	115.81	121.00
2	C	543	PHE	CB-CG-CD1	8.45	126.71	120.80
2	B	596	TYR	CB-CG-CD2	-8.26	116.05	121.00
2	C	543	PHE	CB-CG-CD2	-8.13	115.11	120.80
1	3	136	PHE	CB-CG-CD2	-8.04	115.17	120.80
2	B	701	PHE	CB-CG-CD2	-8.00	115.20	120.80
1	3	155	TYR	CB-CG-CD1	-7.90	116.26	121.00
2	B	358	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	2	136	PHE	CB-CG-CD2	-7.75	115.38	120.80
2	B	701	PHE	CB-CG-CD1	7.74	126.22	120.80
2	C	358	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	2	156	SER	N-CA-CB	7.41	121.62	110.50
1	4	157	PHE	CB-CG-CD2	-7.35	115.65	120.80
2	D	543	PHE	CB-CG-CD1	7.28	125.89	120.80
1	6	136	PHE	CB-CG-CD2	-7.27	115.71	120.80
2	B	760	TYR	CB-CG-CD1	7.25	125.35	121.00
2	B	760	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	B	596	TYR	CB-CG-CD1	7.20	125.32	121.00
2	B	627	PHE	CB-CG-CD1	7.19	125.83	120.80
2	A	358	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	A	711	PHE	CB-CG-CD1	-7.06	115.86	120.80
2	F	627	PHE	CB-CG-CD1	7.05	125.74	120.80
2	C	165	SER	C-N-CA	7.04	139.31	121.70
2	D	358	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	4	155	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	4	199	TYR	CB-CG-CD1	6.96	125.18	121.00
2	D	627	PHE	CB-CG-CD2	-6.96	115.93	120.80
2	D	543	PHE	CB-CG-CD2	-6.95	115.94	120.80
1	5	161	TYR	CA-CB-CG	-6.91	100.27	113.40
2	F	543	PHE	CB-CG-CD1	6.89	125.63	120.80
2	B	201	LYS	N-CA-C	-6.82	92.58	111.00
2	F	563	PHE	CB-CG-CD1	6.82	125.57	120.80
2	A	165	SER	C-N-CA	6.79	138.67	121.70
1	4	199	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	B	672	GLY	N-CA-C	-6.77	96.17	113.10
2	F	167	ALA	N-CA-CB	6.76	119.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	358	TYR	CB-CG-CD1	6.76	125.06	121.00
2	F	627	PHE	CB-CG-CD2	-6.72	116.10	120.80
2	A	543	PHE	CB-CG-CD2	-6.69	116.11	120.80
2	B	627	PHE	CB-CG-CD2	-6.60	116.18	120.80
2	D	165	SER	C-N-CA	6.60	138.19	121.70
2	A	543	PHE	CB-CG-CD1	6.58	125.41	120.80
1	4	157	PHE	CB-CG-CD1	6.57	125.40	120.80
1	2	155	TYR	CB-CG-CD1	-6.57	117.06	121.00
2	B	358	TYR	CB-CG-CD1	6.56	124.94	121.00
1	2	136	PHE	CB-CG-CD1	6.52	125.36	120.80
2	C	539	GLY	N-CA-C	-6.50	96.86	113.10
2	F	611	TYR	CB-CG-CD1	-6.45	117.13	121.00
2	F	165	SER	C-N-CA	6.45	137.81	121.70
2	B	165	SER	C-N-CA	6.44	137.80	121.70
2	B	120	ALA	CB-CA-C	-6.41	100.48	110.10
2	F	543	PHE	CB-CG-CD2	-6.41	116.31	120.80
2	D	360	ALA	N-CA-C	-6.38	93.76	111.00
2	B	516	ALA	CB-CA-C	-6.37	100.55	110.10
1	4	207	HIS	N-CA-C	-6.36	93.83	111.00
2	F	364	VAL	C-N-CA	6.34	137.54	121.70
2	C	382	ILE	C-N-CA	6.32	137.50	121.70
2	E	627	PHE	CB-CG-CD2	6.31	125.22	120.80
2	E	165	SER	C-N-CA	6.30	137.46	121.70
1	1	166	ASP	N-CA-C	-6.30	93.99	111.00
2	C	685	MET	CG-SD-CE	6.29	110.27	100.20
2	D	341	GLN	N-CA-C	-6.25	94.12	111.00
2	F	377	LEU	CB-CA-C	-6.25	98.33	110.20
2	B	543	PHE	CB-CG-CD1	6.24	125.17	120.80
2	E	543	PHE	CB-CG-CD1	6.24	125.16	120.80
1	5	155	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	D	627	PHE	CB-CG-CD1	6.21	125.15	120.80
2	F	120	ALA	CB-CA-C	-6.20	100.80	110.10
2	D	358	TYR	CB-CG-CD1	6.18	124.71	121.00
2	F	358	TYR	CB-CG-CD1	6.18	124.71	121.00
1	4	204	ILE	N-CA-C	-6.16	94.37	111.00
1	6	136	PHE	CB-CG-CD1	6.13	125.09	120.80
2	D	701	PHE	CB-CG-CD2	-6.11	116.53	120.80
2	F	436	PHE	CB-CG-CD1	6.10	125.07	120.80
2	A	711	PHE	CB-CG-CD2	6.06	125.04	120.80
1	5	166	ASP	N-CA-C	-6.03	94.71	111.00
1	4	166	ASP	N-CA-C	-6.01	94.78	111.00
2	B	201	LYS	N-CA-CB	6.00	121.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	627	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	3	156	SER	N-CA-C	-5.98	94.86	111.00
2	A	382	ILE	C-N-CA	5.98	136.64	121.70
2	F	563	PHE	CB-CG-CD2	-5.97	116.62	120.80
2	C	383	SER	N-CA-CB	5.97	119.45	110.50
1	3	204	ILE	N-CA-C	-5.90	95.06	111.00
2	F	323	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	4	156	SER	N-CA-CB	5.85	119.28	110.50
2	A	341	GLN	N-CA-C	-5.85	95.20	111.00
2	E	472	THR	N-CA-CB	5.81	121.34	110.30
1	3	161	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	C	143	GLY	N-CA-C	-5.77	98.67	113.10
1	2	166	ASP	N-CA-C	-5.74	95.50	111.00
2	C	120	ALA	CB-CA-C	-5.72	101.52	110.10
1	2	204	ILE	N-CA-C	-5.72	95.55	111.00
2	B	364	VAL	C-N-CA	5.69	135.93	121.70
2	E	483	TRP	CB-CG-CD2	-5.69	119.20	126.60
1	2	162	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	2	199	TYR	CB-CG-CD2	5.64	124.39	121.00
2	C	270	GLN	C-N-CA	5.64	135.79	121.70
1	3	136	PHE	CB-CG-CD1	5.63	124.74	120.80
2	A	593	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	2	157	PHE	N-CA-C	-5.58	95.93	111.00
1	5	164	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	1	162	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	5	163	LEU	N-CA-C	-5.51	96.12	111.00
2	B	543	PHE	CB-CG-CD2	-5.49	116.96	120.80
2	B	469	SER	N-CA-CB	5.48	118.72	110.50
2	C	460	TRP	CA-CB-CG	-5.48	103.29	113.70
2	E	543	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	F	323	TYR	CB-CA-C	-5.46	99.48	110.40
1	2	199	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	6	156	SER	N-CA-CB	5.45	118.68	110.50
2	D	701	PHE	CB-CG-CD1	5.43	124.60	120.80
2	F	361	HIS	C-N-CA	5.43	135.27	121.70
2	D	120	ALA	N-CA-CB	5.40	117.66	110.10
2	A	717	LYS	C-N-CA	5.39	135.18	121.70
1	1	140	ILE	CA-CB-CG1	5.38	121.23	111.00
2	C	310	GLN	N-CA-C	-5.38	96.47	111.00
2	F	381	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	4	136	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	5	161	TYR	CB-CG-CD1	-5.36	117.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	VAL	C-N-CA	5.36	135.09	121.70
2	E	361	HIS	N-CA-CB	5.35	120.23	110.60
2	F	431	VAL	CG1-CB-CG2	5.35	119.45	110.90
1	1	167	PHE	CB-CG-CD1	5.34	124.54	120.80
2	B	565	ASP	N-CA-C	-5.32	96.63	111.00
2	E	152	ALA	N-CA-CB	5.31	117.54	110.10
2	F	381	TYR	N-CA-CB	5.29	120.12	110.60
2	F	310	GLN	N-CA-C	-5.28	96.76	111.00
2	D	539	GLY	N-CA-C	-5.27	99.92	113.10
1	6	133	PHE	N-CA-C	-5.27	96.78	111.00
1	3	130	VAL	N-CA-C	-5.27	96.78	111.00
2	B	144	SER	N-CA-CB	5.25	118.38	110.50
2	B	574	MET	CG-SD-CE	-5.24	91.82	100.20
2	A	358	TYR	CB-CG-CD1	5.24	124.14	121.00
2	A	471	VAL	C-N-CA	5.24	134.79	121.70
1	3	166	ASP	N-CA-C	-5.23	96.87	111.00
1	2	133	PHE	CB-CG-CD2	5.23	124.46	120.80
2	D	279	ASP	CB-CG-OD2	5.23	123.01	118.30
1	1	133	PHE	CB-CG-CD2	5.23	124.46	120.80
2	C	151	ALA	N-CA-CB	5.22	117.41	110.10
2	C	279	ASP	CB-CG-OD2	5.21	122.99	118.30
2	A	279	ASP	CB-CG-OD2	5.20	122.98	118.30
2	F	279	ASP	CB-CG-OD2	5.20	122.98	118.30
2	C	28	ASN	N-CA-C	-5.20	96.97	111.00
2	B	279	ASP	CB-CG-OD2	5.19	122.97	118.30
1	6	157	PHE	N-CA-C	-5.19	96.99	111.00
1	5	217	ALA	N-CA-CB	5.18	117.36	110.10
2	A	176	GLU	N-CA-C	-5.18	97.01	111.00
2	B	535	LYS	N-CA-CB	5.16	119.89	110.60
1	1	157	PHE	N-CA-C	-5.16	97.06	111.00
1	2	147	VAL	N-CA-C	-5.16	97.08	111.00
1	5	155	TYR	CA-CB-CG	-5.16	103.60	113.40
2	F	682	HIS	N-CA-CB	5.16	119.88	110.60
1	3	157	PHE	CB-CG-CD2	-5.15	117.19	120.80
2	E	279	ASP	CB-CG-OD2	5.15	122.93	118.30
1	3	155	TYR	CA-CB-CG	-5.14	103.63	113.40
2	A	270	GLN	C-N-CA	5.12	134.51	121.70
1	3	157	PHE	N-CA-C	-5.12	97.19	111.00
2	D	120	ALA	CB-CA-C	-5.11	102.43	110.10
2	E	611	TYR	N-CA-CB	5.10	119.78	110.60
2	C	201	LYS	CA-CB-CG	5.09	124.60	113.40
1	1	130	VAL	N-CA-C	-5.09	97.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	216	PHE	N-CA-CB	5.09	119.75	110.60
2	D	30	GLY	N-CA-C	-5.08	100.39	113.10
1	1	167	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	5	136	PHE	CB-CG-CD2	-5.08	117.25	120.80
2	C	114	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	2	132	ARG	N-CA-C	-5.07	97.30	111.00
2	F	92	MET	CG-SD-CE	-5.07	92.09	100.20
2	D	712	HIS	C-N-CA	5.07	134.37	121.70
2	A	610	PRO	C-N-CA	5.07	134.37	121.70
2	B	480	VAL	CB-CA-C	-5.05	101.80	111.40
2	E	102	TYR	C-N-CA	5.05	134.33	121.70
2	D	270	GLN	C-N-CA	5.04	134.31	121.70
2	B	656	MET	N-CA-C	-5.03	97.43	111.00
2	F	397	GLU	N-CA-CB	5.02	119.64	110.60
1	5	164	TYR	CB-CG-CD1	5.02	124.01	121.00
1	4	130	VAL	N-CA-C	-5.02	97.45	111.00
2	A	397	GLU	N-CA-CB	5.02	119.63	110.60
1	3	163	LEU	N-CA-C	-5.01	97.47	111.00
2	C	364	VAL	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (105) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	161	TYR	Sidechain
1	2	162	TYR	Sidechain
1	2	185	TYR	Sidechain
1	3	155	TYR	Sidechain
1	3	161	TYR	Sidechain
1	3	162	TYR	Sidechain
1	3	185	TYR	Sidechain
1	4	155	TYR	Sidechain
1	5	161	TYR	Sidechain
1	5	164	TYR	Sidechain
1	5	185	TYR	Sidechain
1	6	162	TYR	Sidechain
2	A	102	TYR	Sidechain
2	A	199	ARG	Sidechain
2	A	210	PRO	Peptide
2	A	355	ARG	Sidechain
2	A	358	TYR	Sidechain
2	A	381	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	A	40	ARG	Sidechain
2	A	403	ARG	Sidechain
2	A	409	THR	Peptide
2	A	468	ASN	Peptide
2	A	528	ARG	Sidechain
2	A	577	TYR	Sidechain
2	A	592	GLY	Peptide
2	A	627	PHE	Sidechain
2	A	701	PHE	Sidechain
2	A	716	LYS	Mainchain,Peptide
2	A	733	ARG	Sidechain
2	A	756	VAL	Peptide
2	A	9	ARG	Sidechain
2	B	210	PRO	Peptide
2	B	323	TYR	Sidechain
2	B	358	TYR	Sidechain
2	B	381	TYR	Sidechain
2	B	385	ARG	Sidechain
2	B	40	ARG	Sidechain
2	B	409	THR	Peptide
2	B	424	ARG	Sidechain
2	B	468	ASN	Peptide
2	B	536	ARG	Sidechain
2	B	592	GLY	Peptide
2	B	611	TYR	Sidechain
2	B	716	LYS	Peptide
2	B	756	VAL	Peptide
2	C	102	TYR	Sidechain
2	C	210	PRO	Peptide
2	C	381	TYR	Sidechain
2	C	40	ARG	Sidechain
2	C	409	THR	Peptide
2	C	468	ASN	Peptide
2	C	592	GLY	Peptide
2	C	701	PHE	Sidechain
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	83	ARG	Sidechain
2	C	9	ARG	Sidechain
2	D	102	TYR	Sidechain
2	D	122	ARG	Sidechain
2	D	210	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	D	235	ARG	Sidechain
2	D	363	ARG	Sidechain
2	D	385	ARG	Sidechain
2	D	40	ARG	Sidechain
2	D	405	ARG	Sidechain
2	D	409	THR	Peptide
2	D	468	ASN	Peptide
2	D	528	ARG	Sidechain
2	D	577	TYR	Sidechain
2	D	592	GLY	Peptide
2	D	667	ARG	Sidechain
2	D	682	HIS	Sidechain
2	D	716	LYS	Peptide
2	D	756	VAL	Peptide
2	E	23	ARG	Sidechain
2	E	358	TYR	Sidechain
2	E	361	HIS	Sidechain,Peptide
2	E	363	ARG	Sidechain
2	E	381	TYR	Sidechain
2	E	405	ARG	Sidechain
2	E	409	THR	Peptide
2	E	468	ASN	Peptide
2	E	525	ARG	Sidechain
2	E	528	ARG	Sidechain
2	E	577	TYR	Sidechain
2	E	592	GLY	Peptide
2	E	716	LYS	Peptide
2	E	756	VAL	Peptide
2	E	766	ARG	Sidechain
2	F	191	ARG	Sidechain
2	F	198	ARG	Sidechain
2	F	210	PRO	Peptide
2	F	260	ARG	Sidechain
2	F	363	ARG	Sidechain
2	F	381	TYR	Sidechain
2	F	40	ARG	Sidechain
2	F	409	THR	Peptide
2	F	424	ARG	Sidechain
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	670	TYR	Sidechain
2	F	716	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	F	756	VAL	Peptide

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	19	0
1	2	777	0	758	24	0
1	3	777	0	758	29	0
1	4	777	0	758	27	0
1	5	777	0	758	20	0
1	6	777	0	758	22	0
2	A	6200	0	6290	116	0
2	B	6200	0	6290	124	0
2	C	6200	0	6290	101	0
2	D	6200	0	6290	125	0
2	E	6200	0	6290	113	0
2	F	6200	0	6290	127	0
All	All	41862	0	42288	802	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 10.

All (802) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:281:LEU:CD1	2:F:313:GLY:HA3	1.23	1.57
2:D:281:LEU:HD11	2:D:313:GLY:CA	1.23	1.55
2:F:281:LEU:HD11	2:F:313:GLY:CA	1.00	1.47
2:A:277:PHE:CE2	2:A:279:ASP:OD1	1.69	1.45
2:D:281:LEU:CD1	2:D:313:GLY:HA3	1.53	1.38
2:E:278:ILE:HB	2:E:281:LEU:CD2	1.55	1.34
2:E:277:PHE:CE2	2:E:279:ASP:OD1	1.80	1.33
2:C:277:PHE:CZ	2:C:279:ASP:OD1	1.80	1.32
2:D:277:PHE:CE2	2:D:279:ASP:OD1	1.85	1.30
2:D:277:PHE:HE2	2:D:279:ASP:OD1	0.97	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:ILE:HB	2:C:281:LEU:CD2	1.67	1.24
2:B:278:ILE:HB	2:B:281:LEU:CD2	1.71	1.19
2:A:277:PHE:CZ	2:A:279:ASP:OD1	1.97	1.17
2:C:277:PHE:CE1	2:C:279:ASP:OD1	1.98	1.16
2:E:277:PHE:CZ	2:E:279:ASP:OD1	1.98	1.16
2:F:281:LEU:CD1	2:F:313:GLY:CA	1.91	1.15
2:E:278:ILE:HB	2:E:281:LEU:HD21	1.28	1.13
2:D:281:LEU:CD1	2:D:313:GLY:CA	2.18	1.13
2:B:278:ILE:CG2	2:B:281:LEU:HD23	1.82	1.10
2:B:278:ILE:HB	2:B:281:LEU:HD21	1.23	1.09
2:F:281:LEU:HD11	2:F:313:GLY:HA2	1.36	1.03
2:E:278:ILE:CB	2:E:281:LEU:CD2	2.39	1.00
2:A:278:ILE:HB	2:A:281:LEU:CD2	1.92	1.00
2:C:278:ILE:HB	2:C:281:LEU:HD21	1.40	0.99
2:B:278:ILE:HG22	2:B:281:LEU:HD23	1.45	0.98
2:D:281:LEU:HD11	2:D:313:GLY:HA2	1.49	0.95
2:E:278:ILE:CG2	2:E:281:LEU:HD23	1.96	0.94
2:B:278:ILE:CB	2:B:281:LEU:CD2	2.45	0.94
2:A:277:PHE:HE2	2:A:279:ASP:OD1	1.48	0.92
2:A:36:LEU:HD22	2:A:40:ARG:HE	1.33	0.92
2:F:281:LEU:CD1	2:F:313:GLY:HA2	1.96	0.90
2:C:278:ILE:CB	2:C:281:LEU:CD2	2.50	0.90
2:F:281:LEU:HD21	2:F:313:GLY:HA2	1.55	0.89
2:F:281:LEU:CG	2:F:313:GLY:HA2	2.03	0.89
1:3:203:ILE:HG23	2:C:431:VAL:HB	1.56	0.87
2:E:278:ILE:CB	2:E:281:LEU:HD23	2.04	0.86
2:A:277:PHE:CE2	2:A:279:ASP:CG	2.49	0.86
2:D:281:LEU:HD21	2:D:313:GLY:HA2	1.57	0.86
2:E:277:PHE:CE2	2:E:279:ASP:CG	2.49	0.85
2:C:278:ILE:CG2	2:C:281:LEU:HD23	2.06	0.84
2:F:281:LEU:CD2	2:F:313:GLY:HA2	2.10	0.82
2:D:278:ILE:HB	2:D:281:LEU:CD2	2.10	0.81
2:A:278:ILE:HB	2:A:281:LEU:HD21	1.59	0.80
2:F:281:LEU:CG	2:F:313:GLY:CA	2.60	0.80
2:E:277:PHE:HE2	2:E:279:ASP:CG	1.86	0.79
2:A:277:PHE:HE2	2:A:279:ASP:CG	1.84	0.78
2:B:278:ILE:CG2	2:B:281:LEU:CD2	2.60	0.78
2:C:278:ILE:CB	2:C:281:LEU:HD23	2.13	0.78
2:B:278:ILE:CB	2:B:281:LEU:HD21	2.10	0.76
2:F:60:ILE:HG23	2:F:123:VAL:HG11	1.69	0.75
2:E:278:ILE:HG22	2:E:281:LEU:HD23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:GLU:HB2	2:E:123:VAL:HG21	1.69	0.73
2:B:26:HIS:CE1	2:B:64:VAL:HG12	2.23	0.73
2:F:351:LEU:HD11	2:F:375:VAL:HG23	1.70	0.73
2:C:278:ILE:HG22	2:C:281:LEU:HD23	1.71	0.72
2:C:13:VAL:HG11	2:C:38:LEU:HD23	1.73	0.71
2:F:278:ILE:HB	2:F:281:LEU:CD2	2.21	0.70
2:E:100:HIS:CE1	2:E:107:HIS:CE1	2.79	0.70
2:C:278:ILE:O	2:C:281:LEU:CD2	2.40	0.69
2:F:524:VAL:HG11	2:F:562:ILE:HD12	1.73	0.69
2:A:361:HIS:HA	2:B:233:ILE:HG23	1.73	0.69
2:B:278:ILE:CB	2:B:281:LEU:HD23	2.18	0.69
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.28	0.69
2:A:355:ARG:HE	2:A:366:ILE:H	1.39	0.69
2:A:278:ILE:CG2	2:A:281:LEU:HD23	2.23	0.69
2:D:21:ALA:HA	2:D:33:HIS:CE1	2.27	0.68
2:C:416:LEU:HB3	2:C:453:VAL:HG22	1.74	0.68
2:D:281:LEU:HD11	2:D:313:GLY:C	2.12	0.68
2:F:36:LEU:HD21	2:F:61:GLN:HB3	1.76	0.68
2:E:277:PHE:HE2	2:E:279:ASP:OD2	1.77	0.67
2:B:363:ARG:HH21	2:B:402:VAL:HG21	1.60	0.67
2:D:26:HIS:CD2	2:D:68:ILE:HB	2.29	0.67
2:E:39:VAL:HG13	2:E:57:SER:HA	1.76	0.67
1:3:203:ILE:HG22	1:3:204:ILE:HG12	1.76	0.66
2:D:374:ALA:HA	2:D:394:LEU:HD12	1.75	0.66
2:C:38:LEU:HD22	2:C:46:ALA:HB1	1.76	0.66
2:E:33:HIS:CE1	2:E:64:VAL:CG1	2.78	0.66
1:3:133:PHE:CE2	1:3:163:LEU:HB3	2.30	0.66
2:E:33:HIS:CE1	2:E:64:VAL:HG11	2.31	0.65
1:1:139:VAL:HG11	1:1:154:LEU:HD22	1.78	0.65
1:1:203:ILE:HG23	2:A:431:VAL:HB	1.79	0.65
1:3:203:ILE:HG23	2:C:431:VAL:CB	2.26	0.65
2:D:32:GLU:HG2	2:D:64:VAL:HG13	1.76	0.65
2:C:483:TRP:HA	2:D:335:GLN:HE21	1.60	0.64
2:C:21:ALA:HA	2:C:33:HIS:CD2	2.31	0.64
2:D:281:LEU:CD2	2:D:313:GLY:HA2	2.26	0.64
2:C:278:ILE:O	2:C:281:LEU:HD21	1.97	0.64
2:C:402:VAL:HG23	2:C:475:ASP:OD1	1.97	0.64
2:B:39:VAL:HG13	2:B:57:SER:HA	1.80	0.64
1:3:154:LEU:HB2	1:3:208:ALA:HB1	1.80	0.64
2:F:377:LEU:HD21	2:F:496:THR:HG23	1.80	0.64
2:C:377:LEU:HD21	2:C:496:THR:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:GLU:HB2	2:C:64:VAL:HG22	1.80	0.63
2:B:528:ARG:HH11	2:B:562:ILE:HG22	1.64	0.63
2:E:278:ILE:O	2:E:281:LEU:CD2	2.47	0.63
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.80	0.63
2:C:277:PHE:CZ	2:C:279:ASP:CG	2.71	0.63
2:D:281:LEU:HD11	2:D:313:GLY:HA3	0.65	0.63
2:F:26:HIS:H	2:F:26:HIS:CD2	2.17	0.62
1:5:156:SER:HB2	1:5:203:ILE:HD11	1.82	0.62
2:D:13:VAL:HG11	2:D:38:LEU:HD23	1.79	0.62
2:D:503:GLU:HB2	2:D:525:ARG:HH22	1.63	0.62
2:A:277:PHE:HE2	2:A:279:ASP:OD2	1.83	0.62
2:D:476:ILE:O	2:D:480:VAL:HG23	1.99	0.62
1:5:154:LEU:HD12	1:5:203:ILE:HD12	1.81	0.61
2:F:24:LEU:HD21	2:F:61:GLN:HB2	1.83	0.61
1:2:203:ILE:HG23	2:B:431:VAL:HB	1.81	0.61
1:6:203:ILE:HG23	2:F:431:VAL:HB	1.83	0.61
2:E:31:THR:HG22	2:E:120:ALA:HB2	1.82	0.61
2:F:26:HIS:CE1	2:F:64:VAL:HG12	2.35	0.61
2:A:278:ILE:HB	2:A:281:LEU:HD23	1.81	0.61
2:A:747:ALA:HB1	2:A:801:PHE:CE2	2.36	0.61
1:5:136:PHE:CE2	1:5:203:ILE:HG21	2.36	0.61
2:E:31:THR:HB	2:E:120:ALA:H	1.64	0.61
2:D:278:ILE:CG2	2:D:281:LEU:HD23	2.31	0.60
2:C:516:ALA:HB2	2:C:710:VAL:O	2.00	0.60
1:2:154:LEU:HD22	1:2:212:ILE:HD11	1.84	0.60
2:E:26:HIS:CD2	2:E:33:HIS:HE1	2.19	0.60
2:D:278:ILE:HB	2:D:281:LEU:HD21	1.83	0.59
2:E:370:ALA:HB1	2:E:476:ILE:HD12	1.84	0.59
2:B:516:ALA:HB2	2:B:710:VAL:O	2.02	0.59
2:F:32:GLU:HB3	2:F:119:VAL:HB	1.85	0.59
2:B:416:LEU:HB3	2:B:453:VAL:HG22	1.84	0.59
2:B:394:LEU:HD13	2:B:480:VAL:HG22	1.84	0.59
2:F:36:LEU:HD11	2:F:61:GLN:HA	1.83	0.59
2:D:32:GLU:CG	2:D:64:VAL:HG13	2.32	0.59
1:2:132:ARG:HH21	1:2:190:SER:H	1.49	0.59
2:D:24:LEU:HD11	2:D:36:LEU:HD11	1.85	0.59
2:D:96:ARG:HE	2:D:96:ARG:HA	1.67	0.59
1:1:203:ILE:HG22	1:1:204:ILE:HG12	1.85	0.59
2:D:355:ARG:HH22	2:D:368:ASP:HA	1.68	0.58
2:C:31:THR:HB	2:C:120:ALA:HB2	1.83	0.58
2:B:594:VAL:HG21	2:B:626:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:ILE:O	2:E:281:LEU:HD21	2.04	0.58
2:D:39:VAL:HG13	2:D:57:SER:HA	1.85	0.58
2:F:38:LEU:HD22	2:F:46:ALA:HB1	1.85	0.58
2:B:351:LEU:HD11	2:B:375:VAL:HG23	1.85	0.58
2:D:702:ILE:HA	2:D:705:ILE:HD12	1.84	0.58
2:E:734:LEU:HD21	2:F:532:LYS:H	1.68	0.58
2:D:473:VAL:HG23	2:D:474:ASP:H	1.68	0.58
2:B:516:ALA:HB1	2:B:709:ILE:CG2	2.33	0.58
2:C:544:LEU:HB2	2:C:689:VAL:HG13	1.85	0.58
2:E:195:VAL:HA	2:E:198:ARG:HE	1.69	0.58
2:E:351:LEU:HD11	2:E:391:ALA:HB1	1.83	0.58
2:A:355:ARG:HH22	2:A:371:ILE:HD13	1.69	0.58
2:B:46:ALA:H	2:B:105:THR:HB	1.69	0.58
2:B:26:HIS:HA	2:B:68:ILE:HG21	1.85	0.57
2:D:26:HIS:HE1	2:D:64:VAL:HG12	1.69	0.57
2:C:230:VAL:HG22	2:C:231:PRO:HD2	1.86	0.57
1:4:154:LEU:HD12	1:4:162:TYR:O	2.03	0.57
2:A:516:ALA:HB1	2:A:709:ILE:CG2	2.34	0.57
2:A:31:THR:HB	2:A:120:ALA:H	1.68	0.57
2:E:747:ALA:HB1	2:E:801:PHE:CE2	2.39	0.57
2:A:60:ILE:HG23	2:A:123:VAL:HG11	1.85	0.57
2:B:46:ALA:HB2	2:B:105:THR:O	2.05	0.57
2:B:536:ARG:H	2:B:637:GLY:HA3	1.69	0.57
2:D:31:THR:HB	2:D:120:ALA:HB2	1.86	0.57
1:6:139:VAL:HG21	1:6:154:LEU:HD11	1.86	0.56
2:D:633:VAL:HG13	2:D:649:PHE:CG	2.40	0.56
2:E:403:ARG:HH22	2:E:464:GLN:HA	1.69	0.56
2:E:32:GLU:CG	2:E:64:VAL:HG13	2.36	0.56
2:D:26:HIS:CD2	2:D:26:HIS:N	2.72	0.56
2:D:690:MET:HA	2:D:693:LEU:HD23	1.88	0.56
2:A:523:ALA:HA	2:A:526:ARG:HE	1.70	0.56
2:D:26:HIS:CE1	2:D:64:VAL:HG12	2.41	0.56
2:E:32:GLU:HB3	2:E:119:VAL:HG12	1.86	0.56
2:A:278:ILE:CB	2:A:281:LEU:HD23	2.36	0.56
2:B:38:LEU:HD22	2:B:46:ALA:HB1	1.87	0.56
2:F:26:HIS:H	2:F:26:HIS:HD2	1.54	0.56
2:E:474:ASP:O	2:E:477:ALA:HB3	2.06	0.55
2:D:362:HIS:CD2	2:E:232:GLU:HB3	2.41	0.55
2:E:506:LEU:HG	2:E:562:ILE:HD11	1.88	0.55
2:A:38:LEU:HD22	2:A:46:ALA:CB	2.36	0.55
2:D:574:MET:SD	2:D:619:ILE:HG22	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:GLU:HG3	2:E:64:VAL:HG13	1.88	0.55
2:B:13:VAL:HG11	2:B:38:LEU:HD23	1.89	0.55
2:C:398:ALA:HA	2:C:479:VAL:HG11	1.89	0.55
2:E:21:ALA:HB3	2:E:29:ILE:HD12	1.88	0.55
2:E:371:ILE:O	2:E:374:ALA:HB3	2.07	0.55
1:3:142:LEU:HD22	1:3:209:LEU:HD13	1.88	0.55
1:3:164:TYR:HB2	1:3:196:LEU:HD12	1.88	0.55
2:B:477:ALA:HA	2:B:480:VAL:HG23	1.88	0.55
1:6:154:LEU:HD22	1:6:212:ILE:HD11	1.89	0.55
2:B:32:GLU:HB3	2:B:119:VAL:HB	1.87	0.55
1:1:154:LEU:HD12	1:1:162:TYR:O	2.06	0.55
2:A:516:ALA:HB2	2:A:710:VAL:O	2.06	0.55
2:C:281:LEU:HG	2:C:314:ALA:H	1.71	0.55
2:E:367:THR:H	2:E:471:VAL:H	1.55	0.55
1:2:139:VAL:HG21	1:2:154:LEU:HD11	1.88	0.55
2:A:394:LEU:HD13	2:A:480:VAL:CG2	2.36	0.55
2:A:698:ARG:HE	2:A:701:PHE:HB2	1.72	0.55
2:F:509:ARG:HE	2:F:557:ALA:HA	1.72	0.55
1:5:140:ILE:HG12	1:5:212:ILE:HG23	1.87	0.55
2:B:374:ALA:HA	2:B:394:LEU:HD12	1.87	0.55
2:E:747:ALA:HB1	2:E:801:PHE:CZ	2.42	0.55
2:C:39:VAL:HG13	2:C:57:SER:HA	1.88	0.54
2:D:278:ILE:HB	2:D:281:LEU:HD23	1.89	0.54
1:6:131:LEU:HD22	1:6:183:LEU:HD21	1.88	0.54
2:A:278:ILE:HG22	2:A:281:LEU:HD23	1.88	0.54
2:F:516:ALA:HB2	2:F:710:VAL:O	2.08	0.54
1:3:133:PHE:CG	1:3:139:VAL:HG22	2.42	0.54
1:3:207:HIS:CE1	1:3:211:THR:HG21	2.43	0.54
1:5:139:VAL:HG13	1:5:163:LEU:HG	1.88	0.54
2:D:195:VAL:HA	2:D:198:ARG:HE	1.71	0.54
1:4:216:PHE:CE1	2:D:440:ALA:HA	2.42	0.54
2:A:351:LEU:HD11	2:A:375:VAL:HG23	1.90	0.54
2:E:278:ILE:HB	2:E:281:LEU:HD22	1.77	0.54
2:B:355:ARG:HH22	2:B:368:ASP:HA	1.72	0.54
1:5:152:THR:HG23	1:5:209:LEU:H	1.73	0.54
1:4:136:PHE:CZ	1:4:216:PHE:CZ	2.95	0.54
2:A:367:THR:H	2:A:471:VAL:HG12	1.73	0.54
2:B:24:LEU:HD12	2:B:33:HIS:CE1	2.43	0.54
2:B:26:HIS:HE1	2:B:64:VAL:HG12	1.69	0.54
2:A:198:ARG:HH12	2:F:483:TRP:HE1	1.56	0.54
2:A:197:SER:HB2	2:F:400:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:ILE:CB	2:E:281:LEU:HD21	2.18	0.53
2:E:395:ILE:HA	2:E:476:ILE:HD11	1.89	0.53
1:6:133:PHE:CE2	1:6:163:LEU:HB3	2.44	0.53
2:E:106:GLU:HG2	2:E:107:HIS:CD2	2.43	0.53
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.89	0.53
2:A:574:MET:HG3	2:A:619:ILE:HG22	1.89	0.53
2:B:377:LEU:HD22	2:B:495:GLU:HB2	1.90	0.53
2:D:750:LYS:HB2	2:D:796:VAL:HG21	1.89	0.53
2:F:278:ILE:HB	2:F:281:LEU:HD21	1.90	0.53
1:2:202:LEU:HD12	1:2:202:LEU:H	1.73	0.53
2:C:377:LEU:HD22	2:C:495:GLU:CB	2.37	0.53
2:A:524:VAL:HG11	2:A:562:ILE:HD12	1.89	0.53
1:1:183:LEU:HD22	2:A:83:ARG:HH21	1.74	0.53
1:6:202:LEU:HD12	1:6:202:LEU:H	1.73	0.53
2:A:181:PRO:HA	2:A:223:GLN:HE22	1.74	0.53
2:C:63:GLU:HB3	2:C:123:VAL:HG13	1.91	0.53
2:E:39:VAL:HG11	2:E:60:ILE:CG1	2.39	0.53
2:C:195:VAL:HA	2:C:198:ARG:HE	1.74	0.53
2:D:437:GLU:HA	2:D:440:ALA:HB3	1.90	0.53
2:E:477:ALA:HB1	2:E:495:GLU:N	2.23	0.53
2:B:68:ILE:HD12	2:B:68:ILE:H	1.74	0.52
2:E:27:ASN:HD22	2:E:76:GLN:H	1.55	0.52
1:2:154:LEU:HD12	1:2:162:TYR:O	2.09	0.52
1:2:203:ILE:HG23	2:B:431:VAL:CB	2.39	0.52
2:B:520:VAL:HG23	2:B:709:ILE:HD12	1.91	0.52
2:B:714:LEU:HA	2:B:718:HIS:CD2	2.44	0.52
2:C:516:ALA:HB1	2:C:709:ILE:CG2	2.39	0.52
2:D:544:LEU:HD13	2:D:693:LEU:HB3	1.92	0.52
2:D:747:ALA:HB1	2:D:801:PHE:CZ	2.45	0.52
2:F:516:ALA:HB1	2:F:709:ILE:CG2	2.39	0.52
2:F:524:VAL:HG11	2:F:562:ILE:CD1	2.39	0.52
2:E:38:LEU:HD22	2:E:46:ALA:HB1	1.92	0.52
2:F:477:ALA:HB1	2:F:495:GLU:N	2.24	0.52
2:D:281:LEU:CG	2:D:313:GLY:HA2	2.39	0.52
2:A:197:SER:HB3	2:A:233:ILE:HG21	1.90	0.52
2:A:528:ARG:CZ	2:A:562:ILE:HG23	2.40	0.52
2:B:394:LEU:CD1	2:B:480:VAL:HG22	2.39	0.52
2:B:24:LEU:HD22	2:B:65:GLU:HB2	1.91	0.52
2:C:633:VAL:HG13	2:C:649:PHE:CG	2.45	0.52
2:F:750:LYS:HB2	2:F:796:VAL:HG21	1.91	0.52
1:5:152:THR:CG2	1:5:209:LEU:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ALA:HB1	2:B:475:ASP:CG	2.31	0.52
2:C:363:ARG:HD2	2:C:403:ARG:H	1.75	0.52
2:D:747:ALA:HB1	2:D:801:PHE:CE2	2.45	0.52
2:F:473:VAL:HG23	2:F:474:ASP:H	1.75	0.52
2:A:383:SER:H	2:A:390:LYS:HD3	1.75	0.51
2:E:63:GLU:HG3	2:E:123:VAL:HG22	1.91	0.51
2:F:278:ILE:CG2	2:F:281:LEU:HD23	2.40	0.51
1:3:136:PHE:CE1	1:3:212:ILE:CD1	2.93	0.51
1:1:153:THR:HB	1:1:164:TYR:CE2	2.46	0.51
2:C:449:LEU:O	2:C:453:VAL:HG23	2.10	0.51
2:E:380:ARG:HB3	2:E:528:ARG:HE	1.75	0.51
2:A:374:ALA:HA	2:A:394:LEU:HD12	1.93	0.51
1:4:145:LEU:HD13	2:D:27:ASN:HD21	1.76	0.51
2:C:40:ARG:HH11	2:C:57:SER:HB2	1.76	0.51
2:A:361:HIS:CE1	2:B:199:ARG:HD3	2.46	0.51
2:B:32:GLU:CG	2:B:64:VAL:HG13	2.41	0.51
2:E:113:ILE:HG21	2:E:135:ARG:HB2	1.92	0.51
2:E:363:ARG:HH11	2:E:399:GLY:HA2	1.76	0.51
1:2:133:PHE:CE2	1:2:163:LEU:HB3	2.46	0.51
1:3:130:VAL:HG13	1:3:196:LEU:HD11	1.93	0.51
1:3:139:VAL:HG11	1:3:154:LEU:HD22	1.93	0.51
2:A:195:VAL:HG13	2:A:198:ARG:HH21	1.75	0.51
2:E:109:LEU:HB3	2:E:138:VAL:HG11	1.93	0.51
2:F:188:GLU:HG3	2:F:339:VAL:HA	1.94	0.50
1:5:133:PHE:CE2	1:5:163:LEU:HB3	2.46	0.50
2:D:541:PHE:HA	2:D:705:ILE:HG23	1.93	0.50
2:E:394:LEU:CD1	2:E:480:VAL:HG22	2.41	0.50
1:1:142:LEU:HD12	1:1:209:LEU:HD22	1.93	0.50
2:A:38:LEU:HD22	2:A:46:ALA:HB1	1.93	0.50
2:A:520:VAL:HG23	2:A:709:ILE:HD12	1.93	0.50
2:A:20:GLU:HB3	2:A:36:LEU:HD13	1.94	0.50
2:D:38:LEU:HD22	2:D:46:ALA:HB1	1.94	0.50
2:F:46:ALA:HA	2:F:138:VAL:CG1	2.41	0.50
2:F:23:ARG:HH11	2:F:24:LEU:HD23	1.76	0.50
2:B:106:GLU:HG2	2:B:107:HIS:CD2	2.47	0.50
2:E:397:GLU:HB3	2:E:479:VAL:HB	1.92	0.50
1:2:203:ILE:HG22	1:2:204:ILE:HG12	1.94	0.50
1:6:154:LEU:HD12	1:6:162:TYR:O	2.12	0.50
2:B:95:ALA:CB	2:B:103:VAL:HG22	2.41	0.50
2:B:401:LYS:HD2	2:B:479:VAL:HG12	1.94	0.50
2:F:166:LEU:HA	2:F:167:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:GLY:H	2:F:72:GLN:HE22	1.59	0.50
2:E:351:LEU:HD12	2:E:371:ILE:HG23	1.94	0.50
1:4:140:ILE:HA	1:4:212:ILE:HG21	1.94	0.50
2:B:20:GLU:HB3	2:B:36:LEU:HD13	1.94	0.50
2:B:516:ALA:HB1	2:B:709:ILE:HG23	1.94	0.50
1:4:152:THR:HG21	1:4:209:LEU:HG	1.94	0.50
2:C:351:LEU:HG	2:C:392:ILE:HG23	1.94	0.50
2:E:374:ALA:HB1	2:E:391:ALA:O	2.12	0.50
1:3:156:SER:HB3	1:3:203:ILE:HD11	1.94	0.49
2:A:278:ILE:O	2:A:281:LEU:CD2	2.60	0.49
2:D:60:ILE:HG23	2:D:123:VAL:HG11	1.94	0.49
2:E:67:LEU:HD11	2:E:123:VAL:HG23	1.94	0.49
1:4:142:LEU:HD11	1:4:182:LEU:HD23	1.93	0.49
2:B:67:LEU:HD22	2:B:119:VAL:HG22	1.94	0.49
1:1:133:PHE:CD2	1:1:163:LEU:HB3	2.47	0.49
1:4:154:LEU:HD13	1:4:163:LEU:HD23	1.93	0.49
2:B:29:ILE:HG22	2:B:33:HIS:CD2	2.47	0.49
2:C:363:ARG:HB3	2:C:399:GLY:HA2	1.94	0.49
2:C:558:LEU:HD22	2:C:613:VAL:HG22	1.92	0.49
2:D:36:LEU:HD11	2:D:61:GLN:HA	1.93	0.49
2:F:20:GLU:HB3	2:F:36:LEU:HD13	1.93	0.49
2:F:398:ALA:HB2	2:F:479:VAL:HG12	1.94	0.49
2:C:60:ILE:HG23	2:C:123:VAL:HG11	1.94	0.49
1:3:216:PHE:CE1	2:C:440:ALA:HA	2.48	0.49
2:F:498:LYS:HD2	2:F:564:GLY:HA2	1.95	0.49
1:6:216:PHE:CE2	2:F:440:ALA:HA	2.47	0.49
2:C:36:LEU:HD12	2:C:64:VAL:HG21	1.94	0.49
2:C:689:VAL:HB	2:C:710:VAL:HG13	1.93	0.49
2:F:277:PHE:CZ	2:F:279:ASP:OD1	2.66	0.49
1:2:133:PHE:CD2	1:2:163:LEU:HB3	2.48	0.49
2:C:38:LEU:O	2:C:47:ALA:HB2	2.12	0.49
2:D:431:VAL:HG13	2:D:439:ALA:CB	2.43	0.49
2:D:545:GLY:H	2:D:660:VAL:HB	1.77	0.49
2:F:667:ARG:HH21	2:F:681:ASN:HD21	1.61	0.49
1:5:137:GLU:HA	1:5:140:ILE:HD12	1.94	0.49
2:A:370:ALA:HB1	2:A:476:ILE:HD12	1.95	0.49
2:B:449:LEU:O	2:B:453:VAL:HG23	2.13	0.49
2:C:109:LEU:HB3	2:C:138:VAL:HG11	1.95	0.49
2:D:278:ILE:HG22	2:D:281:LEU:HD23	1.93	0.49
1:4:203:ILE:HG23	2:D:431:VAL:HB	1.93	0.49
1:5:136:PHE:HE2	1:5:203:ILE:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:278:ILE:CB	2:A:281:LEU:CD2	2.75	0.49
2:A:26:HIS:CG	2:A:33:HIS:CE1	3.01	0.49
2:A:402:VAL:HG13	2:A:405:ARG:HE	1.78	0.49
2:B:746:ALA:HB1	2:B:796:VAL:H	1.78	0.49
2:E:543:PHE:CZ	2:E:655:ILE:HD13	2.47	0.49
2:F:265:MET:O	2:F:268:ILE:HG22	2.13	0.49
2:F:367:THR:H	2:F:471:VAL:HG12	1.77	0.49
2:F:13:VAL:HG11	2:F:38:LEU:HD23	1.94	0.49
2:F:377:LEU:HD22	2:F:495:GLU:HB2	1.94	0.49
2:A:524:VAL:HG11	2:A:562:ILE:CD1	2.43	0.49
2:A:562:ILE:HG22	2:A:563:PHE:CE1	2.47	0.49
2:B:36:LEU:HD21	2:B:61:GLN:HB3	1.94	0.49
2:C:377:LEU:HD22	2:C:495:GLU:HB3	1.94	0.49
2:E:67:LEU:HD11	2:E:123:VAL:CG2	2.43	0.49
2:F:363:ARG:HG3	2:F:363:ARG:HH11	1.78	0.49
2:F:476:ILE:O	2:F:479:VAL:HG13	2.13	0.49
2:B:394:LEU:HD21	2:B:480:VAL:HA	1.94	0.48
2:C:26:HIS:CG	2:C:33:HIS:CE1	3.01	0.48
2:C:713:SER:O	2:C:718:HIS:CG	2.66	0.48
2:D:398:ALA:HB2	2:D:476:ILE:HA	1.95	0.48
2:D:394:LEU:HD13	2:D:480:VAL:CG2	2.43	0.48
2:E:473:VAL:HG23	2:E:474:ASP:H	1.78	0.48
2:F:32:GLU:HB2	2:F:64:VAL:HG13	1.94	0.48
1:3:139:VAL:HG11	1:3:154:LEU:CD2	2.43	0.48
2:A:371:ILE:O	2:A:374:ALA:HB3	2.14	0.48
2:A:586:LEU:HB3	2:B:594:VAL:H	1.77	0.48
2:D:348:ILE:HG12	2:D:375:VAL:HG21	1.94	0.48
2:E:33:HIS:CD2	2:E:36:LEU:HD13	2.48	0.48
2:A:374:ALA:HB2	2:A:476:ILE:HD13	1.95	0.48
2:C:528:ARG:HD3	2:C:538:ILE:HG21	1.96	0.48
2:E:363:ARG:HE	2:E:467:GLU:HB3	1.79	0.48
2:D:20:GLU:HG3	2:D:36:LEU:HD13	1.95	0.48
2:F:100:HIS:CD2	2:F:145:ASN:HB2	2.48	0.48
2:F:392:ILE:HA	2:F:395:ILE:HD12	1.95	0.48
2:A:281:LEU:HG	2:A:314:ALA:H	1.77	0.48
1:1:136:PHE:CZ	2:A:431:VAL:HG11	2.48	0.48
2:B:398:ALA:HA	2:B:479:VAL:HG11	1.94	0.48
2:D:113:ILE:HG21	2:D:135:ARG:HB2	1.96	0.48
2:F:563:PHE:CG	2:F:611:TYR:CE1	3.02	0.48
2:F:60:ILE:HA	2:F:123:VAL:HG11	1.94	0.48
2:D:476:ILE:O	2:D:479:VAL:HG22	2.14	0.48

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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	0.48
2:B:374:ALA:HB2	2:B:476:ILE:HD13	1.96	0.48
2:C:9:ARG:HH22	2:C:45:ILE:HD12	1.78	0.48
2:E:502:MET:HB3	2:E:525:ARG:HH21	1.79	0.48
2:A:481:SER:HA	2:A:564:GLY:HA3	1.96	0.48
2:F:686:LYS:HA	2:F:712:HIS:CE1	2.49	0.48
1:6:177:ASN:HD21	2:F:67:LEU:HD11	1.79	0.48
2:A:394:LEU:HD22	2:A:480:VAL:HG22	1.96	0.48
2:A:516:ALA:HB1	2:A:709:ILE:HG23	1.94	0.48
2:E:634:LEU:HD21	2:E:701:PHE:CZ	2.49	0.48
1:5:136:PHE:CE2	2:E:431:VAL:HG21	2.49	0.47
1:6:152:THR:HG23	1:6:209:LEU:H	1.79	0.47
2:C:471:VAL:CG1	2:C:476:ILE:HD11	2.44	0.47
1:6:139:VAL:HG21	1:6:154:LEU:CD1	2.44	0.47
1:6:136:PHE:CZ	1:6:216:PHE:CZ	3.02	0.47
2:D:26:HIS:CG	2:D:68:ILE:HB	2.49	0.47
2:E:623:HIS:CD2	2:E:624:PRO:HD2	2.49	0.47
1:3:183:LEU:HB3	2:C:83:ARG:HH21	1.79	0.47
1:4:152:THR:HG23	1:4:208:ALA:N	2.29	0.47
2:B:63:GLU:HB3	2:B:123:VAL:HG13	1.96	0.47
2:B:25:GLY:HA2	2:B:73:GLU:HA	1.95	0.47
2:C:555:ALA:HB1	2:C:569:MET:SD	2.53	0.47
2:E:377:LEU:HD22	2:E:381:TYR:OH	2.15	0.47
2:A:36:LEU:HD21	2:A:61:GLN:CA	2.45	0.47
2:B:60:ILE:HG23	2:B:123:VAL:HG11	1.97	0.47
2:C:277:PHE:HZ	2:C:279:ASP:OD1	1.75	0.47
2:A:24:LEU:HD21	2:A:61:GLN:HG2	1.96	0.47
2:D:53:LEU:HD21	2:D:134:ALA:HA	1.95	0.47
2:A:278:ILE:O	2:A:281:LEU:HD21	2.14	0.47
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.96	0.47
2:D:377:LEU:HD22	2:D:495:GLU:HB2	1.97	0.47
2:E:381:TYR:CD2	2:E:563:PHE:HB3	2.50	0.47
2:E:714:LEU:HA	2:E:718:HIS:CE1	2.49	0.47
2:B:36:LEU:HD11	2:B:61:GLN:HA	1.97	0.47
2:D:370:ALA:O	2:D:373:ALA:HB3	2.14	0.47
2:F:106:GLU:HG2	2:F:107:HIS:CD2	2.49	0.47
2:F:35:LEU:HG	2:F:60:ILE:HD13	1.96	0.47
1:1:154:LEU:HB2	1:1:208:ALA:HB1	1.97	0.47
2:A:747:ALA:HA	2:A:796:VAL:HG23	1.96	0.47
2:C:13:VAL:CG1	2:C:38:LEU:HD23	2.45	0.47
2:D:403:ARG:HH21	2:E:232:GLU:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:ARG:HH22	2:E:100:HIS:CE1	2.33	0.47
2:A:26:HIS:HE1	2:A:67:LEU:HB2	1.80	0.47
2:B:603:THR:HG23	2:B:647:VAL:HG11	1.96	0.47
2:B:543:PHE:CD1	2:B:655:ILE:HG23	2.50	0.47
2:E:53:LEU:HD21	2:E:134:ALA:HA	1.97	0.47
2:F:357:ARG:HE	2:F:360:ALA:HB2	1.80	0.47
1:4:156:SER:CB	1:4:203:ILE:HD11	2.45	0.47
2:B:278:ILE:O	2:B:281:LEU:CD2	2.63	0.47
2:D:278:ILE:CB	2:D:281:LEU:HD23	2.45	0.47
2:D:281:LEU:CG	2:D:313:GLY:CA	2.90	0.47
2:E:374:ALA:HA	2:E:394:LEU:HD12	1.96	0.47
2:E:24:LEU:HD21	2:E:61:GLN:OE1	2.14	0.47
1:4:133:PHE:CE2	1:4:163:LEU:HB3	2.50	0.47
2:B:39:VAL:HG11	2:B:60:ILE:CG1	2.44	0.47
1:1:133:PHE:CE2	1:1:163:LEU:HB3	2.51	0.46
2:B:95:ALA:HB3	2:B:103:VAL:HG22	1.95	0.46
2:C:751:VAL:HG11	2:C:769:ILE:HG13	1.96	0.46
2:F:616:LEU:HD13	2:F:630:LEU:HD22	1.97	0.46
1:6:142:LEU:HD23	1:6:185:TYR:CD2	2.50	0.46
2:A:198:ARG:HH22	2:A:335:GLN:HG3	1.80	0.46
2:D:32:GLU:HB3	2:D:119:VAL:CG1	2.45	0.46
2:D:750:LYS:HG3	2:D:772:HIS:CE1	2.50	0.46
2:E:26:HIS:CG	2:E:33:HIS:CE1	3.02	0.46
2:F:104:GLY:H	2:F:107:HIS:HD1	1.63	0.46
2:A:531:LEU:HA	2:F:737:GLN:HE22	1.80	0.46
1:2:147:VAL:HG13	1:2:148:ASN:H	1.79	0.46
2:A:203:ASN:HD22	2:A:311:CYS:H	1.64	0.46
2:C:202:ASN:HD21	2:C:307:GLY:HA2	1.80	0.46
2:D:18:GLN:O	2:D:21:ALA:HB3	2.15	0.46
2:E:26:HIS:CG	2:E:33:HIS:HE1	2.34	0.46
2:E:473:VAL:HB	2:E:493:GLN:H	1.79	0.46
2:A:39:VAL:HG13	2:A:57:SER:HA	1.97	0.46
2:B:363:ARG:HB3	2:B:399:GLY:HA2	1.97	0.46
2:D:183:ILE:H	2:D:183:ILE:HD12	1.78	0.46
2:E:541:PHE:HA	2:E:705:ILE:HG23	1.98	0.46
1:6:145:LEU:HB3	2:F:72:GLN:HG2	1.97	0.46
2:B:394:LEU:CD2	2:B:483:TRP:CZ2	2.97	0.46
1:2:216:PHE:CE2	2:B:440:ALA:HA	2.51	0.46
2:B:555:ALA:HB1	2:B:615:LEU:HD21	1.98	0.46
2:C:33:HIS:HE2	2:C:64:VAL:HG13	1.81	0.46
2:D:191:ARG:HH22	2:D:335:GLN:HE22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:TYR:CE1	2:D:562:ILE:O	2.69	0.46
2:E:33:HIS:NE2	2:E:64:VAL:HG11	2.30	0.46
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.50	0.46
2:F:395:ILE:HA	2:F:476:ILE:HD11	1.98	0.46
2:A:620:GLU:HG3	2:A:659:ASN:H	1.81	0.46
2:B:63:GLU:OE2	2:B:123:VAL:HG22	2.16	0.46
2:D:373:ALA:HB2	2:D:492:ALA:CB	2.46	0.46
2:E:543:PHE:CD1	2:E:655:ILE:HG23	2.51	0.46
2:A:23:ARG:HH11	2:A:24:LEU:HD23	1.80	0.46
2:A:26:HIS:CE1	2:A:67:LEU:HB2	2.51	0.46
2:B:119:VAL:O	2:B:123:VAL:HG23	2.16	0.46
2:A:555:ALA:HB1	2:A:569:MET:SD	2.55	0.46
2:D:370:ALA:HB1	2:D:476:ILE:HD12	1.98	0.46
2:F:281:LEU:CD1	2:F:313:GLY:C	2.76	0.46
2:D:772:HIS:CD2	2:D:776:ARG:HH21	2.33	0.46
2:A:394:LEU:CD2	2:A:480:VAL:HG13	2.46	0.46
2:A:528:ARG:NH2	2:A:562:ILE:HG23	2.31	0.46
2:C:382:ILE:HG12	2:C:611:TYR:CE2	2.51	0.46
2:D:544:LEU:HD13	2:D:693:LEU:CB	2.47	0.46
2:D:563:PHE:CD1	2:D:611:TYR:CE2	3.04	0.46
1:4:183:LEU:HB3	2:D:83:ARG:HH21	1.80	0.46
2:E:281:LEU:HG	2:E:314:ALA:H	1.79	0.46
2:F:36:LEU:HG	2:F:60:ILE:HG22	1.98	0.46
2:E:10:ALA:HB1	2:E:108:ILE:HD11	1.97	0.45
2:F:35:LEU:HB2	2:F:120:ALA:HB1	1.98	0.45
2:F:723:VAL:HG22	2:F:765:LEU:HD13	1.98	0.45
1:4:210:GLU:CD	1:4:210:GLU:H	2.20	0.45
2:A:371:ILE:HD11	2:A:395:ILE:HG23	1.98	0.45
2:A:385:ARG:HD2	2:A:385:ARG:H	1.81	0.45
2:B:516:ALA:HB1	2:B:709:ILE:HG22	1.99	0.45
2:D:281:LEU:CD1	2:D:313:GLY:HA2	2.20	0.45
2:D:394:LEU:HD23	2:D:483:TRP:CH2	2.52	0.45
2:D:470:GLU:HG2	2:D:472:THR:H	1.81	0.45
2:D:394:LEU:HD22	2:D:480:VAL:HG22	1.97	0.45
2:E:631:LEU:HD13	2:E:701:PHE:HA	1.97	0.45
2:F:46:ALA:HB2	2:F:105:THR:O	2.16	0.45
2:F:38:LEU:HD22	2:F:46:ALA:CB	2.45	0.45
2:F:49:ALA:O	2:F:53:LEU:HD22	2.16	0.45
1:3:136:PHE:CE1	1:3:212:ILE:HD11	2.51	0.45
2:C:606:VAL:HG11	2:C:649:PHE:CD1	2.50	0.45
2:E:191:ARG:HH21	2:E:195:VAL:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ILE:O	2:B:374:ALA:HB3	2.16	0.45
2:E:606:VAL:HG11	2:E:649:PHE:CD1	2.51	0.45
2:F:366:ILE:HB	2:F:367:THR:HA	1.97	0.45
2:B:377:LEU:HD21	2:B:496:THR:HG23	1.98	0.45
2:F:374:ALA:HA	2:F:394:LEU:HD12	1.99	0.45
1:1:136:PHE:CZ	1:1:216:PHE:CE1	3.05	0.45
1:2:145:LEU:HD13	2:B:68:ILE:HG23	1.99	0.45
1:6:155:TYR:CD2	1:6:196:LEU:HB3	2.52	0.45
2:A:544:LEU:HD11	2:A:693:LEU:HD22	1.99	0.45
2:F:363:ARG:HD2	2:F:399:GLY:HA2	1.98	0.45
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.52	0.45
2:B:94:GLU:O	2:B:107:HIS:CD2	2.69	0.45
2:B:363:ARG:HH21	2:B:402:VAL:CG2	2.28	0.45
2:D:506:LEU:HD21	2:D:558:LEU:HD23	1.97	0.45
2:F:281:LEU:HG	2:F:314:ALA:H	1.81	0.45
2:A:40:ARG:HH21	2:A:61:GLN:HB2	1.81	0.45
2:B:603:THR:HG22	2:B:607:ARG:HH12	1.81	0.45
2:C:355:ARG:HE	2:C:371:ILE:HG12	1.82	0.45
1:4:136:PHE:CZ	1:4:203:ILE:CG2	3.00	0.45
2:B:278:ILE:O	2:B:281:LEU:HD21	2.17	0.45
2:B:431:VAL:HG13	2:B:439:ALA:CB	2.47	0.45
2:E:100:HIS:CE1	2:E:107:HIS:HE1	2.29	0.45
2:F:377:LEU:HD22	2:F:495:GLU:CB	2.47	0.45
1:3:136:PHE:CE1	1:3:203:ILE:HG21	2.52	0.45
2:A:26:HIS:CG	2:A:33:HIS:HE1	2.35	0.45
2:B:380:ARG:HG3	2:B:528:ARG:HG3	1.99	0.45
2:B:612:SER:H	2:B:652:THR:HG22	1.83	0.45
2:F:94:GLU:O	2:F:107:HIS:CD2	2.70	0.45
2:F:63:GLU:HB3	2:F:123:VAL:HG13	1.99	0.45
2:B:24:LEU:HD21	2:B:61:GLN:OE1	2.17	0.44
2:B:707:GLU:HB2	2:B:709:ILE:HD11	1.99	0.44
2:F:528:ARG:HH21	2:F:538:ILE:HG12	1.82	0.44
2:F:686:LYS:HA	2:F:712:HIS:HE1	1.82	0.44
2:A:763:ARG:HE	2:B:702:ILE:HD12	1.82	0.44
2:C:27:ASN:H	2:C:72:GLN:HE21	1.65	0.44
2:D:106:GLU:HG2	2:D:107:HIS:H	1.82	0.44
2:D:360:ALA:O	2:D:361:HIS:CG	2.70	0.44
1:6:203:ILE:HG22	1:6:204:ILE:HG12	1.99	0.44
2:A:17:ALA:HB2	2:A:34:ILE:HA	1.99	0.44
2:A:36:LEU:HD11	2:A:61:GLN:HA	1.99	0.44
2:C:723:VAL:HG22	2:C:765:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:747:ALA:HB1	2:C:801:PHE:CZ	2.52	0.44
1:3:142:LEU:HD21	1:3:182:LEU:HD23	1.99	0.44
2:A:281:LEU:HD21	2:A:313:GLY:HA2	1.76	0.44
2:B:281:LEU:HG	2:B:314:ALA:H	1.82	0.44
2:D:26:HIS:HB2	2:D:33:HIS:CE1	2.53	0.44
2:D:26:HIS:ND1	2:D:33:HIS:CE1	2.85	0.44
2:D:33:HIS:CD2	2:D:64:VAL:HG11	2.52	0.44
2:E:477:ALA:HB1	2:E:494:THR:C	2.37	0.44
2:F:21:ALA:HB2	2:F:29:ILE:HG23	1.98	0.44
2:F:36:LEU:HD12	2:F:64:VAL:HG11	1.99	0.44
1:3:142:LEU:HD22	1:3:209:LEU:CD1	2.48	0.44
2:A:355:ARG:NH2	2:A:371:ILE:HD13	2.32	0.44
2:C:395:ILE:HA	2:C:476:ILE:HD12	1.99	0.44
1:3:152:THR:HG23	1:3:209:LEU:H	1.83	0.44
1:3:136:PHE:CE2	1:3:216:PHE:CE1	3.05	0.44
2:A:26:HIS:CE1	2:A:64:VAL:O	2.71	0.44
2:B:751:VAL:HG11	2:B:769:ILE:HG13	1.99	0.44
2:C:685:MET:C	2:C:687:ASP:H	2.21	0.44
2:D:21:ALA:HB2	2:D:29:ILE:HD11	2.00	0.44
2:F:378:SER:HB3	2:F:390:LYS:HB2	1.99	0.44
2:B:473:VAL:HG23	2:B:474:ASP:H	1.83	0.44
2:B:667:ARG:HH21	2:B:681:ASN:HD22	1.66	0.44
2:B:400:SER:HB2	2:C:197:SER:HB3	1.99	0.44
2:C:206:LEU:HB3	2:C:339:VAL:HG21	2.00	0.44
2:E:36:LEU:HD12	2:E:64:VAL:HG11	2.00	0.44
2:F:278:ILE:HB	2:F:281:LEU:HD23	1.99	0.44
2:F:426:GLU:HG3	2:F:427:LYS:H	1.81	0.44
2:F:536:ARG:HG2	2:F:537:PRO:HD2	1.98	0.44
2:A:516:ALA:HB1	2:A:709:ILE:HG22	2.00	0.44
2:B:26:HIS:CE1	2:B:68:ILE:HB	2.53	0.44
2:B:550:GLY:HA3	2:B:711:PHE:CD1	2.53	0.44
2:C:38:LEU:HD13	2:C:109:LEU:HD13	1.99	0.44
2:C:471:VAL:HG13	2:C:476:ILE:HD11	1.99	0.44
2:E:628:ASN:HA	2:E:698:ARG:HH22	1.83	0.44
2:F:627:PHE:HB3	2:F:701:PHE:HB2	2.00	0.44
2:A:31:THR:HG22	2:A:120:ALA:HB2	1.98	0.44
2:B:499:LEU:C	2:B:499:LEU:HD22	2.38	0.44
2:C:362:HIS:CD2	2:D:232:GLU:HB3	2.53	0.44
2:C:381:TYR:HB2	2:C:480:VAL:HG11	1.99	0.44
2:D:18:GLN:HE22	2:D:79:HIS:HA	1.83	0.44
2:E:21:ALA:CB	2:E:29:ILE:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:139:VAL:HG21	1:2:154:LEU:CD1	2.48	0.43
2:A:64:VAL:HG22	2:A:123:VAL:HG21	2.00	0.43
2:B:594:VAL:HG21	2:B:626:VAL:CG1	2.49	0.43
2:D:697:PHE:CD2	2:D:702:ILE:HG21	2.53	0.43
2:F:669:LYS:HZ3	2:F:715:GLU:HG3	1.82	0.43
1:2:181:ILE:HG23	2:B:68:ILE:HG13	1.99	0.43
2:A:39:VAL:HG11	2:A:60:ILE:HG13	2.00	0.43
2:A:669:LYS:HE3	2:A:682:HIS:CE1	2.54	0.43
2:B:198:ARG:HG2	2:B:201:LYS:H	1.83	0.43
2:B:385:ARG:HH11	2:B:390:LYS:HA	1.82	0.43
2:C:524:VAL:HG11	2:C:562:ILE:CG1	2.47	0.43
2:E:26:HIS:CE1	2:E:64:VAL:O	2.71	0.43
1:3:136:PHE:CZ	1:3:203:ILE:HG21	2.53	0.43
2:B:381:TYR:HA	2:B:611:TYR:CE1	2.53	0.43
2:C:543:PHE:CZ	2:C:655:ILE:HD13	2.53	0.43
2:A:355:ARG:HB2	2:A:364:VAL:HG12	2.00	0.43
2:A:701:PHE:CE2	2:A:705:ILE:HD11	2.54	0.43
2:D:109:LEU:HB3	2:D:138:VAL:HG11	2.01	0.43
2:E:21:ALA:HA	2:E:33:HIS:NE2	2.33	0.43
2:F:355:ARG:HH22	2:F:368:ASP:HA	1.83	0.43
2:F:431:VAL:HG22	2:F:439:ALA:HB2	2.01	0.43
2:F:7:THR:HG21	2:F:9:ARG:HH21	1.83	0.43
1:4:156:SER:HB3	1:4:203:ILE:HD11	2.01	0.43
1:4:207:HIS:CG	1:4:210:GLU:HB2	2.53	0.43
2:A:794:LEU:HG	2:A:803:VAL:HG22	2.01	0.43
2:D:20:GLU:CB	2:D:36:LEU:HD13	2.48	0.43
1:3:156:SER:CB	1:3:203:ILE:HD11	2.49	0.43
2:C:21:ALA:HA	2:C:33:HIS:CG	2.54	0.43
2:C:38:LEU:HD22	2:C:46:ALA:CB	2.45	0.43
1:4:133:PHE:CD2	1:4:163:LEU:HB3	2.54	0.43
2:A:60:ILE:O	2:A:64:VAL:HG23	2.18	0.43
2:C:278:ILE:CB	2:C:281:LEU:HD21	2.27	0.43
2:C:477:ALA:HB2	2:C:492:ALA:C	2.39	0.43
2:D:541:PHE:O	2:D:656:MET:HE2	2.19	0.43
2:D:382:ILE:HG12	2:D:611:TYR:CE1	2.53	0.43
1:2:144:LYS:HG2	1:2:217:ALA:HB1	2.01	0.43
1:2:204:ILE:HG22	1:2:208:ALA:HA	2.00	0.43
2:B:476:ILE:O	2:B:479:VAL:HG22	2.19	0.43
2:B:361:HIS:CG	2:C:233:ILE:HG23	2.53	0.43
2:C:751:VAL:HG22	2:C:772:HIS:HB2	1.99	0.43
2:F:199:ARG:HH12	2:F:233:ILE:HD13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:613:VAL:CG1	2:F:655:ILE:HD12	2.49	0.43
2:A:506:LEU:HD21	2:A:558:LEU:HD23	2.00	0.43
2:B:606:VAL:HG11	2:B:649:PHE:CD1	2.54	0.43
2:C:278:ILE:HB	2:C:281:LEU:HD22	1.85	0.43
2:C:516:ALA:HB1	2:C:709:ILE:HG22	2.01	0.43
1:5:145:LEU:HD13	2:E:68:ILE:HD13	2.01	0.43
2:F:516:ALA:HB1	2:F:709:ILE:HG22	2.01	0.43
1:5:133:PHE:CD2	1:5:163:LEU:HB3	2.53	0.42
2:A:36:LEU:HG	2:A:60:ILE:HG22	2.01	0.42
2:C:26:HIS:CB	2:C:33:HIS:CE1	3.02	0.42
2:E:385:ARG:HH21	2:F:201:LYS:NZ	2.17	0.42
2:F:26:HIS:CG	2:F:33:HIS:HE1	2.36	0.42
1:3:136:PHE:CZ	1:3:203:ILE:CG2	3.01	0.42
1:6:203:ILE:HG23	2:F:431:VAL:CB	2.47	0.42
2:A:543:PHE:HA	2:A:709:ILE:HB	2.02	0.42
2:D:498:LYS:HD3	2:D:564:GLY:HA2	2.00	0.42
2:E:481:SER:HA	2:E:564:GLY:HA2	2.01	0.42
2:F:278:ILE:HG22	2:F:281:LEU:HD23	2.01	0.42
2:F:39:VAL:HG13	2:F:57:SER:HA	2.00	0.42
1:5:157:PHE:HB3	1:5:162:TYR:CE2	2.55	0.42
1:6:152:THR:CG2	1:6:209:LEU:H	2.33	0.42
2:D:638:ARG:HE	2:D:650:ARG:HD3	1.83	0.42
2:F:26:HIS:ND1	2:F:33:HIS:CE1	2.87	0.42
2:B:38:LEU:HD22	2:B:46:ALA:CB	2.50	0.42
2:B:542:ILE:HG13	2:B:705:ILE:HG21	2.00	0.42
2:D:46:ALA:H	2:D:105:THR:HB	1.84	0.42
2:E:366:ILE:HB	2:E:367:THR:HA	2.01	0.42
1:1:136:PHE:HB2	1:1:161:TYR:CZ	2.54	0.42
2:A:437:GLU:HA	2:A:440:ALA:HB3	2.02	0.42
2:E:106:GLU:HA	2:E:138:VAL:HG12	2.02	0.42
2:F:106:GLU:CD	2:F:106:GLU:H	2.23	0.42
2:A:53:LEU:HD21	2:A:134:ALA:HA	2.02	0.42
2:A:544:LEU:HD22	2:A:693:LEU:HB2	2.01	0.42
2:B:382:ILE:HG22	2:B:382:ILE:O	2.20	0.42
2:B:39:VAL:HG11	2:B:60:ILE:HB	2.00	0.42
2:B:689:VAL:HG21	2:B:710:VAL:HG13	2.00	0.42
2:B:551:LYS:HA	2:B:711:PHE:CE2	2.55	0.42
2:D:394:LEU:HD13	2:D:480:VAL:HG21	2.02	0.42
1:4:137:GLU:HA	2:D:443:ARG:HE	1.85	0.42
1:4:152:THR:HG23	1:4:208:ALA:H	1.83	0.42
1:4:142:LEU:CD2	1:4:182:LEU:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:94:GLU:O	2:A:107:HIS:CD2	2.73	0.42
2:F:431:VAL:HG13	2:F:439:ALA:CB	2.49	0.42
1:4:130:VAL:HG13	1:4:196:LEU:HD11	2.01	0.42
2:A:36:LEU:HD21	2:A:61:GLN:N	2.35	0.42
2:D:667:ARG:HH21	2:D:681:ASN:HB2	1.85	0.42
1:3:152:THR:CG2	1:3:209:LEU:H	2.33	0.42
1:4:142:LEU:CD1	1:4:147:VAL:HG11	2.50	0.42
2:B:544:LEU:HB2	2:B:689:VAL:HG12	2.02	0.42
2:C:118:GLY:H	2:C:122:ARG:HE	1.68	0.42
2:F:202:ASN:HD22	2:F:310:GLN:NE2	2.18	0.42
2:B:395:ILE:HA	2:B:476:ILE:HD11	2.01	0.42
2:B:669:LYS:HB2	2:B:716:LYS:H	1.84	0.42
2:D:395:ILE:HA	2:D:476:ILE:CD1	2.49	0.42
2:F:394:LEU:HD23	2:F:479:VAL:HG22	2.02	0.42
2:F:747:ALA:HB1	2:F:801:PHE:CE1	2.54	0.42
1:1:133:PHE:CE2	1:1:186:ALA:HB2	2.55	0.41
1:3:133:PHE:CD2	1:3:133:PHE:N	2.88	0.41
1:6:133:PHE:CD2	1:6:163:LEU:HB3	2.54	0.41
1:6:136:PHE:CZ	1:6:216:PHE:CE2	3.08	0.41
2:A:63:GLU:HB3	2:A:123:VAL:HG13	2.02	0.41
2:A:354:LEU:HD13	2:A:358:TYR:CE2	2.55	0.41
2:B:106:GLU:CD	2:B:106:GLU:H	2.23	0.41
2:D:26:HIS:NE2	2:D:65:GLU:HA	2.35	0.41
2:D:544:LEU:HD11	2:D:708:ILE:HG23	2.02	0.41
2:E:502:MET:HE2	2:E:562:ILE:HG21	2.02	0.41
2:E:566:GLU:HB2	2:E:567:GLU:H	1.74	0.41
2:F:747:ALA:HB1	2:F:801:PHE:CZ	2.55	0.41
1:5:204:ILE:HG22	1:5:207:HIS:CD2	2.56	0.41
2:A:106:GLU:HG2	2:A:107:HIS:CD2	2.55	0.41
2:B:91:SER:HB3	2:B:108:ILE:HA	2.03	0.41
2:B:746:ALA:CB	2:B:796:VAL:H	2.33	0.41
2:C:577:TYR:CG	2:C:597:ASP:HB3	2.56	0.41
2:D:38:LEU:O	2:D:47:ALA:HB2	2.20	0.41
2:A:233:ILE:HG23	2:F:361:HIS:CG	2.55	0.41
1:1:136:PHE:CE1	1:1:212:ILE:CD1	3.03	0.41
1:5:216:PHE:CD2	2:E:440:ALA:HA	2.54	0.41
2:B:394:LEU:HD21	2:B:483:TRP:CZ2	2.56	0.41
2:C:94:GLU:O	2:C:107:HIS:CD2	2.73	0.41
2:D:544:LEU:HD13	2:D:693:LEU:HD22	2.02	0.41
2:E:36:LEU:HD21	2:E:61:GLN:HB3	2.02	0.41
2:F:524:VAL:CG1	2:F:562:ILE:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:VAL:CG1	2:F:60:ILE:HD12	2.50	0.41
1:2:152:THR:HG23	1:2:209:LEU:H	1.84	0.41
1:5:140:ILE:HG21	2:E:443:ARG:HE	1.86	0.41
2:A:473:VAL:HG23	2:A:493:GLN:HE22	1.85	0.41
2:B:68:ILE:HD11	2:B:119:VAL:HG21	2.02	0.41
2:C:351:LEU:HA	2:C:392:ILE:HG23	2.01	0.41
2:C:558:LEU:HD13	2:C:655:ILE:HD11	2.03	0.41
2:D:477:ALA:HB1	2:D:495:GLU:N	2.35	0.41
2:E:470:GLU:HG2	2:E:472:THR:H	1.85	0.41
1:3:142:LEU:HD23	1:3:142:LEU:O	2.20	0.41
1:4:164:TYR:CD1	1:4:193:ILE:HD13	2.55	0.41
1:5:142:LEU:HD21	1:5:146:ASN:HD21	1.86	0.41
2:A:496:THR:HA	2:A:499:LEU:HD23	2.01	0.41
2:B:106:GLU:HG3	2:B:143:GLY:H	1.84	0.41
2:B:20:GLU:HB3	2:B:33:HIS:CE1	2.55	0.41
2:C:536:ARG:HH22	2:C:540:SER:HB2	1.85	0.41
2:D:39:VAL:HG11	2:D:60:ILE:HB	2.02	0.41
2:D:751:VAL:HG11	2:D:769:ILE:HG13	2.02	0.41
2:E:13:VAL:CG1	2:E:38:LEU:HD23	2.50	0.41
1:3:202:LEU:HD12	1:3:202:LEU:H	1.85	0.41
1:6:205:SER:O	1:6:207:HIS:CD2	2.73	0.41
2:C:106:GLU:HG2	2:C:107:HIS:CD2	2.55	0.41
2:D:363:ARG:HD2	2:D:403:ARG:H	1.85	0.41
2:E:94:GLU:O	2:E:107:HIS:CD2	2.74	0.41
2:E:38:LEU:HD13	2:E:109:LEU:HD13	2.02	0.41
1:5:203:ILE:HG23	2:E:431:VAL:C	2.41	0.41
2:F:709:ILE:HG22	2:F:711:PHE:CE2	2.55	0.41
2:F:747:ALA:HA	2:F:796:VAL:HG23	2.01	0.41
1:1:136:PHE:CE1	1:1:212:ILE:HD11	2.55	0.41
1:2:140:ILE:HG13	1:2:212:ILE:HG23	2.03	0.41
2:A:714:LEU:HA	2:A:718:HIS:CG	2.56	0.41
2:B:563:PHE:CZ	2:B:613:VAL:HG22	2.55	0.41
2:D:697:PHE:CE2	2:D:702:ILE:HG21	2.56	0.41
2:F:544:LEU:HD21	2:F:693:LEU:HD13	2.02	0.41
1:2:153:THR:HB	1:2:164:TYR:CD2	2.56	0.41
1:6:147:VAL:HG13	1:6:148:ASN:H	1.85	0.41
2:A:394:LEU:N	2:A:394:LEU:HD23	2.36	0.41
2:B:354:LEU:HD13	2:B:358:TYR:CE2	2.55	0.41
2:C:620:GLU:HB3	2:C:696:ALA:HB1	2.03	0.41
2:E:382:ILE:HG12	2:E:484:THR:HG23	2.03	0.41
2:E:361:HIS:CD2	2:F:197:SER:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:212:ILE:HA	1:1:216:PHE:CD2	2.55	0.41
1:2:141:SER:HA	1:2:144:LYS:HE2	2.03	0.41
2:A:13:VAL:HG12	2:A:41:GLU:HB2	2.03	0.41
2:B:39:VAL:HG11	2:B:60:ILE:HG13	2.03	0.41
2:C:22:LEU:HD13	2:C:78:ILE:HG21	2.03	0.41
2:D:351:LEU:HD13	2:D:374:ALA:HB3	2.03	0.41
2:D:558:LEU:O	2:D:562:ILE:HB	2.21	0.41
2:E:431:VAL:HG22	2:E:439:ALA:CB	2.51	0.41
2:E:545:GLY:HA2	2:E:689:VAL:HG12	2.02	0.41
2:F:373:ALA:HB1	2:F:492:ALA:HA	2.03	0.41
1:2:131:LEU:HD11	1:2:165:VAL:HG22	2.02	0.41
2:B:26:HIS:HE2	2:B:65:GLU:HA	1.85	0.41
2:C:709:ILE:HG22	2:C:711:PHE:CE2	2.56	0.41
2:D:394:LEU:HD13	2:D:480:VAL:HG22	2.03	0.41
2:F:26:HIS:ND1	2:F:33:HIS:HE1	2.19	0.41
1:2:205:SER:O	1:2:207:HIS:CD2	2.74	0.41
2:A:473:VAL:CG2	2:A:493:GLN:HE22	2.34	0.41
2:F:363:ARG:NH1	2:F:403:ARG:H	2.19	0.41
1:5:179:LEU:HA	1:5:182:LEU:HD12	2.02	0.40
2:C:26:HIS:CE1	2:C:64:VAL:O	2.74	0.40
2:C:524:VAL:HG11	2:C:562:ILE:HG12	2.03	0.40
2:C:767:ARG:HH12	2:C:771:LYS:HZ2	1.69	0.40
2:D:39:VAL:HG11	2:D:60:ILE:CG1	2.51	0.40
2:D:431:VAL:HG13	2:D:439:ALA:HB2	2.02	0.40
2:F:371:ILE:O	2:F:374:ALA:HB3	2.21	0.40
1:4:203:ILE:HG23	2:D:431:VAL:CB	2.51	0.40
2:A:206:LEU:HB3	2:A:339:VAL:HG21	2.04	0.40
2:A:495:GLU:OE2	2:A:495:GLU:HA	2.21	0.40
2:B:380:ARG:HD3	2:B:380:ARG:H	1.86	0.40
2:D:49:ALA:O	2:D:53:LEU:HD22	2.22	0.40
2:F:38:LEU:HD13	2:F:109:LEU:HD13	2.04	0.40
2:F:516:ALA:HB1	2:F:709:ILE:HG23	2.03	0.40
2:F:544:LEU:HD22	2:F:693:LEU:HB3	2.03	0.40
1:2:154:LEU:HD13	1:2:163:LEU:HD23	2.02	0.40
2:B:499:LEU:HD21	2:B:529:ALA:HB2	2.04	0.40
2:C:499:LEU:HD22	2:C:502:MET:HE3	2.03	0.40
2:C:677:ASP:HA	2:C:680:GLN:HB3	2.04	0.40
2:D:669:LYS:H	2:D:716:LYS:HB2	1.87	0.40
2:F:417:GLU:HG3	2:F:453:VAL:HG13	2.03	0.40
2:F:524:VAL:HG13	2:F:538:ILE:HG12	2.04	0.40
1:1:136:PHE:CE1	1:1:203:ILE:CG2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:154:LEU:HD22	1:4:212:ILE:HD11	2.04	0.40
2:C:58:GLU:HA	2:C:61:GLN:HG2	2.02	0.40
2:D:22:LEU:CD2	2:D:78:ILE:HG21	2.52	0.40
2:D:35:LEU:HD23	2:D:123:VAL:HB	2.03	0.40
2:D:714:LEU:HA	2:D:718:HIS:CG	2.57	0.40
2:E:698:ARG:HE	2:E:701:PHE:HB2	1.87	0.40
2:E:714:LEU:HD12	2:E:718:HIS:CG	2.56	0.40
2:F:370:ALA:HB1	2:F:476:ILE:HD12	2.03	0.40
1:1:142:LEU:HG	1:1:182:LEU:HA	2.04	0.40
1:4:132:ARG:HB2	1:4:160:ARG:HH11	1.87	0.40
2:B:750:LYS:HD2	2:B:776:ARG:HH12	1.87	0.40
2:C:347:SER:HA	2:C:388:PRO:HB3	2.03	0.40
2:D:351:LEU:CD1	2:D:375:VAL:HG23	2.51	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	1	92/218 (42%)	76 (83%)	10 (11%)	6 (6%)	1	22
1	2	92/218 (42%)	78 (85%)	9 (10%)	5 (5%)	2	25
1	3	92/218 (42%)	76 (83%)	10 (11%)	6 (6%)	1	22
1	4	92/218 (42%)	77 (84%)	13 (14%)	2 (2%)	8	44
1	5	92/218 (42%)	78 (85%)	7 (8%)	7 (8%)	1	18
1	6	92/218 (42%)	79 (86%)	9 (10%)	4 (4%)	3	29
2	A	794/810 (98%)	630 (79%)	110 (14%)	54 (7%)	1	20
2	B	794/810 (98%)	634 (80%)	101 (13%)	59 (7%)	1	18
2	C	794/810 (98%)	627 (79%)	122 (15%)	45 (6%)	2	24
2	D	794/810 (98%)	632 (80%)	117 (15%)	45 (6%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	794/810 (98%)	632 (80%)	115 (14%)	47 (6%)	2	23
2	F	794/810 (98%)	623 (78%)	115 (14%)	56 (7%)	1	19
All	All	5316/6168 (86%)	4242 (80%)	738 (14%)	336 (6%)	3	22

All (336) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	2	147	VAL
1	2	216	PHE
1	3	147	VAL
1	5	148	ASN
1	5	207	HIS
1	6	147	VAL
2	A	100	HIS
2	A	142	LEU
2	A	362	HIS
2	A	363	ARG
2	A	366	ILE
2	A	410	PRO
2	A	412	ASN
2	A	468	ASN
2	A	472	THR
2	A	532	LYS
2	A	533	ASP
2	A	549	VAL
2	A	581	HIS
2	A	612	SER
2	A	670	TYR
2	A	673	PHE
2	A	739	LEU
2	B	294	ILE
2	B	362	HIS
2	B	366	ILE
2	B	410	PRO
2	B	468	ASN
2	B	472	THR
2	B	549	VAL
2	B	568	SER
2	B	714	LEU
2	B	715	GLU

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Mol	Chain	Res	Type
2	B	717	LYS
2	C	72	GLN
2	C	103	VAL
2	C	366	ILE
2	C	468	ASN
2	C	472	THR
2	C	493	GLN
2	C	587	VAL
2	C	738	ASP
2	C	757	ASP
2	D	361	HIS
2	D	366	ILE
2	D	410	PRO
2	D	468	ASN
2	D	472	THR
2	D	535	LYS
2	D	582	SER
2	D	713	SER
2	D	715	GLU
2	D	738	ASP
2	E	69	GLY
2	E	103	VAL
2	E	152	ALA
2	E	294	ILE
2	E	361	HIS
2	E	366	ILE
2	E	410	PRO
2	E	468	ASN
2	E	568	SER
2	F	103	VAL
2	F	142	LEU
2	F	183	ILE
2	F	294	ILE
2	F	365	SER
2	F	366	ILE
2	F	410	PRO
2	F	412	ASN
2	F	468	ASN
2	F	472	THR
2	F	532	LYS
2	F	584	SER
2	F	673	PHE

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Mol	Chain	Res	Type
2	F	717	LYS
2	F	738	ASP
1	1	145	LEU
1	2	145	LEU
1	2	177	ASN
1	3	145	LEU
1	3	148	ASN
1	6	145	LEU
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	473	VAL
2	A	493	GLN
2	A	579	GLU
2	A	600	GLY
2	A	611	TYR
2	A	618	GLU
2	A	659	ASN
2	A	662	ALA
2	B	76	GLN
2	B	100	HIS
2	B	142	LEU
2	B	144	SER
2	B	165	SER
2	B	493	GLN
2	B	535	LYS
2	B	566	GLU
2	B	652	THR
2	B	662	ALA
2	B	696	ALA
2	C	100	HIS
2	C	151	ALA
2	C	165	SER
2	C	271	ALA
2	C	469	SER
2	C	470	GLU
2	C	662	ALA
2	D	5	ARG
2	D	152	ALA
2	D	165	SER
2	D	271	ALA
2	D	413	LEU

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Mol	Chain	Res	Type
2	D	470	GLU
2	D	493	GLN
2	D	549	VAL
2	D	662	ALA
2	D	669	LYS
2	D	670	TYR
2	D	717	LYS
2	D	757	ASP
2	E	77	THR
2	E	165	SER
2	E	391	ALA
2	E	413	LEU
2	E	470	GLU
2	E	493	GLN
2	E	535	LYS
2	E	547	THR
2	E	584	SER
2	E	662	ALA
2	E	714	LEU
2	E	715	GLU
2	E	738	ASP
2	F	74	MET
2	F	144	SER
2	F	165	SER
2	F	169	ASP
2	F	363	ARG
2	F	471	VAL
2	F	493	GLN
2	F	600	GLY
2	F	652	THR
2	F	662	ALA
2	F	757	ASP
1	1	177	ASN
1	2	144	LYS
1	3	177	ASN
1	4	177	ASN
1	5	144	LYS
1	5	145	LEU
1	5	146	ASN
1	5	177	ASN
1	5	217	ALA
1	6	177	ASN

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Mol	Chain	Res	Type
2	A	117	GLU
2	A	162	THR
2	A	271	ALA
2	A	391	ALA
2	A	413	LEU
2	A	585	ARG
2	A	590	PRO
2	A	660	VAL
2	A	690	MET
2	A	755	GLY
2	A	799	GLY
2	B	4	GLY
2	B	145	ASN
2	B	157	ASN
2	B	162	THR
2	B	163	LEU
2	B	166	LEU
2	B	168	ARG
2	B	391	ALA
2	B	413	LEU
2	B	434	GLN
2	B	471	VAL
2	B	536	ARG
2	B	578	MET
2	B	600	GLY
2	B	690	MET
2	B	706	ASP
2	B	755	GLY
2	C	4	GLY
2	C	162	THR
2	C	163	LEU
2	C	166	LEU
2	C	391	ALA
2	C	408	THR
2	C	413	LEU
2	C	546	PRO
2	C	707	GLU
2	D	74	MET
2	D	162	THR
2	D	163	LEU
2	D	166	LEU
2	D	360	ALA

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Mol	Chain	Res	Type
2	D	391	ALA
2	D	600	GLY
2	D	755	GLY
2	E	162	THR
2	E	163	LEU
2	E	412	ASN
2	E	472	THR
2	E	550	GLY
2	E	755	GLY
2	F	68	ILE
2	F	147	THR
2	F	162	THR
2	F	163	LEU
2	F	167	ALA
2	F	343	SER
2	F	362	HIS
2	F	391	ALA
2	F	413	LEU
2	F	667	ARG
2	F	713	SER
1	1	126	LYS
1	3	144	LYS
1	4	144	LYS
1	6	144	LYS
2	A	4	GLY
2	A	152	ALA
2	A	342	PRO
2	A	375	VAL
2	A	383	SER
2	A	385	ARG
2	A	388	PRO
2	A	400	SER
2	A	591	PRO
2	A	686	LYS
2	A	738	ASP
2	B	341	GLN
2	B	363	ARG
2	B	375	VAL
2	B	388	PRO
2	B	400	SER
2	B	408	THR
2	B	412	ASN

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Mol	Chain	Res	Type
2	B	473	VAL
2	B	533	ASP
2	B	584	SER
2	B	686	LYS
2	B	713	SER
2	B	798	ASP
2	C	145	ASN
2	C	167	ALA
2	C	375	VAL
2	C	383	SER
2	C	388	PRO
2	C	400	SER
2	C	534	PRO
2	C	583	THR
2	C	673	PHE
2	D	329	ALA
2	D	375	VAL
2	D	388	PRO
2	D	400	SER
2	D	412	ASN
2	D	473	VAL
2	D	568	SER
2	D	591	PRO
2	D	612	SER
2	D	675	VAL
2	E	117	GLU
2	E	166	LEU
2	E	271	ALA
2	E	375	VAL
2	E	388	PRO
2	E	400	SER
2	E	690	MET
2	F	149	SER
2	F	166	LEU
2	F	168	ARG
2	F	226	ILE
2	F	271	ALA
2	F	375	VAL
2	F	388	PRO
2	F	400	SER
2	F	408	THR
2	F	434	GLN

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Mol	Chain	Res	Type
2	F	580	LYS
2	F	670	TYR
1	1	144	LYS
1	1	146	ASN
2	A	144	SER
2	A	226	ILE
2	B	226	ILE
2	B	293	ALA
2	B	567	GLU
2	C	78	ILE
2	C	152	ALA
2	C	226	ILE
2	C	412	ASN
2	C	549	VAL
2	C	579	GLU
2	C	659	ASN
2	C	686	LYS
2	D	226	ILE
2	D	384	ASP
2	E	183	ILE
2	E	209	GLU
2	E	226	ILE
2	E	293	ALA
2	E	549	VAL
2	E	686	LYS
2	F	440	ALA
2	F	686	LYS
2	F	690	MET
2	F	714	LEU
2	F	715	GLU
1	3	169	ASN
2	A	757	ASP
2	B	382	ILE
2	B	440	ALA
2	C	382	ILE
2	D	686	LYS
2	E	440	ALA
2	E	536	ARG
2	E	592	GLY
2	F	293	ALA
2	A	534	PRO
2	E	210	PRO

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Mol	Chain	Res	Type
2	E	382	ILE
2	E	600	GLY
2	B	160	THR
2	C	212	VAL
2	C	671	VAL
2	D	382	ILE
2	F	382	ILE
2	B	210	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%)	83 (94%)	5 (6%)	24	56
1	2	88/201 (44%)	80 (91%)	8 (9%)	11	38
1	3	88/201 (44%)	79 (90%)	9 (10%)	8	33
1	4	88/201 (44%)	82 (93%)	6 (7%)	18	51
1	5	88/201 (44%)	80 (91%)	8 (9%)	11	38
1	6	88/201 (44%)	83 (94%)	5 (6%)	24	56
2	A	667/686 (97%)	613 (92%)	54 (8%)	14	44
2	B	667/686 (97%)	607 (91%)	60 (9%)	11	38
2	C	667/686 (97%)	613 (92%)	54 (8%)	14	44
2	D	667/686 (97%)	608 (91%)	59 (9%)	12	39
2	E	667/686 (97%)	591 (89%)	76 (11%)	7	28
2	F	667/686 (97%)	617 (92%)	50 (8%)	16	48
All	All	4530/5322 (85%)	4136 (91%)	394 (9%)	16	40

All (394) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	140	ILE
1	1	164	TYR

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Mol	Chain	Res	Type
1	1	176	GLU
1	1	207	HIS
1	1	216	PHE
1	2	136	PHE
1	2	137	GLU
1	2	145	LEU
1	2	147	VAL
1	2	164	TYR
1	2	182	LEU
1	2	207	HIS
1	2	216	PHE
1	3	131	LEU
1	3	136	PHE
1	3	137	GLU
1	3	154	LEU
1	3	164	TYR
1	3	166	ASP
1	3	207	HIS
1	3	215	HIS
1	3	216	PHE
1	4	126	LYS
1	4	129	PHE
1	4	136	PHE
1	4	157	PHE
1	4	204	ILE
1	4	207	HIS
1	5	130	VAL
1	5	135	ASP
1	5	137	GLU
1	5	145	LEU
1	5	154	LEU
1	5	164	TYR
1	5	176	GLU
1	5	207	HIS
1	6	136	PHE
1	6	145	LEU
1	6	160	ARG
1	6	164	TYR
1	6	207	HIS
2	A	8	GLU
2	A	23	ARG
2	A	29	ILE

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Mol	Chain	Res	Type
2	A	31	THR
2	A	41	GLU
2	A	53	LEU
2	A	73	GLU
2	A	105	THR
2	A	106	GLU
2	A	119	VAL
2	A	135	ARG
2	A	138	VAL
2	A	139	LEU
2	A	187	LYS
2	A	200	THR
2	A	237	LYS
2	A	238	ARG
2	A	253	TYR
2	A	269	ARG
2	A	318	ASP
2	A	364	VAL
2	A	366	ILE
2	A	385	ARG
2	A	397	GLU
2	A	402	VAL
2	A	416	LEU
2	A	417	GLU
2	A	427	LYS
2	A	431	VAL
2	A	446	GLU
2	A	448	ARG
2	A	452	GLN
2	A	461	LYS
2	A	469	SER
2	A	472	THR
2	A	473	VAL
2	A	475	ASP
2	A	476	ILE
2	A	480	VAL
2	A	535	LYS
2	A	577	TYR
2	A	580	LYS
2	A	602	LEU
2	A	624	PRO
2	A	647	VAL

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Mol	Chain	Res	Type
2	A	676	GLN
2	A	678	GLU
2	A	680	GLN
2	A	681	ASN
2	A	704	ARG
2	A	707	GLU
2	A	766	ARG
2	A	787	HIS
2	A	797	GLU
2	B	8	GLU
2	B	23	ARG
2	B	32	GLU
2	B	36	LEU
2	B	63	GLU
2	B	76	GLN
2	B	78	ILE
2	B	81	THR
2	B	83	ARG
2	B	92	MET
2	B	105	THR
2	B	106	GLU
2	B	115	GLU
2	B	117	GLU
2	B	138	VAL
2	B	139	LEU
2	B	188	GLU
2	B	195	VAL
2	B	235	ARG
2	B	238	ARG
2	B	267	GLU
2	B	268	ILE
2	B	321	ARG
2	B	338	GLN
2	B	345	ASP
2	B	357	ARG
2	B	363	ARG
2	B	364	VAL
2	B	376	LYS
2	B	380	ARG
2	B	381	TYR
2	B	385	ARG
2	B	402	VAL

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Mol	Chain	Res	Type
2	B	404	LEU
2	B	418	GLN
2	B	424	ARG
2	B	425	LYS
2	B	431	VAL
2	B	437	GLU
2	B	443	ARG
2	B	447	GLN
2	B	449	LEU
2	B	472	THR
2	B	473	VAL
2	B	476	ILE
2	B	483	TRP
2	B	499	LEU
2	B	542	ILE
2	B	567	GLU
2	B	579	GLU
2	B	580	LYS
2	B	596	TYR
2	B	621	LYS
2	B	634	LEU
2	B	643	LYS
2	B	648	ASP
2	B	664	GLU
2	B	685	MET
2	B	697	PHE
2	B	736	GLU
2	C	5	ARG
2	C	8	GLU
2	C	20	GLU
2	C	23	ARG
2	C	28	ASN
2	C	36	LEU
2	C	48	LYS
2	C	51	GLN
2	C	63	GLU
2	C	105	THR
2	C	106	GLU
2	C	119	VAL
2	C	122	ARG
2	C	135	ARG
2	C	138	VAL

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Mol	Chain	Res	Type
2	C	185	ARG
2	C	187	LYS
2	C	254	ARG
2	C	299	ILE
2	C	318	ASP
2	C	335	GLN
2	C	364	VAL
2	C	367	THR
2	C	380	ARG
2	C	382	ILE
2	C	385	ARG
2	C	392	ILE
2	C	400	SER
2	C	403	ARG
2	C	431	VAL
2	C	443	ARG
2	C	449	LEU
2	C	452	GLN
2	C	470	GLU
2	C	472	THR
2	C	480	VAL
2	C	500	LEU
2	C	569	MET
2	C	585	ARG
2	C	586	LEU
2	C	587	VAL
2	C	597	ASP
2	C	638	ARG
2	C	641	ASP
2	C	647	VAL
2	C	678	GLU
2	C	681	ASN
2	C	700	GLU
2	C	707	GLU
2	C	716	LYS
2	C	766	ARG
2	C	771	LYS
2	C	794	LEU
2	C	801	PHE
2	D	6	PHE
2	D	8	GLU
2	D	19	GLU

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Mol	Chain	Res	Type
2	D	23	ARG
2	D	26	HIS
2	D	32	GLU
2	D	36	LEU
2	D	53	LEU
2	D	78	ILE
2	D	92	MET
2	D	96	ARG
2	D	105	THR
2	D	124	LEU
2	D	138	VAL
2	D	146	GLU
2	D	155	ASN
2	D	187	LYS
2	D	200	THR
2	D	231	PRO
2	D	238	ARG
2	D	268	ILE
2	D	341	GLN
2	D	345	ASP
2	D	364	VAL
2	D	366	ILE
2	D	380	ARG
2	D	385	ARG
2	D	387	LEU
2	D	397	GLU
2	D	403	ARG
2	D	414	LYS
2	D	431	VAL
2	D	432	GLN
2	D	447	GLN
2	D	449	LEU
2	D	450	ARG
2	D	466	GLN
2	D	472	THR
2	D	475	ASP
2	D	499	LEU
2	D	542	ILE
2	D	565	ASP
2	D	566	GLU
2	D	590	PRO
2	D	611	TYR

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Mol	Chain	Res	Type
2	D	613	VAL
2	D	621	LYS
2	D	647	VAL
2	D	690	MET
2	D	694	LYS
2	D	695	ARG
2	D	700	GLU
2	D	701	PHE
2	D	712	HIS
2	D	730	LEU
2	D	736	GLU
2	D	742	GLU
2	D	774	GLU
2	D	780	GLU
2	E	8	GLU
2	E	19	GLU
2	E	22	LEU
2	E	31	THR
2	E	32	GLU
2	E	48	LYS
2	E	51	GLN
2	E	53	LEU
2	E	61	GLN
2	E	62	LYS
2	E	72	GLN
2	E	76	GLN
2	E	90	LEU
2	E	96	ARG
2	E	105	THR
2	E	106	GLU
2	E	112	LEU
2	E	119	VAL
2	E	122	ARG
2	E	138	VAL
2	E	155	ASN
2	E	179	LEU
2	E	185	ARG
2	E	187	LYS
2	E	188	GLU
2	E	191	ARG
2	E	230	VAL
2	E	244	MET

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Mol	Chain	Res	Type
2	E	251	THR
2	E	262	LYS
2	E	263	LYS
2	E	269	ARG
2	E	316	THR
2	E	318	ASP
2	E	319	GLU
2	E	338	GLN
2	E	345	ASP
2	E	364	VAL
2	E	367	THR
2	E	376	LYS
2	E	392	ILE
2	E	395	ILE
2	E	424	ARG
2	E	427	LYS
2	E	431	VAL
2	E	443	ARG
2	E	448	ARG
2	E	449	LEU
2	E	452	GLN
2	E	470	GLU
2	E	472	THR
2	E	476	ILE
2	E	480	VAL
2	E	500	LEU
2	E	520	VAL
2	E	531	LEU
2	E	536	ARG
2	E	549	VAL
2	E	556	ARG
2	E	566	GLU
2	E	581	HIS
2	E	593	TYR
2	E	610	PRO
2	E	624	PRO
2	E	634	LEU
2	E	647	VAL
2	E	654	LEU
2	E	678	GLU
2	E	682	HIS
2	E	697	PHE

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Mol	Chain	Res	Type
2	E	706	ASP
2	E	712	HIS
2	E	715	GLU
2	E	736	GLU
2	E	772	HIS
2	E	780	GLU
2	F	22	LEU
2	F	23	ARG
2	F	26	HIS
2	F	74	MET
2	F	105	THR
2	F	106	GLU
2	F	122	ARG
2	F	138	VAL
2	F	196	LEU
2	F	200	THR
2	F	231	PRO
2	F	254	ARG
2	F	308	GLU
2	F	357	ARG
2	F	361	HIS
2	F	363	ARG
2	F	364	VAL
2	F	385	ARG
2	F	414	LYS
2	F	425	LYS
2	F	431	VAL
2	F	443	ARG
2	F	449	LEU
2	F	450	ARG
2	F	452	GLN
2	F	457	LYS
2	F	472	THR
2	F	475	ASP
2	F	476	ILE
2	F	479	VAL
2	F	480	VAL
2	F	499	LEU
2	F	586	LEU
2	F	593	TYR
2	F	619	ILE
2	F	624	PRO

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Mol	Chain	Res	Type
2	F	634	LEU
2	F	647	VAL
2	F	650	ARG
2	F	653	ILE
2	F	667	ARG
2	F	681	ASN
2	F	683	LYS
2	F	689	VAL
2	F	697	PHE
2	F	700	GLU
2	F	702	ILE
2	F	706	ASP
2	F	766	ARG
2	F	801	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	3	207	HIS
1	6	177	ASN
2	A	26	HIS
2	A	223	GLN
2	A	282	HIS
2	A	361	HIS
2	A	493	GLN
2	A	680	GLN
2	A	681	ASN
2	A	718	HIS
2	A	729	GLN
2	A	787	HIS
2	B	270	GLN
2	B	349	GLN
2	B	362	HIS
2	B	632	GLN
2	B	659	ASN
2	B	676	GLN
2	B	712	HIS
2	B	718	HIS
2	B	787	HIS
2	C	26	HIS
2	C	223	GLN

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Mol	Chain	Res	Type
2	C	310	GLN
2	C	362	HIS
2	C	434	GLN
2	C	632	GLN
2	C	651	ASN
2	C	737	GLN
2	C	791	HIS
2	D	26	HIS
2	D	27	ASN
2	D	33	HIS
2	D	623	HIS
2	D	632	GLN
2	D	772	HIS
2	D	791	HIS
2	E	27	ASN
2	E	33	HIS
2	E	100	HIS
2	E	107	HIS
2	E	310	GLN
2	E	507	HIS
2	E	601	GLN
2	E	623	HIS
2	E	718	HIS
2	E	787	HIS
2	F	26	HIS
2	F	27	ASN
2	F	33	HIS
2	F	126	ASN
2	F	310	GLN
2	F	361	HIS
2	F	362	HIS
2	F	682	HIS
2	F	737	GLN
2	F	772	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.