wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:53 PM BST

PDB ID	:	3J3U
EMDB ID:	:	EMD-5609
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	:	10.00 Å(reported)
Based on PDB ID	:	3PXI

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

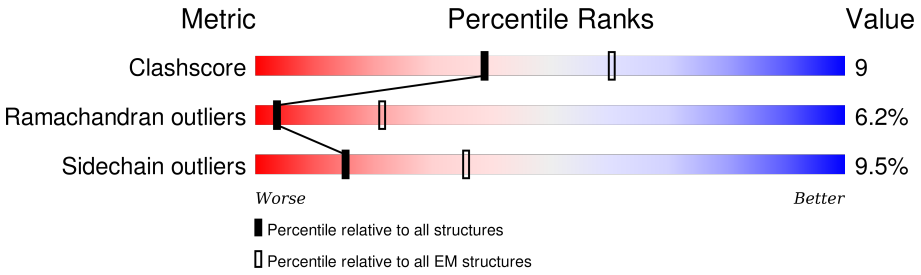
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 10.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	1	218	30% 10% • 57%
1	2	218	28% 11% • 57%
1	3	218	28% 13% • 57%
1	4	218	30% 11% • • 57%
1	5	218	31% 10% •• 57%
1	6	218	31% 11% • 57%
2	A	810	69% 24% • ••
2	B	810	71% 23% • ••
2	C	810	72% 23% • ••

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Mol	Chain	Length	Quality of chain
2	D	810	
2	E	810	
2	F	810	

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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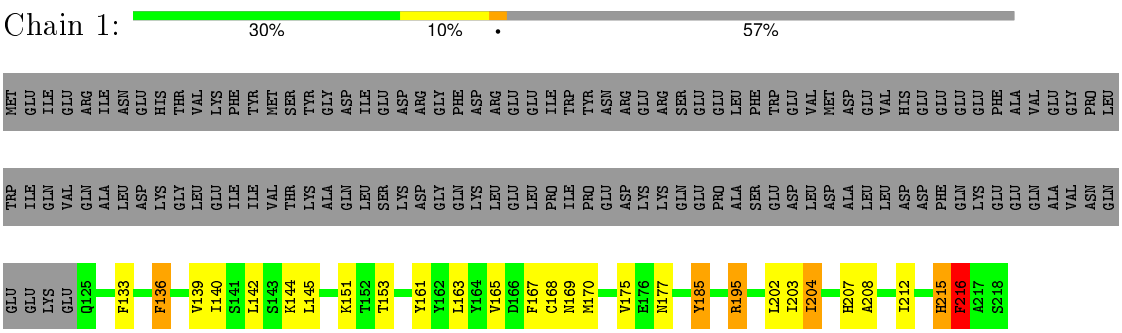
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	618	ALA	GLU	ENGINEERED MUTATION	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 (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

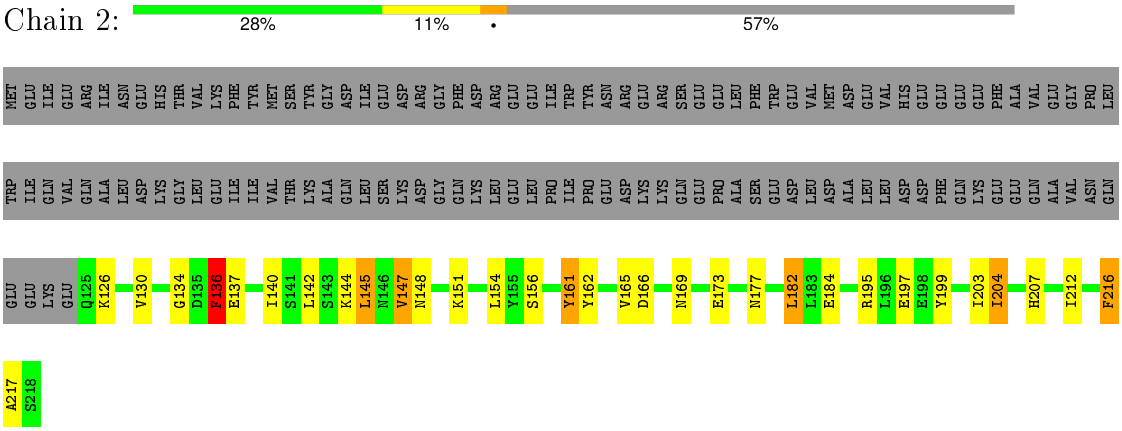
- Molecule 1: Adapter protein MecA 1

Chain 1:



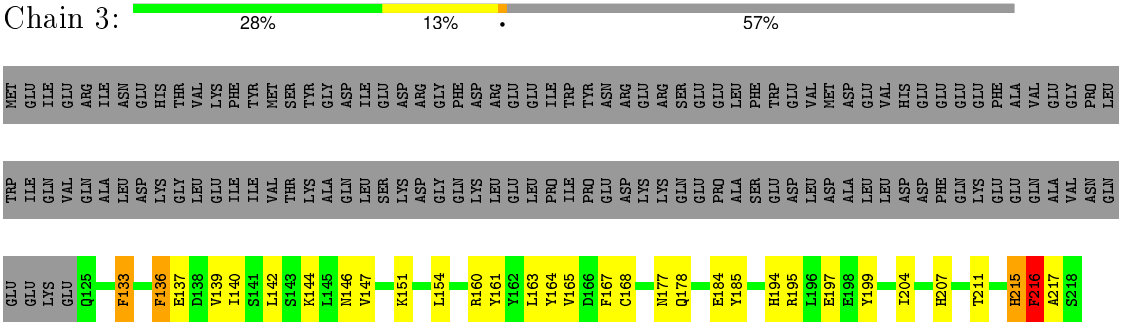
- Molecule 1: Adapter protein MecA 1

Chain 2:



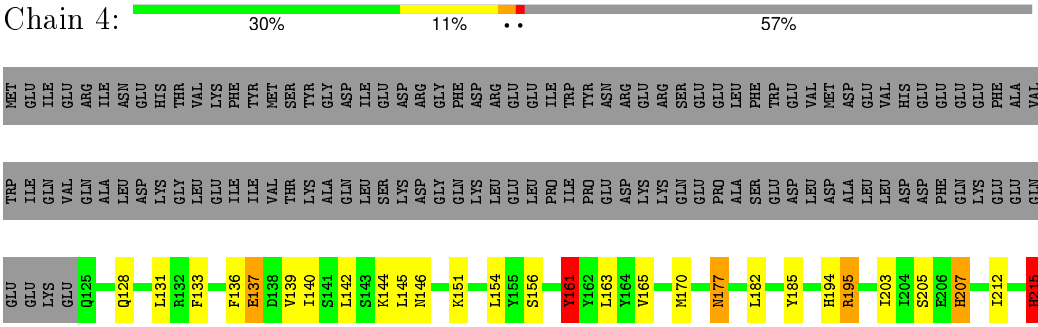
- Molecule 1: Adapter protein MecA 1

Chain 3:



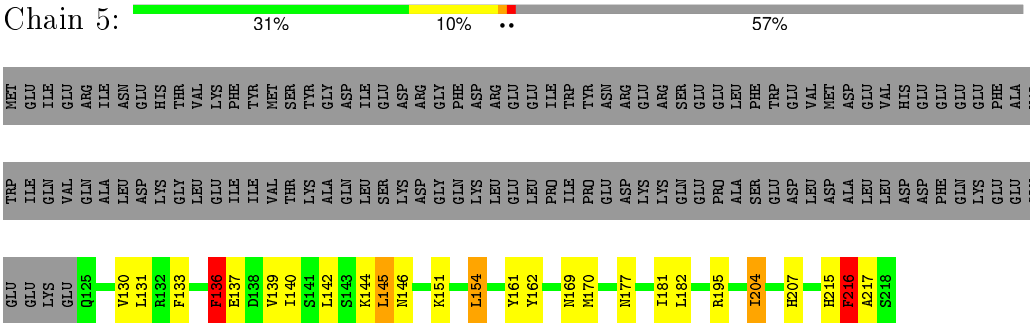
- Molecule 1: Adapter protein MecA 1

Chain 4:



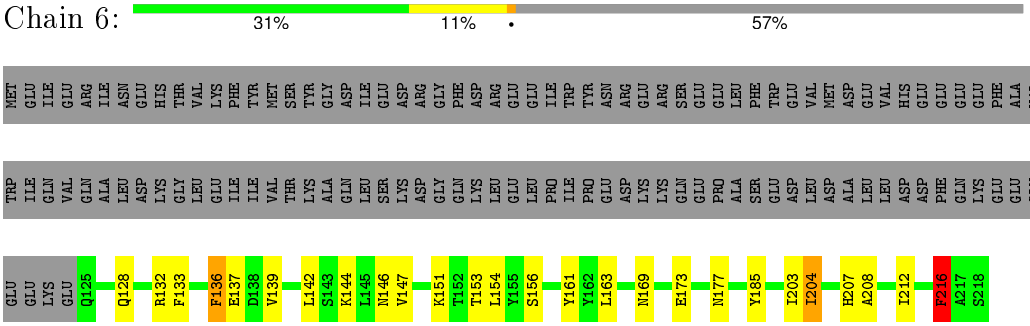
- Molecule 1: Adapter protein MecA 1

Chain 5:



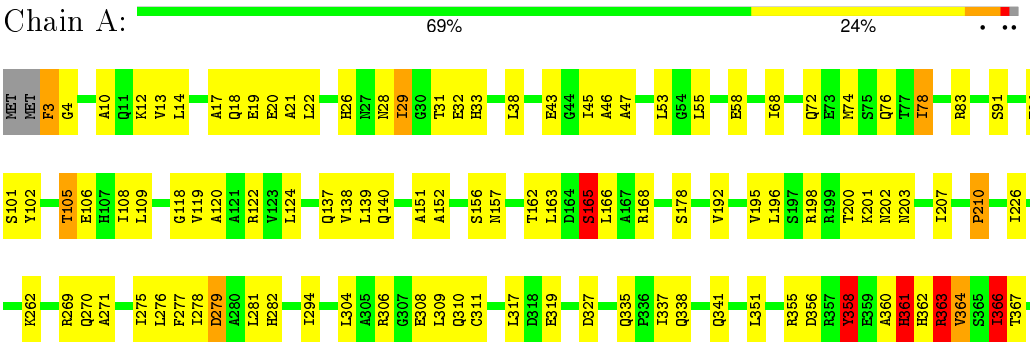
- Molecule 1: Adapter protein MecA 1

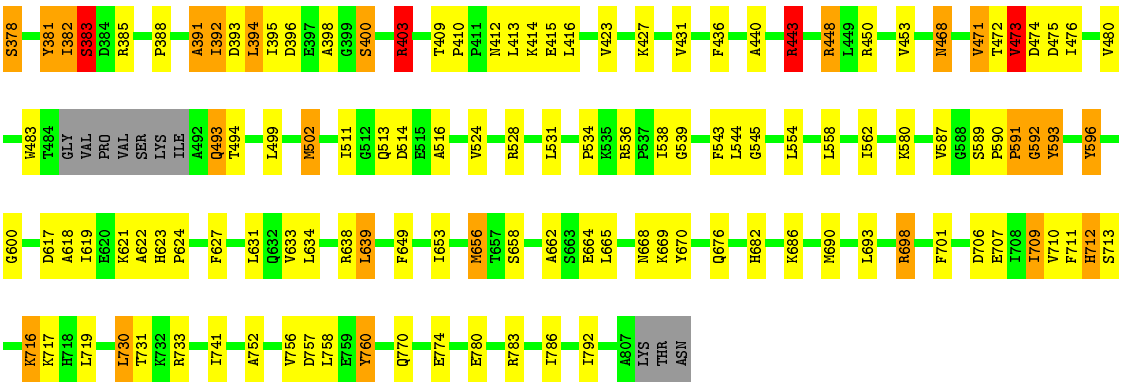
Chain 6:



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

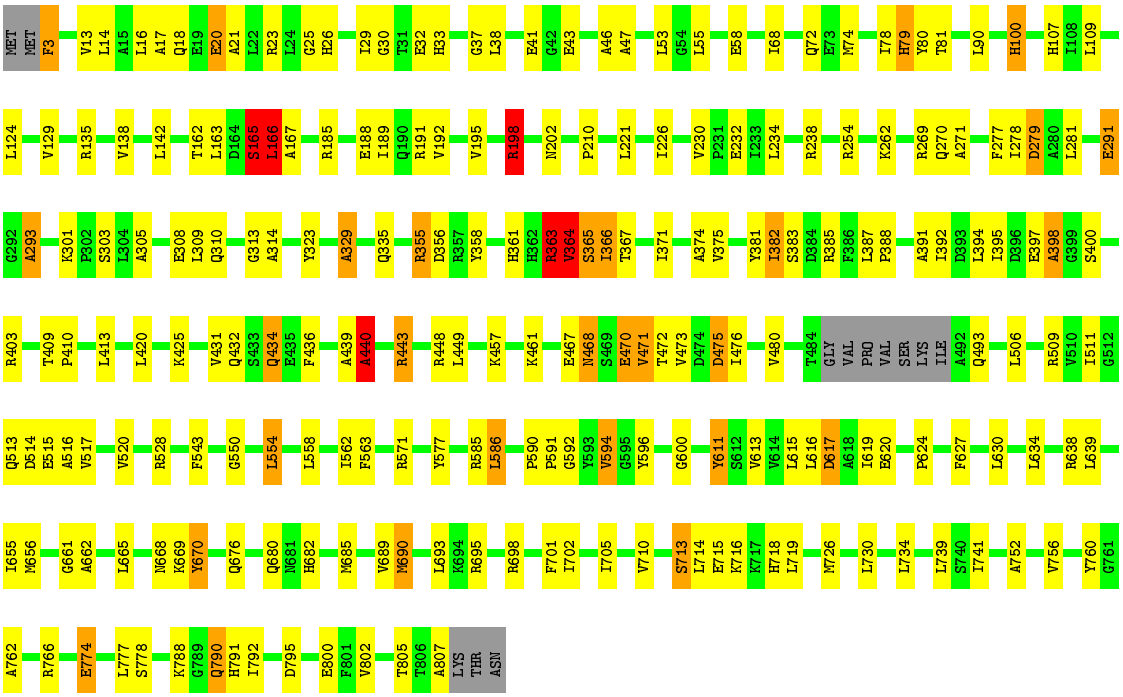
Chain A:





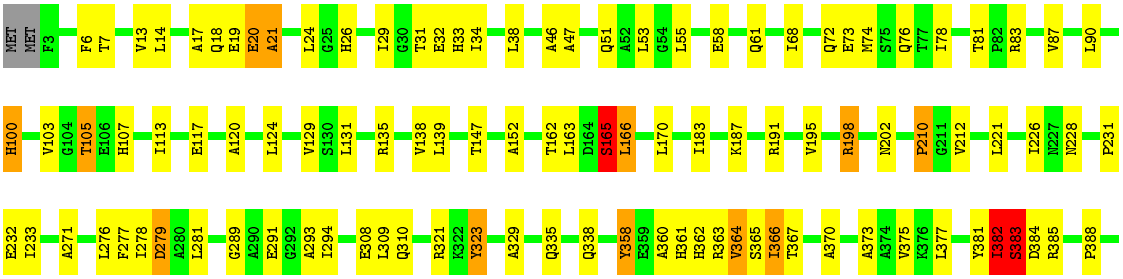
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

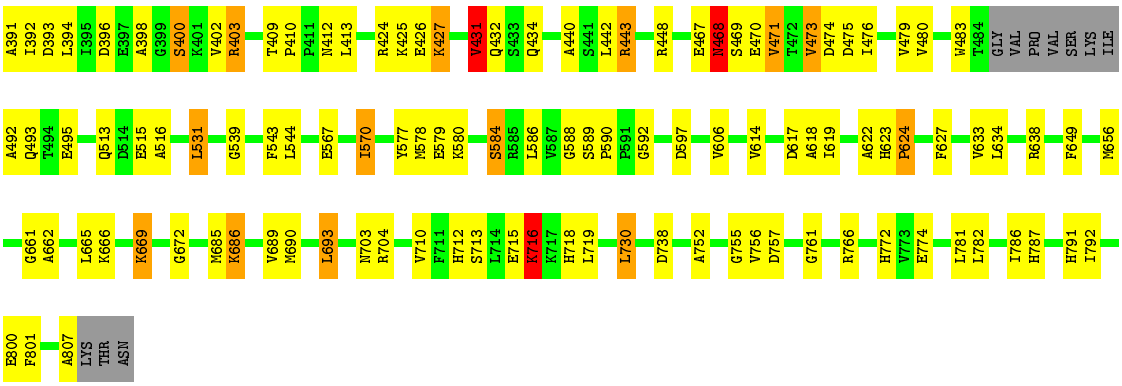
Chain B:



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

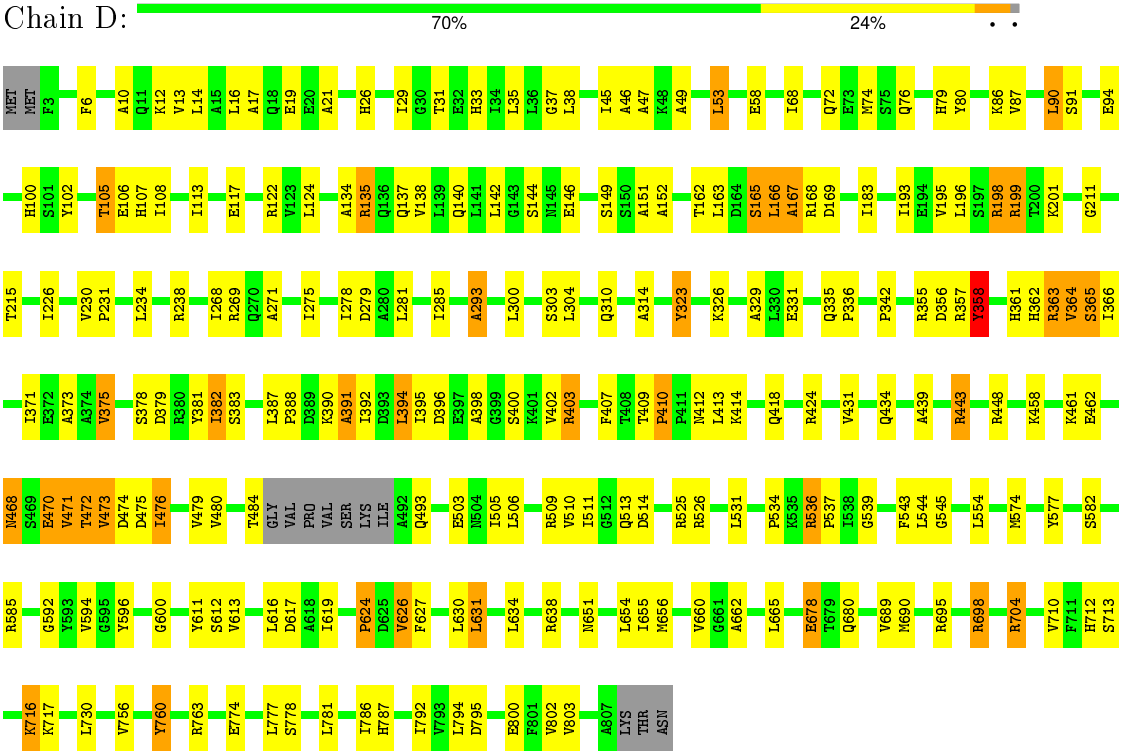
Chain C:





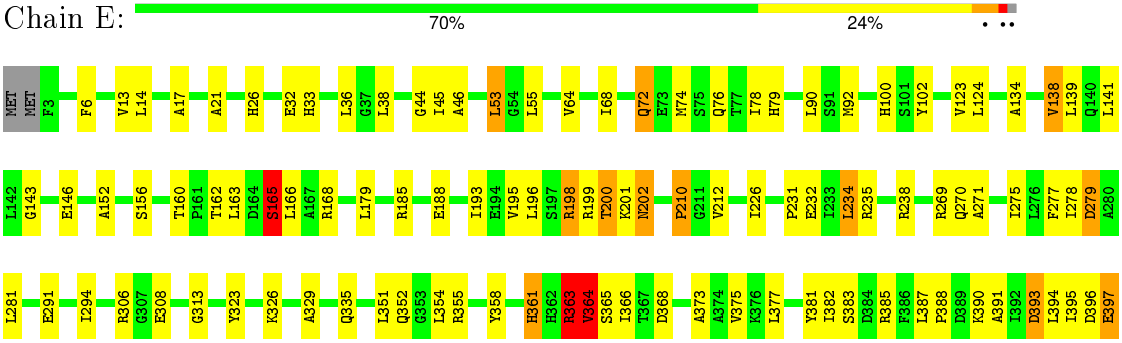
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

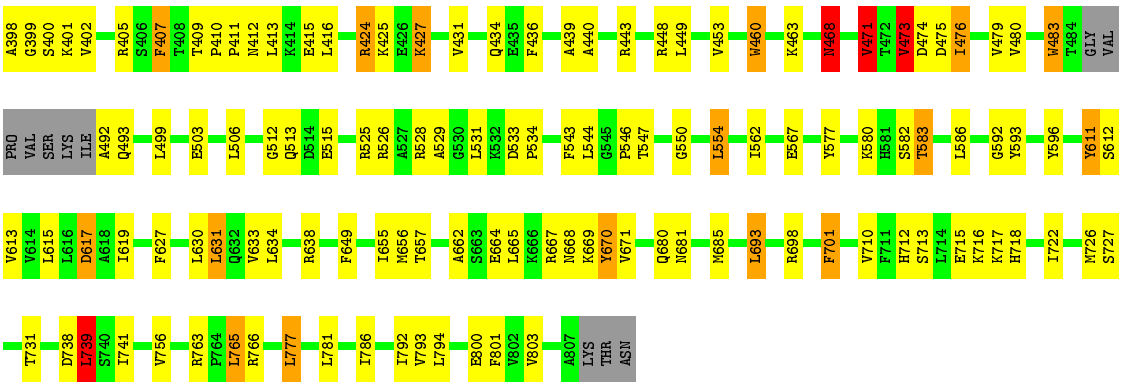
Chain D:



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

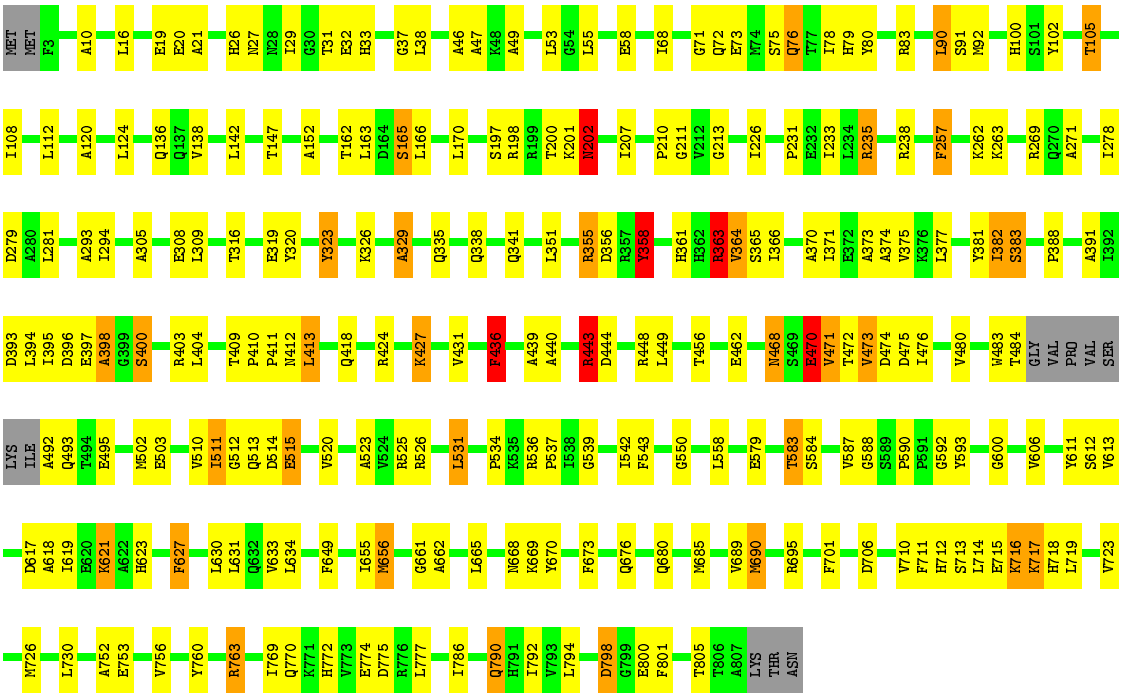
Chain E:





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

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	36688	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 ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1700	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	0.97	0/791	1.22	1/1064 (0.1%)
1	2	0.98	0/791	1.26	3/1064 (0.3%)
1	3	0.97	0/791	1.28	2/1064 (0.2%)
1	4	0.95	0/791	1.24	2/1064 (0.2%)
1	5	0.97	0/791	1.26	5/1064 (0.5%)
1	6	0.96	0/791	1.18	0/1064
2	A	0.99	0/6265	1.23	20/8436 (0.2%)
2	B	0.98	0/6265	1.24	23/8436 (0.3%)
2	C	0.99	0/6265	1.23	20/8436 (0.2%)
2	D	0.99	0/6265	1.25	30/8436 (0.4%)
2	E	0.99	0/6265	1.27	30/8436 (0.4%)
2	F	0.99	0/6265	1.25	30/8436 (0.4%)
All	All	0.99	0/42336	1.24	166/57000 (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	3
1	2	0	3
1	3	0	6
1	4	0	2
1	5	0	1
1	6	0	3
2	A	0	18
2	B	0	18
2	C	0	13
2	D	0	13
2	E	0	14
2	F	0	12
All	All	0	106

There are no bond length outliers.

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	611	TYR	CB-CG-CD2	-10.85	114.49	121.00
2	E	611	TYR	CB-CG-CD1	10.46	127.27	121.00
2	B	543	PHE	CB-CG-CD2	-9.50	114.15	120.80
2	D	358	TYR	CB-CG-CD2	-9.00	115.60	121.00
2	D	543	PHE	CB-CG-CD2	-8.68	114.72	120.80
2	B	670	TYR	CB-CG-CD1	8.61	126.17	121.00
2	D	543	PHE	CB-CG-CD1	8.52	126.77	120.80
2	B	670	TYR	CB-CG-CD2	-8.52	115.89	121.00
2	D	611	TYR	CB-CG-CD2	-8.52	115.89	121.00
2	E	543	PHE	CB-CG-CD2	-8.47	114.87	120.80
2	B	543	PHE	CB-CG-CD1	8.38	126.66	120.80
2	E	543	PHE	CB-CG-CD1	8.22	126.56	120.80
2	F	358	TYR	CB-CG-CD2	-8.18	116.09	121.00
2	D	596	TYR	CB-CG-CD2	-8.15	116.11	121.00
2	A	760	TYR	CB-CG-CD2	8.14	125.88	121.00
2	D	611	TYR	CB-CG-CD1	8.11	125.87	121.00
2	A	760	TYR	CB-CG-CD1	-7.97	116.22	121.00
2	A	543	PHE	CB-CG-CD2	-7.93	115.25	120.80
2	C	383	SER	N-CA-CB	7.70	122.04	110.50
2	A	543	PHE	CB-CG-CD1	7.63	126.14	120.80
2	D	596	TYR	CB-CG-CD1	7.60	125.56	121.00
2	F	627	PHE	CB-CG-CD2	7.43	126.00	120.80
2	F	543	PHE	CB-CG-CD1	7.33	125.93	120.80
2	F	364	VAL	C-N-CA	7.30	139.96	121.70
2	C	165	SER	C-N-CA	7.28	139.91	121.70
2	C	543	PHE	CB-CG-CD2	-7.21	115.75	120.80
2	F	502	MET	CG-SD-CE	-7.19	88.69	100.20
2	F	358	TYR	CB-CG-CD1	7.18	125.31	121.00
2	C	21	ALA	CB-CA-C	-7.17	99.35	110.10
2	B	596	TYR	CB-CG-CD2	-7.13	116.72	121.00
2	F	257	PHE	CB-CG-CD2	7.10	125.77	120.80
2	B	165	SER	C-N-CA	7.03	139.28	121.70
2	F	510	VAL	C-N-CA	6.97	139.13	121.70
2	F	257	PHE	CB-CG-CD1	-6.92	115.96	120.80
2	E	165	SER	C-N-CA	6.89	138.93	121.70
2	F	543	PHE	CB-CG-CD2	-6.87	115.99	120.80
2	F	627	PHE	CB-CG-CD1	-6.82	116.03	120.80
2	E	596	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	A	165	SER	C-N-CA	6.80	138.70	121.70
2	F	323	TYR	CB-CG-CD1	-6.79	116.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	102	TYR	CB-CG-CD2	6.79	125.07	121.00
2	E	407	PHE	CB-CG-CD1	6.78	125.55	120.80
2	E	407	PHE	CB-CG-CD2	-6.76	116.06	120.80
2	C	669	LYS	N-CA-C	-6.73	92.82	111.00
2	A	443	ARG	N-CA-CB	6.73	122.72	110.60
2	F	102	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	5	136	PHE	CB-CG-CD2	6.70	125.49	120.80
2	D	358	TYR	CB-CG-CD1	6.67	125.00	121.00
2	C	543	PHE	CB-CG-CD1	6.65	125.45	120.80
2	D	167	ALA	N-CA-CB	6.64	119.39	110.10
2	E	364	VAL	C-N-CA	6.60	138.20	121.70
2	A	3	PHE	CB-CG-CD1	6.57	125.40	120.80
2	B	364	VAL	C-N-CA	6.55	138.08	121.70
1	5	215	HIS	CA-CB-CG	6.48	124.62	113.60
2	E	44	GLY	N-CA-C	-6.48	96.90	113.10
2	F	165	SER	C-N-CA	6.47	137.87	121.70
2	D	760	TYR	CB-CG-CD1	-6.43	117.14	121.00
2	D	760	TYR	CB-CG-CD2	6.43	124.86	121.00
1	2	136	PHE	CB-CG-CD1	6.42	125.30	120.80
2	A	656	MET	CG-SD-CE	-6.38	90.00	100.20
2	A	383	SER	N-CA-CB	6.36	120.04	110.50
2	E	669	LYS	C-N-CA	6.36	137.59	121.70
2	A	3	PHE	CB-CG-CD2	-6.32	116.38	120.80
2	D	166	LEU	C-N-CA	6.26	137.34	121.70
2	F	364	VAL	N-CA-C	-6.25	94.14	111.00
2	D	704	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	E	439	ALA	N-CA-CB	6.19	118.77	110.10
2	E	6	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	3	215	HIS	CA-CB-CG	6.16	124.07	113.60
2	A	539	GLY	N-CA-C	-6.15	97.72	113.10
2	F	383	SER	N-CA-CB	6.15	119.72	110.50
2	E	79	HIS	N-CA-C	-6.13	94.45	111.00
2	D	293	ALA	N-CA-CB	6.09	118.63	110.10
2	C	323	TYR	CB-CA-C	-6.07	98.26	110.40
2	D	364	VAL	C-N-CA	6.05	136.84	121.70
2	E	363	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	F	436	PHE	CB-CG-CD1	6.01	125.00	120.80
2	D	323	TYR	CB-CG-CD1	-5.95	117.43	121.00
2	E	483	TRP	CB-CG-CD2	-5.93	118.89	126.60
2	B	79	HIS	N-CA-C	-5.91	95.06	111.00
1	5	136	PHE	CB-CG-CD1	-5.88	116.68	120.80
2	E	397	GLU	N-CA-CB	5.86	121.15	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	439	ALA	N-CA-CB	5.84	118.28	110.10
2	C	431	VAL	CA-CB-CG1	-5.84	102.14	110.90
2	E	701	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	5	170	MET	CG-SD-CE	-5.81	90.91	100.20
2	E	6	PHE	CB-CG-CD2	5.81	124.87	120.80
1	2	136	PHE	CB-CG-CD2	-5.80	116.74	120.80
2	B	3	PHE	CB-CG-CD1	5.79	124.86	120.80
1	1	215	HIS	CA-CB-CG	5.78	123.42	113.60
2	D	536	ARG	N-CA-C	-5.78	95.41	111.00
2	B	270	GLN	C-N-CA	5.76	136.09	121.70
2	A	361	HIS	CA-CB-CG	-5.74	103.84	113.60
2	D	358	TYR	CA-CB-CG	5.74	124.31	113.40
2	C	539	GLY	N-CA-C	-5.72	98.80	113.10
2	B	198	ARG	CD-NE-CZ	-5.67	115.67	123.60
2	C	364	VAL	C-N-CA	5.64	135.81	121.70
2	C	382	ILE	C-N-CA	5.64	135.80	121.70
2	B	596	TYR	CB-CG-CD1	5.62	124.37	121.00
2	B	398	ALA	C-N-CA	5.61	134.08	122.30
2	D	536	ARG	CB-CA-C	-5.59	99.22	110.40
2	F	120	ALA	CB-CA-C	-5.58	101.72	110.10
2	B	383	SER	N-CA-CB	5.58	118.87	110.50
2	A	593	TYR	CB-CG-CD1	5.57	124.34	121.00
2	E	793	VAL	N-CA-C	-5.55	96.01	111.00
2	C	310	GLN	N-CA-C	-5.53	96.07	111.00
2	E	596	TYR	CB-CG-CD1	5.52	124.31	121.00
2	A	358	TYR	CA-CB-CG	5.50	123.86	113.40
2	D	165	SER	C-N-CA	5.50	135.46	121.70
2	F	439	ALA	N-CA-CB	5.49	117.79	110.10
1	5	216	PHE	N-CA-CB	5.49	120.49	110.60
2	B	382	ILE	C-N-CA	5.47	135.38	121.70
2	C	21	ALA	N-CA-CB	5.46	117.74	110.10
2	E	72	GLN	N-CA-CB	5.46	120.42	110.60
2	F	323	TYR	CB-CG-CD2	5.44	124.27	121.00
2	F	436	PHE	CB-CG-CD2	-5.43	117.00	120.80
2	E	92	MET	CG-SD-CE	-5.43	91.52	100.20
2	D	358	TYR	N-CA-CB	5.39	120.31	110.60
2	A	364	VAL	N-CA-C	-5.39	96.44	111.00
2	C	323	TYR	N-CA-CB	5.39	120.30	110.60
2	F	470	GLU	N-CA-CB	5.38	120.29	110.60
1	4	215	HIS	CA-CB-CG	5.37	122.73	113.60
2	B	440	ALA	CB-CA-C	-5.37	102.05	110.10
2	D	439	ALA	N-CA-CB	5.36	117.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	589	SER	N-CA-C	-5.36	96.54	111.00
2	B	166	LEU	N-CA-CB	5.34	121.09	110.40
2	D	802	VAL	N-CA-C	-5.34	96.57	111.00
2	B	3	PHE	CB-CG-CD2	-5.33	117.07	120.80
2	D	539	GLY	N-CA-C	-5.33	99.78	113.10
2	F	398	ALA	C-N-CA	5.31	133.45	122.30
2	E	739	LEU	C-N-CA	5.30	134.94	121.70
1	4	161	TYR	CA-CB-CG	-5.29	103.35	113.40
2	E	669	LYS	N-CA-C	-5.28	96.74	111.00
2	C	590	PRO	CA-C-N	5.28	131.88	117.10
2	A	270	GLN	C-N-CA	5.27	134.88	121.70
2	D	310	GLN	N-CA-C	-5.26	96.79	111.00
2	D	358	TYR	CB-CA-C	-5.23	99.95	110.40
2	B	279	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	279	ASP	CB-CG-OD2	5.21	122.99	118.30
2	A	617	ASP	CB-CG-OD2	5.21	122.98	118.30
2	C	617	ASP	CB-CG-OD2	5.20	122.98	118.30
2	D	279	ASP	CB-CG-OD2	5.20	122.98	118.30
2	A	28	ASN	N-CA-C	-5.19	96.99	111.00
2	F	279	ASP	CB-CG-OD2	5.19	122.97	118.30
2	D	617	ASP	CB-CG-OD2	5.18	122.97	118.30
2	F	617	ASP	CB-CG-OD2	5.18	122.96	118.30
2	A	279	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	617	ASP	CB-CG-OD2	5.17	122.95	118.30
1	2	166	ASP	N-CA-C	-5.16	97.06	111.00
2	E	279	ASP	CB-CG-OD2	5.16	122.94	118.30
2	C	578	MET	CG-SD-CE	-5.16	91.95	100.20
1	3	216	PHE	N-CA-CB	5.16	119.88	110.60
2	E	471	VAL	N-CA-C	-5.15	97.10	111.00
2	F	539	GLY	N-CA-C	-5.15	100.23	113.10
2	E	801	PHE	CB-CG-CD1	5.14	124.40	120.80
2	E	617	ASP	CB-CG-OD2	5.14	122.92	118.30
2	A	210	PRO	C-N-CA	5.14	133.09	122.30
2	F	711	PHE	CB-CG-CD2	5.12	124.39	120.80
2	D	471	VAL	CA-CB-CG1	5.09	118.54	110.90
2	B	310	GLN	N-CA-C	-5.08	97.28	111.00
2	D	383	SER	N-CA-CB	5.08	118.11	110.50
2	E	270	GLN	C-N-CA	5.06	134.35	121.70
2	B	802	VAL	N-CA-C	-5.04	97.41	111.00
2	C	393	ASP	CB-CA-C	-5.02	100.37	110.40
2	F	443	ARG	N-CA-CB	5.02	119.63	110.60
2	F	656	MET	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (106) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	136	PHE	Sidechain
1	1	161	TYR	Sidechain
1	1	185	TYR	Sidechain
1	2	161	TYR	Sidechain
1	2	162	TYR	Sidechain
1	2	199	TYR	Sidechain
1	3	133	PHE	Sidechain
1	3	164	TYR	Sidechain
1	3	185	TYR	Sidechain
1	3	199	TYR	Sidechain
1	3	215	HIS	Sidechain
1	3	216	PHE	Sidechain
1	4	161	TYR	Sidechain
1	4	185	TYR	Sidechain
1	5	162	TYR	Sidechain
1	6	136	PHE	Sidechain
1	6	161	TYR	Sidechain
1	6	185	TYR	Sidechain
2	A	102	TYR	Sidechain
2	A	122	ARG	Sidechain
2	A	210	PRO	Peptide
2	A	361	HIS	Peptide
2	A	363	ARG	Sidechain
2	A	381	TYR	Sidechain
2	A	403	ARG	Sidechain
2	A	409	THR	Peptide
2	A	448	ARG	Sidechain
2	A	450	ARG	Sidechain
2	A	468	ASN	Peptide
2	A	592	GLY	Peptide
2	A	596	TYR	Sidechain
2	A	670	TYR	Sidechain
2	A	698	ARG	Sidechain
2	A	713	SER	Peptide
2	A	716	LYS	Peptide
2	A	756	VAL	Peptide
2	B	135	ARG	Sidechain
2	B	185	ARG	Sidechain
2	B	191	ARG	Sidechain
2	B	198	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	210	PRO	Peptide
2	B	355	ARG	Sidechain
2	B	358	TYR	Sidechain
2	B	381	TYR	Sidechain
2	B	409	THR	Peptide
2	B	468	ASN	Peptide
2	B	577	TYR	Sidechain
2	B	585	ARG	Sidechain
2	B	592	GLY	Peptide
2	B	611	TYR	Sidechain
2	B	713	SER	Peptide
2	B	716	LYS	Peptide
2	B	756	VAL	Peptide
2	B	80	TYR	Sidechain
2	C	135	ARG	Sidechain
2	C	198	ARG	Sidechain
2	C	210	PRO	Peptide
2	C	323	TYR	Sidechain
2	C	358	TYR	Sidechain
2	C	403	ARG	Sidechain
2	C	409	THR	Peptide
2	C	468	ASN	Peptide
2	C	592	GLY	Peptide
2	C	713	SER	Peptide
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	83	ARG	Sidechain
2	D	102	TYR	Sidechain
2	D	198	ARG	Sidechain
2	D	358	TYR	Sidechain
2	D	409	THR	Peptide
2	D	468	ASN	Peptide
2	D	577	TYR	Sidechain
2	D	592	GLY	Peptide
2	D	6	PHE	Sidechain
2	D	651	ASN	Peptide
2	D	698	ARG	Sidechain
2	D	713	SER	Peptide
2	D	716	LYS	Peptide
2	D	756	VAL	Peptide
2	E	102	TYR	Sidechain
2	E	198	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	210	PRO	Peptide
2	E	363	ARG	Sidechain
2	E	385	ARG	Sidechain
2	E	409	THR	Peptide
2	E	424	ARG	Sidechain
2	E	460	TRP	Peptide
2	E	468	ASN	Peptide
2	E	592	GLY	Peptide
2	E	593	TYR	Sidechain
2	E	713	SER	Peptide
2	E	716	LYS	Peptide
2	E	756	VAL	Peptide
2	F	235	ARG	Sidechain
2	F	320	TYR	Sidechain
2	F	323	TYR	Sidechain
2	F	358	TYR	Sidechain
2	F	409	THR	Peptide
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	593	TYR	Sidechain
2	F	611	TYR	Sidechain
2	F	716	LYS	Peptide
2	F	756	VAL	Peptide
2	F	763	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	777	0	758	18	0
1	2	777	0	758	12	0
1	3	777	0	758	19	0
1	4	777	0	758	19	0
1	5	777	0	758	12	0
1	6	777	0	758	16	0
2	A	6196	0	6289	133	0
2	B	6196	0	6289	119	0
2	C	6196	0	6289	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6196	0	6289	116	0
2	E	6196	0	6289	144	0
2	F	6196	0	6289	130	0
All	All	41838	0	42282	790	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 9.

All (790) 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:E:281:LEU:CD1	2:E:313:GLY:HA3	1.25	1.60
2:E:281:LEU:HD11	2:E:313:GLY:CA	1.17	1.57
2:C:278:ILE:HB	2:C:281:LEU:CD2	1.34	1.52
2:F:278:ILE:CG2	2:F:281:LEU:HD23	1.37	1.50
2:A:278:ILE:HB	2:A:281:LEU:CD2	1.41	1.50
2:B:277:PHE:CE2	2:B:279:ASP:OD1	1.74	1.38
2:C:277:PHE:CE2	2:C:279:ASP:OD1	1.78	1.35
2:F:278:ILE:HB	2:F:281:LEU:CD2	1.60	1.30
2:B:571:ARG:HD3	2:B:617:ASP:OD2	1.29	1.30
2:C:278:ILE:CB	2:C:281:LEU:CD2	2.10	1.29
2:F:278:ILE:CG2	2:F:281:LEU:CD2	2.08	1.29
2:A:277:PHE:CE2	2:A:279:ASP:OD1	1.85	1.28
2:F:278:ILE:CB	2:F:281:LEU:HD21	1.63	1.26
2:C:277:PHE:HE2	2:C:279:ASP:OD1	0.94	1.25
2:B:619:ILE:HG23	2:B:627:PHE:CE1	1.72	1.25
2:F:278:ILE:CB	2:F:281:LEU:CD2	2.17	1.22
2:C:278:ILE:CG2	2:C:281:LEU:HD23	1.67	1.22
2:A:278:ILE:CG2	2:A:281:LEU:HD23	1.71	1.21
2:E:281:LEU:CD1	2:E:313:GLY:CA	1.92	1.20
2:B:619:ILE:HD12	2:B:656:MET:HB3	1.24	1.20
2:A:278:ILE:CB	2:A:281:LEU:CD2	2.21	1.18
2:B:277:PHE:CZ	2:B:279:ASP:OD1	1.96	1.16
2:E:278:ILE:HB	2:E:281:LEU:HD21	1.27	1.13
2:A:278:ILE:CB	2:A:281:LEU:HD21	1.81	1.10
2:C:619:ILE:HD12	2:C:656:MET:HB3	1.22	1.10
2:E:281:LEU:HD11	2:E:313:GLY:HA2	1.25	1.08
2:E:281:LEU:HD12	2:E:313:GLY:HA3	1.30	1.08
2:E:619:ILE:HD12	2:E:656:MET:HB3	1.11	1.07
2:D:619:ILE:HD12	2:D:656:MET:HB3	1.37	1.07
2:C:278:ILE:CB	2:C:281:LEU:HD21	1.74	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:ILE:HG22	2:C:281:LEU:HD23	1.32	1.05
2:B:278:ILE:HB	2:B:281:LEU:HD21	1.36	1.04
2:F:278:ILE:HG22	2:F:281:LEU:HD23	1.03	1.02
2:E:278:ILE:HB	2:E:281:LEU:CD2	1.92	0.99
2:F:278:ILE:HG21	2:F:281:LEU:HD23	1.43	0.98
2:E:619:ILE:HD12	2:E:656:MET:CB	1.92	0.98
2:C:619:ILE:CG2	2:C:627:PHE:CE1	2.47	0.97
2:E:278:ILE:CG2	2:E:281:LEU:HD23	1.95	0.97
2:D:278:ILE:HB	2:D:281:LEU:CD2	1.94	0.97
2:E:619:ILE:HG23	2:E:627:PHE:CE1	1.99	0.96
2:B:278:ILE:HB	2:B:281:LEU:CD2	1.93	0.96
2:C:619:ILE:CG2	2:C:627:PHE:CZ	2.48	0.95
2:B:619:ILE:CD1	2:B:656:MET:HB3	1.97	0.95
2:D:619:ILE:HD13	2:D:630:LEU:CD1	1.97	0.94
2:C:278:ILE:HB	2:C:281:LEU:HD21	0.94	0.94
2:E:615:LEU:HD22	2:E:617:ASP:OD1	1.68	0.94
2:B:277:PHE:HE2	2:B:279:ASP:OD1	1.46	0.94
2:C:619:ILE:HG21	2:C:627:PHE:CE1	2.04	0.93
2:A:278:ILE:HG22	2:A:281:LEU:HD23	1.48	0.93
2:D:619:ILE:HD13	2:D:630:LEU:HD11	1.51	0.92
2:D:278:ILE:HB	2:D:281:LEU:HD21	1.52	0.91
2:A:277:PHE:HE2	2:A:279:ASP:OD1	1.40	0.91
2:C:278:ILE:HB	2:C:281:LEU:HD22	1.53	0.90
2:A:277:PHE:CZ	2:A:279:ASP:OD1	2.24	0.90
2:C:278:ILE:CG2	2:C:281:LEU:CD2	2.42	0.89
2:B:619:ILE:HD12	2:B:656:MET:CB	2.03	0.88
2:C:619:ILE:HG21	2:C:627:PHE:HE1	1.38	0.88
2:B:619:ILE:HG23	2:B:627:PHE:HE1	1.24	0.88
2:C:619:ILE:HD12	2:C:656:MET:CB	2.04	0.88
2:A:278:ILE:HB	2:A:281:LEU:HD21	0.90	0.88
2:F:278:ILE:HB	2:F:281:LEU:HD21	0.86	0.84
2:F:278:ILE:HG22	2:F:281:LEU:CD2	1.91	0.84
2:F:278:ILE:HG21	2:F:281:LEU:CD2	2.03	0.84
2:C:619:ILE:CD1	2:C:656:MET:HB3	2.05	0.83
2:E:281:LEU:CG	2:E:313:GLY:HA2	2.09	0.83
2:E:619:ILE:CD1	2:E:656:MET:HB3	2.05	0.82
2:A:278:ILE:CB	2:A:281:LEU:HD23	1.96	0.82
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.16	0.81
2:C:781:LEU:HD13	2:D:531:LEU:HD21	1.63	0.81
2:A:277:PHE:HE2	2:A:279:ASP:CG	1.86	0.80
2:B:277:PHE:HE2	2:B:279:ASP:CG	1.84	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:CG2	2:B:627:PHE:CE1	2.60	0.80
2:B:277:PHE:CE2	2:B:279:ASP:CG	2.55	0.79
2:E:619:ILE:HD11	2:E:656:MET:HG2	1.64	0.79
2:E:619:ILE:HG23	2:E:627:PHE:HE1	1.45	0.79
2:D:619:ILE:HG22	2:D:627:PHE:CE1	2.18	0.79
2:E:281:LEU:CD1	2:E:313:GLY:HA2	1.87	0.78
2:B:571:ARG:CD	2:B:617:ASP:OD2	2.22	0.77
2:C:619:ILE:HG23	2:C:627:PHE:CE1	2.21	0.76
2:B:615:LEU:HD22	2:B:617:ASP:OD1	1.86	0.75
2:C:394:LEU:HD22	2:C:480:VAL:HA	1.68	0.75
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.68	0.75
2:E:278:ILE:HG22	2:E:281:LEU:HD23	1.67	0.75
2:E:278:ILE:CB	2:E:281:LEU:CD2	2.64	0.75
2:E:781:LEU:HD13	2:F:531:LEU:HD11	1.69	0.75
2:E:619:ILE:HG21	2:E:701:PHE:CE2	2.22	0.74
2:C:619:ILE:HG23	2:C:627:PHE:CZ	2.22	0.74
1:3:194:HIS:CE1	2:D:45:ILE:HD12	2.21	0.74
2:C:619:ILE:CG2	2:C:627:PHE:HE1	1.94	0.74
2:C:619:ILE:CG2	2:C:627:PHE:HZ	1.97	0.73
2:F:394:LEU:HD13	2:F:480:VAL:HG22	1.68	0.73
2:B:777:LEU:HD22	2:B:792:ILE:HG21	1.70	0.73
2:F:619:ILE:HG22	2:F:619:ILE:O	1.86	0.73
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.69	0.73
2:C:619:ILE:O	2:C:619:ILE:HG22	1.88	0.72
2:E:619:ILE:HG22	2:E:619:ILE:O	1.90	0.72
2:E:619:ILE:CG2	2:E:627:PHE:CE1	2.72	0.72
2:F:619:ILE:HD13	2:F:630:LEU:CD1	2.19	0.72
2:A:619:ILE:HD12	2:A:656:MET:HB3	1.70	0.72
2:A:278:ILE:CG2	2:A:281:LEU:CD2	2.52	0.71
2:C:619:ILE:HG23	2:C:622:ALA:HB3	1.73	0.71
2:B:278:ILE:CG2	2:B:281:LEU:HD23	2.20	0.70
2:A:619:ILE:O	2:A:619:ILE:HG22	1.90	0.70
2:E:619:ILE:CD1	2:E:656:MET:HG2	2.21	0.69
2:A:17:ALA:HB1	2:A:29:ILE:HD11	1.74	0.69
2:A:395:ILE:HA	2:A:476:ILE:HD12	1.73	0.69
2:E:278:ILE:CG2	2:E:281:LEU:CD2	2.69	0.69
2:C:619:ILE:CD1	2:C:656:MET:CG	2.71	0.68
2:E:281:LEU:HD11	2:E:313:GLY:HA3	0.79	0.68
2:D:619:ILE:HD13	2:D:630:LEU:HD13	1.74	0.67
2:C:278:ILE:O	2:C:281:LEU:CD2	2.42	0.67
2:D:21:ALA:HA	2:D:33:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:HG21	2:B:701:PHE:HE2	1.60	0.67
2:C:619:ILE:HG22	2:C:627:PHE:HZ	1.59	0.67
2:D:476:ILE:O	2:D:480:VAL:HG23	1.95	0.67
2:A:26:HIS:CG	2:A:33:HIS:CE1	2.82	0.67
2:E:619:ILE:CD1	2:E:656:MET:CG	2.73	0.67
2:F:511:ILE:HG22	2:F:512:GLY:H	1.60	0.66
2:D:10:ALA:HB1	2:D:108:ILE:HD11	1.76	0.66
2:B:513:GLN:HE21	2:B:714:LEU:HD11	1.59	0.66
2:E:619:ILE:HD13	2:E:630:LEU:HD12	1.77	0.66
2:E:619:ILE:CD1	2:E:630:LEU:CD1	2.73	0.66
2:F:394:LEU:HD22	2:F:480:VAL:HA	1.76	0.65
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.79	0.65
1:4:136:PHE:CZ	2:D:431:VAL:HG11	2.32	0.65
2:E:281:LEU:CG	2:E:313:GLY:CA	2.69	0.65
1:6:216:PHE:CD1	2:F:440:ALA:HA	2.32	0.65
2:E:26:HIS:CE1	2:E:68:ILE:HB	2.33	0.64
2:A:29:ILE:O	2:A:29:ILE:HD13	1.98	0.64
2:F:197:SER:O	2:F:233:ILE:HG21	1.97	0.64
2:D:619:ILE:HD12	2:D:656:MET:CB	2.22	0.64
2:D:631:LEU:HD13	2:D:698:ARG:HH22	1.63	0.63
2:E:619:ILE:HD13	2:E:630:LEU:CD1	2.29	0.63
2:B:278:ILE:CB	2:B:281:LEU:CD2	2.74	0.63
2:D:394:LEU:HD13	2:D:480:VAL:HG22	1.80	0.63
2:E:38:LEU:HD22	2:E:46:ALA:CB	2.29	0.62
2:F:38:LEU:HD11	2:F:112:LEU:HD12	1.81	0.62
2:C:619:ILE:HD11	2:C:656:MET:CG	2.29	0.62
2:B:619:ILE:HD11	2:B:656:MET:HG2	1.81	0.62
2:F:476:ILE:O	2:F:480:VAL:HG23	1.99	0.62
2:E:45:ILE:HG23	2:E:141:LEU:HB2	1.81	0.62
2:D:619:ILE:HG23	2:D:626:VAL:CG1	2.29	0.62
2:A:10:ALA:HB1	2:A:108:ILE:HD11	1.81	0.62
1:4:142:LEU:HD12	1:4:146:ASN:HD22	1.64	0.61
2:E:544:LEU:HD11	2:E:693:LEU:HD13	1.80	0.61
2:E:619:ILE:HG21	2:E:701:PHE:HE2	1.63	0.61
2:E:792:ILE:HG23	2:E:803:VAL:CG1	2.31	0.61
2:F:370:ALA:O	2:F:373:ALA:HB3	2.01	0.61
2:D:90:LEU:HG	2:E:156:SER:H	1.64	0.61
2:F:665:LEU:HD21	2:F:710:VAL:HB	1.82	0.61
2:C:570:ILE:HD12	2:C:614:VAL:HG22	1.83	0.61
1:3:216:PHE:CD1	2:C:440:ALA:HA	2.36	0.61
2:D:619:ILE:HG21	2:D:630:LEU:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:CD1	2:B:656:MET:HG2	2.31	0.61
2:B:21:ALA:HA	2:B:33:HIS:CE1	2.35	0.61
2:B:619:ILE:HG21	2:B:701:PHE:CE2	2.35	0.60
2:F:619:ILE:HD13	2:F:630:LEU:HD12	1.82	0.60
2:F:26:HIS:CE1	2:F:68:ILE:HB	2.37	0.60
2:C:619:ILE:CD1	2:C:656:MET:HG2	2.31	0.60
2:C:277:PHE:HE2	2:C:279:ASP:CG	1.95	0.60
2:E:361:HIS:O	2:F:233:ILE:HG23	2.02	0.60
2:D:38:LEU:O	2:D:47:ALA:HB2	2.01	0.60
2:D:278:ILE:CG2	2:D:281:LEU:HD23	2.32	0.60
2:C:278:ILE:O	2:C:281:LEU:HD21	2.02	0.60
2:E:277:PHE:HE2	2:E:279:ASP:OD2	1.84	0.59
2:F:10:ALA:HB1	2:F:108:ILE:HD11	1.84	0.59
2:F:38:LEU:O	2:F:47:ALA:HB2	2.03	0.59
2:A:524:VAL:HG13	2:A:538:ILE:HD12	1.84	0.59
2:F:777:LEU:HD11	2:F:794:LEU:HD11	1.85	0.59
2:C:619:ILE:O	2:C:619:ILE:CG2	2.50	0.59
2:D:665:LEU:HD21	2:D:689:VAL:HG11	1.85	0.59
2:F:473:VAL:HG23	2:F:474:ASP:H	1.67	0.59
2:C:21:ALA:HB2	2:C:29:ILE:CG1	2.32	0.59
2:B:571:ARG:HD3	2:B:617:ASP:CG	2.19	0.59
2:C:619:ILE:CD1	2:C:656:MET:CB	2.75	0.59
2:E:786:ILE:HG21	2:E:803:VAL:HG12	1.84	0.59
2:D:26:HIS:CE1	2:D:68:ILE:HB	2.38	0.58
2:A:427:LYS:O	2:A:431:VAL:HG23	2.03	0.58
2:F:619:ILE:CG2	2:F:627:PHE:CD2	2.87	0.58
2:B:714:LEU:HD13	2:B:762:ALA:HB2	1.86	0.58
2:B:374:ALA:HA	2:B:394:LEU:HD12	1.85	0.58
2:F:395:ILE:HA	2:F:476:ILE:HD11	1.84	0.58
2:C:38:LEU:O	2:C:47:ALA:HB2	2.04	0.58
2:E:619:ILE:HG23	2:E:627:PHE:CD1	2.38	0.58
2:D:38:LEU:HD22	2:D:46:ALA:CB	2.34	0.58
2:F:305:ALA:HB2	2:F:329:ALA:HB1	1.84	0.58
2:D:619:ILE:HG22	2:D:627:PHE:HE1	1.64	0.58
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.39	0.58
2:C:278:ILE:O	2:C:281:LEU:HG	2.04	0.57
2:B:109:LEU:HD23	2:B:138:VAL:HG22	1.86	0.57
2:C:278:ILE:CA	2:C:281:LEU:HD21	2.33	0.57
2:B:619:ILE:CD1	2:B:656:MET:CB	2.70	0.57
2:D:278:ILE:CB	2:D:281:LEU:CD2	2.76	0.57
2:A:278:ILE:HG21	2:A:281:LEU:HD23	1.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:665:LEU:HD23	2:F:685:MET:HB3	1.85	0.57
2:C:38:LEU:HD22	2:C:46:ALA:CB	2.34	0.57
2:B:619:ILE:HD13	2:B:701:PHE:HZ	1.69	0.57
2:F:351:LEU:HB3	2:F:395:ILE:HD11	1.87	0.57
2:B:777:LEU:CD2	2:B:792:ILE:HG21	2.35	0.57
2:D:373:ALA:HB3	2:D:476:ILE:HG21	1.86	0.57
2:D:619:ILE:HG23	2:D:626:VAL:HG11	1.86	0.57
2:C:476:ILE:O	2:C:480:VAL:HG23	2.04	0.57
2:C:21:ALA:HB2	2:C:29:ILE:HG12	1.85	0.57
2:D:730:LEU:HD21	2:D:774:GLU:HB3	1.86	0.57
2:A:46:ALA:H	2:A:105:THR:HB	1.70	0.57
2:A:277:PHE:CE2	2:A:279:ASP:CG	2.66	0.56
2:F:358:TYR:HB3	2:F:361:HIS:CE1	2.40	0.56
2:F:198:ARG:HH12	2:F:335:GLN:HG3	1.70	0.56
2:A:361:HIS:CE1	2:B:234:LEU:HD11	2.41	0.56
1:6:154:LEU:HB3	1:6:204:ILE:HD12	1.85	0.56
2:B:30:GLY:H	2:B:33:HIS:CE1	2.24	0.56
2:A:633:VAL:HG23	2:A:639:LEU:HD23	1.86	0.56
2:D:382:ILE:HB	2:D:484:THR:HG23	1.88	0.56
2:A:619:ILE:O	2:A:619:ILE:CG2	2.53	0.56
2:D:278:ILE:HG22	2:D:281:LEU:HD23	1.87	0.56
2:E:398:ALA:HB1	2:E:475:ASP:CG	2.26	0.56
2:E:26:HIS:CD2	2:E:33:HIS:HE2	2.24	0.56
2:A:619:ILE:CD1	2:A:656:MET:HG2	2.36	0.56
2:C:606:VAL:HG21	2:C:649:PHE:CE1	2.40	0.56
2:A:203:ASN:HD21	2:A:304:LEU:HD22	1.71	0.56
2:D:616:LEU:HB2	2:D:619:ILE:HD11	1.88	0.55
2:B:739:LEU:HD11	2:B:792:ILE:HD11	1.87	0.55
2:C:730:LEU:HD11	2:C:774:GLU:HG2	1.88	0.55
2:C:623:HIS:CD2	2:C:624:PRO:HD2	2.41	0.55
2:D:357:ARG:HH21	2:E:200:THR:HA	1.70	0.55
2:F:619:ILE:CD1	2:F:630:LEU:CD1	2.83	0.55
2:C:26:HIS:CG	2:C:33:HIS:CE1	2.94	0.55
2:A:631:LEU:HD22	2:A:698:ARG:HH22	1.70	0.55
2:E:731:THR:HG22	2:E:741:ILE:HB	1.88	0.55
2:D:364:VAL:HG12	2:D:365:SER:HA	1.87	0.55
2:B:619:ILE:HD11	2:B:656:MET:CG	2.36	0.55
2:B:38:LEU:HD22	2:B:46:ALA:CB	2.37	0.55
1:5:216:PHE:CD1	2:E:440:ALA:HA	2.42	0.55
2:E:506:LEU:HD13	2:E:554:LEU:HD11	1.88	0.55
2:E:278:ILE:HG21	2:E:281:LEU:HD23	1.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:18:GLN:OE1	2:A:29:ILE:HD12	2.07	0.55
2:B:682:HIS:CE1	2:B:718:HIS:CE1	2.95	0.55
1:4:154:LEU:HD22	1:4:212:ILE:HD11	1.88	0.54
2:C:772:HIS:CE1	2:C:801:PHE:CE2	2.95	0.54
2:D:362:HIS:CD2	2:E:232:GLU:HB2	2.42	0.54
2:E:26:HIS:CG	2:E:33:HIS:CE1	2.94	0.54
2:E:513:GLN:HE22	2:E:550:GLY:HA3	1.72	0.54
2:C:31:THR:HB	2:C:120:ALA:H	1.72	0.54
2:E:739:LEU:CD2	2:F:531:LEU:HD12	2.37	0.54
2:E:667:ARG:HB2	2:E:681:ASN:HD21	1.72	0.54
2:C:276:LEU:HD23	2:C:309:LEU:HA	1.89	0.54
2:D:281:LEU:HG	2:D:314:ALA:H	1.73	0.54
1:3:140:ILE:HG12	1:3:216:PHE:HB3	1.89	0.54
2:A:398:ALA:HB1	2:A:475:ASP:CG	2.27	0.54
2:F:373:ALA:HB2	2:F:492:ALA:N	2.23	0.54
1:2:216:PHE:CD1	2:B:440:ALA:HA	2.43	0.54
2:D:198:ARG:HH12	2:D:335:GLN:HG3	1.72	0.54
2:B:303:SER:HB3	2:B:309:LEU:HB2	1.90	0.54
1:6:133:PHE:CE2	1:6:163:LEU:HB2	2.42	0.54
2:D:526:ARG:O	2:D:531:LEU:HD23	2.08	0.53
2:E:38:LEU:HD22	2:E:46:ALA:HB1	1.90	0.53
2:B:26:HIS:CE1	2:B:68:ILE:HB	2.44	0.53
2:F:377:LEU:HD13	2:F:495:GLU:HB2	1.90	0.53
2:B:790:GLN:HE21	2:B:805:THR:HG23	1.72	0.53
2:F:16:LEU:HB3	2:F:37:GLY:HA2	1.91	0.53
2:C:373:ALA:HB2	2:C:492:ALA:N	2.24	0.53
2:B:713:SER:HA	2:B:714:LEU:HD12	1.90	0.53
2:A:544:LEU:HB2	2:A:710:VAL:HG22	1.90	0.53
2:E:198:ARG:HH12	2:E:335:GLN:HG3	1.72	0.53
2:A:587:VAL:HA	2:B:594:VAL:H	1.74	0.53
2:F:27:ASN:HA	2:F:75:SER:HA	1.89	0.53
2:A:278:ILE:O	2:A:281:LEU:HG	2.09	0.53
2:D:91:SER:CB	2:D:108:ILE:HD13	2.39	0.53
2:F:503:GLU:H	2:F:525:ARG:HH21	1.56	0.53
2:E:198:ARG:HH11	2:E:201:LYS:HB2	1.74	0.53
2:C:665:LEU:HD21	2:C:710:VAL:CG1	2.39	0.53
2:A:55:LEU:HD13	2:A:124:LEU:HD22	1.90	0.53
2:B:613:VAL:CG1	2:B:655:ILE:HD12	2.38	0.53
2:E:416:LEU:HB3	2:E:453:VAL:HG22	1.90	0.53
2:F:665:LEU:HD11	2:F:689:VAL:HG11	1.91	0.53
2:A:13:VAL:HB	2:A:38:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ASP:HB3	2:D:198:ARG:HD3	1.90	0.53
2:E:619:ILE:CD1	2:E:656:MET:CB	2.74	0.53
1:1:136:PHE:CE2	1:1:216:PHE:CD2	2.97	0.53
1:3:204:ILE:HG21	1:3:211:THR:CB	2.39	0.53
2:E:402:VAL:HG13	2:E:405:ARG:HE	1.73	0.53
1:2:156:SER:HB2	1:2:203:ILE:HD11	1.91	0.53
2:A:619:ILE:HG23	2:A:627:PHE:CE1	2.44	0.52
2:F:31:THR:H	2:F:83:ARG:HH21	1.57	0.52
2:E:64:VAL:HG22	2:E:123:VAL:HG21	1.92	0.52
1:3:136:PHE:CE1	2:C:431:VAL:HG11	2.45	0.52
1:3:133:PHE:CD2	1:3:139:VAL:HG22	2.43	0.52
2:D:473:VAL:HG23	2:D:474:ASP:H	1.73	0.52
2:E:619:ILE:CG2	2:E:619:ILE:O	2.56	0.52
1:4:136:PHE:CZ	1:4:161:TYR:CE1	2.97	0.52
1:6:216:PHE:CZ	2:F:431:VAL:HG22	2.45	0.52
2:D:168:ARG:HE	2:D:169:ASP:H	1.57	0.52
2:E:281:LEU:HG	2:E:313:GLY:HA2	1.90	0.52
2:F:91:SER:CB	2:F:108:ILE:HD13	2.40	0.52
2:E:17:ALA:HA	2:E:33:HIS:HB3	1.91	0.52
2:F:723:VAL:HA	2:F:769:ILE:HD11	1.92	0.52
2:A:558:LEU:HD13	2:A:653:ILE:HG21	1.90	0.52
2:E:14:LEU:O	2:E:17:ALA:HB3	2.10	0.52
2:B:55:LEU:HD13	2:B:124:LEU:HD22	1.92	0.52
2:E:665:LEU:HD22	2:E:712:HIS:HA	1.92	0.52
2:E:547:THR:H	2:E:763:ARG:HE	1.56	0.52
2:A:26:HIS:CD2	2:A:33:HIS:CE1	2.98	0.52
2:B:665:LEU:HD21	2:B:710:VAL:HB	1.90	0.52
1:6:203:ILE:HG22	2:F:436:PHE:CZ	2.45	0.52
2:D:278:ILE:O	2:D:281:LEU:HD21	2.10	0.52
2:E:377:LEU:HD12	2:E:480:VAL:HG21	1.92	0.52
2:E:387:LEU:H	2:E:387:LEU:HD22	1.74	0.52
1:1:216:PHE:CD1	2:A:440:ALA:HA	2.45	0.52
2:A:38:LEU:O	2:A:47:ALA:HB2	2.10	0.52
2:D:31:THR:HG23	2:D:87:VAL:HG21	1.90	0.52
2:A:156:SER:H	2:F:90:LEU:HG	1.75	0.52
2:B:616:LEU:HD13	2:B:630:LEU:HD22	1.92	0.51
2:D:363:ARG:HD2	2:D:403:ARG:H	1.75	0.51
2:B:619:ILE:CD1	2:B:656:MET:CG	2.88	0.51
2:B:26:HIS:CG	2:B:33:HIS:CE1	2.98	0.51
2:D:786:ILE:HD13	2:D:792:ILE:HG23	1.91	0.51
2:D:619:ILE:CG2	2:D:626:VAL:HG13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:615:LEU:CD2	2:E:617:ASP:OD1	2.51	0.51
1:1:216:PHE:CZ	2:A:431:VAL:HG22	2.45	0.51
2:E:168:ARG:HH22	2:E:179:LEU:HD13	1.75	0.51
2:C:619:ILE:HG22	2:C:627:PHE:CZ	2.35	0.51
2:D:14:LEU:O	2:D:17:ALA:HB3	2.11	0.51
2:E:722:ILE:HG23	2:E:765:LEU:HD22	1.91	0.51
2:F:26:HIS:CG	2:F:33:HIS:CE1	2.98	0.51
2:F:790:GLN:HE21	2:F:805:THR:HG23	1.75	0.51
2:C:46:ALA:HB2	2:C:105:THR:O	2.10	0.51
2:B:361:HIS:CD2	2:B:363:ARG:HB2	2.46	0.51
2:D:278:ILE:O	2:D:281:LEU:CD2	2.58	0.51
2:A:17:ALA:CB	2:A:29:ILE:HD11	2.40	0.51
2:B:192:VAL:CG1	2:B:221:LEU:HD21	2.40	0.51
2:F:665:LEU:HA	2:F:685:MET:HG2	1.93	0.51
1:5:216:PHE:HA	2:E:440:ALA:HA	1.93	0.51
2:A:619:ILE:HG21	2:A:701:PHE:CE2	2.45	0.50
2:D:505:ILE:HG22	2:D:509:ARG:HH22	1.75	0.50
2:C:17:ALA:HB1	2:C:29:ILE:CG2	2.41	0.50
2:A:476:ILE:O	2:A:480:VAL:HG23	2.11	0.50
2:F:427:LYS:HG3	2:F:443:ARG:HA	1.92	0.50
2:D:660:VAL:HG21	2:D:695:ARG:HH22	1.76	0.50
2:C:513:GLN:H	2:C:718:HIS:CD2	2.29	0.50
2:F:211:GLY:H	2:F:213:GLY:H	1.59	0.50
2:A:528:ARG:HE	2:A:562:ILE:HG23	1.77	0.50
2:F:382:ILE:HB	2:F:484:THR:HG23	1.93	0.50
1:1:133:PHE:CE2	1:1:163:LEU:HB2	2.46	0.50
2:F:619:ILE:O	2:F:619:ILE:CG2	2.59	0.50
2:B:46:ALA:HB1	2:B:109:LEU:HB2	1.93	0.50
2:A:96:ARG:HE	2:A:101:SER:HA	1.76	0.50
2:D:613:VAL:CG1	2:D:655:ILE:HD12	2.42	0.50
2:B:100:HIS:CD2	2:B:107:HIS:CE1	2.99	0.50
2:A:31:THR:HB	2:A:120:ALA:H	1.76	0.50
2:A:378:SER:OG	2:A:394:LEU:HD11	2.12	0.50
2:D:31:THR:CG2	2:D:87:VAL:HG21	2.42	0.50
2:B:506:LEU:HD13	2:B:554:LEU:HD11	1.93	0.50
2:F:786:ILE:HD13	2:F:792:ILE:HD11	1.94	0.50
2:D:545:GLY:HA2	2:D:665:LEU:HD22	1.94	0.50
2:C:730:LEU:HD11	2:C:774:GLU:CG	2.42	0.50
2:B:277:PHE:HE2	2:B:279:ASP:OD2	1.95	0.49
2:D:619:ILE:HG22	2:D:619:ILE:O	2.12	0.49
2:C:278:ILE:O	2:C:281:LEU:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:786:ILE:HD13	2:A:792:ILE:HG23	1.93	0.49
2:E:281:LEU:HD11	2:E:313:GLY:N	2.09	0.49
2:E:619:ILE:HG21	2:E:701:PHE:CZ	2.47	0.49
2:C:198:ARG:HH12	2:C:335:GLN:HG3	1.78	0.49
2:A:619:ILE:HD12	2:A:656:MET:CB	2.41	0.49
2:A:536:ARG:HH22	2:F:770:GLN:HG3	1.77	0.49
2:B:619:ILE:HD13	2:B:701:PHE:CZ	2.47	0.49
2:D:619:ILE:CG2	2:D:626:VAL:CG1	2.90	0.49
2:C:100:HIS:CD2	2:C:107:HIS:CE1	3.01	0.49
2:E:361:HIS:CD2	2:F:233:ILE:HG22	2.48	0.49
2:E:397:GLU:HA	2:F:198:ARG:HE	1.78	0.49
1:5:136:PHE:CD1	1:5:161:TYR:CE1	3.00	0.49
2:D:398:ALA:HB1	2:D:475:ASP:CG	2.33	0.49
2:C:278:ILE:CB	2:C:281:LEU:HD23	1.94	0.49
2:A:46:ALA:HB2	2:A:105:THR:O	2.13	0.49
2:B:278:ILE:HG22	2:B:281:LEU:HD23	1.94	0.49
2:C:370:ALA:O	2:C:373:ALA:HB3	2.12	0.49
1:5:133:PHE:CG	1:5:139:VAL:HG22	2.48	0.49
2:C:786:ILE:HD12	2:C:792:ILE:HD13	1.95	0.49
2:B:398:ALA:HB1	2:B:475:ASP:HB3	1.95	0.49
2:A:394:LEU:HD22	2:A:480:VAL:HA	1.93	0.48
1:3:140:ILE:CB	2:C:443:ARG:HE	2.26	0.48
2:B:20:GLU:HB3	2:B:33:HIS:CG	2.47	0.48
2:F:371:ILE:O	2:F:374:ALA:HB3	2.12	0.48
2:C:716:LYS:H	2:C:719:LEU:HD12	1.78	0.48
2:D:371:ILE:HD12	2:D:395:ILE:HD13	1.95	0.48
2:D:387:LEU:H	2:D:387:LEU:HD22	1.78	0.48
2:B:281:LEU:HG	2:B:314:ALA:H	1.78	0.48
2:B:714:LEU:HD23	2:B:718:HIS:CG	2.48	0.48
2:C:685:MET:HG3	2:C:712:HIS:CD2	2.47	0.48
2:E:26:HIS:CG	2:E:33:HIS:HE1	2.30	0.48
2:F:46:ALA:HB2	2:F:105:THR:O	2.13	0.48
2:B:29:ILE:HG23	2:B:33:HIS:HD1	1.78	0.48
2:C:46:ALA:H	2:C:105:THR:HB	1.78	0.48
2:F:363:ARG:CG	2:F:403:ARG:HE	2.26	0.48
2:C:619:ILE:HD11	2:C:656:MET:HG3	1.95	0.48
2:E:394:LEU:HD22	2:E:480:VAL:HA	1.96	0.48
1:5:136:PHE:CZ	1:5:154:LEU:HD22	2.49	0.48
2:C:289:GLY:H	2:C:321:ARG:HH12	1.60	0.48
2:C:370:ALA:HB1	2:C:476:ILE:HD12	1.96	0.48
2:C:394:LEU:HD21	2:C:483:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:216:PHE:CE1	2:F:440:ALA:HA	2.47	0.48
2:F:631:LEU:HD23	2:F:701:PHE:HA	1.96	0.48
2:A:355:ARG:HA	2:A:358:TYR:CE1	2.49	0.48
1:1:140:ILE:HD13	1:1:216:PHE:O	2.12	0.48
2:B:364:VAL:HG23	2:B:365:SER:HA	1.95	0.48
2:E:619:ILE:HD12	2:E:656:MET:CG	2.37	0.48
2:D:396:ASP:HB3	2:E:198:ARG:HD3	1.94	0.48
2:D:355:ARG:HD3	2:D:371:ILE:HD11	1.95	0.48
1:4:215:HIS:O	1:4:216:PHE:CD1	2.67	0.48
2:C:18:GLN:O	2:C:21:ALA:HB3	2.14	0.48
2:E:352:GLN:HE22	2:E:368:ASP:HA	1.79	0.48
2:C:584:SER:HB3	2:D:582:SER:H	1.79	0.48
2:D:619:ILE:HG23	2:D:626:VAL:HG13	1.96	0.47
2:B:278:ILE:CB	2:B:281:LEU:HD23	2.44	0.47
2:E:13:VAL:HG11	2:E:38:LEU:HD23	1.96	0.47
2:B:394:LEU:HD22	2:B:480:VAL:HG22	1.96	0.47
2:E:427:LYS:HG3	2:E:443:ARG:HA	1.95	0.47
1:3:136:PHE:CE1	1:3:161:TYR:CE1	3.01	0.47
2:E:476:ILE:O	2:E:480:VAL:HG23	2.15	0.47
2:D:689:VAL:HG11	2:D:710:VAL:HG13	1.96	0.47
2:C:730:LEU:HD21	2:C:774:GLU:HG3	1.95	0.47
2:A:730:LEU:HA	2:A:733:ARG:HE	1.79	0.47
2:D:678:GLU:CD	2:D:678:GLU:H	2.17	0.47
2:C:398:ALA:HB1	2:C:475:ASP:CG	2.34	0.47
2:C:719:LEU:HD21	2:C:755:GLY:HA3	1.96	0.47
2:F:665:LEU:CD1	2:F:689:VAL:HG11	2.44	0.47
2:B:32:GLU:HG3	2:B:33:HIS:CD2	2.50	0.47
2:D:16:LEU:HB3	2:D:37:GLY:HA2	1.96	0.47
2:F:719:LEU:HD22	2:F:752:ALA:O	2.14	0.47
2:E:619:ILE:HD13	2:E:701:PHE:HZ	1.79	0.47
2:B:665:LEU:HD23	2:B:685:MET:HB3	1.97	0.47
2:A:382:ILE:HA	2:A:383:SER:HB3	1.96	0.47
2:E:739:LEU:HD13	2:E:741:ILE:HD11	1.97	0.47
2:E:741:ILE:HD12	2:E:777:LEU:HG	1.97	0.47
2:A:619:ILE:HG21	2:A:701:PHE:HE2	1.80	0.47
2:D:46:ALA:H	2:D:105:THR:HB	1.79	0.47
2:C:26:HIS:CE1	2:C:68:ILE:HB	2.50	0.47
2:C:473:VAL:HG23	2:C:474:ASP:H	1.80	0.47
2:E:399:GLY:CA	2:E:471:VAL:HG13	2.45	0.47
2:C:791:HIS:H	2:C:807:ALA:HB2	1.80	0.47
2:A:196:LEU:HD12	2:A:275:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:140:ILE:HD12	2:A:443:ARG:CZ	2.44	0.47
2:F:363:ARG:CG	2:F:403:ARG:HB2	2.45	0.47
1:3:184:GLU:HA	2:C:81:THR:HG22	1.96	0.47
2:B:739:LEU:HD13	2:B:788:LYS:HA	1.97	0.47
2:E:46:ALA:HA	2:E:138:VAL:HG13	1.96	0.47
2:E:398:ALA:HA	2:E:401:LYS:HB3	1.97	0.47
1:3:146:ASN:HB2	1:3:178:GLN:HE22	1.80	0.47
2:A:589:SER:H	2:B:591:PRO:HA	1.80	0.47
2:A:18:GLN:O	2:A:21:ALA:HB3	2.15	0.47
2:F:777:LEU:HD22	2:F:792:ILE:HG21	1.96	0.47
2:D:168:ARG:NE	2:D:169:ASP:H	2.13	0.47
2:E:685:MET:O	2:E:710:VAL:HG11	2.15	0.47
2:E:278:ILE:CB	2:E:281:LEU:HD23	2.39	0.46
2:F:38:LEU:HD13	2:F:46:ALA:HB1	1.96	0.46
2:F:716:LYS:H	2:F:717:LYS:HB3	1.79	0.46
2:A:26:HIS:CE1	2:A:68:ILE:HB	2.50	0.46
2:C:6:PHE:HA	2:C:103:VAL:H	1.81	0.46
2:E:777:LEU:HG	2:E:792:ILE:HG21	1.96	0.46
2:F:665:LEU:HG	2:F:689:VAL:HG21	1.97	0.46
2:F:363:ARG:HH22	2:F:470:GLU:CD	2.19	0.46
2:F:726:MET:HB2	2:F:769:ILE:HD13	1.97	0.46
2:B:668:ASN:HB3	2:B:715:GLU:HB2	1.97	0.46
2:F:613:VAL:CG1	2:F:655:ILE:HD12	2.46	0.46
2:D:786:ILE:HD13	2:D:803:VAL:HG11	1.97	0.46
2:F:772:HIS:CE1	2:F:801:PHE:CD1	3.03	0.46
2:F:370:ALA:HB1	2:F:476:ILE:HD12	1.97	0.46
2:F:619:ILE:HG23	2:F:627:PHE:CD2	2.50	0.46
2:B:305:ALA:HB2	2:B:329:ALA:CB	2.45	0.46
2:E:727:SER:O	2:E:731:THR:HG23	2.16	0.46
2:C:20:GLU:HB3	2:C:33:HIS:CD2	2.51	0.46
2:A:232:GLU:H	2:F:403:ARG:HD2	1.80	0.46
1:2:140:ILE:HB	2:B:443:ARG:HH11	1.81	0.46
1:1:153:THR:HG23	1:1:202:LEU:HD21	1.98	0.46
2:C:14:LEU:O	2:C:17:ALA:HB3	2.15	0.46
2:D:506:LEU:HD13	2:D:554:LEU:HD11	1.97	0.46
2:F:713:SER:HA	2:F:718:HIS:CG	2.50	0.46
2:F:395:ILE:HA	2:F:476:ILE:CD1	2.46	0.46
1:1:216:PHE:CE1	2:A:443:ARG:HB2	2.50	0.46
2:E:36:LEU:HD11	2:E:64:VAL:HG11	1.98	0.46
2:A:165:SER:HB2	2:A:166:LEU:HB2	1.98	0.46
2:A:385:ARG:HH22	2:B:335:GLN:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:LEU:HB2	2:B:741:ILE:HD11	1.98	0.46
2:A:780:GLU:HG2	2:A:783:ARG:HH21	1.81	0.46
2:E:411:PRO:HA	2:E:460:TRP:CE2	2.51	0.46
2:E:739:LEU:HD22	2:E:741:ILE:HD11	1.97	0.46
2:A:91:SER:CB	2:A:108:ILE:HD13	2.46	0.46
2:E:613:VAL:CG1	2:E:655:ILE:HD12	2.46	0.46
2:E:383:SER:H	2:E:390:LYS:HD3	1.82	0.46
2:E:619:ILE:CG2	2:E:701:PHE:HE2	2.26	0.45
1:1:202:LEU:HD23	1:1:203:ILE:N	2.31	0.45
2:A:83:ARG:HH21	2:A:119:VAL:HG22	1.81	0.45
2:C:13:VAL:HB	2:C:38:LEU:HD23	1.99	0.45
2:C:361:HIS:CD2	2:D:234:LEU:HD12	2.51	0.45
2:A:416:LEU:HB3	2:A:453:VAL:HG22	1.96	0.45
2:C:703:ASN:HB2	2:C:704:ARG:HH11	1.80	0.45
2:A:198:ARG:CD	2:A:201:LYS:HB2	2.46	0.45
2:D:17:ALA:HA	2:D:33:HIS:HB3	1.99	0.45
2:E:45:ILE:HG22	2:E:138:VAL:HG12	1.99	0.45
2:B:41:GLU:HG2	2:B:47:ALA:HB2	1.98	0.45
1:1:142:LEU:HA	1:1:185:TYR:CD2	2.51	0.45
2:B:730:LEU:CD2	2:B:774:GLU:HG3	2.47	0.45
2:F:523:ALA:HA	2:F:526:ARG:HE	1.80	0.45
2:B:615:LEU:CD2	2:B:617:ASP:OD1	2.59	0.45
2:C:26:HIS:HB2	2:C:33:HIS:CE1	2.51	0.45
2:C:20:GLU:HB3	2:C:33:HIS:CG	2.51	0.45
2:E:358:TYR:CE2	2:F:200:THR:HA	2.51	0.45
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.51	0.45
2:A:355:ARG:HE	2:A:395:ILE:HG21	1.82	0.45
1:6:216:PHE:CE2	2:F:431:VAL:HG22	2.52	0.45
1:4:142:LEU:HD11	1:4:182:LEU:HD22	1.99	0.45
2:B:558:LEU:CD1	2:B:655:ILE:HD11	2.47	0.45
1:4:212:ILE:HD12	1:4:216:PHE:CD2	2.52	0.45
2:B:26:HIS:CD2	2:B:33:HIS:NE2	2.85	0.45
2:E:373:ALA:HB2	2:E:492:ALA:HA	1.98	0.45
2:F:55:LEU:HD13	2:F:124:LEU:HD22	1.99	0.45
2:D:777:LEU:HD21	2:D:794:LEU:HB2	1.99	0.45
2:E:499:LEU:HD11	2:E:529:ALA:HB2	1.99	0.45
2:D:394:LEU:HG	2:D:394:LEU:H	1.60	0.45
1:4:194:HIS:CE1	2:E:141:LEU:O	2.70	0.45
1:2:203:ILE:HG21	2:B:434:GLN:HE21	1.82	0.45
2:B:476:ILE:O	2:B:480:VAL:HG23	2.16	0.45
2:B:558:LEU:HD12	2:B:655:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:689:VAL:HG11	2:B:710:VAL:HG12	1.98	0.45
2:E:460:TRP:CG	2:E:463:LYS:HB2	2.52	0.45
2:B:528:ARG:CZ	2:B:562:ILE:HA	2.47	0.45
2:D:361:HIS:CE1	2:E:234:LEU:HD12	2.52	0.45
2:B:38:LEU:O	2:B:47:ALA:HB2	2.17	0.45
2:C:515:GLU:OE2	2:C:712:HIS:CD2	2.70	0.45
2:A:198:ARG:HH12	2:A:335:GLN:HG3	1.81	0.45
2:F:520:VAL:HG11	2:F:558:LEU:HD11	1.98	0.45
2:B:702:ILE:HA	2:B:705:ILE:HD12	1.97	0.45
2:A:366:ILE:HB	2:A:367:THR:HA	1.99	0.45
2:C:382:ILE:HA	2:C:383:SER:CB	2.47	0.45
2:C:367:THR:O	2:C:370:ALA:HB3	2.17	0.45
2:F:661:GLY:HA3	2:F:689:VAL:HG13	1.99	0.45
2:F:713:SER:HA	2:F:718:HIS:CD2	2.52	0.45
1:2:136:PHE:HA	1:2:161:TYR:CD2	2.52	0.45
2:A:317:LEU:H	2:A:317:LEU:HD12	1.82	0.45
2:D:574:MET:SD	2:D:619:ILE:HG12	2.57	0.44
2:A:20:GLU:HB3	2:A:33:HIS:CD2	2.52	0.44
2:E:411:PRO:HA	2:E:460:TRP:CD2	2.52	0.44
2:B:730:LEU:HD23	2:B:774:GLU:HG3	1.99	0.44
2:F:27:ASN:HB2	2:F:76:GLN:H	1.83	0.44
2:D:137:GLN:HA	2:D:140:GLN:HG2	1.99	0.44
2:C:55:LEU:HD13	2:C:124:LEU:HD22	1.99	0.44
2:A:278:ILE:O	2:A:281:LEU:CD2	2.65	0.44
2:D:619:ILE:HG21	2:D:630:LEU:HD11	1.98	0.44
2:E:394:LEU:HA	2:E:479:VAL:HG11	2.00	0.44
2:E:277:PHE:CE2	2:E:279:ASP:OD2	2.59	0.44
2:C:21:ALA:HA	2:C:33:HIS:CE1	2.53	0.44
2:E:449:LEU:O	2:E:453:VAL:HG23	2.17	0.44
1:1:133:PHE:CD2	1:1:139:VAL:HG22	2.51	0.44
2:D:503:GLU:H	2:D:525:ARG:HH21	1.65	0.44
2:F:583:THR:HG23	2:F:584:SER:H	1.82	0.44
1:5:204:ILE:HD13	1:5:204:ILE:N	2.32	0.44
2:A:14:LEU:O	2:A:17:ALA:HB3	2.18	0.44
2:D:113:ILE:HG21	2:D:135:ARG:HB2	1.99	0.44
2:E:631:LEU:HD13	2:E:698:ARG:HH22	1.82	0.44
1:2:184:GLU:HA	2:B:81:THR:HG22	2.00	0.44
2:F:278:ILE:HD11	2:F:309:LEU:HD11	1.99	0.44
1:5:139:VAL:HG21	1:5:154:LEU:HD11	1.98	0.44
2:D:624:PRO:HA	2:D:627:PHE:CD2	2.53	0.44
2:B:25:GLY:O	2:B:26:HIS:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:LEU:HD11	2:D:124:LEU:HD21	1.99	0.44
2:D:458:LYS:HA	2:D:461:LYS:HG2	2.00	0.44
1:3:194:HIS:HE1	2:D:45:ILE:HD12	1.79	0.44
2:A:21:ALA:HB2	2:A:29:ILE:CG2	2.48	0.44
1:4:136:PHE:CE2	2:D:431:VAL:HG11	2.52	0.44
2:B:395:ILE:HA	2:B:476:ILE:CD1	2.48	0.44
2:C:686:LYS:HA	2:C:710:VAL:HG11	2.00	0.44
1:4:133:PHE:CD2	1:4:139:VAL:HG22	2.53	0.44
1:4:133:PHE:CE2	1:4:163:LEU:HB2	2.53	0.44
2:E:55:LEU:HD13	2:E:124:LEU:HD22	2.00	0.44
2:C:781:LEU:HD12	2:C:787:HIS:HA	1.99	0.44
2:A:351:LEU:HD22	2:A:392:ILE:HG12	1.99	0.44
1:4:137:GLU:CD	2:D:443:ARG:HE	2.21	0.44
1:3:140:ILE:HD12	1:3:140:ILE:H	1.82	0.44
2:C:17:ALA:HB2	2:C:34:ILE:HA	2.00	0.44
2:B:397:GLU:HA	2:C:198:ARG:CZ	2.48	0.44
2:F:715:GLU:H	2:F:718:HIS:HB3	1.83	0.44
2:A:198:ARG:CZ	2:F:397:GLU:HA	2.48	0.44
2:E:196:LEU:HD11	2:E:275:ILE:HD12	2.00	0.44
2:E:281:LEU:HD12	2:E:313:GLY:CA	2.10	0.44
2:B:619:ILE:HG22	2:B:619:ILE:O	2.18	0.44
2:F:394:LEU:CD2	2:F:480:VAL:HA	2.46	0.44
2:C:198:ARG:HH22	2:C:335:GLN:NE2	2.16	0.44
2:B:719:LEU:HD13	2:B:752:ALA:O	2.18	0.44
2:A:394:LEU:HG	2:A:394:LEU:H	1.57	0.43
2:A:394:LEU:HD21	2:A:483:TRP:CE3	2.53	0.43
1:3:204:ILE:HG21	1:3:211:THR:HB	2.00	0.43
2:B:517:VAL:HG22	2:B:554:LEU:HD23	2.00	0.43
2:C:198:ARG:HB2	2:C:202:ASN:HA	2.00	0.43
2:F:730:LEU:HD23	2:F:774:GLU:HG2	1.99	0.43
2:A:282:HIS:CG	2:A:319:GLU:HB3	2.53	0.43
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.53	0.43
2:A:391:ALA:HA	2:A:394:LEU:HD12	2.00	0.43
2:F:26:HIS:H	2:F:26:HIS:CD2	2.37	0.43
2:A:633:VAL:HG13	2:A:649:PHE:CG	2.53	0.43
1:3:133:PHE:CE2	1:3:163:LEU:HB2	2.52	0.43
1:3:195:ARG:HH11	2:D:146:GLU:H	1.65	0.43
1:2:204:ILE:HD11	1:2:212:ILE:CD1	2.48	0.43
1:2:142:LEU:HD21	1:2:182:LEU:HA	2.00	0.43
2:C:358:TYR:CZ	2:C:364:VAL:HG21	2.53	0.43
2:E:633:VAL:HG13	2:E:649:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:137:GLU:CB	2:F:443:ARG:HD3	2.49	0.43
2:C:633:VAL:HG13	2:C:649:PHE:CG	2.53	0.43
1:2:140:ILE:HG12	1:2:216:PHE:HB3	1.99	0.43
2:D:29:ILE:HB	2:D:80:TYR:HA	2.00	0.43
2:A:545:GLY:H	2:A:665:LEU:HD13	1.84	0.43
2:B:366:ILE:HB	2:B:367:THR:HA	1.99	0.43
1:6:137:GLU:HB2	2:F:443:ARG:HH11	1.84	0.43
1:3:140:ILE:CG1	1:3:216:PHE:HB3	2.49	0.43
2:B:17:ALA:HA	2:B:33:HIS:HB3	2.00	0.43
2:F:316:THR:H	2:F:319:GLU:HB2	1.82	0.43
1:5:140:ILE:HG12	1:5:216:PHE:CB	2.49	0.43
1:2:161:TYR:CE1	2:B:431:VAL:HG11	2.54	0.43
2:F:413:LEU:HD13	2:F:456:THR:HB	2.01	0.43
1:4:156:SER:HB2	1:4:203:ILE:HD11	1.98	0.43
1:4:136:PHE:CE2	1:4:161:TYR:CD1	3.07	0.43
2:F:363:ARG:HG2	2:F:403:ARG:HB2	2.00	0.43
2:E:397:GLU:HB2	2:F:198:ARG:HH21	1.84	0.43
2:D:777:LEU:O	2:D:781:LEU:HG	2.19	0.43
2:A:362:HIS:CE1	2:B:232:GLU:HB3	2.53	0.43
1:5:146:ASN:HD21	1:5:181:ILE:HG22	1.84	0.43
2:E:739:LEU:HD21	2:F:531:LEU:HD12	2.00	0.43
2:A:536:ARG:HH12	2:F:770:GLN:HB2	1.84	0.43
2:A:276:LEU:HD23	2:A:309:LEU:HA	2.01	0.43
2:B:563:PHE:CD1	2:B:611:TYR:HB2	2.53	0.43
2:F:49:ALA:O	2:F:53:LEU:HD22	2.18	0.43
1:1:195:ARG:HE	1:1:195:ARG:HA	1.84	0.43
2:C:577:TYR:CD1	2:C:597:ASP:HB2	2.54	0.43
1:6:139:VAL:HG13	1:6:154:LEU:HD13	2.01	0.43
2:C:361:HIS:CE1	2:D:198:ARG:O	2.72	0.43
2:A:516:ALA:HB2	2:A:710:VAL:O	2.19	0.43
2:D:778:SER:HA	2:D:781:LEU:HD12	2.01	0.43
2:E:363:ARG:HG2	2:E:364:VAL:HG23	2.00	0.43
2:F:398:ALA:HB1	2:F:475:ASP:CG	2.39	0.43
2:D:278:ILE:CB	2:D:281:LEU:HD23	2.47	0.43
2:A:619:ILE:HG23	2:A:627:PHE:HE1	1.83	0.43
2:C:570:ILE:HD12	2:C:606:VAL:HG22	2.00	0.43
2:C:665:LEU:HD23	2:C:685:MET:HB2	2.00	0.43
2:C:358:TYR:CE2	2:C:364:VAL:HG21	2.54	0.43
2:A:731:THR:HG22	2:A:741:ILE:HB	2.01	0.43
2:D:704:ARG:HH11	2:D:704:ARG:HG3	1.84	0.43
2:C:377:LEU:HD13	2:C:495:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:136:PHE:CD1	2:F:431:VAL:HG21	2.54	0.42
2:D:26:HIS:HB2	2:D:33:HIS:HE1	1.83	0.42
2:F:633:VAL:HG13	2:F:649:PHE:CG	2.54	0.42
2:D:513:GLN:HG3	2:D:712:HIS:H	1.84	0.42
1:2:147:VAL:HG13	1:2:148:ASN:H	1.83	0.42
2:C:113:ILE:HG23	2:C:131:LEU:HB3	2.01	0.42
2:B:281:LEU:HD21	2:B:313:GLY:HA2	1.89	0.42
1:4:136:PHE:CD2	1:4:216:PHE:CE2	3.07	0.42
2:E:53:LEU:HD21	2:E:134:ALA:HA	2.00	0.42
2:B:739:LEU:HD11	2:B:792:ILE:CD1	2.49	0.42
2:A:233:ILE:H	2:F:403:ARG:NH1	2.17	0.42
2:E:363:ARG:HH21	2:E:468:ASN:HA	1.84	0.42
2:C:385:ARG:HH21	2:D:331:GLU:HA	1.85	0.42
2:A:17:ALA:HA	2:A:33:HIS:HB3	2.00	0.42
2:B:661:GLY:CA	2:B:689:VAL:HG13	2.50	0.42
2:D:510:VAL:HG21	2:D:554:LEU:HA	2.02	0.42
1:1:204:ILE:HD11	1:1:212:ILE:HD11	2.02	0.42
2:C:363:ARG:HD3	2:C:400:SER:HA	2.01	0.42
1:6:212:ILE:HG23	1:6:216:PHE:HB3	2.02	0.42
2:F:382:ILE:HA	2:F:383:SER:HB2	2.00	0.42
2:E:503:GLU:H	2:E:525:ARG:NH2	2.17	0.42
2:A:686:LYS:HB2	2:A:712:HIS:CE1	2.55	0.42
2:D:53:LEU:HD21	2:D:134:ALA:HA	2.01	0.42
2:C:476:ILE:HA	2:C:479:VAL:HG22	2.01	0.42
2:A:21:ALA:HA	2:A:33:HIS:CE1	2.54	0.42
2:B:516:ALA:HB2	2:B:710:VAL:O	2.20	0.42
2:A:192:VAL:O	2:A:196:LEU:HD22	2.19	0.42
1:1:216:PHE:CE2	2:A:431:VAL:HG22	2.55	0.42
2:A:370:ALA:CB	2:A:471:VAL:HG13	2.50	0.42
2:F:53:LEU:H	2:F:53:LEU:HD22	1.85	0.42
2:E:528:ARG:HD2	2:E:562:ILE:HD12	2.01	0.42
2:B:16:LEU:HB3	2:B:37:GLY:HA2	2.02	0.42
2:C:544:LEU:HD21	2:C:693:LEU:HD12	2.02	0.42
2:B:14:LEU:O	2:B:17:ALA:HB3	2.19	0.42
2:F:21:ALA:CB	2:F:29:ILE:HG12	2.50	0.42
2:F:20:GLU:HB2	2:F:33:HIS:CG	2.55	0.42
2:B:371:ILE:O	2:B:374:ALA:HB3	2.19	0.42
2:B:791:HIS:H	2:B:807:ALA:HB3	1.85	0.42
1:6:132:ARG:HH22	2:A:151:ALA:H	1.68	0.42
2:A:427:LYS:HE2	2:A:443:ARG:HA	2.02	0.42
1:3:136:PHE:CZ	1:3:154:LEU:CD2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:515:GLU:CD	2:E:712:HIS:CD2	2.93	0.42
2:D:387:LEU:HA	2:D:390:LYS:HE2	2.02	0.42
2:A:770:GLN:HA	2:A:774:GLU:HG2	2.02	0.42
1:1:202:LEU:HD23	1:1:203:ILE:H	1.84	0.42
2:A:719:LEU:HD13	2:A:752:ALA:O	2.20	0.42
2:F:515:GLU:H	2:F:515:GLU:CD	2.23	0.42
2:C:483:TRP:HE1	2:D:336:PRO:HD2	1.85	0.41
2:A:619:ILE:HD12	2:A:656:MET:CG	2.50	0.41
2:D:26:HIS:CG	2:D:33:HIS:CE1	3.08	0.41
1:4:136:PHE:HB3	2:D:443:ARG:HG3	2.02	0.41
2:F:361:HIS:HD2	2:F:403:ARG:HH21	1.68	0.41
2:C:366:ILE:O	2:C:471:VAL:HG13	2.20	0.41
1:1:133:PHE:CZ	1:1:142:LEU:HD13	2.55	0.41
2:F:772:HIS:HE1	2:F:801:PHE:CD1	2.37	0.41
1:1:153:THR:HA	1:1:208:ALA:HB2	2.01	0.41
2:C:363:ARG:HG2	2:C:403:ARG:HH21	1.84	0.41
2:E:792:ILE:HG23	2:E:803:VAL:HG13	2.02	0.41
2:A:38:LEU:HD22	2:A:46:ALA:CB	2.50	0.41
2:D:777:LEU:HD11	2:D:794:LEU:HB2	2.02	0.41
2:E:503:GLU:H	2:E:525:ARG:HH21	1.68	0.41
2:E:512:GLY:HA3	2:E:718:HIS:CD2	2.55	0.41
2:A:46:ALA:HB1	2:A:109:LEU:HB2	2.03	0.41
2:A:203:ASN:HA	2:A:311:CYS:O	2.20	0.41
2:B:189:ILE:HG23	2:B:221:LEU:HD23	2.02	0.41
2:C:719:LEU:HD13	2:C:752:ALA:O	2.20	0.41
2:B:165:SER:HB2	2:B:166:LEU:HB2	2.02	0.41
2:A:499:LEU:O	2:A:502:MET:HB2	2.21	0.41
2:F:427:LYS:O	2:F:431:VAL:HG23	2.20	0.41
2:A:398:ALA:C	2:A:400:SER:H	2.24	0.41
1:6:156:SER:HB2	1:6:203:ILE:HD11	2.01	0.41
2:F:542:ILE:HD13	2:F:656:MET:HB2	2.02	0.41
2:B:778:SER:HA	2:C:531:LEU:HD23	2.03	0.41
2:A:351:LEU:HD11	2:A:391:ALA:HB1	2.02	0.41
1:4:131:LEU:HD11	1:4:182:LEU:HD13	2.01	0.41
2:A:544:LEU:HD21	2:A:693:LEU:CD1	2.50	0.41
2:C:515:GLU:HG3	2:C:516:ALA:H	1.85	0.41
2:A:396:ASP:HB3	2:B:198:ARG:HD3	2.03	0.41
2:C:588:GLY:H	2:D:594:VAL:HG13	1.84	0.41
2:B:714:LEU:HD23	2:B:718:HIS:CD2	2.56	0.41
2:A:524:VAL:CG1	2:A:538:ILE:HD12	2.49	0.41
1:5:216:PHE:CD1	2:E:443:ARG:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:360:ALA:HA	2:A:362:HIS:CE1	2.55	0.41
2:F:606:VAL:HG11	2:F:649:PHE:CD1	2.54	0.41
2:D:49:ALA:O	2:D:53:LEU:HD22	2.21	0.41
2:D:787:HIS:CE1	2:E:531:LEU:HD11	2.56	0.41
2:E:619:ILE:HD11	2:E:630:LEU:HD13	2.03	0.41
2:F:198:ARG:HB2	2:F:202:ASN:HA	2.02	0.41
2:F:355:ARG:NH1	2:F:371:ILE:HD13	2.36	0.41
2:E:619:ILE:CD1	2:E:630:LEU:HD13	2.50	0.41
2:E:615:LEU:HD21	2:E:657:THR:HG23	2.01	0.41
1:6:136:PHE:CD2	1:6:216:PHE:CE1	3.09	0.41
1:5:136:PHE:CZ	1:5:154:LEU:CD2	3.04	0.41
2:E:664:GLU:HG3	2:E:685:MET:HA	2.02	0.41
2:A:709:ILE:HG21	2:A:711:PHE:CE2	2.55	0.41
2:C:426:GLU:HB3	2:C:442:LEU:HD13	2.03	0.41
2:A:137:GLN:HA	2:A:140:GLN:HG2	2.02	0.41
2:D:470:GLU:HG2	2:D:472:THR:HG23	2.03	0.41
1:4:195:ARG:HE	2:E:143:GLY:N	2.19	0.41
1:5:131:LEU:HD11	1:5:182:LEU:HD13	2.03	0.41
2:A:202:ASN:HA	2:A:310:GLN:HE21	1.86	0.41
1:3:165:VAL:HG11	1:3:167:PHE:CZ	2.56	0.41
2:E:281:LEU:CD2	2:E:313:GLY:HA2	2.51	0.41
2:D:619:ILE:CG2	2:D:619:ILE:O	2.69	0.41
2:D:394:LEU:O	2:D:479:VAL:HG21	2.21	0.41
1:4:136:PHE:CD2	1:4:216:PHE:CZ	3.08	0.41
2:F:198:ARG:HH11	2:F:201:LYS:HB3	1.86	0.41
2:D:403:ARG:HH21	2:E:231:PRO:HA	1.85	0.41
2:A:730:LEU:HD11	2:A:774:GLU:HB3	2.03	0.41
2:A:45:ILE:HB	2:A:106:GLU:HB3	2.03	0.41
1:6:153:THR:HA	1:6:208:ALA:HB2	2.03	0.41
2:D:375:VAL:HG12	2:D:379:ASP:OD1	2.21	0.41
2:F:630:LEU:O	2:F:634:LEU:HD13	2.21	0.40
2:E:393:ASP:HB2	2:F:335:GLN:HG3	2.02	0.40
2:B:363:ARG:HG2	2:B:403:ARG:HB2	2.03	0.40
2:A:366:ILE:O	2:A:471:VAL:HG12	2.21	0.40
2:A:474:ASP:HA	2:A:494:THR:H	1.85	0.40
2:B:627:PHE:HB2	2:B:698:ARG:HE	1.86	0.40
2:F:29:ILE:HB	2:F:80:TYR:HA	2.02	0.40
1:2:154:LEU:CD2	1:2:212:ILE:HD11	2.50	0.40
2:D:94:GLU:O	2:D:107:HIS:CD2	2.74	0.40
2:E:199:ARG:HA	2:E:202:ASN:HB3	2.03	0.40
2:A:363:ARG:HB2	2:A:403:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:358:TYR:CE2	2:D:364:VAL:HG21	2.57	0.40
2:E:667:ARG:CB	2:E:681:ASN:HD21	2.32	0.40
2:D:375:VAL:HA	2:D:391:ALA:HB2	2.04	0.40
2:C:402:VAL:HG21	2:C:470:GLU:HB3	2.03	0.40
2:C:24:LEU:HD11	2:C:61:GLN:HE22	1.86	0.40
2:B:291:GLU:HG2	2:B:293:ALA:H	1.86	0.40
2:A:351:LEU:HD23	2:A:351:LEU:N	2.36	0.40
2:F:685:MET:HB2	2:F:712:HIS:CE1	2.57	0.40
2:C:427:LYS:HG3	2:C:443:ARG:HA	2.04	0.40
2:F:363:ARG:HD2	2:F:403:ARG:H	1.85	0.40
2:A:232:GLU:N	2:F:403:ARG:HH11	2.20	0.40
2:A:633:VAL:HG22	2:A:649:PHE:CE2	2.56	0.40
2:B:364:VAL:HA	2:B:365:SER:O	2.22	0.40
2:C:661:GLY:HA3	2:C:689:VAL:HG13	2.03	0.40
2:E:473:VAL:HG23	2:E:474:ASP:H	1.87	0.40
1:1:167:PHE:CD1	1:1:175:VAL:HG22	2.56	0.40
2:E:165:SER:HB2	2:E:166:LEU:HB2	2.02	0.40
1:3:194:HIS:NE2	2:D:45:ILE:HD12	2.35	0.40
2:D:13:VAL:HG21	2:D:38:LEU:HD23	2.02	0.40
2:A:361:HIS:HE1	2:B:234:LEU:HD11	1.83	0.40
2:C:165:SER:HB2	2:C:166:LEU:HB2	2.04	0.40
2:A:473:VAL:HB	2:A:493:GLN:H	1.86	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%)	77 (84%)	10 (11%)	5 (5%)	2 29
1	2	92/218 (42%)	76 (83%)	8 (9%)	8 (9%)	1 17
1	3	92/218 (42%)	79 (86%)	9 (10%)	4 (4%)	3 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	4	92/218 (42%)	77 (84%)	10 (11%)	5 (5%)	2 29
1	5	92/218 (42%)	76 (83%)	10 (11%)	6 (6%)	1 25
1	6	92/218 (42%)	76 (83%)	11 (12%)	5 (5%)	2 29
2	A	794/810 (98%)	632 (80%)	113 (14%)	49 (6%)	2 26
2	B	794/810 (98%)	634 (80%)	118 (15%)	42 (5%)	2 29
2	C	794/810 (98%)	630 (79%)	110 (14%)	54 (7%)	1 23
2	D	794/810 (98%)	624 (79%)	121 (15%)	49 (6%)	2 26
2	E	794/810 (98%)	628 (79%)	120 (15%)	46 (6%)	2 27
2	F	794/810 (98%)	629 (79%)	106 (13%)	59 (7%)	1 21
All	All	5316/6168 (86%)	4238 (80%)	746 (14%)	332 (6%)	4 26

All (332) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	147	VAL
1	3	147	VAL
1	4	207	HIS
1	6	147	VAL
2	A	76	GLN
2	A	78	ILE
2	A	271	ALA
2	A	294	ILE
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	468	ASN
2	A	472	THR
2	A	473	VAL
2	A	591	PRO
2	A	669	LYS
2	A	712	HIS
2	A	757	ASP
2	B	100	HIS
2	B	129	VAL
2	B	230	VAL
2	B	271	ALA
2	B	365	SER
2	B	366	ILE
2	B	382	ILE

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Mol	Chain	Res	Type
2	B	468	ASN
2	B	472	THR
2	B	473	VAL
2	C	76	GLN
2	C	78	ILE
2	C	100	HIS
2	C	117	GLU
2	C	183	ILE
2	C	294	ILE
2	C	383	SER
2	C	468	ASN
2	C	471	VAL
2	C	473	VAL
2	C	669	LYS
2	C	757	ASP
2	D	76	GLN
2	D	167	ALA
2	D	183	ILE
2	D	293	ALA
2	D	382	ILE
2	D	468	ASN
2	D	472	THR
2	D	473	VAL
2	D	493	GLN
2	D	716	LYS
2	D	717	LYS
2	E	72	GLN
2	E	271	ALA
2	E	294	ILE
2	E	363	ARG
2	E	365	SER
2	E	410	PRO
2	E	412	ASN
2	E	468	ASN
2	E	473	VAL
2	E	670	TYR
2	E	739	LEU
2	F	100	HIS
2	F	202	ASN
2	F	294	ILE
2	F	364	VAL
2	F	365	SER

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Mol	Chain	Res	Type
2	F	366	ILE
2	F	382	ILE
2	F	468	ASN
2	F	472	THR
2	F	473	VAL
2	F	511	ILE
2	F	579	GLU
2	F	583	THR
2	F	587	VAL
2	F	618	ALA
2	F	621	LYS
2	F	668	ASN
2	F	760	TYR
1	3	217	ALA
1	4	145	LEU
1	4	205	SER
1	5	217	ALA
2	A	100	HIS
2	A	118	GLY
2	A	165	SER
2	A	327	ASP
2	A	493	GLN
2	A	590	PRO
2	A	592	GLY
2	A	662	ALA
2	A	668	ASN
2	A	716	LYS
2	B	72	GLN
2	B	165	SER
2	B	202	ASN
2	B	363	ARG
2	B	470	GLU
2	B	471	VAL
2	B	493	GLN
2	C	73	GLU
2	C	129	VAL
2	C	165	SER
2	C	212	VAL
2	C	360	ALA
2	C	366	ILE
2	C	375	VAL
2	C	412	ASN

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Mol	Chain	Res	Type
2	C	493	GLN
2	C	580	LYS
2	C	618	ALA
2	D	151	ALA
2	D	163	LEU
2	D	165	SER
2	D	201	LYS
2	D	365	SER
2	D	366	ILE
2	D	412	ASN
2	D	470	GLU
2	D	662	ALA
2	E	100	HIS
2	E	165	SER
2	E	200	THR
2	E	202	ASN
2	E	366	ILE
2	E	413	LEU
2	E	471	VAL
2	E	493	GLN
2	E	662	ALA
2	E	738	ASP
2	F	78	ILE
2	F	165	SER
2	F	271	ALA
2	F	375	VAL
2	F	471	VAL
2	F	493	GLN
2	F	534	PRO
2	F	669	LYS
2	F	714	LEU
2	F	717	LYS
1	1	144	LYS
1	1	145	LEU
1	1	169	ASN
1	1	177	ASN
1	1	216	PHE
1	2	144	LYS
1	2	145	LEU
1	2	169	ASN
1	2	177	ASN
1	2	217	ALA

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Mol	Chain	Res	Type
1	3	144	LYS
1	3	177	ASN
1	4	144	LYS
1	4	177	ASN
1	5	144	LYS
1	5	169	ASN
1	5	177	ASN
1	5	216	PHE
1	6	144	LYS
1	6	177	ASN
1	6	216	PHE
2	A	4	GLY
2	A	152	ALA
2	A	162	THR
2	A	375	VAL
2	A	391	ALA
2	A	413	LEU
2	A	580	LYS
2	A	600	GLY
2	A	618	ALA
2	A	690	MET
2	B	162	THR
2	B	329	ALA
2	B	391	ALA
2	B	413	LEU
2	B	434	GLN
2	B	550	GLY
2	B	586	LEU
2	B	662	ALA
2	B	669	LYS
2	B	690	MET
2	C	152	ALA
2	C	163	LEU
2	C	271	ALA
2	C	365	SER
2	C	384	ASP
2	C	391	ALA
2	C	413	LEU
2	C	662	ALA
2	C	672	GLY
2	C	716	LYS
2	C	761	GLY

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Mol	Chain	Res	Type
2	D	149	SER
2	D	166	LEU
2	D	211	GLY
2	D	231	PRO
2	D	271	ALA
2	D	326	LYS
2	D	375	VAL
2	D	388	PRO
2	D	391	ALA
2	D	410	PRO
2	D	413	LEU
2	D	434	GLN
2	D	600	GLY
2	D	612	SER
2	E	152	ALA
2	E	162	THR
2	E	212	VAL
2	E	364	VAL
2	E	375	VAL
2	E	391	ALA
2	E	434	GLN
2	E	580	LYS
2	E	582	SER
2	E	583	THR
2	E	612	SER
2	E	668	ASN
2	F	71	GLY
2	F	73	GLU
2	F	142	LEU
2	F	147	THR
2	F	152	ALA
2	F	162	THR
2	F	163	LEU
2	F	210	PRO
2	F	391	ALA
2	F	550	GLY
2	F	588	GLY
2	F	590	PRO
2	F	662	ALA
1	2	216	PHE
1	5	145	LEU
2	A	388	PRO

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Mol	Chain	Res	Type
2	A	400	SER
2	A	412	ASN
2	A	534	PRO
2	A	622	ALA
2	A	717	LYS
2	B	163	LEU
2	B	375	VAL
2	B	388	PRO
2	B	400	SER
2	B	410	PRO
2	B	760	TYR
2	C	162	THR
2	C	232	GLU
2	C	293	ALA
2	C	329	ALA
2	C	362	HIS
2	C	382	ILE
2	C	388	PRO
2	C	400	SER
2	C	410	PRO
2	C	579	GLU
2	C	586	LEU
2	C	686	LYS
2	C	690	MET
2	D	117	GLU
2	D	152	ALA
2	D	162	THR
2	D	199	ARG
2	D	329	ALA
2	D	342	PRO
2	D	400	SER
2	D	690	MET
2	E	163	LEU
2	E	329	ALA
2	E	388	PRO
2	E	400	SER
2	F	166	LEU
2	F	293	ALA
2	F	329	ALA
2	F	363	ARG
2	F	388	PRO
2	F	400	SER

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Mol	Chain	Res	Type
2	F	412	ASN
2	F	413	LEU
2	F	600	GLY
2	F	612	SER
2	F	623	HIS
2	F	673	PHE
2	F	690	MET
1	6	169	ASN
2	A	163	LEU
2	A	178	SER
2	A	226	ILE
2	A	410	PRO
2	A	623	HIS
2	A	707	GLU
2	B	590	PRO
2	C	166	LEU
2	C	226	ILE
2	C	434	GLN
2	C	584	SER
2	C	738	ASP
2	D	215	THR
2	D	226	ILE
2	D	534	PRO
2	E	226	ILE
2	E	326	LYS
2	F	226	ILE
2	F	326	LYS
2	F	798	ASP
2	A	383	SER
2	A	471	VAL
2	B	166	LEU
2	B	167	ALA
2	B	226	ILE
2	B	293	ALA
2	B	323	TYR
2	B	440	ALA
2	B	670	TYR
2	C	147	THR
2	D	144	SER
2	D	323	TYR
2	E	323	TYR
2	E	717	LYS

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Mol	Chain	Res	Type
2	D	536	ARG
2	E	534	PRO
2	F	537	PRO
2	B	600	GLY
2	E	210	PRO
2	A	423	VAL
2	C	210	PRO
2	E	160	THR
2	E	671	VAL
2	F	410	PRO
1	2	134	GLY
2	D	537	PRO
2	E	546	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	88/201 (44%)	79 (90%)	9 (10%)	9 37
1	2	88/201 (44%)	75 (85%)	13 (15%)	4 24
1	3	88/201 (44%)	80 (91%)	8 (9%)	12 43
1	4	88/201 (44%)	78 (89%)	10 (11%)	7 33
1	5	88/201 (44%)	78 (89%)	10 (11%)	7 33
1	6	88/201 (44%)	80 (91%)	8 (9%)	12 43
2	A	666/685 (97%)	597 (90%)	69 (10%)	9 36
2	B	666/685 (97%)	601 (90%)	65 (10%)	10 39
2	C	666/685 (97%)	616 (92%)	50 (8%)	17 53
2	D	666/685 (97%)	602 (90%)	64 (10%)	10 40
2	E	666/685 (97%)	603 (90%)	63 (10%)	11 41
2	F	666/685 (97%)	603 (90%)	63 (10%)	11 41
All	All	4524/5316 (85%)	4092 (90%)	432 (10%)	15 41

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	151	LYS
1	1	165	VAL
1	1	168	CYS
1	1	170	MET
1	1	195	ARG
1	1	204	ILE
1	1	207	HIS
1	1	215	HIS
1	1	216	PHE
1	2	126	LYS
1	2	130	VAL
1	2	136	PHE
1	2	137	GLU
1	2	145	LEU
1	2	151	LYS
1	2	165	VAL
1	2	173	GLU
1	2	182	LEU
1	2	195	ARG
1	2	197	GLU
1	2	204	ILE
1	2	207	HIS
1	3	136	PHE
1	3	137	GLU
1	3	142	LEU
1	3	151	LYS
1	3	160	ARG
1	3	168	CYS
1	3	197	GLU
1	3	207	HIS
1	4	128	GLN
1	4	137	GLU
1	4	140	ILE
1	4	151	LYS
1	4	165	VAL
1	4	170	MET
1	4	177	ASN
1	4	195	ARG
1	4	207	HIS
1	4	215	HIS
1	5	130	VAL
1	5	136	PHE

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Mol	Chain	Res	Type
1	5	137	GLU
1	5	142	LEU
1	5	145	LEU
1	5	151	LYS
1	5	154	LEU
1	5	195	ARG
1	5	204	ILE
1	5	207	HIS
1	6	128	GLN
1	6	142	LEU
1	6	146	ASN
1	6	151	LYS
1	6	173	GLU
1	6	204	ILE
1	6	207	HIS
1	6	216	PHE
2	A	3	PHE
2	A	12	LYS
2	A	19	GLU
2	A	22	LEU
2	A	29	ILE
2	A	32	GLU
2	A	43	GLU
2	A	53	LEU
2	A	58	GLU
2	A	72	GLN
2	A	74	MET
2	A	78	ILE
2	A	94	GLU
2	A	100	HIS
2	A	105	THR
2	A	138	VAL
2	A	139	LEU
2	A	157	ASN
2	A	168	ARG
2	A	195	VAL
2	A	200	THR
2	A	207	ILE
2	A	230	VAL
2	A	262	LYS
2	A	269	ARG
2	A	306	ARG

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Mol	Chain	Res	Type
2	A	308	GLU
2	A	337	ILE
2	A	338	GLN
2	A	341	GLN
2	A	356	ASP
2	A	358	TYR
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	378	SER
2	A	381	TYR
2	A	392	ILE
2	A	393	ASP
2	A	394	LEU
2	A	403	ARG
2	A	414	LYS
2	A	415	GLU
2	A	436	PHE
2	A	443	ARG
2	A	448	ARG
2	A	473	VAL
2	A	502	MET
2	A	511	ILE
2	A	513	GLN
2	A	514	ASP
2	A	531	LEU
2	A	554	LEU
2	A	591	PRO
2	A	593	TYR
2	A	596	TYR
2	A	621	LYS
2	A	634	LEU
2	A	638	ARG
2	A	639	LEU
2	A	658	SER
2	A	664	GLU
2	A	676	GLN
2	A	682	HIS
2	A	706	ASP
2	A	709	ILE
2	A	730	LEU
2	A	758	LEU

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Mol	Chain	Res	Type
2	A	760	TYR
2	B	3	PHE
2	B	13	VAL
2	B	18	GLN
2	B	20	GLU
2	B	23	ARG
2	B	43	GLU
2	B	53	LEU
2	B	58	GLU
2	B	74	MET
2	B	78	ILE
2	B	79	HIS
2	B	90	LEU
2	B	142	LEU
2	B	188	GLU
2	B	195	VAL
2	B	238	ARG
2	B	254	ARG
2	B	262	LYS
2	B	269	ARG
2	B	291	GLU
2	B	301	LYS
2	B	308	GLU
2	B	355	ARG
2	B	356	ASP
2	B	363	ARG
2	B	364	VAL
2	B	385	ARG
2	B	387	LEU
2	B	392	ILE
2	B	420	LEU
2	B	425	LYS
2	B	432	GLN
2	B	436	PHE
2	B	443	ARG
2	B	448	ARG
2	B	449	LEU
2	B	457	LYS
2	B	461	LYS
2	B	467	GLU
2	B	470	GLU
2	B	471	VAL

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Mol	Chain	Res	Type
2	B	475	ASP
2	B	509	ARG
2	B	511	ILE
2	B	514	ASP
2	B	515	GLU
2	B	520	VAL
2	B	554	LEU
2	B	586	LEU
2	B	594	VAL
2	B	620	GLU
2	B	634	LEU
2	B	638	ARG
2	B	639	LEU
2	B	676	GLN
2	B	680	GLN
2	B	690	MET
2	B	693	LEU
2	B	695	ARG
2	B	726	MET
2	B	766	ARG
2	B	774	GLU
2	B	790	GLN
2	B	795	ASP
2	B	800	GLU
2	C	7	THR
2	C	19	GLU
2	C	20	GLU
2	C	32	GLU
2	C	51	GLN
2	C	53	LEU
2	C	58	GLU
2	C	72	GLN
2	C	74	MET
2	C	87	VAL
2	C	90	LEU
2	C	105	THR
2	C	138	VAL
2	C	139	LEU
2	C	170	LEU
2	C	187	LYS
2	C	191	ARG
2	C	195	VAL

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Mol	Chain	Res	Type
2	C	221	LEU
2	C	228	ASN
2	C	231	PRO
2	C	233	ILE
2	C	291	GLU
2	C	308	GLU
2	C	338	GLN
2	C	381	TYR
2	C	392	ILE
2	C	424	ARG
2	C	425	LYS
2	C	427	LYS
2	C	431	VAL
2	C	432	GLN
2	C	443	ARG
2	C	448	ARG
2	C	467	GLU
2	C	468	ASN
2	C	469	SER
2	C	531	LEU
2	C	567	GLU
2	C	570	ILE
2	C	624	PRO
2	C	634	LEU
2	C	638	ARG
2	C	666	LYS
2	C	693	LEU
2	C	715	GLU
2	C	730	LEU
2	C	766	ARG
2	C	782	LEU
2	C	800	GLU
2	D	12	LYS
2	D	19	GLU
2	D	53	LEU
2	D	58	GLU
2	D	72	GLN
2	D	74	MET
2	D	79	HIS
2	D	86	LYS
2	D	90	LEU
2	D	100	HIS

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Mol	Chain	Res	Type
2	D	105	THR
2	D	106	GLU
2	D	122	ARG
2	D	135	ARG
2	D	138	VAL
2	D	142	LEU
2	D	193	ILE
2	D	195	VAL
2	D	196	LEU
2	D	199	ARG
2	D	230	VAL
2	D	238	ARG
2	D	268	ILE
2	D	269	ARG
2	D	275	ILE
2	D	285	ILE
2	D	300	LEU
2	D	303	SER
2	D	304	LEU
2	D	356	ASP
2	D	358	TYR
2	D	363	ARG
2	D	378	SER
2	D	381	TYR
2	D	392	ILE
2	D	394	LEU
2	D	402	VAL
2	D	403	ARG
2	D	407	PHE
2	D	410	PRO
2	D	414	LYS
2	D	418	GLN
2	D	424	ARG
2	D	443	ARG
2	D	448	ARG
2	D	462	GLU
2	D	471	VAL
2	D	476	ILE
2	D	511	ILE
2	D	514	ASP
2	D	544	LEU
2	D	585	ARG

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Mol	Chain	Res	Type
2	D	624	PRO
2	D	626	VAL
2	D	631	LEU
2	D	634	LEU
2	D	638	ARG
2	D	654	LEU
2	D	678	GLU
2	D	680	GLN
2	D	760	TYR
2	D	763	ARG
2	D	795	ASP
2	D	800	GLU
2	E	32	GLU
2	E	53	LEU
2	E	74	MET
2	E	76	GLN
2	E	78	ILE
2	E	90	LEU
2	E	138	VAL
2	E	139	LEU
2	E	146	GLU
2	E	185	ARG
2	E	188	GLU
2	E	193	ILE
2	E	195	VAL
2	E	234	LEU
2	E	235	ARG
2	E	238	ARG
2	E	269	ARG
2	E	291	GLU
2	E	306	ARG
2	E	308	GLU
2	E	351	LEU
2	E	354	LEU
2	E	355	ARG
2	E	361	HIS
2	E	381	TYR
2	E	382	ILE
2	E	393	ASP
2	E	395	ILE
2	E	396	ASP
2	E	407	PHE

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Mol	Chain	Res	Type
2	E	415	GLU
2	E	424	ARG
2	E	425	LYS
2	E	427	LYS
2	E	431	VAL
2	E	436	PHE
2	E	448	ARG
2	E	471	VAL
2	E	473	VAL
2	E	476	ILE
2	E	483	TRP
2	E	526	ARG
2	E	533	ASP
2	E	554	LEU
2	E	567	GLU
2	E	577	TYR
2	E	583	THR
2	E	586	LEU
2	E	611	TYR
2	E	631	LEU
2	E	634	LEU
2	E	638	ARG
2	E	670	TYR
2	E	680	GLN
2	E	693	LEU
2	E	715	GLU
2	E	726	MET
2	E	739	LEU
2	E	765	LEU
2	E	766	ARG
2	E	777	LEU
2	E	794	LEU
2	E	800	GLU
2	F	19	GLU
2	F	32	GLU
2	F	58	GLU
2	F	72	GLN
2	F	76	GLN
2	F	79	HIS
2	F	90	LEU
2	F	92	MET
2	F	105	THR

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Mol	Chain	Res	Type
2	F	136	GLN
2	F	138	VAL
2	F	170	LEU
2	F	202	ASN
2	F	207	ILE
2	F	231	PRO
2	F	235	ARG
2	F	238	ARG
2	F	257	PHE
2	F	262	LYS
2	F	263	LYS
2	F	269	ARG
2	F	308	GLU
2	F	338	GLN
2	F	341	GLN
2	F	355	ARG
2	F	356	ASP
2	F	363	ARG
2	F	381	TYR
2	F	393	ASP
2	F	396	ASP
2	F	400	SER
2	F	404	LEU
2	F	411	PRO
2	F	418	GLN
2	F	424	ARG
2	F	427	LYS
2	F	436	PHE
2	F	443	ARG
2	F	444	ASP
2	F	448	ARG
2	F	449	LEU
2	F	462	GLU
2	F	470	GLU
2	F	471	VAL
2	F	483	TRP
2	F	513	GLN
2	F	514	ASP
2	F	515	GLU
2	F	531	LEU
2	F	536	ARG
2	F	621	LYS

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Mol	Chain	Res	Type
2	F	670	TYR
2	F	676	GLN
2	F	680	GLN
2	F	690	MET
2	F	695	ARG
2	F	706	ASP
2	F	753	GLU
2	F	763	ARG
2	F	775	ASP
2	F	790	GLN
2	F	798	ASP
2	F	800	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	3	178	GLN
1	3	207	HIS
1	4	146	ASN
1	4	178	GLN
1	4	207	HIS
1	5	146	ASN
1	5	178	GLN
1	5	194	HIS
1	6	128	GLN
1	6	194	HIS
2	A	79	HIS
2	A	100	HIS
2	A	228	ASN
2	A	273	ASN
2	A	310	GLN
2	A	341	GLN
2	A	772	HIS
2	A	791	HIS
2	B	26	HIS
2	B	100	HIS
2	B	464	GLN
2	B	513	GLN
2	B	623	HIS
2	B	682	HIS
2	B	703	ASN

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Mol	Chain	Res	Type
2	B	718	HIS
2	B	729	GLN
2	B	737	GLN
2	C	33	HIS
2	C	100	HIS
2	C	273	ASN
2	C	703	ASN
2	C	712	HIS
2	C	718	HIS
2	C	729	GLN
2	C	772	HIS
2	C	791	HIS
2	D	76	GLN
2	D	79	HIS
2	D	136	GLN
2	D	273	ASN
2	D	282	HIS
2	D	361	HIS
2	D	623	HIS
2	D	682	HIS
2	D	791	HIS
2	E	11	GLN
2	E	26	HIS
2	E	100	HIS
2	E	140	GLN
2	E	228	ASN
2	E	282	HIS
2	E	310	GLN
2	E	352	GLN
2	E	681	ASN
2	E	712	HIS
2	E	729	GLN
2	F	33	HIS
2	F	100	HIS
2	F	140	GLN
2	F	270	GLN
2	F	310	GLN
2	F	362	HIS
2	F	718	HIS
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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.